wwPDB X-ray Structure Validation Summary Report (i)

Aug 13, 2026 – 01:46 PM JST

PDB ID	:	9IKI / pdb_00009iki
Title	:	Bovine Heart Cytochrome c Oxidase in the Nitrous Oxide-bound Fully Reduced State
Authors	:	Muramoto, K.; Ide, T.; Shinzawa-Itoh, K.
Deposited on	:	2024-06-27
Resolution	:	1.75 Å(reported)

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

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

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

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

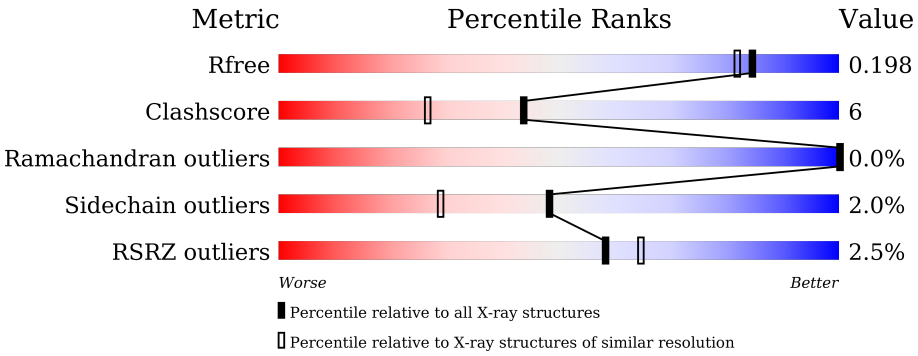
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
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	87% 11%
1	N	514	87% 12%
2	B	227	5% 80% 17%
2	O	227	3% 80% 18%
3	C	261	86% 13%
3	P	261	84% 15%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	147	2% 90% 7%
4	Q	147	5% 87% 7%
5	E	109	89% 5% 6%
5	R	109	2% 86% 7% 6%
6	F	98	% 76% 15% 7%
6	S	98	2% 78% 12% 7%
7	G	85	5% 75% 7% 15%
7	T	85	2% 76% 7% 15%
8	H	85	5% 79% 7% 12%
8	U	85	7% 78% 8% 12%
9	I	73	12% 86% 7%
9	V	73	5% 81% 14%
10	J	59	3% 85% 8% 5%
10	W	59	3% 83% 8% 5%
11	K	56	5% 79% 7% 12%
11	X	56	5% 88% 12%
12	L	47	81% 11% 6%
12	Y	47	85% 6% 6%
13	M	46	2% 78% 9% 13%
13	Z	46	2% 76% 9% 13%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	LFA	P	310	-	-	-	X
26	CDL	C	304	-	-	X	-

2 Entry composition (i)

There are 29 unique types of molecules in this entry. The entry contains 33027 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			

Continued on next page...

Continued from previous page...

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

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

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

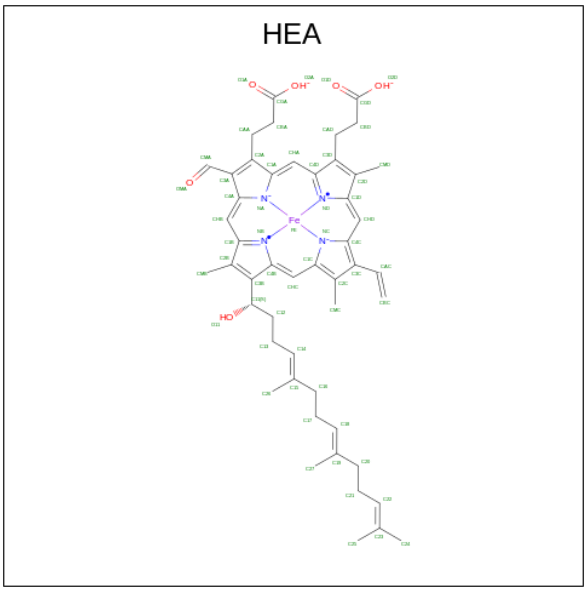
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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

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

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

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



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

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

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

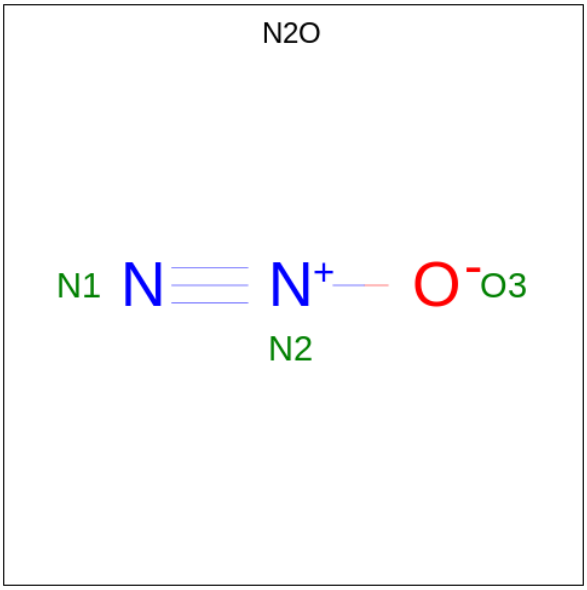
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

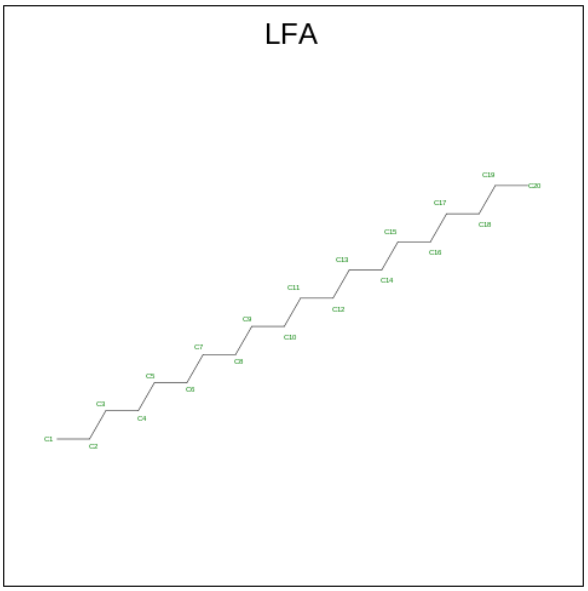
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Na 1 1	0	0
17	N	1	Total Na 1 1	0	0

- Molecule 18 is NITROUS OXIDE (CCD ID: N2O) (formula: N_2O) (labeled as "Ligand of Interest" by depositor).



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

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



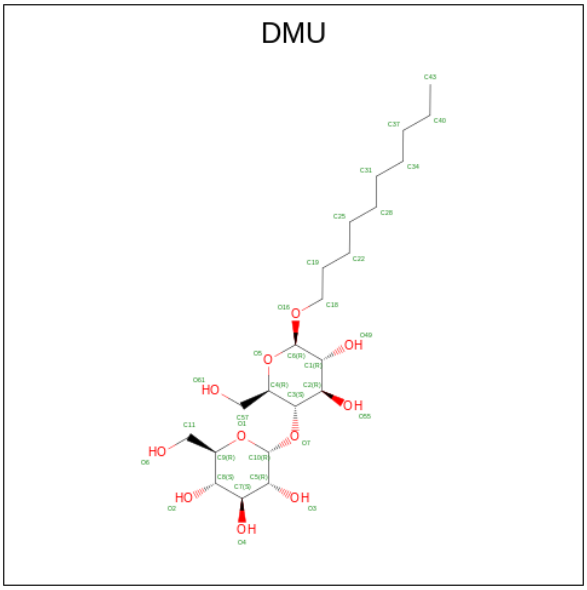
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	A	1	Total C 14 14	0	0
19	B	1	Total C 17 17	0	0
19	C	1	Total C 11 11	0	0
19	C	1	Total C 6 6	0	0
19	C	1	Total C 18 18	0	0
19	C	1	Total C 15 15	0	0
19	C	1	Total C 11 11	0	0
19	C	1	Total C 14 14	0	0
19	C	1	Total C 11 11	0	0
19	C	1	Total C 15 15	0	0
19	C	1	Total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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	O	1	Total C 17 17	0	0
19	O	1	Total C 11 11	0	0
19	P	1	Total C 11 11	0	0
19	P	1	Total C 6 6	0	0
19	P	1	Total C 18 18	0	0
19	P	1	Total C 11 11	0	0
19	P	1	Total C 11 11	0	0
19	P	1	Total C 15 15	0	0
19	P	1	Total C 13 13	0	0
19	T	1	Total C 14 14	0	0
19	T	1	Total C 14 14	0	0
19	T	1	Total C 11 11	0	0

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



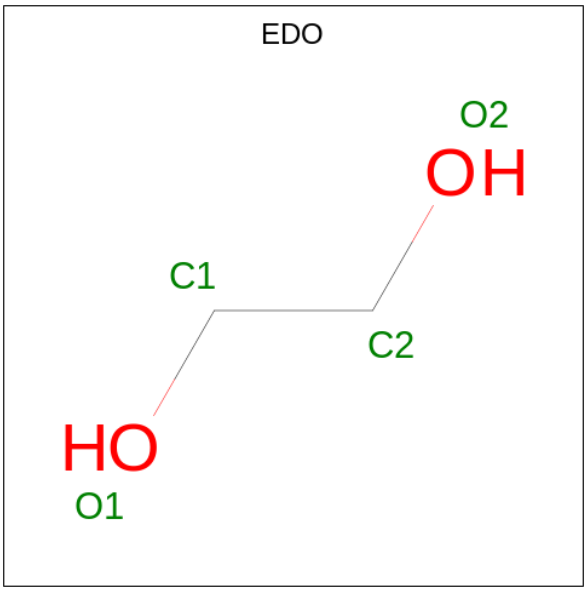
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	A	1	Total C 7 7	0	0
20	A	1	Total C O 33 22 11	0	0
20	A	1	Total C O 11 10 1	0	0
20	B	1	Total C O 11 10 1	0	0
20	B	1	Total C O 11 10 1	0	0
20	B	1	Total C O 22 16 6	0	0
20	B	1	Total C O 22 16 6	0	0
20	C	1	Total C O 11 10 1	0	0
20	C	1	Total C O 33 22 11	0	0
20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

Continued on next page...

Continued from previous page...

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

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



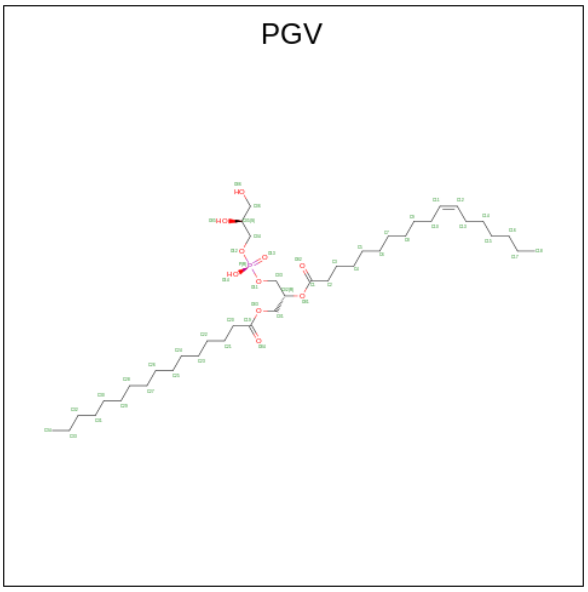
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	B	1	Total	C	O	0	0
			4	2	2		
21	C	1	Total	C	O	0	0
			4	2	2		
21	C	1	Total	C	O	0	0
			4	2	2		
21	C	1	Total	C	O	0	0
			4	2	2		
21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

Continued on next page...

Continued from previous page...

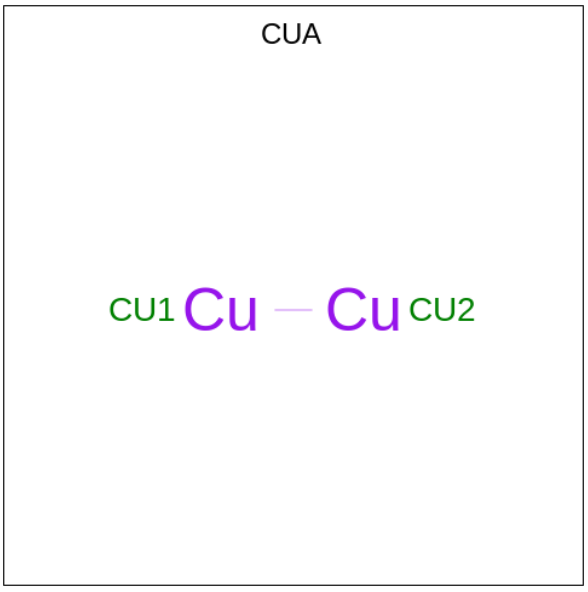
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	N	1	Total C O 4 2 2	0	0
21	N	1	Total C O 4 2 2	0	0
21	N	1	Total C O 4 2 2	0	0
21	N	1	Total C O 4 2 2	0	0
21	N	1	Total C O 4 2 2	0	0
21	O	1	Total C O 4 2 2	0	0
21	P	1	Total C O 4 2 2	0	0
21	P	1	Total C O 4 2 2	0	0
21	P	1	Total C O 4 2 2	0	0
21	R	1	Total C O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

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



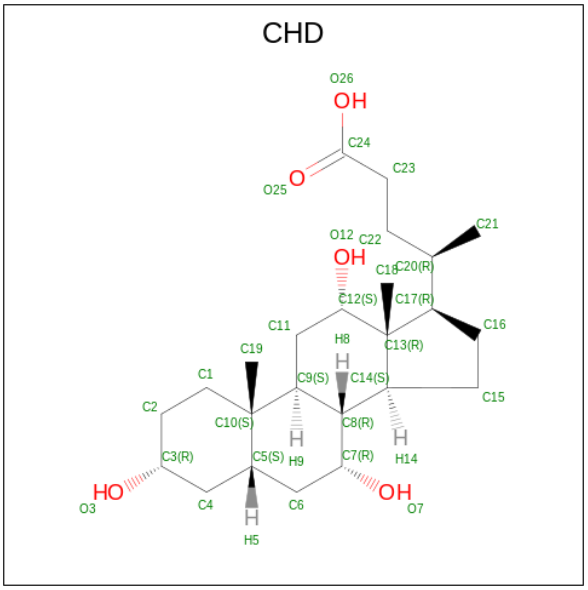
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
22	A	1	Total	C	O	P	0	0
			51	40	10	1		
22	C	1	Total	C	O	P	0	0
			51	40	10	1		
22	N	1	Total	C	O	P	0	0
			51	40	10	1		
22	P	1	Total	C	O	P	0	0
			51	40	10	1		

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



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

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

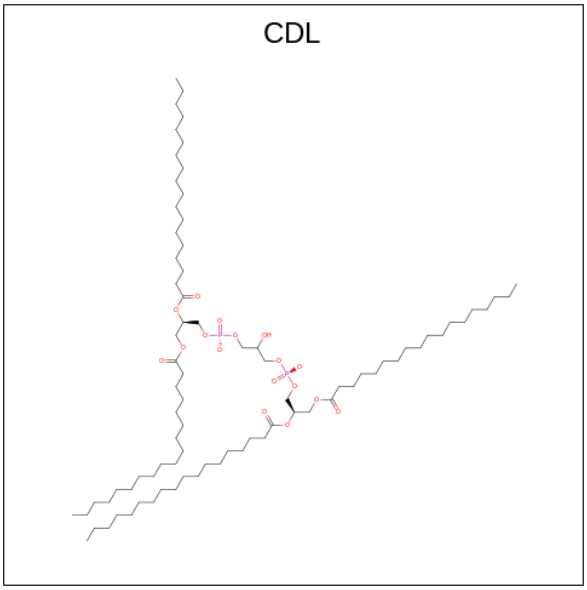


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	B	1	Total C O 29 24 5	0	0
24	C	1	Total C O 29 24 5	0	0
24	C	1	Total C O 29 24 5	0	0
24	O	1	Total C O 29 24 5	0	0
24	P	1	Total C O 29 24 5	0	0
24	P	1	Total C O 29 24 5	0	0

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

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

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

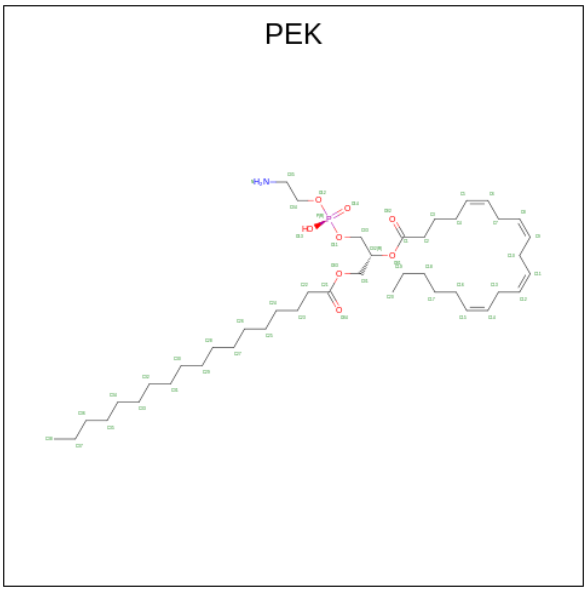


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	C	1	Total	C	O	P	0	0
			87	68	17	2		
26	I	1	Total	C	O	P	0	0
			64	45	17	2		
26	L	1	Total	C	O	P	0	0
			94	75	17	2		
26	N	1	Total	C	O	P	0	0
			64	45	17	2		
26	P	1	Total	C	O	P	0	0
			87	68	17	2		
26	Y	1	Total	C	O	P	0	0
			94	75	17	2		

- Molecule 27 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 28 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
28	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 29 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	A	235	Total	O	0	11
			246	246		
29	B	167	Total	O	0	2
			169	169		
29	C	107	Total	O	0	1
			108	108		
29	D	136	Total	O	0	8
			144	144		
29	E	108	Total	O	0	8
			116	116		
29	F	103	Total	O	0	7
			110	110		
29	G	43	Total	O	0	1
			44	44		
29	H	62	Total	O	0	0
			62	62		
29	I	41	Total	O	0	0
			41	41		
29	J	20	Total	O	0	0
			20	20		

Continued on next page...

Continued from previous page...

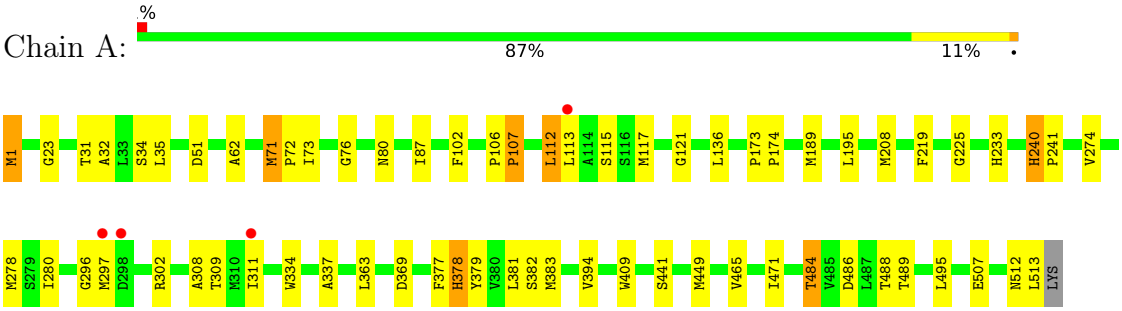
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	K	21	Total O 21 21	0	0
29	L	26	Total O 28 28	0	2
29	M	21	Total O 21 21	0	0
29	N	221	Total O 231 231	0	10
29	O	147	Total O 148 148	0	1
29	P	101	Total O 102 102	0	1
29	Q	78	Total O 83 83	0	5
29	R	87	Total O 93 93	0	6
29	S	91	Total O 98 98	0	7
29	T	40	Total O 41 41	0	1
29	U	51	Total O 51 51	0	0
29	V	22	Total O 22 22	0	0
29	W	15	Total O 15 15	0	0
29	X	17	Total O 17 17	0	0
29	Y	24	Total O 26 26	0	2
29	Z	17	Total O 17 17	0	0

3 Residue-property plots (i)

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

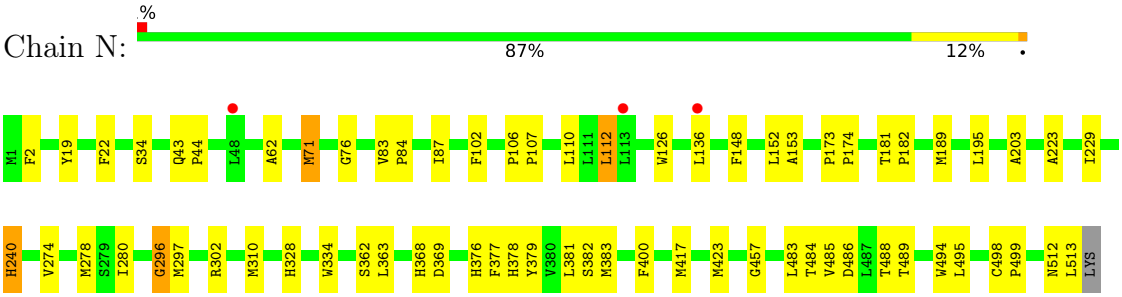
• Molecule 1: Cytochrome c oxidase subunit 1

Chain A:



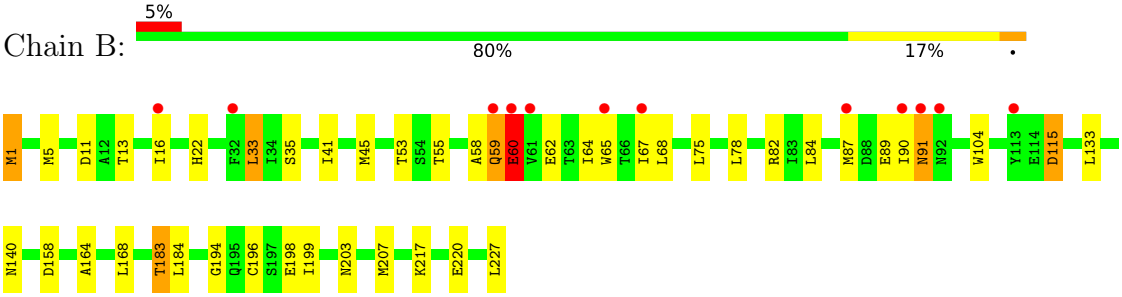
• Molecule 1: Cytochrome c oxidase subunit 1

Chain N:



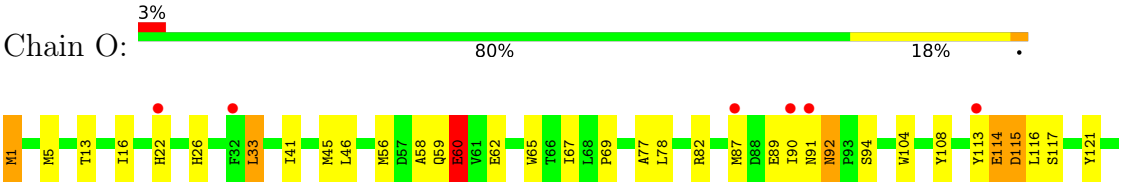
• Molecule 2: Cytochrome c oxidase subunit 2

Chain B:



• Molecule 2: Cytochrome c oxidase subunit 2

Chain O:



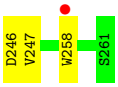


• Molecule 3: Cytochrome c oxidase subunit 3

Chain C:



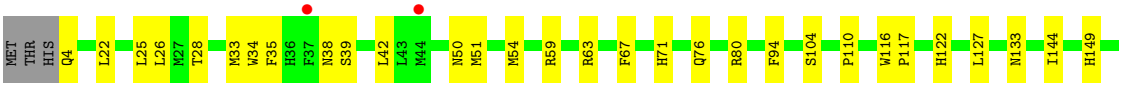




• Molecule 3: Cytochrome c oxidase subunit 3

Chain P:



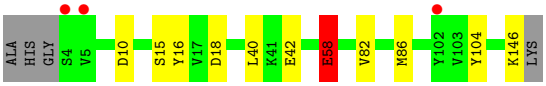




• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain D:





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

Chain Q:

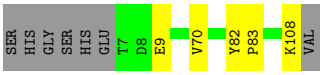




• Molecule 5: Cytochrome c oxidase subunit 5A

Chain E:

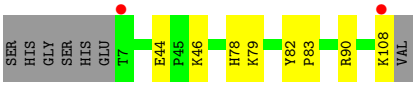




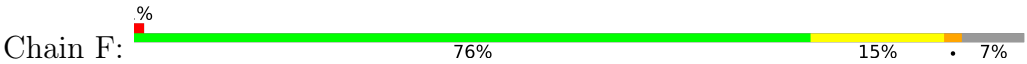
• Molecule 5: Cytochrome c oxidase subunit 5A

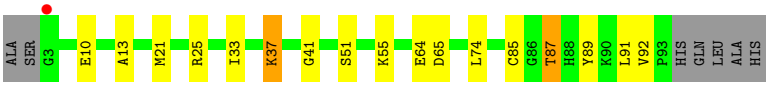
Chain R:



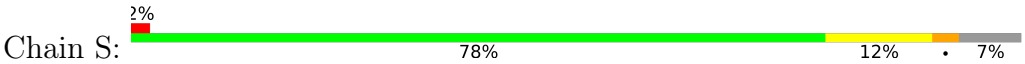


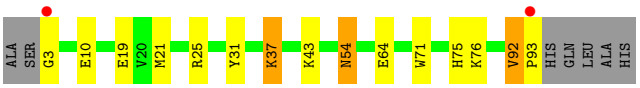
• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



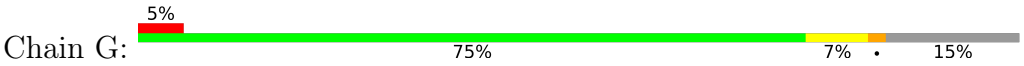


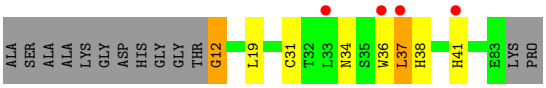
• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



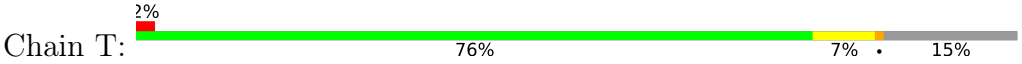


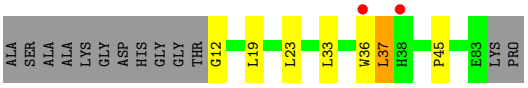
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



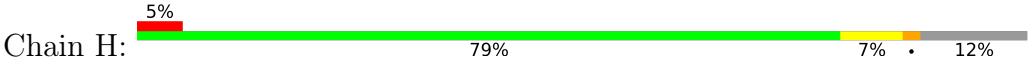


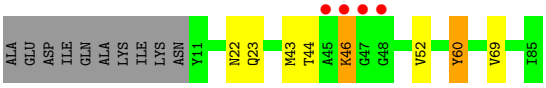
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



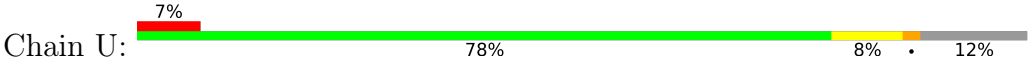


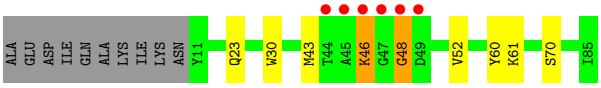
• Molecule 8: Cytochrome c oxidase subunit 6B1





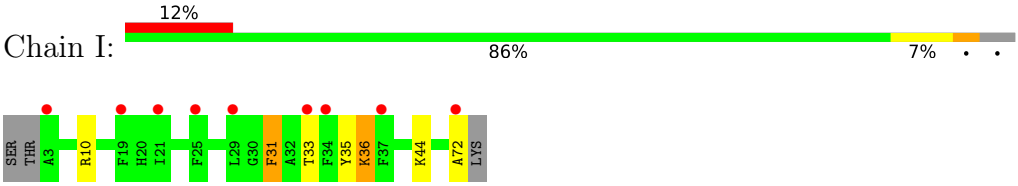
• Molecule 8: Cytochrome c oxidase subunit 6B1





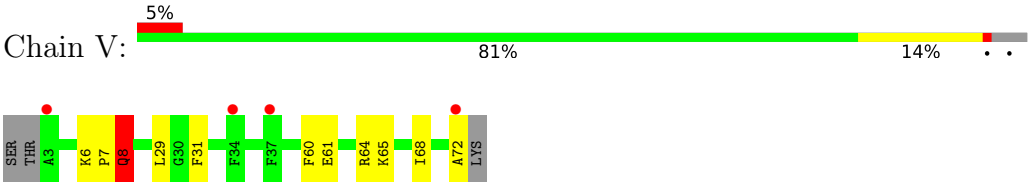
• Molecule 9: Cytochrome c oxidase subunit 6C

Chain I:



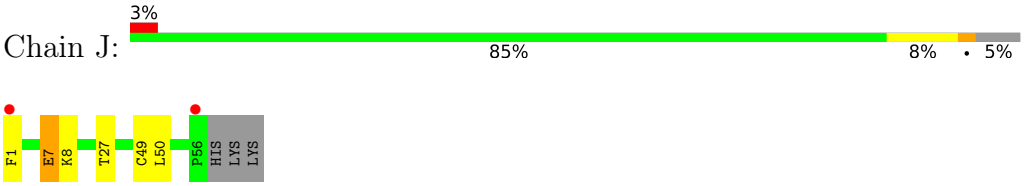
• Molecule 9: Cytochrome c oxidase subunit 6C

Chain V:



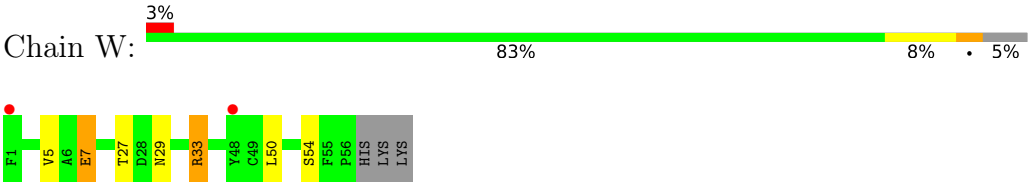
• Molecule 10: Cytochrome c oxidase subunit 7A1

Chain J:



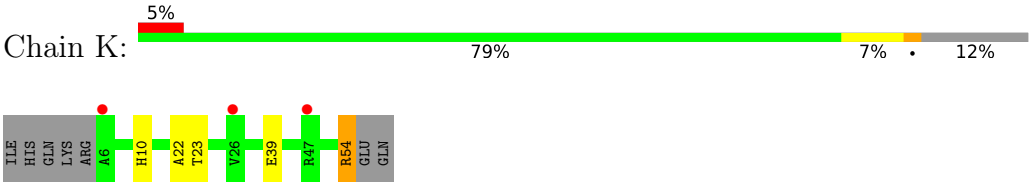
• Molecule 10: Cytochrome c oxidase subunit 7A1

Chain W:



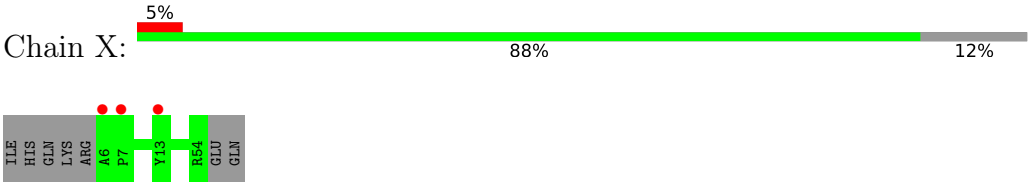
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

Chain K:



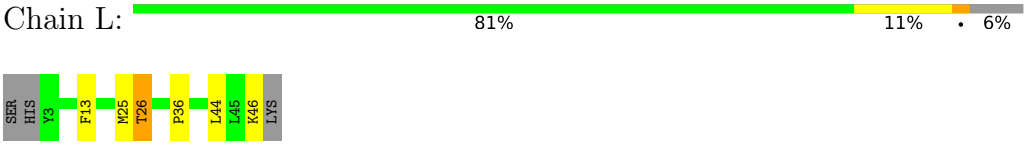
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

Chain X:



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

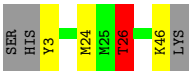
Chain L:



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

Chain Y:

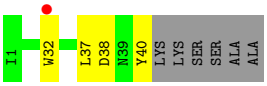




• Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

Chain M:

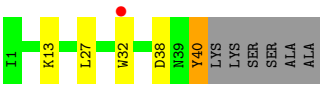




• Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

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	181.90Å 204.00Å 177.70Å 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]	2.19 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.153 , 0.189 0.165 , 0.198	Depositor DCC
R_{free} test set	32776 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	30.8	Xtriage
Anisotropy	0.779	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 60.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	33027	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

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

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: UNX, CHD, NA, N2O, CDL, ZN, HEA, CUA, DMU, EDO, MG, LFA, PGV, FME, CU, PEK

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	1.17	4/4259 (0.1%)	1.30	9/5816 (0.2%)
1	N	1.16	6/4259 (0.1%)	1.31	13/5816 (0.2%)
2	B	1.25	4/1908 (0.2%)	1.40	15/2598 (0.6%)
2	O	1.22	7/1908 (0.4%)	1.35	5/2598 (0.2%)
3	C	1.15	2/2258 (0.1%)	1.26	3/3084 (0.1%)
3	P	1.18	4/2258 (0.2%)	1.27	8/3084 (0.3%)
4	D	1.18	2/1226 (0.2%)	1.36	2/1657 (0.1%)
4	Q	1.16	2/1182 (0.2%)	1.39	3/1598 (0.2%)
5	E	1.16	0/843	1.33	2/1145 (0.2%)
5	R	1.22	0/843	1.37	2/1145 (0.2%)
6	F	1.17	0/724	1.35	0/983
6	S	1.31	4/724 (0.6%)	1.34	3/983 (0.3%)
7	G	1.27	3/633 (0.5%)	1.30	0/864
7	T	1.24	2/633 (0.3%)	1.32	0/864
8	H	1.14	2/648 (0.3%)	1.42	0/877
8	U	1.13	1/648 (0.2%)	1.41	0/877
9	I	1.25	1/588 (0.2%)	1.46	2/781 (0.3%)
9	V	1.19	0/588	1.50	3/781 (0.4%)
10	J	1.15	0/451	1.29	1/610 (0.2%)
10	W	1.21	0/451	1.36	3/610 (0.5%)
11	K	1.20	2/398 (0.5%)	1.45	2/546 (0.4%)
11	X	1.15	0/398	1.32	0/546
12	L	1.12	0/372	1.41	4/500 (0.8%)
12	Y	1.14	1/372 (0.3%)	1.37	1/500 (0.2%)
13	M	1.11	0/321	1.35	0/440
13	Z	1.09	0/321	1.40	0/440
All	All	1.18	47/29214 (0.2%)	1.34	81/39743 (0.2%)

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

sidechain that are expected to be planar.

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

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	198	GLU	C-O	9.10	1.34	1.23
2	B	198	GLU	C-O	8.24	1.33	1.23
2	O	60	GLU	CD-OE1	8.13	1.40	1.25
4	D	58	GLU	CD-OE1	7.83	1.40	1.25
2	B	90	ILE	C-O	7.57	1.32	1.24

The worst 5 of 81 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	240	HIS	CA-CB-CG	-10.22	103.58	113.80
9	I	72	ALA	CA-C-O	-10.09	103.64	120.80
1	N	240	HIS	CA-CB-CG	-9.68	104.12	113.80
2	B	183	THR	CA-CB-OG1	-9.53	95.31	109.60
4	Q	146	LYS	CA-C-O	-9.29	105.01	120.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	296	GLY	Mainchain
1	N	296	GLY	Mainchain
6	S	92	VAL	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4130	0	4102	54	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	4130	0	4102	60	0
2	B	1870	0	1870	35	0
2	O	1870	0	1870	36	0
3	C	2171	0	2080	32	0
3	P	2172	0	2081	26	0
4	D	1192	0	1178	7	0
4	Q	1148	0	1131	5	0
5	E	825	0	823	1	0
5	R	825	0	823	5	0
6	F	709	0	691	14	0
6	S	709	0	691	9	0
7	G	606	0	577	5	0
7	T	606	0	577	3	0
8	H	628	0	580	12	0
8	U	628	0	580	8	0
9	I	575	0	584	6	0
9	V	575	0	584	5	0
10	J	441	0	439	6	0
10	W	441	0	439	3	0
11	K	384	0	366	1	0
11	X	384	0	366	0	0
12	L	360	0	360	3	0
12	Y	360	0	360	5	0
13	M	311	0	321	2	0
13	Z	311	0	321	2	0
14	A	120	0	108	6	0
14	N	120	0	108	4	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	3	0	0	0	0
18	N	3	0	0	0	0
19	A	14	0	27	7	0
19	B	17	0	33	4	0
19	C	129	0	234	9	0
19	G	14	0	27	5	0
19	N	14	0	27	5	0
19	O	28	0	54	4	0
19	P	85	0	145	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	T	39	0	75	6	0
20	A	51	0	75	3	0
20	B	66	0	104	0	0
20	C	194	0	261	5	0
20	D	33	0	41	2	0
20	G	11	0	21	0	0
20	H	33	0	29	1	0
20	J	11	0	21	0	0
20	L	22	0	31	0	0
20	M	41	0	56	0	0
20	N	40	0	54	0	0
20	O	66	0	104	1	0
20	P	172	0	231	2	0
20	Q	33	0	42	3	0
20	T	22	0	31	1	0
20	U	33	0	26	0	0
20	W	11	0	21	0	0
20	Z	63	0	87	4	0
21	A	16	0	24	1	0
21	B	4	0	6	0	0
21	C	12	0	17	0	0
21	D	4	0	6	0	0
21	E	8	0	12	0	0
21	F	8	0	12	0	0
21	G	4	0	6	0	0
21	N	20	0	29	1	0
21	O	4	0	6	0	0
21	P	12	0	18	0	0
21	R	12	0	18	0	0
21	S	8	0	12	0	0
21	T	4	0	6	0	0
22	A	51	0	76	0	0
22	C	51	0	76	2	0
22	N	51	0	76	2	0
22	P	51	0	76	1	0
23	B	2	0	0	0	0
23	O	2	0	0	0	0
24	B	29	0	39	0	0
24	C	58	0	78	2	0
24	O	29	0	39	1	0
24	P	58	0	78	5	0
25	C	1	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	P	1	0	0	1	0
26	C	87	0	124	24	0
26	I	64	0	72	3	0
26	L	94	0	141	4	0
26	N	64	0	72	6	0
26	P	87	0	124	16	0
26	Y	94	0	141	10	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	G	53	0	77	0	0
28	T	53	0	77	4	0
29	A	246	0	0	10	0
29	B	169	0	0	6	0
29	C	108	0	0	5	0
29	D	144	0	0	3	0
29	E	116	0	0	0	0
29	F	110	0	0	1	0
29	G	44	0	0	1	0
29	H	62	0	0	6	0
29	I	41	0	0	2	0
29	J	20	0	0	0	0
29	K	21	0	0	0	0
29	L	28	0	0	1	0
29	M	21	0	0	0	0
29	N	231	0	0	7	0
29	O	148	0	0	3	0
29	P	102	0	0	4	0
29	Q	83	0	0	3	0
29	R	93	0	0	2	0
29	S	98	0	0	1	0
29	T	41	0	0	1	0
29	U	51	0	0	2	0
29	V	22	0	0	1	0
29	W	15	0	0	0	0
29	X	17	0	0	0	0
29	Y	26	0	0	2	0
29	Z	17	0	0	0	0
All	All	33027	0	31507	384	0

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

The worst 5 of 384 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:N:112:LEU:HG	29:N:914:HOH:O	1.15	1.28
1:A:112:LEU:HG	29:A:922:HOH:O	1.13	1.28
2:B:16[A]:ILE:HG21	2:B:87[A]:MET:HE3	1.23	1.11
19:C:309:LFA:H12	29:H:228:HOH:O	1.46	1.11
2:B:16[A]:ILE:CG2	2:B:87[A]:MET:HE3	1.82	1.08

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%)	512 (97%)	14 (3%)	0	100	100
1	N	526/514 (102%)	511 (97%)	15 (3%)	0	100	100
2	B	230/227 (101%)	223 (97%)	7 (3%)	0	100	100
2	O	230/227 (101%)	223 (97%)	7 (3%)	0	100	100
3	C	265/261 (102%)	261 (98%)	4 (2%)	0	100	100
3	P	265/261 (102%)	261 (98%)	4 (2%)	0	100	100
4	D	142/147 (97%)	139 (98%)	3 (2%)	0	100	100
4	Q	136/147 (92%)	133 (98%)	3 (2%)	0	100	100
5	E	100/109 (92%)	100 (100%)	0	0	100	100
5	R	100/109 (92%)	99 (99%)	1 (1%)	0	100	100
6	F	91/98 (93%)	91 (100%)	0	0	100	100
6	S	91/98 (93%)	88 (97%)	3 (3%)	0	100	100
7	G	71/85 (84%)	67 (94%)	4 (6%)	0	100	100
7	T	71/85 (84%)	69 (97%)	2 (3%)	0	100	100
8	H	73/85 (86%)	71 (97%)	2 (3%)	0	100	100
8	U	73/85 (86%)	71 (97%)	1 (1%)	1 (1%)	9	2

Continued on next page...

Continued from previous page...

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%)	38 (100%)	0	0	100	100
All	All	3488/3614 (96%)	3411 (98%)	76 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	U	48	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	440/426 (103%)	437 (99%)	3 (1%)	76	67
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%)	209 (97%)	6 (3%)	38	18
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%)	120 (98%)	2 (2%)	55	38

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	E	89/95 (94%)	88 (99%)	1 (1%)	65 52
5	R	89/95 (94%)	88 (99%)	1 (1%)	65 52
6	F	78/81 (96%)	75 (96%)	3 (4%)	29 10
6	S	78/81 (96%)	75 (96%)	3 (4%)	29 10
7	G	63/69 (91%)	61 (97%)	2 (3%)	34 14
7	T	63/69 (91%)	60 (95%)	3 (5%)	23 6
8	H	67/75 (89%)	65 (97%)	2 (3%)	36 16
8	U	67/75 (89%)	64 (96%)	3 (4%)	24 7
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%)	36 (97%)	1 (3%)	39 19
12	Y	37/40 (92%)	36 (97%)	1 (3%)	39 19
13	M	34/38 (90%)	33 (97%)	1 (3%)	37 17
13	Z	34/38 (90%)	31 (91%)	3 (9%)	9 1
All	All	3042/3086 (99%)	2980 (98%)	62 (2%)	48 29

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

Mol	Chain	Res	Type
1	N	112	LEU
9	V	68	ILE
2	O	92	ASN
9	V	65	LYS
13	Z	13	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
2	O	59	GLN
4	Q	76	ASN
8	U	22	ASN

Continued on next page...

Continued from previous page...

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FME	B	1	2	8,9,10	1.00	1 (12%)	7,9,11	1.18	1 (14%)
1	FME	A	1	1	8,9,10	0.60	0	7,9,11	1.24	1 (14%)
1	FME	N	1	1	8,9,10	0.82	0	7,9,11	1.07	0
2	FME	O	1	2	8,9,10	0.71	0	7,9,11	1.08	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	B	1	2	-	0/7/9/11	-
1	FME	A	1	1	-	2/7/9/11	-
1	FME	N	1	1	-	3/7/9/11	-
2	FME	O	1	2	-	0/7/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	CG-SD	-2.33	1.69	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	FME	CG-CB-CA	-2.30	106.57	112.95
1	A	1	FME	CE-SD-CG	2.16	107.82	100.40
2	O	1	FME	O-C-CA	-2.09	119.30	124.78

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

There are no ring outliers.

3 monomers are involved in 4 short contacts:

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 133 ligands modelled in this entry, 8 are monoatomic and 2 are unknown - leaving 123 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	LFA	C	307	-	10,10,19	0.19	0	9,9,18	0.21	0
18	N2O	A	606	-	0,2,2	-	-	0,1,1	-	-
19	LFA	T	101	-	13,13,19	0.66	0	12,12,18	0.43	0
21	EDO	R	203	-	3,3,3	0.64	0	2,2,2	0.39	0
20	DMU	C	318	-	22,22,34	0.93	2 (9%)	27,27,45	1.29	4 (14%)
20	DMU	B	304	-	22,22,34	1.19	2 (9%)	27,27,45	1.18	3 (11%)
21	EDO	C	323	-	3,3,3	0.78	0	2,2,2	0.73	0
22	PGV	P	303	-	50,50,50	0.93	2 (4%)	53,56,56	1.04	2 (3%)
20	DMU	D	201	-	34,34,34	1.54	7 (20%)	45,45,45	1.39	5 (11%)
20	DMU	C	319	-	34,34,34	1.00	3 (8%)	45,45,45	1.22	3 (6%)
20	DMU	L	102	-	22,22,34	0.72	0	27,27,45	0.99	1 (3%)
21	EDO	N	613	-	3,3,3	0.36	0	2,2,2	0.30	0
21	EDO	R	201	-	3,3,3	0.73	0	2,2,2	0.35	0
24	CHD	C	305	-	32,32,32	0.80	1 (3%)	51,51,51	1.66	7 (13%)
22	PGV	C	303	-	50,50,50	0.83	3 (6%)	53,56,56	0.94	1 (1%)
21	EDO	A	611	-	3,3,3	0.36	0	2,2,2	0.26	0
22	PGV	A	614	-	50,50,50	0.93	2 (4%)	53,56,56	1.20	3 (5%)
26	CDL	N	606	-	63,63,99	0.72	0	69,75,111	1.22	6 (8%)
20	DMU	U	101	19	34,34,34	1.03	3 (8%)	45,45,45	1.48	5 (11%)
20	DMU	Q	201	-	34,34,34	1.42	7 (20%)	45,45,45	1.64	6 (13%)
20	DMU	P	318	-	34,34,34	1.11	3 (8%)	45,45,45	1.33	3 (6%)
20	DMU	Z	103	-	7,7,34	0.33	0	6,6,45	0.64	0
20	DMU	B	302	-	10,10,34	0.23	0	9,9,45	0.57	0
20	DMU	P	314	-	34,34,34	0.88	2 (5%)	45,45,45	1.44	6 (13%)
21	EDO	B	305	-	3,3,3	0.17	0	2,2,2	0.39	0
20	DMU	M	102	-	7,7,34	0.31	0	6,6,45	0.38	0
23	CUA	B	301	2	0,1,1	-	-	-		
14	HEA	A	602	1	66,67,67	2.21	24 (36%)	78,103,103	2.37	30 (38%)
14	HEA	N	601	1	66,67,67	1.95	22 (33%)	78,103,103	2.86	37 (47%)
21	EDO	R	202	-	3,3,3	0.19	0	2,2,2	0.09	0
24	CHD	B	306	-	32,32,32	0.83	0	51,51,51	0.93	3 (5%)
21	EDO	C	322	-	3,3,3	0.45	0	2,2,2	0.06	0
21	EDO	A	613	-	3,3,3	0.46	0	2,2,2	0.37	0
19	LFA	B	307	-	16,16,19	0.43	0	15,15,18	0.26	0
19	LFA	C	308	-	5,5,19	0.28	0	4,4,18	0.19	0
21	EDO	A	612	-	3,3,3	0.73	0	2,2,2	0.21	0
21	EDO	G	103	-	3,3,3	0.16	0	2,2,2	0.05	0
21	EDO	C	321	-	3,3,3	0.13	0	2,2,2	0.29	0
20	DMU	P	317	-	34,34,34	1.11	3 (8%)	45,45,45	1.35	5 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	DMU	P	315	-	6,6,34	0.29	0	5,5,45	0.52	0
24	CHD	C	301	-	32,32,32	0.88	2 (6%)	51,51,51	0.87	1 (1%)
19	LFA	O	303	-	10,10,19	0.30	0	9,9,18	0.19	0
21	EDO	O	309	-	3,3,3	0.27	0	2,2,2	0.18	0
20	DMU	C	317	-	6,6,34	0.36	0	5,5,45	0.44	0
19	LFA	P	309	20	17,17,19	0.30	0	16,16,18	0.25	0
28	PEK	T	102	-	52,52,52	0.77	2 (3%)	55,57,57	1.07	4 (7%)
21	EDO	F	102	-	3,3,3	0.36	0	2,2,2	0.22	0
19	LFA	C	314	-	14,14,19	0.29	0	13,13,18	0.44	0
20	DMU	P	316	-	22,22,34	0.88	2 (9%)	27,27,45	1.12	2 (7%)
21	EDO	E	202	-	3,3,3	0.29	0	2,2,2	0.01	0
28	PEK	G	101	-	52,52,52	0.70	1 (1%)	55,57,57	0.74	2 (3%)
20	DMU	O	306	-	10,10,34	0.12	0	9,9,45	0.55	0
26	CDL	P	304	-	86,86,99	0.82	2 (2%)	92,98,111	1.47	14 (15%)
20	DMU	H	101	19	34,34,34	1.21	5 (14%)	45,45,45	1.40	6 (13%)
19	LFA	C	313	-	10,10,19	0.33	0	9,9,18	0.23	0
20	DMU	O	307	-	10,10,34	0.26	0	9,9,45	0.62	0
20	DMU	C	324	-	22,22,34	0.84	1 (4%)	27,27,45	1.04	2 (7%)
20	DMU	P	306	-	10,10,34	0.29	0	9,9,45	0.66	0
21	EDO	T	106	-	3,3,3	0.26	0	2,2,2	0.18	0
19	LFA	P	308	-	5,5,19	0.21	0	4,4,18	0.17	0
20	DMU	J	101	-	10,10,34	0.27	0	9,9,45	0.71	0
14	HEA	N	602	1	66,67,67	2.19	23 (34%)	78,103,103	2.69	33 (42%)
19	LFA	C	309	20	17,17,19	0.32	0	16,16,18	0.19	0
20	DMU	C	320	-	34,34,34	0.92	1 (2%)	45,45,45	1.31	5 (11%)
19	LFA	C	315	-	12,12,19	0.21	0	11,11,18	0.14	0
19	LFA	C	311	-	10,10,19	0.24	0	9,9,18	0.16	0
19	LFA	P	307	-	10,10,19	0.26	0	9,9,18	0.21	0
21	EDO	N	612	-	3,3,3	0.23	0	2,2,2	0.22	0
21	EDO	E	201	-	3,3,3	0.24	0	2,2,2	0.16	0
20	DMU	P	322	-	34,34,34	0.94	2 (5%)	45,45,45	1.69	10 (22%)
24	CHD	P	305	-	32,32,32	0.85	0	51,51,51	1.73	10 (19%)
20	DMU	B	308	-	22,22,34	0.73	0	27,27,45	1.55	5 (18%)
14	HEA	A	601	1	66,67,67	2.10	25 (37%)	78,103,103	2.60	28 (35%)
20	DMU	A	615	-	10,10,34	0.43	0	9,9,45	0.58	0
21	EDO	F	103	-	3,3,3	0.39	0	2,2,2	0.57	0
19	LFA	O	302	-	16,16,19	0.24	0	15,15,18	0.24	0
19	LFA	N	608	-	13,13,19	0.29	0	12,12,18	0.29	0
18	N2O	N	607	-	0,2,2	-	-	0,1,1	-	-
20	DMU	Z	102	-	22,22,34	0.63	0	27,27,45	1.02	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	DMU	A	609	-	34,34,34	1.41	5 (14%)	45,45,45	1.20	5 (11%)
19	LFA	T	104	-	10,10,19	0.34	0	9,9,18	0.31	0
19	LFA	P	310	-	10,10,19	0.22	0	9,9,18	0.13	0
20	DMU	O	308	-	22,22,34	0.87	1 (4%)	27,27,45	1.40	4 (14%)
21	EDO	P	321	-	3,3,3	0.42	0	2,2,2	1.01	0
21	EDO	N	614	-	3,3,3	0.24	0	2,2,2	0.16	0
19	LFA	T	103	-	13,13,19	0.20	0	12,12,18	0.16	0
26	CDL	I	101	-	63,63,99	0.73	0	69,75,111	1.38	10 (14%)
21	EDO	N	615	-	3,3,3	0.73	0	2,2,2	0.31	0
20	DMU	T	105	-	22,22,34	0.74	0	27,27,45	1.71	4 (14%)
26	CDL	L	101	-	93,93,99	0.65	2 (2%)	99,105,111	0.91	8 (8%)
20	DMU	N	610	-	34,34,34	1.63	9 (26%)	45,45,45	1.15	3 (6%)
20	DMU	M	101	-	34,34,34	1.45	4 (11%)	45,45,45	1.01	2 (4%)
19	LFA	A	607	-	13,13,19	0.37	0	12,12,18	0.24	0
21	EDO	D	202	-	3,3,3	0.21	0	2,2,2	0.13	0
21	EDO	A	610	-	3,3,3	0.32	0	2,2,2	0.21	0
19	LFA	C	326	-	14,14,19	0.27	0	13,13,18	0.18	0
20	DMU	B	303	-	10,10,34	0.29	0	9,9,45	0.72	0
21	EDO	S	102	-	3,3,3	0.41	0	2,2,2	0.54	0
19	LFA	P	311	-	10,10,19	0.24	0	9,9,18	0.28	0
19	LFA	P	313	-	12,12,19	0.32	0	11,11,18	0.29	0
24	CHD	O	301	-	32,32,32	0.69	0	51,51,51	0.99	2 (3%)
20	DMU	C	316	-	34,34,34	0.99	3 (8%)	45,45,45	1.57	6 (13%)
19	LFA	C	310	-	14,14,19	0.26	0	13,13,18	0.10	0
20	DMU	A	608	-	6,6,34	0.60	0	5,5,45	0.31	0
20	DMU	G	102	-	10,10,34	0.40	0	9,9,45	0.50	0
21	EDO	N	611	-	3,3,3	0.50	0	2,2,2	0.07	0
22	PGV	N	616	-	50,50,50	0.93	3 (6%)	53,56,56	1.28	4 (7%)
26	CDL	C	304	-	86,86,99	0.81	3 (3%)	92,98,111	1.31	11 (11%)
19	LFA	C	312	-	13,13,19	0.25	0	12,12,18	0.19	0
26	CDL	Y	101	-	93,93,99	0.56	0	99,105,111	0.83	6 (6%)
20	DMU	Z	101	-	34,34,34	1.02	3 (8%)	45,45,45	1.23	5 (11%)
20	DMU	C	306	-	10,10,34	0.27	0	9,9,45	0.61	0
21	EDO	S	103	-	3,3,3	0.39	0	2,2,2	0.24	0
21	EDO	P	320	-	3,3,3	0.46	0	2,2,2	0.22	0
19	LFA	P	312	-	14,14,19	0.61	0	13,13,18	0.28	0
21	EDO	P	319	-	3,3,3	0.33	0	2,2,2	0.19	0
20	DMU	W	101	-	10,10,34	0.24	0	9,9,45	0.57	0
23	CUA	O	305	2	0,1,1	-	-	-		
20	DMU	C	325	-	34,34,34	0.95	1 (2%)	45,45,45	1.19	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	DMU	O	304	-	22,22,34	0.95	1 (4%)	27,27,45	1.50	4 (14%)
24	CHD	P	301	-	32,32,32	0.91	1 (3%)	51,51,51	0.93	3 (5%)
20	DMU	N	609	-	6,6,34	0.22	0	5,5,45	0.40	0
19	LFA	G	104	-	13,13,19	0.52	0	12,12,18	0.27	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	LFA	C	307	-	-	5/8/8/17	-
19	LFA	T	101	-	-	6/11/11/17	-
21	EDO	R	203	-	-	1/1/1/1	-
20	DMU	C	318	-	-	9/13/33/59	0/1/1/2
20	DMU	B	304	-	-	6/13/33/59	0/1/1/2
21	EDO	C	323	-	-	1/1/1/1	-
22	PGV	P	303	-	-	10/55/55/55	-
20	DMU	D	201	-	-	9/19/59/59	0/2/2/2
20	DMU	C	319	-	-	12/19/59/59	0/2/2/2
20	DMU	L	102	-	-	9/13/33/59	0/1/1/2
21	EDO	N	613	-	-	1/1/1/1	-
21	EDO	R	201	-	-	1/1/1/1	-
24	CHD	C	305	-	-	7/9/74/74	0/4/4/4
22	PGV	C	303	-	-	13/55/55/55	-
21	EDO	A	611	-	-	1/1/1/1	-
22	PGV	A	614	-	-	7/55/55/55	-
26	CDL	N	606	-	-	45/74/74/110	-
20	DMU	U	101	19	-	7/19/59/59	0/2/2/2
20	DMU	Q	201	-	-	7/19/59/59	0/2/2/2
20	DMU	P	318	-	-	11/19/59/59	0/2/2/2
20	DMU	Z	103	-	-	3/5/5/59	-
20	DMU	B	302	-	-	5/8/8/59	-
21	EDO	B	305	-	-	0/1/1/1	-
20	DMU	P	314	-	-	8/19/59/59	0/2/2/2
20	DMU	M	102	-	-	3/5/5/59	-
14	HEA	A	602	1	-	6/36/76/76	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	HEA	N	601	1	-	2/36/76/76	-
21	EDO	R	202	-	-	0/1/1/1	-
24	CHD	B	306	-	-	2/9/74/74	0/4/4/4
21	EDO	C	322	-	-	0/1/1/1	-
21	EDO	A	613	-	-	0/1/1/1	-
19	LFA	B	307	-	-	7/14/14/17	-
19	LFA	C	308	-	-	0/3/3/17	-
21	EDO	A	612	-	-	0/1/1/1	-
21	EDO	G	103	-	-	0/1/1/1	-
21	EDO	C	321	-	-	1/1/1/1	-
20	DMU	P	317	-	-	14/19/59/59	0/2/2/2
20	DMU	P	315	-	-	2/4/4/59	-
24	CHD	C	301	-	-	2/9/74/74	0/4/4/4
19	LFA	O	303	-	-	3/8/8/17	-
21	EDO	O	309	-	-	0/1/1/1	-
20	DMU	C	317	-	-	3/4/4/59	-
19	LFA	P	309	20	-	9/15/15/17	-
28	PEK	T	102	-	-	21/56/56/56	-
21	EDO	F	102	-	-	0/1/1/1	-
19	LFA	C	314	-	-	5/12/12/17	-
20	DMU	P	316	-	-	8/13/33/59	0/1/1/2
21	EDO	E	202	-	-	0/1/1/1	-
28	PEK	G	101	-	-	14/56/56/56	-
20	DMU	O	306	-	-	6/8/8/59	-
26	CDL	P	304	-	-	58/97/97/110	-
20	DMU	H	101	19	-	7/19/59/59	0/2/2/2
19	LFA	C	313	-	-	4/8/8/17	-
20	DMU	O	307	-	-	5/8/8/59	-
20	DMU	C	324	-	-	7/13/33/59	0/1/1/2
20	DMU	P	306	-	-	4/8/8/59	-
21	EDO	T	106	-	-	0/1/1/1	-
19	LFA	P	308	-	-	0/3/3/17	-
20	DMU	J	101	-	-	3/8/8/59	-
14	HEA	N	602	1	-	6/36/76/76	-
19	LFA	C	309	20	-	10/15/15/17	-
20	DMU	C	320	-	-	11/19/59/59	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	LFA	C	315	-	-	3/10/10/17	-
19	LFA	C	311	-	-	7/8/8/17	-
19	LFA	P	307	-	-	2/8/8/17	-
21	EDO	N	612	-	-	0/1/1/1	-
21	EDO	E	201	-	-	0/1/1/1	-
20	DMU	P	322	-	-	4/19/59/59	0/2/2/2
24	CHD	P	305	-	-	7/9/74/74	0/4/4/4
20	DMU	B	308	-	-	9/13/33/59	0/1/1/2
14	HEA	A	601	1	-	4/36/76/76	-
20	DMU	A	615	-	-	5/8/8/59	-
21	EDO	F	103	-	-	1/1/1/1	-
19	LFA	O	302	-	-	5/14/14/17	-
19	LFA	N	608	-	-	4/11/11/17	-
20	DMU	Z	102	-	-	11/13/33/59	0/1/1/2
20	DMU	A	609	-	-	5/19/59/59	0/2/2/2
19	LFA	T	104	-	-	4/8/8/17	-
19	LFA	P	310	-	-	5/8/8/17	-
20	DMU	O	308	-	-	3/13/33/59	0/1/1/2
21	EDO	P	321	-	-	1/1/1/1	-
21	EDO	N	614	-	-	0/1/1/1	-
19	LFA	T	103	-	-	5/11/11/17	-
26	CDL	I	101	-	-	36/74/74/110	-
21	EDO	N	615	-	-	0/1/1/1	-
20	DMU	T	105	-	-	10/13/33/59	0/1/1/2
26	CDL	L	101	-	-	49/104/104/110	-
20	DMU	N	610	-	-	5/19/59/59	0/2/2/2
20	DMU	M	101	-	-	5/19/59/59	0/2/2/2
19	LFA	A	607	-	-	3/11/11/17	-
21	EDO	D	202	-	-	0/1/1/1	-
21	EDO	A	610	-	-	0/1/1/1	-
19	LFA	C	326	-	-	8/12/12/17	-
20	DMU	B	303	-	-	5/8/8/59	-
21	EDO	S	102	-	-	0/1/1/1	-
19	LFA	P	311	-	-	3/8/8/17	-
19	LFA	P	313	-	-	2/10/10/17	-
24	CHD	O	301	-	-	2/9/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	DMU	C	316	-	-	12/19/59/59	0/2/2/2
19	LFA	C	310	-	-	8/12/12/17	-
20	DMU	A	608	-	-	2/4/4/59	-
20	DMU	G	102	-	-	2/8/8/59	-
21	EDO	N	611	-	-	0/1/1/1	-
22	PGV	N	616	-	-	10/55/55/55	-
26	CDL	C	304	-	-	49/97/97/110	-
19	LFA	C	312	-	-	6/11/11/17	-
26	CDL	Y	101	-	-	47/104/104/110	-
20	DMU	Z	101	-	-	6/19/59/59	0/2/2/2
20	DMU	C	306	-	-	1/8/8/59	-
21	EDO	S	103	-	-	0/1/1/1	-
21	EDO	P	320	-	-	0/1/1/1	-
19	LFA	P	312	-	-	7/12/12/17	-
21	EDO	P	319	-	-	1/1/1/1	-
20	DMU	W	101	-	-	2/8/8/59	-
20	DMU	C	325	-	-	6/19/59/59	0/2/2/2
20	DMU	O	304	-	-	6/13/33/59	0/1/1/2
24	CHD	P	301	-	-	2/9/74/74	0/4/4/4
20	DMU	N	609	-	-	1/4/4/59	-
19	LFA	G	104	-	-	7/11/11/17	-

The worst 5 of 188 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	602	HEA	C1D-ND	-5.92	1.30	1.40
14	A	602	HEA	C1D-ND	-5.75	1.30	1.40
14	N	602	HEA	CHB-C4A	5.35	1.48	1.38
14	A	601	HEA	C3A-C2A	5.29	1.48	1.36
14	A	601	HEA	C1D-ND	-5.08	1.31	1.40

The worst 5 of 334 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	N	601	HEA	C3C-C4C-NC	8.55	115.51	110.25
14	A	601	HEA	C3C-C4C-NC	8.41	115.42	110.25
14	N	602	HEA	C3C-C4C-NC	7.98	115.16	110.25
14	N	601	HEA	C2B-C1B-NB	7.50	118.87	109.88
14	N	602	HEA	C3D-C4D-ND	7.18	117.31	110.36

There are no chirality outliers.

5 of 795 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	B	304	DMU	C1-C6-O16-C18
20	B	304	DMU	O5-C6-O16-C18
20	B	304	DMU	C19-C18-O16-C6
20	B	308	DMU	O5-C6-O16-C18
20	B	308	DMU	C19-C18-O16-C6

There are no ring outliers.

50 monomers are involved in 154 short contacts:

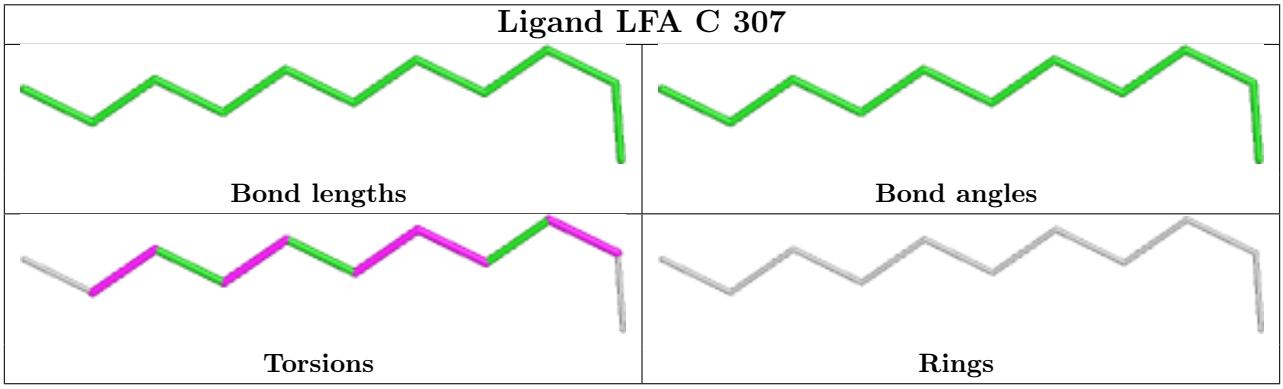
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	C	307	LFA	3	0
19	T	101	LFA	6	0
22	P	303	PGV	1	0
20	D	201	DMU	2	0
24	C	305	CHD	2	0
22	C	303	PGV	2	0
21	A	611	EDO	1	0
26	N	606	CDL	6	0
20	Q	201	DMU	3	0
14	A	602	HEA	2	0
14	N	601	HEA	2	0
19	B	307	LFA	4	0
19	O	303	LFA	1	0
19	P	309	LFA	2	0
28	T	102	PEK	4	0
19	C	314	LFA	3	0
26	P	304	CDL	16	0
20	H	101	DMU	1	0
19	C	313	LFA	1	0
20	C	324	DMU	1	0
14	N	602	HEA	2	0
19	C	309	LFA	2	0
20	C	320	DMU	1	0
19	C	315	LFA	1	0
19	P	307	LFA	1	0
20	P	322	DMU	2	0
24	P	305	CHD	3	0
14	A	601	HEA	4	0
20	A	615	DMU	1	0
19	O	302	LFA	3	0

Continued on next page...

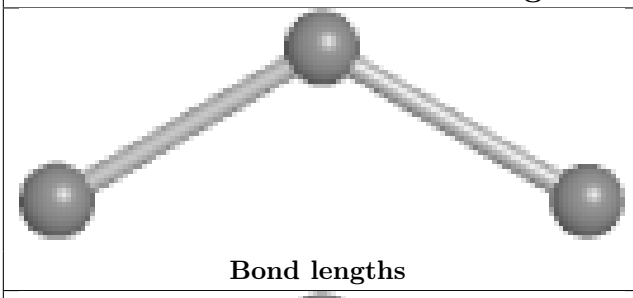
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	N	608	LFA	5	0
20	Z	102	DMU	3	0
20	A	609	DMU	1	0
26	I	101	CDL	3	0
21	N	615	EDO	1	0
20	T	105	DMU	1	0
26	L	101	CDL	4	0
19	A	607	LFA	7	0
19	P	311	LFA	1	0
24	O	301	CHD	1	0
20	A	608	DMU	1	0
22	N	616	PGV	2	0
26	C	304	CDL	24	0
26	Y	101	CDL	10	0
20	Z	101	DMU	1	0
19	P	312	LFA	2	0
20	C	325	DMU	3	0
20	O	304	DMU	1	0
24	P	301	CHD	2	0
19	G	104	LFA	5	0

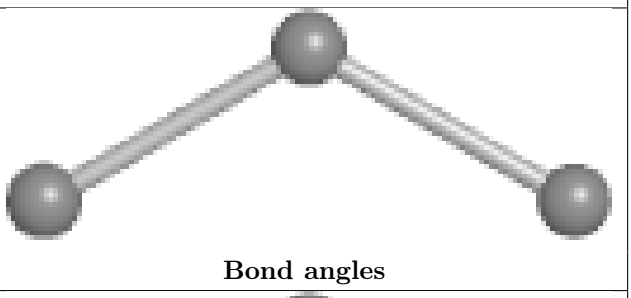
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



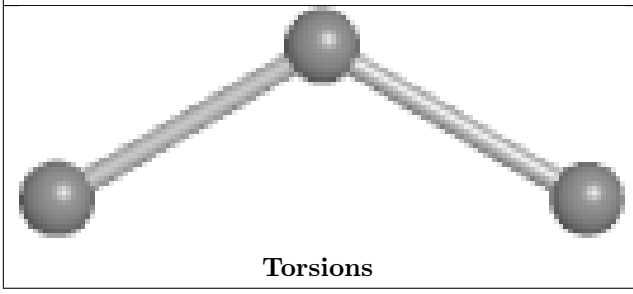
Ligand N2O A 606



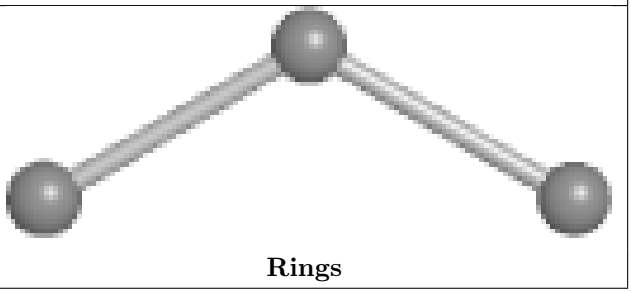
Bond lengths



Bond angles

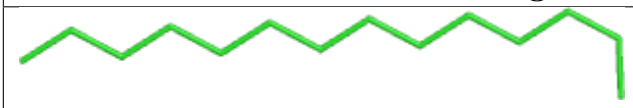


Torsions

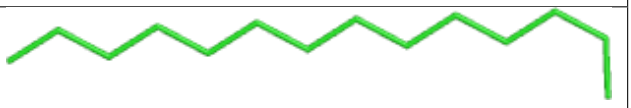


Rings

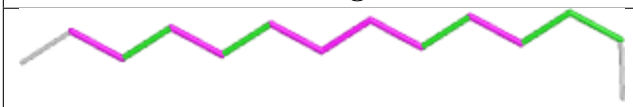
Ligand LFA T 101



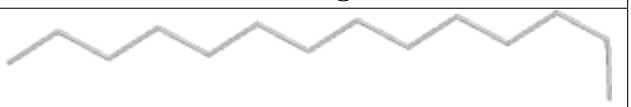
Bond lengths



Bond angles

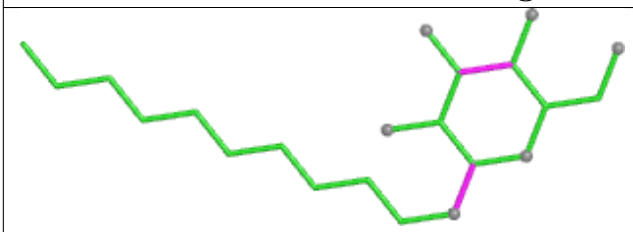


Torsions

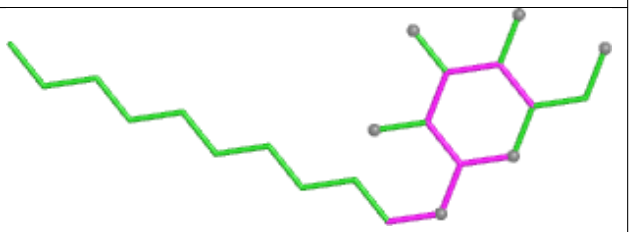


Rings

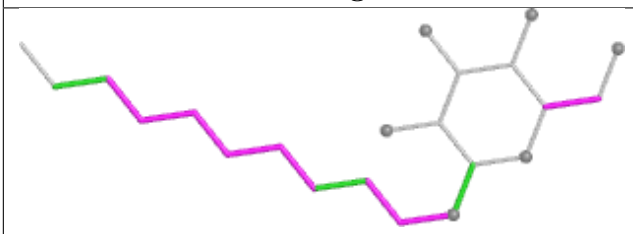
Ligand DMU C 318



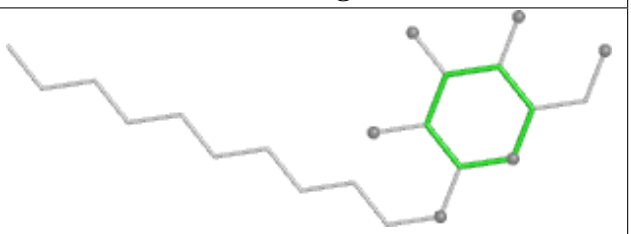
Bond lengths



Bond angles

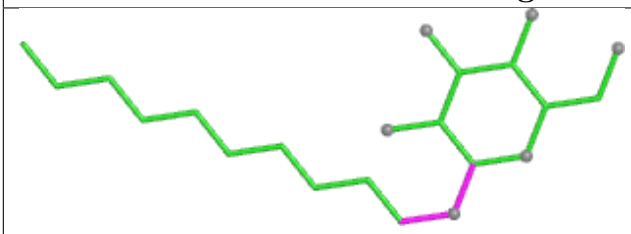


Torsions

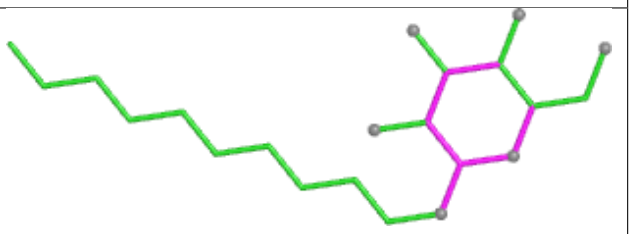


Rings

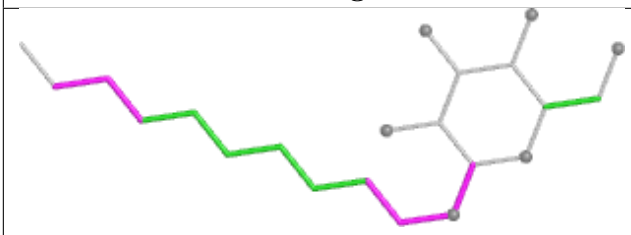
Ligand DMU B 304



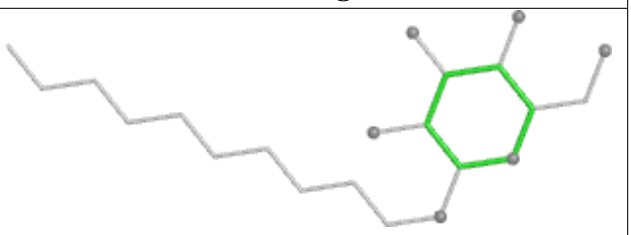
Bond lengths



Bond angles

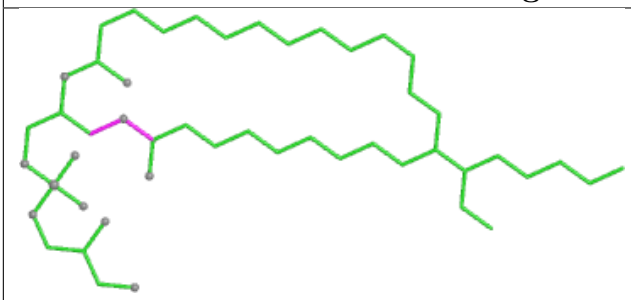


Torsions

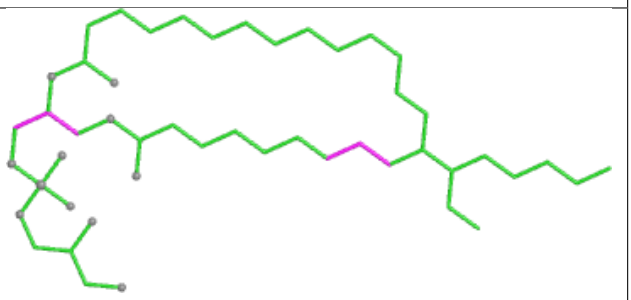


Rings

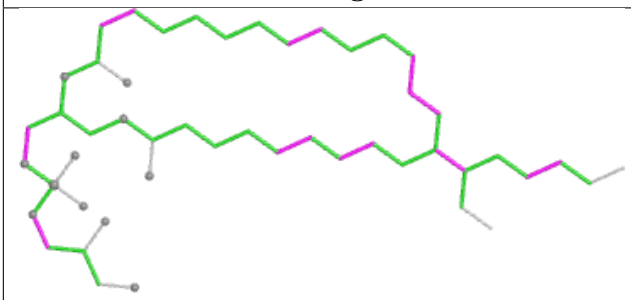
Ligand PGV P 303



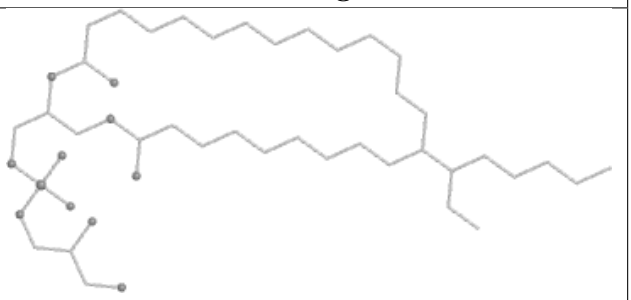
Bond lengths



Bond angles

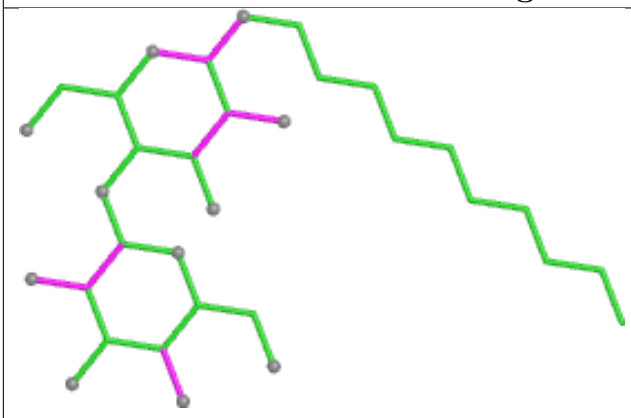


Torsions

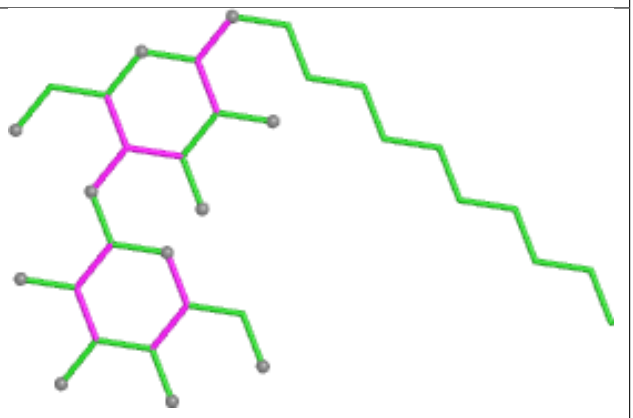


Rings

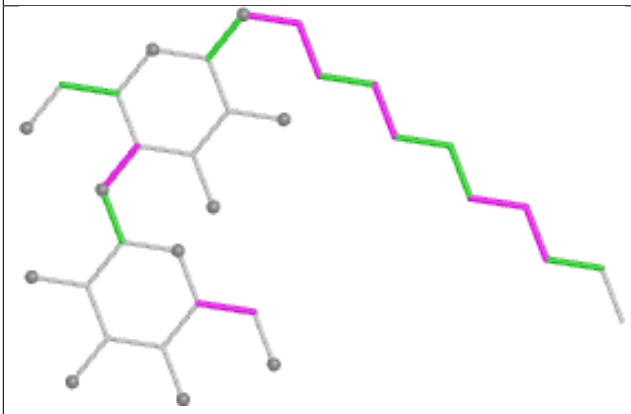
Ligand DMU D 201



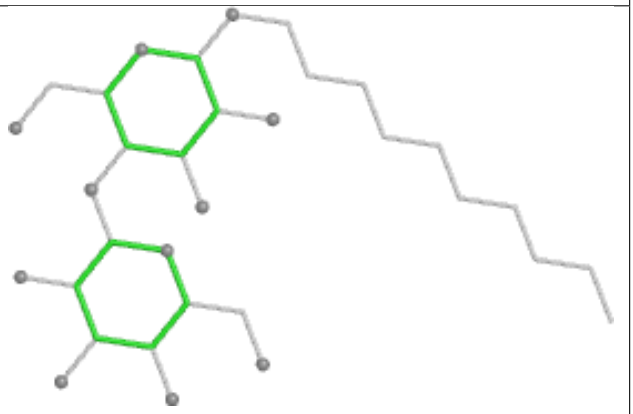
Bond lengths



Bond angles

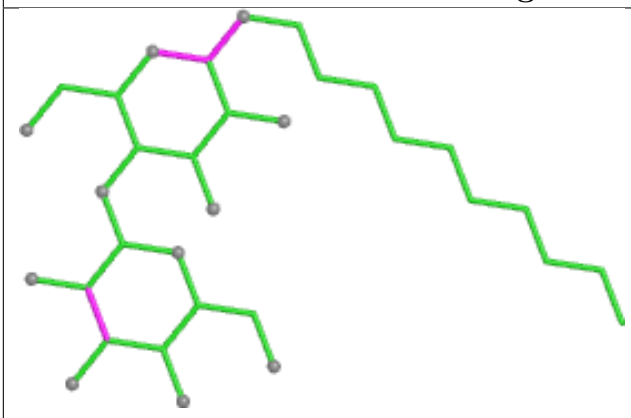


Torsions

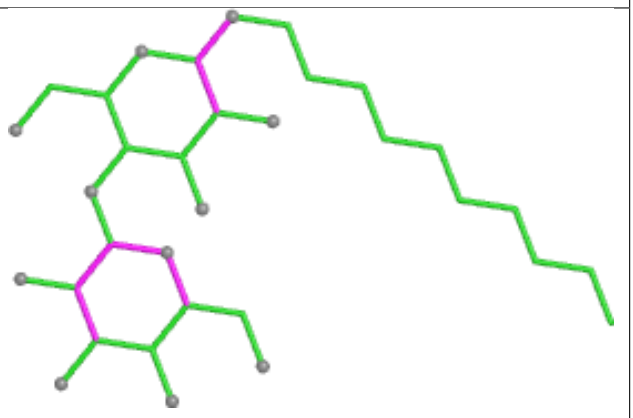


Rings

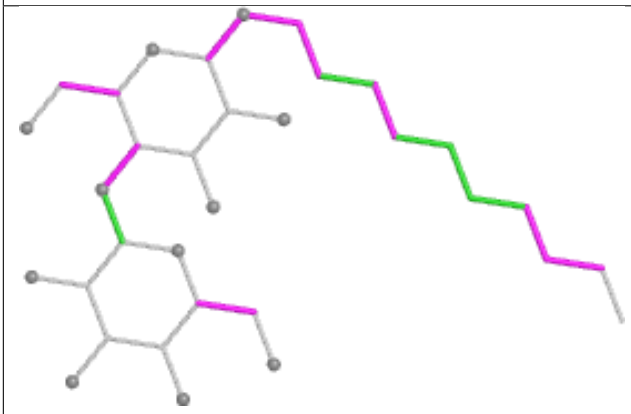
Ligand DMU C 319



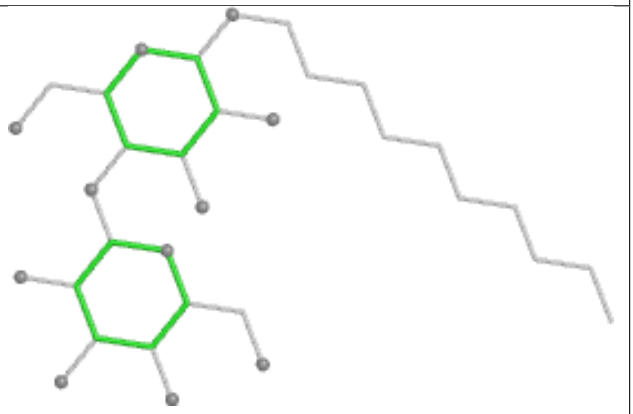
Bond lengths



Bond angles

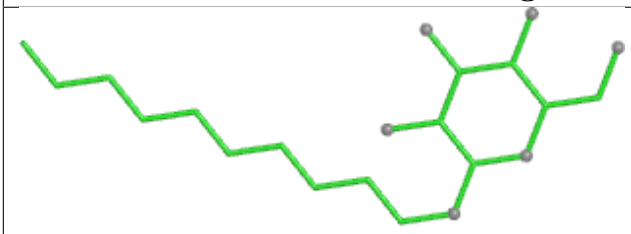


Torsions

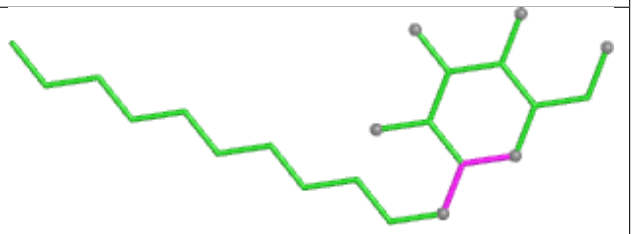


Rings

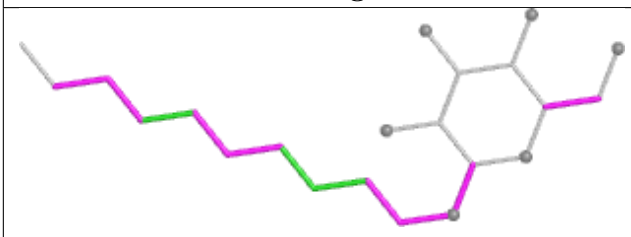
Ligand DMU L 102



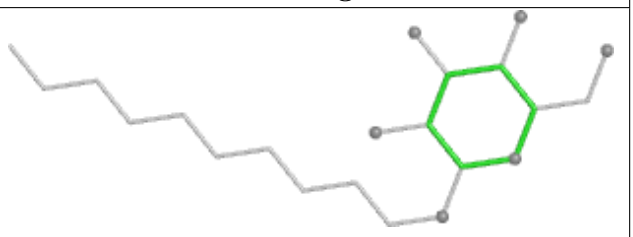
Bond lengths



Bond angles

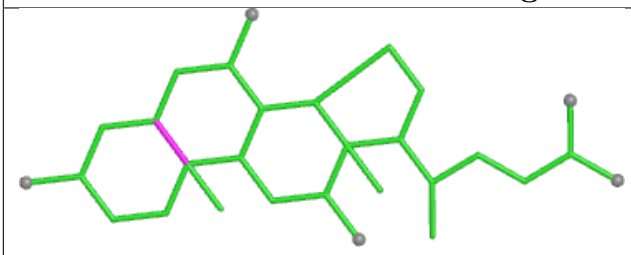


Torsions

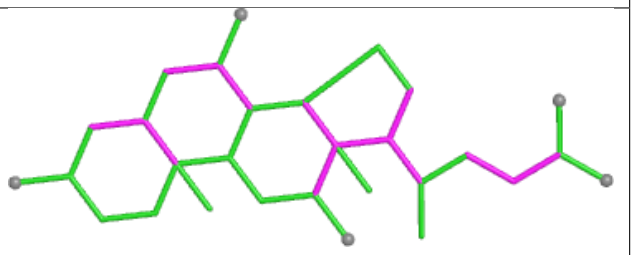


Rings

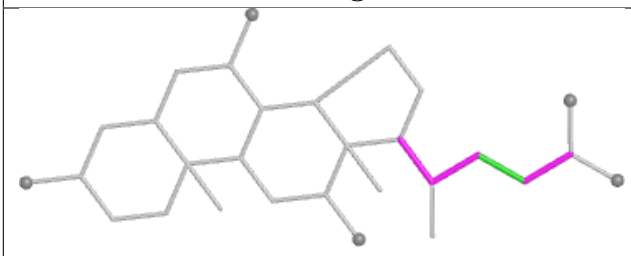
Ligand CHD C 305



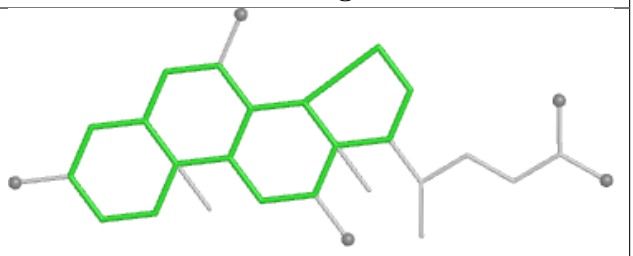
Bond lengths



Bond angles

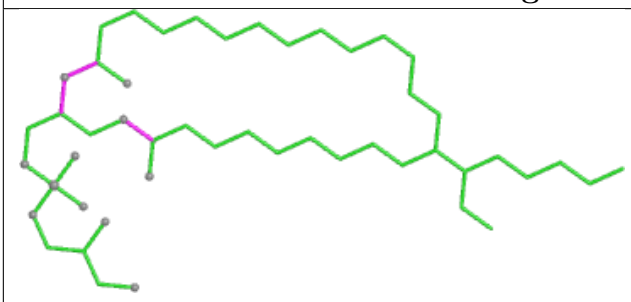


Torsions

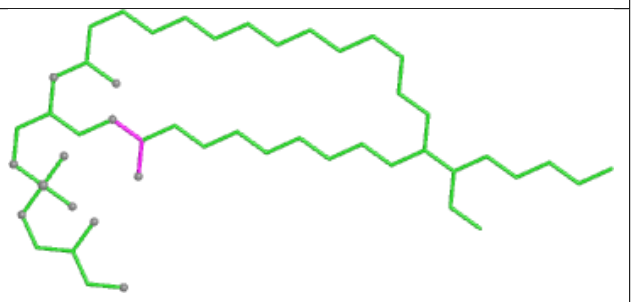


Rings

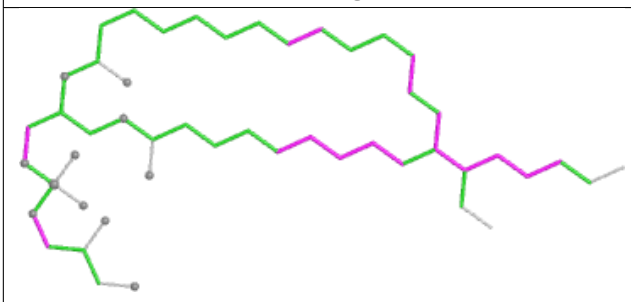
Ligand PGV C 303



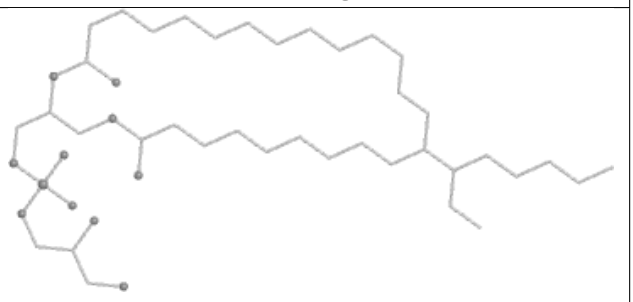
Bond lengths



Bond angles

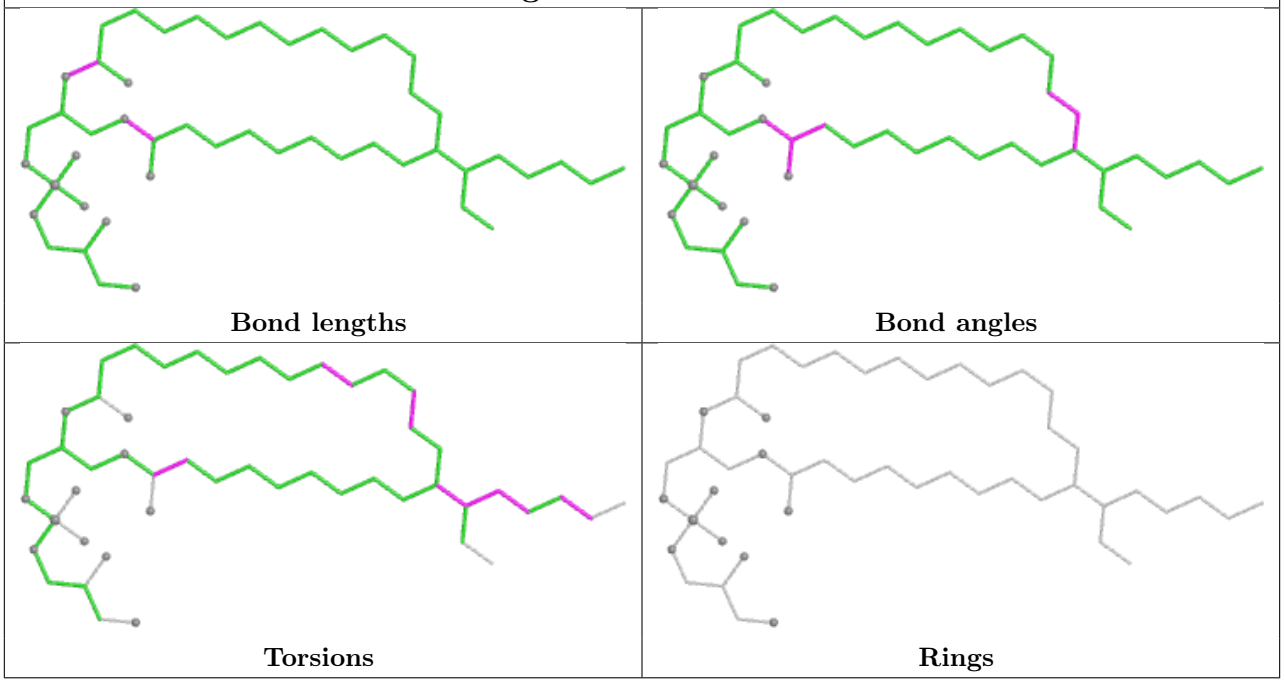


Torsions

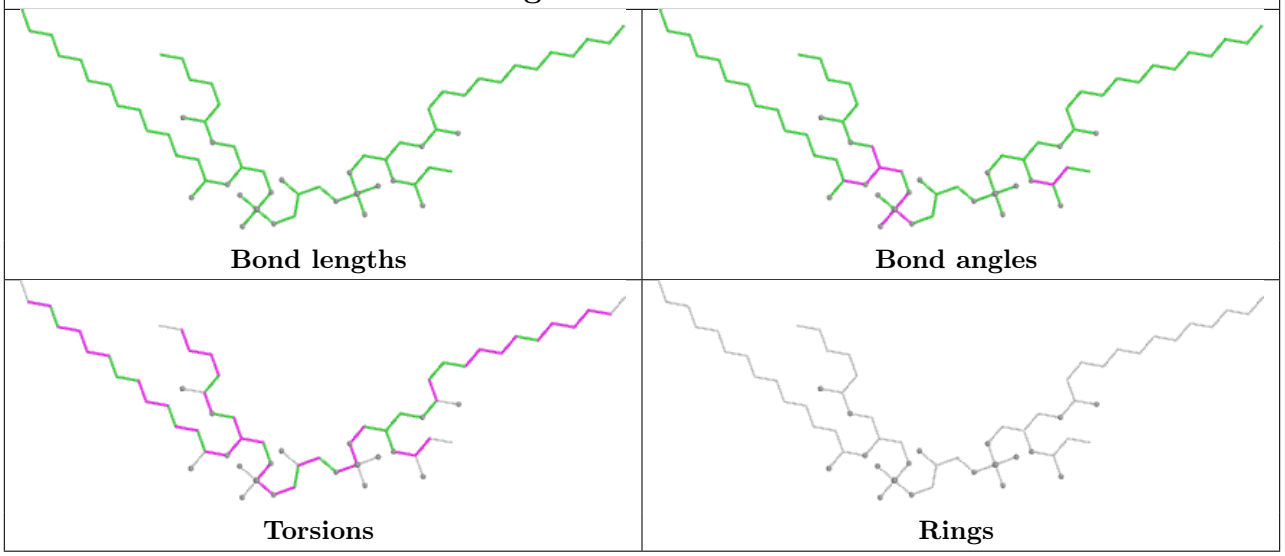


Rings

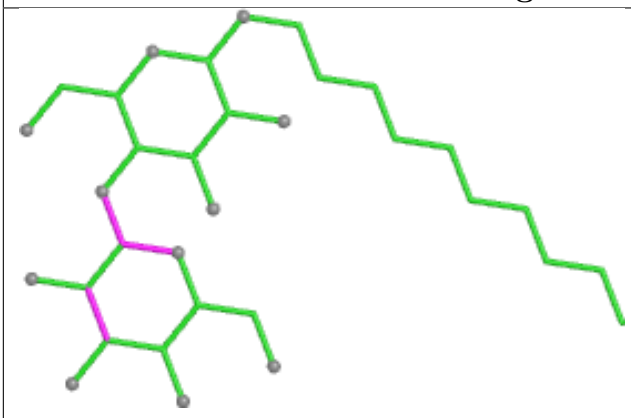
Ligand PGV A 614



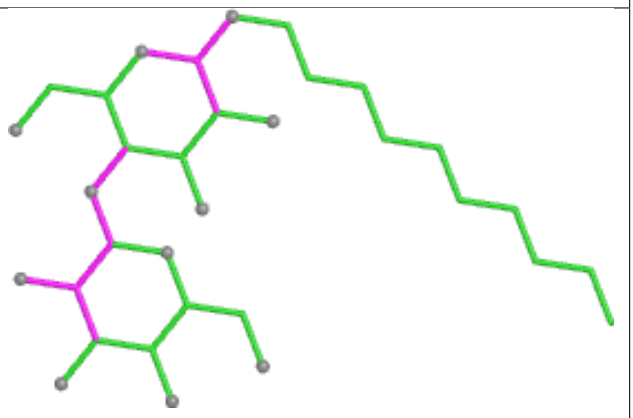
Ligand CDL N 606



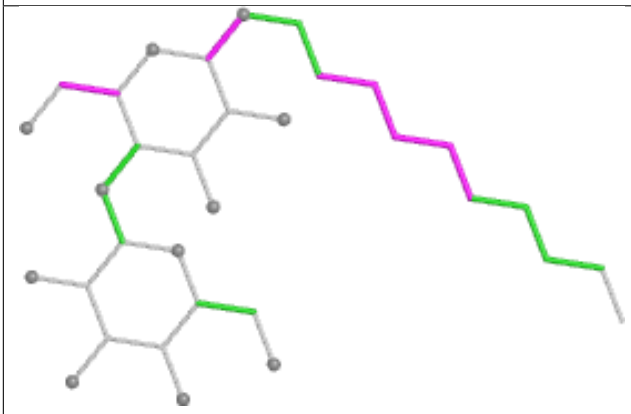
Ligand DMU U 101



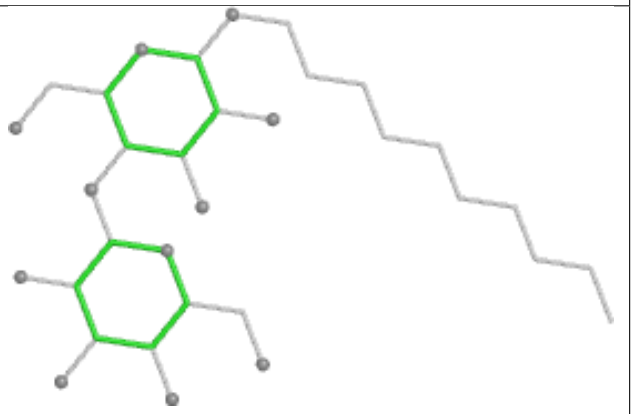
Bond lengths



Bond angles

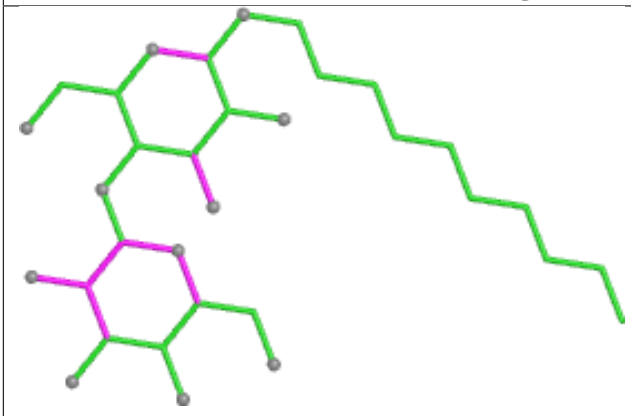


Torsions

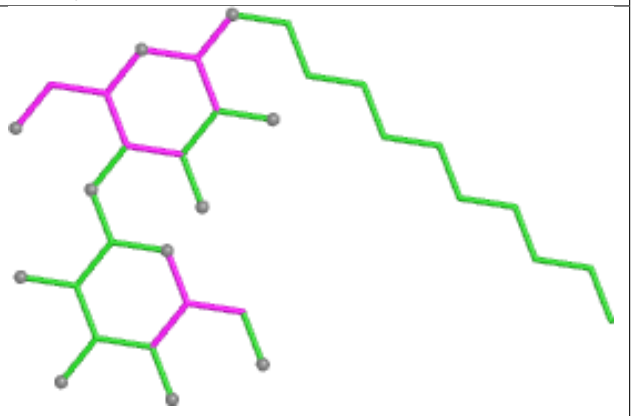


Rings

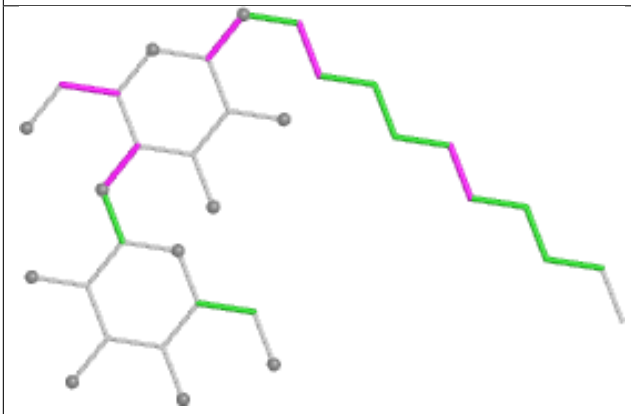
Ligand DMU Q 201



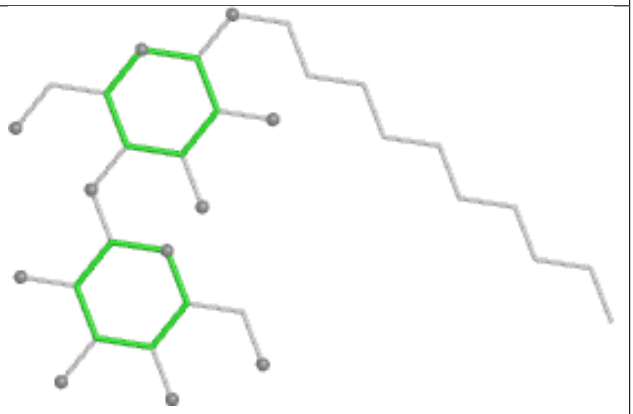
Bond lengths



Bond angles

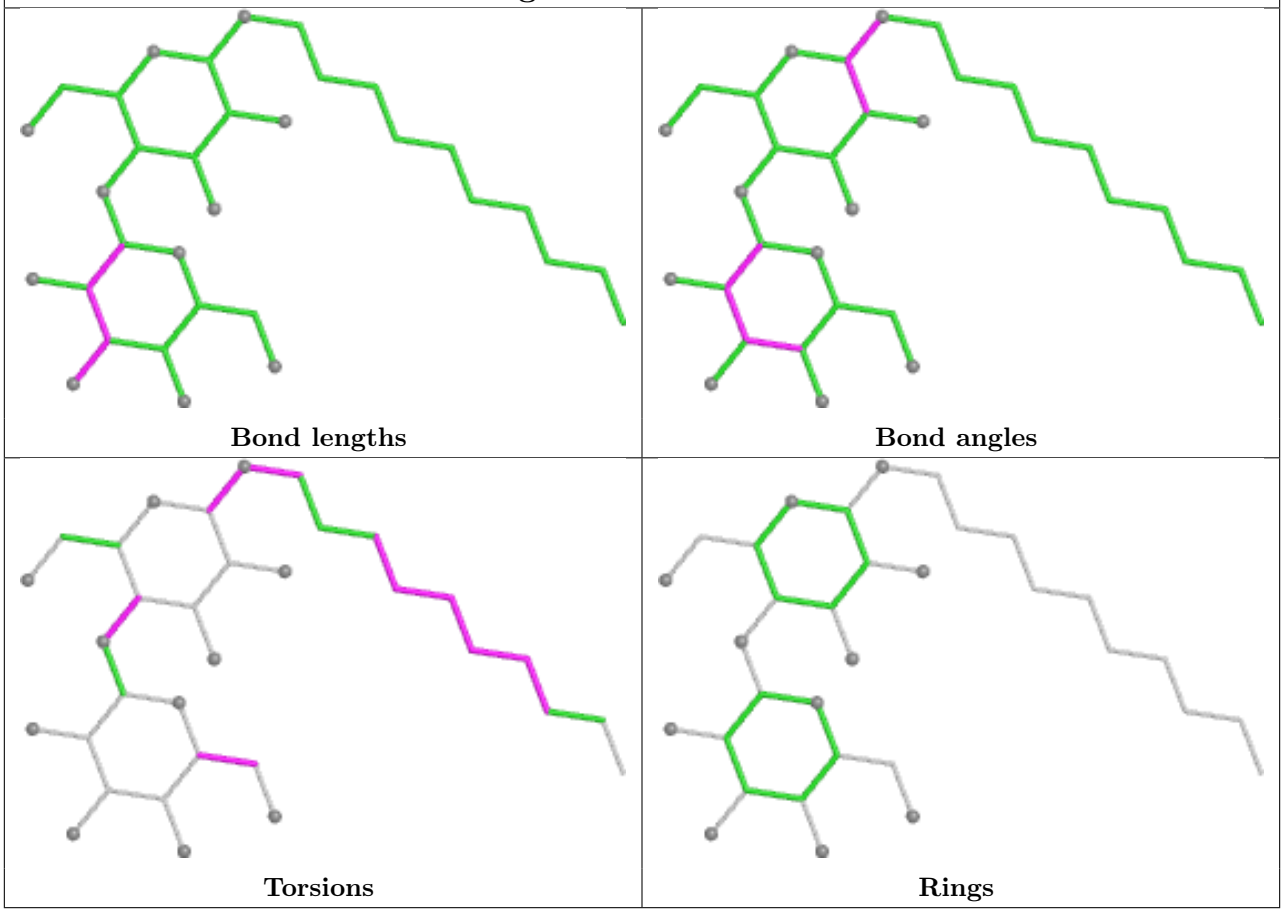


Torsions

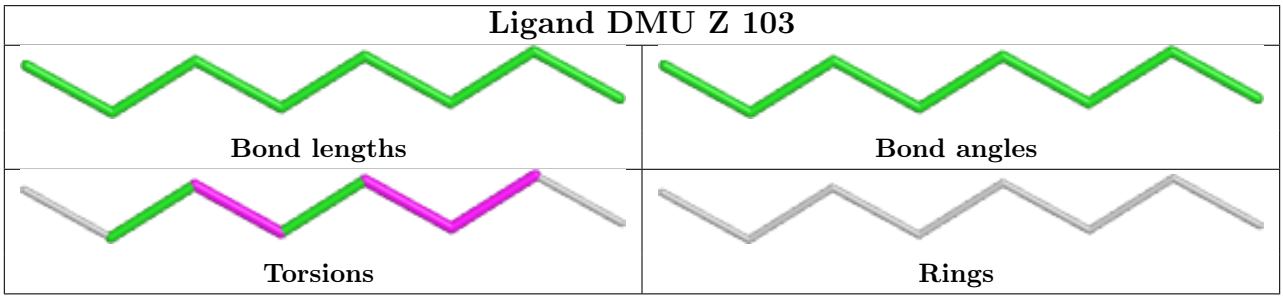


Rings

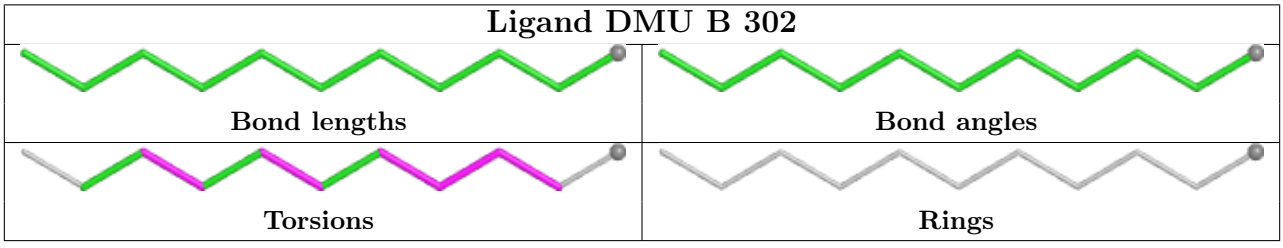
Ligand DMU P 318



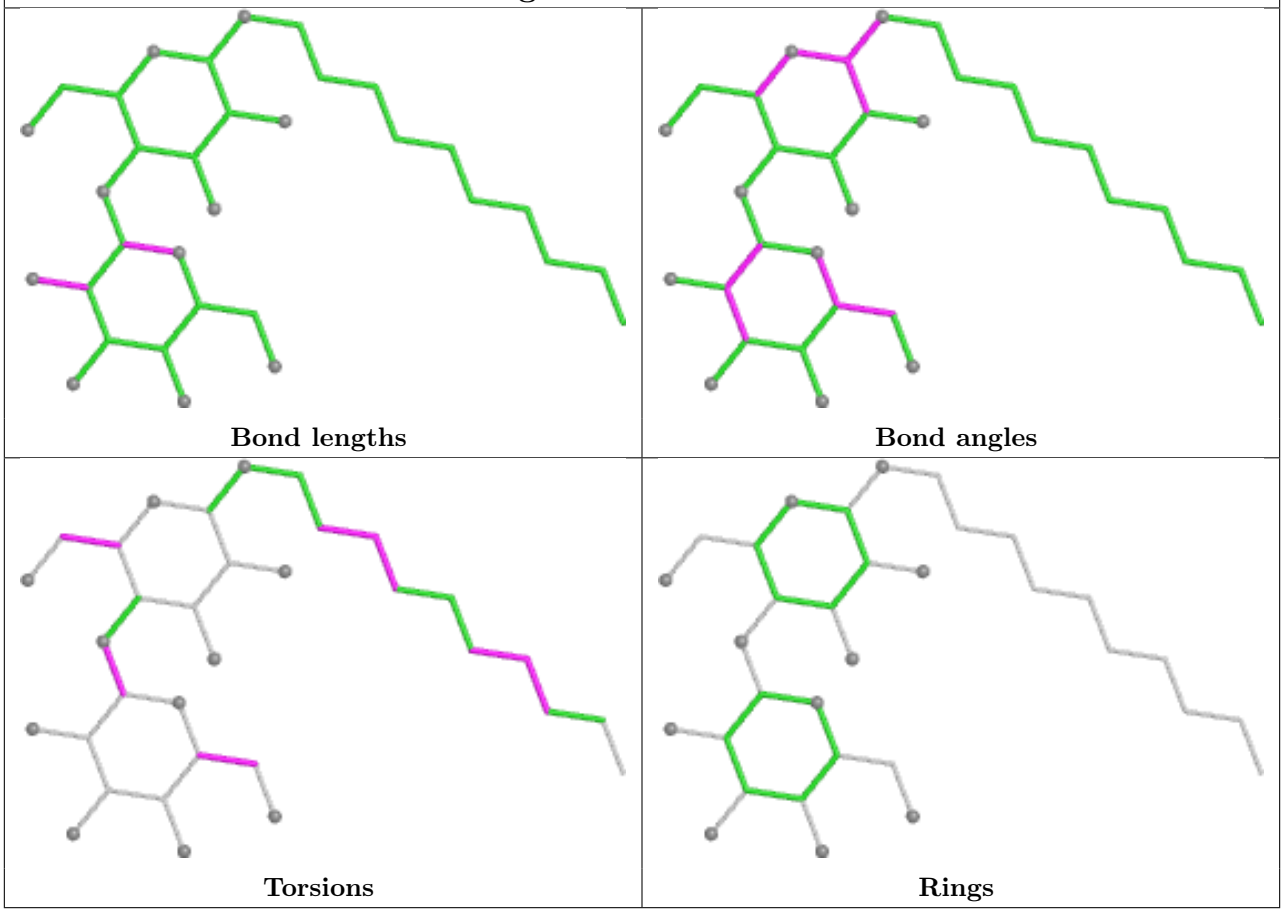
Ligand DMU Z 103



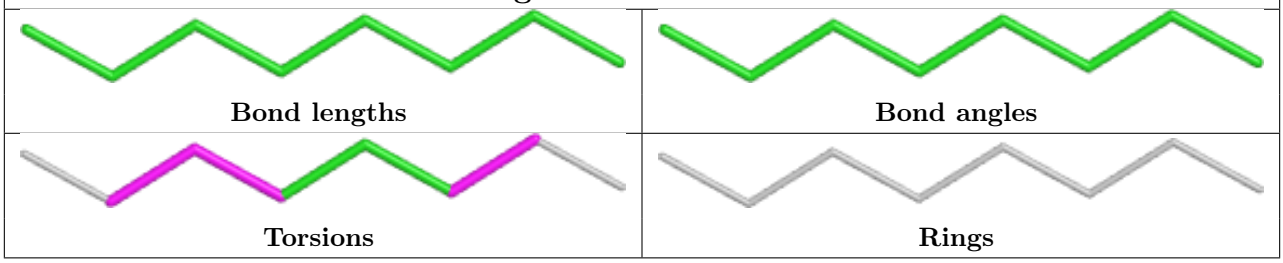
Ligand DMU B 302



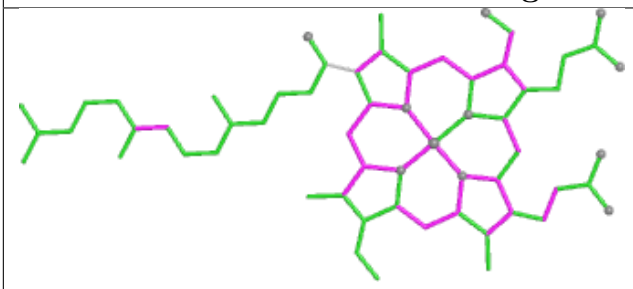
Ligand DMU P 314



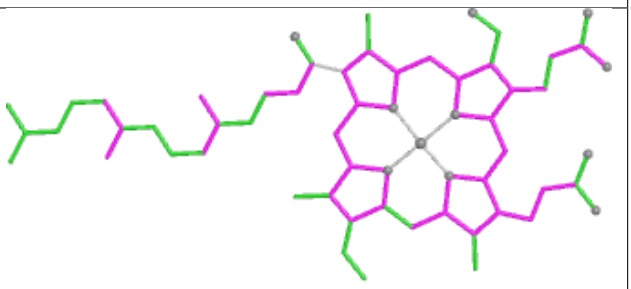
Ligand DMU M 102



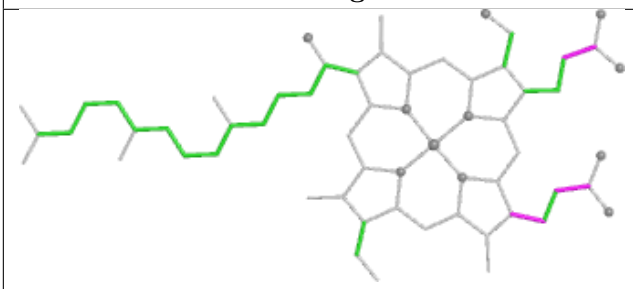
Ligand HEA A 602



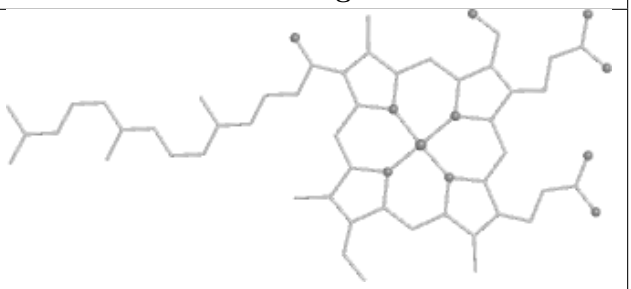
Bond lengths



Bond angles

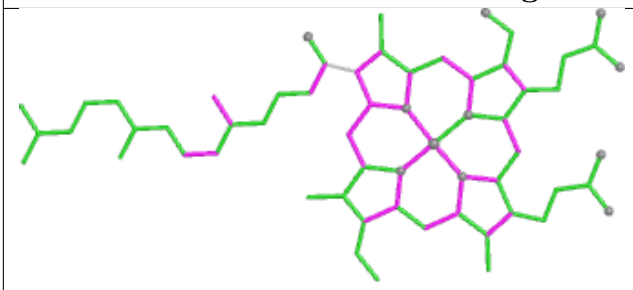


Torsions

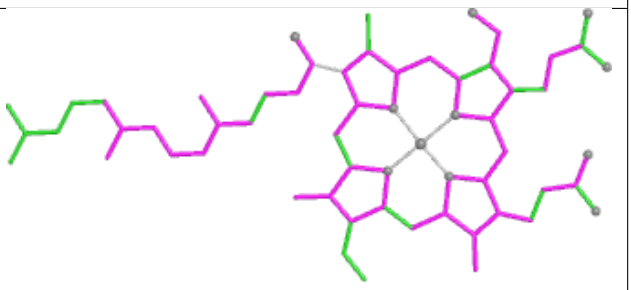


Rings

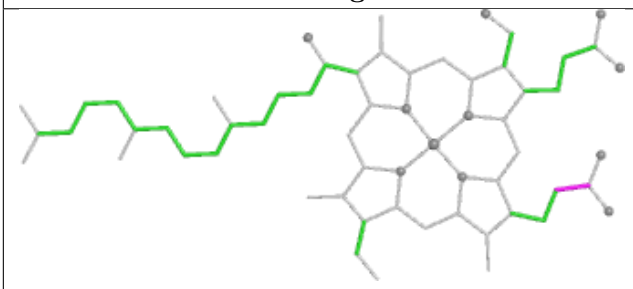
Ligand HEA N 601



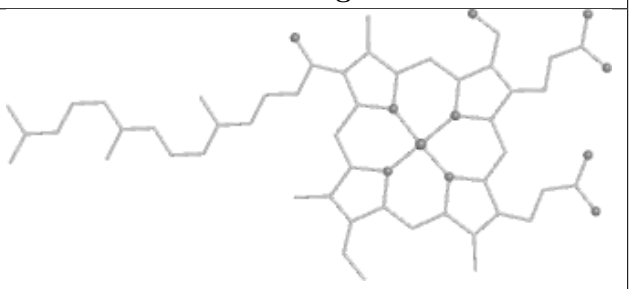
Bond lengths



Bond angles

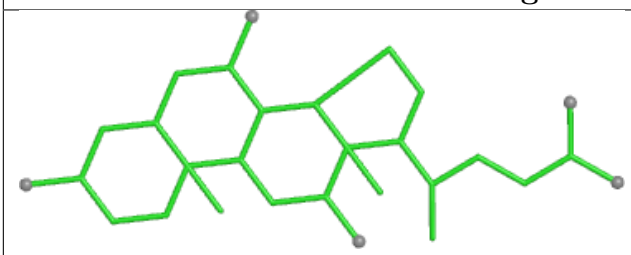


Torsions

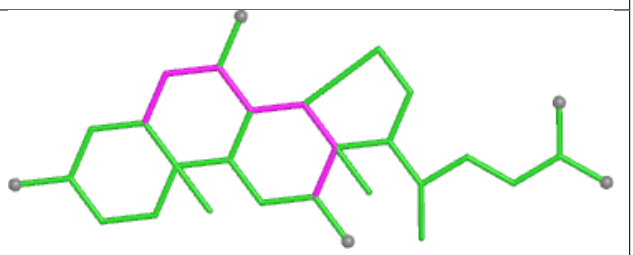


Rings

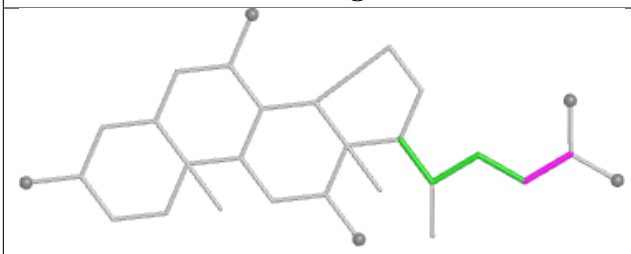
Ligand CHD B 306



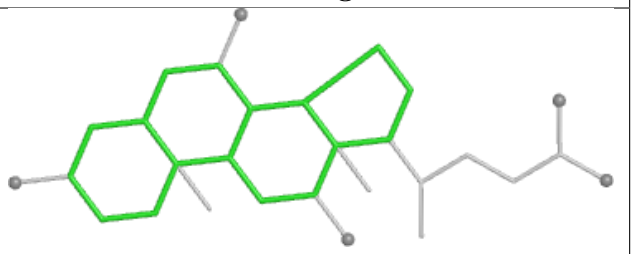
Bond lengths



Bond angles

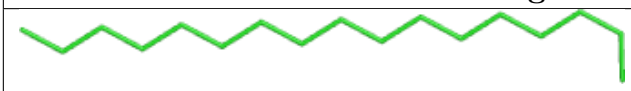


Torsions

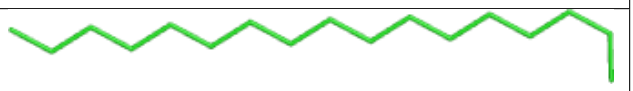


Rings

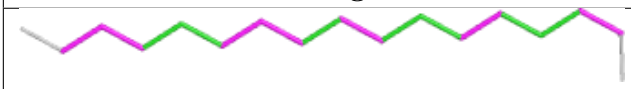
Ligand LFA B 307



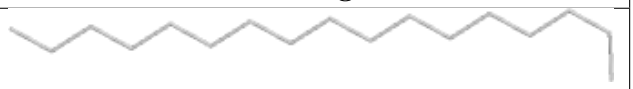
Bond lengths



Bond angles

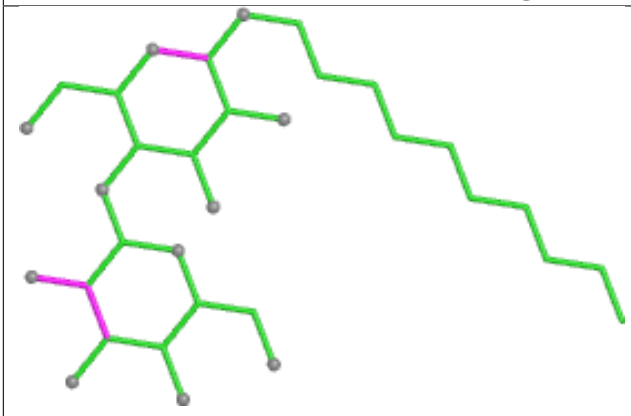


Torsions

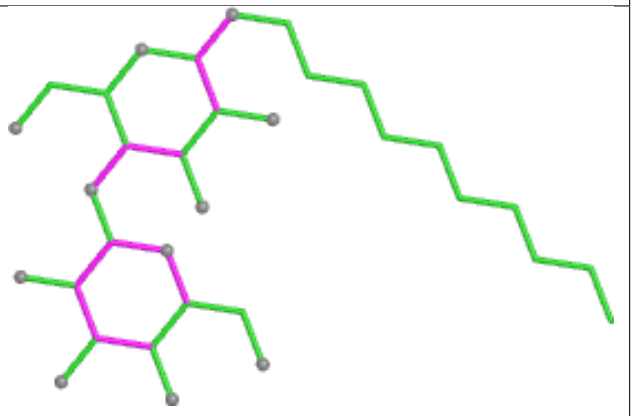


Rings

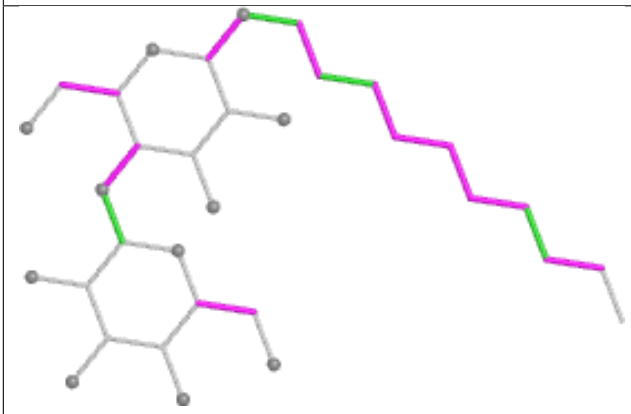
Ligand DMU P 317



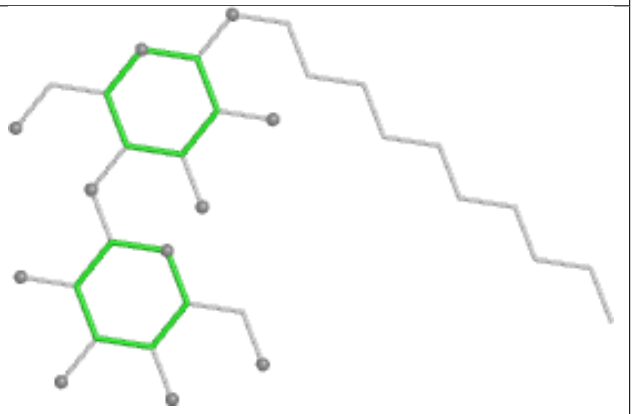
Bond lengths



Bond angles



Torsions



Rings

Ligand DMU P 315



Bond lengths



Bond angles

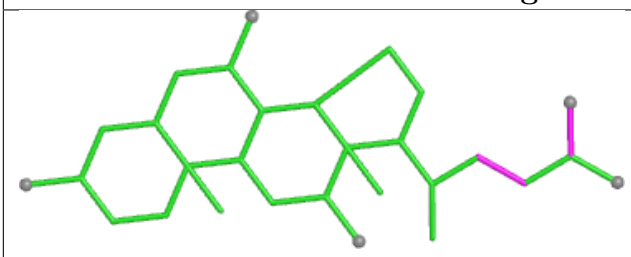


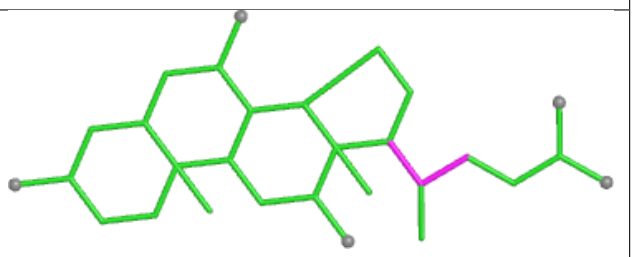
Torsions

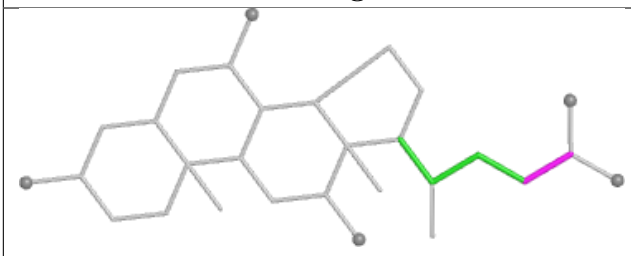


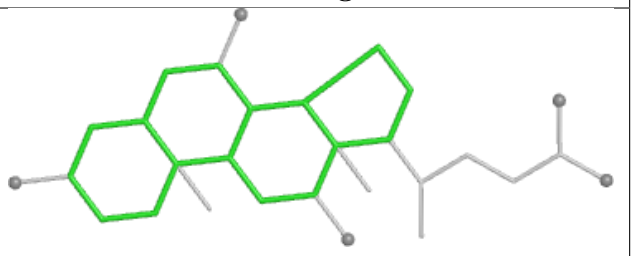
Rings

Ligand CHD C 301

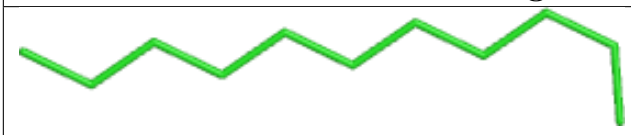

Bond lengths

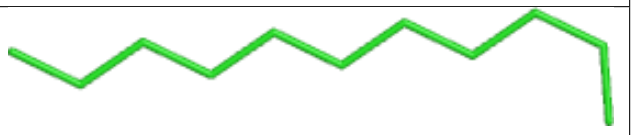

Bond angles

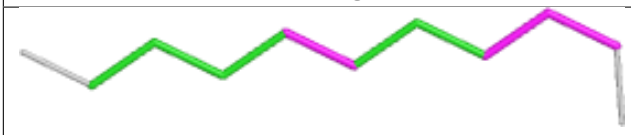

Torsions

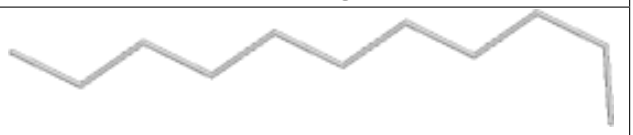

Rings

Ligand LFA O 303

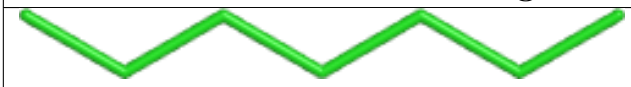

Bond lengths

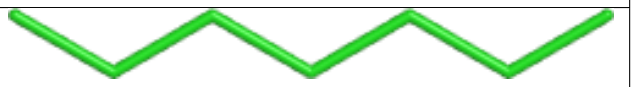

Bond angles


Torsions


Rings

Ligand DMU C 317


Bond lengths


Bond angles

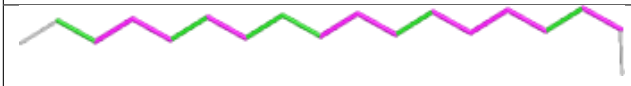

Torsions

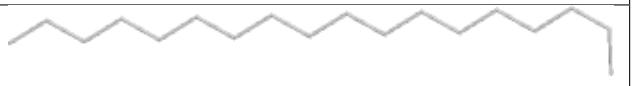

Rings

Ligand LFA P 309

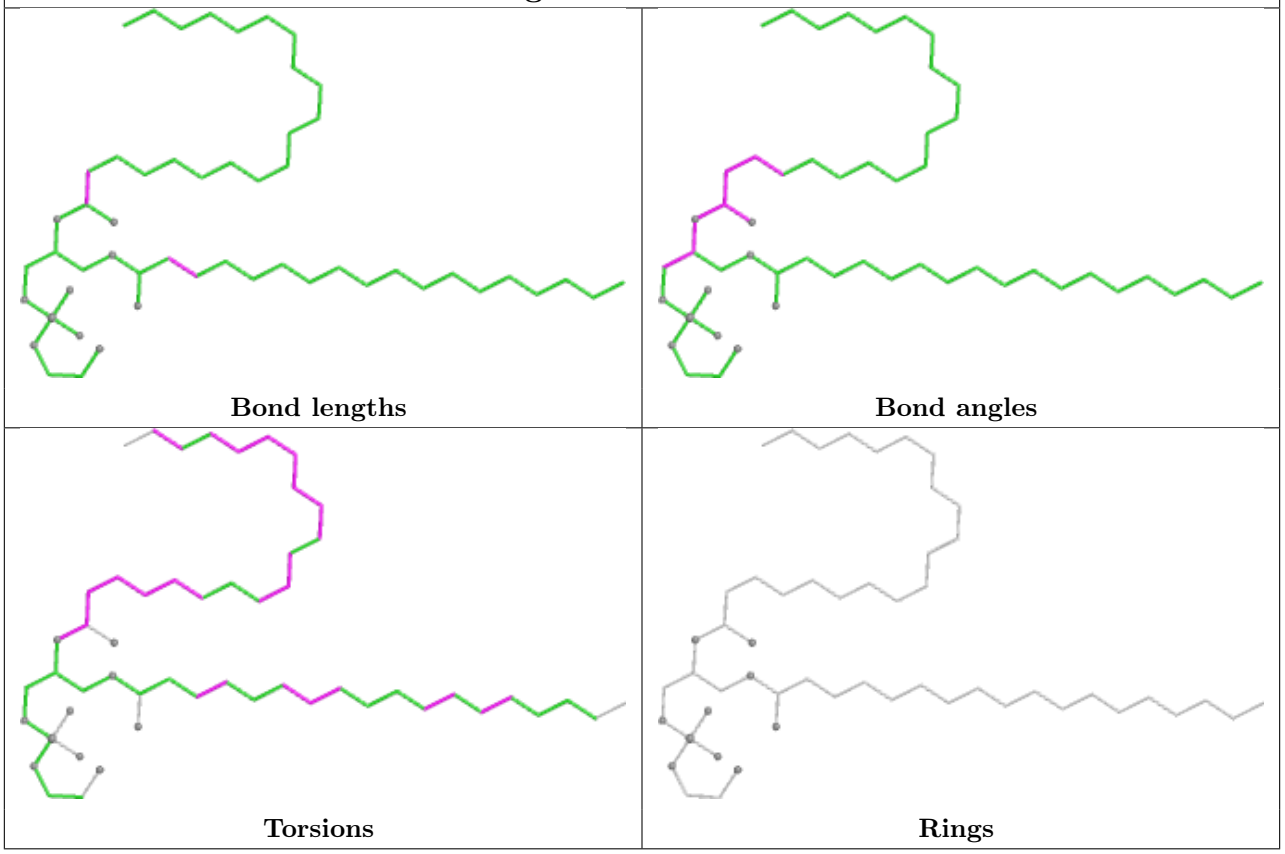

Bond lengths


Bond angles

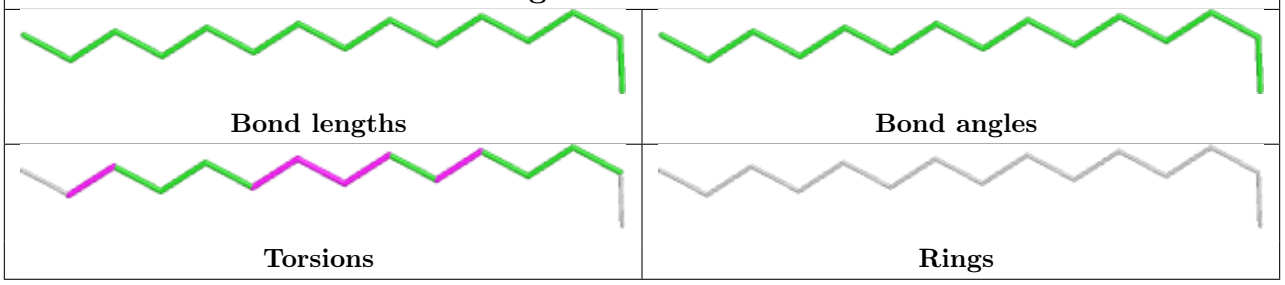

Torsions


Rings

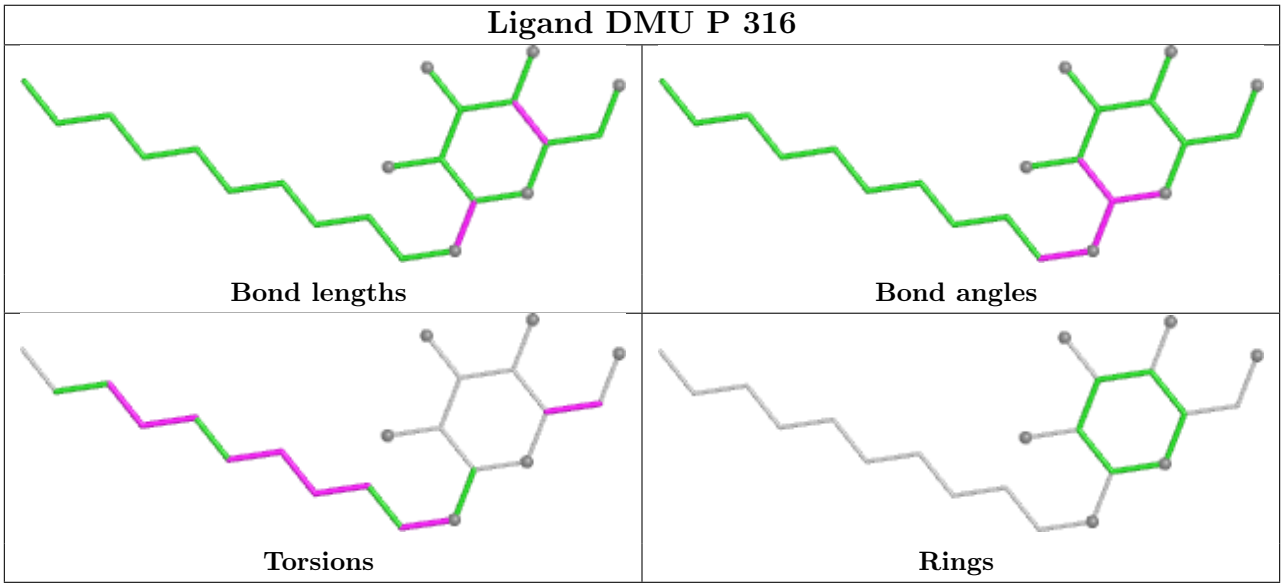
Ligand PEK T 102



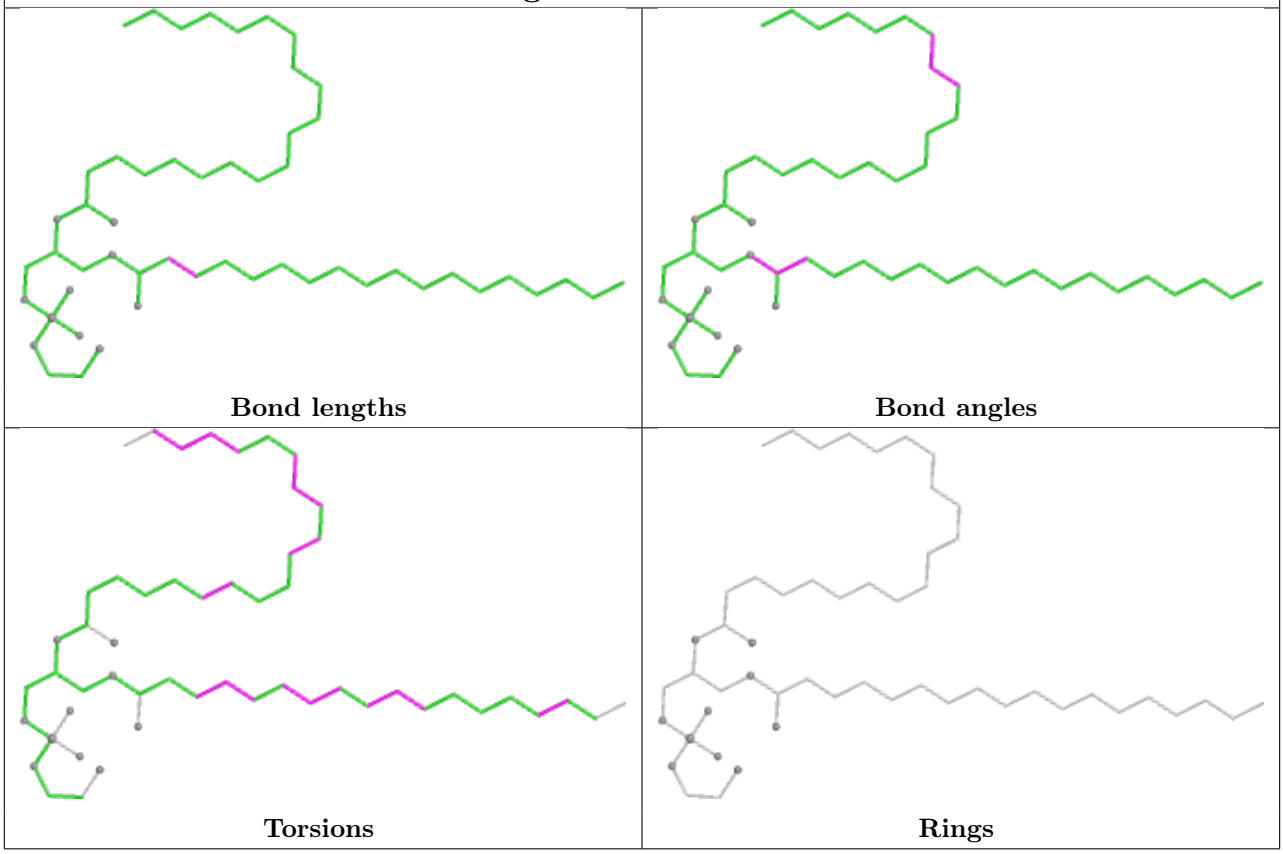
Ligand LFA C 314



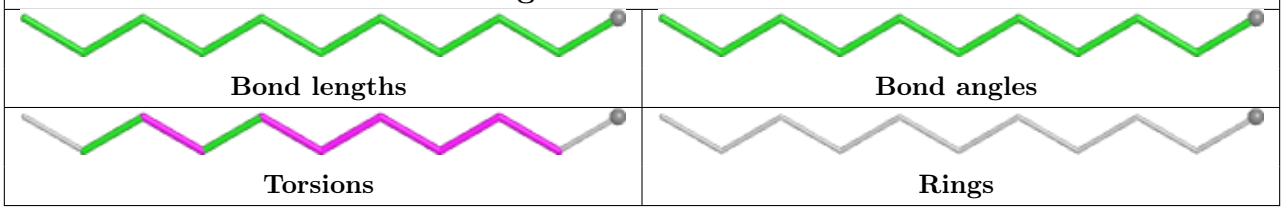
Ligand DMU P 316



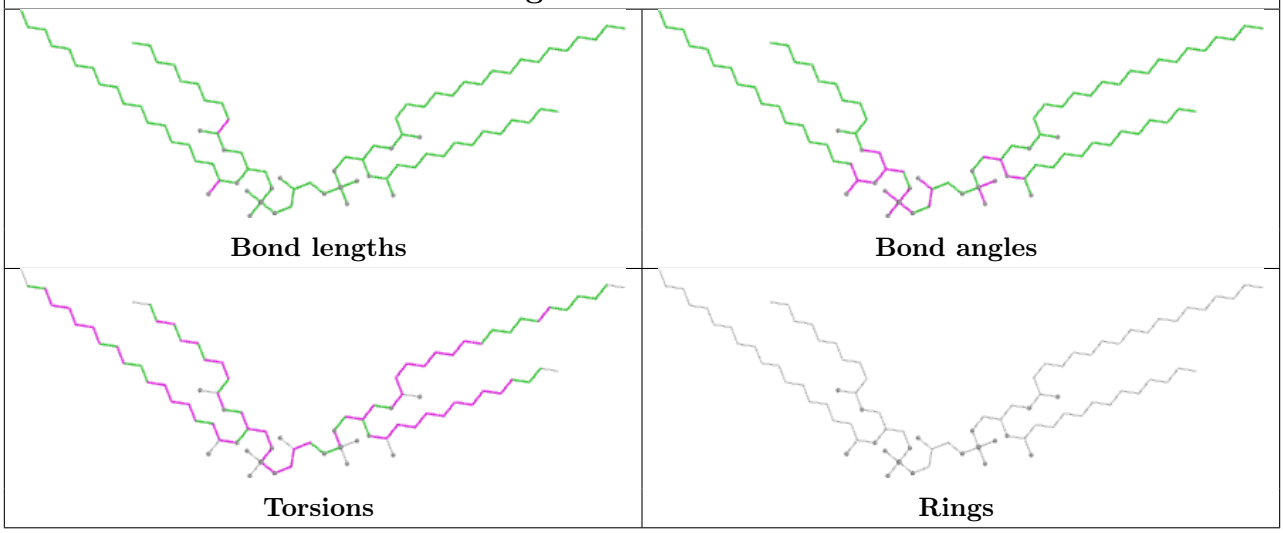
Ligand PEK G 101



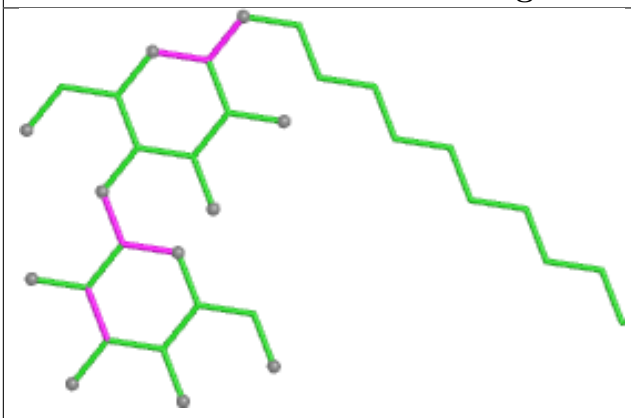
Ligand DMU O 306



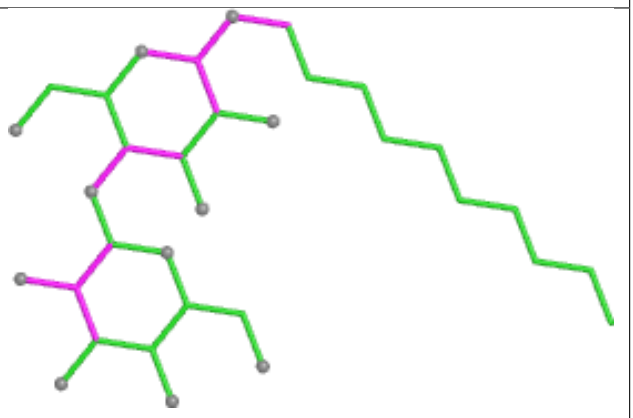
Ligand CDL P 304



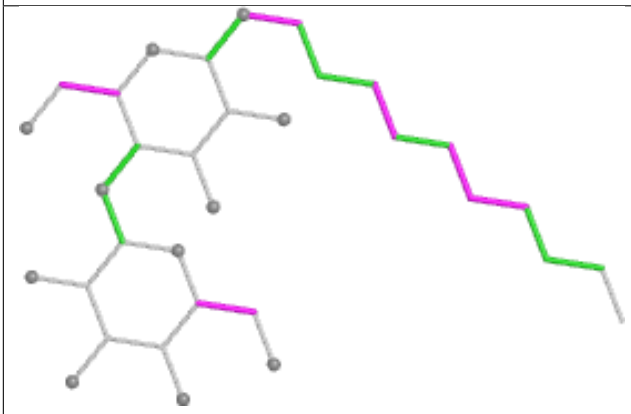
Ligand DMU H 101



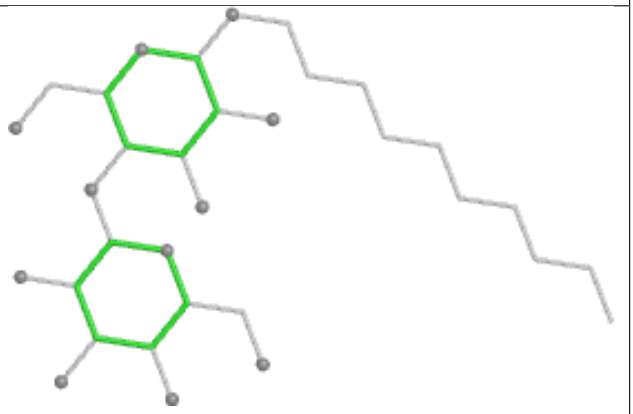
Bond lengths



Bond angles

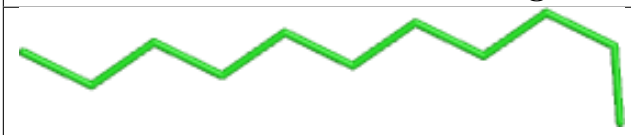


Torsions



Rings

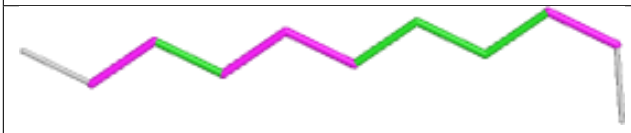
Ligand LFA C 313



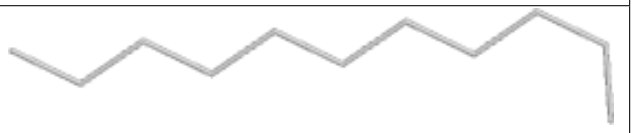
Bond lengths



Bond angles



Torsions



Rings

Ligand DMU O 307



Bond lengths



Bond angles

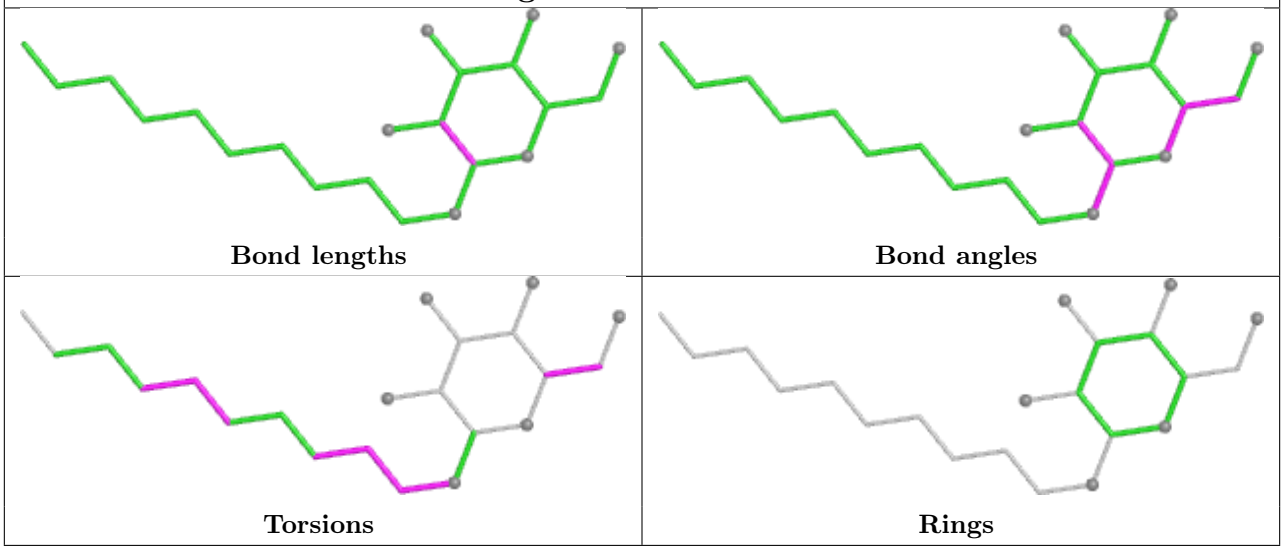


Torsions

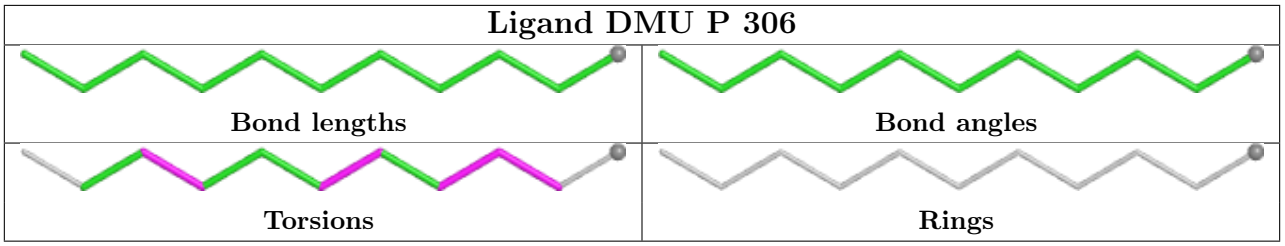


Rings

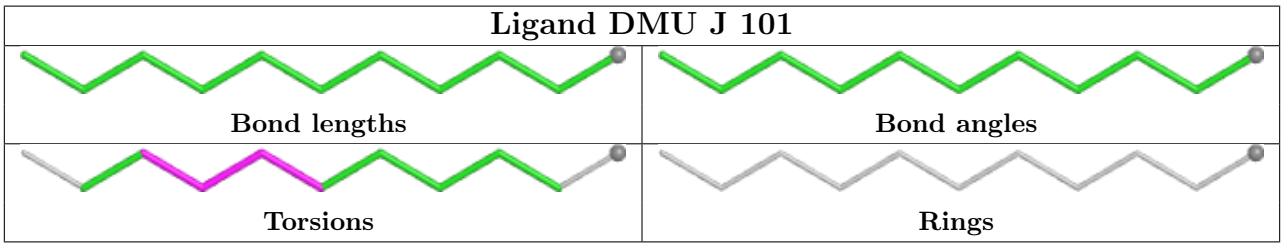
Ligand DMU C 324



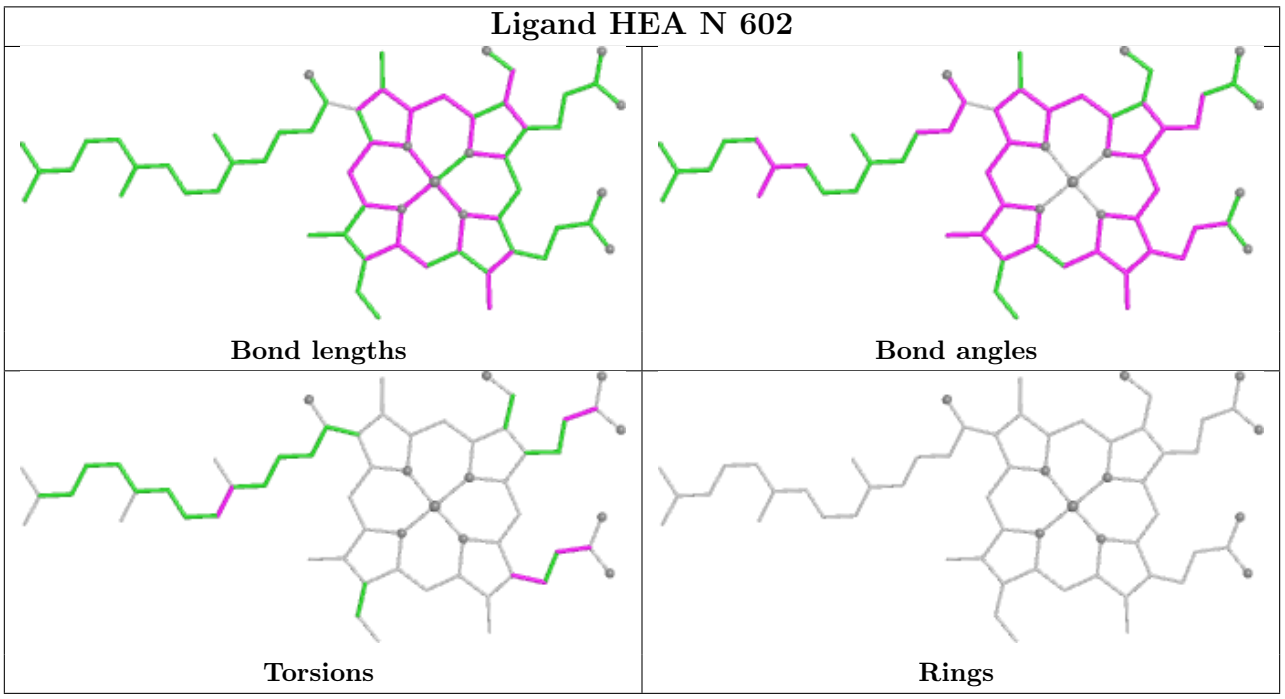
Ligand DMU P 306



Ligand DMU J 101

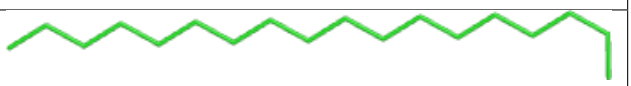


Ligand HEA N 602



Ligand LFA C 309

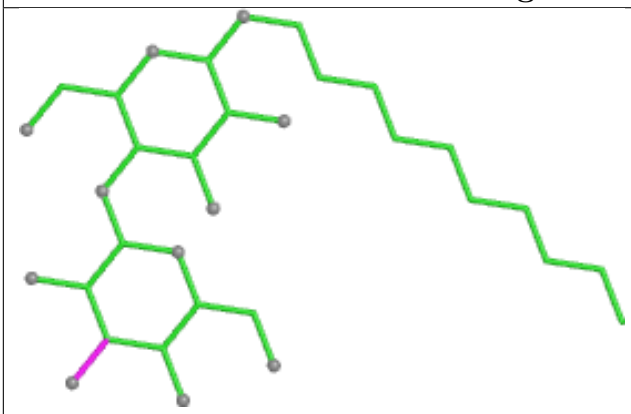

Bond lengths

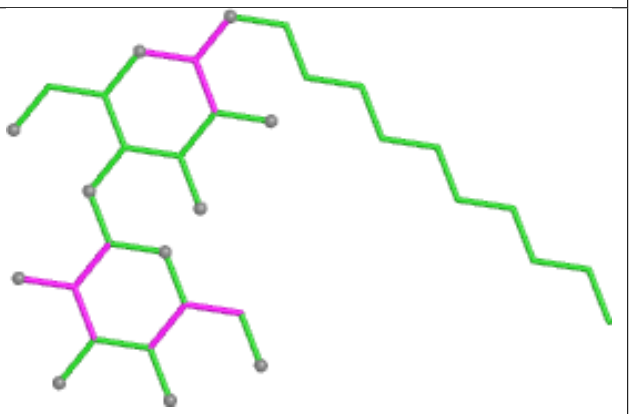

Bond angles

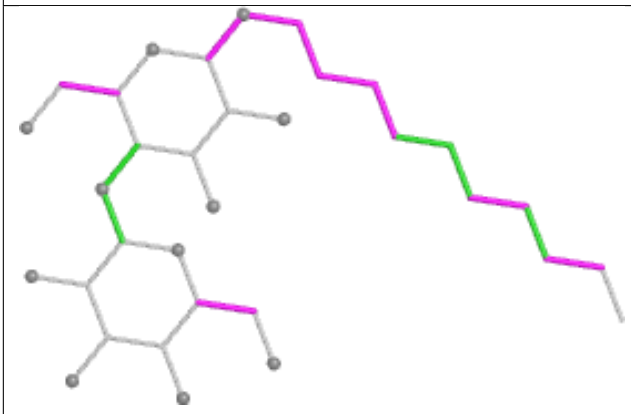

Torsions

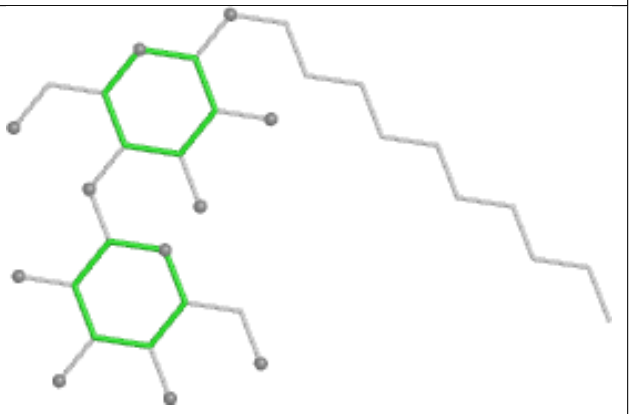

Rings

Ligand DMU C 320

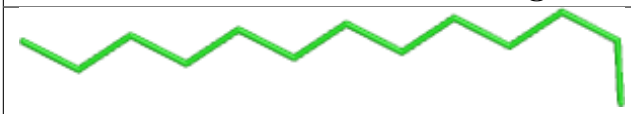

Bond lengths

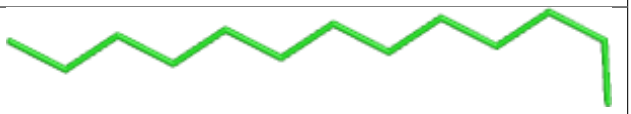

Bond angles

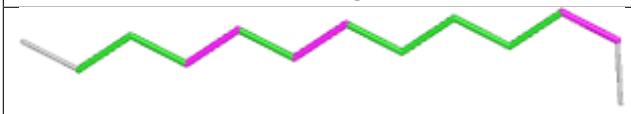

Torsions

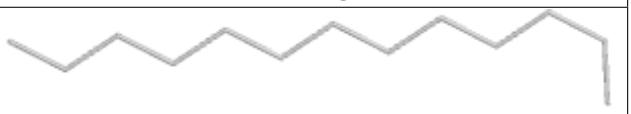

Rings

Ligand LFA C 315

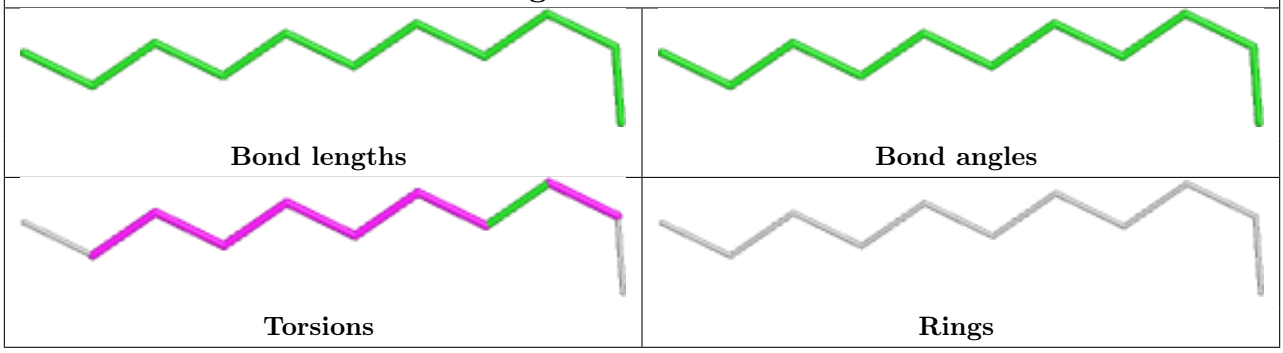

Bond lengths


Bond angles

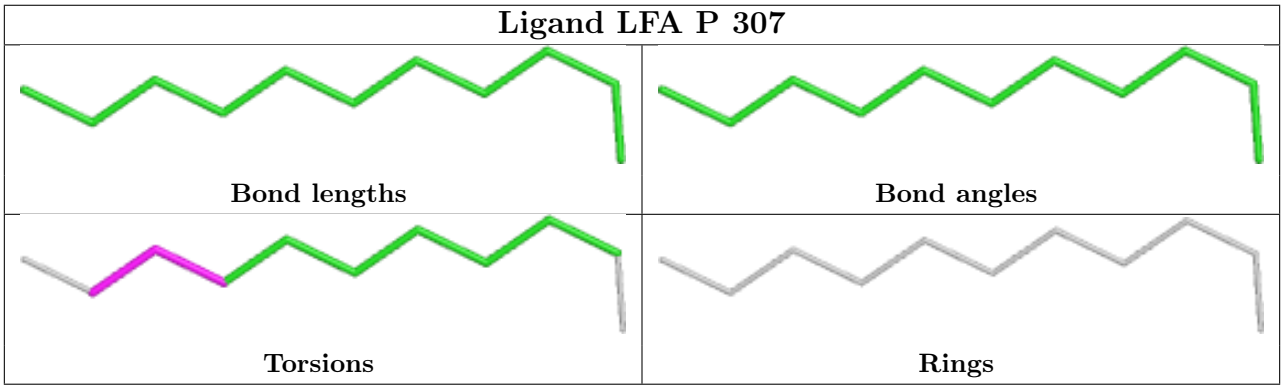

Torsions


Rings

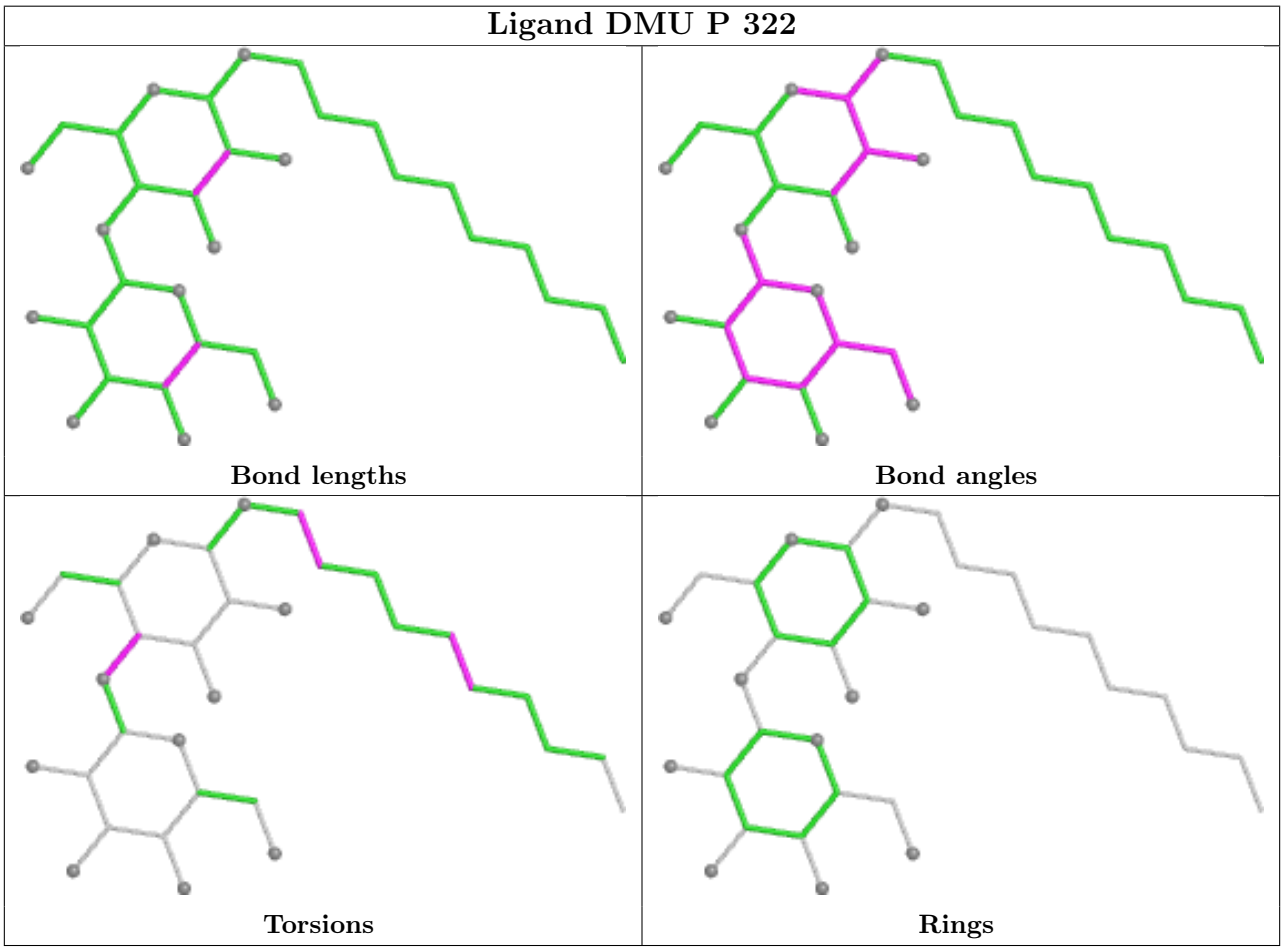
Ligand LFA C 311



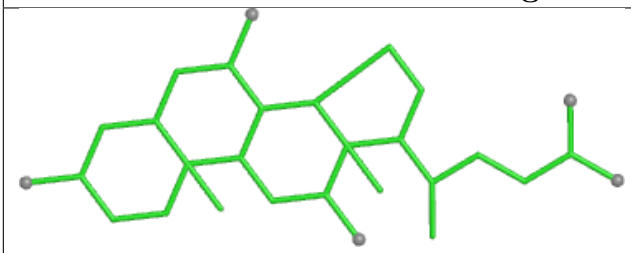
Ligand LFA P 307



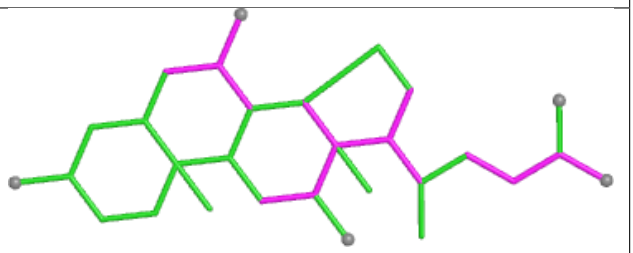
Ligand DMU P 322



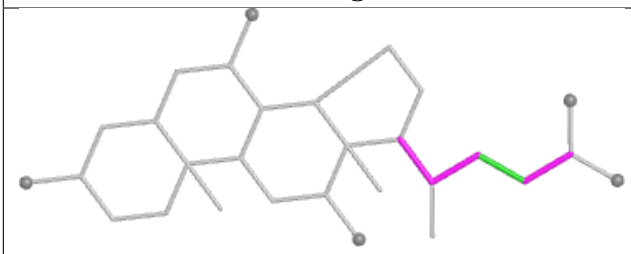
Ligand CHD P 305



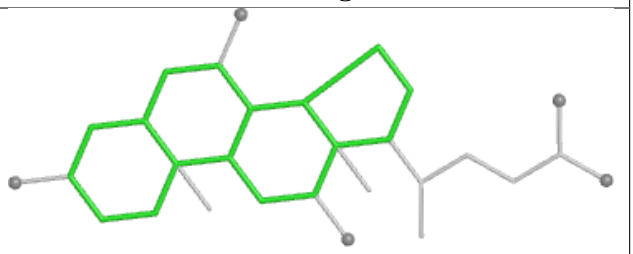
Bond lengths



Bond angles

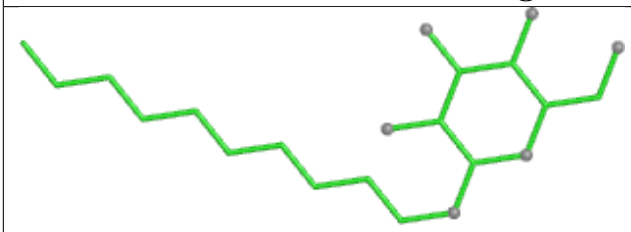


Torsions

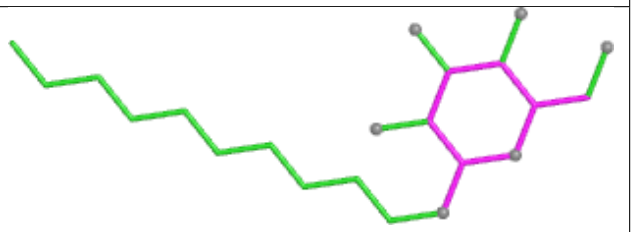


Rings

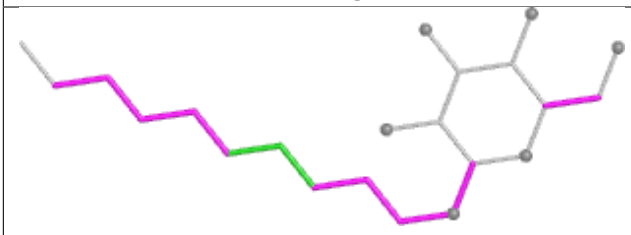
Ligand DMU B 308



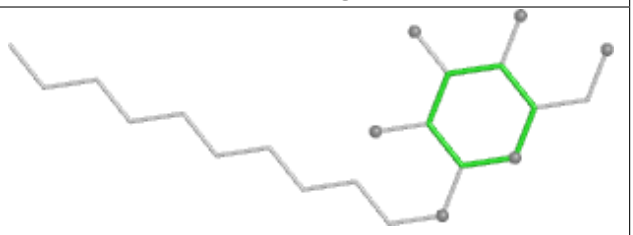
Bond lengths



Bond angles

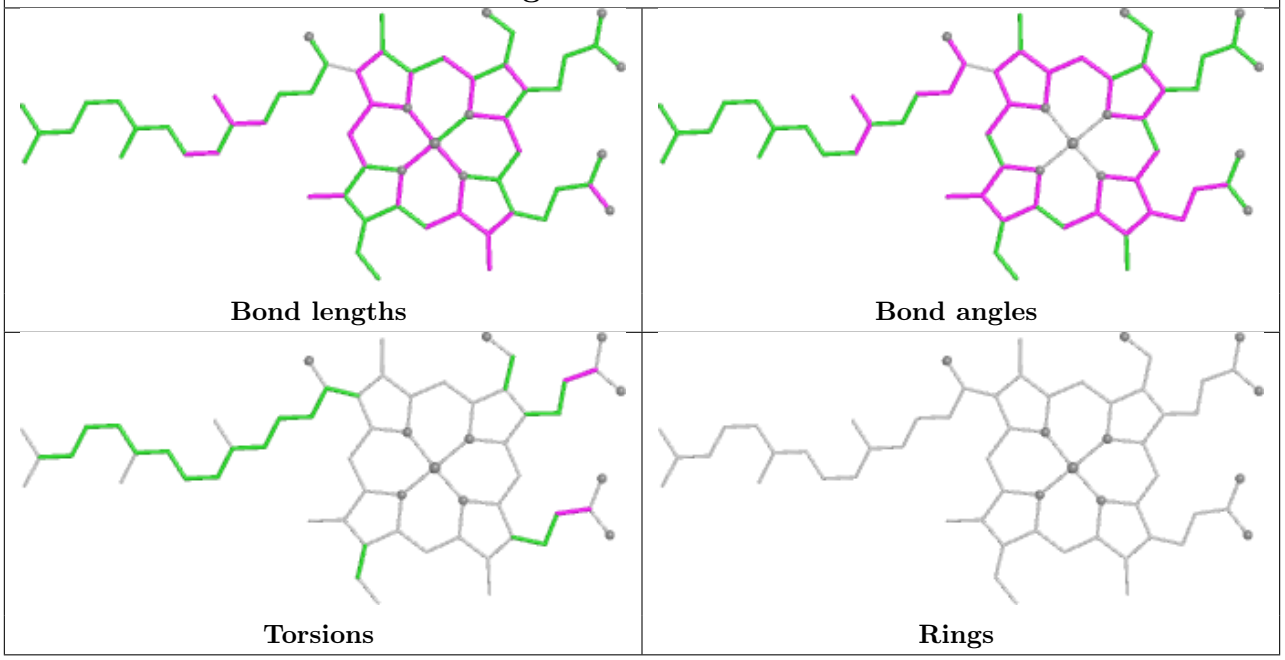


Torsions

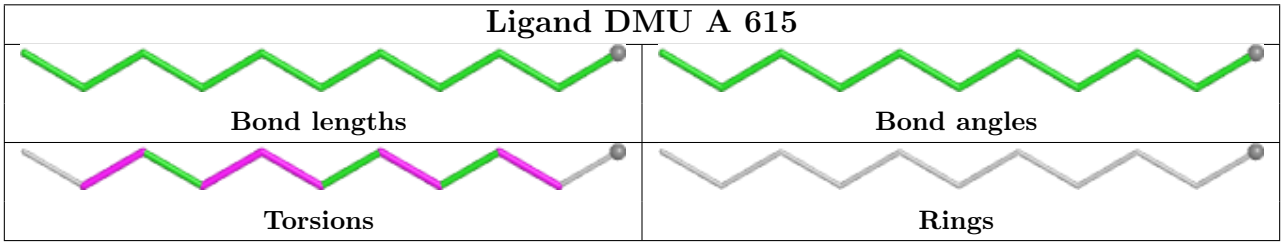


Rings

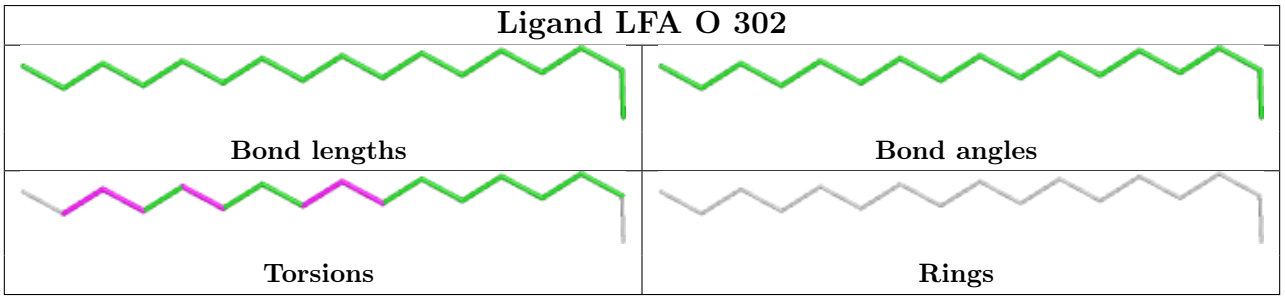
Ligand HEA A 601



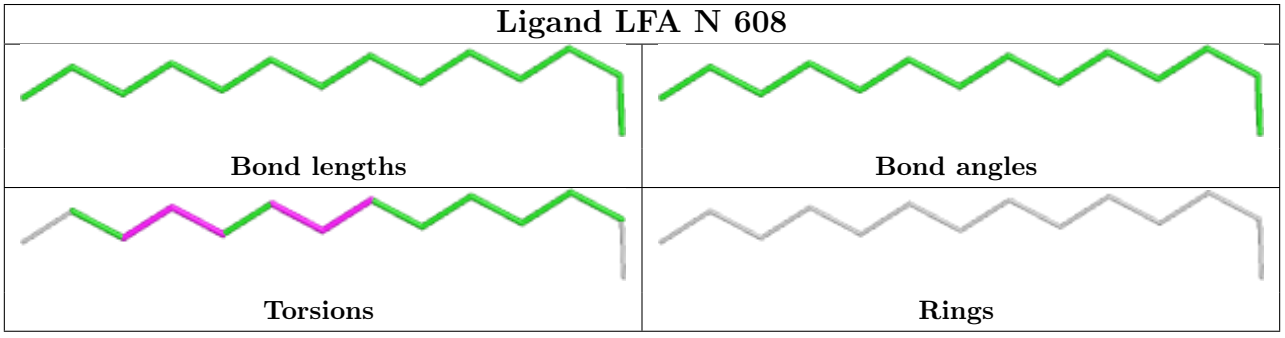
Ligand DMU A 615



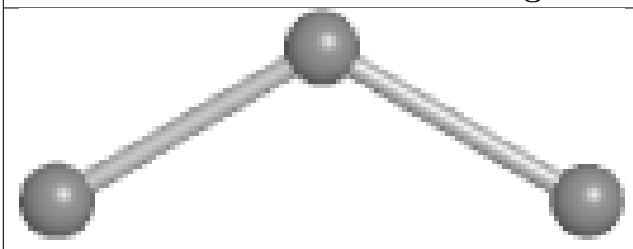
Ligand LFA O 302



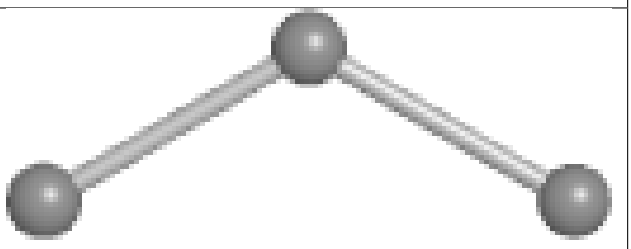
Ligand LFA N 608



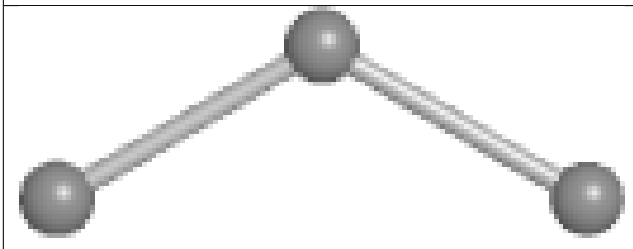
Ligand N2O N 607



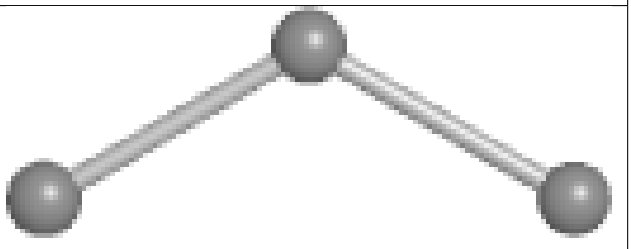
Bond lengths



Bond angles

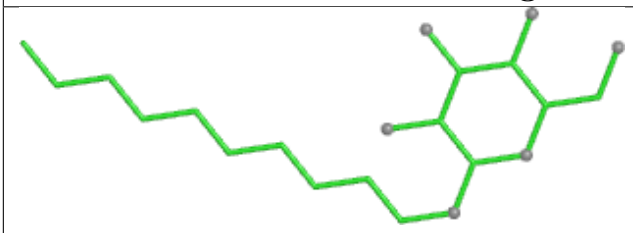


Torsions

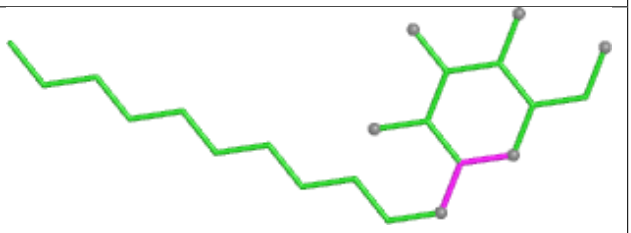


Rings

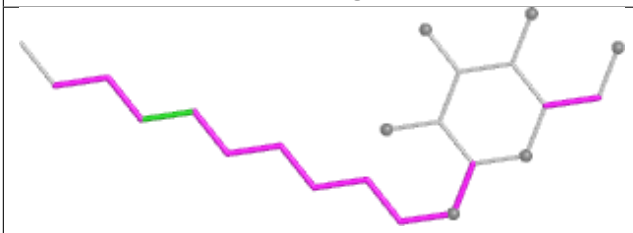
Ligand DMU Z 102



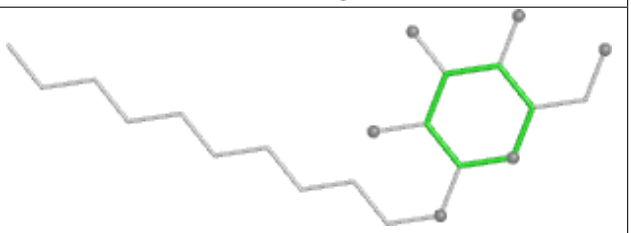
Bond lengths



Bond angles

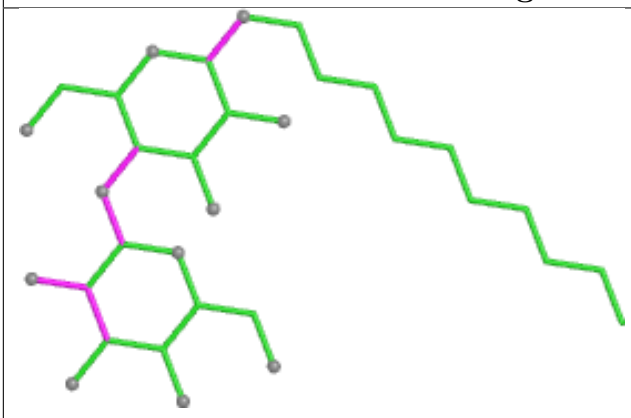


Torsions

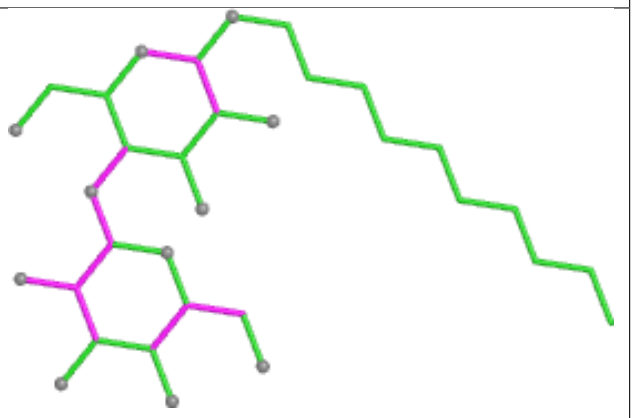


Rings

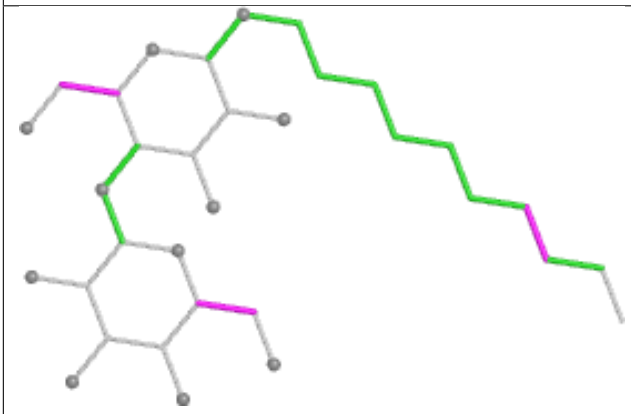
Ligand DMU A 609



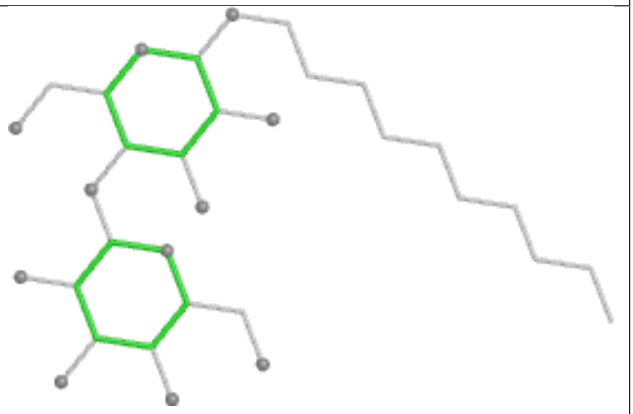
Bond lengths



Bond angles

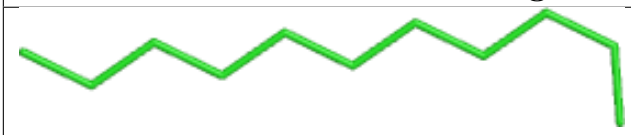


Torsions



Rings

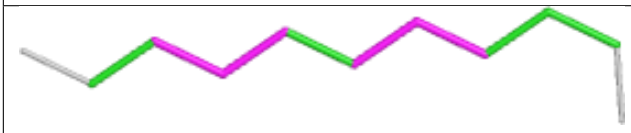
Ligand LFA T 104



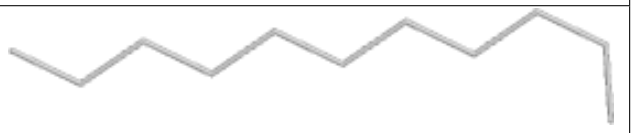
Bond lengths



Bond angles

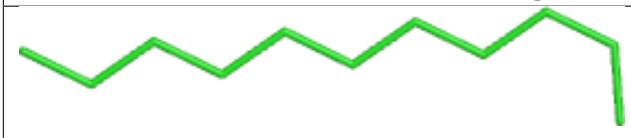


Torsions

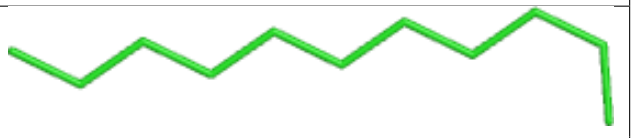


Rings

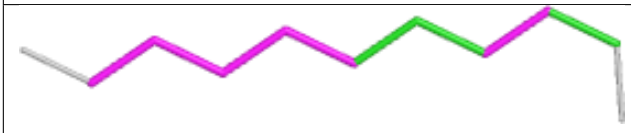
Ligand LFA P 310



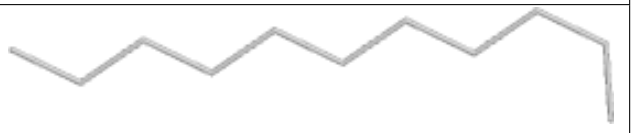
Bond lengths



Bond angles

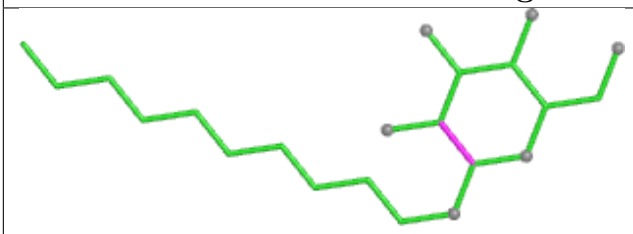


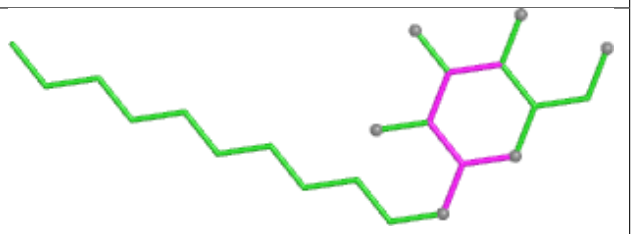
Torsions

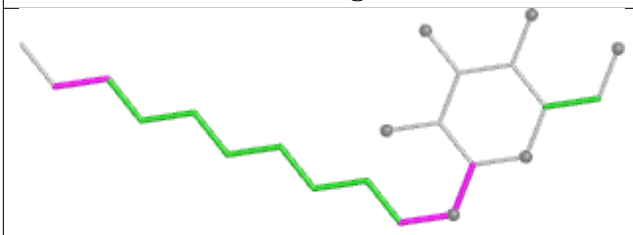


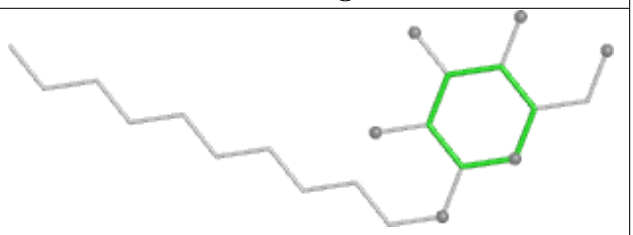
Rings

Ligand DMU O 308

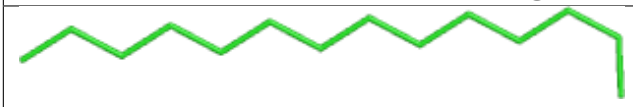

Bond lengths

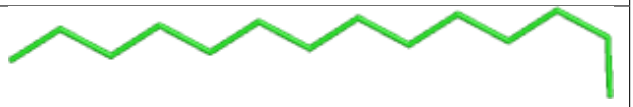

Bond angles


Torsions

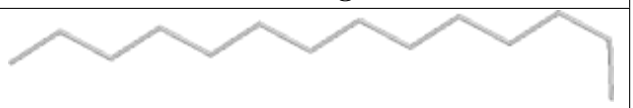

Rings

Ligand LFA T 103

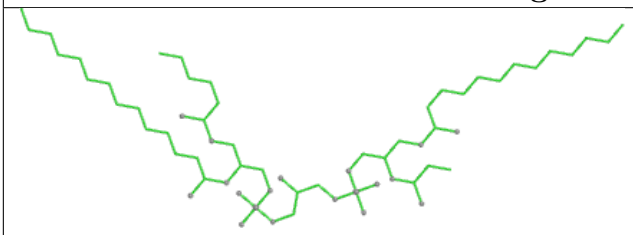

Bond lengths

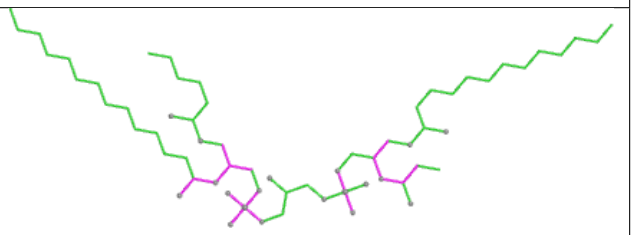

Bond angles

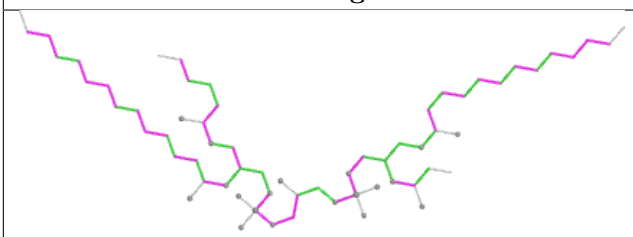

Torsions

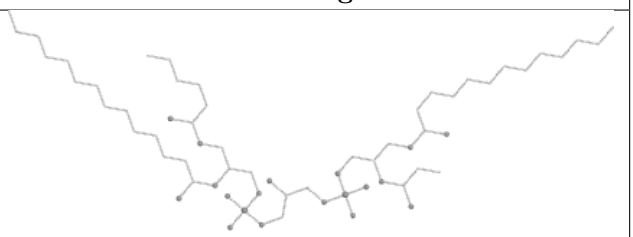

Rings

Ligand CDL I 101

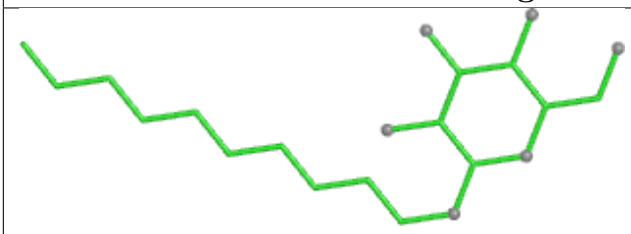

Bond lengths


Bond angles

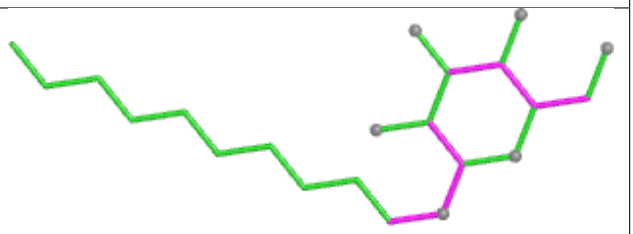

Torsions


Rings

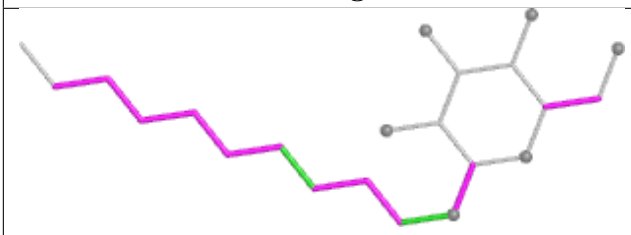
Ligand DMU T 105



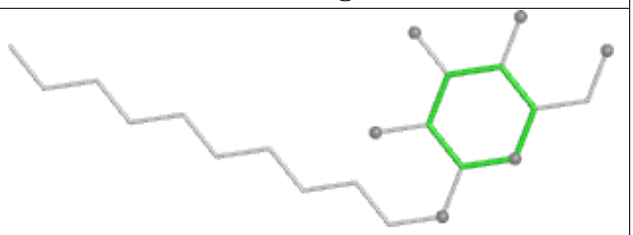
Bond lengths



Bond angles

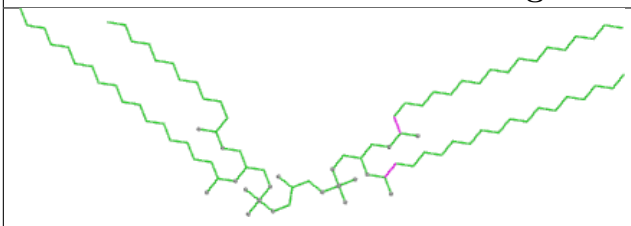


Torsions

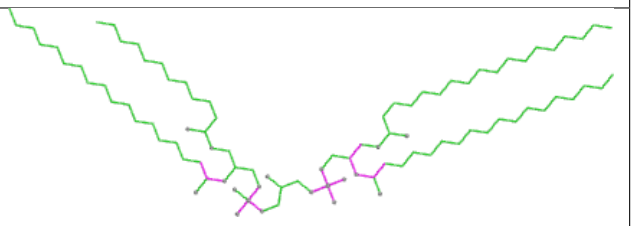


Rings

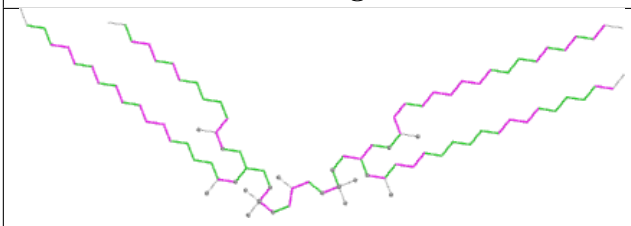
Ligand CDL L 101



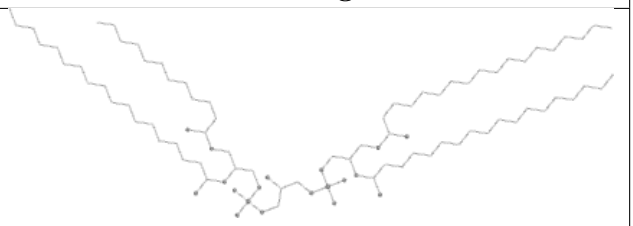
Bond lengths



Bond angles

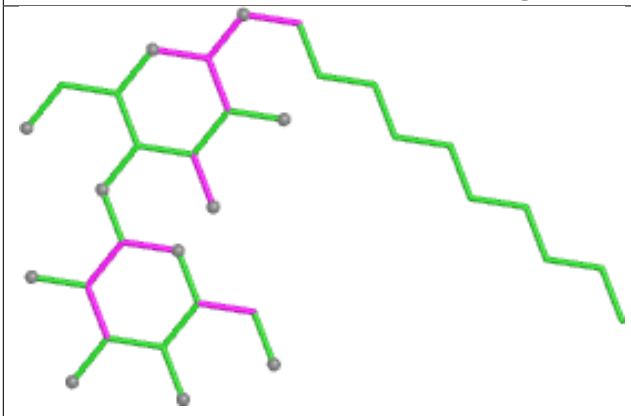


Torsions

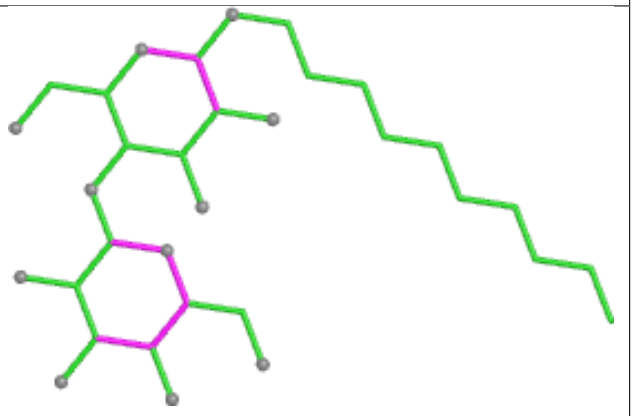


Rings

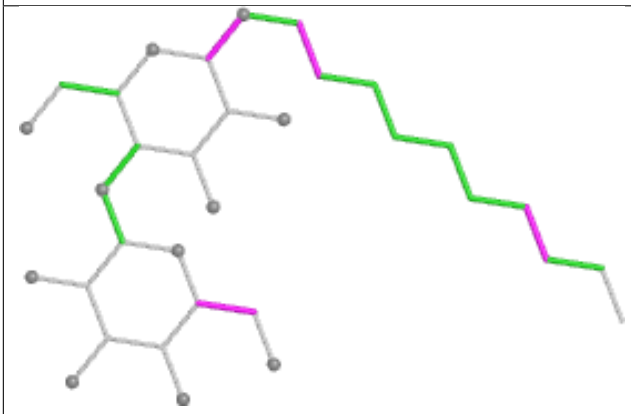
Ligand DMU N 610



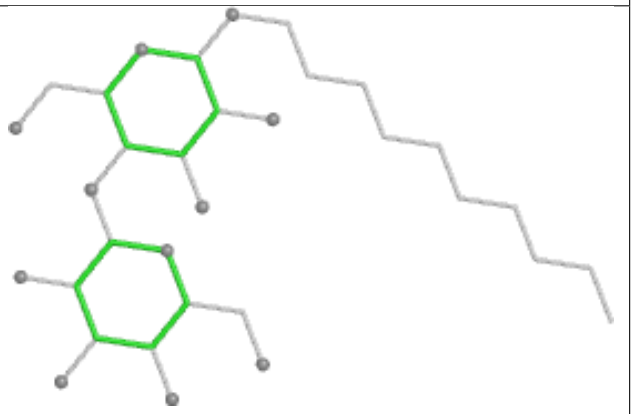
Bond lengths



Bond angles

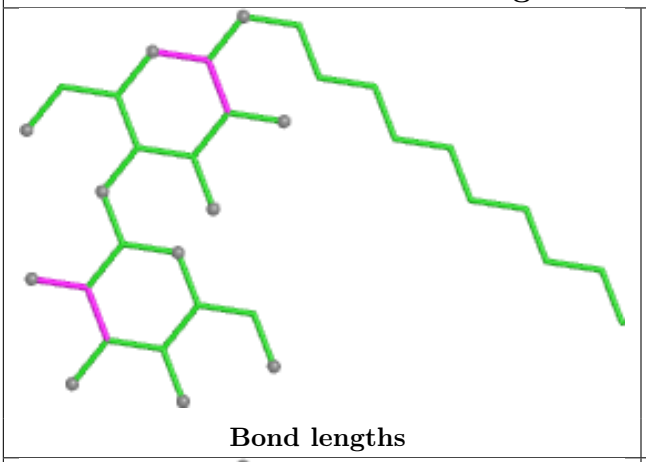


Torsions

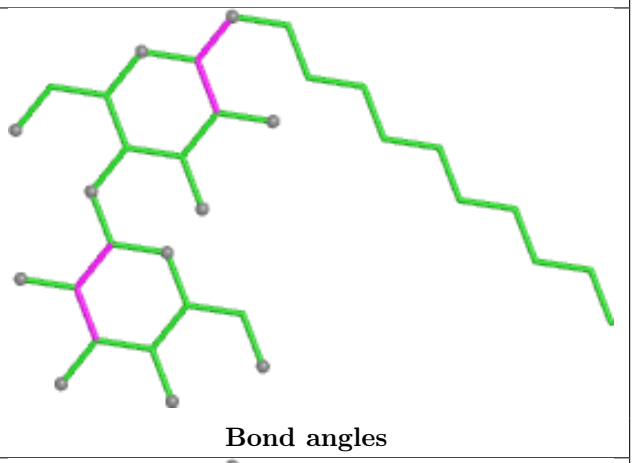


Rings

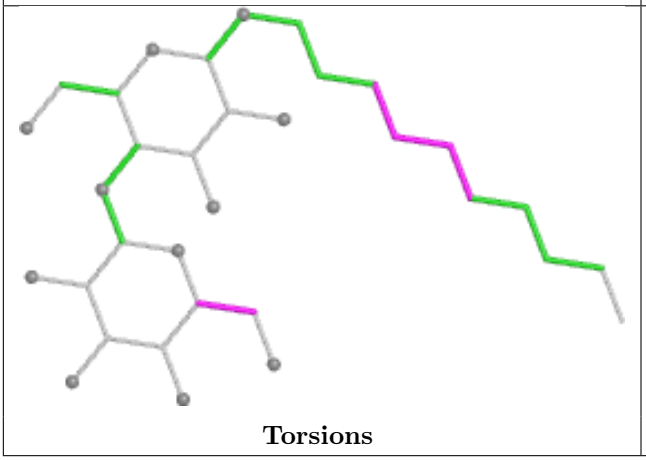
Ligand DMU M 101



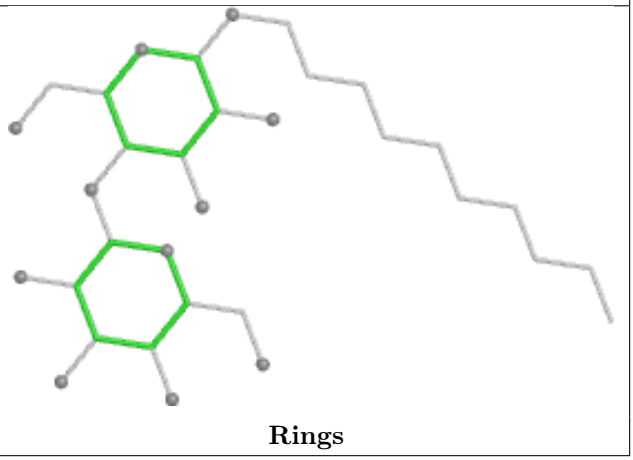
Bond lengths



Bond angles

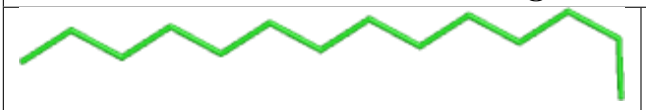


Torsions

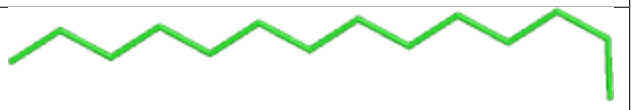


Rings

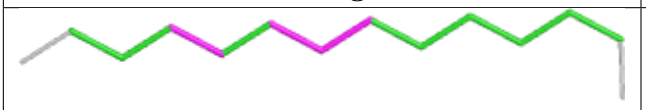
Ligand LFA A 607



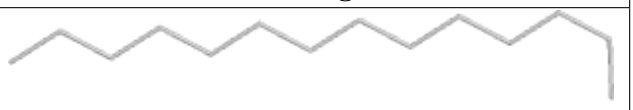
Bond lengths



Bond angles

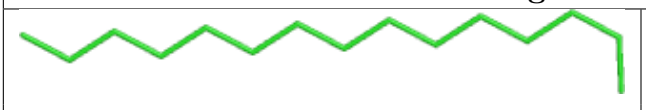


Torsions

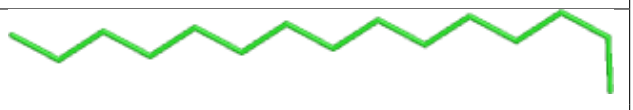


Rings

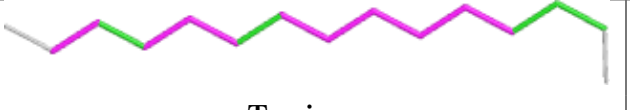
Ligand LFA C 326



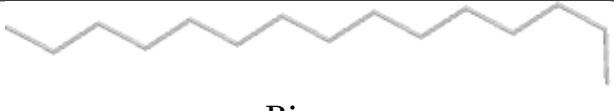
Bond lengths



Bond angles

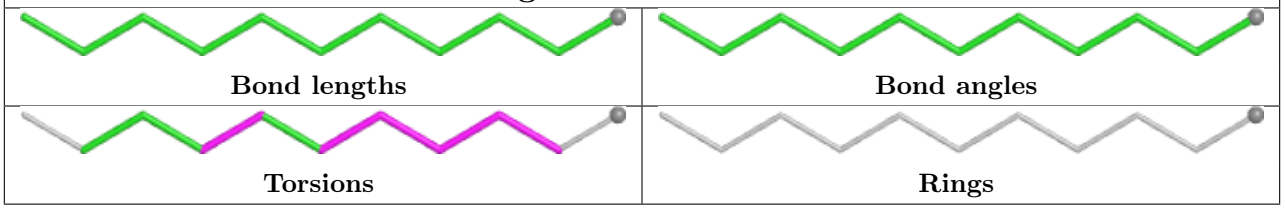


Torsions

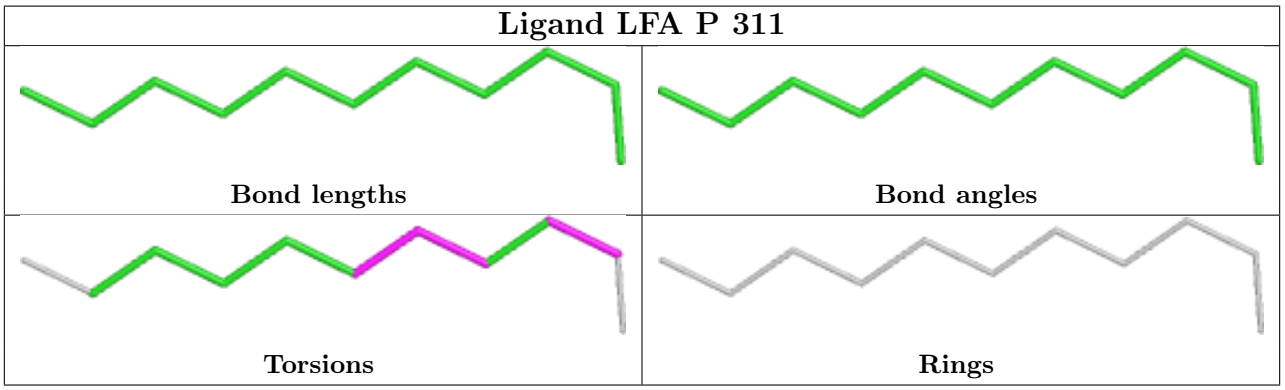


Rings

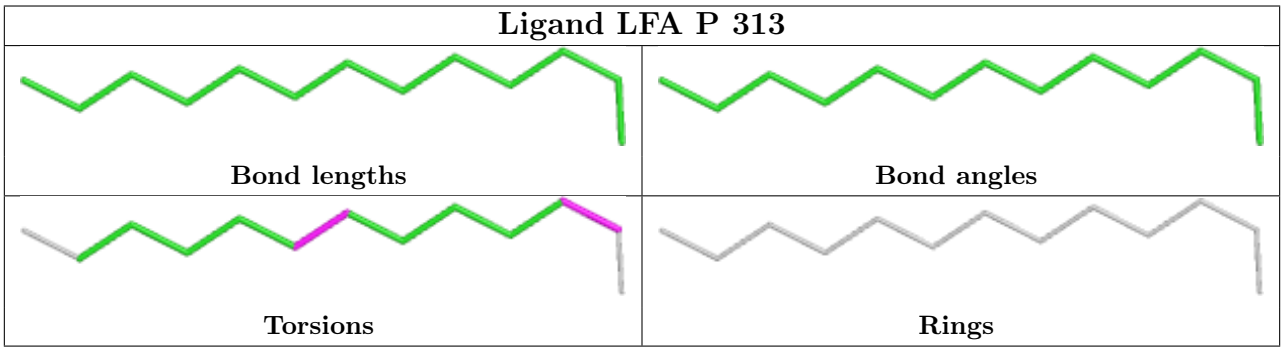
Ligand DMU B 303



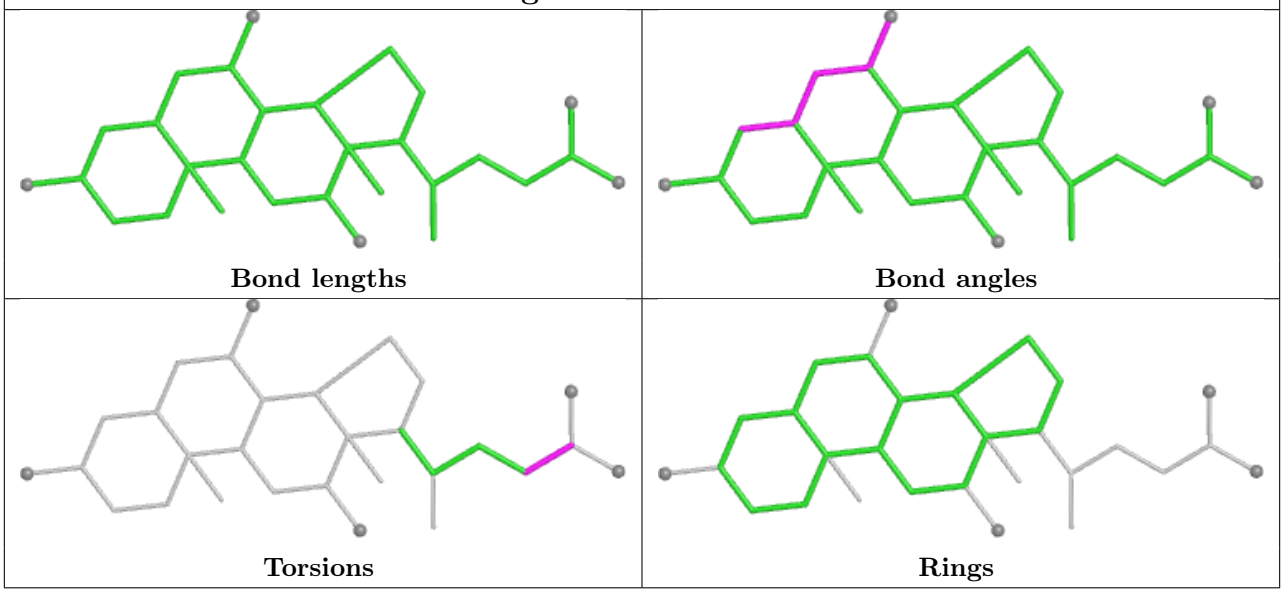
Ligand LFA P 311



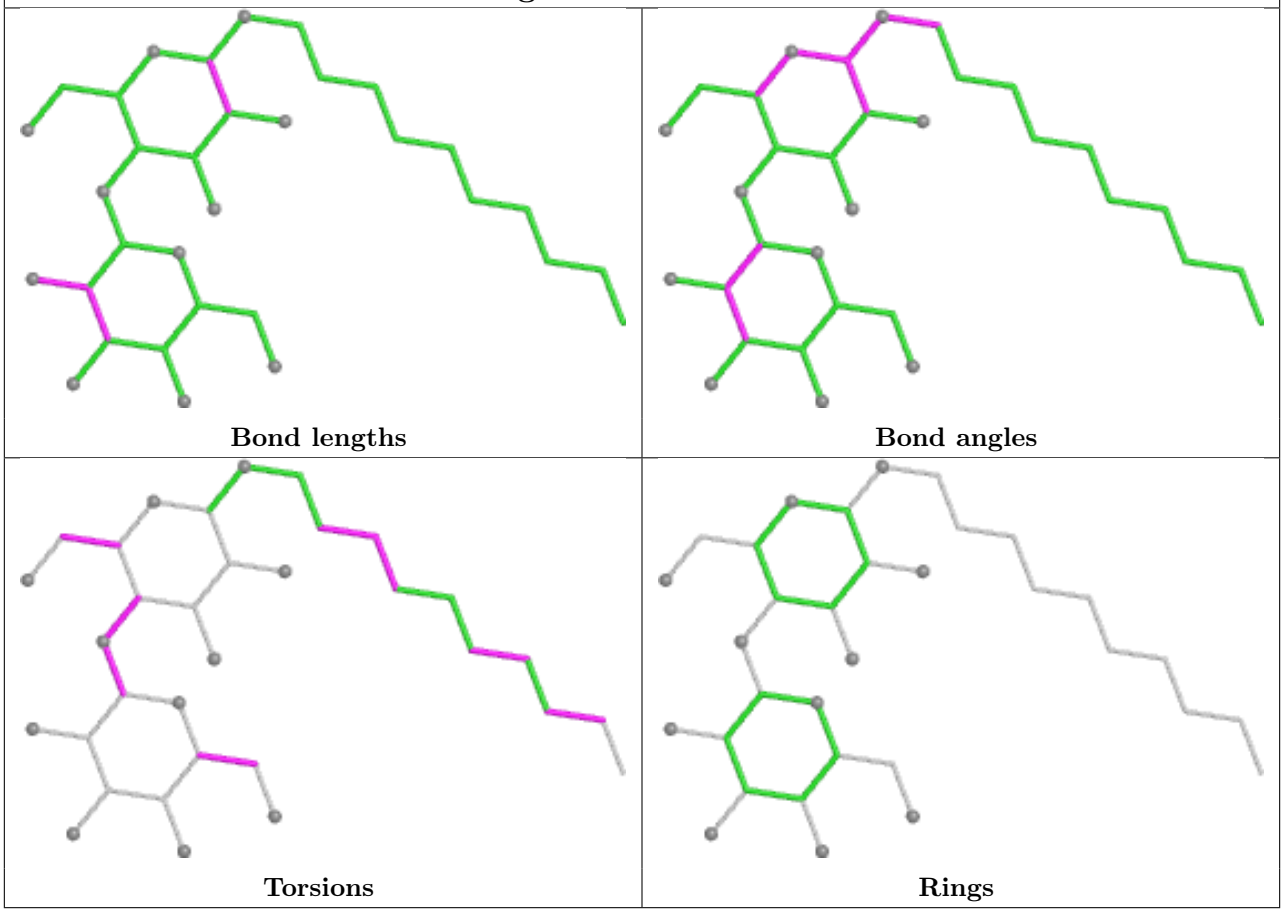
Ligand LFA P 313



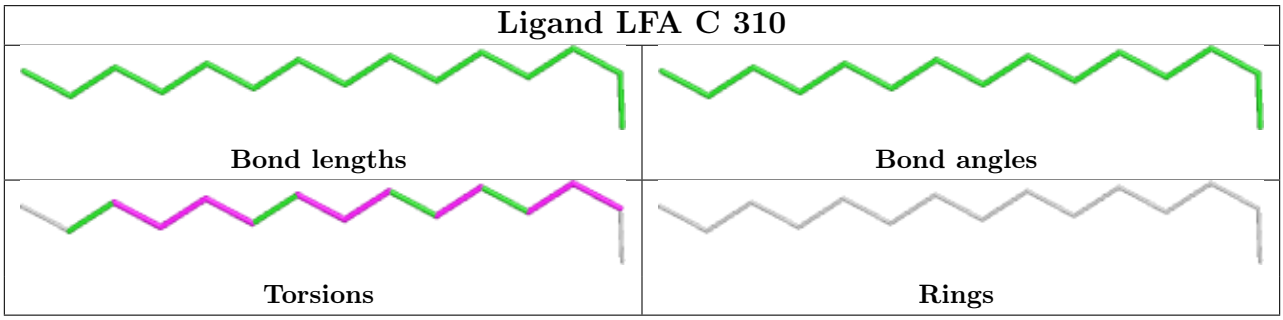
Ligand CHD O 301



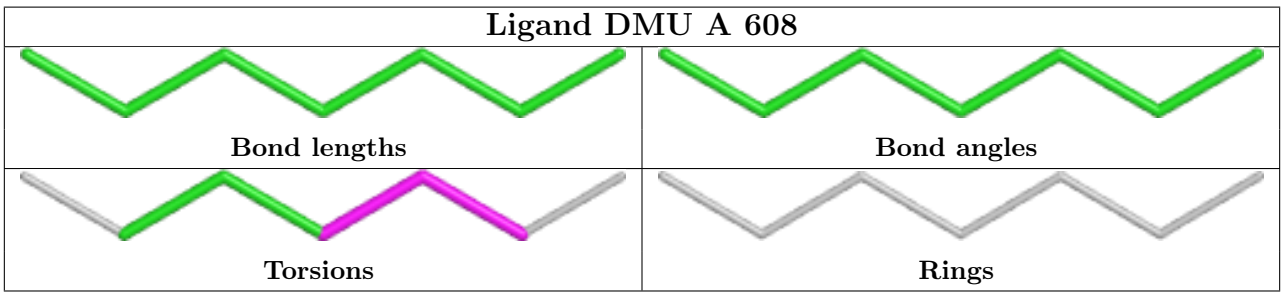
Ligand DMU C 316



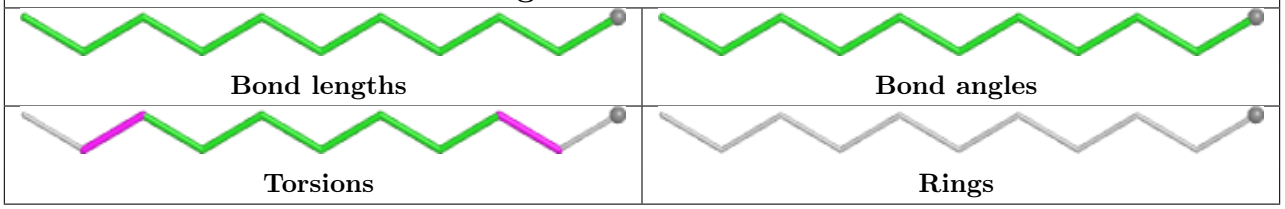
Ligand LFA C 310



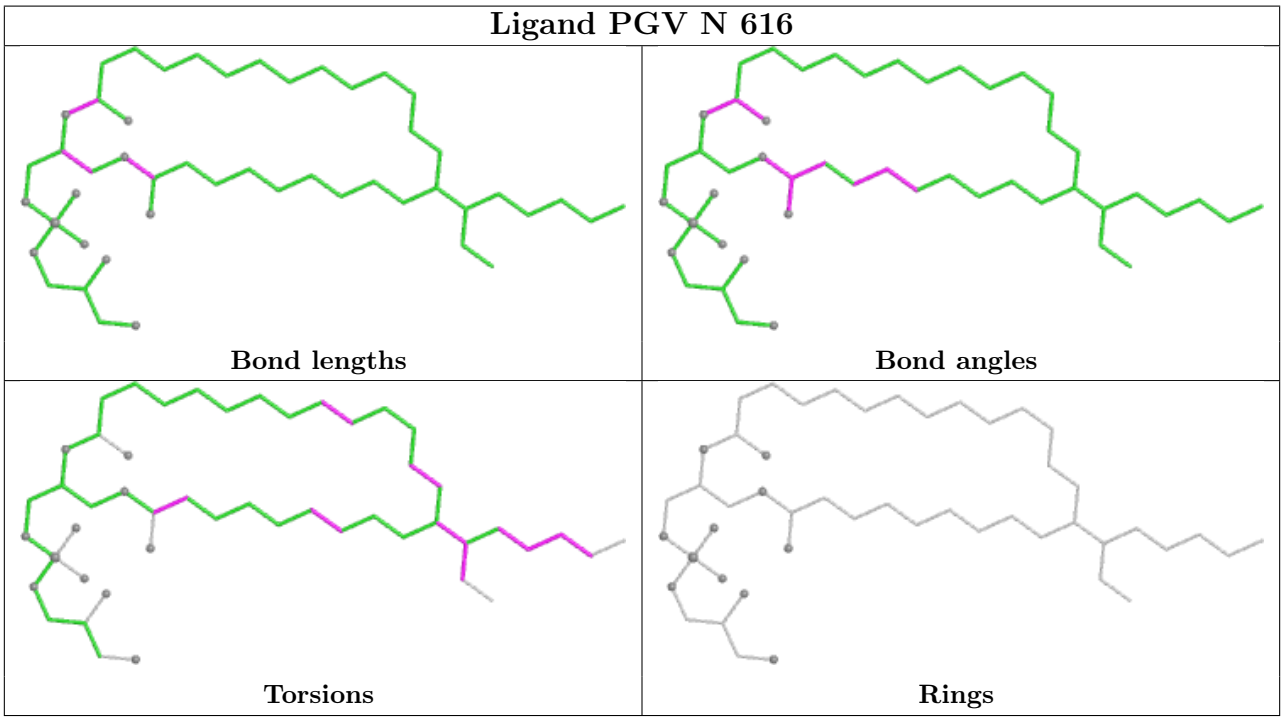
Ligand DMU A 608



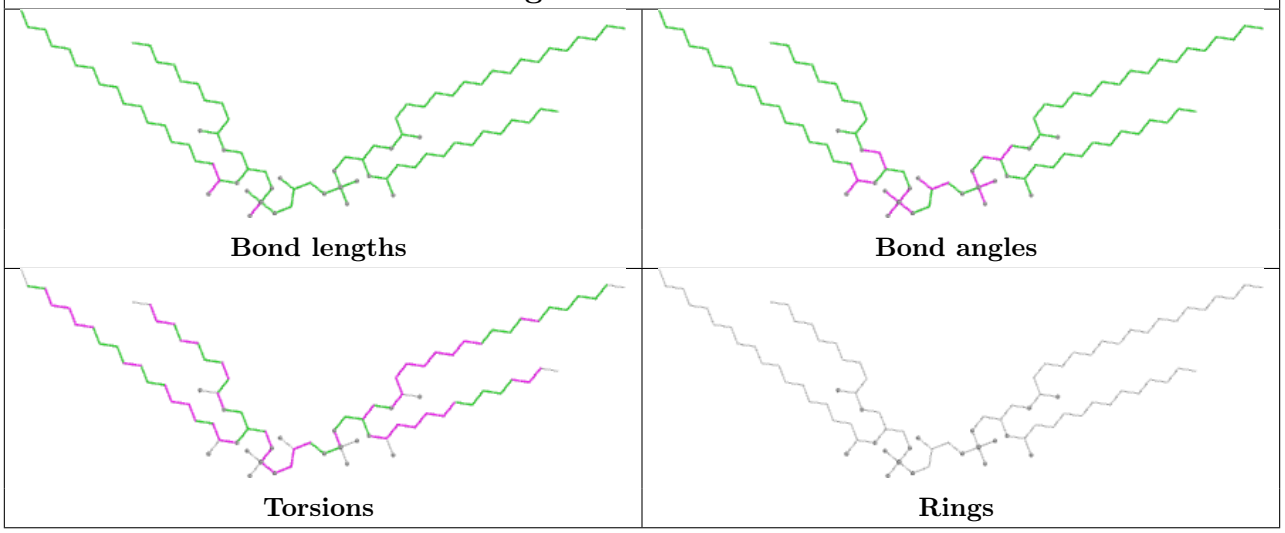
Ligand DMU G 102



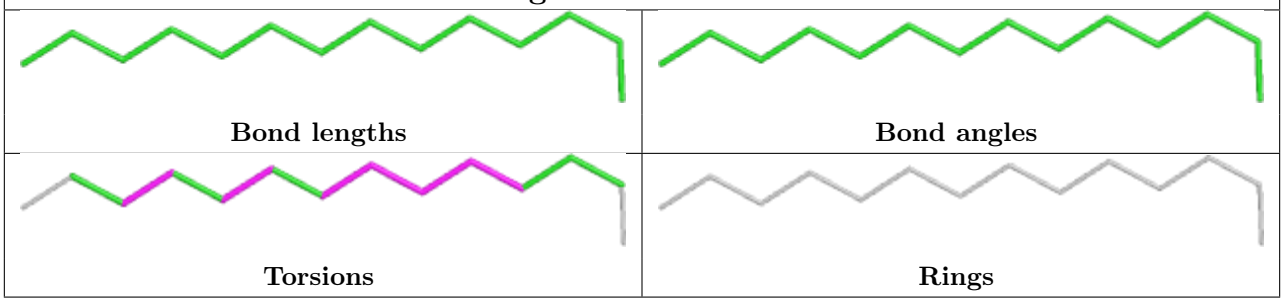
Ligand PGV N 616



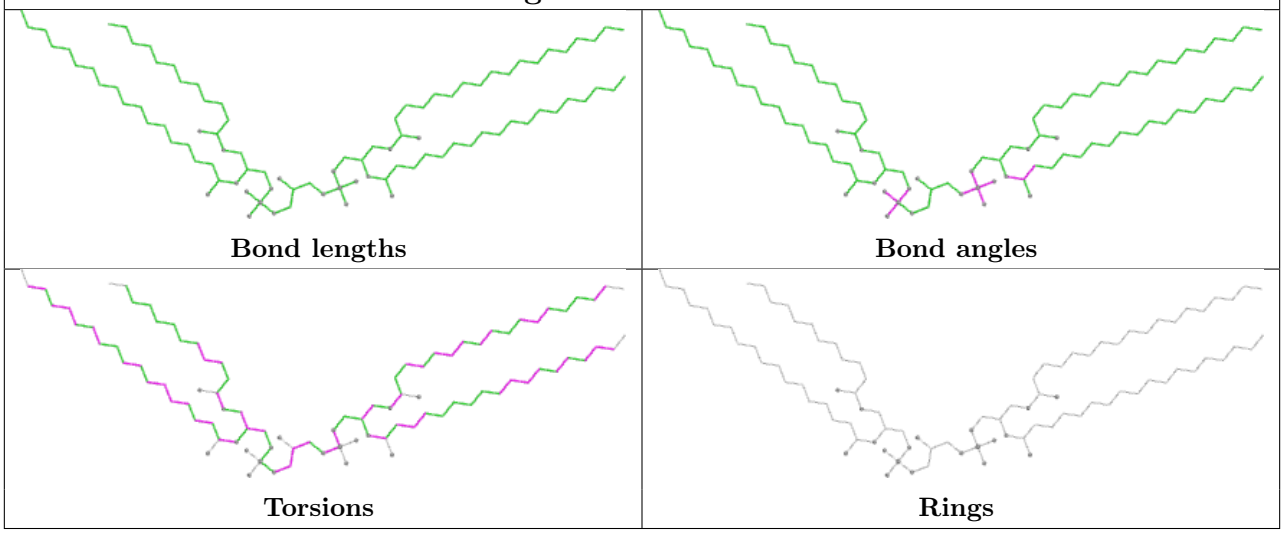
Ligand CDL C 304



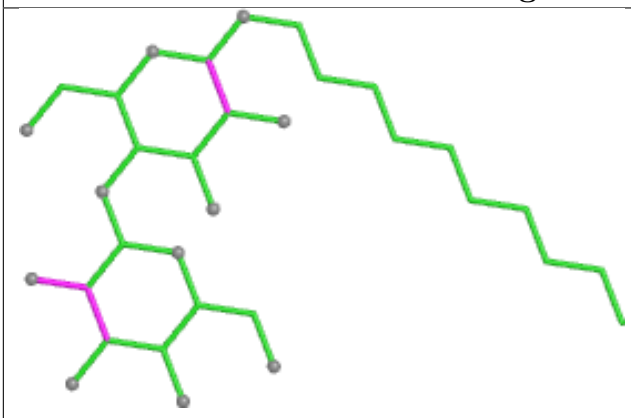
Ligand LFA C 312



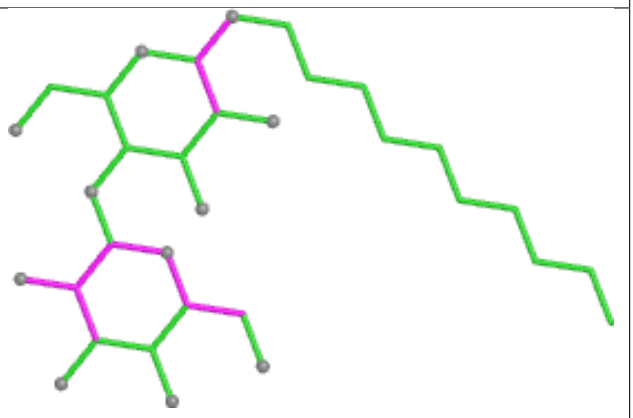
Ligand CDL Y 101



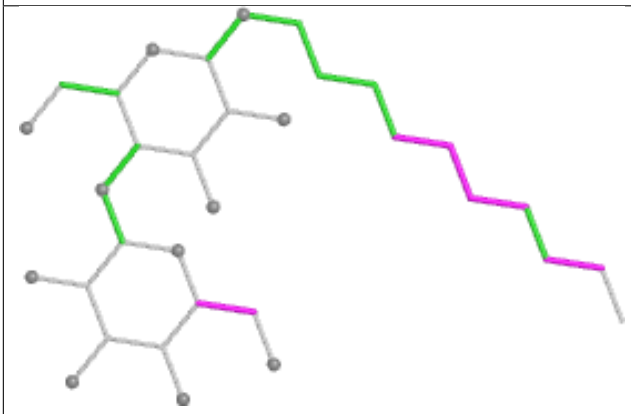
Ligand DMU Z 101



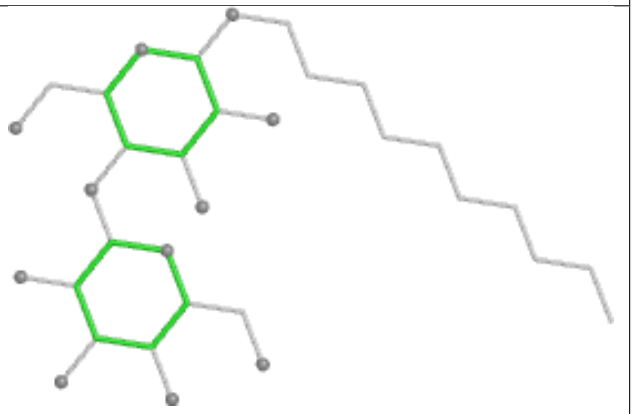
Bond lengths



Bond angles



Torsions



Rings

Ligand DMU C 306



Bond lengths



Bond angles

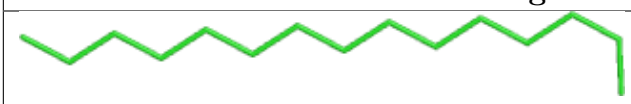


Torsions

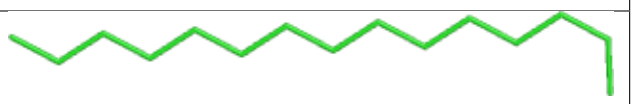


Rings

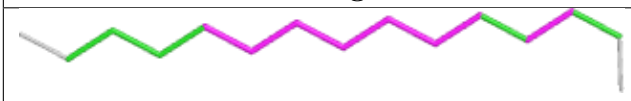
Ligand LFA P 312



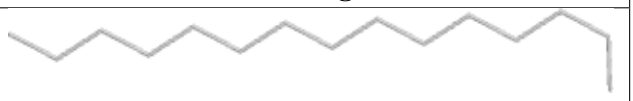
Bond lengths



Bond angles



Torsions



Rings

Ligand DMU W 101



Bond lengths



Bond angles

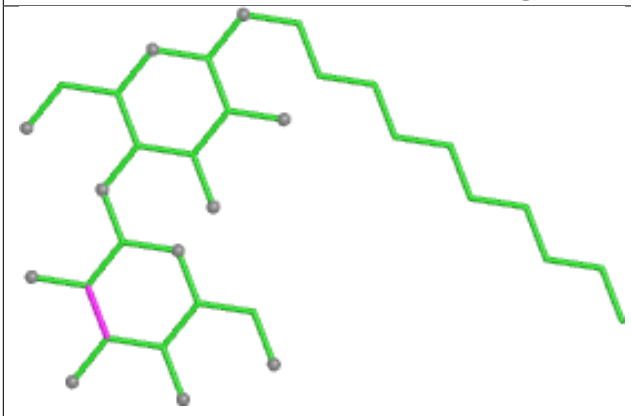


Torsions

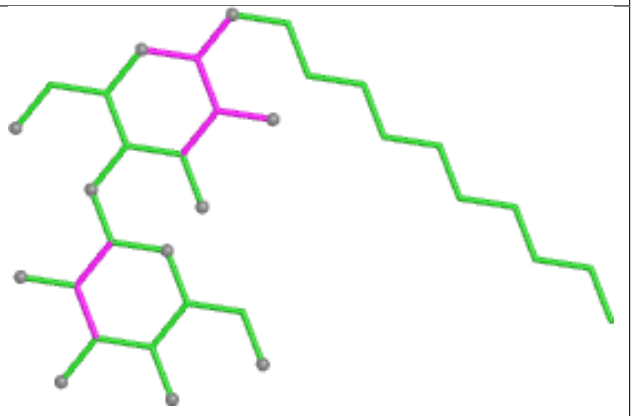


Rings

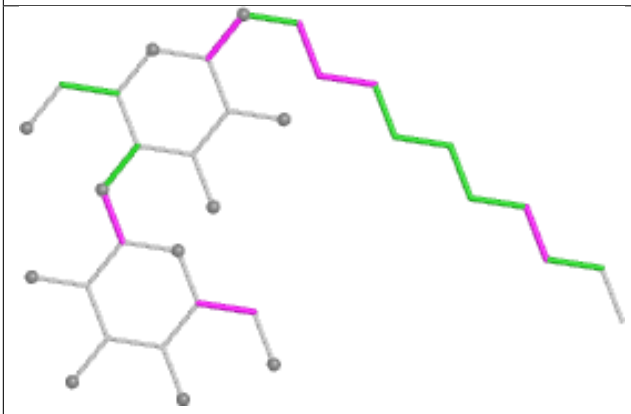
Ligand DMU C 325



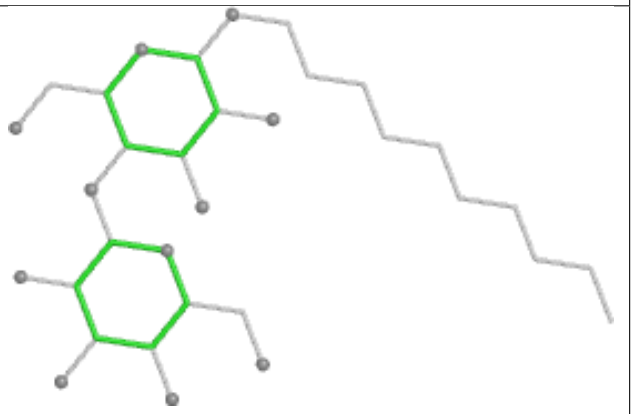
Bond lengths



Bond angles

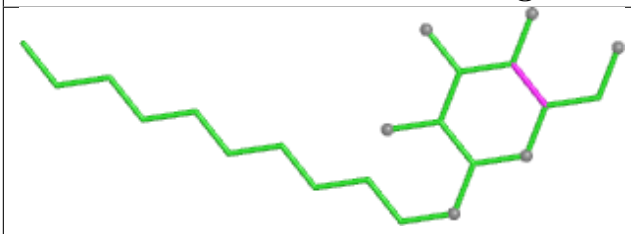


Torsions

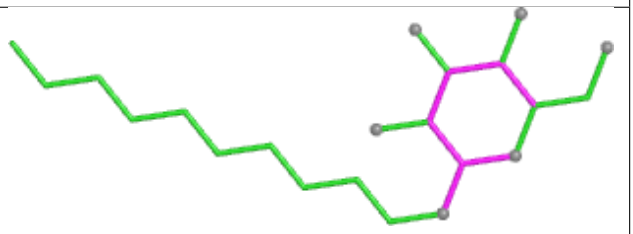


Rings

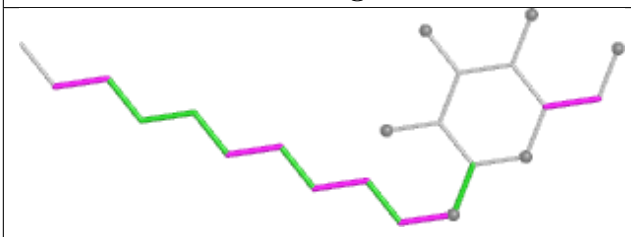
Ligand DMU O 304



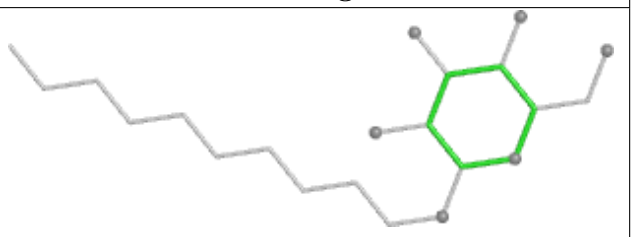
Bond lengths



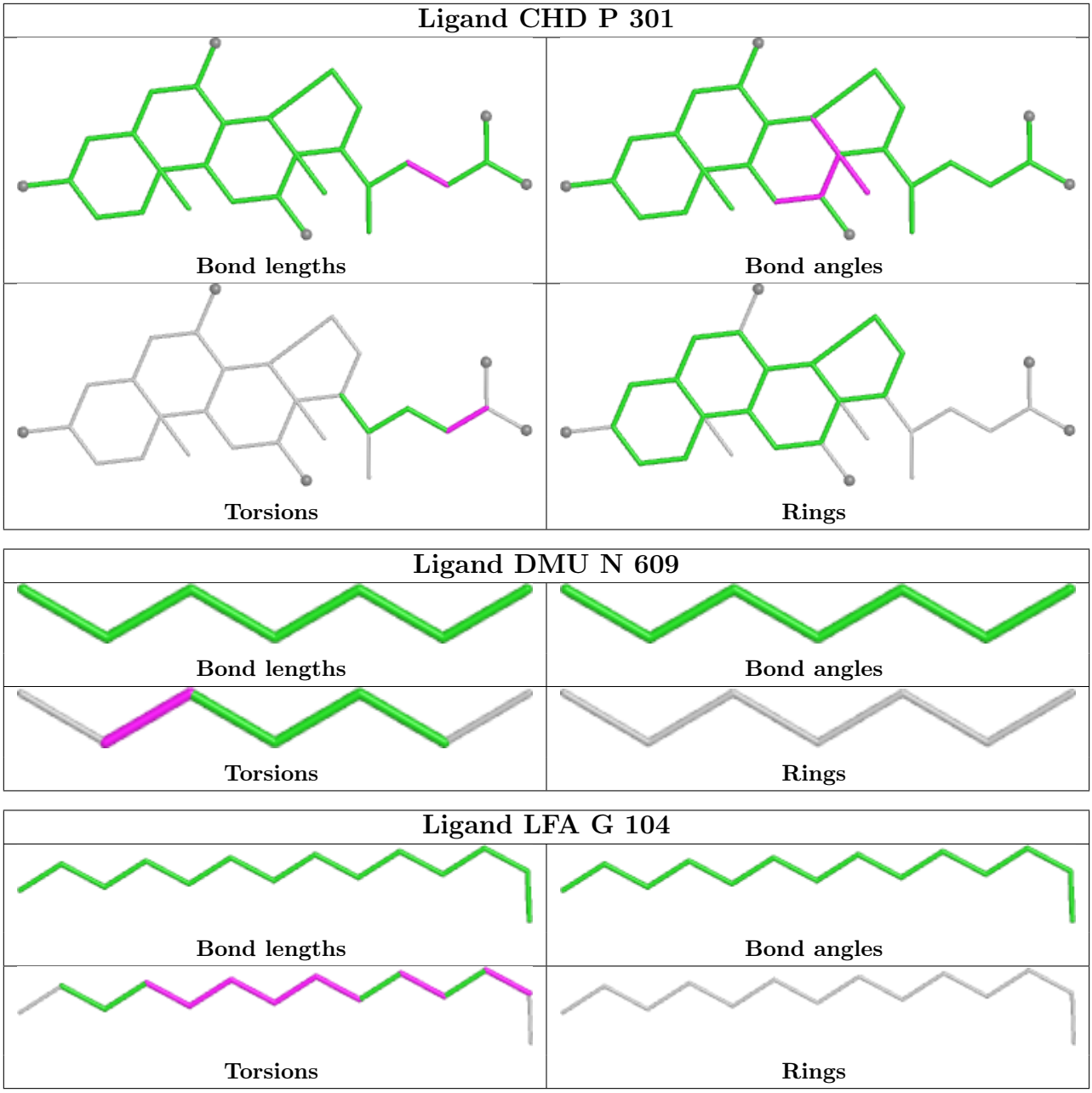
Bond angles



Torsions



Rings



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.03	4 (0%) 82 86	16, 34, 40, 50	15 (2%)
1	N	512/514 (99%)	0.03	3 (0%) 85 89	17, 36, 43, 54	15 (2%)
2	B	226/227 (99%)	0.32	12 (5%) 32 36	21, 41, 53, 64	5 (2%)
2	O	226/227 (99%)	0.31	7 (3%) 51 58	22, 44, 62, 73	5 (2%)
3	C	258/261 (98%)	0.02	2 (0%) 82 86	16, 37, 44, 53	9 (3%)
3	P	258/261 (98%)	-0.02	2 (0%) 82 86	16, 37, 45, 57	9 (3%)
4	D	143/147 (97%)	0.17	3 (2%) 63 70	20, 42, 52, 64	1 (0%)
4	Q	137/147 (93%)	0.48	8 (5%) 29 33	23, 51, 67, 74	1 (0%)
5	E	102/109 (93%)	0.06	0 100 100	37, 43, 51, 60	0
5	R	102/109 (93%)	0.12	2 (1%) 65 71	38, 48, 59, 68	0
6	F	91/98 (92%)	0.09	1 (1%) 78 83	20, 41, 53, 65	2 (2%)
6	S	91/98 (92%)	0.21	2 (2%) 62 69	19, 40, 53, 59	2 (2%)
7	G	72/85 (84%)	0.46	4 (5%) 30 34	21, 42, 65, 72	1 (1%)
7	T	72/85 (84%)	0.50	2 (2%) 55 61	22, 44, 66, 78	1 (1%)
8	H	75/85 (88%)	0.45	4 (5%) 32 36	38, 45, 70, 79	0
8	U	75/85 (88%)	0.63	6 (8%) 18 22	42, 48, 75, 87	0
9	I	70/73 (95%)	0.70	9 (12%) 7 8	38, 49, 60, 69	0
9	V	70/73 (95%)	0.55	4 (5%) 29 33	38, 55, 65, 76	0
10	J	56/59 (94%)	0.32	2 (3%) 46 52	37, 45, 57, 64	0
10	W	56/59 (94%)	0.32	2 (3%) 46 52	38, 45, 58, 64	0
11	K	49/56 (87%)	0.47	3 (6%) 27 31	41, 46, 57, 64	0
11	X	49/56 (87%)	0.84	3 (6%) 27 31	46, 53, 66, 74	0
12	L	44/47 (93%)	0.03	0 100 100	35, 38, 46, 51	0
12	Y	44/47 (93%)	0.22	0 100 100	38, 43, 52, 56	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	40/46 (86%)	0.29	1 (2%) 58 64	37, 40, 51, 57	0
13	Z	40/46 (86%)	0.48	1 (2%) 58 64	43, 47, 62, 64	0
All	All	3470/3614 (96%)	0.19	87 (2%) 58 64	16, 40, 58, 87	66 (1%)

The worst 5 of 87 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	U	48	GLY	7.0
7	T	36	TRP	6.9
11	X	6	ALA	5.4
2	O	113	TYR	5.4
2	O	90	ILE	5.2

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	0.91	0.14	41,47,64,69	0
1	FME	N	1	10/11	0.92	0.14	44,49,65,75	0
2	FME	B	1	10/11	0.97	0.08	38,41,48,68	0
2	FME	O	1	10/11	0.97	0.10	43,46,54,63	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	DMU	C	318	22/33	0.68	0.29	39,46,54,64	22

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	DMU	P	316	22/33	0.68	0.33	36,50,58,64	22
19	LFA	P	310	11/20	0.74	0.40	42,50,57,64	11
19	LFA	C	312	14/20	0.75	0.39	38,49,56,56	14
20	DMU	A	608	7/33	0.76	0.35	40,44,47,47	7
21	EDO	P	321	4/4	0.78	0.37	35,36,37,42	4
19	LFA	P	311	11/20	0.79	0.30	38,43,51,51	11
20	DMU	C	319	33/33	0.79	0.32	36,48,58,66	33
20	DMU	C	316	33/33	0.80	0.33	40,46,56,57	33
24	CHD	C	305	29/29	0.80	0.17	54,62,74,90	0
24	CHD	P	305	29/29	0.80	0.17	54,62,74,103	0
26	CDL	N	606	64/100	0.80	0.19	48,66,80,96	0
19	LFA	P	308	6/20	0.81	0.35	38,41,43,44	6
26	CDL	I	101	64/100	0.81	0.19	41,63,73,83	0
19	LFA	C	326	15/20	0.81	0.38	40,47,55,57	15
19	LFA	C	308	6/20	0.82	0.42	40,45,46,48	6
19	LFA	T	101	14/20	0.82	0.26	36,41,49,51	14
19	LFA	G	104	14/20	0.82	0.27	34,42,51,51	14
20	DMU	O	304	22/33	0.83	0.27	46,59,68,69	22
20	DMU	P	314	33/33	0.83	0.28	39,48,56,66	33
19	LFA	O	303	11/20	0.83	0.33	43,50,58,59	11
20	DMU	P	317	33/33	0.83	0.29	39,50,56,61	33
20	DMU	Q	201	33/33	0.83	0.23	40,50,59,62	33
20	DMU	Z	102	22/33	0.83	0.38	46,57,63,72	22
19	LFA	C	313	11/20	0.83	0.28	37,41,51,54	11
19	LFA	C	315	13/20	0.83	0.26	41,46,54,59	13
20	DMU	C	320	33/33	0.83	0.23	40,55,60,62	33
26	CDL	C	304	87/100	0.83	0.20	43,61,77,82	0
20	DMU	G	102	11/33	0.83	0.38	43,51,56,58	11
20	DMU	M	102	8/33	0.83	0.26	39,43,45,51	8
26	CDL	P	304	87/100	0.83	0.20	42,63,83,88	0
26	CDL	Y	101	94/100	0.83	0.18	46,63,81,92	0
19	LFA	P	307	11/20	0.84	0.33	41,45,48,51	11
19	LFA	P	313	13/20	0.84	0.27	39,45,53,58	13
21	EDO	A	611	4/4	0.84	0.31	35,41,42,45	4
21	EDO	D	202	4/4	0.84	0.36	40,40,42,43	4
20	DMU	C	324	22/33	0.84	0.28	41,51,59,60	22
20	DMU	P	318	33/33	0.84	0.24	47,57,67,74	33
19	LFA	C	314	15/20	0.85	0.23	38,42,53,54	15
21	EDO	C	323	4/4	0.85	0.32	35,38,38,42	4
20	DMU	C	317	7/33	0.85	0.26	41,43,47,49	7
21	EDO	N	612	4/4	0.85	0.29	39,40,42,44	4
19	LFA	C	307	11/20	0.85	0.30	42,46,51,51	11

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
21	EDO	R	203	4/4	0.85	0.28	39,40,45,50	4
19	LFA	T	103	14/20	0.85	0.31	41,50,54,58	14
19	LFA	T	104	11/20	0.85	0.30	45,47,61,63	11
19	LFA	C	311	11/20	0.85	0.28	42,52,56,57	11
20	DMU	B	308	22/33	0.85	0.30	48,64,72,73	22
20	DMU	Z	101	33/33	0.85	0.14	48,58,70,73	0
20	DMU	H	101	33/33	0.85	0.25	36,45,51,60	33
21	EDO	A	610	4/4	0.85	0.24	31,33,34,34	4
20	DMU	N	609	7/33	0.86	0.34	47,48,50,53	7
20	DMU	N	610	33/33	0.86	0.21	38,52,65,67	33
19	LFA	P	309	18/20	0.86	0.24	36,44,48,48	18
21	EDO	C	321	4/4	0.86	0.29	46,47,48,57	4
20	DMU	A	615	11/33	0.86	0.35	43,51,57,57	11
20	DMU	U	101	33/33	0.86	0.26	36,46,57,65	33
20	DMU	W	101	11/33	0.86	0.32	50,56,61,66	11
20	DMU	P	315	7/33	0.86	0.29	44,46,53,61	7
20	DMU	T	105	22/33	0.87	0.24	44,50,56,65	22
19	LFA	C	309	18/20	0.87	0.23	35,41,47,49	18
26	CDL	L	101	94/100	0.87	0.16	40,59,75,80	0
19	LFA	O	302	17/20	0.87	0.28	43,54,60,68	17
19	LFA	C	310	15/20	0.87	0.32	38,50,54,54	15
20	DMU	C	325	33/33	0.87	0.16	39,47,63,68	33
20	DMU	A	609	33/33	0.88	0.19	33,44,52,57	33
20	DMU	P	322	33/33	0.88	0.16	38,52,69,74	33
19	LFA	P	312	15/20	0.89	0.17	36,41,46,51	15
19	LFA	B	307	17/20	0.89	0.28	42,53,63,63	17
20	DMU	L	102	22/33	0.89	0.30	40,48,54,59	22
20	DMU	B	302	11/33	0.89	0.27	39,43,51,58	11
20	DMU	B	304	22/33	0.89	0.20	36,52,58,70	22
20	DMU	M	101	33/33	0.90	0.11	46,52,64,74	0
21	EDO	E	202	4/4	0.90	0.24	36,37,41,44	4
20	DMU	J	101	11/33	0.90	0.29	48,52,55,68	11
21	EDO	N	613	4/4	0.90	0.18	31,31,32,33	4
20	DMU	O	306	11/33	0.90	0.27	38,41,49,53	11
20	DMU	O	308	22/33	0.90	0.20	33,47,51,52	22
20	DMU	D	201	33/33	0.90	0.16	29,42,50,55	33
20	DMU	P	306	11/33	0.91	0.27	40,46,49,56	11
21	EDO	P	319	4/4	0.91	0.22	46,48,55,63	4
21	EDO	N	611	4/4	0.91	0.16	30,31,32,34	4
20	DMU	B	303	11/33	0.91	0.22	38,45,55,56	11
21	EDO	C	322	4/4	0.92	0.24	35,37,38,39	4
21	EDO	R	202	4/4	0.92	0.20	34,35,39,42	4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
19	LFA	A	607	14/20	0.92	0.21	34,40,57,57	14
20	DMU	C	306	11/33	0.92	0.22	43,49,53,57	11
20	DMU	Z	103	8/33	0.92	0.20	42,45,47,49	8
25	UNX	P	302	1/1	0.92	0.28	44,44,44,44	0
21	EDO	A	613	4/4	0.93	0.19	39,40,41,45	4
21	EDO	N	615	4/4	0.93	0.22	32,32,32,34	4
21	EDO	A	612	4/4	0.93	0.20	30,30,30,31	4
21	EDO	N	614	4/4	0.94	0.19	34,34,35,39	4
21	EDO	G	103	4/4	0.94	0.16	38,38,39,41	4
19	LFA	N	608	14/20	0.94	0.17	34,40,52,53	14
21	EDO	E	201	4/4	0.94	0.21	34,34,34,37	4
20	DMU	O	307	11/33	0.94	0.21	38,44,50,56	11
28	PEK	T	102	53/53	0.94	0.12	38,48,67,69	0
21	EDO	F	103	4/4	0.95	0.11	31,34,35,36	4
21	EDO	R	201	4/4	0.95	0.25	54,59,60,62	4
21	EDO	F	102	4/4	0.95	0.12	27,27,31,32	4
21	EDO	P	320	4/4	0.95	0.23	33,35,36,38	4
28	PEK	G	101	53/53	0.95	0.11	36,46,68,76	0
21	EDO	T	106	4/4	0.95	0.12	40,40,40,43	4
25	UNX	C	302	1/1	0.96	0.15	45,45,45,45	0
24	CHD	C	301	29/29	0.96	0.07	34,37,39,42	0
22	PGV	N	616	51/51	0.97	0.08	33,38,55,62	0
22	PGV	P	303	51/51	0.97	0.08	33,39,63,67	0
24	CHD	B	306	29/29	0.97	0.07	35,39,41,47	0
21	EDO	S	103	4/4	0.97	0.09	31,37,37,38	4
21	EDO	O	309	4/4	0.97	0.12	35,37,37,40	4
24	CHD	O	301	29/29	0.97	0.07	35,39,41,47	0
24	CHD	P	301	29/29	0.97	0.07	34,38,41,44	0
22	PGV	A	614	51/51	0.97	0.09	32,38,55,59	0
22	PGV	C	303	51/51	0.97	0.09	33,40,64,68	0
14	HEA	N	602	60/60	0.98	0.06	32,34,38,43	0
21	EDO	B	305	4/4	0.98	0.08	32,33,35,36	4
17	NA	A	605	1/1	0.98	0.07	36,36,36,36	0
18	N2O	A	606	3/3	0.98	0.10	33,33,35,38	0
18	N2O	N	607	3/3	0.98	0.13	36,36,41,41	0
21	EDO	S	102	4/4	0.98	0.07	26,28,29,29	4
14	HEA	A	602	60/60	0.98	0.06	29,32,37,42	0
14	HEA	A	601	60/60	0.99	0.06	28,32,41,47	0
15	CU	A	603	1/1	0.99	0.02	31,31,31,31	0
16	MG	A	604	1/1	0.99	0.04	31,31,31,31	0
23	CUA	B	301	2/2	0.99	0.03	33,33,33,34	0
23	CUA	O	305	2/2	0.99	0.03	37,37,37,38	0

Continued on next page...

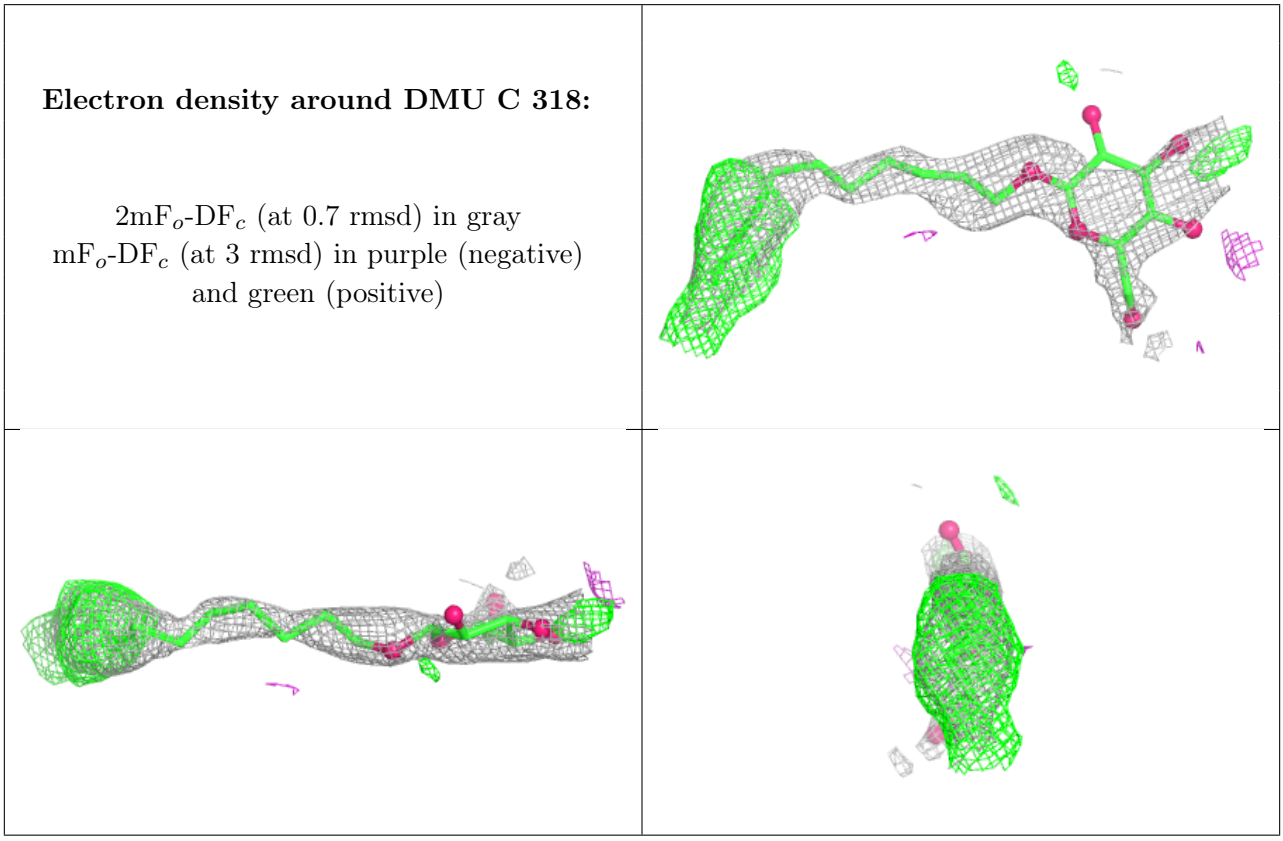
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
27	ZN	F	101	1/1	0.99	0.02	37,37,37,37	0
27	ZN	S	101	1/1	0.99	0.03	37,37,37,37	0
14	HEA	N	601	60/60	0.99	0.06	31,35,44,52	0
17	NA	N	605	1/1	0.99	0.04	41,41,41,41	0
16	MG	N	604	1/1	1.00	0.04	36,36,36,36	0
15	CU	N	603	1/1	1.00	0.02	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.

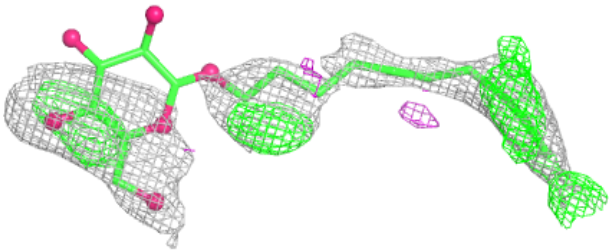
Electron density around DMU C 318:

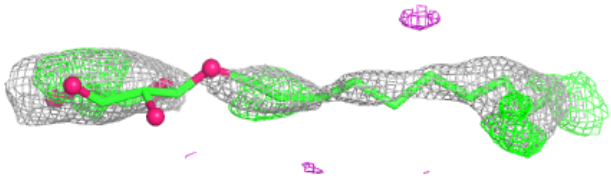
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

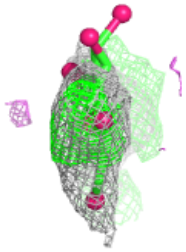


Electron density around DMU P 316:

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

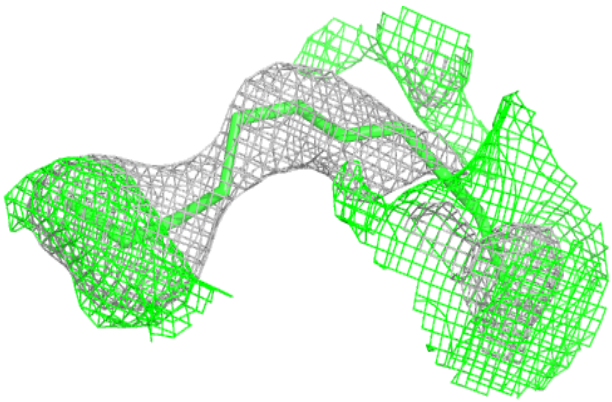


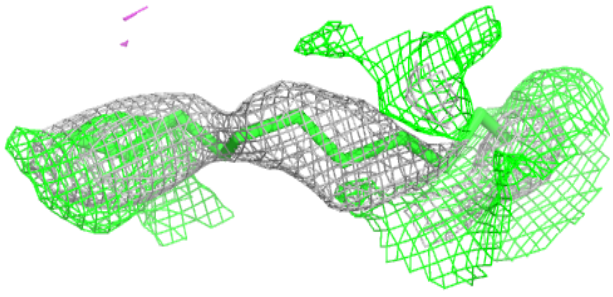


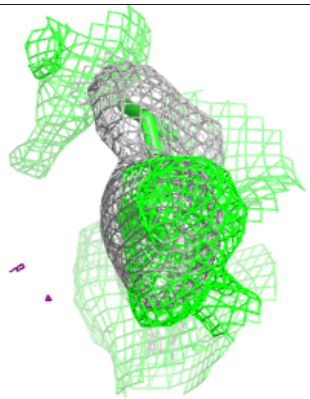


Electron density around LFA P 310:

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

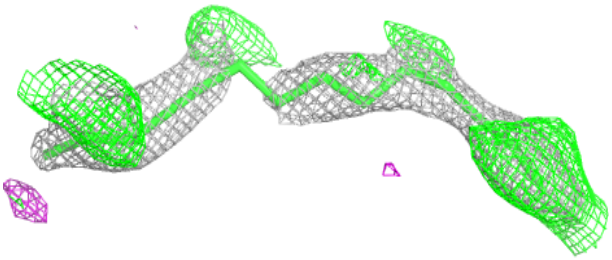


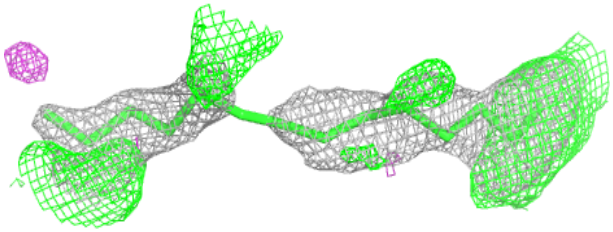


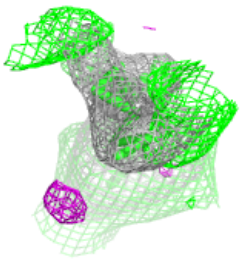


Electron density around LFA C 312:

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

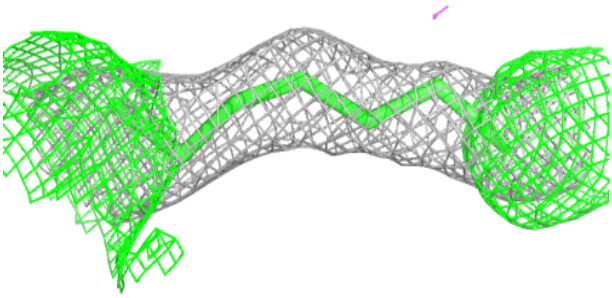


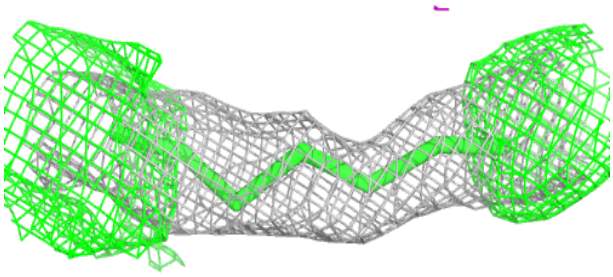


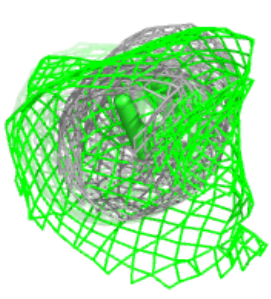


Electron density around DMU A 608:

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

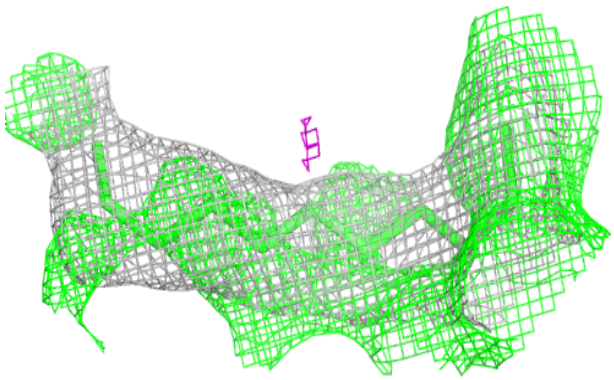


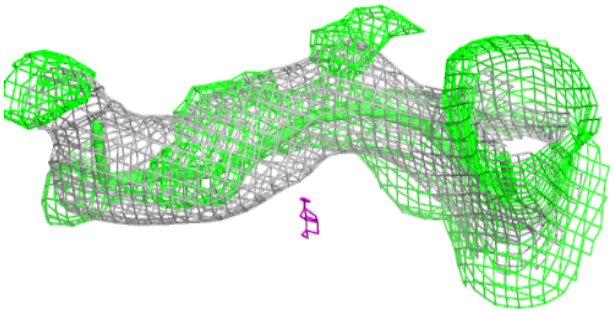


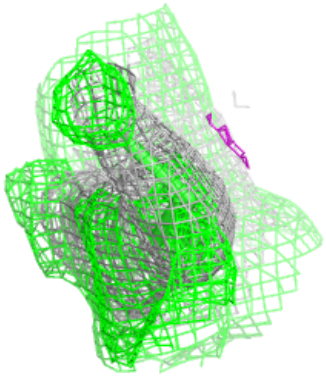


Electron density around LFA P 311:

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

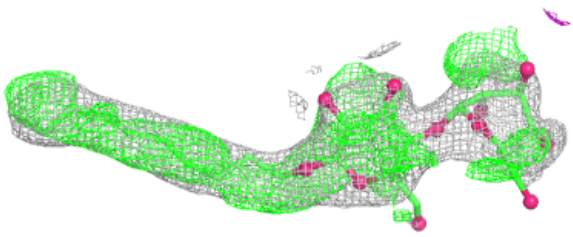


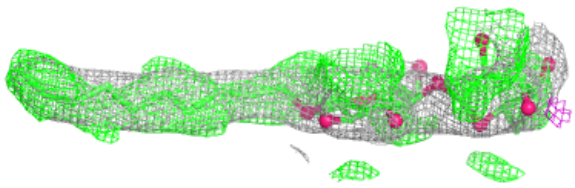


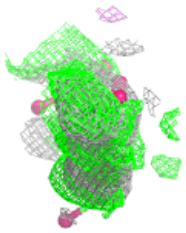


Electron density around DMU C 319:

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

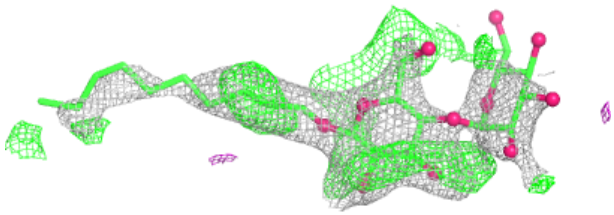


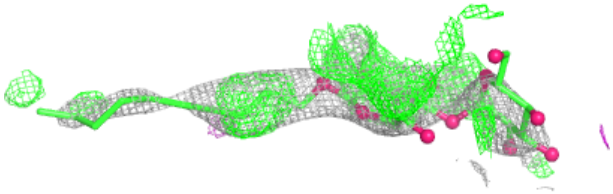


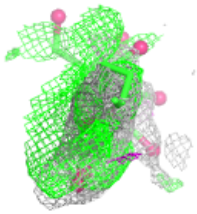


Electron density around DMU C 316:

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

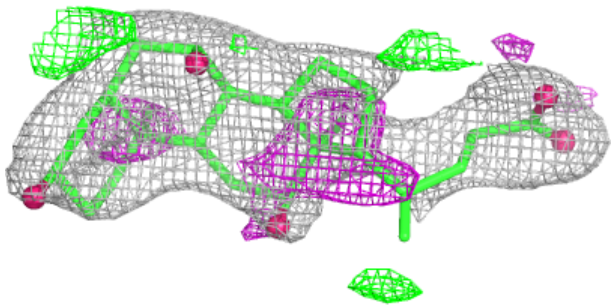


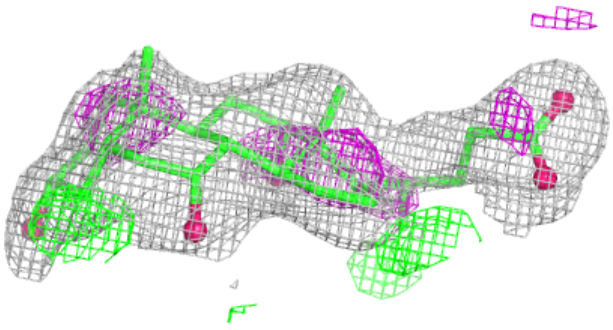


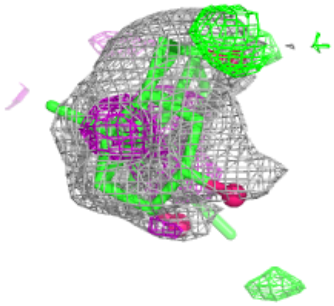


Electron density around CHD C 305:

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

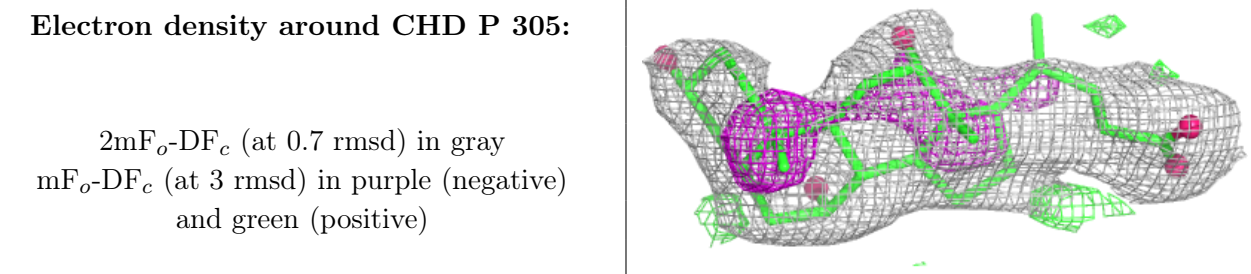


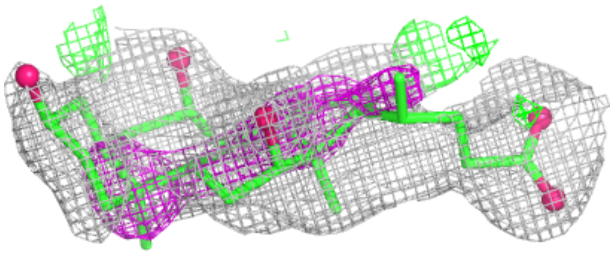


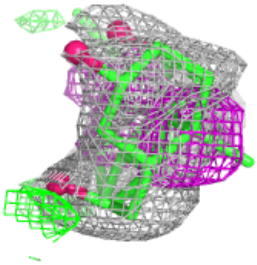


Electron density around CHD P 305:

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

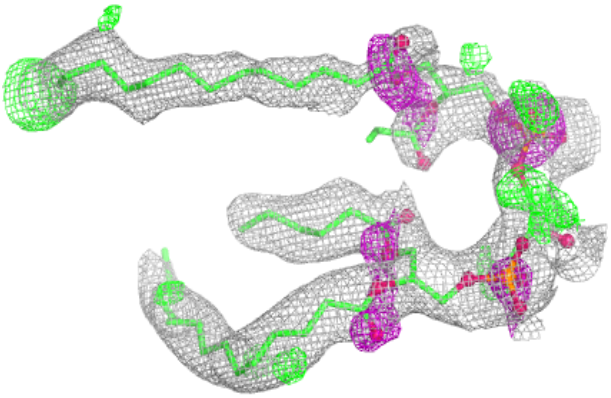


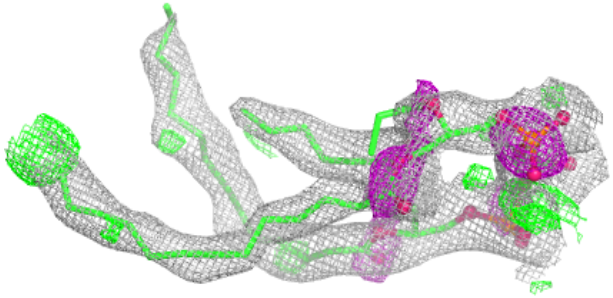


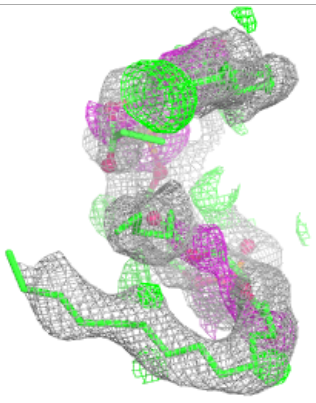


Electron density around CDL N 606:

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

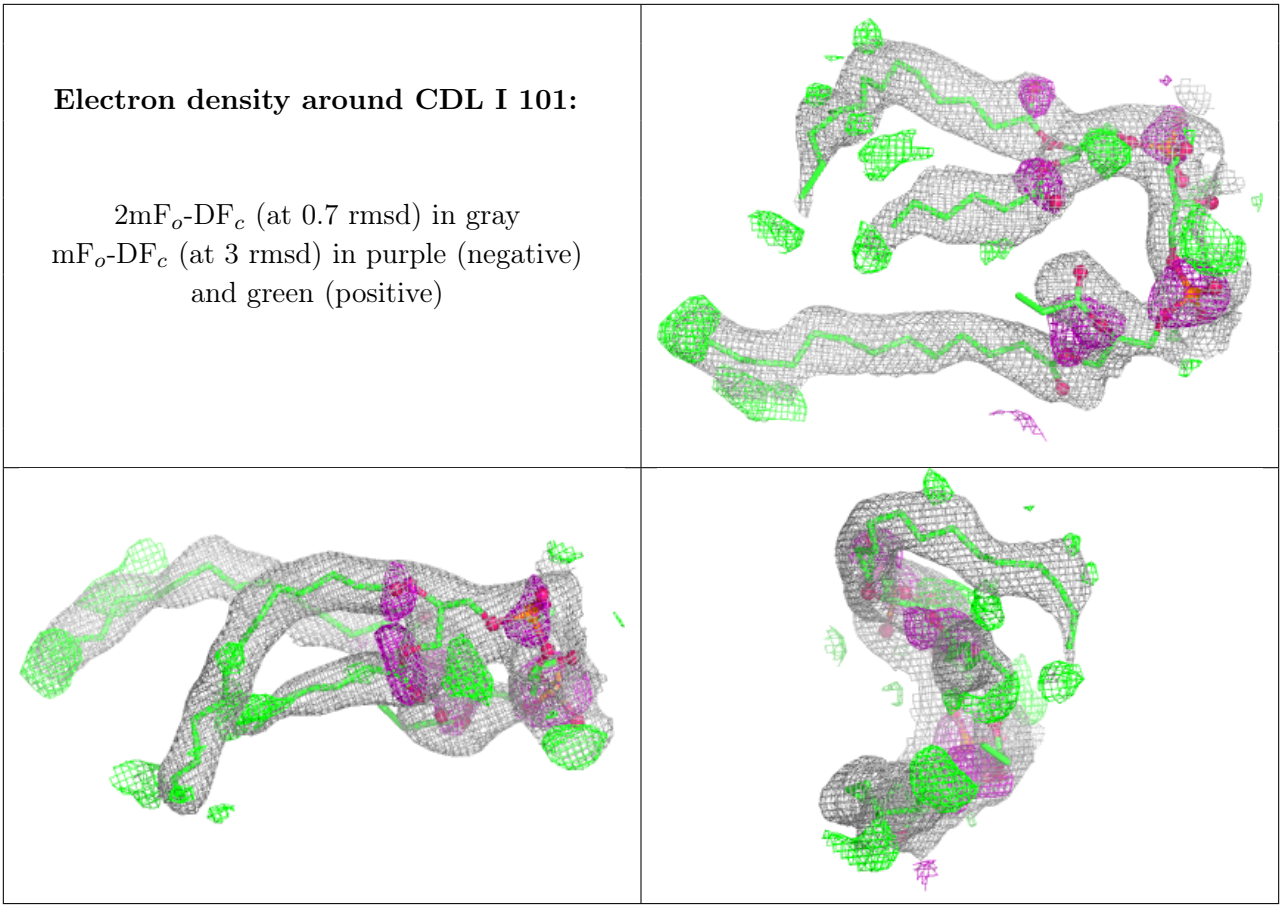






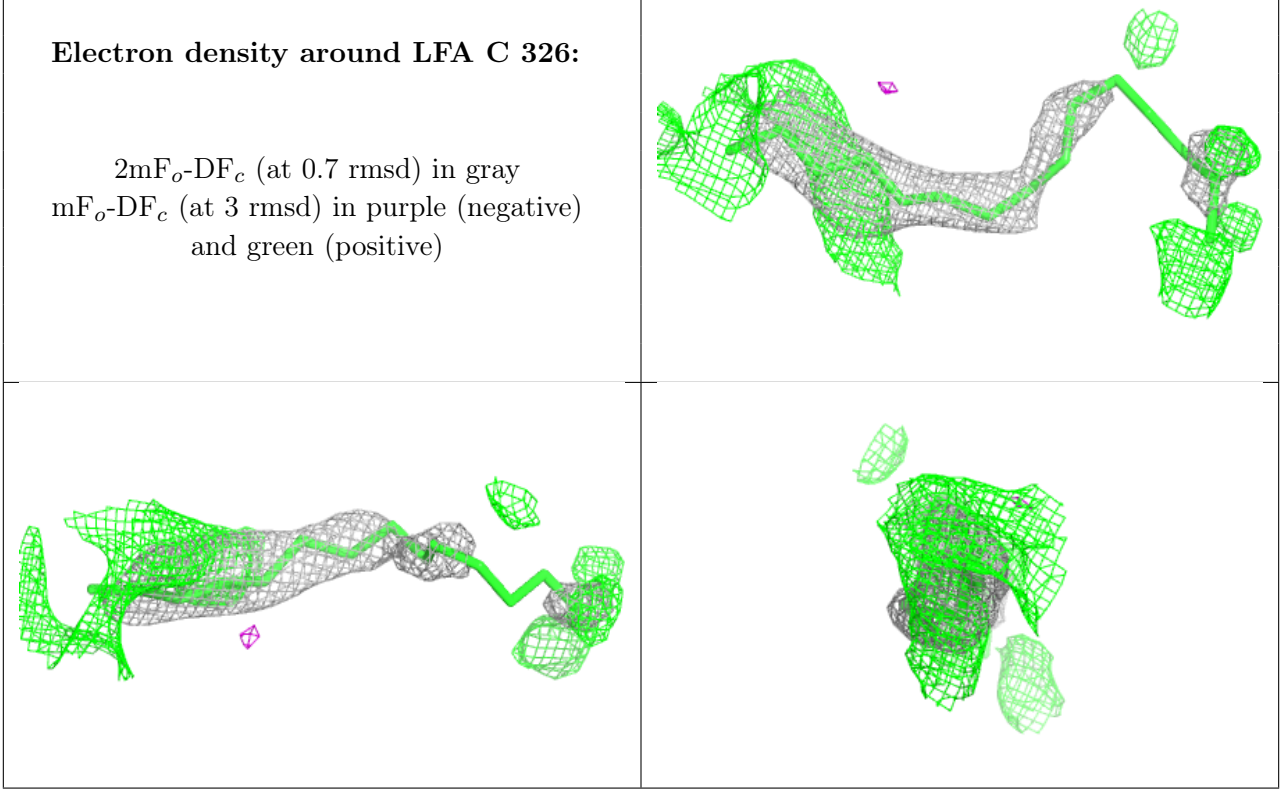
Electron density around CDL I 101:

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



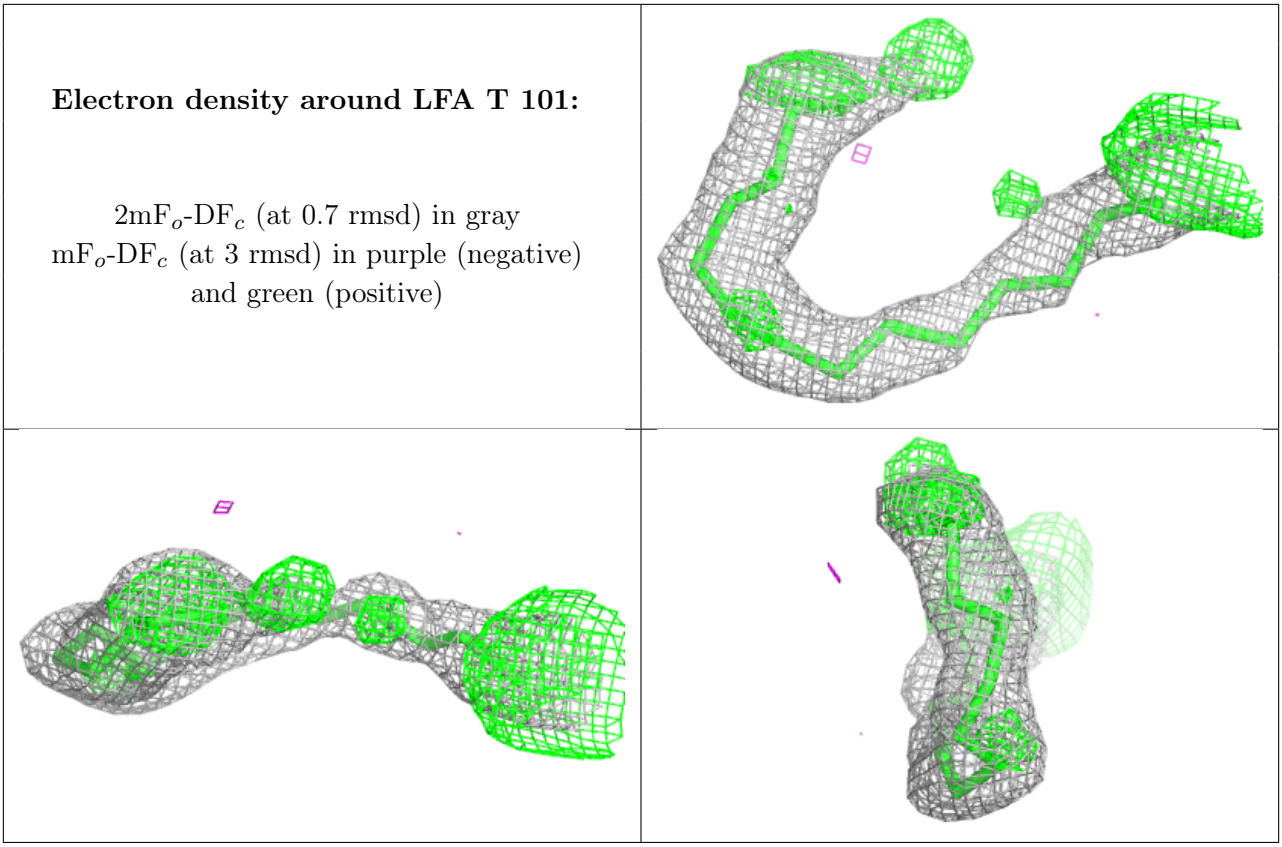
Electron density around LFA C 326:

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



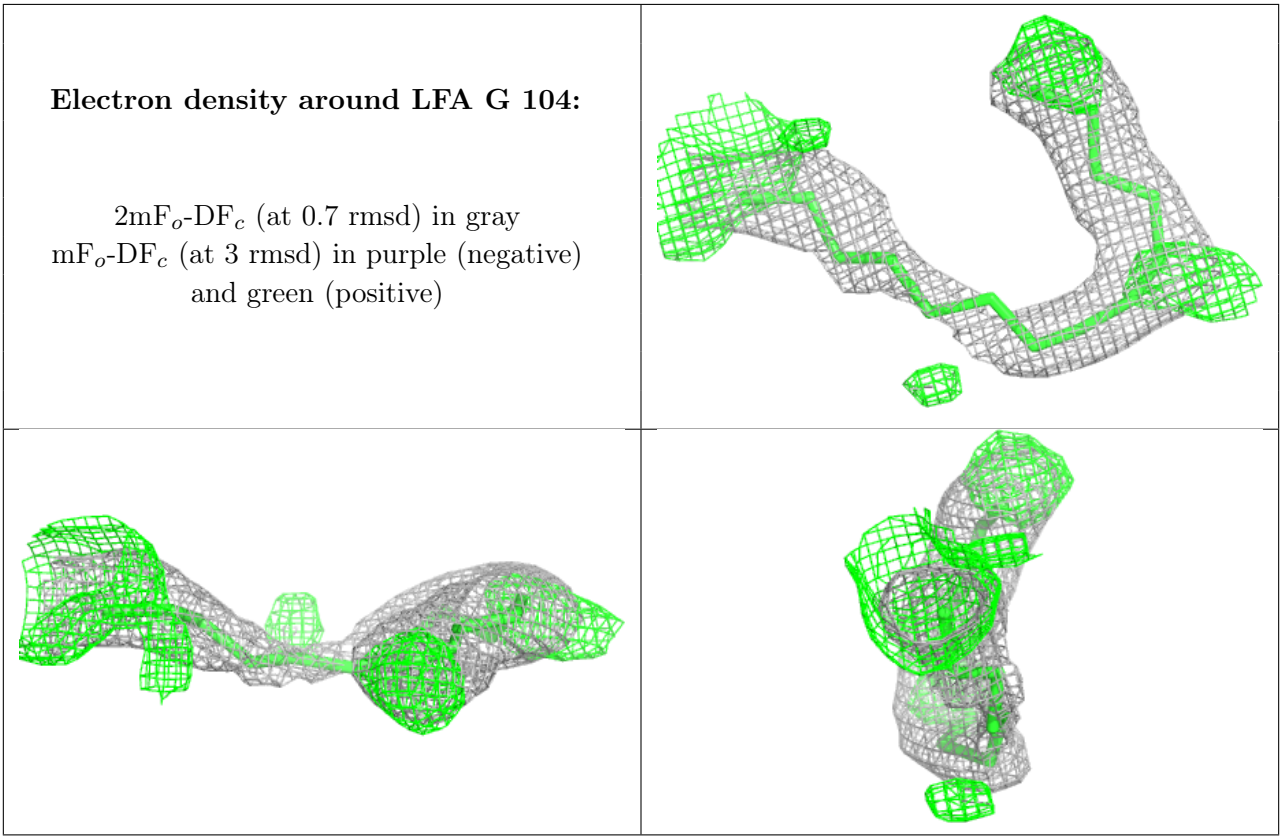
Electron density around LFA T 101:

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



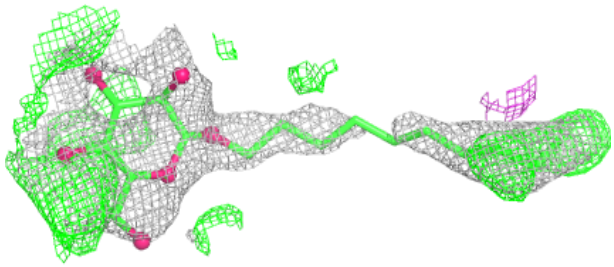
Electron density around LFA G 104:

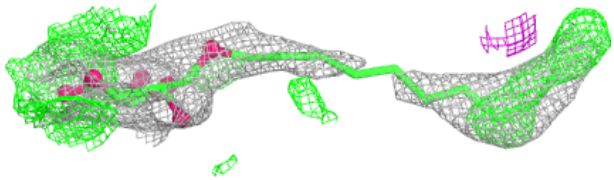
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

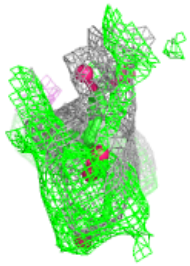


Electron density around DMU O 304:

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

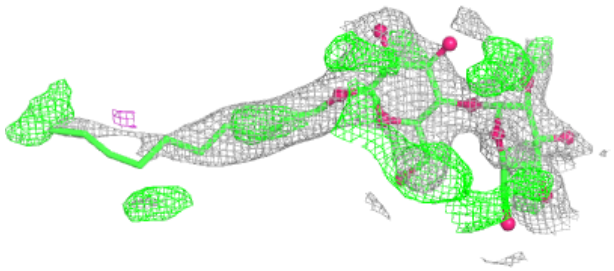


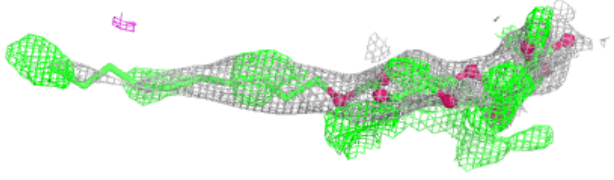


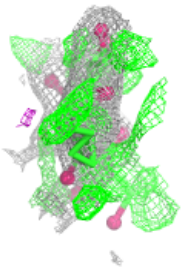


Electron density around DMU P 314:

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

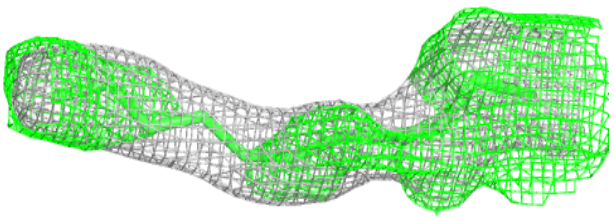


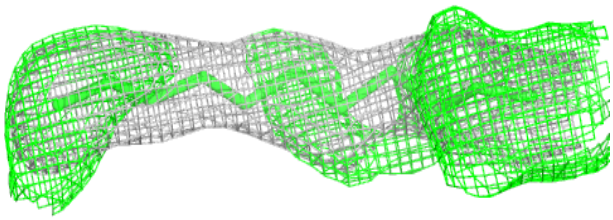


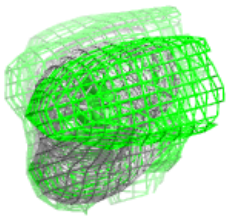


Electron density around LFA O 303:

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

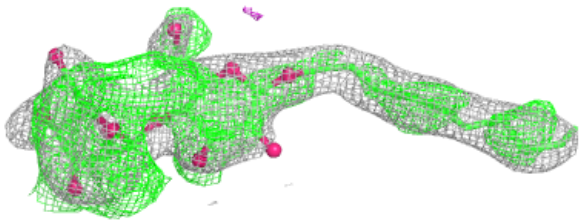


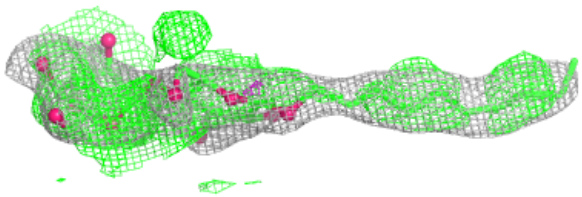


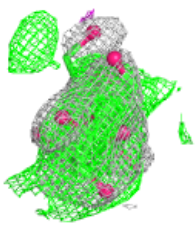


Electron density around DMU P 317:

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

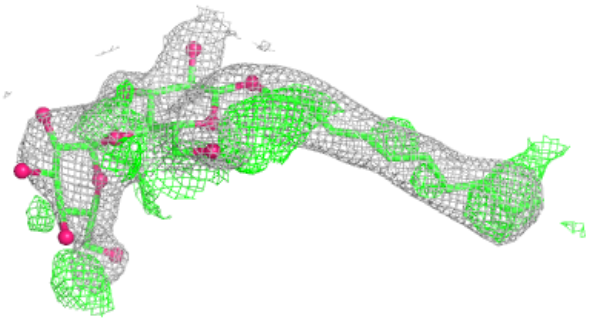


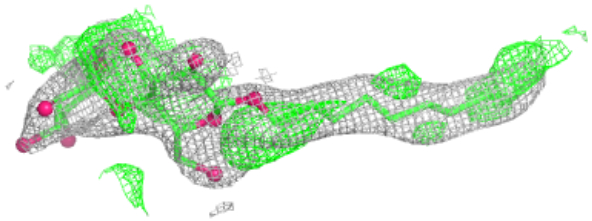


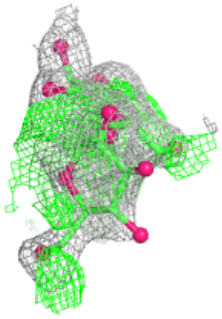


Electron density around DMU Q 201:

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

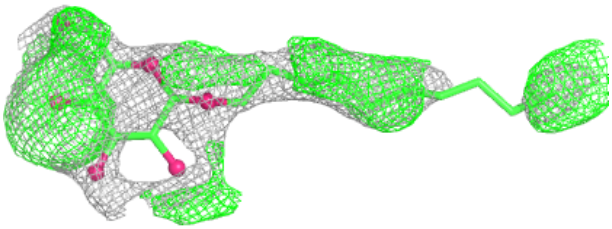


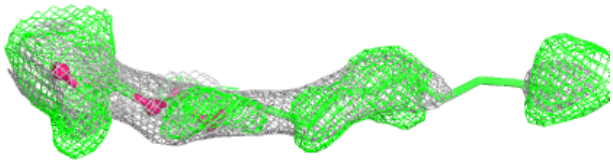


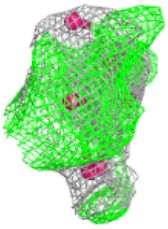


Electron density around DMU Z 102:

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

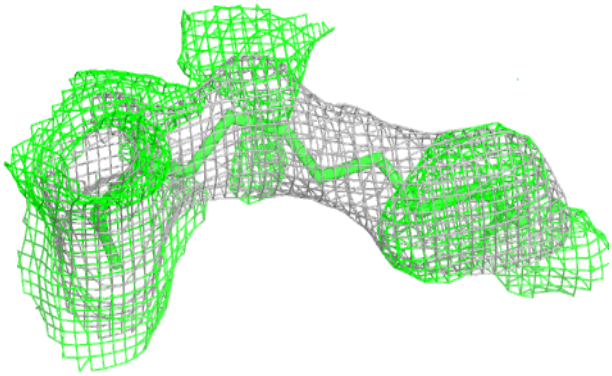


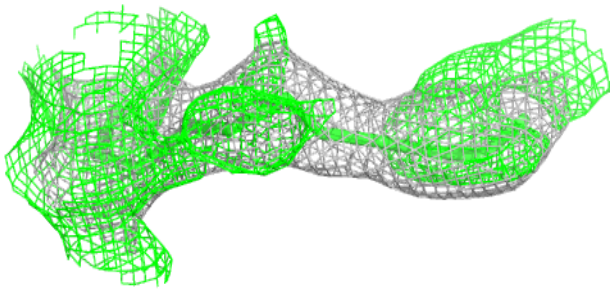


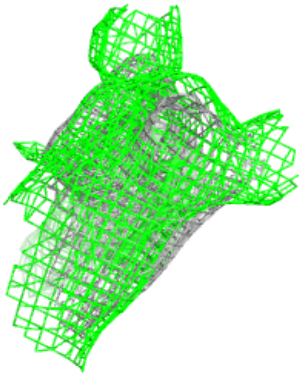


Electron density around LFA C 313:

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

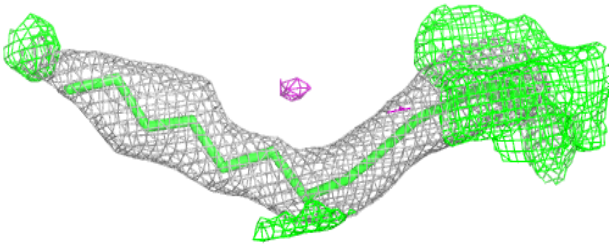


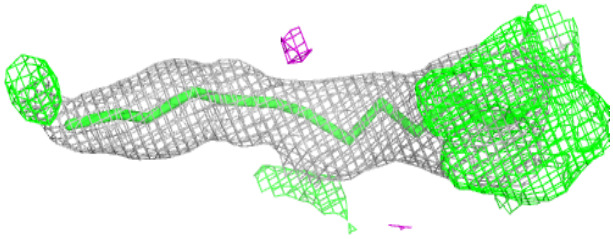


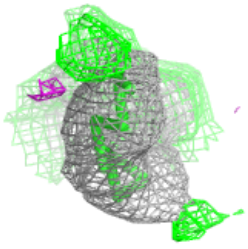


Electron density around LFA C 315:

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

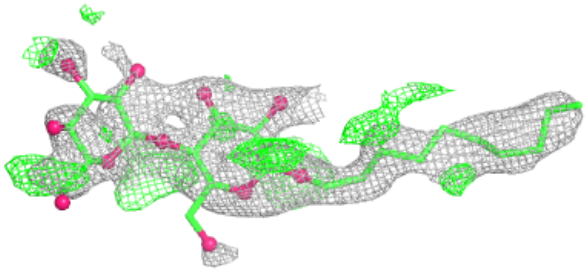


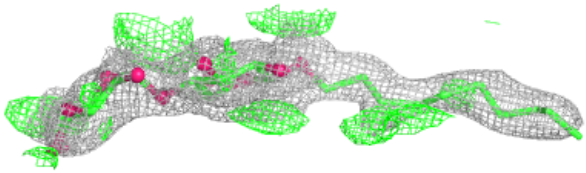


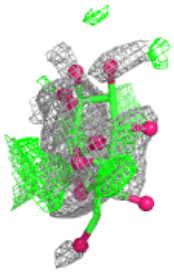


Electron density around DMU C 320:

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

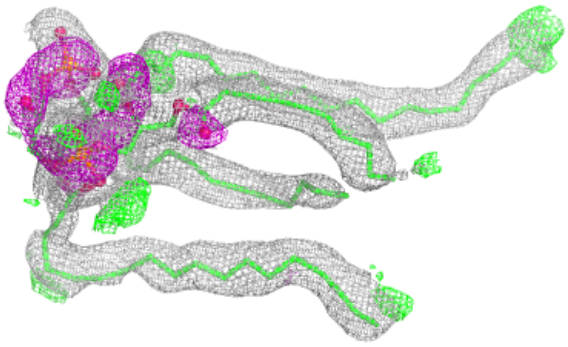


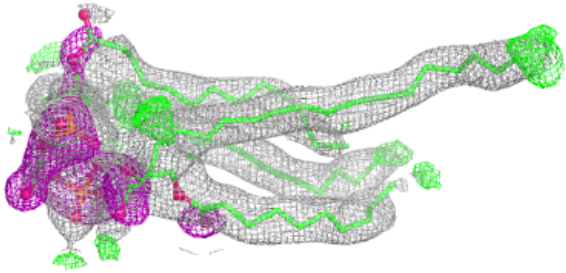


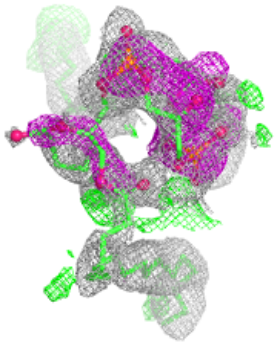


Electron density around CDL C 304:

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

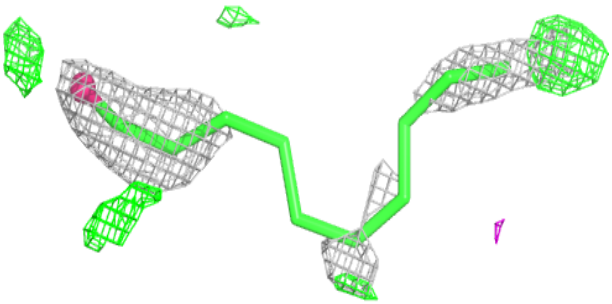


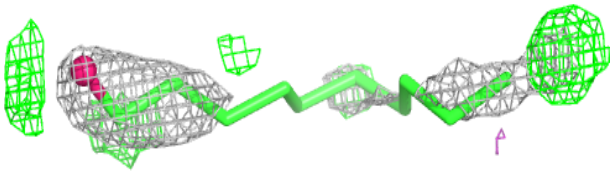


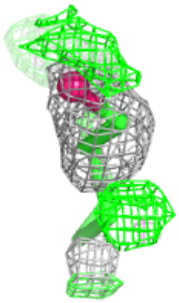


Electron density around DMU G 102:

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

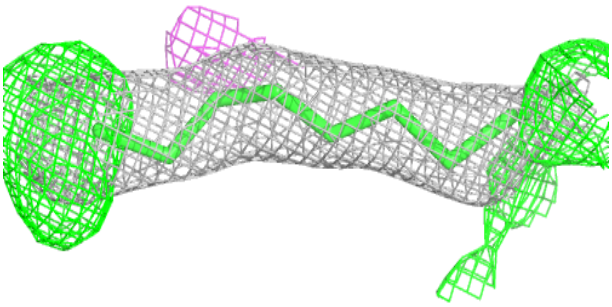


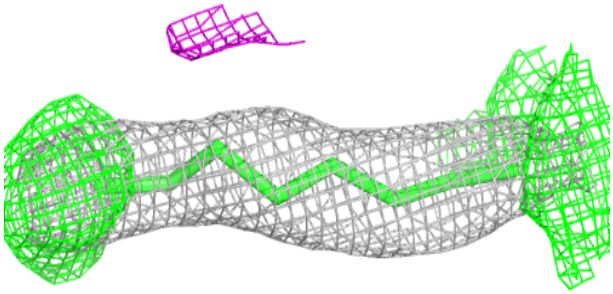


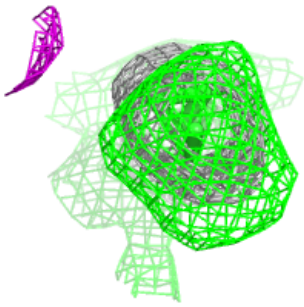


Electron density around DMU M 102:

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

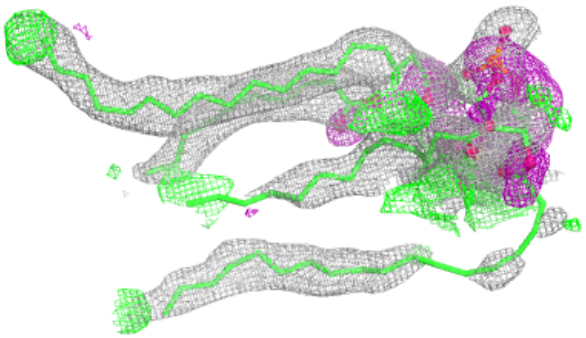


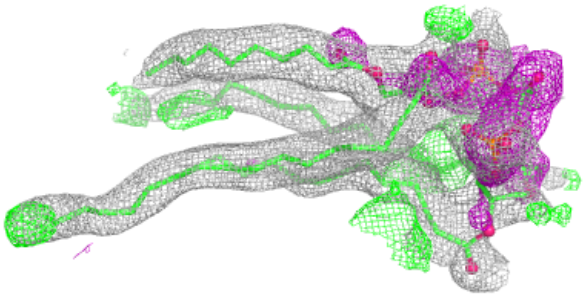


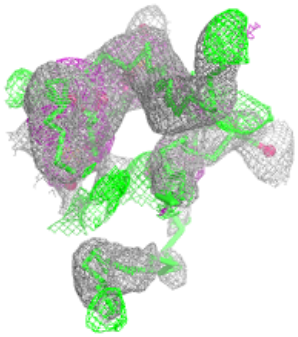


Electron density around CDL P 304:

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

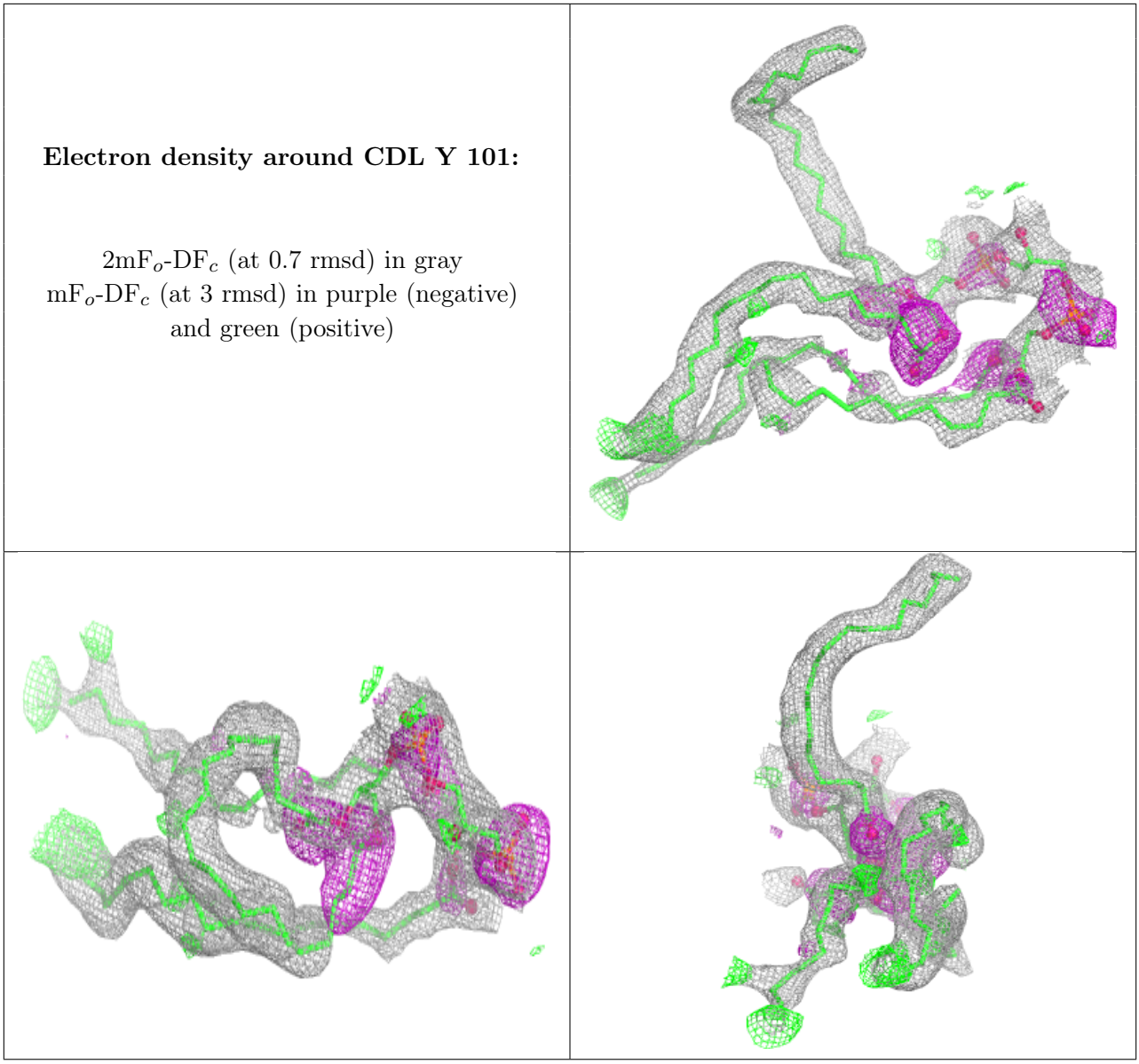






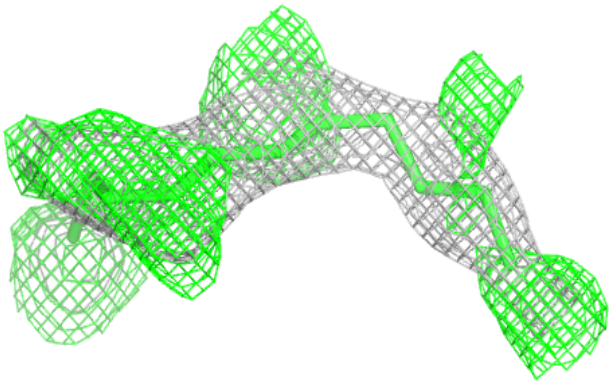
Electron density around CDL Y 101:

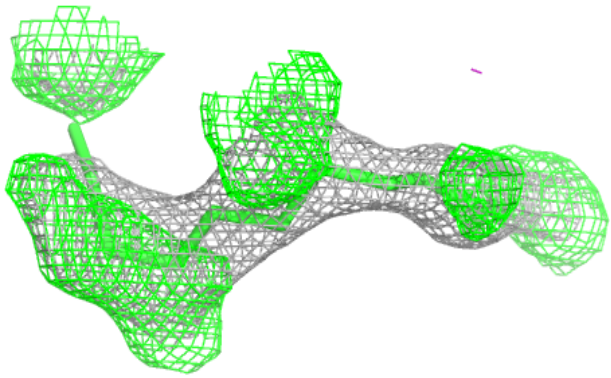
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

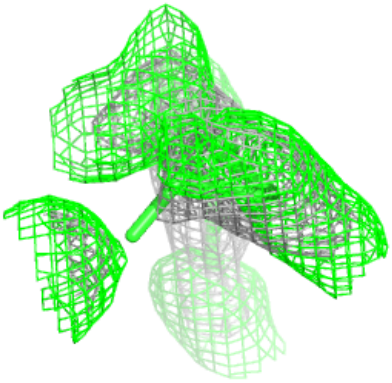


Electron density around LFA P 307:

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

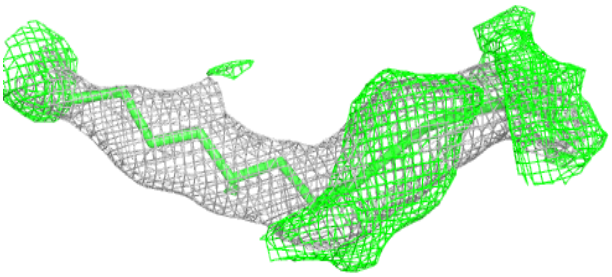


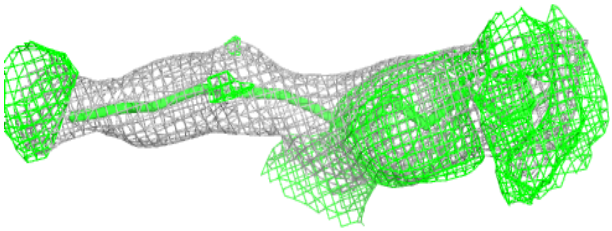


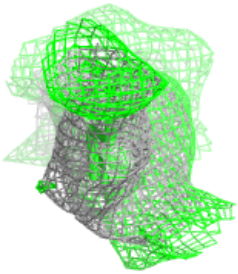


Electron density around LFA P 313:

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

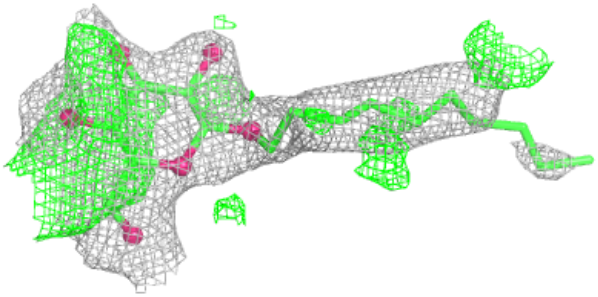


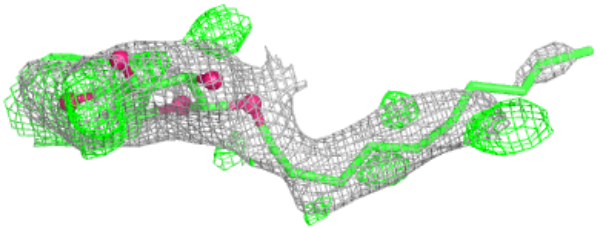


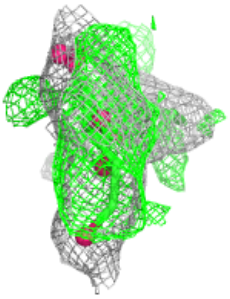


Electron density around DMU C 324:

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

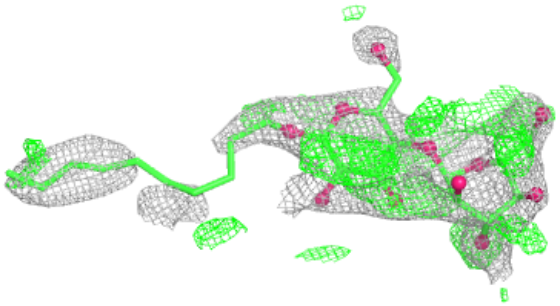


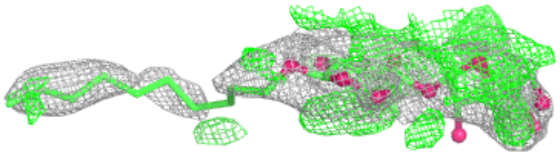


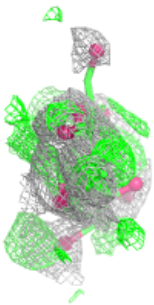


Electron density around DMU P 318:

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

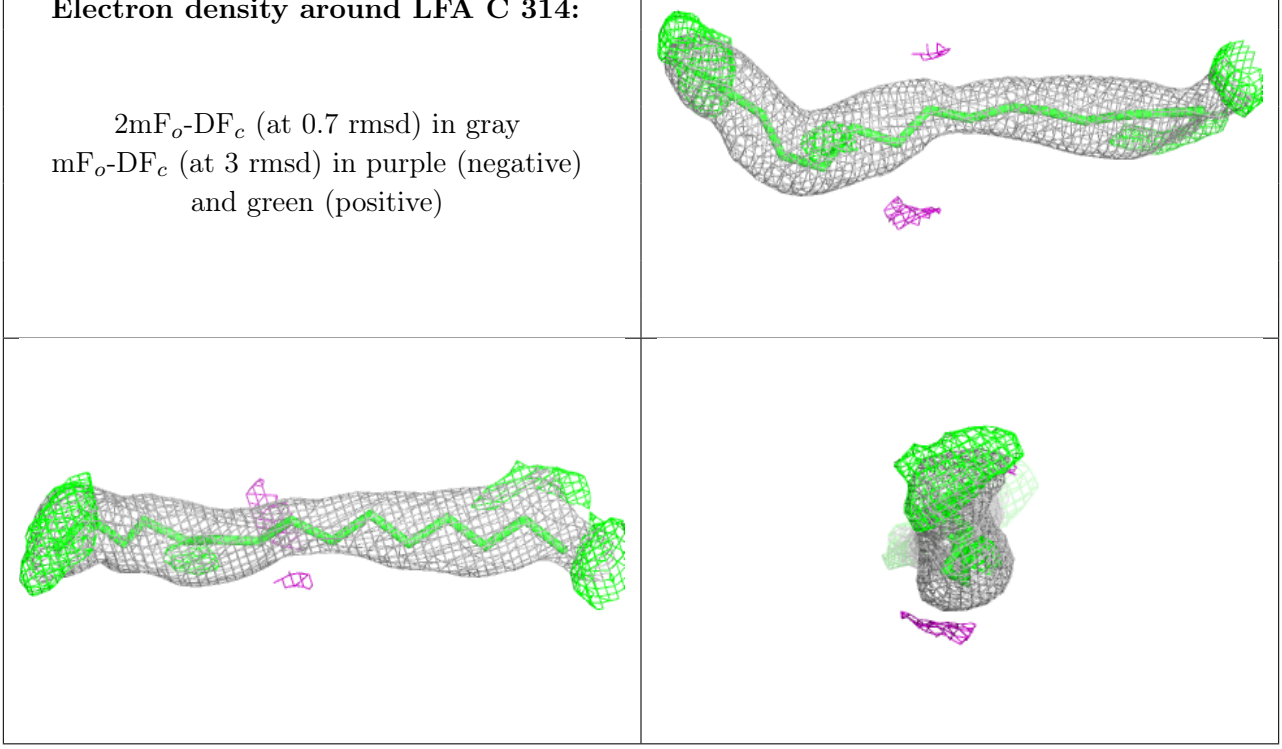






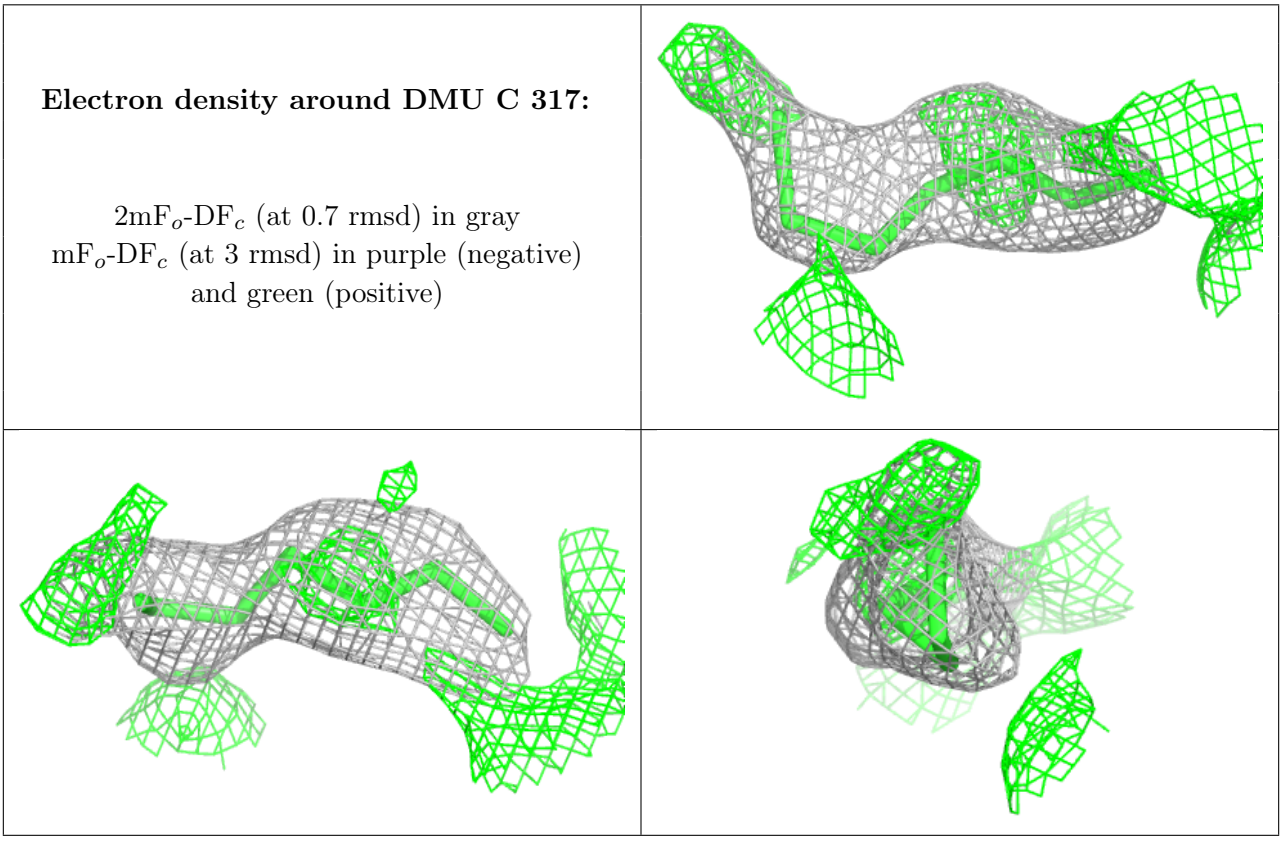
Electron density around LFA C 314:

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



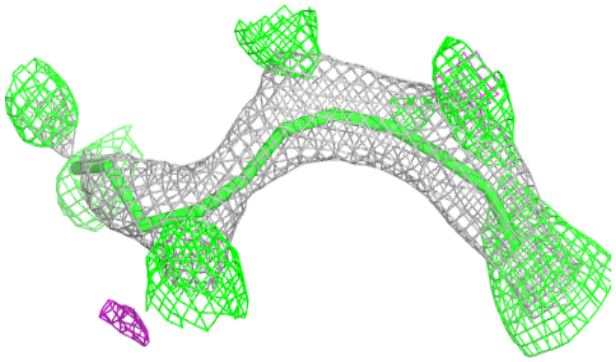
Electron density around DMU C 317:

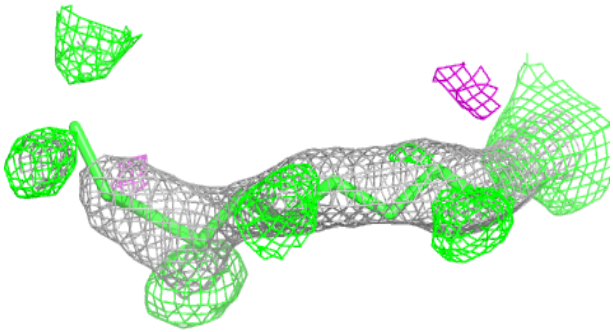
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

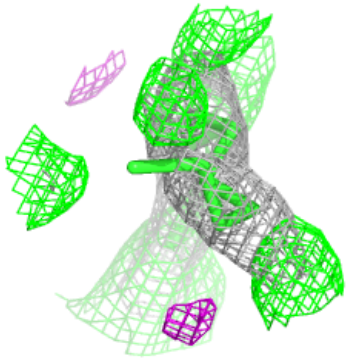


Electron density around LFA C 307:

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

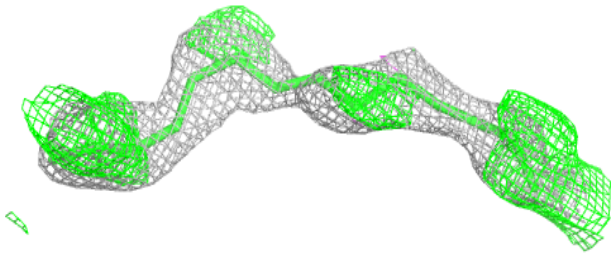


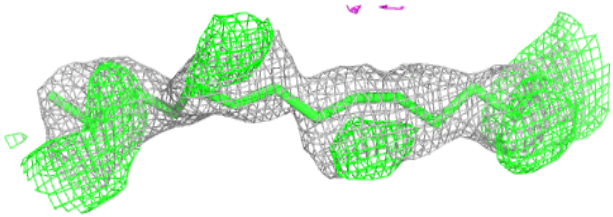


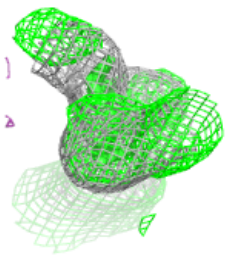


Electron density around LFA T 103:

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

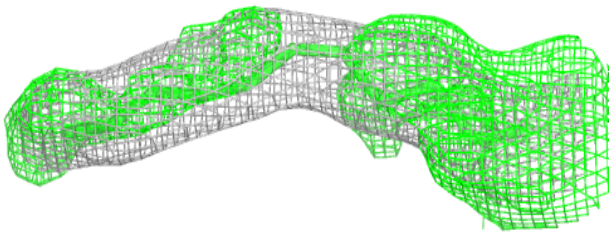


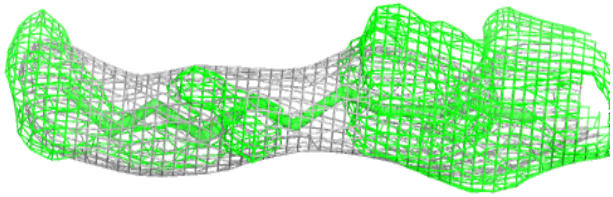


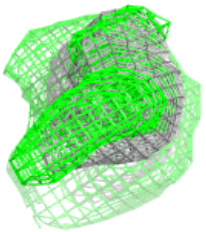


Electron density around LFA T 104:

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

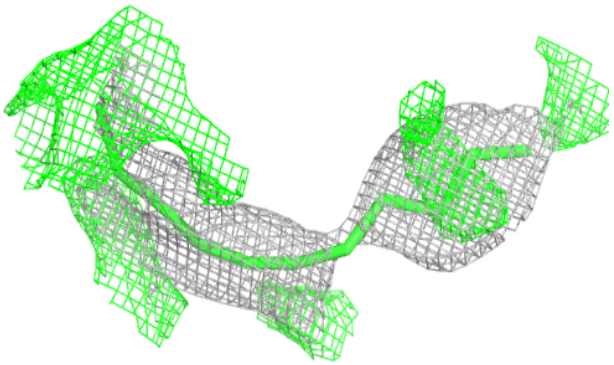


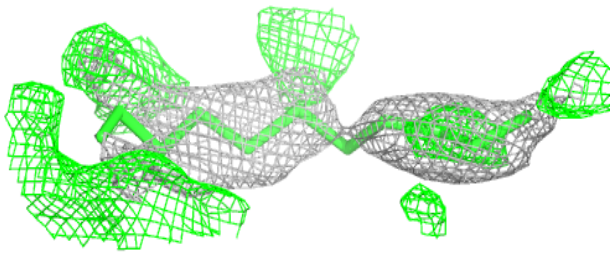


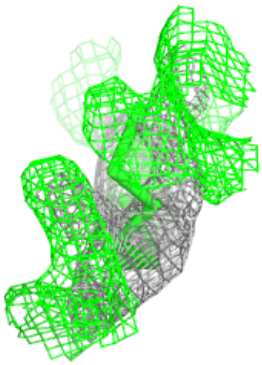


Electron density around LFA C 311:

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

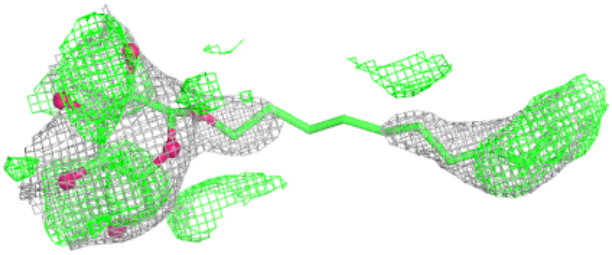


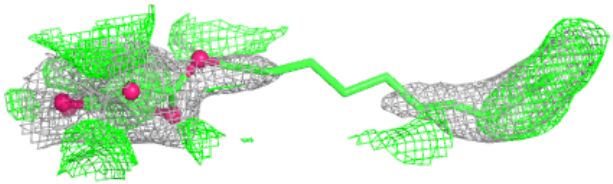


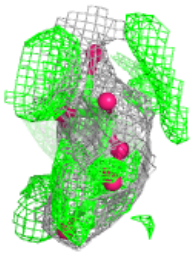


Electron density around DMU B 308:

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

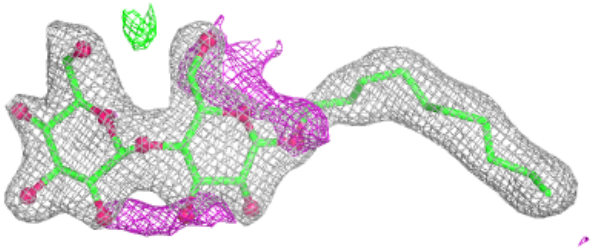


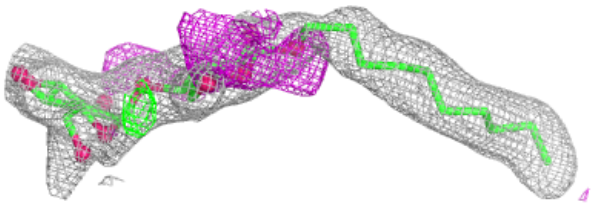


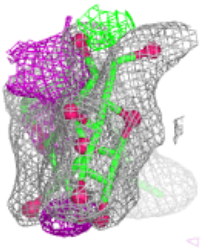


Electron density around DMU Z 101:

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

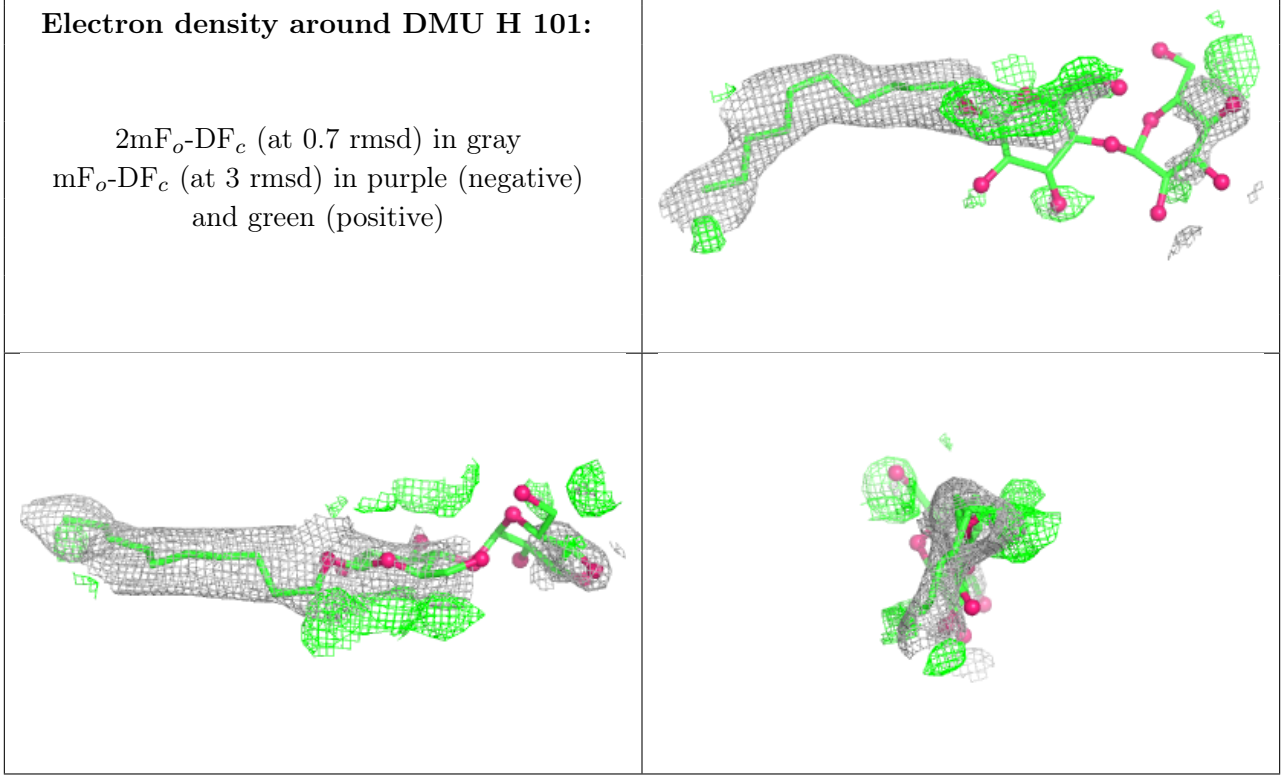






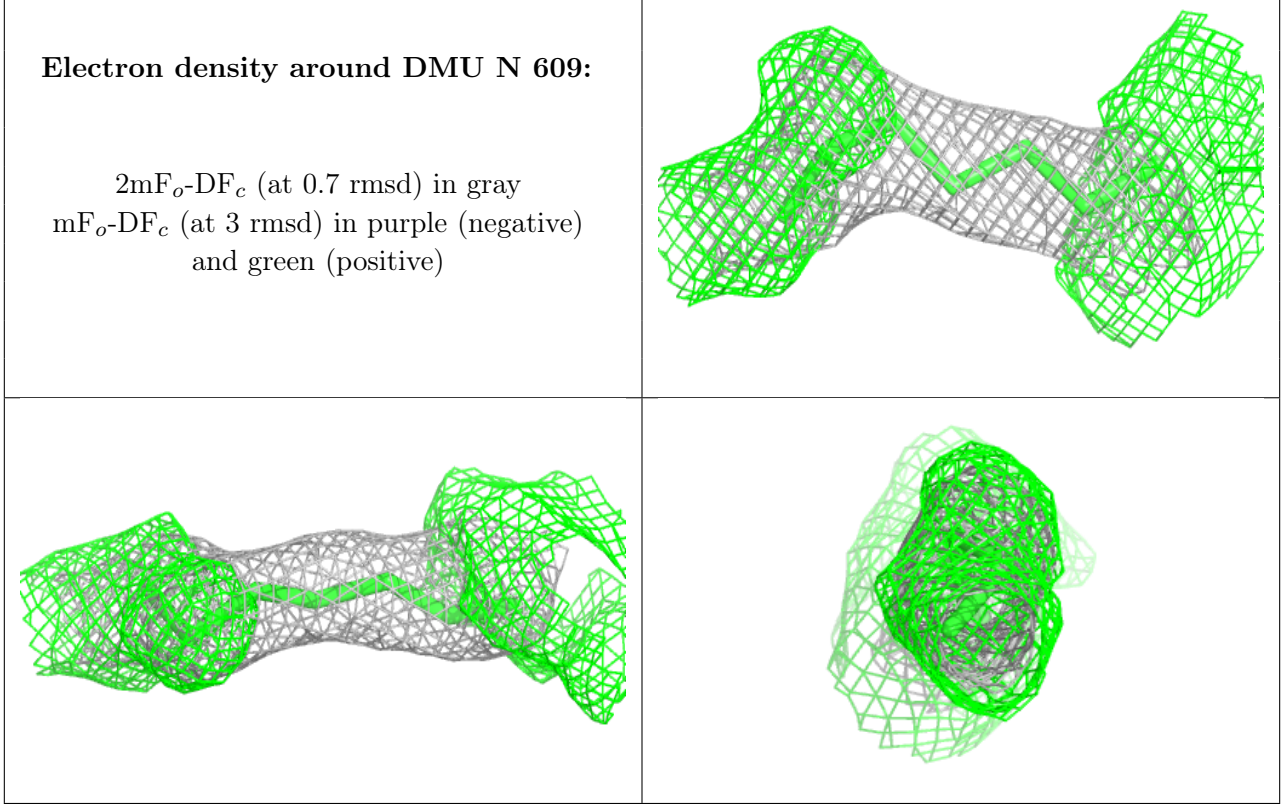
Electron density around DMU H 101:

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



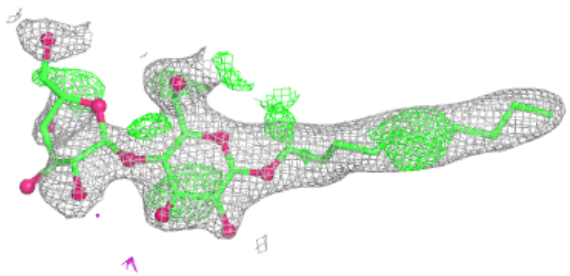
Electron density around DMU N 609:

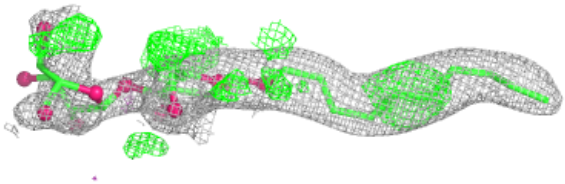
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

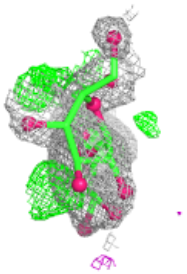


Electron density around DMU N 610:

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

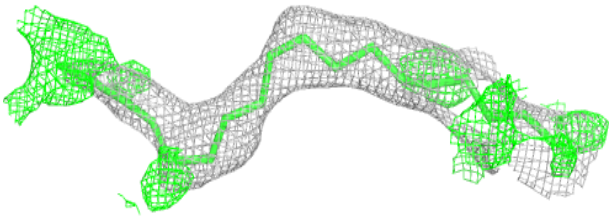


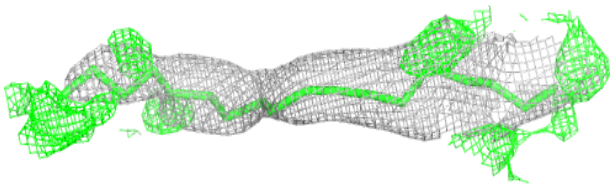


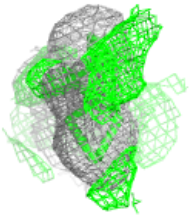


Electron density around LFA P 309:

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

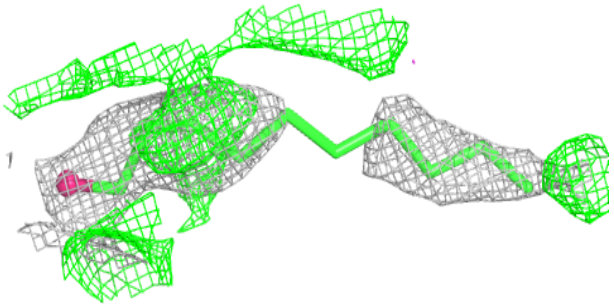


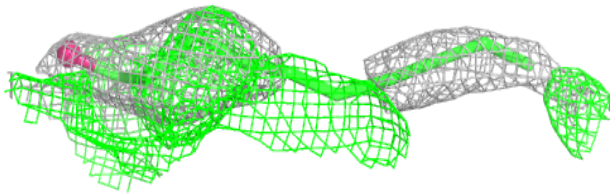


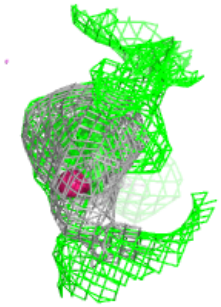


Electron density around DMU A 615:

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

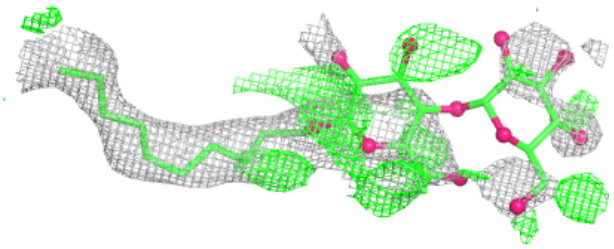


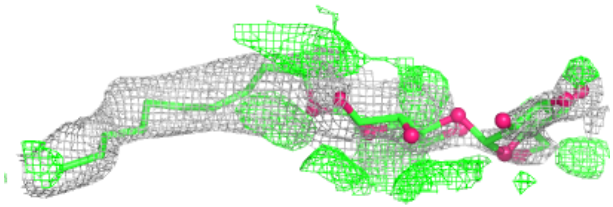


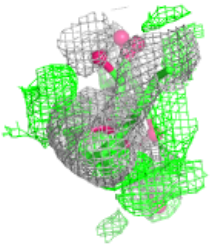


Electron density around DMU U 101:

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

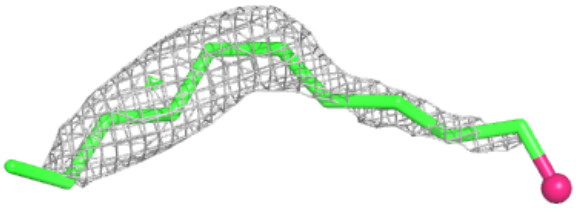


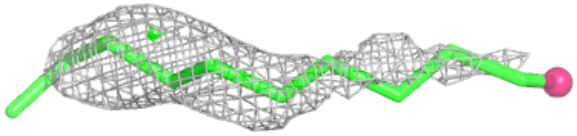


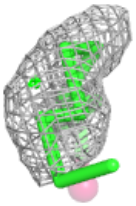


Electron density around DMU W 101:

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

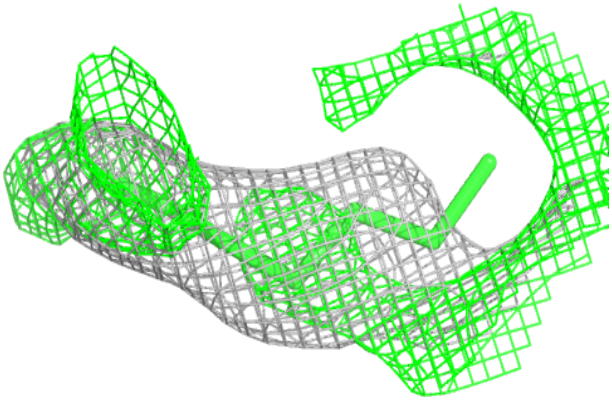


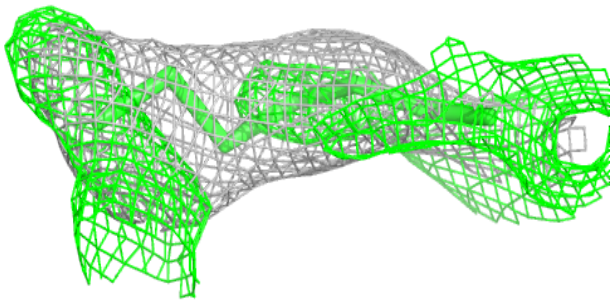


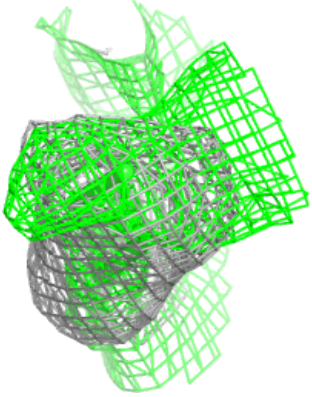


Electron density around DMU P 315:

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

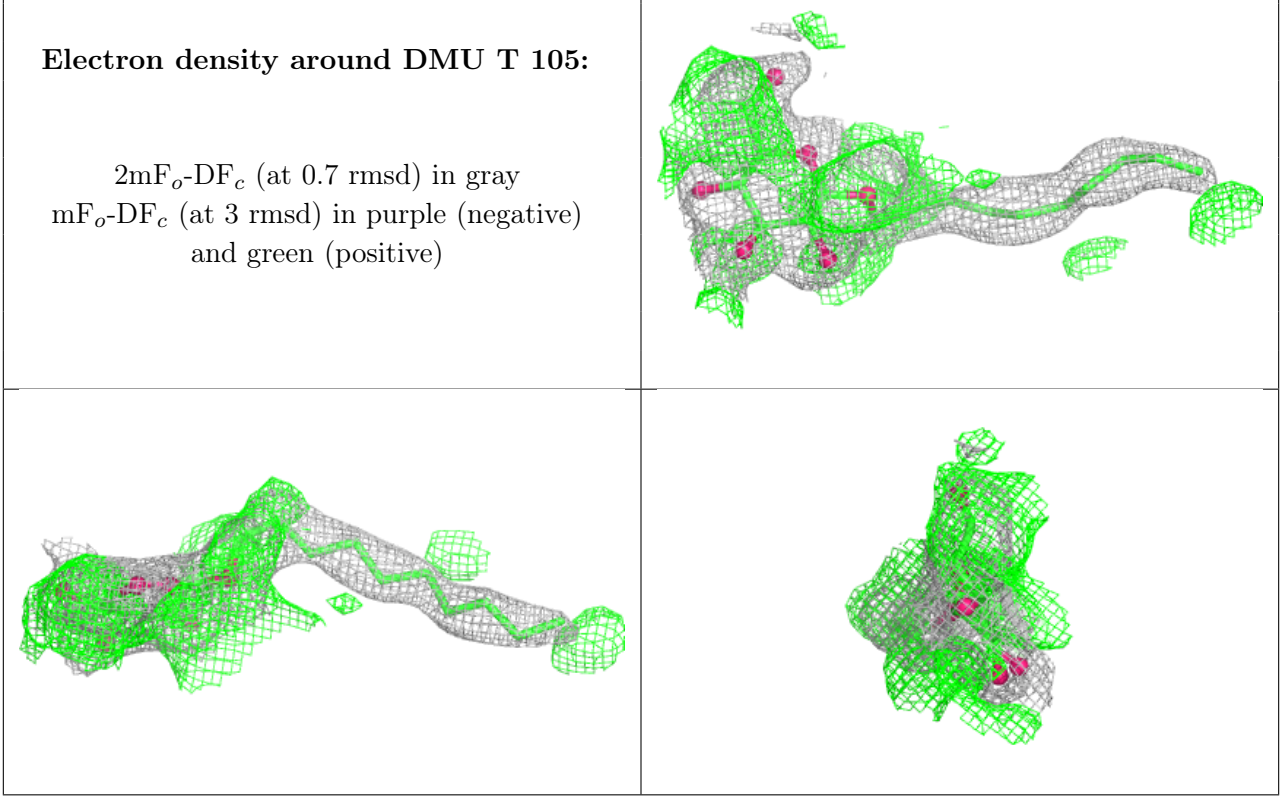






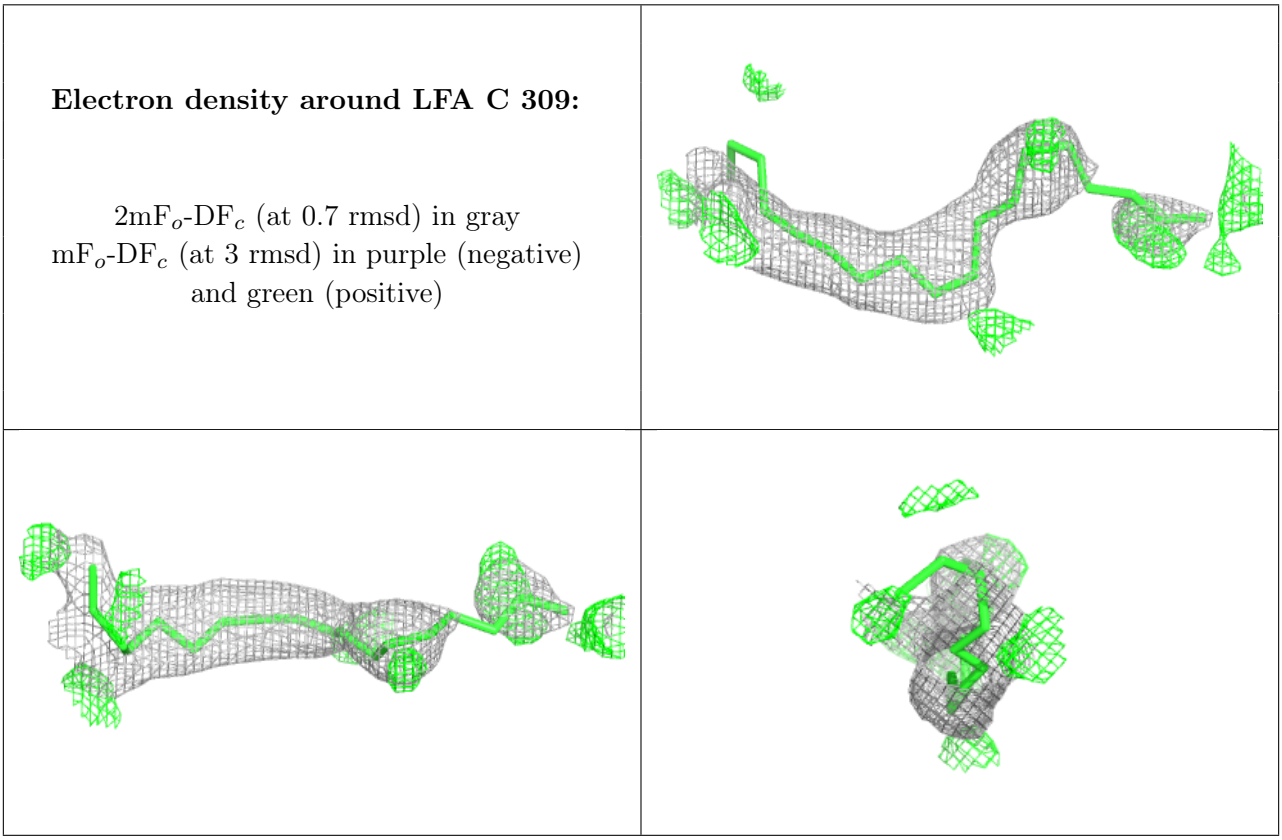
Electron density around DMU T 105:

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



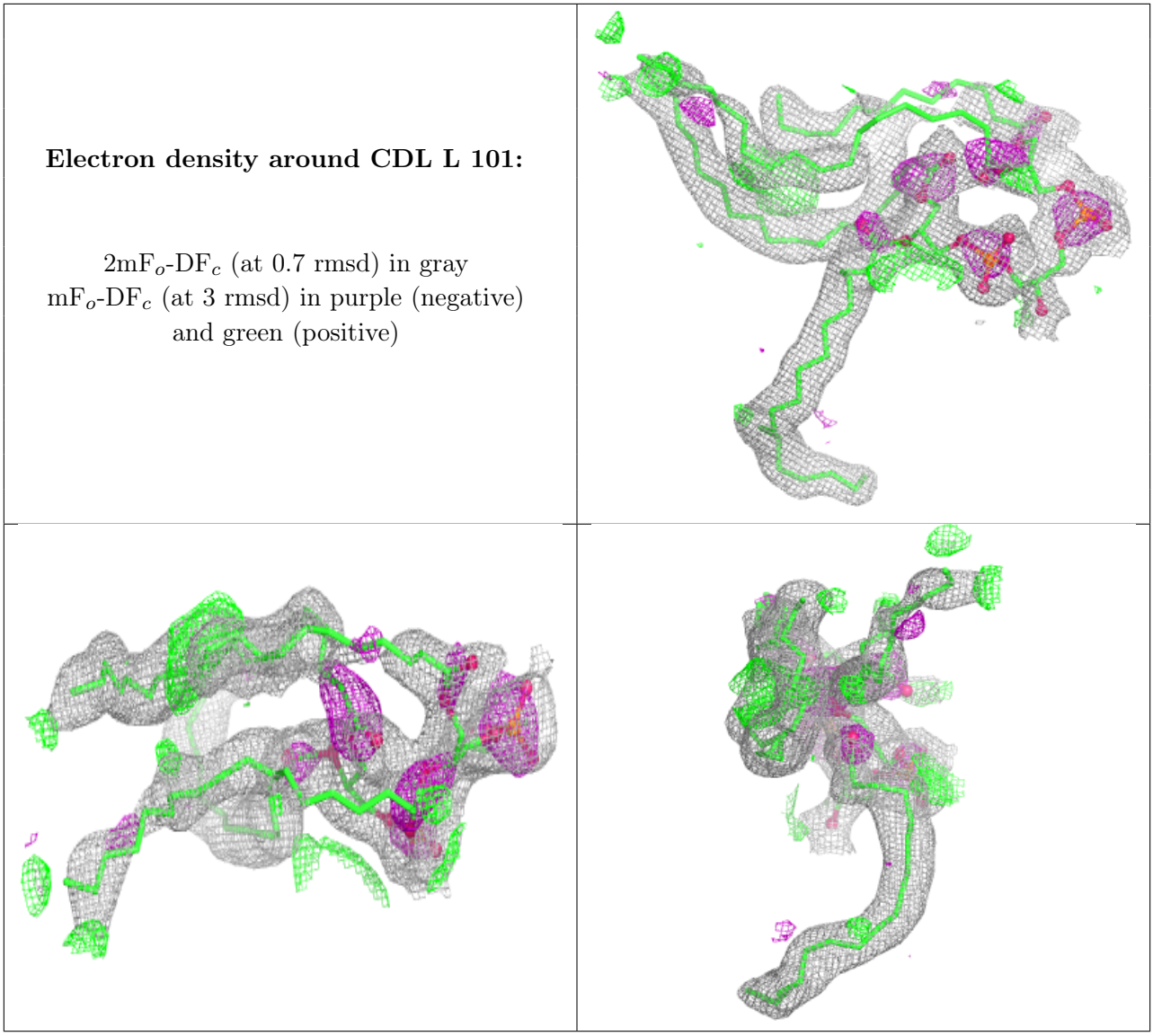
Electron density around LFA C 309:

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



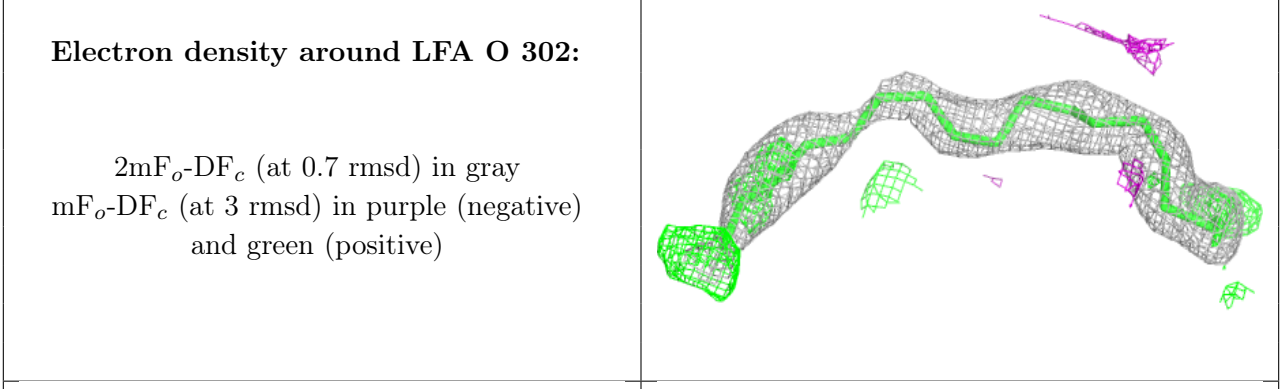
Electron density around CDL L 101:

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



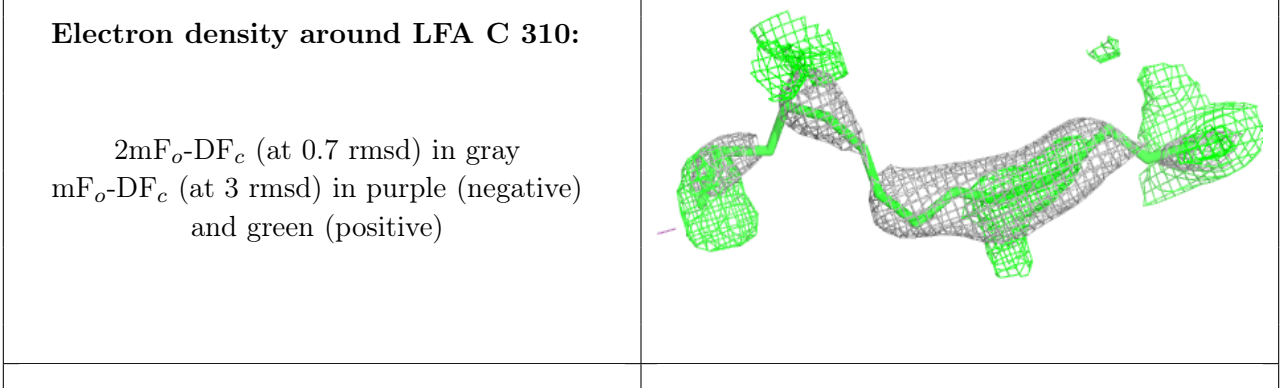
Electron density around LFA O 302:

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



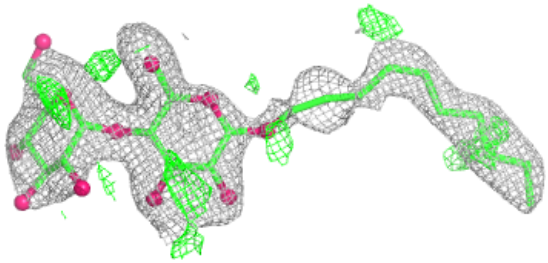
Electron density around LFA C 310:

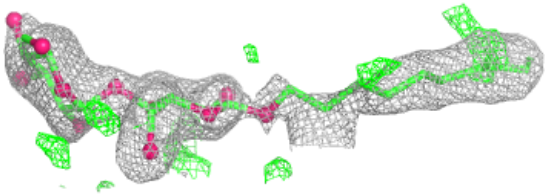
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

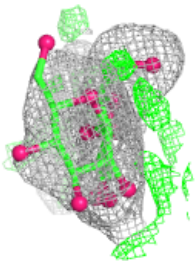


Electron density around DMU C 325:

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

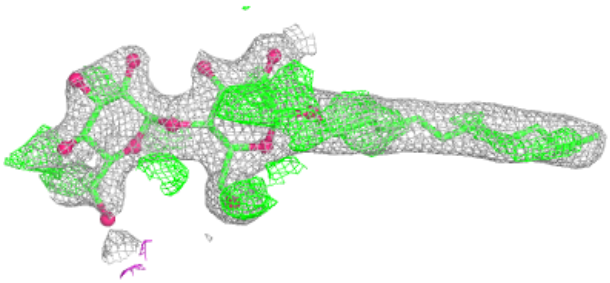


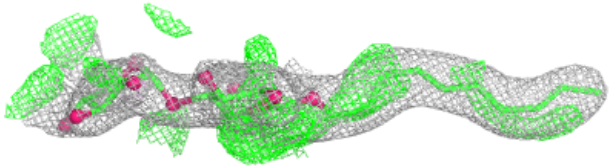


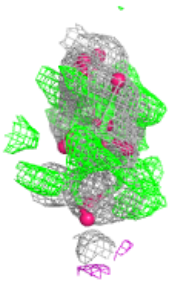


Electron density around DMU A 609:

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

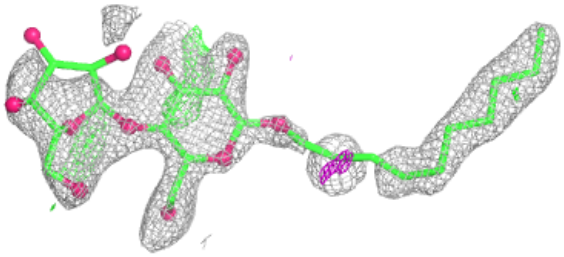


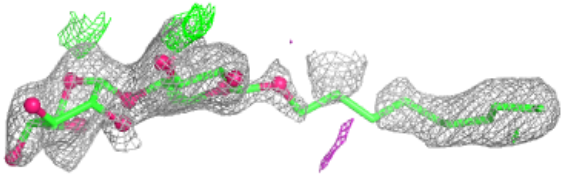


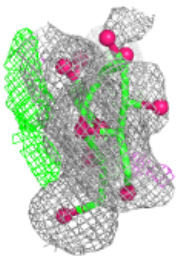


Electron density around DMU P 322:

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

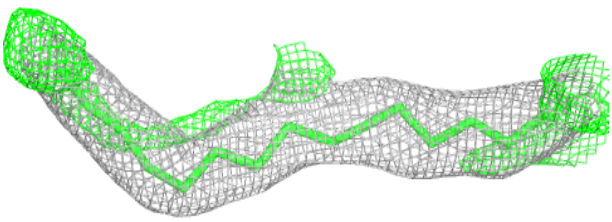


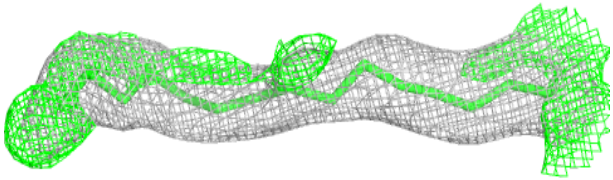


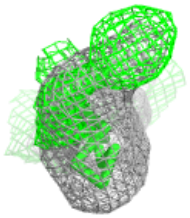


Electron density around LFA P 312:

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

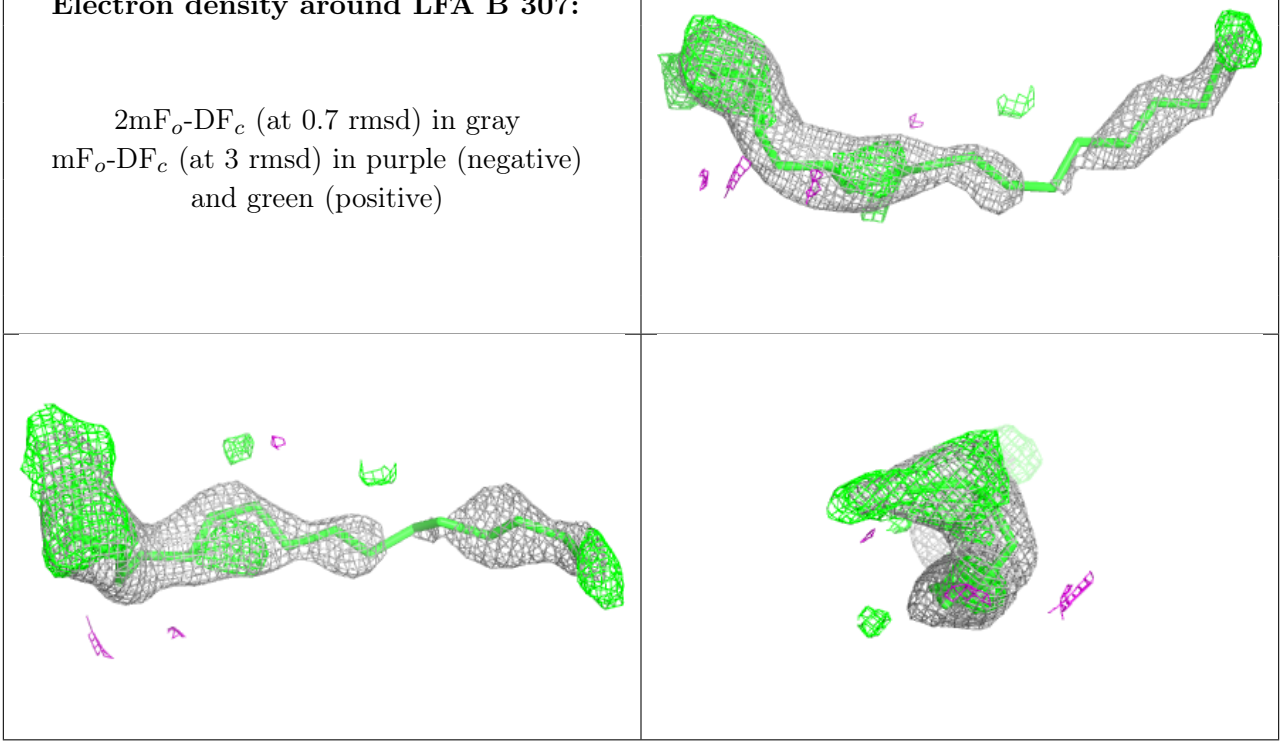






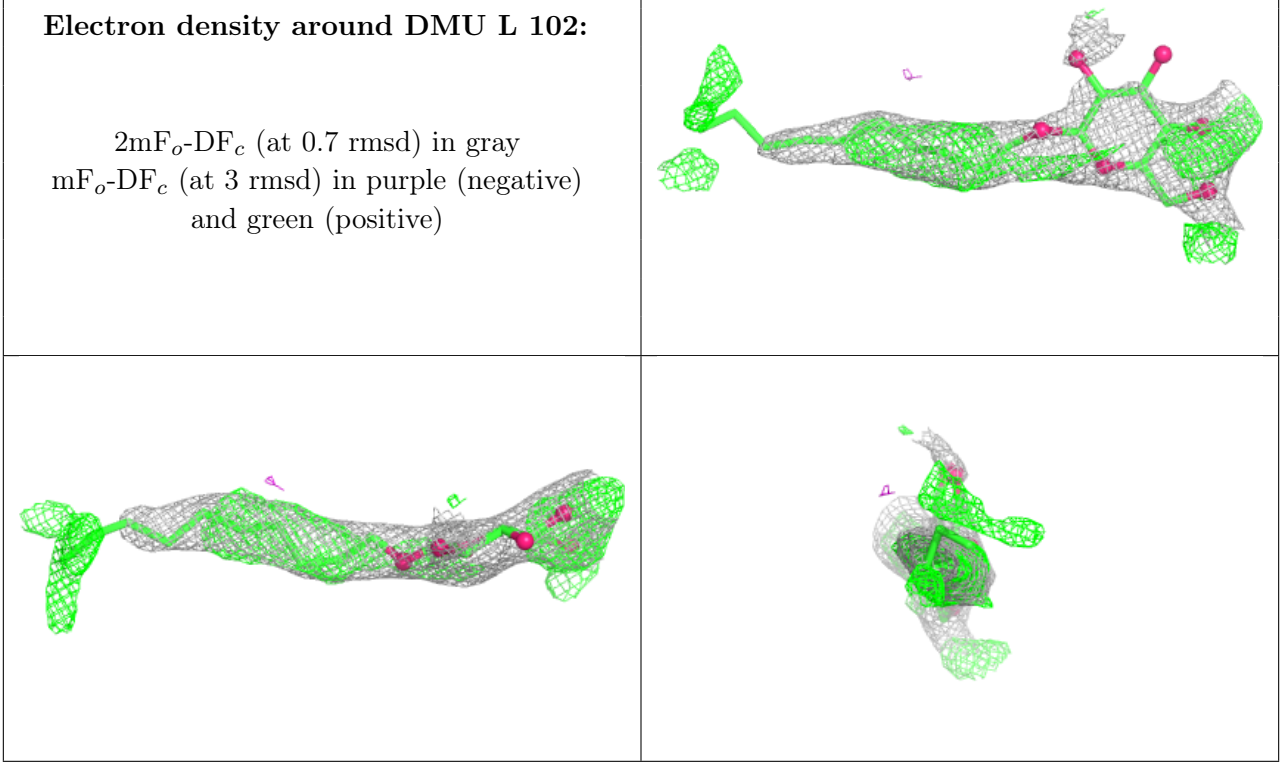
Electron density around LFA B 307:

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



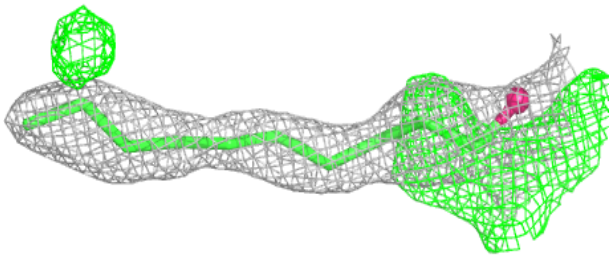
Electron density around DMU L 102:

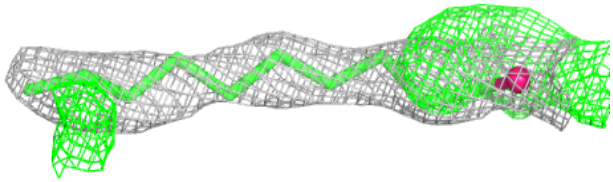
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

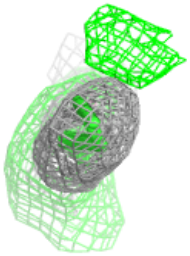


Electron density around DMU B 302:

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

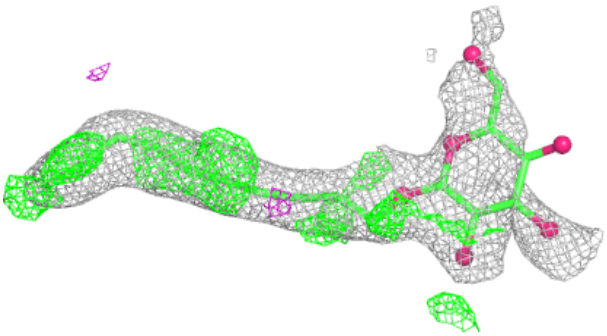


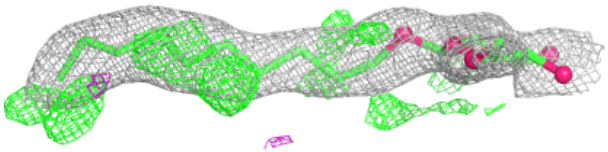


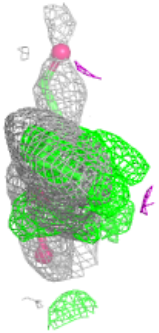


Electron density around DMU B 304:

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

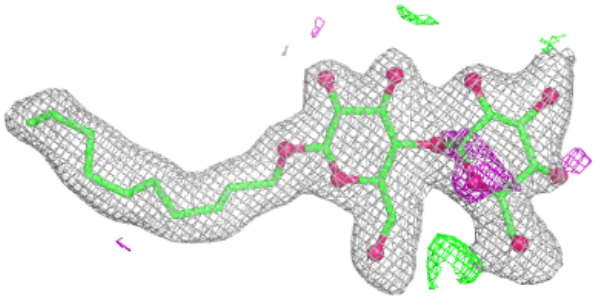


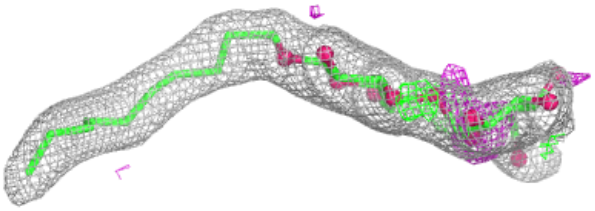


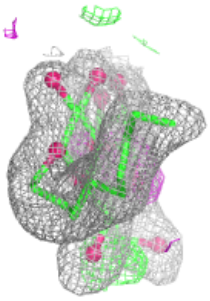


Electron density around DMU M 101:

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

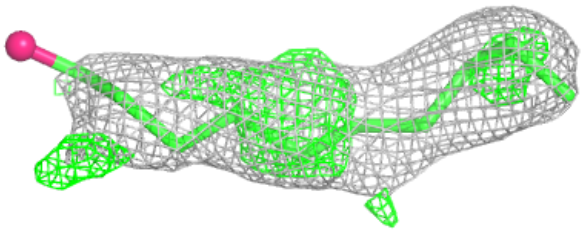


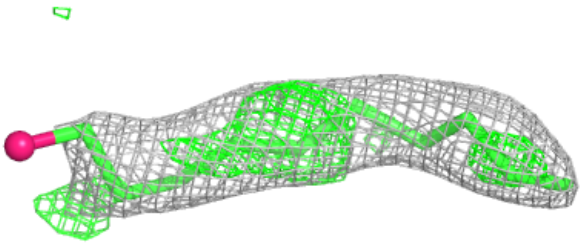


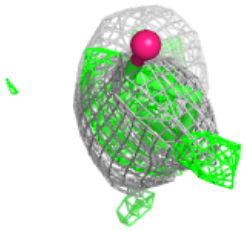


Electron density around DMU J 101:

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

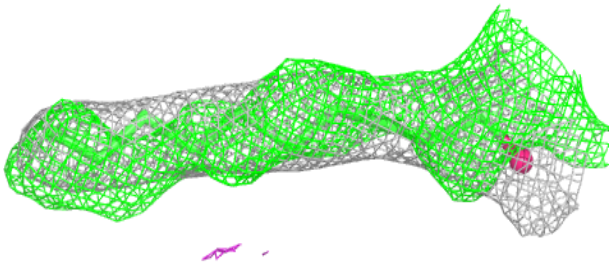


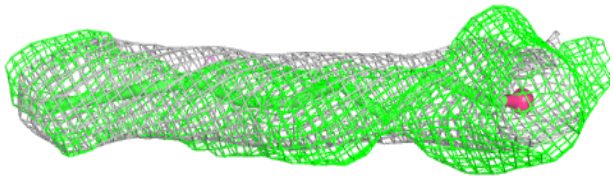


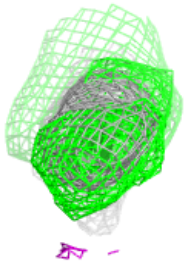


Electron density around DMU O 306:

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

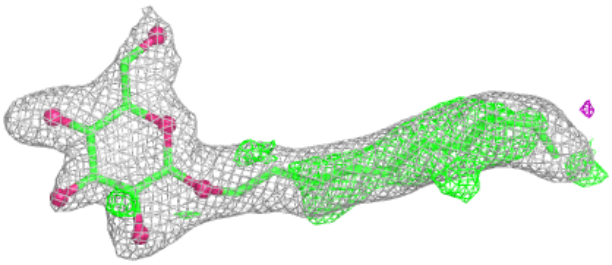


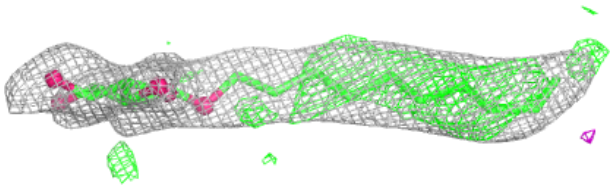


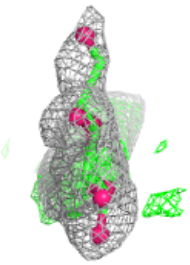


Electron density around DMU O 308:

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

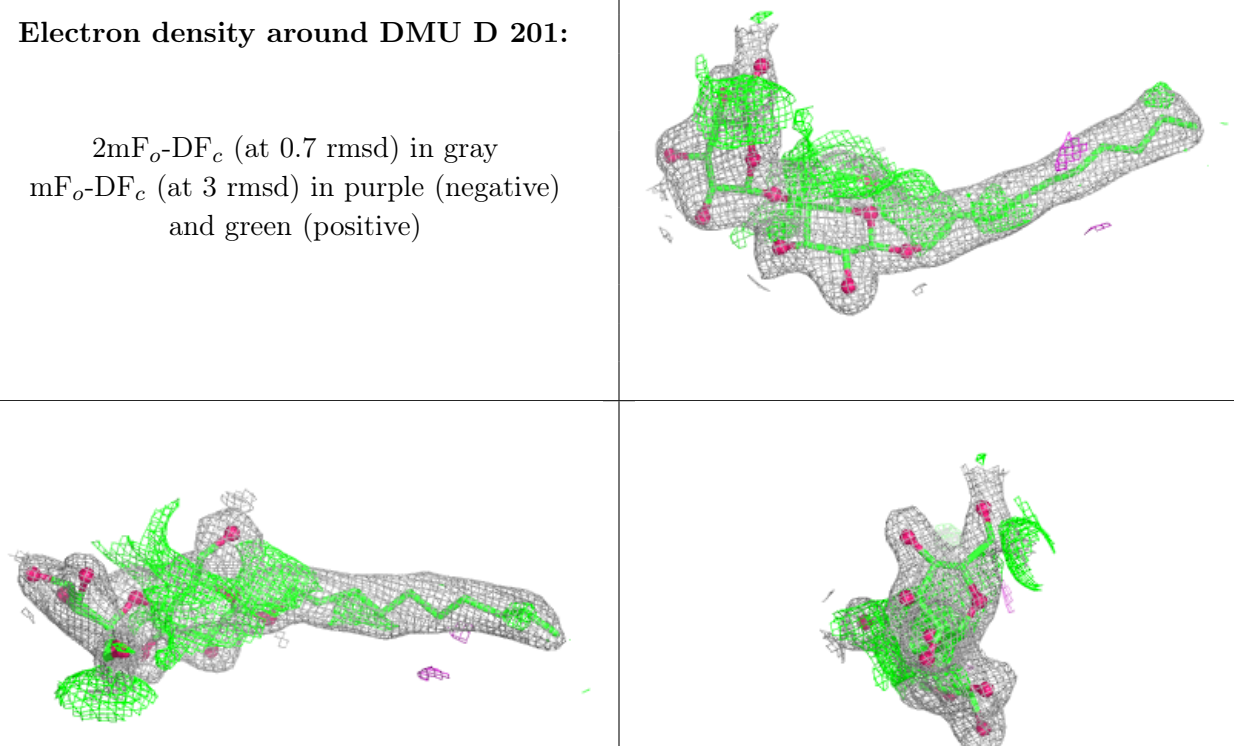






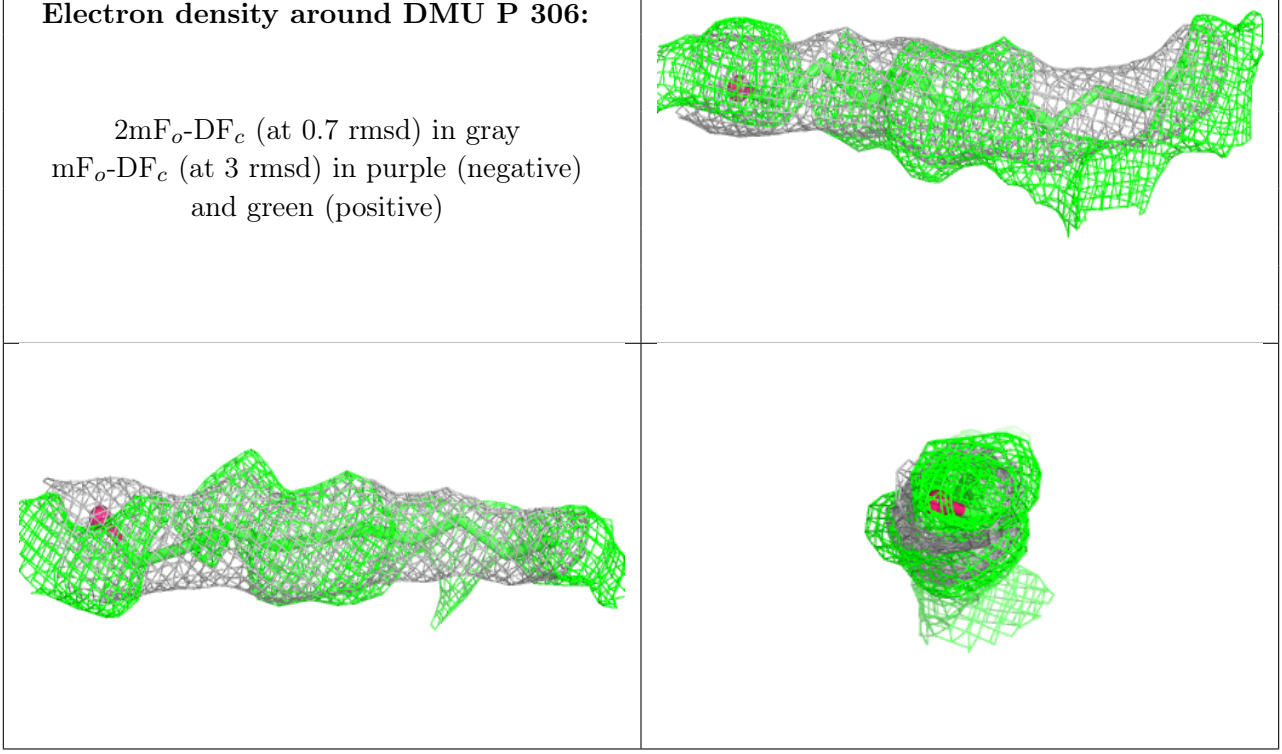
Electron density around DMU D 201:

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



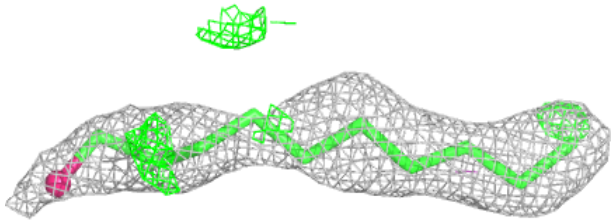
Electron density around DMU P 306:

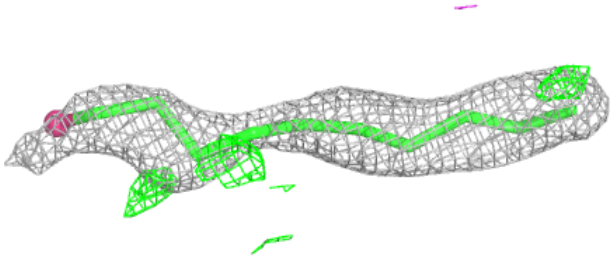
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

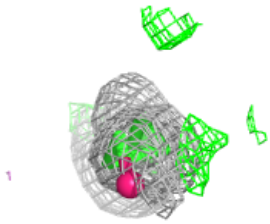


Electron density around DMU B 303:

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

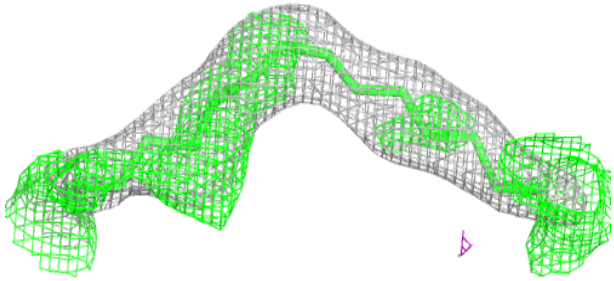


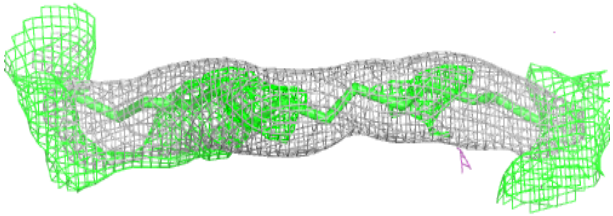


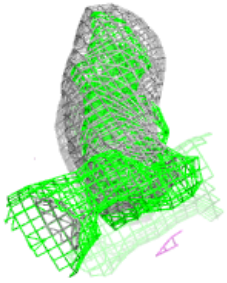


Electron density around LFA A 607:

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

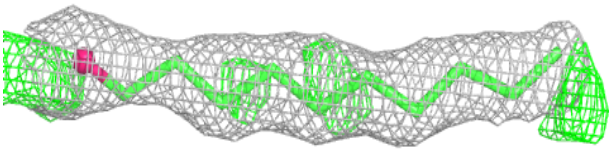


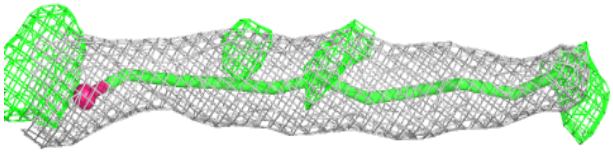


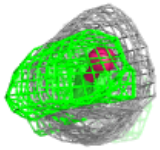


Electron density around DMU C 306:

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

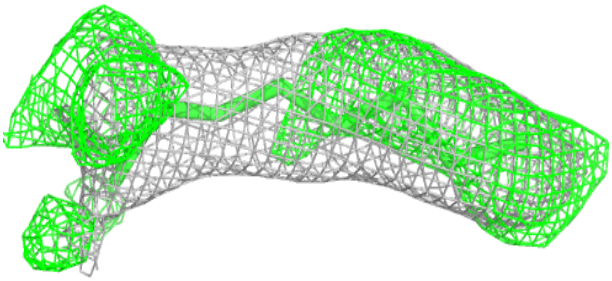


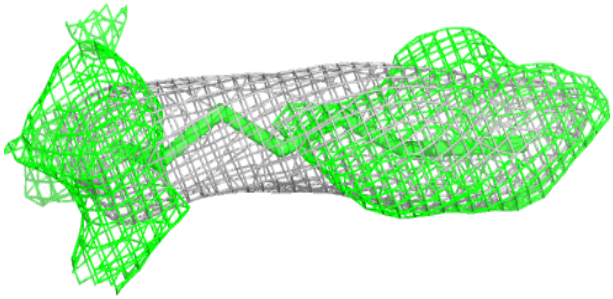


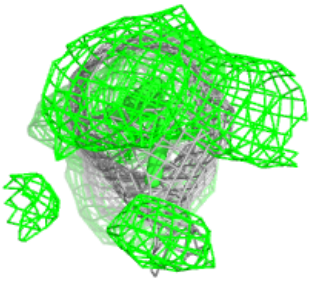


Electron density around DMU Z 103:

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

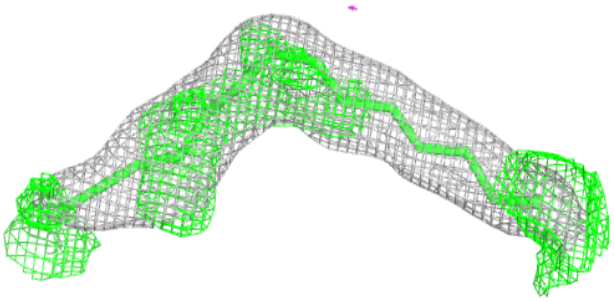


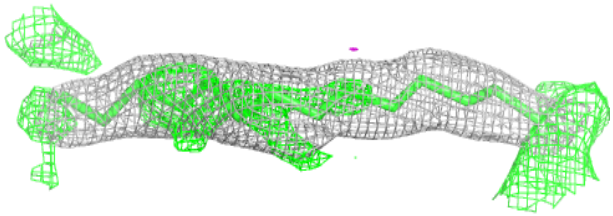


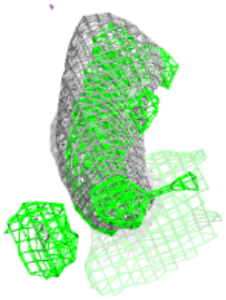


Electron density around LFA N 608:

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

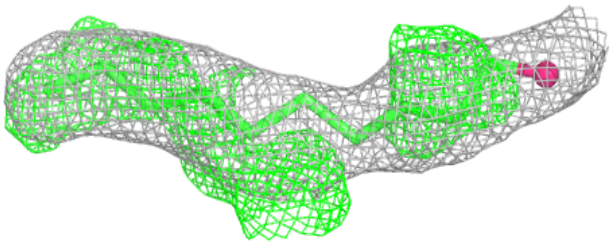


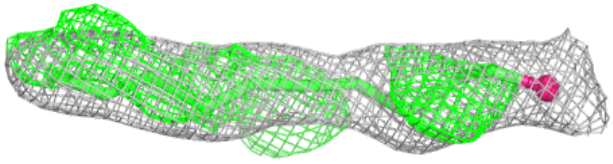


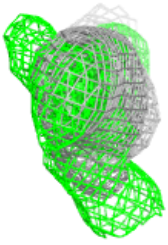


Electron density around DMU O 307:

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

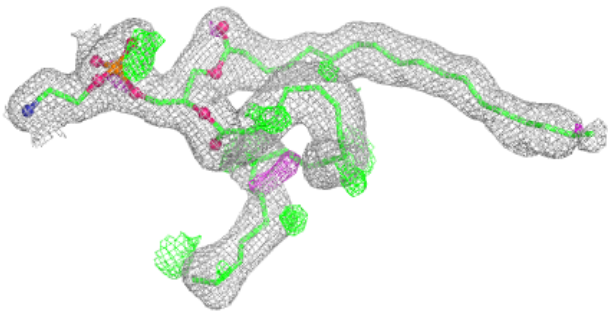


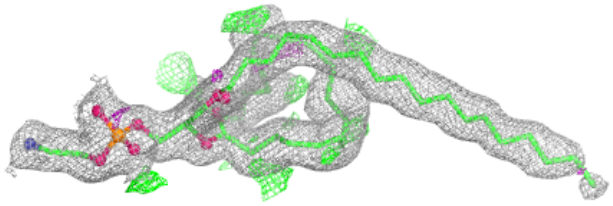


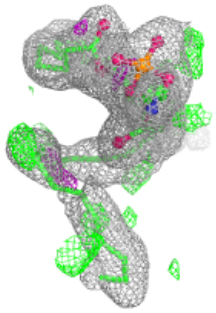


Electron density around PEK T 102:

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

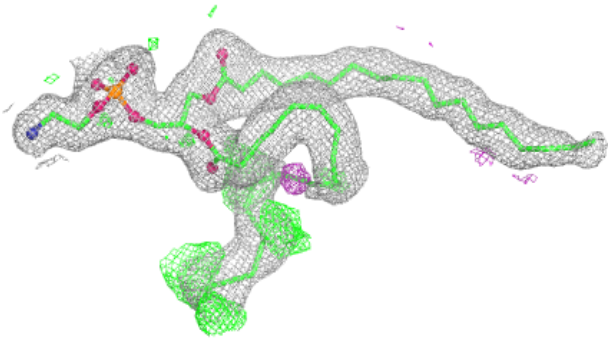


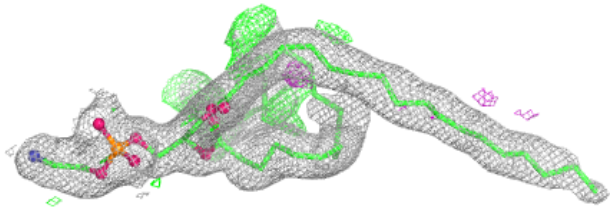


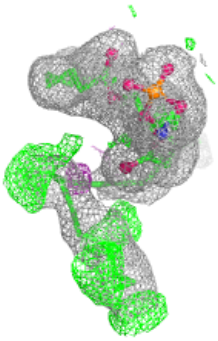


Electron density around PEK G 101:

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

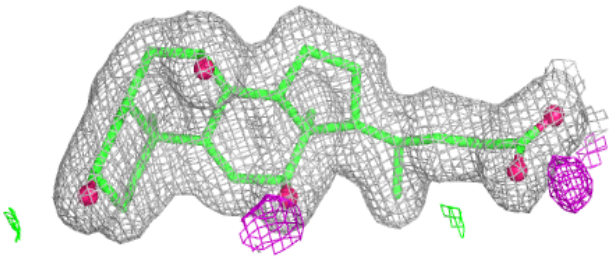


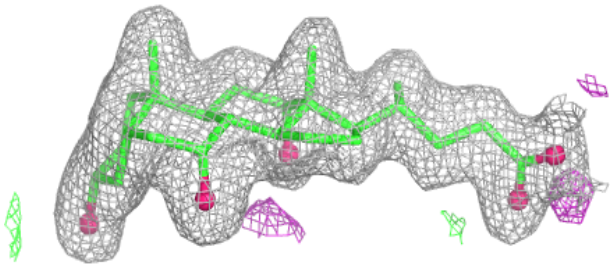


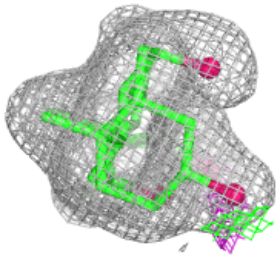


Electron density around CHD C 301:

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

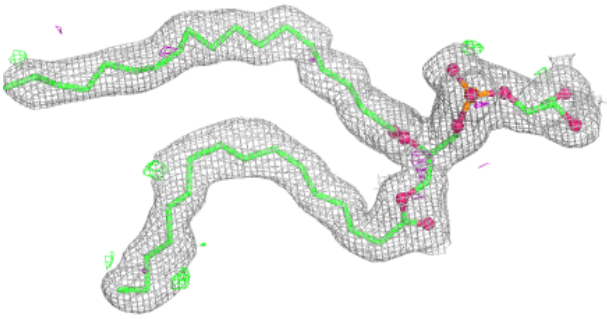


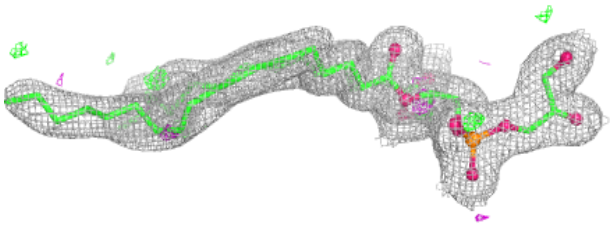


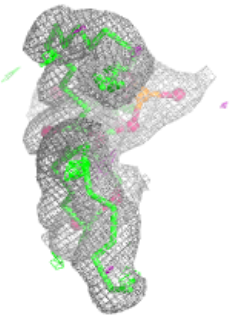


Electron density around PGV N 616:

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

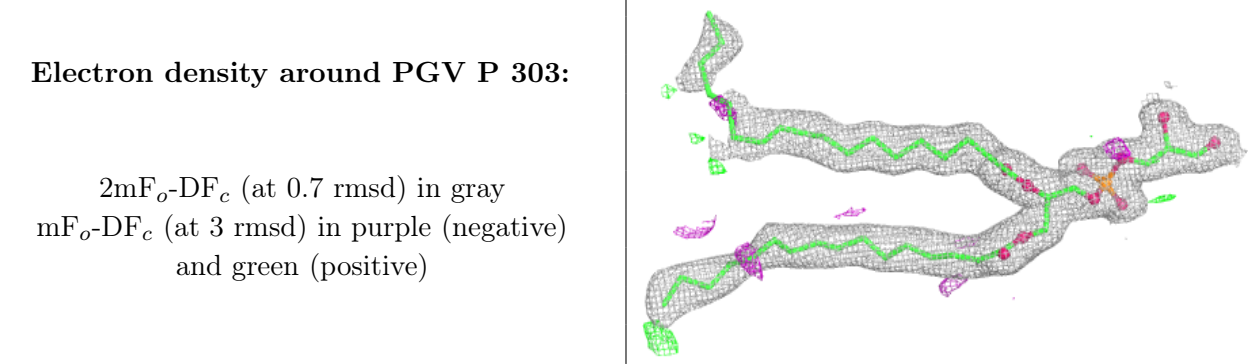


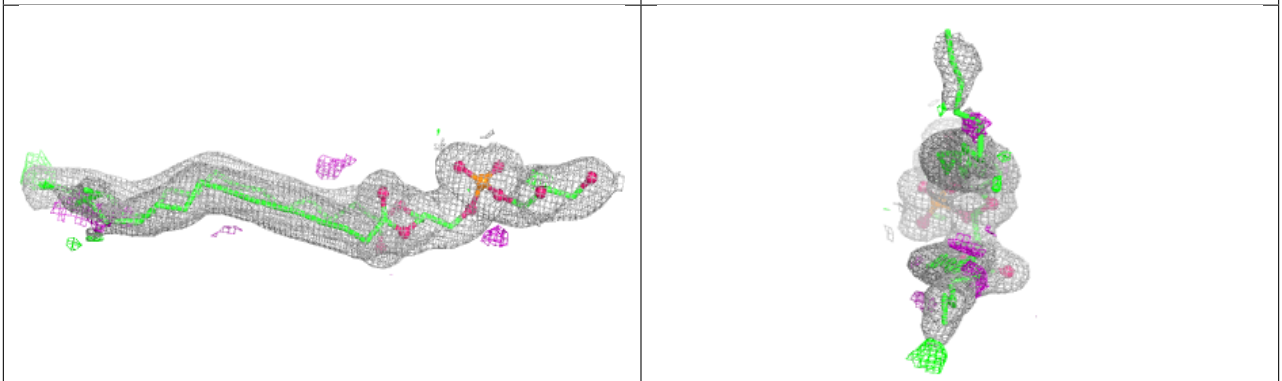




Electron density around PGV P 303:

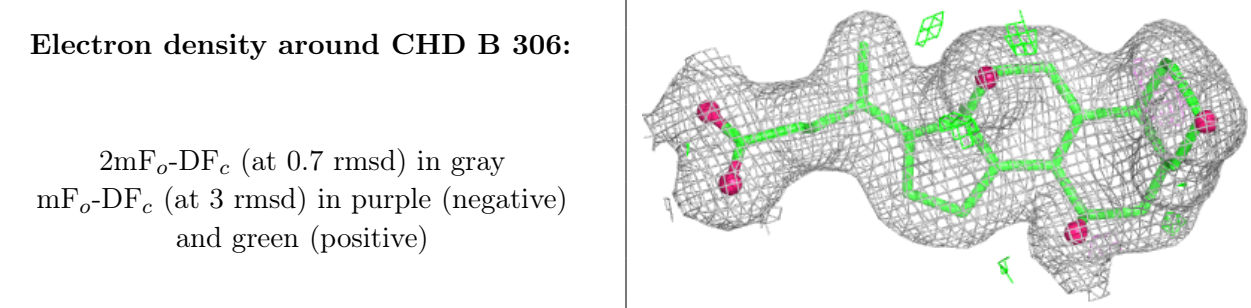
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

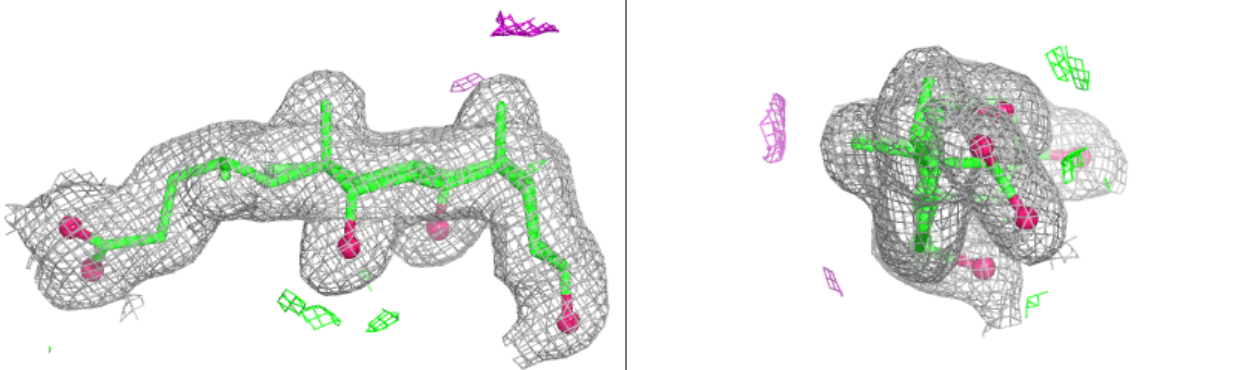




Electron density around CHD B 306:

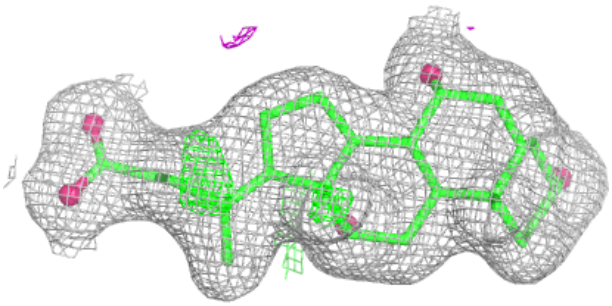
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

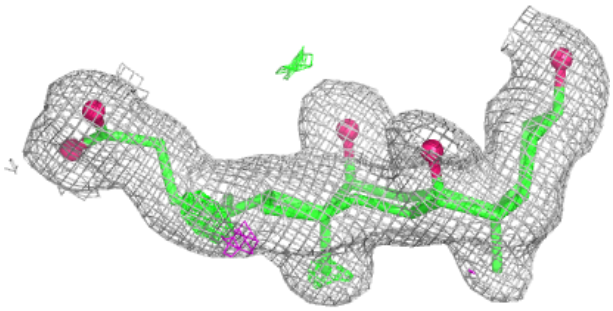


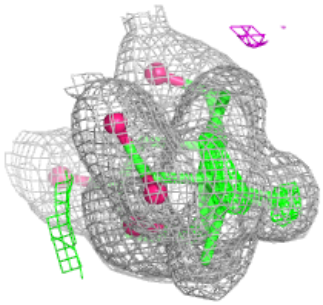


Electron density around CHD O 301:

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

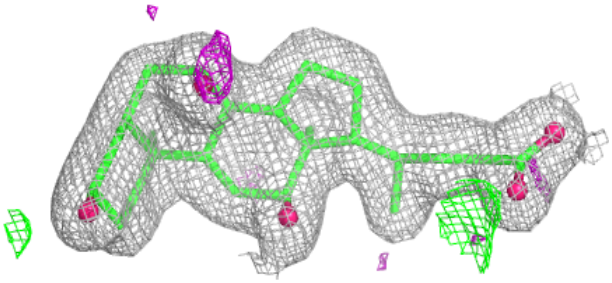


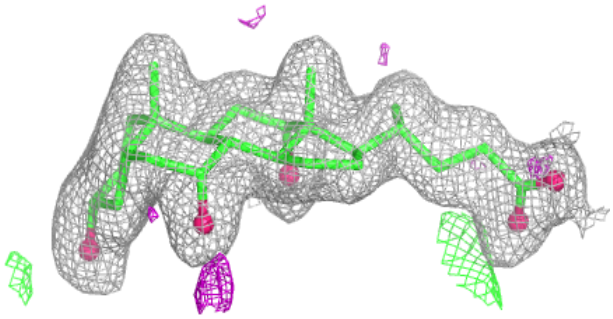


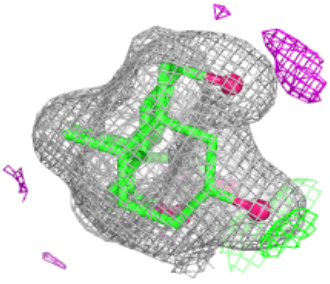


Electron density around CHD P 301:

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

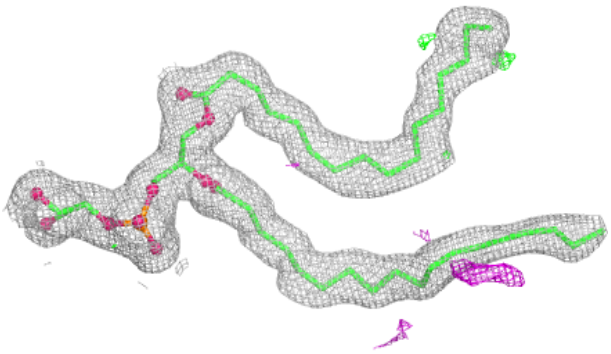


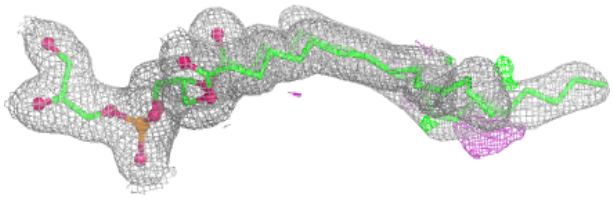


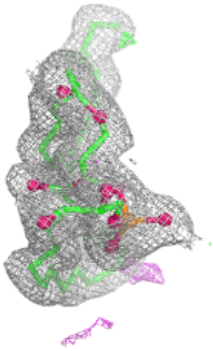


Electron density around PGV A 614:

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

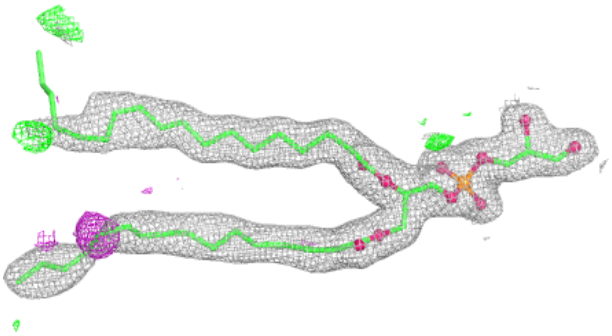


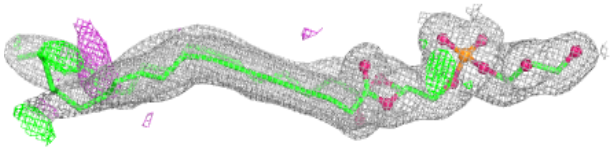


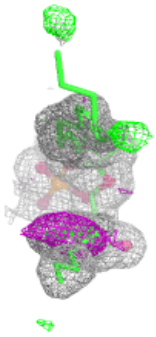


Electron density around PGV C 303:

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

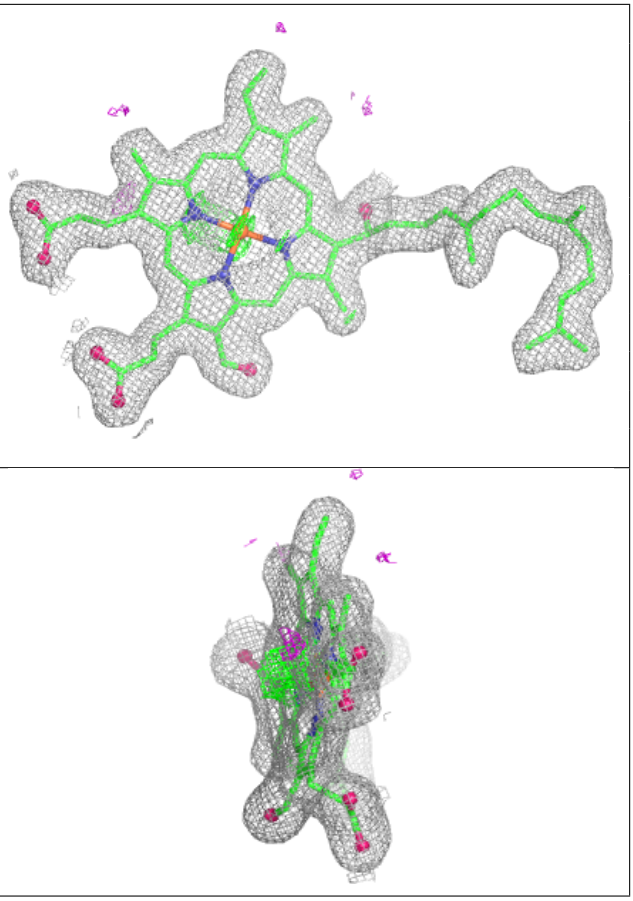






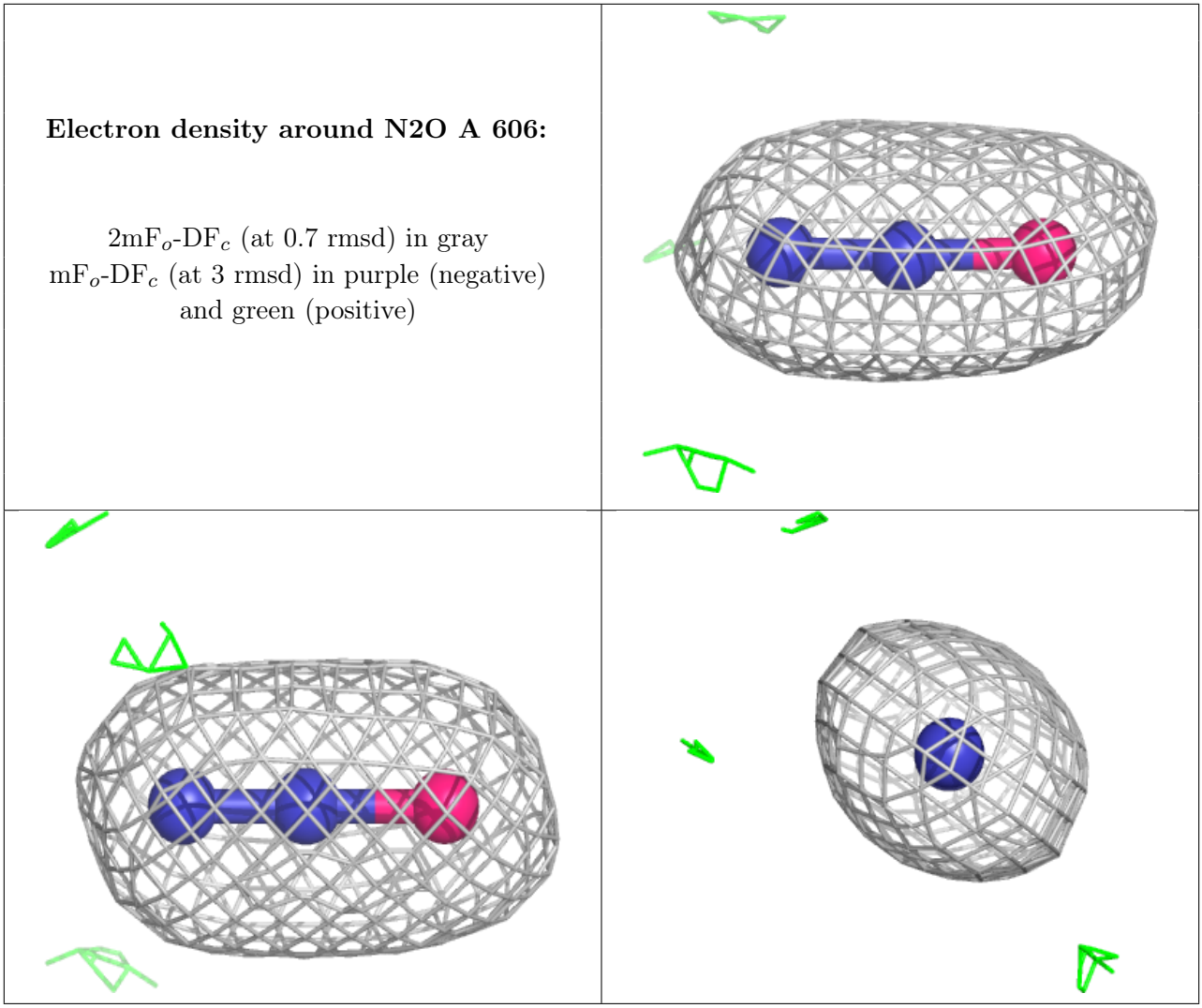
Electron density around HEA N 602:

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



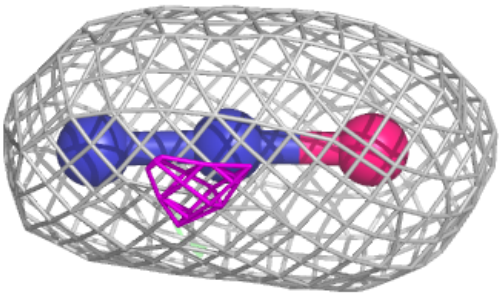
Electron density around N2O A 606:

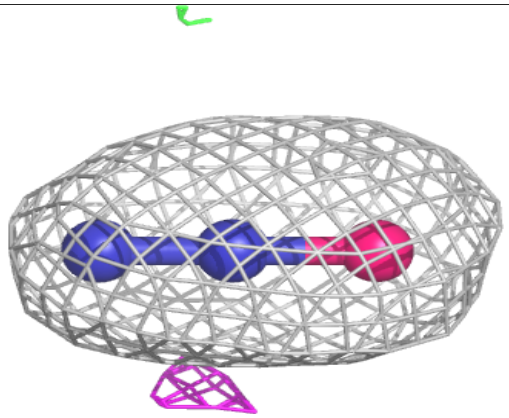
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

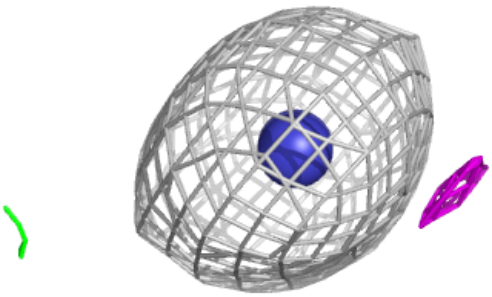


Electron density around N2O N 607:

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

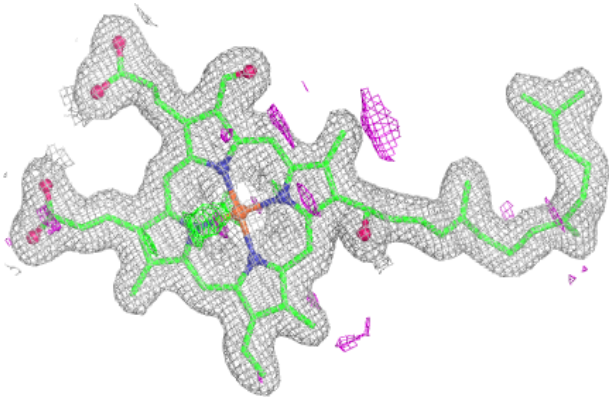


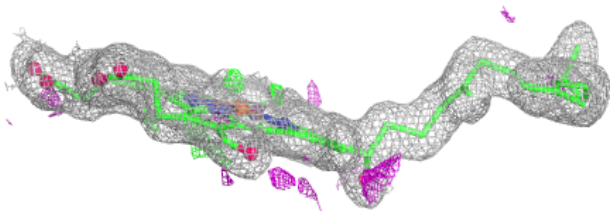


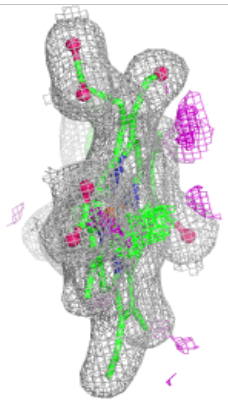


Electron density around HEA A 602:

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

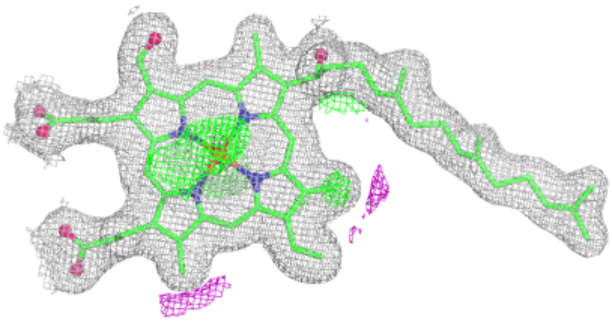


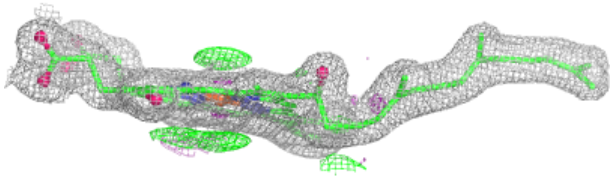


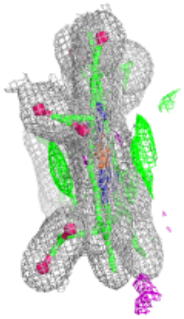


Electron density around HEA A 601:

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

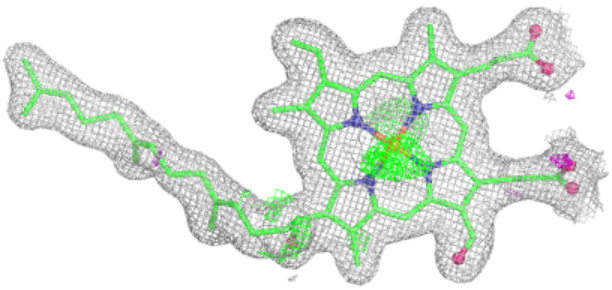


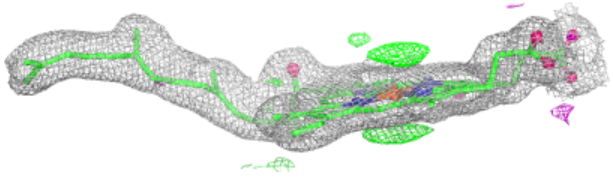


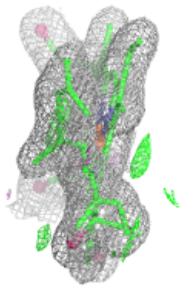


Electron density around HEA N 601:

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







6.5 Other polymers (i)

There are no such residues in this entry.