Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2024 – 05:09 PM JST

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

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

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

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

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

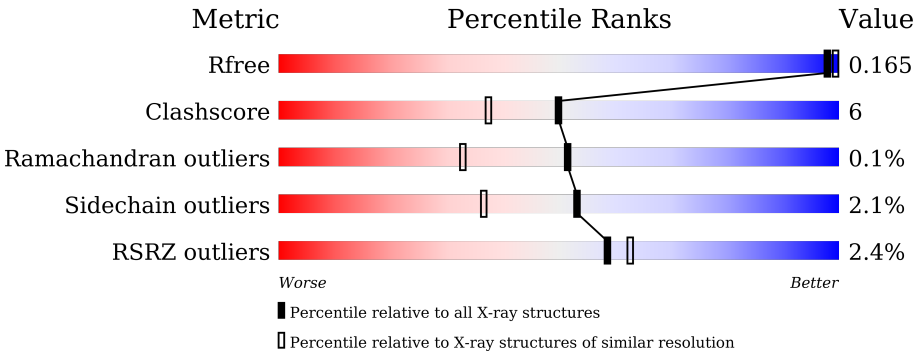
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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

Mol	Chain	Length	Quality of chain
1	A	514	90% 9%
1	N	514	92% 8%
2	B	227	3% 85% 13%
2	O	227	3% 85% 15%
3	C	261	88% 11%
3	P	261	% 89% 10%

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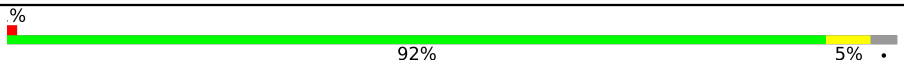
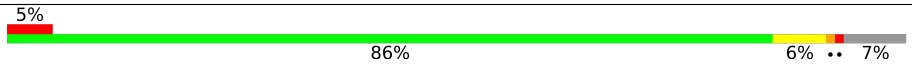
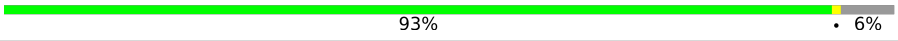
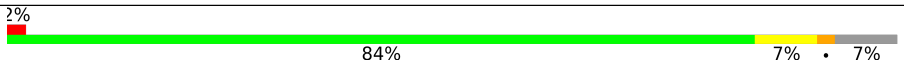
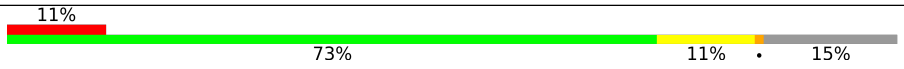
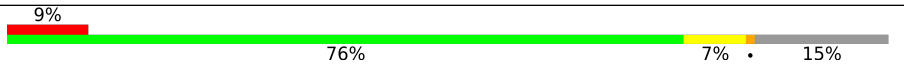
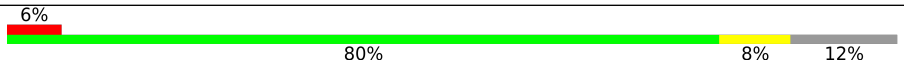
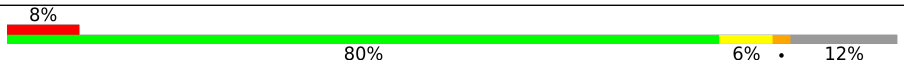
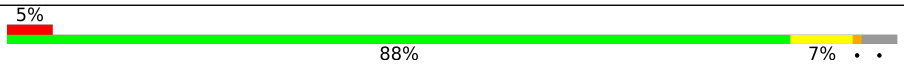
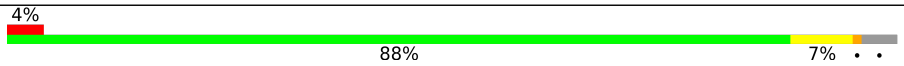
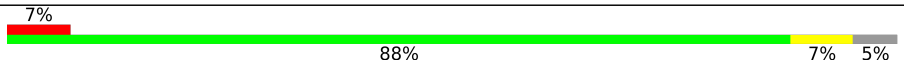
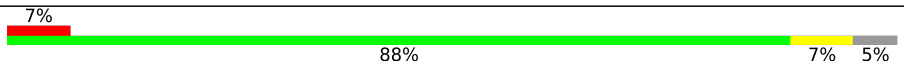
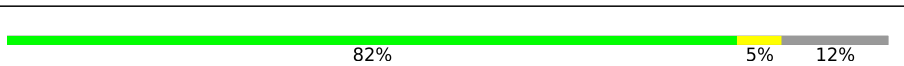
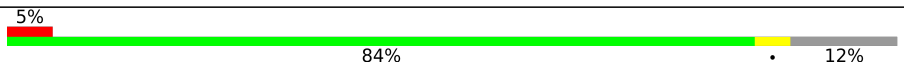
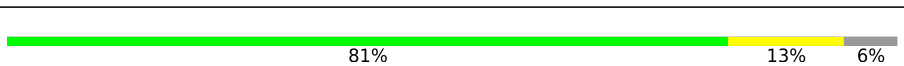
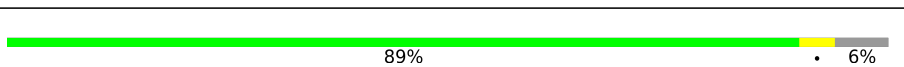
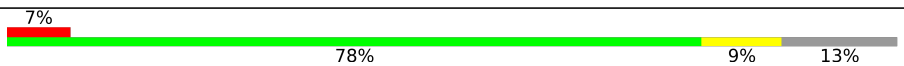
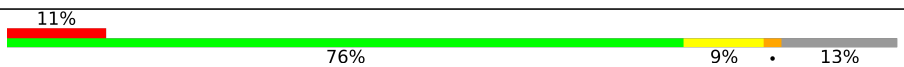
Mol	Chain	Length	Quality of chain
4	D	147	
4	Q	147	
5	E	109	
5	R	109	
6	F	98	
6	S	98	
7	G	85	
7	T	85	
8	H	85	
8	U	85	
9	I	73	
9	V	73	
10	J	59	
10	W	59	
11	K	56	
11	X	56	
12	L	47	
12	Y	47	
13	M	46	
13	Z	46	

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

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

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

2 Entry composition (i)

There are 29 unique types of molecules in this entry. The entry contains 33049 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

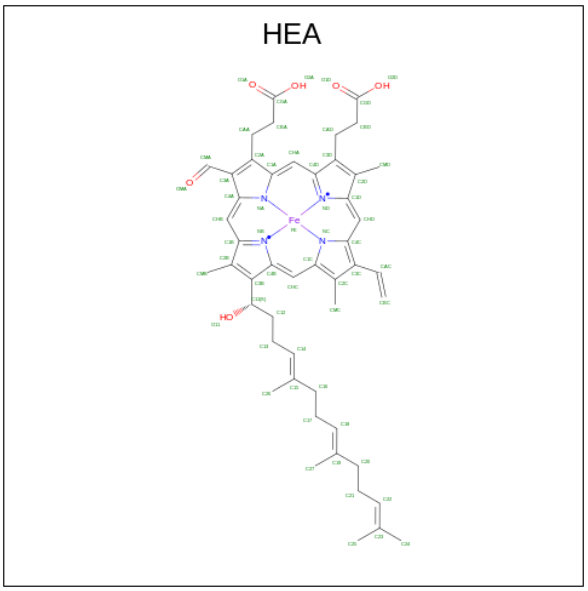
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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

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

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

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



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

- Molecule 15 is COPPER (II) ION (three-letter code: 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		

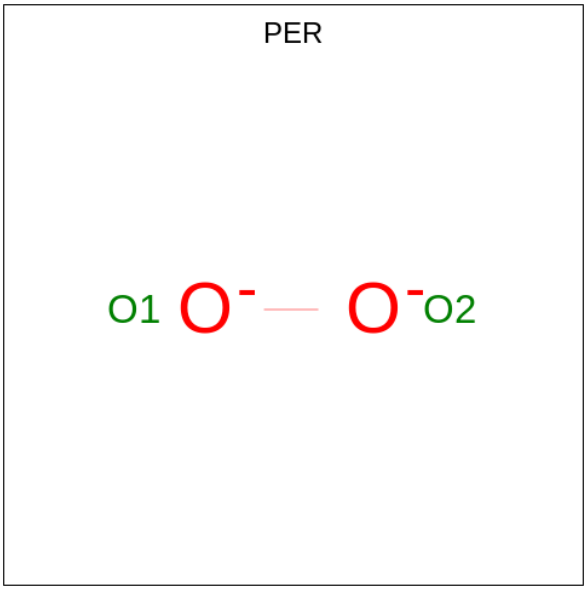
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

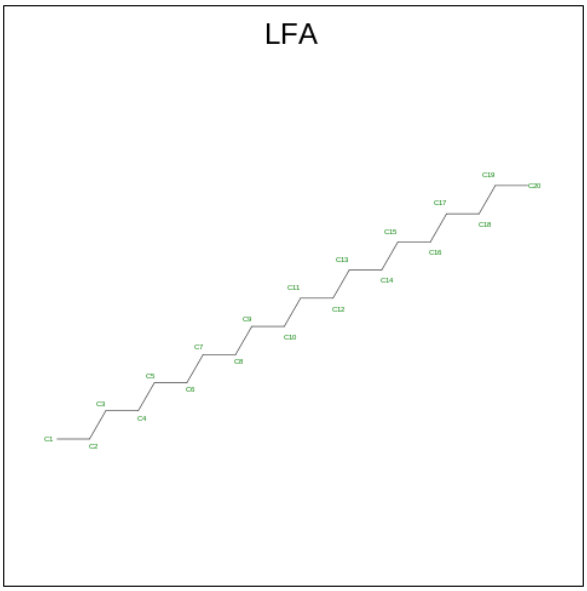
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Ca 1 1	0	0
17	N	1	Total Ca 1 1	0	0

- Molecule 18 is PEROXIDE ION (three-letter code: PER) (formula: O_2).



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

- Molecule 19 is EICOSANE (three-letter code: LFA) (formula: $C_{20}H_{42}$).



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

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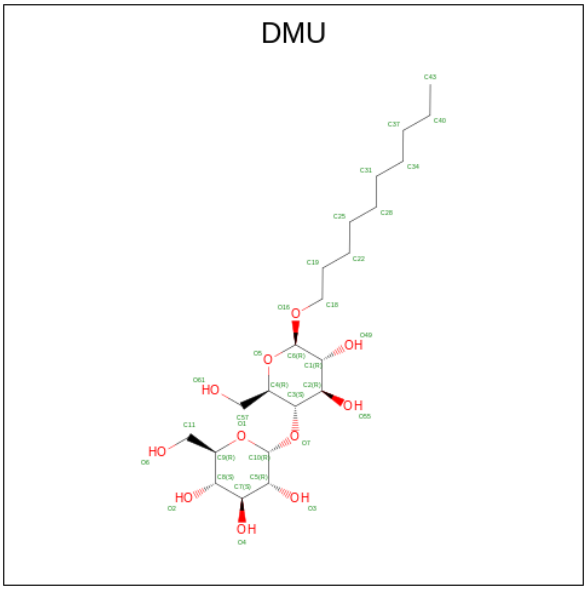
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	N	1	Total C 14 14	0	0
19	O	1	Total C 11 11	0	0
19	P	1	Total C 15 15	0	0
19	P	1	Total C 11 11	0	0
19	P	1	Total C 6 6	0	0
19	P	1	Total C 18 18	0	0
19	P	1	Total C 11 11	0	0
19	P	1	Total C 11 11	0	0
19	P	1	Total C 15 15	0	0
19	P	1	Total C 13 13	0	0
19	T	1	Total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

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



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

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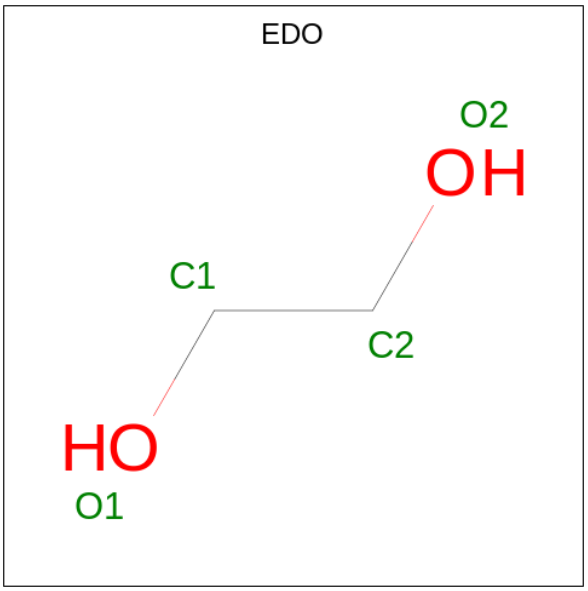
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	N	1	Total C 7 7	0	0
20	N	1	Total C O 33 22 11	0	0
20	N	1	Total C O 33 22 11	0	0
20	O	1	Total C O 22 16 6	0	0
20	O	1	Total C O 11 10 1	0	0
20	O	1	Total C O 11 10 1	0	0
20	O	1	Total C O 22 16 6	0	0
20	P	1	Total C O 11 10 1	0	0
20	P	1	Total C O 33 22 11	0	0
20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

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



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

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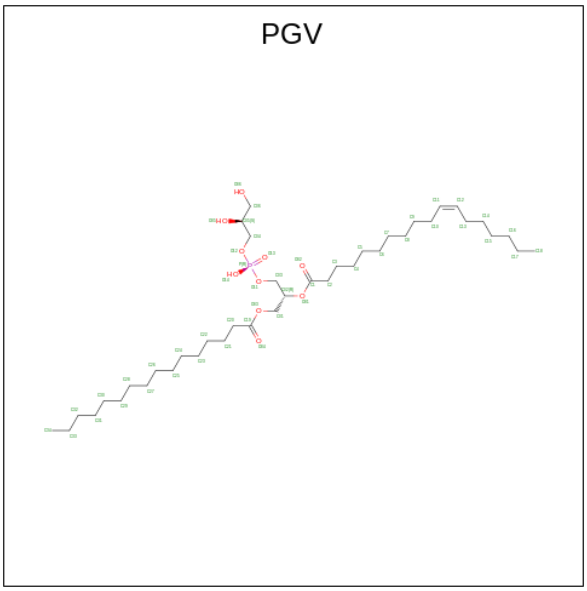
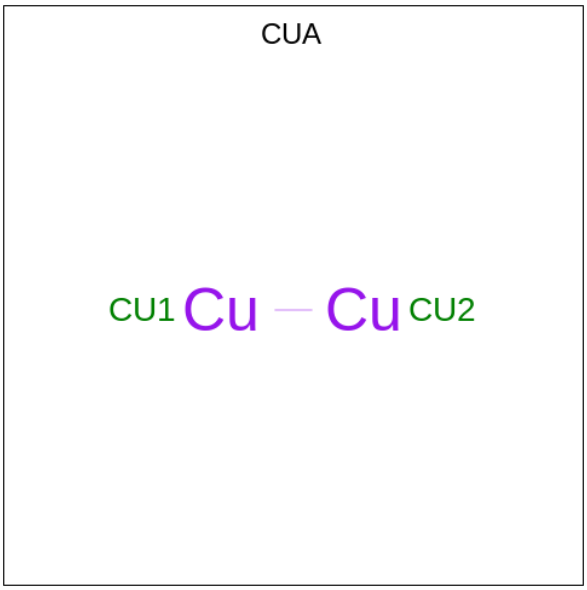
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	N	1	Total	C	O	0	0
			4	2	2		
21	N	1	Total	C	O	0	0
			4	2	2		
21	N	1	Total	C	O	0	0
			4	2	2		
21	N	1	Total	C	O	0	0
			4	2	2		
21	N	1	Total	C	O	0	0
			4	2	2		
21	O	1	Total	C	O	0	0
			4	2	2		
21	P	1	Total	C	O	0	0
			4	2	2		
21	P	1	Total	C	O	0	0
			4	2	2		
21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

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



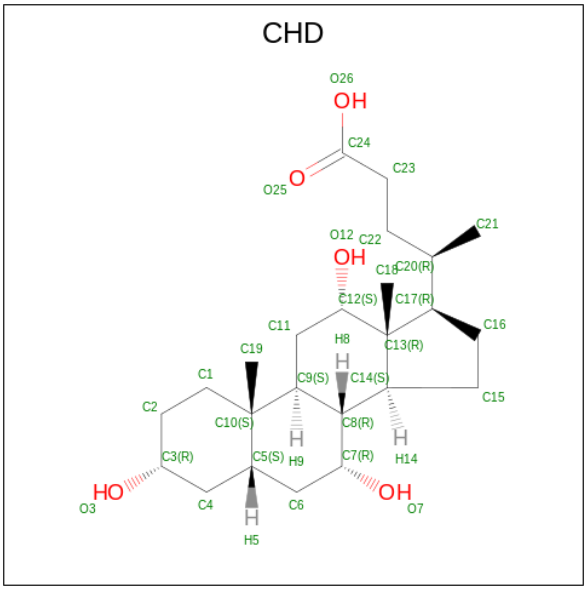
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
22	A	1	Total	C	O	P	0	0
			51	40	10	1		
22	C	1	Total	C	O	P	0	0
			51	40	10	1		
22	N	1	Total	C	O	P	0	0
			51	40	10	1		
22	P	1	Total	C	O	P	0	0
			51	40	10	1		

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



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

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

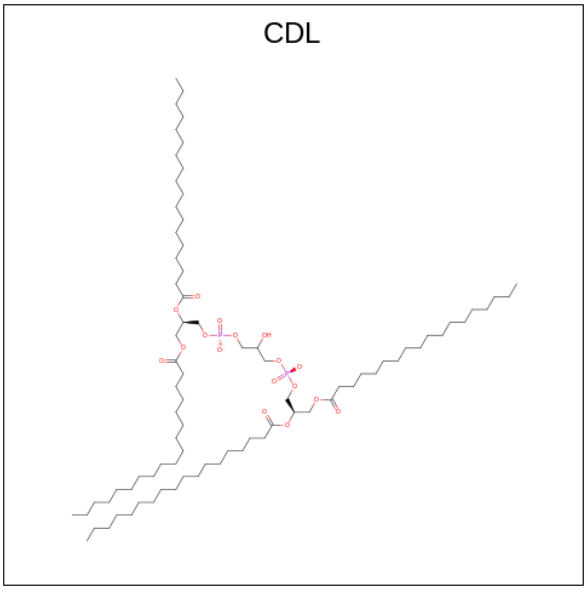


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	B	1	Total C O 29 24 5	0	0
24	C	1	Total C O 29 24 5	0	0
24	C	1	Total C O 29 24 5	0	0
24	O	1	Total C O 29 24 5	0	0
24	P	1	Total C O 29 24 5	0	0
24	P	1	Total C O 29 24 5	0	0

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

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

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

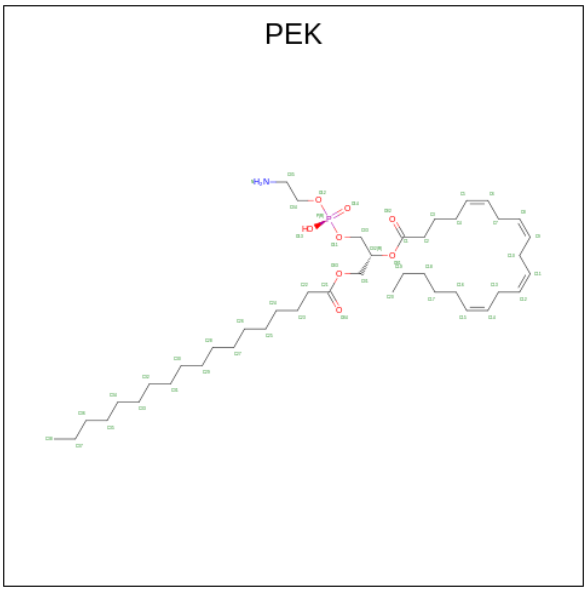


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	C	1	Total	C	O	P	0	0
			87	68	17	2		
26	I	1	Total	C	O	P	0	0
			64	45	17	2		
26	L	1	Total	C	O	P	0	0
			94	75	17	2		
26	O	1	Total	C	O	P	0	0
			64	45	17	2		
26	P	1	Total	C	O	P	0	0
			87	68	17	2		
26	Y	1	Total	C	O	P	0	0
			94	75	17	2		

- Molecule 27 is ZINC ION (three-letter code: 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 (three-letter code: 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	239	Total	O	0	11
			250	250		
29	B	175	Total	O	0	2
			177	177		
29	C	102	Total	O	0	1
			103	103		
29	D	135	Total	O	0	9
			144	144		
29	E	109	Total	O	0	7
			116	116		
29	F	104	Total	O	0	7
			111	111		
29	G	42	Total	O	0	1
			43	43		
29	H	61	Total	O	0	0
			61	61		
29	I	41	Total	O	0	0
			41	41		
29	J	20	Total	O	0	0
			20	20		

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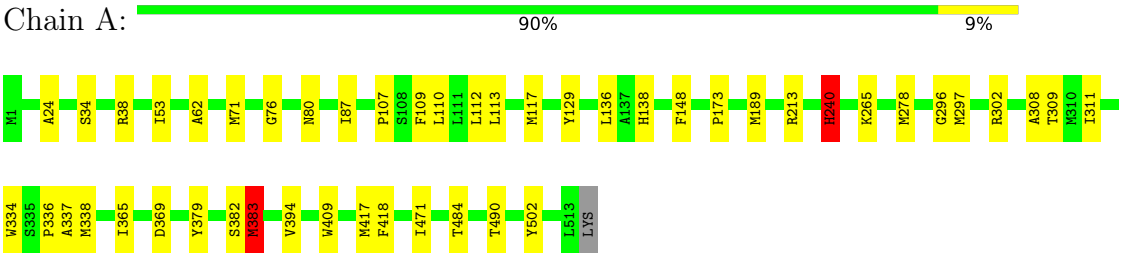
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	K	22	Total O 22 22	0	0
29	L	25	Total O 27 27	0	2
29	M	21	Total O 21 21	0	0
29	N	227	Total O 237 237	0	10
29	O	148	Total O 149 149	0	1
29	P	101	Total O 102 102	0	1
29	Q	81	Total O 86 86	0	5
29	R	87	Total O 94 94	0	7
29	S	87	Total O 93 93	0	6
29	T	37	Total O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

3 Residue-property plots (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.

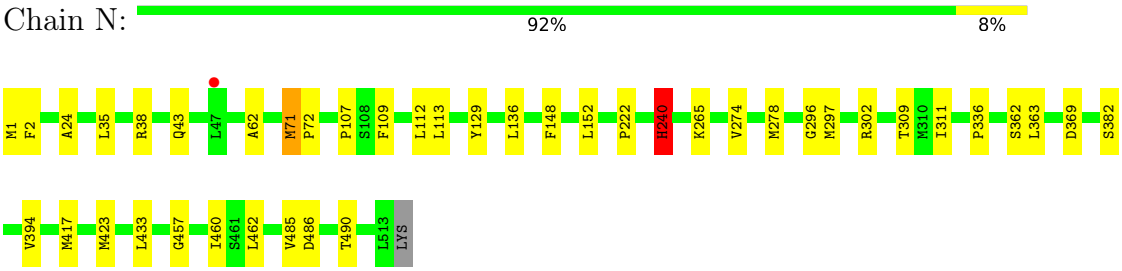
• Molecule 1: Cytochrome c oxidase subunit 1

Chain A:



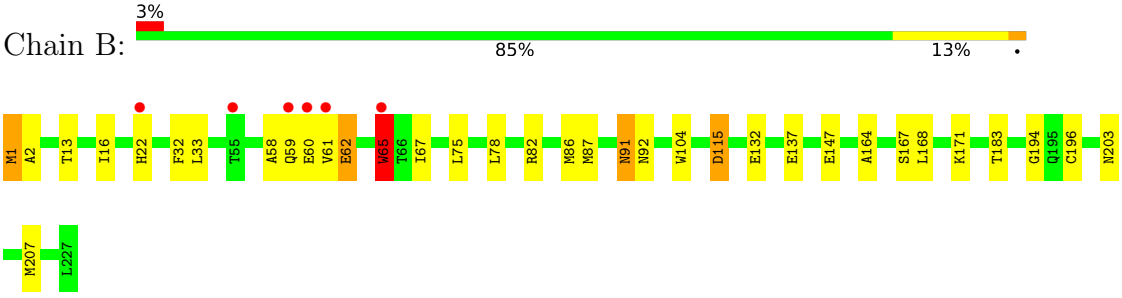
• Molecule 1: Cytochrome c oxidase subunit 1

Chain N:



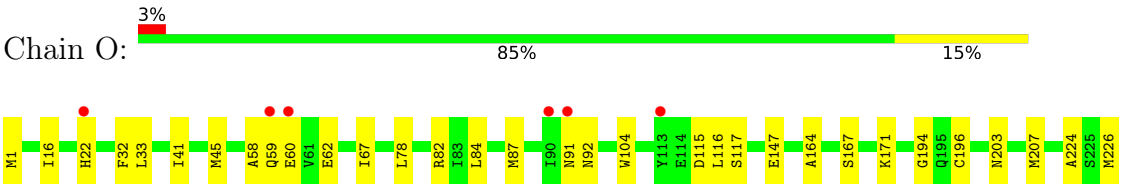
• Molecule 2: Cytochrome c oxidase subunit 2

Chain B:

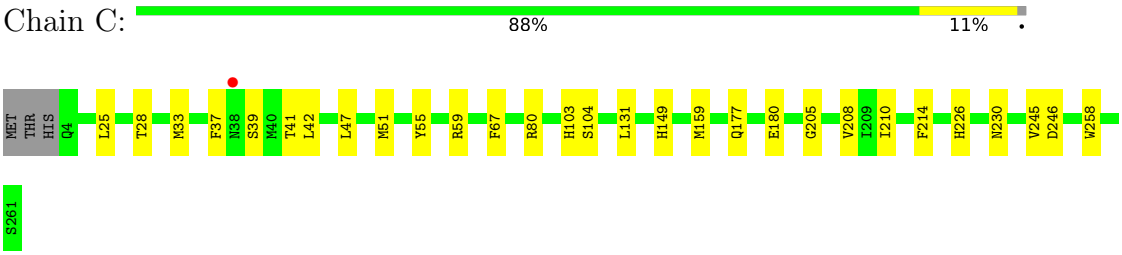


• Molecule 2: Cytochrome c oxidase subunit 2

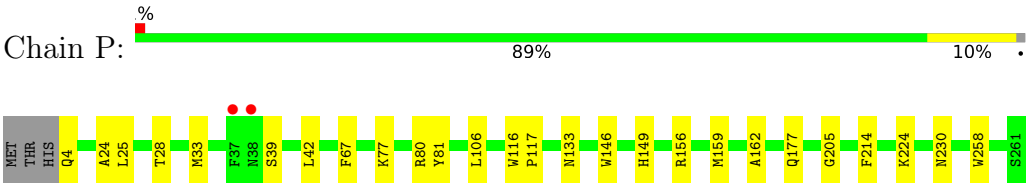
Chain O:



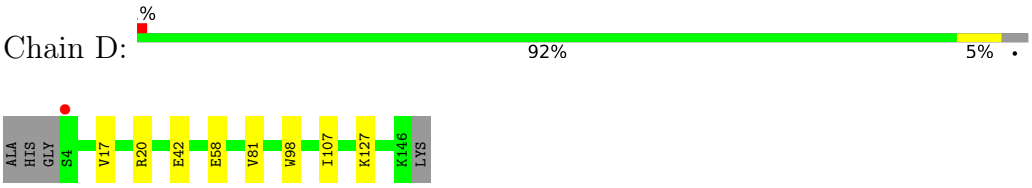
• Molecule 3: Cytochrome c oxidase subunit 3



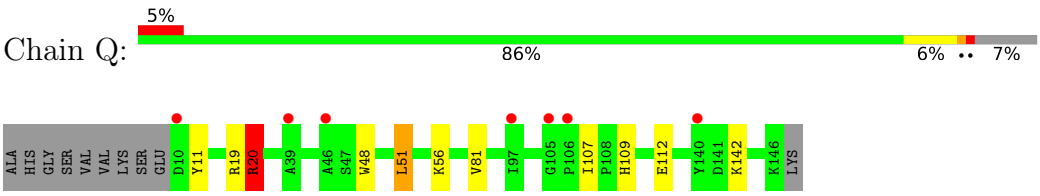
• Molecule 3: Cytochrome c oxidase subunit 3



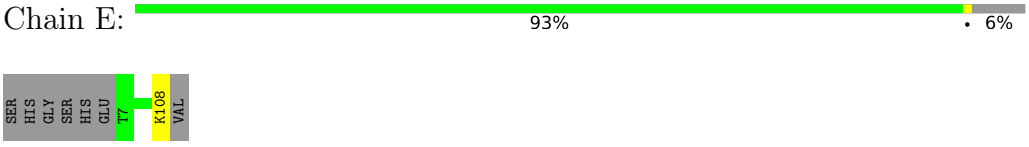
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



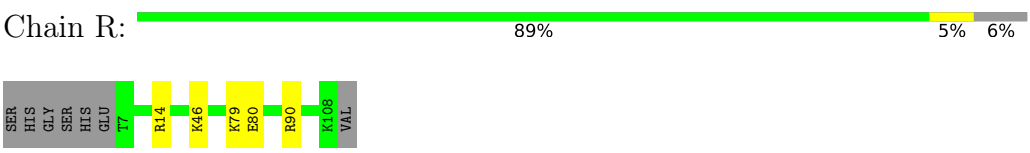
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



• Molecule 5: Cytochrome c oxidase subunit 5A

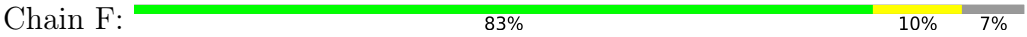


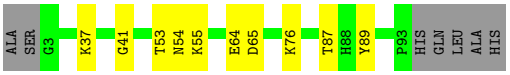
• Molecule 5: Cytochrome c oxidase subunit 5A



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

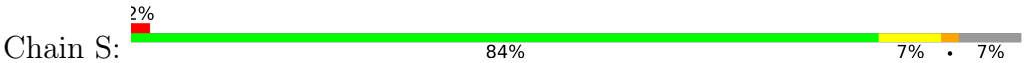
Chain F:

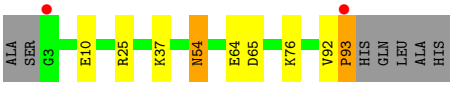




• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

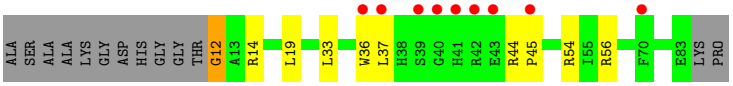
Chain S:





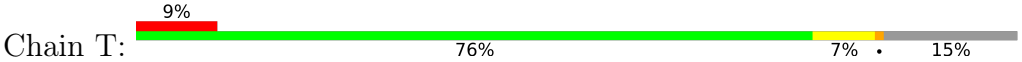
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

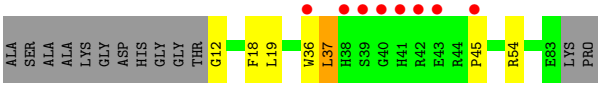
Chain G:



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

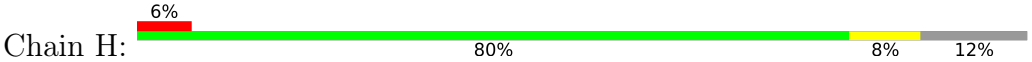
Chain T:

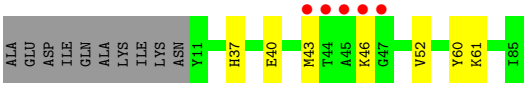




• Molecule 8: Cytochrome c oxidase subunit 6B1

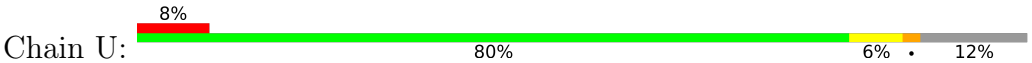
Chain H:

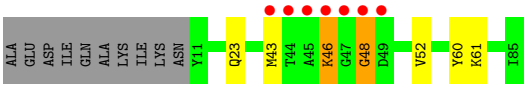




• Molecule 8: Cytochrome c oxidase subunit 6B1

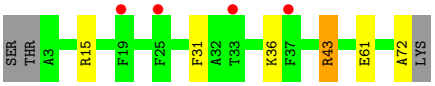
Chain U:



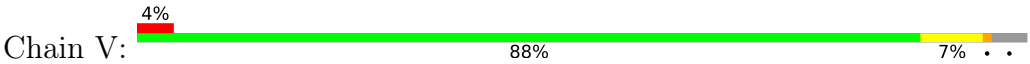


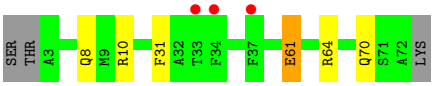
• Molecule 9: Cytochrome c oxidase subunit 6C

Chain I:

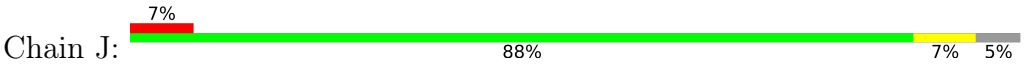


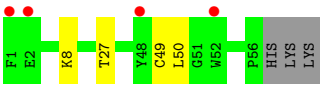
• Molecule 9: Cytochrome c oxidase subunit 6C



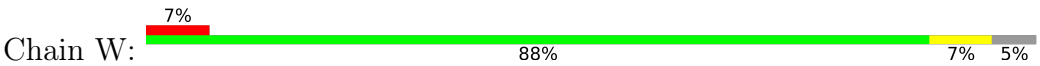


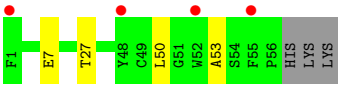
• Molecule 10: Cytochrome c oxidase subunit 7A1



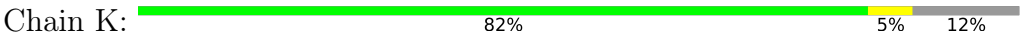


• Molecule 10: Cytochrome c oxidase subunit 7A1

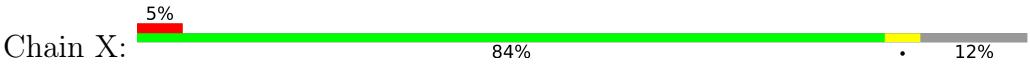


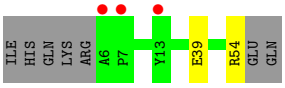


• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

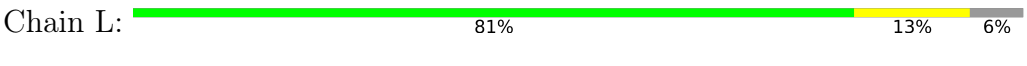


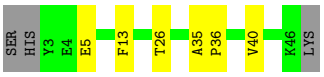
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial





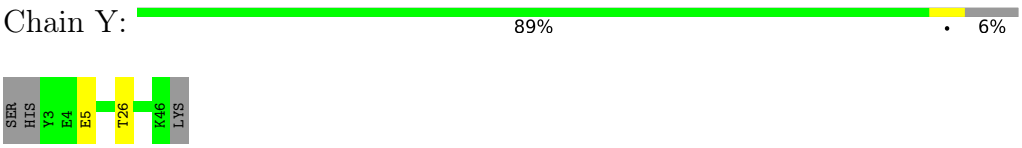
• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial





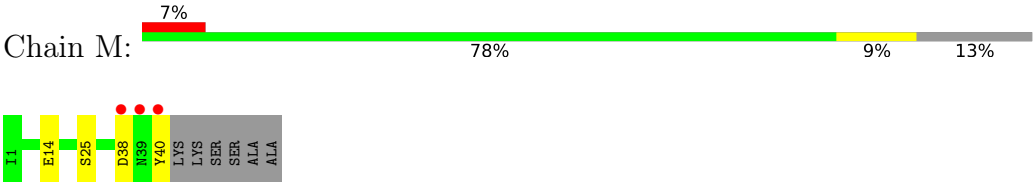
• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain Y:



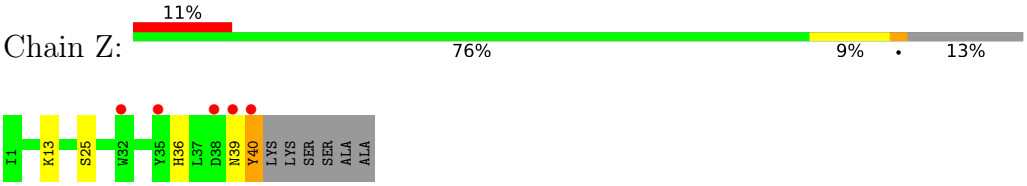
• Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

Chain M:



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

Chain Z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	182.80Å 205.70Å 177.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.70 136.64 – 1.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.00-1.70) 99.9 (136.64-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.07 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.123 , 0.153 0.139 , 0.165	Depositor DCC
R_{free} test set	36325 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	30.8	Xtriage
Anisotropy	0.586	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 64.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.006 for l,-k,h	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	33049	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

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

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

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

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

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

sidechain that are expected to be planar.

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

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	58	GLU	CD-OE1	13.48	1.40	1.25
5	R	80	GLU	CD-OE1	11.61	1.38	1.25
12	L	5	GLU	CD-OE2	-8.74	1.16	1.25
9	I	72	ALA	C-O	7.29	1.37	1.23
1	A	382	SER	CB-OG	-6.98	1.33	1.42
9	I	61	GLU	CD-OE2	-6.84	1.18	1.25
12	Y	5	GLU	CD-OE2	-6.67	1.18	1.25
1	A	189	MET	CB-CG	6.45	1.72	1.51
5	E	108	LYS	C-O	6.40	1.35	1.23
13	M	14	GLU	CD-OE1	-6.34	1.18	1.25
1	A	383	MET	C-O	6.28	1.35	1.23
2	B	167	SER	CB-OG	-6.24	1.34	1.42
2	O	167	SER	CB-OG	-5.92	1.34	1.42
7	G	12	GLY	N-CA	-5.81	1.37	1.46
2	O	147	GLU	CD-OE1	-5.65	1.19	1.25
2	B	147	GLU	CD-OE1	-5.48	1.19	1.25
6	S	93	PRO	C-O	5.40	1.34	1.23
4	Q	142	LYS	C-O	5.37	1.33	1.23
7	G	12	GLY	C-O	5.19	1.31	1.23
1	A	34	SER	CA-CB	5.15	1.60	1.52
2	B	147	GLU	CD-OE2	-5.15	1.20	1.25
2	B	62	GLU	CD-OE1	-5.12	1.20	1.25

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	Q	20	ARG	NE-CZ-NH1	14.28	127.44	120.30
9	V	10	ARG	NE-CZ-NH2	-11.91	114.34	120.30
4	Q	20	ARG	NE-CZ-NH2	-11.61	114.49	120.30
2	B	65	TRP	CA-CB-CG	10.74	134.10	113.70
2	B	65	TRP	CB-CG-CD1	-9.24	114.99	127.00
1	A	71	MET	CG-SD-CE	-8.84	86.06	100.20
2	B	65	TRP	CB-CA-C	-8.68	93.03	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	82	ARG	NE-CZ-NH2	-8.37	116.11	120.30
2	B	65	TRP	CB-CG-CD2	8.11	137.15	126.60
7	G	44	ARG	NE-CZ-NH1	8.05	124.33	120.30
9	V	10	ARG	NE-CZ-NH1	8.03	124.31	120.30
1	N	71	MET	CG-SD-CE	-7.50	88.21	100.20
2	B	82	ARG	CG-CD-NE	-7.19	96.71	111.80
2	O	82	ARG	NE-CZ-NH2	-6.82	116.89	120.30
9	I	72	ALA	CA-C-O	-6.69	106.05	120.10
3	C	80	ARG	CG-CD-NE	-6.33	98.52	111.80
3	P	80	ARG	CG-CD-NE	-6.29	98.59	111.80
1	N	240	HIS	CA-CB-CG	-6.15	103.14	113.60
4	Q	20	ARG	CG-CD-NE	-6.15	98.88	111.80
1	A	240	HIS	CA-CB-CG	-5.94	103.50	113.60
2	B	115	ASP	CB-CA-C	5.91	122.22	110.40
9	I	15	ARG	NE-CZ-NH1	5.85	123.22	120.30
6	S	93	PRO	N-CA-C	-5.73	97.21	112.10
1	A	129	TYR	CB-CG-CD1	5.72	124.43	121.00
9	I	43	ARG	CG-CD-NE	5.62	123.60	111.80
4	D	58	GLU	CB-CG-CD	5.56	129.21	114.20
1	A	213	ARG	NE-CZ-NH2	-5.50	117.55	120.30
4	D	20	ARG	NE-CZ-NH1	-5.45	117.58	120.30
11	K	47	ARG	NE-CZ-NH2	5.40	123.00	120.30
1	N	43	GLN	CB-CA-C	5.38	121.15	110.40
7	G	56	ARG	NE-CZ-NH2	-5.34	117.63	120.30
5	R	14	ARG	NE-CZ-NH1	5.23	122.91	120.30
4	D	20	ARG	NE-CZ-NH2	5.19	122.89	120.30
7	G	14	ARG	NE-CZ-NH1	-5.17	117.71	120.30
1	N	129	TYR	CB-CG-CD1	5.17	124.10	121.00
1	A	502	TYR	CB-CG-CD1	-5.11	117.93	121.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

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

5.2 Too-close contacts (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	50	0
1	N	4130	0	4102	44	0
2	B	1870	0	1870	20	0
2	O	1870	0	1870	23	0
3	C	2171	0	2080	32	0
3	P	2172	0	2081	24	0
4	D	1192	0	1178	6	0
4	Q	1148	0	1131	9	0
5	E	825	0	823	0	0
5	R	825	0	823	2	0
6	F	709	0	691	8	0
6	S	709	0	691	5	0
7	G	606	0	577	4	0
7	T	606	0	577	5	0
8	H	628	0	580	7	0
8	U	628	0	580	9	0
9	I	575	0	584	1	0
9	V	575	0	584	4	0
10	J	441	0	439	4	0
10	W	441	0	439	5	0
11	K	384	0	366	1	0
11	X	384	0	366	1	0
12	L	360	0	360	7	0
12	Y	360	0	360	4	0
13	M	311	0	321	2	0
13	Z	311	0	321	4	0
14	A	129	0	88	4	0
14	N	129	0	88	4	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	2	0	0	1	0
18	N	2	0	0	1	0
19	A	28	0	54	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	B	17	0	33	3	0
19	C	114	0	203	31	0
19	N	45	0	87	5	0
19	O	11	0	21	4	0
19	P	100	0	174	22	0
19	T	25	0	48	1	0
20	A	62	0	96	11	0
20	B	55	0	83	1	0
20	C	194	0	262	21	0
20	D	33	0	41	4	0
20	H	33	0	26	9	0
20	J	11	0	21	0	0
20	L	22	0	31	2	0
20	M	41	0	57	1	0
20	N	84	0	100	4	0
20	O	66	0	104	2	0
20	P	194	0	262	13	0
20	Q	33	0	41	2	0
20	W	11	0	21	0	0
20	Y	22	0	31	4	0
20	Z	41	0	56	0	0
21	A	16	0	24	0	0
21	B	4	0	6	0	0
21	C	12	0	17	1	0
21	E	12	0	18	0	0
21	F	8	0	12	1	0
21	G	4	0	6	0	0
21	N	20	0	30	3	0
21	O	4	0	6	0	0
21	P	12	0	18	1	0
21	R	12	0	18	0	0
21	S	8	0	12	1	0
21	T	4	0	6	0	0
22	A	51	0	76	1	0
22	C	51	0	76	1	0
22	N	51	0	76	1	0
22	P	51	0	76	0	0
23	B	2	0	0	0	0
23	O	2	0	0	0	0
24	B	29	0	39	0	0
24	C	58	0	78	1	0
24	O	29	0	39	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	P	58	0	78	4	0
25	C	1	0	0	1	0
25	P	1	0	0	1	0
26	C	87	0	124	16	0
26	I	64	0	72	0	0
26	L	94	0	141	3	0
26	O	64	0	72	1	0
26	P	87	0	124	10	0
26	Y	94	0	141	4	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	G	53	0	77	2	0
28	T	53	0	77	4	0
29	A	250	0	0	9	0
29	B	177	0	0	3	0
29	C	103	0	0	7	0
29	D	144	0	0	2	0
29	E	116	0	0	0	0
29	F	111	0	0	2	0
29	G	43	0	0	2	0
29	H	61	0	0	0	0
29	I	41	0	0	1	0
29	J	20	0	0	0	0
29	K	22	0	0	0	0
29	L	27	0	0	1	0
29	M	21	0	0	0	0
29	N	237	0	0	11	0
29	O	149	0	0	2	0
29	P	102	0	0	8	0
29	Q	86	0	0	3	0
29	R	94	0	0	2	0
29	S	93	0	0	1	0
29	T	38	0	0	2	0
29	U	46	0	0	0	0
29	V	22	0	0	0	0
29	W	15	0	0	0	0
29	X	18	0	0	0	0
29	Y	27	0	0	1	0
29	Z	17	0	0	1	0
All	All	33049	0	31463	358	0

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

All (358) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:C:314:LFA:H12	29:C:423:HOH:O	1.38	1.24
20:P:318:DMU:O3	20:P:319:DMU:H29	1.36	1.23
1:A:297[B]:MET:HB2	29:A:804:HOH:O	1.41	1.18
8:H:52:VAL:HG12	8:U:46:LYS:HG2	1.23	1.14
18:N:608:PER:O2	18:N:608:PER:O1	1.64	1.14
18:A:606:PER:O2	18:A:606:PER:O1	1.68	1.10
3:P:4:GLN:N	29:P:402:HOH:O	1.88	1.07
19:C:309:LFA:H11	20:H:101:DMU:H3	1.37	1.06
20:P:318:DMU:O3	20:P:319:DMU:C57	2.07	1.02
3:C:33[A]:MET:HE1	3:C:42:LEU:H	1.21	0.99
19:A:607:LFA:H12	19:A:608:LFA:H11	1.45	0.99
1:A:136[B]:LEU:HD11	29:A:931:HOH:O	1.61	0.98
2:B:16[B]:ILE:HG23	29:B:531:HOH:O	1.64	0.97
1:A:297[B]:MET:CB	29:A:804:HOH:O	1.99	0.96
1:N:297[B]:MET:CB	29:N:2915:HOH:O	2.15	0.95
20:P:319:DMU:H36	20:P:319:DMU:O55	1.66	0.95
19:C:325:LFA:H12	19:P:311:LFA:H12	1.47	0.95
19:C:309:LFA:H11	20:H:101:DMU:C3	1.98	0.93
6:S:76:LYS:HE2	6:S:93:PRO:HG2	1.52	0.91
19:P:314:LFA:H13	29:P:416:HOH:O	1.69	0.91
25:C:302:UNX:UNK	29:C:496:HOH:O	1.52	0.90
3:C:245:VAL:C	3:C:246[B]:ASP:CA	2.39	0.89
19:C:309:LFA:C1	20:H:101:DMU:C2	2.30	0.89
3:P:149:HIS:NE2	19:P:312:LFA:H11	1.86	0.89
1:N:297[B]:MET:SD	1:N:302:ARG:HG2	2.13	0.88
24:P:306:CHD:H162	24:P:306:CHD:H231	1.57	0.86
19:P:314:LFA:C1	29:P:416:HOH:O	2.21	0.86
1:A:297[B]:MET:SD	1:A:302:ARG:HG2	2.17	0.85
19:C:309:LFA:H11	20:H:101:DMU:C2	2.06	0.85
25:P:303:UNX:UNK	29:P:497:HOH:O	1.57	0.84
1:N:297[B]:MET:HB3	29:N:2915:HOH:O	1.72	0.84
20:N:612:DMU:H41	29:Z:208:HOH:O	1.78	0.84
3:C:67:PHE:CE2	26:C:304:CDL:O1	2.32	0.81
20:C:323:DMU:H20	20:N:602:DMU:H21	1.62	0.80
1:N:297[B]:MET:HB2	29:N:2915:HOH:O	1.81	0.79
7:G:19:LEU:HD23	19:N:610:LFA:H61	1.65	0.78
1:N:311[A]:ILE:HD11	20:N:602:DMU:H22	1.63	0.78
4:Q:20:ARG:HG2	29:Q:348:HOH:O	1.84	0.78
3:P:67:PHE:CE2	26:P:305:CDL:O1	2.36	0.77
8:H:52:VAL:HG12	8:U:46:LYS:CG	2.09	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278[B]:MET:SD	19:A:607:LFA:H51	2.26	0.76
1:A:53:ILE:HD11	12:L:40:VAL:HG13	1.70	0.74
8:H:52:VAL:CG1	8:U:46:LYS:HG2	2.10	0.74
1:N:297[B]:MET:SD	1:N:302:ARG:CG	2.75	0.74
19:C:309:LFA:H122	19:P:301:LFA:H92	1.69	0.74
19:C:312:LFA:H102	20:C:316:DMU:C43	2.18	0.74
2:O:59:GLN:HE22	19:O:302:LFA:H32	1.53	0.74
1:A:278[A]:MET:CE	19:A:608:LFA:H51	2.18	0.73
3:C:33[A]:MET:HE1	3:C:42:LEU:N	2.02	0.73
2:B:13:THR:OG1	29:B:402:HOH:O	2.08	0.72
14:N:604:HEA:HBC1	14:N:604:HEA:HMC1	1.70	0.72
2:O:84:LEU:HA	2:O:87[A]:MET:HE2	1.70	0.72
4:Q:112:GLU:OE2	29:Q:301:HOH:O	2.07	0.72
24:P:306:CHD:H162	24:P:306:CHD:C23	2.19	0.70
1:N:423[B]:MET:HE2	1:N:457:GLY:HA2	1.73	0.70
21:F:103:EDO:O1	29:F:201[A]:HOH:O	0.70	0.69
26:L:101:CDL:O1	29:L:222[B]:HOH:O	1.85	0.69
28:T:101:PEK:H32	28:T:101:PEK:H71	1.75	0.69
1:A:278[A]:MET:HE3	19:A:608:LFA:H51	1.74	0.69
1:A:112:LEU:HG	29:A:919:HOH:O	1.92	0.69
1:A:297[B]:MET:SD	1:A:302:ARG:CG	2.81	0.69
19:C:325:LFA:C1	19:P:311:LFA:H12	2.21	0.68
12:L:26:THR:HG21	20:L:102:DMU:H26	1.74	0.68
3:P:258:TRP:CE2	19:P:308:LFA:H32	2.27	0.68
1:A:112:LEU:C	1:A:112:LEU:HD23	2.13	0.68
14:A:602:HEA:HBC1	14:A:602:HEA:HMC1	1.77	0.67
20:A:610:DMU:O6	29:A:706:HOH:O	2.12	0.66
3:C:149:HIS:NE2	19:C:312:LFA:H11	2.10	0.66
3:C:180[A]:GLU:OE2	29:C:404:HOH:O	2.13	0.66
1:A:113[B]:LEU:HD11	1:A:117[B]:MET:SD	2.36	0.66
20:P:319:DMU:O55	20:P:319:DMU:C10	2.42	0.66
24:C:305:CHD:H162	24:C:305:CHD:H231	1.77	0.65
1:N:136[B]:LEU:HD11	29:N:3025:HOH:O	1.96	0.65
3:P:4:GLN:CA	29:P:402:HOH:O	2.32	0.65
26:C:304:CDL:H752	10:J:27:THR:HG21	1.79	0.65
1:A:311[A]:ILE:HD12	20:A:617:DMU:H23	1.78	0.65
7:G:12:GLY:HA3	29:G:235:HOH:O	1.97	0.65
19:C:312:LFA:H102	20:C:316:DMU:H26	1.78	0.65
9:V:61:GLU:OE1	9:V:64:ARG:NH2	2.28	0.64
3:P:33[B]:MET:HE3	3:P:42:LEU:HD12	1.78	0.64
8:U:43:MET:O	8:U:48:GLY:N	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:485:VAL:HG13	21:N:617:EDO:H21	1.80	0.64
19:C:309:LFA:C1	20:H:101:DMU:C3	2.64	0.63
4:Q:48:TRP:HA	4:Q:51:LEU:HD22	1.80	0.63
26:Y:101:CDL:O1	29:Y:216[B]:HOH:O	2.16	0.63
2:O:116:LEU:CD1	2:O:226:MET:HG2	2.28	0.63
20:Y:102:DMU:H6	20:Y:102:DMU:O49	1.99	0.62
6:F:37:LYS:HG2	29:F:297:HOH:O	1.99	0.62
1:A:365:ILE:HD11	29:A:715:HOH:O	2.00	0.62
3:C:33[B]:MET:HE2	20:C:324:DMU:H12	1.82	0.61
21:N:617:EDO:O1	29:N:2805:HOH:O	2.16	0.61
26:P:305:CDL:HB61	26:P:305:CDL:HB22	1.82	0.61
9:V:61:GLU:OE1	9:V:64:ARG:NE	2.30	0.60
3:P:33[B]:MET:CE	3:P:42:LEU:HD12	2.32	0.60
22:N:618:PGV:H183	28:T:101:PEK:H331	1.84	0.60
1:A:278[A]:MET:HE3	19:A:608:LFA:C5	2.31	0.60
19:C:309:LFA:C1	20:H:101:DMU:O55	2.50	0.60
1:N:486:ASP:OD2	4:Q:19:ARG:NE	2.35	0.59
2:O:116:LEU:HD13	2:O:226:MET:HG2	1.82	0.59
26:C:304:CDL:OA3	26:C:304:CDL:H1	2.03	0.59
20:Y:102:DMU:O49	20:Y:102:DMU:C18	2.50	0.59
3:C:33[B]:MET:CE	20:C:324:DMU:H12	2.31	0.59
26:C:304:CDL:HB61	26:C:304:CDL:HB21	1.84	0.59
12:Y:26:THR:HG23	13:Z:25:SER:CB	2.33	0.59
1:A:278[A]:MET:SD	19:A:608:LFA:H51	2.43	0.59
19:C:325:LFA:H12	19:P:311:LFA:C1	2.26	0.59
26:P:305:CDL:H121	26:P:305:CDL:HA62	1.85	0.58
2:O:59:GLN:HE22	19:O:302:LFA:C3	2.16	0.58
1:A:297[B]:MET:HG2	1:A:302:ARG:HG3	1.84	0.58
2:B:16[A]:ILE:HG21	2:B:87[A]:MET:CE	2.32	0.58
1:N:417[B]:MET:CE	29:N:2932:HOH:O	2.49	0.58
2:O:92:ASN:ND2	29:O:403:HOH:O	2.36	0.58
1:A:297[B]:MET:CG	1:A:302:ARG:HG3	2.34	0.58
26:C:304:CDL:HB21	26:C:304:CDL:HB32	1.86	0.58
20:P:318:DMU:C5	20:P:319:DMU:H29	2.34	0.57
19:C:312:LFA:H102	20:C:316:DMU:H25	1.86	0.57
19:C:307:LFA:C11	19:C:307:LFA:H72	2.35	0.57
6:F:64:GLU:O	6:F:65:ASP:HB2	2.05	0.57
3:C:59:ARG:HB2	26:C:304:CDL:OA9	2.04	0.57
12:L:13:PHE:HB3	26:L:101:CDL:H512	1.87	0.57
3:C:258:TRP:CE2	19:C:307:LFA:H32	2.40	0.57
20:C:324:DMU:H20	10:J:50:LEU:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:278[B]:MET:SD	19:N:609:LFA:H51	2.45	0.56
7:G:19:LEU:CD2	19:N:610:LFA:H61	2.35	0.56
1:N:297[B]:MET:HG2	1:N:302:ARG:HG3	1.88	0.56
3:P:205:GLY:HA3	28:T:101:PEK:H182	1.86	0.56
1:N:297[B]:MET:CG	1:N:302:ARG:HG3	2.36	0.56
4:Q:48:TRP:O	4:Q:51:LEU:HB2	2.04	0.56
12:Y:26:THR:HG23	13:Z:25:SER:HB3	1.87	0.56
26:P:305:CDL:C75	10:W:27:THR:HG21	2.35	0.56
19:C:307:LFA:H91	20:C:323:DMU:C31	2.36	0.56
1:N:112:LEU:HD23	1:N:112:LEU:C	2.27	0.56
3:P:156:ARG:HE	24:P:306:CHD:C24	2.19	0.56
1:A:334:TRP:CE3	20:A:609:DMU:H19	2.41	0.56
4:D:17[A]:VAL:HG12	29:D:302:HOH:O	2.06	0.55
1:A:311[A]:ILE:CD1	20:A:617:DMU:C40	2.85	0.55
4:Q:107:ILE:HD13	11:X:39:GLU:HB2	1.86	0.55
19:C:310:LFA:H12	19:P:301:LFA:H11	1.87	0.55
6:S:76:LYS:CE	6:S:93:PRO:HG2	2.33	0.55
20:C:323:DMU:O61	20:O:303:DMU:O55	2.19	0.55
2:B:67:ILE:HD11	19:B:306:LFA:H42	1.89	0.54
1:A:110:LEU:HD21	20:C:324:DMU:H24	1.89	0.54
1:A:278[A]:MET:CE	19:A:608:LFA:C5	2.84	0.54
4:D:42:GLU:OE2	29:D:301:HOH:O	2.18	0.54
2:O:58:ALA:O	2:O:62:GLU:HG3	2.08	0.54
3:P:133:ASN:ND2	29:P:404:HOH:O	2.34	0.54
4:Q:81:VAL:HG11	20:Q:201:DMU:H11	1.90	0.54
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.90	0.54
1:N:311[A]:ILE:CD1	20:N:602:DMU:H22	2.37	0.54
1:N:296:GLY:HA2	8:U:23:GLN:OE1	2.08	0.54
29:P:453[B]:HOH:O	10:W:27:THR:HG22	2.09	0.53
20:A:617:DMU:H13	20:P:323:DMU:H11	1.91	0.53
1:N:2:PHE:CE2	26:Y:101:CDL:H712	2.44	0.53
1:N:423[B]:MET:HE2	1:N:460:ILE:HD12	1.90	0.53
3:P:224:LYS:HE3	26:P:305:CDL:HB31	1.88	0.53
19:C:313:LFA:H21	19:C:314:LFA:H71	1.89	0.53
4:D:107:ILE:HD13	11:K:39:GLU:HB2	1.90	0.53
3:C:180[B]:GLU:HG2	29:C:428:HOH:O	2.08	0.53
19:C:310:LFA:H12	19:P:301:LFA:C1	2.39	0.53
20:C:324:DMU:H11	10:J:49:CYS:HB3	1.91	0.53
28:T:101:PEK:H32	28:T:101:PEK:C7	2.36	0.53
6:F:87[A]:THR:HG22	6:F:89:TYR:CE1	2.44	0.52
1:A:24:ALA:HB2	14:A:601[B]:HEA:H253	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:423[B]:MET:CE	1:N:460:ILE:HD12	2.40	0.52
2:B:91:ASN:OD1	2:B:183:THR:HG21	2.10	0.52
26:C:304:CDL:HB21	26:C:304:CDL:CB3	2.40	0.51
26:P:305:CDL:H752	10:W:27:THR:HG21	1.91	0.51
20:P:324:DMU:H10	10:W:53:ALA:HB2	1.92	0.51
2:B:91:ASN:HD22	2:B:92:ASN:N	2.08	0.51
3:C:37:PHE:CE2	20:C:324:DMU:H13	2.45	0.51
20:A:617:DMU:O16	20:P:323:DMU:O61	2.22	0.51
19:N:601:LFA:H42	2:O:67:ILE:HD11	1.91	0.51
26:P:305:CDL:HB61	26:P:305:CDL:CB2	2.41	0.51
1:A:297[B]:MET:HB3	29:A:804:HOH:O	1.85	0.51
7:T:45:PRO:HD2	29:T:218:HOH:O	2.10	0.51
3:P:258:TRP:CZ2	19:P:308:LFA:H32	2.46	0.51
1:A:484:THR:HG22	29:A:864:HOH:O	2.09	0.51
2:O:16[B]:ILE:HG23	29:O:517:HOH:O	2.10	0.51
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.92	0.50
12:L:26:THR:CG2	20:L:102:DMU:H26	2.41	0.50
1:A:311[A]:ILE:CD1	20:A:617:DMU:H23	2.40	0.50
12:Y:26:THR:CG2	20:Y:102:DMU:H26	2.41	0.50
2:B:58:ALA:O	2:B:62:GLU:HG3	2.11	0.50
1:N:417[B]:MET:HE2	29:N:2932:HOH:O	2.11	0.50
1:N:35:LEU:HD11	1:N:462:LEU:HB2	1.93	0.50
26:P:305:CDL:HB32	26:P:305:CDL:HB21	1.94	0.49
6:F:41:GLY:HA3	6:F:87[B]:THR:CG2	2.42	0.49
1:N:297[B]:MET:SD	1:N:302:ARG:HG3	2.50	0.49
2:B:61:VAL:HG22	2:B:65:TRP:CZ3	2.47	0.49
2:O:22[B]:HIS:O	2:O:22[B]:HIS:CG	2.65	0.49
26:C:304:CDL:H121	26:C:304:CDL:CA6	2.43	0.49
6:F:41:GLY:HA3	6:F:87[B]:THR:HG22	1.94	0.49
20:A:617:DMU:H8	20:P:323:DMU:H11	1.93	0.49
1:N:113[A]:LEU:HD12	26:Y:101:CDL:C87	2.42	0.49
2:O:224:ALA:O	2:O:227:LEU:HD12	2.12	0.49
19:C:309:LFA:C1	20:H:101:DMU:H3	2.23	0.49
5:R:46:LYS:NZ	29:R:303:HOH:O	2.46	0.49
22:A:616:PGV:H183	28:G:101:PEK:H322	1.94	0.49
29:N:2884:HOH:O	19:P:310:LFA:H51	2.11	0.49
3:C:33[B]:MET:HE2	3:C:33[B]:MET:CA	2.43	0.48
20:C:323:DMU:O61	20:O:303:DMU:C2	2.61	0.48
2:O:59:GLN:NE2	19:O:302:LFA:C3	2.76	0.48
20:P:318:DMU:C11	20:P:324:DMU:H40	2.43	0.48
19:C:309:LFA:H122	19:P:301:LFA:C9	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:362[A]:SER:HA	2:O:87[A]:MET:HE1	1.94	0.48
19:A:607:LFA:C1	19:A:608:LFA:H11	2.32	0.48
1:N:112:LEU:HG	29:N:3010:HOH:O	2.13	0.48
6:S:54:ASN:HD22	6:S:54:ASN:C	2.17	0.48
1:A:336:PRO:HB2	1:A:394[B]:VAL:HG11	1.95	0.48
1:N:24:ALA:HB2	14:N:603[B]:HEA:H253	1.95	0.48
20:Q:201:DMU:O55	20:Q:201:DMU:H36	2.14	0.48
19:P:301:LFA:H51	19:P:301:LFA:H21	1.57	0.47
3:C:210:ILE:HD13	22:C:303:PGV:H312	1.95	0.47
2:B:67:ILE:CD1	19:B:306:LFA:H61	2.44	0.47
1:A:311[A]:ILE:HD11	20:A:617:DMU:H22	1.96	0.47
1:N:278[B]:MET:SD	19:N:609:LFA:C5	3.02	0.47
26:P:305:CDL:H751	10:W:27:THR:HG21	1.96	0.47
24:P:306:CHD:C23	24:P:306:CHD:C16	2.92	0.47
19:P:314:LFA:H12	29:P:416:HOH:O	1.98	0.47
21:S:102:EDO:O1	29:S:221[B]:HOH:O	0.47	0.47
8:U:46:LYS:HG3	8:U:48:GLY:N	2.30	0.47
1:A:110:LEU:CD2	20:C:324:DMU:H24	2.44	0.47
2:B:32[B]:PHE:CD2	9:I:31:PHE:CZ	3.03	0.47
8:H:43:MET:CE	8:U:52:VAL:HG11	2.44	0.47
3:C:226:HIS:HE1	26:C:304:CDL:H111	1.79	0.47
3:P:33[A]:MET:HG2	3:P:39:SER:O	2.14	0.47
20:D:201:DMU:H36	20:D:201:DMU:O55	2.15	0.46
19:P:312:LFA:H12	19:P:312:LFA:H42	1.65	0.46
19:C:307:LFA:H91	20:C:323:DMU:H21	1.98	0.46
20:C:315:DMU:H36	20:C:315:DMU:O55	2.16	0.46
3:C:104:SER:OG	29:C:405:HOH:O	2.20	0.46
4:D:98:TRP:CE2	20:M:101:DMU:H11	2.50	0.46
3:P:177:GLN:OE1	3:P:177:GLN:HA	2.16	0.46
1:A:311[A]:ILE:CD1	20:A:617:DMU:H22	2.45	0.46
3:C:205:GLY:HA3	28:G:101:PEK:H192	1.98	0.46
2:B:16[A]:ILE:HD11	2:B:86:MET:HG2	1.97	0.46
2:B:22[B]:HIS:HD2	29:B:447:HOH:O	1.97	0.46
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.96	0.46
24:O:301:CHD:H212	24:O:301:CHD:H12	1.96	0.46
2:B:16[A]:ILE:HG21	2:B:87[A]:MET:HG2	1.97	0.46
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.51	0.46
12:L:26:THR:HG23	13:M:25:SER:CB	2.46	0.46
4:Q:109:HIS:HD2	29:Q:347:HOH:O	1.98	0.46
21:C:321:EDO:C2	29:C:403:HOH:O	2.33	0.45
3:P:106:LEU:HD22	19:P:311:LFA:H21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:32[B]:PHE:CD2	9:V:31:PHE:CZ	3.04	0.45
4:Q:51:LEU:HB3	4:Q:56:LYS:HG3	1.97	0.45
19:A:608:LFA:C6	7:T:19:LEU:HD23	2.47	0.45
2:O:116:LEU:HD12	2:O:117:SER:N	2.31	0.45
19:C:325:LFA:C1	19:P:311:LFA:C1	2.91	0.45
6:F:53:THR:HG23	6:F:55:LYS:H	1.82	0.45
19:C:325:LFA:H82	19:P:310:LFA:H122	1.99	0.45
3:C:51[B]:MET:HB3	3:C:51[B]:MET:HE2	1.80	0.45
20:P:315:DMU:H16	20:P:315:DMU:H22	1.55	0.45
20:P:318:DMU:O3	20:P:319:DMU:H30	2.05	0.45
1:A:311[A]:ILE:HD12	20:A:617:DMU:C40	2.45	0.45
4:D:81:VAL:HG11	20:D:201:DMU:H11	1.99	0.45
26:C:304:CDL:CA5	26:C:304:CDL:OB4	2.65	0.45
9:V:61:GLU:OE1	9:V:64:ARG:CZ	2.65	0.45
1:A:53:ILE:HG22	29:A:819:HOH:O	2.16	0.44
1:A:311[B]:ILE:HG22	20:B:307:DMU:H25	1.99	0.44
3:C:67:PHE:HE2	26:C:304:CDL:O1	1.93	0.44
3:C:131:LEU:CD2	20:C:323:DMU:H18	2.47	0.44
3:C:47:LEU:O	3:C:51[A]:MET:HG2	2.17	0.44
3:P:224:LYS:CE	26:P:305:CDL:HB31	2.48	0.44
1:A:418:PHE:CD1	20:D:201:DMU:H24	2.51	0.44
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.99	0.44
3:C:55:TYR:OH	26:C:304:CDL:HA61	2.18	0.44
2:O:22[B]:HIS:O	2:O:22[B]:HIS:ND1	2.50	0.44
13:Z:36:HIS:HD2	13:Z:39:ASN:ND2	2.16	0.44
1:A:309:THR:HG22	14:A:602:HEA:HMB2	2.00	0.44
3:P:146:TRP:CD2	3:P:162:ALA:HB2	2.53	0.44
19:C:314:LFA:C1	29:C:423:HOH:O	2.20	0.44
3:C:33[A]:MET:CE	3:C:41:THR:HB	2.48	0.44
26:L:101:CDL:OB9	26:L:101:CDL:H122	2.17	0.44
3:C:208:VAL:HG22	3:C:245:VAL:CG1	2.48	0.43
8:U:46:LYS:HE2	8:U:46:LYS:O	2.18	0.43
1:A:297[B]:MET:SD	1:A:302:ARG:HG3	2.58	0.43
19:C:307:LFA:H91	20:C:323:DMU:H17	2.00	0.43
8:H:46:LYS:HE2	8:H:46:LYS:O	2.18	0.43
3:P:116:TRP:HA	3:P:117:PRO:C	2.39	0.43
1:A:87:ILE:O	1:A:173:PRO:HD3	2.18	0.43
6:S:10:GLU:OE2	6:S:25:ARG:NH1	2.43	0.43
1:A:409:TRP:HB3	1:A:471:ILE:HG12	2.00	0.43
1:N:240:HIS:C	1:N:240:HIS:CD2	2.91	0.43
1:N:423[B]:MET:HE3	1:N:457:GLY:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:39:SER:HB2	20:C:318:DMU:O55	2.18	0.43
1:N:265:LYS:HB2	1:N:490:THR:HG21	2.01	0.43
29:N:2884:HOH:O	19:P:310:LFA:C3	2.66	0.43
1:N:222:PRO:HB2	21:P:321:EDO:H22	2.01	0.43
19:P:312:LFA:C11	19:T:102:LFA:H91	2.48	0.43
8:H:37:HIS:HD2	8:H:40:GLU:OE2	2.02	0.43
2:O:164:ALA:O	2:O:194:GLY:HA3	2.19	0.43
6:F:64:GLU:O	6:F:65:ASP:CB	2.67	0.42
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.54	0.42
1:A:76:GLY:O	1:A:80:ASN:HB2	2.20	0.42
3:C:177:GLN:HA	3:C:177:GLN:OE1	2.19	0.42
26:C:304:CDL:H121	26:C:304:CDL:HA62	2.01	0.42
1:A:337:ALA:HB2	1:A:394[A]:VAL:HG23	2.01	0.42
19:P:301:LFA:H101	19:P:301:LFA:H131	1.53	0.42
1:A:240:HIS:C	1:A:240:HIS:CD2	2.92	0.42
1:A:334:TRP:HB2	20:D:201:DMU:C57	2.49	0.42
2:B:164:ALA:O	2:B:194:GLY:HA3	2.19	0.42
7:T:12:GLY:HA3	29:T:228:HOH:O	2.18	0.42
3:P:77:LYS:NZ	3:P:81:TYR:OH	2.52	0.42
19:A:608:LFA:H92	19:A:608:LFA:H121	1.82	0.42
2:B:13:THR:HB	2:B:168:LEU:HD23	2.01	0.42
26:C:304:CDL:H121	26:C:304:CDL:OA8	2.20	0.42
3:C:33[B]:MET:HG3	3:C:37:PHE:HB2	2.00	0.42
4:D:127:LYS:HD2	29:I:239:HOH:O	2.19	0.42
1:N:148:PHE:HB3	3:P:28:THR:HB	2.01	0.42
2:O:196:CYS:HB2	2:O:207:MET:HG3	2.01	0.42
1:A:379:TYR:O	1:A:383:MET:HB2	2.20	0.42
26:C:304:CDL:H531	26:C:304:CDL:HB4	2.00	0.42
8:H:46:LYS:HD3	8:U:52:VAL:HG22	2.01	0.42
26:C:304:CDL:HB22	10:J:8:LYS:HE3	2.02	0.41
1:N:71:MET:HB2	1:N:72:PRO:HD3	2.01	0.41
1:N:136[B]:LEU:CD1	29:N:3025:HOH:O	2.61	0.41
1:N:433:LEU:HD11	26:O:304:CDL:OA7	2.20	0.41
19:C:312:LFA:C10	20:C:316:DMU:C43	2.94	0.41
1:N:336:PRO:HB2	1:N:394[B]:VAL:HG11	2.02	0.41
12:Y:26:THR:HG21	20:Y:102:DMU:H26	2.01	0.41
1:A:265:LYS:HB2	1:A:490:THR:HG21	2.02	0.41
3:C:103:HIS:HA	20:H:101:DMU:H11	2.01	0.41
19:C:309:LFA:H13	20:H:101:DMU:O55	2.18	0.41
20:C:316:DMU:H15	20:C:317:DMU:H1	2.03	0.41
2:O:16[A]:ILE:HG21	2:O:87[A]:MET:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Z:40:TYR:CD1	13:Z:40:TYR:N	2.88	0.41
7:G:45:PRO:HD2	29:G:220:HOH:O	2.19	0.41
1:A:308:ALA:O	1:A:311[B]:ILE:HG12	2.21	0.41
6:F:54:ASN:ND2	6:F:76:LYS:HD2	2.35	0.41
12:L:35:ALA:HB3	12:L:36:PRO:HD3	2.02	0.41
3:P:33[B]:MET:CE	20:P:324:DMU:H12	2.50	0.41
2:B:67:ILE:HD11	19:B:306:LFA:H61	2.01	0.41
12:L:26:THR:HG23	13:M:25:SER:HB3	2.03	0.41
1:N:485:VAL:CG1	21:N:617:EDO:H21	2.48	0.41
1:A:112:LEU:C	1:A:112:LEU:CD2	2.86	0.41
1:N:274:VAL:HG12	1:N:278[A]:MET:CE	2.51	0.41
6:S:64:GLU:O	6:S:65:ASP:HB2	2.20	0.41
1:A:148:PHE:HB3	3:C:28:THR:HB	2.03	0.40
3:C:258:TRP:NE1	19:C:307:LFA:H12	2.36	0.40
2:O:59:GLN:NE2	19:O:302:LFA:H31	2.36	0.40
19:A:608:LFA:H61	7:T:19:LEU:HD23	2.04	0.40
2:B:1:FME:HE2	2:B:2:ALA:O	2.21	0.40
2:O:41:ILE:O	2:O:45:MET:HG2	2.21	0.40
5:R:90:ARG:NH1	29:R:308:HOH:O	2.49	0.40
1:N:113[A]:LEU:HD12	26:Y:101:CDL:H871	2.03	0.40
14:N:603[A]:HEA:H271	14:N:603[A]:HEA:H212	1.85	0.40
2:O:116:LEU:HD13	2:O:226:MET:CG	2.51	0.40
7:T:37:LEU:HD12	7:T:37:LEU:HA	1.82	0.40
14:A:601[A]:HEA:H271	14:A:601[A]:HEA:H212	1.90	0.40
1:N:309:THR:HG22	14:N:604:HEA:HMB2	2.03	0.40
3:C:33[B]:MET:HB2	3:C:33[B]:MET:HE3	0.89	0.40
1:N:152:LEU:CD2	3:P:24:ALA:HB1	2.52	0.40
3:P:33[B]:MET:HE2	3:P:33[B]:MET:HB2	1.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	526/514 (102%)	512 (97%)	14 (3%)	0	100 100
1	N	526/514 (102%)	514 (98%)	12 (2%)	0	100 100
2	B	230/227 (101%)	224 (97%)	6 (3%)	0	100 100
2	O	230/227 (101%)	225 (98%)	5 (2%)	0	100 100
3	C	265/261 (102%)	261 (98%)	4 (2%)	0	100 100
3	P	265/261 (102%)	261 (98%)	4 (2%)	0	100 100
4	D	142/147 (97%)	139 (98%)	3 (2%)	0	100 100
4	Q	136/147 (92%)	132 (97%)	3 (2%)	1 (1%)	22 8
5	E	100/109 (92%)	100 (100%)	0	0	100 100
5	R	100/109 (92%)	100 (100%)	0	0	100 100
6	F	91/98 (93%)	90 (99%)	1 (1%)	0	100 100
6	S	91/98 (93%)	90 (99%)	1 (1%)	0	100 100
7	G	71/85 (84%)	67 (94%)	4 (6%)	0	100 100
7	T	71/85 (84%)	68 (96%)	3 (4%)	0	100 100
8	H	73/85 (86%)	70 (96%)	3 (4%)	0	100 100
8	U	73/85 (86%)	71 (97%)	1 (1%)	1 (1%)	11 2
9	I	68/73 (93%)	67 (98%)	1 (2%)	0	100 100
9	V	68/73 (93%)	67 (98%)	1 (2%)	0	100 100
10	J	54/59 (92%)	54 (100%)	0	0	100 100
10	W	54/59 (92%)	54 (100%)	0	0	100 100
11	K	47/56 (84%)	46 (98%)	1 (2%)	0	100 100
11	X	47/56 (84%)	46 (98%)	1 (2%)	0	100 100
12	L	42/47 (89%)	41 (98%)	1 (2%)	0	100 100
12	Y	42/47 (89%)	41 (98%)	1 (2%)	0	100 100
13	M	38/46 (83%)	38 (100%)	0	0	100 100
13	Z	38/46 (83%)	37 (97%)	1 (3%)	0	100 100
All	All	3488/3614 (96%)	3415 (98%)	71 (2%)	2 (0%)	51 33

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (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%)	435 (99%)	5 (1%)	73 63
1	N	440/426 (103%)	435 (99%)	5 (1%)	73 63
2	B	215/210 (102%)	206 (96%)	9 (4%)	30 12
2	O	215/210 (102%)	209 (97%)	6 (3%)	43 25
3	C	232/226 (103%)	229 (99%)	3 (1%)	69 56
3	P	232/226 (103%)	229 (99%)	3 (1%)	69 56
4	D	128/129 (99%)	128 (100%)	0	100 100
4	Q	122/129 (95%)	120 (98%)	2 (2%)	62 48
5	E	89/95 (94%)	89 (100%)	0	100 100
5	R	89/95 (94%)	88 (99%)	1 (1%)	73 63
6	F	78/81 (96%)	78 (100%)	0	100 100
6	S	78/81 (96%)	76 (97%)	2 (3%)	46 28
7	G	63/69 (91%)	59 (94%)	4 (6%)	18 5
7	T	63/69 (91%)	59 (94%)	4 (6%)	18 5
8	H	67/75 (89%)	65 (97%)	2 (3%)	41 22
8	U	67/75 (89%)	64 (96%)	3 (4%)	27 10
9	I	55/58 (95%)	53 (96%)	2 (4%)	35 16
9	V	55/58 (95%)	52 (94%)	3 (6%)	21 7
10	J	47/50 (94%)	47 (100%)	0	100 100
10	W	47/50 (94%)	45 (96%)	2 (4%)	29 11
11	K	39/46 (85%)	38 (97%)	1 (3%)	46 28
11	X	39/46 (85%)	38 (97%)	1 (3%)	46 28
12	L	37/40 (92%)	37 (100%)	0	100 100
12	Y	37/40 (92%)	37 (100%)	0	100 100
13	M	34/38 (90%)	32 (94%)	2 (6%)	19 6
13	Z	34/38 (90%)	32 (94%)	2 (6%)	19 6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3042/3086 (99%)	2980 (98%)	62 (2%)	53 38

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	109	PHE
1	A	138	HIS
1	A	338	MET
1	A	369	ASP
2	B	33	LEU
2	B	59	GLN
2	B	60	GLU
2	B	65	TRP
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
2	B	115	ASP
2	B	171	LYS
3	C	159	MET
3	C	214	PHE
3	C	230	ASN
7	G	33	LEU
7	G	36	TRP
7	G	37	LEU
7	G	54	ARG
8	H	60	TYR
8	H	61	LYS
9	I	36	LYS
9	I	43	ARG
11	K	54	ARG
13	M	38	ASP
13	M	40	TYR
1	N	38	ARG
1	N	109	PHE
1	N	363	LEU
1	N	369	ASP
1	N	382	SER
2	O	33	LEU
2	O	60	GLU
2	O	78	LEU
2	O	91	ASN

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Mol	Chain	Res	Type
2	O	115	ASP
2	O	171	LYS
3	P	159	MET
3	P	214	PHE
3	P	230	ASN
4	Q	20	ARG
4	Q	51	LEU
5	R	79	LYS
6	S	37	LYS
6	S	54	ASN
7	T	18	PHE
7	T	36	TRP
7	T	37	LEU
7	T	54	ARG
8	U	46	LYS
8	U	60	TYR
8	U	61	LYS
9	V	8	GLN
9	V	61	GLU
9	V	70	GLN
10	W	7	GLU
10	W	50	LEU
11	X	54	ARG
13	Z	13	LYS
13	Z	40	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	10	GLN
2	B	52	HIS
2	B	59	GLN
2	B	195	GLN
3	C	38	ASN
3	C	50	ASN
4	D	109	HIS
4	D	143	ASN
5	E	94	ASN
6	F	54	ASN
8	H	22	ASN
8	H	37	HIS
10	J	29	ASN

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Mol	Chain	Res	Type
2	O	10	GLN
2	O	59	GLN
2	O	92	ASN
3	P	50	ASN
4	Q	101	HIS
4	Q	109	HIS
5	R	94	ASN
6	S	54	ASN
8	U	22	ASN
9	V	8	GLN
10	W	29	ASN
13	Z	39	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

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

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

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

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

All (1) bond length outliers are listed below:

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

All (3) bond angle outliers are listed below:

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

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	LFA	P	313	-	14,14,19	0.27	0	13,13,18	0.22	0
20	DMU	Q	201	-	34,34,34	1.31	5 (14%)	45,45,45	1.46	4 (8%)
23	CUA	O	305	2	0,1,1	-	-	-		
19	LFA	C	307	-	10,10,19	0.14	0	9,9,18	0.19	0
21	EDO	P	320	-	3,3,3	0.20	0	2,2,2	0.06	0
20	DMU	C	316	-	6,6,34	0.28	0	5,5,45	0.47	0
20	DMU	M	102	-	7,7,34	0.26	0	6,6,45	0.53	0
20	DMU	C	317	-	22,22,34	0.57	0	27,27,45	1.26	4 (14%)
18	PER	N	608	15,14	0,1,1	-	-	-		
21	EDO	T	104	-	3,3,3	0.18	0	2,2,2	0.23	0
14	HEA	A	602	18,1	57,67,67	1.50	10 (17%)	61,103,103	2.45	24 (39%)
18	PER	A	606	15,14	0,1,1	-	-	-		
20	DMU	P	307	-	10,10,34	0.33	0	9,9,45	0.55	0
21	EDO	C	321	-	3,3,3	0.30	0	2,2,2	0.44	0
21	EDO	O	309	-	3,3,3	0.44	0	2,2,2	0.30	0
20	DMU	A	617	-	10,10,34	0.25	0	9,9,45	0.56	0
20	DMU	P	317	-	22,22,34	0.92	1 (4%)	27,27,45	1.32	2 (7%)
19	LFA	T	102	-	13,13,19	0.23	0	12,12,18	0.13	0
20	DMU	C	323	-	22,22,34	0.67	1 (4%)	27,27,45	1.02	2 (7%)
28	PEK	G	101	-	52,52,52	0.56	1 (1%)	55,57,57	0.61	0
19	LFA	P	309	-	5,5,19	0.17	0	4,4,18	0.07	0
21	EDO	R	203	-	3,3,3	0.26	0	2,2,2	0.61	0
20	DMU	O	307	-	10,10,34	0.50	0	9,9,45	0.44	0
24	CHD	C	301	-	32,32,32	0.85	1 (3%)	51,51,51	0.72	0
26	CDL	C	304	-	86,86,99	0.53	0	92,98,111	1.11	8 (8%)
21	EDO	N	616	-	3,3,3	0.21	0	2,2,2	0.10	0
21	EDO	A	612	-	3,3,3	0.07	0	2,2,2	0.13	0
21	EDO	C	322	-	3,3,3	0.81	0	2,2,2	0.70	0
21	EDO	N	617	-	3,3,3	0.38	0	2,2,2	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	DMU	Z	102	-	7,7,34	0.26	0	6,6,45	0.45	0
21	EDO	N	613	-	3,3,3	0.17	0	2,2,2	0.13	0
14	HEA	N	603[A]	-	57,67,67	1.74	12 (21%)	61,103,103	2.46	23 (37%)
19	LFA	P	312	-	10,10,19	0.20	0	9,9,18	0.30	0
24	CHD	P	302	-	32,32,32	0.75	1 (3%)	51,51,51	0.85	0
24	CHD	O	301	-	32,32,32	0.72	0	51,51,51	0.77	0
21	EDO	E	201	-	3,3,3	0.07	0	2,2,2	0.21	0
14	HEA	N	603[B]	-	57,67,67	1.75	12 (21%)	61,103,103	2.38	22 (36%)
21	EDO	E	203	-	3,3,3	0.44	0	2,2,2	0.43	0
20	DMU	L	102	-	22,22,34	0.73	1 (4%)	27,27,45	1.21	4 (14%)
20	DMU	P	316	-	6,6,34	0.29	0	5,5,45	0.47	0
20	DMU	P	318	-	34,34,34	0.93	3 (8%)	45,45,45	1.15	3 (6%)
21	EDO	S	103	-	3,3,3	0.14	0	2,2,2	0.05	0
21	EDO	G	102	-	3,3,3	0.27	0	2,2,2	0.20	0
20	DMU	O	303	-	22,22,34	0.74	0	27,27,45	1.44	3 (11%)
20	DMU	P	324	-	34,34,34	0.68	0	45,45,45	1.54	4 (8%)
22	PGV	A	616	-	50,50,50	0.69	0	53,56,56	1.19	4 (7%)
24	CHD	P	306	-	32,32,32	0.79	1 (3%)	51,51,51	1.31	5 (9%)
20	DMU	B	303	-	22,22,34	0.90	1 (4%)	27,27,45	0.86	1 (3%)
20	DMU	N	602	-	10,10,34	0.28	0	9,9,45	0.52	0
19	LFA	B	306	-	16,16,19	0.34	0	15,15,18	0.17	0
28	PEK	T	101	-	52,52,52	0.61	2 (3%)	55,57,57	1.00	3 (5%)
20	DMU	C	324	-	34,34,34	0.84	1 (2%)	45,45,45	1.15	3 (6%)
26	CDL	L	101	-	93,93,99	0.42	0	99,105,111	0.62	2 (2%)
19	LFA	C	314	-	12,12,19	0.30	0	11,11,18	0.25	0
21	EDO	N	614	-	3,3,3	0.20	0	2,2,2	0.40	0
19	LFA	C	309	20	17,17,19	0.22	0	16,16,18	0.19	0
20	DMU	B	307	-	22,22,34	0.49	0	27,27,45	1.23	2 (7%)
14	HEA	N	604	18,1	57,67,67	1.63	9 (15%)	61,103,103	2.35	23 (37%)
19	LFA	N	601	-	16,16,19	0.28	0	15,15,18	0.21	0
21	EDO	R	202	-	3,3,3	0.20	0	2,2,2	0.36	0
21	EDO	S	102	-	3,3,3	0.39	0	2,2,2	0.30	0
19	LFA	C	313	-	14,14,19	0.27	0	13,13,18	0.41	0
26	CDL	Y	101	-	93,93,99	0.33	0	99,105,111	0.43	1 (1%)
19	LFA	C	311	-	13,13,19	0.23	0	12,12,18	0.12	0
20	DMU	A	609	-	6,6,34	0.59	0	5,5,45	0.29	0
19	LFA	P	310	20	17,17,19	0.19	0	16,16,18	0.16	0
20	DMU	C	306	-	10,10,34	0.42	0	9,9,45	0.58	0
20	DMU	M	101	-	34,34,34	0.85	1 (2%)	45,45,45	1.14	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	DMU	A	610	-	34,34,34	1.27	6 (17%)	45,45,45	1.18	5 (11%)
26	CDL	O	304	-	63,63,99	0.40	0	69,75,111	0.70	1 (1%)
20	DMU	W	101	-	10,10,34	0.29	0	9,9,45	0.56	0
21	EDO	P	321	-	3,3,3	0.19	0	2,2,2	0.17	0
21	EDO	B	304	-	3,3,3	0.40	0	2,2,2	0.21	0
21	EDO	F	103	-	3,3,3	0.20	0	2,2,2	0.36	0
22	PGV	P	304	-	50,50,50	0.76	1 (2%)	53,56,56	0.94	3 (5%)
23	CUA	B	301	2	0,1,1	-	-	-		
20	DMU	C	318	-	34,34,34	0.89	2 (5%)	45,45,45	1.24	2 (4%)
24	CHD	C	305	-	32,32,32	0.69	1 (3%)	51,51,51	1.57	9 (17%)
20	DMU	P	319	-	34,34,34	0.79	2 (5%)	45,45,45	1.20	3 (6%)
20	DMU	A	615	-	10,10,34	0.29	0	9,9,45	0.53	0
20	DMU	P	315	-	34,34,34	0.82	2 (5%)	45,45,45	1.33	3 (6%)
19	LFA	P	308	-	10,10,19	0.22	0	9,9,18	0.26	0
21	EDO	A	614	-	3,3,3	0.30	0	2,2,2	0.17	0
21	EDO	F	102	-	3,3,3	0.19	0	2,2,2	0.04	0
20	DMU	O	306	-	10,10,34	0.14	0	9,9,45	0.63	0
20	DMU	O	308	-	22,22,34	0.68	0	27,27,45	1.08	2 (7%)
19	LFA	C	325	-	14,14,19	0.14	0	13,13,18	0.10	0
20	DMU	C	319	-	34,34,34	0.85	1 (2%)	45,45,45	1.29	5 (11%)
20	DMU	J	101	-	10,10,34	0.21	0	9,9,45	0.58	0
19	LFA	C	308	-	5,5,19	0.19	0	4,4,18	0.05	0
19	LFA	N	610	-	13,13,19	0.55	0	12,12,18	0.38	0
19	LFA	P	314	-	12,12,19	0.31	0	11,11,18	0.25	0
21	EDO	P	322	-	3,3,3	0.38	0	2,2,2	0.78	0
20	DMU	D	201	-	34,34,34	1.48	8 (23%)	45,45,45	1.51	5 (11%)
21	EDO	R	201	-	3,3,3	0.17	0	2,2,2	0.13	0
19	LFA	N	609	-	13,13,19	0.35	0	12,12,18	0.40	0
20	DMU	N	611	-	6,6,34	0.35	0	5,5,45	0.36	0
19	LFA	C	310	-	10,10,19	0.13	0	9,9,18	0.10	0
20	DMU	N	619	19	34,34,34	0.83	1 (2%)	45,45,45	1.31	6 (13%)
19	LFA	O	302	-	10,10,19	0.23	0	9,9,18	0.15	0
19	LFA	A	608	-	13,13,19	0.64	0	12,12,18	0.54	0
19	LFA	P	301	-	14,14,19	0.23	0	13,13,18	0.16	0
26	CDL	I	101	-	63,63,99	0.46	0	69,75,111	1.02	4 (5%)
20	DMU	P	323	-	22,22,34	0.76	0	27,27,45	1.46	1 (3%)
21	EDO	C	320	-	3,3,3	0.06	0	2,2,2	0.10	0
19	LFA	A	607	-	13,13,19	0.36	0	12,12,18	0.25	0
20	DMU	C	315	-	34,34,34	1.00	1 (2%)	45,45,45	1.64	10 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	HEA	A	601[A]	-	57,67,67	1.75	11 (19%)	61,103,103	2.61	23 (37%)
20	DMU	Y	102	-	22,22,34	0.57	0	27,27,45	1.00	1 (3%)
19	LFA	C	312	-	10,10,19	0.23	0	9,9,18	0.17	0
20	DMU	B	302	-	10,10,34	0.21	0	9,9,45	0.58	0
22	PGV	C	303	-	50,50,50	0.77	2 (4%)	53,56,56	1.06	3 (5%)
26	CDL	P	305	-	86,86,99	0.48	0	92,98,111	0.83	5 (5%)
22	PGV	N	618	-	50,50,50	0.76	1 (2%)	53,56,56	1.21	3 (5%)
19	LFA	T	103	-	10,10,19	0.23	0	9,9,18	0.13	0
20	DMU	H	101	19	34,34,34	0.91	2 (5%)	45,45,45	1.10	3 (6%)
20	DMU	Z	101	-	34,34,34	1.00	3 (8%)	45,45,45	0.97	3 (6%)
14	HEA	A	601[B]	-	57,67,67	1.76	11 (19%)	61,103,103	2.59	24 (39%)
19	LFA	P	311	-	10,10,19	0.16	0	9,9,18	0.09	0
20	DMU	N	612	-	34,34,34	1.32	4 (11%)	45,45,45	1.00	3 (6%)
21	EDO	A	613	-	3,3,3	0.38	0	2,2,2	0.19	0
24	CHD	B	305	-	32,32,32	0.65	0	51,51,51	0.90	1 (1%)
21	EDO	E	202	-	3,3,3	0.17	0	2,2,2	0.12	0
21	EDO	A	611	-	3,3,3	0.33	0	2,2,2	0.54	0
21	EDO	N	615	-	3,3,3	0.46	0	2,2,2	0.41	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	LFA	P	313	-	-	5/12/12/17	-
20	DMU	Q	201	-	-	8/19/59/59	0/2/2/2
19	LFA	C	307	-	-	7/8/8/17	-
21	EDO	P	320	-	-	1/1/1/1	-
20	DMU	C	316	-	-	3/4/4/59	-
20	DMU	M	102	-	-	5/5/5/59	-
20	DMU	C	317	-	-	7/13/33/59	0/1/1/2
21	EDO	T	104	-	-	0/1/1/1	-
14	HEA	A	602	18,1	-	4/32/76/76	-
20	DMU	P	307	-	-	2/8/8/59	-
21	EDO	C	321	-	-	0/1/1/1	-
21	EDO	O	309	-	-	0/1/1/1	-
20	DMU	A	617	-	-	6/8/8/59	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	DMU	P	317	-	-	8/13/33/59	0/1/1/2
19	LFA	T	102	-	-	6/11/11/17	-
20	DMU	C	323	-	-	10/13/33/59	0/1/1/2
28	PEK	G	101	-	-	15/56/56/56	-
19	LFA	P	309	-	-	1/3/3/17	-
21	EDO	R	203	-	-	1/1/1/1	-
20	DMU	O	307	-	-	5/8/8/59	-
24	CHD	C	301	-	-	2/9/74/74	0/4/4/4
26	CDL	C	304	-	-	41/97/97/110	-
21	EDO	N	616	-	-	0/1/1/1	-
21	EDO	A	612	-	-	1/1/1/1	-
21	EDO	C	322	-	-	0/1/1/1	-
21	EDO	N	617	-	-	0/1/1/1	-
20	DMU	Z	102	-	-	2/5/5/59	-
21	EDO	N	613	-	-	0/1/1/1	-
14	HEA	N	603[A]	-	-	6/32/76/76	-
19	LFA	P	312	-	-	5/8/8/17	-
24	CHD	P	302	-	-	2/9/74/74	0/4/4/4
24	CHD	O	301	-	-	2/9/74/74	0/4/4/4
21	EDO	E	201	-	-	0/1/1/1	-
14	HEA	N	603[B]	-	-	2/32/76/76	-
21	EDO	E	203	-	-	1/1/1/1	-
20	DMU	L	102	-	-	11/13/33/59	0/1/1/2
20	DMU	P	316	-	-	3/4/4/59	-
20	DMU	P	318	-	-	15/19/59/59	0/2/2/2
21	EDO	S	103	-	-	0/1/1/1	-
21	EDO	G	102	-	-	0/1/1/1	-
20	DMU	O	303	-	-	7/13/33/59	0/1/1/2
20	DMU	P	324	-	-	7/19/59/59	0/2/2/2
22	PGV	A	616	-	-	10/55/55/55	-
24	CHD	P	306	-	-	9/9/74/74	0/4/4/4
20	DMU	B	303	-	-	7/13/33/59	0/1/1/2
20	DMU	N	602	-	-	4/8/8/59	-
19	LFA	B	306	-	-	11/14/14/17	-
28	PEK	T	101	-	-	21/56/56/56	-
20	DMU	C	324	-	-	4/19/59/59	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CDL	L	101	-	-	56/104/104/110	-
19	LFA	C	314	-	-	5/10/10/17	-
21	EDO	N	614	-	-	1/1/1/1	-
19	LFA	C	309	20	-	9/15/15/17	-
20	DMU	B	307	-	-	9/13/33/59	0/1/1/2
14	HEA	N	604	18,1	-	4/32/76/76	-
19	LFA	N	601	-	-	10/14/14/17	-
21	EDO	R	202	-	-	0/1/1/1	-
21	EDO	S	102	-	-	0/1/1/1	-
19	LFA	C	313	-	-	4/12/12/17	-
26	CDL	Y	101	-	-	55/104/104/110	-
19	LFA	C	311	-	-	5/11/11/17	-
20	DMU	A	609	-	-	3/4/4/59	-
19	LFA	P	310	20	-	6/15/15/17	-
20	DMU	C	306	-	-	3/8/8/59	-
20	DMU	M	101	-	-	3/19/59/59	0/2/2/2
20	DMU	A	610	-	-	7/19/59/59	0/2/2/2
26	CDL	O	304	-	-	41/74/74/110	-
20	DMU	W	101	-	-	5/8/8/59	-
21	EDO	P	321	-	-	1/1/1/1	-
21	EDO	B	304	-	-	0/1/1/1	-
21	EDO	F	103	-	-	1/1/1/1	-
22	PGV	P	304	-	-	11/55/55/55	-
20	DMU	C	318	-	-	13/19/59/59	0/2/2/2
24	CHD	C	305	-	-	8/9/74/74	0/4/4/4
20	DMU	P	319	-	-	9/19/59/59	0/2/2/2
20	DMU	A	615	-	-	6/8/8/59	-
20	DMU	P	315	-	-	5/19/59/59	0/2/2/2
19	LFA	P	308	-	-	4/8/8/17	-
21	EDO	A	614	-	-	1/1/1/1	-
21	EDO	F	102	-	-	0/1/1/1	-
20	DMU	O	306	-	-	5/8/8/59	-
20	DMU	O	308	-	-	5/13/33/59	0/1/1/2
19	LFA	C	325	-	-	7/12/12/17	-
20	DMU	C	319	-	-	10/19/59/59	0/2/2/2
20	DMU	J	101	-	-	6/8/8/59	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	LFA	C	308	-	-	1/3/3/17	-
19	LFA	N	610	-	-	7/11/11/17	-
19	LFA	P	314	-	-	3/10/10/17	-
21	EDO	P	322	-	-	0/1/1/1	-
20	DMU	D	201	-	-	7/19/59/59	0/2/2/2
21	EDO	R	201	-	-	1/1/1/1	-
19	LFA	N	609	-	-	4/11/11/17	-
20	DMU	N	611	-	-	2/4/4/59	-
19	LFA	C	310	-	-	8/8/8/17	-
20	DMU	N	619	19	-	5/19/59/59	0/2/2/2
19	LFA	O	302	-	-	3/8/8/17	-
19	LFA	A	608	-	-	5/11/11/17	-
19	LFA	P	301	-	-	7/12/12/17	-
26	CDL	I	101	-	-	43/74/74/110	-
20	DMU	P	323	-	-	6/13/33/59	0/1/1/2
21	EDO	C	320	-	-	0/1/1/1	-
19	LFA	A	607	-	-	3/11/11/17	-
20	DMU	C	315	-	-	11/19/59/59	0/2/2/2
14	HEA	A	601[A]	-	-	6/32/76/76	-
20	DMU	Y	102	-	-	9/13/33/59	0/1/1/2
19	LFA	C	312	-	-	4/8/8/17	-
20	DMU	B	302	-	-	5/8/8/59	-
22	PGV	C	303	-	-	14/55/55/55	-
26	CDL	P	305	-	-	46/97/97/110	-
22	PGV	N	618	-	-	8/55/55/55	-
19	LFA	T	103	-	-	3/8/8/17	-
20	DMU	H	101	19	-	5/19/59/59	0/2/2/2
20	DMU	Z	101	-	-	6/19/59/59	0/2/2/2
14	HEA	A	601[B]	-	-	2/32/76/76	-
19	LFA	P	311	-	-	5/8/8/17	-
20	DMU	N	612	-	-	5/19/59/59	0/2/2/2
21	EDO	A	613	-	-	0/1/1/1	-
24	CHD	B	305	-	-	2/9/74/74	0/4/4/4
21	EDO	E	202	-	-	0/1/1/1	-
21	EDO	A	611	-	-	0/1/1/1	-
21	EDO	N	615	-	-	0/1/1/1	-

All (122) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	603[A]	HEA	C1D-ND	-5.11	1.31	1.40
14	N	603[B]	HEA	C1D-ND	-5.11	1.31	1.40
20	N	612	DMU	O16-C6	-4.74	1.32	1.40
14	N	603[A]	HEA	C3B-C2B	4.58	1.45	1.34
14	N	603[B]	HEA	C3B-C2B	4.58	1.45	1.34
14	A	602	HEA	CHD-C1D	4.48	1.46	1.35
14	N	604	HEA	C3B-C2B	4.42	1.44	1.34
14	A	601[A]	HEA	C1D-ND	-4.35	1.32	1.40
14	A	601[B]	HEA	C1D-ND	-4.35	1.32	1.40
14	A	601[A]	HEA	CHD-C1D	4.24	1.45	1.35
14	A	601[B]	HEA	CHD-C1D	4.24	1.45	1.35
14	A	601[A]	HEA	C16-C17	-4.19	1.39	1.53
14	A	601[B]	HEA	C16-C17	-4.19	1.39	1.53
14	N	603[A]	HEA	CHD-C1D	4.19	1.45	1.35
14	N	603[B]	HEA	CHD-C1D	4.19	1.45	1.35
14	N	604	HEA	C3D-C2D	4.12	1.45	1.36
14	A	601[A]	HEA	C3B-C2B	4.07	1.43	1.34
14	A	601[B]	HEA	C3B-C2B	4.07	1.43	1.34
14	N	604	HEA	CHD-C1D	4.04	1.45	1.35
14	A	601[A]	HEA	C3D-C2D	3.90	1.45	1.36
14	A	601[B]	HEA	C3D-C2D	3.90	1.45	1.36
14	N	604	HEA	C1D-ND	-3.90	1.33	1.40
20	Q	201	DMU	O3-C5	-3.76	1.34	1.43
14	N	604	HEA	C3A-C2A	3.73	1.45	1.40
20	P	317	DMU	O16-C6	3.72	1.46	1.40
14	N	603[A]	HEA	CHC-C4B	3.61	1.44	1.35
14	N	603[B]	HEA	CHC-C4B	3.61	1.44	1.35
14	A	602	HEA	CHC-C4B	3.58	1.44	1.35
14	A	601[A]	HEA	C1B-NB	-3.55	1.31	1.38
14	A	601[B]	HEA	C1B-NB	-3.55	1.31	1.38
14	A	601[A]	HEA	CHC-C4B	3.52	1.44	1.35
14	A	601[B]	HEA	CHC-C4B	3.52	1.44	1.35
14	A	602	HEA	C3B-C2B	3.45	1.42	1.34
20	D	201	DMU	O61-C57	3.38	1.56	1.42
14	N	603[A]	HEA	C3D-C2D	3.34	1.43	1.36
14	N	603[B]	HEA	C3D-C2D	3.34	1.43	1.36
20	Q	201	DMU	C10-C5	-3.22	1.43	1.52
20	C	315	DMU	C7-C5	-3.22	1.44	1.52
14	N	604	HEA	CHC-C4B	3.20	1.43	1.35
20	A	610	DMU	O3-C5	-3.16	1.35	1.43
20	Z	101	DMU	O3-C5	-3.12	1.35	1.43
14	N	603[A]	HEA	C1B-NB	-3.04	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	603[B]	HEA	C1B-NB	-3.04	1.32	1.38
14	N	604	HEA	C2A-C1A	3.04	1.49	1.42
14	A	601[A]	HEA	C3A-C2A	3.00	1.44	1.40
14	A	601[B]	HEA	C3A-C2A	3.00	1.44	1.40
20	D	201	DMU	O5-C6	-2.94	1.34	1.41
28	G	101	PEK	C23-C22	-2.90	1.41	1.52
20	D	201	DMU	O3-C5	-2.87	1.36	1.43
20	N	612	DMU	C10-C5	-2.83	1.44	1.52
14	A	602	HEA	C3D-C2D	2.78	1.42	1.36
20	C	318	DMU	O5-C6	-2.77	1.34	1.41
14	N	603[A]	HEA	C2A-C1A	2.75	1.48	1.42
14	N	603[B]	HEA	C2A-C1A	2.75	1.48	1.42
14	N	603[A]	HEA	C16-C17	-2.74	1.44	1.53
14	N	603[B]	HEA	C16-C17	-2.74	1.44	1.53
14	A	602	HEA	C1D-ND	-2.72	1.35	1.40
22	P	304	PGV	O03-C19	2.71	1.41	1.33
22	C	303	PGV	O01-C1	2.65	1.41	1.34
20	P	319	DMU	C10-C5	-2.64	1.44	1.52
20	N	619	DMU	C6-C1	-2.63	1.44	1.52
14	A	601[A]	HEA	C2A-C1A	2.59	1.48	1.42
14	A	601[B]	HEA	C2A-C1A	2.59	1.48	1.42
14	A	602	HEA	C1B-NB	-2.57	1.33	1.38
22	N	618	PGV	O03-C19	2.56	1.40	1.33
28	T	101	PEK	C2-C1	2.55	1.58	1.50
20	N	612	DMU	C7-C5	-2.54	1.45	1.52
24	C	301	CHD	O26-C24	-2.53	1.22	1.30
14	A	602	HEA	C2A-C1A	2.52	1.48	1.42
20	P	318	DMU	O5-C6	-2.52	1.35	1.41
20	A	610	DMU	C10-C5	-2.51	1.45	1.52
20	C	319	DMU	O55-C2	-2.50	1.37	1.43
20	N	612	DMU	O3-C5	-2.49	1.37	1.43
14	N	603[A]	HEA	C3A-C2A	2.49	1.43	1.40
14	N	603[B]	HEA	C3A-C2A	2.49	1.43	1.40
14	A	602	HEA	C4D-ND	-2.45	1.33	1.38
24	C	305	CHD	O26-C24	-2.42	1.22	1.30
20	A	610	DMU	O7-C10	2.41	1.48	1.41
20	Q	201	DMU	O5-C6	-2.41	1.35	1.41
20	M	101	DMU	O3-C5	-2.36	1.37	1.43
22	C	303	PGV	O03-C19	2.35	1.40	1.33
20	C	318	DMU	C7-C5	-2.33	1.46	1.52
20	P	319	DMU	C7-C5	-2.32	1.46	1.52
20	P	318	DMU	C7-C5	-2.31	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	610	DMU	O55-C2	2.30	1.48	1.43
20	P	318	DMU	O3-C5	2.30	1.48	1.43
14	N	604	HEA	CMC-C2C	-2.28	1.46	1.51
20	D	201	DMU	O49-C1	-2.28	1.37	1.43
28	T	101	PEK	C23-C22	-2.27	1.43	1.52
20	A	610	DMU	O4-C7	-2.27	1.37	1.43
20	P	315	DMU	C7-C5	-2.26	1.46	1.52
14	N	603[A]	HEA	C12-C11	-2.25	1.48	1.52
14	N	603[B]	HEA	C12-C11	-2.25	1.48	1.52
20	P	315	DMU	O3-C5	-2.24	1.37	1.43
14	A	602	HEA	C4B-NB	-2.22	1.36	1.40
20	D	201	DMU	O5-C4	-2.21	1.39	1.44
20	C	324	DMU	C7-C5	-2.21	1.46	1.52
24	P	306	CHD	O26-C24	-2.20	1.23	1.30
14	A	601[A]	HEA	CBD-CGD	2.18	1.55	1.50
14	A	601[B]	HEA	CBD-CGD	2.18	1.55	1.50
20	D	201	DMU	O55-C2	2.17	1.48	1.43
24	P	302	CHD	O26-C24	-2.17	1.23	1.30
14	N	603[A]	HEA	CBA-CGA	2.15	1.55	1.50
14	N	603[B]	HEA	CBA-CGA	2.15	1.55	1.50
14	N	603[A]	HEA	C4B-NB	-2.15	1.36	1.40
14	N	603[B]	HEA	C4B-NB	-2.15	1.36	1.40
20	D	201	DMU	O1-C10	2.15	1.47	1.41
20	Q	201	DMU	O49-C1	-2.14	1.37	1.43
20	B	303	DMU	O16-C6	2.14	1.43	1.40
20	Q	201	DMU	C7-C5	-2.13	1.46	1.52
14	N	604	HEA	C4B-NB	-2.10	1.36	1.40
20	L	102	DMU	O16-C6	2.10	1.43	1.40
20	A	610	DMU	O16-C6	-2.09	1.36	1.40
20	D	201	DMU	C3-C4	2.08	1.58	1.52
20	H	101	DMU	O16-C6	-2.06	1.36	1.40
20	Z	101	DMU	O16-C6	-2.06	1.36	1.40
20	H	101	DMU	O5-C6	-2.05	1.36	1.41
20	C	323	DMU	C6-C1	-2.05	1.46	1.52
20	Z	101	DMU	C10-C5	-2.03	1.46	1.52
14	A	601[A]	HEA	O1D-CGD	2.02	1.28	1.22
14	A	601[B]	HEA	O1D-CGD	2.02	1.28	1.22
14	A	602	HEA	CMC-C2C	-2.01	1.47	1.51

All (278) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	601[A]	HEA	C3D-C4D-ND	8.02	118.13	110.36
14	A	601[B]	HEA	C3D-C4D-ND	8.02	118.13	110.36
14	N	603[A]	HEA	C3D-C4D-ND	7.32	117.44	110.36
14	N	603[B]	HEA	C3D-C4D-ND	7.32	117.44	110.36
14	A	602	HEA	C2B-C1B-NB	6.62	117.81	109.88
20	D	201	DMU	O16-C6-C1	5.87	117.47	108.30
20	P	323	DMU	O16-C6-C1	5.84	117.42	108.30
14	A	601[A]	HEA	C2B-C1B-NB	5.72	116.74	109.88
14	A	601[B]	HEA	C2B-C1B-NB	5.72	116.74	109.88
14	N	604	HEA	C2D-C1D-ND	5.68	116.57	109.84
20	Q	201	DMU	O16-C6-C1	5.66	117.14	108.30
14	N	604	HEA	C3D-C4D-ND	5.60	115.78	110.36
14	N	603[A]	HEA	C2D-C1D-ND	5.48	116.33	109.84
14	N	603[B]	HEA	C2D-C1D-ND	5.48	116.33	109.84
20	P	315	DMU	O16-C6-C1	5.46	116.83	108.30
14	N	603[A]	HEA	C2B-C1B-NB	5.45	116.42	109.88
14	N	603[B]	HEA	C2B-C1B-NB	5.45	116.42	109.88
24	C	305	CHD	C17-C13-C12	-5.28	112.84	117.67
20	C	315	DMU	O16-C6-C1	5.18	116.39	108.30
20	P	324	DMU	O16-C6-C1	5.13	116.31	108.30
14	A	601[A]	HEA	C27-C19-C20	5.06	123.79	115.27
14	N	604	HEA	C3B-C4B-NB	5.05	115.82	109.84
14	A	601[A]	HEA	C3C-C4C-NC	4.99	115.66	109.21
14	A	601[B]	HEA	C3C-C4C-NC	4.99	115.66	109.21
14	N	604	HEA	C2B-C1B-NB	4.98	115.85	109.88
14	A	602	HEA	C3B-C4B-NB	4.94	115.69	109.84
14	A	602	HEA	C3D-C4D-ND	4.92	115.12	110.36
20	P	324	DMU	C10-C5-C7	4.91	120.22	110.00
24	C	305	CHD	C16-C17-C20	4.89	119.72	112.15
14	A	601[A]	HEA	C13-C12-C11	-4.88	107.02	114.35
14	A	601[B]	HEA	C13-C12-C11	-4.88	107.02	114.35
22	N	618	PGV	O03-C19-O04	-4.82	111.43	123.59
14	A	601[A]	HEA	CHA-C4D-C3D	-4.78	117.81	124.84
14	A	601[B]	HEA	CHA-C4D-C3D	-4.78	117.81	124.84
20	C	324	DMU	O16-C6-C1	4.76	115.73	108.30
14	N	603[A]	HEA	C27-C19-C20	4.75	123.25	115.27
14	A	602	HEA	C13-C12-C11	-4.70	107.29	114.35
20	P	319	DMU	O16-C6-C1	4.66	115.58	108.30
14	A	601[A]	HEA	CHB-C1B-C2B	-4.60	117.79	124.98
14	A	601[B]	HEA	CHB-C1B-C2B	-4.60	117.79	124.98
14	A	601[A]	HEA	C2D-C1D-ND	4.59	115.28	109.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	601[B]	HEA	C2D-C1D-ND	4.59	115.28	109.84
26	C	304	CDL	OA5-PA1-OA3	4.56	126.89	109.07
14	N	603[A]	HEA	CHB-C1B-C2B	-4.47	117.99	124.98
14	N	603[B]	HEA	CHB-C1B-C2B	-4.47	117.99	124.98
22	A	616	PGV	O03-C19-O04	-4.46	112.33	123.59
14	A	601[A]	HEA	C3B-C4B-NB	4.44	115.10	109.84
14	A	601[B]	HEA	C3B-C4B-NB	4.44	115.10	109.84
20	P	317	DMU	O5-C6-C1	4.43	119.73	110.35
26	I	101	CDL	CA4-OA6-CA5	4.41	128.66	117.79
14	N	604	HEA	C1D-C2D-C3D	-4.37	102.36	106.96
14	A	602	HEA	C4B-NB-C1B	-4.35	100.58	105.07
20	C	318	DMU	O16-C6-C1	4.33	115.07	108.30
20	O	303	DMU	O5-C6-C1	4.26	119.36	110.35
14	A	601[A]	HEA	C4D-C3D-C2D	-4.25	100.70	106.90
14	A	601[B]	HEA	C4D-C3D-C2D	-4.25	100.70	106.90
14	N	603[A]	HEA	C3C-C4C-NC	4.24	114.70	109.21
14	N	603[B]	HEA	C3C-C4C-NC	4.24	114.70	109.21
14	A	602	HEA	C2D-C1D-ND	4.22	114.84	109.84
26	C	304	CDL	OA4-PA1-OA5	-4.21	88.21	107.75
14	A	602	HEA	CHB-C1B-C2B	-4.18	118.44	124.98
14	N	603[A]	HEA	C3B-C4B-NB	4.15	114.75	109.84
14	N	603[B]	HEA	C3B-C4B-NB	4.15	114.75	109.84
14	A	602	HEA	CMD-C2D-C1D	4.03	131.18	125.04
28	T	101	PEK	O01-C1-O02	-4.00	114.03	123.70
20	C	318	DMU	C10-C5-C7	4.00	118.32	110.00
20	C	317	DMU	O5-C6-C1	3.96	118.73	110.35
20	N	619	DMU	C10-C5-C7	3.96	118.24	110.00
14	N	603[A]	HEA	C4D-C3D-C2D	-3.93	101.16	106.90
14	N	603[B]	HEA	C4D-C3D-C2D	-3.93	101.16	106.90
24	P	306	CHD	C22-C23-C24	-3.92	102.12	112.51
20	B	307	DMU	O16-C6-C1	3.91	114.41	108.30
20	M	101	DMU	O16-C6-C1	3.80	114.23	108.30
14	N	604	HEA	CHB-C1B-C2B	-3.79	119.05	124.98
26	C	304	CDL	OA6-CA5-C11	-3.79	103.33	111.50
22	N	618	PGV	O03-C19-C20	3.78	123.78	111.91
14	A	602	HEA	CHA-C4D-C3D	-3.78	119.28	124.84
14	A	602	HEA	CMB-C2B-C1B	3.78	130.79	125.04
14	A	601[B]	HEA	C27-C19-C20	3.74	121.57	115.27
14	A	602	HEA	C27-C19-C20	3.73	121.55	115.27
22	C	303	PGV	O03-C19-O04	-3.72	114.21	123.59
14	N	604	HEA	C3C-C4C-NC	3.71	114.01	109.21
20	C	319	DMU	C10-C5-C7	3.71	117.72	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	P	318	DMU	O16-C6-C1	3.69	114.06	108.30
14	N	604	HEA	CAD-CBD-CGD	-3.69	105.66	113.60
20	O	303	DMU	O16-C6-C1	3.67	114.04	108.30
14	N	603[A]	HEA	C1D-ND-C4D	-3.65	101.30	105.07
14	N	603[B]	HEA	C1D-ND-C4D	-3.65	101.30	105.07
14	A	601[A]	HEA	C1D-ND-C4D	-3.63	101.33	105.07
14	A	601[B]	HEA	C1D-ND-C4D	-3.63	101.33	105.07
14	A	602	HEA	C1B-C2B-C3B	-3.61	102.48	106.80
20	P	318	DMU	C10-C5-C7	3.61	117.51	110.00
14	N	604	HEA	C1B-C2B-C3B	-3.56	102.54	106.80
14	N	603[A]	HEA	C20-C19-C18	-3.55	113.93	121.12
14	N	604	HEA	CMD-C2D-C1D	3.49	130.36	125.04
14	N	604	HEA	CAD-C3D-C4D	3.47	130.72	124.66
20	C	315	DMU	C6-O5-C4	3.45	120.47	113.69
26	I	101	CDL	OA6-CA4-CA3	3.45	120.90	108.40
22	A	616	PGV	O03-C19-C20	3.43	122.67	111.91
20	H	101	DMU	C10-C5-C7	3.42	117.12	110.00
20	C	319	DMU	O16-C6-C1	3.38	113.58	108.30
20	C	323	DMU	O16-C6-C1	3.38	113.58	108.30
14	N	603[A]	HEA	C1D-C2D-C3D	-3.37	103.41	106.96
14	N	603[B]	HEA	C1D-C2D-C3D	-3.37	103.41	106.96
28	T	101	PEK	O02-C1-C2	3.37	136.86	123.73
24	P	306	CHD	C16-C17-C20	3.34	117.32	112.15
20	L	102	DMU	O5-C6-O16	3.33	117.87	109.97
26	P	305	CDL	OA5-PA1-OA3	3.33	122.06	109.07
26	C	304	CDL	OB5-PB2-OB3	3.28	121.90	109.07
14	N	604	HEA	CBA-CAA-C2A	-3.26	107.11	112.60
14	N	604	HEA	C4D-CHA-C1A	3.26	126.86	122.56
14	A	602	HEA	CAD-CBD-CGD	-3.24	106.63	113.60
20	M	101	DMU	C18-O16-C6	-3.23	108.48	113.84
26	O	304	CDL	OA6-CA5-C11	3.20	118.41	111.50
24	C	305	CHD	C14-C13-C12	3.20	110.38	107.40
24	C	305	CHD	C22-C23-C24	-3.19	104.04	112.51
26	I	101	CDL	OA8-CA6-CA4	3.18	117.69	108.43
20	O	303	DMU	C6-C1-C2	3.17	116.61	110.00
24	C	305	CHD	C17-C13-C14	-3.17	96.90	100.09
24	P	306	CHD	C17-C13-C12	-3.16	114.78	117.67
14	N	603[A]	HEA	C13-C12-C11	-3.16	109.61	114.35
14	N	603[B]	HEA	C13-C12-C11	-3.16	109.61	114.35
20	N	619	DMU	O16-C6-C1	3.12	113.17	108.30
14	A	601[A]	HEA	C20-C19-C18	-3.10	114.84	121.12
22	P	304	PGV	C27-C26-C25	-3.10	98.67	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	601[A]	HEA	C1B-C2B-C3B	-3.06	103.14	106.80
14	A	601[B]	HEA	C1B-C2B-C3B	-3.06	103.14	106.80
14	A	601[A]	HEA	C4B-NB-C1B	-3.06	101.91	105.07
14	A	601[B]	HEA	C4B-NB-C1B	-3.06	101.91	105.07
20	C	315	DMU	C10-O1-C9	3.05	119.68	113.69
14	N	603[A]	HEA	CHA-C4D-C3D	-3.04	120.38	124.84
14	N	603[B]	HEA	CHA-C4D-C3D	-3.04	120.38	124.84
14	A	601[A]	HEA	CAD-C3D-C4D	3.02	129.94	124.66
14	A	601[B]	HEA	CAD-C3D-C4D	3.02	129.94	124.66
20	Q	201	DMU	C2-C3-C4	-3.01	104.03	110.93
14	N	604	HEA	C13-C12-C11	-3.01	109.83	114.35
20	C	315	DMU	C18-O16-C6	-3.00	108.87	113.84
24	P	306	CHD	C23-C22-C20	-2.99	109.05	114.52
20	C	315	DMU	O1-C9-C8	2.99	115.13	109.69
14	N	603[A]	HEA	C4D-CHA-C1A	2.98	126.50	122.56
14	N	603[B]	HEA	C4D-CHA-C1A	2.98	126.50	122.56
22	A	616	PGV	C25-C24-C23	2.98	129.54	114.42
20	P	324	DMU	C10-O1-C9	-2.97	107.86	113.69
20	B	307	DMU	O5-C6-C1	2.97	116.63	110.35
14	A	602	HEA	CMC-C2C-C3C	2.96	130.21	124.68
14	N	604	HEA	C4B-NB-C1B	-2.94	102.03	105.07
14	N	604	HEA	CHA-C4D-C3D	-2.93	120.53	124.84
20	Z	101	DMU	O16-C6-C1	2.92	112.86	108.30
14	N	603[A]	HEA	C4B-C3B-C2B	-2.91	102.44	107.41
14	N	603[B]	HEA	C4B-C3B-C2B	-2.91	102.44	107.41
14	A	602	HEA	C1D-C2D-C3D	-2.91	103.90	106.96
20	P	315	DMU	C10-C5-C7	2.91	116.05	110.00
26	L	101	CDL	OB4-PB2-OB2	2.89	121.17	107.75
26	P	305	CDL	OB5-PB2-OB3	2.89	120.35	109.07
20	M	101	DMU	O3-C5-C7	2.85	116.93	110.35
14	A	602	HEA	C3C-C4C-NC	2.83	112.88	109.21
14	N	603[A]	HEA	C1B-C2B-C3B	-2.83	103.42	106.80
14	N	603[B]	HEA	C1B-C2B-C3B	-2.83	103.42	106.80
20	N	619	DMU	O5-C6-O16	2.82	116.65	109.97
20	D	201	DMU	C57-C4-C3	2.81	121.51	113.33
20	Y	102	DMU	O5-C6-O16	2.81	116.62	109.97
20	C	315	DMU	O5-C6-C1	2.81	116.29	110.35
14	N	603[A]	HEA	CAD-C3D-C4D	2.77	129.49	124.66
14	N	603[B]	HEA	CAD-C3D-C4D	2.77	129.49	124.66
14	N	604	HEA	C4D-C3D-C2D	-2.75	102.88	106.90
20	Z	101	DMU	O3-C5-C7	2.75	116.71	110.35
26	I	101	CDL	OA6-CA4-CA6	2.73	118.29	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	N	604	HEA	CMB-C2B-C1B	2.71	129.17	125.04
20	A	610	DMU	C10-C5-C7	2.71	115.63	110.00
20	C	315	DMU	O3-C5-C10	2.69	116.57	110.05
26	L	101	CDL	OB5-PB2-OB3	-2.68	98.60	109.07
20	Q	201	DMU	C6-O5-C4	-2.66	108.48	113.69
20	P	315	DMU	C18-O16-C6	-2.64	109.46	113.84
20	C	315	DMU	O5-C6-O16	-2.63	103.74	109.97
20	D	201	DMU	C2-C3-C4	-2.62	104.92	110.93
14	N	604	HEA	C1D-ND-C4D	-2.61	102.38	105.07
14	A	601[A]	HEA	O11-C11-C12	2.60	116.70	109.42
14	A	601[B]	HEA	O11-C11-C12	2.60	116.70	109.42
20	D	201	DMU	C10-C5-C7	2.60	115.41	110.00
24	C	305	CHD	C6-C7-C8	2.58	114.23	111.48
26	C	304	CDL	OA4-PA1-OA3	2.57	124.97	112.24
20	N	619	DMU	C10-O7-C3	-2.57	111.60	117.96
14	A	602	HEA	C4D-C3D-C2D	-2.57	103.15	106.90
28	T	101	PEK	C2-C3-C4	2.57	117.81	113.23
20	A	610	DMU	O3-C5-C7	2.55	116.24	110.35
20	C	317	DMU	C18-O16-C6	-2.54	109.62	113.84
14	A	601[A]	HEA	C4B-C3B-C2B	-2.52	103.10	107.41
14	A	601[B]	HEA	C4B-C3B-C2B	-2.52	103.10	107.41
14	A	602	HEA	CBA-CAA-C2A	-2.52	108.36	112.60
20	C	319	DMU	O3-C5-C10	2.51	116.15	110.05
20	A	610	DMU	C10-O7-C3	-2.51	111.74	117.96
20	O	308	DMU	O5-C6-C1	2.50	115.64	110.35
20	N	612	DMU	C10-O1-C9	2.50	118.59	113.69
20	H	101	DMU	O3-C5-C10	2.50	116.11	110.05
14	A	601[A]	HEA	CMC-C2C-C3C	2.49	129.34	124.68
14	A	601[B]	HEA	CMC-C2C-C3C	2.49	129.34	124.68
14	A	602	HEA	C20-C19-C18	-2.49	116.09	121.12
20	O	308	DMU	C57-C4-C3	-2.46	107.23	113.00
26	P	305	CDL	OA6-CA5-OA7	-2.45	117.79	123.70
22	C	303	PGV	C23-C22-C21	2.43	126.74	114.42
14	A	601[A]	HEA	CHD-C1D-C2D	-2.42	120.02	126.72
14	A	601[B]	HEA	CHD-C1D-C2D	-2.42	120.02	126.72
14	N	603[B]	HEA	C21-C20-C19	-2.41	105.04	112.98
20	C	319	DMU	O3-C5-C7	2.41	115.92	110.35
20	B	303	DMU	O5-C6-C1	2.40	115.44	110.35
14	N	604	HEA	C20-C19-C18	-2.40	116.26	121.12
14	A	601[B]	HEA	C20-C19-C18	-2.40	116.27	121.12
14	N	603[A]	HEA	CHD-C1D-C2D	-2.39	120.10	126.72
14	N	603[B]	HEA	CHD-C1D-C2D	-2.39	120.10	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	P	317	DMU	C18-O16-C6	-2.38	109.89	113.84
26	C	304	CDL	OB6-CB5-C51	2.38	116.63	111.50
14	A	601[A]	HEA	C1D-C2D-C3D	-2.38	104.45	106.96
14	A	601[B]	HEA	C1D-C2D-C3D	-2.38	104.45	106.96
14	N	603[A]	HEA	C25-C23-C24	2.37	119.84	114.60
14	A	602	HEA	O1D-CGD-CBD	-2.36	115.50	123.08
14	A	602	HEA	C4B-C3B-C2B	-2.36	103.39	107.41
20	L	102	DMU	C3-C2-C1	-2.35	106.72	110.82
14	A	602	HEA	O1A-CGA-CBA	-2.35	115.54	123.08
26	C	304	CDL	OA7-CA5-C11	2.35	132.88	123.73
20	C	315	DMU	C7-C8-C9	2.32	114.39	110.24
26	P	305	CDL	OA4-PA1-OA5	-2.32	96.97	107.75
20	C	317	DMU	C2-C3-C4	-2.29	106.15	110.24
20	P	319	DMU	O3-C5-C7	2.28	115.62	110.35
20	C	315	DMU	C10-C5-C7	2.28	114.74	110.00
20	N	612	DMU	O5-C6-C1	2.28	115.17	110.35
22	P	304	PGV	C22-C21-C20	-2.28	105.01	113.19
14	A	602	HEA	C1D-ND-C4D	-2.26	102.74	105.07
22	C	303	PGV	O14-P-O13	2.24	123.30	112.24
20	A	610	DMU	O5-C6-O16	2.23	115.27	109.97
26	C	304	CDL	OB2-PB2-OB3	-2.21	100.44	109.07
14	A	601[A]	HEA	C4D-CHA-C1A	2.20	125.46	122.56
14	A	601[B]	HEA	C4D-CHA-C1A	2.20	125.46	122.56
20	P	319	DMU	C10-C5-C7	2.19	114.56	110.00
14	N	603[A]	HEA	C4A-CHB-C1B	2.19	125.45	122.56
14	N	603[B]	HEA	C4A-CHB-C1B	2.19	125.45	122.56
14	N	604	HEA	CHD-C1D-ND	-2.19	121.68	124.38
20	N	619	DMU	O3-C5-C10	2.18	115.34	110.05
14	A	601[B]	HEA	C21-C22-C23	-2.18	120.31	127.75
20	L	102	DMU	O5-C6-C1	2.18	114.95	110.35
26	P	305	CDL	OA4-PA1-OA3	2.17	122.96	112.24
20	A	610	DMU	O16-C6-C1	2.17	111.68	108.30
20	N	619	DMU	C57-C4-C3	-2.17	107.02	113.33
20	L	102	DMU	C57-C4-C3	-2.16	107.95	113.00
14	N	604	HEA	C4B-C3B-C2B	-2.15	103.74	107.41
24	C	305	CHD	C18-C13-C17	2.15	114.57	111.21
14	A	601[A]	HEA	CHC-C4B-NB	-2.14	121.73	124.38
14	A	601[B]	HEA	CHC-C4B-NB	-2.14	121.73	124.38
24	C	305	CHD	C15-C14-C8	2.14	121.32	118.33
20	P	318	DMU	C1-C2-C3	2.13	114.55	109.68
14	A	601[A]	HEA	CMD-C2D-C1D	2.12	128.27	125.04
14	A	601[B]	HEA	CMD-C2D-C1D	2.12	128.27	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	P	324	DMU	O7-C10-O1	-2.11	104.77	110.67
14	N	603[A]	HEA	CBA-CAA-C2A	-2.11	109.05	112.60
14	N	603[B]	HEA	CBA-CAA-C2A	-2.11	109.05	112.60
20	Z	101	DMU	O5-C6-C1	2.11	114.81	110.35
14	N	603[B]	HEA	C25-C23-C24	2.11	119.26	114.60
22	P	304	PGV	O03-C19-O04	-2.10	118.29	123.59
24	B	305	CHD	C17-C13-C14	2.09	102.20	100.09
14	N	603[A]	HEA	CHA-C4D-ND	-2.09	122.16	124.43
14	N	603[B]	HEA	CHA-C4D-ND	-2.09	122.16	124.43
20	C	317	DMU	C6-C1-C2	2.09	114.35	110.00
20	C	323	DMU	C18-O16-C6	-2.09	110.38	113.84
20	N	612	DMU	O1-C9-C11	2.09	111.62	106.44
20	C	324	DMU	C10-C5-C7	2.08	114.33	110.00
20	C	319	DMU	O5-C6-C1	2.07	114.73	110.35
20	H	101	DMU	C10-O1-C9	2.06	117.72	113.69
22	A	616	PGV	O01-C1-O02	-2.04	118.76	123.70
24	C	305	CHD	O12-C12-C13	-2.04	107.58	111.03
20	Q	201	DMU	C10-C5-C7	2.04	114.25	110.00
14	N	603[A]	HEA	C4B-NB-C1B	-2.04	102.97	105.07
14	N	603[B]	HEA	C4B-NB-C1B	-2.04	102.97	105.07
22	N	618	PGV	O01-C1-O02	-2.03	118.80	123.70
14	A	602	HEA	OMA-CMA-C3A	-2.03	120.49	124.91
24	P	306	CHD	C18-C13-C14	2.03	114.38	111.21
20	D	201	DMU	O5-C4-C3	-2.02	105.50	109.75
26	Y	101	CDL	OA6-CA5-C11	2.01	115.83	111.50
14	N	604	HEA	C27-C19-C20	2.00	118.64	115.27
20	C	324	DMU	O5-C6-C1	2.00	114.59	110.35

There are no chirality outliers.

All (821) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	601[A]	HEA	C18-C19-C20-C21
14	A	601[A]	HEA	C27-C19-C20-C21
14	N	603[A]	HEA	C18-C19-C20-C21
14	N	603[A]	HEA	C27-C19-C20-C21
20	B	303	DMU	C1-C6-O16-C18
20	B	303	DMU	O5-C6-O16-C18
20	B	307	DMU	C19-C18-O16-C6
20	C	318	DMU	C19-C18-O16-C6
20	C	323	DMU	C19-C18-O16-C6
20	D	201	DMU	C19-C18-O16-C6

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Mol	Chain	Res	Type	Atoms
20	L	102	DMU	C19-C18-O16-C6
20	O	303	DMU	C19-C18-O16-C6
20	O	308	DMU	C19-C18-O16-C6
20	P	323	DMU	C1-C6-O16-C18
20	Q	201	DMU	C19-C18-O16-C6
20	Y	102	DMU	O5-C6-O16-C18
20	Y	102	DMU	C19-C18-O16-C6
24	C	305	CHD	C13-C17-C20-C21
24	C	305	CHD	C16-C17-C20-C22
26	C	304	CDL	O1-C1-CB2-OB2
26	C	304	CDL	C1-CA2-OA2-PA1
26	C	304	CDL	OB7-CB5-OB6-CB4
26	C	304	CDL	C51-CB5-OB6-CB4
26	I	101	CDL	CA2-C1-CB2-OB2
26	I	101	CDL	C1-CA2-OA2-PA1
26	I	101	CDL	CA3-OA5-PA1-OA2
26	I	101	CDL	CA3-OA5-PA1-OA3
26	I	101	CDL	CA3-OA5-PA1-OA4
26	I	101	CDL	CB2-OB2-PB2-OB3
26	I	101	CDL	CB2-OB2-PB2-OB4
26	I	101	CDL	CB2-OB2-PB2-OB5
26	I	101	CDL	CB3-OB5-PB2-OB3
26	I	101	CDL	CB3-OB5-PB2-OB4
26	I	101	CDL	C51-CB5-OB6-CB4
26	L	101	CDL	CB2-C1-CA2-OA2
26	L	101	CDL	CA2-OA2-PA1-OA3
26	L	101	CDL	CA2-OA2-PA1-OA4
26	L	101	CDL	CA3-OA5-PA1-OA3
26	L	101	CDL	CB2-OB2-PB2-OB5
26	L	101	CDL	OB6-CB4-CB6-OB8
26	L	101	CDL	OB7-CB5-OB6-CB4
26	L	101	CDL	C51-CB5-OB6-CB4
26	O	304	CDL	CA2-OA2-PA1-OA3
26	O	304	CDL	C11-CA5-OA6-CA4
26	O	304	CDL	CB2-OB2-PB2-OB3
26	P	305	CDL	O1-C1-CB2-OB2
26	P	305	CDL	C1-CA2-OA2-PA1
26	P	305	CDL	CA2-OA2-PA1-OA3
26	P	305	CDL	C11-CA5-OA6-CA4
26	P	305	CDL	CB3-OB5-PB2-OB4
26	P	305	CDL	OB7-CB5-OB6-CB4
26	Y	101	CDL	CA2-OA2-PA1-OA3

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Mol	Chain	Res	Type	Atoms
26	Y	101	CDL	CA3-OA5-PA1-OA2
26	Y	101	CDL	CA3-OA5-PA1-OA3
26	Y	101	CDL	CA3-OA5-PA1-OA4
26	Y	101	CDL	C11-CA5-OA6-CA4
26	Y	101	CDL	CB2-OB2-PB2-OB4
26	Y	101	CDL	C51-CB5-OB6-CB4
28	G	101	PEK	C11-C12-C13-C14
28	T	101	PEK	C11-C12-C13-C14
28	T	101	PEK	C12-C13-C14-C15
20	L	102	DMU	C3-C4-C57-O61
24	C	305	CHD	C16-C17-C20-C21
24	C	305	CHD	C13-C17-C20-C22
26	C	304	CDL	OA7-CA5-OA6-CA4
26	I	101	CDL	OA7-CA5-OA6-CA4
26	I	101	CDL	OB7-CB5-OB6-CB4
26	O	304	CDL	OA7-CA5-OA6-CA4
26	P	305	CDL	OA7-CA5-OA6-CA4
26	Y	101	CDL	OA7-CA5-OA6-CA4
26	Y	101	CDL	OB7-CB5-OB6-CB4
26	O	304	CDL	C31-CA7-OA8-CA6
26	C	304	CDL	C11-CA5-OA6-CA4
26	L	101	CDL	C11-CA5-OA6-CA4
26	P	305	CDL	C51-CB5-OB6-CB4
24	P	306	CHD	C16-C17-C20-C21
24	P	306	CHD	C13-C17-C20-C22
20	D	201	DMU	O6-C11-C9-O1
26	C	304	CDL	C71-CB7-OB8-CB6
20	C	318	DMU	O5-C4-C57-O61
20	L	102	DMU	O5-C4-C57-O61
22	A	616	PGV	C26-C27-C28-C29
26	L	101	CDL	OA7-CA5-OA6-CA4
26	O	304	CDL	OA9-CA7-OA8-CA6
24	P	306	CHD	C13-C17-C20-C21
26	I	101	CDL	O1-C1-CB2-OB2
26	L	101	CDL	O1-C1-CA2-OA2
26	P	305	CDL	C31-CA7-OA8-CA6
19	P	310	LFA	C11-C10-C9-C8
26	L	101	CDL	C72-C73-C74-C75
20	A	610	DMU	O6-C11-C9-O1
20	C	319	DMU	O5-C4-C57-O61
20	C	319	DMU	O6-C11-C9-O1
20	C	323	DMU	O5-C4-C57-O61

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Mol	Chain	Res	Type	Atoms
20	O	303	DMU	O5-C4-C57-O61
20	P	319	DMU	O6-C11-C9-O1
20	N	612	DMU	O6-C11-C9-C8
26	O	304	CDL	C51-CB5-OB6-CB4
19	N	610	LFA	C9-C10-C11-C12
22	A	616	PGV	C23-C24-C25-C26
20	C	315	DMU	O6-C11-C9-O1
20	N	612	DMU	O6-C11-C9-O1
20	P	324	DMU	O6-C11-C9-O1
20	A	610	DMU	O6-C11-C9-C8
20	P	315	DMU	C31-C34-C37-C40
22	C	303	PGV	C28-C29-C30-C31
19	P	301	LFA	C10-C11-C12-C13
20	P	324	DMU	O6-C11-C9-C8
24	P	306	CHD	C16-C17-C20-C22
20	N	619	DMU	O5-C4-C57-O61
20	C	319	DMU	C3-C4-C57-O61
20	C	319	DMU	O6-C11-C9-C8
19	A	608	LFA	C9-C10-C11-C12
26	C	304	CDL	CA4-CA3-OA5-PA1
20	B	307	DMU	C3-C4-C57-O61
20	D	201	DMU	O6-C11-C9-C8
20	O	303	DMU	C3-C4-C57-O61
19	P	301	LFA	C2-C3-C4-C5
26	C	304	CDL	OB9-CB7-OB8-CB6
20	N	612	DMU	O5-C6-O16-C18
20	Q	201	DMU	O5-C6-O16-C18
14	A	601[A]	HEA	C15-C16-C17-C18
14	N	603[A]	HEA	C15-C16-C17-C18
26	C	304	CDL	C31-CA7-OA8-CA6
19	C	309	LFA	C12-C13-C14-C15
19	C	325	LFA	C9-C10-C11-C12
20	C	318	DMU	C3-C4-C57-O61
26	L	101	CDL	C31-CA7-OA8-CA6
26	Y	101	CDL	C31-CA7-OA8-CA6
20	C	324	DMU	O6-C11-C9-C8
26	I	101	CDL	O1-C1-CA2-OA2
26	Y	101	CDL	O1-C1-CA2-OA2
24	P	306	CHD	C21-C20-C22-C23
20	Y	102	DMU	C1-C6-O16-C18
26	L	101	CDL	OA9-CA7-OA8-CA6
20	C	318	DMU	O6-C11-C9-O1

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Mol	Chain	Res	Type	Atoms
20	P	318	DMU	O5-C4-C57-O61
26	O	304	CDL	OB7-CB5-OB6-CB4
20	C	323	DMU	C3-C4-C57-O61
26	P	305	CDL	OA9-CA7-OA8-CA6
20	P	319	DMU	C2-C3-O7-C10
26	L	101	CDL	CA5-C11-C12-C13
20	P	319	DMU	O6-C11-C9-C8
26	C	304	CDL	CB5-C51-C52-C53
26	I	101	CDL	CA5-C11-C12-C13
26	O	304	CDL	CA7-C31-C32-C33
26	P	305	CDL	CB7-C71-C72-C73
20	C	319	DMU	O16-C18-C19-C22
20	Y	102	DMU	O16-C18-C19-C22
19	P	310	LFA	C12-C13-C14-C15
20	C	317	DMU	O16-C18-C19-C22
26	O	304	CDL	C1-CA2-OA2-PA1
26	C	304	CDL	CA7-C31-C32-C33
26	C	304	CDL	OA9-CA7-OA8-CA6
20	B	307	DMU	O5-C4-C57-O61
20	N	619	DMU	C3-C4-C57-O61
20	L	102	DMU	O16-C18-C19-C22
20	B	303	DMU	O16-C18-C19-C22
20	P	319	DMU	C4-C3-O7-C10
26	Y	101	CDL	OA9-CA7-OA8-CA6
19	C	309	LFA	C11-C10-C9-C8
20	Z	101	DMU	O16-C18-C19-C22
20	C	324	DMU	O6-C11-C9-O1
20	A	610	DMU	C3-C4-C57-O61
26	C	304	CDL	CA3-OA5-PA1-OA2
26	I	101	CDL	CB3-OB5-PB2-OB2
26	L	101	CDL	CA2-OA2-PA1-OA5
26	O	304	CDL	CB2-OB2-PB2-OB5
26	O	304	CDL	CB3-OB5-PB2-OB2
26	P	305	CDL	CA2-OA2-PA1-OA5
26	P	305	CDL	CA3-OA5-PA1-OA2
26	Y	101	CDL	CB2-OB2-PB2-OB5
20	A	610	DMU	O5-C4-C57-O61
26	Y	101	CDL	CB2-C1-CA2-OA2
20	C	318	DMU	O16-C18-C19-C22
20	O	308	DMU	O16-C18-C19-C22
26	P	305	CDL	C82-C83-C84-C85
20	P	318	DMU	O1-C10-O7-C3

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Mol	Chain	Res	Type	Atoms
19	T	102	LFA	C10-C11-C12-C13
20	C	323	DMU	O16-C18-C19-C22
26	I	101	CDL	C11-CA5-OA6-CA4
19	T	103	LFA	C3-C4-C5-C6
26	C	304	CDL	C35-C36-C37-C38
26	L	101	CDL	C58-C59-C60-C61
26	Y	101	CDL	C79-C80-C81-C82
20	C	315	DMU	C19-C22-C25-C28
20	P	318	DMU	C25-C28-C31-C34
26	C	304	CDL	C11-C12-C13-C14
26	L	101	CDL	C12-C13-C14-C15
26	O	304	CDL	C17-C18-C19-C20
19	N	601	LFA	C5-C6-C7-C8
26	C	304	CDL	C72-C73-C74-C75
28	T	101	PEK	C7-C8-C9-C10
20	C	317	DMU	C31-C34-C37-C40
22	C	303	PGV	C7-C8-C9-C10
26	O	304	CDL	C31-C32-C33-C34
20	C	315	DMU	O6-C11-C9-C8
26	C	304	CDL	O1-C1-CA2-OA2
26	P	305	CDL	O1-C1-CA2-OA2
20	N	602	DMU	C25-C28-C31-C34
20	P	318	DMU	C22-C25-C28-C31
20	W	101	DMU	C25-C28-C31-C34
26	C	304	CDL	CB7-C71-C72-C73
20	C	318	DMU	C1-C6-O16-C18
20	C	319	DMU	C1-C6-O16-C18
20	L	102	DMU	C1-C6-O16-C18
20	N	619	DMU	C1-C6-O16-C18
20	P	318	DMU	C1-C6-O16-C18
19	N	601	LFA	C13-C14-C15-C16
26	Y	101	CDL	C19-C20-C21-C22
19	B	306	LFA	C13-C14-C15-C16
19	C	309	LFA	C3-C4-C5-C6
19	P	310	LFA	C4-C5-C6-C7
20	M	101	DMU	C19-C22-C25-C28
20	O	306	DMU	C19-C22-C25-C28
26	C	304	CDL	C75-C76-C77-C78
26	I	101	CDL	C31-C32-C33-C34
19	B	306	LFA	C10-C11-C12-C13
19	B	306	LFA	C11-C12-C13-C14
19	C	307	LFA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
19	P	308	LFA	C3-C4-C5-C6
20	A	617	DMU	C19-C22-C25-C28
20	C	318	DMU	C31-C34-C37-C40
20	N	612	DMU	C31-C34-C37-C40
20	Z	101	DMU	C25-C28-C31-C34
22	C	303	PGV	C22-C23-C24-C25
22	C	303	PGV	C25-C26-C27-C28
26	P	305	CDL	C74-C75-C76-C77
20	M	101	DMU	C22-C25-C28-C31
19	C	307	LFA	C4-C5-C6-C7
20	Z	101	DMU	C22-C25-C28-C31
22	C	303	PGV	C14-C15-C16-C17
26	C	304	CDL	C22-C23-C24-C25
20	P	317	DMU	C31-C34-C37-C40
20	P	319	DMU	C22-C25-C28-C31
26	L	101	CDL	C37-C38-C39-C40
26	L	101	CDL	C59-C60-C61-C62
26	O	304	CDL	C78-C79-C80-C81
26	P	305	CDL	C13-C14-C15-C16
26	P	305	CDL	C35-C36-C37-C38
20	P	323	DMU	O5-C6-O16-C18
20	C	316	DMU	C31-C34-C37-C40
20	M	102	DMU	C25-C28-C31-C34
26	L	101	CDL	C74-C75-C76-C77
26	O	304	CDL	C12-C13-C14-C15
19	A	607	LFA	C6-C7-C8-C9
20	A	615	DMU	C25-C28-C31-C34
20	H	101	DMU	C3-C4-C57-O61
26	Y	101	CDL	CA5-C11-C12-C13
28	T	101	PEK	C1-C2-C3-C4
19	C	325	LFA	C4-C5-C6-C7
19	T	102	LFA	C3-C4-C5-C6
20	H	101	DMU	C19-C22-C25-C28
22	C	303	PGV	C13-C14-C15-C16
26	L	101	CDL	C17-C18-C19-C20
19	C	310	LFA	C7-C8-C9-C10
19	P	301	LFA	C4-C5-C6-C7
19	P	311	LFA	C6-C7-C8-C9
26	O	304	CDL	C73-C74-C75-C76
26	Y	101	CDL	C13-C14-C15-C16
20	A	617	DMU	C18-C19-C22-C25
20	Y	102	DMU	C18-C19-C22-C25

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Mol	Chain	Res	Type	Atoms
19	N	609	LFA	C6-C7-C8-C9
20	A	610	DMU	C31-C34-C37-C40
20	P	317	DMU	C28-C31-C34-C37
19	P	311	LFA	C2-C3-C4-C5
26	O	304	CDL	C74-C75-C76-C77
20	A	615	DMU	C19-C22-C25-C28
20	P	316	DMU	C28-C31-C34-C37
26	P	305	CDL	CB5-C51-C52-C53
20	P	307	DMU	C31-C34-C37-C40
26	O	304	CDL	C76-C77-C78-C79
19	A	608	LFA	C2-C3-C4-C5
22	P	304	PGV	C7-C8-C9-C10
20	A	615	DMU	C18-C19-C22-C25
19	C	325	LFA	C7-C8-C9-C10
20	C	317	DMU	C19-C22-C25-C28
26	P	305	CDL	C71-C72-C73-C74
28	T	101	PEK	C26-C27-C28-C29
26	C	304	CDL	C71-C72-C73-C74
24	P	306	CHD	C17-C20-C22-C23
20	P	317	DMU	C18-C19-C22-C25
20	O	306	DMU	C22-C25-C28-C31
20	B	302	DMU	C18-C19-C22-C25
19	C	309	LFA	C5-C6-C7-C8
20	C	317	DMU	C28-C31-C34-C37
20	N	602	DMU	C28-C31-C34-C37
26	L	101	CDL	C51-C52-C53-C54
20	P	323	DMU	C18-C19-C22-C25
26	Y	101	CDL	C14-C15-C16-C17
21	P	320	EDO	O1-C1-C2-O2
19	C	311	LFA	C4-C5-C6-C7
19	C	312	LFA	C1-C2-C3-C4
20	C	315	DMU	C28-C31-C34-C37
20	J	101	DMU	C31-C34-C37-C40
22	N	618	PGV	C29-C30-C31-C32
19	P	301	LFA	C6-C7-C8-C9
20	C	319	DMU	C25-C28-C31-C34
22	C	303	PGV	C30-C31-C32-C33
19	P	313	LFA	C5-C6-C7-C8
20	B	307	DMU	C18-C19-C22-C25
20	L	102	DMU	C22-C25-C28-C31
19	P	312	LFA	C1-C2-C3-C4
19	T	103	LFA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	P	304	PGV	C12-C13-C14-C15
28	G	101	PEK	C15-C16-C17-C18
20	A	609	DMU	C28-C31-C34-C37
26	Y	101	CDL	C31-C32-C33-C34
28	G	101	PEK	C28-C29-C30-C31
26	O	304	CDL	CA5-C11-C12-C13
24	C	305	CHD	C21-C20-C22-C23
19	A	608	LFA	C11-C10-C9-C8
20	C	323	DMU	C19-C22-C25-C28
26	C	304	CDL	C23-C24-C25-C26
19	N	610	LFA	C5-C6-C7-C8
20	C	318	DMU	O5-C6-O16-C18
20	P	318	DMU	O5-C6-O16-C18
19	P	313	LFA	C2-C3-C4-C5
20	L	102	DMU	C31-C34-C37-C40
22	N	618	PGV	C26-C27-C28-C29
26	P	305	CDL	C75-C76-C77-C78
22	A	616	PGV	C29-C30-C31-C32
26	I	101	CDL	C15-C16-C17-C18
20	P	318	DMU	C19-C22-C25-C28
20	J	101	DMU	C18-C19-C22-C25
19	C	311	LFA	C11-C10-C9-C8
19	C	325	LFA	C10-C11-C12-C13
20	O	303	DMU	C34-C37-C40-C43
20	P	319	DMU	C31-C34-C37-C40
19	P	310	LFA	C3-C4-C5-C6
19	C	312	LFA	C5-C6-C7-C8
20	C	323	DMU	C28-C31-C34-C37
26	Y	101	CDL	C72-C73-C74-C75
19	N	601	LFA	C4-C5-C6-C7
19	O	302	LFA	C5-C6-C7-C8
26	I	101	CDL	C76-C77-C78-C79
19	A	607	LFA	C2-C3-C4-C5
19	C	309	LFA	C13-C14-C15-C16
19	N	601	LFA	C6-C7-C8-C9
22	A	616	PGV	C14-C15-C16-C17
22	C	303	PGV	C24-C25-C26-C27
20	P	323	DMU	O16-C18-C19-C22
26	L	101	CDL	C34-C35-C36-C37
26	Y	101	CDL	C51-C52-C53-C54
26	C	304	CDL	C74-C75-C76-C77
26	I	101	CDL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
26	I	101	CDL	C19-C20-C21-C22
26	Y	101	CDL	C80-C81-C82-C83
28	T	101	PEK	C14-C15-C16-C17
26	L	101	CDL	CA3-OA5-PA1-OA2
19	C	309	LFA	C14-C15-C16-C17
26	I	101	CDL	C71-C72-C73-C74
26	O	304	CDL	C77-C78-C79-C80
20	P	318	DMU	O6-C11-C9-O1
20	P	318	DMU	C3-C4-C57-O61
26	P	305	CDL	CA7-C31-C32-C33
20	D	201	DMU	C4-C3-O7-C10
20	W	101	DMU	C31-C34-C37-C40
26	L	101	CDL	C38-C39-C40-C41
26	Y	101	CDL	C59-C60-C61-C62
20	C	319	DMU	C31-C34-C37-C40
26	Y	101	CDL	C63-C64-C65-C66
28	G	101	PEK	C34-C35-C36-C37
28	T	101	PEK	C32-C33-C34-C35
28	T	101	PEK	C2-C3-C4-C5
19	C	310	LFA	C3-C4-C5-C6
19	P	314	LFA	C6-C7-C8-C9
20	O	306	DMU	C25-C28-C31-C34
20	P	315	DMU	C19-C22-C25-C28
19	B	306	LFA	C12-C13-C14-C15
20	C	316	DMU	C28-C31-C34-C37
20	J	101	DMU	C25-C28-C31-C34
20	P	318	DMU	C28-C31-C34-C37
20	A	617	DMU	C28-C31-C34-C37
26	Y	101	CDL	C64-C65-C66-C67
19	C	309	LFA	C2-C3-C4-C5
20	Z	102	DMU	C34-C37-C40-C43
26	C	304	CDL	CB3-CB4-CB6-OB8
26	I	101	CDL	CA3-CA4-CA6-OA8
26	P	305	CDL	CA3-CA4-CA6-OA8
26	I	101	CDL	C31-CA7-OA8-CA6
19	N	601	LFA	C14-C15-C16-C17
26	Y	101	CDL	C84-C85-C86-C87
20	B	302	DMU	O16-C18-C19-C22
20	W	101	DMU	O16-C18-C19-C22
19	N	601	LFA	C11-C12-C13-C14
20	A	617	DMU	C25-C28-C31-C34
20	C	318	DMU	C34-C37-C40-C43

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Mol	Chain	Res	Type	Atoms
28	G	101	PEK	C17-C18-C19-C20
20	C	319	DMU	C19-C22-C25-C28
28	G	101	PEK	C16-C17-C18-C19
20	C	315	DMU	O5-C4-C57-O61
20	P	315	DMU	O6-C11-C9-O1
19	P	314	LFA	C5-C6-C7-C8
19	P	314	LFA	C10-C11-C12-C13
26	I	101	CDL	C12-C13-C14-C15
20	Y	102	DMU	O5-C4-C57-O61
20	W	101	DMU	C34-C37-C40-C43
26	I	101	CDL	C17-C18-C19-C20
22	N	618	PGV	C11-C10-C9-C8
28	T	101	PEK	C15-C16-C17-C18
20	C	318	DMU	C19-C22-C25-C28
19	C	307	LFA	C6-C7-C8-C9
19	P	310	LFA	C5-C6-C7-C8
26	C	304	CDL	C59-C60-C61-C62
20	Z	101	DMU	C34-C37-C40-C43
19	P	301	LFA	C1-C2-C3-C4
26	L	101	CDL	C76-C77-C78-C79
20	N	611	DMU	C34-C37-C40-C43
20	P	307	DMU	O16-C18-C19-C22
20	A	615	DMU	C28-C31-C34-C37
20	C	316	DMU	C34-C37-C40-C43
19	C	310	LFA	C11-C10-C9-C8
19	P	311	LFA	C7-C8-C9-C10
20	B	303	DMU	C34-C37-C40-C43
20	N	602	DMU	C19-C22-C25-C28
22	P	304	PGV	C30-C31-C32-C33
26	C	304	CDL	C33-C34-C35-C36
26	P	305	CDL	C57-C58-C59-C60
20	Z	102	DMU	C31-C34-C37-C40
20	Q	201	DMU	C4-C3-O7-C10
22	A	616	PGV	C28-C29-C30-C31
20	Y	102	DMU	C31-C34-C37-C40
26	P	305	CDL	C19-C20-C21-C22
20	O	303	DMU	C1-C6-O16-C18
20	J	101	DMU	C34-C37-C40-C43
26	I	101	CDL	OA6-CA4-CA6-OA8
26	O	304	CDL	OA6-CA4-CA6-OA8
19	N	610	LFA	C3-C4-C5-C6
19	P	312	LFA	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
26	I	101	CDL	C32-C33-C34-C35
19	C	310	LFA	C1-C2-C3-C4
26	Y	101	CDL	C76-C77-C78-C79
20	N	602	DMU	C34-C37-C40-C43
26	C	304	CDL	C51-C52-C53-C54
26	L	101	CDL	C75-C76-C77-C78
26	P	305	CDL	C21-C22-C23-C24
22	P	304	PGV	C14-C15-C16-C17
26	L	101	CDL	C15-C16-C17-C18
20	M	102	DMU	C22-C25-C28-C31
26	O	304	CDL	C32-C33-C34-C35
26	I	101	CDL	C18-C19-C20-C21
19	B	306	LFA	C9-C10-C11-C12
19	P	311	LFA	C11-C10-C9-C8
26	Y	101	CDL	C73-C74-C75-C76
26	I	101	CDL	C71-CB7-OB8-CB6
20	C	324	DMU	O16-C18-C19-C22
22	A	616	PGV	C30-C31-C32-C33
28	T	101	PEK	C4-C5-C6-C7
20	C	318	DMU	C2-C3-O7-C10
20	L	102	DMU	C34-C37-C40-C43
20	N	611	DMU	C31-C34-C37-C40
20	C	318	DMU	C4-C3-O7-C10
22	N	618	PGV	C30-C31-C32-C33
19	C	310	LFA	C2-C3-C4-C5
19	B	306	LFA	C4-C5-C6-C7
20	L	102	DMU	C25-C28-C31-C34
28	G	101	PEK	C26-C27-C28-C29
20	O	303	DMU	C22-C25-C28-C31
19	B	306	LFA	C3-C4-C5-C6
26	O	304	CDL	C15-C16-C17-C18
26	P	305	CDL	C71-CB7-OB8-CB6
19	P	301	LFA	C11-C12-C13-C14
20	B	303	DMU	C19-C18-O16-C6
20	C	317	DMU	C19-C18-O16-C6
20	P	317	DMU	C19-C18-O16-C6
20	O	307	DMU	C19-C22-C25-C28
22	A	616	PGV	C11-C10-C9-C8
19	C	313	LFA	C4-C5-C6-C7
19	T	102	LFA	C4-C5-C6-C7
20	D	201	DMU	C2-C3-O7-C10
20	Y	102	DMU	C22-C25-C28-C31

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Mol	Chain	Res	Type	Atoms
26	L	101	CDL	C84-C85-C86-C87
20	A	615	DMU	O16-C18-C19-C22
20	J	101	DMU	O16-C18-C19-C22
26	L	101	CDL	CB3-CB4-CB6-OB8
26	P	305	CDL	CB3-CB4-CB6-OB8
19	C	309	LFA	C11-C12-C13-C14
19	N	601	LFA	C12-C13-C14-C15
20	Y	102	DMU	C34-C37-C40-C43
26	L	101	CDL	C21-C22-C23-C24
26	Y	101	CDL	C61-C62-C63-C64
28	T	101	PEK	C10-C11-C12-C13
20	P	316	DMU	C25-C28-C31-C34
20	Q	201	DMU	C28-C31-C34-C37
28	T	101	PEK	C17-C18-C19-C20
19	N	609	LFA	C7-C8-C9-C10
19	P	310	LFA	C13-C14-C15-C16
20	B	302	DMU	C19-C22-C25-C28
26	L	101	CDL	C14-C15-C16-C17
28	G	101	PEK	C9-C10-C11-C12
28	G	101	PEK	C12-C13-C14-C15
28	T	101	PEK	C11-C10-C9-C8
20	P	323	DMU	O5-C4-C57-O61
19	C	308	LFA	C3-C4-C5-C6
20	B	302	DMU	C25-C28-C31-C34
20	P	324	DMU	C25-C28-C31-C34
19	C	312	LFA	C11-C10-C9-C8
26	P	305	CDL	C53-C54-C55-C56
20	A	609	DMU	C34-C37-C40-C43
26	O	304	CDL	C18-C19-C20-C21
19	C	310	LFA	C4-C5-C6-C7
26	Y	101	CDL	OB6-CB4-CB6-OB8
26	O	304	CDL	C72-C73-C74-C75
28	G	101	PEK	C29-C30-C31-C32
19	T	103	LFA	C7-C8-C9-C10
26	Y	101	CDL	C37-C38-C39-C40
26	Y	101	CDL	C1-CA2-OA2-PA1
22	P	304	PGV	C24-C25-C26-C27
19	C	311	LFA	C10-C11-C12-C13
21	N	614	EDO	O1-C1-C2-O2
26	L	101	CDL	C53-C54-C55-C56
20	N	619	DMU	C18-C19-C22-C25
19	A	608	LFA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
19	C	307	LFA	C11-C10-C9-C8
20	P	323	DMU	C22-C25-C28-C31
20	N	612	DMU	O16-C18-C19-C22
26	Y	101	CDL	OA5-CA3-CA4-CA6
20	B	307	DMU	O16-C18-C19-C22
20	P	324	DMU	O16-C18-C19-C22
20	C	324	DMU	C18-C19-C22-C25
19	N	610	LFA	C6-C7-C8-C9
19	P	308	LFA	C2-C3-C4-C5
20	A	617	DMU	C34-C37-C40-C43
20	O	306	DMU	C31-C34-C37-C40
20	P	317	DMU	C22-C25-C28-C31
26	P	305	CDL	C54-C55-C56-C57
20	H	101	DMU	O5-C4-C57-O61
22	A	616	PGV	C31-C32-C33-C34
26	L	101	CDL	C13-C14-C15-C16
26	Y	101	CDL	C71-CB7-OB8-CB6
28	G	101	PEK	C27-C28-C29-C30
19	N	610	LFA	C1-C2-C3-C4
20	P	318	DMU	C31-C34-C37-C40
26	C	304	CDL	C18-C19-C20-C21
26	Y	101	CDL	C22-C23-C24-C25
19	P	308	LFA	C11-C10-C9-C8
19	P	313	LFA	C4-C5-C6-C7
22	C	303	PGV	C21-C22-C23-C24
20	Z	101	DMU	O6-C11-C9-C8
26	O	304	CDL	C71-CB7-OB8-CB6
19	C	307	LFA	C3-C4-C5-C6
20	B	307	DMU	O5-C6-O16-C18
26	I	101	CDL	OB9-CB7-OB8-CB6
26	I	101	CDL	C77-C78-C79-C80
26	C	304	CDL	C12-C11-CA5-OA6
19	N	609	LFA	C11-C12-C13-C14
20	C	315	DMU	C31-C34-C37-C40
20	C	306	DMU	C18-C19-C22-C25
20	C	315	DMU	C18-C19-C22-C25
19	B	306	LFA	C6-C7-C8-C9
26	I	101	CDL	OA9-CA7-OA8-CA6
26	P	305	CDL	OB9-CB7-OB8-CB6
26	Y	101	CDL	OB9-CB7-OB8-CB6
20	O	307	DMU	C18-C19-C22-C25
20	A	617	DMU	O16-C18-C19-C22

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Mol	Chain	Res	Type	Atoms
26	P	305	CDL	OB6-CB4-CB6-OB8
20	C	318	DMU	O6-C11-C9-C8
26	O	304	CDL	C20-C21-C22-C23
26	L	101	CDL	C22-C23-C24-C25
20	B	303	DMU	C31-C34-C37-C40
26	L	101	CDL	C18-C19-C20-C21
20	O	307	DMU	C28-C31-C34-C37
20	Q	201	DMU	C2-C3-O7-C10
24	P	306	CHD	C20-C22-C23-C24
26	I	101	CDL	C73-C74-C75-C76
26	Y	101	CDL	C56-C57-C58-C59
20	C	315	DMU	C25-C28-C31-C34
20	P	319	DMU	C28-C31-C34-C37
20	O	303	DMU	C18-C19-C22-C25
26	C	304	CDL	CA2-OA2-PA1-OA5
26	L	101	CDL	O1-C1-CB2-OB2
20	C	323	DMU	C34-C37-C40-C43
22	C	303	PGV	C02-C03-O11-P
22	P	304	PGV	C02-C03-O11-P
26	P	305	CDL	CA4-CA3-OA5-PA1
26	C	304	CDL	CA3-OA5-PA1-OA3
26	L	101	CDL	CA3-OA5-PA1-OA4
26	L	101	CDL	CB2-OB2-PB2-OB3
26	O	304	CDL	CB2-OB2-PB2-OB4
26	O	304	CDL	CB3-OB5-PB2-OB3
26	O	304	CDL	CB3-OB5-PB2-OB4
26	P	305	CDL	CA2-OA2-PA1-OA4
26	P	305	CDL	CA3-OA5-PA1-OA3
20	C	317	DMU	C25-C28-C31-C34
22	N	618	PGV	C14-C15-C16-C17
19	C	309	LFA	C1-C2-C3-C4
19	C	314	LFA	C6-C7-C8-C9
26	L	101	CDL	C36-C37-C38-C39
26	Y	101	CDL	OA5-CA3-CA4-OA6
19	N	609	LFA	C2-C3-C4-C5
26	O	304	CDL	OB9-CB7-OB8-CB6
19	C	314	LFA	C1-C2-C3-C4
26	O	304	CDL	CA3-CA4-CA6-OA8
26	P	305	CDL	OA6-CA4-CA6-OA8
26	Y	101	CDL	C20-C21-C22-C23
22	P	304	PGV	C11-C12-C13-C14
28	T	101	PEK	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
24	C	305	CHD	C17-C20-C22-C23
19	C	311	LFA	C5-C6-C7-C8
20	M	102	DMU	C31-C34-C37-C40
14	A	601[A]	HEA	C19-C20-C21-C22
20	P	324	DMU	C3-C4-C57-O61
26	Y	101	CDL	C21-C22-C23-C24
20	Z	101	DMU	O6-C11-C9-O1
19	C	307	LFA	C7-C8-C9-C10
28	G	101	PEK	C4-C5-C6-C7
26	P	305	CDL	C72-C73-C74-C75
20	C	323	DMU	C22-C25-C28-C31
19	C	325	LFA	C6-C7-C8-C9
20	C	306	DMU	C31-C34-C37-C40
19	P	313	LFA	C9-C10-C11-C12
20	C	315	DMU	C34-C37-C40-C43
20	O	307	DMU	O16-C18-C19-C22
26	Y	101	CDL	C53-C54-C55-C56
26	C	304	CDL	C20-C21-C22-C23
20	P	317	DMU	C25-C28-C31-C34
20	P	324	DMU	C4-C3-O7-C10
26	L	101	CDL	C71-C72-C73-C74
26	Y	101	CDL	C33-C34-C35-C36
20	Q	201	DMU	C34-C37-C40-C43
20	H	101	DMU	C28-C31-C34-C37
22	P	304	PGV	C28-C29-C30-C31
21	P	321	EDO	O1-C1-C2-O2
21	R	203	EDO	O1-C1-C2-O2
19	N	610	LFA	C2-C3-C4-C5
19	O	302	LFA	C2-C3-C4-C5
20	P	318	DMU	C2-C3-O7-C10
20	P	324	DMU	C2-C3-O7-C10
20	O	308	DMU	C34-C37-C40-C43
20	P	319	DMU	C1-C6-O16-C18
26	Y	101	CDL	CB3-OB5-PB2-OB2
19	T	102	LFA	C2-C3-C4-C5
22	N	618	PGV	C31-C32-C33-C34
26	C	304	CDL	C36-C37-C38-C39
19	P	312	LFA	C11-C10-C9-C8
20	C	306	DMU	C28-C31-C34-C37
20	B	307	DMU	C25-C28-C31-C34
19	N	601	LFA	C2-C3-C4-C5
20	C	315	DMU	C4-C3-O7-C10

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Mol	Chain	Res	Type	Atoms
28	G	101	PEK	C25-C26-C27-C28
26	P	305	CDL	C73-C74-C75-C76
20	B	303	DMU	C18-C19-C22-C25
20	H	101	DMU	C18-C19-C22-C25
26	I	101	CDL	CB2-C1-CA2-OA2
26	L	101	CDL	CA2-C1-CB2-OB2
28	T	101	PEK	O02-C1-O01-C02
19	C	312	LFA	C4-C5-C6-C7
26	O	304	CDL	C11-C12-C13-C14
26	L	101	CDL	C31-C32-C33-C34
26	L	101	CDL	C16-C17-C18-C19
19	C	311	LFA	C6-C7-C8-C9
20	C	323	DMU	C18-C19-C22-C25
19	P	308	LFA	C7-C8-C9-C10
20	C	317	DMU	C22-C25-C28-C31
20	L	102	DMU	C19-C22-C25-C28
26	I	101	CDL	C75-C76-C77-C78
20	C	315	DMU	C2-C3-O7-C10
26	P	305	CDL	C33-C34-C35-C36
20	C	323	DMU	C1-C6-O16-C18
20	P	318	DMU	C4-C3-O7-C10
26	L	101	CDL	C19-C20-C21-C22
24	C	305	CHD	C22-C23-C24-O26
20	Q	201	DMU	O5-C4-C57-O61
26	O	304	CDL	CB4-CB3-OB5-PB2
26	L	101	CDL	C78-C79-C80-C81
22	P	304	PGV	C11-C10-C9-C8
26	Y	101	CDL	C57-C58-C59-C60
19	C	310	LFA	C6-C7-C8-C9
26	C	304	CDL	C79-C80-C81-C82
26	Y	101	CDL	C52-C53-C54-C55
26	P	305	CDL	C12-C11-CA5-OA6
14	A	601[A]	HEA	CAD-CBD-CGD-O1D
14	A	601[B]	HEA	CAD-CBD-CGD-O1D
24	C	305	CHD	C22-C23-C24-O25
24	O	301	CHD	C22-C23-C24-O25
19	C	325	LFA	C12-C13-C14-C15
26	C	304	CDL	C57-C58-C59-C60
20	L	102	DMU	O5-C6-O16-C18
14	A	602	HEA	CAA-CBA-CGA-O1A
24	B	305	CHD	C22-C23-C24-O25
26	I	101	CDL	CA3-CA4-OA6-CA5

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Mol	Chain	Res	Type	Atoms
19	P	311	LFA	C3-C4-C5-C6
20	B	307	DMU	C34-C37-C40-C43
14	N	604	HEA	CAA-CBA-CGA-O1A
14	N	604	HEA	CAA-CBA-CGA-O2A
24	O	301	CHD	C22-C23-C24-O26
28	G	101	PEK	C13-C14-C15-C16
19	C	314	LFA	C10-C11-C12-C13
26	O	304	CDL	OB5-CB3-CB4-CB6
14	A	602	HEA	CAD-CBD-CGD-O2D
20	P	316	DMU	C31-C34-C37-C40
20	A	609	DMU	C31-C34-C37-C40
22	C	303	PGV	C29-C30-C31-C32
26	I	101	CDL	C74-C75-C76-C77
22	N	618	PGV	C15-C16-C17-C18
20	P	317	DMU	O5-C4-C57-O61
14	A	602	HEA	CAA-CBA-CGA-O2A
26	C	304	CDL	OB6-CB4-CB6-OB8
14	N	603[A]	HEA	CAD-CBD-CGD-O1D
14	N	603[B]	HEA	CAD-CBD-CGD-O1D
20	J	101	DMU	C19-C22-C25-C28
19	B	306	LFA	C1-C2-C3-C4
19	N	601	LFA	C11-C10-C9-C8
26	P	305	CDL	CA2-C1-CB2-OB2
14	A	602	HEA	CAD-CBD-CGD-O1D
20	P	318	DMU	C34-C37-C40-C43
20	O	307	DMU	C22-C25-C28-C31
19	B	306	LFA	C11-C10-C9-C8
19	P	312	LFA	C4-C5-C6-C7
22	A	616	PGV	C15-C16-C17-C18
22	P	304	PGV	C27-C28-C29-C30
19	C	325	LFA	C11-C12-C13-C14
26	L	101	CDL	C56-C57-C58-C59
26	Y	101	CDL	CB3-CB4-CB6-OB8
24	P	302	CHD	C22-C23-C24-O26
21	F	103	EDO	O1-C1-C2-O2
21	R	201	EDO	O1-C1-C2-O2
19	B	306	LFA	C14-C15-C16-C17
20	Q	201	DMU	C31-C34-C37-C40
19	A	608	LFA	C6-C7-C8-C9
24	C	301	CHD	C22-C23-C24-O26
19	P	312	LFA	C2-C3-C4-C5
28	T	101	PEK	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
19	P	313	LFA	C11-C10-C9-C8
22	C	303	PGV	C1-C2-C3-C4
19	C	313	LFA	C9-C10-C11-C12
14	N	604	HEA	CAD-CBD-CGD-O2D
24	B	305	CHD	C22-C23-C24-O26
24	P	306	CHD	C22-C23-C24-O25
24	P	306	CHD	C22-C23-C24-O26
20	C	319	DMU	O5-C6-O16-C18
20	B	307	DMU	C31-C34-C37-C40
22	A	616	PGV	O03-C19-C20-C21
22	N	618	PGV	O03-C19-C20-C21
22	C	303	PGV	C05-C04-O12-P
14	N	604	HEA	CAD-CBD-CGD-O1D
19	C	313	LFA	C1-C2-C3-C4
20	B	302	DMU	C31-C34-C37-C40
26	I	101	CDL	C79-C80-C81-C82
26	L	101	CDL	C80-C81-C82-C83
26	O	304	CDL	C32-C31-CA7-OA8
26	O	304	CDL	C72-C71-CB7-OB8
14	N	603[A]	HEA	CAD-CBD-CGD-O2D
14	N	603[B]	HEA	CAD-CBD-CGD-O2D
19	N	601	LFA	C7-C8-C9-C10
19	T	102	LFA	C5-C6-C7-C8
26	P	305	CDL	C17-C18-C19-C20
26	Y	101	CDL	C72-C71-CB7-OB8
20	P	318	DMU	O16-C18-C19-C22
24	C	301	CHD	C22-C23-C24-O25
24	P	302	CHD	C22-C23-C24-O25
14	N	603[A]	HEA	C19-C20-C21-C22
20	M	101	DMU	C25-C28-C31-C34
20	P	315	DMU	C28-C31-C34-C37
26	I	101	CDL	CB4-CB3-OB5-PB2
28	T	101	PEK	C13-C14-C15-C16
26	C	304	CDL	C52-C51-CB5-OB6
19	P	301	LFA	C12-C13-C14-C15
26	L	101	CDL	C64-C65-C66-C67
21	A	612	EDO	O1-C1-C2-O2
21	A	614	EDO	O1-C1-C2-O2
20	D	201	DMU	C19-C22-C25-C28
26	P	305	CDL	C55-C56-C57-C58
26	Y	101	CDL	C32-C33-C34-C35
19	C	310	LFA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
19	P	309	LFA	C2-C3-C4-C5
14	A	601[A]	HEA	CAD-CBD-CGD-O2D
14	A	601[B]	HEA	CAD-CBD-CGD-O2D
26	P	305	CDL	C52-C53-C54-C55
20	D	201	DMU	O16-C18-C19-C22
20	P	317	DMU	C19-C22-C25-C28
20	A	610	DMU	C4-C3-O7-C10
28	T	101	PEK	C2-C1-O01-C02
20	M	102	DMU	C28-C31-C34-C37
22	P	304	PGV	C1-C2-C3-C4
19	N	610	LFA	C11-C10-C9-C8
26	L	101	CDL	C72-C71-CB7-OB8
19	A	607	LFA	C7-C8-C9-C10
20	A	615	DMU	C22-C25-C28-C31
19	C	307	LFA	C2-C3-C4-C5
20	N	619	DMU	C19-C22-C25-C28
26	L	101	CDL	C60-C61-C62-C63
19	C	314	LFA	C2-C3-C4-C5
20	P	315	DMU	C4-C3-O7-C10
26	Y	101	CDL	C77-C78-C79-C80
26	Y	101	CDL	CA2-OA2-PA1-OA5
26	O	304	CDL	C32-C31-CA7-OA9
26	O	304	CDL	C72-C71-CB7-OB9
26	Y	101	CDL	C72-C71-CB7-OB9
20	W	101	DMU	C18-C19-C22-C25
20	O	308	DMU	C1-C6-O16-C18
22	C	303	PGV	C9-C10-C11-C12
26	P	305	CDL	C12-C13-C14-C15
26	I	101	CDL	CA2-OA2-PA1-OA3
26	Y	101	CDL	CB3-OB5-PB2-OB3
28	T	101	PEK	C25-C26-C27-C28
26	C	304	CDL	C52-C51-CB5-OB7
21	E	203	EDO	O1-C1-C2-O2
28	T	101	PEK	O01-C1-C2-C3
20	O	306	DMU	C18-C19-C22-C25
20	O	308	DMU	C18-C19-C22-C25
28	G	101	PEK	C32-C33-C34-C35
19	C	314	LFA	C3-C4-C5-C6
26	Y	101	CDL	C38-C39-C40-C41
20	A	610	DMU	C2-C3-O7-C10
26	L	101	CDL	C72-C71-CB7-OB9
19	O	302	LFA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
26	Y	101	CDL	C34-C35-C36-C37
26	C	304	CDL	CA2-C1-CB2-OB2
19	T	102	LFA	C1-C2-C3-C4
26	L	101	CDL	C32-C31-CA7-OA8
26	O	304	CDL	C52-C51-CB5-OB6
28	T	101	PEK	O02-C1-C2-C3
20	M	102	DMU	C34-C37-C40-C43
26	L	101	CDL	C77-C78-C79-C80
20	P	319	DMU	C19-C18-O16-C6
26	P	305	CDL	C52-C51-CB5-OB6
26	C	304	CDL	C12-C11-CA5-OA7
26	L	101	CDL	C32-C31-CA7-OA9
19	C	313	LFA	C5-C6-C7-C8

There are no ring outliers.

71 monomers are involved in 184 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	Q	201	DMU	2	0
19	C	307	LFA	6	0
20	C	316	DMU	5	0
20	C	317	DMU	1	0
18	N	608	PER	1	0
14	A	602	HEA	2	0
18	A	606	PER	1	0
21	C	321	EDO	1	0
20	A	617	DMU	9	0
19	T	102	LFA	1	0
20	C	323	DMU	7	0
28	G	101	PEK	2	0
26	C	304	CDL	16	0
21	N	617	EDO	3	0
14	N	603[A]	HEA	1	0
19	P	312	LFA	3	0
24	O	301	CHD	1	0
14	N	603[B]	HEA	1	0
20	L	102	DMU	2	0
20	P	318	DMU	5	0
20	O	303	DMU	2	0
20	P	324	DMU	3	0
22	A	616	PGV	1	0
24	P	306	CHD	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	N	602	DMU	3	0
19	B	306	LFA	3	0
28	T	101	PEK	4	0
20	C	324	DMU	7	0
26	L	101	CDL	3	0
19	C	314	LFA	3	0
19	C	309	LFA	10	0
20	B	307	DMU	1	0
14	N	604	HEA	2	0
19	N	601	LFA	1	0
21	S	102	EDO	1	0
19	C	313	LFA	1	0
26	Y	101	CDL	4	0
20	A	609	DMU	1	0
19	P	310	LFA	3	0
20	M	101	DMU	1	0
20	A	610	DMU	1	0
26	O	304	CDL	1	0
21	P	321	EDO	1	0
21	F	103	EDO	1	0
20	C	318	DMU	1	0
24	C	305	CHD	1	0
20	P	319	DMU	6	0
20	P	315	DMU	1	0
19	P	308	LFA	2	0
19	C	325	LFA	5	0
19	N	610	LFA	2	0
19	P	314	LFA	3	0
20	D	201	DMU	4	0
19	N	609	LFA	2	0
19	C	310	LFA	2	0
19	O	302	LFA	4	0
19	A	608	LFA	10	0
19	P	301	LFA	6	0
20	P	323	DMU	3	0
19	A	607	LFA	3	0
20	C	315	DMU	1	0
14	A	601[A]	HEA	1	0
20	Y	102	DMU	4	0
19	C	312	LFA	5	0
22	C	303	PGV	1	0
26	P	305	CDL	10	0

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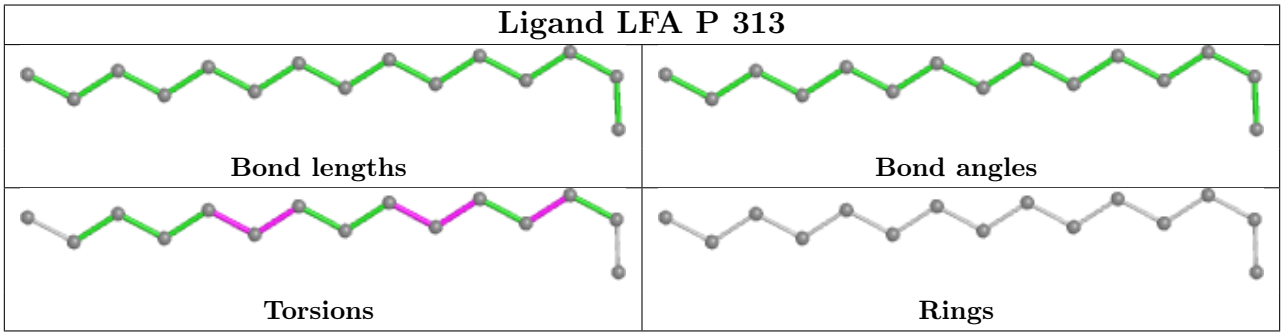
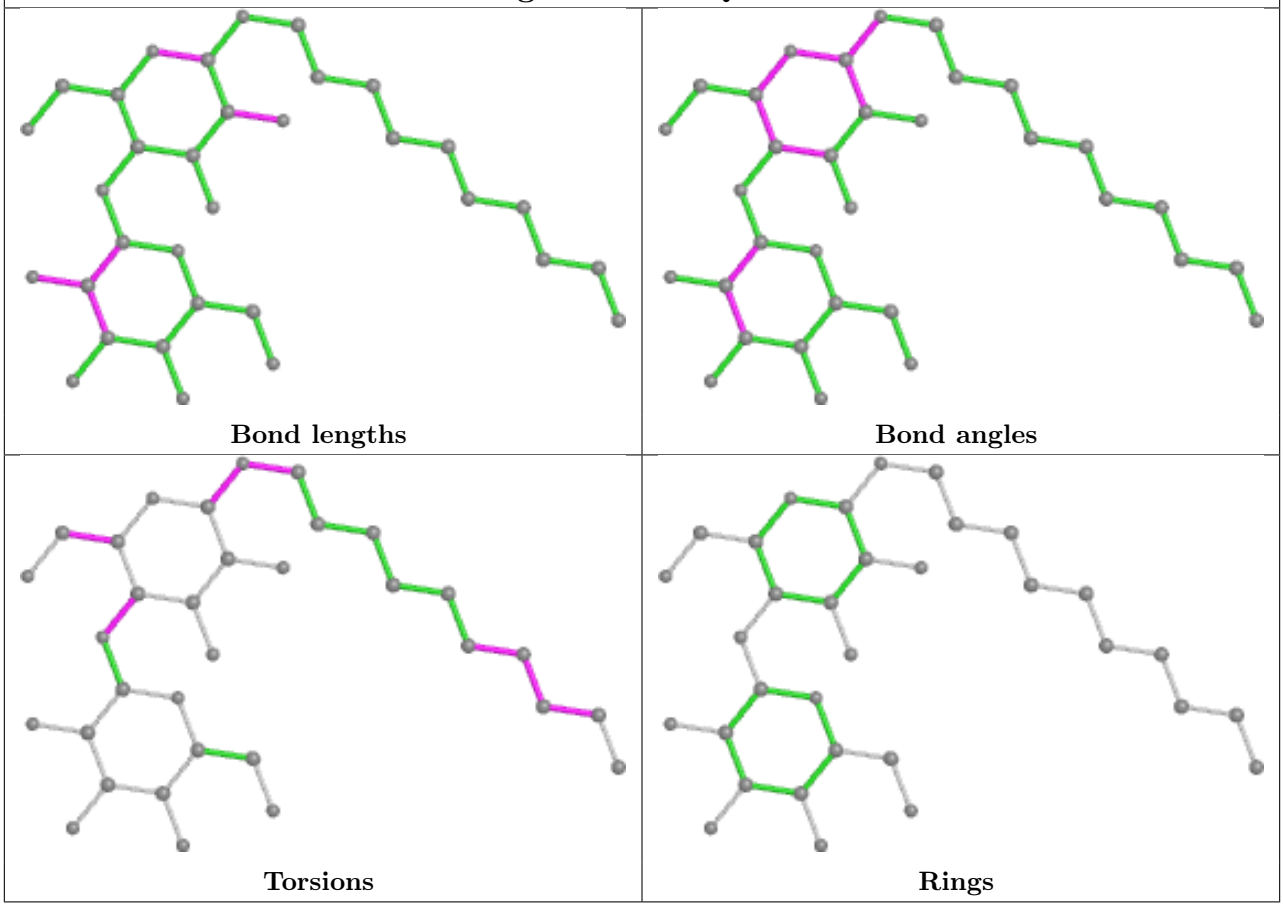
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	N	618	PGV	1	0
20	H	101	DMU	9	0
14	A	601[B]	HEA	1	0
19	P	311	LFA	5	0
20	N	612	DMU	1	0

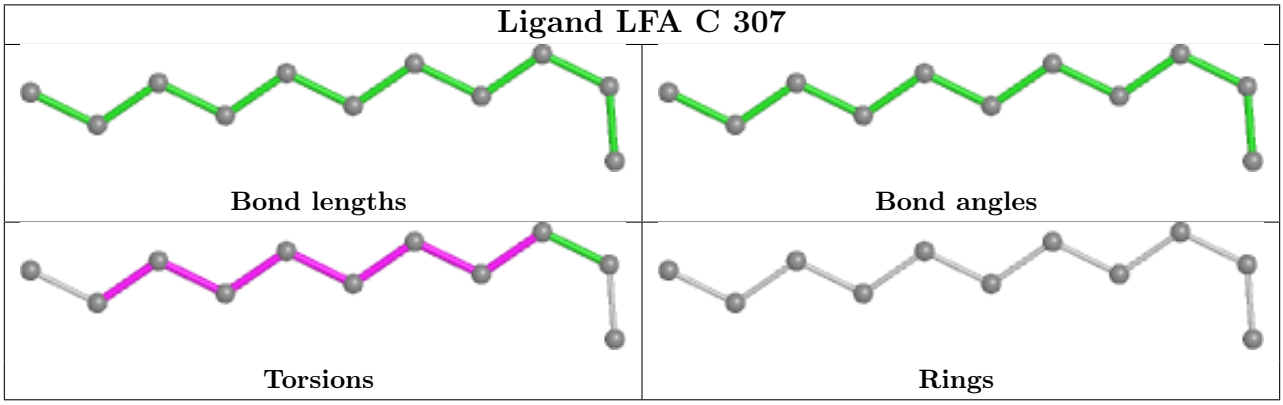
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



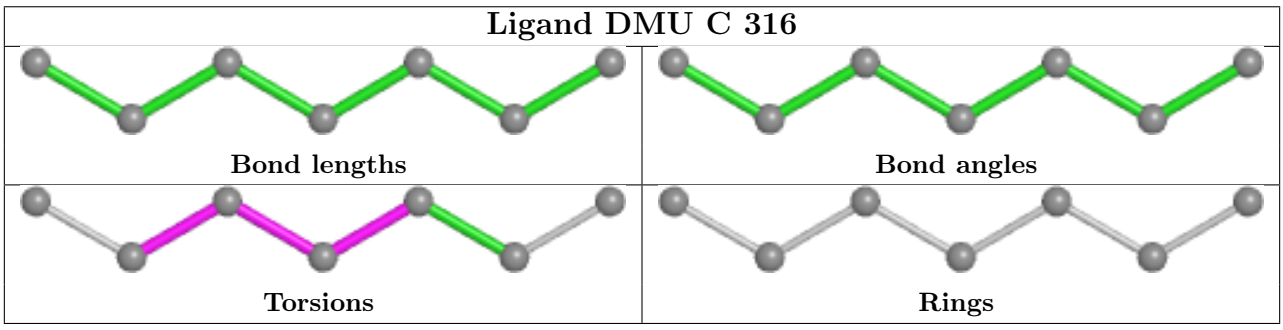
Ligand DMU Q 201



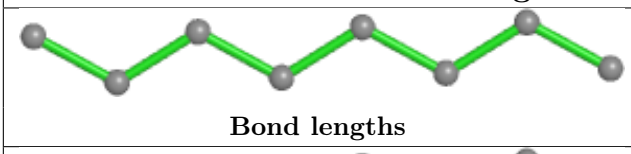
Ligand LFA C 307



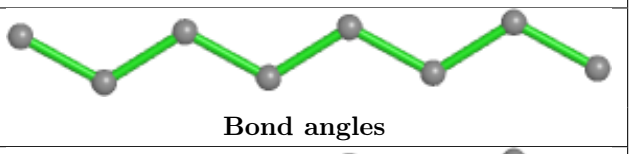
Ligand DMU C 316



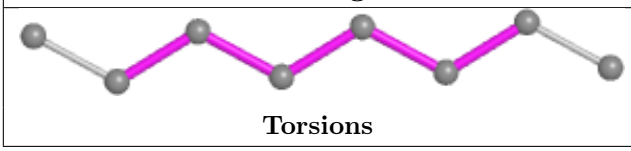
Ligand DMU M 102



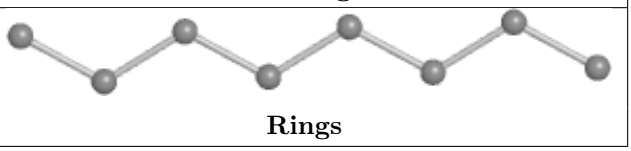
Bond lengths



Bond angles

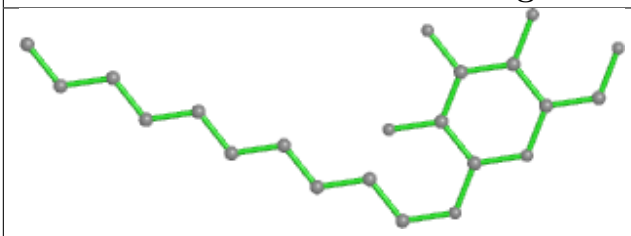


Torsions

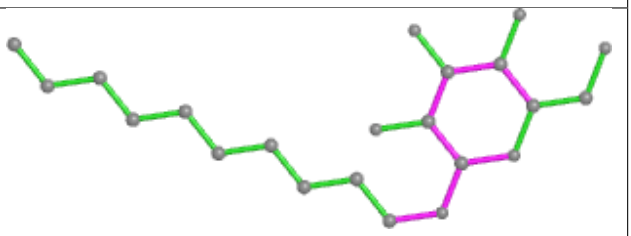


Rings

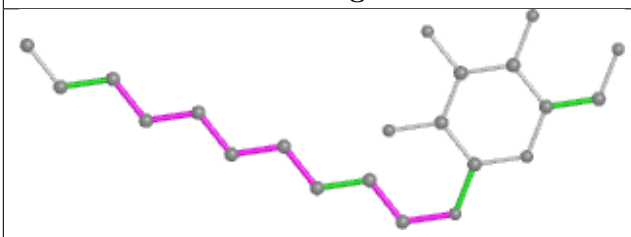
Ligand DMU C 317



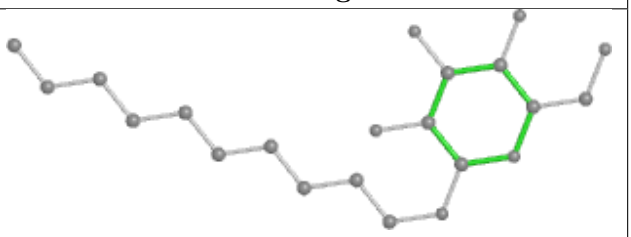
Bond lengths



Bond angles

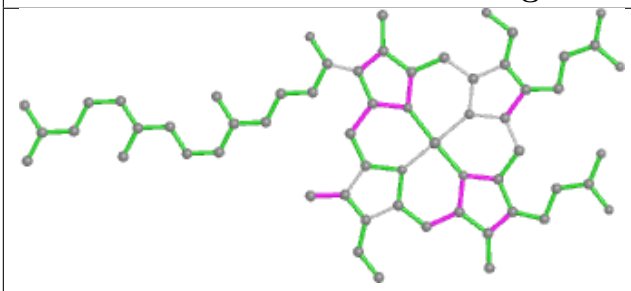


Torsions

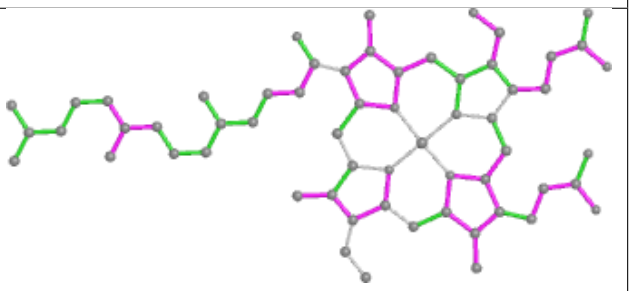


Rings

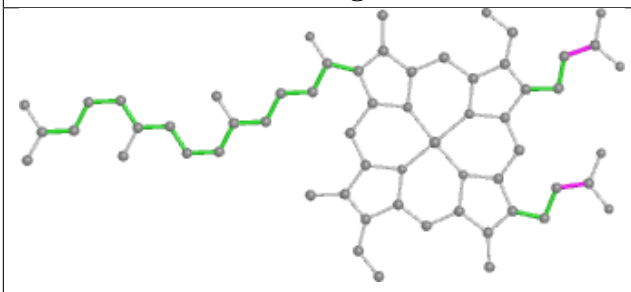
Ligand HEA A 602



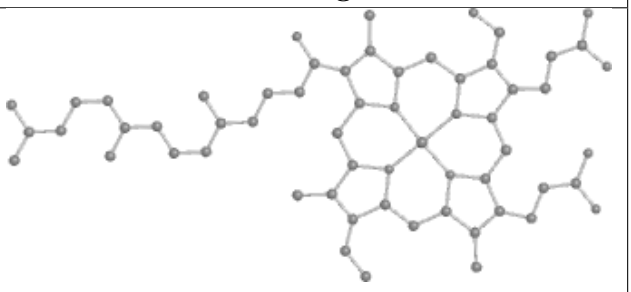
Bond lengths



Bond angles

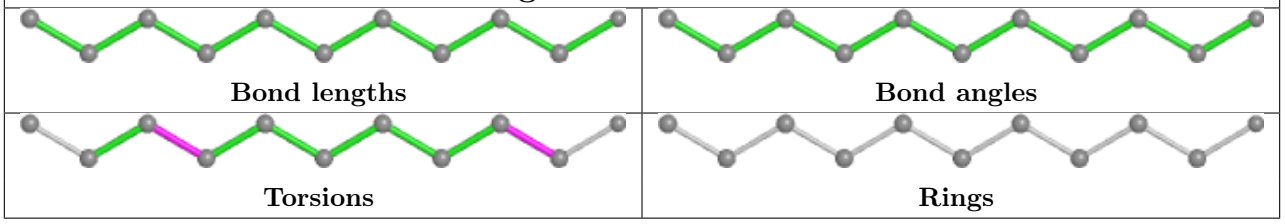


Torsions

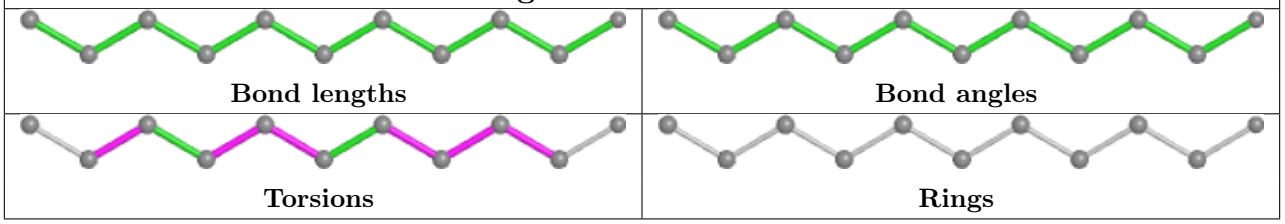


Rings

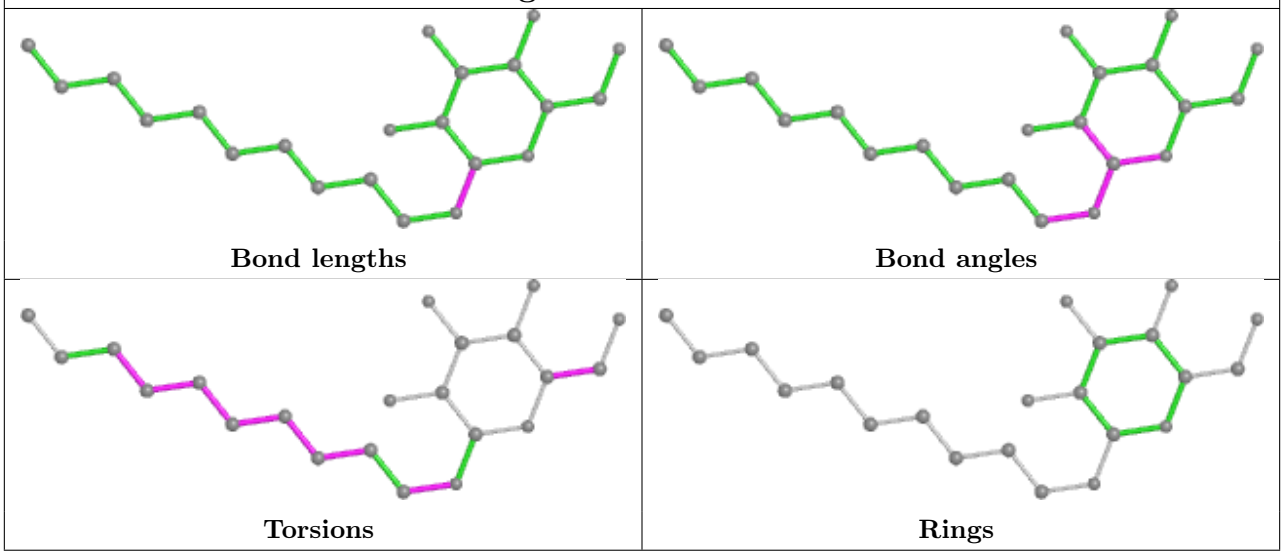
Ligand DMU P 307



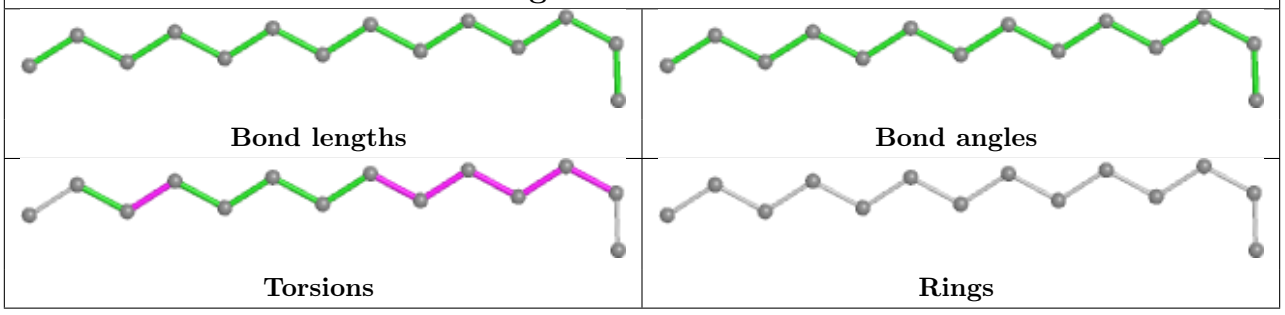
Ligand DMU A 617



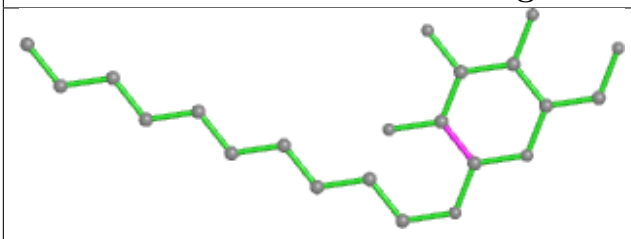
Ligand DMU P 317



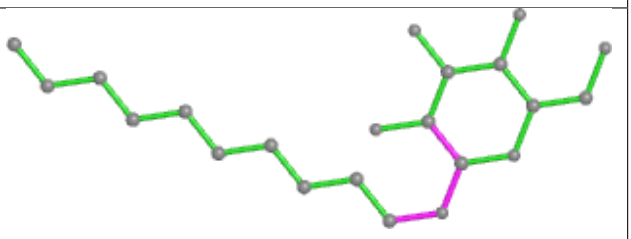
Ligand LFA T 102



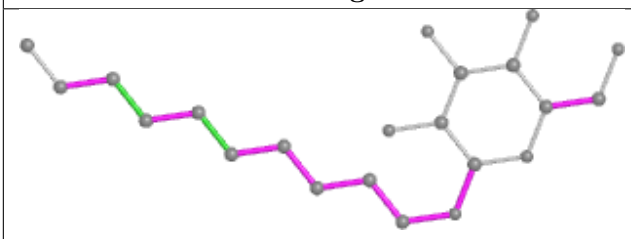
Ligand DMU C 323



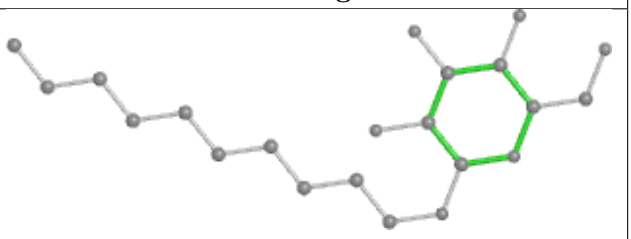
Bond lengths



Bond angles

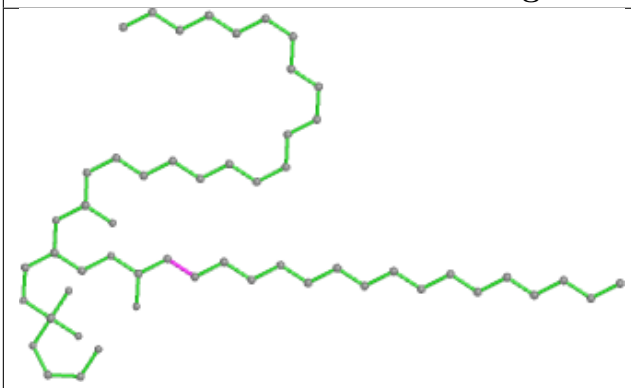


Torsions

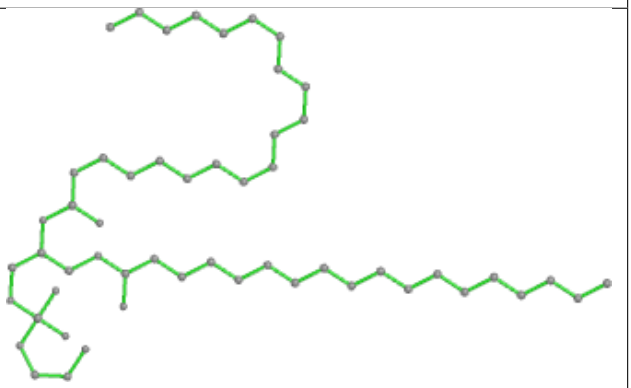


Rings

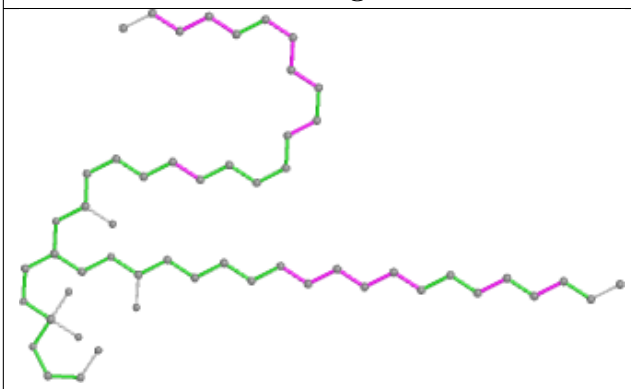
Ligand PEK G 101



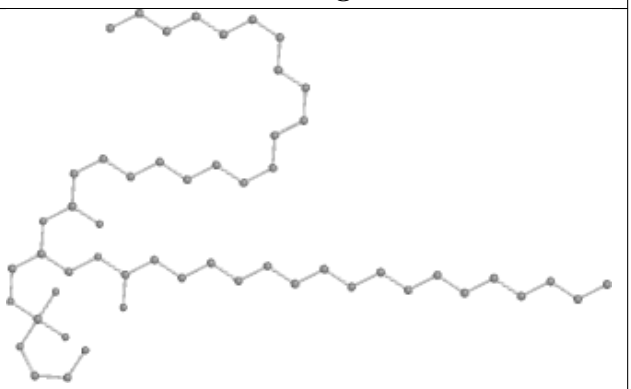
Bond lengths



Bond angles

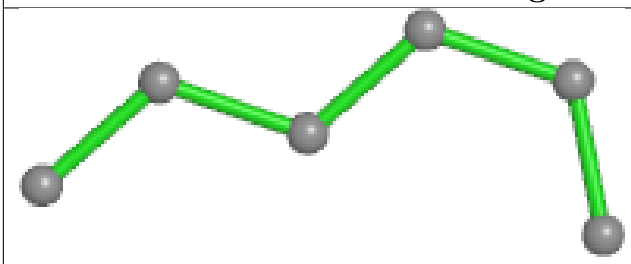


Torsions

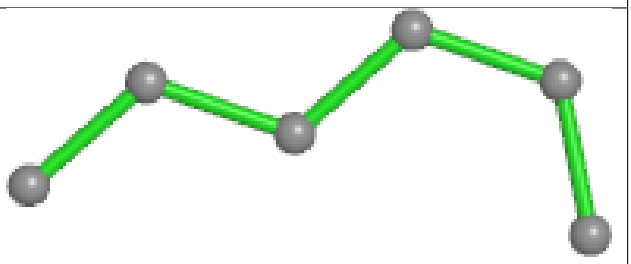


Rings

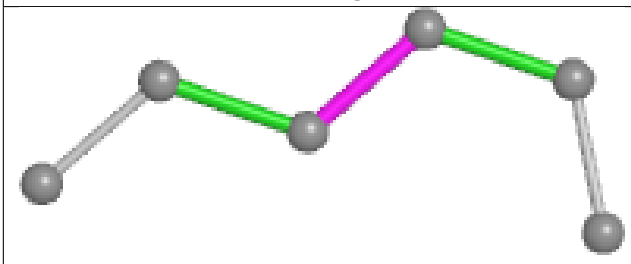
Ligand LFA P 309



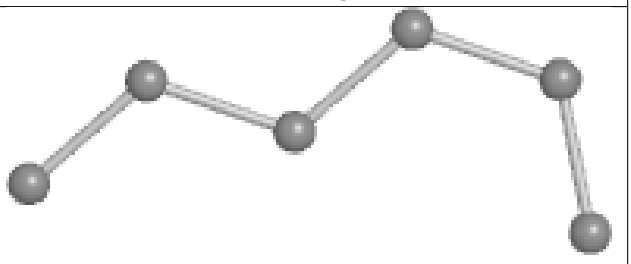
Bond lengths



Bond angles

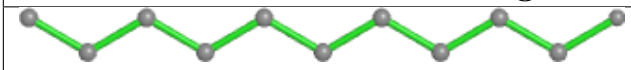


Torsions

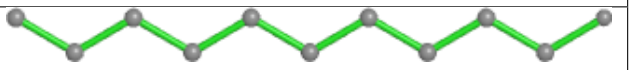


Rings

Ligand DMU O 307



Bond lengths

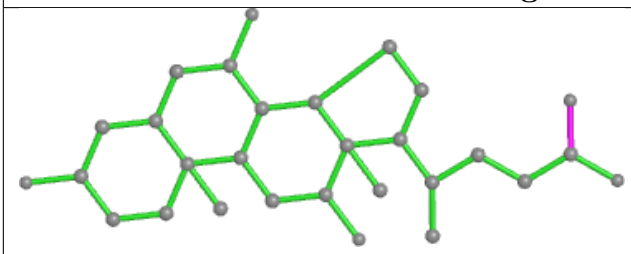


Bond angles

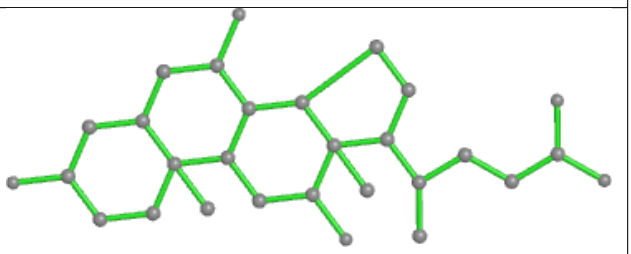
Torsions

Rings

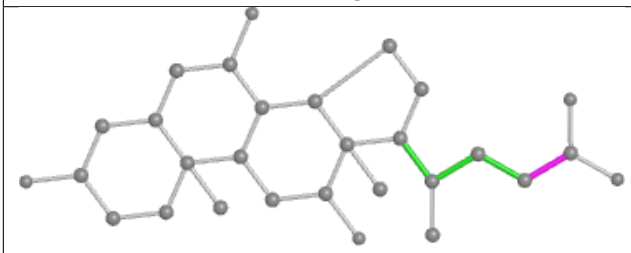
Ligand CHD C 301



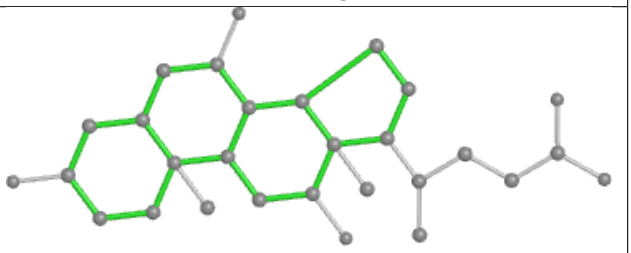
Bond lengths



Bond angles

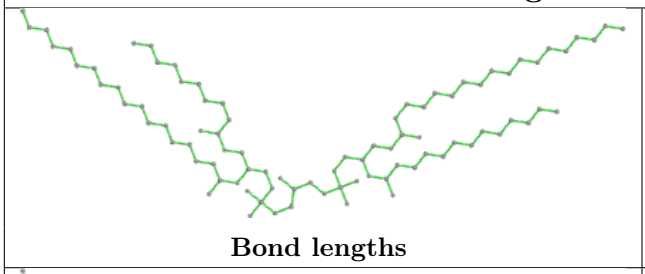


Torsions

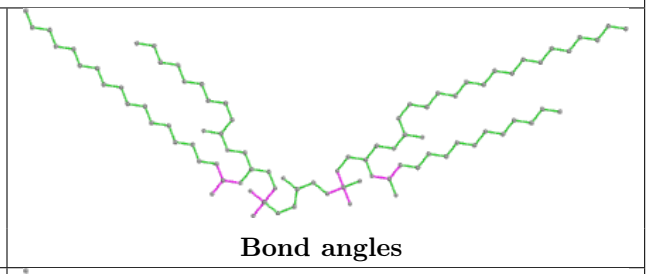


Rings

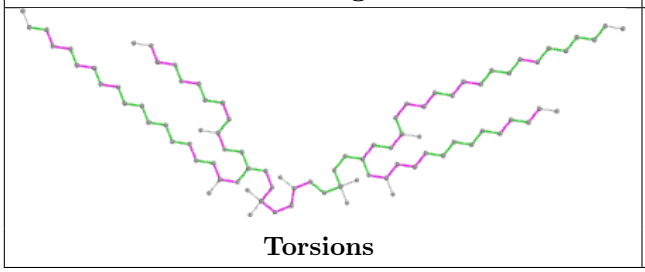
Ligand CDL C 304



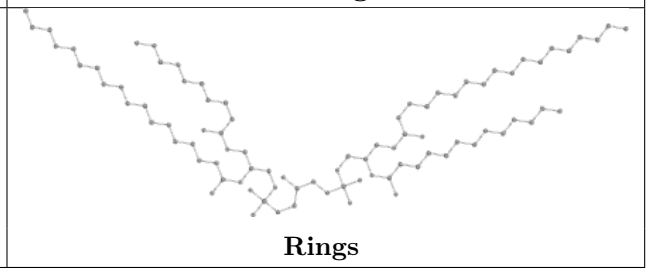
Bond lengths



Bond angles



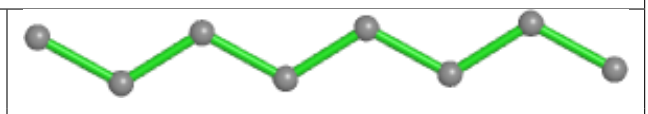
Torsions



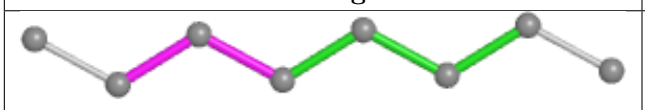
Rings

Ligand DMU Z 102

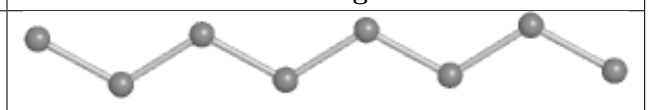
Bond lengths



Bond angles

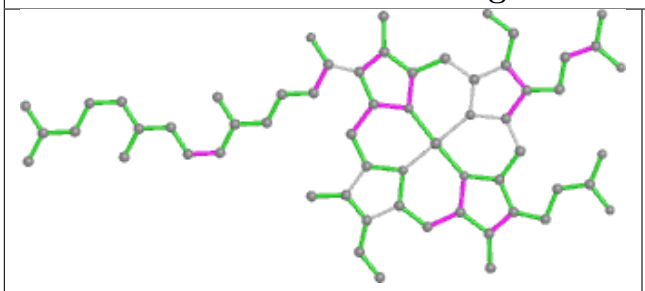


Torsions

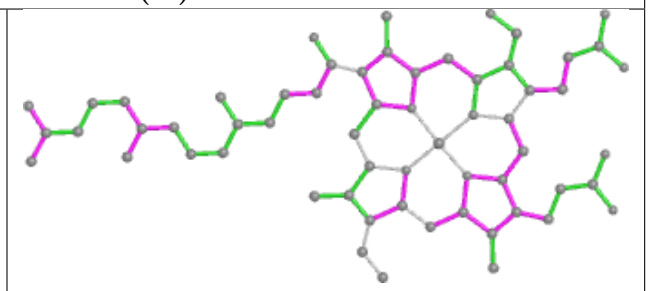


Rings

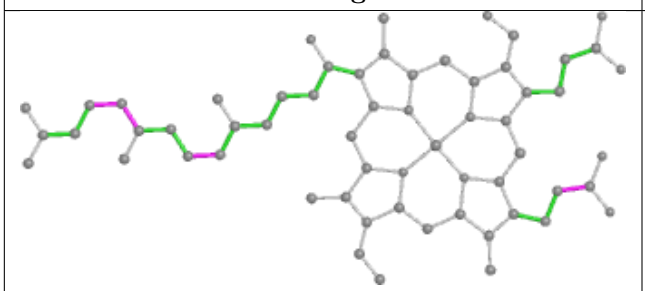
Ligand HEA N 603 (A)



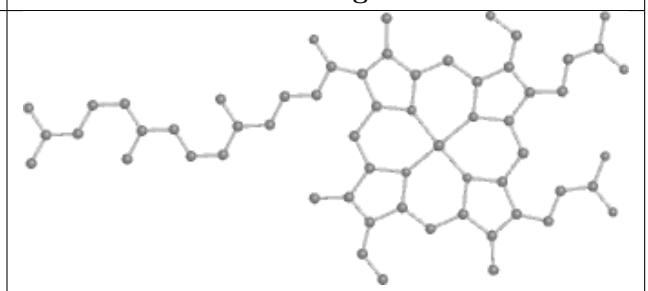
Bond lengths



Bond angles

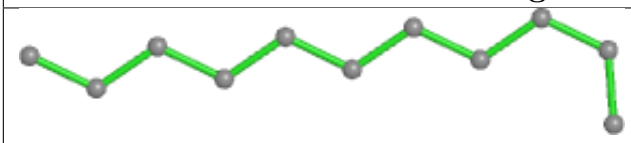


Torsions

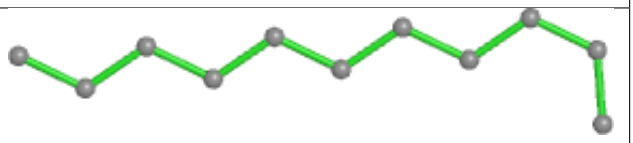


Rings

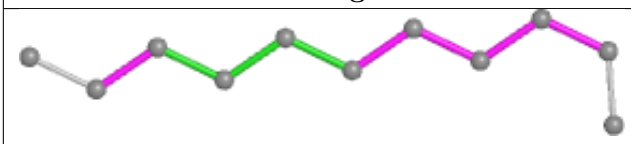
Ligand LFA P 312



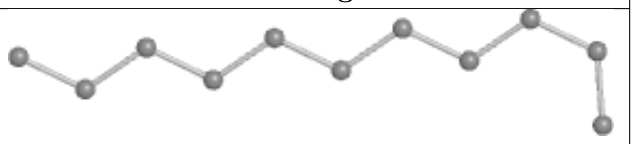
Bond lengths



Bond angles

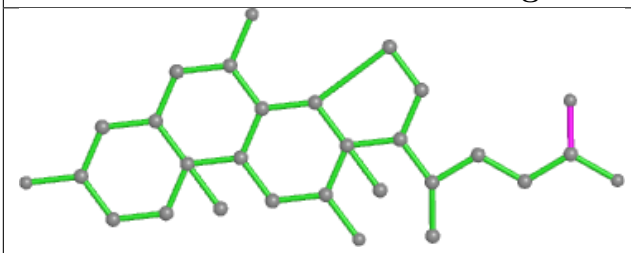


Torsions

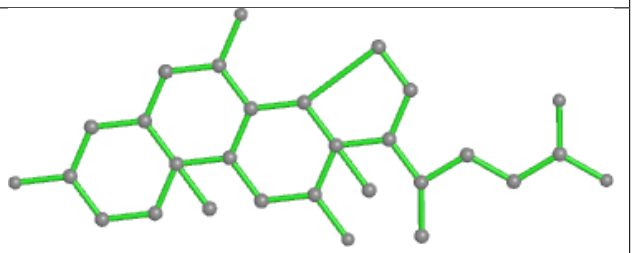


Rings

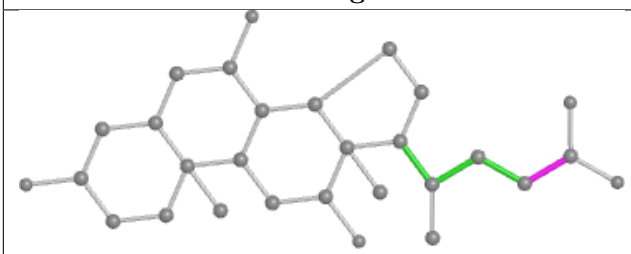
Ligand CHD P 302



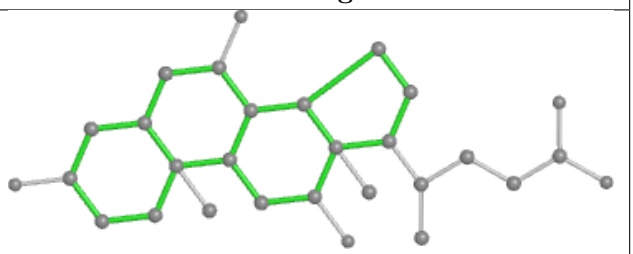
Bond lengths



Bond angles

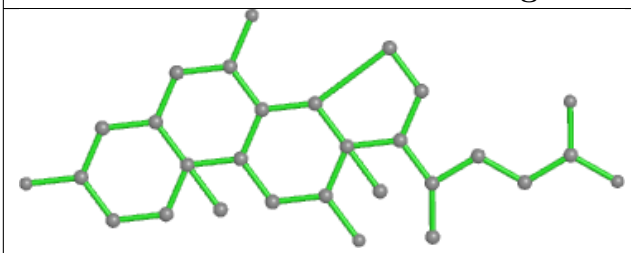


Torsions

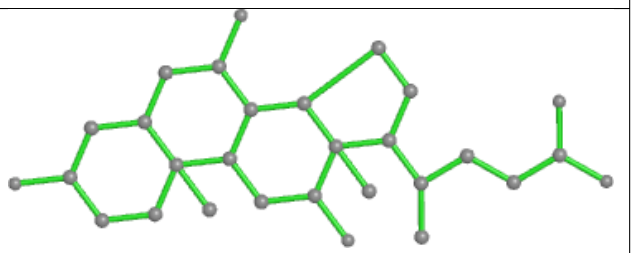


Rings

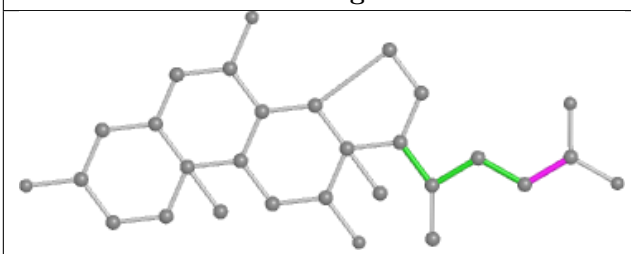
Ligand CHD O 301



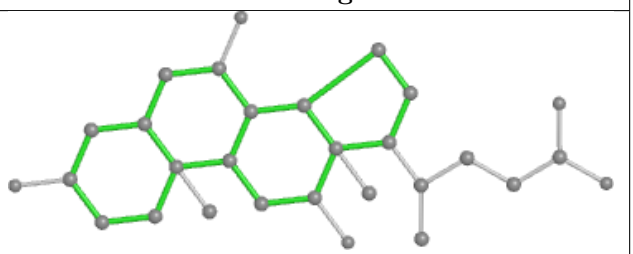
Bond lengths



Bond angles

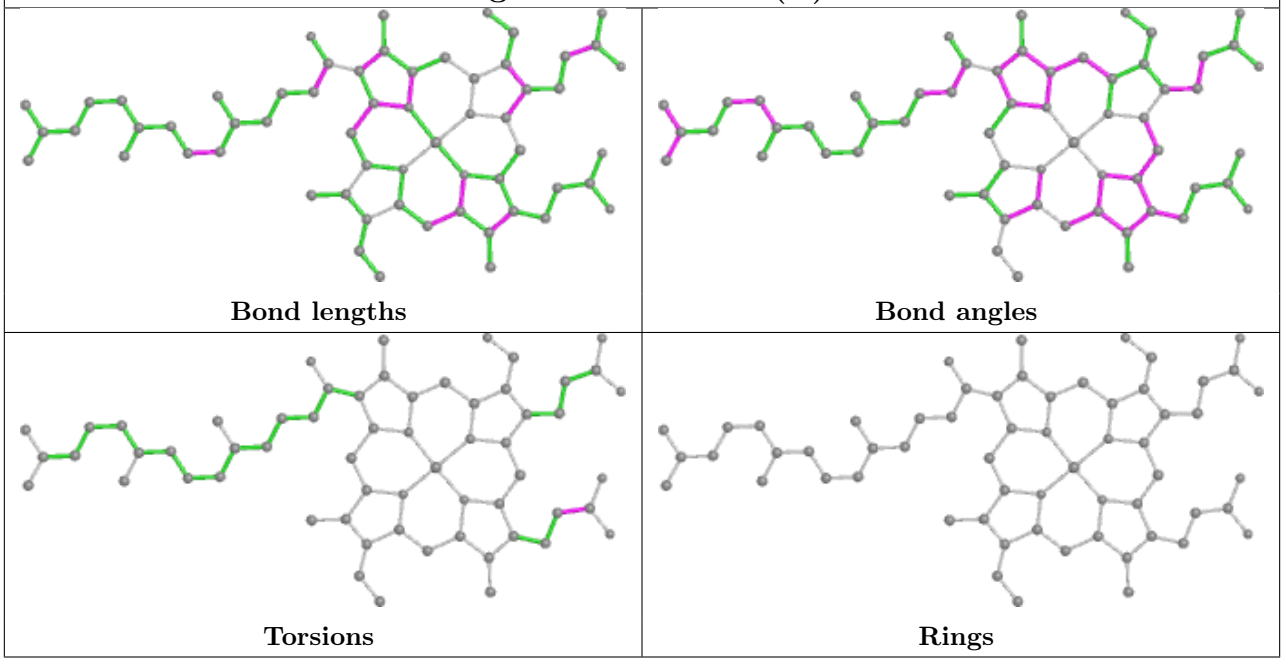


Torsions

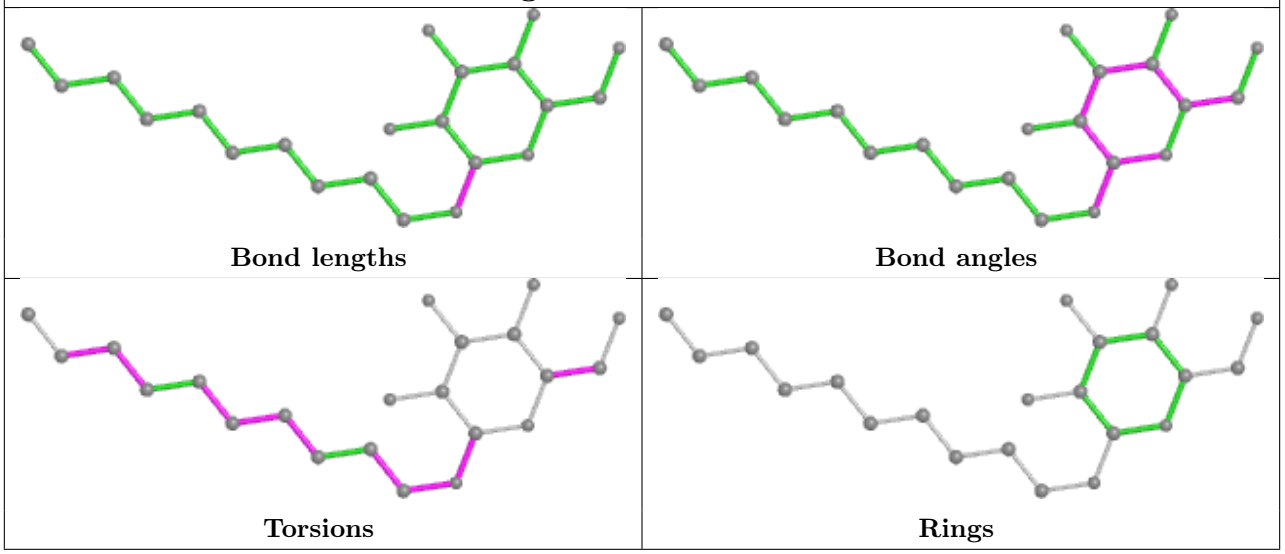


Rings

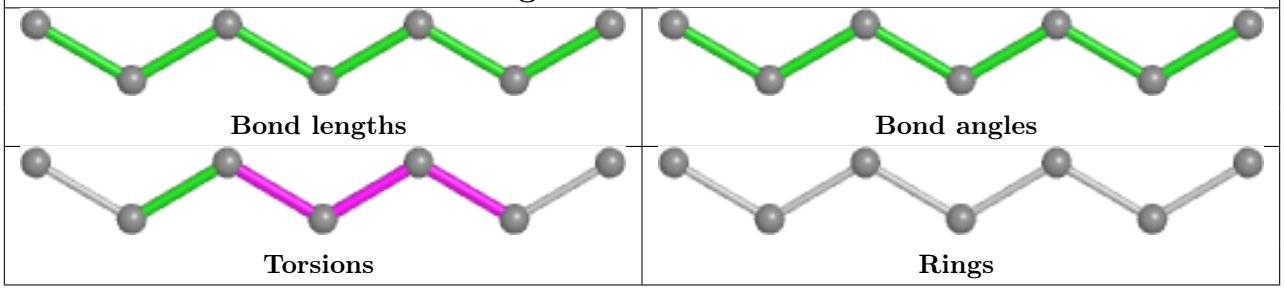
Ligand HEA N 603 (B)



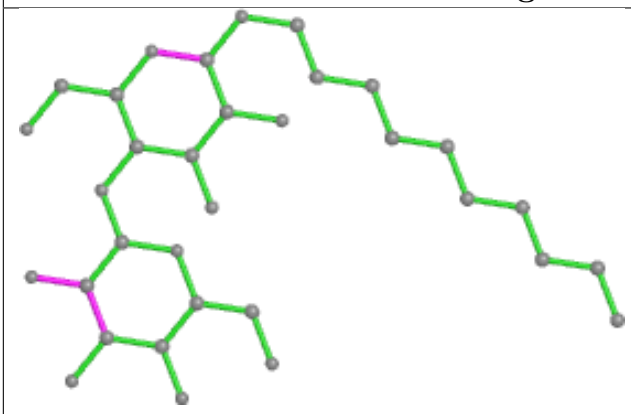
Ligand DMU L 102



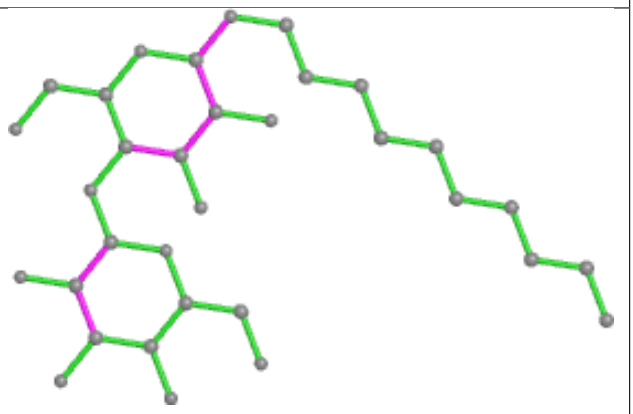
Ligand DMU P 316



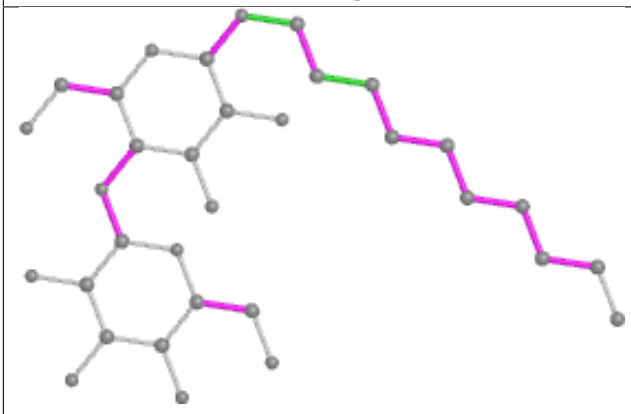
Ligand DMU P 318



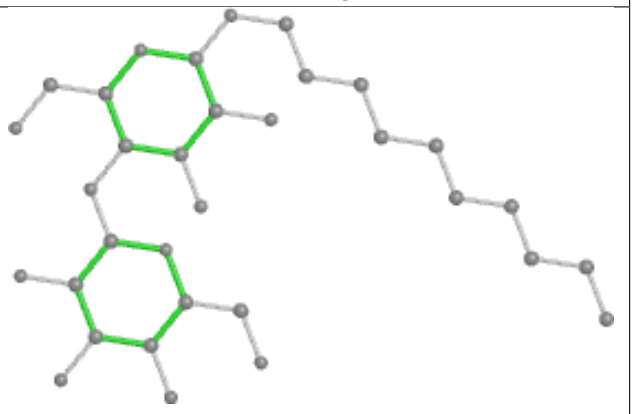
Bond lengths



Bond angles

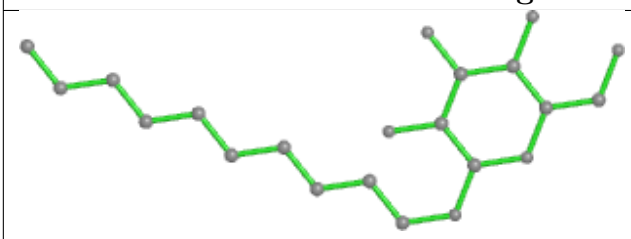


Torsions

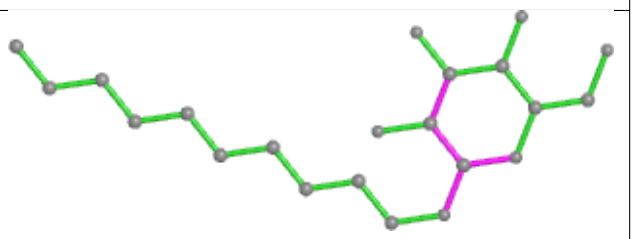


Rings

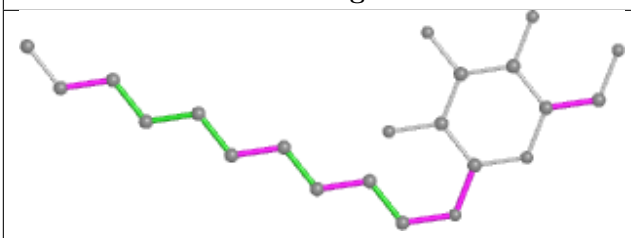
Ligand DMU O 303



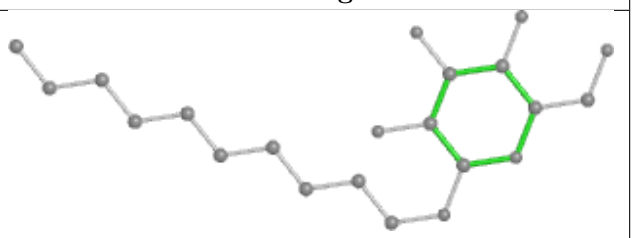
Bond lengths



Bond angles

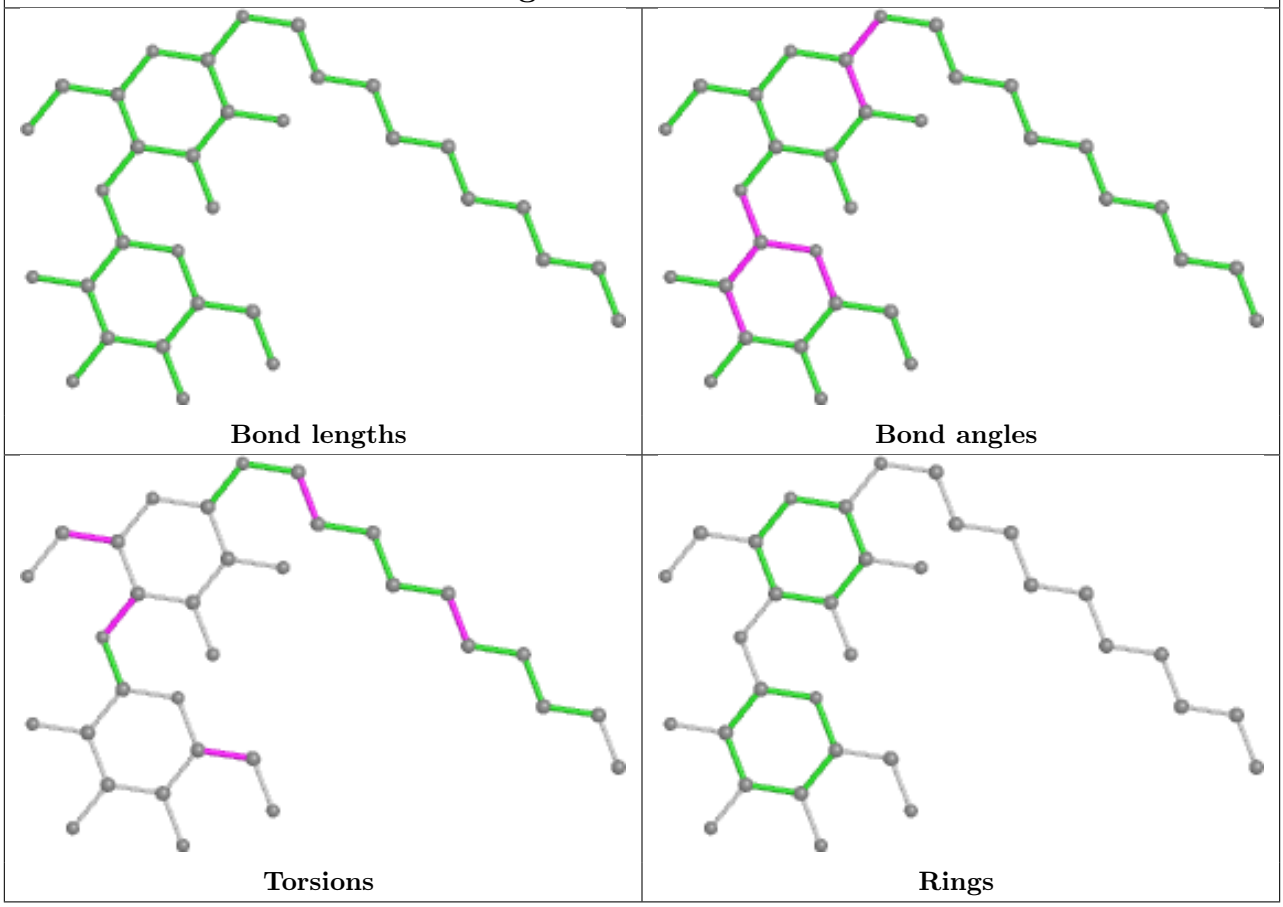


Torsions

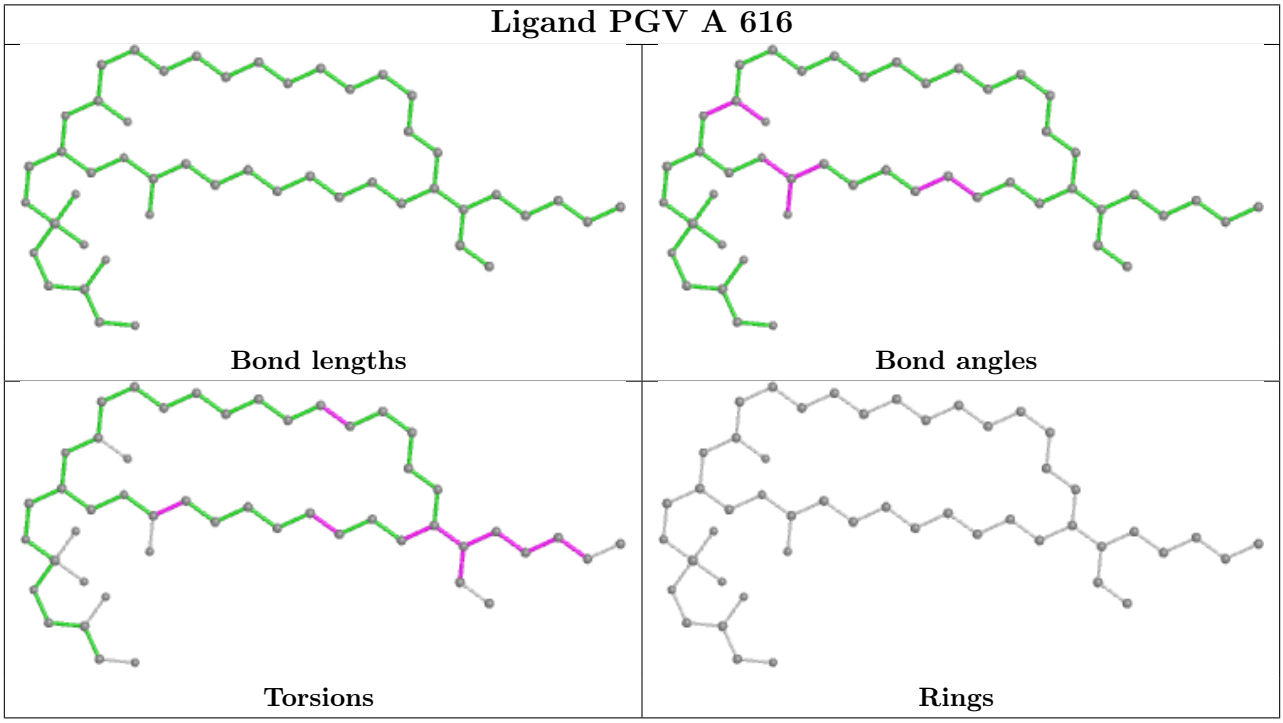


Rings

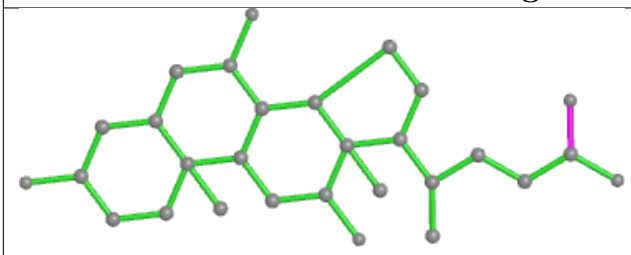
Ligand DMU P 324



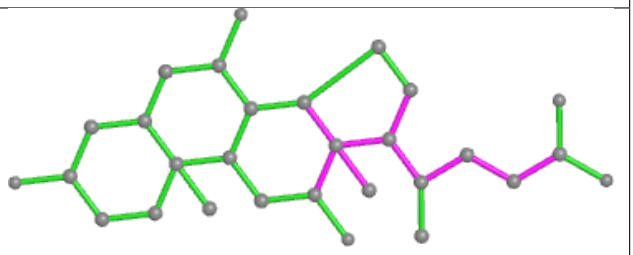
Ligand PGV A 616



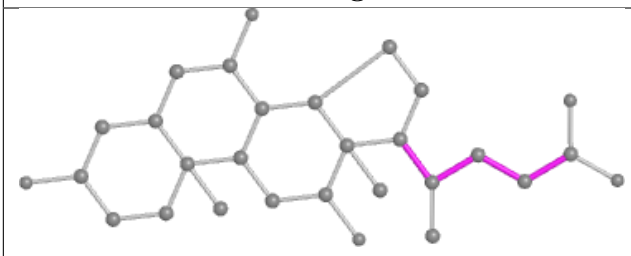
Ligand CHD P 306



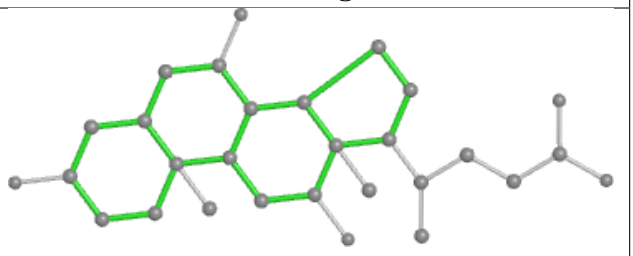
Bond lengths



Bond angles

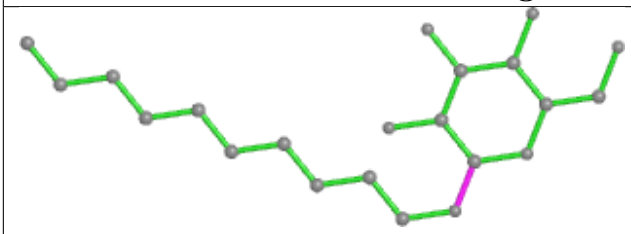


Torsions

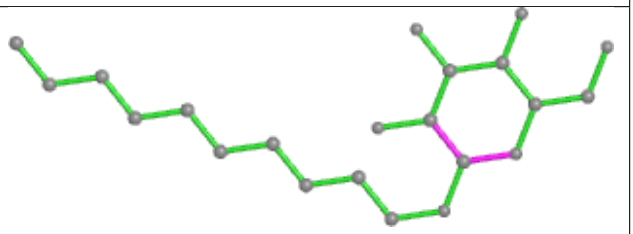


Rings

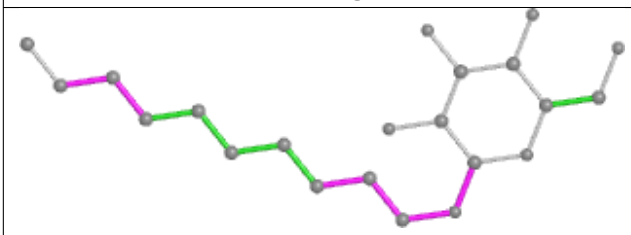
Ligand DMU B 303



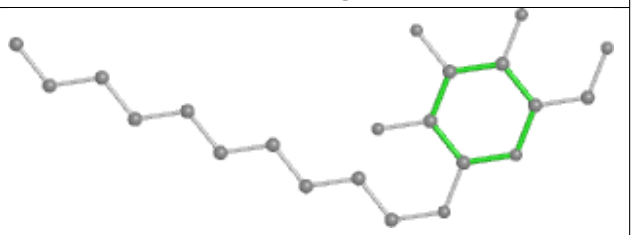
Bond lengths



Bond angles

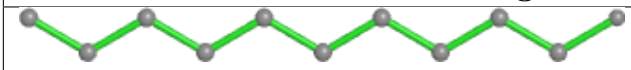


Torsions

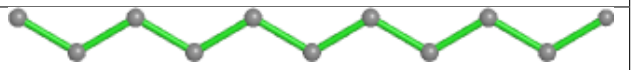


Rings

Ligand DMU N 602



Bond lengths

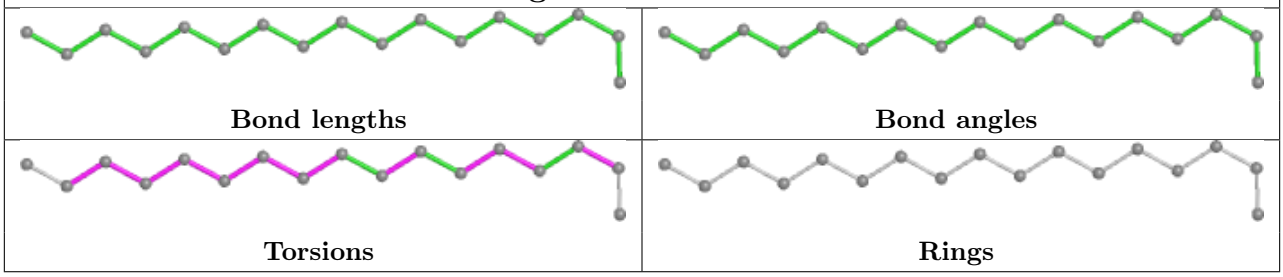


Bond angles

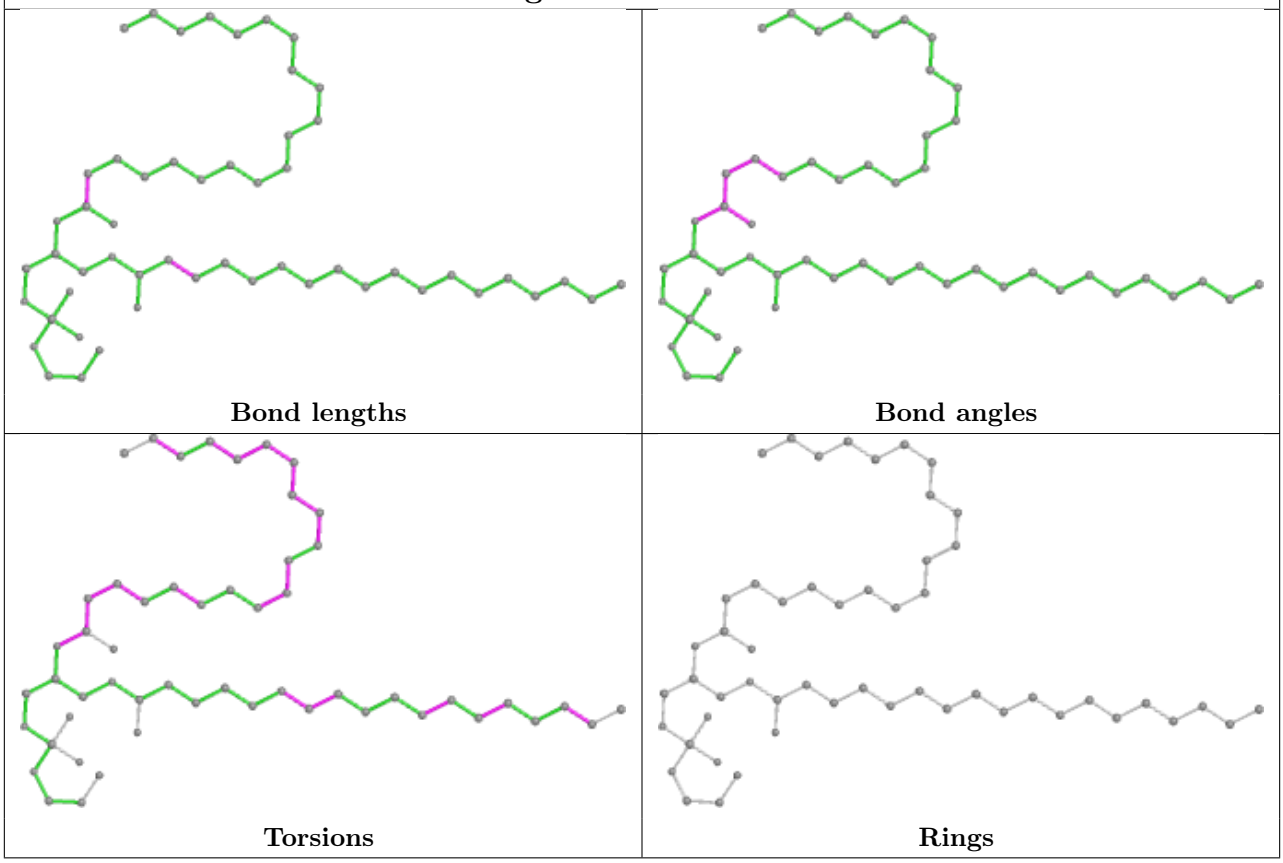
Torsions

Rings

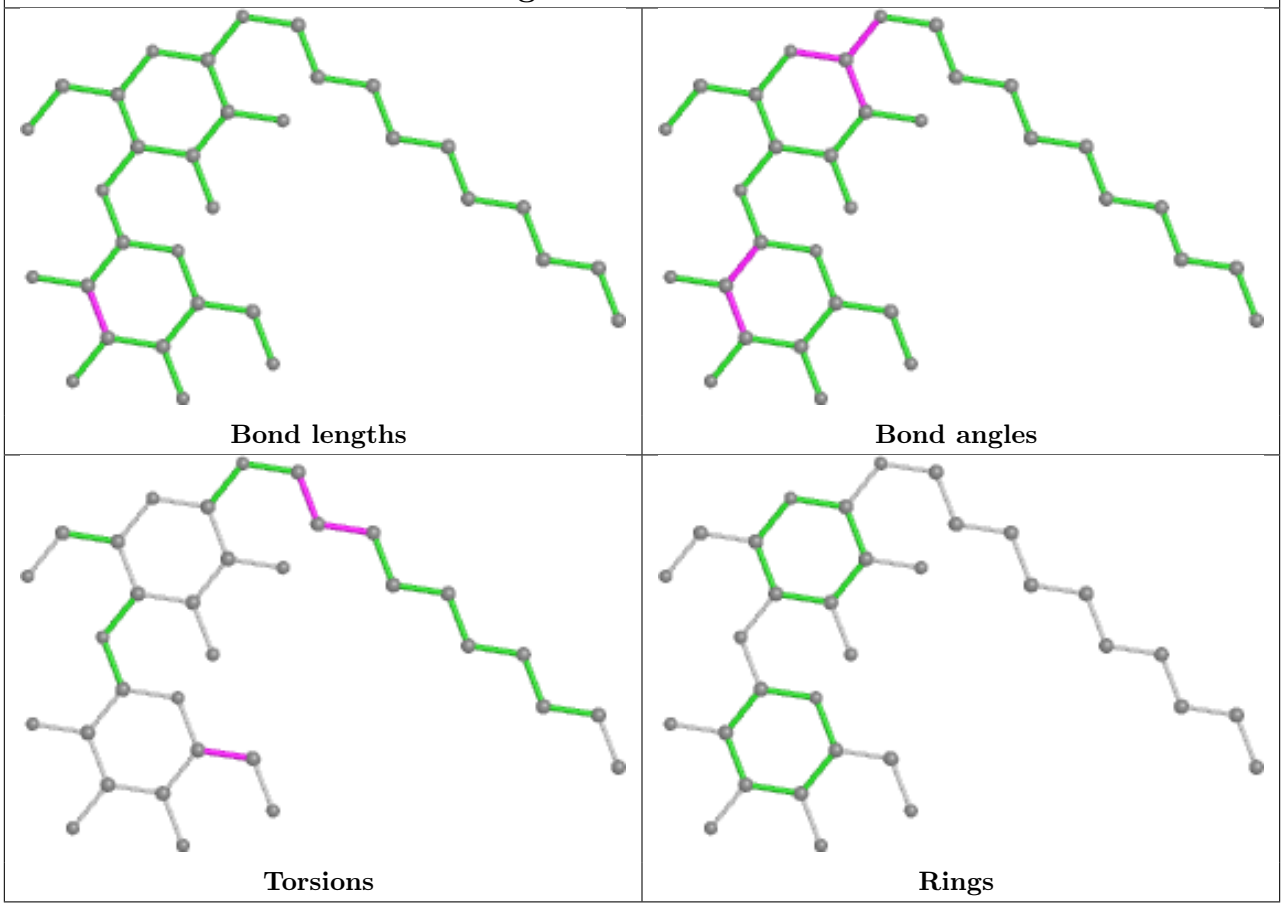
Ligand LFA B 306



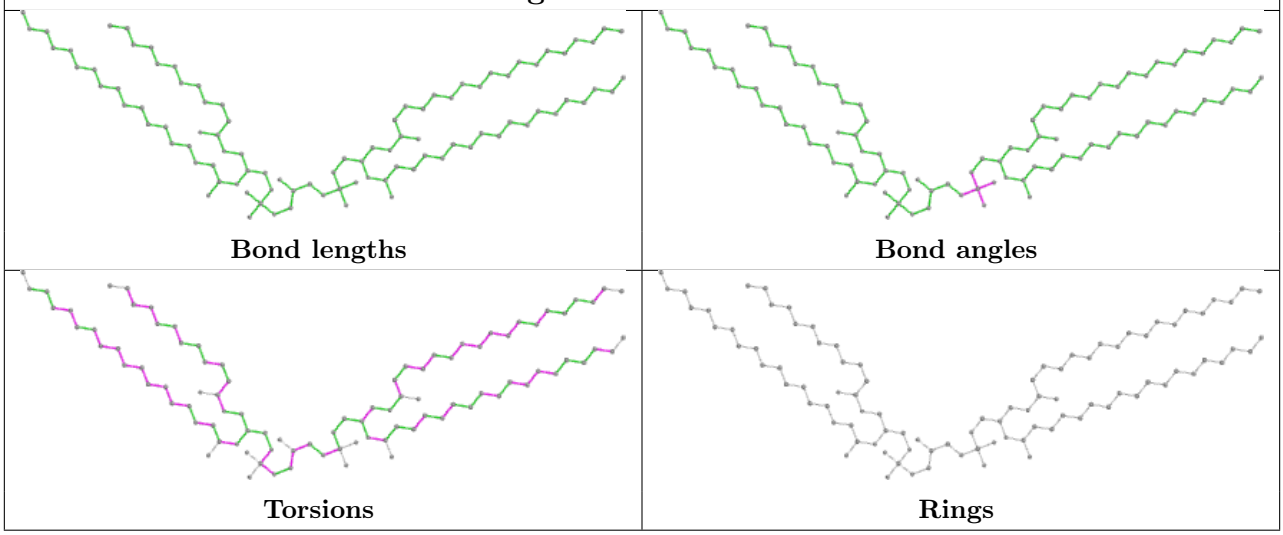
Ligand PEK T 101



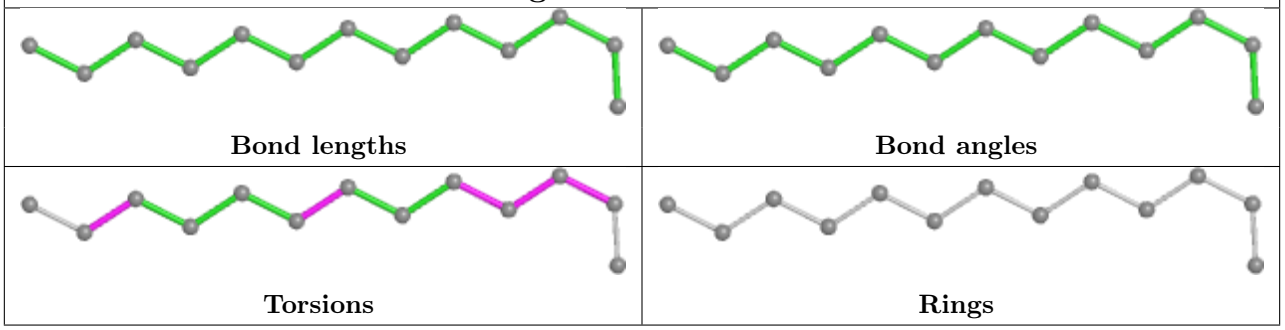
Ligand DMU C 324



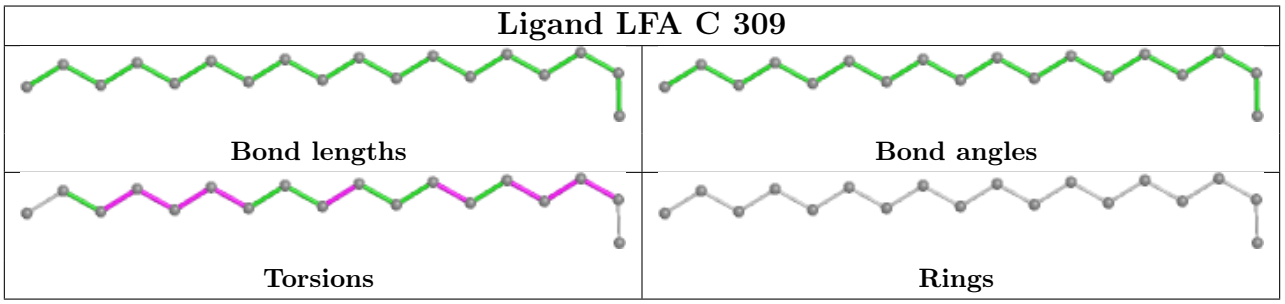
Ligand CDL L 101



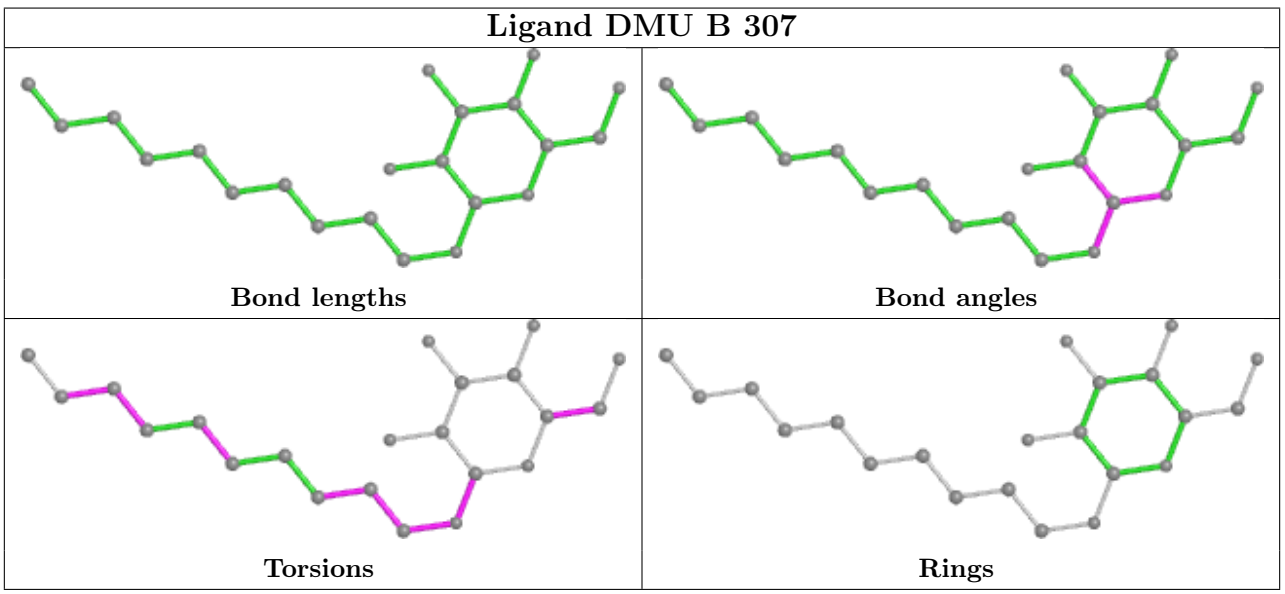
Ligand LFA C 314



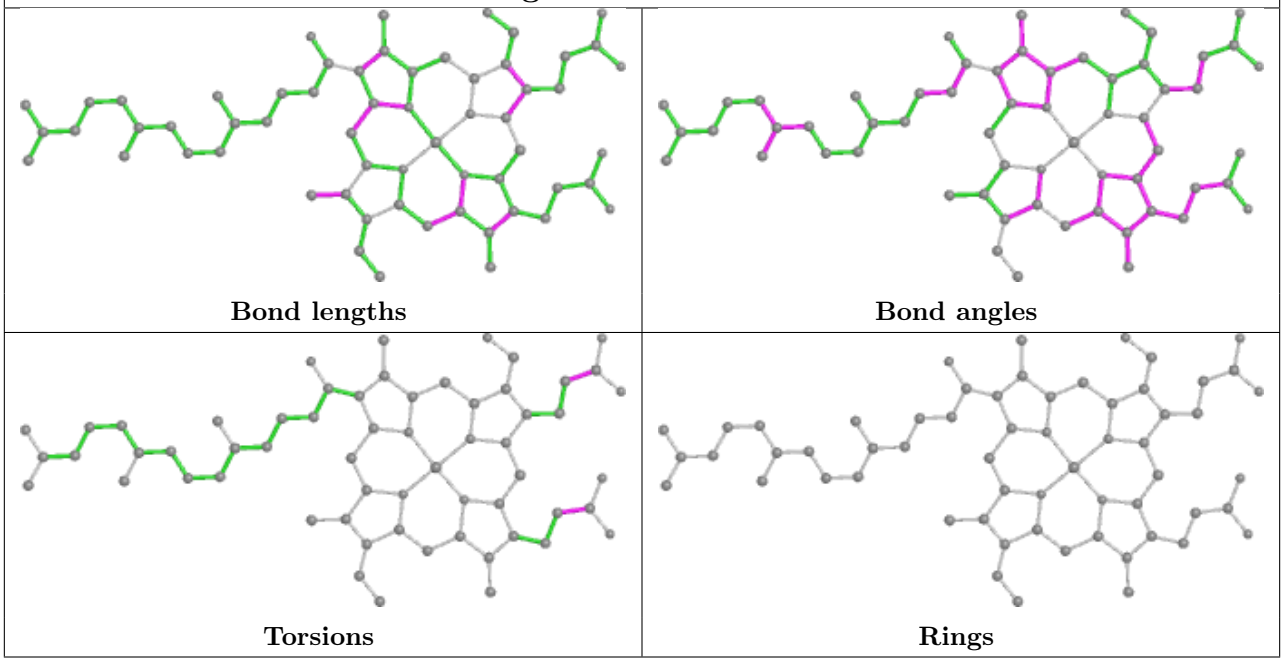
Ligand LFA C 309



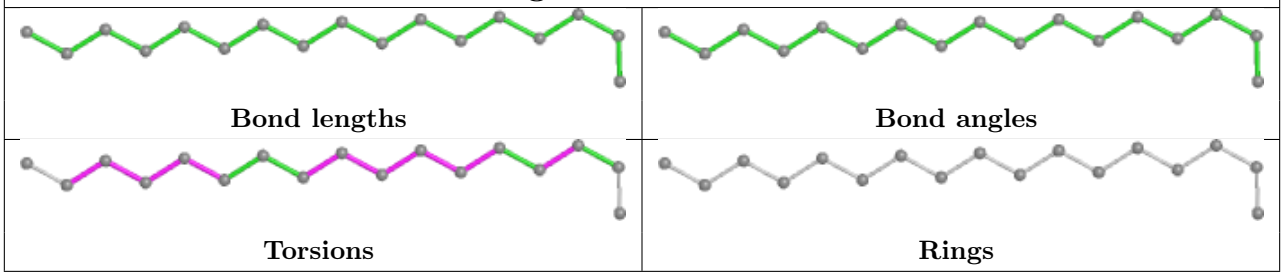
Ligand DMU B 307



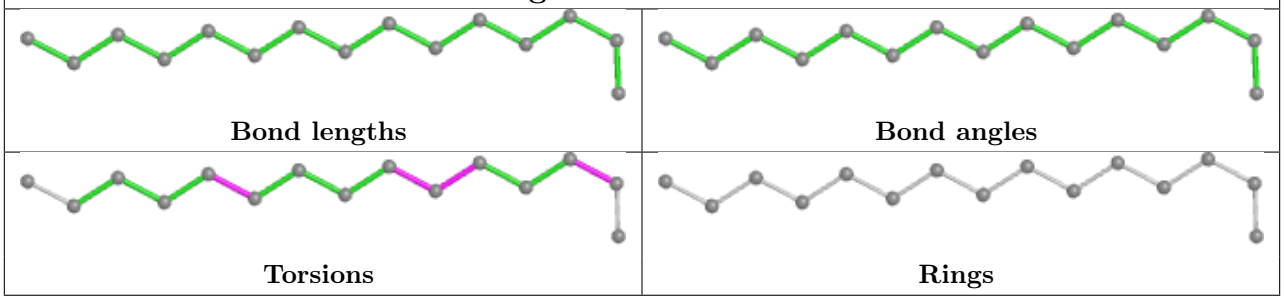
Ligand HEA N 604



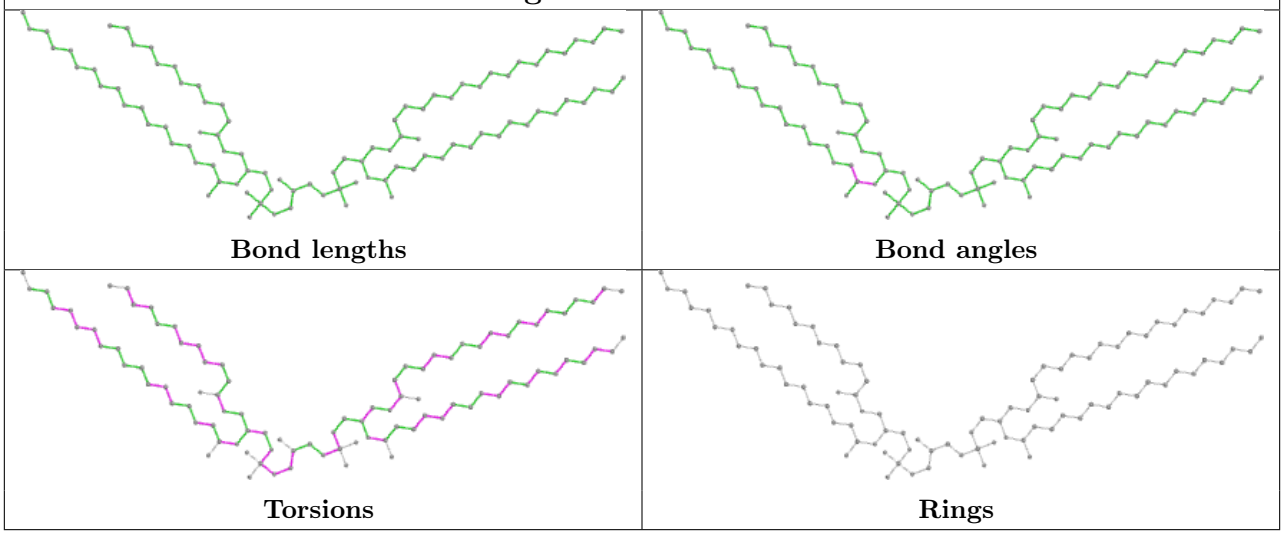
Ligand LFA N 601



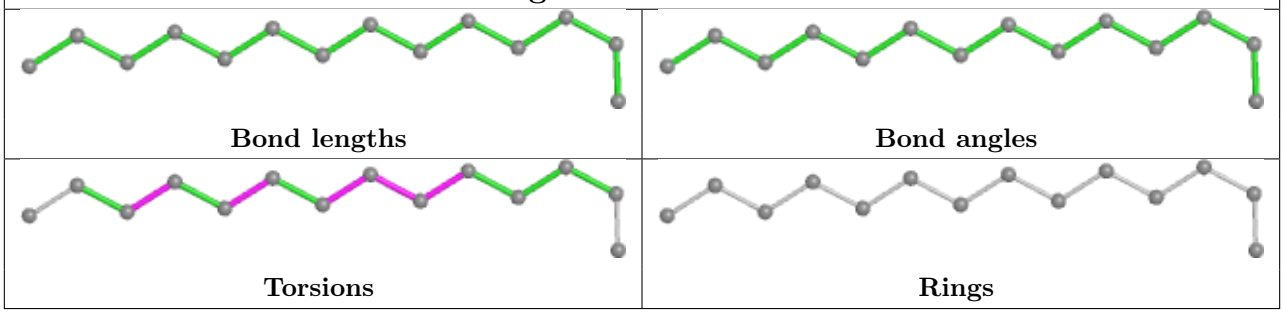
Ligand LFA C 313



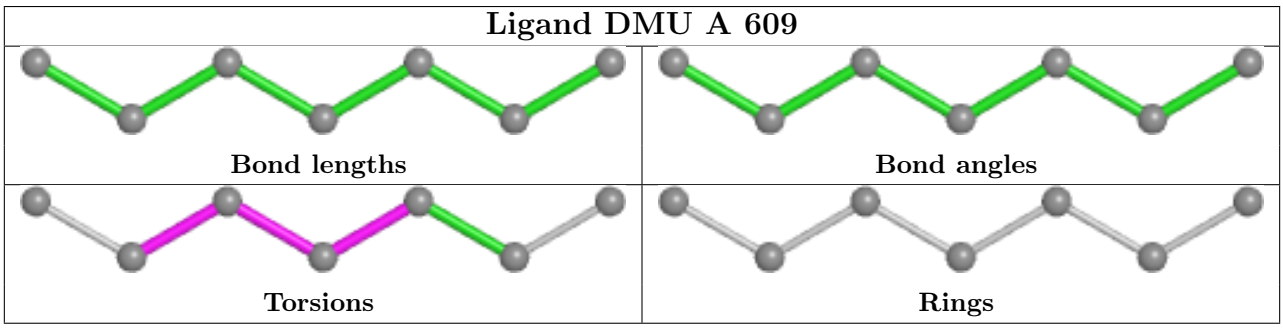
Ligand CDL Y 101



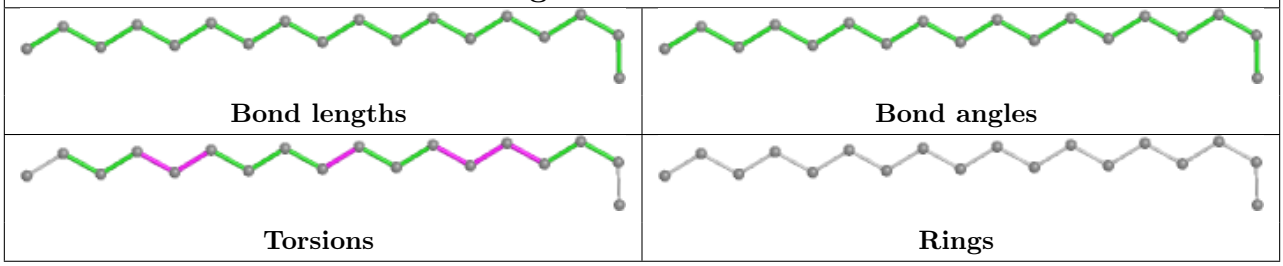
Ligand LFA C 311



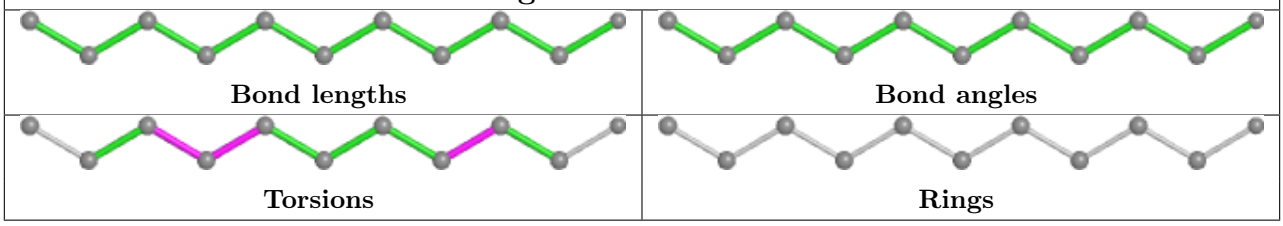
Ligand DMU A 609



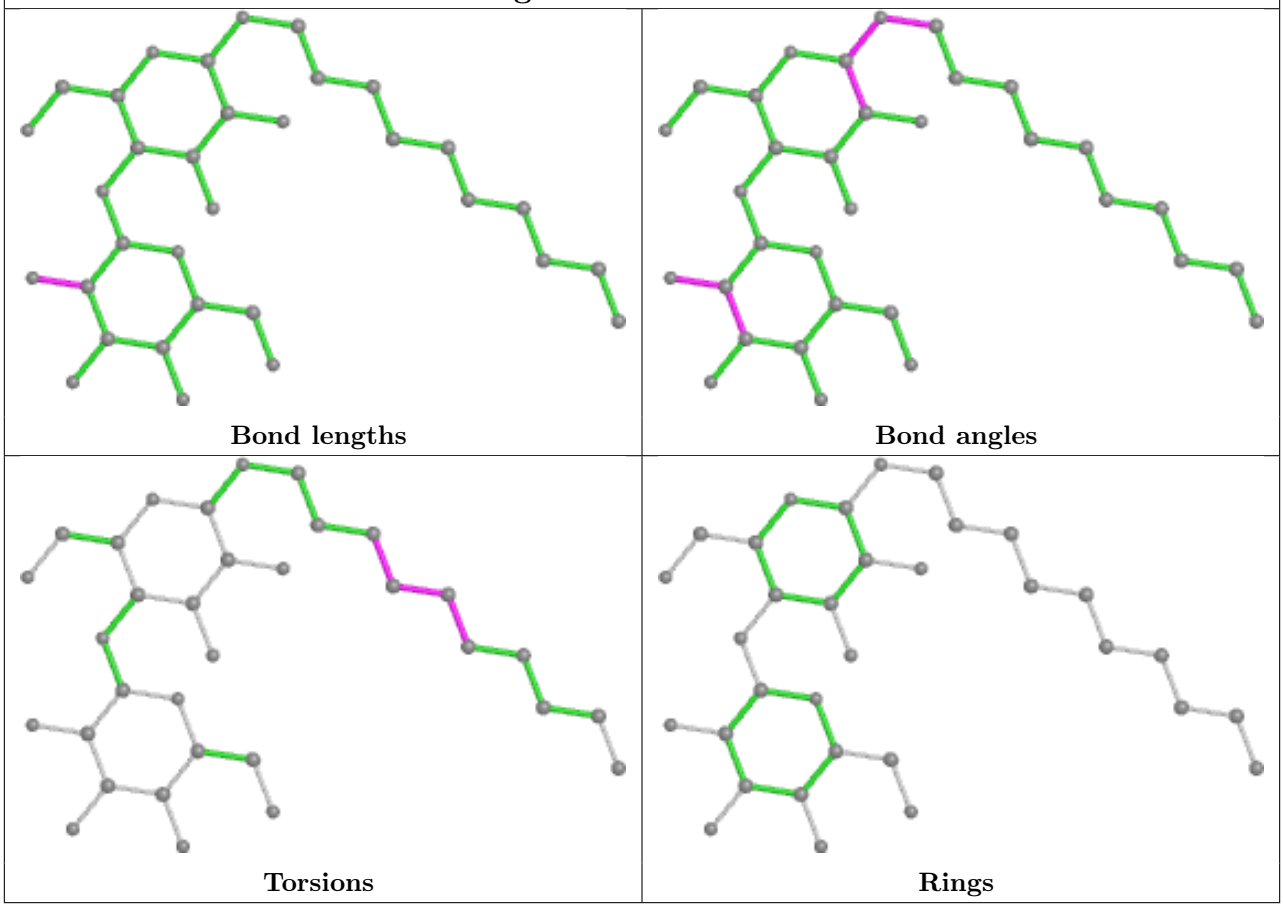
Ligand LFA P 310



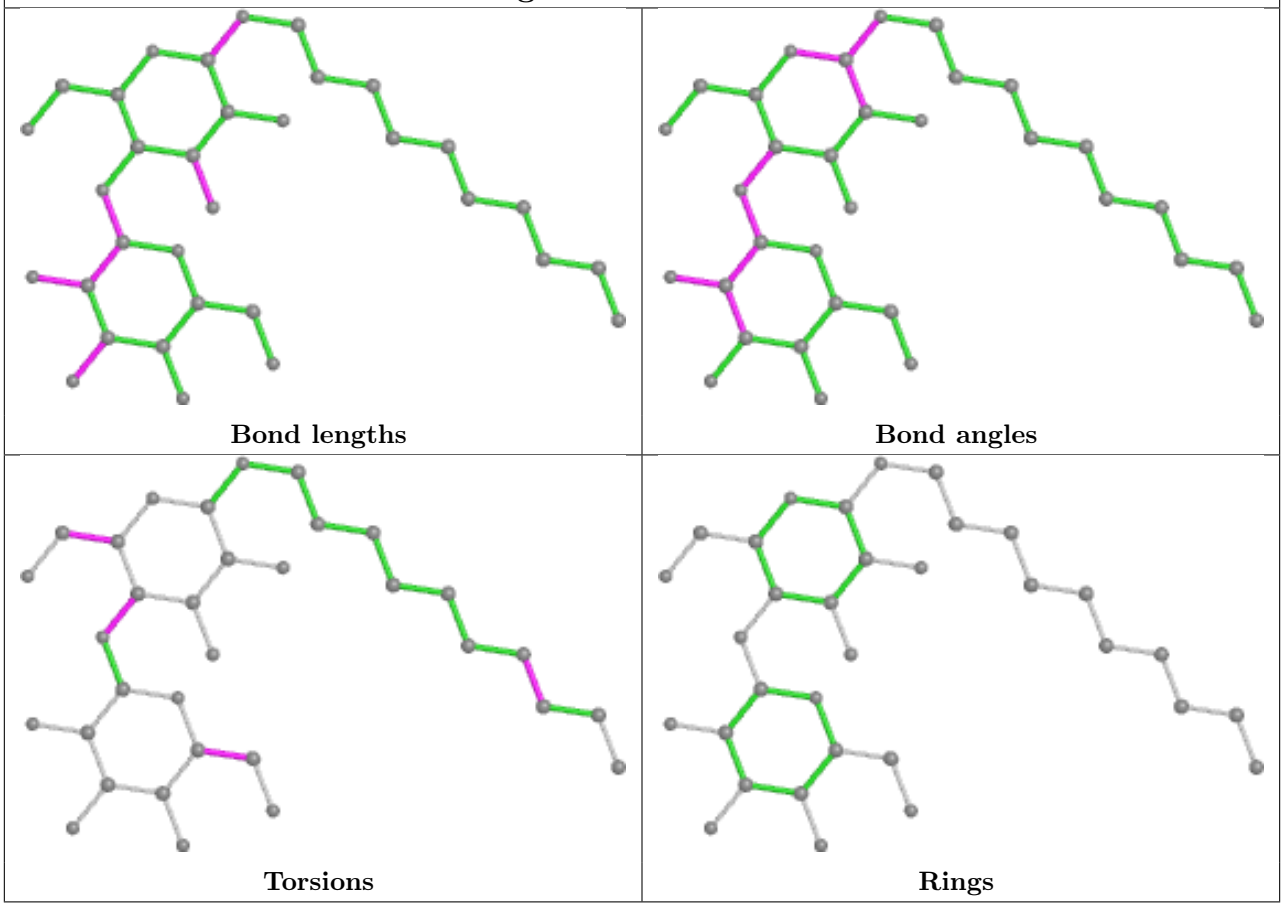
Ligand DMU C 306



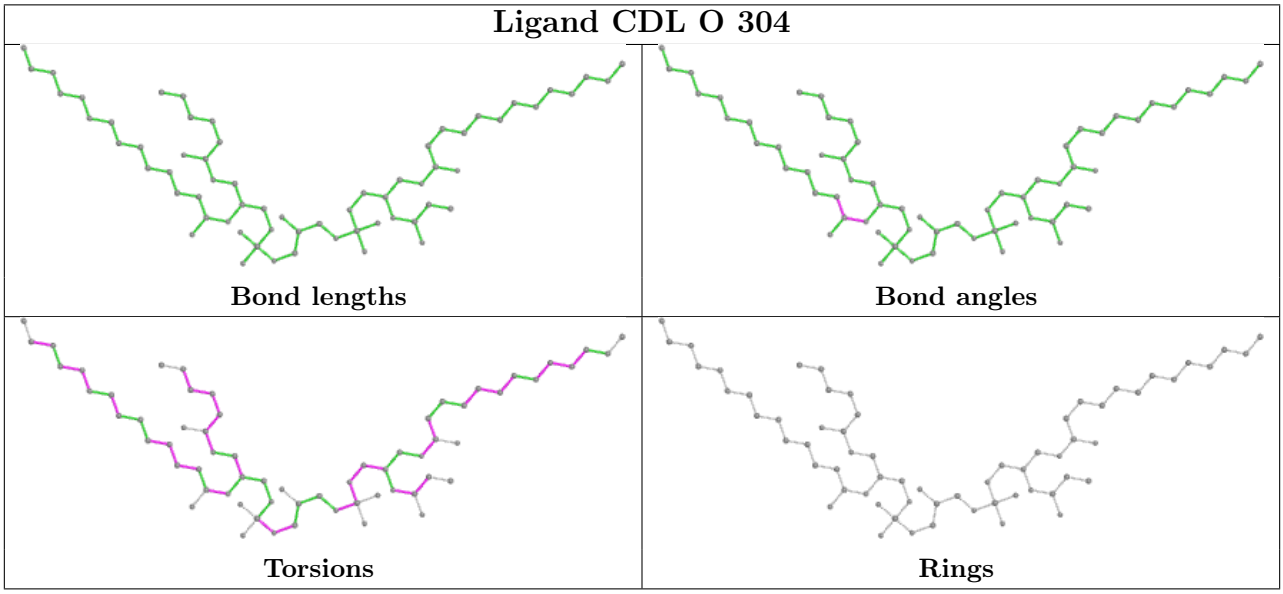
Ligand DMU M 101



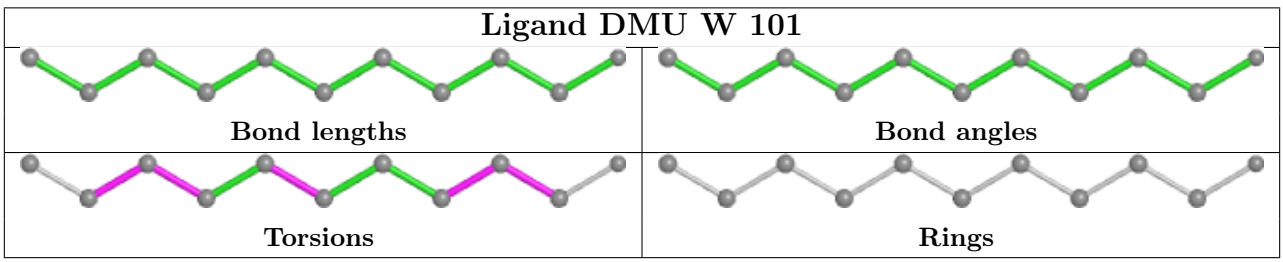
Ligand DMU A 610



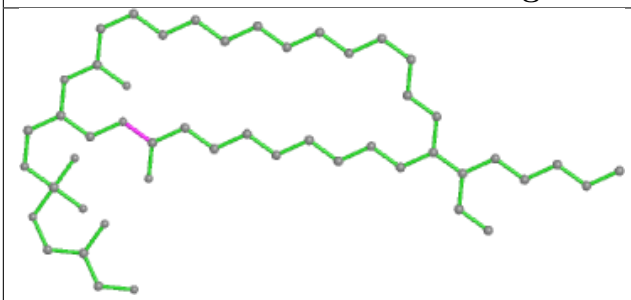
Ligand CDL O 304



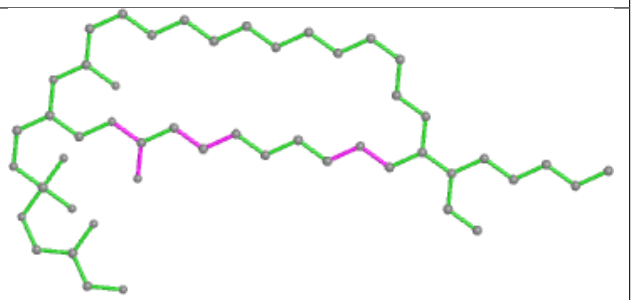
Ligand DMU W 101



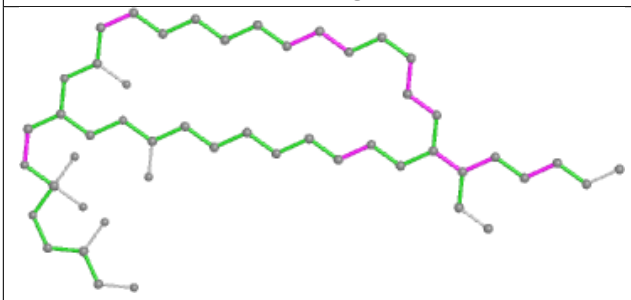
Ligand PGV P 304



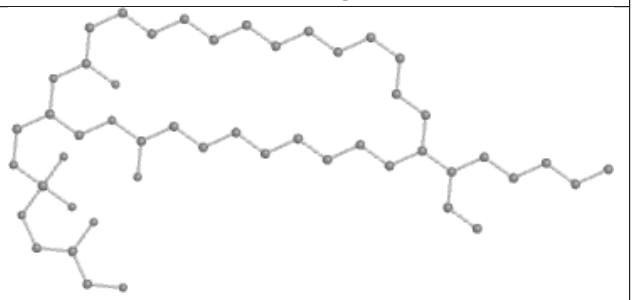
Bond lengths



Bond angles

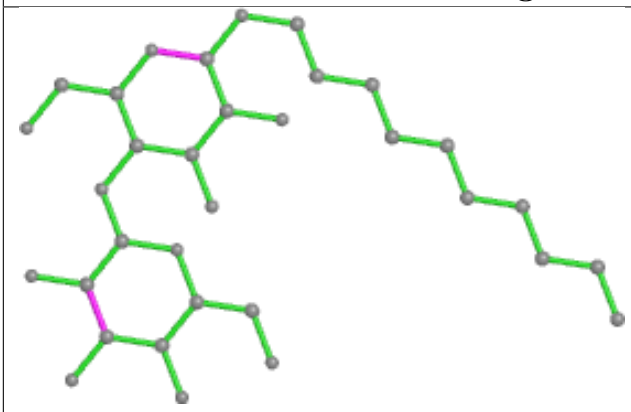


Torsions

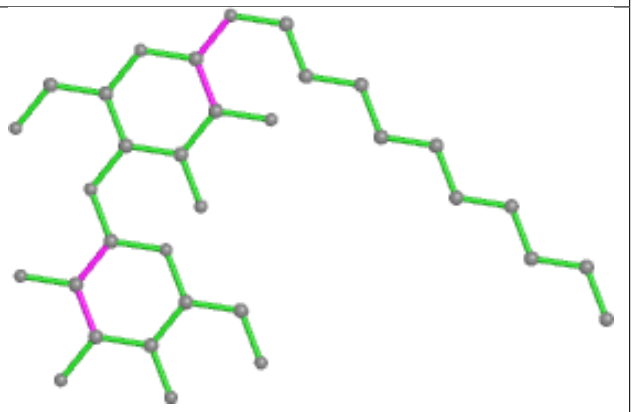


Rings

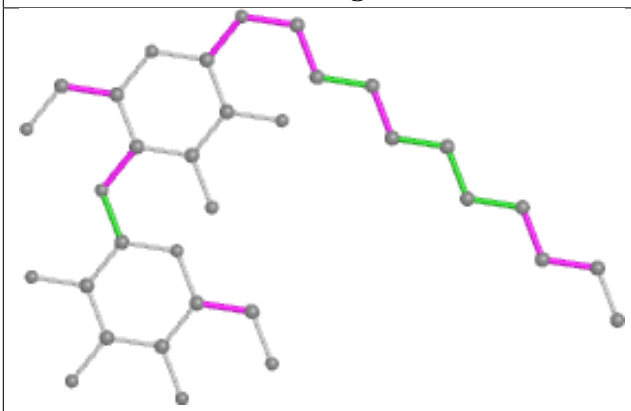
Ligand DMU C 318



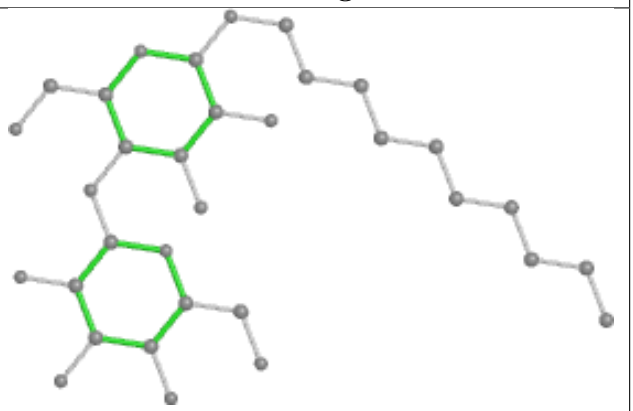
Bond lengths



Bond angles

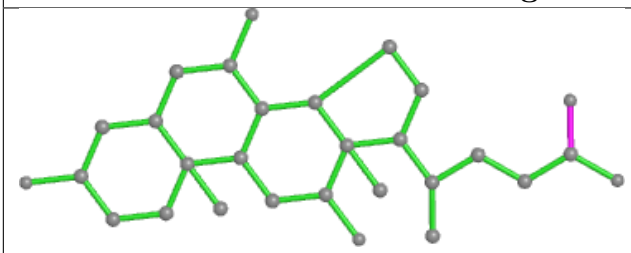


Torsions

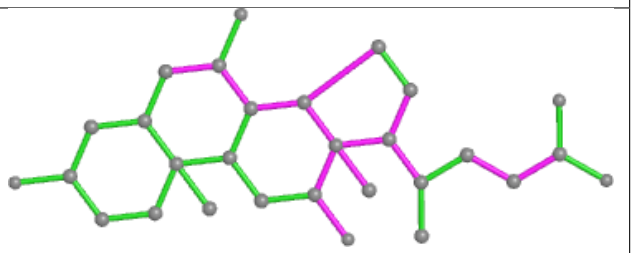


Rings

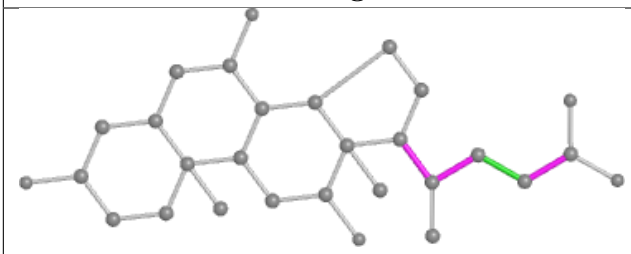
Ligand CHD C 305



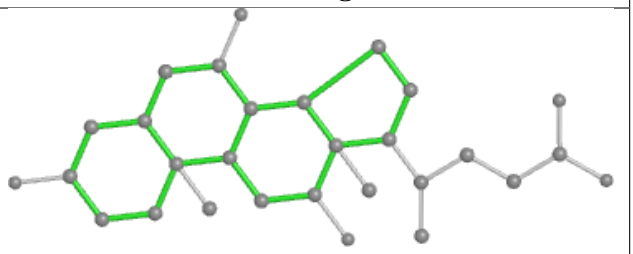
Bond lengths



Bond angles

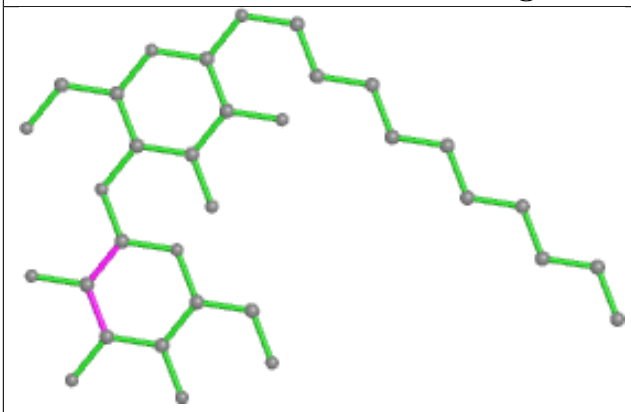


Torsions

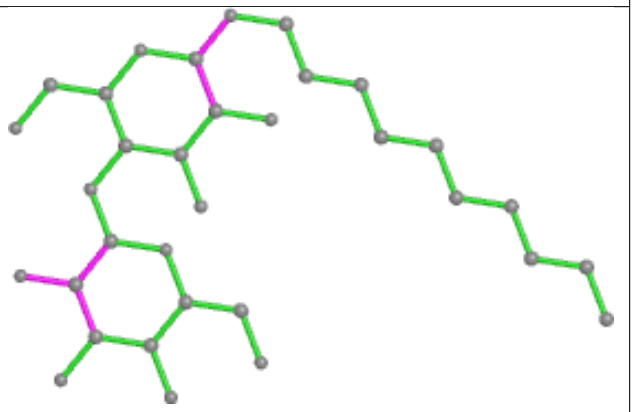


Rings

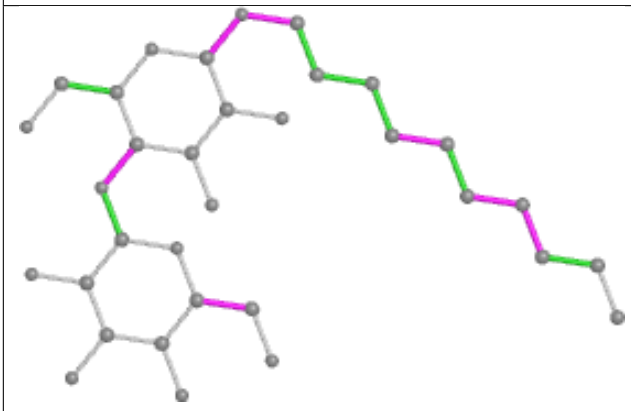
Ligand DMU P 319



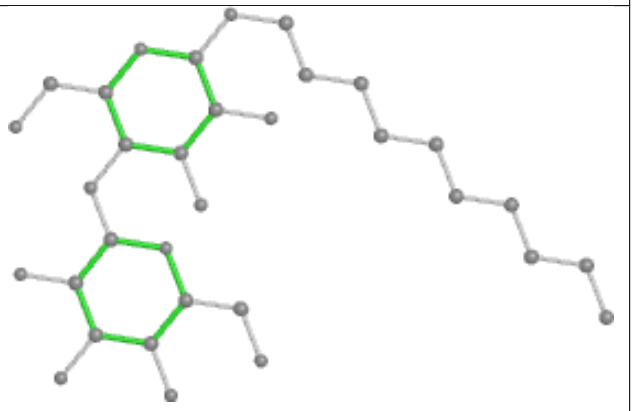
Bond lengths



Bond angles

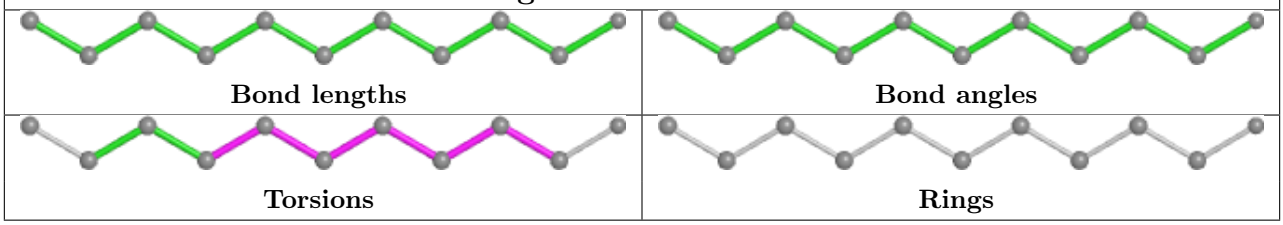


Torsions

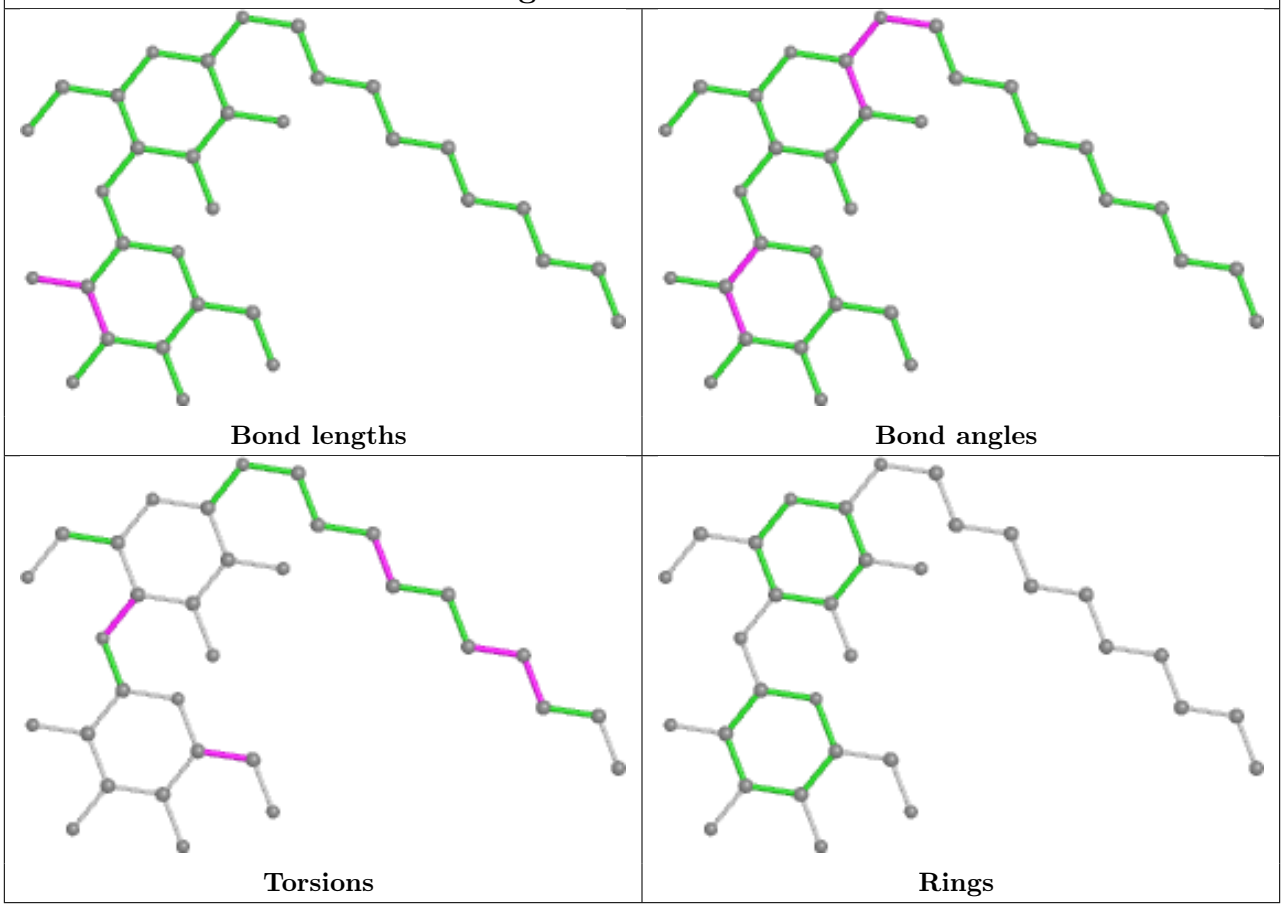


Rings

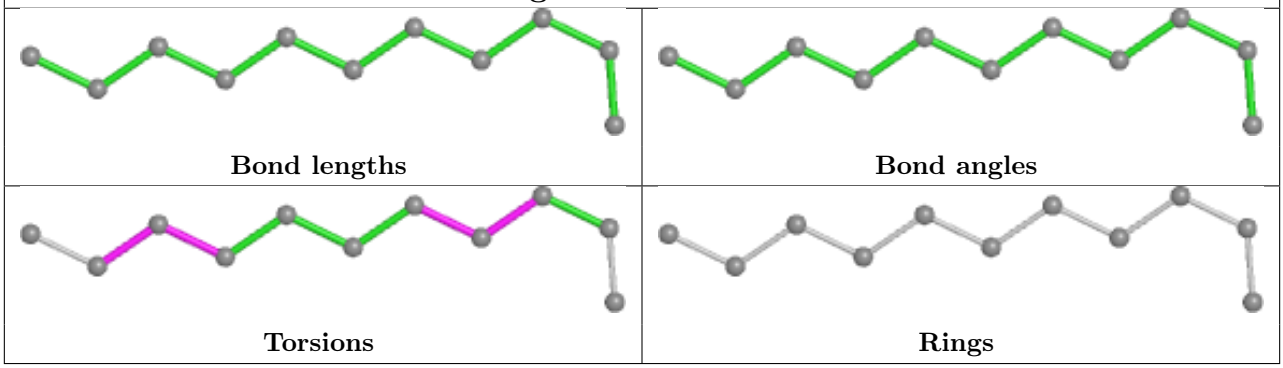
Ligand DMU A 615



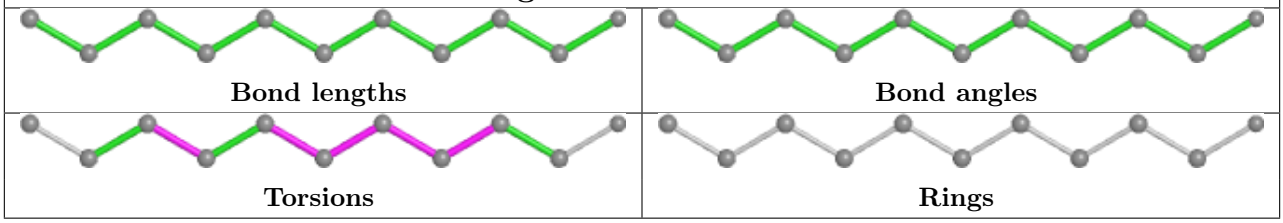
Ligand DMU P 315



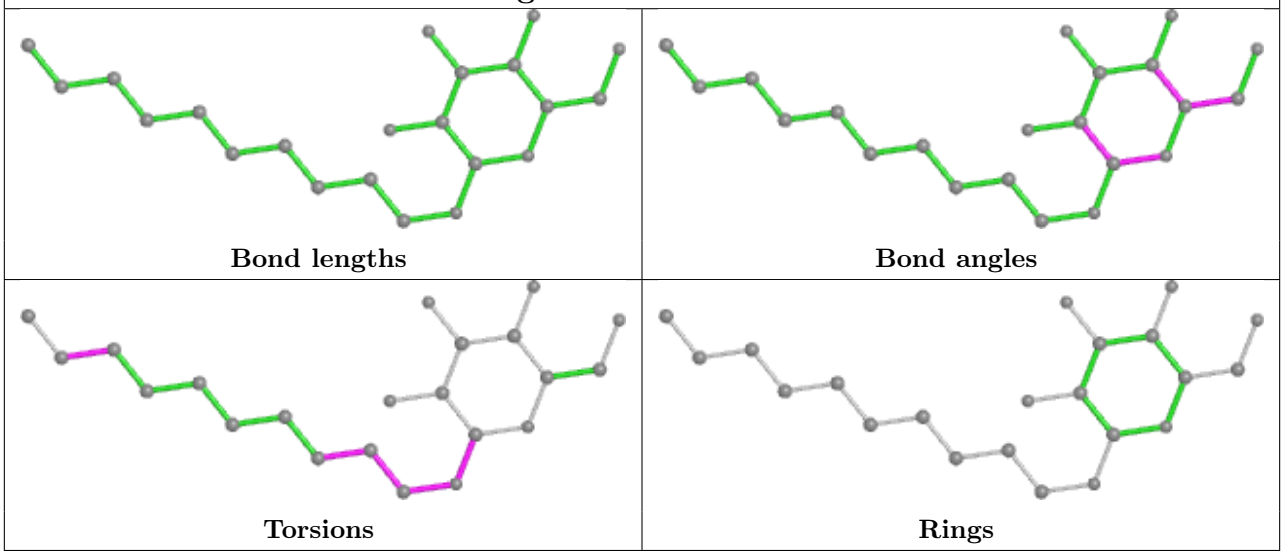
Ligand LFA P 308



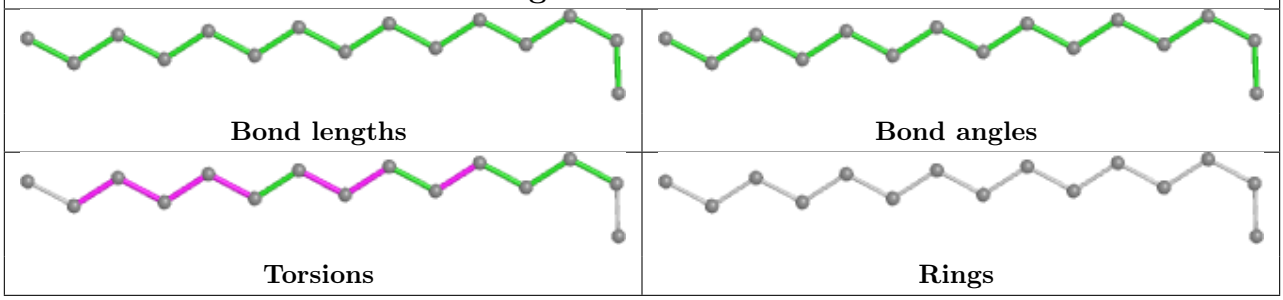
Ligand DMU O 306



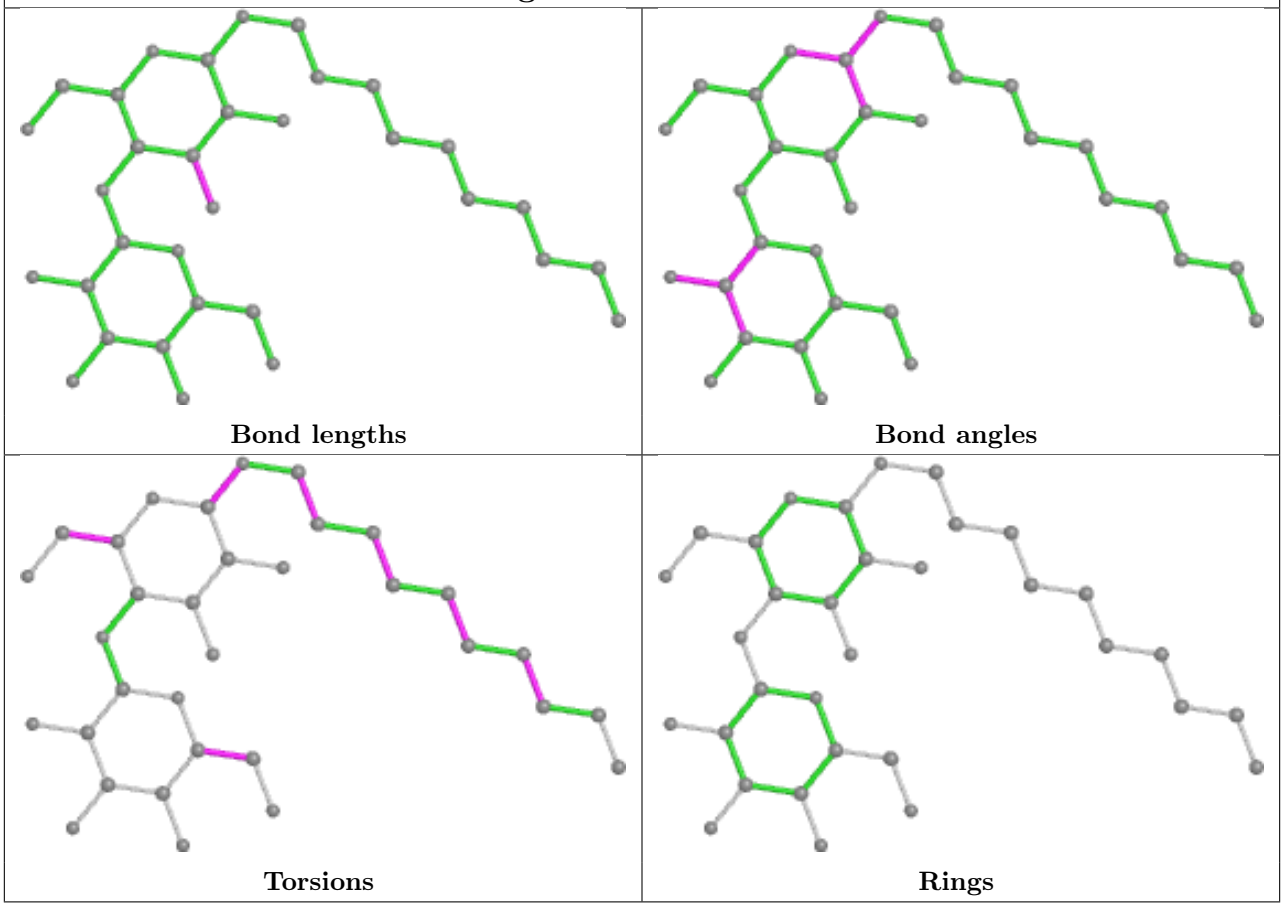
Ligand DMU O 308



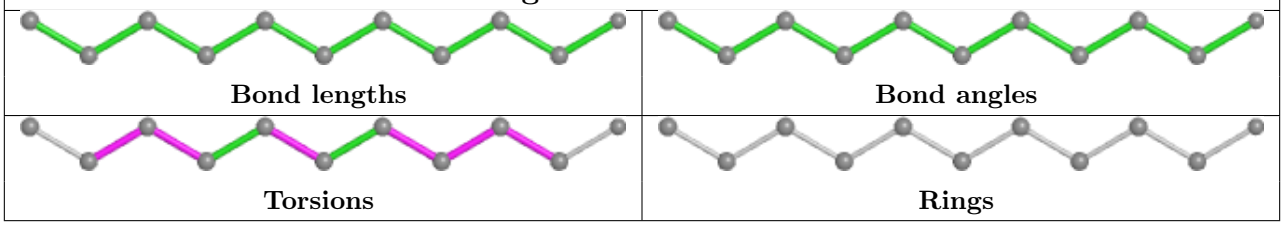
Ligand LFA C 325



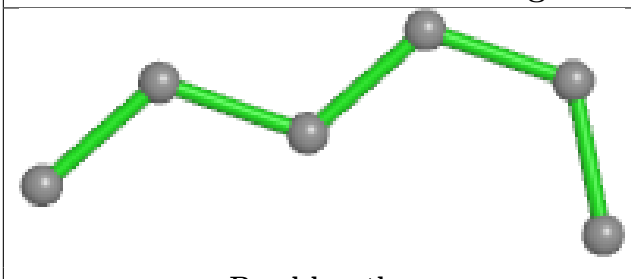
Ligand DMU C 319



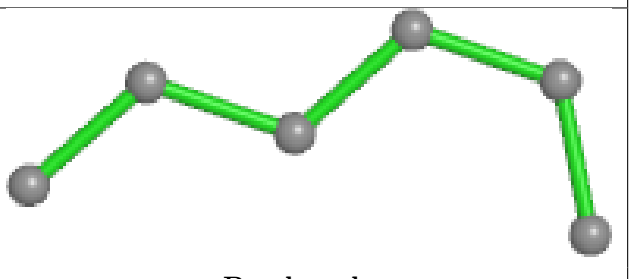
Ligand DMU J 101



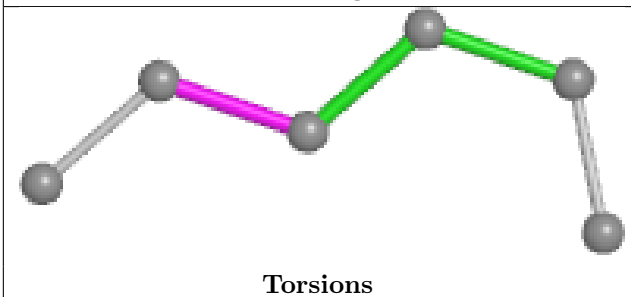
Ligand LFA C 308



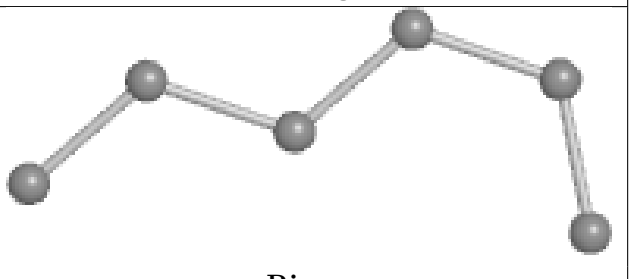
Bond lengths



Bond angles

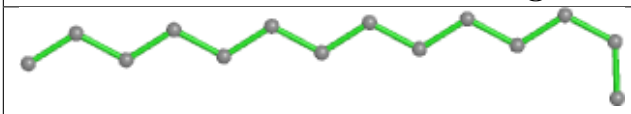


Torsions

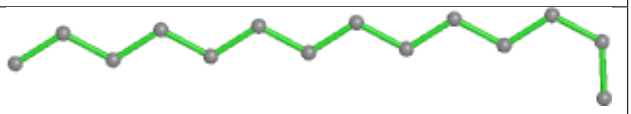


Rings

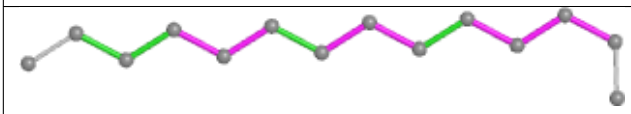
Ligand LFA N 610



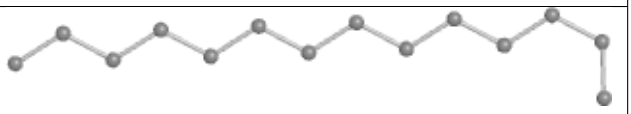
Bond lengths



Bond angles

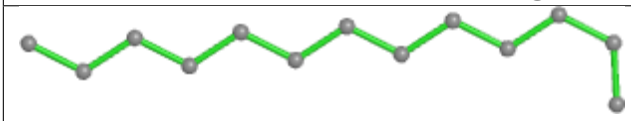


Torsions

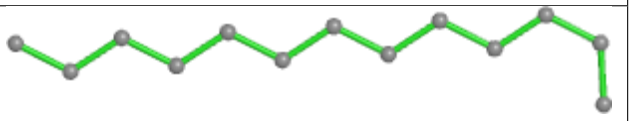


Rings

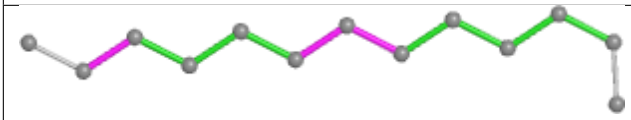
Ligand LFA P 314



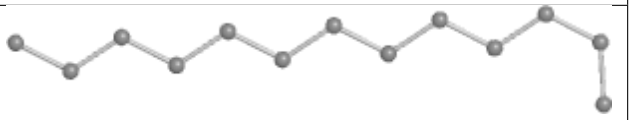
Bond lengths



Bond angles

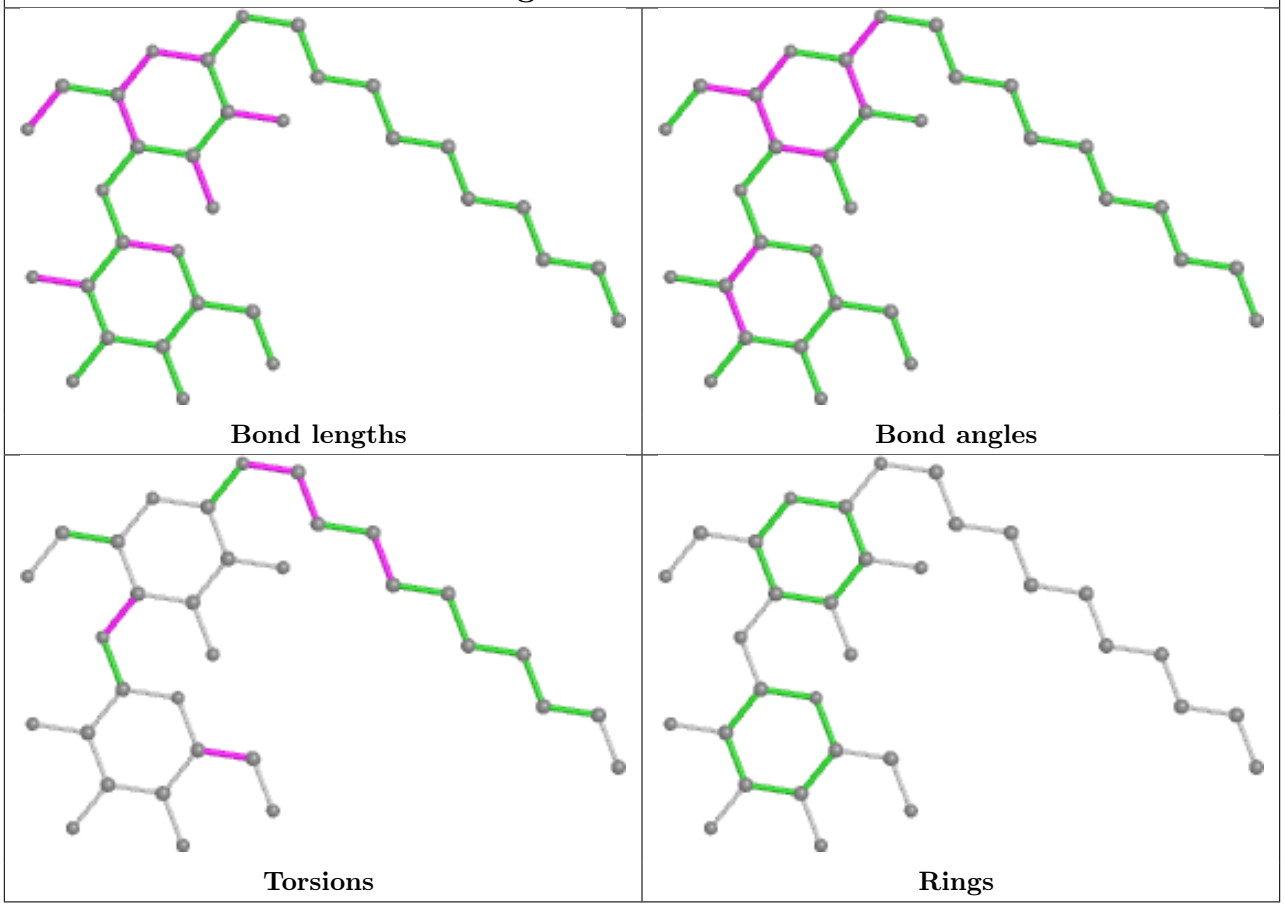


Torsions

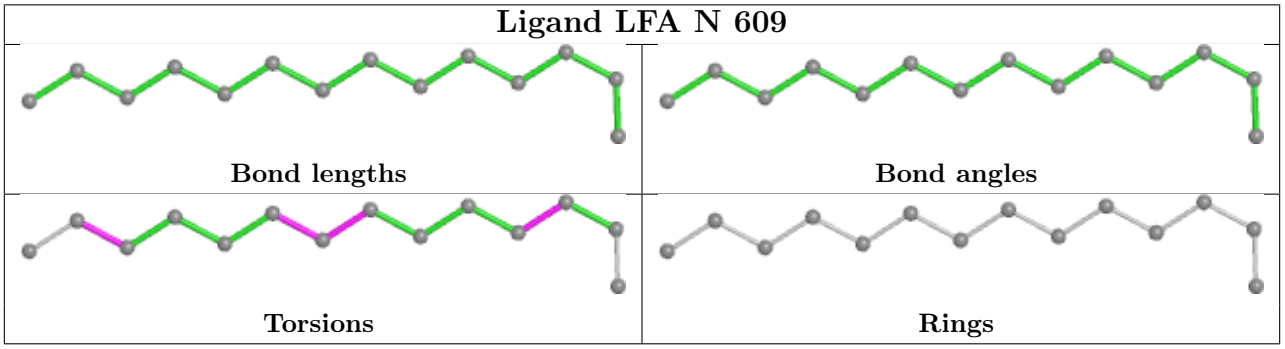


Rings

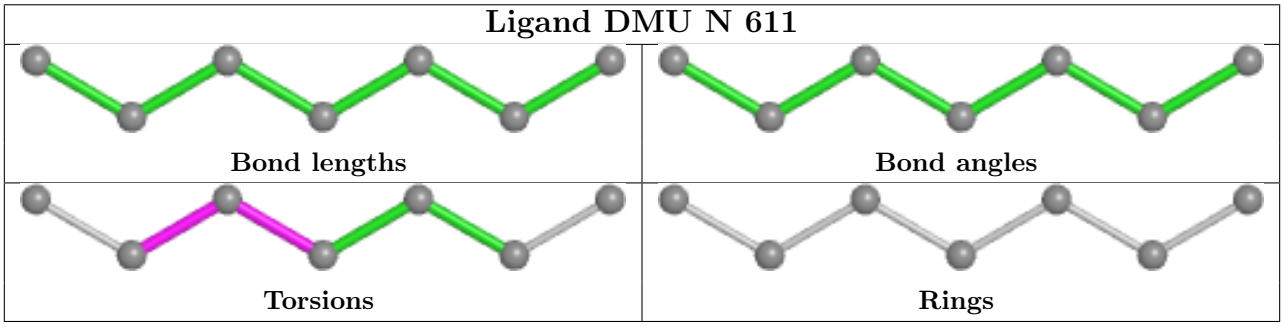
Ligand DMU D 201



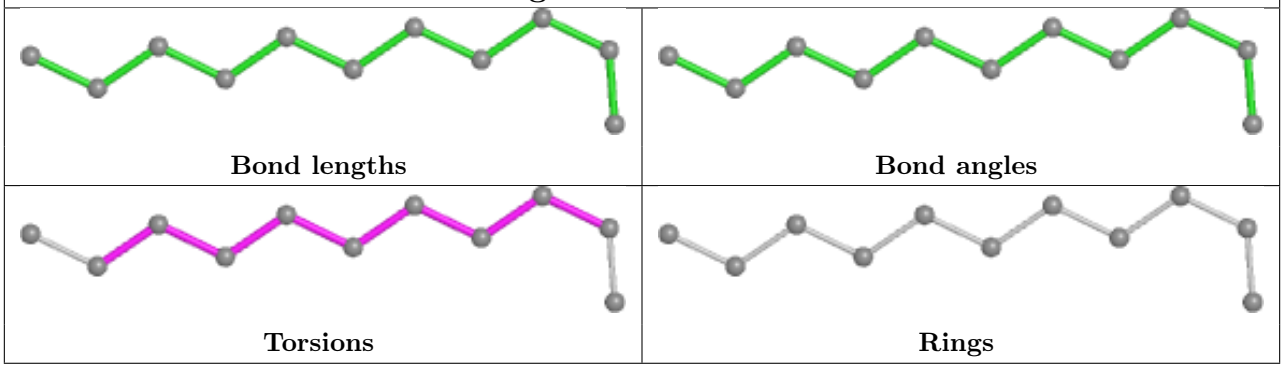
Ligand LFA N 609



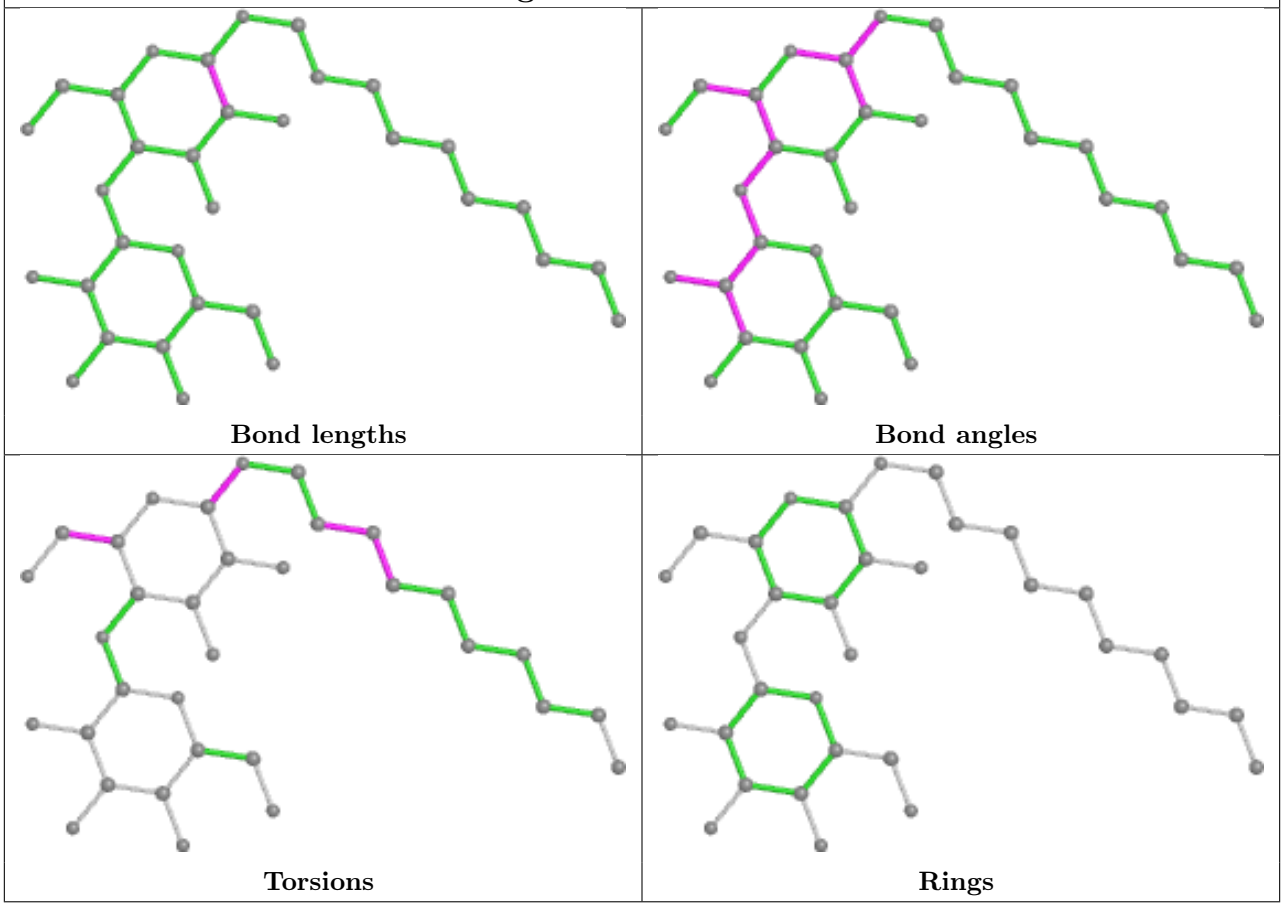
Ligand DMU N 611



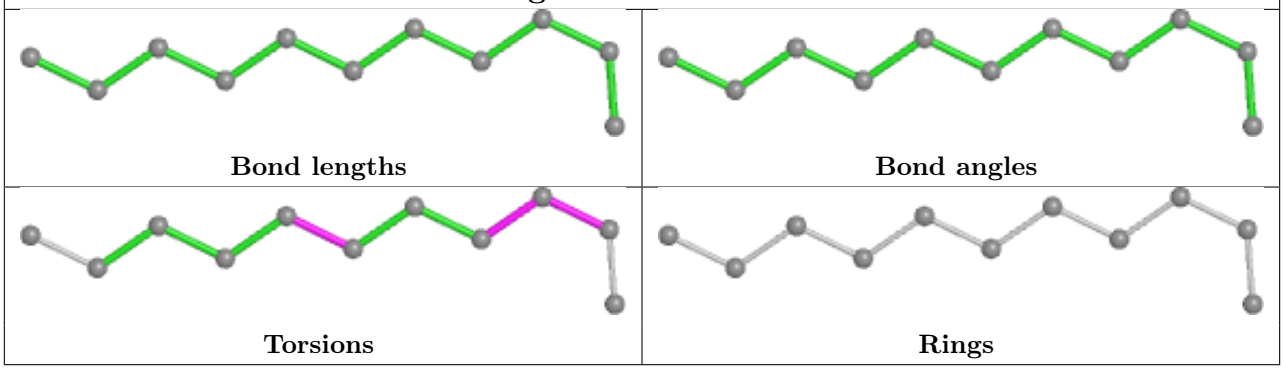
Ligand LFA C 310



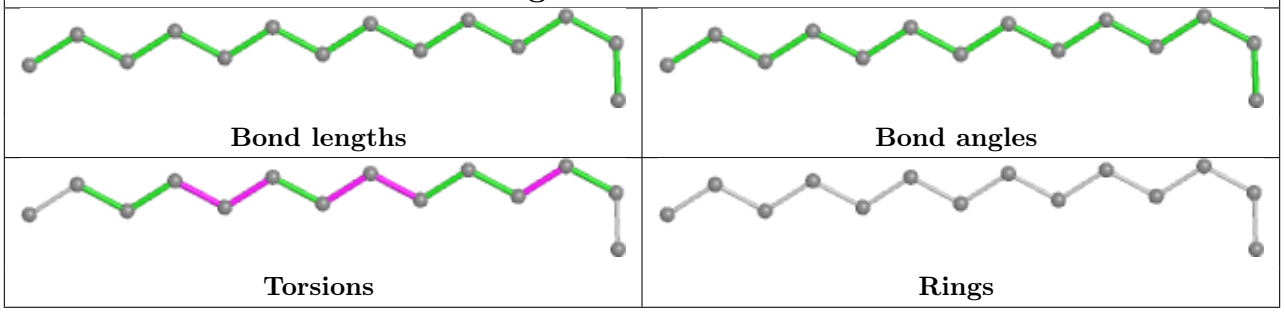
Ligand DMU N 619



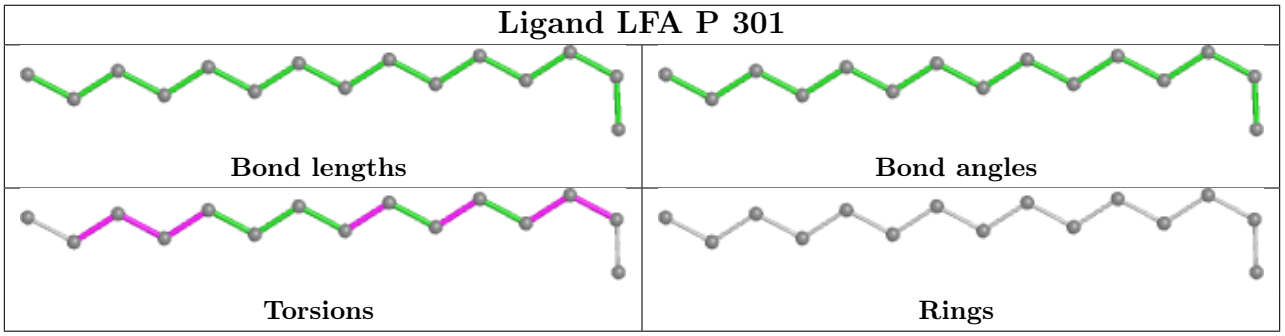
Ligand LFA O 302



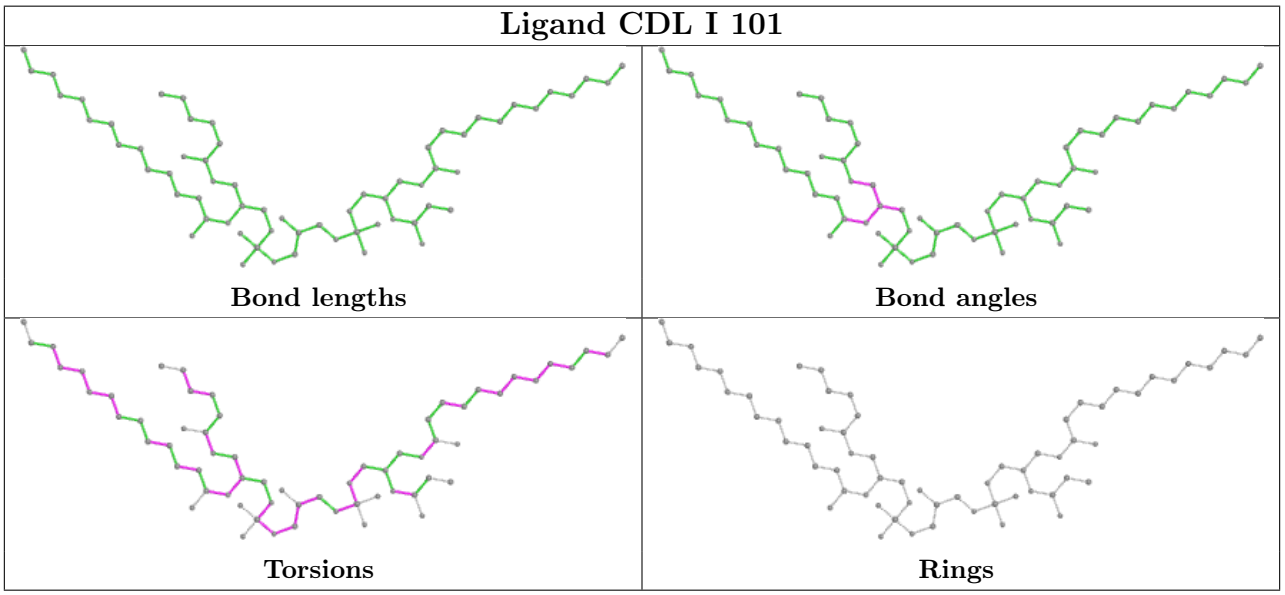
Ligand LFA A 608



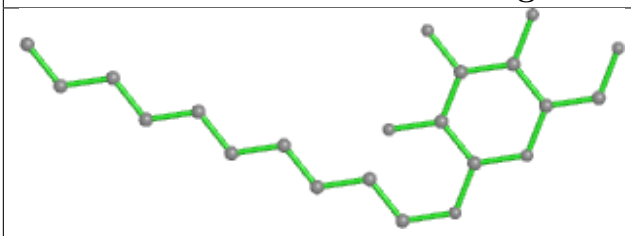
Ligand LFA P 301



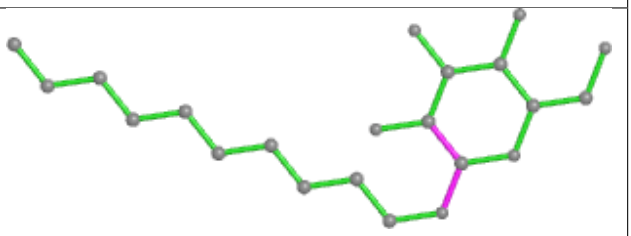
Ligand CDL I 101



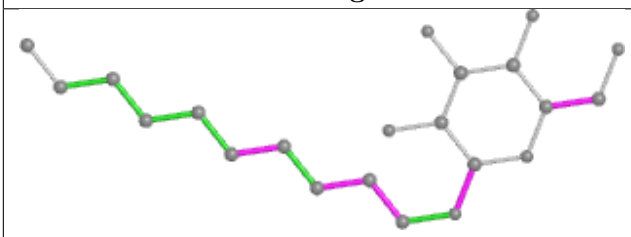
Ligand DMU P 323



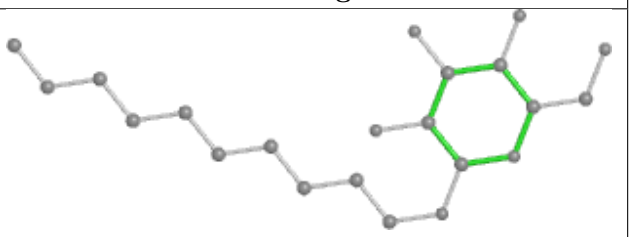
Bond lengths



Bond angles

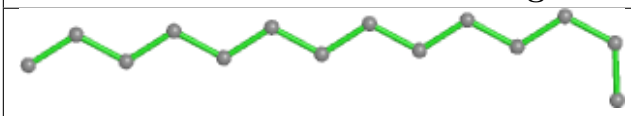


Torsions

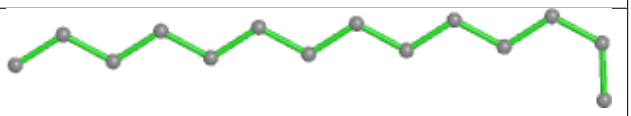


Rings

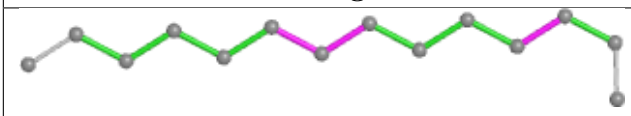
Ligand LFA A 607



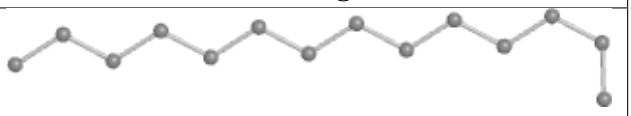
Bond lengths



Bond angles

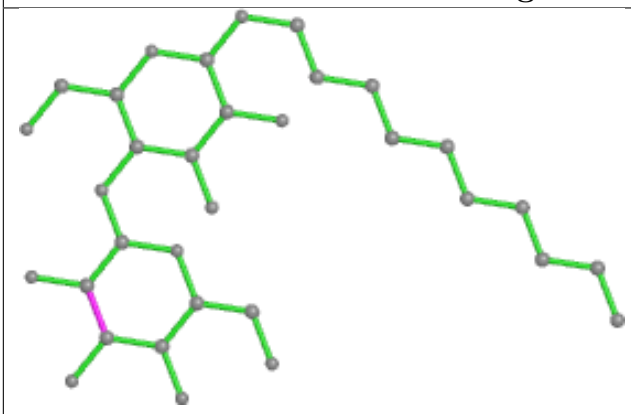


Torsions

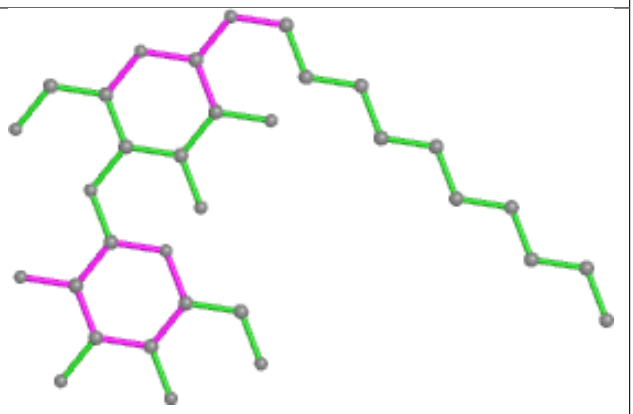


Rings

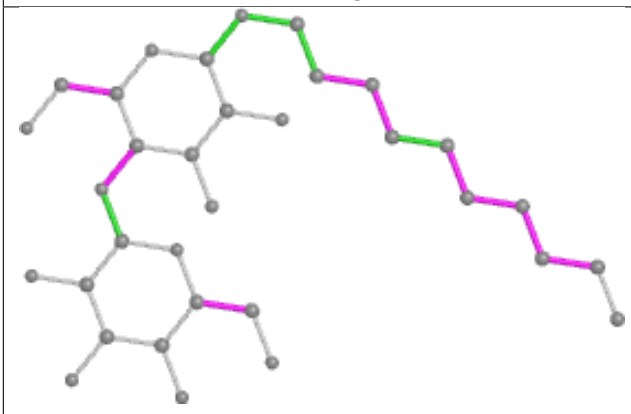
Ligand DMU C 315



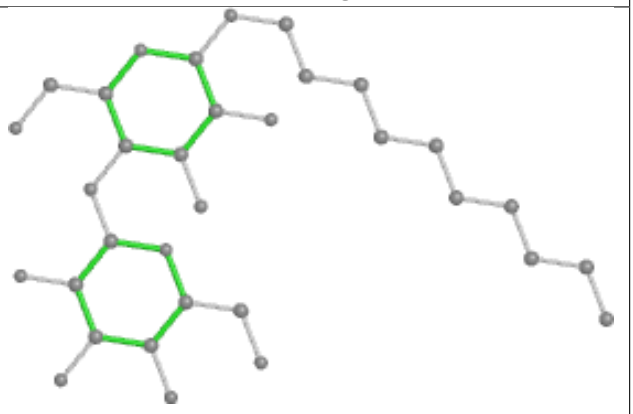
Bond lengths



Bond angles

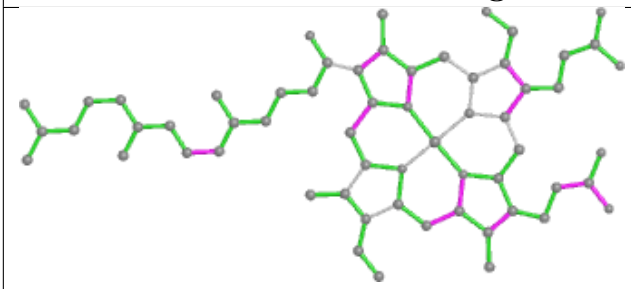


Torsions

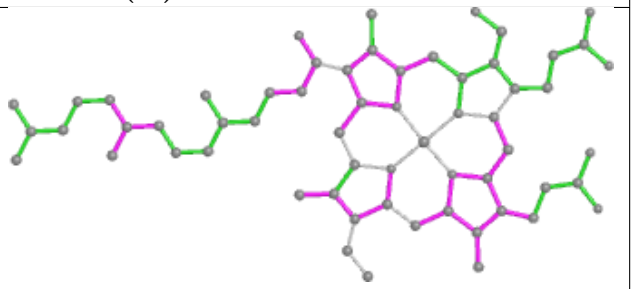


Rings

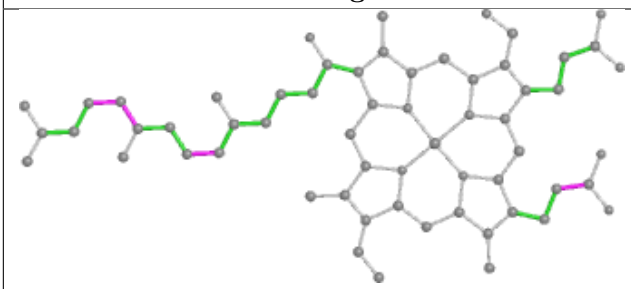
Ligand HEA A 601 (A)



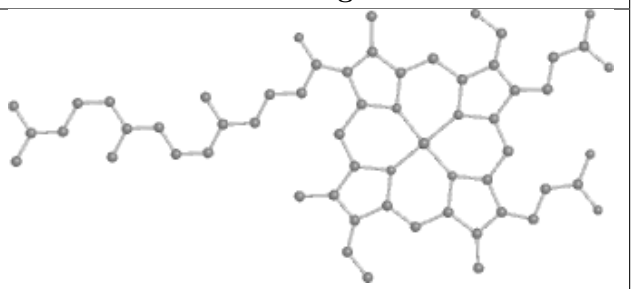
Bond lengths



Bond angles

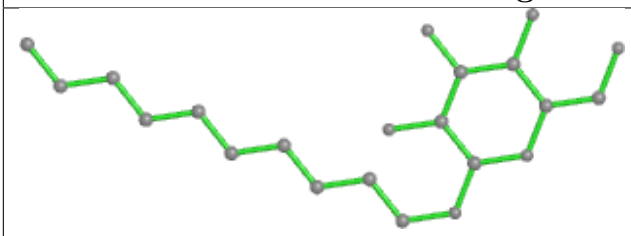


Torsions

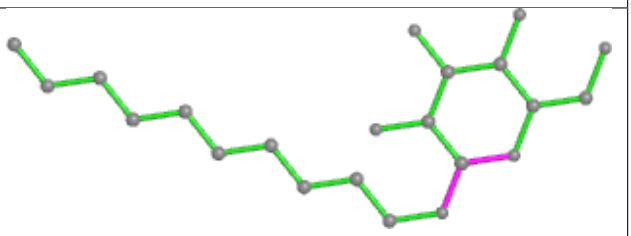


Rings

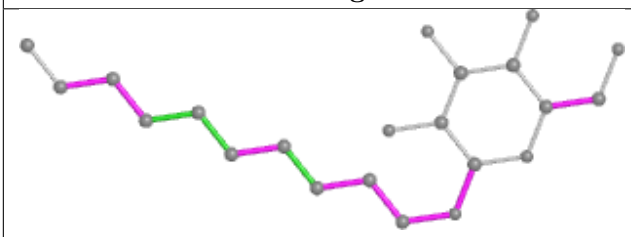
Ligand DMU Y 102



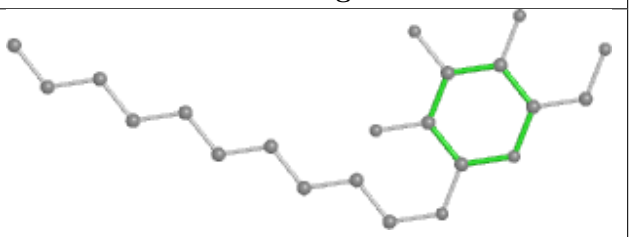
Bond lengths



Bond angles

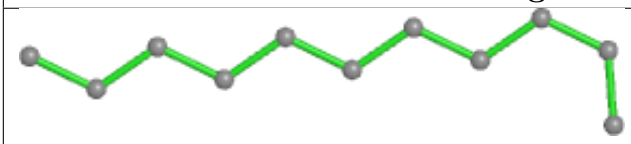


Torsions

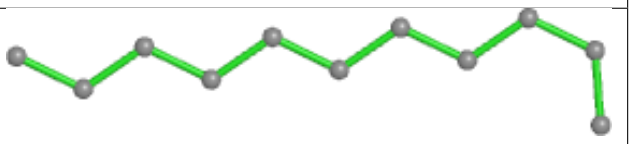


Rings

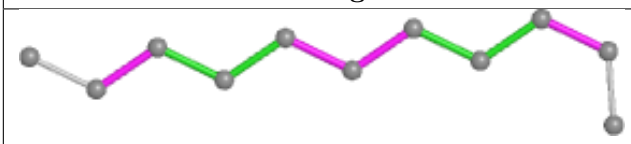
Ligand LFA C 312



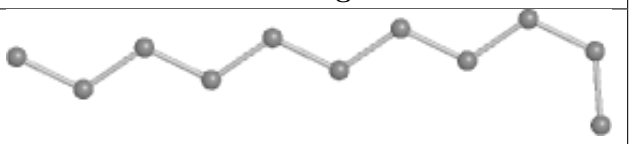
Bond lengths



Bond angles



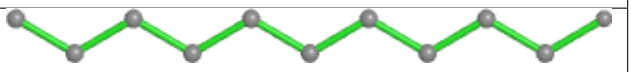
Torsions



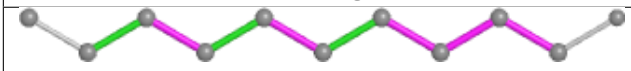
Rings

Ligand DMU B 302

Bond lengths



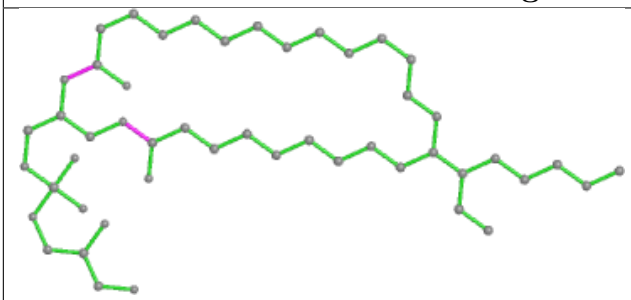
Bond angles



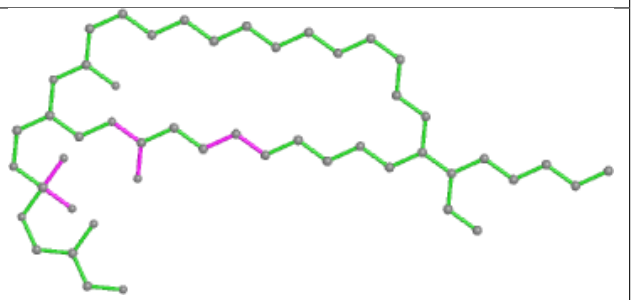
Torsions

Rings

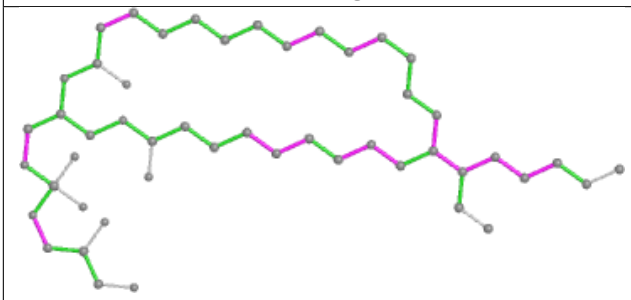
Ligand PGV C 303



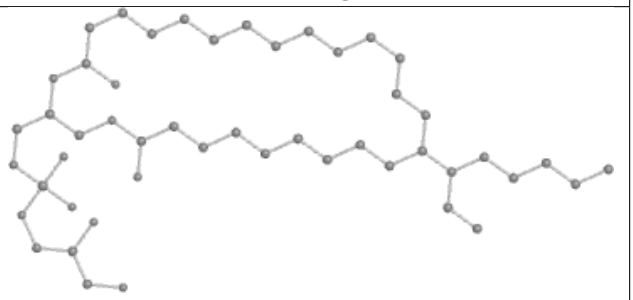
Bond lengths



Bond angles

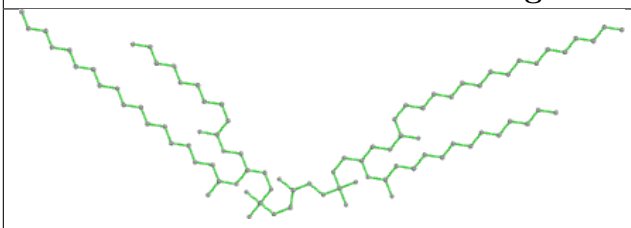


Torsions

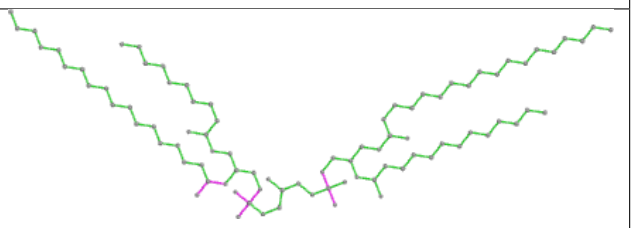


Rings

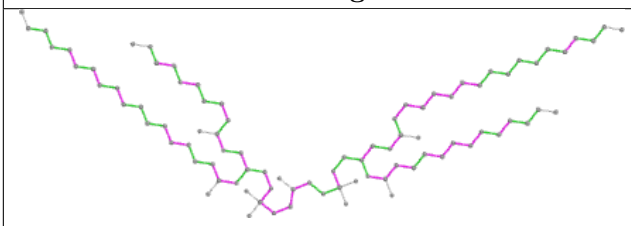
Ligand CDL P 305



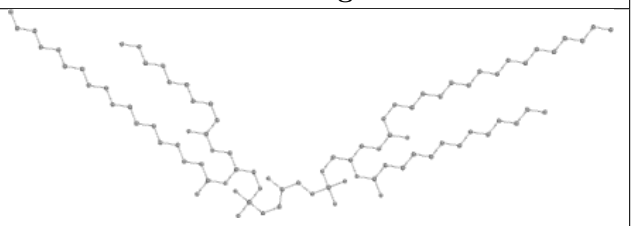
Bond lengths



Bond angles

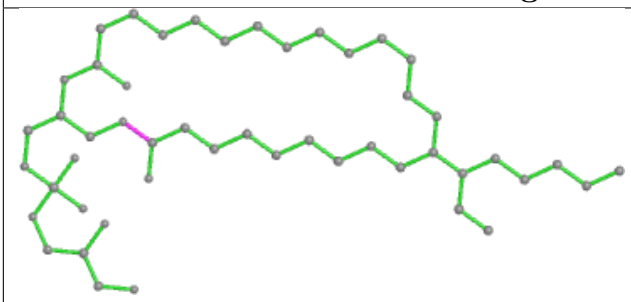


Torsions

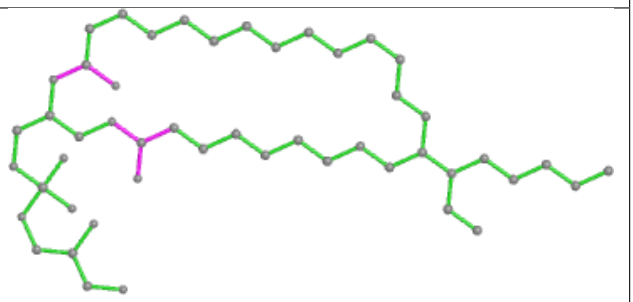


Rings

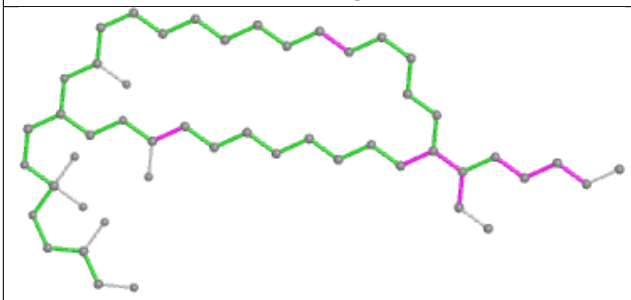
Ligand PGV N 618



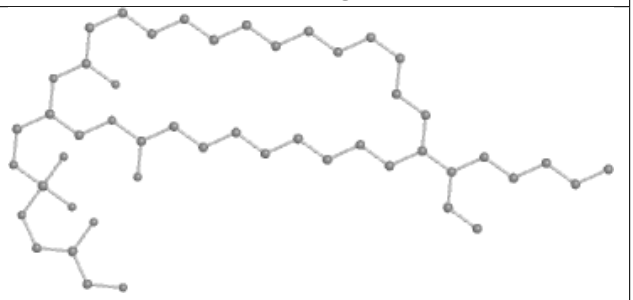
Bond lengths



Bond angles

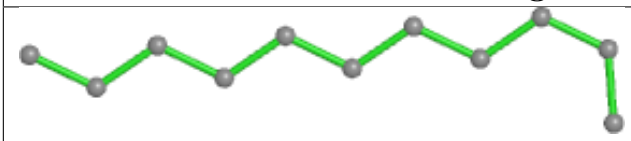


Torsions

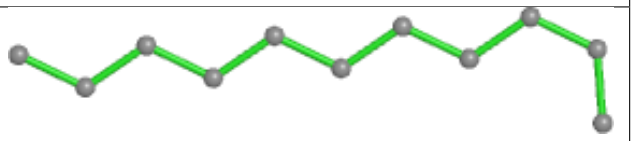


Rings

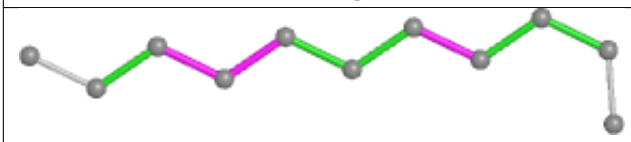
Ligand LFA T 103



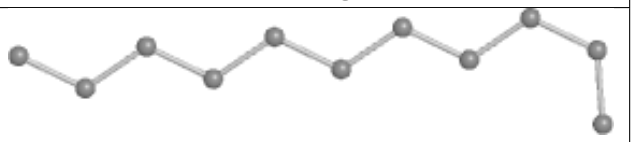
Bond lengths



Bond angles

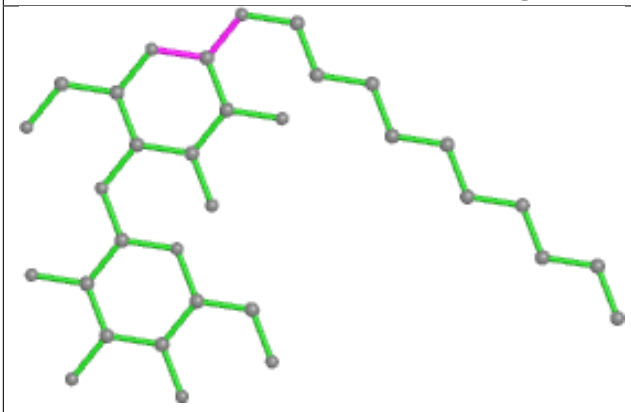


Torsions

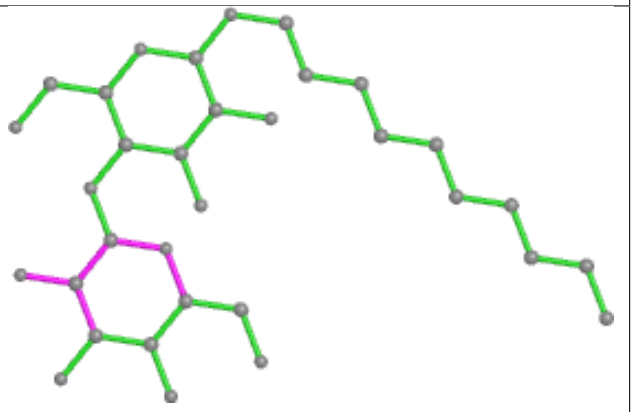


Rings

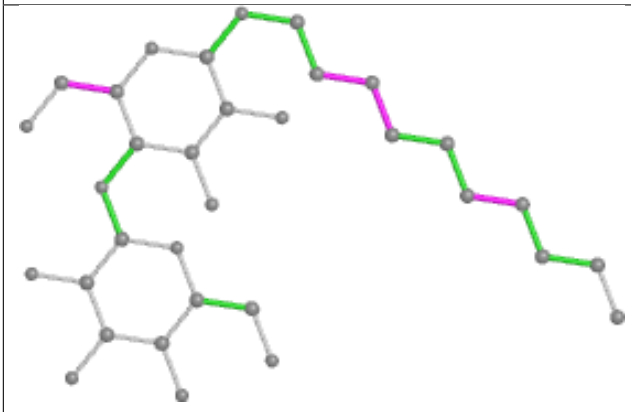
Ligand DMU H 101



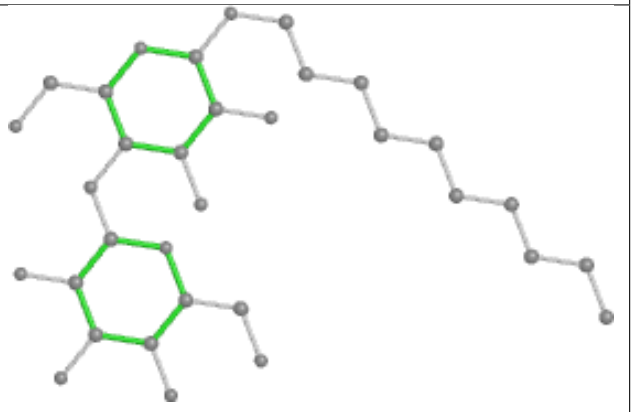
Bond lengths



Bond angles

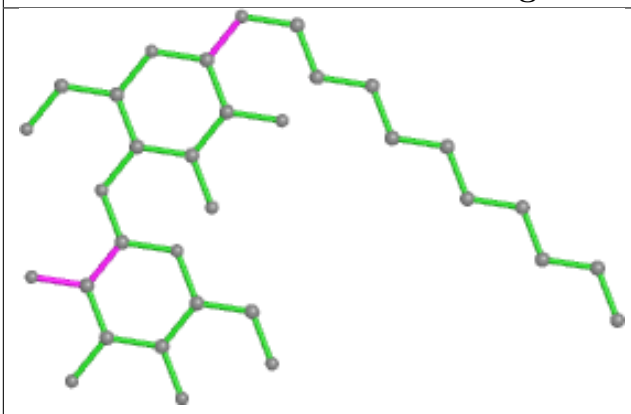


Torsions

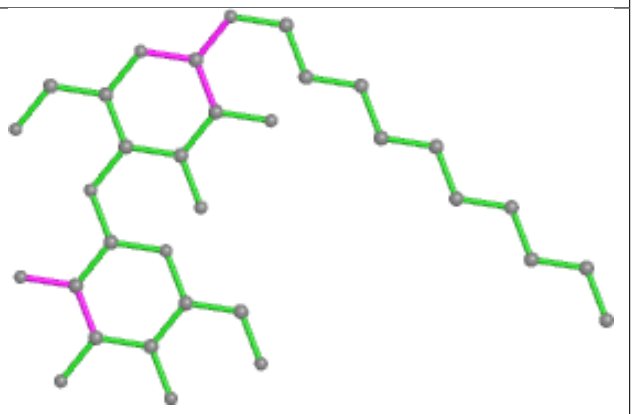


Rings

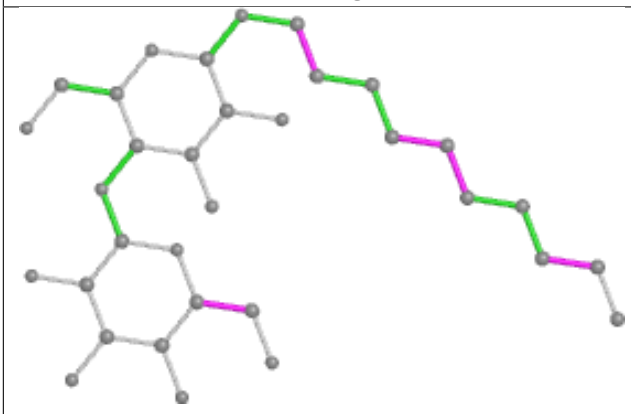
Ligand DMU Z 101



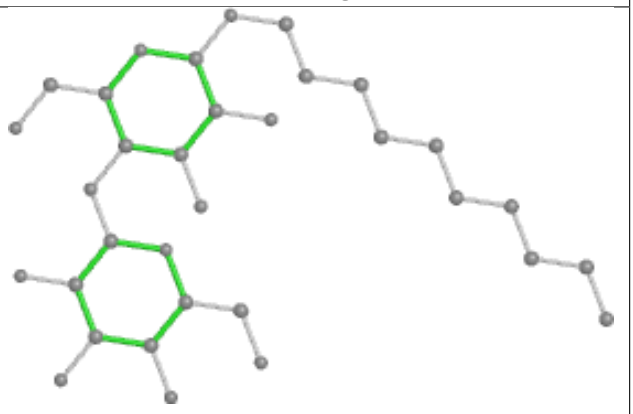
Bond lengths



Bond angles

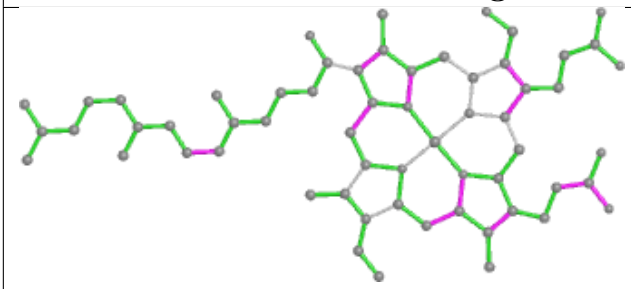


Torsions

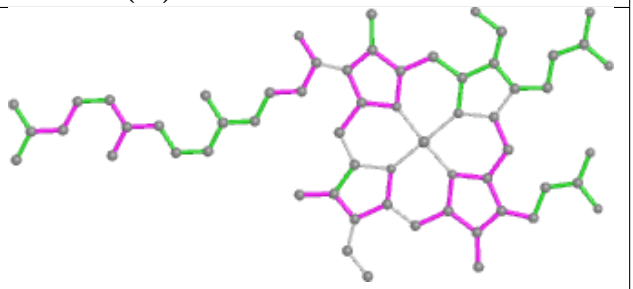


Rings

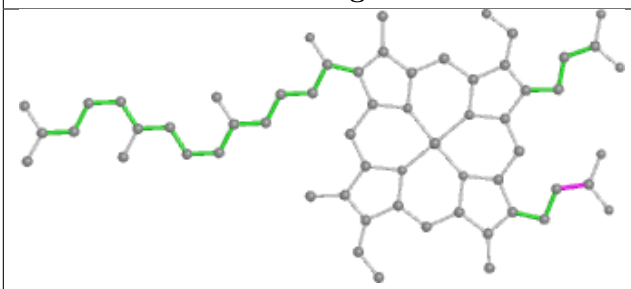
Ligand HEA A 601 (B)



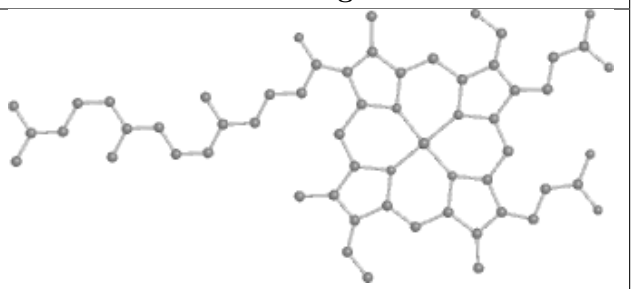
Bond lengths



Bond angles

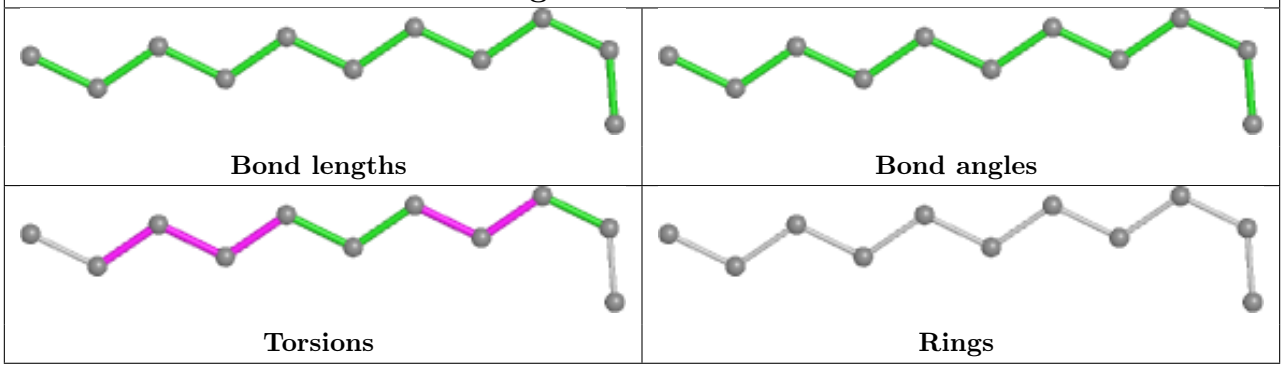


Torsions

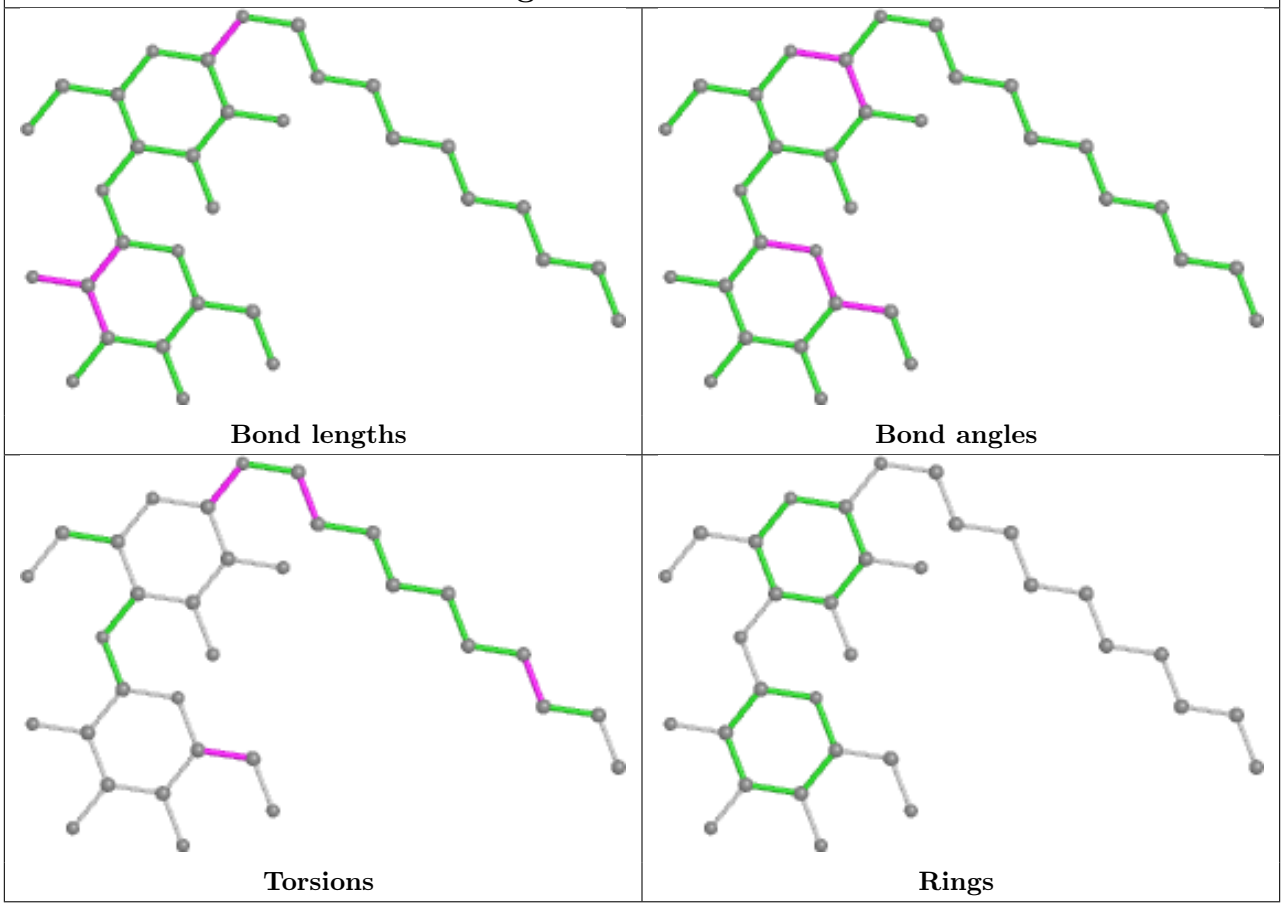


Rings

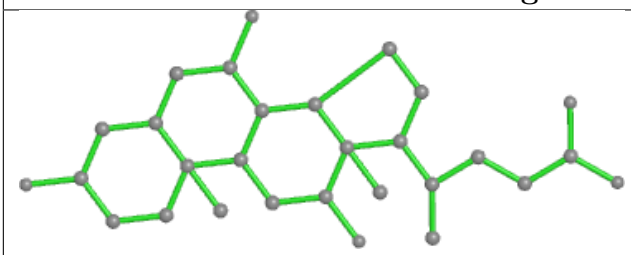
Ligand LFA P 311



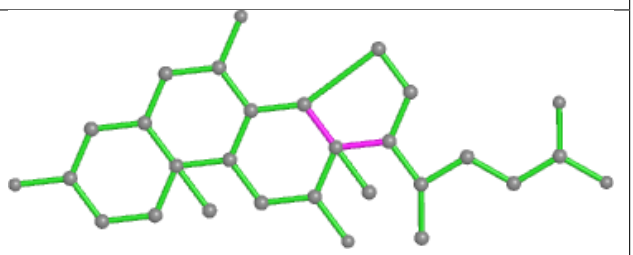
Ligand DMU N 612



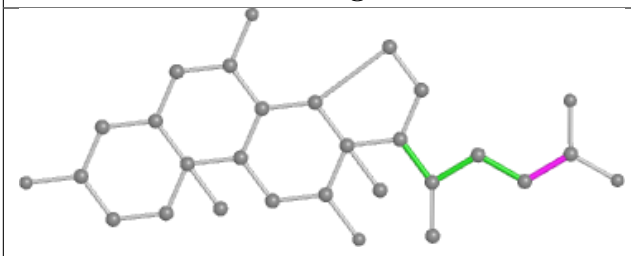
Ligand CHD B 305



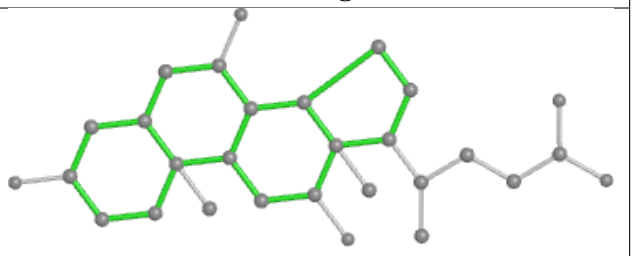
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.13	0 100 100	27, 31, 40, 57	0
1	N	512/514 (99%)	-0.04	1 (0%) 95 95	29, 37, 48, 66	0
2	B	226/227 (99%)	0.10	6 (2%) 54 58	29, 37, 57, 81	0
2	O	226/227 (99%)	0.10	7 (3%) 49 53	36, 47, 74, 84	0
3	C	258/261 (98%)	0.01	1 (0%) 92 93	29, 35, 47, 62	0
3	P	258/261 (98%)	-0.02	2 (0%) 86 88	30, 38, 49, 76	0
4	D	143/147 (97%)	-0.13	1 (0%) 87 90	33, 40, 56, 70	0
4	Q	137/147 (93%)	0.38	7 (5%) 28 31	41, 59, 85, 104	0
5	E	102/109 (93%)	-0.17	0 100 100	33, 39, 56, 74	0
5	R	102/109 (93%)	-0.13	0 100 100	37, 48, 64, 82	0
6	F	91/98 (92%)	-0.05	0 100 100	31, 42, 65, 79	0
6	S	91/98 (92%)	0.05	2 (2%) 62 66	33, 41, 66, 79	0
7	G	72/85 (84%)	0.45	9 (12%) 3 4	33, 41, 96, 108	0
7	T	72/85 (84%)	0.48	8 (11%) 5 6	33, 46, 94, 105	0
8	H	75/85 (88%)	0.26	5 (6%) 17 20	34, 45, 89, 110	0
8	U	75/85 (88%)	0.47	7 (9%) 8 9	42, 50, 89, 114	0
9	I	70/73 (95%)	0.25	4 (5%) 23 26	36, 48, 72, 91	0
9	V	70/73 (95%)	0.46	3 (4%) 35 39	37, 61, 79, 101	0
10	J	56/59 (94%)	0.14	4 (7%) 16 18	36, 45, 66, 78	0
10	W	56/59 (94%)	0.23	4 (7%) 16 18	40, 51, 75, 83	0
11	K	49/56 (87%)	-0.06	0 100 100	38, 45, 60, 76	0
11	X	49/56 (87%)	0.44	3 (6%) 21 23	50, 60, 76, 100	0
12	L	44/47 (93%)	-0.09	0 100 100	32, 37, 50, 60	0
12	Y	44/47 (93%)	-0.08	0 100 100	41, 49, 65, 71	0

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

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	Z	40	TYR	8.4
8	H	45	ALA	7.7
7	G	36	TRP	7.5
9	V	37	PHE	6.7
8	U	45	ALA	6.1
7	G	42	ARG	5.9
2	O	113	TYR	5.8
13	Z	39	ASN	5.7
13	M	40	TYR	5.6
10	W	52	TRP	5.5
7	T	42	ARG	5.3
7	T	36	TRP	5.2
7	T	38	HIS	4.9
6	S	93	PRO	4.9
7	G	40	GLY	4.7
2	O	90	ILE	4.6
2	B	60	GLU	4.6
7	T	43	GLU	4.5
8	U	47	GLY	4.4
7	T	39	SER	4.3
10	W	55	PHE	4.1
2	B	59	GLN	4.1
7	G	37	LEU	4.1
8	H	44	THR	4.0
4	Q	106	PRO	3.9
4	Q	39	ALA	3.9
9	I	25	PHE	3.9
3	P	37	PHE	3.8
10	J	52	TRP	3.7
13	M	39	ASN	3.7
7	T	40	GLY	3.6
9	I	37	PHE	3.6
8	U	44	THR	3.6
7	T	41	HIS	3.6

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Mol	Chain	Res	Type	RSRZ
2	O	91	ASN	3.5
9	V	34	PHE	3.5
2	B	65	TRP	3.4
13	Z	35	TYR	3.4
8	H	46	LYS	3.4
4	Q	140	TYR	3.3
10	J	1	PHE	3.3
7	G	39	SER	3.2
4	Q	105	GLY	3.2
13	Z	38	ASP	3.2
11	X	6	ALA	3.2
10	W	48	TYR	3.2
8	U	48	GLY	3.2
8	U	49	ASP	3.0
8	U	46	LYS	2.9
10	W	1	PHE	2.9
2	B	61	VAL	2.9
2	B	22[A]	HIS	2.9
2	O	59	GLN	2.8
13	M	38	ASP	2.8
2	O	227	LEU	2.8
6	S	3	GLY	2.7
1	N	47	LEU	2.7
2	B	55	THR	2.7
2	O	60	GLU	2.7
11	X	13	TYR	2.7
7	G	41	HIS	2.6
3	C	38	ASN	2.6
2	O	22[A]	HIS	2.6
10	J	48	TYR	2.6
7	T	45	PRO	2.6
8	H	47	GLY	2.5
7	G	43	GLU	2.5
13	Z	32	TRP	2.5
7	G	70[A]	PHE	2.5
9	I	19	PHE	2.5
7	G	45	PRO	2.4
4	D	4	SER	2.4
8	U	43	MET	2.4
9	I	33	THR	2.4
10	J	2	GLU	2.4
4	Q	46	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
4	Q	10	ASP	2.4
9	V	33	THR	2.2
8	H	43	MET	2.2
4	Q	97	ILE	2.1
3	P	38	ASN	2.1
11	X	7	PRO	2.0

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

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	DMU	P	317	22/33	0.47	0.41	50,66,82,91	22
20	DMU	B	307	22/33	0.60	0.24	61,71,81,85	22
20	DMU	C	317	22/33	0.61	0.36	42,65,78,85	22
20	DMU	A	617	11/33	0.61	0.37	47,60,69,72	11
20	DMU	P	318	33/33	0.62	0.35	52,62,77,100	33
19	LFA	P	311	11/20	0.63	0.36	59,67,76,82	11
19	LFA	P	308	11/20	0.65	0.43	36,52,58,59	11
20	DMU	B	303	22/33	0.65	0.27	50,61,72,75	22

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	DMU	O	303	22/33	0.66	0.23	51,76,86,88	22
20	DMU	P	319	33/33	0.66	0.26	55,74,82,94	33
26	CDL	C	304	87/100	0.66	0.24	46,81,122,135	0
20	DMU	C	324	33/33	0.67	0.26	39,54,72,82	33
20	DMU	C	318	33/33	0.68	0.34	46,55,68,81	33
20	DMU	O	308	22/33	0.68	0.22	46,52,59,63	22
20	DMU	N	602	11/33	0.68	0.35	52,67,72,75	11
20	DMU	P	324	33/33	0.69	0.25	50,63,84,91	33
20	DMU	Q	201	33/33	0.70	0.16	39,57,69,89	33
20	DMU	C	319	33/33	0.70	0.22	43,71,86,87	33
20	DMU	P	323	22/33	0.71	0.21	46,60,70,77	22
19	LFA	C	308	6/20	0.71	0.55	49,51,55,59	6
26	CDL	P	305	87/100	0.71	0.24	50,86,130,152	0
20	DMU	A	615	11/33	0.72	0.35	54,63,68,71	11
26	CDL	O	304	64/100	0.73	0.21	62,91,140,180	0
20	DMU	A	609	7/33	0.73	0.47	61,69,77,86	7
20	DMU	C	323	22/33	0.74	0.19	50,62,70,83	22
20	DMU	W	101	11/33	0.74	0.27	68,74,76,78	11
20	DMU	Y	102	22/33	0.74	0.28	55,63,76,86	22
20	DMU	P	316	7/33	0.75	0.41	62,66,71,72	7
20	DMU	P	315	33/33	0.75	0.27	45,54,67,71	33
20	DMU	N	612	33/33	0.76	0.22	40,55,75,86	33
20	DMU	A	610	33/33	0.76	0.21	31,42,53,63	33
19	LFA	T	102	14/20	0.77	0.35	42,70,86,87	14
20	DMU	L	102	22/33	0.77	0.33	49,59,67,70	22
20	DMU	C	315	33/33	0.77	0.29	43,56,69,70	33
20	DMU	N	611	7/33	0.77	0.34	72,76,81,93	7
20	DMU	O	307	11/33	0.78	0.35	47,55,65,70	11
19	LFA	C	313	15/20	0.78	0.28	44,52,70,73	15
19	LFA	C	325	15/20	0.78	0.45	57,66,74,75	15
26	CDL	Y	101	94/100	0.78	0.25	57,95,141,156	0
19	LFA	A	608	14/20	0.79	0.29	37,50,62,63	14
19	LFA	C	310	11/20	0.79	0.36	59,70,85,90	11
19	LFA	N	610	14/20	0.79	0.29	42,51,71,72	14
19	LFA	O	302	11/20	0.79	0.26	49,56,73,80	11
19	LFA	C	311	14/20	0.79	0.34	40,62,72,75	14
26	CDL	I	101	64/100	0.80	0.21	54,87,129,158	0
19	LFA	C	312	11/20	0.80	0.40	53,59,73,76	11
19	LFA	P	309	6/20	0.83	0.55	45,51,54,55	6
19	LFA	P	310	18/20	0.83	0.22	43,52,62,69	18
20	DMU	Z	101	33/33	0.83	0.19	56,67,90,94	0
19	LFA	T	103	11/20	0.83	0.27	55,59,73,75	11

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
21	EDO	N	617	4/4	0.84	0.21	31,39,39,43	4
19	LFA	P	301	15/20	0.84	0.41	51,57,62,64	15
20	DMU	D	201	33/33	0.84	0.16	28,44,51,78	33
26	CDL	L	101	94/100	0.84	0.20	44,85,129,155	0
19	LFA	P	312	11/20	0.84	0.38	47,59,70,74	11
20	DMU	C	306	11/33	0.84	0.26	59,63,70,72	11
19	LFA	P	313	15/20	0.84	0.28	48,53,63,66	15
20	DMU	J	101	11/33	0.85	0.28	63,68,71,82	11
19	LFA	N	601	17/20	0.85	0.27	41,60,75,78	17
21	EDO	P	322	4/4	0.85	0.19	32,36,40,42	4
19	LFA	C	307	11/20	0.86	0.42	41,52,64,70	11
21	EDO	E	201	4/4	0.86	0.23	39,41,48,51	4
19	LFA	P	314	13/20	0.86	0.26	46,63,74,76	13
19	LFA	B	306	17/20	0.86	0.29	43,59,87,90	17
20	DMU	O	306	11/33	0.86	0.37	44,47,72,75	11
20	DMU	C	316	7/33	0.87	0.32	47,51,63,69	7
19	LFA	C	314	13/20	0.87	0.23	56,59,77,86	13
20	DMU	M	102	8/33	0.88	0.23	48,51,58,60	8
19	LFA	C	309	18/20	0.88	0.19	37,45,54,56	18
19	LFA	A	607	14/20	0.89	0.31	36,51,76,78	14
21	EDO	A	611	4/4	0.89	0.18	27,29,29,33	4
20	DMU	P	307	11/33	0.89	0.41	52,53,61,63	11
20	DMU	H	101	33/33	0.89	0.20	31,45,59,68	33
20	DMU	N	619	33/33	0.89	0.22	35,49,63,66	33
24	CHD	P	306	29/29	0.89	0.18	54,60,72,86	0
21	EDO	C	322	4/4	0.90	0.21	36,36,37,38	4
24	CHD	P	302	29/29	0.91	0.08	32,37,41,45	0
21	EDO	P	320	4/4	0.91	0.19	53,60,63,73	4
20	DMU	Z	102	8/33	0.91	0.29	51,57,61,62	8
24	CHD	C	301	29/29	0.91	0.09	32,35,40,43	0
21	EDO	A	614	4/4	0.92	0.10	37,39,40,44	4
20	DMU	M	101	33/33	0.92	0.10	41,52,78,83	0
20	DMU	B	302	11/33	0.92	0.27	47,58,64,68	11
21	EDO	N	613	4/4	0.92	0.15	31,37,37,39	4
21	EDO	O	309	4/4	0.93	0.17	36,37,39,40	4
24	CHD	C	305	29/29	0.93	0.17	50,58,77,111	0
21	EDO	A	612	4/4	0.93	0.16	35,41,50,53	4
19	LFA	N	609	14/20	0.93	0.29	40,50,68,71	14
21	EDO	R	201	4/4	0.93	0.20	63,63,64,70	4
21	EDO	C	320	4/4	0.94	0.29	53,57,58,71	4
25	UNX	P	303	1/1	0.94	0.17	55,55,55,55	0
21	EDO	P	321	4/4	0.94	0.14	42,42,45,45	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	CHD	B	305	29/29	0.94	0.09	30,36,41,50	0
21	EDO	F	102	4/4	0.95	0.18	23,24,31,31	4
21	EDO	E	202	4/4	0.95	0.20	35,35,37,39	4
21	EDO	N	615	4/4	0.95	0.22	31,32,32,33	4
28	PEK	T	101	53/53	0.95	0.12	38,62,110,159	0
21	EDO	G	102	4/4	0.96	0.14	30,34,35,38	4
24	CHD	O	301	29/29	0.96	0.09	32,36,39,47	0
21	EDO	R	202	4/4	0.96	0.14	38,39,41,41	4
21	EDO	S	102	4/4	0.96	0.14	25,25,31,31	4
14	HEA	N	604	60/60	0.96	0.10	28,32,40,43	0
28	PEK	G	101	53/53	0.96	0.12	33,56,90,112	0
21	EDO	N	614	4/4	0.96	0.15	39,40,50,50	4
21	EDO	N	616	4/4	0.97	0.16	37,39,42,45	4
14	HEA	A	601[B]	60/60	0.97	0.11	25,28,45,51	9
14	HEA	A	602	60/60	0.97	0.10	24,27,36,41	0
14	HEA	N	603[A]	60/60	0.97	0.10	31,35,46,52	9
14	HEA	N	603[B]	60/60	0.97	0.10	31,35,49,53	9
21	EDO	A	613	4/4	0.97	0.21	27,28,28,29	4
14	HEA	A	601[A]	60/60	0.97	0.11	25,28,41,47	9
18	PER	N	608	2/2	0.97	0.10	33,33,33,40	0
21	EDO	R	203	4/4	0.97	0.17	44,49,51,58	4
21	EDO	C	321	4/4	0.97	0.14	37,37,39,40	4
21	EDO	T	104	4/4	0.97	0.13	36,37,39,40	4
22	PGV	A	616	51/51	0.97	0.11	29,41,80,92	0
22	PGV	C	303	51/51	0.97	0.10	32,41,90,108	0
22	PGV	N	618	51/51	0.97	0.10	33,46,79,92	0
22	PGV	P	304	51/51	0.97	0.11	34,43,102,119	0
21	EDO	B	304	4/4	0.98	0.18	25,26,27,30	4
18	PER	A	606	2/2	0.98	0.10	29,29,29,34	0
25	UNX	C	302	1/1	0.98	0.11	56,56,56,56	0
21	EDO	E	203	4/4	0.98	0.20	34,35,41,42	4
16	MG	N	606	1/1	0.99	0.07	37,37,37,37	0
21	EDO	S	103	4/4	0.99	0.13	32,36,37,37	4
21	EDO	F	103	4/4	0.99	0.10	32,34,37,38	4
23	CUA	O	305	2/2	0.99	0.12	39,39,39,40	0
16	MG	A	604	1/1	0.99	0.09	30,30,30,30	0
15	CU	N	605	1/1	1.00	0.18	32,32,32,32	0
17	CA	A	605	1/1	1.00	0.12	33,33,33,33	0
23	CUA	B	301	2/2	1.00	0.15	29,29,29,30	0
27	ZN	F	101	1/1	1.00	0.14	36,36,36,36	0
27	ZN	S	101	1/1	1.00	0.12	37,37,37,37	0
17	CA	N	607	1/1	1.00	0.08	45,45,45,45	0

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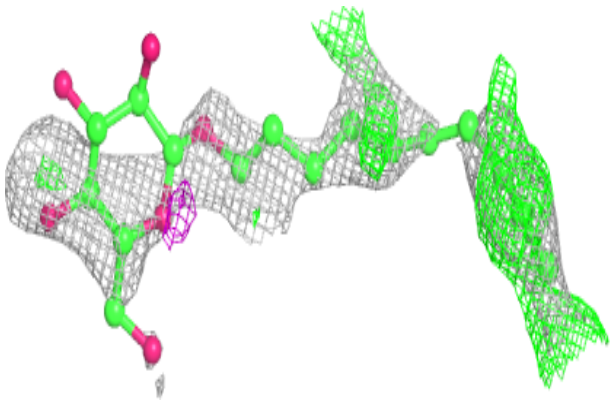
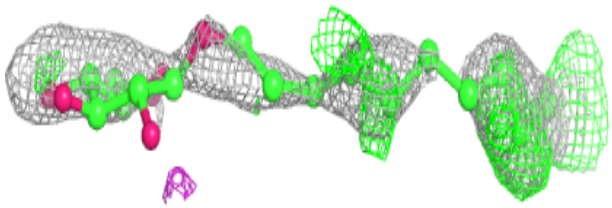
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	CU	A	603	1/1	1.00	0.17	28,28,28,28	0

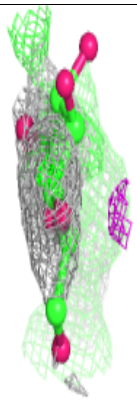
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DMU P 317:

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

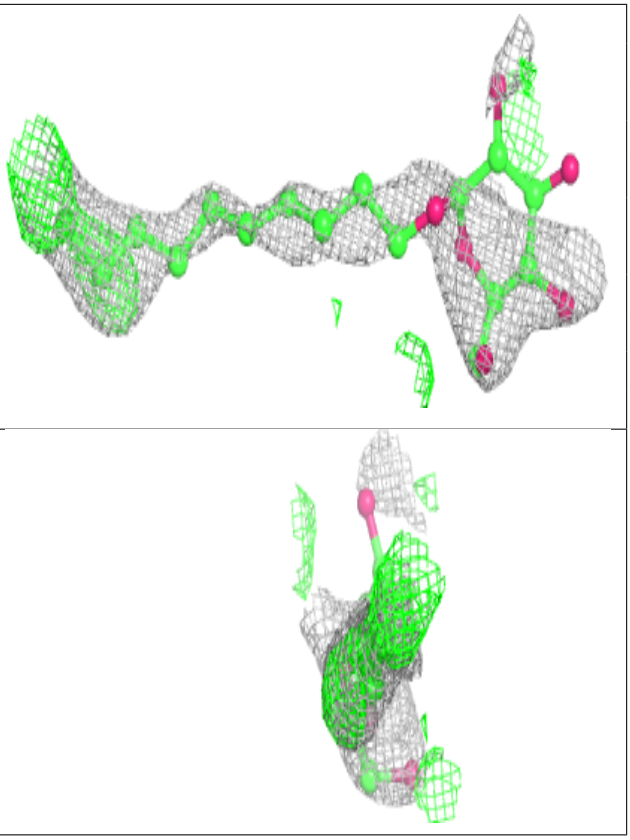






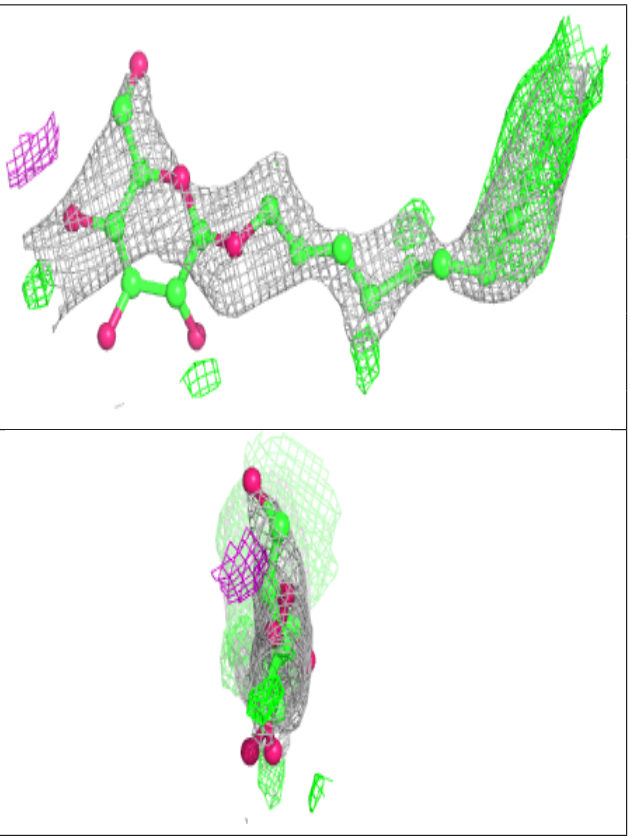
Electron density around DMU B 307:

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



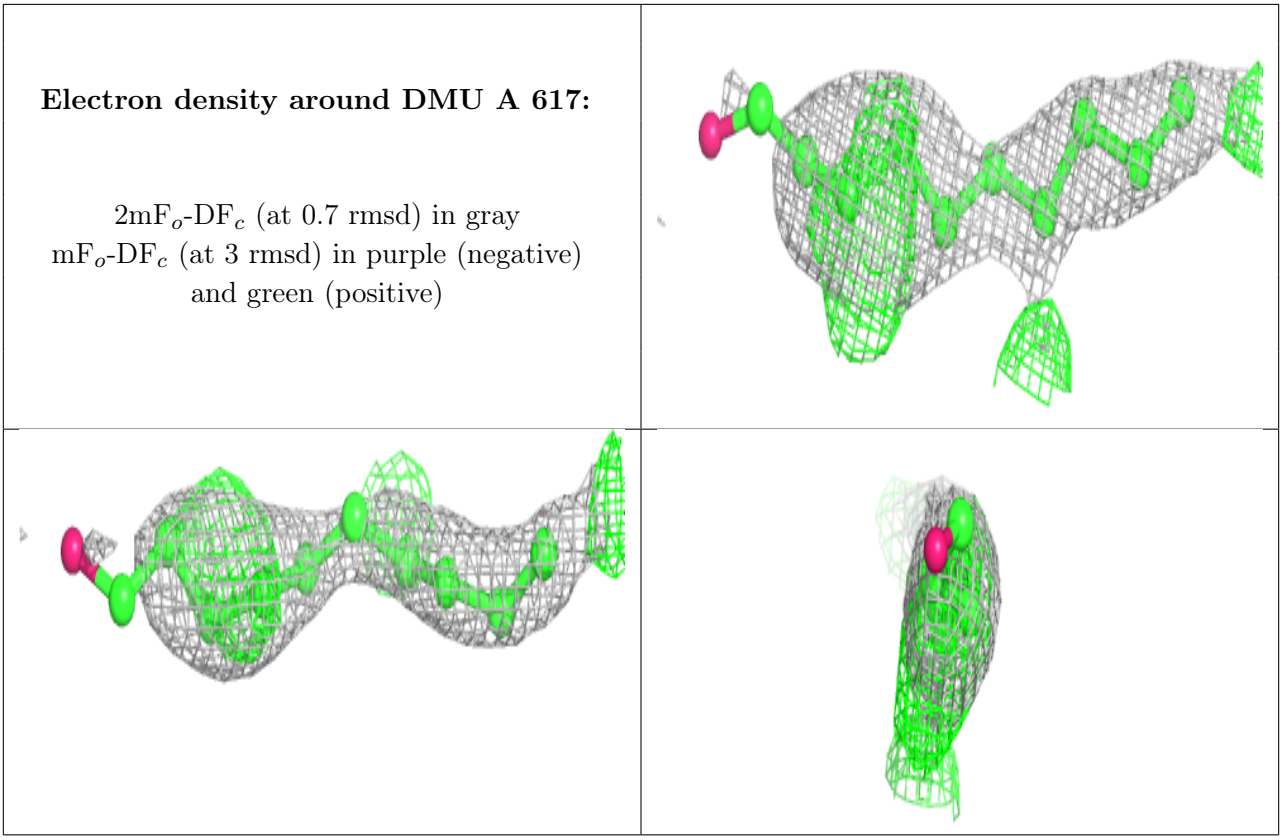
Electron density around DMU C 317:

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



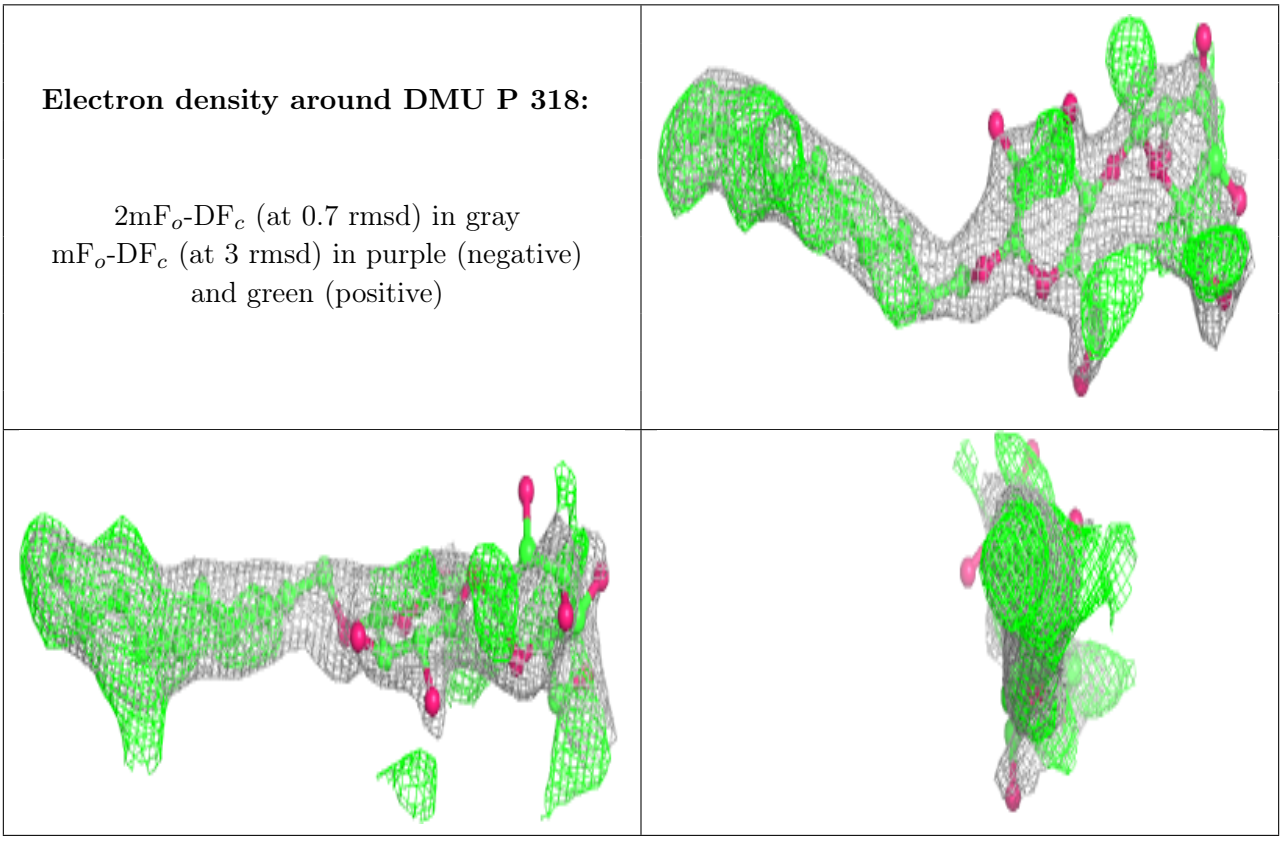
Electron density around DMU A 617:

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



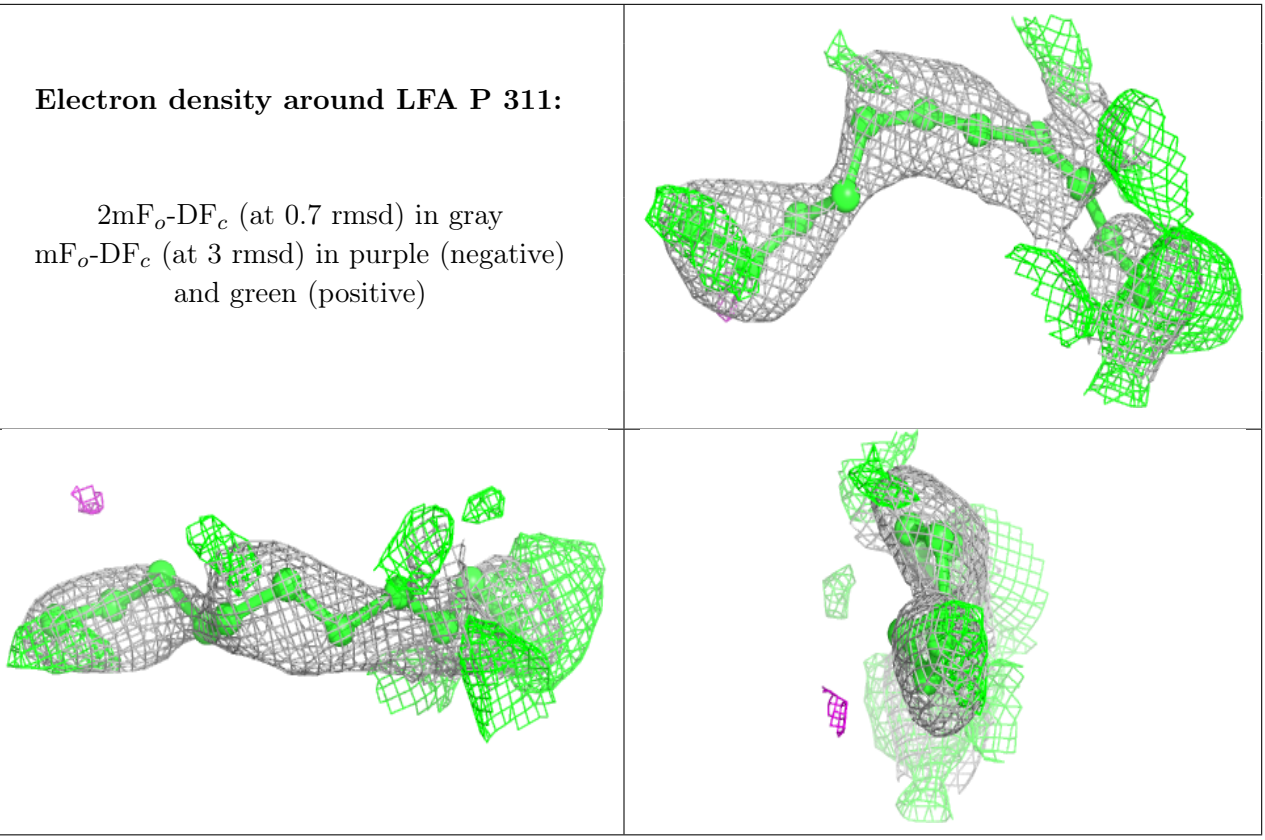
Electron density around DMU P 318:

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



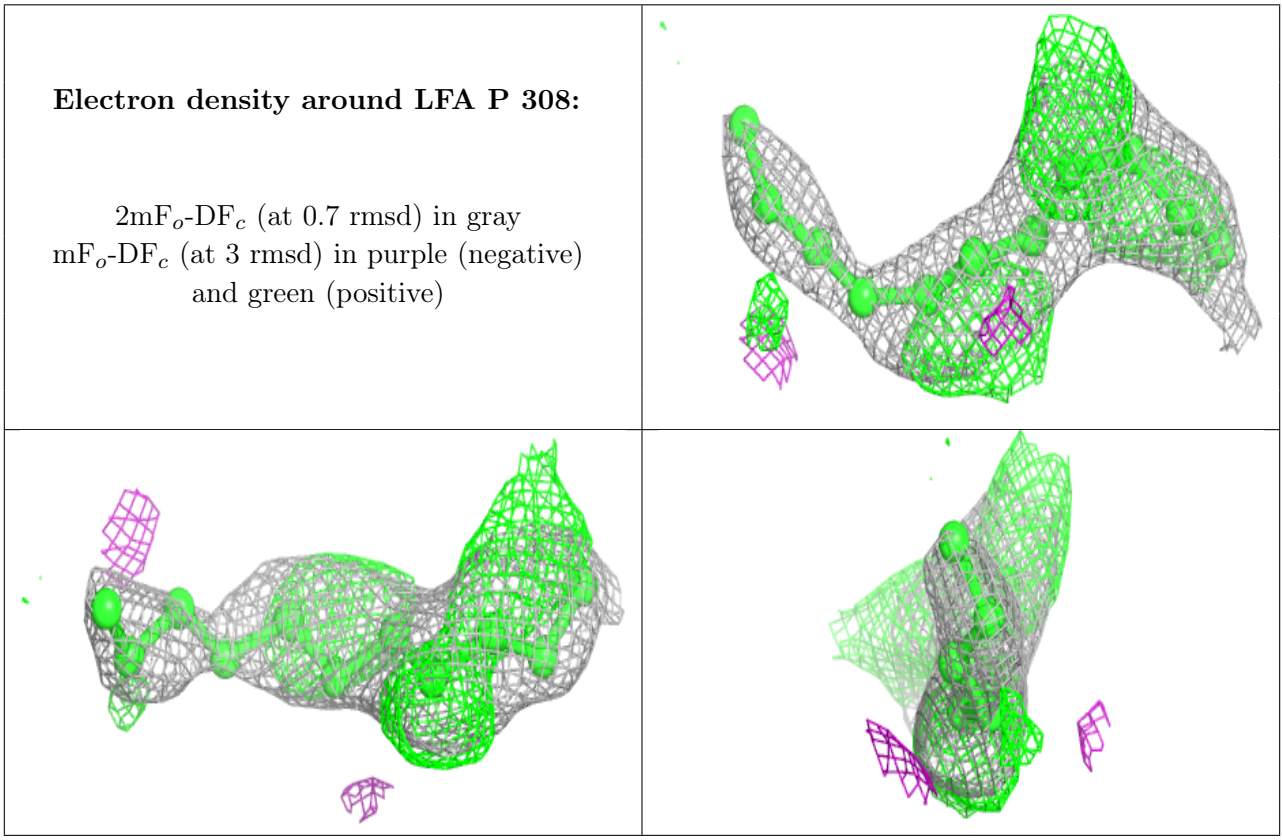
Electron density around LFA P 311:

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



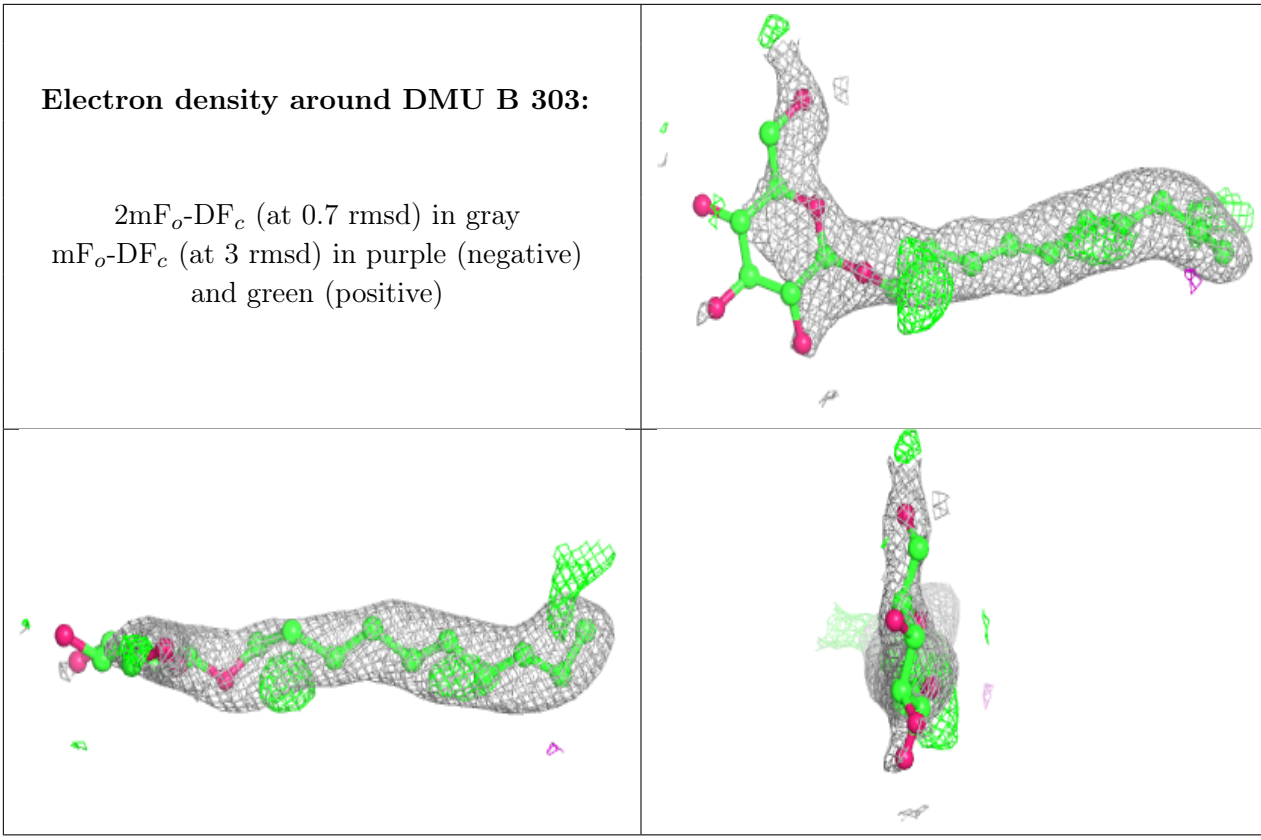
Electron density around LFA P 308:

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



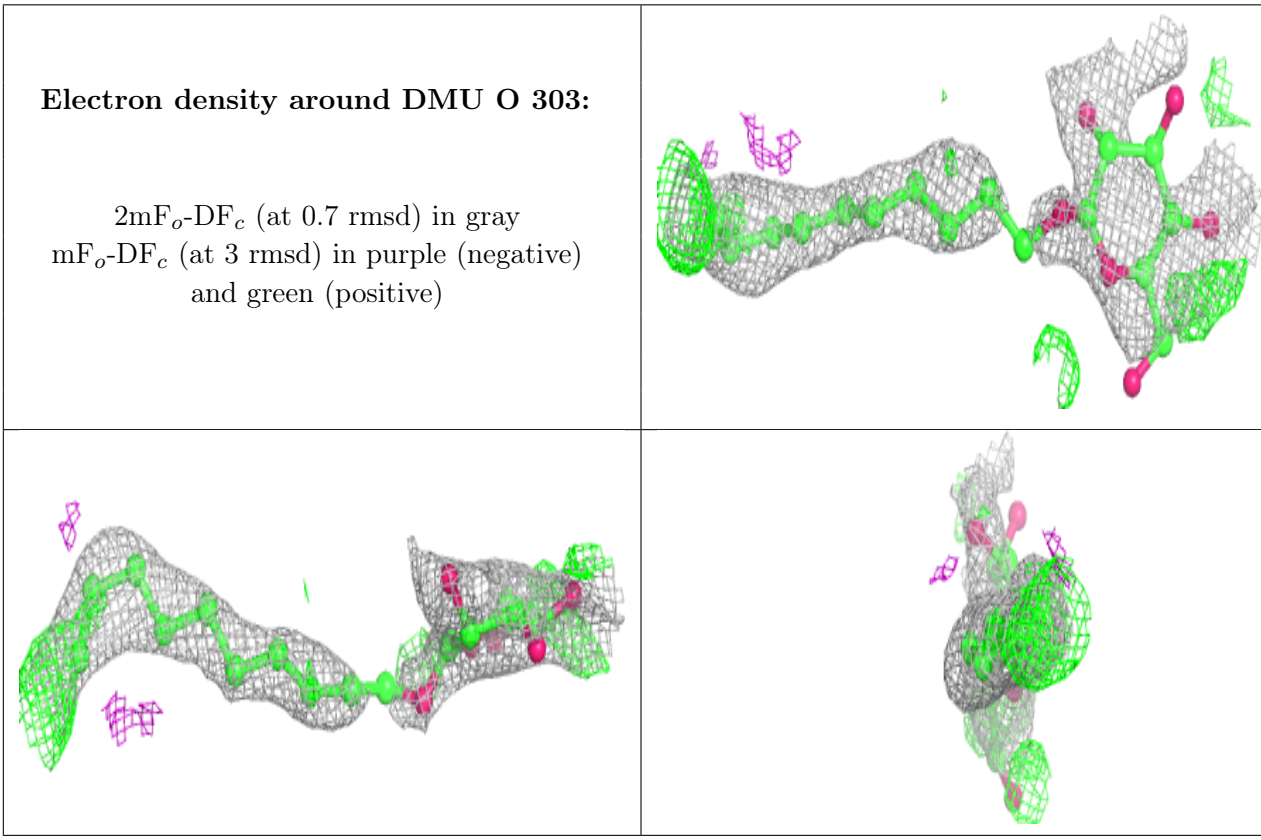
Electron density around DMU B 303:

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



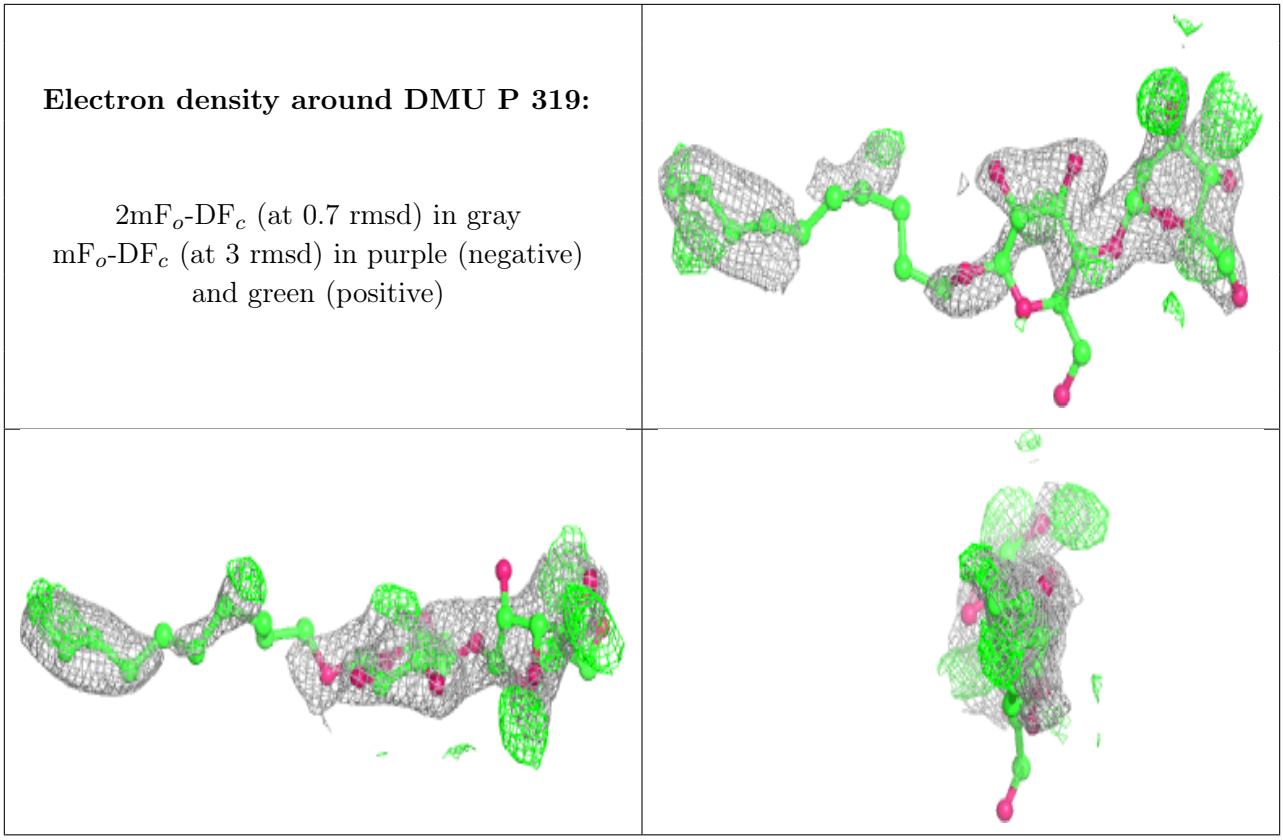
Electron density around DMU O 303:

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



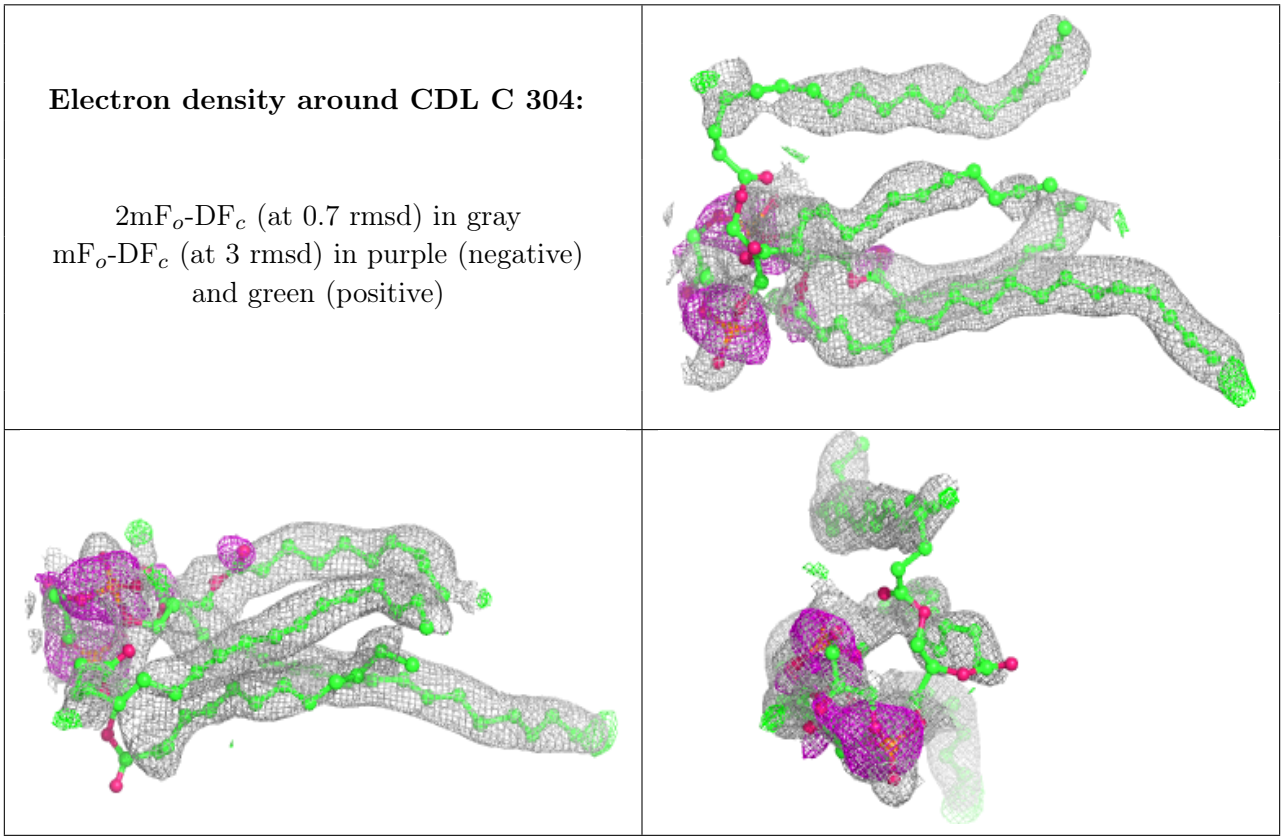
Electron density around DMU P 319:

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



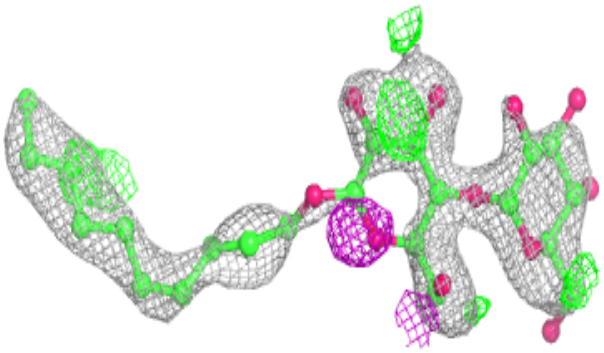
Electron density around CDL C 304:

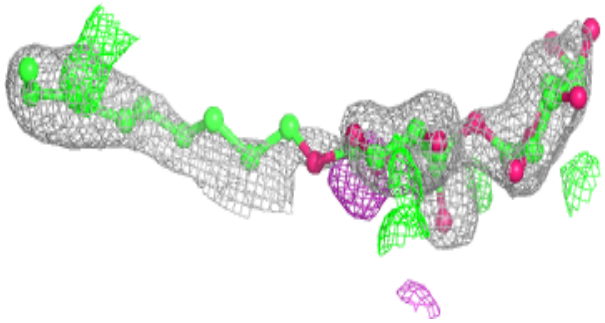
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

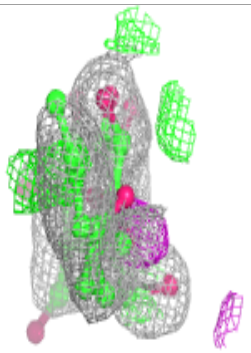


Electron density around DMU C 324:

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

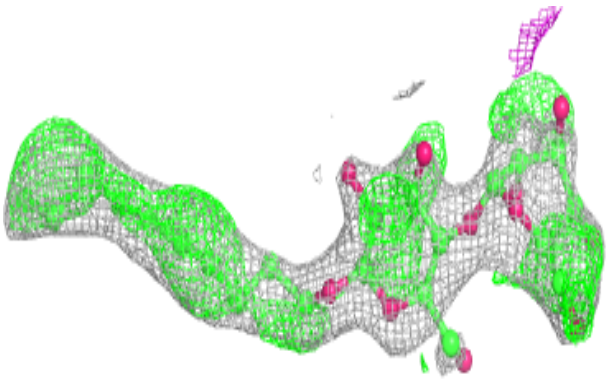


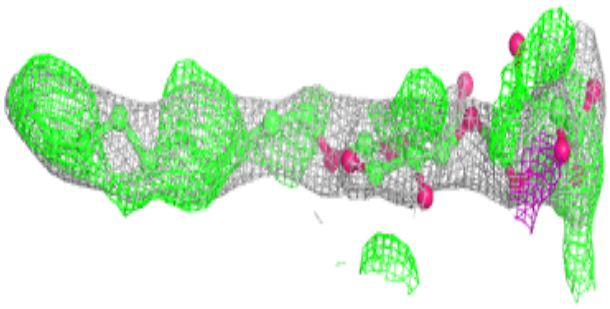


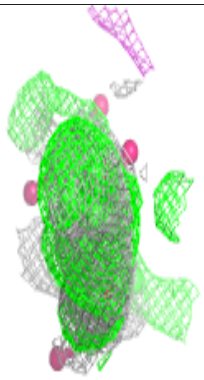


Electron density around DMU C 318:

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

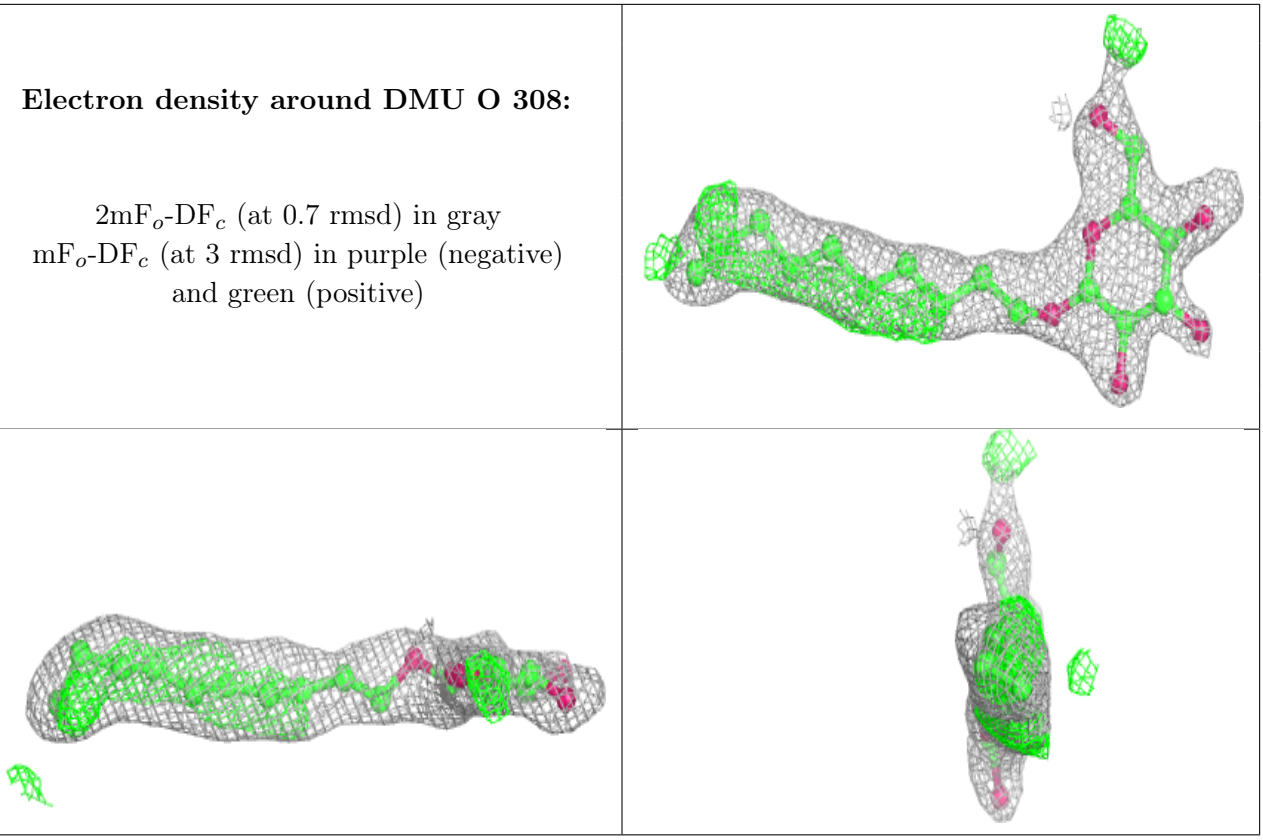






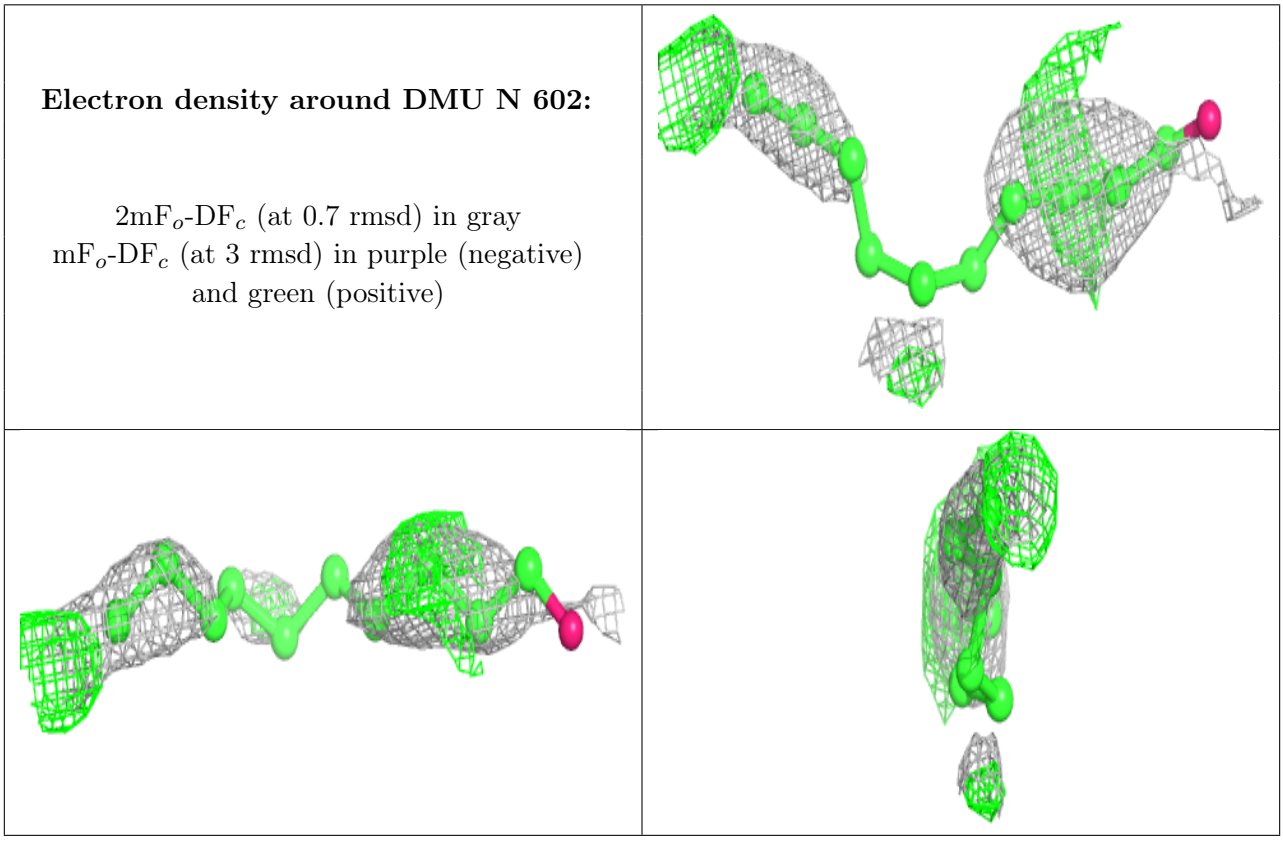
Electron density around DMU O 308:

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



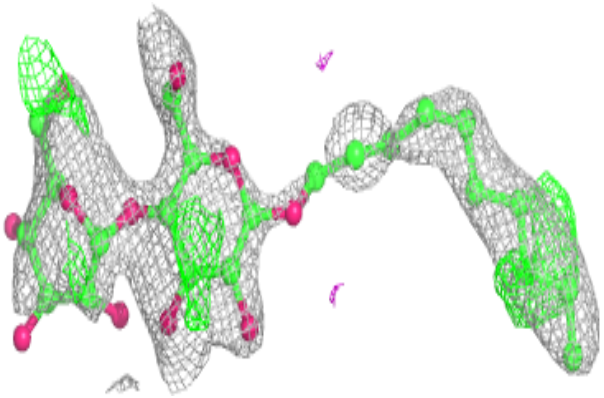
Electron density around DMU N 602:

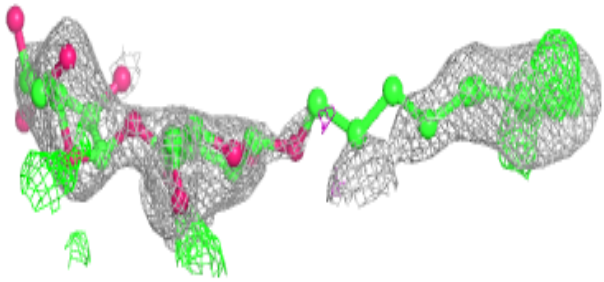
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

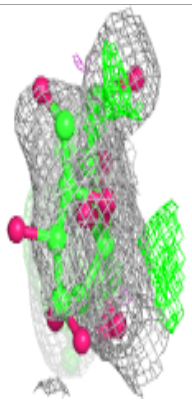


Electron density around DMU P 324:

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

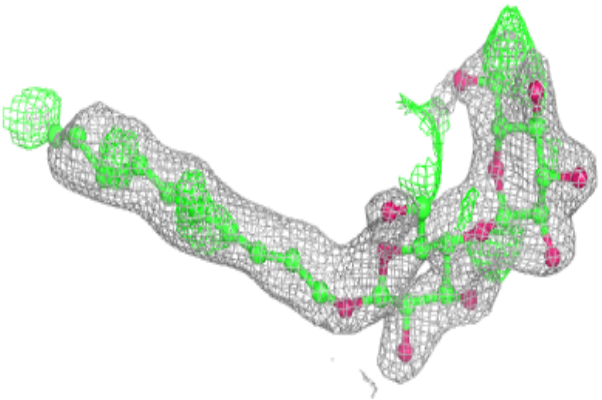


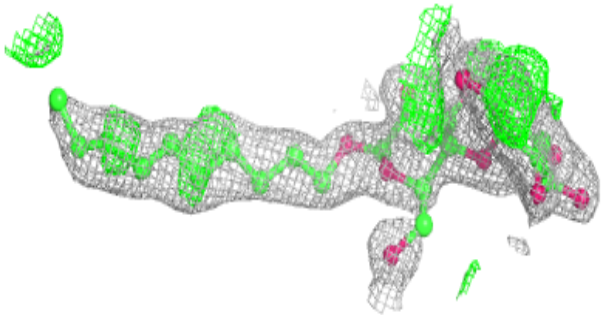


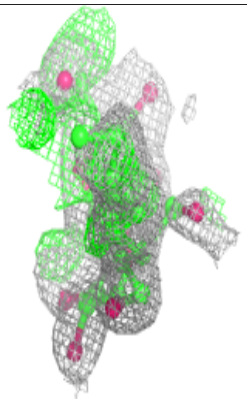


Electron density around DMU Q 201:

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

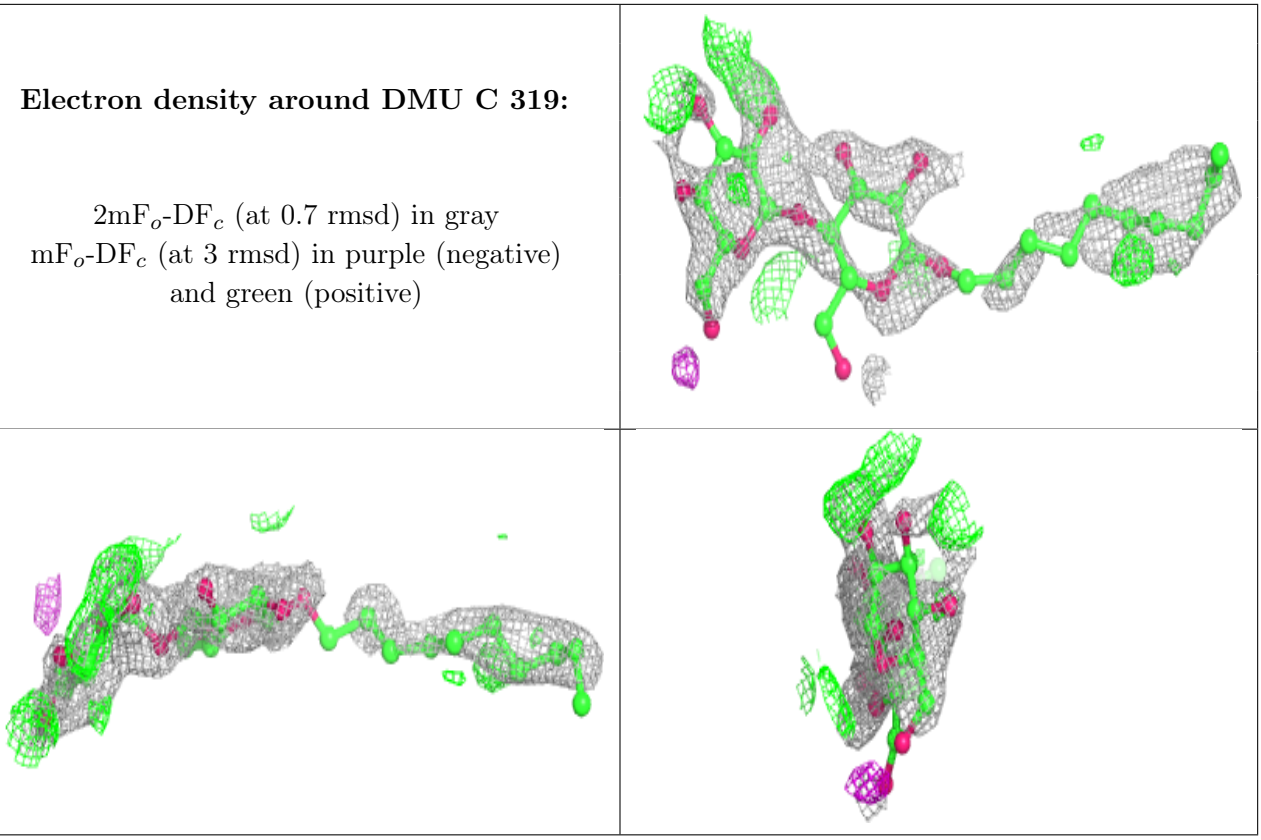






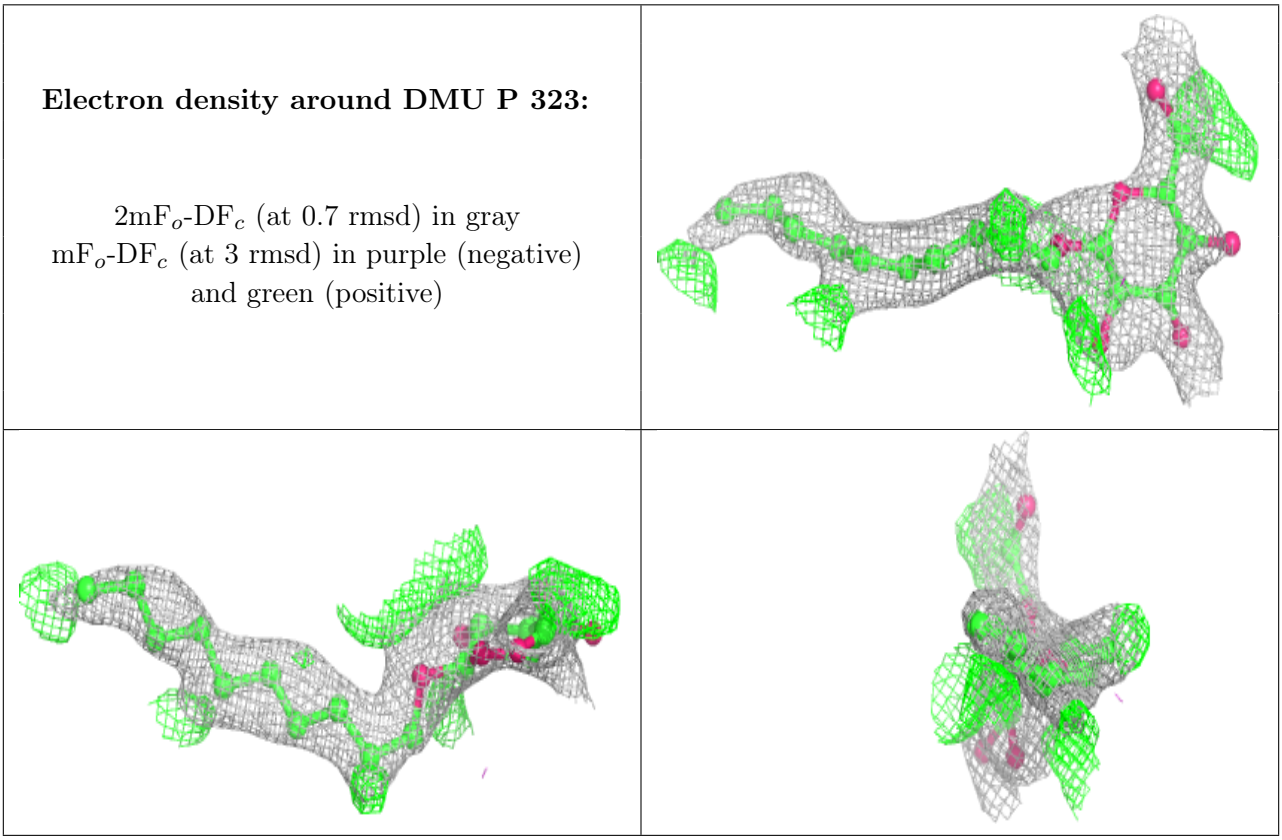
Electron density around DMU C 319:

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



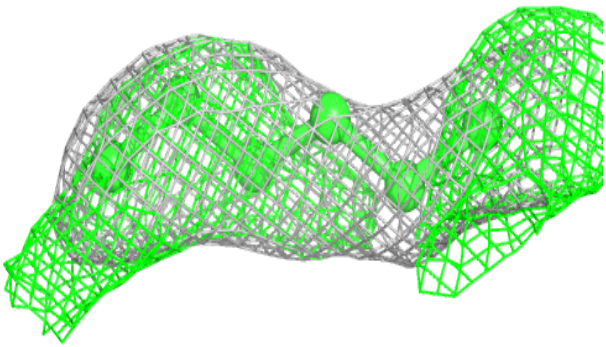
Electron density around DMU P 323:

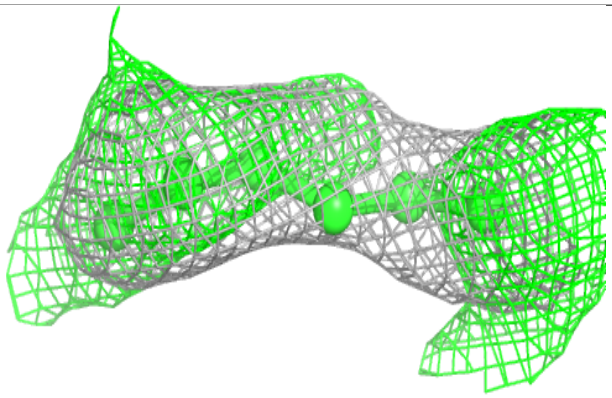
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

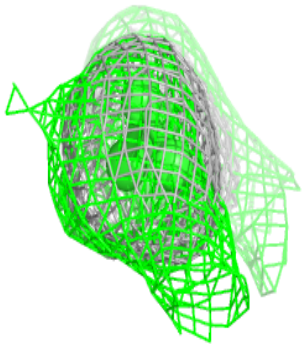


Electron density around LFA C 308:

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

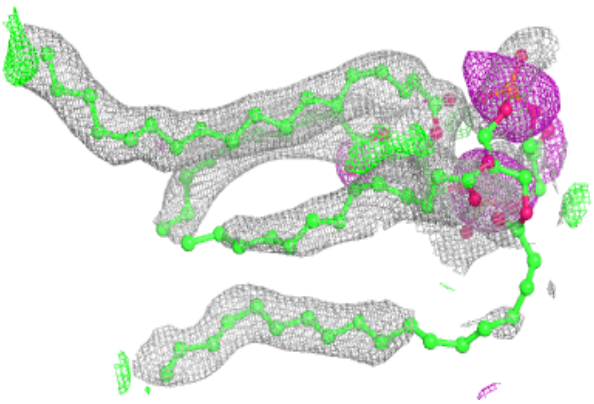


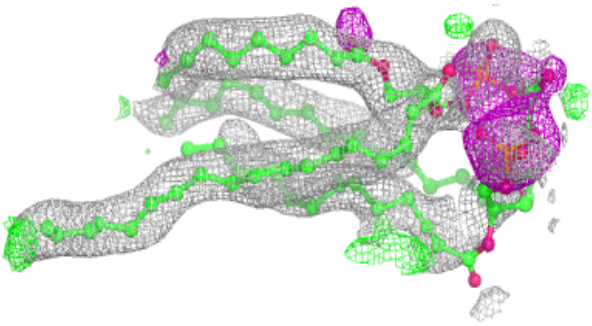


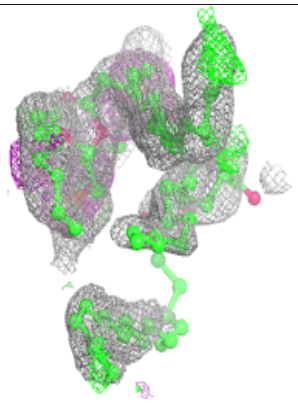


Electron density around CDL P 305:

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

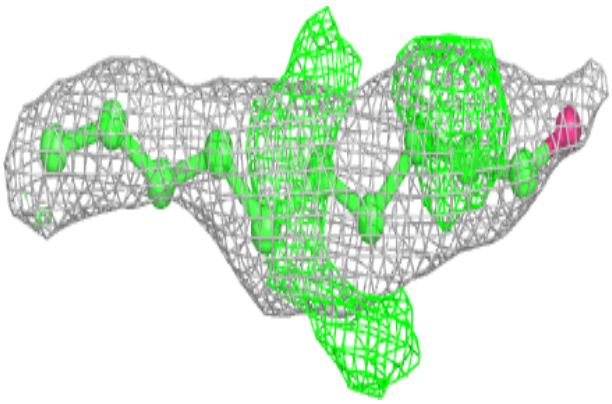


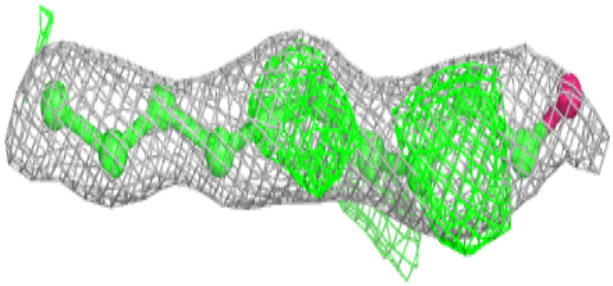


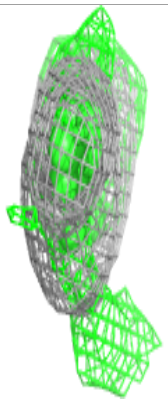


Electron density around DMU A 615:

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

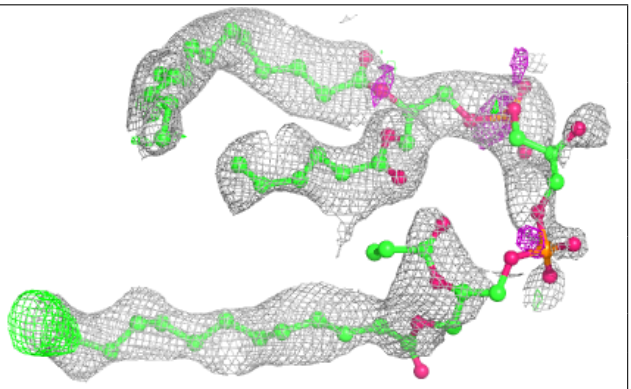


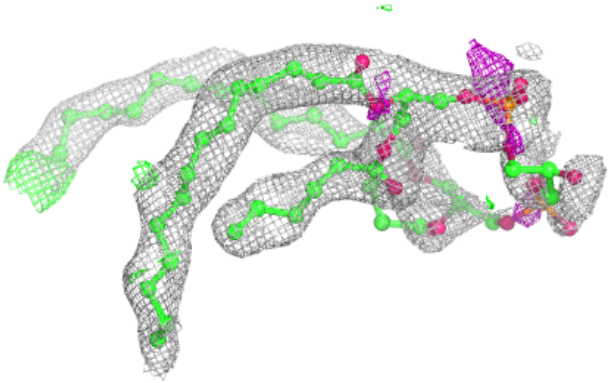


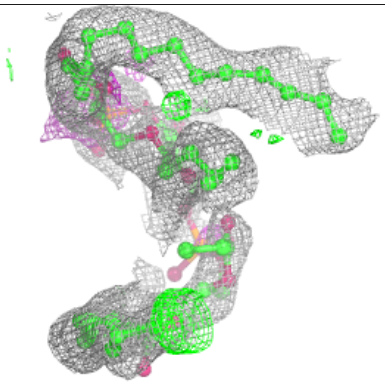


Electron density around CDL O 304:

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

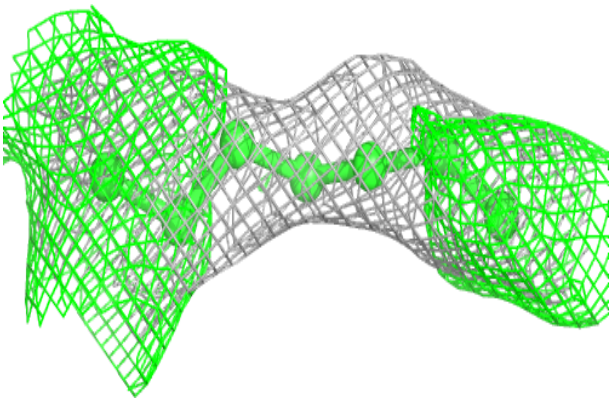


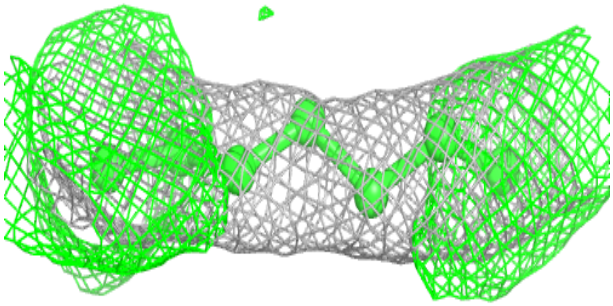


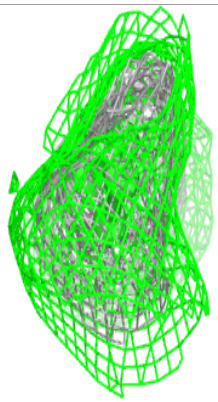


Electron density around DMU A 609:

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

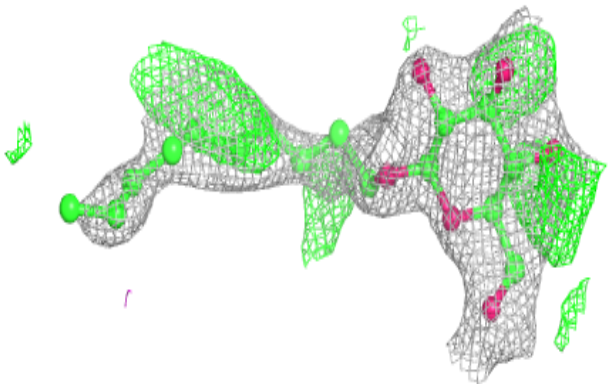


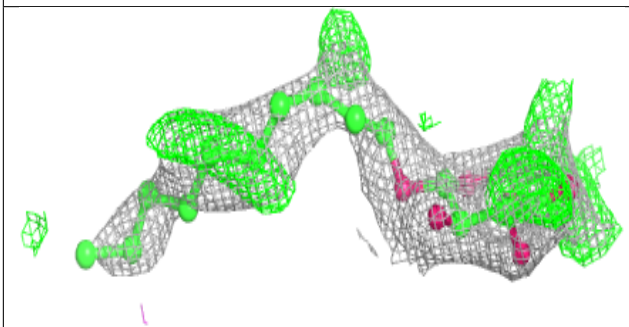


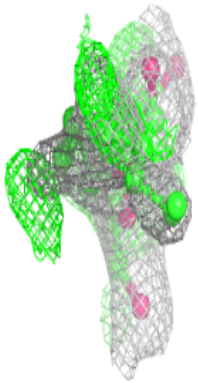


Electron density around DMU C 323:

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

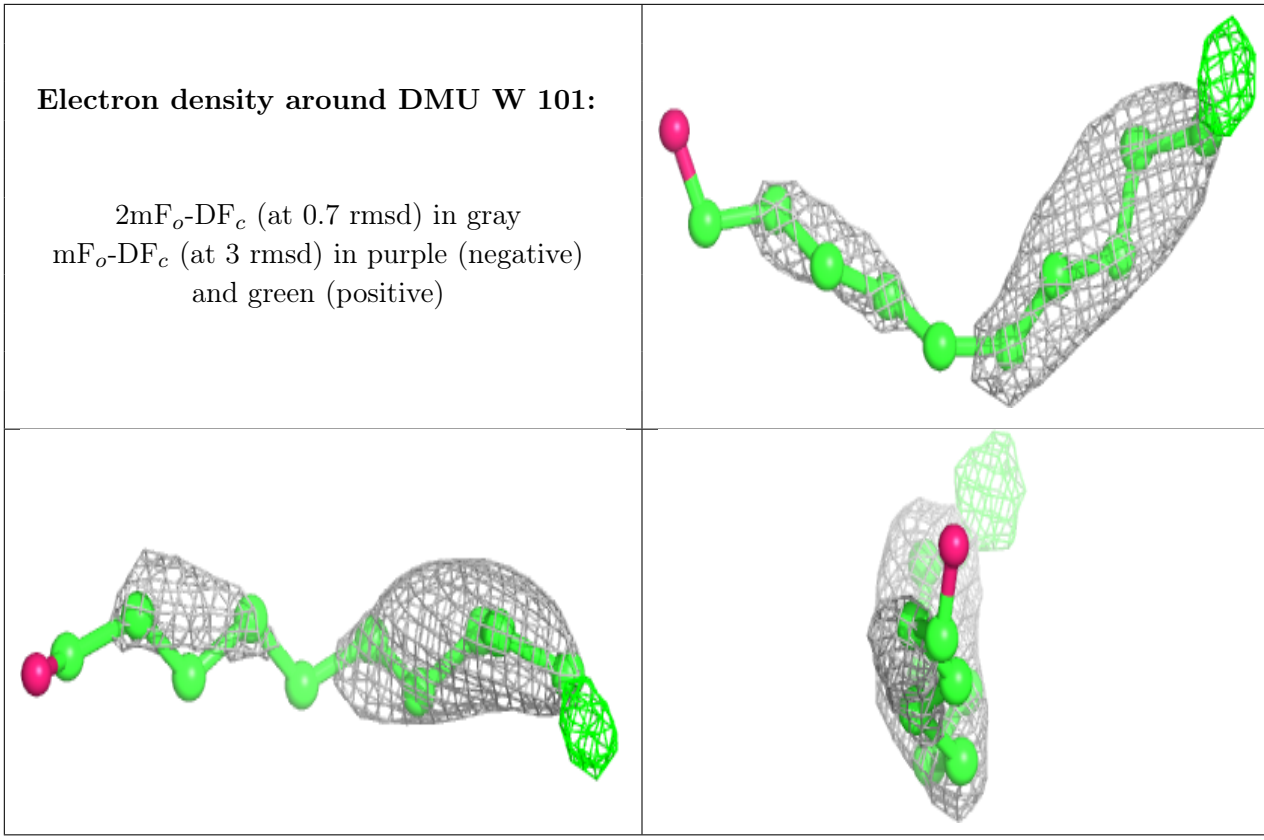






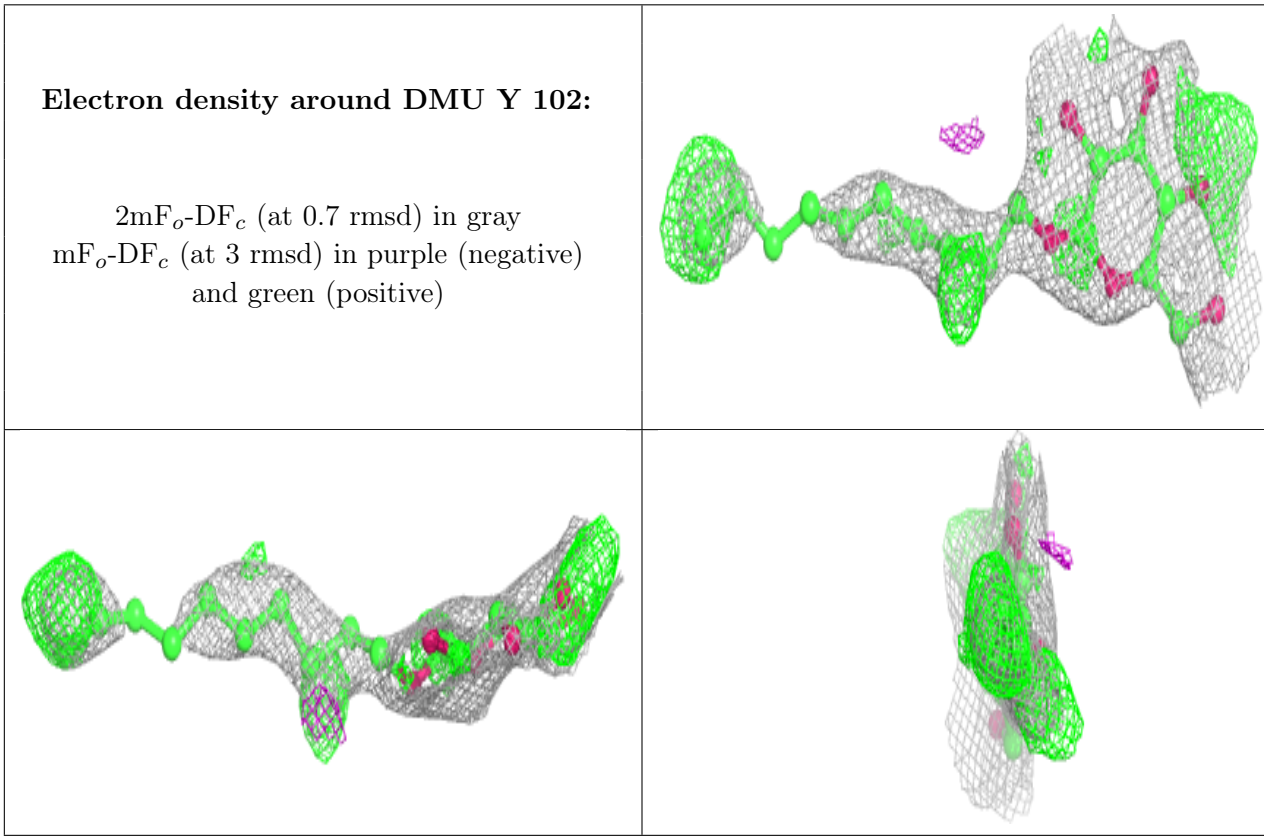
Electron density around DMU W 101:

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



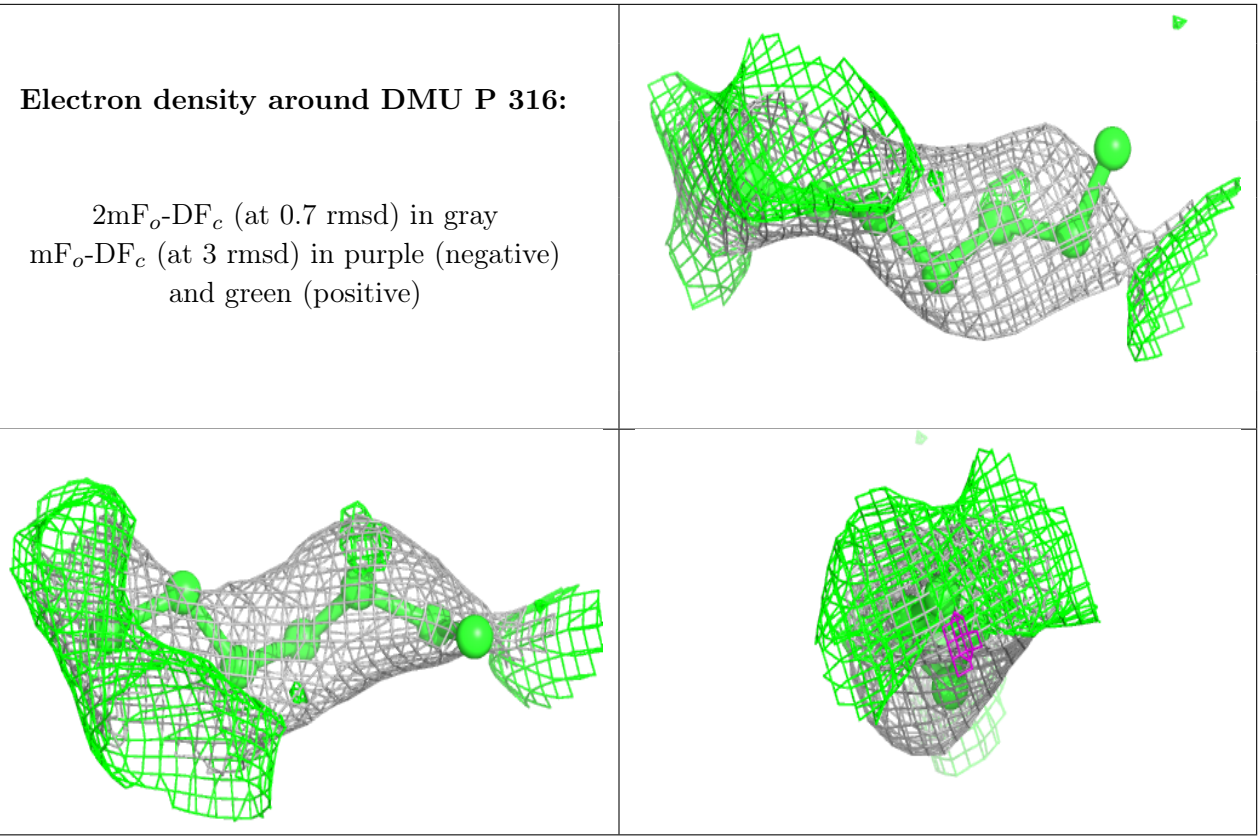
Electron density around DMU Y 102:

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



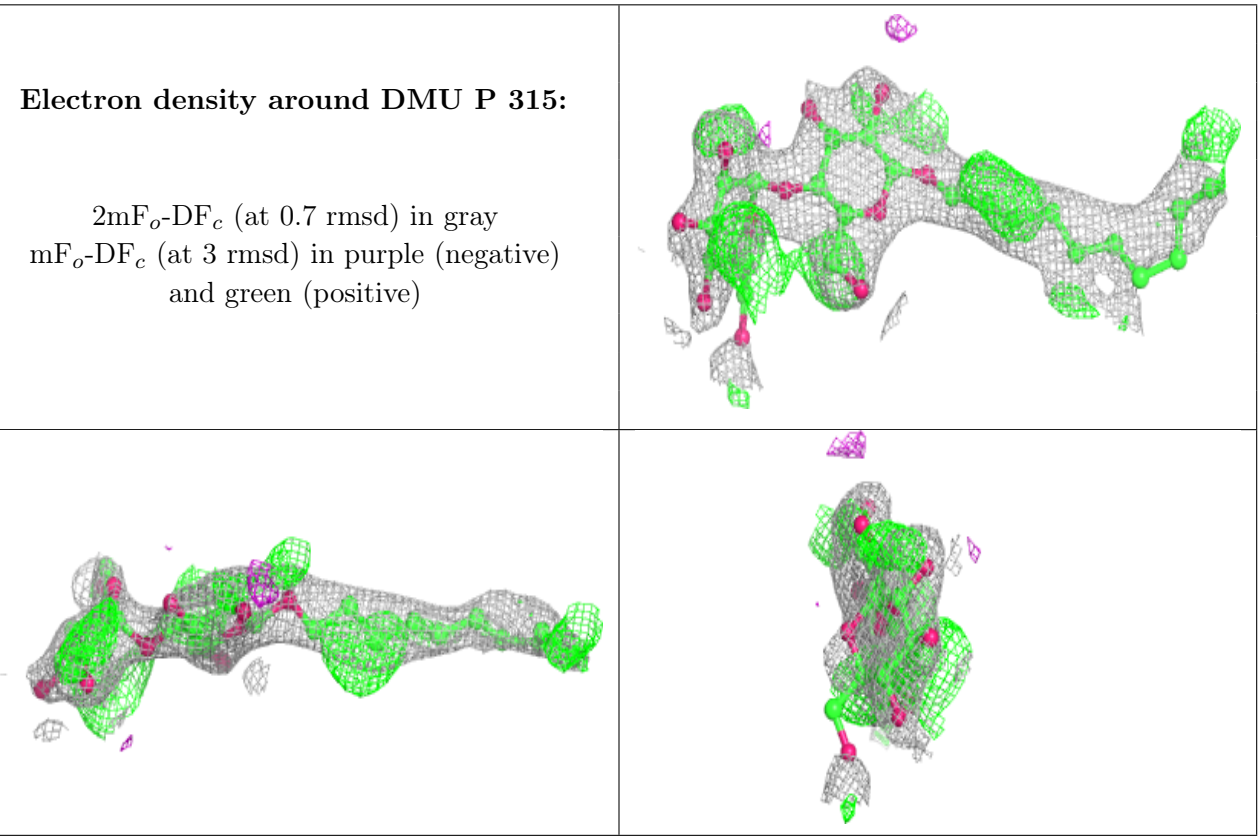
Electron density around DMU P 316:

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



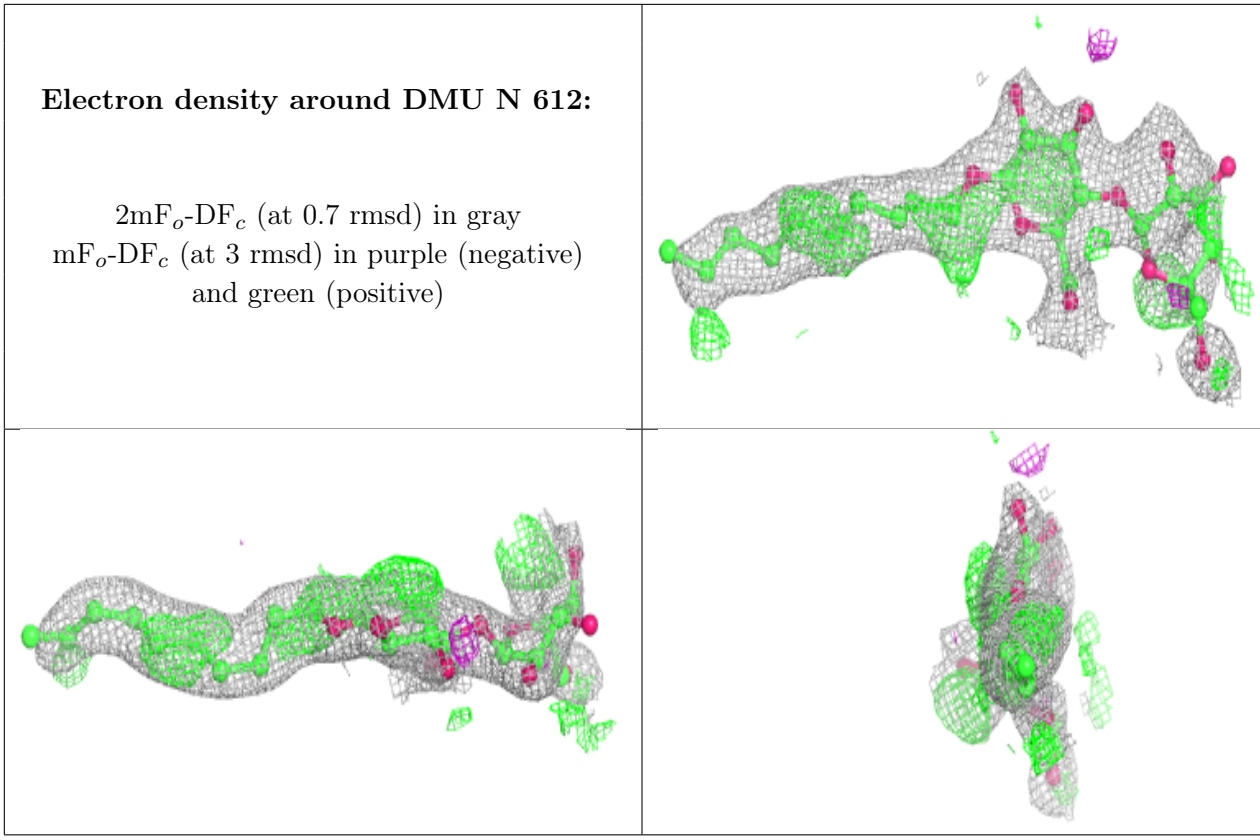
Electron density around DMU P 315:

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



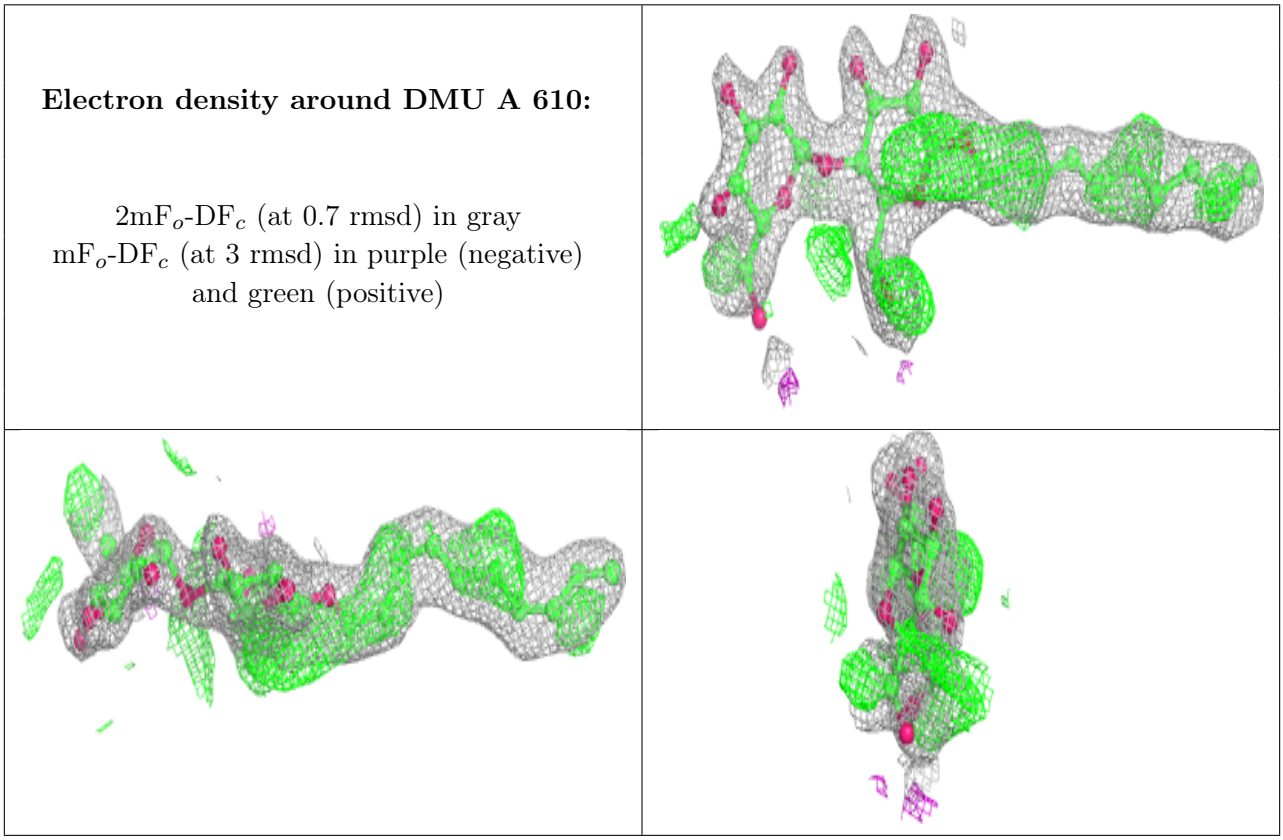
Electron density around DMU N 612:

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



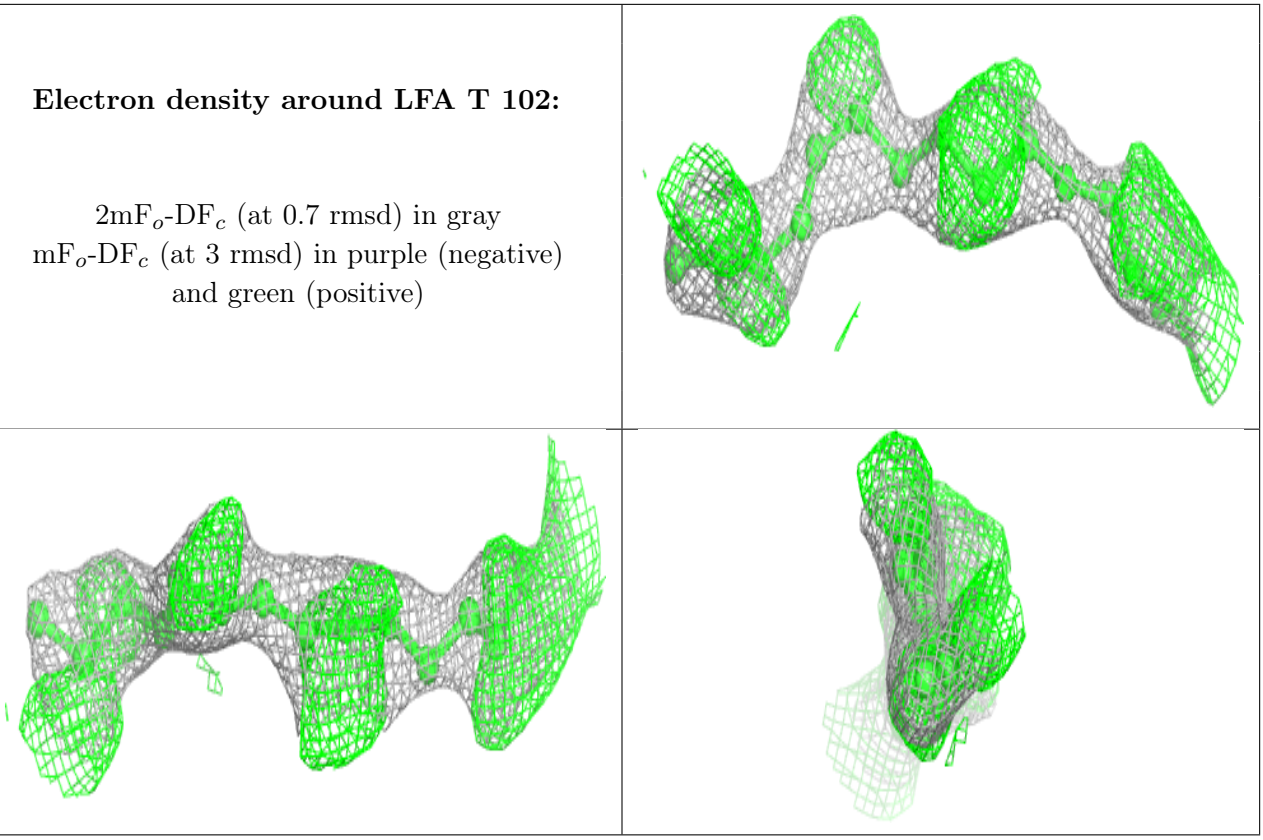
Electron density around DMU A 610:

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



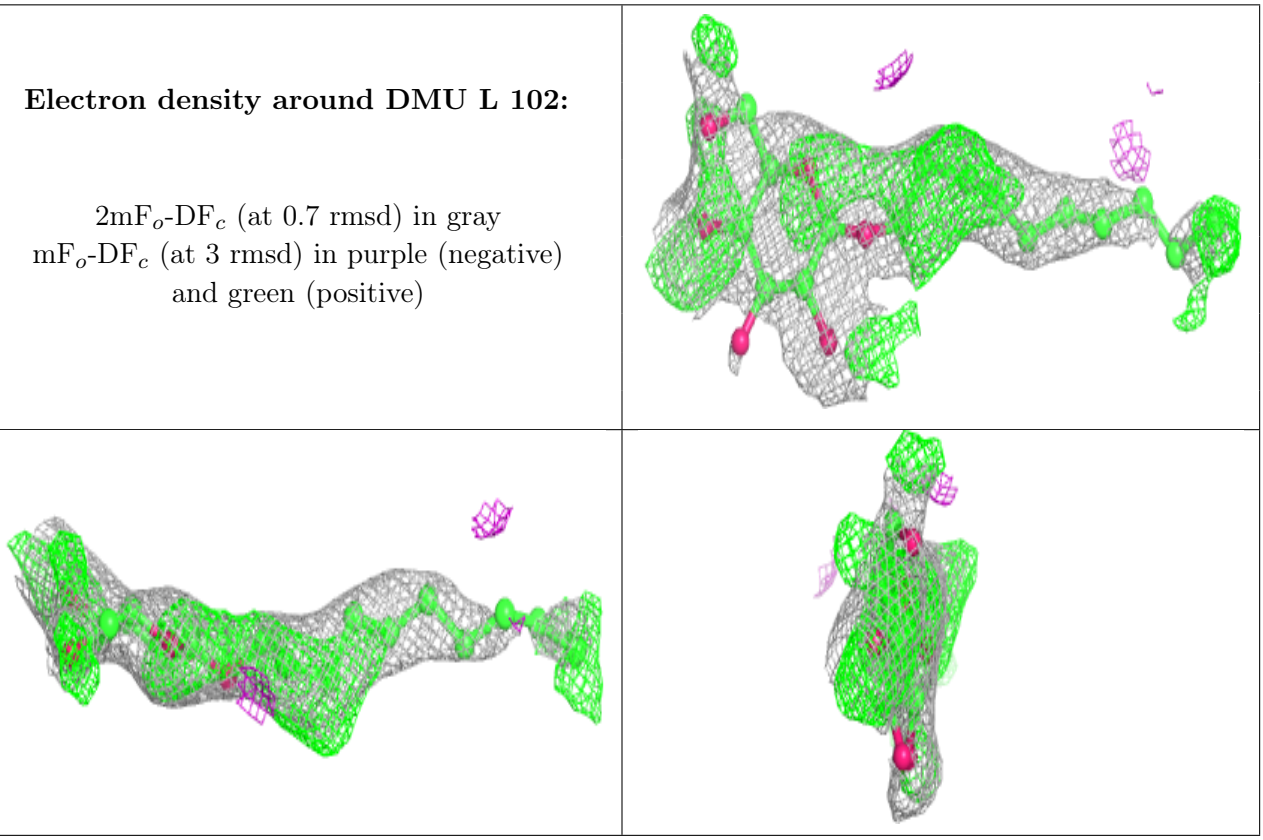
Electron density around LFA T 102:

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



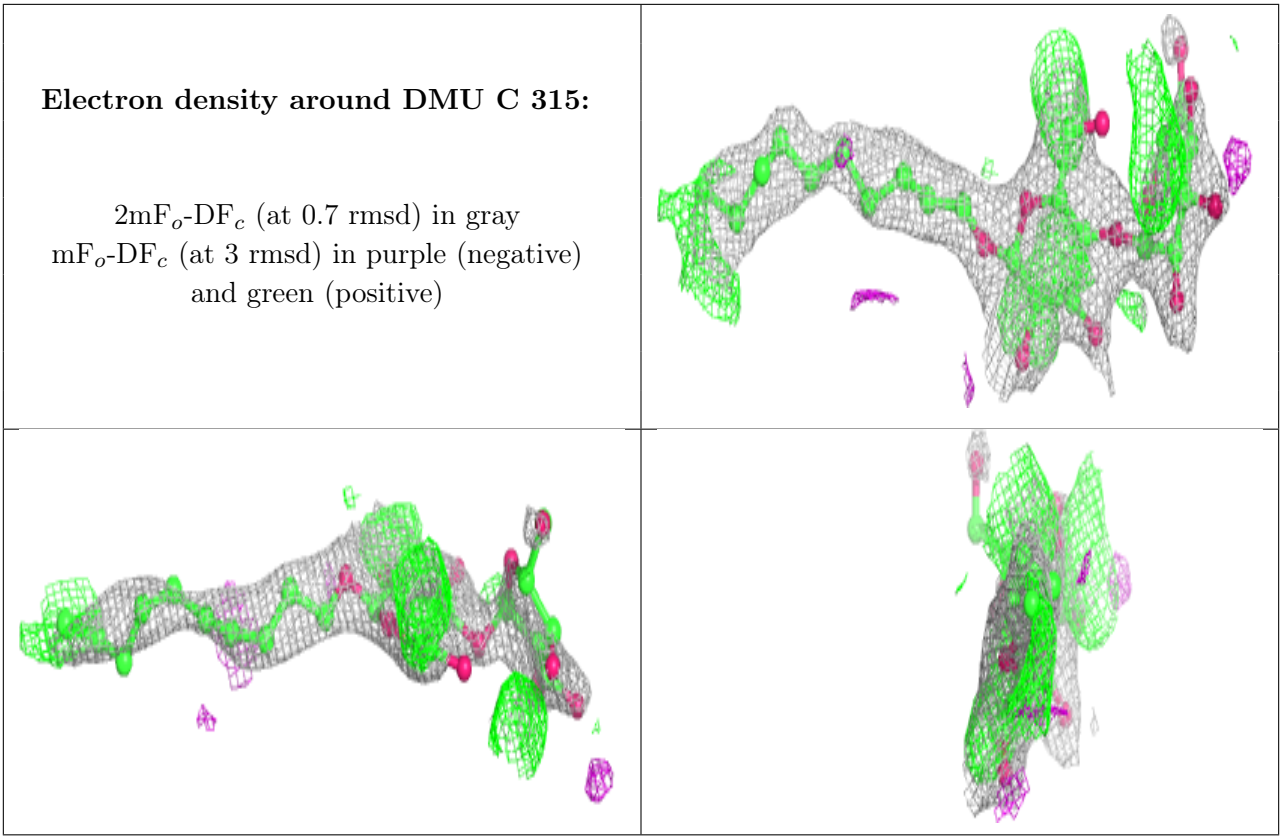
Electron density around DMU L 102:

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



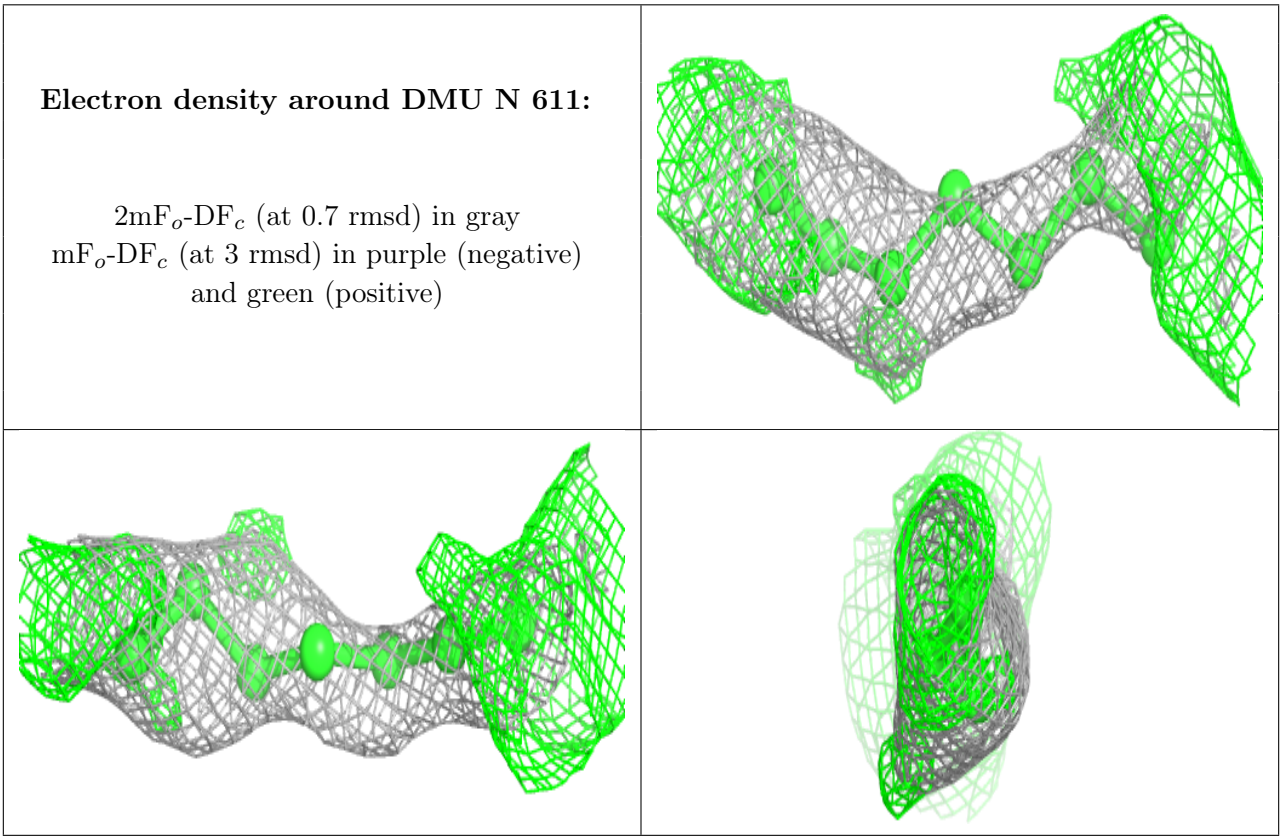
Electron density around DMU C 315:

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



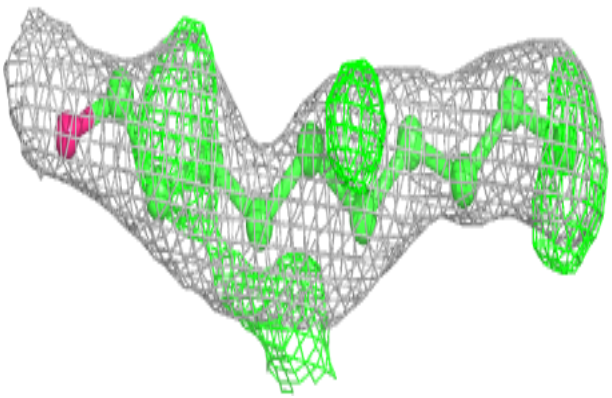
Electron density around DMU N 611:

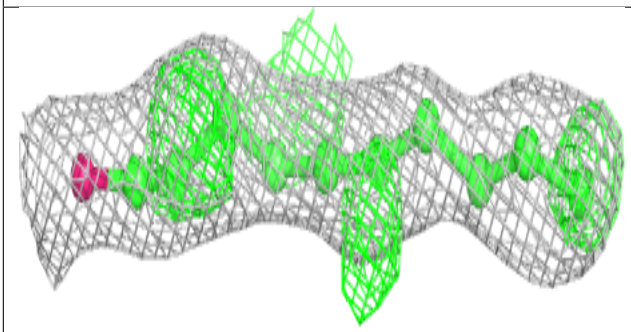
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

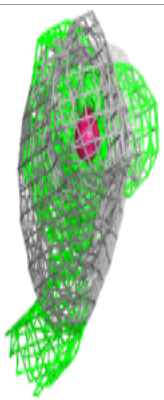


Electron density around DMU O 307:

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

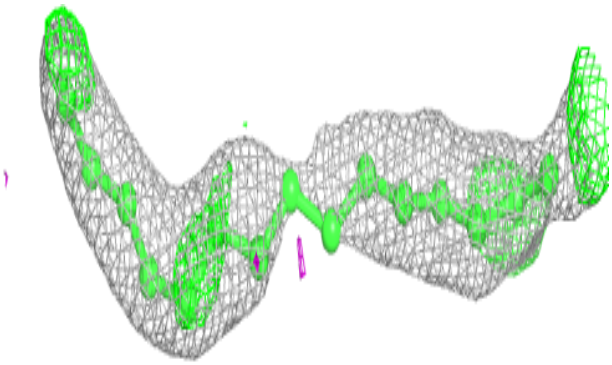


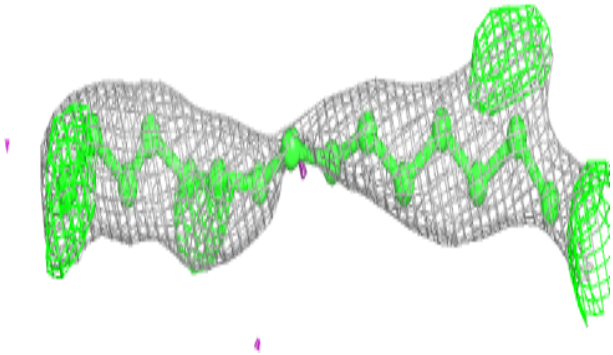


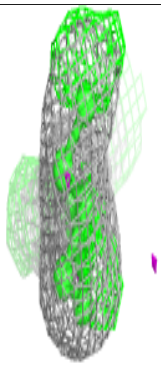


Electron density around LFA C 313:

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

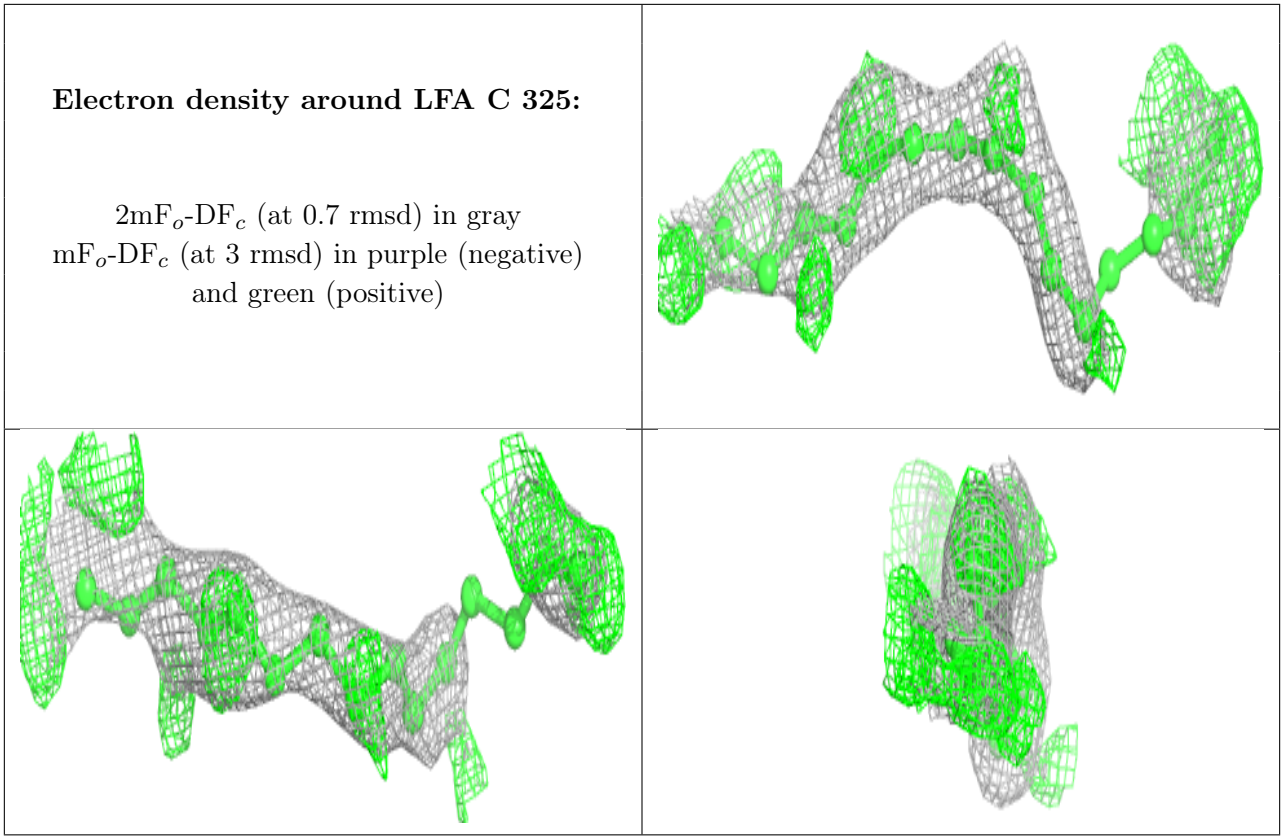






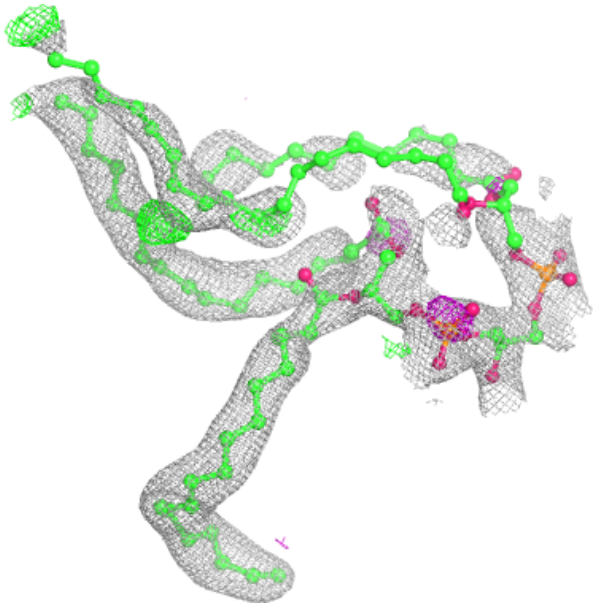
Electron density around LFA C 325:

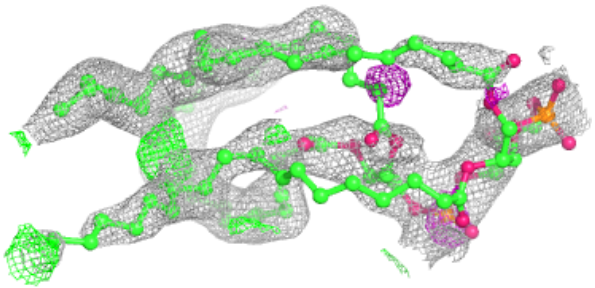
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

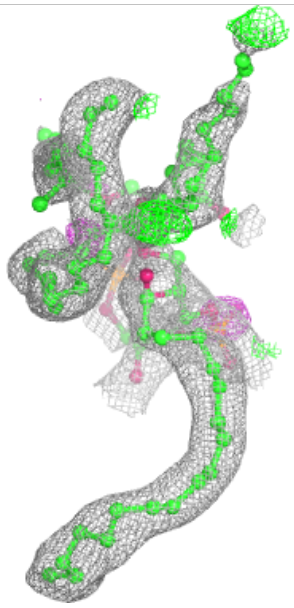


Electron density around CDL Y 101:

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

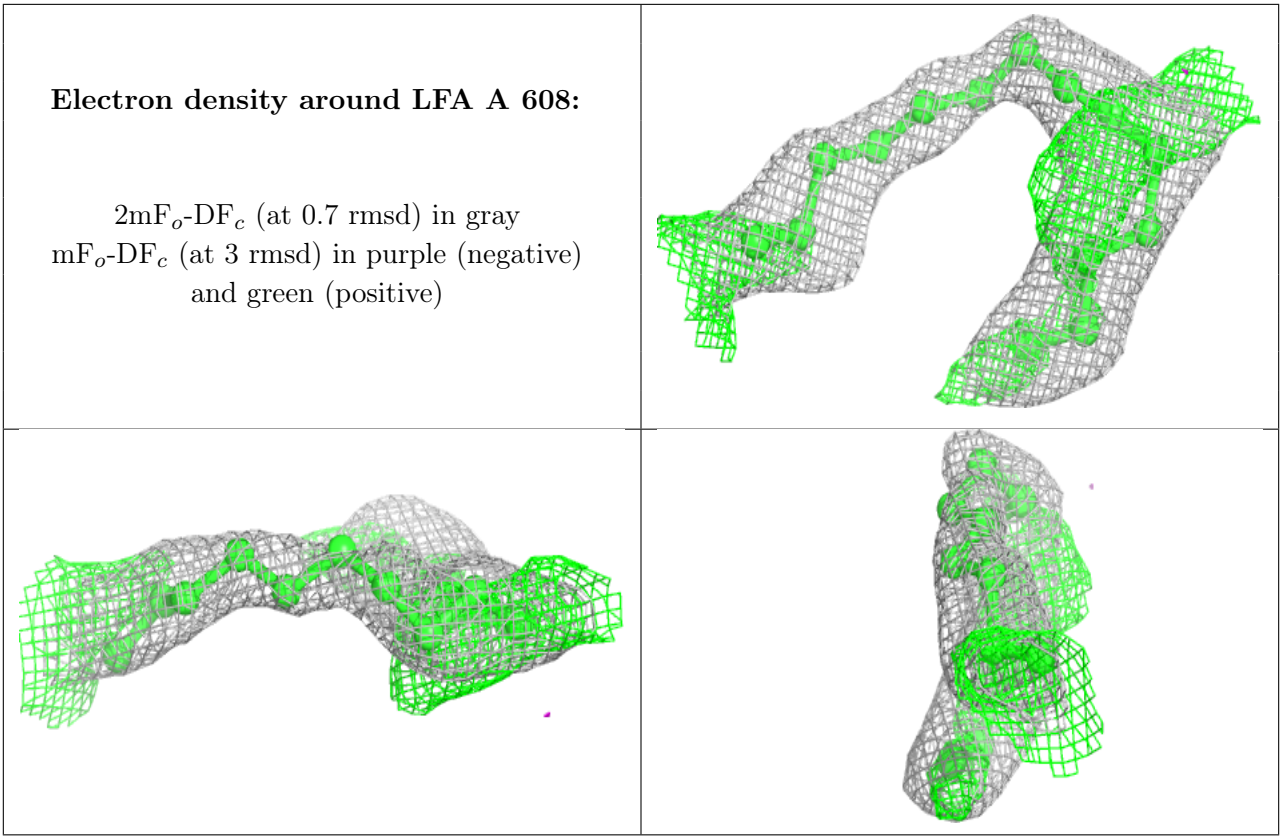






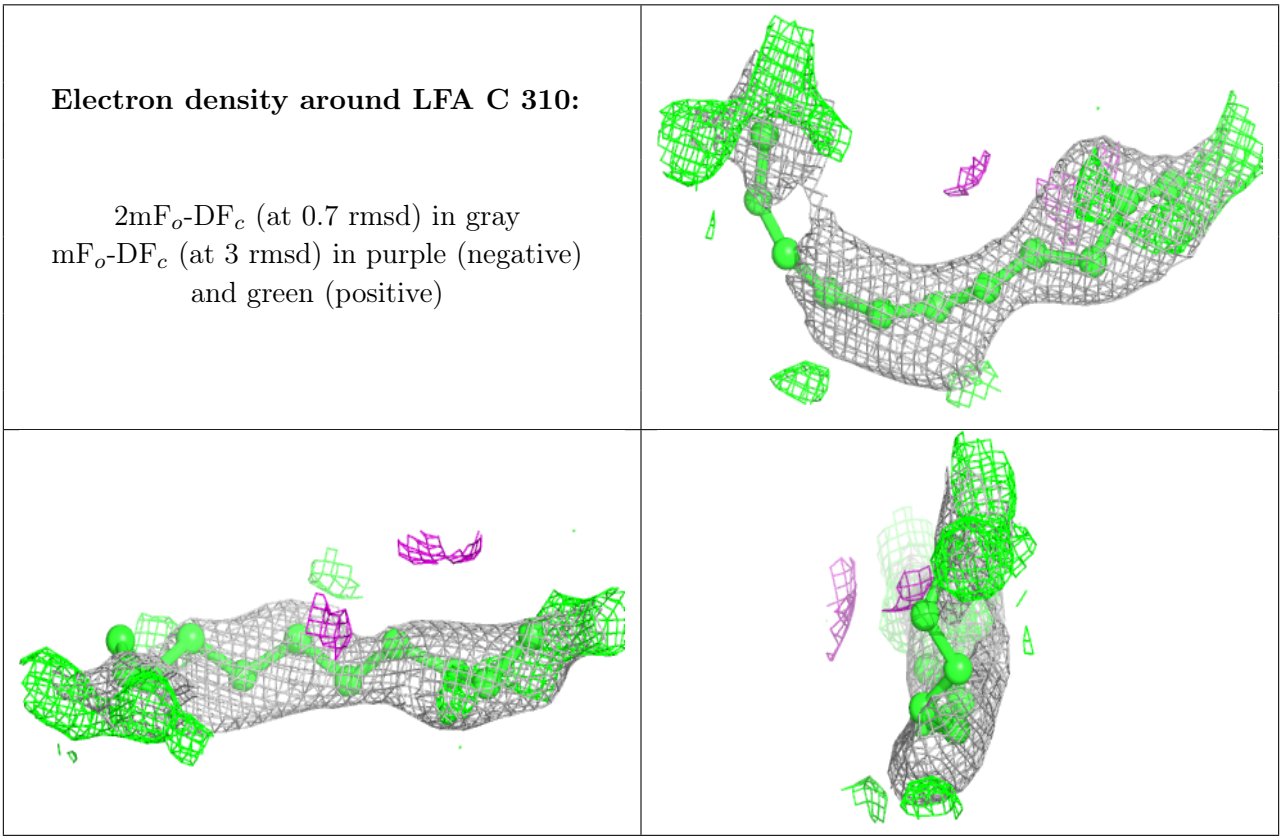
Electron density around LFA A 608:

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



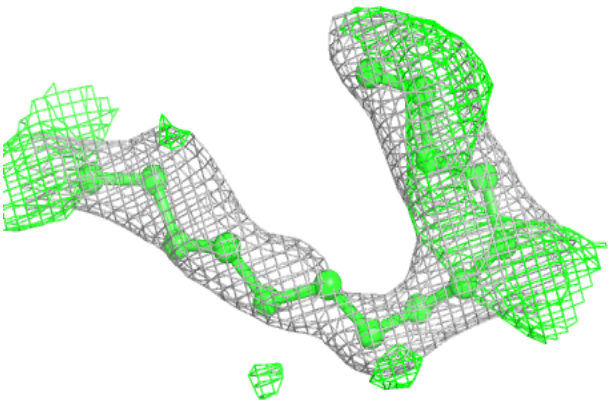
Electron density around LFA C 310:

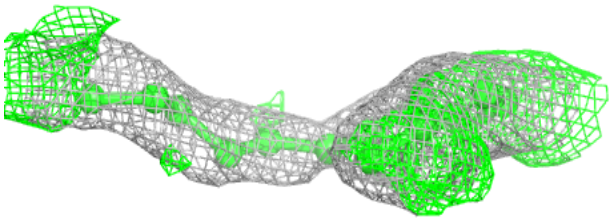
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

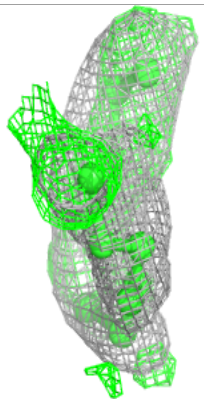


Electron density around LFA N 610:

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

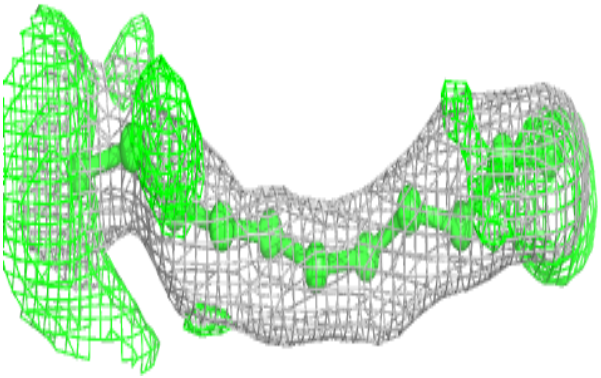


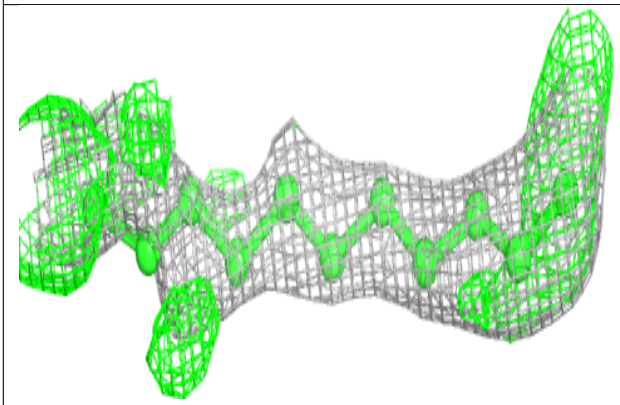


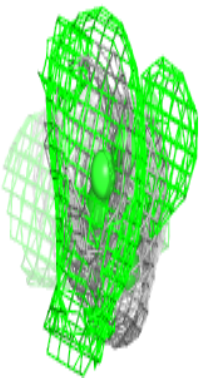


Electron density around LFA O 302:

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

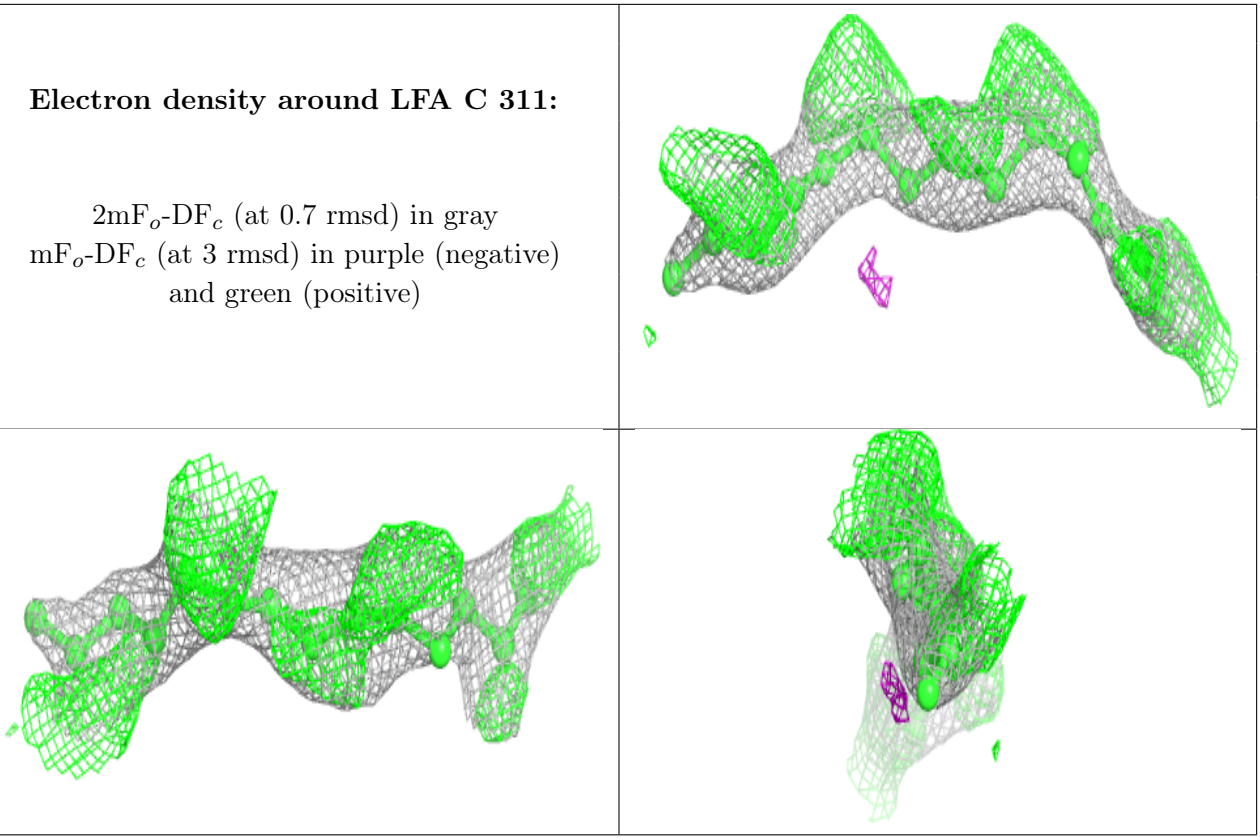






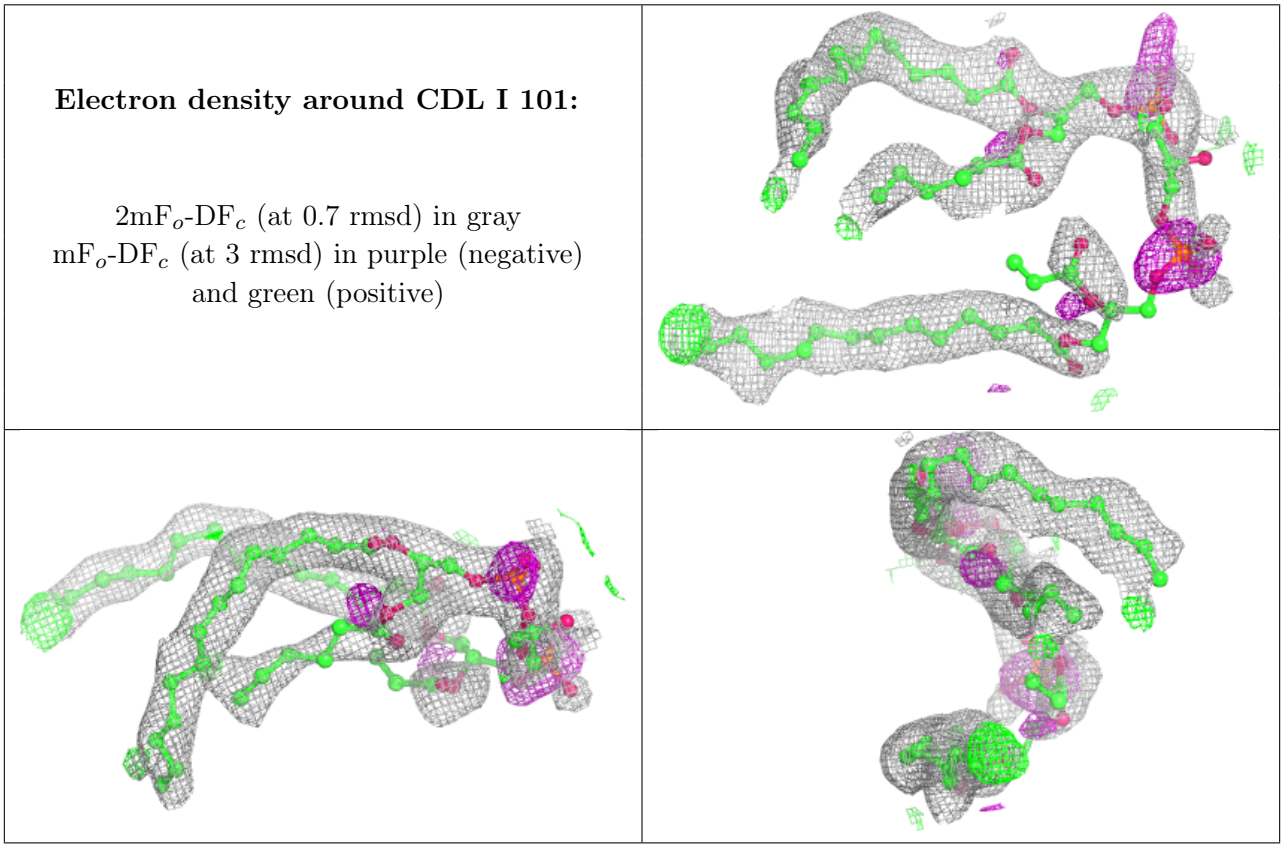
Electron density around LFA C 311:

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



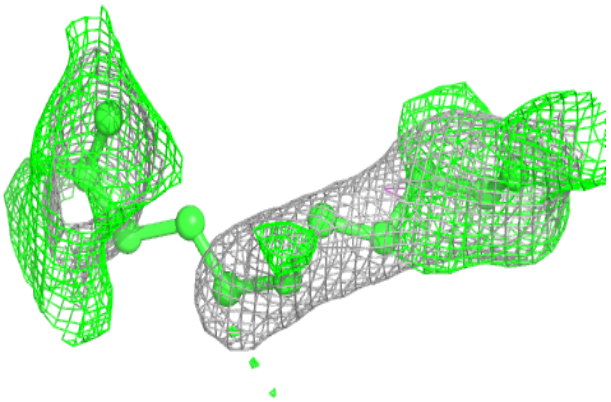
Electron density around CDL I 101:

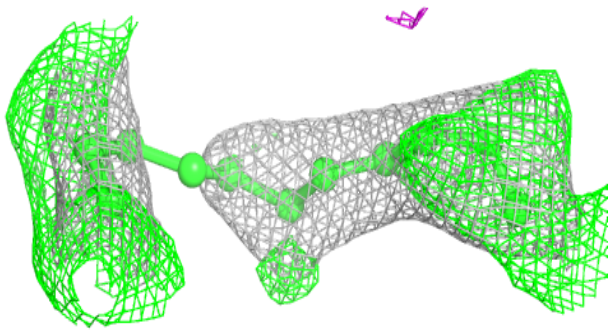
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

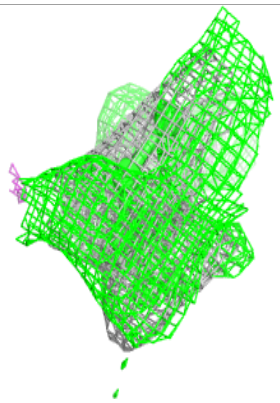


Electron density around LFA C 312:

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

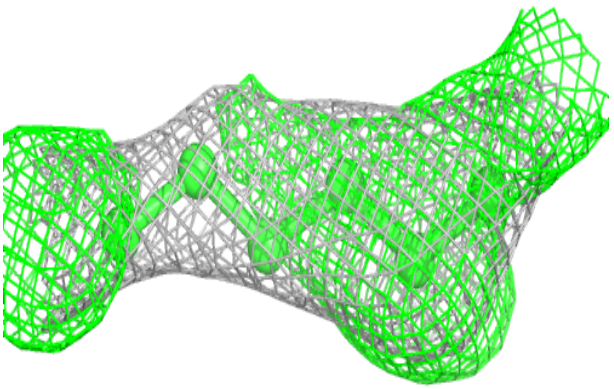


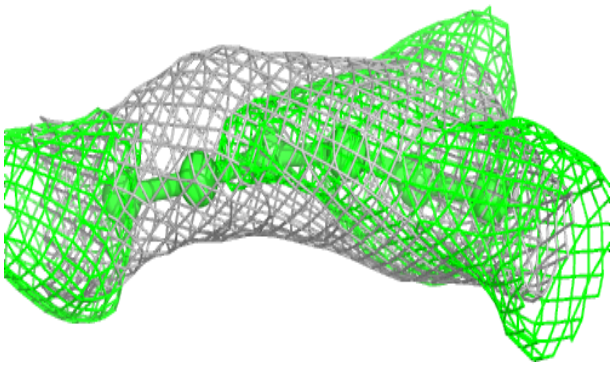


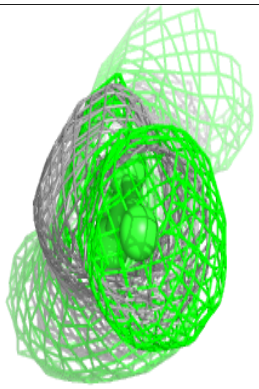


Electron density around LFA P 309:

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

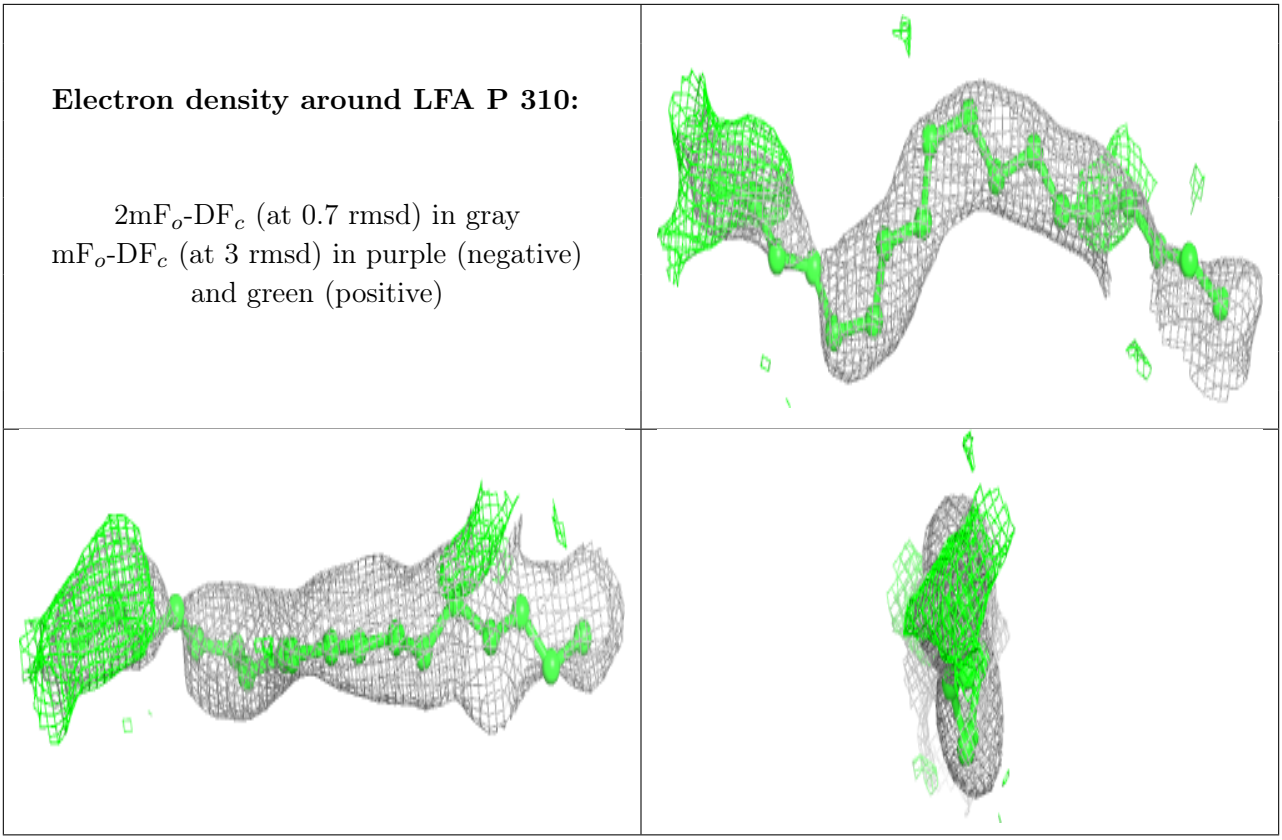






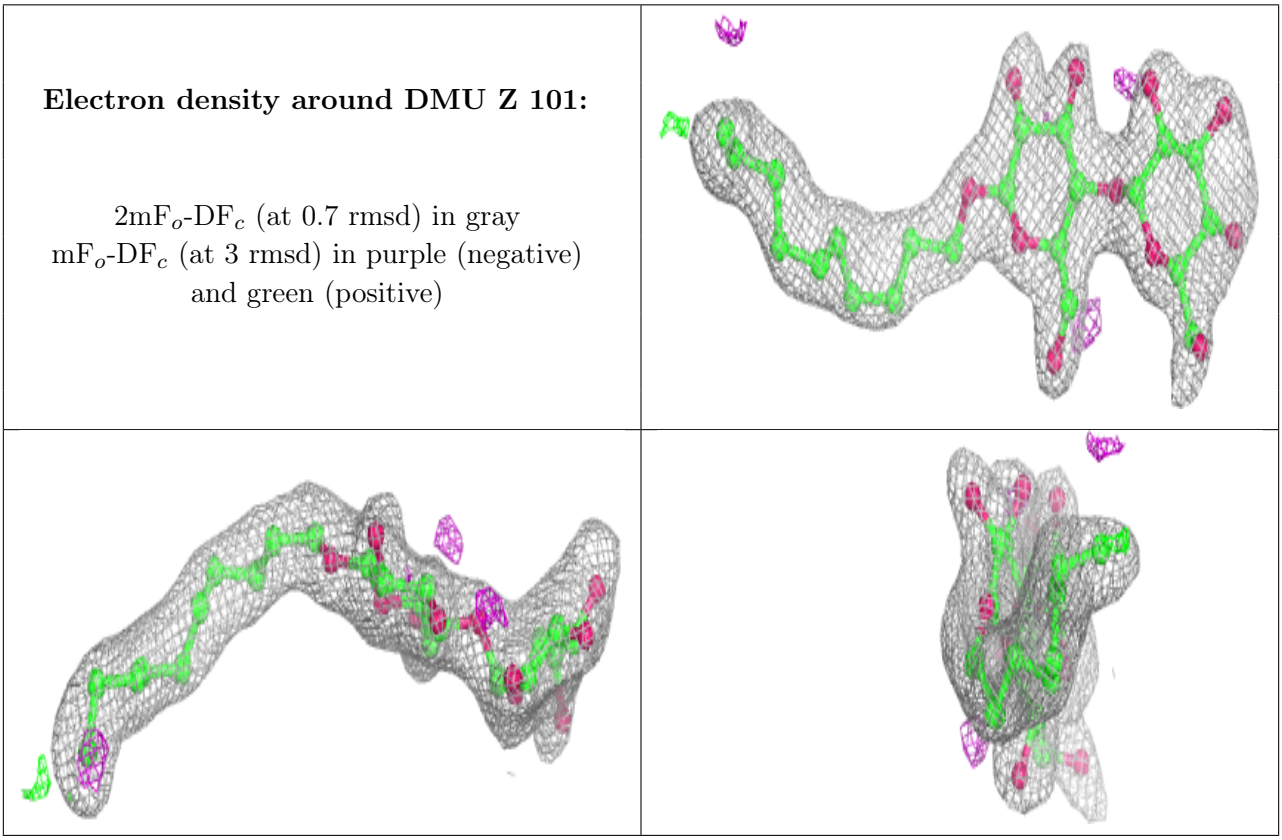
Electron density around LFA P 310:

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



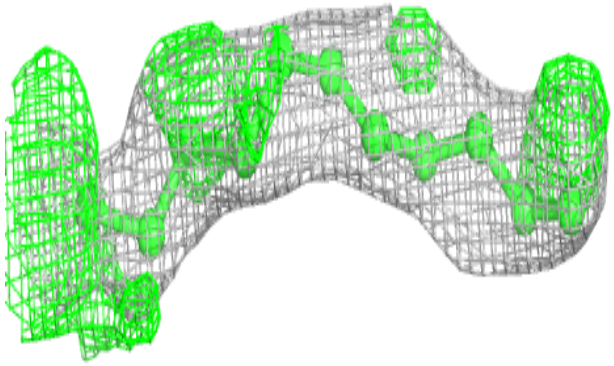
Electron density around DMU Z 101:

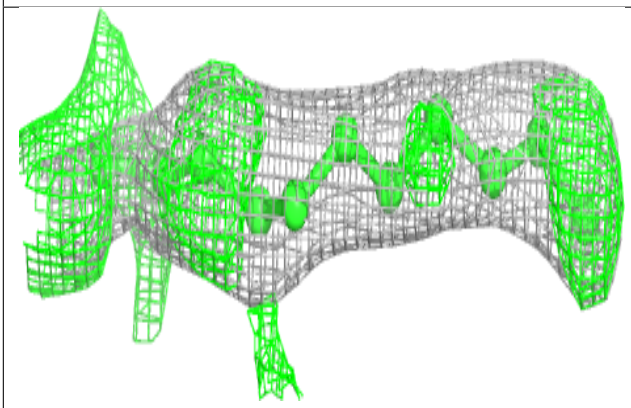
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

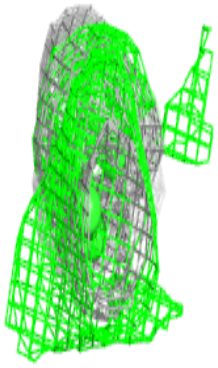


Electron density around LFA T 103:

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

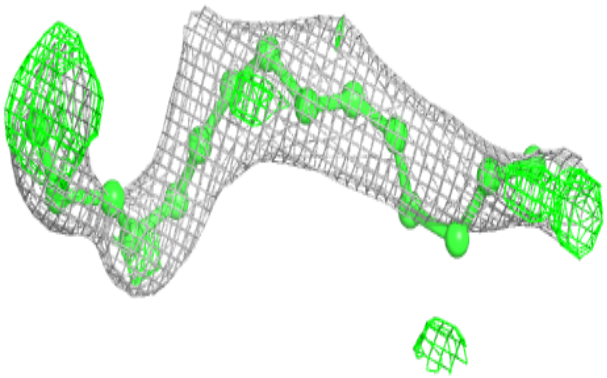


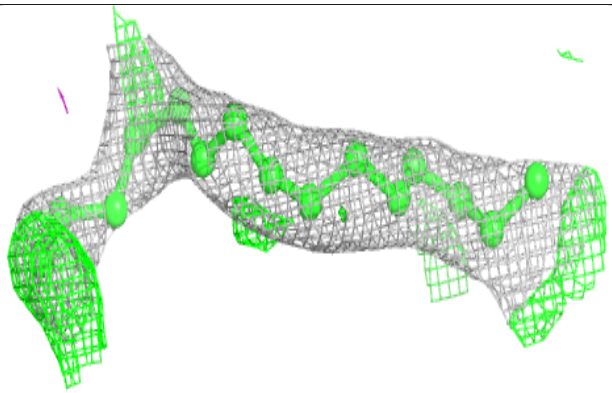


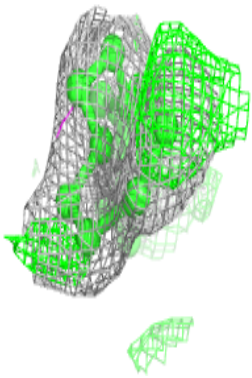


Electron density around LFA P 301:

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

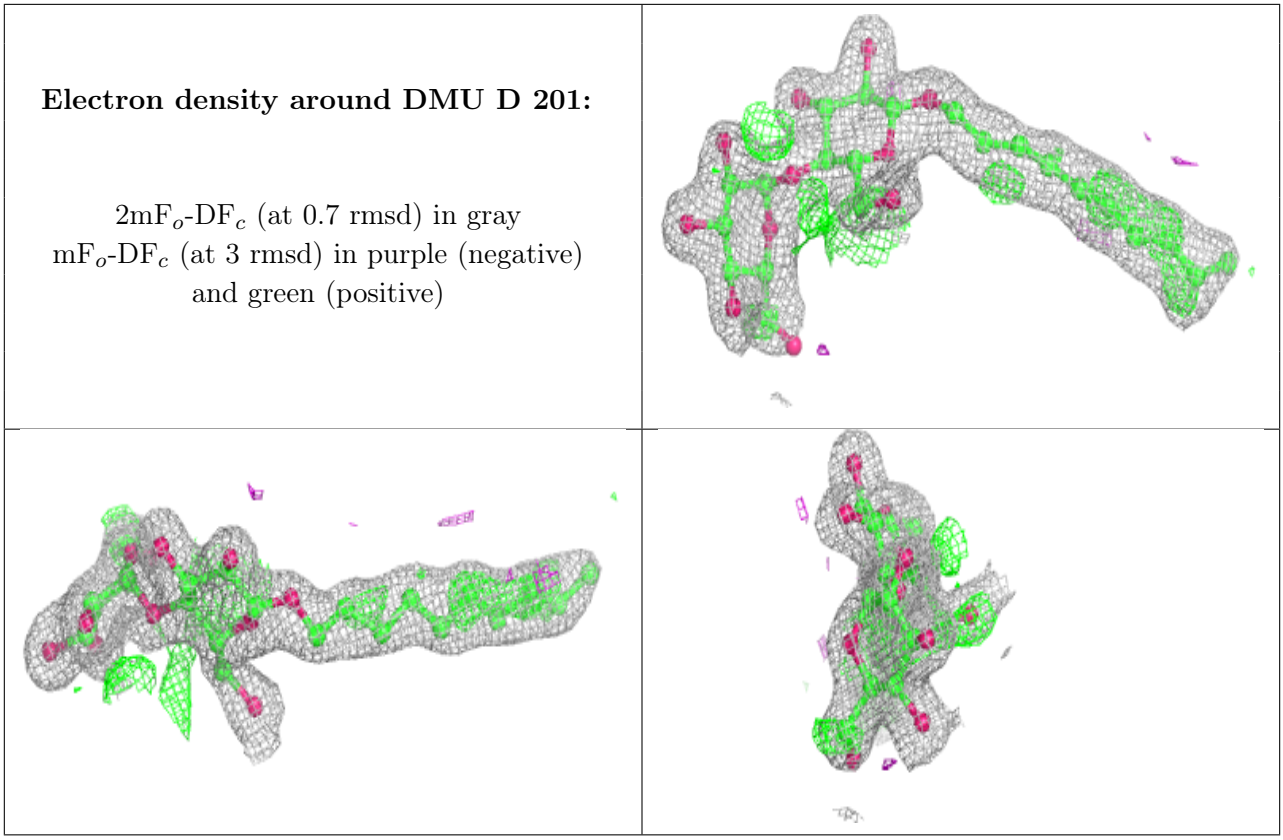






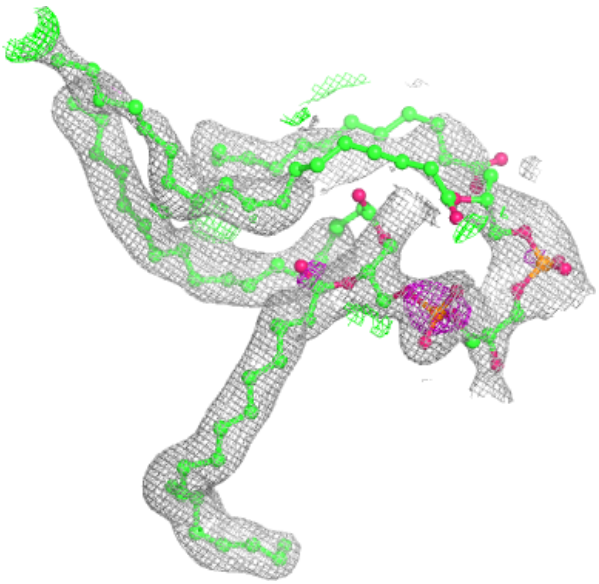
Electron density around DMU D 201:

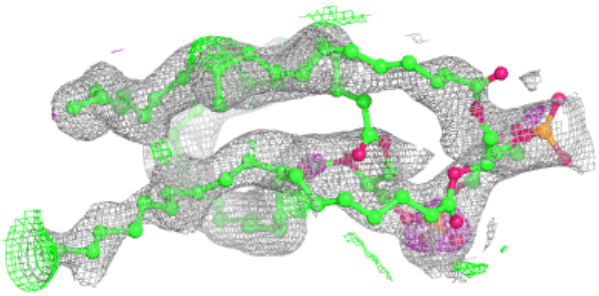
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CDL L 101:

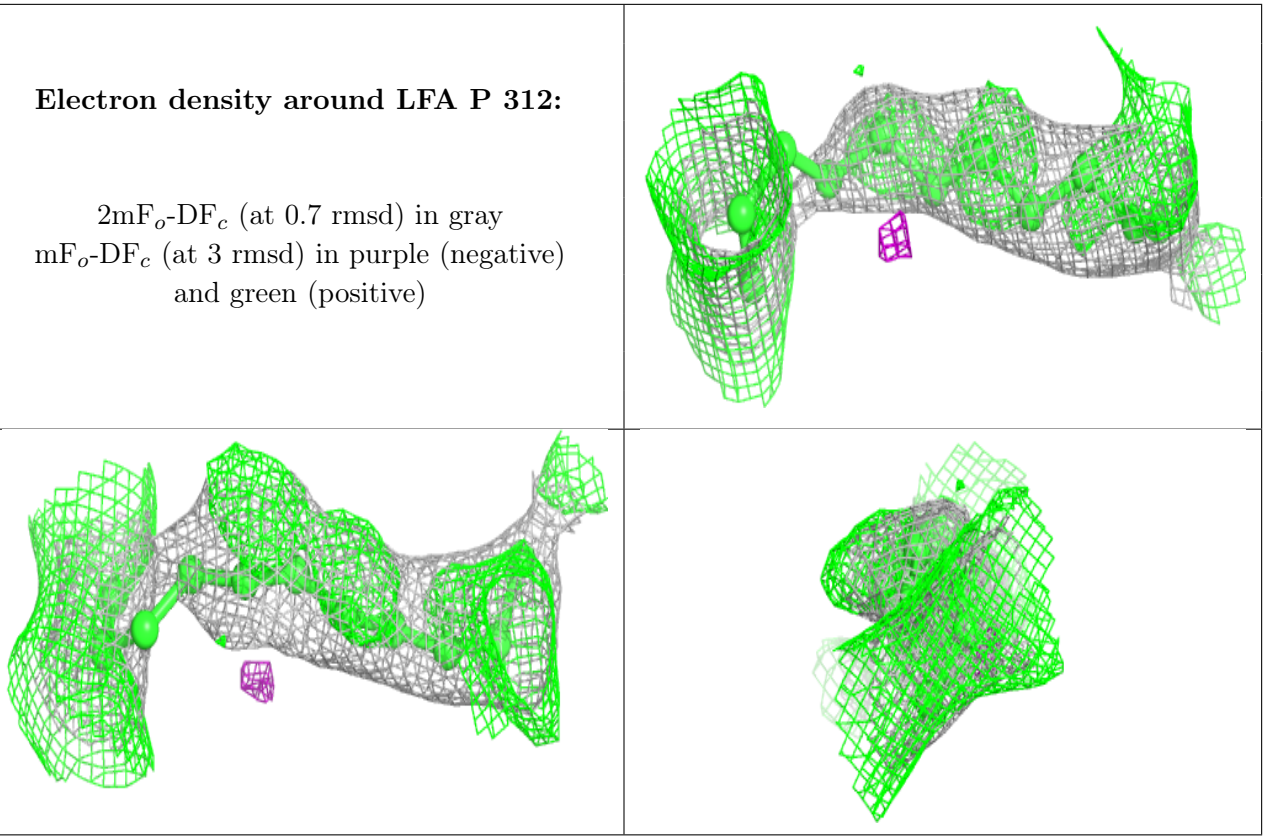
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





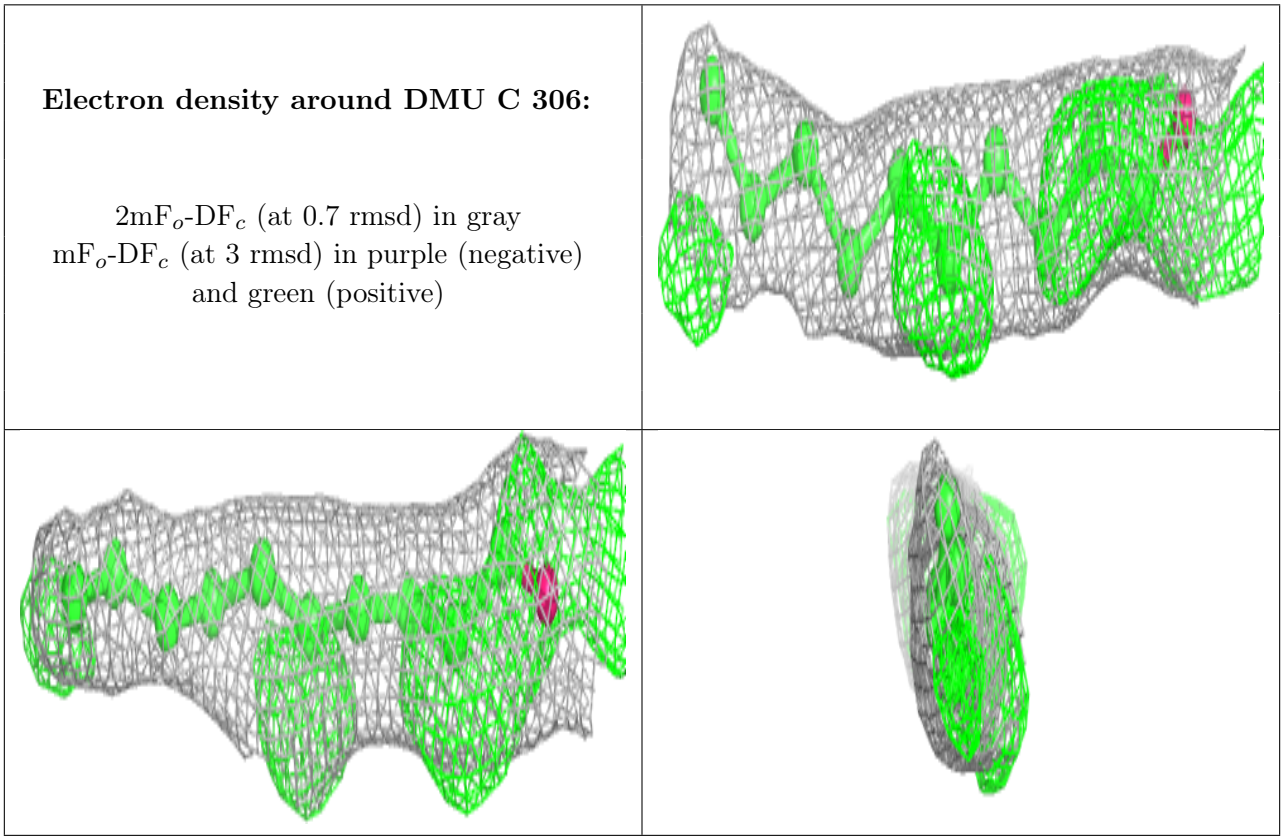
Electron density around LFA P 312:

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



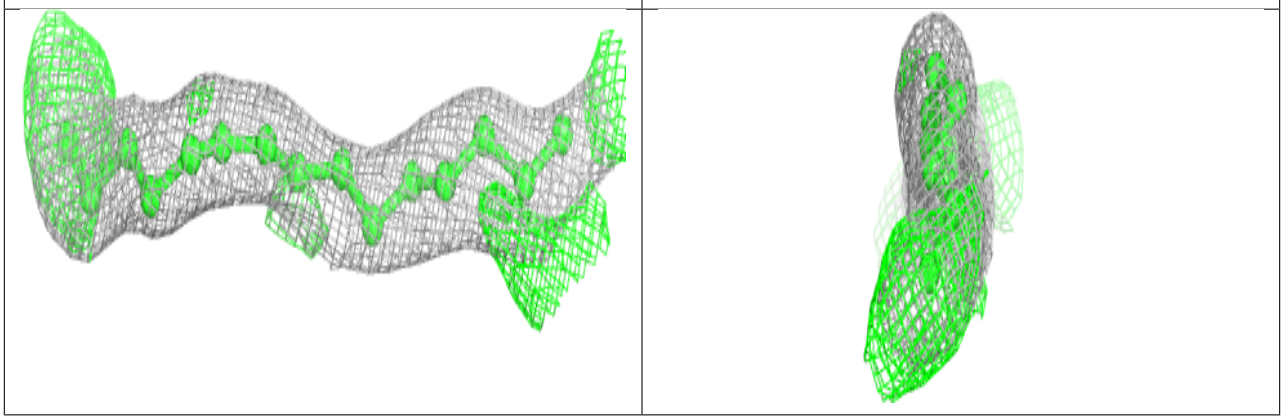
Electron density around DMU C 306:

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



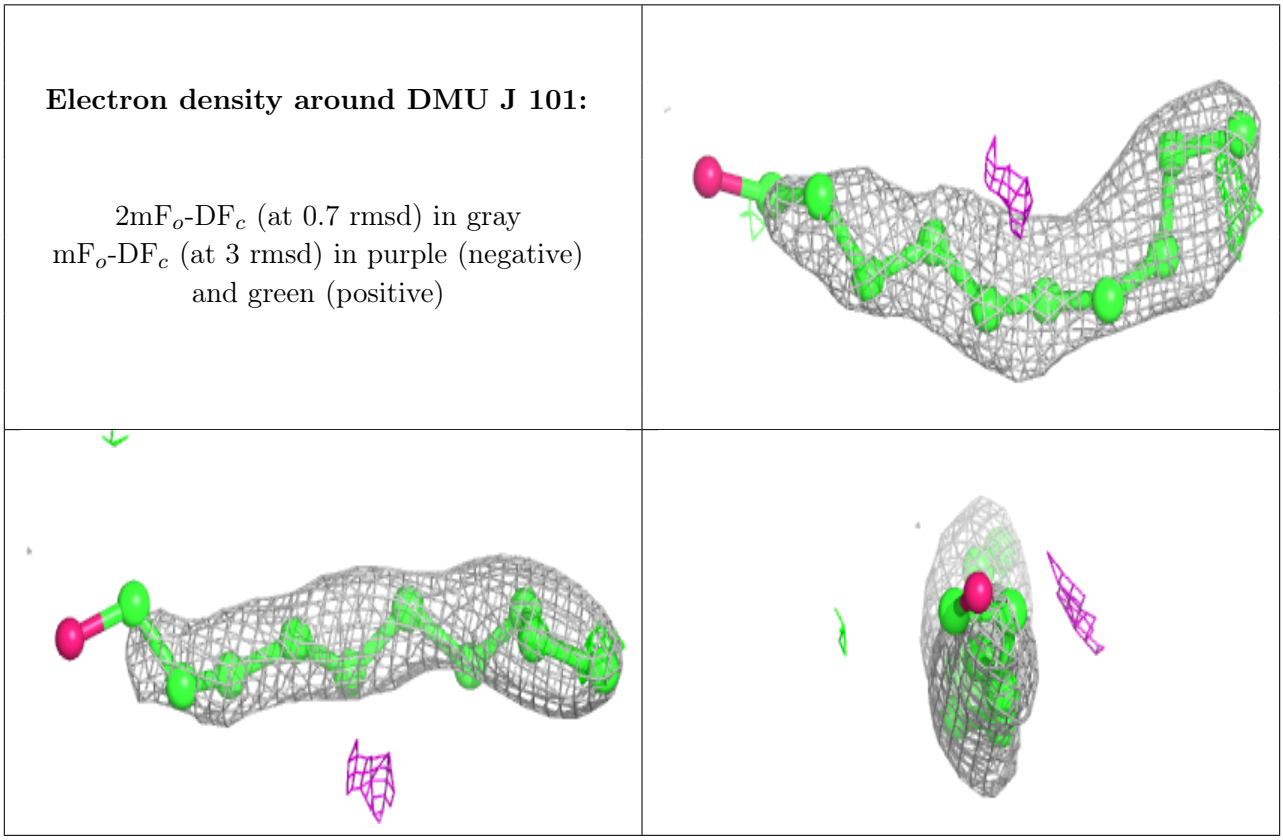
Electron density around LFA P 313:

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



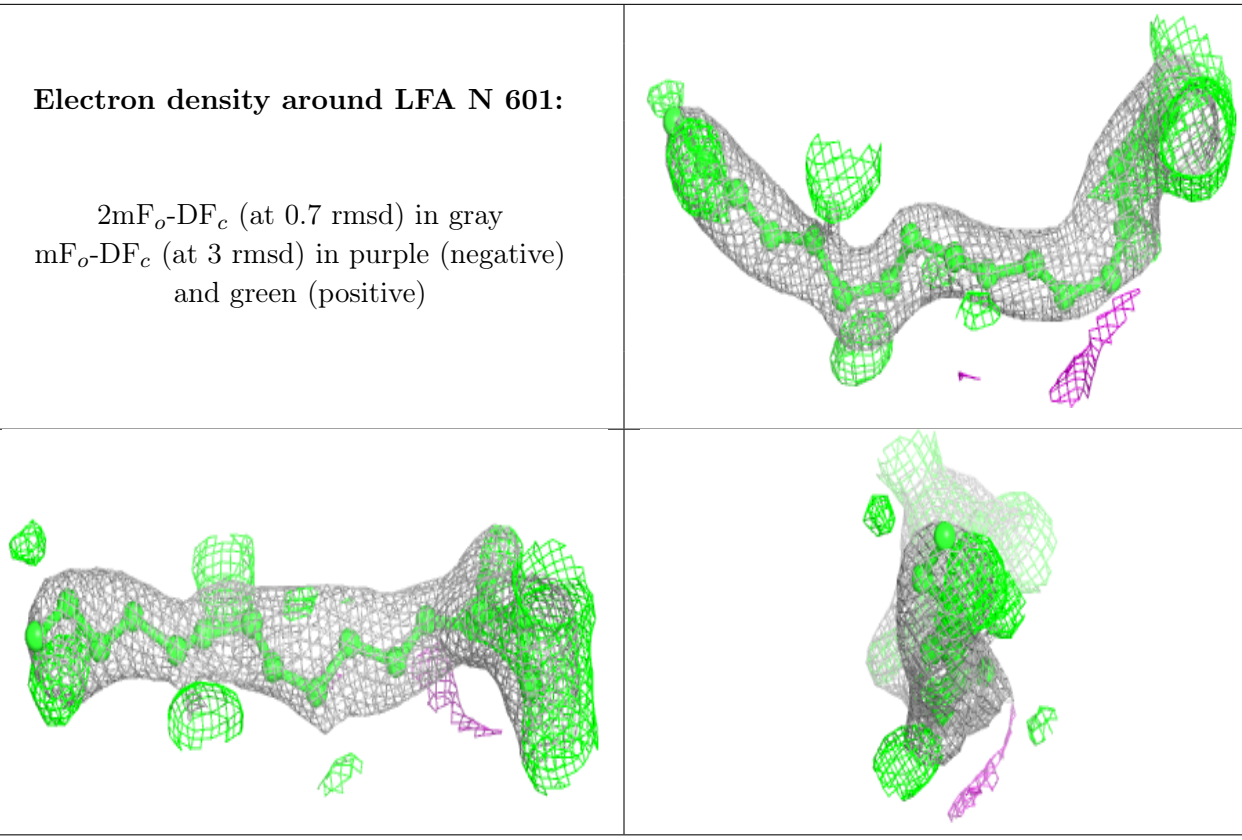
Electron density around DMU J 101:

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



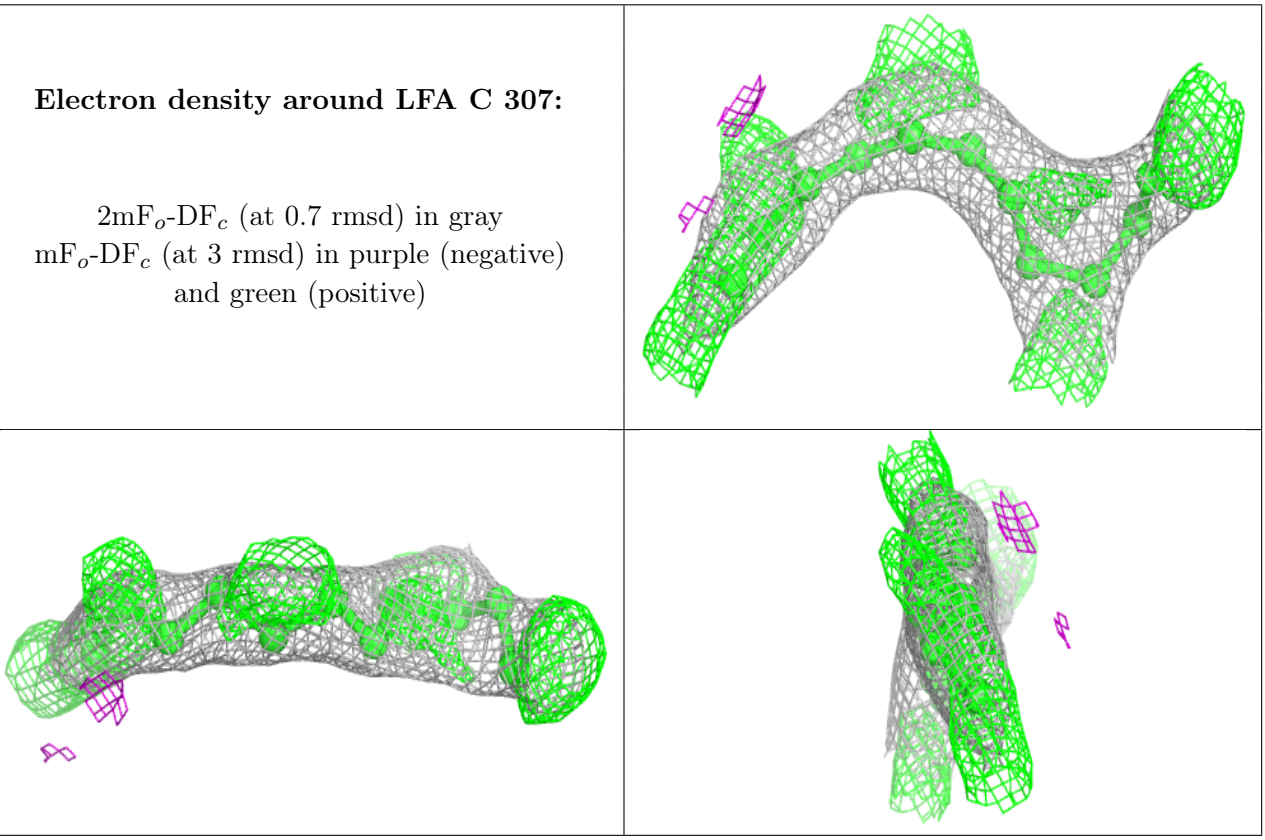
Electron density around LFA N 601:

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



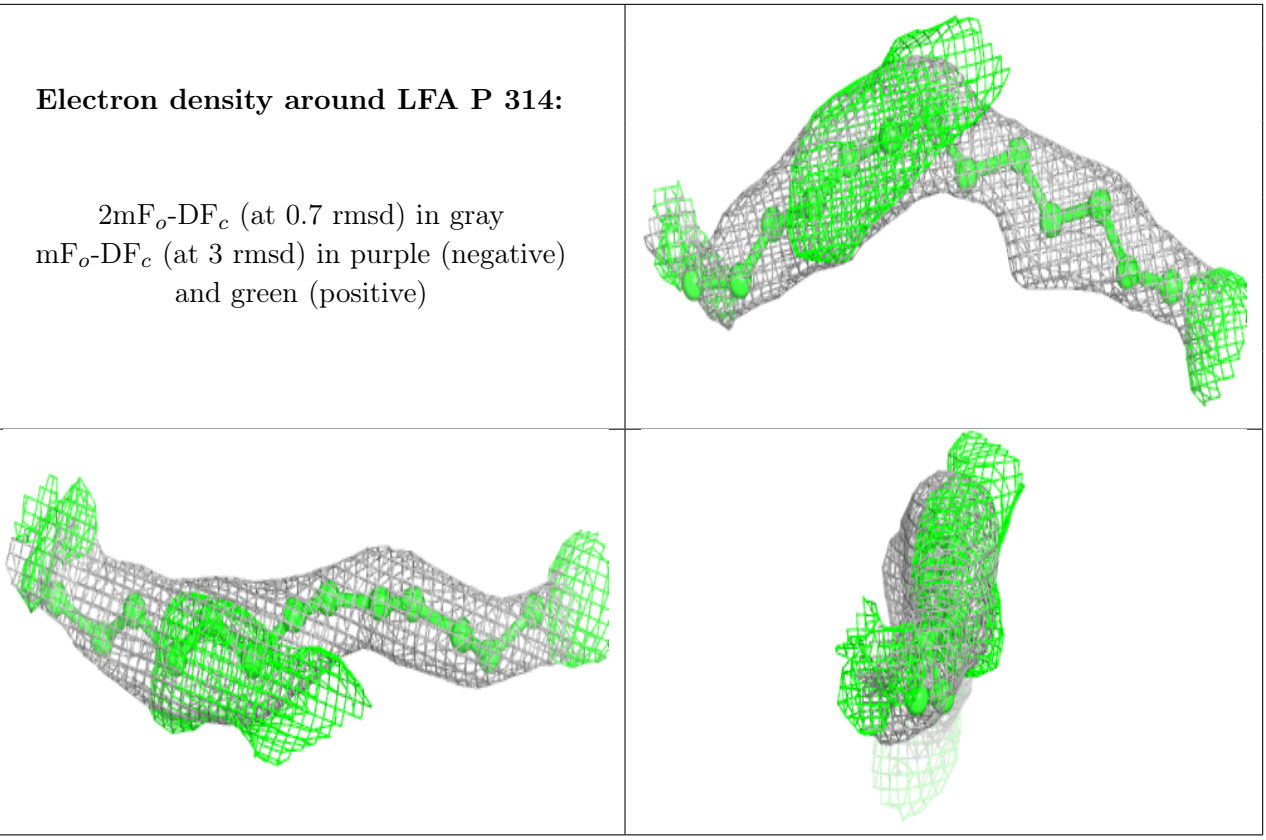
Electron density around LFA C 307:

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



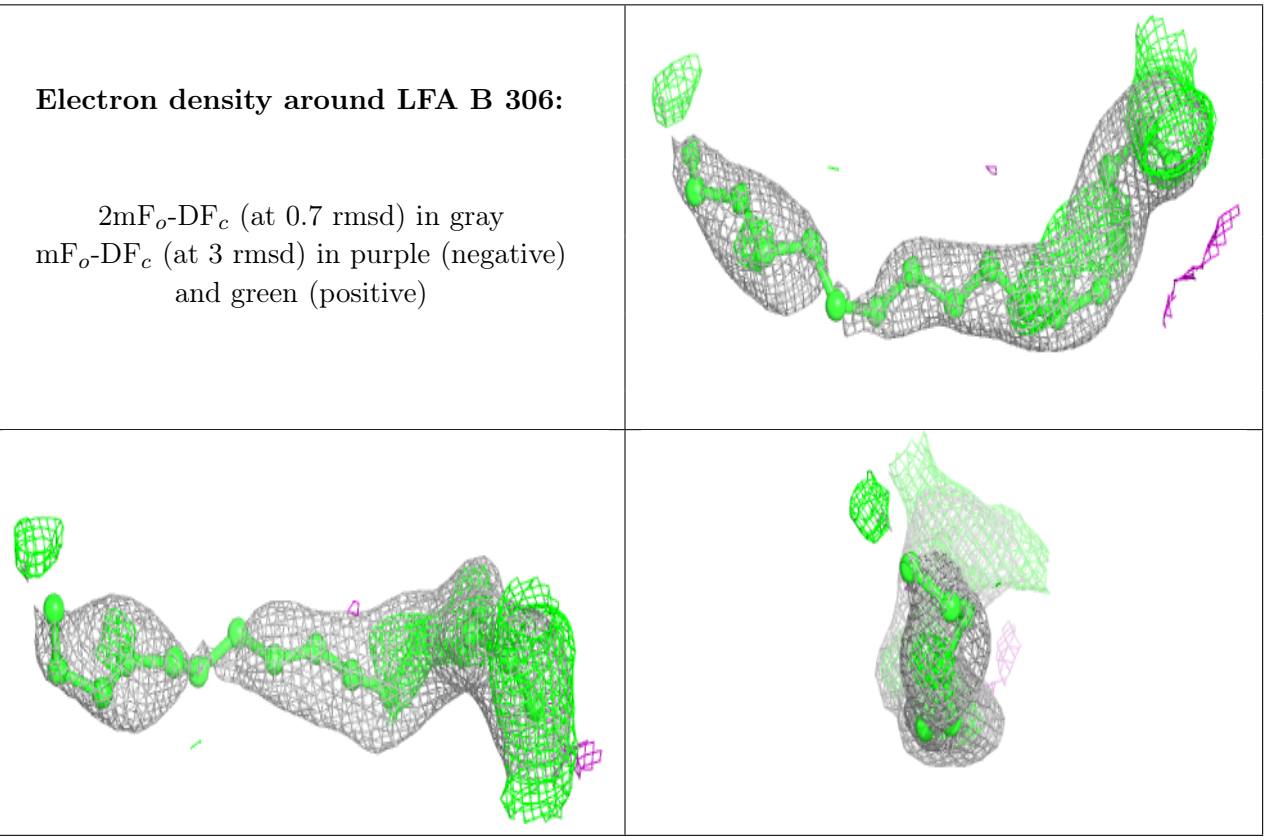
Electron density around LFA P 314:

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



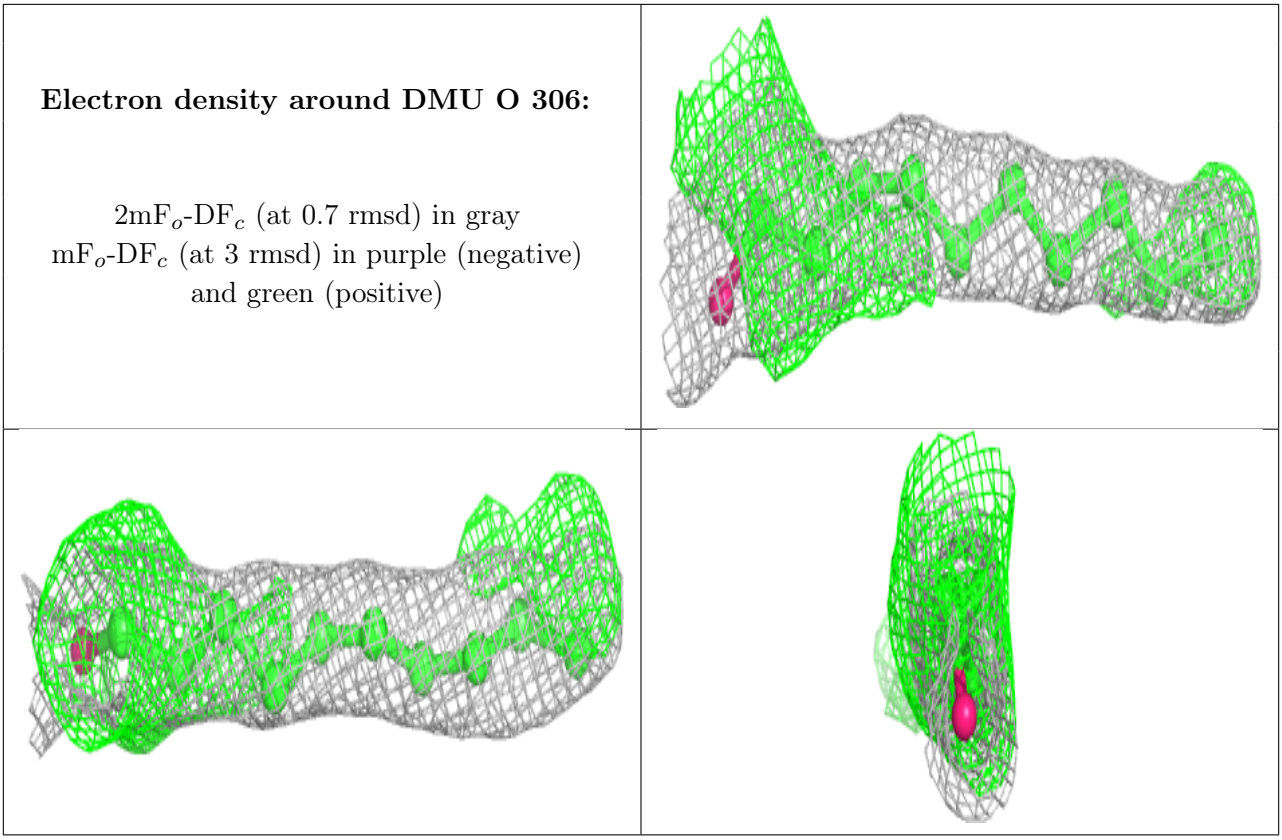
Electron density around LFA B 306:

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



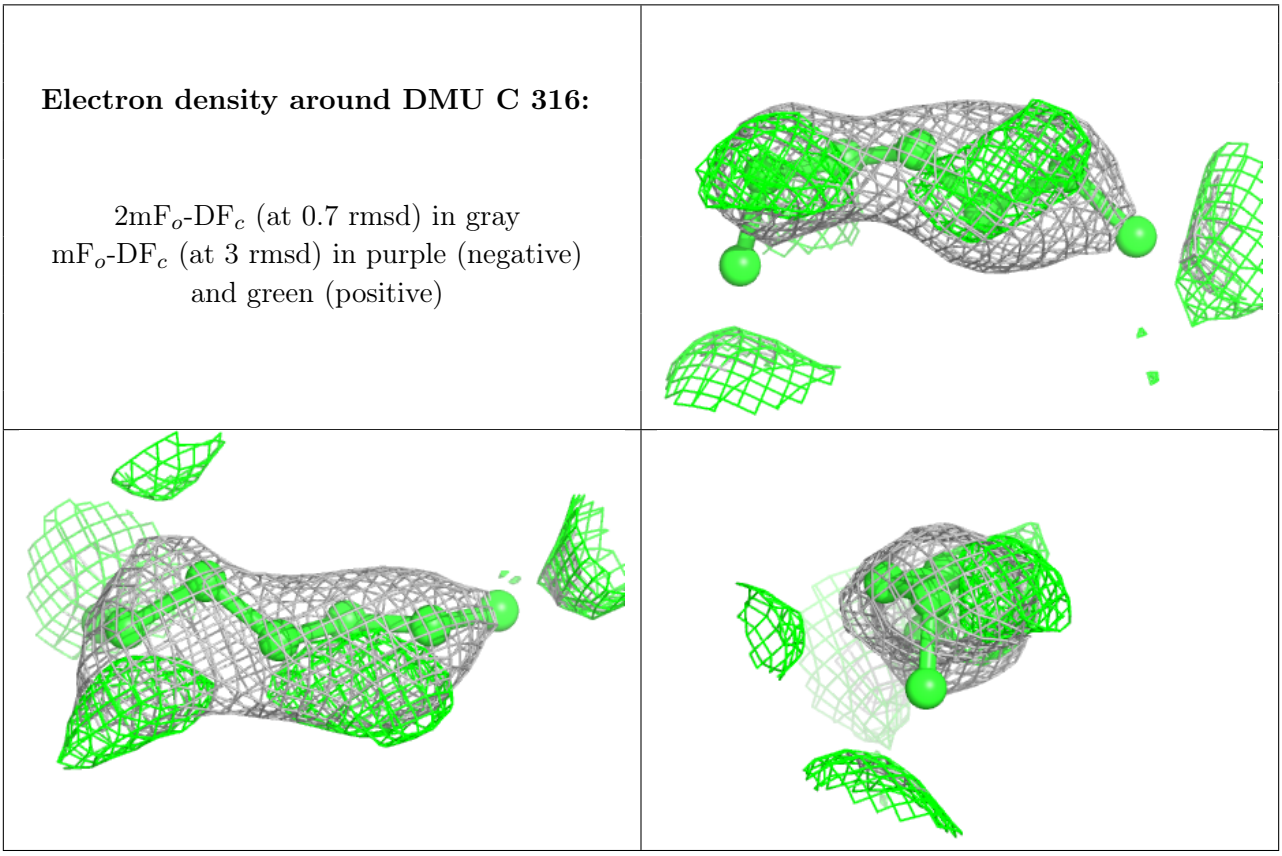
Electron density around DMU O 306:

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



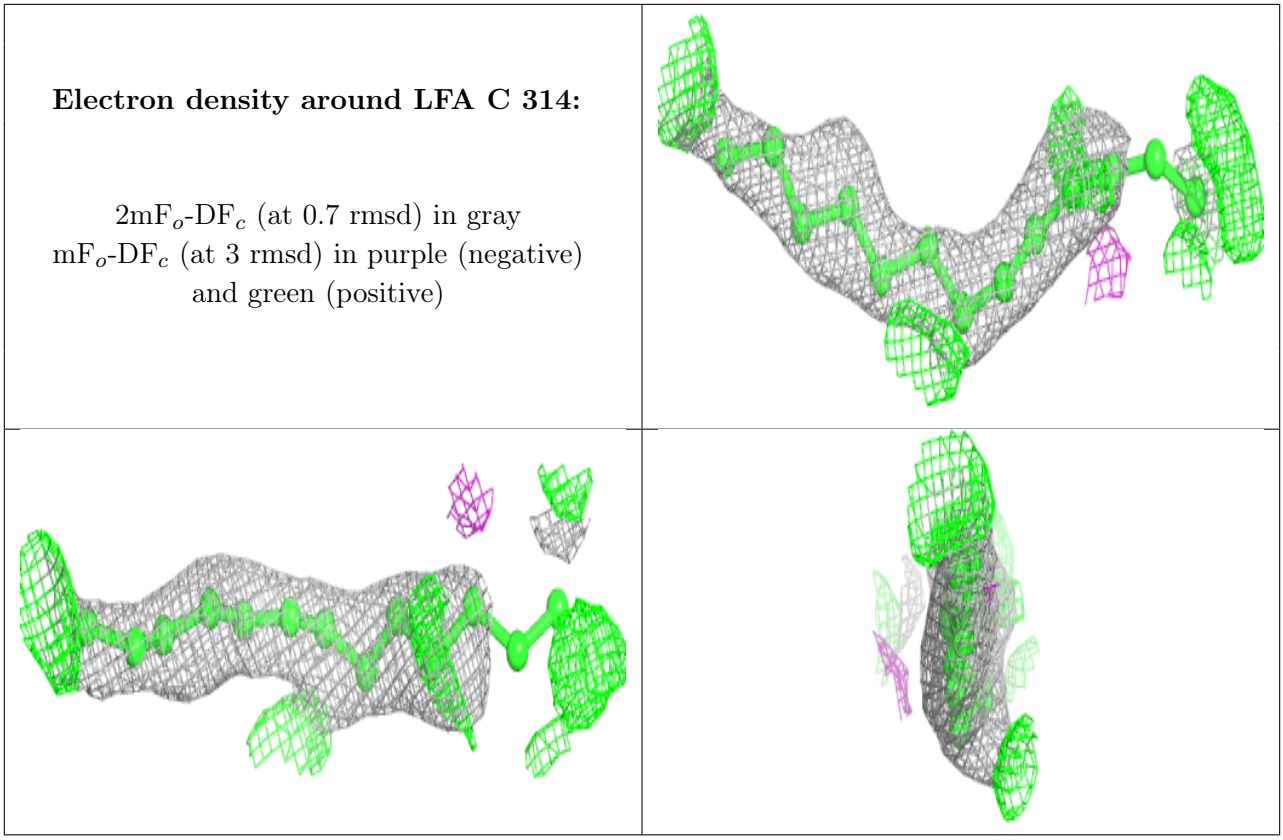
Electron density around DMU C 316:

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



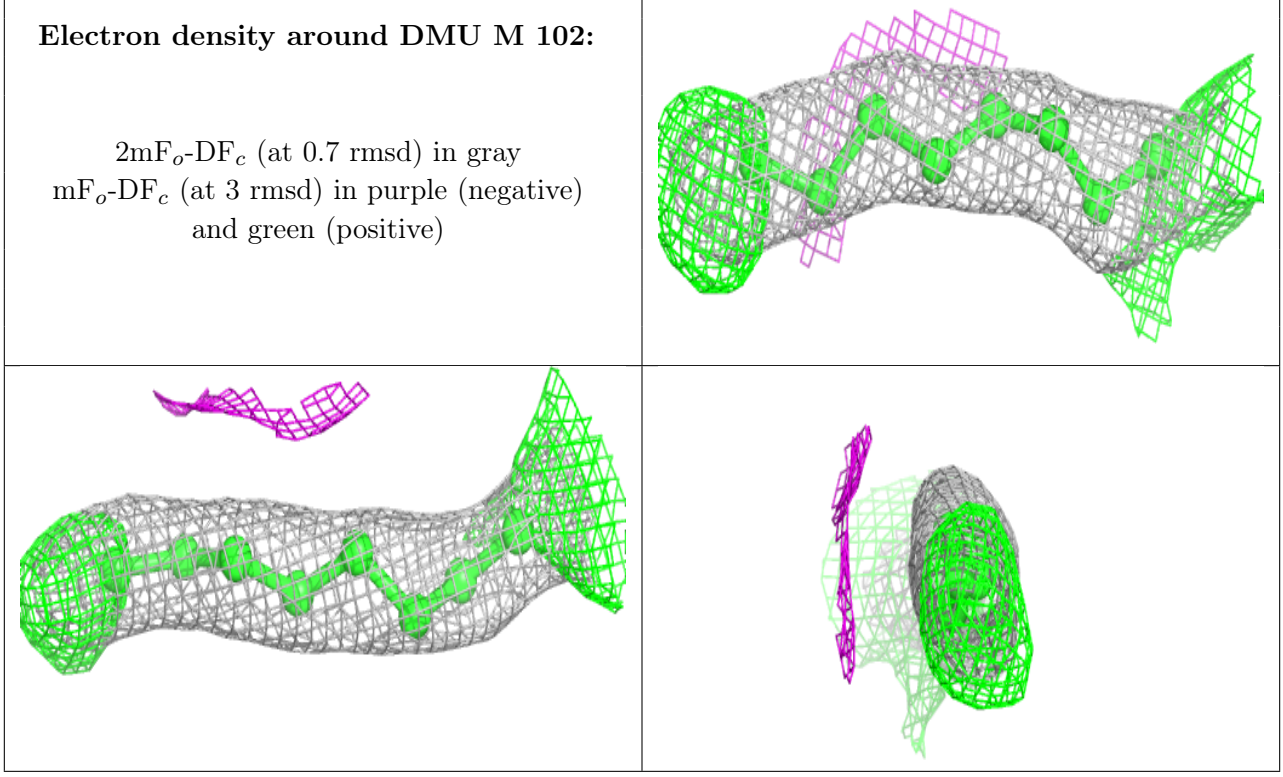
Electron density around LFA C 314:

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



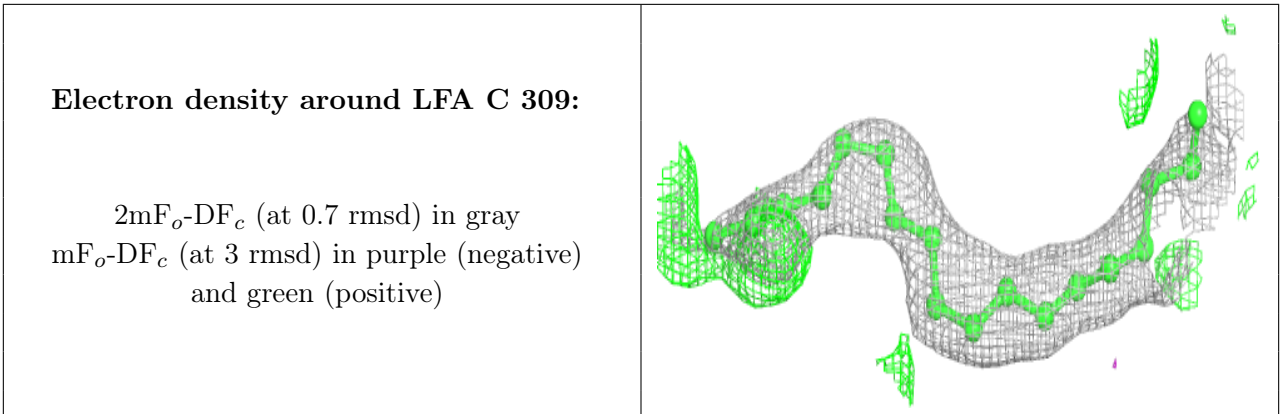
Electron density around DMU M 102:

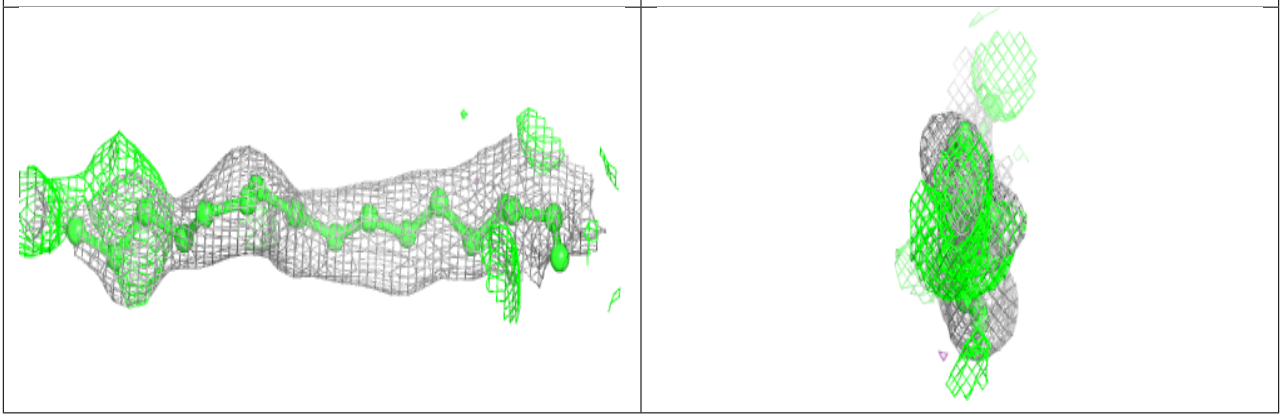
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LFA C 309:

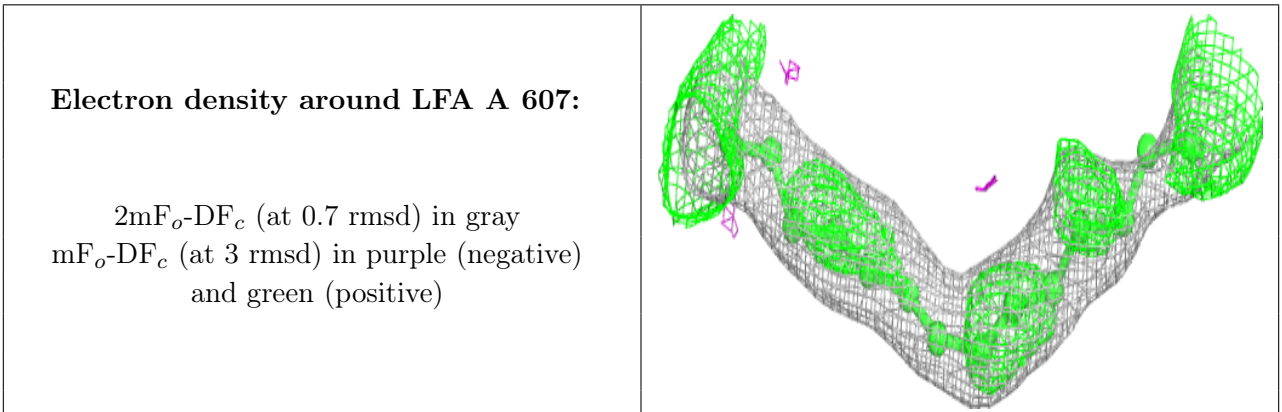
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

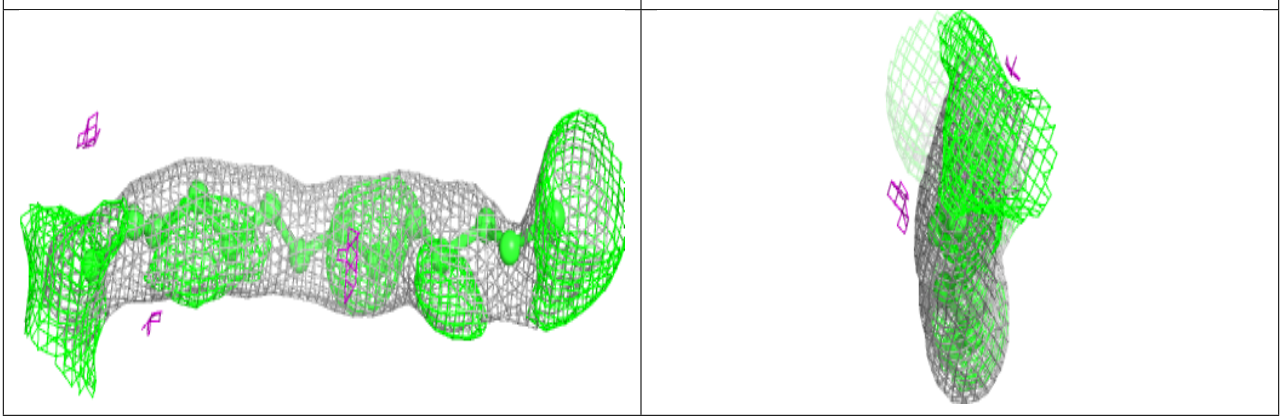




Electron density around LFA A 607:

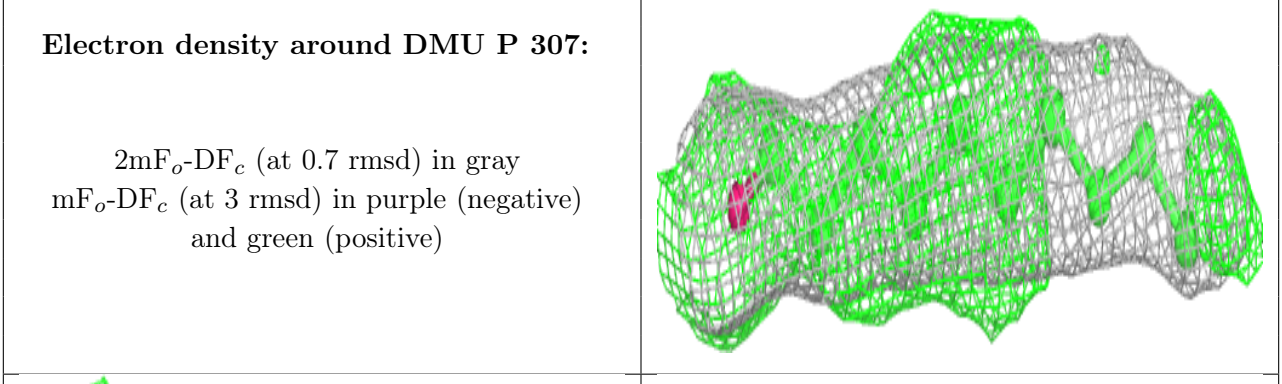
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





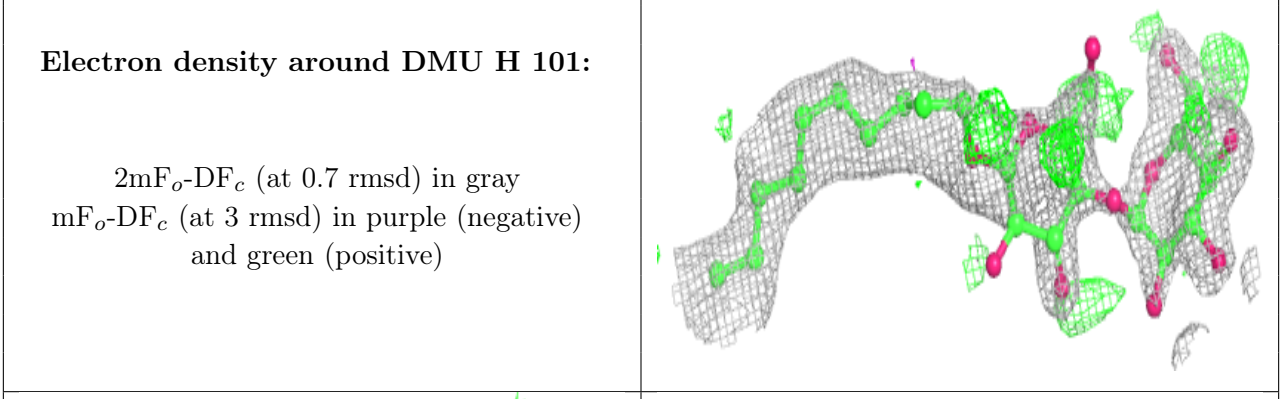
Electron density around DMU P 307:

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



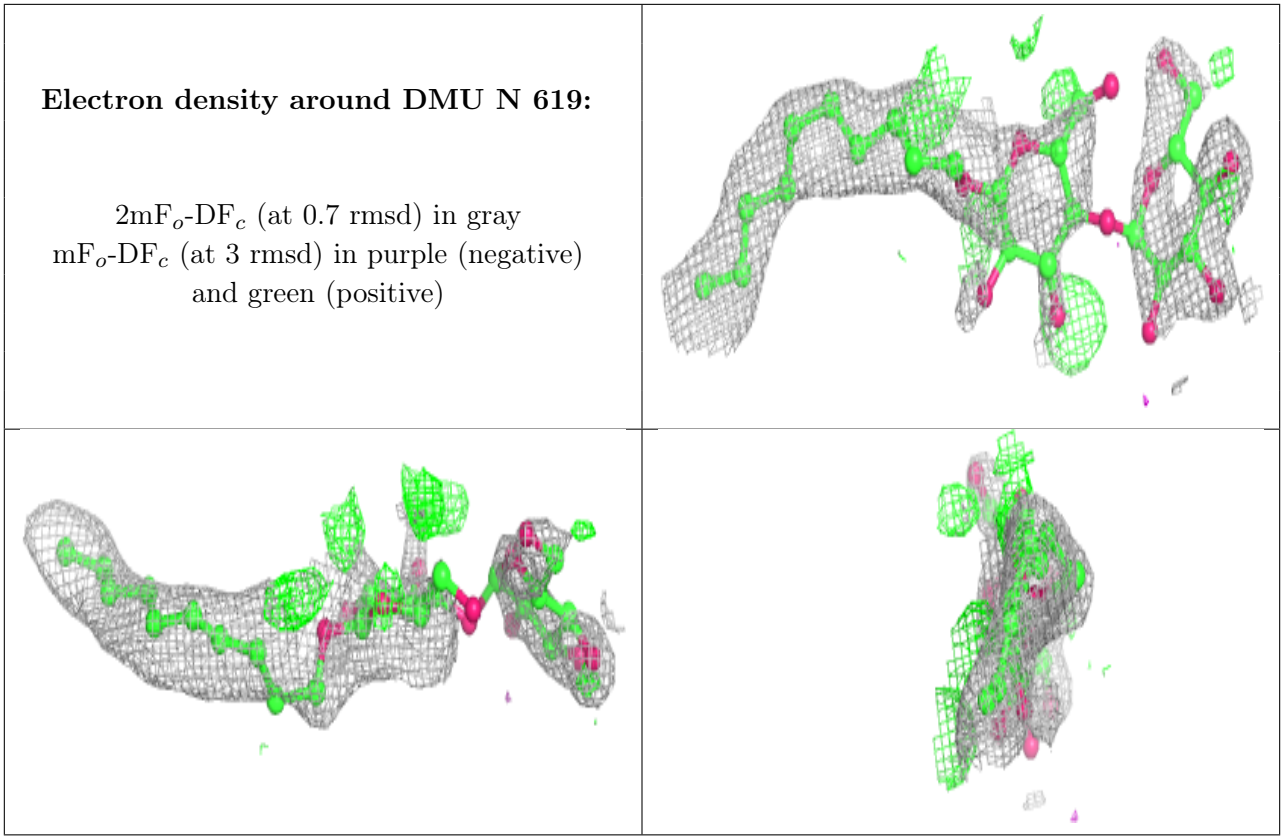
Electron density around DMU H 101:

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



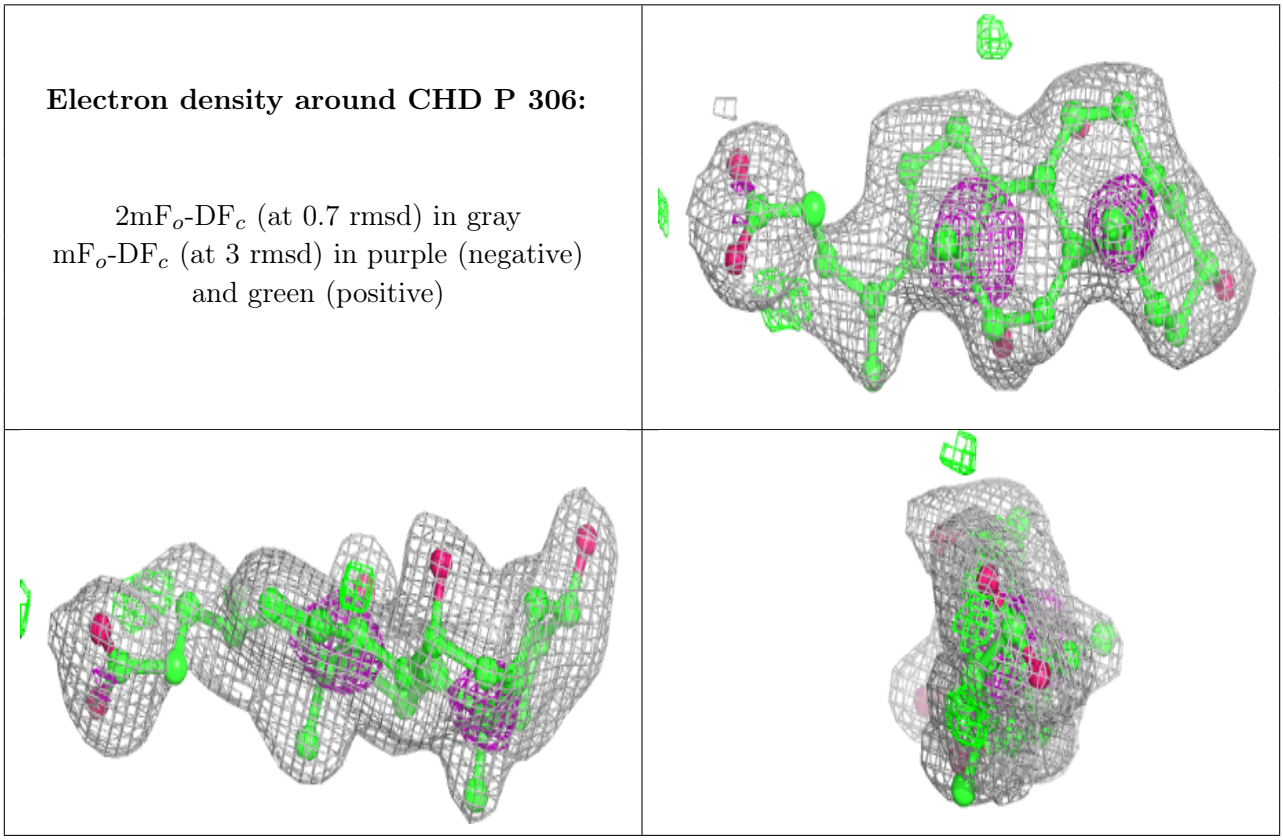
Electron density around DMU N 619:

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



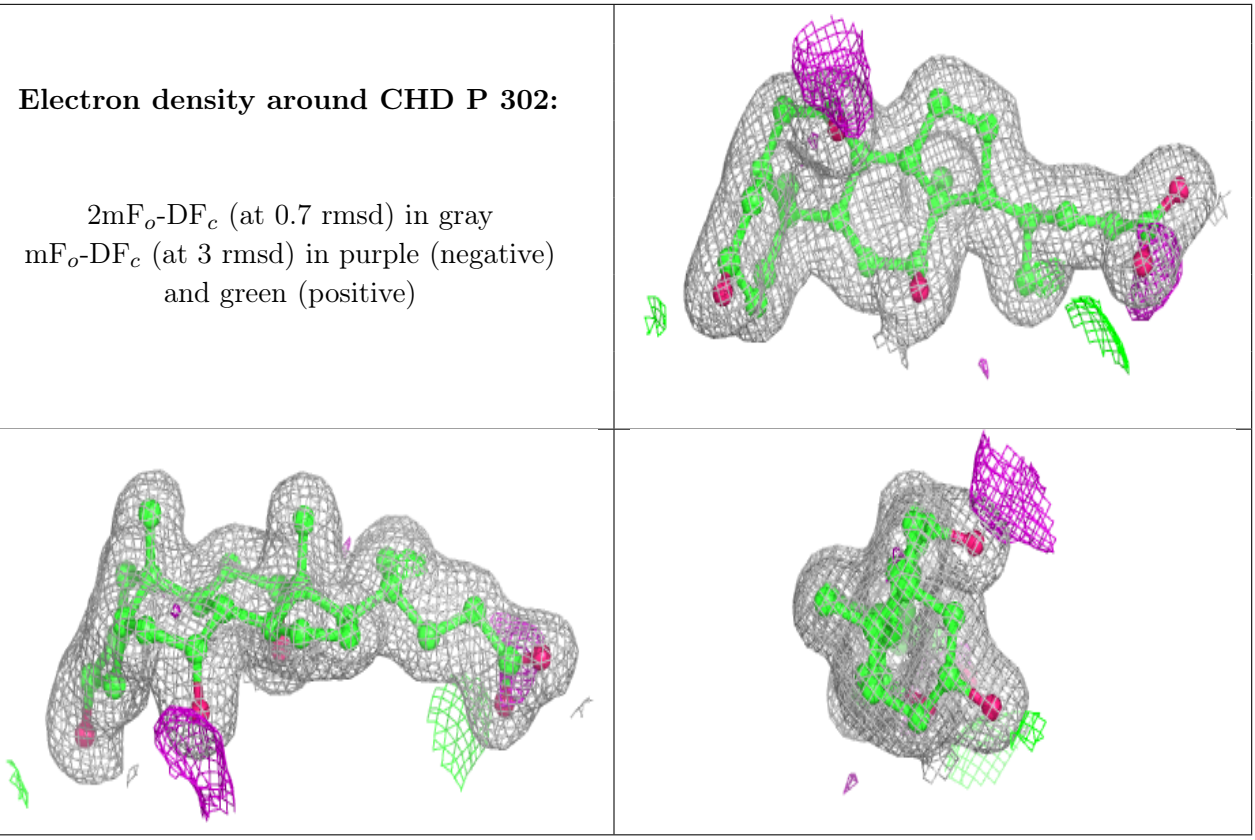
Electron density around CHD P 306:

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



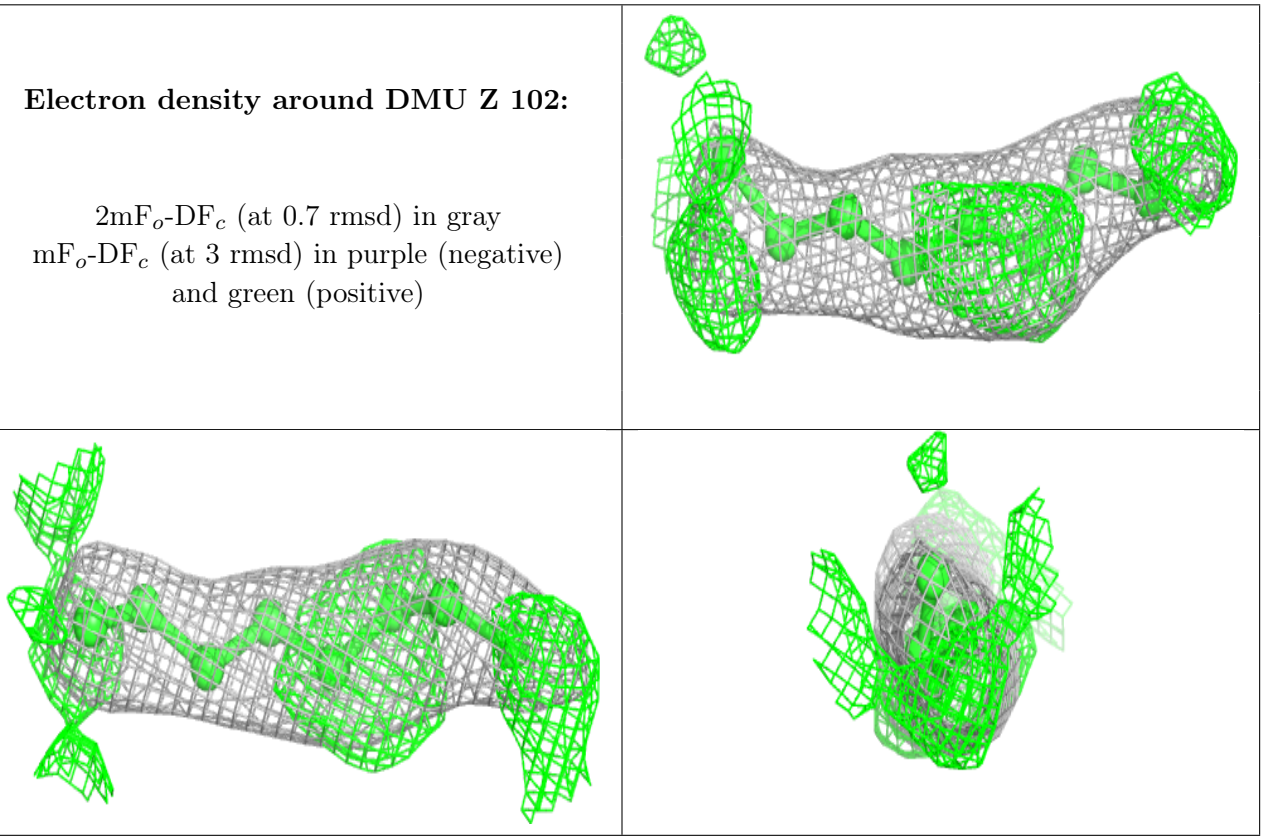
Electron density around CHD P 302:

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



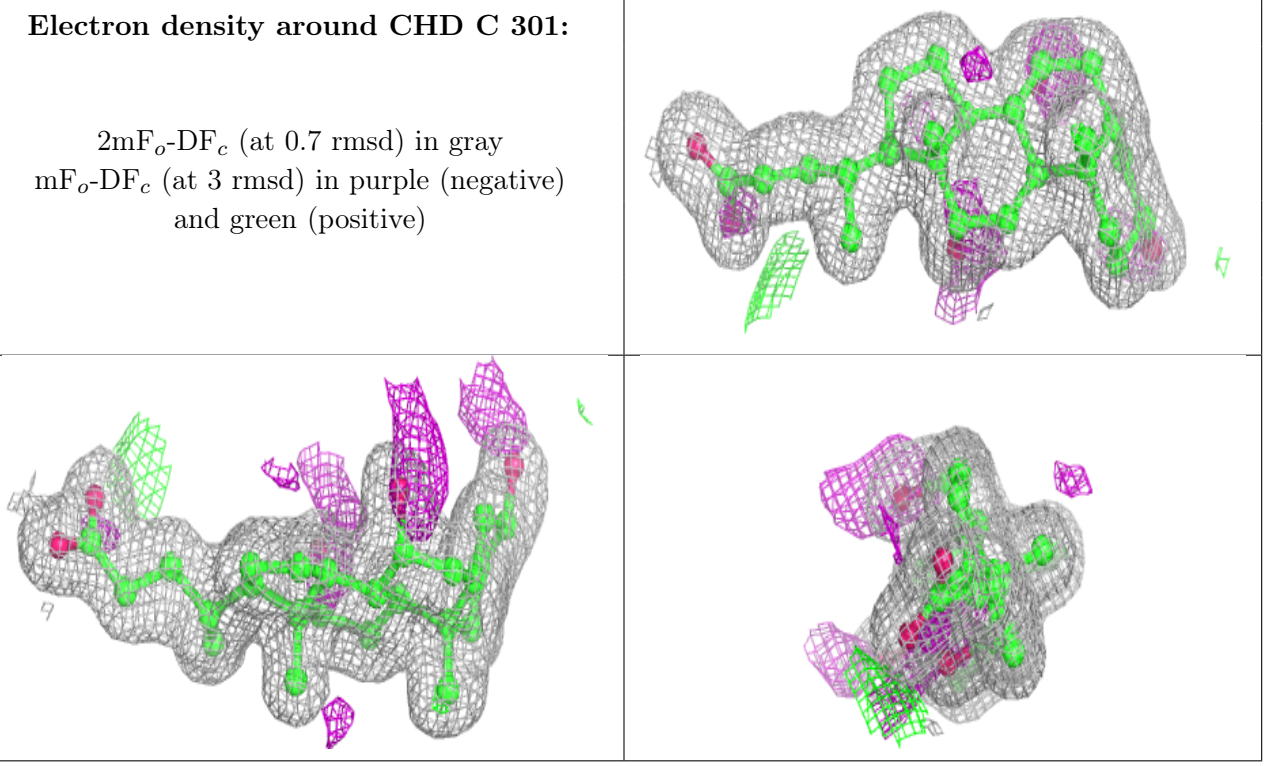
Electron density around DMU Z 102:

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



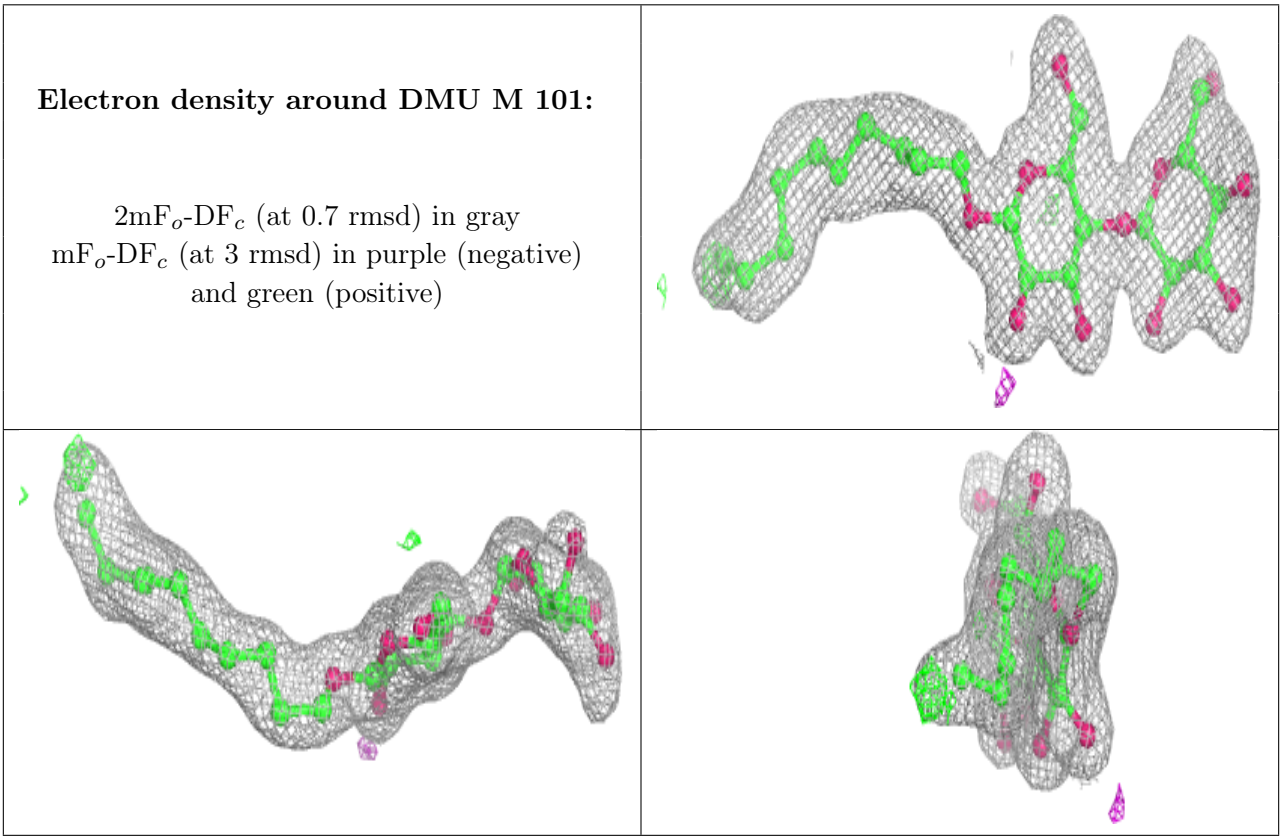
Electron density around CHD C 301:

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



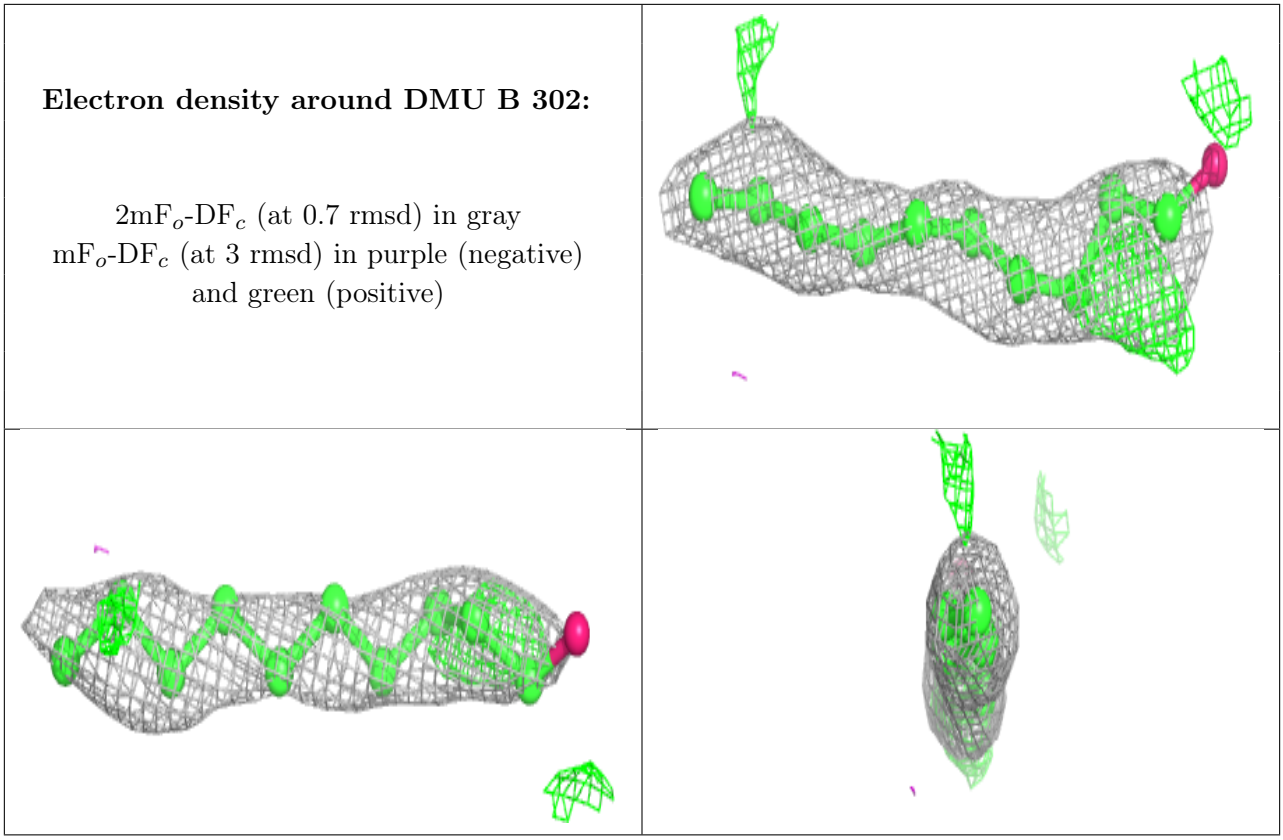
Electron density around DMU M 101:

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



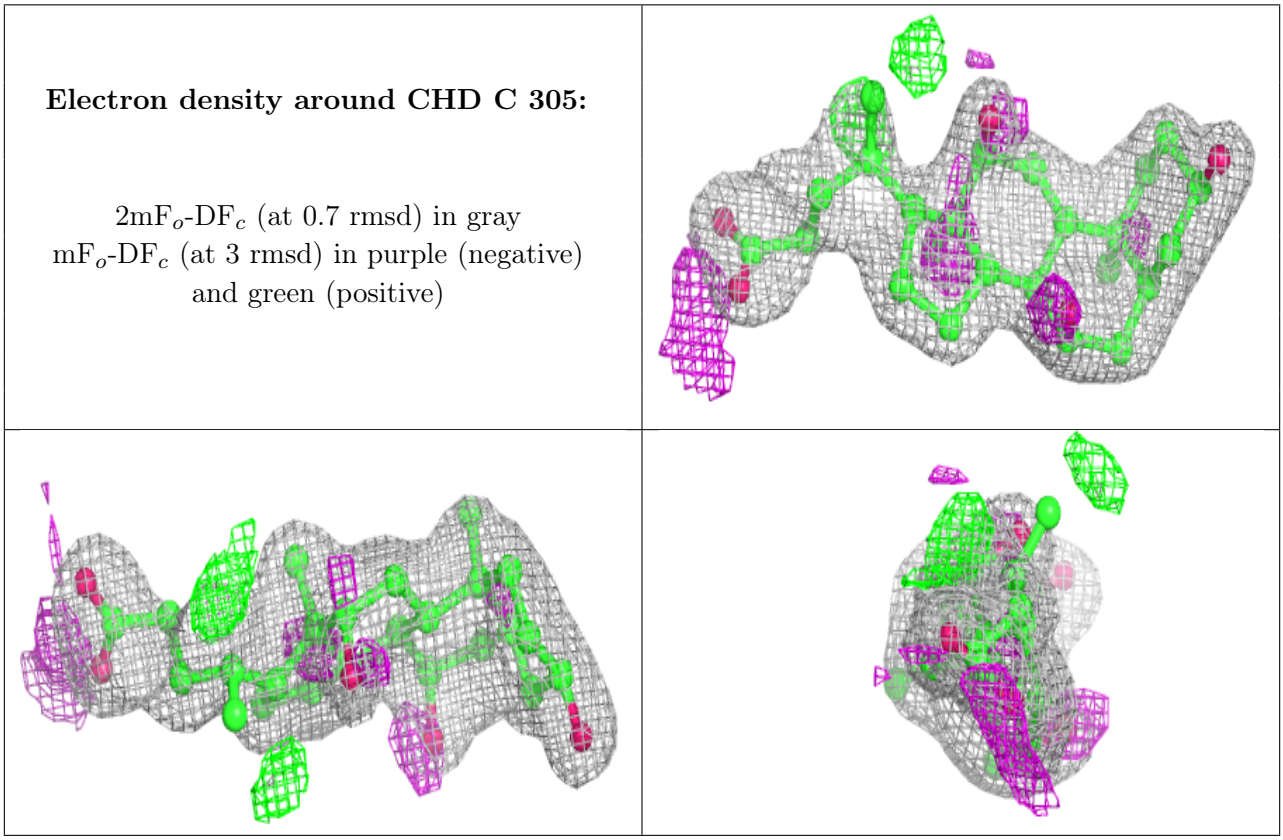
Electron density around DMU B 302:

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



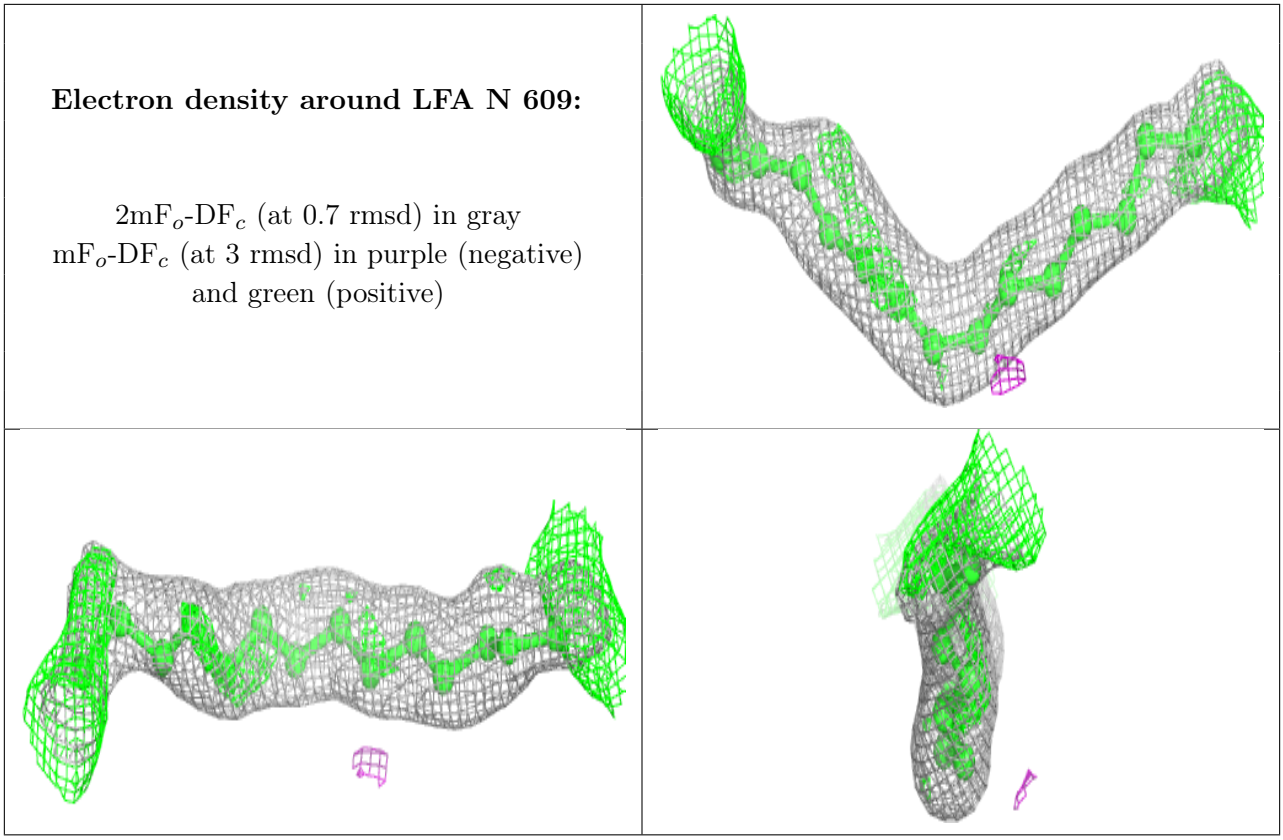
Electron density around CHD C 305:

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



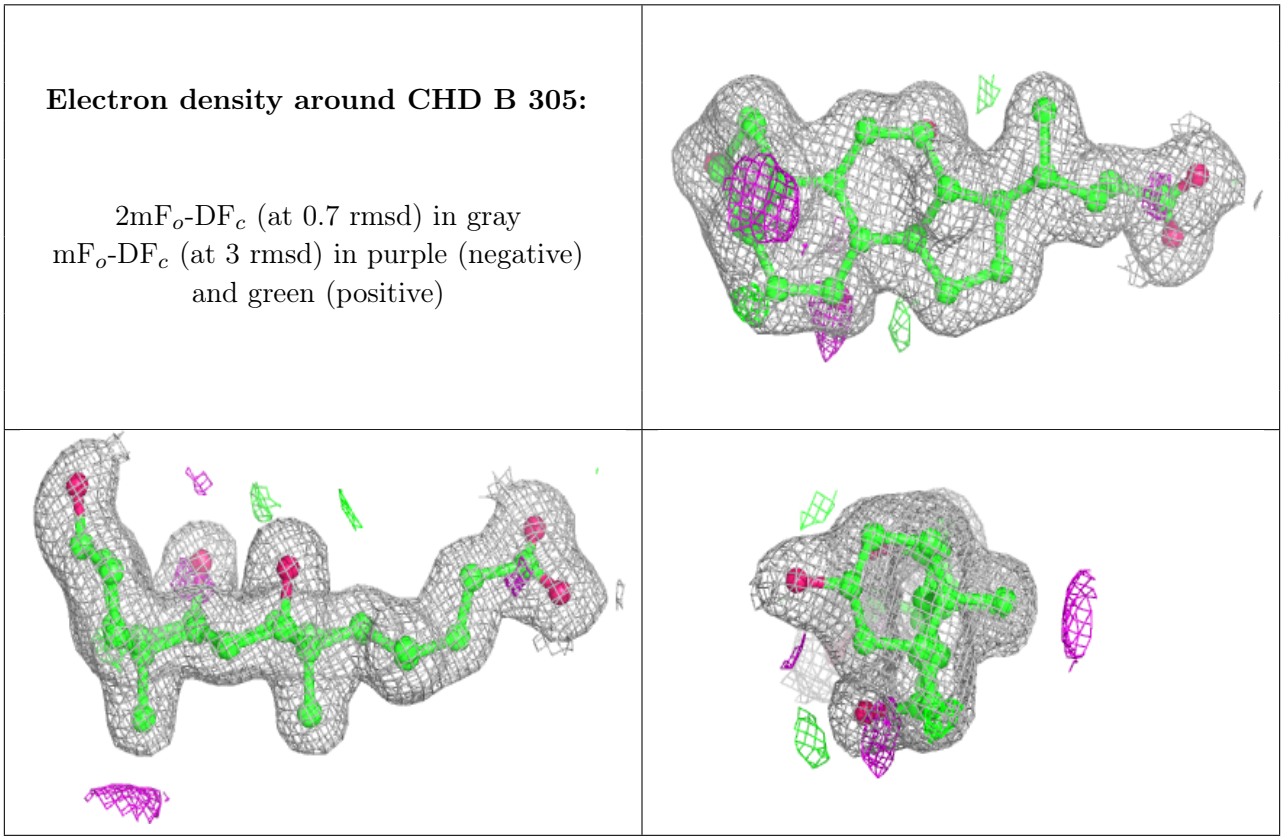
Electron density around LFA N 609:

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



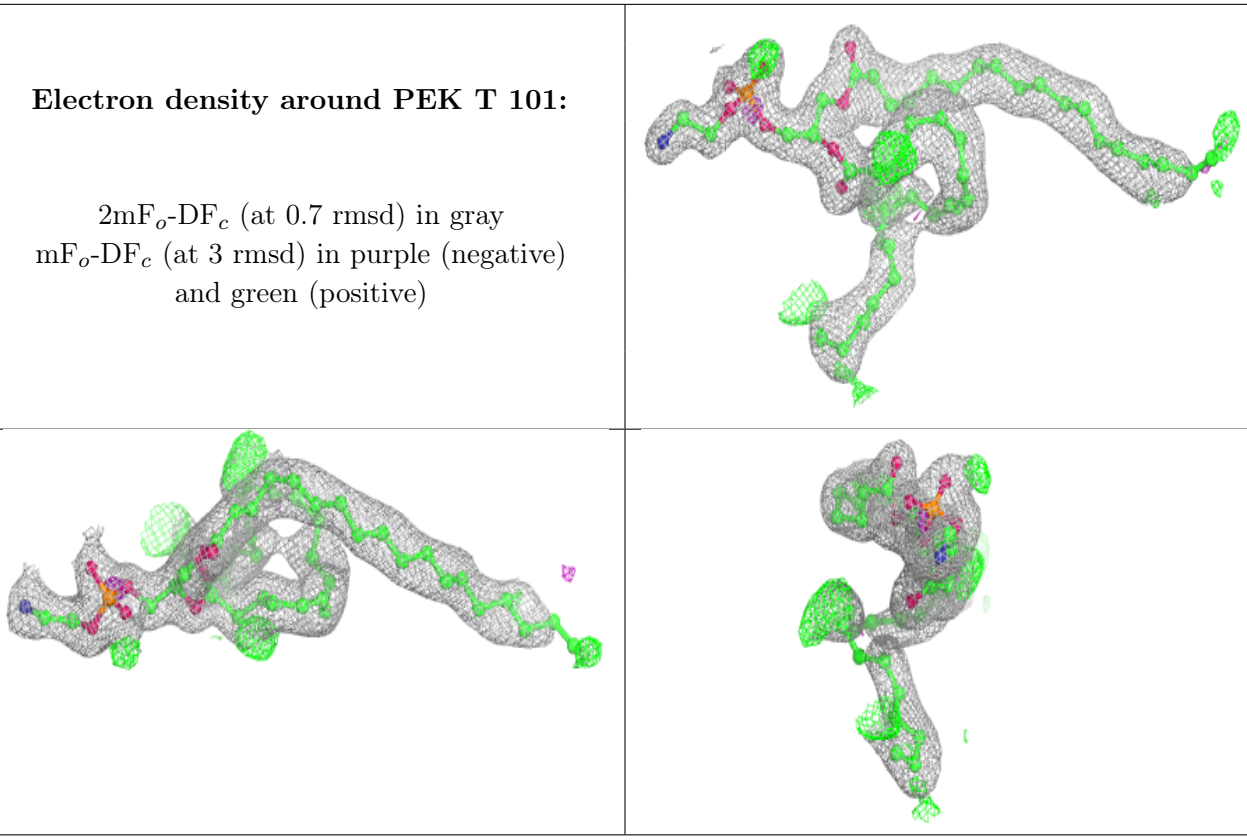
Electron density around CHD B 305:

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



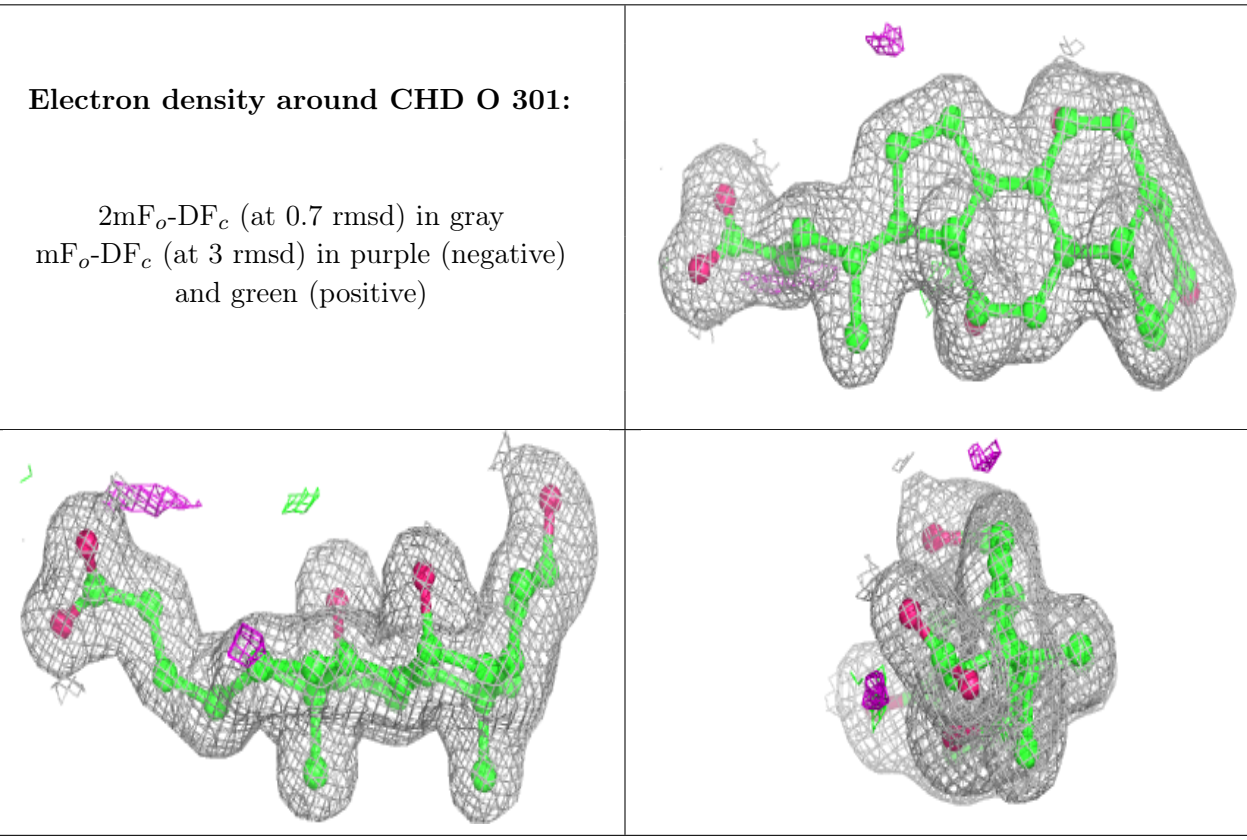
Electron density around PEK T 101:

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



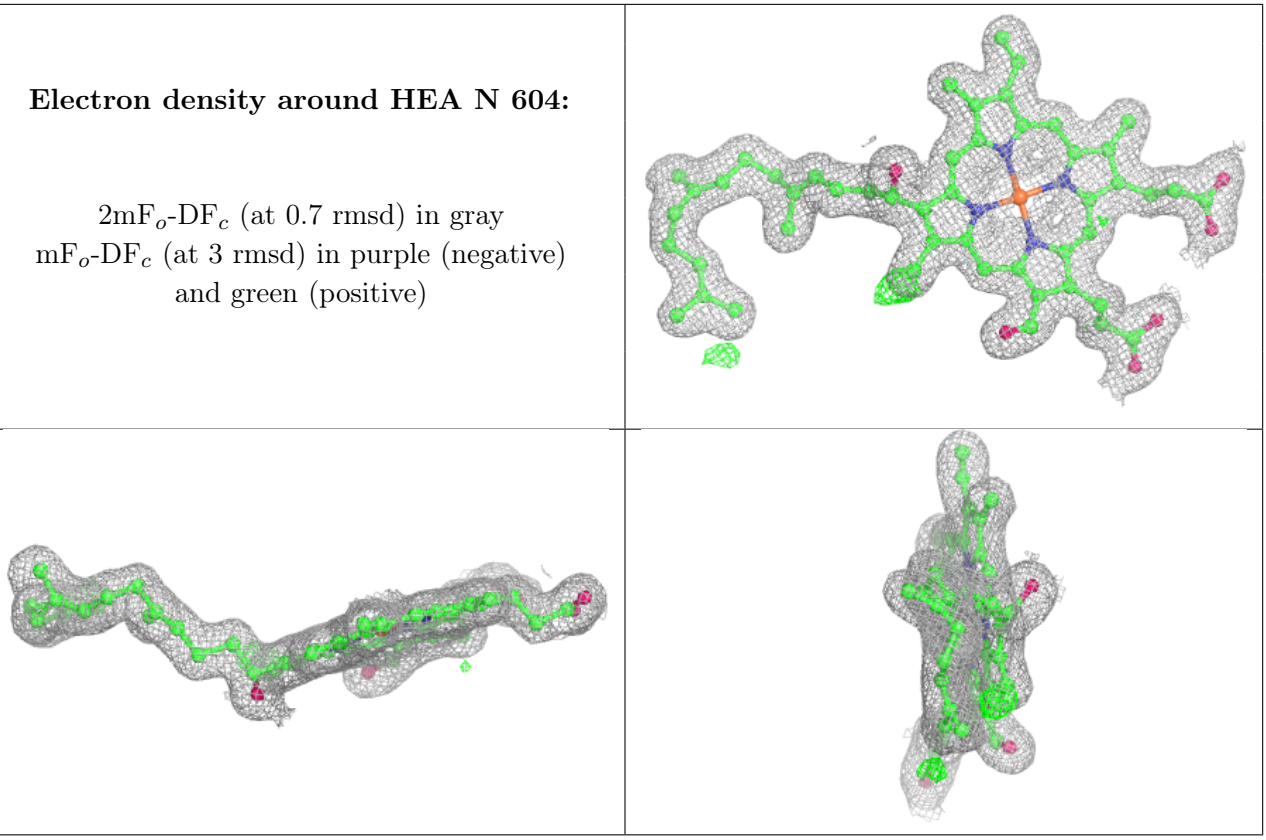
Electron density around CHD O 301:

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



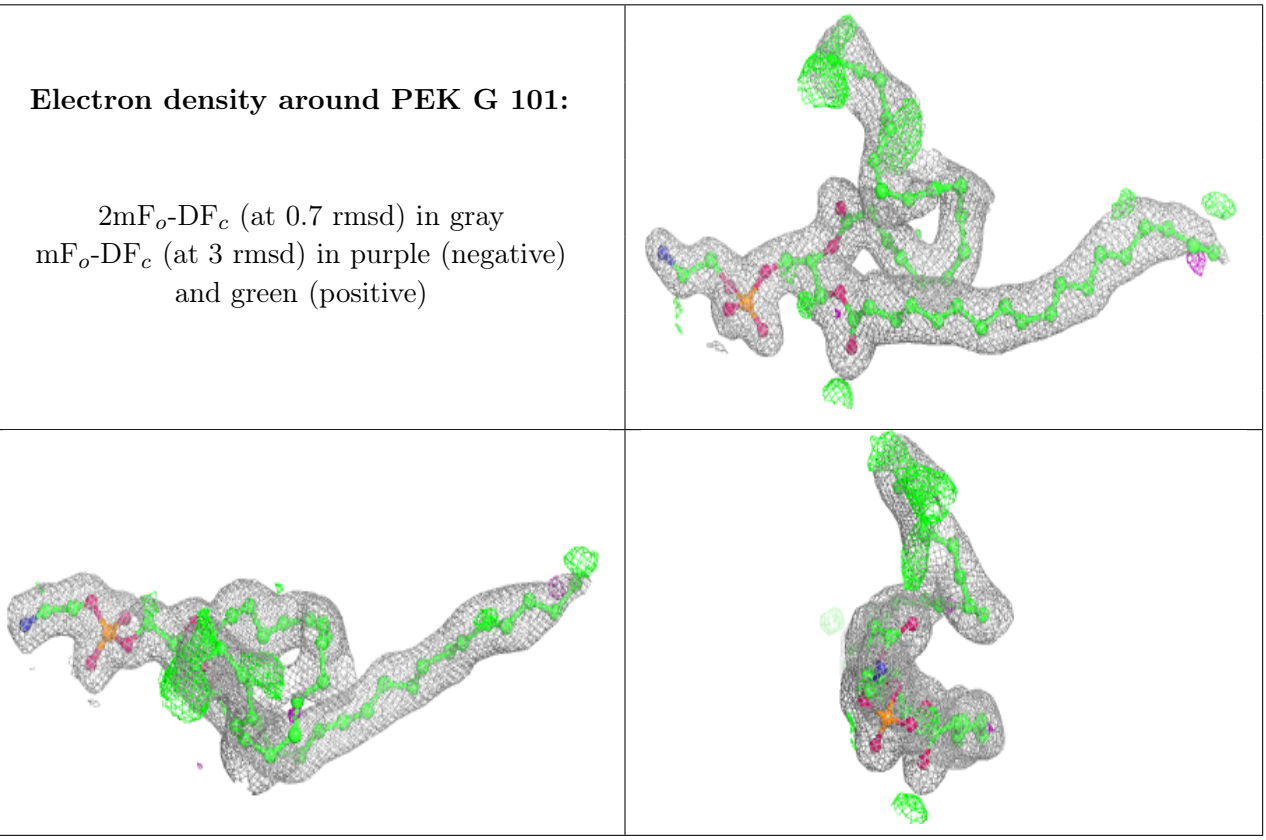
Electron density around HEA N 604:

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



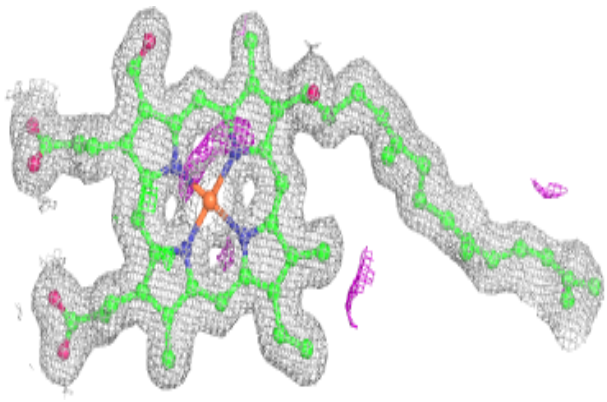
Electron density around PEK G 101:

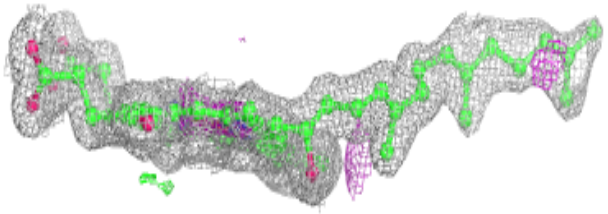
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

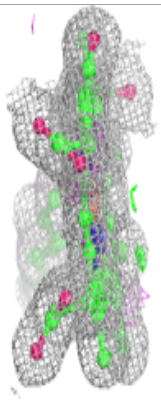


Electron density around HEA A 601 (B):

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

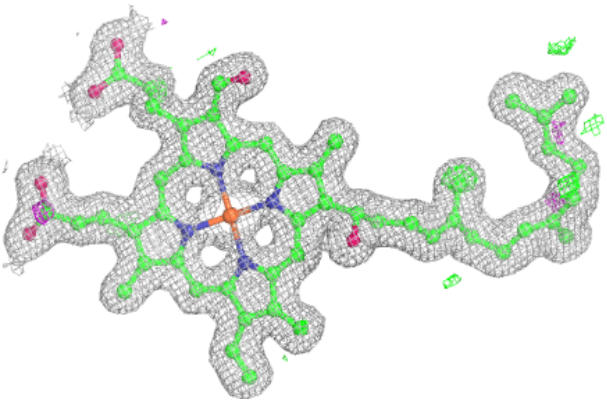


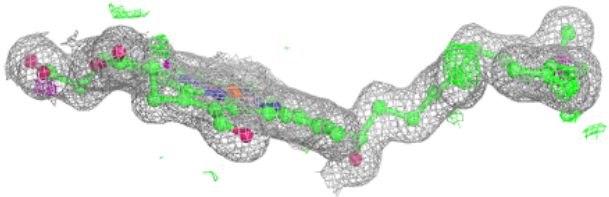


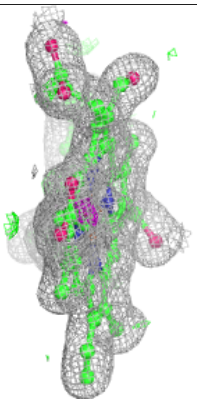


Electron density around HEA A 602:

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

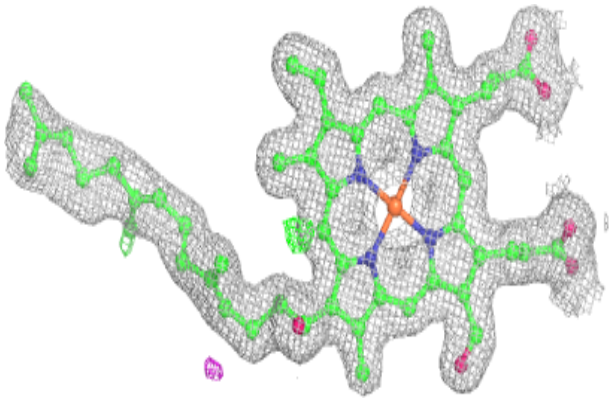


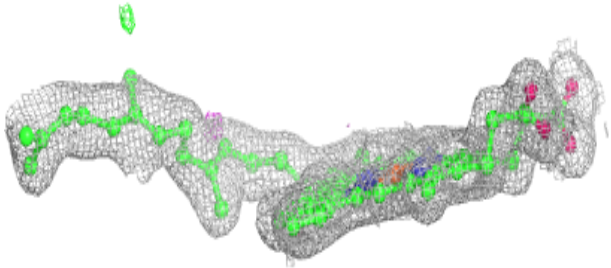


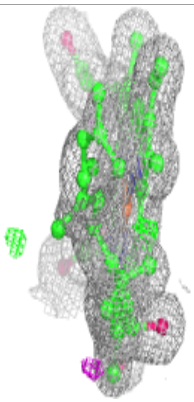


Electron density around HEA N 603 (A):

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

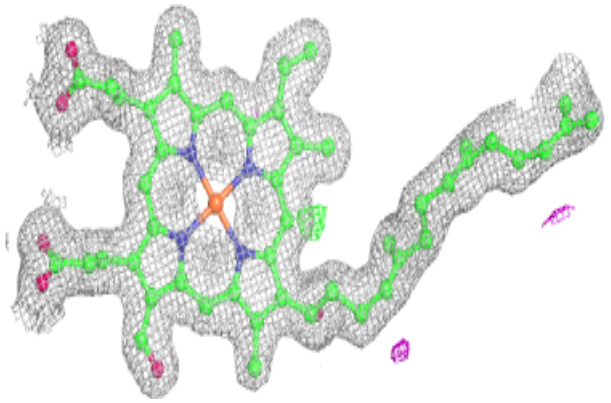


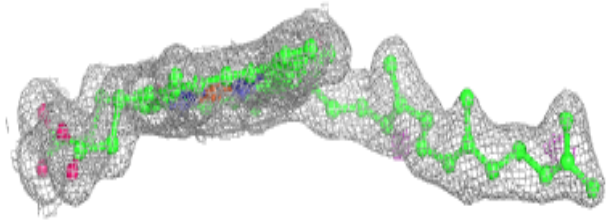


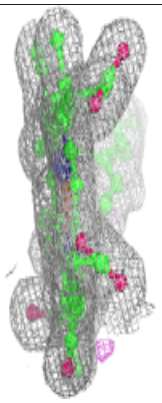


Electron density around HEA N 603 (B):

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

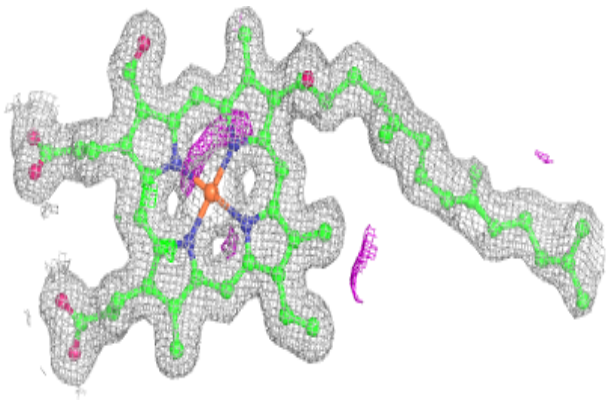


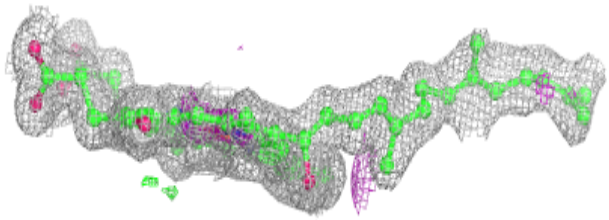


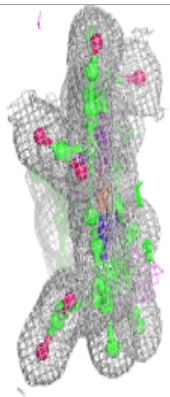


Electron density around HEA A 601 (A):

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

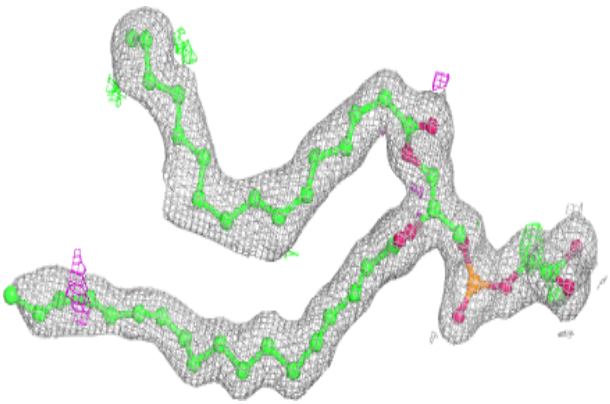


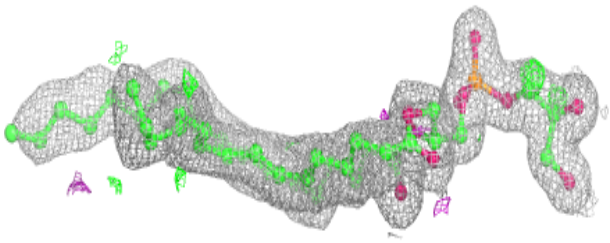


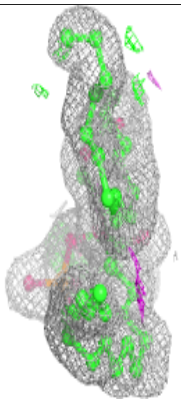


Electron density around PGV A 616:

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

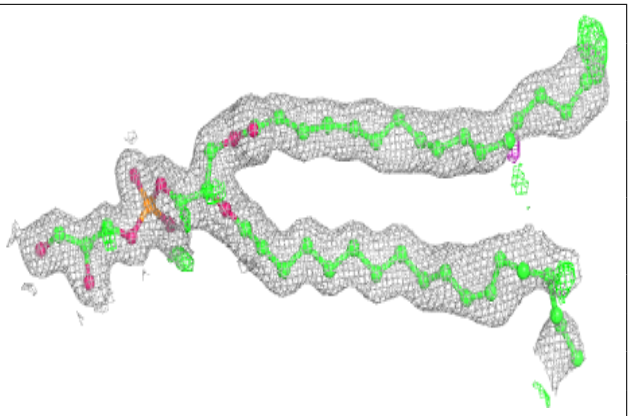


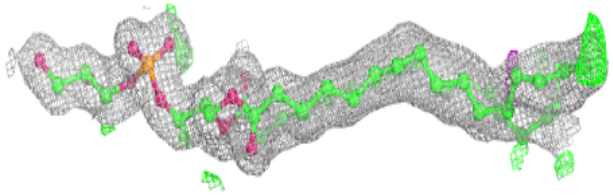


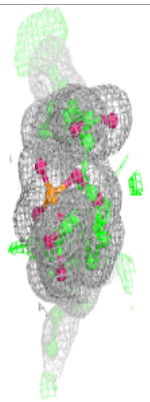


Electron density around PGV C 303:

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

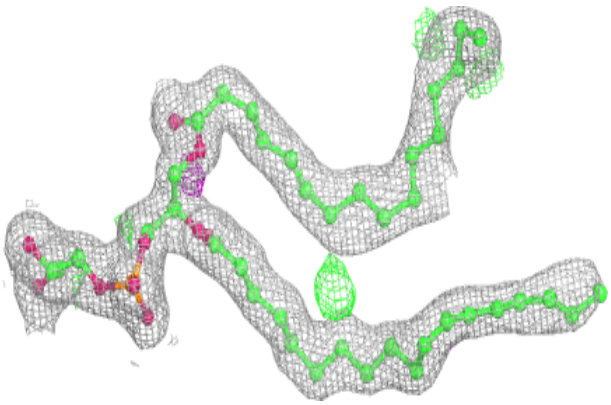


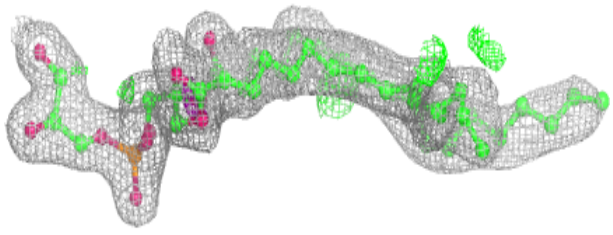


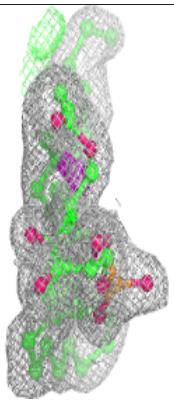


Electron density around PGV N 618:

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

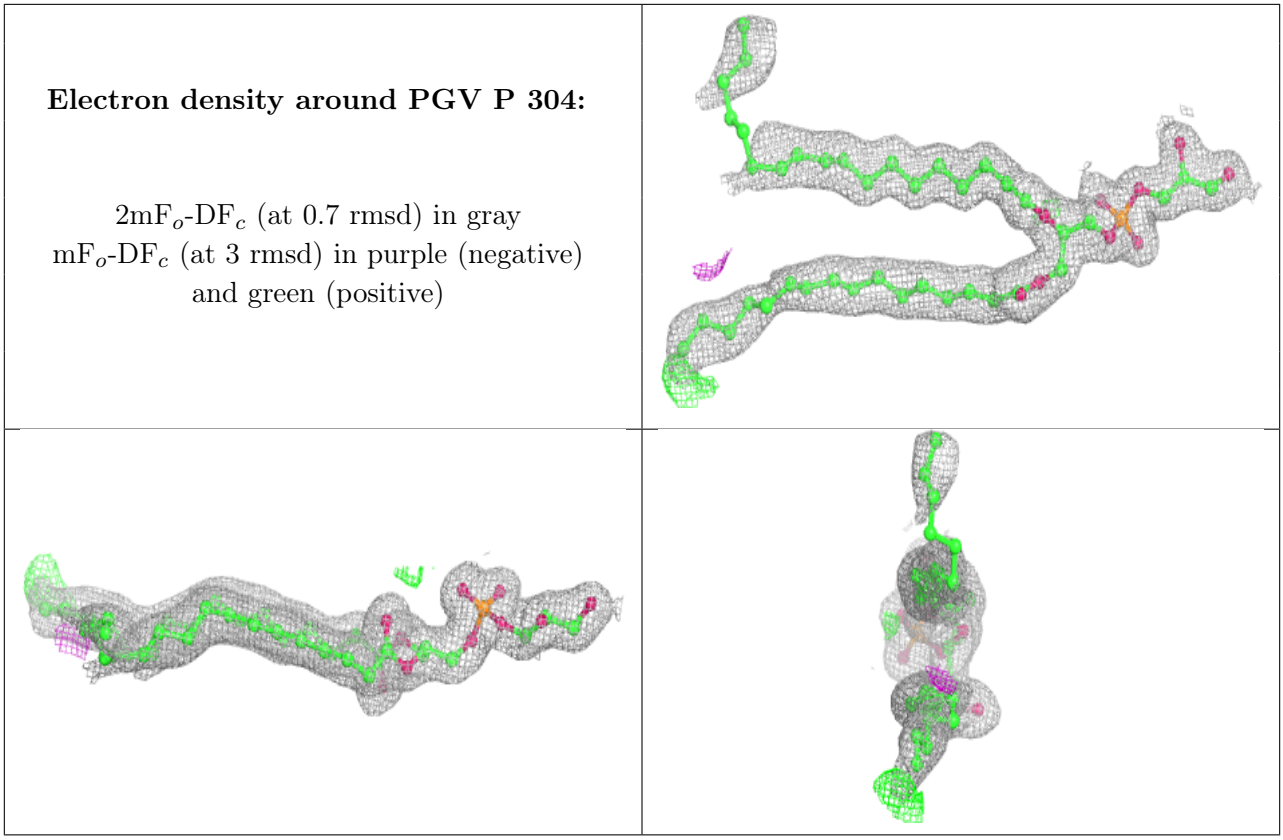






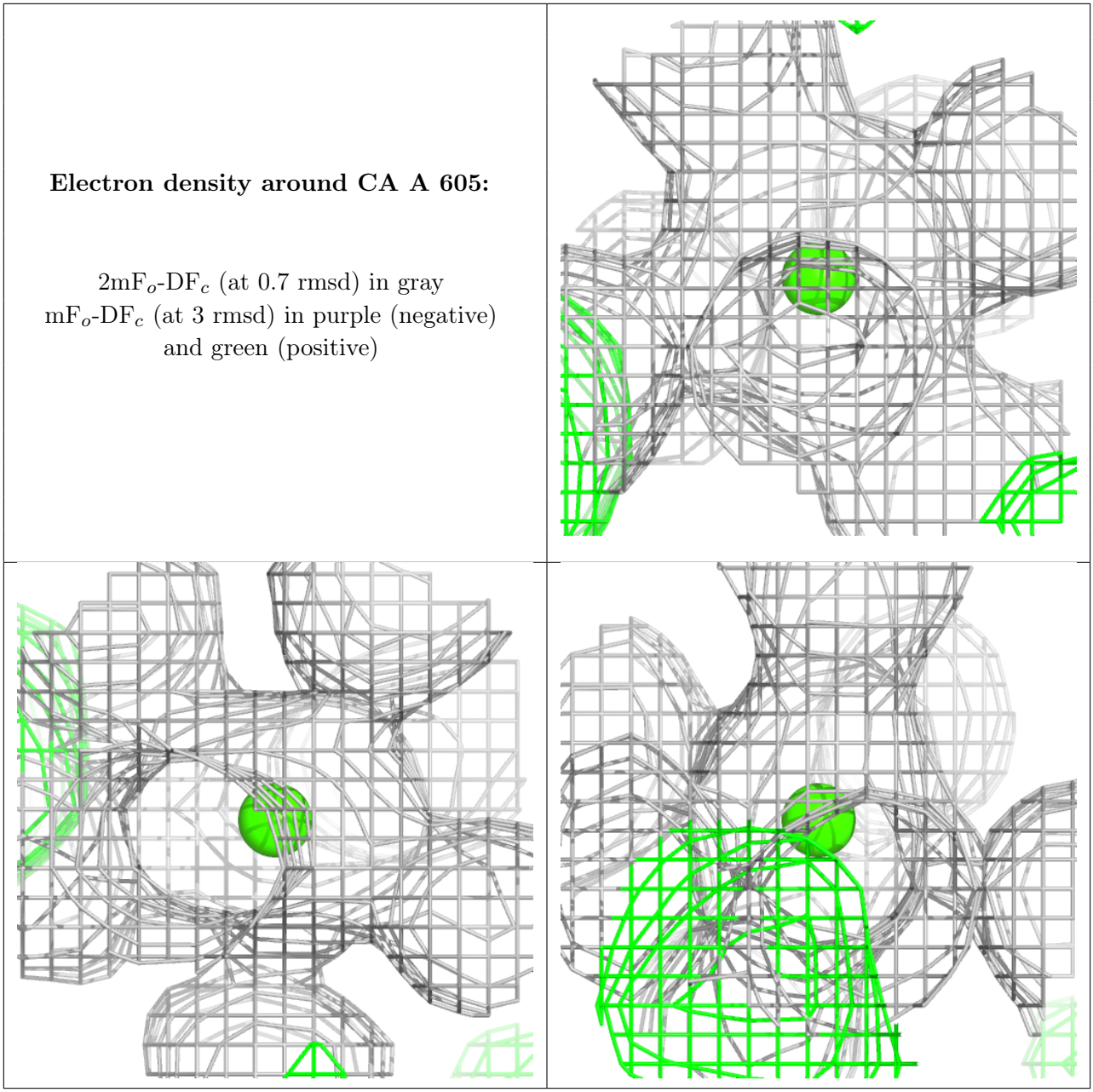
Electron density around PGV P 304:

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



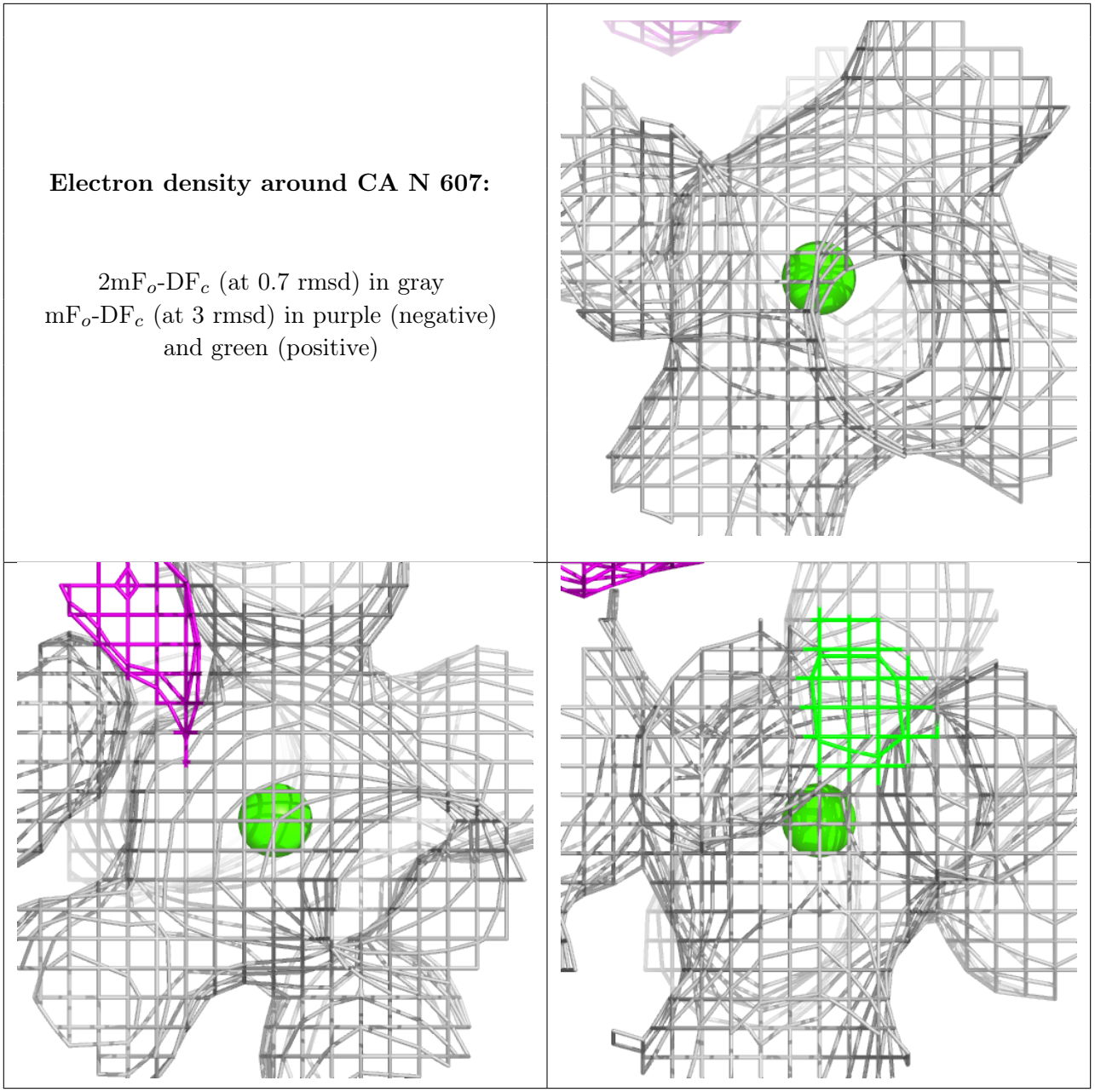
Electron density around CA A 605:

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



Electron density around CA N 607:

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



6.5 Other polymers

There are no such residues in this entry.