Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 07:39 PM UTC

PDB ID	:	8H8S / pdb_00008h8s
Title	:	Bovine Heart Cytochrome c Oxidase in the Calcium-bound Fully Reduced 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:

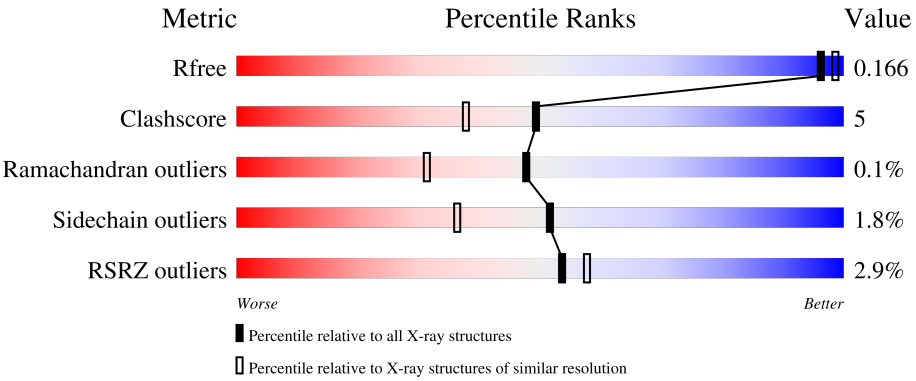
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (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	91% 8%
1	N	514	% 89% 10%
2	B	227	5% 81% 17%
2	O	227	3% 84% 15%
3	C	261	85% 14%

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Mol	Chain	Length	Quality of chain
3	P	261	85% 13%
4	D	147	2% 91% 6%
4	Q	147	7% 86% 5% 7%
5	E	109	% 91% 6%
5	R	109	3% 90% 6%
6	F	98	2% 80% 11% 7%
6	S	98	3% 77% 13% 7%
7	G	85	8% 75% 8% 15%
7	T	85	5% 74% 11% 15%
8	H	85	7% 81% 6% 12%
8	U	85	6% 80% 6% 12%
9	I	73	8% 90%
9	V	73	10% 84% 11%
10	J	59	5% 88% 5% 5%
10	W	59	7% 86% 8% 5%
11	K	56	4% 79% 9% 12%
11	X	56	5% 80% 7% 12%
12	L	47	83% 11% 6%
12	Y	47	2% 83% 9% 6%
13	M	46	2% 85% 13%
13	Z	46	4% 74% 11% 13%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	DMU	A	608	-	-	-	X
20	DMU	N	608	-	-	-	X

2 Entry composition (i)

There are 28 unique types of molecules in this entry. The entry contains 33023 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

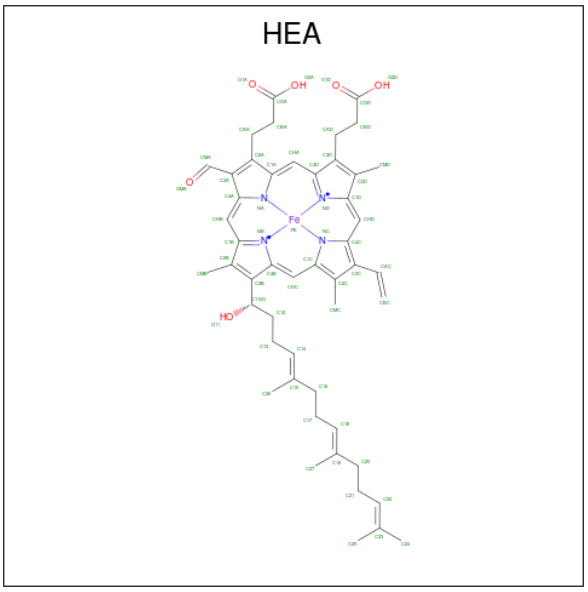
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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

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

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

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



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

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

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

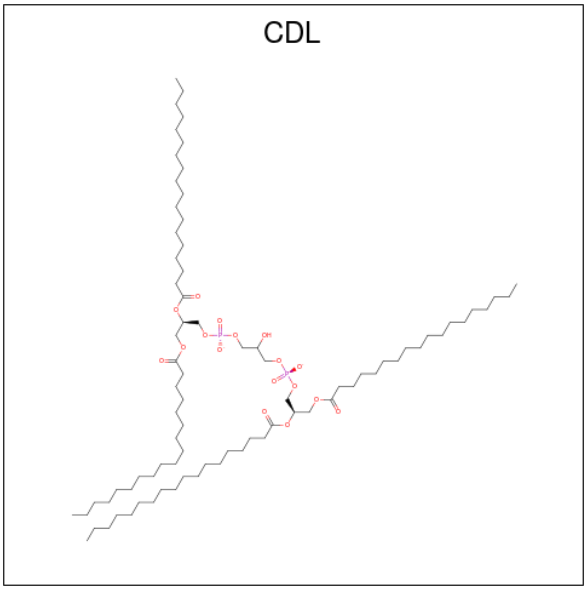
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

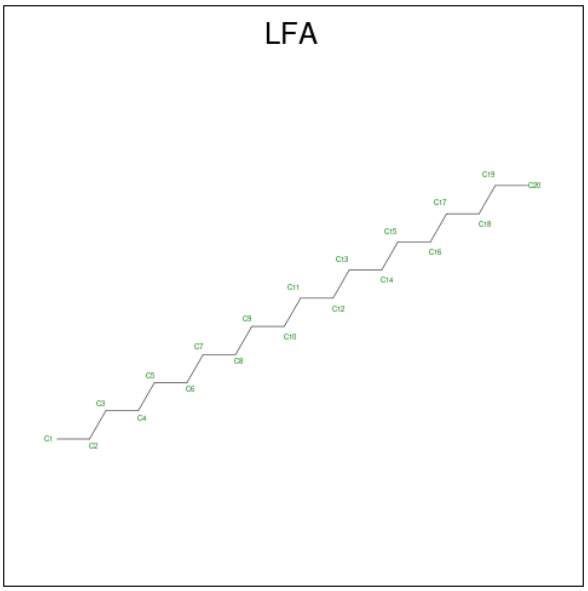
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Ca 1 1	0	0
17	N	1	Total Ca 1 1	0	0

- Molecule 18 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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

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



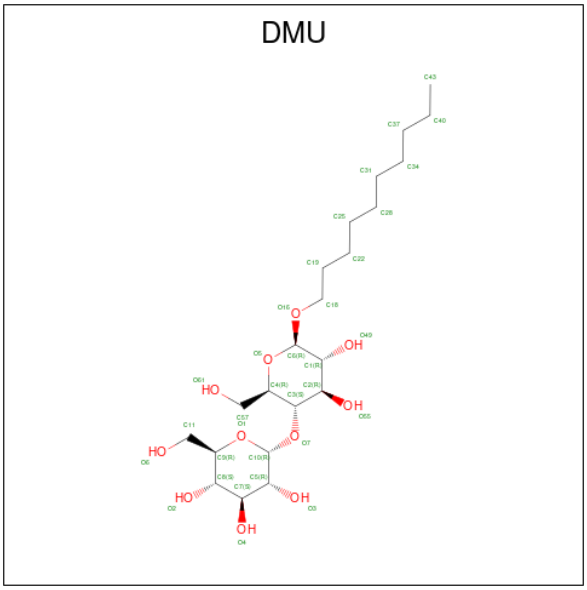
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	A	1	Total C 14 14	0	0
19	B	1	Total C 17 17	0	0
19	C	1	Total C 11 11	0	0
19	C	1	Total C 6 6	0	0
19	C	1	Total C 18 18	0	0
19	C	1	Total C 15 15	0	0
19	C	1	Total C 11 11	0	0
19	C	1	Total C 14 14	0	0
19	C	1	Total C 11 11	0	0
19	C	1	Total C 15 15	0	0
19	C	1	Total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

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

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



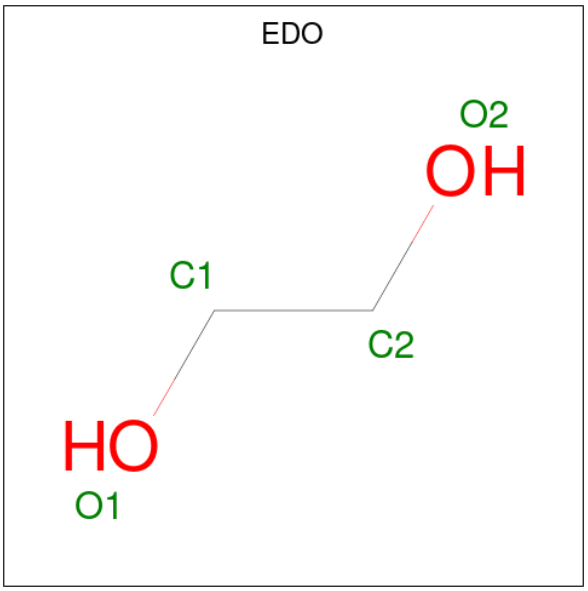
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	A	1	Total C 7 7	0	0
20	A	1	Total C O 33 22 11	0	0
20	A	1	Total C O 11 10 1	0	0
20	B	1	Total C O 11 10 1	0	0
20	B	1	Total C O 11 10 1	0	0
20	B	1	Total C O 22 16 6	0	0
20	B	1	Total C O 22 16 6	0	0
20	C	1	Total C O 11 10 1	0	0
20	C	1	Total C O 33 22 11	0	0
20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

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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 33 22 11	0	0
20	Q	1	Total C O 33 22 11	0	0
20	T	1	Total C O 22 16 6	0	0
20	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 (CCD ID: EDO) (formula: $C_2H_6O_2$).



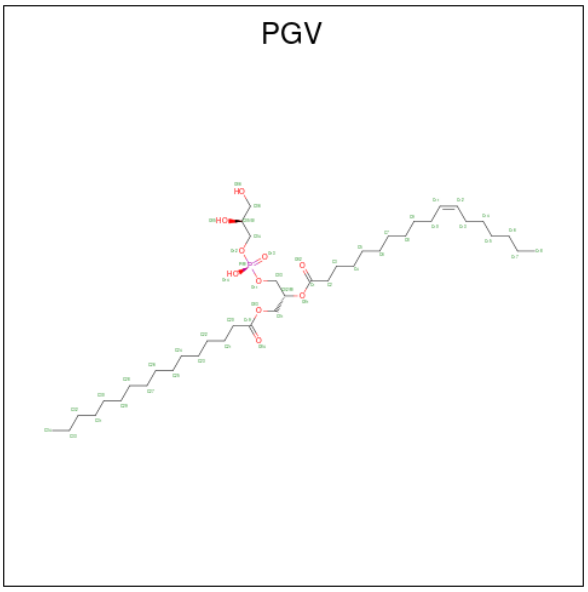
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	B	1	Total	C	O	0	0
			4	2	2		
21	C	1	Total	C	O	0	0
			4	2	2		
21	C	1	Total	C	O	0	0
			4	2	2		
21	C	1	Total	C	O	0	0
			4	2	2		
21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

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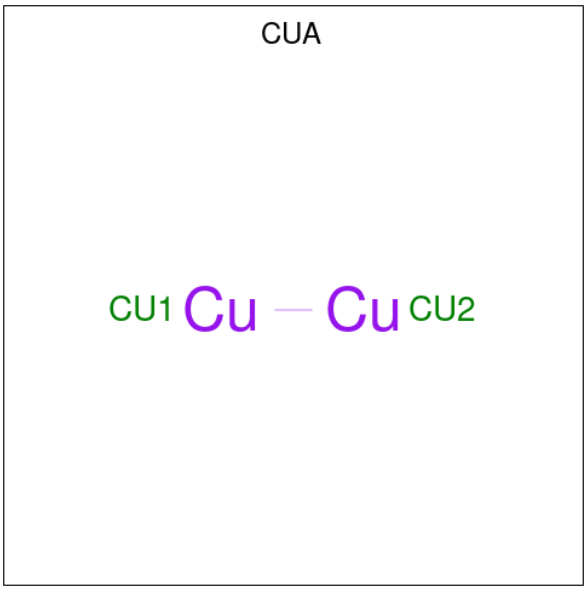
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	N	1	Total	C	O	0	0
			4	2	2		
21	N	1	Total	C	O	0	0
			4	2	2		
21	N	1	Total	C	O	0	0
			4	2	2		
21	N	1	Total	C	O	0	0
			4	2	2		
21	N	1	Total	C	O	0	0
			4	2	2		
21	O	1	Total	C	O	0	0
			4	2	2		
21	P	1	Total	C	O	0	0
			4	2	2		
21	P	1	Total	C	O	0	0
			4	2	2		
21	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 (CCD ID: PGV) (formula: $C_{40}H_{77}O_{10}P$).



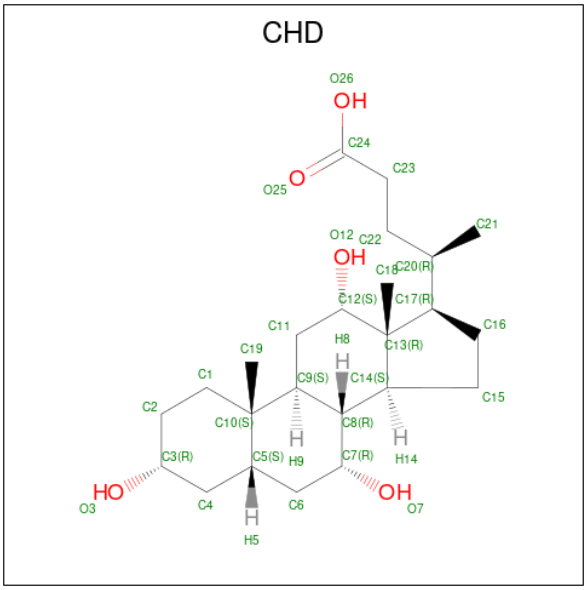
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
22	A	1	Total	C	O	P	0	0
			51	40	10	1		
22	C	1	Total	C	O	P	0	0
			51	40	10	1		
22	N	1	Total	C	O	P	0	0
			51	40	10	1		
22	P	1	Total	C	O	P	0	0
			51	40	10	1		

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



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

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



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

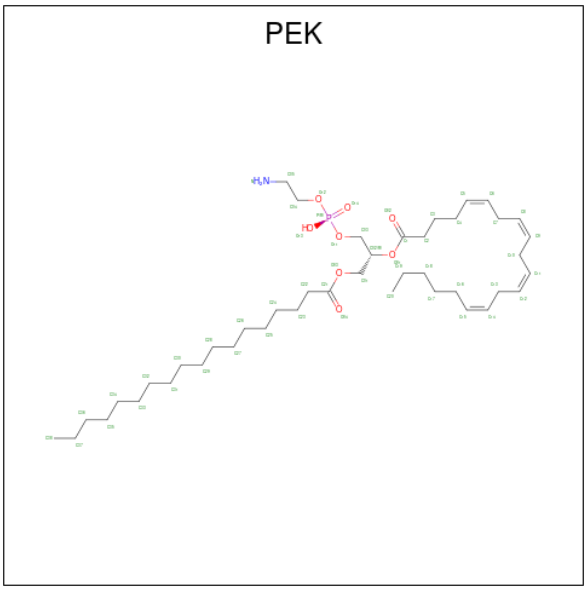
- Molecule 25 is UNKNOWN ATOM OR ION (CCD ID: UNX) (formula: X).

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

- Molecule 26 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 27 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (CCD ID: PEK) (formula: $C_{43}H_{78}NO_8P$).



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

- Molecule 28 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	238	Total O 249 249	0	11
28	B	171	Total O 173 173	0	2
28	C	105	Total O 106 106	0	1
28	D	135	Total O 144 144	0	9

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	E	108	Total O 115 115	0	7
28	F	100	Total O 107 107	0	7
28	G	42	Total O 43 43	0	1
28	H	63	Total O 63 63	0	0
28	I	40	Total O 40 40	0	0
28	J	21	Total O 21 21	0	0
28	K	21	Total O 21 21	0	0
28	L	26	Total O 28 28	0	2
28	M	21	Total O 21 21	0	0
28	N	227	Total O 237 237	0	10
28	O	146	Total O 147 147	0	1
28	P	103	Total O 104 104	0	1
28	Q	79	Total O 84 84	0	5
28	R	87	Total O 94 94	0	7
28	S	89	Total O 95 95	0	6
28	T	37	Total O 38 38	0	1
28	U	47	Total O 47 47	0	0
28	V	24	Total O 24 24	0	0
28	W	15	Total O 15 15	0	0
28	X	18	Total O 18 18	0	0
28	Y	23	Total O 25 25	0	2

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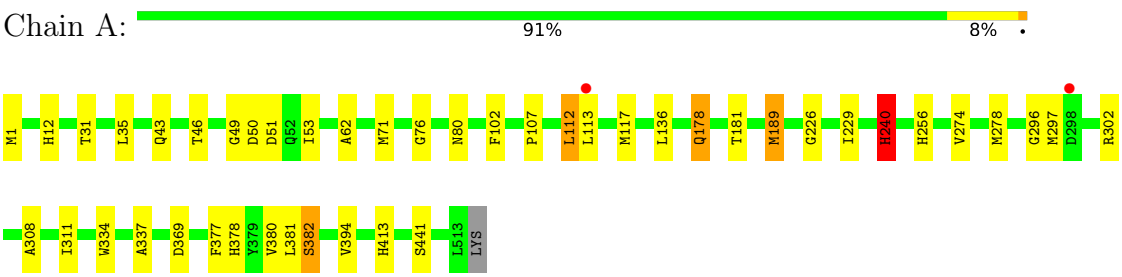
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	Z	17	Total 17	O 17	0	0

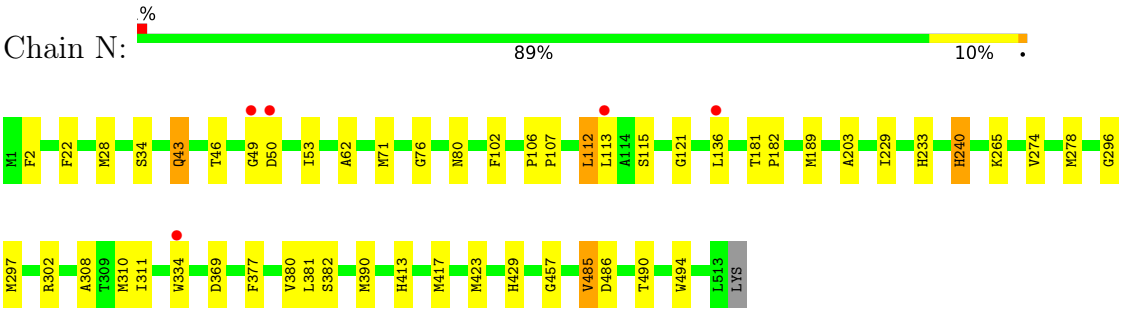
3 Residue-property plots (i)

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

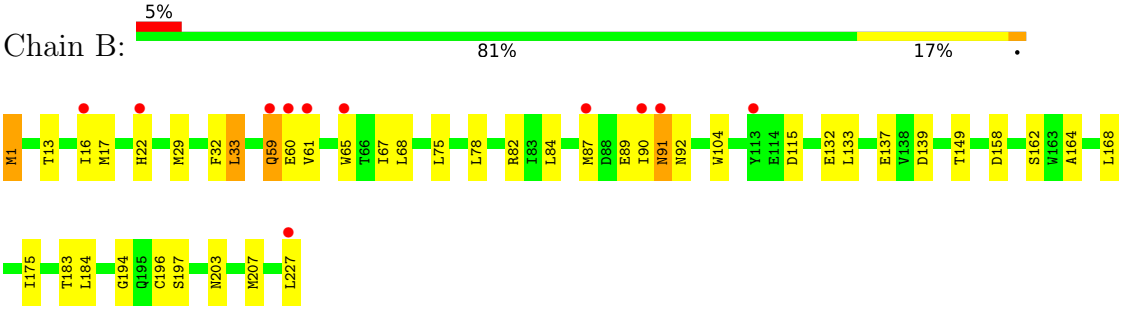
• Molecule 1: Cytochrome c oxidase subunit 1



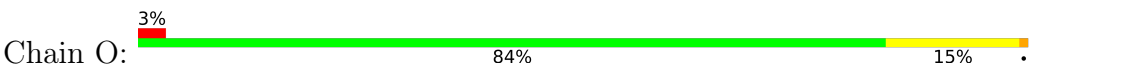
• Molecule 1: Cytochrome c oxidase subunit 1

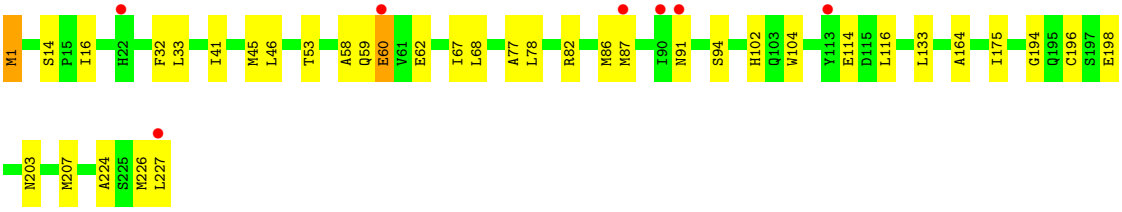


• Molecule 2: Cytochrome c oxidase subunit 2

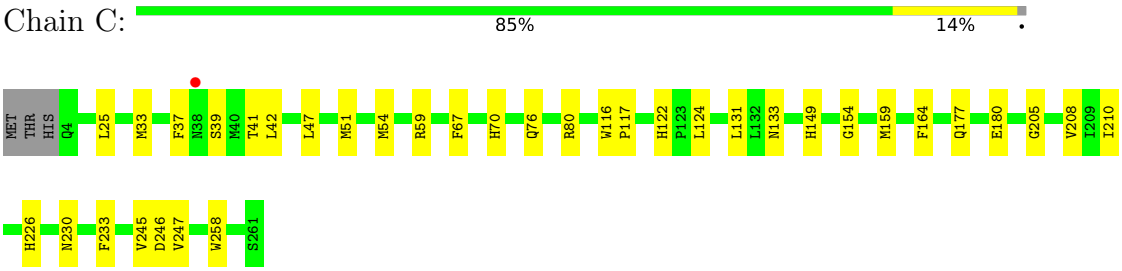


• Molecule 2: Cytochrome c oxidase subunit 2

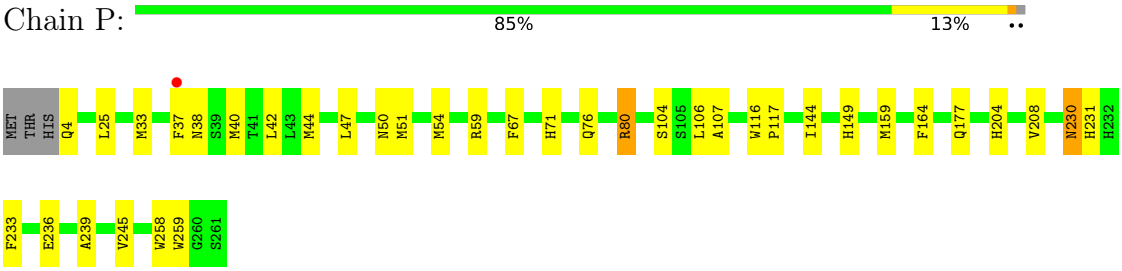




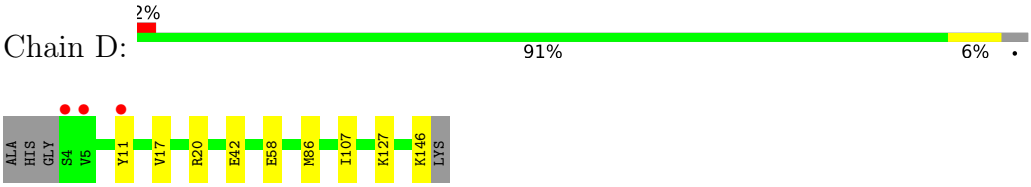
• Molecule 3: Cytochrome c oxidase subunit 3



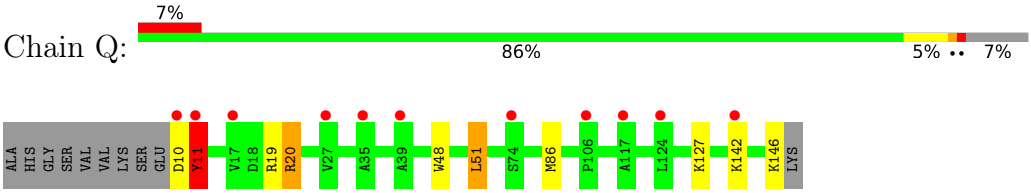
• Molecule 3: Cytochrome c oxidase subunit 3



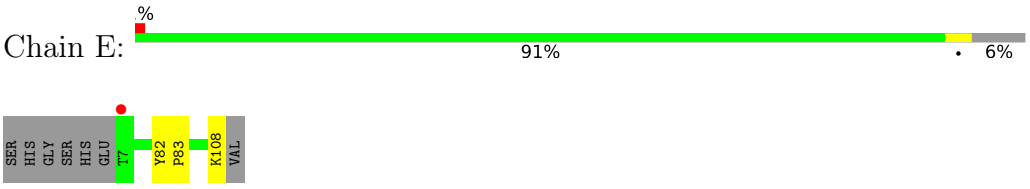
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



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

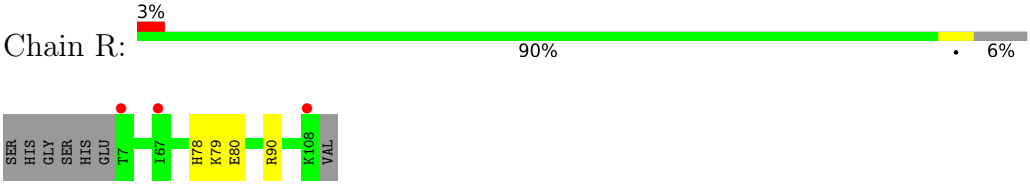


• Molecule 5: Cytochrome c oxidase subunit 5A



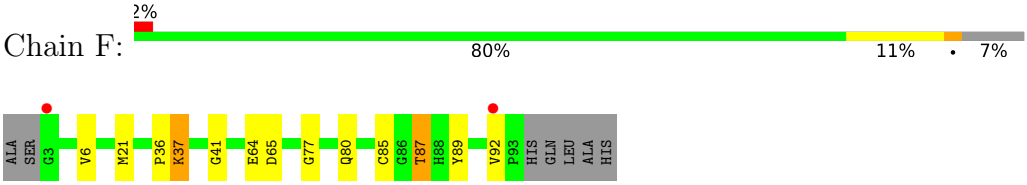
• Molecule 5: Cytochrome c oxidase subunit 5A

Chain R:



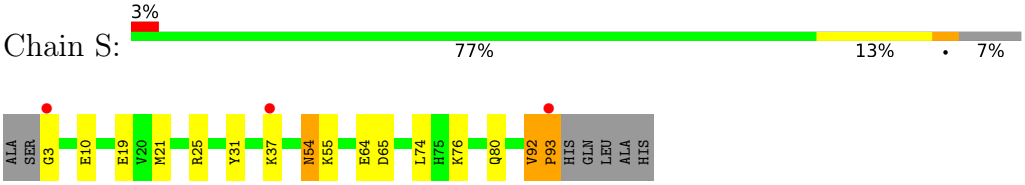
• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

Chain F:



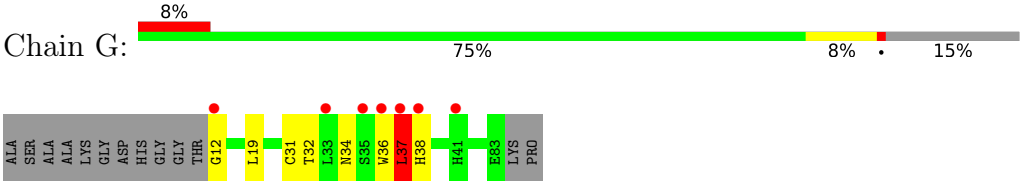
• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

Chain S:



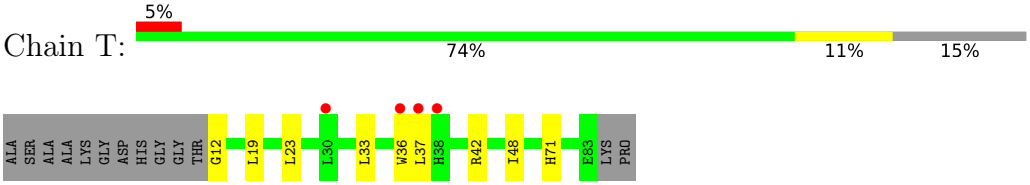
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain G:



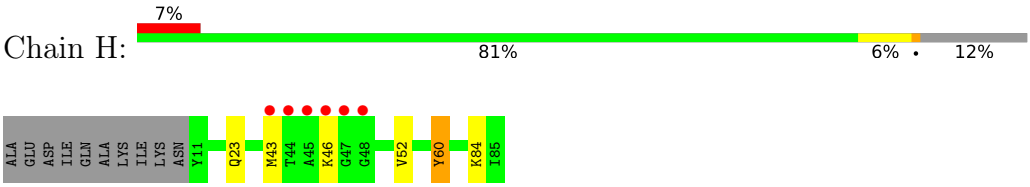
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain T:



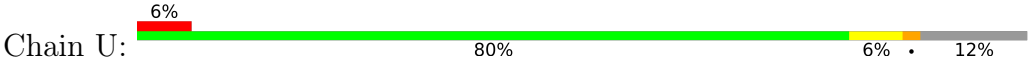
• Molecule 8: Cytochrome c oxidase subunit 6B1

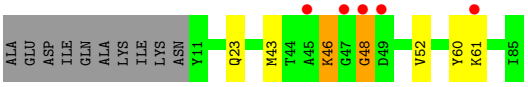
Chain H:



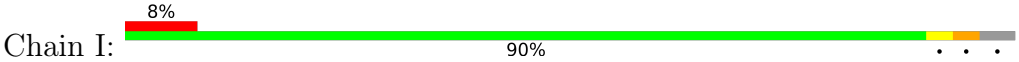
• Molecule 8: Cytochrome c oxidase subunit 6B1

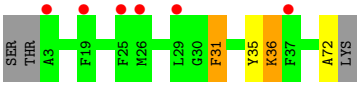
Chain U:



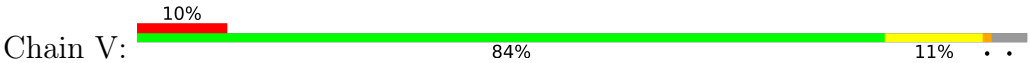


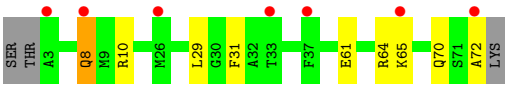
• Molecule 9: Cytochrome c oxidase subunit 6C



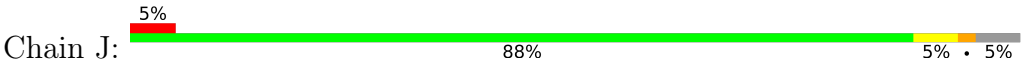


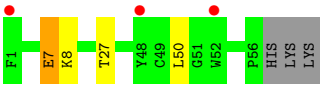
• Molecule 9: Cytochrome c oxidase subunit 6C



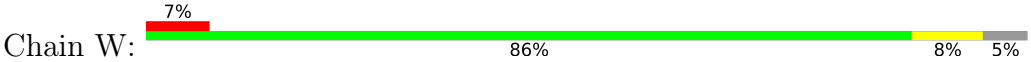


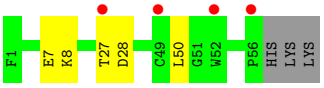
• Molecule 10: Cytochrome c oxidase subunit 7A1



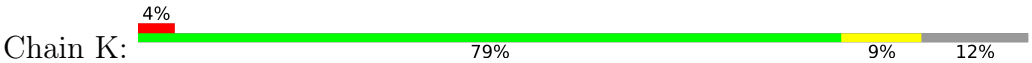


• Molecule 10: Cytochrome c oxidase subunit 7A1



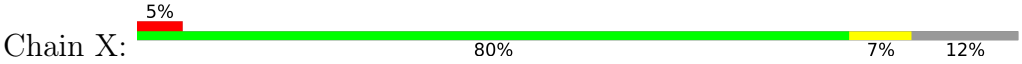


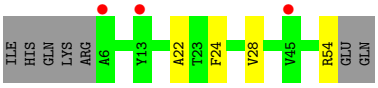
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial





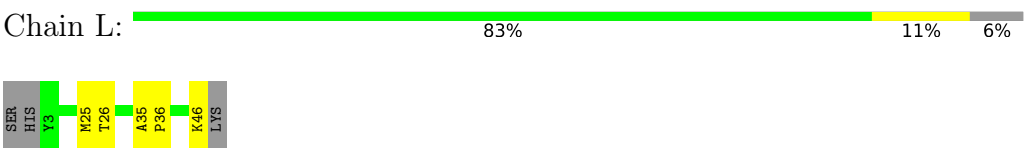
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial





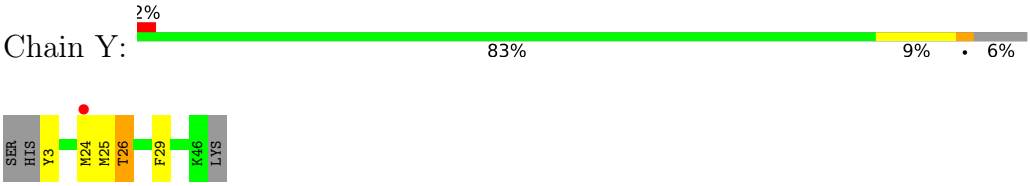
• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain L:



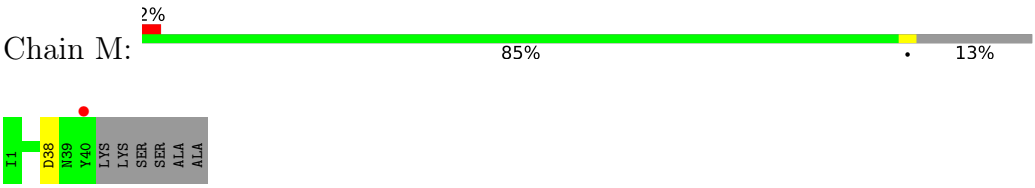
• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain Y:



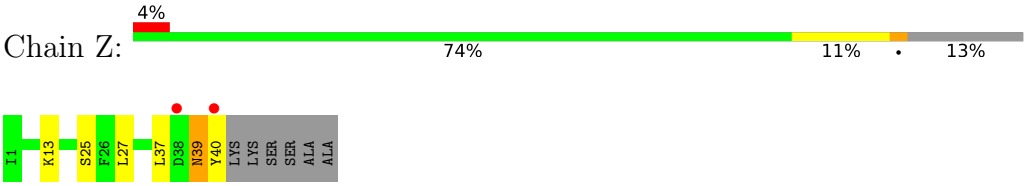
• Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

Chain M:



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

Chain Z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	182.10Å 204.70Å 177.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.70 40.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.00-1.70) 100.0 (40.00-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.124 , 0.156 0.140 , 0.166	Depositor DCC
R_{free} test set	36339 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	32.1	Xtriage
Anisotropy	0.575	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 66.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.006 for l,-k,h	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	33023	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% 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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.08	7/4259 (0.2%)	1.22	7/5816 (0.1%)
1	N	1.09	4/4259 (0.1%)	1.23	7/5816 (0.1%)
2	B	1.13	1/1908 (0.1%)	1.27	12/2598 (0.5%)
2	O	1.08	2/1908 (0.1%)	1.27	2/2598 (0.1%)
3	C	1.07	2/2258 (0.1%)	1.21	4/3084 (0.1%)
3	P	1.09	3/2258 (0.1%)	1.22	6/3084 (0.2%)
4	D	1.15	1/1226 (0.1%)	1.24	4/1657 (0.2%)
4	Q	1.14	2/1182 (0.2%)	1.37	8/1598 (0.5%)
5	E	1.09	0/843	1.22	1/1145 (0.1%)
5	R	1.08	1/843 (0.1%)	1.31	2/1145 (0.2%)
6	F	1.16	2/724 (0.3%)	1.17	0/983
6	S	1.16	0/724	1.24	4/983 (0.4%)
7	G	1.16	1/633 (0.2%)	1.21	0/864
7	T	1.13	2/633 (0.3%)	1.21	0/864
8	H	1.03	0/648	1.30	0/877
8	U	1.08	0/648	1.32	0/877
9	I	1.15	2/588 (0.3%)	1.42	1/781 (0.1%)
9	V	1.10	0/588	1.42	1/781 (0.1%)
10	J	0.98	0/451	1.29	1/610 (0.2%)
10	W	1.09	0/451	1.34	1/610 (0.2%)
11	K	1.19	1/398 (0.3%)	1.31	0/546
11	X	1.11	0/398	1.28	1/546 (0.2%)
12	L	1.12	0/372	1.29	3/500 (0.6%)
12	Y	1.08	0/372	1.28	3/500 (0.6%)
13	M	1.08	0/321	1.13	0/440
13	Z	1.11	0/321	1.37	0/440
All	All	1.10	31/29214 (0.1%)	1.26	68/39743 (0.2%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	N	0	1
6	S	0	1
All	All	0	4

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	58	GLU	CD-OE1	11.06	1.46	1.25
4	Q	142	LYS	C-N	8.72	1.45	1.33
4	Q	142	LYS	C-O	8.34	1.35	1.23
11	K	10	HIS	CE1-NE2	7.55	1.40	1.32
1	A	189	MET	CG-SD	-7.20	1.62	1.80
1	A	413	HIS	CE1-NE2	-7.00	1.25	1.32
1	A	226	GLY	C-O	6.92	1.30	1.23
1	A	413	HIS	CG-ND1	-6.74	1.30	1.38
5	R	80	GLU	CD-OE1	6.60	1.37	1.25
9	I	72	ALA	C-O	6.58	1.36	1.23
3	C	124	LEU	C-O	6.44	1.32	1.23
3	P	71	HIS	CE1-NE2	6.25	1.38	1.32
3	C	70	HIS	CE1-NE2	6.13	1.38	1.32
7	T	71	HIS	CE1-NE2	6.05	1.38	1.32
3	P	204	HIS	CE1-NE2	6.04	1.38	1.32
6	F	77	GLY	C-O	5.79	1.27	1.24
7	G	37	LEU	C-O	-5.71	1.17	1.24
1	N	233	HIS	CE1-NE2	5.66	1.38	1.32
1	N	203	ALA	C-O	5.65	1.30	1.24
1	N	189	MET	CG-SD	-5.56	1.66	1.80
1	A	12	HIS	CE1-NE2	5.45	1.38	1.32
1	A	256	HIS	CE1-NE2	5.37	1.38	1.32
2	B	90	ILE	C-O	5.33	1.29	1.24
9	I	31	PHE	C-O	5.29	1.30	1.24
1	A	189	MET	CB-CG	5.28	1.68	1.52
3	P	231	HIS	CE1-NE2	5.22	1.37	1.32
7	T	48	ILE	N-CA	5.22	1.50	1.45
6	F	36	PRO	C-O	-5.17	1.18	1.23
1	N	189	MET	CB-CG	5.02	1.67	1.52
2	O	102	HIS	CE1-NE2	5.01	1.37	1.32
2	O	198	GLU	C-O	5.00	1.29	1.23

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	I	72	ALA	CA-C-O	-11.52	101.21	120.80
1	N	240	HIS	CA-CB-CG	-11.39	102.41	113.80
1	A	240	HIS	CA-CB-CG	-10.53	103.28	113.80
1	A	71	MET	CG-SD-CE	-10.49	77.82	100.90
4	D	58	GLU	CB-CG-CD	10.15	129.85	112.60
1	N	71	MET	CG-SD-CE	-9.41	80.20	100.90
6	S	93	PRO	CB-CA-C	8.71	126.65	110.10
1	N	43	GLN	CB-CA-C	7.72	120.65	109.45
9	V	72	ALA	CA-C-O	-7.66	107.77	120.80
3	C	80	ARG	CG-CD-NE	-7.23	96.10	112.00
2	B	158	ASP	CA-CB-CG	7.20	119.80	112.60
2	B	65	TRP	CB-CA-C	7.13	123.06	110.37
4	Q	20	ARG	CG-CD-NE	-6.90	96.83	112.00
3	C	233	PHE	CA-CB-CG	-6.87	106.93	113.80
4	Q	20	ARG	NE-CZ-NH1	6.78	128.28	121.50
6	S	93	PRO	N-CA-C	-6.72	95.31	112.10
1	N	240	HIS	N-CA-CB	6.67	116.72	110.39
4	Q	20	ARG	NE-CZ-NH2	-6.56	113.29	119.20
2	B	59	GLN	CB-CG-CD	6.56	123.75	112.60
12	L	25	MET	CA-C-N	6.50	129.31	120.54
12	L	25	MET	C-N-CA	6.50	129.31	120.54
11	X	54	ARG	CA-C-O	-6.42	109.89	120.80
10	J	7	GLU	CB-CA-C	6.34	121.31	110.79
4	Q	10	ASP	CA-C-N	6.33	133.64	121.54
4	Q	10	ASP	C-N-CA	6.33	133.64	121.54
4	D	20	ARG	NE-CZ-NH2	6.24	124.82	119.20
3	P	233	PHE	CA-CB-CG	-6.19	107.61	113.80
1	N	382	SER	CA-C-O	-6.18	114.51	121.00
2	B	82	ARG	CG-CD-NE	-6.17	98.42	112.00
2	O	91	ASN	CB-CA-C	6.16	122.41	109.79
2	B	89	GLU	CA-C-N	6.14	128.80	120.63
2	B	89	GLU	C-N-CA	6.14	128.80	120.63
3	C	122	HIS	CB-CA-C	6.08	116.97	110.65
1	N	102	PHE	CA-CB-CG	-6.07	107.73	113.80
1	A	382	SER	CA-C-O	-6.00	114.46	121.07
4	Q	146	LYS	CA-C-O	-5.95	110.68	120.80
4	Q	10	ASP	CA-C-O	-5.92	110.74	120.80
3	P	76	GLN	CG-CD-NE2	-5.88	107.58	116.40
10	W	28	ASP	CA-CB-CG	5.75	118.36	112.60
3	P	230	ASN	CA-CB-CG	-5.71	106.89	112.60
5	R	78	HIS	CA-C-N	5.67	128.44	120.28
5	R	78	HIS	C-N-CA	5.67	128.44	120.28
3	P	37	PHE	CA-C-N	5.62	130.38	122.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	P	37	PHE	C-N-CA	5.62	130.38	122.46
4	D	146	LYS	CA-C-O	-5.61	111.26	120.80
4	D	11	TYR	N-CA-CB	5.59	118.45	110.06
2	O	53	THR	CA-CB-OG1	-5.56	101.26	109.60
2	B	89	GLU	CA-C-O	-5.46	115.77	121.55
3	C	76	GLN	CG-CD-NE2	-5.45	108.23	116.40
1	A	181	THR	CA-CB-OG1	-5.42	101.48	109.60
1	A	189	MET	CA-CB-CG	-5.40	103.29	114.10
12	Y	26	THR	CA-CB-OG1	-5.39	101.52	109.60
5	E	108	LYS	CA-C-O	-5.36	111.68	120.80
2	B	115	ASP	CB-CA-C	5.32	120.32	112.03
1	A	178	GLN	CB-CG-CD	5.30	121.61	112.60
2	B	184	LEU	N-CA-CB	-5.27	101.68	110.80
12	L	46	LYS	CA-C-O	-5.25	111.88	120.80
1	N	106	PRO	CB-CA-C	5.16	117.22	110.92
2	B	139	ASP	CA-CB-CG	5.16	117.76	112.60
6	S	3	GLY	CA-C-N	5.13	131.47	121.41
6	S	3	GLY	C-N-CA	5.13	131.47	121.41
4	Q	11	TYR	CA-C-O	-5.10	113.21	120.51
3	P	80	ARG	CG-CD-NE	-5.09	100.81	112.00
1	A	102	PHE	CA-CB-CG	-5.07	108.73	113.80
2	B	59	GLN	N-CA-CB	5.05	117.39	110.07
12	Y	25	MET	CA-C-N	5.03	126.97	120.44
12	Y	25	MET	C-N-CA	5.03	126.97	120.44
2	B	149	THR	CA-CB-OG1	-5.02	102.08	109.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

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

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4130	0	4102	34	0
1	N	4130	0	4102	51	0
2	B	1870	0	1870	32	0
2	O	1870	0	1870	37	0
3	C	2171	0	2080	37	0
3	P	2172	0	2081	30	0
4	D	1192	0	1178	5	0
4	Q	1148	0	1131	8	0
5	E	825	0	823	1	0
5	R	825	0	823	1	0
6	F	709	0	691	9	0
6	S	709	0	691	9	0
7	G	606	0	577	7	0
7	T	606	0	577	4	0
8	H	628	0	580	8	0
8	U	628	0	580	10	0
9	I	575	0	584	4	0
9	V	575	0	584	3	0
10	J	441	0	439	5	0
10	W	441	0	439	4	0
11	K	384	0	366	2	0
11	X	384	0	366	3	0
12	L	360	0	360	1	0
12	Y	360	0	360	7	0
13	M	311	0	321	0	0
13	Z	311	0	321	6	0
14	A	120	0	108	3	0
14	N	120	0	108	3	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	64	0	72	0	0
18	C	87	0	124	18	0
18	L	94	0	141	2	0
18	P	87	0	124	14	0
18	V	64	0	72	2	0
18	Y	94	0	141	5	0
19	A	14	0	27	5	0
19	B	17	0	33	1	0
19	C	129	0	235	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	N	28	0	54	11	0
19	O	28	0	54	5	0
19	P	85	0	144	7	0
19	T	39	0	75	6	0
20	A	51	0	76	2	0
20	B	66	0	104	0	0
20	C	172	0	230	4	0
20	D	33	0	41	1	0
20	G	33	0	52	2	0
20	H	33	0	28	0	0
20	J	11	0	21	0	0
20	L	22	0	31	0	0
20	M	41	0	56	0	0
20	N	73	0	80	2	0
20	O	66	0	104	1	0
20	P	172	0	230	2	0
20	Q	33	0	41	1	0
20	T	22	0	31	0	0
20	W	11	0	21	0	0
20	Y	22	0	31	1	0
20	Z	41	0	56	1	0
21	A	16	0	24	0	0
21	B	4	0	6	0	0
21	C	12	0	17	0	0
21	E	12	0	18	0	0
21	F	8	0	12	0	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	0	0
21	R	12	0	18	0	0
21	S	8	0	12	0	0
21	T	4	0	6	0	0
22	A	51	0	76	0	0
22	C	51	0	76	2	0
22	N	51	0	76	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	2	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	2	0
25	C	1	0	0	1	0
25	P	1	0	0	1	0
26	F	1	0	0	0	0
26	S	1	0	0	0	0
27	G	53	0	77	3	0
27	T	53	0	77	5	0
28	A	249	0	0	3	0
28	B	173	0	0	4	0
28	C	106	0	0	4	0
28	D	144	0	0	2	0
28	E	115	0	0	0	0
28	F	107	0	0	1	0
28	G	43	0	0	1	0
28	H	63	0	0	6	0
28	I	40	0	0	1	0
28	J	21	0	0	0	0
28	K	21	0	0	0	0
28	L	28	0	0	0	0
28	M	21	0	0	0	0
28	N	237	0	0	9	0
28	O	147	0	0	2	0
28	P	104	0	0	5	0
28	Q	84	0	0	1	0
28	R	94	0	0	1	0
28	S	95	0	0	0	0
28	T	38	0	0	1	0
28	U	47	0	0	1	0
28	V	24	0	0	1	0
28	W	15	0	0	0	0
28	X	18	0	0	0	0
28	Y	25	0	0	2	0
28	Z	17	0	0	0	0
All	All	33023	0	31506	339	0

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

All (339) 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)
2:B:16[A]:ILE:CG2	2:B:87[A]:MET:HE3	1.53	1.36
1:A:112:LEU:HG	28:A:926:HOH:O	1.36	1.22
2:B:16[A]:ILE:HG21	2:B:87[A]:MET:CE	1.68	1.22
19:C:309:LFA:H12	28:H:217:HOH:O	1.41	1.15
1:A:31:THR:O	1:A:35:LEU:HD23	1.49	1.11
1:A:51:ASP:OD2	1:A:441:SER:OG	1.70	1.08
6:S:76:LYS:HE2	6:S:93:PRO:HG2	1.40	1.03
1:N:112:LEU:HG	28:N:3015:HOH:O	1.58	1.01
8:H:52:VAL:HG12	8:U:46:LYS:HG2	1.41	0.97
3:P:4:GLN:N	28:P:403:HOH:O	1.96	0.97
4:Q:20:ARG:HG2	28:Q:342:HOH:O	1.66	0.96
3:P:67:PHE:CE2	18:P:304:CDL:O1	2.17	0.95
25:P:302:UNX:UNK	28:P:494:HOH:O	1.45	0.94
3:C:67:PHE:CE2	18:C:304:CDL:O1	2.22	0.92
1:A:112:LEU:C	1:A:112:LEU:HD23	1.97	0.90
3:C:245:VAL:C	3:C:246[B]:ASP:CA	2.44	0.90
1:A:278[A]:MET:HE1	19:T:101:LFA:H51	1.52	0.90
2:B:16[B]:ILE:HG23	28:B:516:HOH:O	1.70	0.89
2:O:16[A]:ILE:HD12	2:O:87[A]:MET:CG	2.03	0.89
20:A:609:DMU:O6	28:A:706:HOH:O	1.90	0.88
2:B:16[A]:ILE:HG21	2:B:87[A]:MET:HE3	0.89	0.88
1:N:417[B]:MET:CE	28:N:2948:HOH:O	2.20	0.88
6:S:76:LYS:CE	6:S:93:PRO:HG2	2.01	0.87
8:H:52:VAL:HG21	8:U:43:MET:HE1	1.58	0.84
2:B:16[A]:ILE:HD12	2:B:87[A]:MET:HG3	1.57	0.84
2:O:16[A]:ILE:HG21	2:O:87[A]:MET:SD	2.18	0.83
3:P:67:PHE:HE2	18:P:304:CDL:O1	1.60	0.83
28:N:2935:HOH:O	19:P:309:LFA:H41	1.79	0.82
24:P:305:CHD:H231	24:P:305:CHD:H162	1.62	0.81
7:G:19:LEU:HD23	19:N:607:LFA:H61	1.62	0.81
25:C:302:UNX:UNK	28:C:496:HOH:O	1.62	0.80
2:B:16[A]:ILE:HD12	2:B:87[A]:MET:CG	2.12	0.80
2:O:16[A]:ILE:HD12	2:O:87[A]:MET:HG2	1.62	0.79
1:N:278[A]:MET:HE1	19:N:607:LFA:H51	1.65	0.79
2:B:16[A]:ILE:HG22	2:B:87[A]:MET:HE3	1.62	0.78
4:D:42:GLU:OE2	28:D:301:HOH:O	2.02	0.77
3:C:33[A]:MET:CE	3:C:42:LEU:H	1.98	0.76
1:N:112:LEU:HD23	1:N:112:LEU:C	2.11	0.76
8:H:23:GLN:NE2	28:H:201:HOH:O	2.19	0.76
3:C:33[A]:MET:HE2	3:C:42:LEU:H	1.51	0.75
1:N:46:THR:HG22	1:N:49:GLY:H	1.52	0.75
2:O:16[A]:ILE:HD12	2:O:87[A]:MET:HG3	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:43:MET:O	8:U:48:GLY:N	2.20	0.75
1:N:423[B]:MET:HE2	1:N:457:GLY:HA2	1.69	0.73
2:O:16[B]:ILE:HG23	28:O:500:HOH:O	1.88	0.73
18:C:304:CDL:HB61	18:C:304:CDL:HB21	1.70	0.73
6:F:37:LYS:HG2	28:F:291:HOH:O	1.89	0.72
28:N:2935:HOH:O	19:P:309:LFA:C4	2.36	0.72
1:N:22:PHE:HA	18:Y:101:CDL:H802	1.71	0.72
2:O:114:GLU:HG3	28:O:535:HOH:O	1.90	0.71
1:A:112:LEU:HD23	1:A:112:LEU:O	1.91	0.71
2:O:224:ALA:O	2:O:227:LEU:HD12	1.90	0.71
3:P:149:HIS:NE2	19:P:311:LFA:H11	2.06	0.70
1:A:46:THR:HG22	1:A:49:GLY:H	1.57	0.70
1:N:274:VAL:HG12	1:N:278[A]:MET:HE2	1.73	0.70
3:P:104:SER:OG	28:P:404:HOH:O	2.09	0.70
19:A:607:LFA:H12	19:T:101:LFA:H11	1.74	0.70
7:G:12:GLY:HA3	28:G:235:HOH:O	1.90	0.70
8:H:23:GLN:CD	28:H:201:HOH:O	2.35	0.69
19:C:314:LFA:H21	19:C:315:LFA:H71	1.73	0.68
12:Y:24:MET:HG3	28:Y:212:HOH:O	1.93	0.68
1:N:297[B]:MET:SD	1:N:302:ARG:HG2	2.33	0.68
3:P:33[B]:MET:CE	3:P:42:LEU:HD12	2.24	0.67
28:N:2803:HOH:O	4:Q:11:TYR:HB3	1.94	0.67
1:A:136[B]:LEU:HD11	28:A:932:HOH:O	1.94	0.66
19:N:606:LFA:H12	19:N:607:LFA:H11	1.77	0.66
7:T:19:LEU:HD23	19:T:101:LFA:H61	1.78	0.66
27:T:102:PEK:H71	27:T:102:PEK:H32	1.78	0.66
1:A:278[B]:MET:SD	19:A:607:LFA:H52	2.35	0.66
1:A:278[A]:MET:CE	19:T:101:LFA:H51	2.26	0.65
3:P:59:ARG:HG3	18:P:304:CDL:HA4	1.78	0.65
3:C:67:PHE:HE2	18:C:304:CDL:O1	1.72	0.65
6:F:41:GLY:HA3	6:F:87[B]:THR:HG22	1.78	0.65
18:P:304:CDL:OA3	18:P:304:CDL:H1	1.97	0.65
8:H:23:GLN:NE2	28:H:202:HOH:O	2.29	0.64
22:N:615:PGV:H183	27:T:102:PEK:H331	1.79	0.64
2:O:14:SER:OG	2:O:16[B]:ILE:HG12	1.97	0.64
18:P:304:CDL:H752	10:W:27:THR:HG21	1.80	0.64
20:C:324:DMU:H20	10:J:50:LEU:HB2	1.80	0.64
1:A:112:LEU:C	1:A:112:LEU:CD2	2.70	0.63
3:C:33[A]:MET:HE3	3:C:39:SER:OG	1.98	0.62
3:C:33[A]:MET:HE1	3:C:41:THR:HB	1.82	0.62
2:O:16[A]:ILE:HG21	2:O:87[A]:MET:CG	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:C:304:CDL:OA3	18:C:304:CDL:H1	1.98	0.62
14:A:601:HEA:HMC1	14:A:601:HEA:HBC1	1.81	0.61
2:B:227:LEU:HD21	28:B:484:HOH:O	1.99	0.61
2:O:60:GLU:CD	2:O:60:GLU:H	2.08	0.61
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.36	0.60
18:C:304:CDL:HB61	18:C:304:CDL:CB2	2.30	0.60
2:O:16[A]:ILE:CG2	2:O:87[A]:MET:SD	2.88	0.60
18:C:304:CDL:CA3	18:C:304:CDL:OB9	2.50	0.60
1:A:46:THR:CG2	1:A:49:GLY:H	2.15	0.60
18:P:304:CDL:HA62	18:P:304:CDL:H121	1.83	0.60
1:N:423[B]:MET:HE2	1:N:457:GLY:CA	2.32	0.60
1:N:278[B]:MET:HE1	19:N:606:LFA:H52	1.85	0.59
1:N:112:LEU:HD23	1:N:112:LEU:O	2.02	0.59
27:T:102:PEK:C15	27:T:102:PEK:C11	2.75	0.59
1:N:50:ASP:HB3	1:N:53:ILE:HD12	1.86	0.58
1:N:485:VAL:HG13	21:N:614:EDO:H21	1.85	0.58
3:C:33[B]:MET:HG3	3:C:37:PHE:HB2	1.85	0.58
1:N:46:THR:CG2	1:N:49:GLY:H	2.16	0.57
2:O:16[A]:ILE:HG21	2:O:87[A]:MET:HG2	1.86	0.57
27:T:102:PEK:H32	27:T:102:PEK:C7	2.33	0.57
6:F:64:GLU:O	6:F:65:ASP:HB2	2.05	0.57
1:A:31:THR:O	1:A:35:LEU:CD2	2.39	0.56
9:V:8:GLN:OE1	9:V:10:ARG:O	2.24	0.56
2:B:13:THR:HB	2:B:168:LEU:HD23	1.87	0.56
1:A:334:TRP:CZ3	20:A:608:DMU:H19	2.40	0.56
3:C:54[A]:MET:HE1	22:C:303:PGV:H141	1.88	0.56
1:N:136[B]:LEU:HD11	28:N:3025:HOH:O	2.04	0.56
24:C:305:CHD:H162	24:C:305:CHD:H231	1.88	0.55
18:C:304:CDL:HB22	10:J:8:LYS:HE3	1.89	0.55
4:D:17[A]:VAL:HG12	28:D:306:HOH:O	2.07	0.55
8:H:23:GLN:HG3	28:H:238:HOH:O	2.06	0.55
3:P:50:ASN:ND2	3:P:54[A]:MET:HE2	2.22	0.55
6:F:41:GLY:HA3	6:F:87[B]:THR:CG2	2.35	0.55
3:C:258:TRP:CD2	19:C:307:LFA:H32	2.42	0.55
12:Y:26:THR:HG23	13:Z:25:SER:CB	2.36	0.55
1:N:278[A]:MET:CE	19:N:607:LFA:H51	2.35	0.55
1:N:417[B]:MET:HE1	28:N:2948:HOH:O	1.98	0.54
8:U:46:LYS:CG	8:U:46:LYS:O	2.56	0.54
2:B:16[A]:ILE:HD12	2:B:87[A]:MET:HG2	1.88	0.54
2:B:91:ASN:OD1	2:B:183:THR:HG21	2.07	0.54
18:C:304:CDL:HA62	18:C:304:CDL:H121	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:259:TRP:CD1	20:P:314:DMU:O61	2.61	0.54
1:A:278[B]:MET:HE1	19:A:607:LFA:H52	1.90	0.54
3:C:226:HIS:HE1	18:C:304:CDL:H111	1.73	0.54
6:F:87[A]:THR:HG22	6:F:89:TYR:CE1	2.43	0.54
7:G:31:CYS:SG	20:G:103:DMU:H26	2.48	0.53
1:N:113[A]:LEU:HD12	18:Y:101:CDL:C87	2.38	0.53
3:C:149:HIS:NE2	19:C:313:LFA:H11	2.22	0.53
6:S:54:ASN:HD22	6:S:54:ASN:C	2.17	0.53
2:B:32[B]:PHE:CD2	9:I:31:PHE:CZ	2.97	0.53
1:A:43:GLN:CG	4:D:107:ILE:HG22	2.39	0.53
7:T:12:GLY:HA3	28:T:231:HOH:O	2.07	0.53
28:C:481[B]:HOH:O	10:J:27:THR:HG22	2.08	0.53
3:P:67:PHE:HE2	18:P:304:CDL:H1O1	1.37	0.53
2:B:33:LEU:HD13	9:I:31:PHE:CD2	2.44	0.53
18:P:304:CDL:H121	18:P:304:CDL:CA6	2.39	0.53
8:U:23:GLN:NE2	28:U:102:HOH:O	2.41	0.52
1:N:297[B]:MET:SD	1:N:302:ARG:CG	2.97	0.52
3:C:33[B]:MET:HE1	20:C:324:DMU:H12	1.91	0.52
2:B:67:ILE:HD11	19:B:307:LFA:H42	1.92	0.52
3:C:33[B]:MET:CE	20:C:324:DMU:H12	2.40	0.52
2:B:84:LEU:O	2:B:87[B]:MET:HB2	2.10	0.52
1:N:112:LEU:C	1:N:112:LEU:CD2	2.82	0.52
1:N:278[B]:MET:SD	19:N:606:LFA:C5	2.97	0.52
3:C:258:TRP:CE2	19:C:307:LFA:H32	2.45	0.52
2:O:82:ARG:O	2:O:86:MET:HG3	2.09	0.51
1:A:1:FME:HE2	1:A:1:FME:HA	1.92	0.51
2:B:87[B]:MET:HB3	28:B:502:HOH:O	2.09	0.51
4:Q:48:TRP:O	4:Q:51:LEU:HB2	2.11	0.51
12:Y:26:THR:HG23	13:Z:25:SER:HB3	1.91	0.51
1:A:274:VAL:HG12	1:A:278[A]:MET:HE2	1.93	0.51
3:C:59:ARG:HB2	18:C:304:CDL:OA9	2.11	0.51
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.93	0.51
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.46	0.51
4:D:86:MET:HE1	11:K:22:ALA:HB2	1.93	0.51
1:A:46:THR:HG21	1:A:49:GLY:HA2	1.93	0.50
3:C:133:ASN:ND2	28:C:405:HOH:O	2.33	0.50
2:O:116:LEU:CD1	2:O:226:MET:HG2	2.42	0.50
3:C:164:PHE:CD1	24:C:305:CHD:H192	2.46	0.50
12:Y:3:TYR:N	28:Y:202:HOH:O	2.44	0.50
18:L:101:CDL:OB9	18:L:101:CDL:H122	2.11	0.50
2:B:16[A]:ILE:CG2	2:B:87[A]:MET:CE	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:164:PHE:CD1	24:P:305:CHD:H192	2.46	0.50
14:N:601:HEA:HBC1	14:N:601:HEA:HMC1	1.93	0.50
12:L:35:ALA:HB3	12:L:36:PRO:HD3	1.92	0.50
2:O:32[B]:PHE:CD2	9:V:31:PHE:CZ	3.00	0.50
3:P:149:HIS:NE2	19:P:311:LFA:C1	2.75	0.50
8:U:46:LYS:O	8:U:46:LYS:HG3	2.09	0.50
1:A:113[B]:LEU:HD11	1:A:117[B]:MET:SD	2.52	0.50
1:A:62:ALA:HB2	14:A:601:HEA:HBD1	1.94	0.50
2:O:1:FME:HE1	2:O:133:LEU:HD22	1.94	0.50
2:O:58:ALA:O	2:O:62:GLU:HG3	2.12	0.50
7:G:32:THR:O	7:G:36:TRP:HB2	2.12	0.49
7:G:34:ASN:O	7:G:38:HIS:HD2	1.95	0.49
3:P:116:TRP:HA	3:P:117:PRO:C	2.38	0.49
11:X:24:PHE:O	11:X:28:VAL:HG12	2.13	0.49
20:D:201:DMU:H36	20:D:201:DMU:O55	2.13	0.49
3:C:47:LEU:O	3:C:51[A]:MET:HG2	2.13	0.49
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.95	0.49
1:N:485:VAL:CG1	21:N:614:EDO:H21	2.43	0.49
3:C:180[B]:GLU:HG2	28:C:419:HOH:O	2.12	0.49
1:N:377:PHE:O	1:N:381:LEU:HB3	2.13	0.49
20:N:609:DMU:H29	20:N:609:DMU:O1	2.13	0.49
4:Q:127:LYS:HD2	28:V:221:HOH:O	2.13	0.49
1:N:494:TRP:O	21:N:614:EDO:H22	2.13	0.48
20:Q:201:DMU:O55	20:Q:201:DMU:H36	2.13	0.48
8:U:46:LYS:NZ	8:U:48:GLY:HA2	2.28	0.48
28:N:2935:HOH:O	19:P:309:LFA:C5	2.60	0.48
4:Q:86:MET:HE2	11:X:22:ALA:HA	1.95	0.48
18:P:304:CDL:HB32	18:P:304:CDL:HB21	1.96	0.48
1:N:278[B]:MET:SD	19:N:606:LFA:H52	2.53	0.48
2:B:91:ASN:HD22	2:B:92:ASN:N	2.12	0.47
7:G:19:LEU:CD2	19:N:607:LFA:H61	2.40	0.47
2:B:22[B]:HIS:HD2	28:B:505:HOH:O	1.98	0.47
4:Q:48:TRP:HA	4:Q:51:LEU:HD22	1.95	0.47
3:C:131:LEU:HD21	20:G:103:DMU:H21	1.95	0.47
1:N:278[B]:MET:SD	19:N:606:LFA:H51	2.54	0.47
2:O:67:ILE:HD11	19:O:302:LFA:H42	1.95	0.47
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.96	0.47
1:N:310:MET:HE1	2:O:77:ALA:HB2	1.96	0.47
1:A:337:ALA:HB2	1:A:394[A]:VAL:HG23	1.97	0.47
3:C:210:ILE:HD13	22:C:303:PGV:H312	1.96	0.47
2:O:59:GLN:NE2	19:O:303:LFA:H31	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:33[A]:MET:HE1	3:C:42:LEU:H	1.76	0.46
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.98	0.46
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.98	0.46
1:A:76:GLY:O	1:A:80:ASN:HB2	2.16	0.46
4:D:127:LYS:HD2	28:I:138:HOH:O	2.16	0.46
1:A:278[B]:MET:CE	19:A:607:LFA:H52	2.46	0.46
2:B:164:ALA:O	2:B:194:GLY:HA3	2.16	0.46
1:N:28:MET:HE3	12:Y:29:PHE:CD1	2.51	0.46
1:N:76:GLY:O	1:N:80:ASN:HB2	2.16	0.46
18:C:304:CDL:H531	18:C:304:CDL:HB4	1.98	0.46
1:A:377:PHE:O	1:A:381:LEU:HB3	2.15	0.46
2:O:116:LEU:CD2	2:O:226:MET:HG2	2.45	0.45
1:N:62:ALA:HB2	14:N:601:HEA:HBD1	1.97	0.45
3:C:116:TRP:HA	3:C:117:PRO:C	2.40	0.45
1:N:240:HIS:C	1:N:240:HIS:CD2	2.94	0.45
2:B:104:TRP:CD2	2:B:203:ASN:HB2	2.52	0.45
19:C:309:LFA:C1	28:H:217:HOH:O	2.20	0.45
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.99	0.45
1:N:278[B]:MET:HE3	19:N:607:LFA:H122	1.98	0.45
18:V:101:CDL:C52	18:V:101:CDL:H312	2.47	0.45
1:N:417[B]:MET:HE2	28:N:2948:HOH:O	2.03	0.45
6:S:64:GLU:O	6:S:65:ASP:HB2	2.15	0.45
3:C:33[B]:MET:CA	3:C:33[B]:MET:HE2	2.17	0.45
3:C:33[B]:MET:HE3	3:C:42:LEU:HD12	1.99	0.45
8:H:60:TYR:CD1	8:H:60:TYR:C	2.95	0.45
3:P:51[B]:MET:HE3	18:P:304:CDL:H873	1.98	0.45
5:R:90:ARG:NH1	28:R:304:HOH:O	2.41	0.45
4:Q:86:MET:CE	11:X:22:ALA:HA	2.47	0.44
2:O:60:GLU:CD	2:O:60:GLU:N	2.74	0.44
1:A:378:HIS:HA	1:A:382:SER:HB2	2.00	0.44
2:B:16[A]:ILE:HG21	2:B:87[A]:MET:SD	2.57	0.44
2:B:91:ASN:HD22	2:B:91:ASN:C	2.25	0.44
3:P:208:VAL:HG22	3:P:245:VAL:CG1	2.48	0.44
7:T:23:LEU:HB2	19:T:101:LFA:C9	2.47	0.44
6:S:19:GLU:OE1	6:S:31:TYR:OH	2.21	0.44
8:U:43:MET:HE2	8:U:43:MET:HA	2.00	0.44
3:C:149:HIS:NE2	19:C:313:LFA:C1	2.80	0.44
18:C:304:CDL:H752	10:J:27:THR:HG21	2.00	0.44
3:P:40:MET:O	3:P:44[B]:MET:HG3	2.17	0.44
1:N:46:THR:HG21	1:N:49:GLY:HA2	2.00	0.44
1:N:390:MET:HE2	1:N:413:HIS:HE1	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:O:301:CHD:H212	24:O:301:CHD:H12	1.98	0.44
3:C:247:VAL:CG1	19:C:314:LFA:H71	2.48	0.43
3:C:247:VAL:HG11	19:C:314:LFA:H71	2.00	0.43
1:N:34:SER:HB2	14:N:601:HEA:C2B	2.48	0.43
1:A:297[B]:MET:SD	1:A:302:ARG:HG2	2.59	0.43
18:P:304:CDL:HB22	10:W:8:LYS:HE3	2.00	0.43
8:U:46:LYS:HZ3	8:U:48:GLY:HA2	1.83	0.43
18:C:304:CDL:H121	18:C:304:CDL:CA6	2.48	0.43
3:P:51[A]:MET:SD	18:P:304:CDL:C39	3.07	0.43
3:P:258:TRP:CE2	19:P:307:LFA:H32	2.54	0.43
27:T:102:PEK:H242	27:T:102:PEK:H12	1.99	0.43
18:C:304:CDL:HB4	18:C:304:CDL:C52	2.49	0.43
1:N:486:ASP:OD2	4:Q:19:ARG:NE	2.52	0.43
2:B:60:GLU:HG2	2:B:61:VAL:N	2.33	0.43
3:P:47:LEU:O	3:P:51[A]:MET:HG2	2.19	0.43
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.99	0.43
1:N:278[B]:MET:CE	19:N:606:LFA:H52	2.48	0.43
2:O:59:GLN:HE22	19:O:303:LFA:H32	1.84	0.43
1:N:229:ILE:HD11	2:O:175:ILE:HD13	2.01	0.42
18:P:304:CDL:OA3	18:P:304:CDL:C1	2.65	0.42
1:A:50:ASP:HB3	1:A:53:ILE:HD12	2.01	0.42
2:O:82:ARG:HA	20:O:304:DMU:H30	2.01	0.42
18:P:304:CDL:C75	10:W:27:THR:HG21	2.49	0.42
3:C:177:GLN:HA	3:C:177:GLN:OE1	2.18	0.42
7:G:37:LEU:HD12	7:G:37:LEU:HA	1.83	0.42
27:G:101:PEK:C12	27:G:101:PEK:H161	2.50	0.42
1:A:308:ALA:O	1:A:311[B]:ILE:HG12	2.20	0.42
2:B:1:FME:HE1	2:B:133:LEU:HD22	2.01	0.42
20:C:306:DMU:H16	27:G:101:PEK:H252	2.00	0.42
2:B:16[B]:ILE:HG13	2:B:17:MET:N	2.34	0.42
3:C:51[B]:MET:HE2	18:C:304:CDL:H861	2.02	0.42
3:C:59:ARG:HG3	18:C:304:CDL:HA4	2.02	0.42
3:C:154:GLY:HA2	6:F:6:VAL:HB	2.02	0.42
6:S:21[B]:MET:HB2	6:S:21[B]:MET:HE2	1.69	0.42
18:L:101:CDL:H522	18:L:101:CDL:H552	1.91	0.42
3:P:4:GLN:CA	28:P:403:HOH:O	2.54	0.42
3:P:80:ARG:NH2	3:P:236:GLU:OE1	2.48	0.42
13:Z:39:ASN:OD1	13:Z:39:ASN:N	2.52	0.42
2:B:162:SER:HB3	2:B:197:SER:C	2.45	0.42
11:K:6:ALA:HA	11:K:7:PRO:HD3	1.91	0.42
3:P:106:LEU:HD22	19:P:310:LFA:H21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:N:616:DMU:H29	3:P:107:ALA:HB1	2.02	0.42
3:P:38:ASN:HD21	20:P:318:DMU:H41	1.85	0.42
1:A:240:HIS:CD2	1:A:240:HIS:C	2.98	0.41
6:F:92:VAL:HG23	6:F:92:VAL:O	2.19	0.41
1:N:115[B]:SER:O	1:N:121:GLY:HA2	2.20	0.41
1:N:334:TRP:HH2	2:O:46:LEU:HD13	1.85	0.41
2:O:59:GLN:NE2	19:O:303:LFA:C3	2.84	0.41
2:O:104:TRP:CD2	2:O:203:ASN:HB2	2.55	0.41
3:P:50:ASN:HD22	3:P:51[A]:MET:HE2	1.85	0.41
12:Y:26:THR:HG23	13:Z:25:SER:HB2	2.00	0.41
13:Z:27:LEU:HD22	20:Z:101:DMU:H14	2.02	0.41
18:Y:101:CDL:OA8	18:Y:101:CDL:OA5	2.38	0.41
13:Z:37:LEU:HD23	13:Z:37:LEU:HA	1.89	0.41
6:S:55:LYS:HA	6:S:74:LEU:O	2.21	0.41
1:A:229:ILE:HD11	2:B:175:ILE:HD13	2.02	0.41
1:N:377:PHE:HA	1:N:380:VAL:HG12	2.01	0.41
3:P:33[B]:MET:HB2	3:P:33[B]:MET:HE2	1.46	0.41
3:P:144[A]:ILE:HD13	3:P:239:ALA:HA	2.03	0.41
14:A:601:HEA:HBC1	14:A:601:HEA:CMC	2.48	0.41
18:C:304:CDL:HB22	10:J:8:LYS:CE	2.50	0.41
18:Y:101:CDL:H362	18:Y:101:CDL:H711	2.02	0.41
2:B:29:MET:HB2	9:I:35:TYR:CE1	2.56	0.41
3:P:33[B]:MET:HE2	3:P:42:LEU:HD12	2.02	0.41
6:S:92:VAL:O	6:S:93:PRO:C	2.62	0.41
3:C:205:GLY:HA3	27:G:101:PEK:H192	2.03	0.41
1:N:429:HIS:HB3	18:V:101:CDL:H122	2.03	0.41
28:P:448[B]:HOH:O	10:W:27:THR:HG22	2.21	0.41
9:V:61:GLU:OE1	9:V:64:ARG:NH2	2.43	0.41
3:C:33[A]:MET:CE	3:C:41:THR:HB	2.50	0.41
18:C:304:CDL:HB21	18:C:304:CDL:CB3	2.51	0.41
1:N:308:ALA:O	1:N:311[B]:ILE:HG12	2.21	0.41
2:O:16[A]:ILE:CD1	2:O:87[A]:MET:HG2	2.43	0.41
6:F:21[B]:MET:HE2	6:F:21[B]:MET:HB2	1.89	0.40
6:F:85:CYS:SG	6:F:87[B]:THR:OG1	2.77	0.40
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.56	0.40
2:O:164:ALA:O	2:O:194:GLY:HA3	2.21	0.40
3:P:177:GLN:OE1	3:P:177:GLN:HA	2.20	0.40
7:T:23:LEU:HB2	19:T:101:LFA:H91	2.03	0.40
12:Y:26:THR:CG2	20:Y:102:DMU:H26	2.51	0.40
1:A:377:PHE:HA	1:A:380:VAL:HG12	2.03	0.40
8:H:43:MET:HE1	8:U:52:VAL:HG11	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:181:THR:HA	1:N:182:PRO:HD3	1.95	0.40
1:N:334:TRP:CZ2	2:O:46:LEU:HB3	2.56	0.40
2:O:41:ILE:O	2:O:45:MET:HG2	2.21	0.40
2:O:59:GLN:HE22	19:O:303:LFA:C3	2.35	0.40
6:S:10:GLU:OE2	6:S:25:ARG:NH1	2.51	0.40
1:A:189:MET:HE3	19:A:607:LFA:H31	2.02	0.40
9:I:36:LYS:HE3	9:I:36:LYS:HA	2.04	0.40
3:C:208:VAL:HG22	3:C:245:VAL:CG1	2.51	0.40
1:N:2:PHE:HZ	18:Y:101:CDL:H721	1.85	0.40
2:O:116:LEU:HD13	2:O:226:MET:CG	2.51	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%)	513 (98%)	13 (2%)	0	100	100
1	N	526/514 (102%)	513 (98%)	13 (2%)	0	100	100
2	B	230/227 (101%)	224 (97%)	6 (3%)	0	100	100
2	O	230/227 (101%)	226 (98%)	4 (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%)	131 (96%)	4 (3%)	1 (1%)	18	7
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%)	91 (100%)	0	0	100	100
6	S	91/98 (93%)	90 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	71/85 (84%)	64 (90%)	7 (10%)	0	100	100
7	T	71/85 (84%)	68 (96%)	3 (4%)	0	100	100
8	H	73/85 (86%)	72 (99%)	1 (1%)	0	100	100
8	U	73/85 (86%)	71 (97%)	1 (1%)	1 (1%)	9	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%)	37 (97%)	1 (3%)	0	100	100
13	Z	38/46 (83%)	38 (100%)	0	0	100	100
All	All	3488/3614 (96%)	3415 (98%)	71 (2%)	2 (0%)	48	31

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	440/426 (103%)	437 (99%)	3 (1%)	76	69
1	N	440/426 (103%)	436 (99%)	4 (1%)	70	62
2	B	215/210 (102%)	209 (97%)	6 (3%)	38	21
2	O	215/210 (102%)	210 (98%)	5 (2%)	44	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	C	232/226 (103%)	230 (99%)	2 (1%)	70 62
3	P	232/226 (103%)	230 (99%)	2 (1%)	70 62
4	D	128/129 (99%)	128 (100%)	0	100 100
4	Q	122/129 (95%)	121 (99%)	1 (1%)	73 65
5	E	89/95 (94%)	89 (100%)	0	100 100
5	R	89/95 (94%)	88 (99%)	1 (1%)	65 54
6	F	78/81 (96%)	74 (95%)	4 (5%)	21 7
6	S	78/81 (96%)	75 (96%)	3 (4%)	29 13
7	G	63/69 (91%)	62 (98%)	1 (2%)	55 41
7	T	63/69 (91%)	59 (94%)	4 (6%)	16 5
8	H	67/75 (89%)	64 (96%)	3 (4%)	24 9
8	U	67/75 (89%)	64 (96%)	3 (4%)	24 9
9	I	55/58 (95%)	54 (98%)	1 (2%)	51 36
9	V	55/58 (95%)	51 (93%)	4 (7%)	13 3
10	J	47/50 (94%)	46 (98%)	1 (2%)	47 30
10	W	47/50 (94%)	45 (96%)	2 (4%)	26 10
11	K	39/46 (85%)	38 (97%)	1 (3%)	40 23
11	X	39/46 (85%)	39 (100%)	0	100 100
12	L	37/40 (92%)	36 (97%)	1 (3%)	39 23
12	Y	37/40 (92%)	37 (100%)	0	100 100
13	M	34/38 (90%)	33 (97%)	1 (3%)	37 20
13	Z	34/38 (90%)	31 (91%)	3 (9%)	9 2
All	All	3042/3086 (99%)	2986 (98%)	56 (2%)	51 36

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	LEU
1	A	178	GLN
1	A	369	ASP
2	B	33	LEU
2	B	59	GLN
2	B	68	LEU
2	B	75	LEU

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Mol	Chain	Res	Type
2	B	78	LEU
2	B	91	ASN
3	C	159	MET
3	C	230	ASN
6	F	37	LYS
6	F	80	GLN
6	F	87[A]	THR
6	F	87[B]	THR
7	G	37	LEU
8	H	46	LYS
8	H	60	TYR
8	H	84	LYS
9	I	36	LYS
10	J	7	GLU
11	K	54	ARG
12	L	26	THR
13	M	38	ASP
1	N	43	GLN
1	N	112	LEU
1	N	369	ASP
1	N	485	VAL
2	O	33	LEU
2	O	60	GLU
2	O	68	LEU
2	O	78	LEU
2	O	94	SER
3	P	159	MET
3	P	230	ASN
4	Q	51	LEU
5	R	79	LYS
6	S	37	LYS
6	S	54	ASN
6	S	80	GLN
7	T	33	LEU
7	T	36	TRP
7	T	37	LEU
7	T	42	ARG
8	U	46	LYS
8	U	60	TYR
8	U	61	LYS
9	V	8	GLN
9	V	29	LEU

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Mol	Chain	Res	Type
9	V	65	LYS
9	V	70	GLN
10	W	7	GLU
10	W	50	LEU
13	Z	13	LYS
13	Z	39	ASN
13	Z	40	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	ASN
1	A	422	ASN
2	B	59	GLN
2	B	203	ASN
3	C	50	ASN
3	C	76	GLN
4	D	76	ASN
4	D	119	GLN
5	E	94	ASN
6	F	54	ASN
7	G	38	HIS
8	H	37	HIS
10	J	29	ASN
11	K	35	GLN
1	N	170	ASN
1	N	422	ASN
2	O	10	GLN
2	O	59	GLN
3	P	38	ASN
3	P	50	ASN
4	Q	101	HIS
4	Q	109	HIS
4	Q	119	GLN
5	R	94	ASN
6	S	54	ASN
7	T	34	ASN
8	U	28	ASN
8	U	31	GLN
8	U	32	ASN
8	U	37	HIS
10	W	29	ASN

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Mol	Chain	Res	Type
11	X	35	GLN

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	$\#\|Z\| > 2$
1	FME	A	1	1	8,9,10	0.50	0	8,9,11	0.87	0
1	FME	N	1	1	8,9,10	0.68	0	8,9,11	0.73	0
2	FME	O	1	2	8,9,10	0.66	0	8,9,11	1.25	2 (25%)
2	FME	B	1	2	8,9,10	1.14	1 (12%)	8,9,11	1.14	1 (12%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	CG-SD	-2.44	1.68	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	-2.46	105.33	112.87
2	O	1	FME	CA-N-CN	2.45	126.59	122.82
2	O	1	FME	O-C-CA	-2.08	119.41	124.77

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

There are no ring outliers.

3 monomers are involved in 3 short contacts:

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 131 ligands modelled in this entry, 8 are monoatomic and 2 are unknown - leaving 121 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	$\#\|Z\|>2$
21	EDO	A	611	-	3,3,3	0.18	0	2,2,2	0.33	0
18	CDL	Y	101	-	93,93,99	0.35	0	99,105,111	0.46	1 (1%)
19	LFA	O	302	-	16,16,19	0.30	0	15,15,18	0.26	0
21	EDO	F	103	-	3,3,3	0.27	0	2,2,2	0.28	0
20	DMU	J	101	-	10,10,34	0.27	0	9,9,45	0.58	0
20	DMU	B	303	-	10,10,34	0.31	0	9,9,45	0.64	0
23	CUA	O	305	2	0,1,1	-	-	-		
21	EDO	A	613	-	3,3,3	0.38	0	2,2,2	0.24	0
27	PEK	T	102	-	52,52,52	0.72	2 (3%)	55,57,57	1.05	3 (5%)
20	DMU	T	105	-	22,22,34	0.78	0	27,27,45	1.54	4 (14%)
20	DMU	O	307	-	10,10,34	0.35	0	9,9,45	0.56	0
21	EDO	R	202	-	3,3,3	0.43	0	2,2,2	0.10	0
20	DMU	A	609	-	34,34,34	1.12	5 (14%)	45,45,45	1.25	5 (11%)
21	EDO	A	610	-	3,3,3	0.53	0	2,2,2	0.33	0
19	LFA	C	310	-	14,14,19	0.21	0	13,13,18	0.14	0
21	EDO	C	322	-	3,3,3	0.13	0	2,2,2	0.11	0
20	DMU	L	102	-	22,22,34	0.47	0	27,27,45	1.09	3 (11%)
21	EDO	S	103	-	3,3,3	0.21	0	2,2,2	0.23	0
14	HEA	N	602	1	67,67,67	1.81	21 (31%)	81,103,103	2.34	31 (38%)
21	EDO	N	614	-	3,3,3	0.65	0	2,2,2	1.42	0
19	LFA	C	315	-	12,12,19	0.22	0	11,11,18	0.18	0
19	LFA	C	311	-	10,10,19	0.22	0	9,9,18	0.13	0
20	DMU	Y	102	-	22,22,34	0.58	0	27,27,45	1.13	3 (11%)
20	DMU	B	302	-	10,10,34	0.18	0	9,9,45	0.60	0
20	DMU	H	101	19	34,34,34	1.24	5 (14%)	45,45,45	1.45	6 (13%)
20	DMU	P	322	-	34,34,34	0.74	0	45,45,45	1.64	6 (13%)
21	EDO	N	613	-	3,3,3	0.18	0	2,2,2	0.15	0
19	LFA	A	607	-	13,13,19	0.37	0	12,12,18	0.26	0
19	LFA	C	325	-	14,14,19	0.26	0	13,13,18	0.15	0
18	CDL	V	101	-	63,63,99	0.41	0	69,75,111	0.71	2 (2%)
21	EDO	P	321	-	3,3,3	0.54	0	2,2,2	1.02	0
21	EDO	S	102	-	3,3,3	0.35	0	2,2,2	0.28	0
20	DMU	P	314	-	34,34,34	0.88	2 (5%)	45,45,45	1.83	9 (20%)
19	LFA	C	307	-	10,10,19	0.14	0	9,9,18	0.15	0
19	LFA	O	303	-	10,10,19	0.21	0	9,9,18	0.15	0
19	LFA	C	309	20	17,17,19	0.30	0	16,16,18	0.30	0
18	CDL	L	101	-	93,93,99	0.44	0	99,105,111	0.59	2 (2%)
19	LFA	C	312	-	13,13,19	0.35	0	12,12,18	0.12	0
21	EDO	F	102	-	3,3,3	0.49	0	2,2,2	0.21	0
20	DMU	N	609	-	34,34,34	1.37	5 (14%)	45,45,45	1.12	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	DMU	B	304	-	22,22,34	0.96	1 (4%)	27,27,45	1.04	1 (3%)
18	CDL	C	304	-	86,86,99	0.57	1 (1%)	92,98,111	1.14	9 (9%)
19	LFA	N	606	-	13,13,19	0.37	0	12,12,18	0.32	0
19	LFA	C	313	-	10,10,19	0.20	0	9,9,18	0.13	0
19	LFA	T	103	-	13,13,19	0.23	0	12,12,18	0.11	0
18	CDL	A	606	-	63,63,99	0.50	0	69,75,111	1.07	4 (5%)
19	LFA	C	308	-	5,5,19	0.25	0	4,4,18	0.08	0
19	LFA	P	312	-	14,14,19	0.44	0	13,13,18	0.18	0
20	DMU	O	308	-	22,22,34	0.66	0	27,27,45	1.11	3 (11%)
21	EDO	C	323	-	3,3,3	0.86	0	2,2,2	0.87	0
21	EDO	R	203	-	3,3,3	0.35	0	2,2,2	0.45	0
24	CHD	P	305	-	32,32,32	0.76	0	51,51,51	1.49	5 (9%)
20	DMU	C	324	-	34,34,34	0.71	0	45,45,45	1.24	4 (8%)
21	EDO	B	305	-	3,3,3	0.21	0	2,2,2	0.34	0
21	EDO	O	309	-	3,3,3	0.22	0	2,2,2	0.21	0
19	LFA	P	309	20	17,17,19	0.22	0	16,16,18	0.23	0
23	CUA	B	301	2	0,1,1	-	-	-		
21	EDO	P	319	-	3,3,3	0.25	0	2,2,2	0.04	0
20	DMU	N	608	-	6,6,34	0.54	0	5,5,45	0.29	0
20	DMU	O	304	-	22,22,34	0.84	0	27,27,45	1.53	4 (14%)
22	PGV	P	303	-	50,50,50	0.78	1 (2%)	53,56,56	0.95	2 (3%)
20	DMU	Z	101	-	34,34,34	1.00	3 (8%)	45,45,45	1.09	3 (6%)
14	HEA	N	601	1	67,67,67	1.84	19 (28%)	81,103,103	2.54	28 (34%)
21	EDO	N	611	-	3,3,3	0.23	0	2,2,2	0.36	0
19	LFA	B	307	-	16,16,19	0.30	0	15,15,18	0.19	0
20	DMU	C	316	-	34,34,34	1.03	2 (5%)	45,45,45	1.67	12 (26%)
24	CHD	P	301	-	32,32,32	0.88	2 (6%)	51,51,51	0.79	0
22	PGV	N	615	-	50,50,50	0.83	2 (4%)	53,56,56	1.22	3 (5%)
22	PGV	C	303	-	50,50,50	0.71	0	53,56,56	0.97	4 (7%)
19	LFA	P	311	-	10,10,19	0.31	0	9,9,18	0.23	0
21	EDO	A	612	-	3,3,3	0.72	0	2,2,2	0.28	0
20	DMU	C	320	-	34,34,34	0.82	0	45,45,45	1.27	7 (15%)
20	DMU	N	616	19	34,34,34	1.02	2 (5%)	45,45,45	1.68	9 (20%)
21	EDO	E	202	-	3,3,3	0.22	0	2,2,2	0.25	0
20	DMU	B	308	-	22,22,34	0.58	0	27,27,45	1.35	5 (18%)
18	CDL	P	304	-	86,86,99	0.54	1 (1%)	92,98,111	0.87	4 (4%)
20	DMU	P	315	-	6,6,34	0.33	0	5,5,45	0.48	0
20	DMU	D	201	-	34,34,34	1.53	9 (26%)	45,45,45	1.57	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	PGV	A	614	-	50,50,50	0.84	1 (2%)	53,56,56	1.07	3 (5%)
14	HEA	A	602	1	67,67,67	1.86	19 (28%)	81,103,103	2.26	27 (33%)
19	LFA	P	308	-	5,5,19	0.19	0	4,4,18	0.11	0
21	EDO	P	320	-	3,3,3	0.34	0	2,2,2	0.14	0
21	EDO	T	106	-	3,3,3	0.08	0	2,2,2	0.15	0
20	DMU	P	317	-	34,34,34	0.89	3 (8%)	45,45,45	1.17	4 (8%)
19	LFA	T	101	-	13,13,19	0.77	0	12,12,18	0.36	0
19	LFA	T	104	-	10,10,19	0.18	0	9,9,18	0.18	0
19	LFA	N	607	-	13,13,19	0.48	0	12,12,18	0.34	0
20	DMU	M	102	-	7,7,34	0.28	0	6,6,45	0.37	0
21	EDO	C	321	-	3,3,3	0.04	0	2,2,2	0.17	0
20	DMU	O	306	-	10,10,34	0.21	0	9,9,45	0.61	0
20	DMU	M	101	-	34,34,34	0.98	2 (5%)	45,45,45	0.98	3 (6%)
21	EDO	R	201	-	3,3,3	0.28	0	2,2,2	0.48	0
21	EDO	N	610	-	3,3,3	0.33	0	2,2,2	0.02	0
19	LFA	P	313	-	12,12,19	0.35	0	11,11,18	0.21	0
24	CHD	C	305	-	32,32,32	0.72	0	51,51,51	1.54	7 (13%)
27	PEK	G	101	-	52,52,52	0.61	1 (1%)	55,57,57	0.67	1 (1%)
20	DMU	C	319	-	34,34,34	0.90	2 (5%)	45,45,45	1.34	4 (8%)
24	CHD	C	301	-	32,32,32	1.02	2 (6%)	51,51,51	0.72	0
20	DMU	C	318	-	22,22,34	0.80	1 (4%)	27,27,45	1.25	3 (11%)
20	DMU	P	306	-	10,10,34	0.33	0	9,9,45	0.54	0
19	LFA	P	307	-	10,10,19	0.25	0	9,9,18	0.28	0
20	DMU	G	103	-	22,22,34	0.67	1 (4%)	27,27,45	0.88	2 (7%)
21	EDO	G	104	-	3,3,3	0.26	0	2,2,2	0.09	0
19	LFA	C	314	-	14,14,19	0.33	0	13,13,18	0.43	0
20	DMU	W	101	-	10,10,34	0.19	0	9,9,45	0.63	0
21	EDO	E	203	-	3,3,3	0.22	0	2,2,2	0.18	0
20	DMU	P	318	-	34,34,34	0.71	0	45,45,45	1.19	3 (6%)
21	EDO	E	201	-	3,3,3	0.34	0	2,2,2	0.55	0
24	CHD	O	301	-	32,32,32	0.78	0	51,51,51	0.90	1 (1%)
20	DMU	G	102	-	10,10,34	0.45	0	9,9,45	0.48	0
20	DMU	P	316	-	22,22,34	0.79	1 (4%)	27,27,45	1.42	3 (11%)
20	DMU	C	306	-	10,10,34	0.34	0	9,9,45	0.49	0
20	DMU	Z	102	-	7,7,34	0.29	0	6,6,45	0.63	0
20	DMU	A	615	-	10,10,34	0.35	0	9,9,45	0.51	0
20	DMU	Q	201	-	34,34,34	1.25	7 (20%)	45,45,45	1.67	6 (13%)
21	EDO	N	612	-	3,3,3	0.43	0	2,2,2	0.08	0
20	DMU	A	608	-	6,6,34	0.76	0	5,5,45	0.30	0
24	CHD	B	306	-	32,32,32	0.76	0	51,51,51	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	LFA	P	310	-	10,10,19	0.12	0	9,9,18	0.13	0
14	HEA	A	601	1	67,67,67	1.99	21 (31%)	81,103,103	2.58	24 (29%)
20	DMU	C	317	-	6,6,34	0.25	0	5,5,45	0.45	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
21	EDO	A	611	-	-	1/1/1/1	-
18	CDL	Y	101	-	-	54/104/104/110	-
19	LFA	O	302	-	-	7/14/14/17	-
21	EDO	F	103	-	-	1/1/1/1	-
20	DMU	J	101	-	-	3/8/8/59	-
20	DMU	B	303	-	-	5/8/8/59	-
21	EDO	A	613	-	-	0/1/1/1	-
27	PEK	T	102	-	-	17/56/56/56	-
20	DMU	T	105	-	-	7/13/33/59	0/1/1/2
20	DMU	O	307	-	-	5/8/8/59	-
21	EDO	R	202	-	-	0/1/1/1	-
20	DMU	A	609	-	-	7/19/59/59	0/2/2/2
21	EDO	A	610	-	-	0/1/1/1	-
19	LFA	C	310	-	-	7/12/12/17	-
21	EDO	C	322	-	-	0/1/1/1	-
20	DMU	L	102	-	-	10/13/33/59	0/1/1/2
21	EDO	S	103	-	-	0/1/1/1	-
14	HEA	N	602	1	-	4/36/76/76	-
21	EDO	N	614	-	-	0/1/1/1	-
19	LFA	C	315	-	-	2/10/10/17	-
19	LFA	C	311	-	-	7/8/8/17	-
20	DMU	Y	102	-	-	11/13/33/59	0/1/1/2
20	DMU	B	302	-	-	5/8/8/59	-
20	DMU	H	101	19	-	8/19/59/59	0/2/2/2
20	DMU	P	322	-	-	6/19/59/59	0/2/2/2
21	EDO	N	613	-	-	1/1/1/1	-
19	LFA	A	607	-	-	4/11/11/17	-
19	LFA	C	325	-	-	6/12/12/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CDL	V	101	-	-	42/74/74/110	-
21	EDO	P	321	-	-	0/1/1/1	-
21	EDO	S	102	-	-	0/1/1/1	-
20	DMU	P	314	-	-	7/19/59/59	0/2/2/2
19	LFA	C	307	-	-	6/8/8/17	-
19	LFA	O	303	-	-	4/8/8/17	-
19	LFA	C	309	20	-	9/15/15/17	-
18	CDL	L	101	-	-	48/104/104/110	-
19	LFA	C	312	-	-	5/11/11/17	-
21	EDO	F	102	-	-	0/1/1/1	-
20	DMU	N	609	-	-	4/19/59/59	0/2/2/2
20	DMU	B	304	-	-	7/13/33/59	0/1/1/2
18	CDL	C	304	-	-	48/97/97/110	-
19	LFA	N	606	-	-	3/11/11/17	-
19	LFA	C	313	-	-	3/8/8/17	-
19	LFA	T	103	-	-	6/11/11/17	-
18	CDL	A	606	-	-	41/74/74/110	-
19	LFA	C	308	-	-	0/3/3/17	-
19	LFA	P	312	-	-	4/12/12/17	-
20	DMU	O	308	-	-	5/13/33/59	0/1/1/2
21	EDO	C	323	-	-	0/1/1/1	-
21	EDO	R	203	-	-	1/1/1/1	-
24	CHD	P	305	-	-	7/9/74/74	0/4/4/4
20	DMU	C	324	-	-	3/19/59/59	0/2/2/2
21	EDO	B	305	-	-	0/1/1/1	-
21	EDO	O	309	-	-	0/1/1/1	-
19	LFA	P	309	20	-	9/15/15/17	-
21	EDO	P	319	-	-	1/1/1/1	-
20	DMU	N	608	-	-	2/4/4/59	-
20	DMU	O	304	-	-	4/13/33/59	0/1/1/2
22	PGV	P	303	-	-	9/55/55/55	-
20	DMU	Z	101	-	-	7/19/59/59	0/2/2/2
14	HEA	N	601	1	-	4/36/76/76	-
21	EDO	N	611	-	-	1/1/1/1	-
19	LFA	B	307	-	-	10/14/14/17	-
20	DMU	C	316	-	-	12/19/59/59	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHD	P	301	-	-	2/9/74/74	0/4/4/4
22	PGV	N	615	-	-	10/55/55/55	-
22	PGV	C	303	-	-	15/55/55/55	-
19	LFA	P	311	-	-	5/8/8/17	-
21	EDO	A	612	-	-	0/1/1/1	-
20	DMU	C	320	-	-	10/19/59/59	0/2/2/2
20	DMU	N	616	19	-	7/19/59/59	0/2/2/2
21	EDO	E	202	-	-	0/1/1/1	-
20	DMU	B	308	-	-	9/13/33/59	0/1/1/2
18	CDL	P	304	-	-	52/97/97/110	-
20	DMU	P	315	-	-	2/4/4/59	-
20	DMU	D	201	-	-	8/19/59/59	0/2/2/2
22	PGV	A	614	-	-	9/55/55/55	-
14	HEA	A	602	1	-	6/36/76/76	-
19	LFA	P	308	-	-	0/3/3/17	-
21	EDO	P	320	-	-	0/1/1/1	-
21	EDO	T	106	-	-	0/1/1/1	-
20	DMU	P	317	-	-	16/19/59/59	0/2/2/2
19	LFA	T	101	-	-	2/11/11/17	-
19	LFA	T	104	-	-	5/8/8/17	-
19	LFA	N	607	-	-	6/11/11/17	-
20	DMU	M	102	-	-	4/5/5/59	-
21	EDO	C	321	-	-	1/1/1/1	-
20	DMU	O	306	-	-	6/8/8/59	-
20	DMU	M	101	-	-	3/19/59/59	0/2/2/2
21	EDO	R	201	-	-	1/1/1/1	-
21	EDO	N	610	-	-	0/1/1/1	-
19	LFA	P	313	-	-	2/10/10/17	-
24	CHD	C	305	-	-	8/9/74/74	0/4/4/4
27	PEK	G	101	-	-	14/56/56/56	-
20	DMU	C	319	-	-	16/19/59/59	0/2/2/2
24	CHD	C	301	-	-	2/9/74/74	0/4/4/4
20	DMU	C	318	-	-	9/13/33/59	0/1/1/2
20	DMU	P	306	-	-	2/8/8/59	-
19	LFA	P	307	-	-	3/8/8/17	-
20	DMU	G	103	-	-	8/13/33/59	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	EDO	G	104	-	-	0/1/1/1	-
19	LFA	C	314	-	-	4/12/12/17	-
20	DMU	W	101	-	-	3/8/8/59	-
21	EDO	E	203	-	-	0/1/1/1	-
20	DMU	P	318	-	-	8/19/59/59	0/2/2/2
21	EDO	E	201	-	-	0/1/1/1	-
24	CHD	O	301	-	-	2/9/74/74	0/4/4/4
20	DMU	G	102	-	-	3/8/8/59	-
20	DMU	P	316	-	-	8/13/33/59	0/1/1/2
20	DMU	C	306	-	-	2/8/8/59	-
20	DMU	Z	102	-	-	2/5/5/59	-
20	DMU	A	615	-	-	5/8/8/59	-
20	DMU	Q	201	-	-	5/19/59/59	0/2/2/2
21	EDO	N	612	-	-	0/1/1/1	-
20	DMU	A	608	-	-	2/4/4/59	-
24	CHD	B	306	-	-	2/9/74/74	0/4/4/4
19	LFA	P	310	-	-	6/8/8/17	-
14	HEA	A	601	1	-	3/36/76/76	-
20	DMU	C	317	-	-	2/4/4/59	-

All (144) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	601	HEA	CHD-C1D	5.42	1.49	1.38
14	N	601	HEA	C3B-C2B	5.12	1.46	1.34
20	N	609	DMU	O16-C6	-4.81	1.32	1.40
14	A	601	HEA	C1D-ND	-4.80	1.31	1.40
14	A	601	HEA	C3B-C2B	4.67	1.45	1.34
14	N	602	HEA	C3B-C2B	4.67	1.45	1.34
14	A	601	HEA	C3D-C2D	4.53	1.46	1.36
14	N	601	HEA	C1D-ND	-4.47	1.32	1.40
14	A	601	HEA	C3A-C2A	4.38	1.47	1.37
14	N	601	HEA	C3D-C2D	4.07	1.45	1.36
14	A	602	HEA	CHB-C4A	4.00	1.46	1.38
14	N	601	HEA	CHD-C1D	3.94	1.46	1.38
14	N	602	HEA	CHB-C4A	3.92	1.46	1.38
14	A	602	HEA	FE-NC	3.86	2.07	1.95
14	A	602	HEA	C3B-C2B	3.78	1.43	1.34
20	D	201	DMU	O61-C57	3.56	1.57	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	602	HEA	FE-ND	3.56	2.05	1.94
14	A	602	HEA	FE-ND	3.55	2.05	1.94
20	D	201	DMU	O5-C6	-3.54	1.32	1.41
14	A	602	HEA	C1B-NB	-3.52	1.31	1.38
14	A	601	HEA	C16-C17	-3.46	1.42	1.53
14	A	601	HEA	C12-C11	-3.43	1.47	1.53
14	N	602	HEA	FE-NB	3.41	2.05	1.94
20	B	304	DMU	O16-C6	3.38	1.45	1.40
14	N	602	HEA	C3A-C2A	3.37	1.44	1.37
20	H	101	DMU	O49-C1	3.35	1.51	1.43
14	A	602	HEA	C3A-C2A	3.33	1.44	1.37
14	A	602	HEA	C1C-NC	-3.31	1.33	1.39
14	A	602	HEA	C3D-C2D	3.27	1.43	1.36
14	N	601	HEA	C4D-ND	-3.19	1.32	1.38
14	A	602	HEA	C1D-ND	-3.16	1.34	1.40
24	C	301	CHD	O26-C24	-3.15	1.20	1.30
14	N	602	HEA	C1A-NA	3.11	1.45	1.39
27	G	101	PEK	C23-C22	-3.11	1.40	1.52
22	A	614	PGV	O01-C1	3.10	1.43	1.34
20	C	316	DMU	O3-C5	-3.09	1.35	1.43
27	T	102	PEK	C23-C22	-3.04	1.41	1.52
20	P	316	DMU	O16-C6	3.03	1.45	1.40
14	N	601	HEA	C3A-C2A	3.03	1.44	1.37
20	C	316	DMU	C7-C5	-2.96	1.44	1.52
14	N	602	HEA	C4B-NB	-2.95	1.35	1.40
14	N	602	HEA	CHC-C4B	2.92	1.44	1.38
14	A	602	HEA	C4C-NC	-2.92	1.34	1.39
14	A	602	HEA	CBD-CAD	-2.91	1.41	1.51
14	N	602	HEA	C3D-C2D	2.89	1.43	1.36
24	P	301	CHD	O26-C24	-2.89	1.21	1.30
14	A	602	HEA	FE-NB	2.88	2.03	1.94
24	C	301	CHD	C22-C23	-2.87	1.44	1.52
20	Q	201	DMU	O3-C5	-2.85	1.35	1.43
14	A	602	HEA	CHA-C1A	2.84	1.43	1.38
14	A	601	HEA	CMD-C2D	-2.80	1.45	1.50
14	N	601	HEA	CHB-C4A	2.80	1.43	1.38
14	N	602	HEA	C1C-NC	-2.78	1.34	1.39
14	A	602	HEA	CHC-C4B	2.78	1.44	1.38
14	N	602	HEA	C1B-NB	-2.75	1.33	1.38
14	N	602	HEA	CHD-C1D	2.75	1.44	1.38
14	N	601	HEA	C4B-NB	-2.73	1.35	1.40
20	C	318	DMU	O16-C6	2.73	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	601	HEA	C1C-NC	-2.72	1.34	1.39
20	M	101	DMU	O3-C5	-2.72	1.36	1.43
20	Z	101	DMU	O3-C5	-2.71	1.36	1.43
14	N	602	HEA	C4D-ND	-2.71	1.33	1.38
20	H	101	DMU	O16-C6	-2.71	1.35	1.40
24	P	301	CHD	C22-C23	-2.70	1.44	1.52
20	N	609	DMU	C10-C5	-2.69	1.44	1.52
22	N	615	PGV	O03-C19	2.67	1.41	1.33
14	N	602	HEA	FE-NC	2.66	2.03	1.95
14	A	602	HEA	C3A-C4A	2.66	1.50	1.46
14	N	601	HEA	CHC-C4B	2.65	1.43	1.38
14	N	602	HEA	C3C-C4C	2.64	1.50	1.42
22	P	303	PGV	O03-C19	2.62	1.41	1.33
20	Q	201	DMU	O16-C18	2.62	1.50	1.43
20	C	319	DMU	C7-C5	-2.62	1.45	1.52
14	N	601	HEA	FE-ND	2.61	2.02	1.94
20	D	201	DMU	O49-C1	-2.60	1.36	1.43
14	N	601	HEA	FE-NC	2.59	2.03	1.95
14	A	602	HEA	CHD-C1D	2.59	1.43	1.38
14	N	601	HEA	C11-C3B	-2.58	1.48	1.51
14	N	601	HEA	C1B-NB	-2.57	1.33	1.38
14	A	602	HEA	C4D-ND	-2.56	1.33	1.38
20	P	314	DMU	O3-C5	-2.54	1.36	1.43
20	P	317	DMU	O3-C5	2.53	1.49	1.43
20	N	616	DMU	O1-C10	2.50	1.48	1.41
20	G	103	DMU	C6-C1	-2.50	1.45	1.52
27	T	102	PEK	C2-C1	2.49	1.57	1.50
14	A	601	HEA	C4C-NC	-2.47	1.35	1.39
14	A	601	HEA	C1B-NB	-2.47	1.34	1.38
14	N	602	HEA	C1D-ND	-2.47	1.36	1.40
20	D	201	DMU	C3-C4	2.47	1.59	1.52
20	A	609	DMU	O7-C10	2.46	1.48	1.41
14	N	601	HEA	CHA-C1A	2.44	1.43	1.38
20	C	319	DMU	O5-C6	-2.43	1.35	1.41
20	P	314	DMU	C7-C5	-2.42	1.46	1.52
14	N	602	HEA	C20-C21	-2.40	1.45	1.53
14	A	601	HEA	C26-C15	-2.39	1.44	1.50
20	A	609	DMU	O4-C7	-2.37	1.37	1.43
14	A	601	HEA	C4D-ND	-2.37	1.34	1.38
20	D	201	DMU	O3-C5	-2.36	1.37	1.43
20	M	101	DMU	C7-C5	-2.36	1.46	1.52
20	D	201	DMU	C2-C1	2.35	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	Q	201	DMU	C10-C5	-2.35	1.45	1.52
18	C	304	CDL	C31-CA7	-2.34	1.43	1.50
14	N	602	HEA	O1A-CGA	2.34	1.29	1.22
14	A	602	HEA	C1C-C2C	2.33	1.48	1.43
14	A	601	HEA	FE-NC	2.32	2.02	1.95
14	N	601	HEA	C4C-NC	-2.32	1.35	1.39
20	N	609	DMU	O5-C6	-2.31	1.35	1.41
14	A	601	HEA	FE-ND	2.31	2.02	1.94
20	A	609	DMU	C10-C5	-2.30	1.45	1.52
20	H	101	DMU	C10-C5	-2.29	1.45	1.52
14	N	601	HEA	C26-C15	-2.27	1.45	1.50
20	Z	101	DMU	O5-C6	-2.25	1.36	1.41
20	Q	201	DMU	O61-C57	2.24	1.51	1.42
20	Z	101	DMU	C10-C5	-2.22	1.46	1.52
14	N	601	HEA	O2D-CGD	-2.22	1.23	1.30
14	A	601	HEA	C1B-C2B	2.21	1.49	1.44
14	A	602	HEA	CHD-C4C	2.20	1.44	1.39
20	D	201	DMU	O1-C10	2.20	1.47	1.41
20	Q	201	DMU	O5-C6	-2.20	1.36	1.41
14	N	602	HEA	CHD-C4C	2.19	1.44	1.39
20	N	609	DMU	C7-C5	-2.19	1.46	1.52
14	A	601	HEA	C1C-C2C	2.19	1.48	1.43
20	H	101	DMU	O1-C10	2.19	1.47	1.41
22	N	615	PGV	O01-C1	2.19	1.40	1.34
14	A	601	HEA	CHB-C4A	2.18	1.42	1.38
20	D	201	DMU	O55-C2	2.18	1.48	1.43
20	H	101	DMU	O5-C6	-2.18	1.36	1.41
20	Q	201	DMU	C7-C5	-2.17	1.46	1.52
20	P	317	DMU	C7-C5	-2.16	1.46	1.52
20	P	317	DMU	O5-C6	-2.15	1.36	1.41
14	N	601	HEA	CBA-CGA	2.14	1.55	1.50
14	N	601	HEA	O1A-CGA	2.13	1.29	1.22
18	P	304	CDL	C31-CA7	-2.12	1.44	1.50
14	N	602	HEA	CHB-C1B	2.12	1.44	1.39
20	Q	201	DMU	O49-C1	-2.11	1.37	1.43
14	N	602	HEA	CHA-C1A	2.11	1.42	1.38
20	N	609	DMU	O1-C10	2.08	1.47	1.41
14	A	601	HEA	CHC-C4B	2.08	1.42	1.38
14	A	601	HEA	CBA-CGA	2.08	1.55	1.50
20	A	609	DMU	O5-C6	-2.06	1.36	1.41
20	D	201	DMU	C10-C5	-2.06	1.46	1.52
20	N	616	DMU	O4-C7	2.05	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	609	DMU	O55-C2	2.03	1.48	1.43
14	A	601	HEA	O1A-CGA	2.00	1.28	1.22

All (281) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	N	601	HEA	C3D-C4D-ND	8.46	118.53	110.35
14	A	601	HEA	C3D-C4D-ND	7.70	117.79	110.35
14	A	601	HEA	C2B-C1B-NB	7.61	118.70	109.90
20	P	314	DMU	O16-C6-C1	7.51	119.68	108.27
14	A	602	HEA	C2B-C1B-NB	7.42	118.48	109.90
14	A	601	HEA	C3C-C4C-NC	6.87	115.59	109.80
14	A	601	HEA	C13-C12-C11	-6.59	103.86	114.39
20	Q	201	DMU	O16-C6-C1	6.58	118.26	108.27
14	N	602	HEA	C2B-C1B-NB	6.47	117.38	109.90
20	D	201	DMU	O16-C6-C1	6.40	118.00	108.27
14	N	601	HEA	C3C-C4C-NC	6.26	115.07	109.80
14	N	601	HEA	C2B-C1B-NB	6.09	116.95	109.90
14	A	601	HEA	C1B-C2B-C3B	-5.95	99.91	106.80
20	T	105	DMU	O16-C6-C1	5.79	117.07	108.27
14	N	602	HEA	C2D-C1D-ND	5.77	116.47	109.84
14	A	602	HEA	C3D-C4D-ND	5.69	115.85	110.35
14	A	601	HEA	C3B-C4B-NB	5.41	116.06	109.84
14	N	601	HEA	C13-C12-C11	-5.41	105.76	114.39
14	N	601	HEA	C2D-C1D-ND	5.34	115.98	109.84
20	C	324	DMU	O16-C6-C1	5.28	116.30	108.27
18	A	606	CDL	CA4-OA6-CA5	5.24	130.34	117.80
24	C	305	CHD	C16-C17-C20	5.18	120.02	112.18
20	P	316	DMU	O5-C6-C1	5.14	120.94	110.37
14	N	602	HEA	C1B-C2B-C3B	-5.11	100.88	106.80
14	A	601	HEA	CHB-C1B-C2B	-5.11	116.96	125.03
14	N	602	HEA	C3D-C4D-ND	5.09	115.27	110.35
14	N	602	HEA	C3B-C4B-NB	5.06	115.66	109.84
20	C	316	DMU	O16-C6-C1	4.95	115.79	108.27
24	C	305	CHD	C17-C13-C14	-4.95	95.15	100.11
14	A	602	HEA	C3B-C4B-NB	4.95	115.53	109.84
14	A	601	HEA	C2D-C1D-ND	4.93	115.51	109.84
20	P	322	DMU	C10-C5-C7	4.89	120.30	110.01
14	N	601	HEA	C3B-C4B-NB	4.87	115.44	109.84
20	P	322	DMU	O16-C6-C1	4.79	115.55	108.27
20	H	101	DMU	O16-C6-C1	4.75	115.49	108.27
20	C	319	DMU	O16-C6-C1	4.75	115.49	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	N	601	HEA	C4D-C3D-C2D	-4.68	100.09	106.89
24	P	305	CHD	C16-C17-C20	4.65	119.21	112.18
20	O	304	DMU	O5-C6-C1	4.65	119.92	110.37
20	P	322	DMU	C10-O1-C9	-4.57	104.79	113.72
20	N	616	DMU	O16-C6-C1	4.52	115.14	108.27
14	N	602	HEA	CMB-C2B-C1B	4.49	132.05	125.03
14	N	602	HEA	CHB-C4A-NA	-4.41	119.65	124.45
27	T	102	PEK	O01-C1-O02	-4.39	113.44	123.70
14	A	601	HEA	CHA-C4D-C3D	-4.35	118.43	124.77
20	P	314	DMU	C18-O16-C6	-4.35	106.26	113.68
20	P	318	DMU	O16-C6-C1	4.34	114.87	108.27
20	C	316	DMU	C6-O5-C4	4.32	122.15	113.72
22	N	615	PGV	O03-C19-O04	-4.27	112.94	123.63
14	N	602	HEA	C1D-C2D-C3D	-4.24	102.52	106.98
20	Z	101	DMU	O16-C6-C1	4.21	114.66	108.27
14	A	601	HEA	C4D-C3D-C2D	-4.19	100.80	106.89
20	N	616	DMU	C10-C5-C7	4.19	118.82	110.01
18	C	304	CDL	OA4-PA1-OA5	-4.17	88.65	107.57
14	N	601	HEA	C1B-C2B-C3B	-4.17	101.97	106.80
14	N	601	HEA	C3A-C2A-C1A	-4.16	103.11	107.05
14	N	601	HEA	C3C-C2C-C1C	-4.15	102.28	107.17
20	O	304	DMU	O16-C6-C1	4.10	114.50	108.27
14	A	601	HEA	C4C-C3C-C2C	-4.07	102.23	107.30
14	A	601	HEA	C4B-NB-C1B	-4.07	100.39	105.21
18	C	304	CDL	OA6-CA5-C11	-4.07	102.68	111.48
14	A	602	HEA	C4B-NB-C1B	-3.99	100.48	105.21
14	N	601	HEA	C2C-C1C-NC	3.97	116.51	110.14
14	A	602	HEA	C3C-C2C-C1C	-3.97	102.49	107.17
14	N	601	HEA	C2A-C1A-NA	3.97	114.15	110.32
22	A	614	PGV	O03-C19-O04	-3.91	113.84	123.63
20	C	318	DMU	O5-C6-C1	3.90	118.39	110.37
18	C	304	CDL	OA5-PA1-OA3	3.90	124.40	108.94
24	C	305	CHD	C14-C13-C12	3.86	110.94	107.42
14	N	601	HEA	O11-C11-C3B	-3.84	104.21	111.26
20	P	317	DMU	O16-C6-C1	3.84	114.11	108.27
14	A	602	HEA	C2D-C1D-ND	3.83	114.24	109.84
20	N	616	DMU	C18-O16-C6	-3.81	107.17	113.68
14	A	602	HEA	CHB-C1B-C2B	-3.81	119.02	125.03
20	M	101	DMU	O16-C6-C1	3.79	114.02	108.27
18	A	606	CDL	OA6-CA4-CA3	3.78	121.91	108.34
20	C	319	DMU	C10-C5-C7	3.77	117.94	110.01
20	B	308	DMU	O16-C6-C1	3.76	113.98	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	N	601	HEA	CHB-C1B-C2B	-3.75	119.10	125.03
20	C	320	DMU	C10-C5-C7	3.72	117.84	110.01
14	A	601	HEA	CAD-C3D-C4D	3.67	131.09	124.70
14	N	601	HEA	CAD-C3D-C4D	3.61	130.98	124.70
14	N	602	HEA	CHA-C4D-C3D	-3.60	119.53	124.77
14	A	602	HEA	C1B-C2B-C3B	-3.55	102.68	106.80
18	P	304	CDL	O1-C1-CB2	3.55	121.97	109.70
24	P	305	CHD	C17-C13-C14	-3.55	96.55	100.11
14	A	602	HEA	CHA-C4D-C3D	-3.54	119.61	124.77
20	H	101	DMU	C18-O16-C6	-3.50	107.71	113.68
14	N	602	HEA	C2C-C1C-NC	3.49	115.74	110.14
20	P	317	DMU	C10-C5-C7	3.49	117.34	110.01
14	A	601	HEA	C26-C15-C16	3.44	121.20	115.23
14	A	602	HEA	C27-C19-C20	3.42	121.16	115.23
14	N	602	HEA	CHB-C1B-C2B	-3.39	119.68	125.03
14	N	602	HEA	C3C-C4C-NC	3.38	112.65	109.80
20	N	616	DMU	O5-C6-O16	3.34	117.93	110.04
14	A	601	HEA	C1D-C2D-C3D	-3.33	103.47	106.98
14	N	601	HEA	C1D-C2D-C3D	-3.32	103.49	106.98
14	A	602	HEA	CMB-C2B-C1B	3.30	130.19	125.03
22	N	615	PGV	O03-C19-C20	3.30	121.88	111.83
18	C	304	CDL	OA4-PA1-OA3	3.27	127.66	112.44
20	N	609	DMU	C10-O1-C9	3.26	120.09	113.72
14	A	602	HEA	C4A-C3A-C2A	-3.25	103.99	106.81
20	P	314	DMU	C10-C5-C7	3.24	116.84	110.01
14	A	602	HEA	C3C-C4C-NC	3.24	112.53	109.80
20	H	101	DMU	C10-C5-C7	3.20	116.75	110.01
14	A	602	HEA	C1D-C2D-C3D	-3.20	103.62	106.98
20	Q	201	DMU	C2-C3-C4	-3.19	103.87	110.93
24	P	305	CHD	C14-C13-C12	3.18	110.33	107.42
20	Z	101	DMU	O3-C5-C7	3.17	117.84	110.38
20	H	101	DMU	O5-C6-C1	3.16	116.86	110.37
14	N	601	HEA	CHA-C4D-C3D	-3.16	120.17	124.77
20	P	318	DMU	C10-C5-C7	3.14	116.62	110.01
14	A	602	HEA	CMD-C2D-C1D	3.11	129.89	125.03
14	N	602	HEA	C3C-C2C-C1C	-3.11	103.51	107.17
22	P	303	PGV	C27-C26-C25	-3.10	98.69	114.37
20	D	201	DMU	C57-C4-C3	3.07	122.00	113.38
14	N	602	HEA	C3A-C2A-C1A	-3.05	104.16	107.05
20	Y	102	DMU	O5-C6-O16	3.01	117.15	110.04
20	N	616	DMU	O3-C5-C10	3.00	117.23	110.08
20	N	616	DMU	C6-O5-C4	-2.99	107.88	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	C	316	DMU	C10-C5-C7	2.99	116.30	110.01
27	T	102	PEK	O02-C1-C2	2.98	135.44	123.78
24	P	305	CHD	C22-C23-C24	-2.96	104.60	112.49
14	N	601	HEA	CHA-C4D-ND	-2.95	121.25	124.42
14	N	602	HEA	C4B-NB-C1B	-2.95	101.71	105.21
22	C	303	PGV	O03-C19-O04	-2.95	116.25	123.63
24	P	305	CHD	C17-C13-C12	-2.89	115.06	117.67
20	P	314	DMU	C6-O5-C4	2.88	119.34	113.72
14	N	602	HEA	CMD-C2D-C1D	2.87	129.52	125.03
20	C	320	DMU	O16-C6-C1	2.86	112.61	108.27
20	Q	201	DMU	C6-O5-C4	-2.85	108.14	113.72
14	A	602	HEA	C13-C12-C11	-2.85	109.84	114.39
14	A	602	HEA	C4D-C3D-C2D	-2.84	102.75	106.89
14	A	601	HEA	C3A-C2A-C1A	-2.84	104.36	107.05
20	L	102	DMU	O5-C6-O16	2.82	116.70	110.04
14	N	601	HEA	C1D-ND-C4D	-2.82	101.87	105.21
14	N	602	HEA	C1D-ND-C4D	-2.81	101.87	105.21
27	T	102	PEK	C2-C3-C4	2.80	119.47	113.35
20	B	308	DMU	O5-C6-C1	2.80	116.12	110.37
14	N	601	HEA	C4C-C3C-C2C	-2.78	103.85	107.30
14	N	601	HEA	CHA-C1A-NA	-2.77	121.44	124.45
14	A	602	HEA	C4B-C3B-C2B	-2.76	102.80	107.44
20	P	314	DMU	O3-C5-C10	2.74	116.61	110.08
20	P	314	DMU	C2-C3-C4	-2.74	104.86	110.93
14	A	601	HEA	O11-C11-C12	2.74	116.41	109.14
20	N	616	DMU	C10-O1-C9	2.73	119.06	113.72
18	C	304	CDL	O1-C1-CB2	2.72	119.09	109.70
20	D	201	DMU	C2-C3-C4	-2.71	104.91	110.93
20	Q	201	DMU	C18-O16-C6	2.71	118.31	113.68
20	C	316	DMU	C7-C8-C9	2.70	115.13	110.23
24	C	305	CHD	C16-C17-C13	-2.70	100.92	103.54
14	A	602	HEA	C2C-C1C-NC	2.69	114.45	110.14
24	C	305	CHD	C17-C13-C12	-2.66	115.27	117.67
20	N	616	DMU	O5-C4-C57	2.65	113.01	106.44
14	A	602	HEA	C12-C11-C3B	-2.64	107.99	112.12
20	H	101	DMU	C10-O1-C9	2.62	118.83	113.72
20	C	316	DMU	C18-O16-C6	-2.61	109.22	113.68
14	A	602	HEA	CHC-C1C-C2C	-2.61	119.86	127.43
22	A	614	PGV	O03-C19-C20	2.60	119.78	111.83
14	N	601	HEA	C26-C15-C16	2.60	119.74	115.23
18	C	304	CDL	OA7-CA5-C11	2.59	133.90	123.78
14	N	602	HEA	C4A-NA-C1A	-2.58	101.61	105.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	P	322	DMU	O1-C9-C8	-2.58	105.05	109.70
14	N	602	HEA	CBD-CAD-C3D	2.58	119.66	112.53
18	A	606	CDL	OA6-CA5-OA7	2.57	129.72	123.70
20	O	304	DMU	C6-C1-C2	2.57	115.42	110.01
14	N	601	HEA	C4B-C3B-C2B	-2.56	103.14	107.44
20	P	314	DMU	O5-C6-O16	-2.55	104.01	110.04
20	A	609	DMU	O16-C6-C1	2.55	112.14	108.27
22	N	615	PGV	O01-C1-O02	-2.54	117.77	123.70
20	C	318	DMU	C18-O16-C6	-2.54	109.34	113.68
20	C	316	DMU	O5-C6-C1	2.54	115.58	110.37
20	C	316	DMU	O7-C3-C2	2.54	113.68	107.23
20	C	324	DMU	C10-C5-C7	2.54	115.34	110.01
20	P	322	DMU	O7-C10-O1	-2.53	104.03	110.69
20	B	308	DMU	C3-C2-C1	-2.53	106.39	110.83
14	N	602	HEA	CAD-CBD-CGD	-2.51	107.00	113.67
14	N	602	HEA	C27-C19-C20	2.51	119.58	115.23
18	C	304	CDL	OB5-PB2-OB3	2.51	118.88	108.94
18	P	304	CDL	OB5-PB2-OB3	2.50	118.83	108.94
20	A	609	DMU	C18-O16-C6	2.49	117.94	113.68
18	V	101	CDL	OA6-CA4-CA6	-2.49	99.42	108.34
20	M	101	DMU	O3-C5-C7	2.48	116.22	110.38
20	P	316	DMU	C18-O16-C6	-2.48	109.45	113.68
20	B	308	DMU	O5-C6-O16	2.47	115.87	110.04
20	P	316	DMU	C6-C1-C2	2.47	115.20	110.01
20	Y	102	DMU	O5-C6-C1	2.47	115.44	110.37
20	T	105	DMU	C57-C4-C3	-2.46	106.97	113.02
20	C	316	DMU	O1-C9-C8	2.46	114.13	109.70
14	N	602	HEA	CAD-C3D-C4D	2.46	128.98	124.70
18	P	304	CDL	OA5-PA1-OA3	2.44	118.59	108.94
22	C	303	PGV	C24-C23-C22	2.44	126.69	114.37
14	A	601	HEA	CMB-C2B-C1B	2.43	128.84	125.03
14	A	601	HEA	C13-C14-C15	-2.43	122.07	127.62
14	A	601	HEA	C1D-ND-C4D	-2.42	102.34	105.21
14	N	602	HEA	CMC-C2C-C1C	2.42	129.10	125.42
22	C	303	PGV	C23-C22-C21	2.41	126.57	114.37
20	O	308	DMU	O5-C6-C1	2.41	115.32	110.37
20	N	609	DMU	O5-C6-C1	2.40	115.29	110.37
22	P	303	PGV	C22-C21-C20	-2.38	104.37	113.13
14	A	602	HEA	CBD-CAD-C3D	2.38	119.12	112.53
20	O	308	DMU	C57-C4-C3	-2.37	107.20	113.02
18	L	101	CDL	OB4-PB2-OB2	2.37	118.29	107.57
20	D	201	DMU	C10-C5-C7	2.36	114.98	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	N	602	HEA	C25-C23-C22	-2.36	115.57	122.66
20	B	308	DMU	C6-O5-C4	2.36	118.33	113.72
14	A	601	HEA	CHD-C1D-C2D	-2.35	120.26	126.95
14	N	601	HEA	CHC-C4B-C3B	-2.33	119.91	125.80
24	C	305	CHD	C18-C13-C17	2.33	114.86	111.20
14	N	602	HEA	CHC-C1C-C2C	-2.33	120.68	127.43
20	P	314	DMU	O5-C6-C1	2.32	115.15	110.37
20	A	609	DMU	O3-C5-C7	2.32	115.85	110.38
14	N	602	HEA	O11-C11-C12	2.30	115.23	109.14
20	G	103	DMU	O5-C6-O16	2.29	115.47	110.04
20	B	304	DMU	O5-C6-C1	2.29	115.08	110.37
14	N	601	HEA	C4C-NC-C1C	-2.29	102.09	105.82
14	N	601	HEA	C4B-NB-C1B	-2.29	102.50	105.21
14	A	602	HEA	C3A-C2A-C1A	-2.29	104.88	107.05
14	A	602	HEA	CHB-C4A-C3A	-2.29	121.36	125.21
18	V	101	CDL	OA6-CA5-C11	2.28	116.41	111.48
20	P	317	DMU	O3-C5-C10	2.28	115.50	110.08
14	N	602	HEA	CHD-C1D-C2D	-2.28	120.47	126.95
14	N	602	HEA	C2A-C1A-NA	2.28	112.52	110.32
20	Q	201	DMU	O7-C3-C2	2.27	113.00	107.23
20	A	609	DMU	C10-C5-C7	2.27	114.78	110.01
20	C	318	DMU	C6-C1-C2	2.26	114.76	110.01
14	N	602	HEA	C20-C19-C18	-2.26	116.10	121.17
24	O	301	CHD	C11-C9-C10	-2.25	111.42	113.70
20	P	318	DMU	C10-O1-C9	-2.24	109.34	113.72
20	D	201	DMU	O5-C4-C3	-2.24	105.09	109.72
18	L	101	CDL	OA6-CA5-C11	2.24	116.32	111.48
14	A	601	HEA	CMD-C2D-C1D	2.23	128.52	125.03
20	G	103	DMU	O16-C6-C1	2.23	111.66	108.27
20	C	319	DMU	C6-O5-C4	2.22	118.06	113.72
20	C	316	DMU	O4-C7-C8	-2.22	105.14	110.38
20	C	320	DMU	O3-C5-C10	2.22	115.36	110.08
14	A	602	HEA	CHD-C1D-C2D	-2.21	120.66	126.95
20	O	304	DMU	C6-O5-C4	2.21	118.03	113.72
14	A	601	HEA	CHC-C4B-NB	-2.21	121.63	124.37
20	Q	201	DMU	C10-C5-C7	2.20	114.65	110.01
20	Z	101	DMU	O5-C6-C1	2.20	114.90	110.37
27	G	101	PEK	O04-C21-C22	2.20	132.39	123.78
20	H	101	DMU	O3-C5-C7	2.20	115.56	110.38
20	T	105	DMU	C2-C3-C4	2.19	114.20	110.23
20	C	320	DMU	O5-C6-C1	2.18	114.85	110.37
20	C	319	DMU	C10-O1-C9	-2.18	109.47	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	N	616	DMU	C10-O7-C3	-2.17	112.83	117.98
14	N	601	HEA	CMD-C2D-C1D	2.17	128.42	125.03
20	C	320	DMU	O3-C5-C7	2.17	115.49	110.38
18	A	606	CDL	OA6-CA4-CA6	2.16	116.09	108.34
20	P	322	DMU	C7-C8-C9	-2.16	106.32	110.23
20	C	324	DMU	O5-C6-C1	2.16	114.80	110.37
18	P	304	CDL	OA4-PA1-OA3	2.16	122.47	112.44
14	N	602	HEA	C4D-C3D-C2D	-2.14	103.78	106.89
20	L	102	DMU	O5-C6-C1	2.14	114.76	110.37
14	N	602	HEA	C13-C12-C11	-2.13	110.99	114.39
20	C	316	DMU	C10-O1-C9	2.12	117.87	113.72
18	Y	101	CDL	OA6-CA5-C11	2.12	116.07	111.48
20	C	320	DMU	O5-C6-O16	2.11	115.03	110.04
20	D	201	DMU	C11-C9-C8	-2.11	107.84	113.02
20	O	308	DMU	O5-C6-O16	2.11	115.02	110.04
20	P	314	DMU	O7-C3-C2	2.10	112.58	107.23
20	M	101	DMU	C10-C5-C7	2.10	114.42	110.01
20	C	324	DMU	O3-C5-C10	2.10	115.07	110.08
20	C	316	DMU	O3-C5-C10	2.09	115.05	110.08
20	A	609	DMU	C10-O7-C3	-2.08	113.05	117.98
20	L	102	DMU	C3-C2-C1	-2.07	107.20	110.83
14	N	601	HEA	CHD-C1D-C2D	-2.06	121.08	126.95
14	A	602	HEA	C20-C19-C18	-2.06	116.54	121.17
20	C	316	DMU	O5-C4-C3	2.05	113.97	109.72
18	C	304	CDL	OB6-CB5-C51	2.04	115.88	111.48
20	Y	102	DMU	O16-C6-C1	-2.02	105.20	108.27
24	C	305	CHD	O25-C24-C23	-2.02	116.67	123.09
14	A	602	HEA	O11-C11-C12	2.02	114.50	109.14
22	C	303	PGV	C25-C24-C23	2.02	124.57	114.37
22	A	614	PGV	C15-C14-C13	-2.02	104.16	113.86
18	C	304	CDL	OB4-PB2-OB3	2.01	121.82	112.44
14	A	601	HEA	C2C-C1C-NC	2.01	113.36	110.14
20	T	105	DMU	O5-C6-O16	2.00	114.78	110.04
20	C	320	DMU	O5-C4-C57	2.00	111.40	106.44
20	P	317	DMU	C6-C1-C2	2.00	114.22	110.01

There are no chirality outliers.

All (790) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	606	CDL	C1-CA2-OA2-PA1
18	A	606	CDL	CA3-OA5-PA1-OA2

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Mol	Chain	Res	Type	Atoms
18	A	606	CDL	CA3-OA5-PA1-OA3
18	A	606	CDL	CA3-OA5-PA1-OA4
18	A	606	CDL	OA6-CA4-CA6-OA8
18	A	606	CDL	CB2-OB2-PB2-OB3
18	A	606	CDL	CB2-OB2-PB2-OB5
18	A	606	CDL	CB3-OB5-PB2-OB2
18	A	606	CDL	CB3-OB5-PB2-OB3
18	A	606	CDL	CB3-OB5-PB2-OB4
18	A	606	CDL	C51-CB5-OB6-CB4
18	C	304	CDL	O1-C1-CB2-OB2
18	C	304	CDL	C1-CA2-OA2-PA1
18	C	304	CDL	CA3-OA5-PA1-OA2
18	C	304	CDL	CA3-OA5-PA1-OA3
18	C	304	CDL	C11-CA5-OA6-CA4
18	C	304	CDL	CB3-OB5-PB2-OB4
18	C	304	CDL	OB7-CB5-OB6-CB4
18	C	304	CDL	C51-CB5-OB6-CB4
18	L	101	CDL	CB2-C1-CA2-OA2
18	L	101	CDL	CA2-OA2-PA1-OA3
18	L	101	CDL	CA3-OA5-PA1-OA2
18	L	101	CDL	CA3-OA5-PA1-OA3
18	L	101	CDL	CA3-OA5-PA1-OA4
18	L	101	CDL	C11-CA5-OA6-CA4
18	L	101	CDL	CB2-OB2-PB2-OB3
18	L	101	CDL	CB2-OB2-PB2-OB5
18	L	101	CDL	C51-CB5-OB6-CB4
18	P	304	CDL	C1-CA2-OA2-PA1
18	P	304	CDL	CA2-OA2-PA1-OA3
18	P	304	CDL	CA2-OA2-PA1-OA5
18	P	304	CDL	CA3-OA5-PA1-OA2
18	P	304	CDL	CA3-OA5-PA1-OA3
18	P	304	CDL	CB3-OB5-PB2-OB4
18	P	304	CDL	C51-CB5-OB6-CB4
18	V	101	CDL	CA3-OA5-PA1-OA2
18	V	101	CDL	CA3-OA5-PA1-OA4
18	V	101	CDL	C11-CA5-OA6-CA4
18	V	101	CDL	CB2-OB2-PB2-OB3
18	V	101	CDL	CB2-OB2-PB2-OB5
18	V	101	CDL	CB3-OB5-PB2-OB2
18	V	101	CDL	CB3-OB5-PB2-OB3
18	V	101	CDL	CB3-OB5-PB2-OB4
18	V	101	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
18	Y	101	CDL	CA2-OA2-PA1-OA3
18	Y	101	CDL	CA2-OA2-PA1-OA5
18	Y	101	CDL	CB2-OB2-PB2-OB3
18	Y	101	CDL	CB2-OB2-PB2-OB4
18	Y	101	CDL	CB2-OB2-PB2-OB5
18	Y	101	CDL	CB3-OB5-PB2-OB3
18	Y	101	CDL	CB3-OB5-PB2-OB4
18	Y	101	CDL	C51-CB5-OB6-CB4
20	B	308	DMU	O5-C6-O16-C18
20	B	308	DMU	C19-C18-O16-C6
20	C	319	DMU	C19-C18-O16-C6
20	D	201	DMU	C19-C18-O16-C6
20	L	102	DMU	C1-C6-O16-C18
20	O	308	DMU	C19-C18-O16-C6
20	Q	201	DMU	O5-C6-O16-C18
20	Y	102	DMU	C1-C6-O16-C18
20	Y	102	DMU	C19-C18-O16-C6
24	C	305	CHD	C13-C17-C20-C21
24	C	305	CHD	C13-C17-C20-C22
24	C	305	CHD	C16-C17-C20-C21
24	P	305	CHD	C13-C17-C20-C21
24	P	305	CHD	C13-C17-C20-C22
24	P	305	CHD	C16-C17-C20-C22
27	G	101	PEK	C12-C13-C14-C15
27	T	102	PEK	C12-C13-C14-C15
24	P	305	CHD	C16-C17-C20-C21
24	C	305	CHD	C16-C17-C20-C22
18	A	606	CDL	OB7-CB5-OB6-CB4
18	C	304	CDL	OA7-CA5-OA6-CA4
18	L	101	CDL	OA7-CA5-OA6-CA4
18	L	101	CDL	OB7-CB5-OB6-CB4
18	P	304	CDL	OA7-CA5-OA6-CA4
18	P	304	CDL	OB7-CB5-OB6-CB4
18	V	101	CDL	OA7-CA5-OA6-CA4
18	V	101	CDL	OB7-CB5-OB6-CB4
18	Y	101	CDL	OB7-CB5-OB6-CB4
18	P	304	CDL	C11-CA5-OA6-CA4
20	L	102	DMU	C3-C4-C57-O61
20	O	304	DMU	O5-C4-C57-O61
20	C	318	DMU	O5-C4-C57-O61
18	V	101	CDL	OA9-CA7-OA8-CA6
20	C	316	DMU	O6-C11-C9-O1

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Mol	Chain	Res	Type	Atoms
20	P	316	DMU	O5-C4-C57-O61
20	B	308	DMU	C3-C4-C57-O61
22	C	303	PGV	C28-C29-C30-C31
18	A	606	CDL	O1-C1-CB2-OB2
18	P	304	CDL	O1-C1-CB2-OB2
18	V	101	CDL	C31-CA7-OA8-CA6
20	A	609	DMU	O6-C11-C9-C8
20	C	318	DMU	C3-C4-C57-O61
20	N	609	DMU	O6-C11-C9-C8
18	Y	101	CDL	C11-CA5-OA6-CA4
20	A	609	DMU	O6-C11-C9-O1
20	N	609	DMU	O6-C11-C9-O1
20	Z	101	DMU	O6-C11-C9-O1
20	C	320	DMU	O6-C11-C9-O1
20	O	304	DMU	C3-C4-C57-O61
20	D	201	DMU	O6-C11-C9-O1
20	P	318	DMU	O6-C11-C9-O1
20	Y	102	DMU	O5-C4-C57-O61
20	B	304	DMU	O5-C6-O16-C18
20	Y	102	DMU	O5-C6-O16-C18
20	C	319	DMU	O6-C11-C9-O1
18	Y	101	CDL	C31-CA7-OA8-CA6
19	C	325	LFA	C9-C10-C11-C12
20	L	102	DMU	O5-C4-C57-O61
18	Y	101	CDL	OA9-CA7-OA8-CA6
20	B	308	DMU	O5-C4-C57-O61
19	P	307	LFA	C7-C8-C9-C10
20	C	316	DMU	O6-C11-C9-C8
18	Y	101	CDL	OA7-CA5-OA6-CA4
18	A	606	CDL	CA2-C1-CB2-OB2
18	P	304	CDL	CA2-C1-CB2-OB2
18	C	304	CDL	C31-CA7-OA8-CA6
22	A	614	PGV	C26-C27-C28-C29
20	P	316	DMU	C3-C4-C57-O61
19	C	309	LFA	C11-C10-C9-C8
19	C	309	LFA	C12-C13-C14-C15
20	C	320	DMU	O5-C4-C57-O61
20	D	201	DMU	O6-C11-C9-C8
20	Z	101	DMU	O6-C11-C9-C8
20	B	304	DMU	C1-C6-O16-C18
20	C	319	DMU	C1-C6-O16-C18
20	N	616	DMU	C1-C6-O16-C18

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Mol	Chain	Res	Type	Atoms
20	T	105	DMU	C1-C6-O16-C18
18	C	304	CDL	O1-C1-CA2-OA2
18	L	101	CDL	O1-C1-CA2-OA2
20	C	319	DMU	C3-C4-C57-O61
18	C	304	CDL	OA9-CA7-OA8-CA6
20	C	324	DMU	O6-C11-C9-O1
20	G	103	DMU	O5-C4-C57-O61
18	P	304	CDL	C31-CA7-OA8-CA6
20	P	318	DMU	C2-C3-O7-C10
20	P	317	DMU	O5-C4-C57-O61
20	C	320	DMU	O6-C11-C9-C8
18	A	606	CDL	CA5-C11-C12-C13
20	P	318	DMU	C4-C3-O7-C10
22	N	615	PGV	C26-C27-C28-C29
20	G	103	DMU	C3-C4-C57-O61
19	T	101	LFA	C9-C10-C11-C12
20	C	318	DMU	O16-C18-C19-C22
20	D	201	DMU	O16-C18-C19-C22
18	C	304	CDL	CA7-C31-C32-C33
18	Y	101	CDL	CA5-C11-C12-C13
20	P	317	DMU	C3-C4-C57-O61
20	Y	102	DMU	O16-C18-C19-C22
18	C	304	CDL	CB5-C51-C52-C53
18	C	304	CDL	CB7-C71-C72-C73
18	L	101	CDL	CB7-C71-C72-C73
20	C	320	DMU	O16-C18-C19-C22
20	L	102	DMU	O16-C18-C19-C22
18	P	304	CDL	CB5-C51-C52-C53
18	V	101	CDL	CA5-C11-C12-C13
18	V	101	CDL	CA7-C31-C32-C33
20	T	105	DMU	O5-C6-O16-C18
19	O	302	LFA	C5-C6-C7-C8
19	O	302	LFA	C7-C8-C9-C10
18	P	304	CDL	O1-C1-CA2-OA2
18	V	101	CDL	O1-C1-CB2-OB2
18	Y	101	CDL	O1-C1-CA2-OA2
20	P	322	DMU	C4-C3-O7-C10
20	G	103	DMU	O16-C18-C19-C22
20	P	317	DMU	O16-C18-C19-C22
27	T	102	PEK	C7-C8-C9-C10
18	C	304	CDL	C71-CB7-OB8-CB6
18	A	606	CDL	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
18	P	304	CDL	CB7-C71-C72-C73
18	V	101	CDL	CA2-C1-CB2-OB2
18	Y	101	CDL	CB2-C1-CA2-OA2
20	C	320	DMU	C1-C6-O16-C18
20	P	317	DMU	C1-C6-O16-C18
18	V	101	CDL	C1-CA2-OA2-PA1
20	C	319	DMU	O5-C4-C57-O61
18	P	304	CDL	OA9-CA7-OA8-CA6
20	C	319	DMU	O6-C11-C9-C8
18	C	304	CDL	OB9-CB7-OB8-CB6
20	C	319	DMU	O5-C6-O16-C18
20	L	102	DMU	O5-C6-O16-C18
18	L	101	CDL	C72-C73-C74-C75
18	L	101	CDL	OB6-CB4-CB6-OB8
20	P	317	DMU	O6-C11-C9-O1
20	G	103	DMU	C25-C28-C31-C34
20	N	609	DMU	C31-C34-C37-C40
18	A	606	CDL	C19-C20-C21-C22
18	A	606	CDL	C78-C79-C80-C81
18	Y	101	CDL	C63-C64-C65-C66
19	N	607	LFA	C5-C6-C7-C8
18	V	101	CDL	C78-C79-C80-C81
18	Y	101	CDL	C13-C14-C15-C16
18	P	304	CDL	C11-C12-C13-C14
20	C	318	DMU	C31-C34-C37-C40
20	C	319	DMU	C31-C34-C37-C40
22	C	303	PGV	C22-C23-C24-C25
18	A	606	CDL	OA7-CA5-OA6-CA4
20	L	102	DMU	C19-C18-O16-C6
20	Q	201	DMU	C19-C18-O16-C6
20	C	320	DMU	C3-C4-C57-O61
19	B	307	LFA	C13-C14-C15-C16
19	N	607	LFA	C11-C10-C9-C8
20	Z	101	DMU	C22-C25-C28-C31
20	A	615	DMU	C19-C22-C25-C28
22	A	614	PGV	C14-C15-C16-C17
27	T	102	PEK	C26-C27-C28-C29
20	J	101	DMU	C25-C28-C31-C34
20	P	322	DMU	C2-C3-O7-C10
20	Y	102	DMU	C18-C19-C22-C25
18	C	304	CDL	C35-C36-C37-C38
18	V	101	CDL	C74-C75-C76-C77

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Mol	Chain	Res	Type	Atoms
20	L	102	DMU	C22-C25-C28-C31
20	P	318	DMU	O6-C11-C9-C8
19	O	302	LFA	C13-C14-C15-C16
22	C	303	PGV	C30-C31-C32-C33
20	B	303	DMU	C18-C19-C22-C25
19	C	325	LFA	C7-C8-C9-C10
20	T	105	DMU	O16-C18-C19-C22
20	O	307	DMU	C18-C19-C22-C25
19	P	310	LFA	C6-C7-C8-C9
18	C	304	CDL	C72-C73-C74-C75
18	V	101	CDL	C31-C32-C33-C34
19	C	309	LFA	C5-C6-C7-C8
19	C	310	LFA	C6-C7-C8-C9
18	P	304	CDL	C52-C53-C54-C55
19	P	309	LFA	C13-C14-C15-C16
20	C	316	DMU	C28-C31-C34-C37
20	P	314	DMU	C28-C31-C34-C37
18	L	101	CDL	C37-C38-C39-C40
18	L	101	CDL	C80-C81-C82-C83
18	Y	101	CDL	C71-C72-C73-C74
19	P	309	LFA	C4-C5-C6-C7
19	T	101	LFA	C5-C6-C7-C8
22	C	303	PGV	C7-C8-C9-C10
20	Q	201	DMU	O5-C4-C57-O61
20	C	317	DMU	C28-C31-C34-C37
21	P	319	EDO	O1-C1-C2-O2
20	M	101	DMU	C22-C25-C28-C31
18	P	304	CDL	C56-C57-C58-C59
19	O	303	LFA	C5-C6-C7-C8
18	C	304	CDL	C22-C23-C24-C25
18	C	304	CDL	C75-C76-C77-C78
18	L	101	CDL	C34-C35-C36-C37
18	L	101	CDL	C14-C15-C16-C17
19	B	307	LFA	C9-C10-C11-C12
19	C	310	LFA	C10-C11-C12-C13
20	A	608	DMU	C28-C31-C34-C37
20	C	320	DMU	C19-C22-C25-C28
18	P	304	CDL	C35-C36-C37-C38
19	P	309	LFA	C3-C4-C5-C6
19	P	311	LFA	C1-C2-C3-C4
20	C	316	DMU	C19-C22-C25-C28
20	M	102	DMU	C31-C34-C37-C40

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Mol	Chain	Res	Type	Atoms
19	C	307	LFA	C4-C5-C6-C7
20	P	318	DMU	C22-C25-C28-C31
22	C	303	PGV	C14-C15-C16-C17
19	C	313	LFA	C1-C2-C3-C4
19	P	309	LFA	C5-C6-C7-C8
27	G	101	PEK	C28-C29-C30-C31
19	T	103	LFA	C10-C11-C12-C13
20	A	609	DMU	C31-C34-C37-C40
22	C	303	PGV	C25-C26-C27-C28
22	P	303	PGV	C7-C8-C9-C10
20	N	616	DMU	O5-C6-O16-C18
20	P	317	DMU	C28-C31-C34-C37
22	A	614	PGV	C29-C30-C31-C32
27	T	102	PEK	C17-C18-C19-C20
20	N	616	DMU	C18-C19-C22-C25
18	V	101	CDL	C17-C18-C19-C20
19	C	312	LFA	C4-C5-C6-C7
19	P	310	LFA	C7-C8-C9-C10
20	C	319	DMU	O16-C18-C19-C22
18	A	606	CDL	C11-CA5-OA6-CA4
22	C	303	PGV	C13-C14-C15-C16
20	B	303	DMU	C19-C22-C25-C28
20	C	319	DMU	C19-C22-C25-C28
22	A	614	PGV	C11-C10-C9-C8
20	C	318	DMU	C28-C31-C34-C37
20	O	308	DMU	C34-C37-C40-C43
22	N	615	PGV	C27-C28-C29-C30
18	L	101	CDL	C13-C14-C15-C16
22	N	615	PGV	C14-C15-C16-C17
20	P	316	DMU	C31-C34-C37-C40
20	B	304	DMU	C18-C19-C22-C25
20	O	306	DMU	C18-C19-C22-C25
20	P	316	DMU	C18-C19-C22-C25
19	C	312	LFA	C10-C11-C12-C13
20	B	302	DMU	C18-C19-C22-C25
27	T	102	PEK	C1-C2-C3-C4
18	V	101	CDL	C77-C78-C79-C80
24	C	305	CHD	C21-C20-C22-C23
20	P	315	DMU	C28-C31-C34-C37
18	A	606	CDL	C17-C18-C19-C20
20	Q	201	DMU	C4-C3-O7-C10
18	V	101	CDL	C73-C74-C75-C76

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Mol	Chain	Res	Type	Atoms
19	T	104	LFA	C6-C7-C8-C9
20	A	609	DMU	C3-C4-C57-O61
19	C	309	LFA	C3-C4-C5-C6
18	Y	101	CDL	OB6-CB4-CB6-OB8
22	P	303	PGV	C12-C13-C14-C15
19	P	312	LFA	C2-C3-C4-C5
19	T	103	LFA	C3-C4-C5-C6
20	C	324	DMU	O6-C11-C9-C8
19	C	325	LFA	C6-C7-C8-C9
20	G	103	DMU	C28-C31-C34-C37
22	A	614	PGV	C30-C31-C32-C33
20	D	201	DMU	C4-C3-O7-C10
22	P	303	PGV	C11-C12-C13-C14
20	B	302	DMU	C19-C22-C25-C28
20	Y	102	DMU	C3-C4-C57-O61
20	A	615	DMU	O16-C18-C19-C22
18	C	304	CDL	C71-C72-C73-C74
18	L	101	CDL	C17-C18-C19-C20
19	C	311	LFA	C7-C8-C9-C10
27	G	101	PEK	C26-C27-C28-C29
20	P	314	DMU	O6-C11-C9-O1
19	B	307	LFA	C4-C5-C6-C7
27	G	101	PEK	C16-C17-C18-C19
20	P	315	DMU	C31-C34-C37-C40
18	P	304	CDL	C73-C74-C75-C76
19	O	303	LFA	C2-C3-C4-C5
20	Y	102	DMU	C31-C34-C37-C40
18	A	606	CDL	C75-C76-C77-C78
19	N	606	LFA	C10-C11-C12-C13
20	B	303	DMU	O16-C18-C19-C22
20	O	307	DMU	O16-C18-C19-C22
20	W	101	DMU	O16-C18-C19-C22
19	P	309	LFA	C11-C10-C9-C8
20	H	101	DMU	C19-C22-C25-C28
19	T	104	LFA	C3-C4-C5-C6
20	Z	101	DMU	C25-C28-C31-C34
27	T	102	PEK	C32-C33-C34-C35
18	Y	101	CDL	C21-C22-C23-C24
18	Y	101	CDL	C61-C62-C63-C64
20	L	102	DMU	C31-C34-C37-C40
18	Y	101	CDL	C19-C20-C21-C22
18	A	606	CDL	CA3-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
18	L	101	CDL	CB3-CB4-CB6-OB8
18	P	304	CDL	CB3-CB4-CB6-OB8
27	T	102	PEK	C2-C3-C4-C5
20	D	201	DMU	C19-C22-C25-C28
18	L	101	CDL	C31-CA7-OA8-CA6
20	P	306	DMU	O16-C18-C19-C22
20	H	101	DMU	O5-C4-C57-O61
20	N	616	DMU	O5-C4-C57-O61
19	N	606	LFA	C6-C7-C8-C9
19	P	312	LFA	C5-C6-C7-C8
20	M	101	DMU	C19-C22-C25-C28
20	P	318	DMU	C25-C28-C31-C34
19	C	309	LFA	C2-C3-C4-C5
20	B	304	DMU	C31-C34-C37-C40
18	C	304	CDL	CA4-CA3-OA5-PA1
18	C	304	CDL	C55-C56-C57-C58
22	A	614	PGV	C28-C29-C30-C31
20	H	101	DMU	C28-C31-C34-C37
20	C	316	DMU	O5-C4-C57-O61
20	C	318	DMU	C25-C28-C31-C34
20	P	316	DMU	C22-C25-C28-C31
18	Y	101	CDL	CB5-C51-C52-C53
18	P	304	CDL	C72-C73-C74-C75
19	B	307	LFA	C7-C8-C9-C10
18	V	101	CDL	C72-C73-C74-C75
19	C	309	LFA	C11-C12-C13-C14
19	C	310	LFA	C9-C10-C11-C12
27	G	101	PEK	C15-C16-C17-C18
20	Y	102	DMU	C25-C28-C31-C34
27	G	101	PEK	C13-C14-C15-C16
19	O	302	LFA	C9-C10-C11-C12
20	C	316	DMU	C34-C37-C40-C43
18	L	101	CDL	CB5-C51-C52-C53
20	N	616	DMU	C19-C22-C25-C28
27	G	101	PEK	C25-C26-C27-C28
18	P	304	CDL	C57-C58-C59-C60
19	C	311	LFA	C3-C4-C5-C6
18	Y	101	CDL	C14-C15-C16-C17
18	Y	101	CDL	C32-C33-C34-C35
19	C	307	LFA	C2-C3-C4-C5
19	C	313	LFA	C5-C6-C7-C8
19	C	325	LFA	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
20	P	322	DMU	C25-C28-C31-C34
18	Y	101	CDL	C84-C85-C86-C87
19	B	307	LFA	C1-C2-C3-C4
19	O	302	LFA	C14-C15-C16-C17
20	P	317	DMU	C34-C37-C40-C43
20	N	609	DMU	O16-C18-C19-C22
18	L	101	CDL	C76-C77-C78-C79
19	P	311	LFA	C3-C4-C5-C6
20	O	307	DMU	C19-C22-C25-C28
20	B	308	DMU	C18-C19-C22-C25
20	C	320	DMU	C18-C19-C22-C25
20	C	319	DMU	C34-C37-C40-C43
18	P	304	CDL	C53-C54-C55-C56
18	Y	101	CDL	C57-C58-C59-C60
20	D	201	DMU	C2-C3-O7-C10
20	P	317	DMU	C2-C3-O7-C10
18	Y	101	CDL	C64-C65-C66-C67
18	C	304	CDL	C74-C75-C76-C77
18	L	101	CDL	C58-C59-C60-C61
20	P	316	DMU	C28-C31-C34-C37
19	C	311	LFA	C11-C10-C9-C8
20	A	608	DMU	C25-C28-C31-C34
20	P	317	DMU	C4-C3-O7-C10
20	G	102	DMU	O16-C18-C19-C22
19	A	607	LFA	C9-C10-C11-C12
20	C	317	DMU	C31-C34-C37-C40
20	B	308	DMU	C34-C37-C40-C43
20	C	318	DMU	C19-C22-C25-C28
18	L	101	CDL	C15-C16-C17-C18
22	N	615	PGV	C30-C31-C32-C33
18	V	101	CDL	C20-C21-C22-C23
19	P	307	LFA	C11-C10-C9-C8
18	C	304	CDL	C23-C24-C25-C26
20	Z	101	DMU	C28-C31-C34-C37
18	P	304	CDL	C54-C55-C56-C57
20	C	320	DMU	C34-C37-C40-C43
27	T	102	PEK	C4-C5-C6-C7
18	V	101	CDL	C13-C14-C15-C16
14	A	602	HEA	C4D-C3D-CAD-CBD
20	L	102	DMU	C34-C37-C40-C43
19	O	302	LFA	C11-C12-C13-C14
22	N	615	PGV	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
18	P	304	CDL	C75-C76-C77-C78
20	Q	201	DMU	C2-C3-O7-C10
20	C	318	DMU	C22-C25-C28-C31
18	A	606	CDL	C31-CA7-OA8-CA6
22	N	615	PGV	C12-C13-C14-C15
19	B	307	LFA	C14-C15-C16-C17
20	T	105	DMU	C34-C37-C40-C43
20	N	616	DMU	C22-C25-C28-C31
20	P	314	DMU	C19-C22-C25-C28
20	P	317	DMU	O1-C10-O7-C3
20	H	101	DMU	C1-C6-O16-C18
18	P	304	CDL	C13-C14-C15-C16
20	B	304	DMU	C34-C37-C40-C43
19	C	310	LFA	C4-C5-C6-C7
19	P	309	LFA	C14-C15-C16-C17
27	G	101	PEK	C29-C30-C31-C32
27	T	102	PEK	C30-C31-C32-C33
20	Z	101	DMU	C34-C37-C40-C43
18	Y	101	CDL	C79-C80-C81-C82
20	M	102	DMU	C34-C37-C40-C43
18	L	101	CDL	OA9-CA7-OA8-CA6
20	P	314	DMU	C18-C19-C22-C25
19	C	325	LFA	C12-C13-C14-C15
18	C	304	CDL	C20-C21-C22-C23
19	P	307	LFA	C3-C4-C5-C6
20	M	102	DMU	C22-C25-C28-C31
20	Y	102	DMU	C34-C37-C40-C43
20	L	102	DMU	C25-C28-C31-C34
18	Y	101	CDL	C51-C52-C53-C54
18	L	101	CDL	C51-C52-C53-C54
18	Y	101	CDL	C59-C60-C61-C62
19	N	606	LFA	C7-C8-C9-C10
20	O	306	DMU	C25-C28-C31-C34
18	C	304	CDL	CB3-CB4-CB6-OB8
18	Y	101	CDL	CB3-CB4-CB6-OB8
19	C	313	LFA	C11-C10-C9-C8
19	P	310	LFA	C11-C10-C9-C8
18	P	304	CDL	C17-C18-C19-C20
18	P	304	CDL	C21-C22-C23-C24
19	T	104	LFA	C7-C8-C9-C10
20	W	101	DMU	C34-C37-C40-C43
19	C	314	LFA	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
18	Y	101	CDL	OA5-CA3-CA4-OA6
20	G	102	DMU	C34-C37-C40-C43
22	N	615	PGV	C11-C10-C9-C8
19	T	103	LFA	C4-C5-C6-C7
20	P	322	DMU	O16-C18-C19-C22
19	T	103	LFA	C5-C6-C7-C8
18	C	304	CDL	C12-C11-CA5-OA6
20	Z	101	DMU	O16-C18-C19-C22
27	G	101	PEK	C9-C10-C11-C12
27	T	102	PEK	C11-C10-C9-C8
27	T	102	PEK	C11-C12-C13-C14
20	M	102	DMU	C25-C28-C31-C34
22	P	303	PGV	C30-C31-C32-C33
18	C	304	CDL	C16-C17-C18-C19
18	C	304	CDL	C58-C59-C60-C61
18	V	101	CDL	C12-C13-C14-C15
20	P	317	DMU	C18-C19-C22-C25
20	O	306	DMU	C19-C22-C25-C28
20	N	608	DMU	C34-C37-C40-C43
20	A	615	DMU	C25-C28-C31-C34
20	P	316	DMU	C19-C22-C25-C28
18	Y	101	CDL	C74-C75-C76-C77
19	P	312	LFA	C6-C7-C8-C9
20	B	308	DMU	C31-C34-C37-C40
14	A	602	HEA	C2D-C3D-CAD-CBD
18	A	606	CDL	C32-C33-C34-C35
18	V	101	CDL	C79-C80-C81-C82
20	C	319	DMU	C2-C3-O7-C10
18	C	304	CDL	C59-C60-C61-C62
19	C	311	LFA	C6-C7-C8-C9
18	Y	101	CDL	C58-C59-C60-C61
20	C	316	DMU	C4-C3-O7-C10
24	P	305	CHD	C21-C20-C22-C23
20	C	306	DMU	C28-C31-C34-C37
18	V	101	CDL	OA5-CA3-CA4-CA6
22	C	303	PGV	C02-C03-O11-P
18	L	101	CDL	C59-C60-C61-C62
18	L	101	CDL	C74-C75-C76-C77
20	M	101	DMU	C25-C28-C31-C34
18	L	101	CDL	C57-C58-C59-C60
19	C	311	LFA	C4-C5-C6-C7
18	L	101	CDL	C84-C85-C86-C87

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Mol	Chain	Res	Type	Atoms
20	P	306	DMU	C31-C34-C37-C40
19	P	312	LFA	C9-C10-C11-C12
20	B	308	DMU	C25-C28-C31-C34
20	H	101	DMU	O6-C11-C9-O1
20	H	101	DMU	C18-C19-C22-C25
19	P	310	LFA	C2-C3-C4-C5
19	P	309	LFA	C1-C2-C3-C4
18	C	304	CDL	C33-C34-C35-C36
19	P	313	LFA	C6-C7-C8-C9
18	V	101	CDL	OA5-CA3-CA4-OA6
20	C	316	DMU	C2-C3-O7-C10
22	P	303	PGV	C24-C25-C26-C27
19	B	307	LFA	C11-C12-C13-C14
22	P	303	PGV	C27-C28-C29-C30
20	T	105	DMU	C18-C19-C22-C25
27	T	102	PEK	C10-C11-C12-C13
21	A	611	EDO	O1-C1-C2-O2
18	P	304	CDL	C19-C20-C21-C22
19	C	315	LFA	C6-C7-C8-C9
18	P	304	CDL	C71-C72-C73-C74
22	C	303	PGV	C29-C30-C31-C32
19	C	311	LFA	C5-C6-C7-C8
19	C	314	LFA	C4-C5-C6-C7
20	O	306	DMU	C31-C34-C37-C40
18	A	606	CDL	C18-C19-C20-C21
18	Y	101	CDL	C22-C23-C24-C25
18	Y	101	CDL	C73-C74-C75-C76
20	P	317	DMU	C25-C28-C31-C34
19	C	307	LFA	C3-C4-C5-C6
20	B	302	DMU	C25-C28-C31-C34
20	C	319	DMU	C4-C3-O7-C10
18	C	304	CDL	C13-C14-C15-C16
20	O	307	DMU	C28-C31-C34-C37
18	A	606	CDL	OA9-CA7-OA8-CA6
18	A	606	CDL	C71-C72-C73-C74
20	A	615	DMU	C28-C31-C34-C37
22	A	614	PGV	C15-C16-C17-C18
20	B	304	DMU	C19-C18-O16-C6
20	C	318	DMU	C19-C18-O16-C6
20	G	103	DMU	C19-C18-O16-C6
20	O	304	DMU	C19-C18-O16-C6
19	T	103	LFA	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
19	C	325	LFA	C3-C4-C5-C6
20	G	103	DMU	C31-C34-C37-C40
18	L	101	CDL	C21-C22-C23-C24
18	Y	101	CDL	OA5-CA3-CA4-CA6
19	C	314	LFA	C2-C3-C4-C5
22	N	615	PGV	C15-C16-C17-C18
27	G	101	PEK	C17-C18-C19-C20
18	C	304	CDL	C52-C53-C54-C55
18	P	304	CDL	C55-C56-C57-C58
19	C	309	LFA	C13-C14-C15-C16
20	B	308	DMU	O16-C18-C19-C22
18	P	304	CDL	OB5-CB3-CB4-OB6
22	C	303	PGV	C21-C22-C23-C24
18	C	304	CDL	OB6-CB4-CB6-OB8
18	P	304	CDL	OB6-CB4-CB6-OB8
18	A	606	CDL	C77-C78-C79-C80
27	G	101	PEK	C4-C5-C6-C7
19	B	307	LFA	C6-C7-C8-C9
19	N	607	LFA	C9-C10-C11-C12
20	Z	102	DMU	C34-C37-C40-C43
18	L	101	CDL	C36-C37-C38-C39
19	C	307	LFA	C6-C7-C8-C9
18	A	606	CDL	CA7-C31-C32-C33
18	L	101	CDL	C73-C74-C75-C76
19	C	307	LFA	C7-C8-C9-C10
18	A	606	CDL	CA2-OA2-PA1-OA3
18	A	606	CDL	CB2-OB2-PB2-OB4
18	C	304	CDL	CA2-OA2-PA1-OA5
18	C	304	CDL	CB3-OB5-PB2-OB2
18	L	101	CDL	CA2-OA2-PA1-OA5
18	P	304	CDL	CA2-OA2-PA1-OA4
18	V	101	CDL	CA3-OA5-PA1-OA3
18	V	101	CDL	CB2-OB2-PB2-OB4
18	Y	101	CDL	CA2-OA2-PA1-OA4
18	Y	101	CDL	CB3-OB5-PB2-OB2
22	C	303	PGV	C24-C25-C26-C27
22	P	303	PGV	C14-C15-C16-C17
18	P	304	CDL	C33-C34-C35-C36
19	P	309	LFA	C11-C12-C13-C14
18	A	606	CDL	CB4-CB3-OB5-PB2
18	P	304	CDL	CA4-CA3-OA5-PA1
22	P	303	PGV	C02-C03-O11-P

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Mol	Chain	Res	Type	Atoms
19	C	312	LFA	C11-C10-C9-C8
19	N	607	LFA	C1-C2-C3-C4
20	W	101	DMU	C25-C28-C31-C34
18	A	606	CDL	C31-C32-C33-C34
18	P	304	CDL	CA7-C31-C32-C33
20	A	609	DMU	O5-C4-C57-O61
18	P	304	CDL	C18-C19-C20-C21
20	B	304	DMU	O16-C18-C19-C22
18	A	606	CDL	CA3-CA4-OA6-CA5
19	B	307	LFA	C10-C11-C12-C13
18	L	101	CDL	C22-C23-C24-C25
18	V	101	CDL	C15-C16-C17-C18
20	C	316	DMU	O5-C6-O16-C18
18	L	101	CDL	C72-C71-CB7-OB8
19	A	607	LFA	C6-C7-C8-C9
19	P	309	LFA	C15-C16-C17-C18
20	O	308	DMU	C1-C6-O16-C18
19	C	311	LFA	C1-C2-C3-C4
19	T	104	LFA	C11-C10-C9-C8
20	O	308	DMU	C22-C25-C28-C31
19	C	309	LFA	C15-C16-C17-C18
20	O	307	DMU	C22-C25-C28-C31
19	C	307	LFA	C11-C10-C9-C8
20	P	322	DMU	O6-C11-C9-C8
27	T	102	PEK	C13-C14-C15-C16
18	V	101	CDL	C16-C17-C18-C19
18	C	304	CDL	C12-C13-C14-C15
19	T	104	LFA	C4-C5-C6-C7
18	P	304	CDL	C12-C11-CA5-OA6
21	N	611	EDO	O1-C1-C2-O2
20	C	320	DMU	C28-C31-C34-C37
20	P	316	DMU	C19-C18-O16-C6
18	Y	101	CDL	OB9-CB7-OB8-CB6
20	P	314	DMU	C4-C3-O7-C10
20	P	317	DMU	C19-C22-C25-C28
18	Y	101	CDL	C23-C24-C25-C26
20	T	105	DMU	C22-C25-C28-C31
20	O	306	DMU	C22-C25-C28-C31
18	P	304	CDL	OA5-CA3-CA4-OA6
14	A	602	HEA	CAD-CBD-CGD-O2D
18	L	101	CDL	C75-C76-C77-C78
20	C	319	DMU	C25-C28-C31-C34

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Mol	Chain	Res	Type	Atoms
20	O	308	DMU	C18-C19-C22-C25
27	T	102	PEK	C14-C15-C16-C17
19	O	303	LFA	C1-C2-C3-C4
18	A	606	CDL	C16-C17-C18-C19
19	C	314	LFA	C7-C8-C9-C10
20	P	322	DMU	O1-C10-O7-C3
19	C	315	LFA	C11-C10-C9-C8
20	B	302	DMU	C31-C34-C37-C40
27	G	101	PEK	C27-C28-C29-C30
19	P	311	LFA	C11-C10-C9-C8
20	G	102	DMU	C19-C22-C25-C28
24	P	305	CHD	C22-C23-C24-O26
14	A	602	HEA	CAD-CBD-CGD-O1D
18	Y	101	CDL	C80-C81-C82-C83
20	P	317	DMU	C22-C25-C28-C31
18	Y	101	CDL	C15-C16-C17-C18
19	N	607	LFA	C2-C3-C4-C5
24	O	301	CHD	C22-C23-C24-O25
20	O	306	DMU	O16-C18-C19-C22
20	D	201	DMU	C28-C31-C34-C37
20	G	103	DMU	C18-C19-C22-C25
18	P	304	CDL	C74-C75-C76-C77
14	N	602	HEA	CAD-CBD-CGD-O1D
20	C	324	DMU	O16-C18-C19-C22
20	B	302	DMU	O16-C18-C19-C22
19	C	312	LFA	C6-C7-C8-C9
24	O	301	CHD	C22-C23-C24-O26
24	P	305	CHD	C22-C23-C24-O25
20	P	317	DMU	C5-C10-O7-C3
20	P	314	DMU	C34-C37-C40-C43
20	A	609	DMU	C4-C3-O7-C10
14	A	601	HEA	CAD-CBD-CGD-O1D
14	N	601	HEA	CAD-CBD-CGD-O1D
14	N	602	HEA	CAA-CBA-CGA-O1A
24	B	306	CHD	C22-C23-C24-O25
18	C	304	CDL	C53-C54-C55-C56
18	V	101	CDL	OA6-CA4-CA6-OA8
18	Y	101	CDL	OA6-CA4-CA6-OA8
14	A	602	HEA	CAA-CBA-CGA-O1A
14	N	602	HEA	CAD-CBD-CGD-O2D
18	A	606	CDL	C73-C74-C75-C76
19	C	312	LFA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
27	T	102	PEK	C6-C7-C8-C9
19	T	103	LFA	C1-C2-C3-C4
20	J	101	DMU	C18-C19-C22-C25
18	L	101	CDL	C32-C33-C34-C35
24	C	305	CHD	C22-C23-C24-O25
18	P	304	CDL	C51-C52-C53-C54
24	B	306	CHD	C22-C23-C24-O26
20	Y	102	DMU	C19-C22-C25-C28
20	T	105	DMU	C28-C31-C34-C37
20	N	616	DMU	C28-C31-C34-C37
20	C	319	DMU	C5-C10-O7-C3
19	O	303	LFA	C6-C7-C8-C9
20	H	101	DMU	C25-C28-C31-C34
20	N	608	DMU	C31-C34-C37-C40
20	H	101	DMU	C22-C25-C28-C31
14	N	601	HEA	CAD-CBD-CGD-O2D
20	B	303	DMU	C22-C25-C28-C31
14	A	602	HEA	CAA-CBA-CGA-O2A
24	C	305	CHD	C22-C23-C24-O26
18	C	304	CDL	C12-C11-CA5-OA7
20	C	316	DMU	C18-C19-C22-C25
21	N	613	EDO	O1-C1-C2-O2
18	V	101	CDL	C32-C33-C34-C35
14	A	601	HEA	CAD-CBD-CGD-O2D
24	C	301	CHD	C22-C23-C24-O26
27	G	101	PEK	C10-C11-C12-C13
19	A	607	LFA	C7-C8-C9-C10
27	G	101	PEK	C34-C35-C36-C37
20	B	303	DMU	C25-C28-C31-C34
20	P	317	DMU	O5-C6-O16-C18
18	P	304	CDL	C23-C24-C25-C26
19	C	310	LFA	C7-C8-C9-C10
14	N	602	HEA	CAA-CBA-CGA-O2A
19	O	302	LFA	C2-C3-C4-C5
18	L	101	CDL	O1-C1-CB2-OB2
19	P	313	LFA	C1-C2-C3-C4
27	T	102	PEK	C15-C16-C17-C18
19	C	310	LFA	C1-C2-C3-C4
18	C	304	CDL	C18-C19-C20-C21
24	P	301	CHD	C22-C23-C24-O26
22	C	303	PGV	C23-C24-C25-C26
18	Y	101	CDL	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
18	Y	101	CDL	C71-CB7-OB8-CB6
22	A	614	PGV	O03-C19-C20-C21
20	C	316	DMU	O16-C18-C19-C22
22	A	614	PGV	C12-C13-C14-C15
18	P	304	CDL	C80-C81-C82-C83
20	O	304	DMU	C18-C19-C22-C25
19	B	307	LFA	C12-C13-C14-C15
22	C	303	PGV	C05-C04-O12-P
18	C	304	CDL	C73-C74-C75-C76
22	P	303	PGV	C28-C29-C30-C31
18	V	101	CDL	C72-C71-CB7-OB8
24	C	301	CHD	C22-C23-C24-O25
24	P	301	CHD	C22-C23-C24-O25
18	L	101	CDL	C16-C17-C18-C19
21	F	103	EDO	O1-C1-C2-O2
21	R	203	EDO	O1-C1-C2-O2
19	P	311	LFA	C4-C5-C6-C7
18	Y	101	CDL	C38-C39-C40-C41
19	N	607	LFA	C6-C7-C8-C9
20	A	609	DMU	C2-C3-O7-C10
19	C	309	LFA	C6-C7-C8-C9
18	V	101	CDL	CB4-CB3-OB5-PB2
20	C	306	DMU	C31-C34-C37-C40
18	C	304	CDL	C52-C51-CB5-OB6
20	P	318	DMU	C19-C22-C25-C28
18	L	101	CDL	C32-C31-CA7-OA8
20	C	319	DMU	O1-C10-O7-C3
18	L	101	CDL	C18-C19-C20-C21
18	P	304	CDL	C52-C51-CB5-OB6
18	P	304	CDL	C82-C83-C84-C85
24	C	305	CHD	C17-C20-C22-C23
18	C	304	CDL	C57-C58-C59-C60
18	A	606	CDL	C72-C71-CB7-OB8
22	N	615	PGV	O03-C19-C20-C21
18	P	304	CDL	C12-C13-C14-C15
18	Y	101	CDL	C83-C84-C85-C86
19	P	310	LFA	C3-C4-C5-C6
20	P	318	DMU	C28-C31-C34-C37
19	P	310	LFA	C1-C2-C3-C4
19	P	311	LFA	C5-C6-C7-C8
20	Z	102	DMU	C25-C28-C31-C34
21	R	201	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
18	A	606	CDL	C32-C31-CA7-OA8
20	A	615	DMU	C18-C19-C22-C25
18	V	101	CDL	C52-C51-CB5-OB6
18	Y	101	CDL	C32-C31-CA7-OA8
20	J	101	DMU	C31-C34-C37-C40
18	L	101	CDL	C32-C31-CA7-OA9
18	P	304	CDL	C52-C51-CB5-OB7
22	C	303	PGV	C1-C2-C3-C4
19	C	310	LFA	C2-C3-C4-C5
18	L	101	CDL	C56-C57-C58-C59
18	C	304	CDL	C11-C12-C13-C14
18	A	606	CDL	C72-C71-CB7-OB9
18	C	304	CDL	C52-C51-CB5-OB7
14	A	601	HEA	CAA-CBA-CGA-O2A
20	P	314	DMU	C31-C34-C37-C40
18	V	101	CDL	C72-C71-CB7-OB9
18	C	304	CDL	C72-C71-CB7-OB8
14	N	601	HEA	CAA-CBA-CGA-O2A
20	C	316	DMU	O1-C10-O7-C3
18	V	101	CDL	O1-C1-CA2-OA2
18	P	304	CDL	OB5-CB3-CB4-CB6
22	N	615	PGV	C31-C32-C33-C34
22	C	303	PGV	C9-C10-C11-C12
19	A	607	LFA	C4-C5-C6-C7
18	Y	101	CDL	C76-C77-C78-C79
21	C	321	EDO	O1-C1-C2-O2
18	L	101	CDL	C61-C62-C63-C64
18	Y	101	CDL	C16-C17-C18-C19
14	N	601	HEA	CAA-CBA-CGA-O1A
18	A	606	CDL	C32-C31-CA7-OA9
18	Y	101	CDL	C32-C31-CA7-OA9
27	T	102	PEK	O01-C1-C2-C3

There are no ring outliers.

45 monomers are involved in 124 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	Y	101	CDL	5	0
19	O	302	LFA	1	0
27	T	102	PEK	5	0
20	A	609	DMU	1	0
21	N	614	EDO	3	0

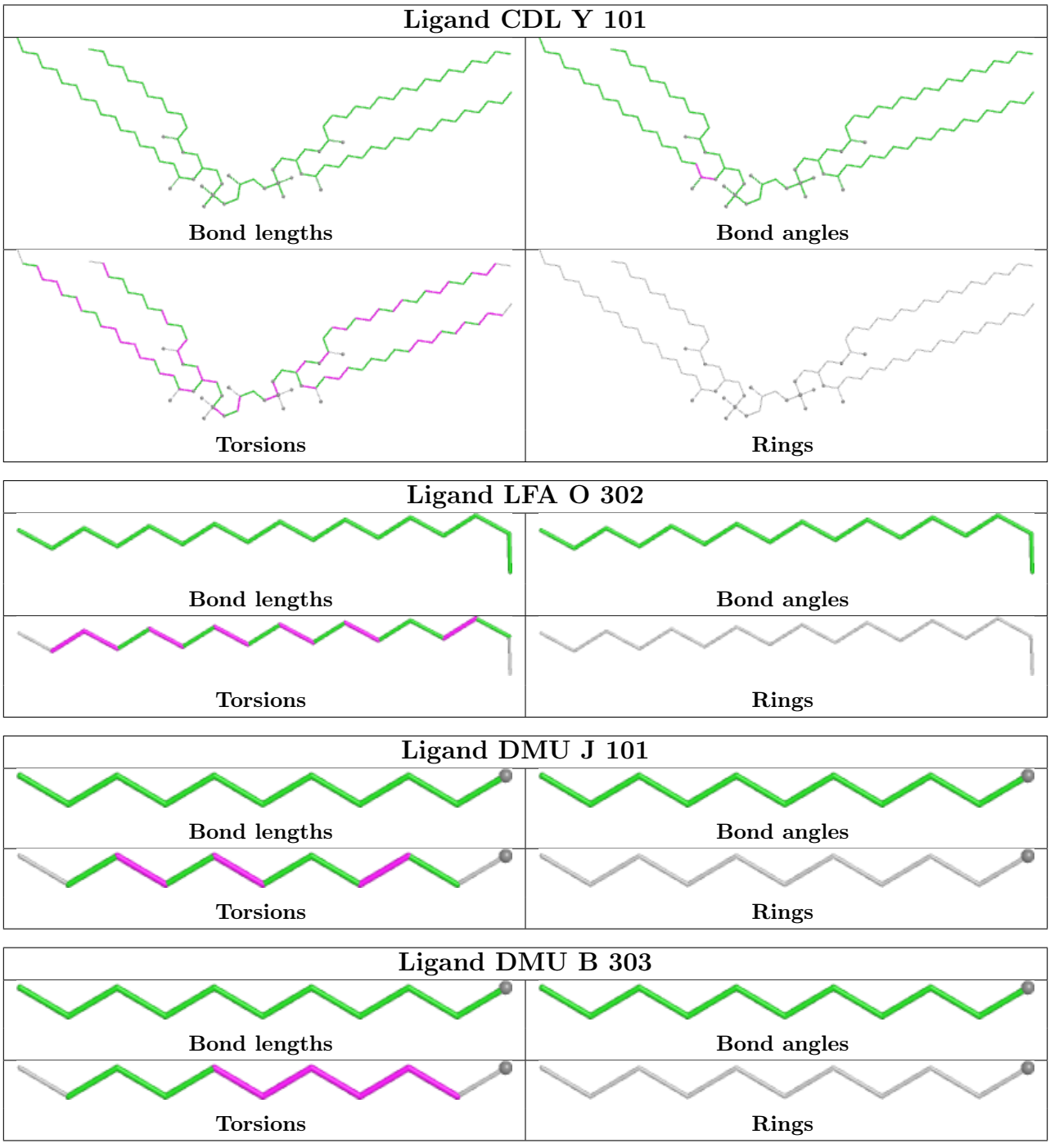
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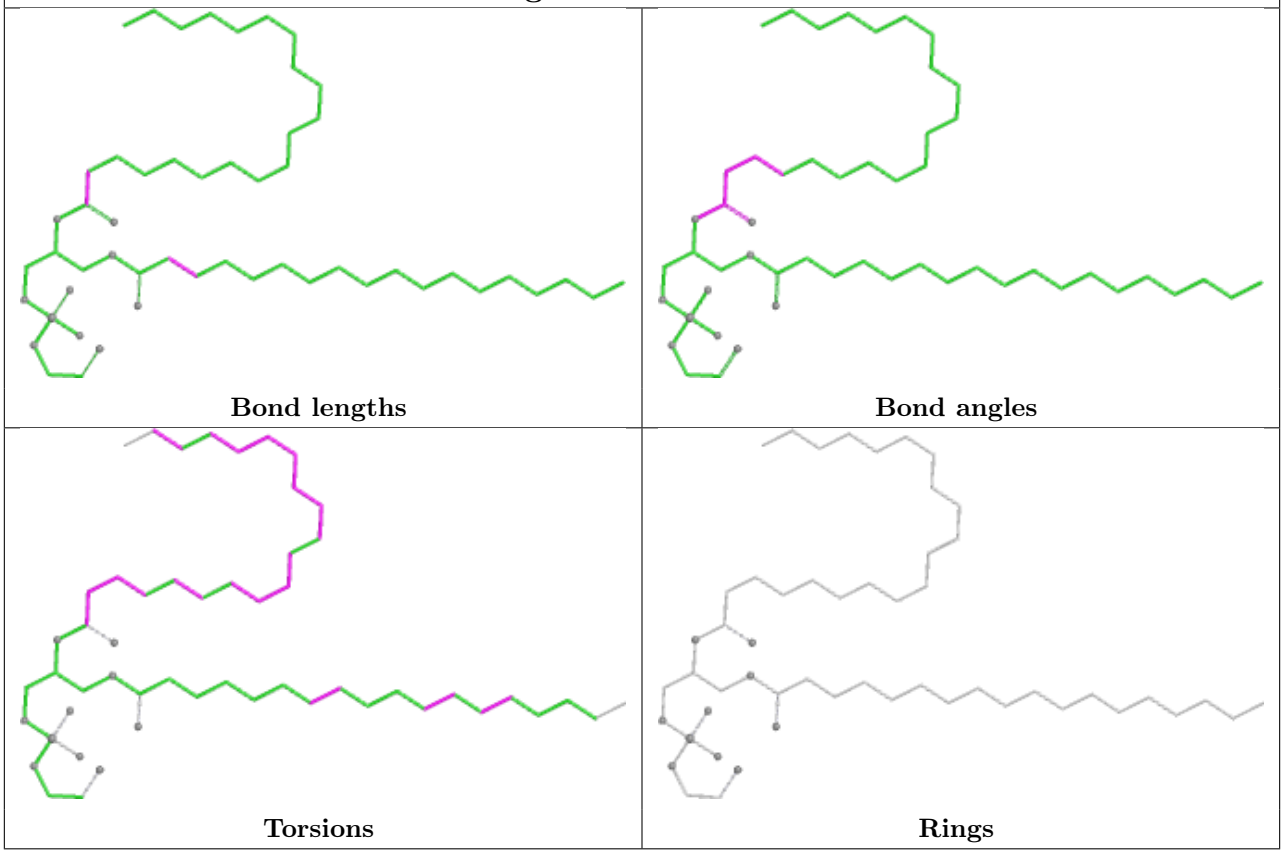
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	C	315	LFA	1	0
20	Y	102	DMU	1	0
19	A	607	LFA	5	0
18	V	101	CDL	2	0
20	P	314	DMU	1	0
19	C	307	LFA	2	0
19	O	303	LFA	4	0
19	C	309	LFA	2	0
18	L	101	CDL	2	0
20	N	609	DMU	1	0
18	C	304	CDL	18	0
19	N	606	LFA	6	0
19	C	313	LFA	2	0
24	P	305	CHD	2	0
20	C	324	DMU	3	0
19	P	309	LFA	3	0
20	O	304	DMU	1	0
20	Z	101	DMU	1	0
14	N	601	HEA	3	0
19	B	307	LFA	1	0
22	N	615	PGV	1	0
22	C	303	PGV	2	0
19	P	311	LFA	2	0
20	N	616	DMU	1	0
18	P	304	CDL	14	0
20	D	201	DMU	1	0
19	T	101	LFA	6	0
19	N	607	LFA	6	0
24	C	305	CHD	2	0
27	G	101	PEK	3	0
19	P	307	LFA	1	0
20	G	103	DMU	2	0
19	C	314	LFA	3	0
20	P	318	DMU	1	0
24	O	301	CHD	1	0
20	C	306	DMU	1	0
20	Q	201	DMU	1	0
20	A	608	DMU	1	0
19	P	310	LFA	1	0
14	A	601	HEA	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

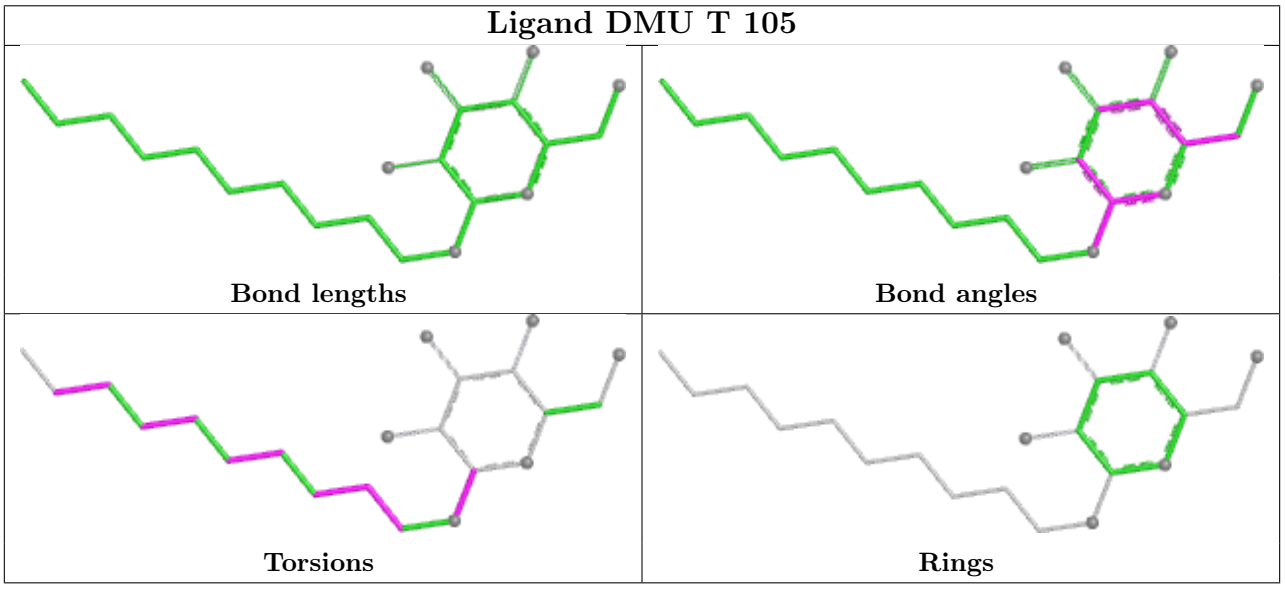
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.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



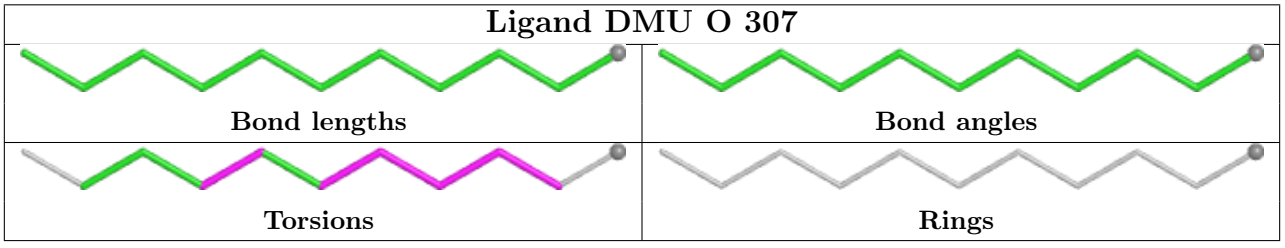
Ligand PEK T 102



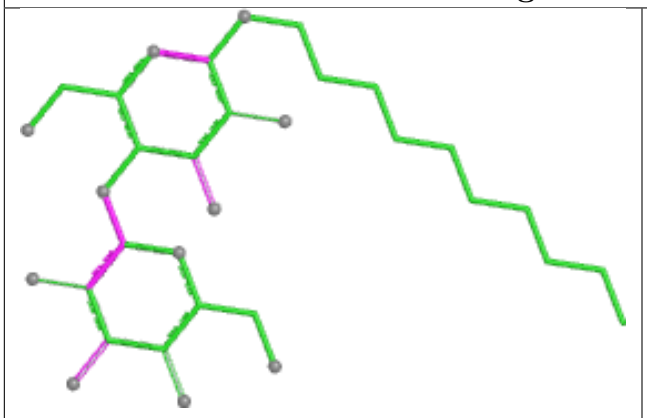
Ligand DMU T 105



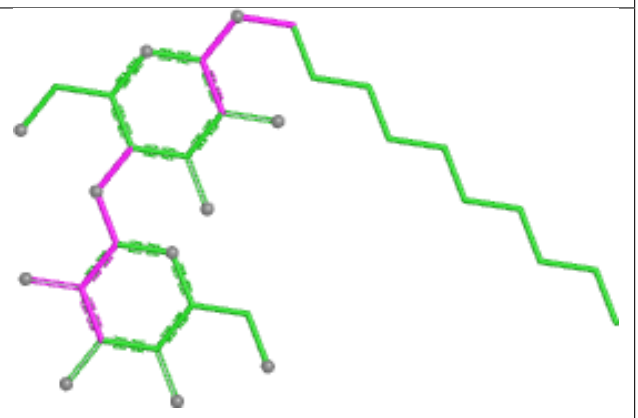
Ligand DMU O 307



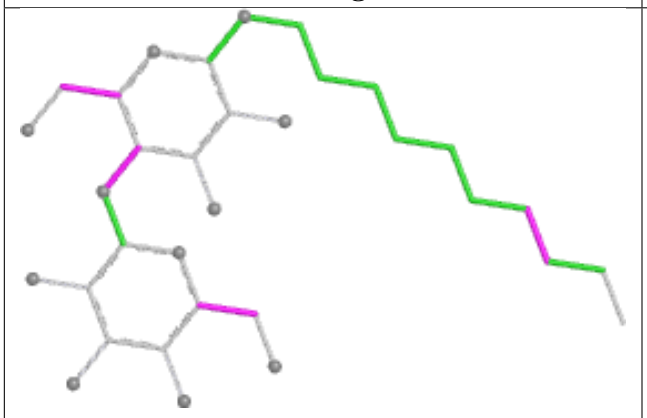
Ligand DMU A 609



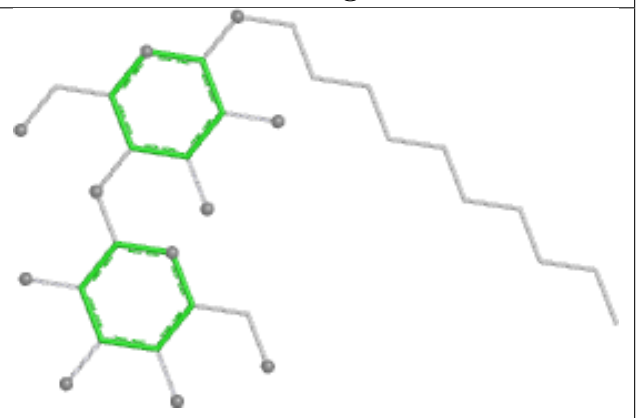
Bond lengths



Bond angles



Torsions



Rings

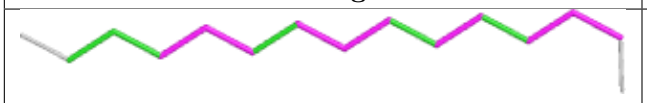
Ligand LFA C 310



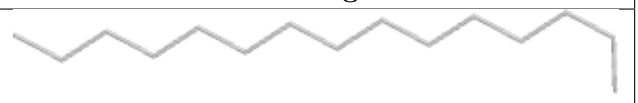
Bond lengths



Bond angles

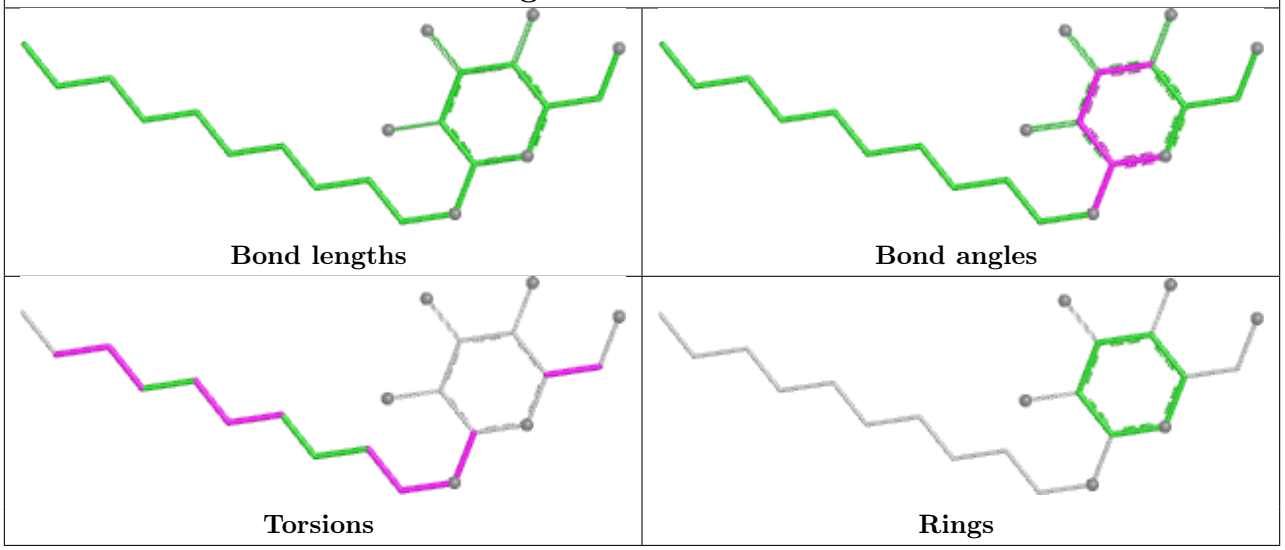


Torsions

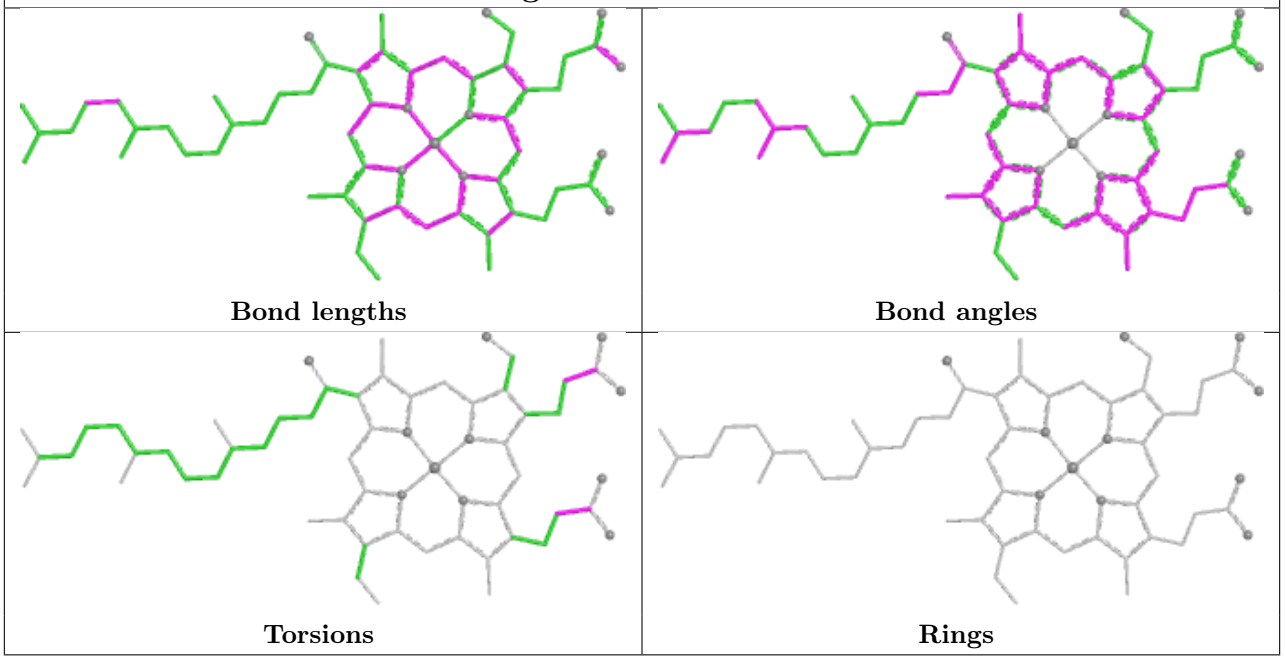


Rings

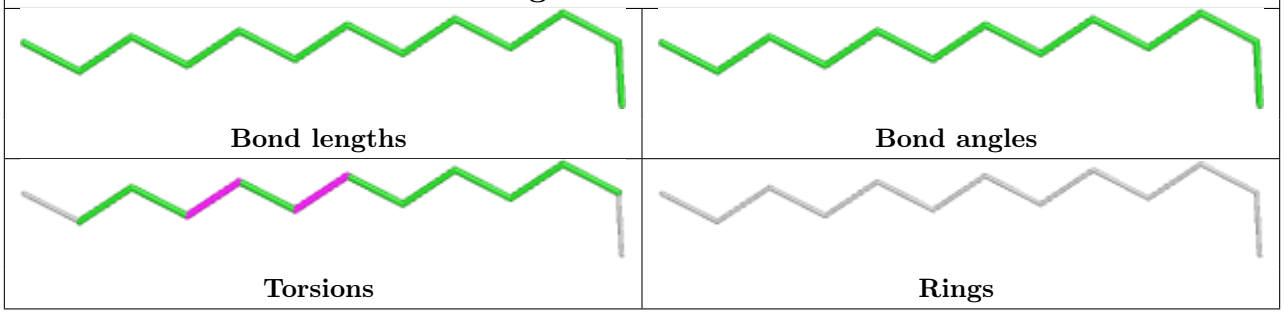
Ligand DMU L 102



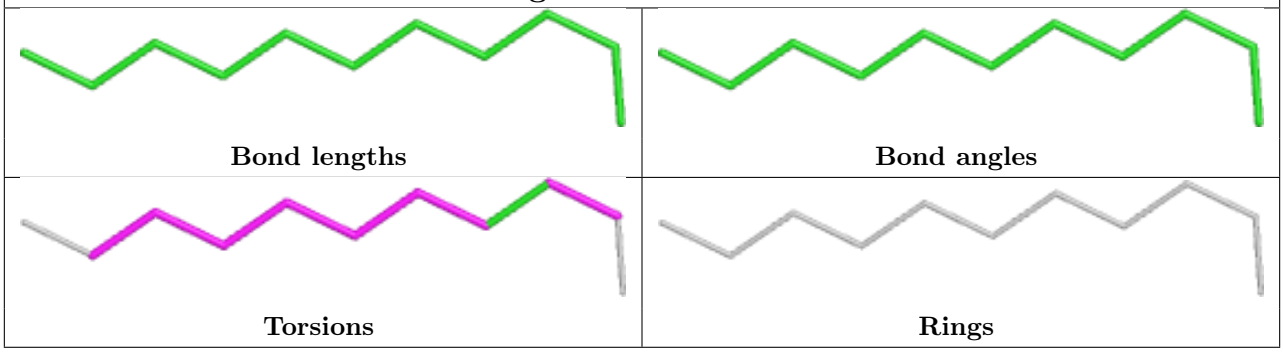
Ligand HEA N 602



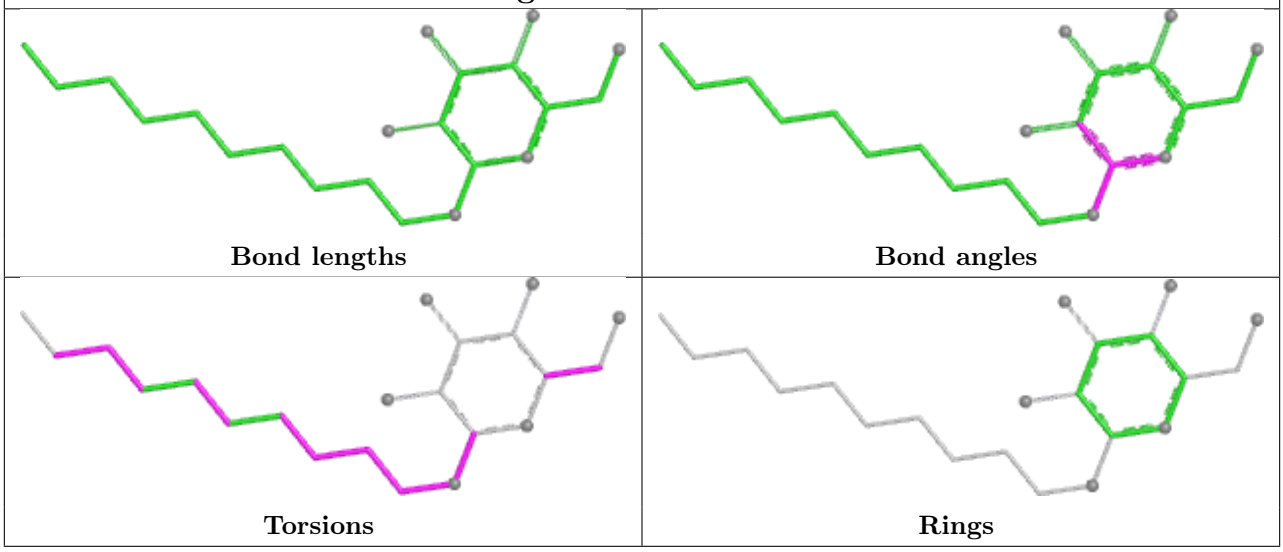
Ligand LFA C 315



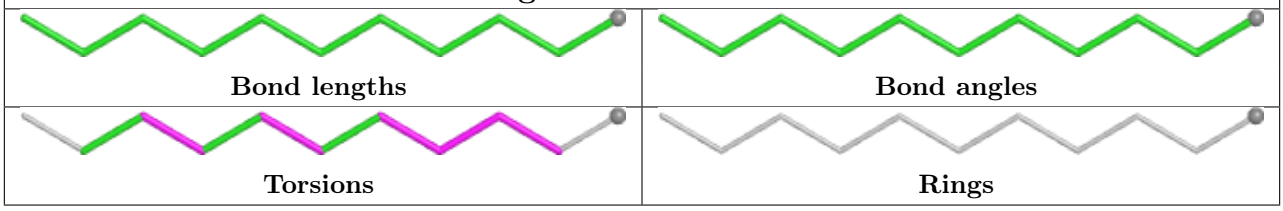
Ligand LFA C 311



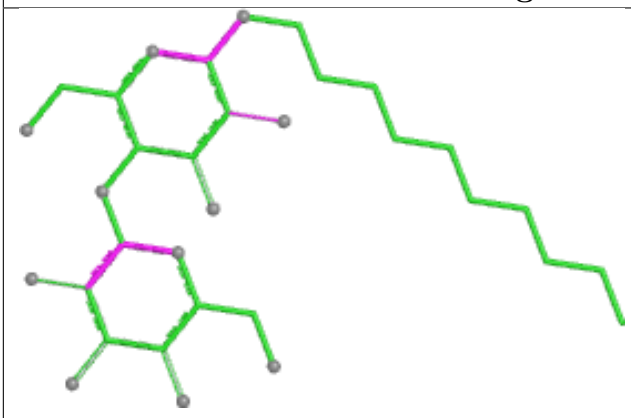
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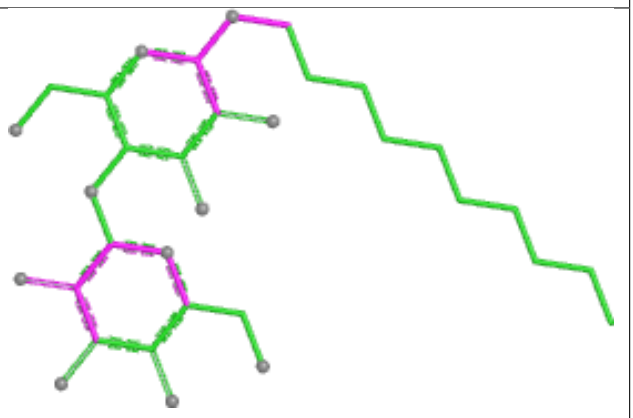
Ligand DMU B 302



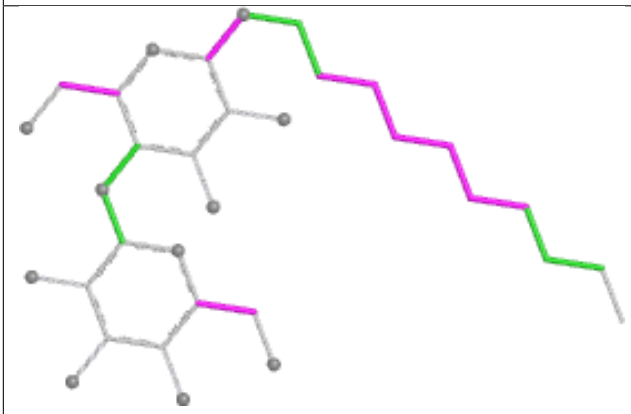
Ligand DMU H 101



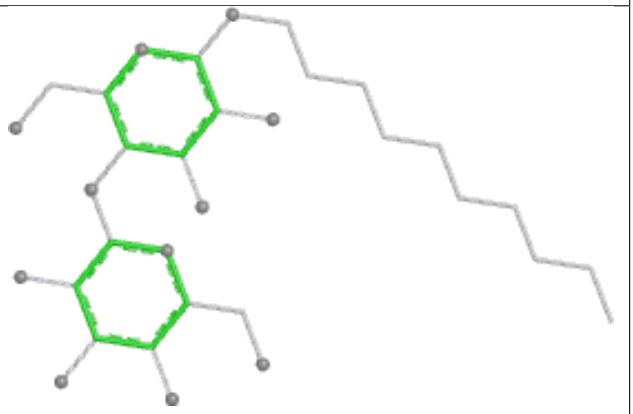
Bond lengths



Bond angles

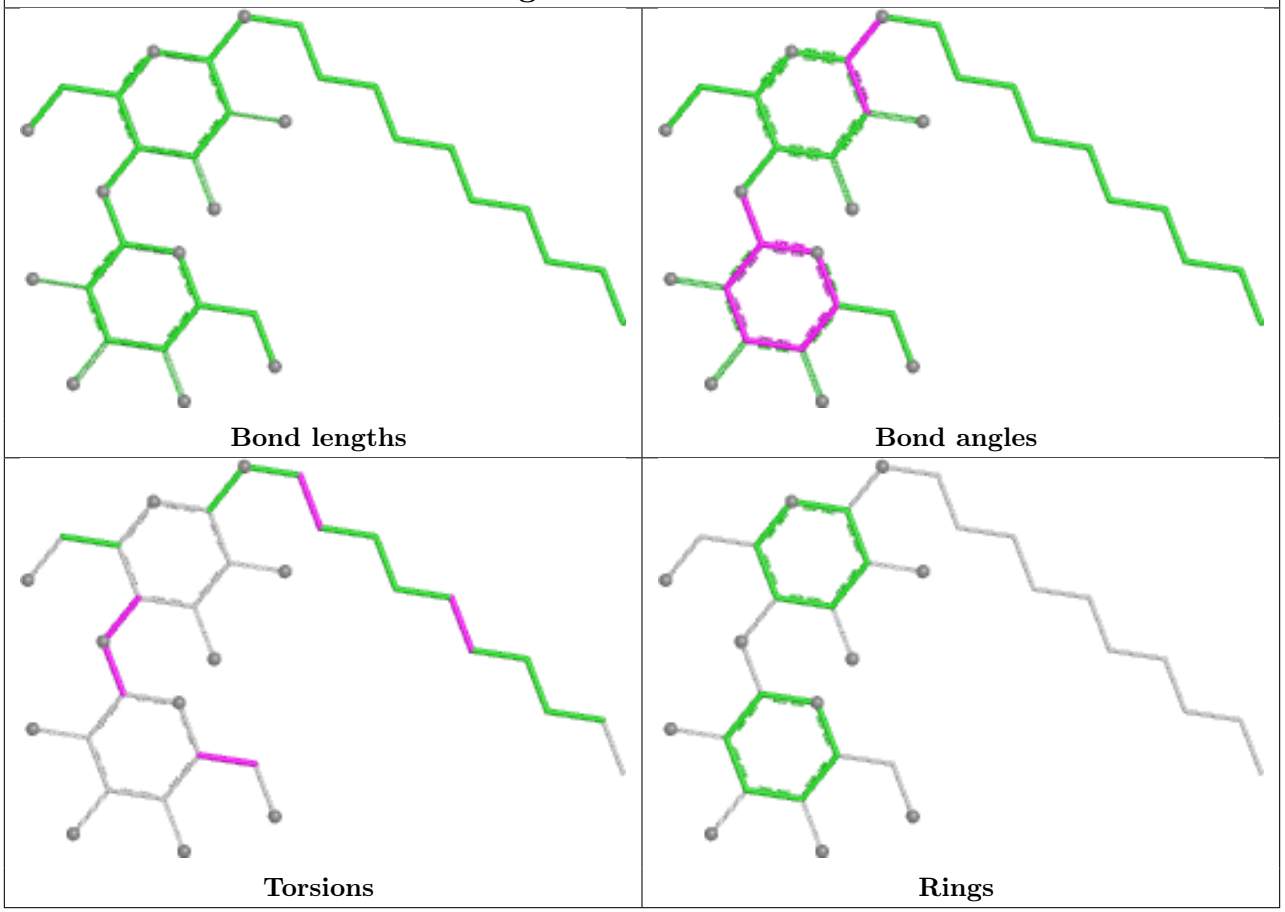


Torsions

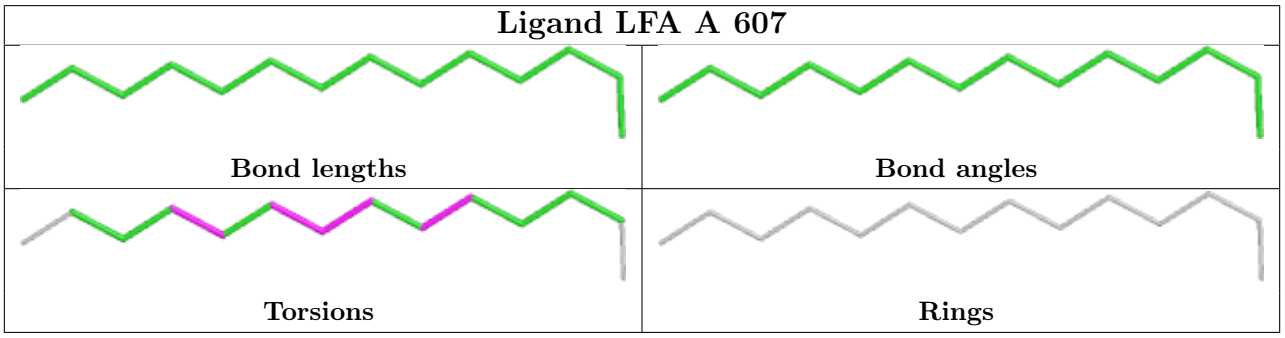


Rings

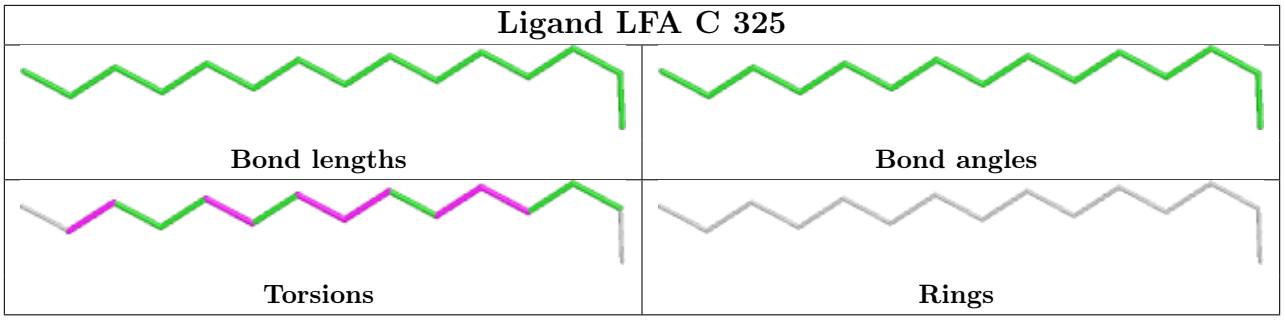
Ligand DMU P 322



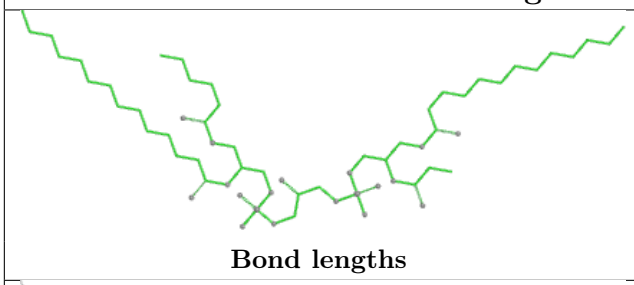
Ligand LFA A 607



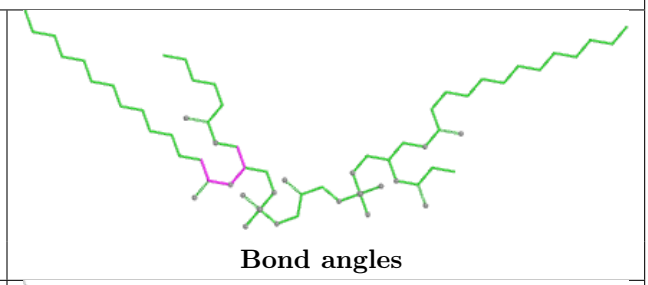
Ligand LFA C 325



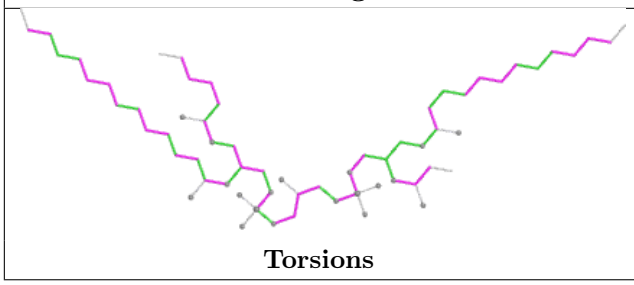
Ligand CDL V 101



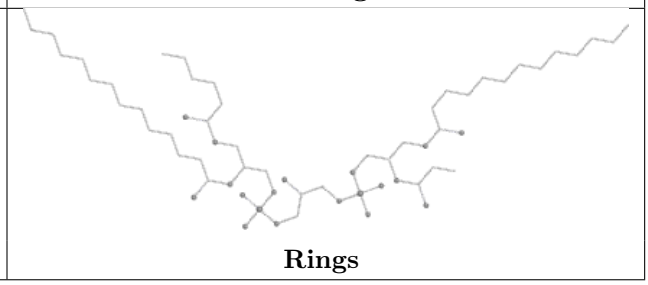
Bond lengths



Bond angles

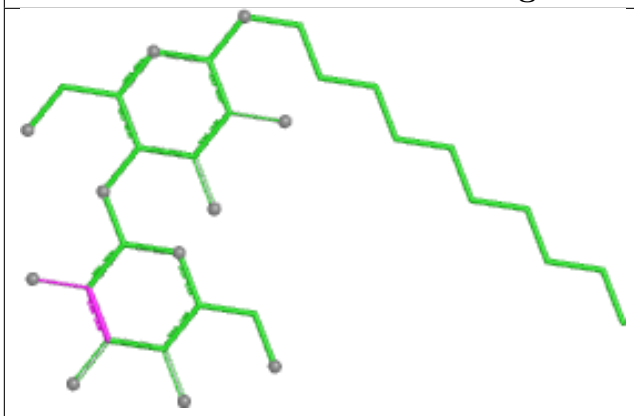


Torsions

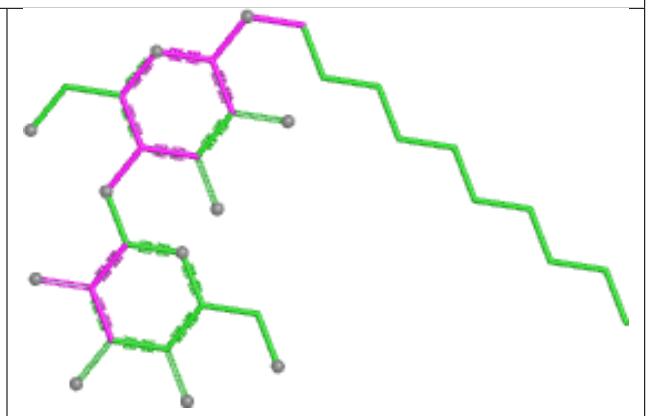


Rings

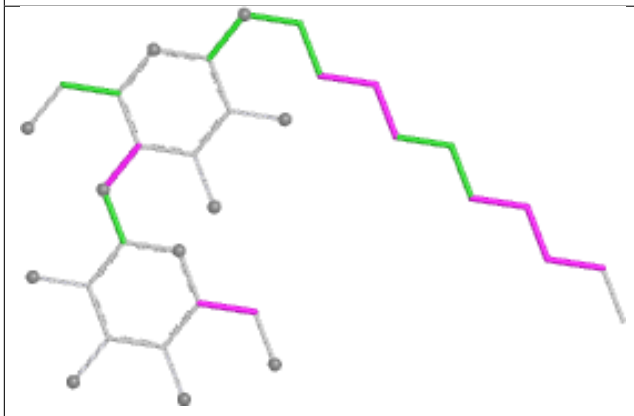
Ligand DMU P 314



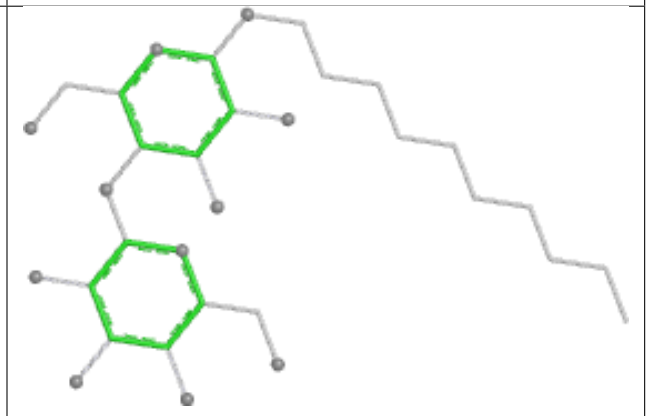
Bond lengths



Bond angles

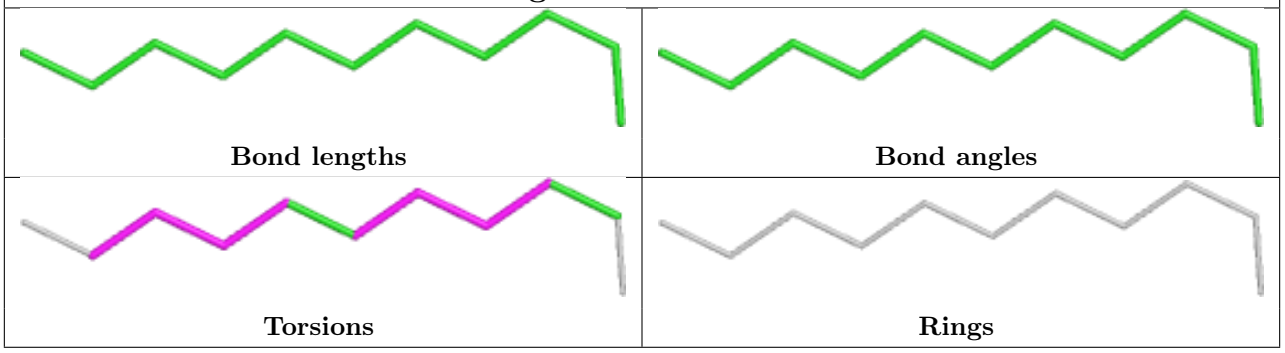


Torsions

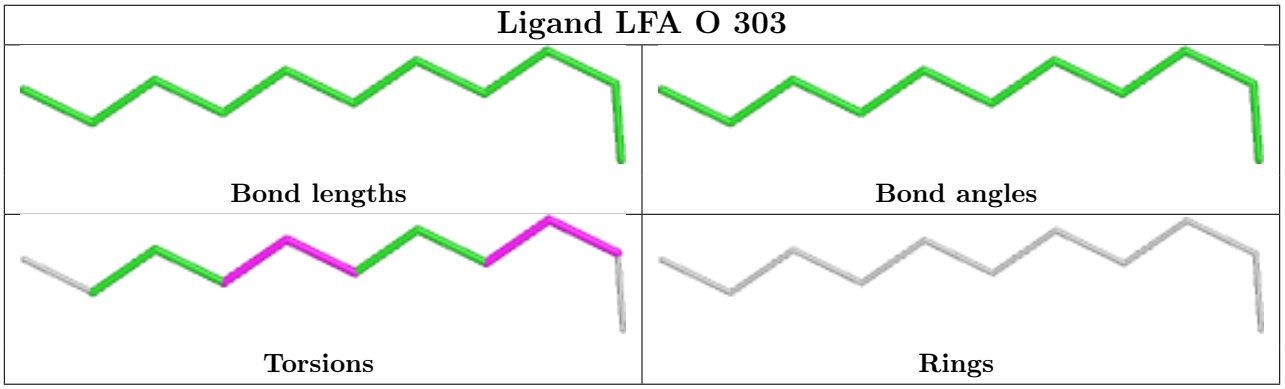


Rings

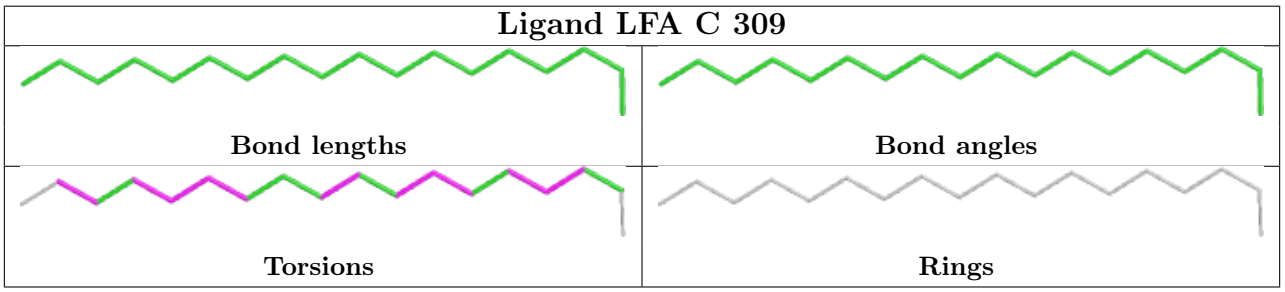
Ligand LFA C 307



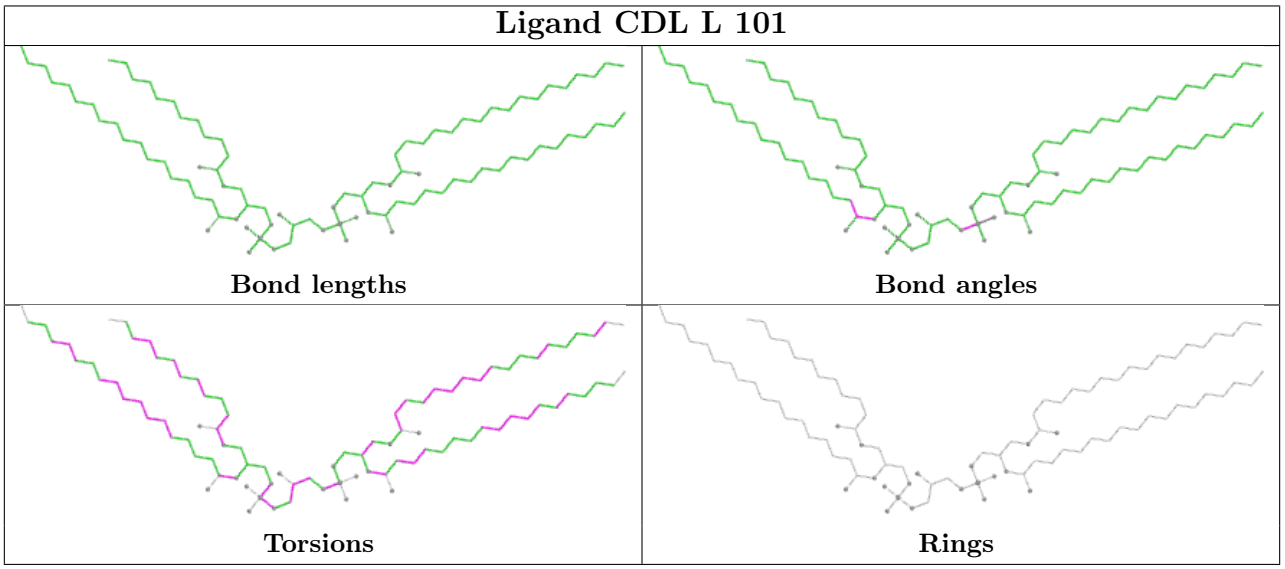
Ligand LFA O 303



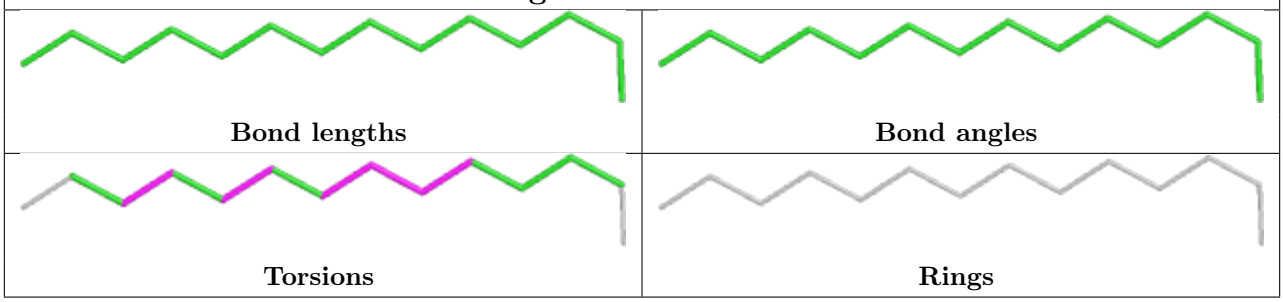
Ligand LFA C 309



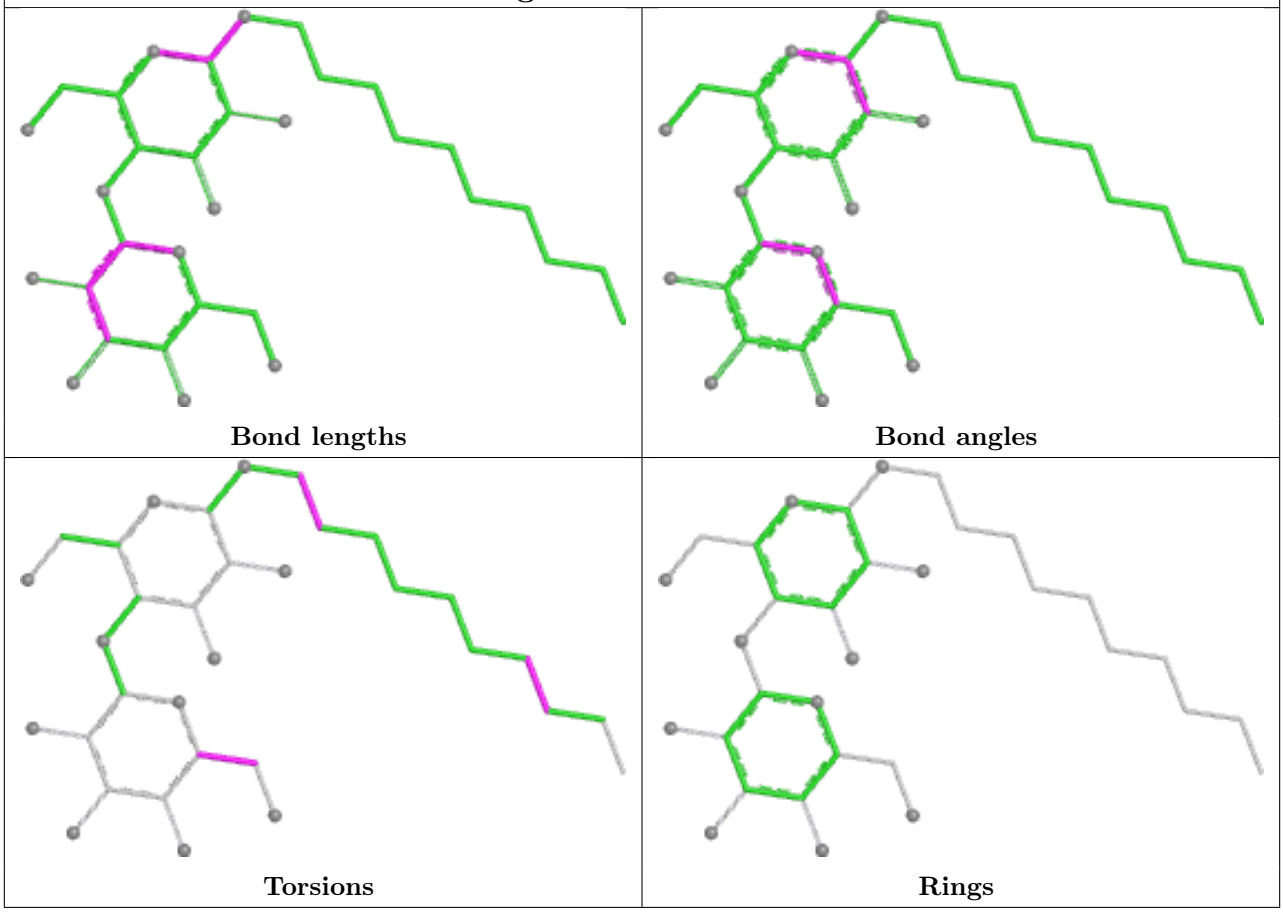
Ligand CDL L 101



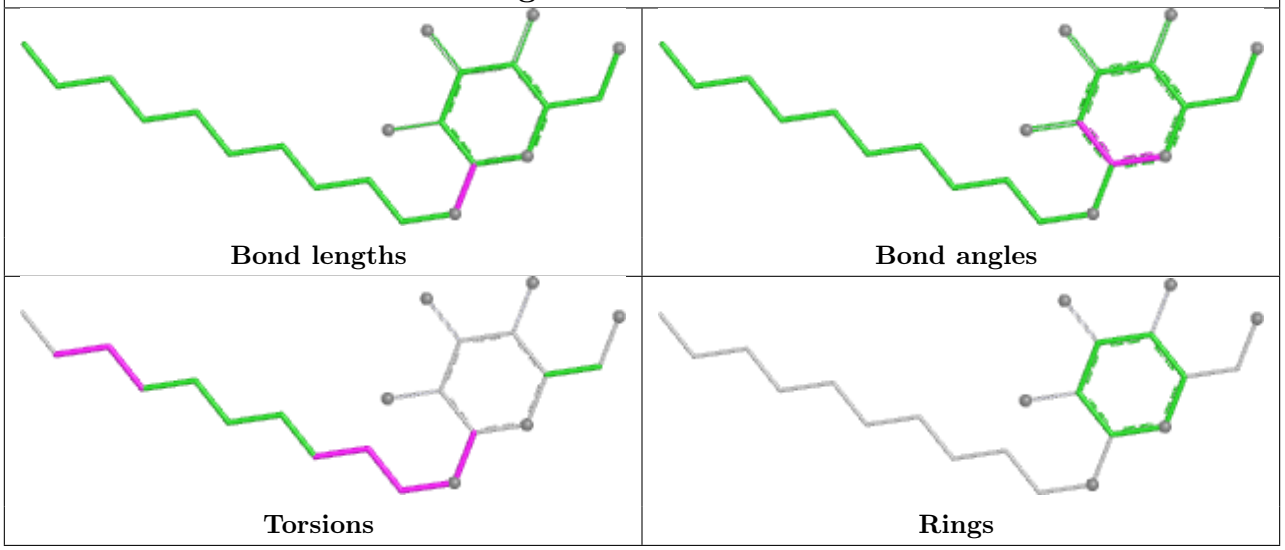
Ligand LFA C 312



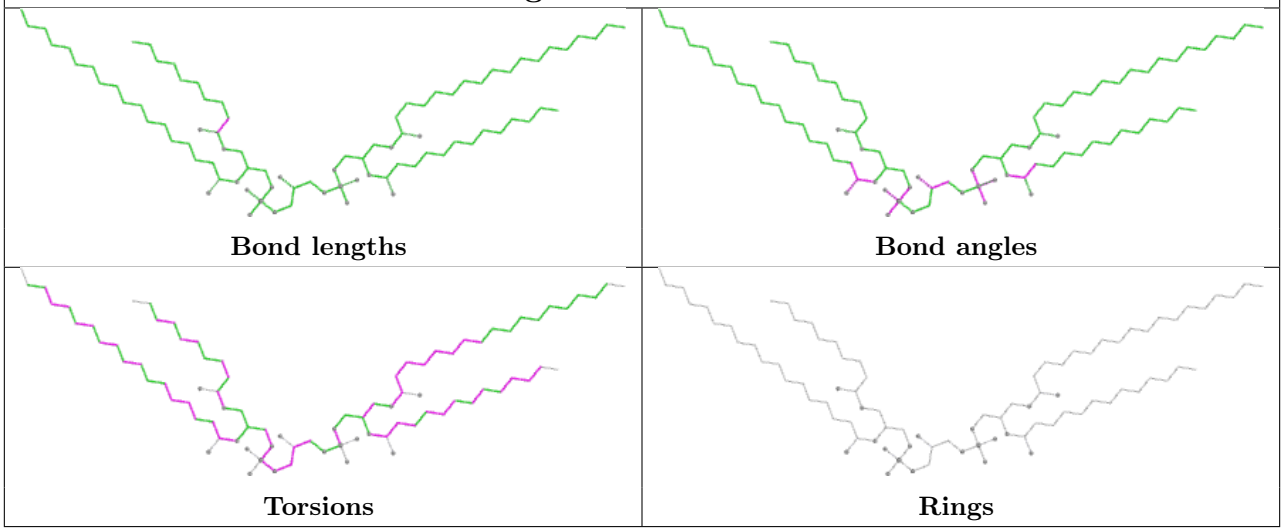
Ligand DMU N 609



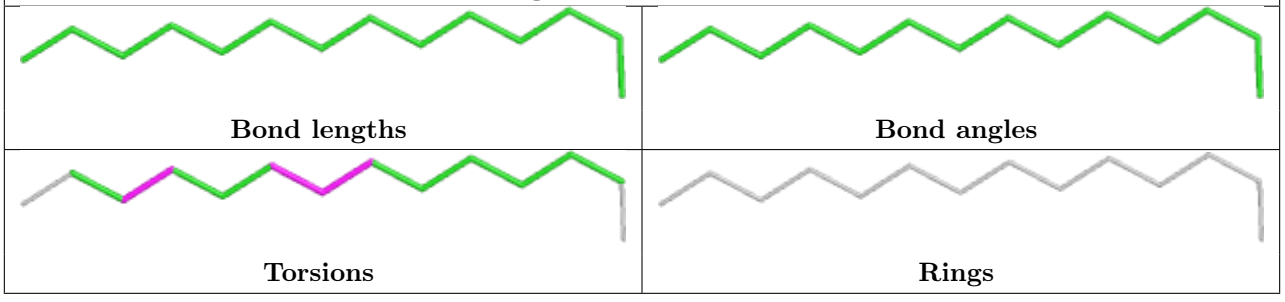
Ligand DMU B 304



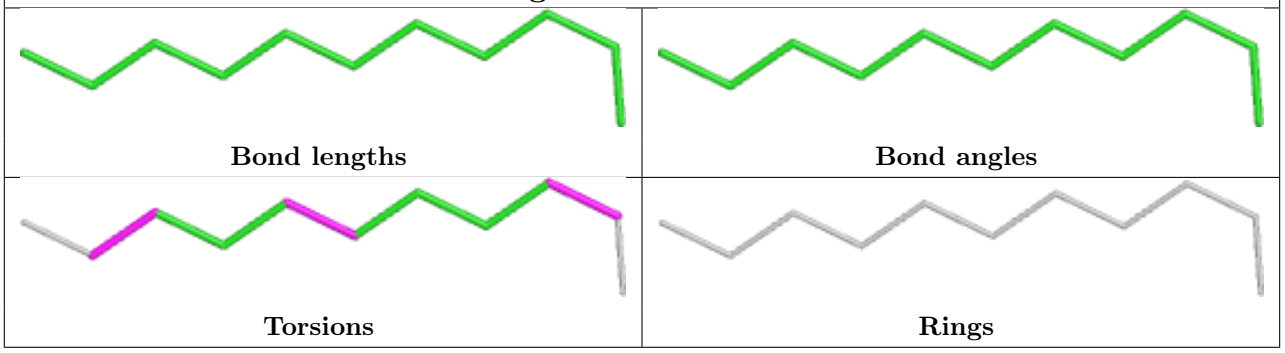
Ligand CDL C 304



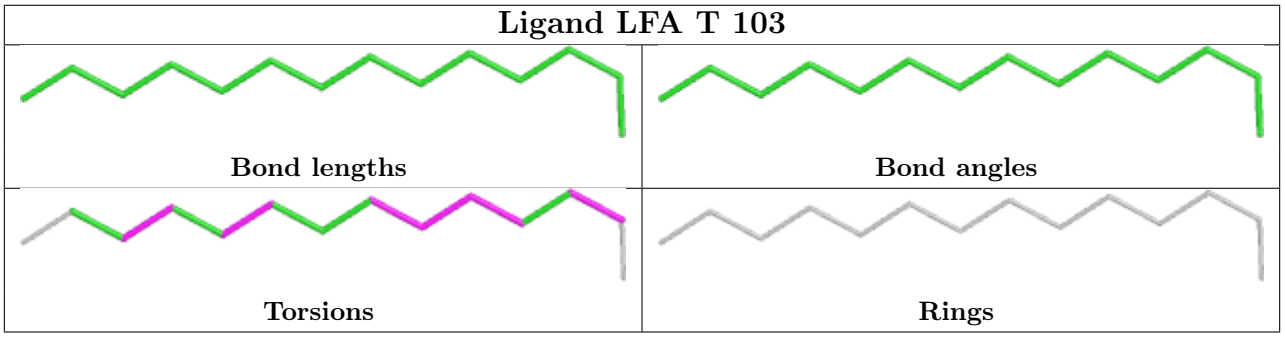
Ligand LFA N 606



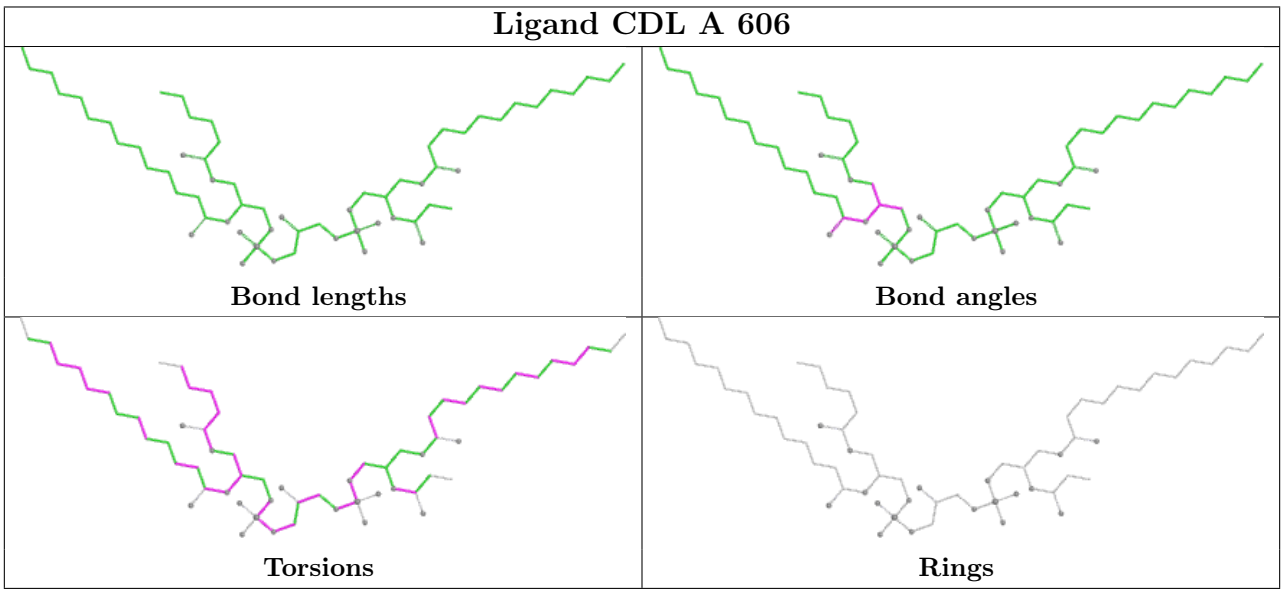
Ligand LFA C 313



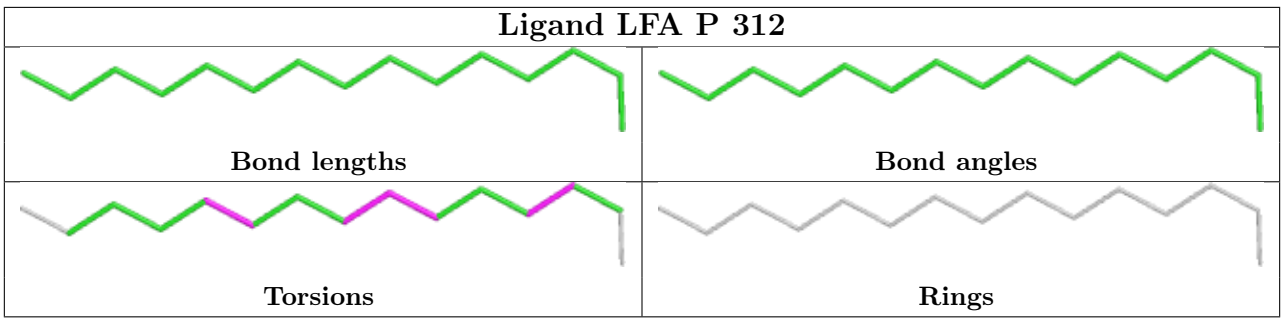
Ligand LFA T 103



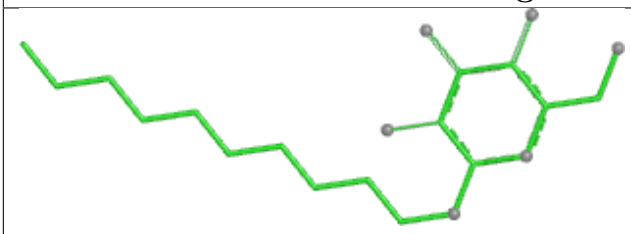
Ligand CDL A 606



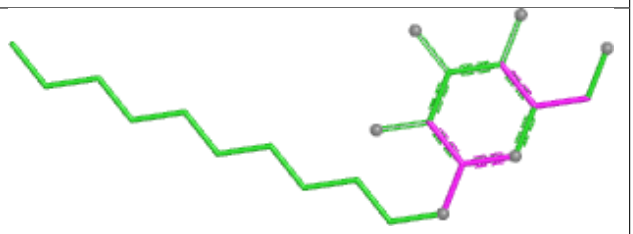
Ligand LFA P 312



Ligand DMU O 308



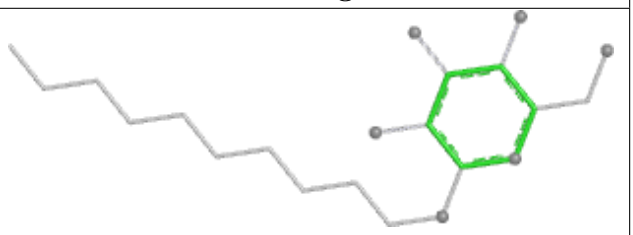
Bond lengths



Bond angles

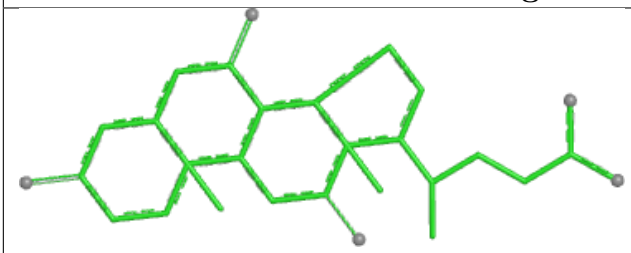


Torsions

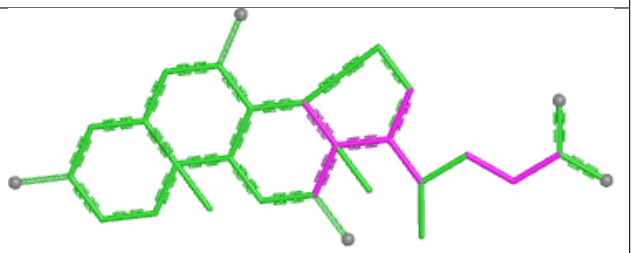


Rings

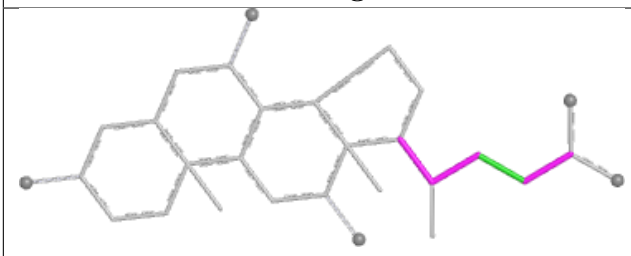
Ligand CHD P 305



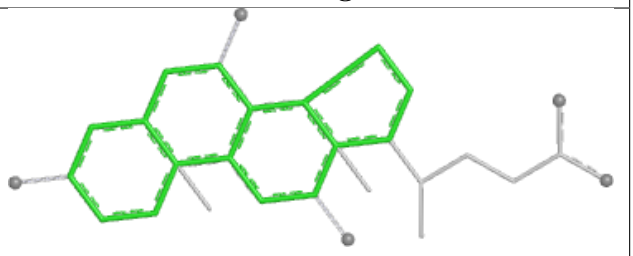
Bond lengths



Bond angles

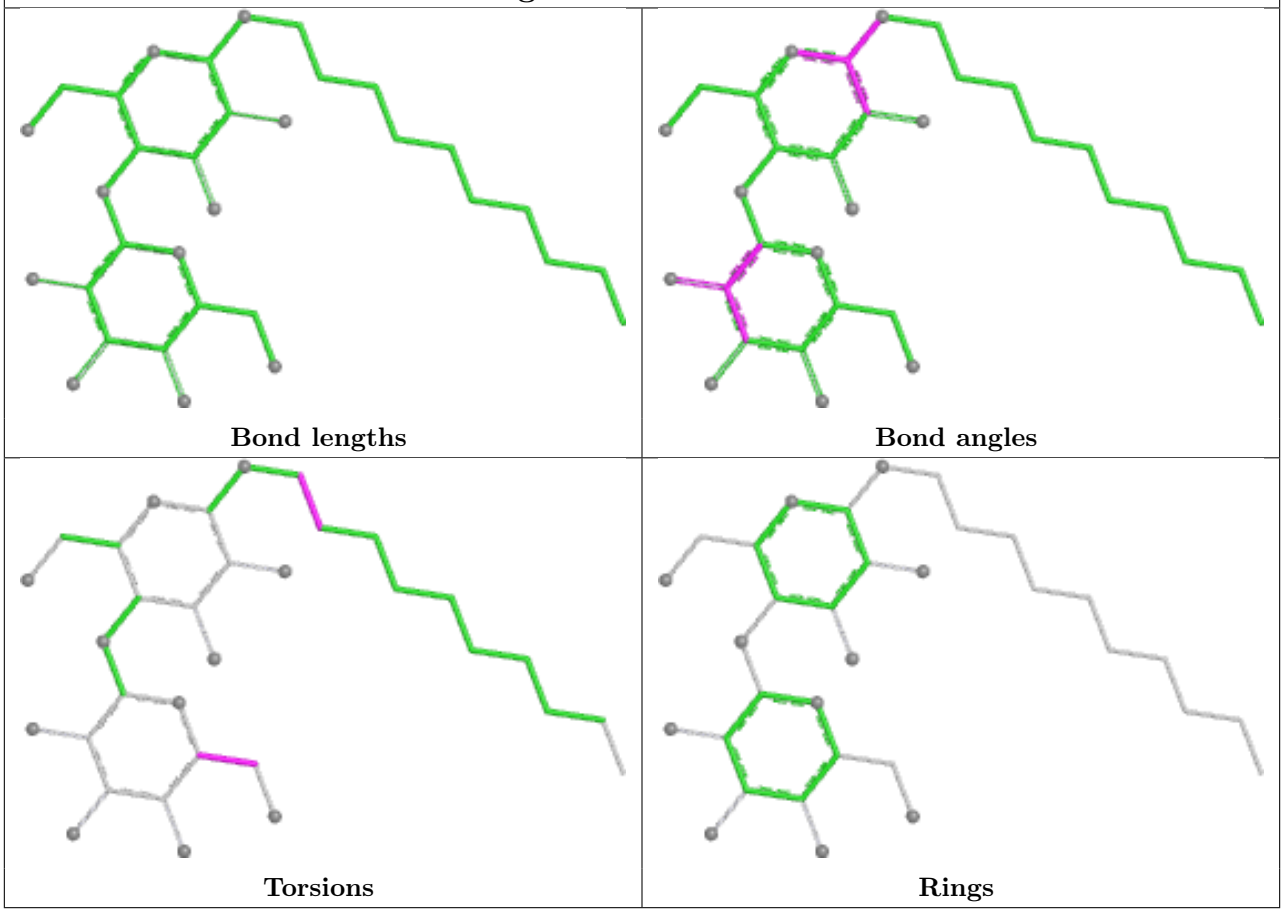


Torsions

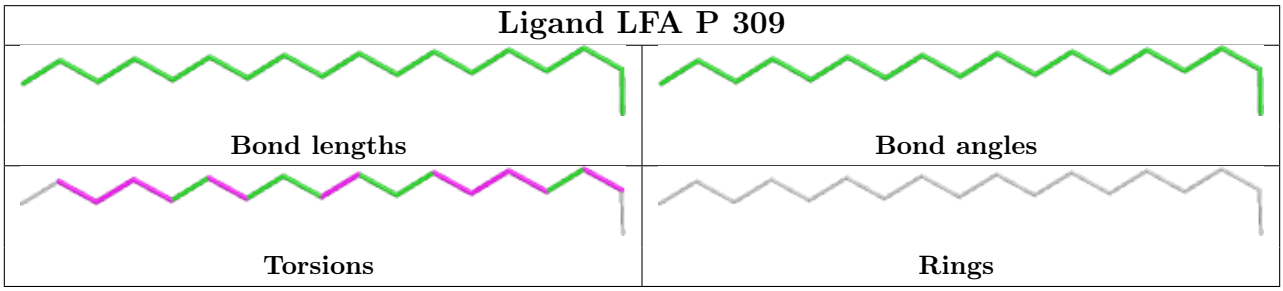


Rings

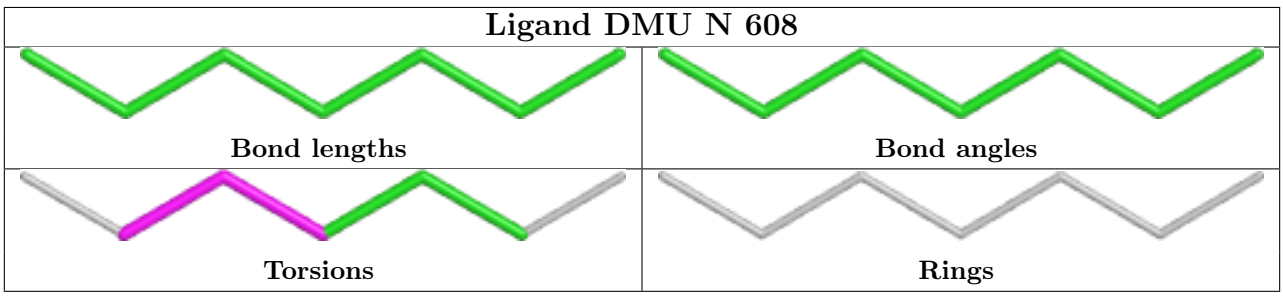
Ligand DMU C 324



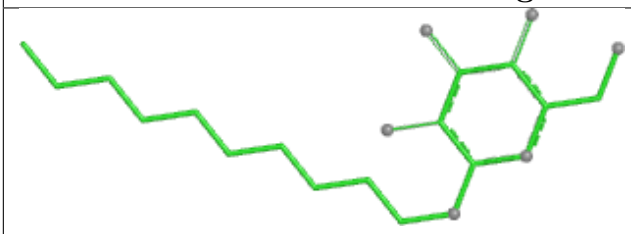
Ligand LFA P 309



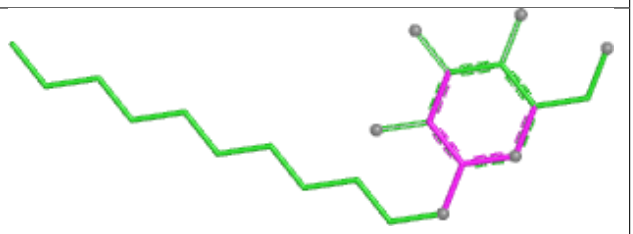
Ligand DMU N 608



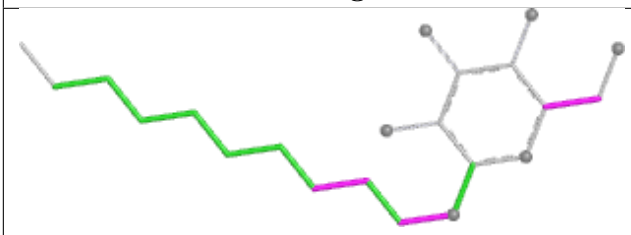
Ligand DMU O 304



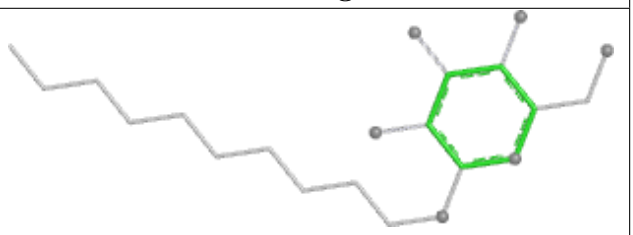
Bond lengths



Bond angles

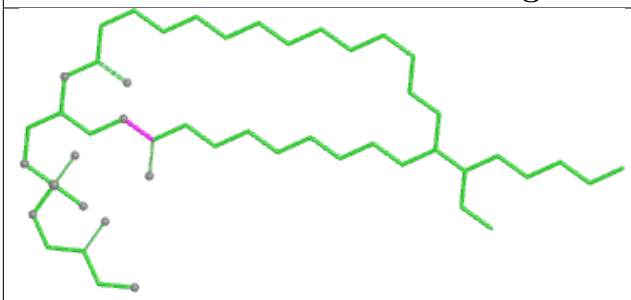


Torsions

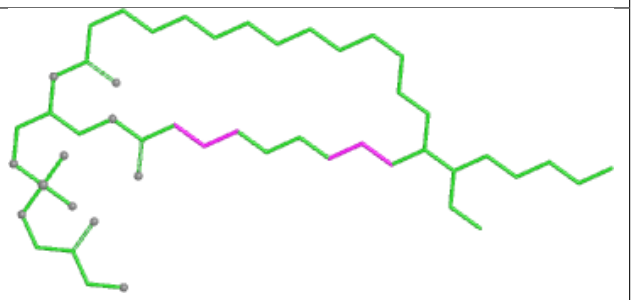


Rings

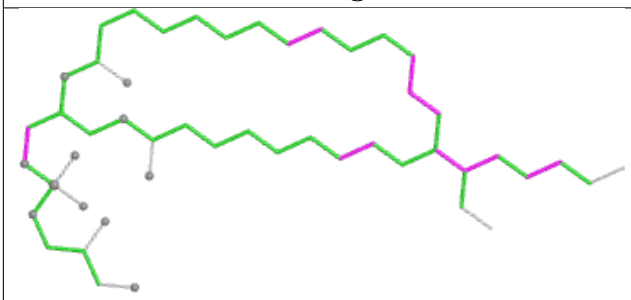
Ligand PGV P 303



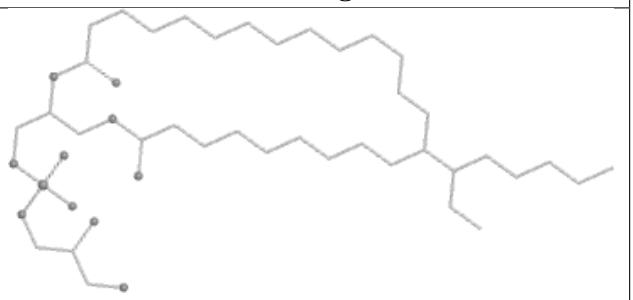
Bond lengths



Bond angles

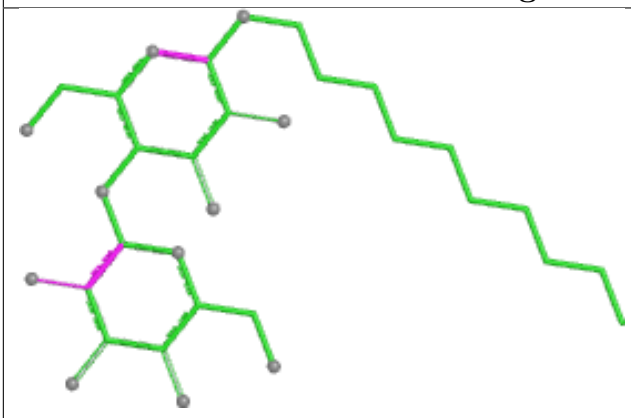


Torsions

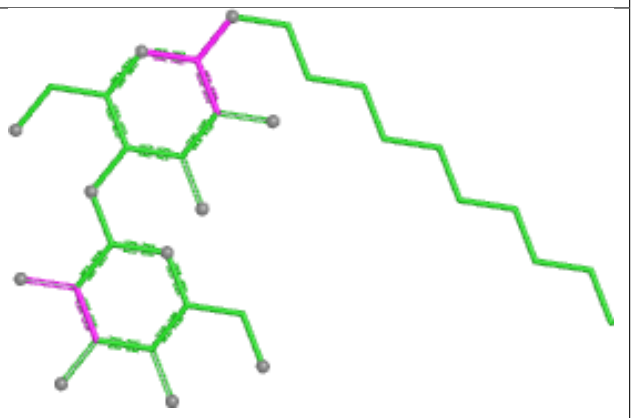


Rings

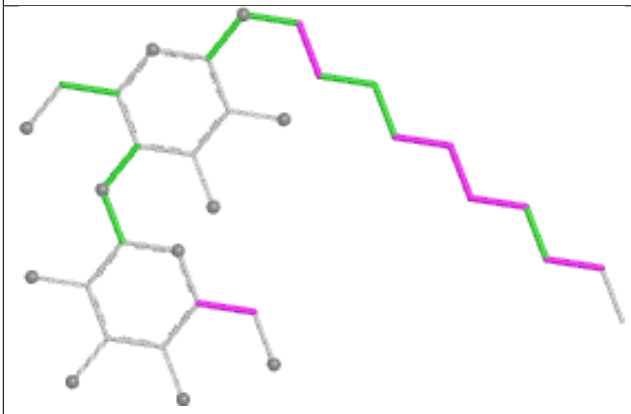
Ligand DMU Z 101



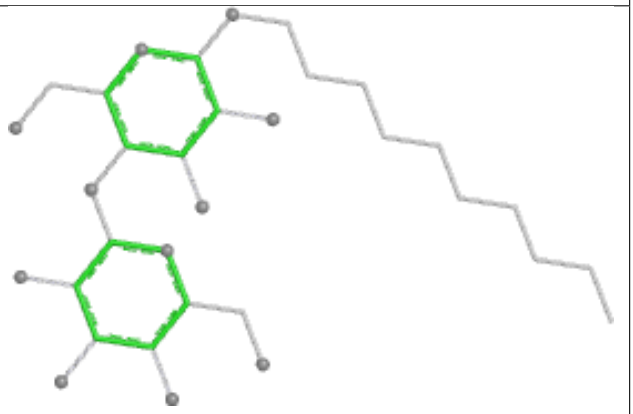
Bond lengths



Bond angles

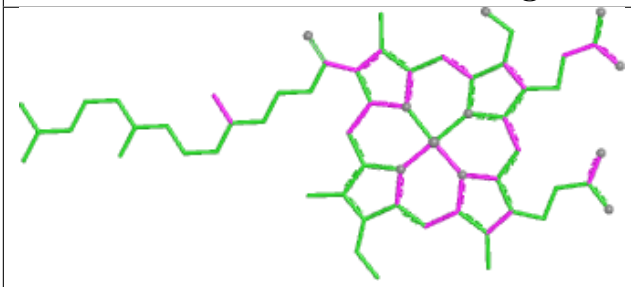


Torsions

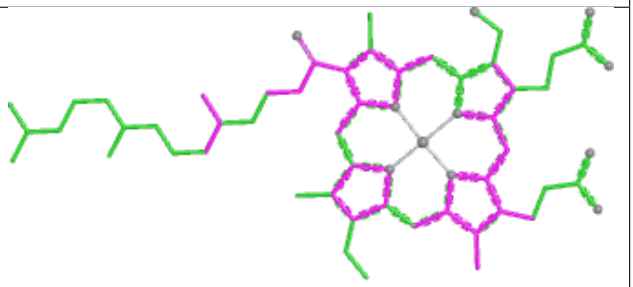


Rings

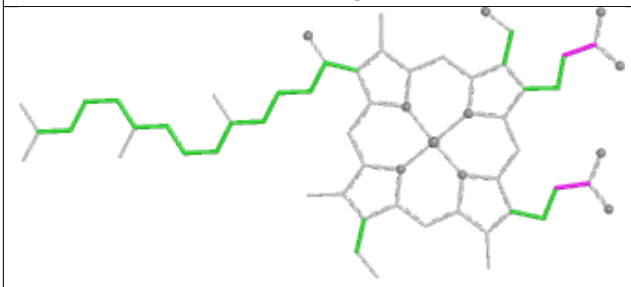
Ligand HEA N 601



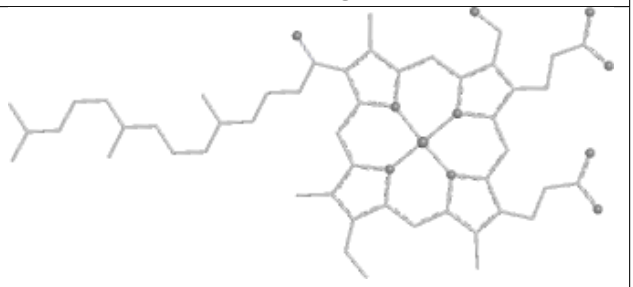
Bond lengths



Bond angles

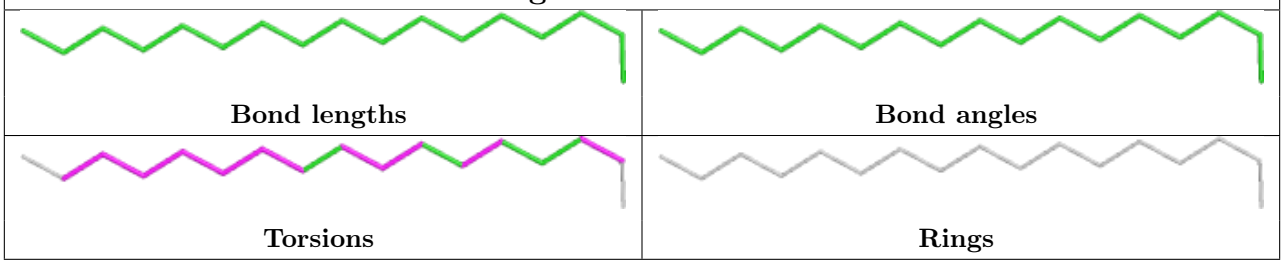


Torsions



Rings

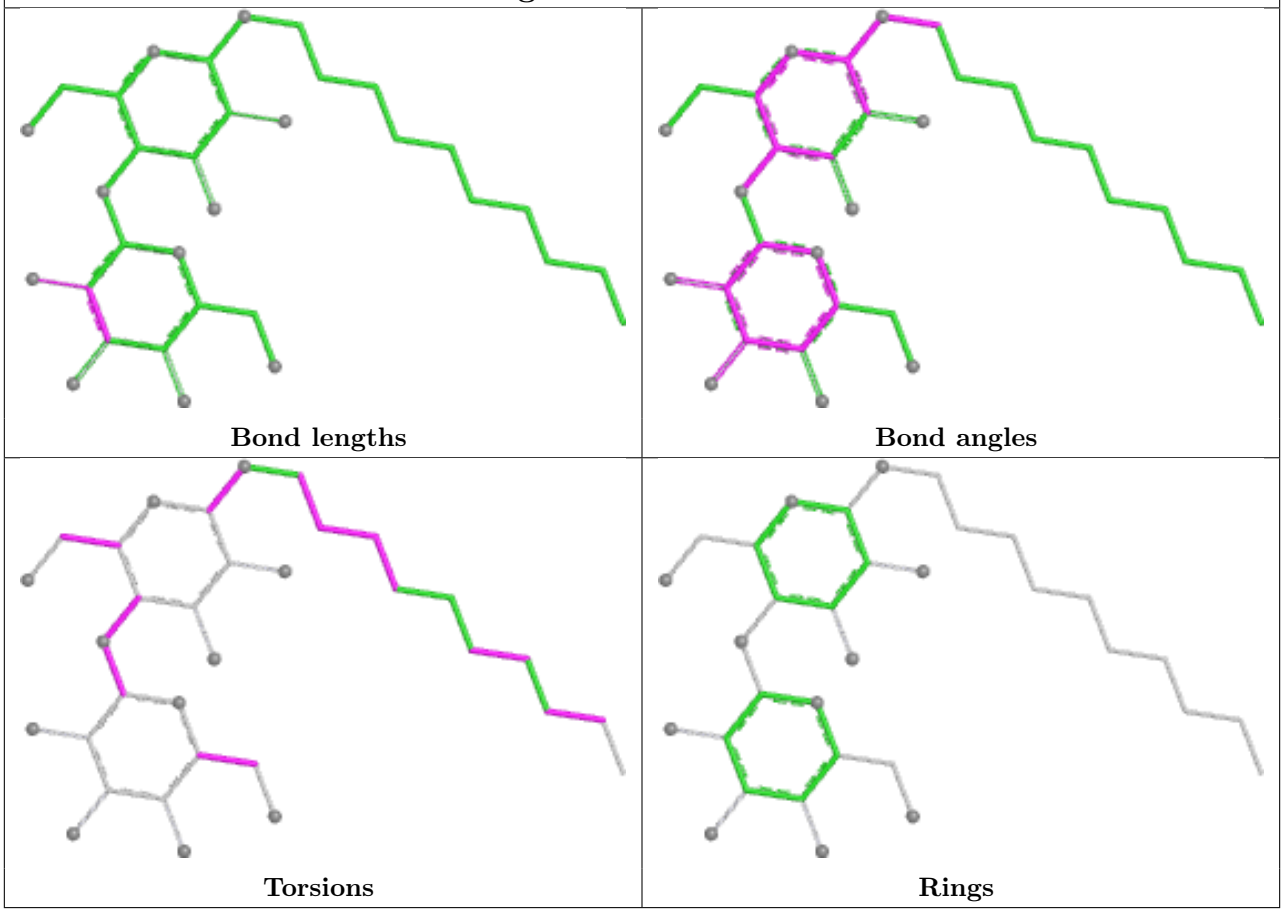
Ligand LFA B 307



Bond lengths | Bond angles

Torsions | Rings

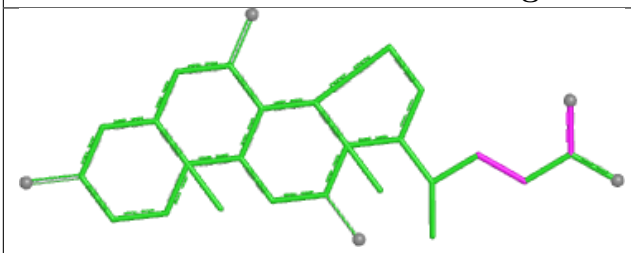
Ligand DMU C 316



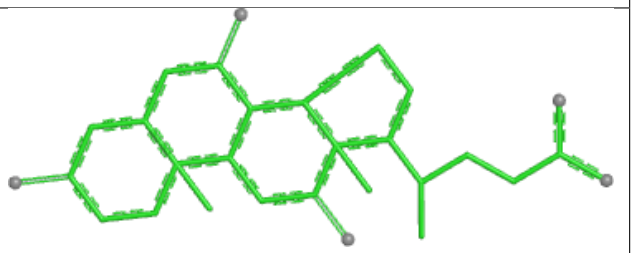
Bond lengths | Bond angles

Torsions | Rings

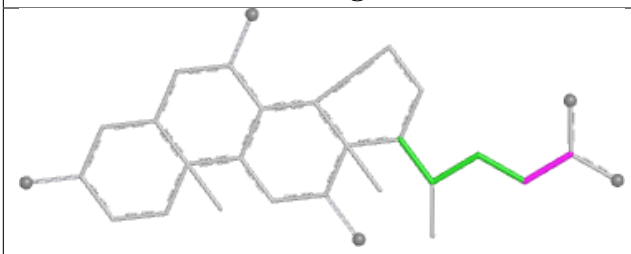
Ligand CHD P 301



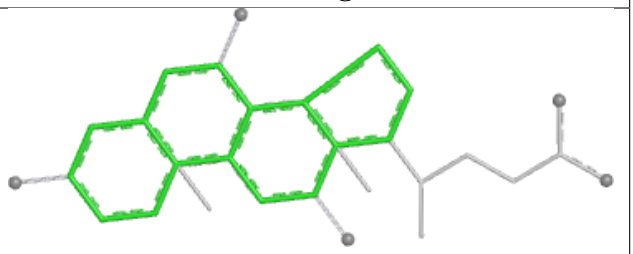
Bond lengths



Bond angles

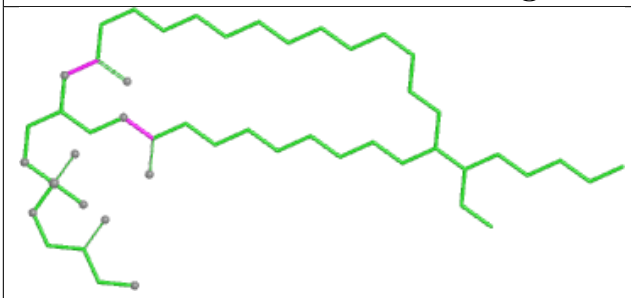


Torsions

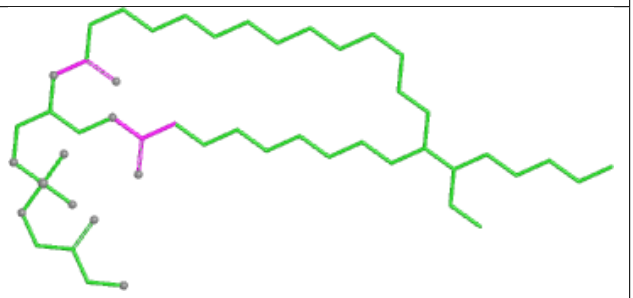


Rings

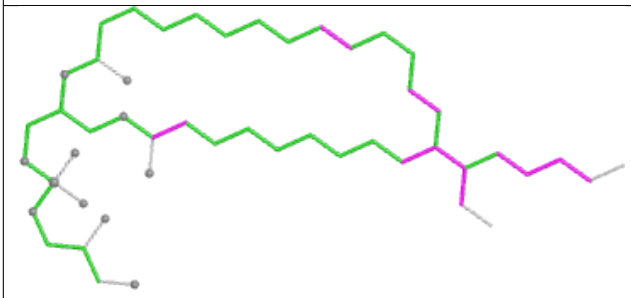
Ligand PGV N 615



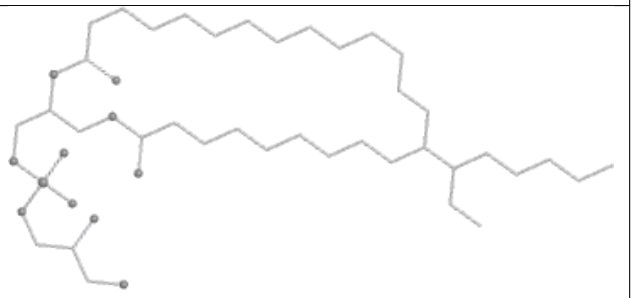
Bond lengths



Bond angles

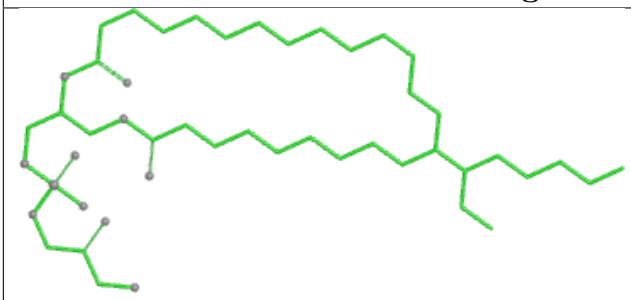


Torsions

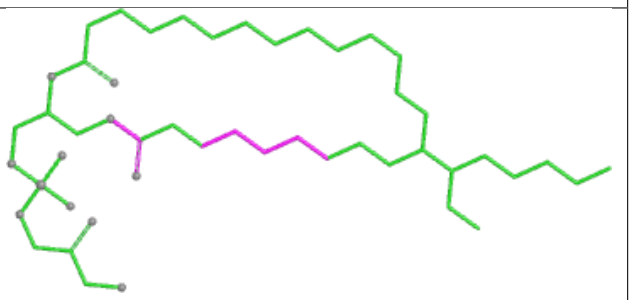


Rings

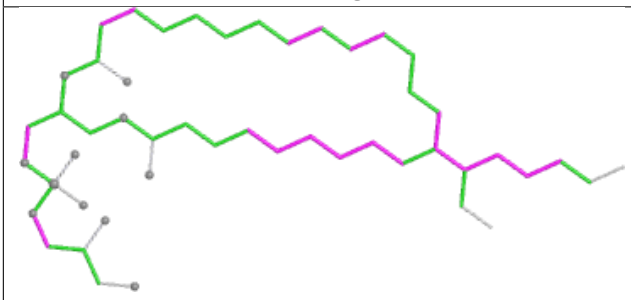
Ligand PGV C 303



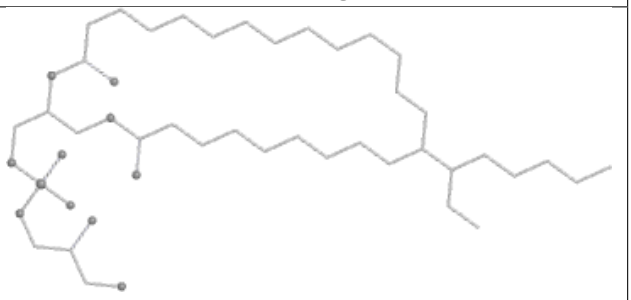
Bond lengths



Bond angles



Torsions



Rings

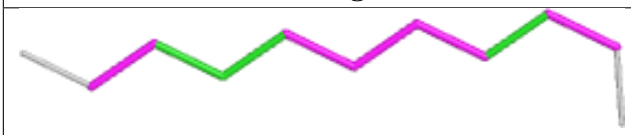
Ligand LFA P 311



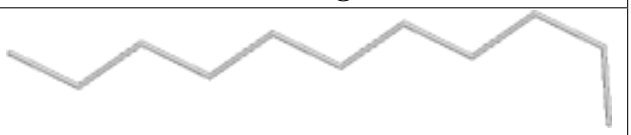
Bond lengths



Bond angles

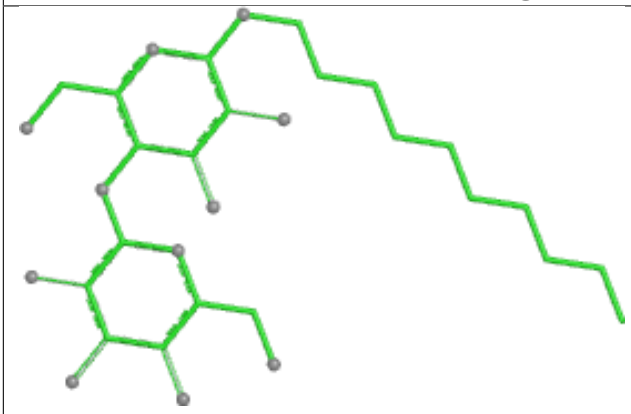


Torsions

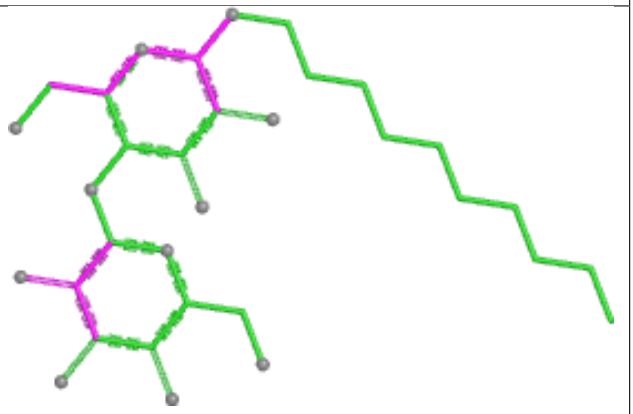


Rings

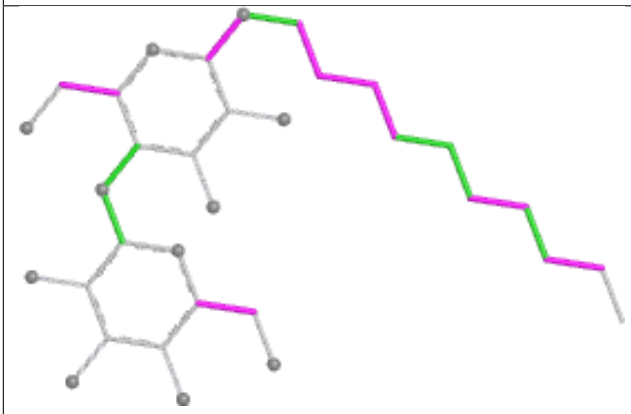
Ligand DMU C 320



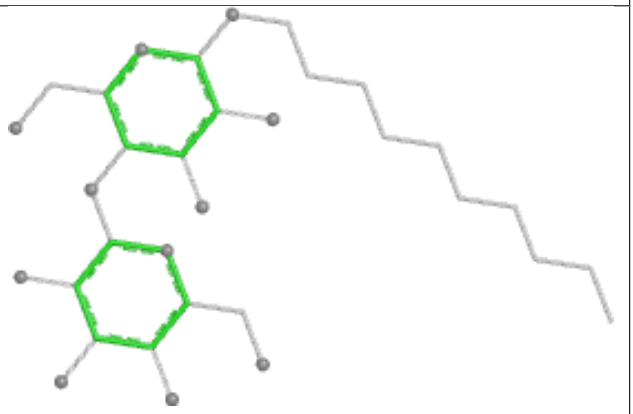
Bond lengths



Bond angles

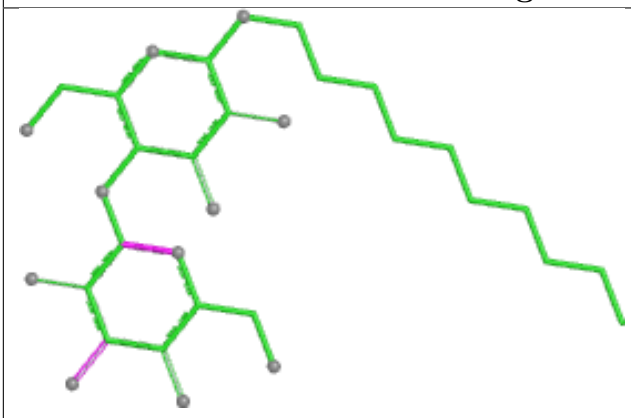


Torsions

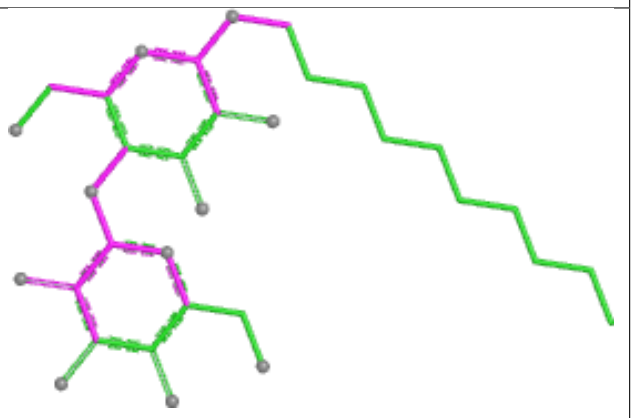


Rings

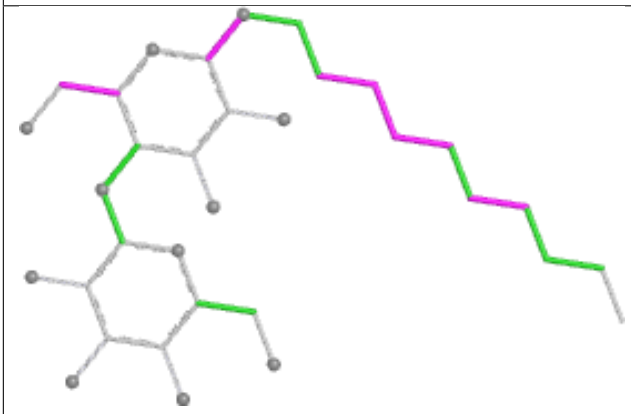
Ligand DMU N 616



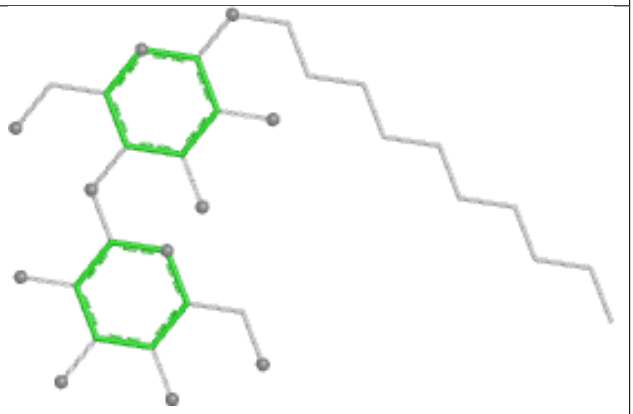
Bond lengths



Bond angles

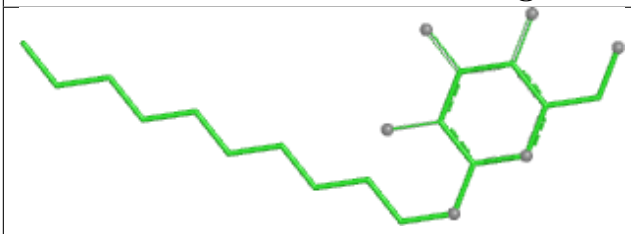


Torsions

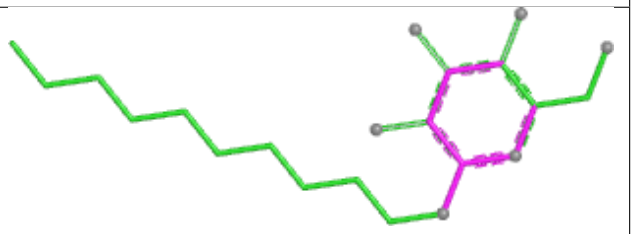


Rings

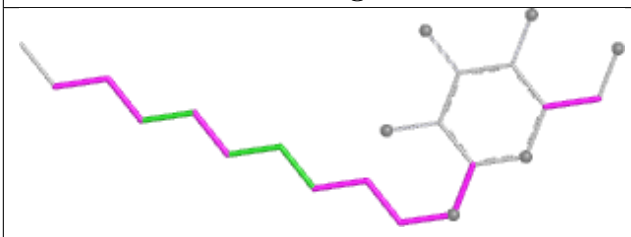
Ligand DMU B 308



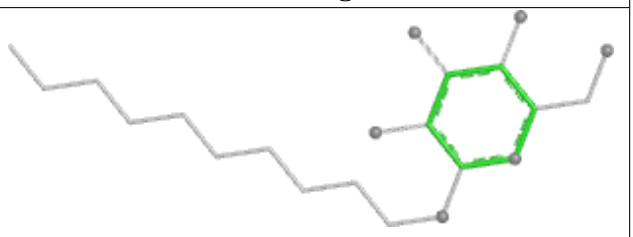
Bond lengths



Bond angles

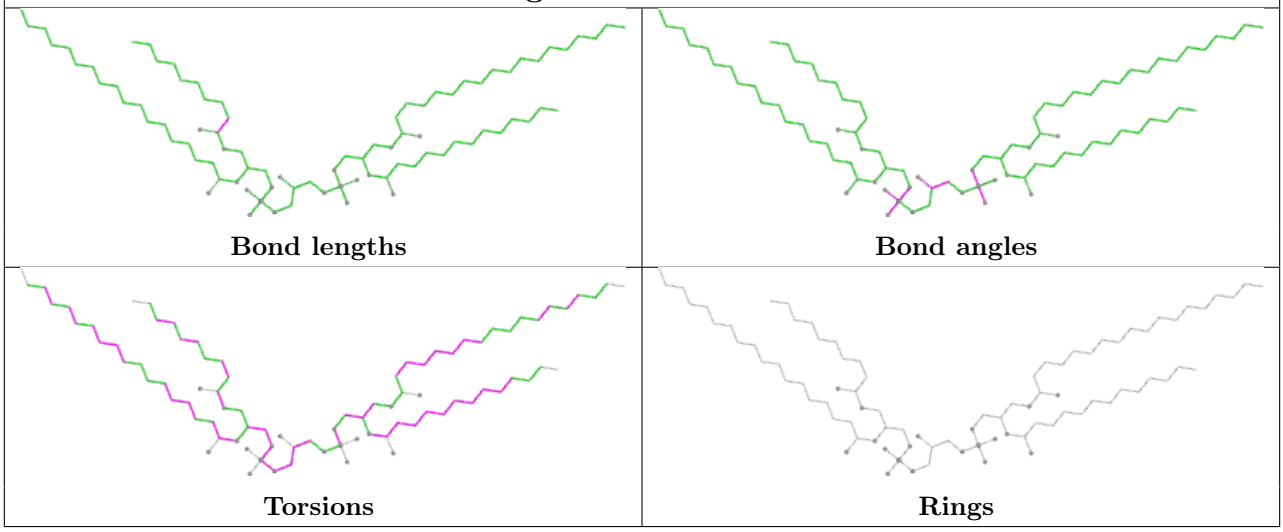


Torsions

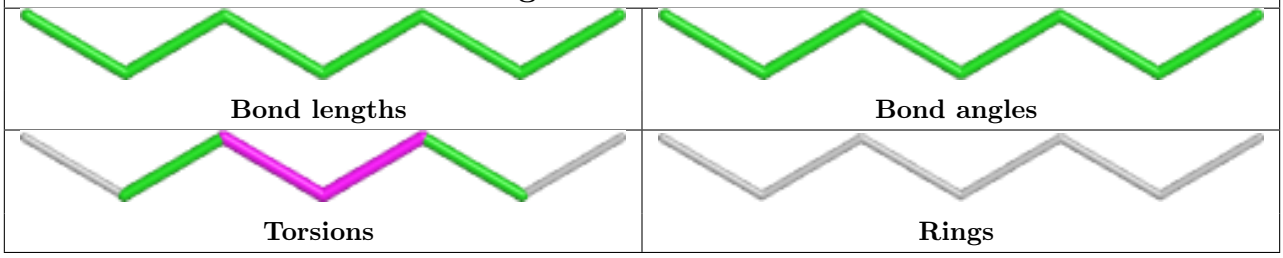


Rings

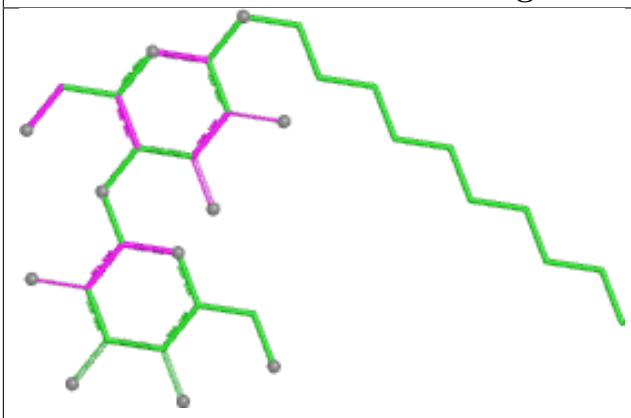
Ligand CDL P 304



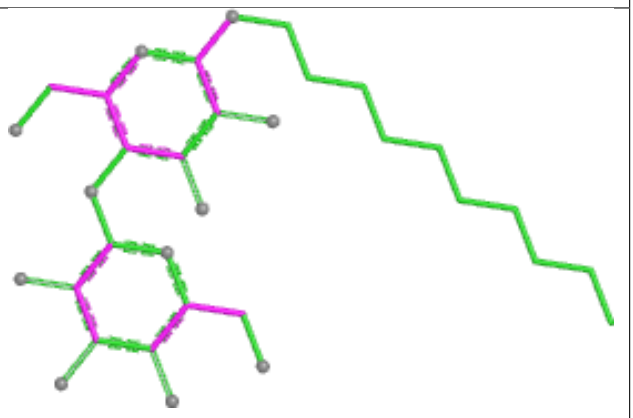
Ligand DMU P 315



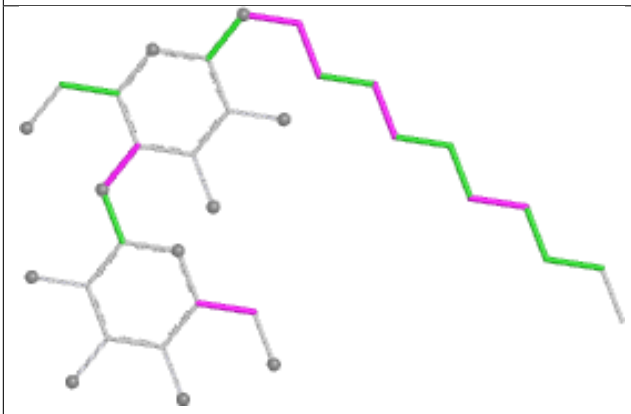
Ligand DMU D 201



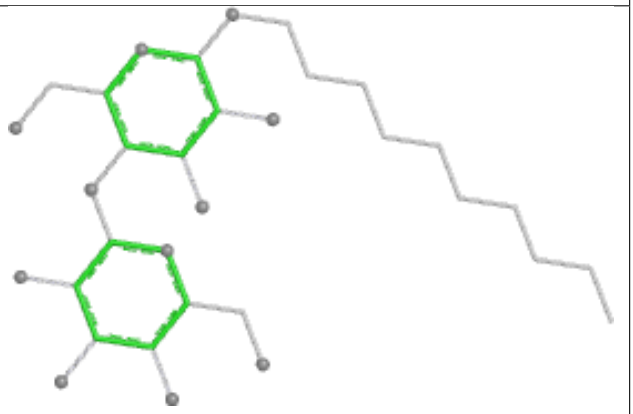
Bond lengths



Bond angles

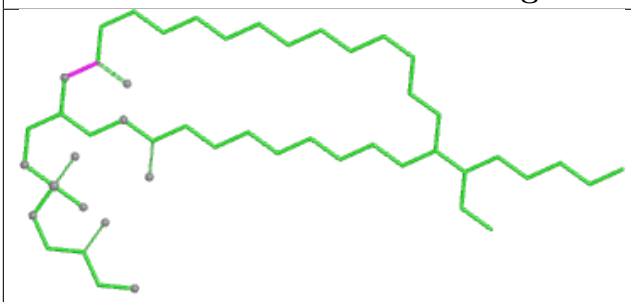


Torsions



Rings

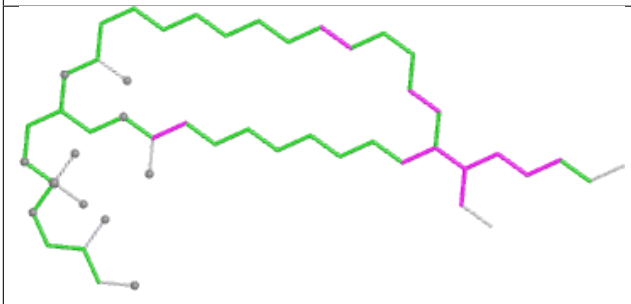
Ligand PGV A 614



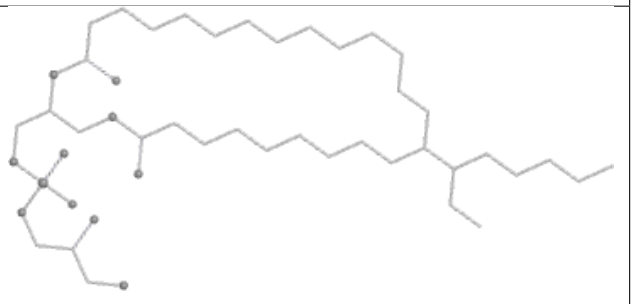
Bond lengths



Bond angles

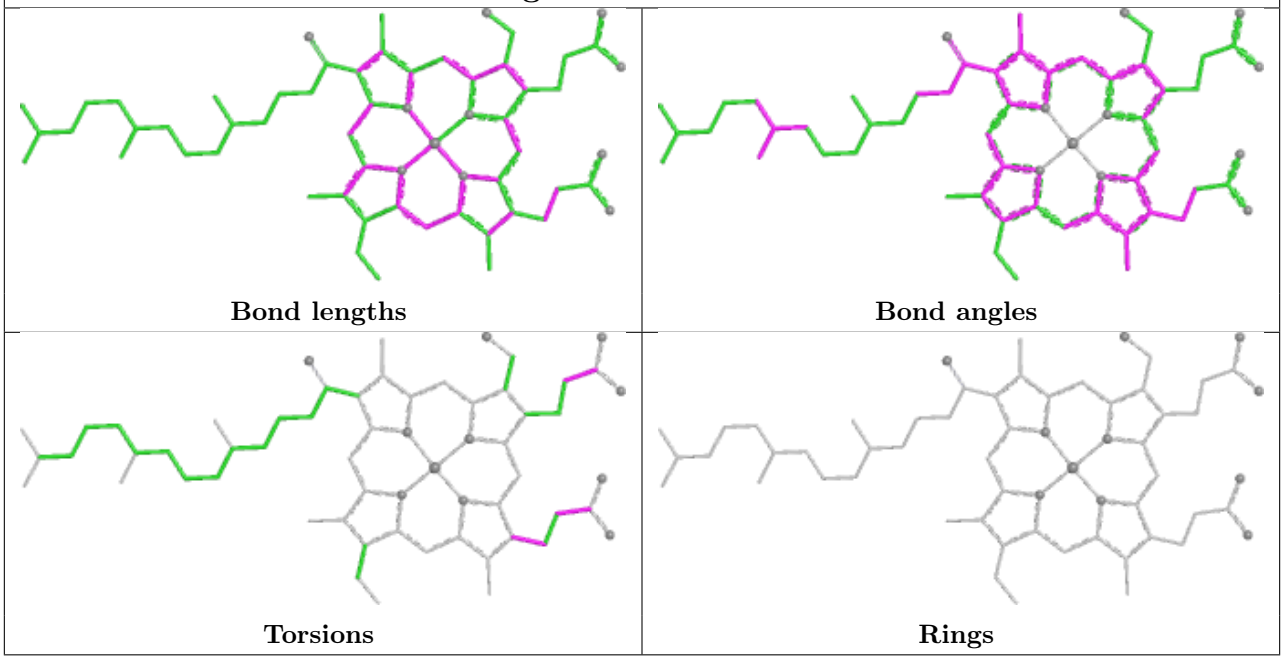


Torsions

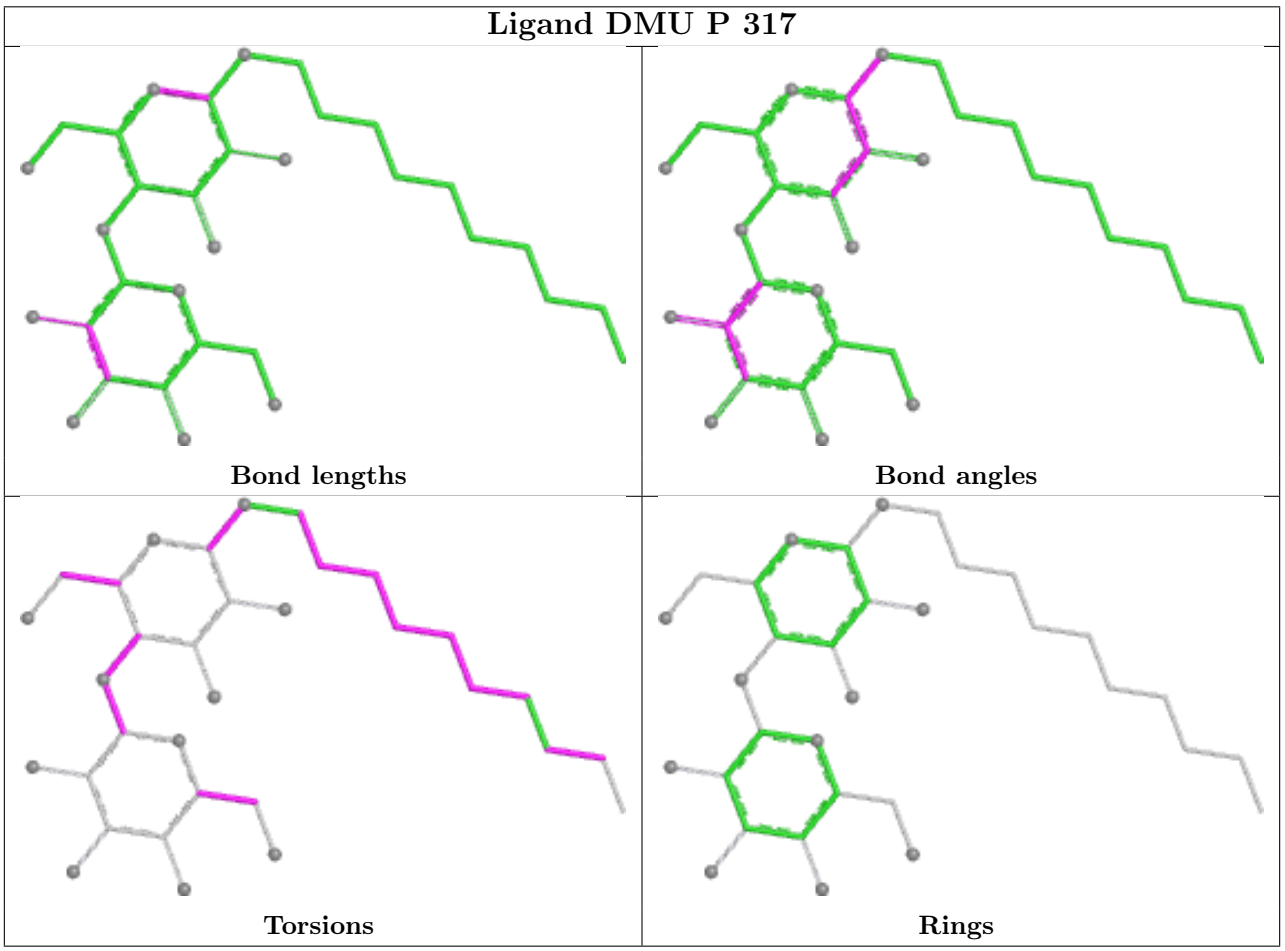


Rings

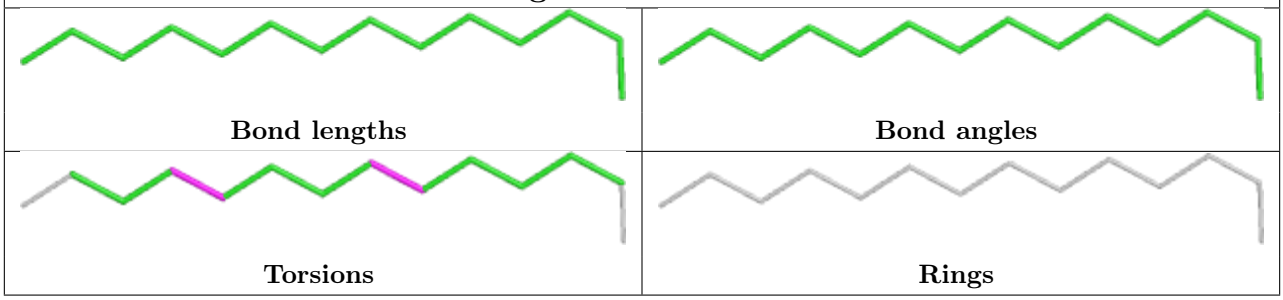
Ligand HEA A 602



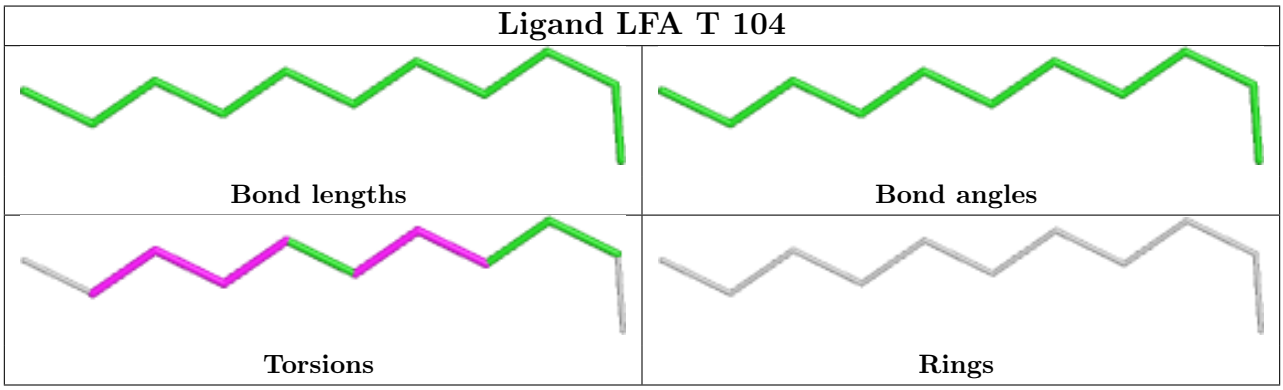
Ligand DMU P 317



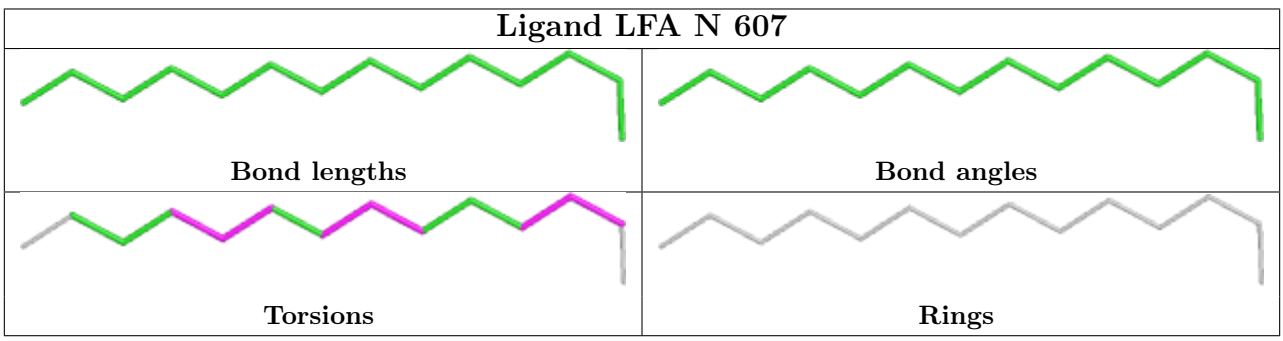
Ligand LFA T 101



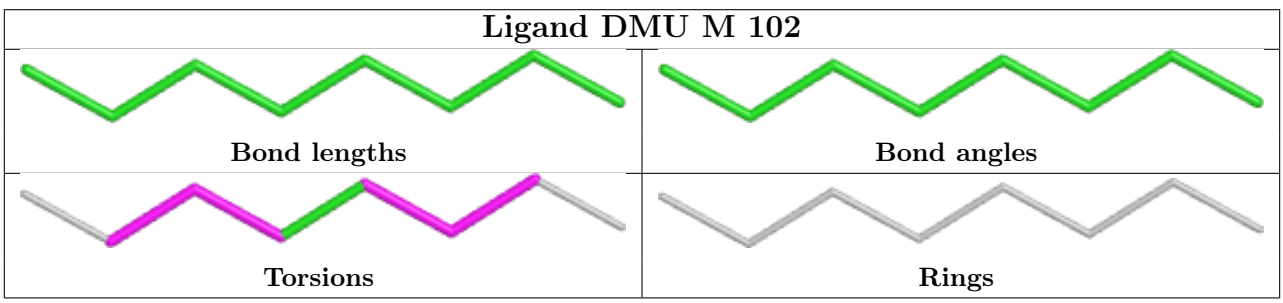
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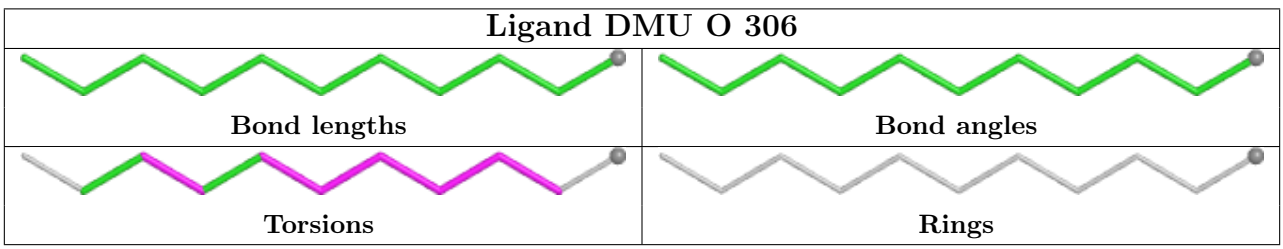
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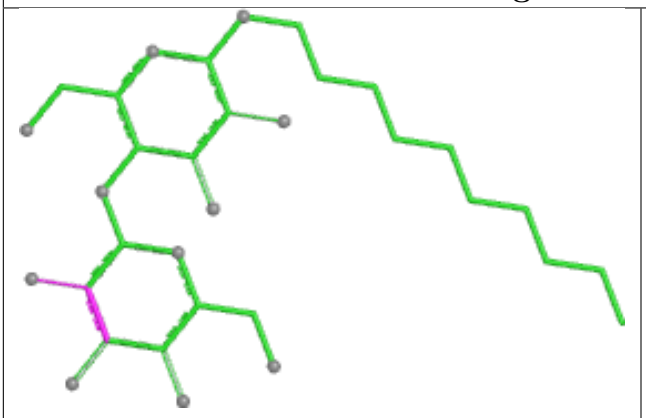
Ligand DMU M 102



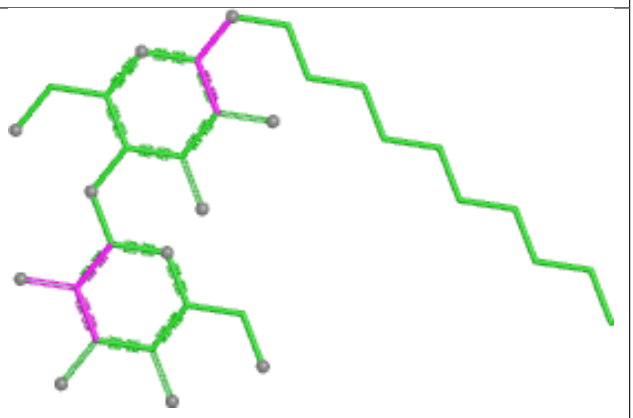
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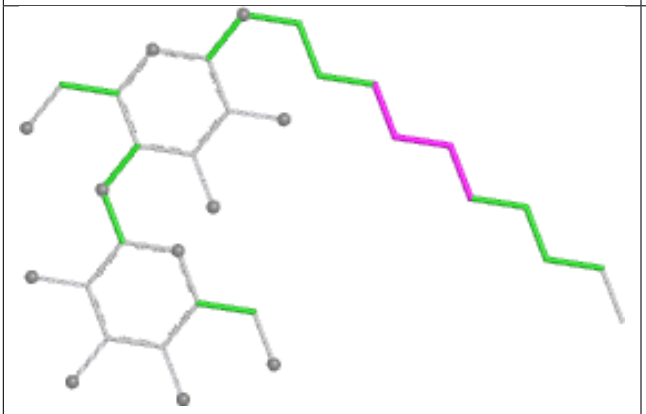
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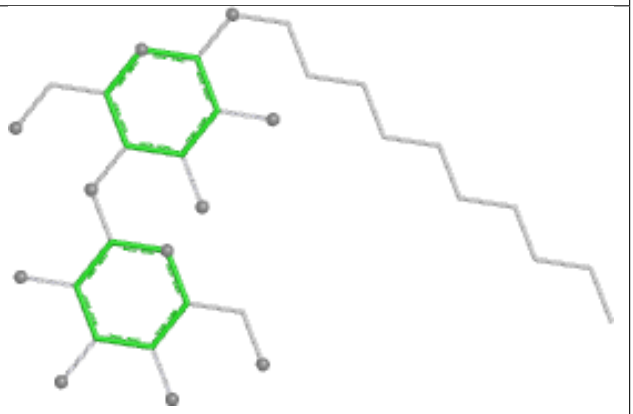
Bond lengths



Bond angles

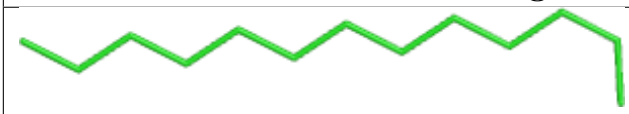


Torsions

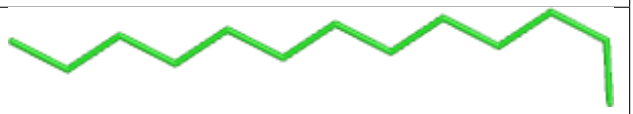


Rings

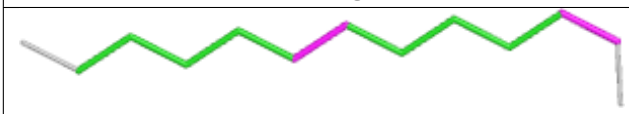
Ligand LFA P 313



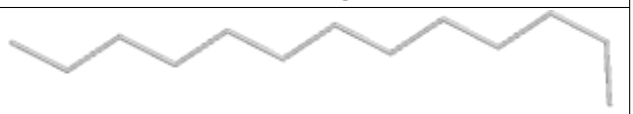
Bond lengths



Bond angles

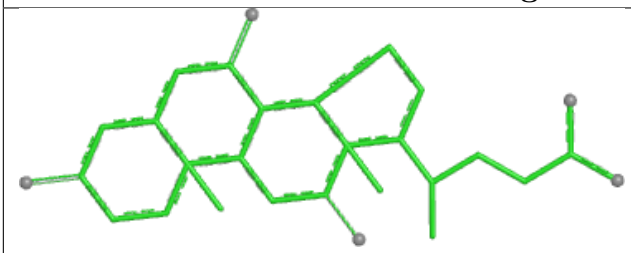


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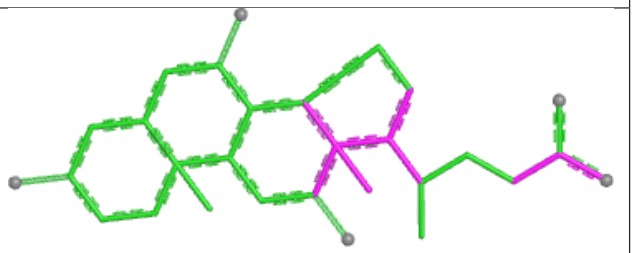


Rings

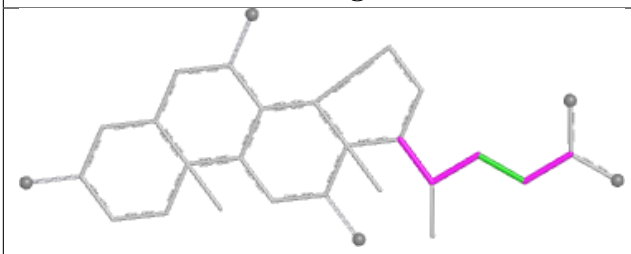
Ligand CHD C 305



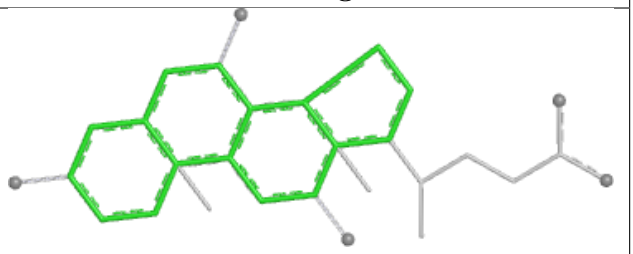
Bond lengths



Bond angles

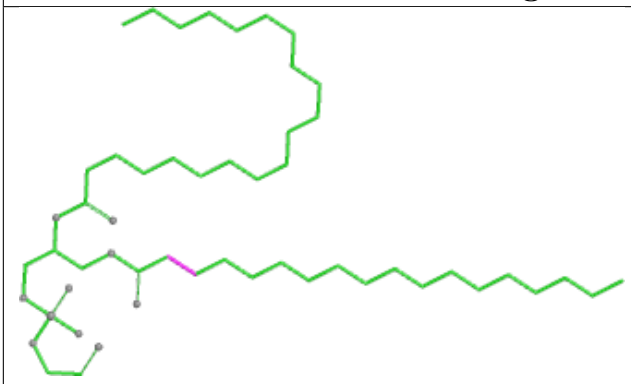


Torsions

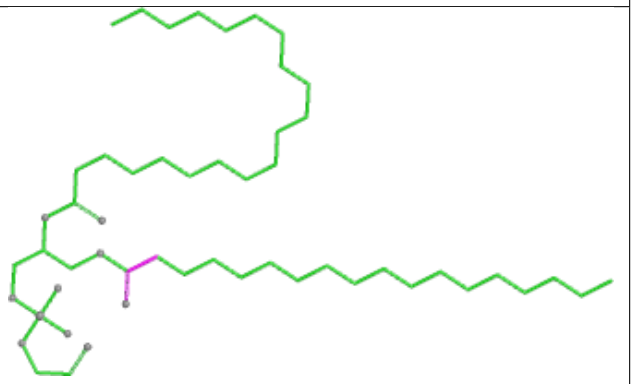


Rings

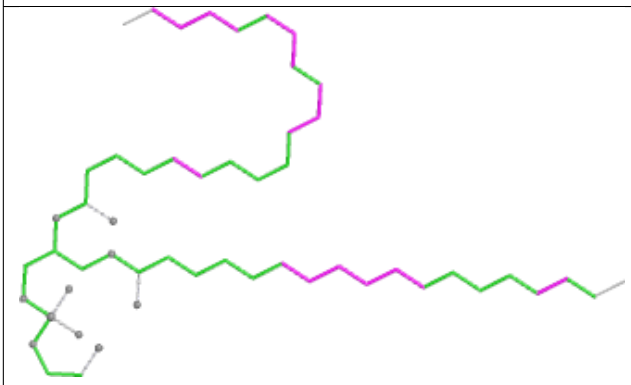
Ligand PEK G 101



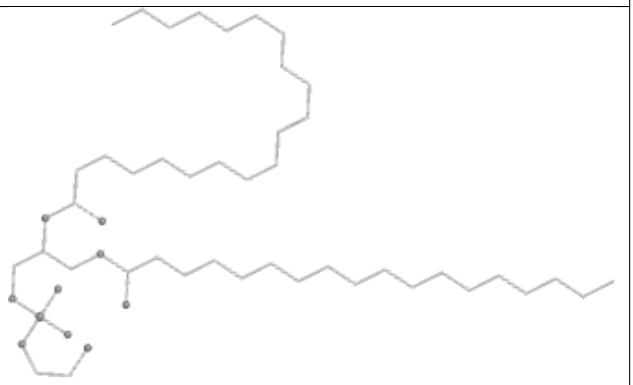
Bond lengths



Bond angles

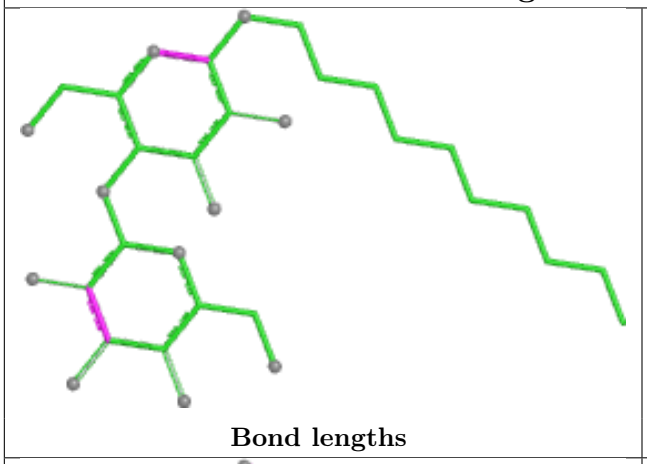


Torsions

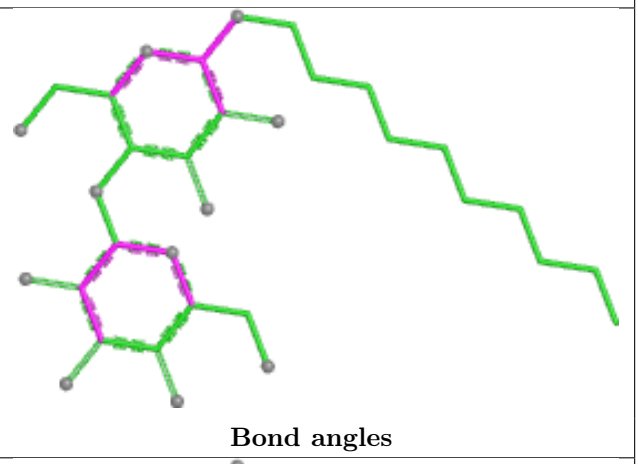


Rings

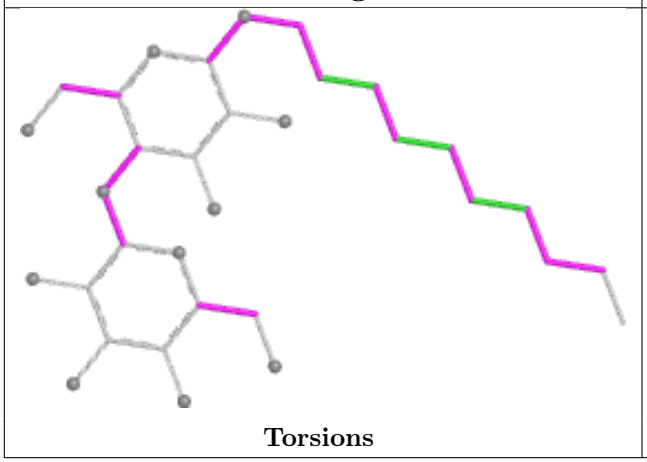
Ligand DMU C 319



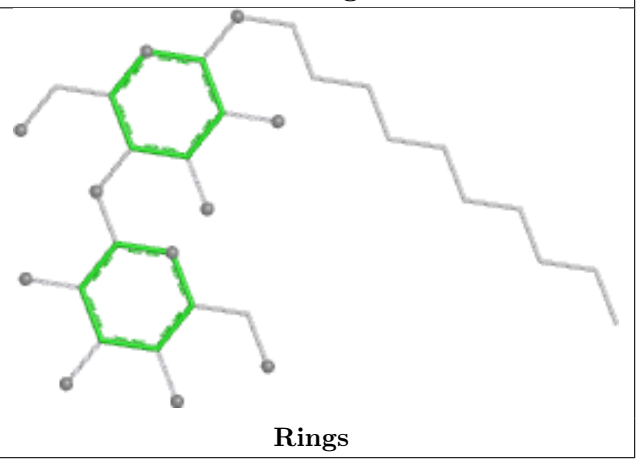
Bond lengths



Bond angles

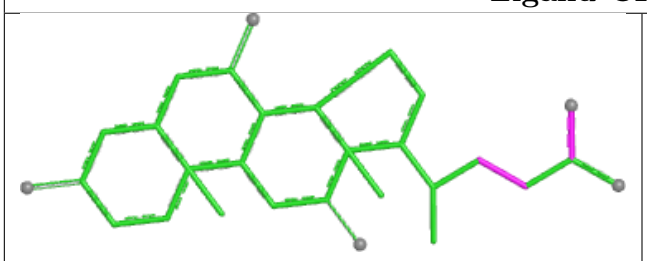


Torsions

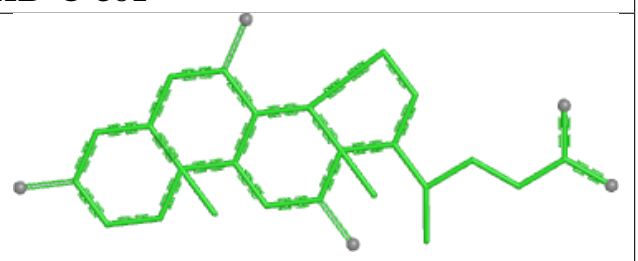


Rings

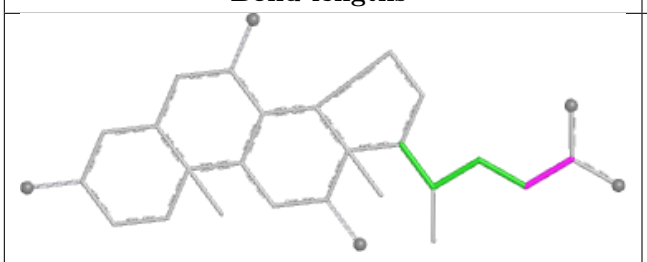
Ligand CHD C 301



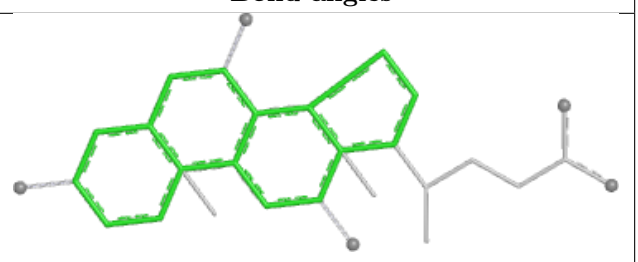
Bond lengths



Bond angles

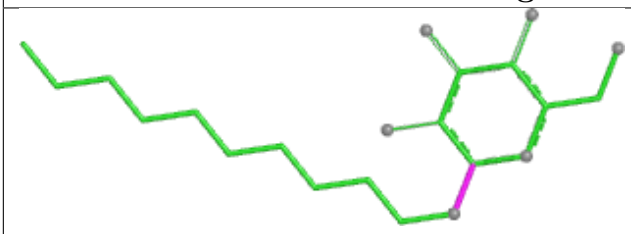


Torsions

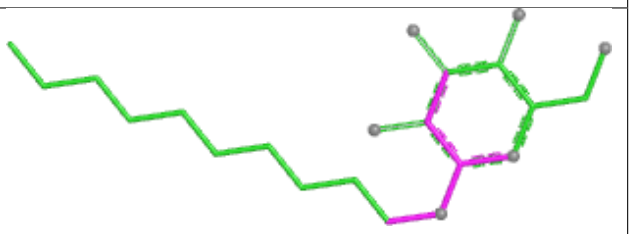


Rings

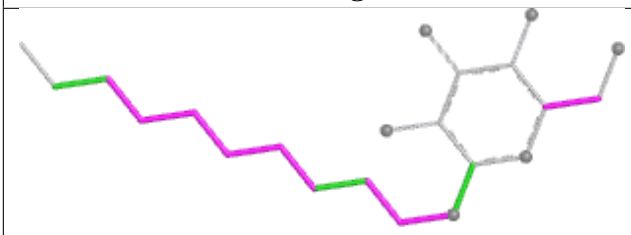
Ligand DMU C 318



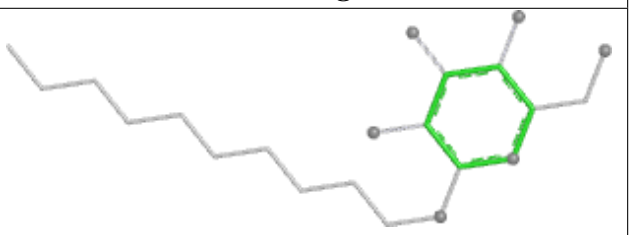
Bond lengths



Bond angles

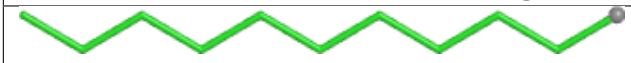


Torsions

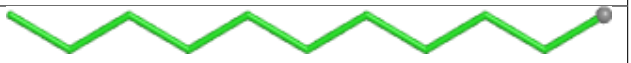


Rings

Ligand DMU P 306



Bond lengths



Bond angles

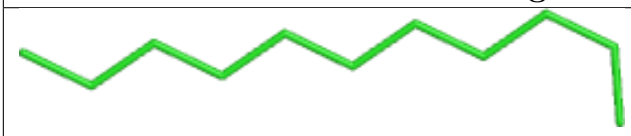


Torsions

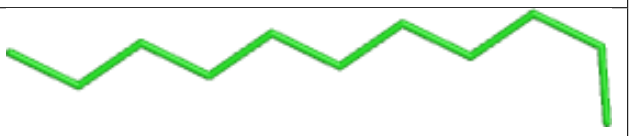


Rings

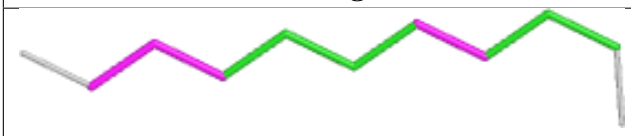
Ligand LFA P 307



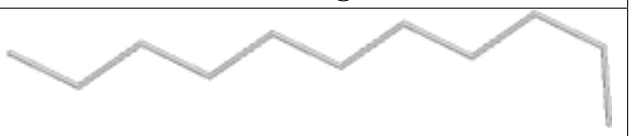
Bond lengths



Bond angles

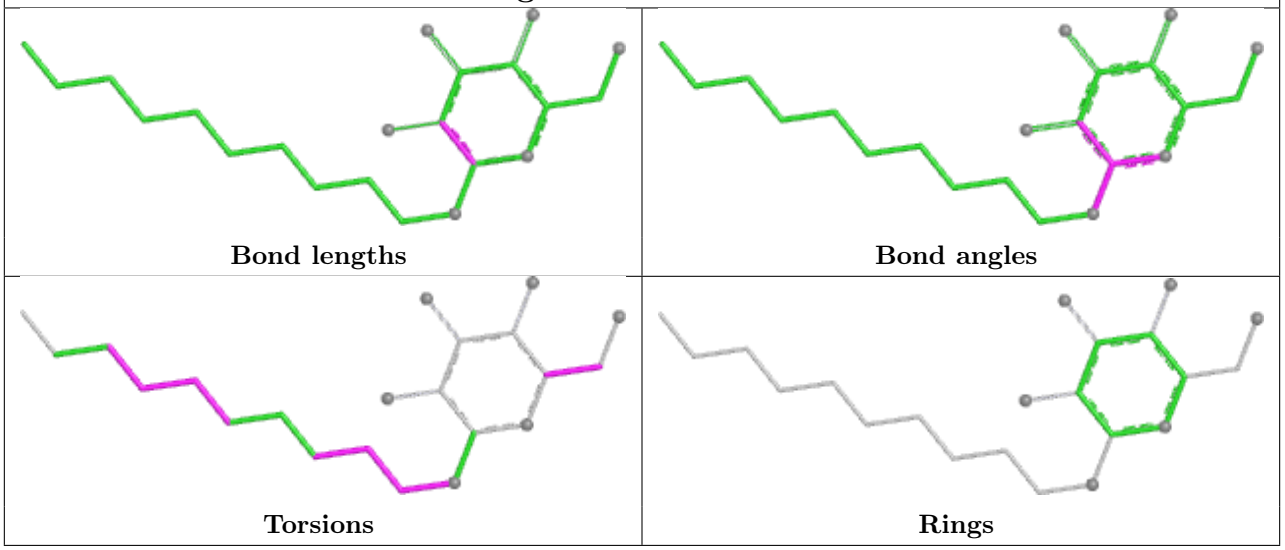


Torsions

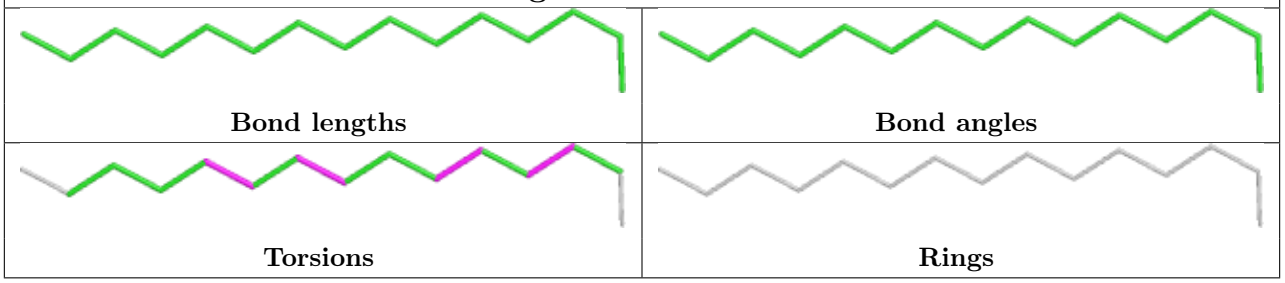


Rings

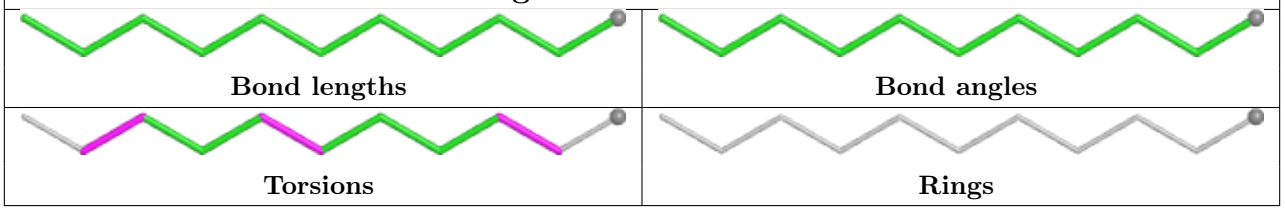
Ligand DMU G 103



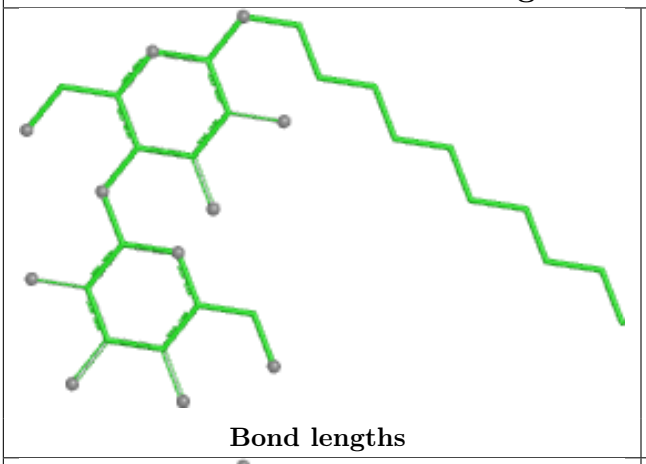
Ligand LFA C 314



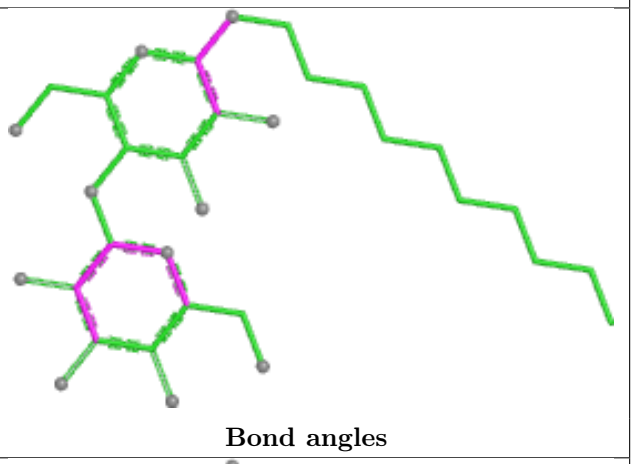
Ligand DMU W 101



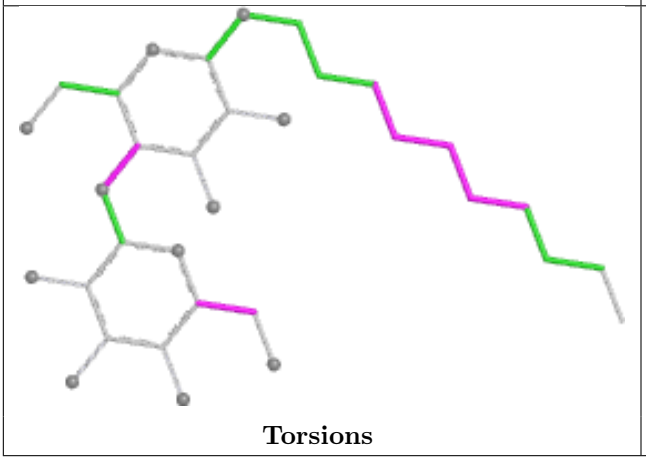
Ligand DMU P 318



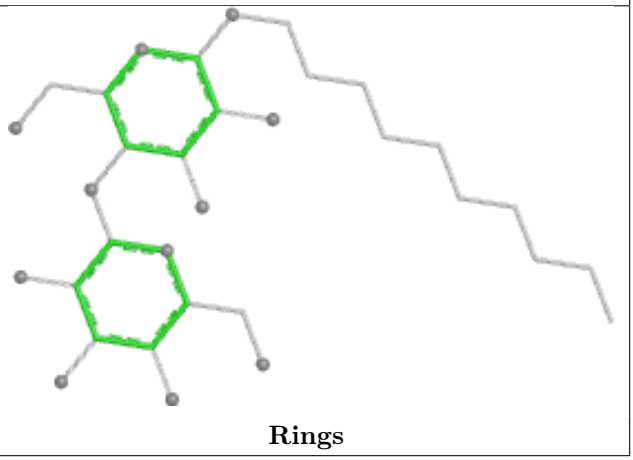
Bond lengths



Bond angles

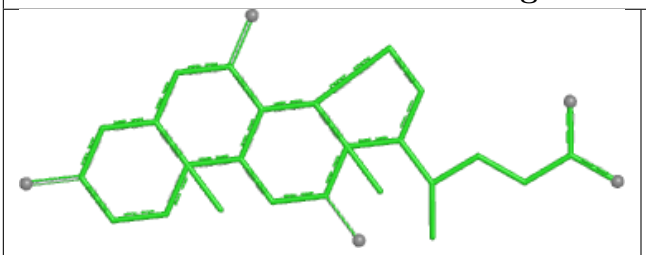


Torsions

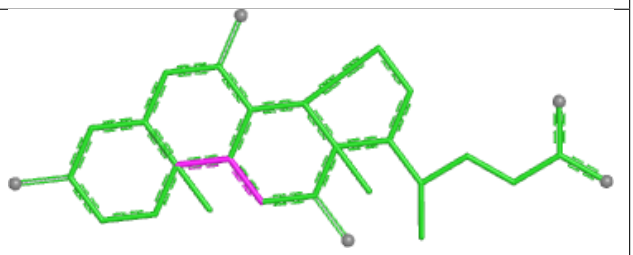


Rings

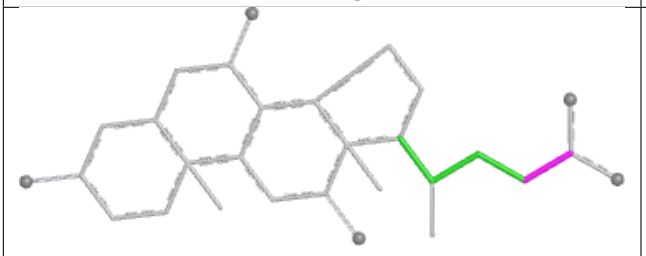
Ligand CHD O 301



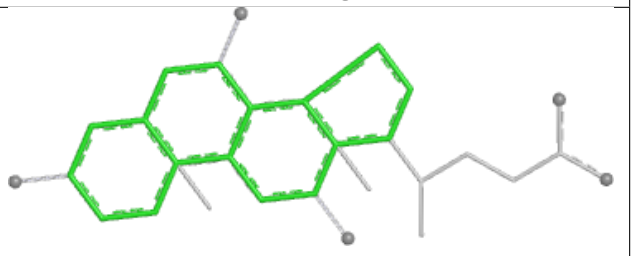
Bond lengths



Bond angles

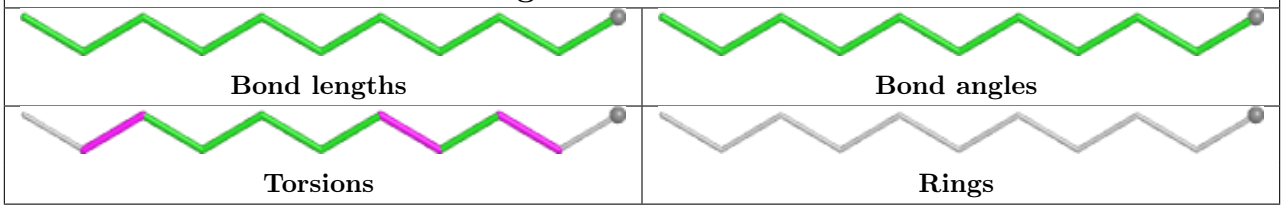


Torsions

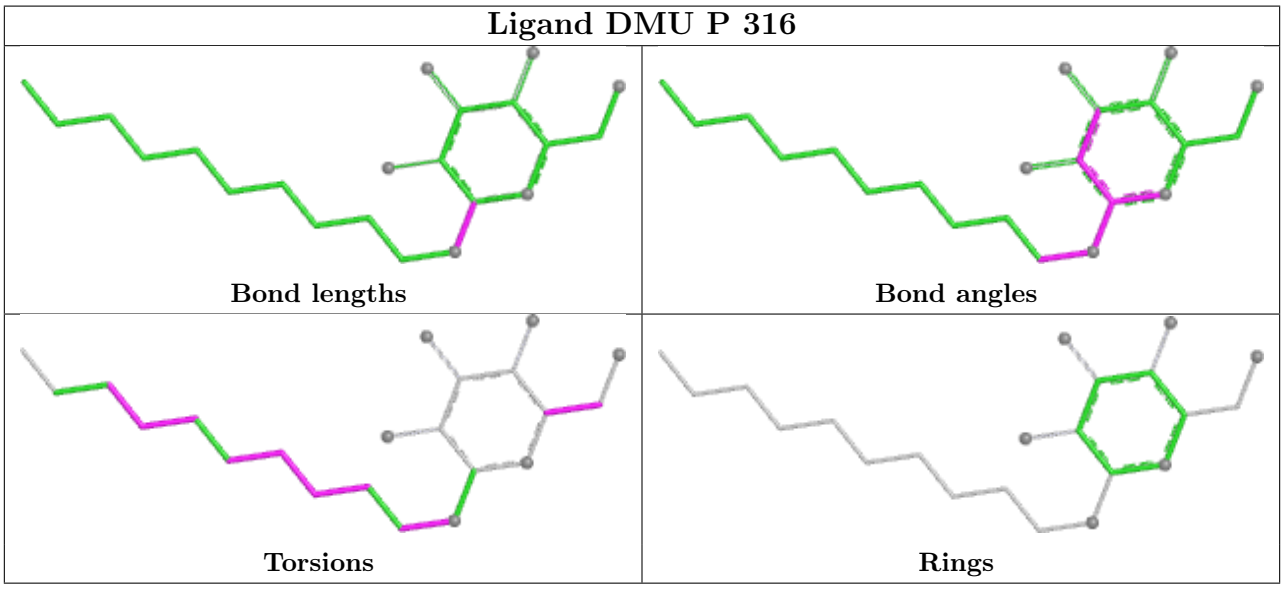


Rings

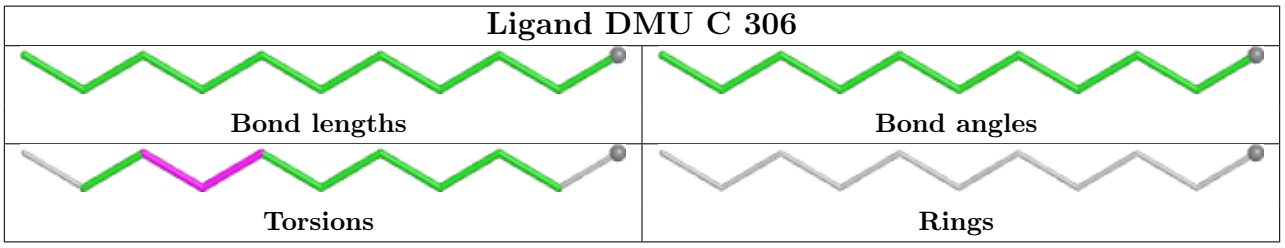
Ligand DMU G 102



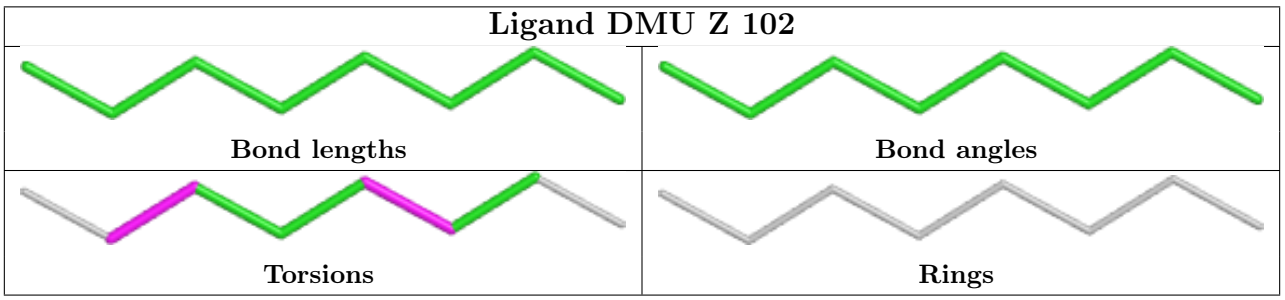
Ligand DMU P 316



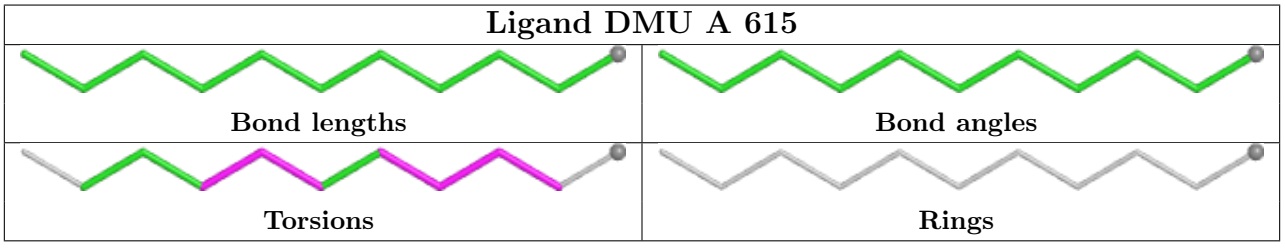
Ligand DMU C 306



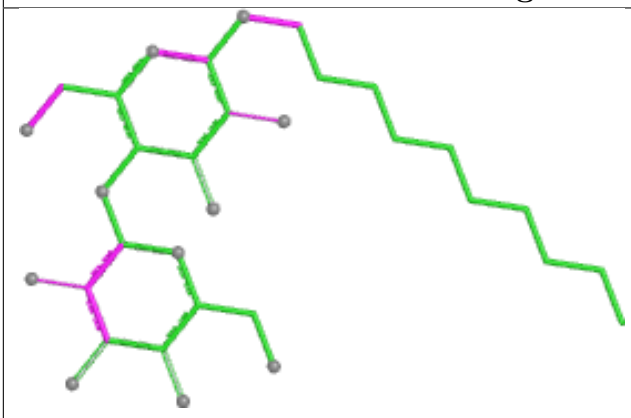
Ligand DMU Z 102



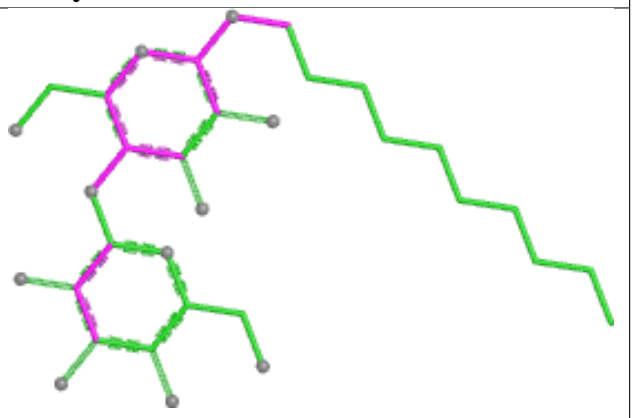
Ligand DMU A 615



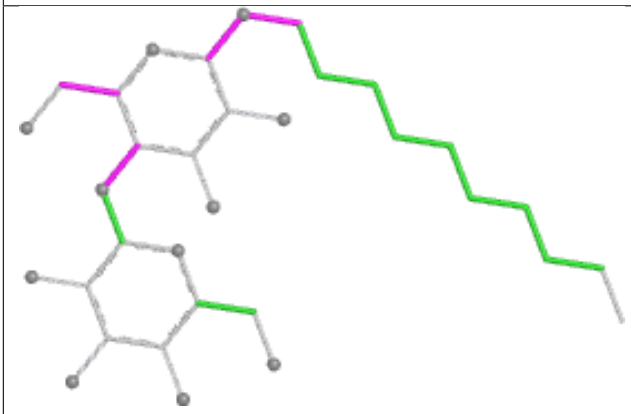
Ligand DMU Q 201



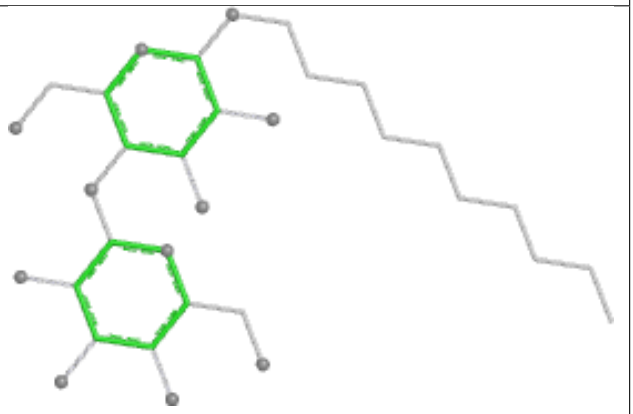
Bond lengths



Bond angles



Torsions



Rings

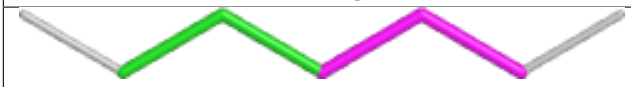
Ligand DMU A 608



Bond lengths



Bond angles

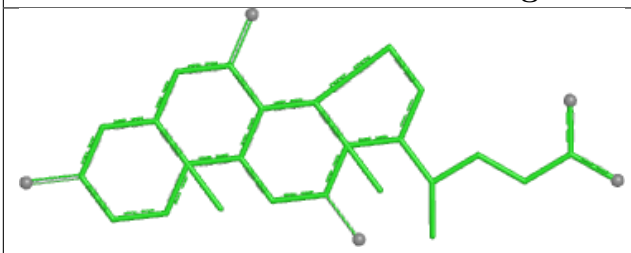


Torsions

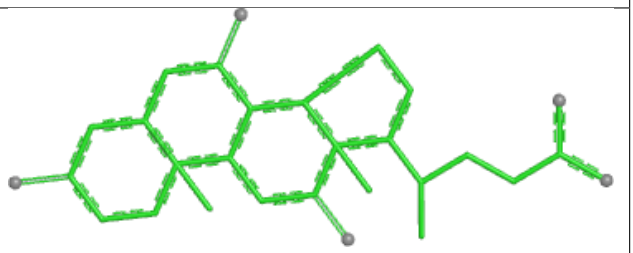


Rings

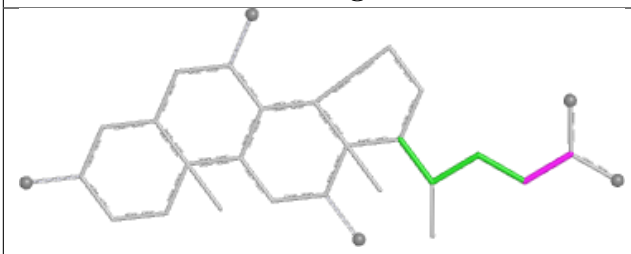
Ligand CHD B 306



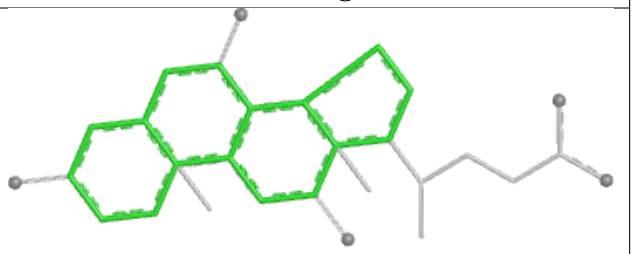
Bond lengths



Bond angles

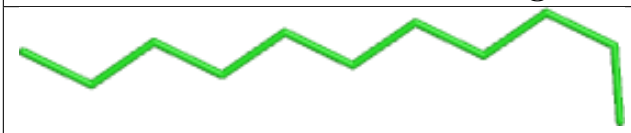


Torsions

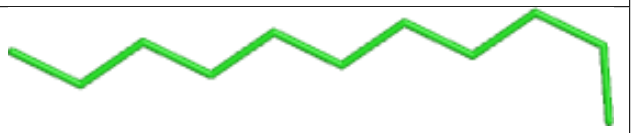


Rings

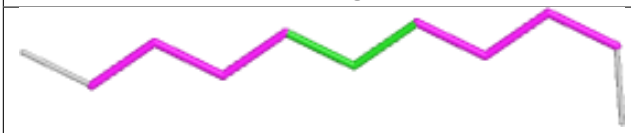
Ligand LFA P 310



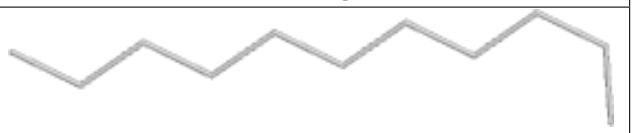
Bond lengths



Bond angles

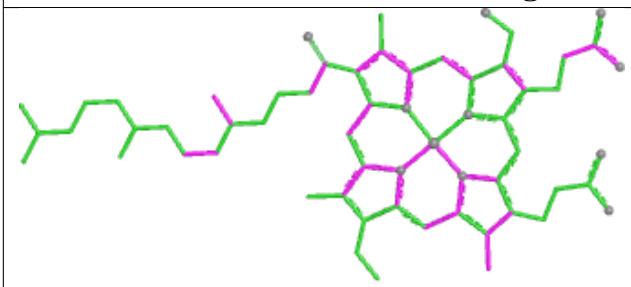


Torsions

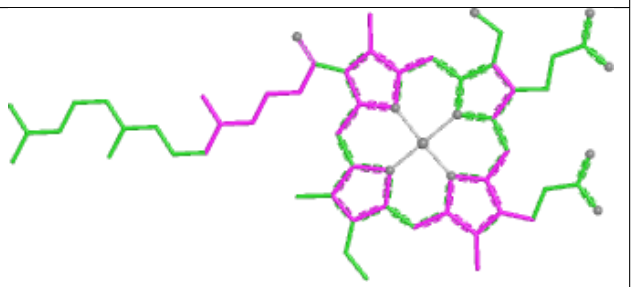


Rings

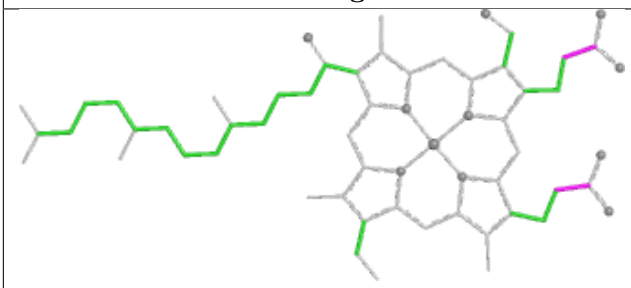
Ligand HEA A 601



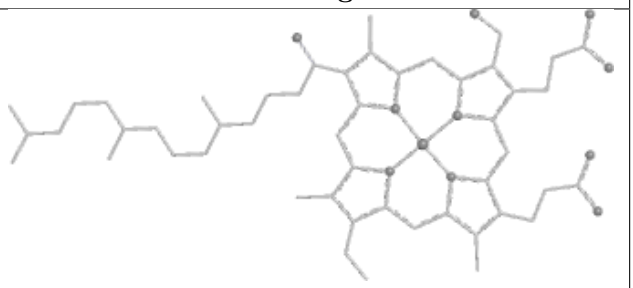
Bond lengths



Bond angles



Torsions



Rings

Ligand DMU C 317	
 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%)	-0.27	2 (0%)	88	90	15, 32, 40, 57	15 (2%)
1	N	512/514 (99%)	-0.07	5 (0%)	79	82	17, 37, 46, 64	15 (2%)
2	B	226/227 (99%)	0.14	11 (4%)	35	38	21, 39, 63, 80	5 (2%)
2	O	226/227 (99%)	0.29	7 (3%)	51	55	23, 46, 72, 93	5 (2%)
3	C	258/261 (98%)	-0.15	1 (0%)	88	90	16, 36, 48, 67	9 (3%)
3	P	258/261 (98%)	-0.07	1 (0%)	88	90	16, 37, 51, 74	9 (3%)
4	D	143/147 (97%)	0.13	3 (2%)	63	68	20, 42, 56, 74	1 (0%)
4	Q	137/147 (93%)	0.58	11 (8%)	18	19	24, 56, 80, 107	1 (0%)
5	E	102/109 (93%)	-0.08	1 (0%)	79	82	35, 42, 56, 73	0
5	R	102/109 (93%)	0.20	3 (2%)	53	58	38, 49, 66, 85	0
6	F	91/98 (92%)	0.17	2 (2%)	62	66	20, 42, 67, 76	2 (2%)
6	S	91/98 (92%)	0.23	3 (3%)	49	53	20, 42, 65, 75	2 (2%)
7	G	72/85 (84%)	0.37	7 (9%)	13	14	21, 43, 88, 110	1 (1%)
7	T	72/85 (84%)	0.44	4 (5%)	30	33	22, 45, 93, 104	1 (1%)
8	H	75/85 (88%)	0.42	6 (8%)	18	19	36, 46, 104, 113	0
8	U	75/85 (88%)	0.60	5 (6%)	24	26	42, 50, 95, 128	0
9	I	70/73 (95%)	0.53	6 (8%)	16	17	38, 50, 74, 92	0
9	V	70/73 (95%)	0.70	7 (10%)	12	13	38, 59, 76, 100	0
10	J	56/59 (94%)	0.36	3 (5%)	31	34	37, 46, 69, 79	0
10	W	56/59 (94%)	0.51	4 (7%)	22	24	40, 50, 74, 82	0
11	K	49/56 (87%)	0.47	2 (4%)	41	45	39, 47, 66, 80	0
11	X	49/56 (87%)	0.83	3 (6%)	27	29	49, 60, 76, 104	0
12	L	44/47 (93%)	0.03	0	100	100	33, 38, 50, 59	0
12	Y	44/47 (93%)	0.41	1 (2%)	61	65	41, 48, 64, 71	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	40/46 (86%)	0.29	1 (2%) 58 62	36, 39, 62, 76	0
13	Z	40/46 (86%)	0.66	2 (5%) 34 38	46, 52, 83, 92	0
All	All	3470/3614 (96%)	0.12	101 (2%) 53 58	15, 40, 68, 128	66 (1%)

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	S	93	PRO	6.1
7	T	36	TRP	5.7
8	U	48	GLY	5.4
6	S	3	GLY	5.3
6	F	3	GLY	5.0
2	O	90	ILE	4.9
2	O	113	TYR	4.7
2	B	59	GLN	4.7
1	N	113[A]	LEU	4.6
11	X	6	ALA	4.4
4	D	4	SER	4.4
2	B	16[A]	ILE	4.3
9	V	72	ALA	4.1
7	G	36	TRP	4.1
9	V	3	ALA	4.0
3	P	37	PHE	4.0
11	K	6	ALA	3.8
2	B	90	ILE	3.8
4	Q	10	ASP	3.7
8	H	48	GLY	3.6
8	H	45	ALA	3.5
7	T	38	HIS	3.5
9	I	29	LEU	3.5
4	Q	11	TYR	3.5
2	O	227	LEU	3.4
1	A	113[A]	LEU	3.4
9	V	37	PHE	3.4
4	D	5	VAL	3.3
10	J	52	TRP	3.3
5	R	7	THR	3.3
2	B	87[A]	MET	3.2
2	B	65	TRP	3.2
8	U	45	ALA	3.2
12	Y	24	MET	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	60	GLU	3.1
10	W	52	TRP	3.1
2	O	91	ASN	3.0
9	I	19	PHE	3.0
3	C	38	ASN	3.0
11	X	13	TYR	3.0
8	U	47	GLY	3.0
5	E	7	THR	2.9
2	B	113	TYR	2.8
4	D	11	TYR	2.8
9	V	26	MET	2.8
4	Q	142	LYS	2.8
13	M	40	TYR	2.7
2	O	22[A]	HIS	2.7
8	U	49	ASP	2.7
8	H	43	MET	2.7
9	I	26	MET	2.7
1	N	50	ASP	2.7
4	Q	35	ALA	2.7
8	H	44	THR	2.6
9	I	25	PHE	2.6
10	J	1	PHE	2.6
2	B	227	LEU	2.6
13	Z	40	TYR	2.6
2	O	87[A]	MET	2.5
1	A	298[A]	ASP	2.5
9	I	37	PHE	2.5
8	H	47	GLY	2.4
4	Q	117	ALA	2.4
9	I	3	ALA	2.4
8	H	46	LYS	2.4
7	T	37	LEU	2.4
4	Q	74	SER	2.4
4	Q	27	VAL	2.4
5	R	108	LYS	2.4
1	N	334	TRP	2.3
11	X	45	VAL	2.3
2	B	91	ASN	2.3
4	Q	106	PRO	2.3
10	W	56	PRO	2.3
9	V	8	GLN	2.3
7	G	37	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
6	S	37	LYS	2.3
4	Q	17[A]	VAL	2.3
11	K	26	VAL	2.3
10	J	48	TYR	2.2
2	B	22[A]	HIS	2.2
2	B	61	VAL	2.2
10	W	27	THR	2.2
10	W	49	CYS	2.2
5	R	67	ILE	2.2
9	V	65	LYS	2.2
7	G	41	HIS	2.1
7	G	35	SER	2.1
1	N	49	GLY	2.1
7	T	30	LEU	2.1
9	V	33	THR	2.1
7	G	38	HIS	2.1
13	Z	38	ASP	2.1
4	Q	124	LEU	2.1
7	G	33	LEU	2.1
1	N	136[A]	LEU	2.0
2	O	60	GLU	2.0
7	G	12	GLY	2.0
4	Q	39	ALA	2.0
6	F	92	VAL	2.0
8	U	61	LYS	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	0.95	0.12	43,51,90,112	0
1	FME	N	1	10/11	0.95	0.13	48,55,93,98	0
2	FME	B	1	10/11	0.98	0.07	35,38,48,89	0
2	FME	O	1	10/11	0.98	0.09	42,47,56,72	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	C	318	22/33	0.69	0.34	42,69,83,94	22
20	DMU	P	316	22/33	0.71	0.36	43,68,80,89	22
20	DMU	A	608	7/33	0.73	0.42	56,60,67,70	7
19	LFA	P	310	11/20	0.75	0.35	57,63,70,74	11
20	DMU	N	608	7/33	0.76	0.48	65,70,75,79	7
20	DMU	P	318	33/33	0.76	0.26	52,79,92,119	33
20	DMU	P	315	7/33	0.79	0.33	54,62,69,70	7
20	DMU	P	314	33/33	0.80	0.29	45,56,69,70	33
19	LFA	C	325	15/20	0.80	0.35	51,56,68,69	15
19	LFA	C	314	15/20	0.81	0.29	44,52,64,74	15
19	LFA	P	307	11/20	0.81	0.34	39,53,63,70	11
19	LFA	P	311	11/20	0.82	0.29	48,57,67,69	11
19	LFA	C	311	11/20	0.82	0.35	60,70,83,84	11
20	DMU	C	316	33/33	0.82	0.29	45,55,70,77	33
19	LFA	N	607	14/20	0.82	0.30	44,54,75,75	14
20	DMU	C	319	33/33	0.82	0.31	45,58,74,94	33
19	LFA	P	308	6/20	0.83	0.42	43,51,54,58	6
20	DMU	O	304	22/33	0.83	0.29	50,68,93,101	22
20	DMU	M	102	8/33	0.83	0.27	45,53,59,60	8
20	DMU	T	105	22/33	0.83	0.27	47,59,71,82	22
21	EDO	E	201	4/4	0.83	0.34	40,41,41,49	4
21	EDO	P	321	4/4	0.83	0.32	33,34,39,44	4
24	CHD	P	305	29/29	0.83	0.16	59,72,91,113	0
20	DMU	C	320	33/33	0.84	0.24	41,75,84,87	33
20	DMU	H	101	33/33	0.84	0.24	32,48,57,68	33
21	EDO	C	323	4/4	0.84	0.31	36,37,37,42	4
19	LFA	C	312	14/20	0.84	0.34	43,69,75,78	14
19	LFA	T	101	14/20	0.84	0.27	44,52,64,64	14
20	DMU	P	317	33/33	0.84	0.28	51,61,77,95	33
19	LFA	C	310	15/20	0.85	0.27	51,57,70,73	15
20	DMU	C	324	33/33	0.85	0.19	43,57,83,92	33
19	LFA	T	104	11/20	0.85	0.31	58,63,71,75	11

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	DMU	P	322	33/33	0.85	0.21	49,60,94,102	33
18	CDL	P	304	87/100	0.85	0.21	46,94,131,157	0
20	DMU	B	308	22/33	0.85	0.26	58,69,83,83	22
19	LFA	P	309	18/20	0.85	0.26	38,50,62,64	18
19	LFA	C	307	11/20	0.85	0.32	53,59,67,69	11
19	LFA	O	303	11/20	0.85	0.31	51,58,64,69	11
20	DMU	W	101	11/33	0.86	0.33	65,69,75,75	11
19	LFA	T	103	14/20	0.86	0.33	42,67,74,74	14
19	LFA	C	308	6/20	0.86	0.39	43,51,53,55	6
21	EDO	N	611	4/4	0.86	0.24	40,42,50,52	4
19	LFA	C	309	18/20	0.86	0.23	34,42,64,70	18
24	CHD	C	305	29/29	0.86	0.15	61,73,97,119	0
18	CDL	V	101	64/100	0.86	0.17	60,96,128,162	0
18	CDL	C	304	87/100	0.87	0.19	47,86,125,131	0
19	LFA	C	313	11/20	0.87	0.28	46,57,69,74	11
20	DMU	Q	201	33/33	0.87	0.22	42,61,74,101	33
21	EDO	N	614	4/4	0.87	0.26	26,41,41,49	4
18	CDL	A	606	64/100	0.87	0.18	53,91,124,151	0
20	DMU	G	102	11/33	0.87	0.32	51,58,65,65	11
21	EDO	A	611	4/4	0.87	0.25	36,41,48,49	4
21	EDO	C	321	4/4	0.88	0.29	56,57,59,83	4
20	DMU	A	609	33/33	0.88	0.20	35,46,61,84	33
20	DMU	N	609	33/33	0.88	0.21	42,60,79,91	33
20	DMU	N	616	33/33	0.88	0.23	33,49,66,73	33
19	LFA	A	607	14/20	0.88	0.24	35,46,69,79	14
19	LFA	C	315	13/20	0.88	0.26	55,58,73,77	13
19	LFA	P	312	15/20	0.88	0.22	43,54,67,67	15
19	LFA	P	313	13/20	0.88	0.26	46,60,74,76	13
21	EDO	A	610	4/4	0.89	0.17	27,28,30,34	4
20	DMU	C	317	7/33	0.89	0.26	52,54,66,68	7
19	LFA	B	307	17/20	0.89	0.28	41,66,83,84	17
20	DMU	A	615	11/33	0.89	0.34	52,61,72,72	11
20	DMU	B	302	11/33	0.89	0.27	48,57,65,70	11
18	CDL	Y	101	94/100	0.89	0.17	53,95,142,162	0
19	LFA	O	302	17/20	0.89	0.25	43,58,72,73	17
20	DMU	O	306	11/33	0.89	0.27	44,47,65,70	11
20	DMU	G	103	22/33	0.89	0.26	47,63,72,73	22
20	DMU	Y	102	22/33	0.89	0.34	59,69,77,82	22
19	LFA	N	606	14/20	0.90	0.23	40,52,61,65	14
20	DMU	B	303	11/33	0.90	0.24	45,58,66,66	11
20	DMU	C	306	11/33	0.91	0.23	53,57,70,71	11
20	DMU	D	201	33/33	0.91	0.17	30,50,58,74	33

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
21	EDO	P	319	4/4	0.91	0.21	50,63,64,80	4
20	DMU	J	101	11/33	0.91	0.33	59,65,71,82	11
20	DMU	L	102	22/33	0.91	0.32	48,66,72,77	22
20	DMU	B	304	22/33	0.91	0.20	49,62,69,77	22
18	CDL	L	101	94/100	0.92	0.15	44,87,132,145	0
25	UNX	P	302	1/1	0.92	0.23	48,48,48,48	0
21	EDO	N	610	4/4	0.93	0.13	30,32,34,35	4
20	DMU	P	306	11/33	0.93	0.26	52,55,62,68	11
20	DMU	Z	101	33/33	0.93	0.11	55,64,80,90	0
20	DMU	Z	102	8/33	0.93	0.21	53,55,60,61	8
20	DMU	O	308	22/33	0.93	0.17	38,52,59,62	22
21	EDO	E	203	4/4	0.93	0.25	37,40,44,48	4
21	EDO	F	102	4/4	0.93	0.15	24,24,31,32	4
21	EDO	G	104	4/4	0.93	0.17	35,35,36,39	4
20	DMU	M	101	33/33	0.95	0.09	44,52,77,80	0
21	EDO	O	309	4/4	0.95	0.15	38,39,39,40	4
21	EDO	C	322	4/4	0.95	0.15	36,36,40,41	4
20	DMU	O	307	11/33	0.95	0.22	49,57,64,69	11
21	EDO	R	201	4/4	0.95	0.24	60,62,63,63	4
21	EDO	R	202	4/4	0.95	0.17	39,39,39,40	4
24	CHD	C	301	29/29	0.95	0.08	33,36,40,45	0
21	EDO	A	613	4/4	0.95	0.15	38,41,41,43	4
21	EDO	E	202	4/4	0.95	0.23	33,34,37,39	4
21	EDO	N	612	4/4	0.95	0.18	31,31,32,33	4
21	EDO	P	320	4/4	0.96	0.16	40,40,42,47	4
21	EDO	A	612	4/4	0.96	0.17	27,28,28,29	4
21	EDO	R	203	4/4	0.96	0.14	44,48,52,58	4
25	UNX	C	302	1/1	0.96	0.23	48,48,48,48	0
21	EDO	S	102	4/4	0.96	0.11	23,25,31,32	4
27	PEK	G	101	53/53	0.96	0.11	33,56,100,125	0
27	PEK	T	102	53/53	0.96	0.12	36,59,107,115	0
21	EDO	S	103	4/4	0.97	0.12	31,36,36,38	4
24	CHD	O	301	29/29	0.97	0.06	32,35,38,46	0
24	CHD	P	301	29/29	0.97	0.07	35,38,42,47	0
21	EDO	T	106	4/4	0.97	0.10	39,40,41,42	4
22	PGV	C	303	51/51	0.97	0.09	32,42,107,117	0
22	PGV	N	615	51/51	0.97	0.08	33,43,76,89	0
24	CHD	B	306	29/29	0.97	0.06	30,35,40,44	0
21	EDO	N	613	4/4	0.97	0.12	41,42,43,46	4
21	EDO	F	103	4/4	0.98	0.11	33,36,37,38	4
22	PGV	P	303	51/51	0.98	0.09	34,43,98,112	0
22	PGV	A	614	51/51	0.98	0.08	31,39,82,96	0

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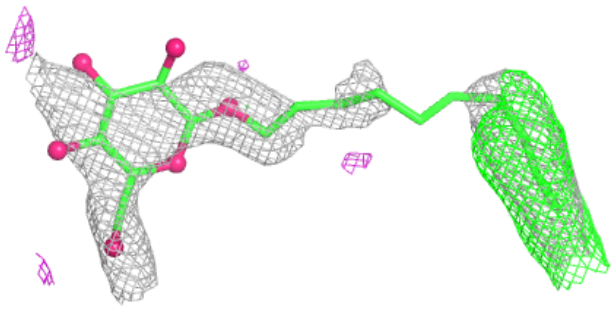
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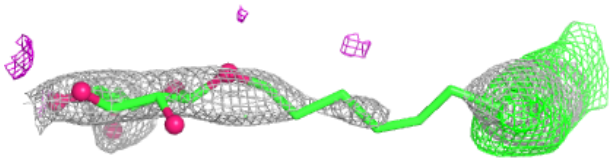
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
21	EDO	B	305	4/4	0.98	0.06	27,30,31,33	4
14	HEA	N	602	60/60	0.99	0.05	29,33,39,43	0
16	MG	A	604	1/1	0.99	0.02	30,30,30,30	0
17	CA	A	605	1/1	0.99	0.07	41,41,41,41	0
14	HEA	A	601	60/60	0.99	0.05	25,29,43,53	0
14	HEA	A	602	60/60	0.99	0.05	26,29,36,43	0
14	HEA	N	601	60/60	0.99	0.06	30,35,48,60	0
23	CUA	B	301	2/2	1.00	0.02	31,31,31,31	0
23	CUA	O	305	2/2	1.00	0.02	38,38,38,38	0
17	CA	N	605	1/1	1.00	0.04	47,47,47,47	0
15	CU	A	603	1/1	1.00	0.01	28,28,28,28	0
26	ZN	F	101	1/1	1.00	0.01	37,37,37,37	0
26	ZN	S	101	1/1	1.00	0.01	39,39,39,39	0
16	MG	N	604	1/1	1.00	0.02	35,35,35,35	0
15	CU	N	603	1/1	1.00	0.02	32,32,32,32	0

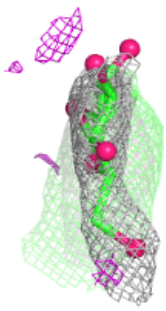
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DMU C 318:

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

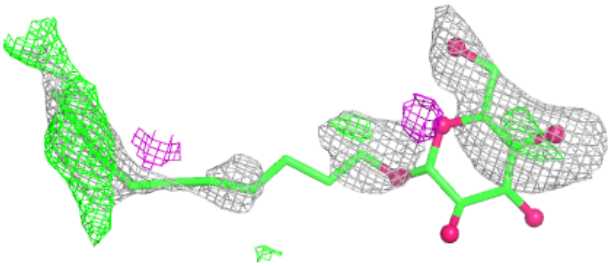


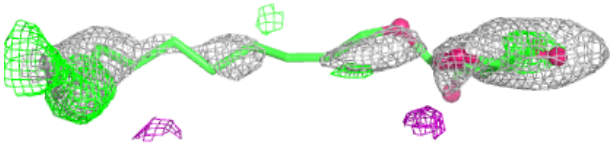


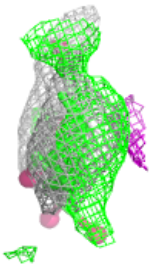


Electron density around DMU P 316:

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

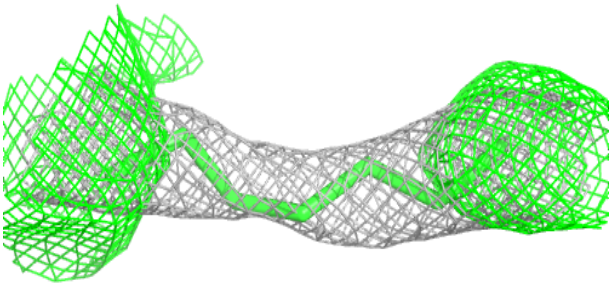


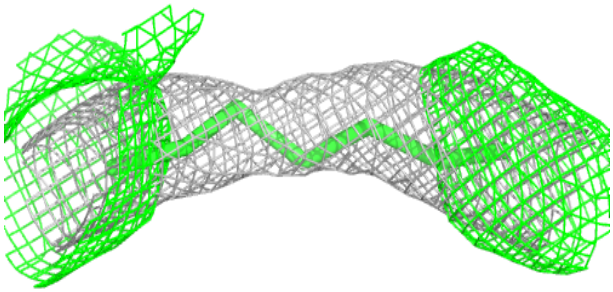


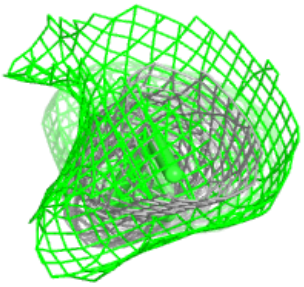


Electron density around DMU A 608:

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

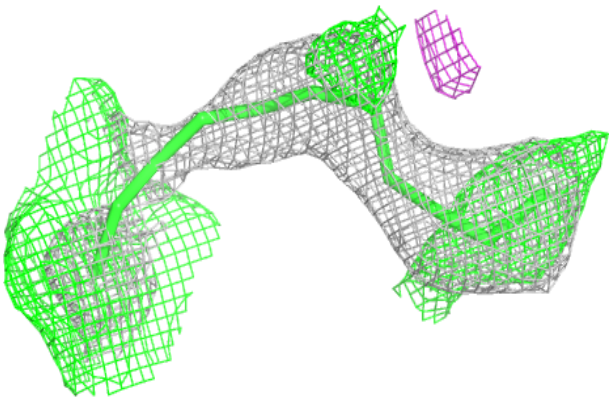


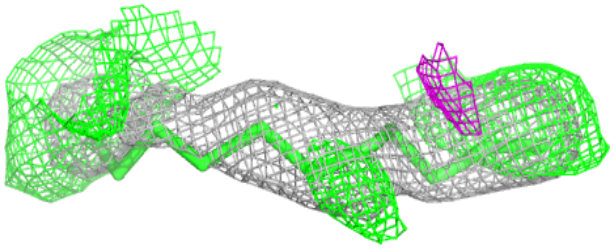


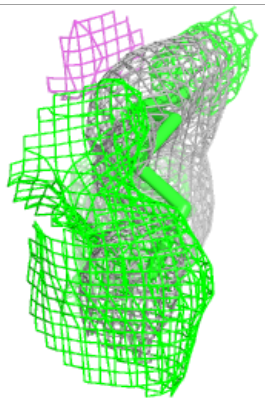


Electron density around LFA P 310:

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

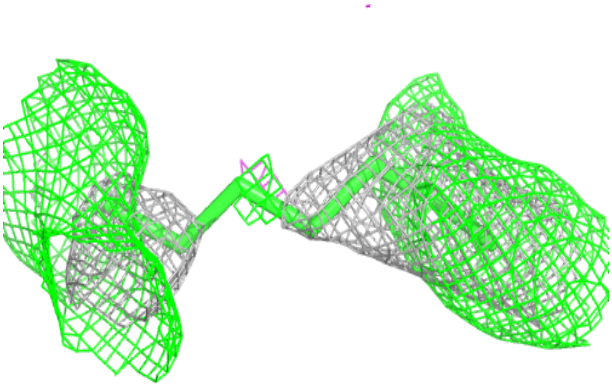


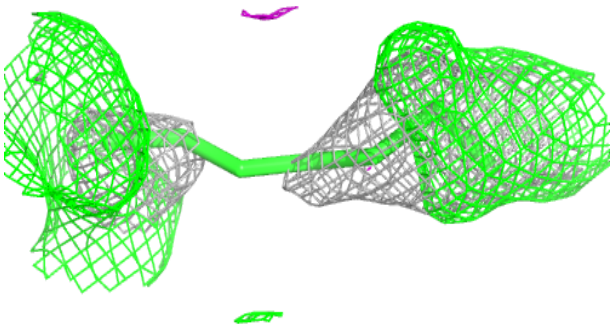


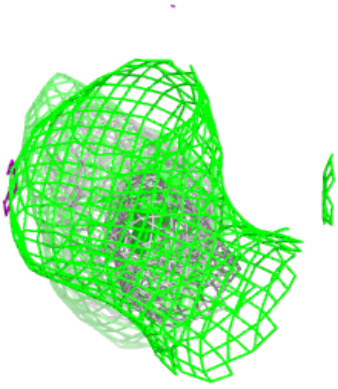


Electron density around DMU N 608:

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

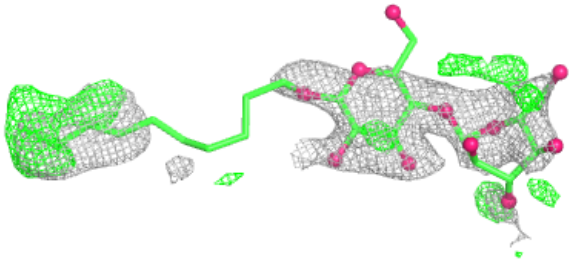


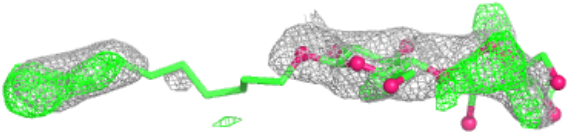


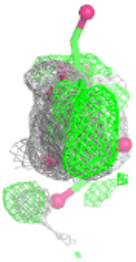


Electron density around DMU P 318:

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

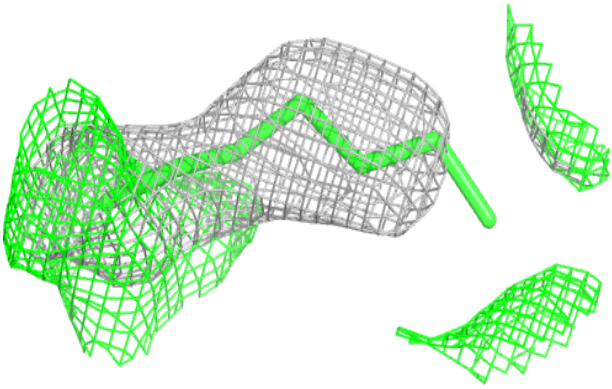


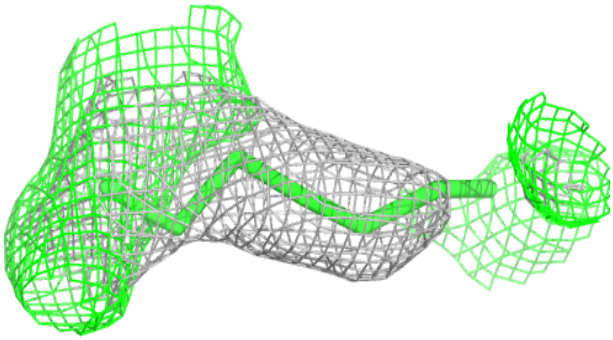


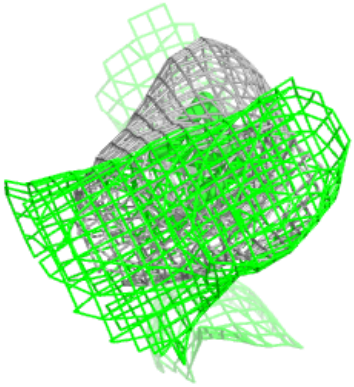


Electron density around DMU P 315:

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

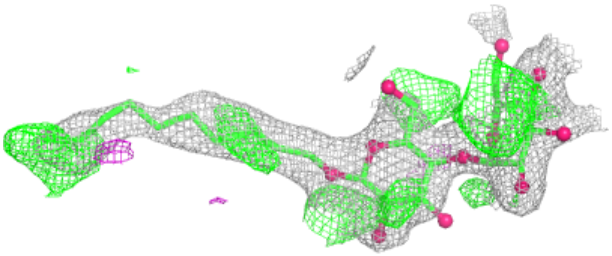


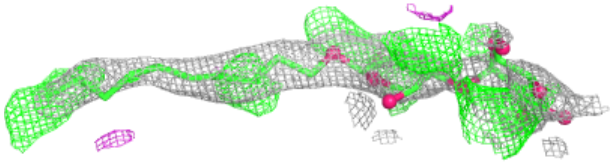


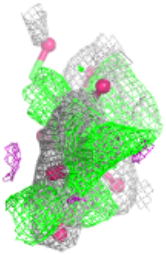


Electron density around DMU P 314:

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

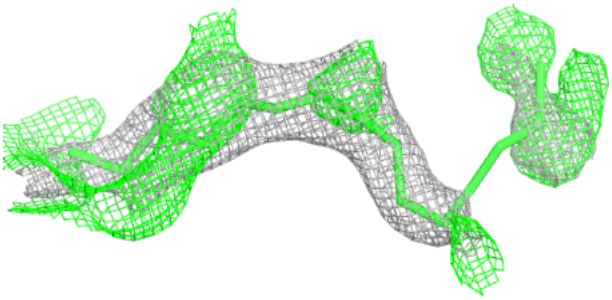


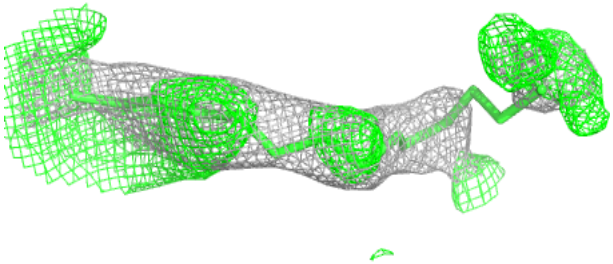


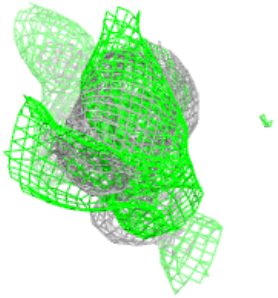


Electron density around LFA C 325:

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

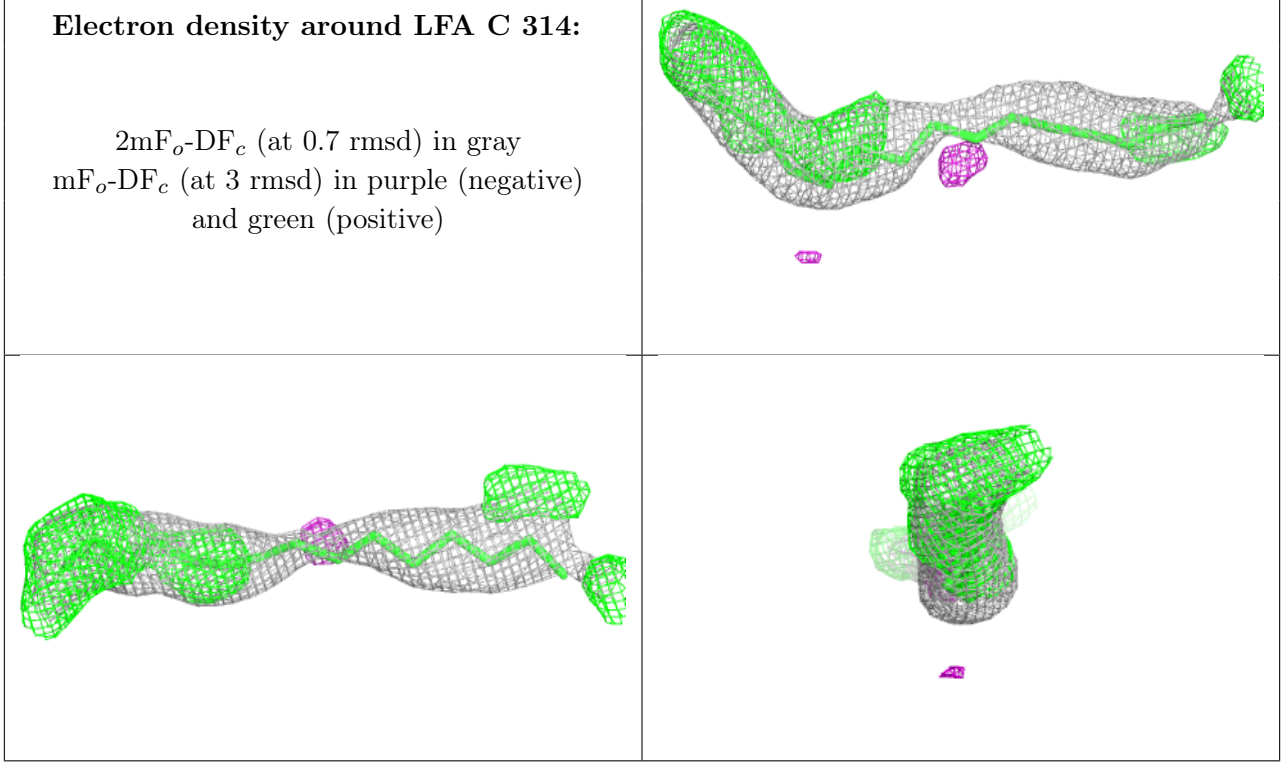






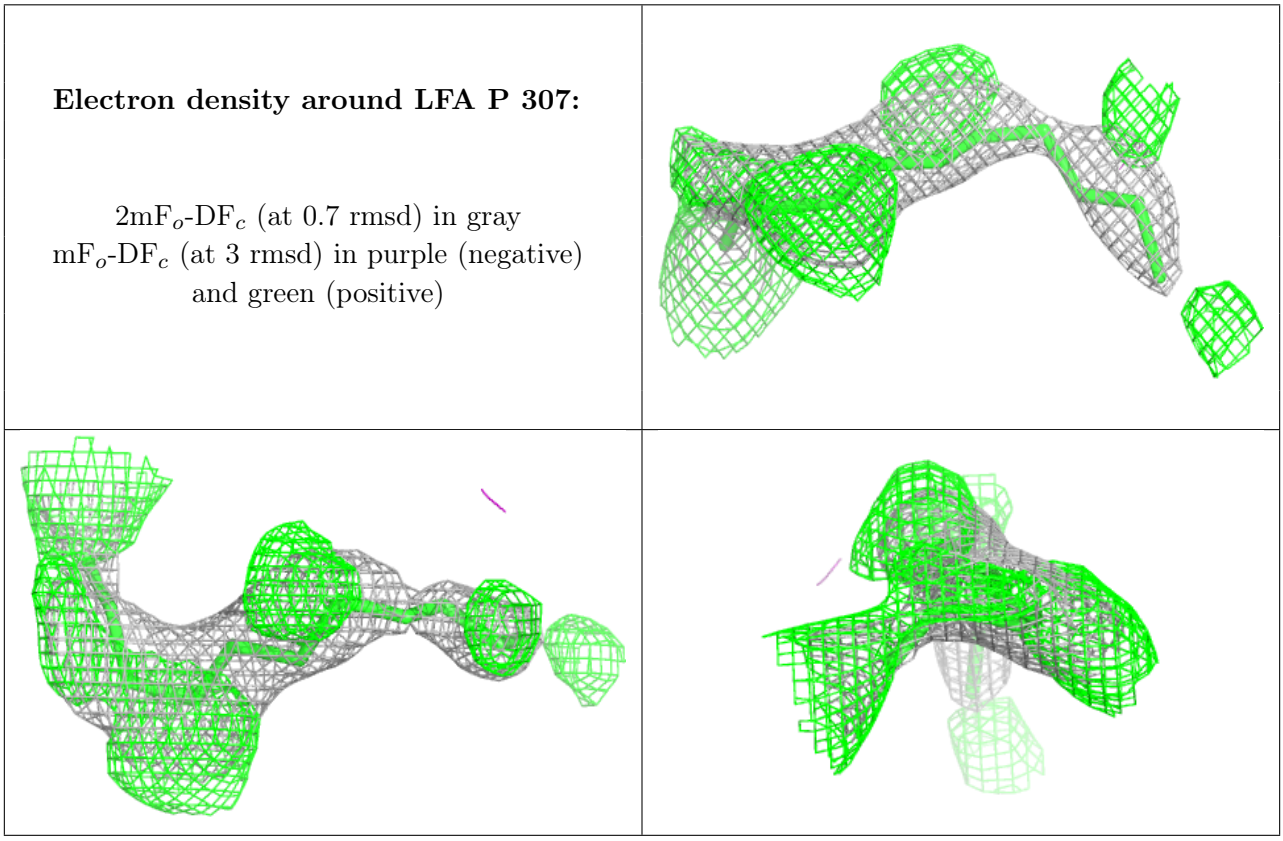
Electron density around LFA C 314:

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



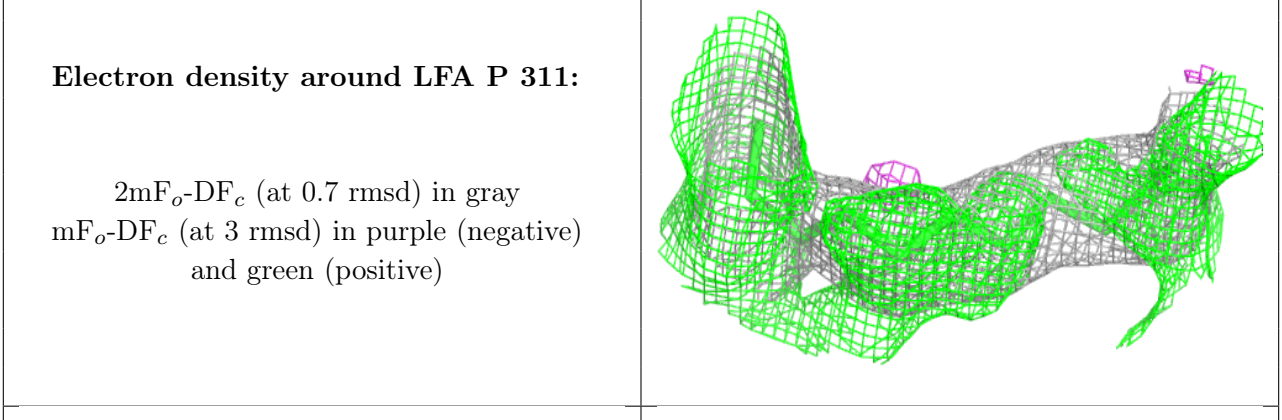
Electron density around LFA P 307:

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



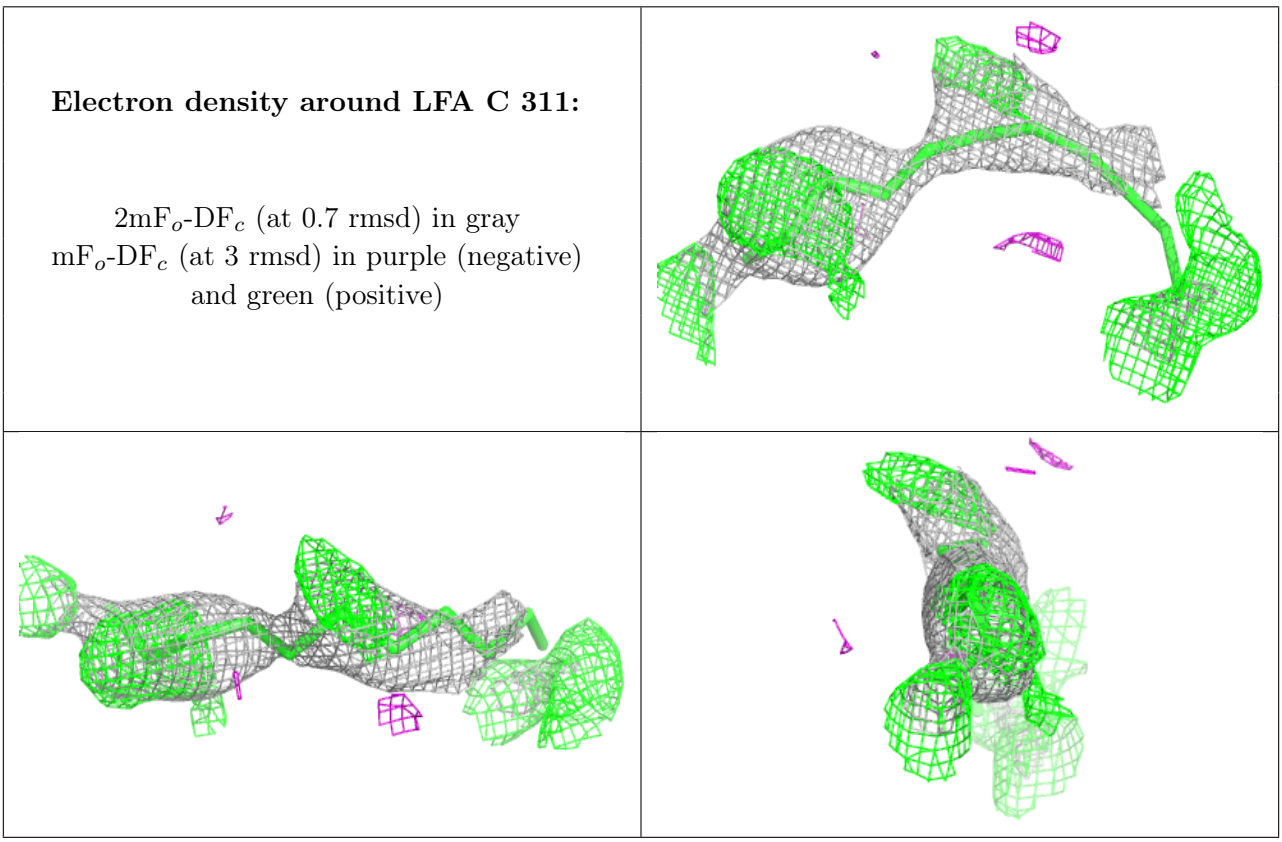
Electron density around LFA P 311:

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



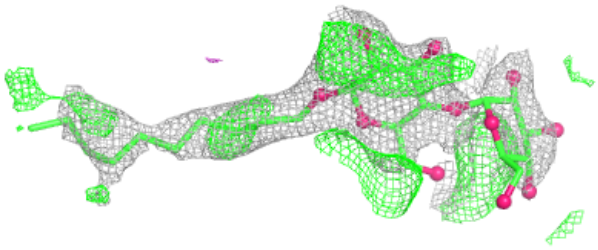
Electron density around LFA C 311:

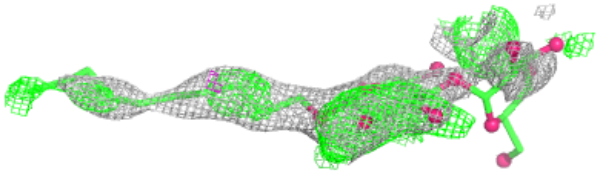
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

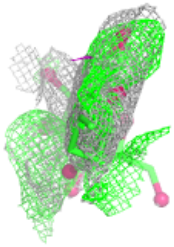


Electron density around DMU C 316:

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

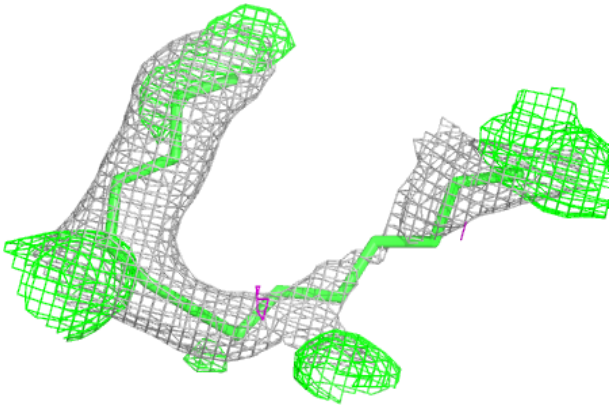


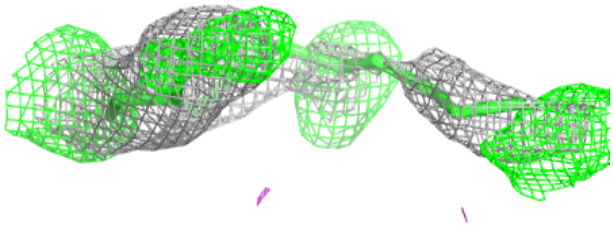


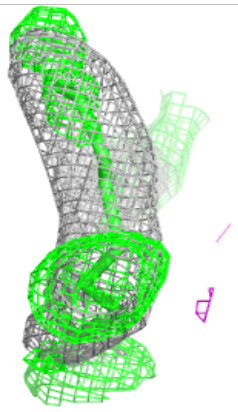


Electron density around LFA N 607:

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

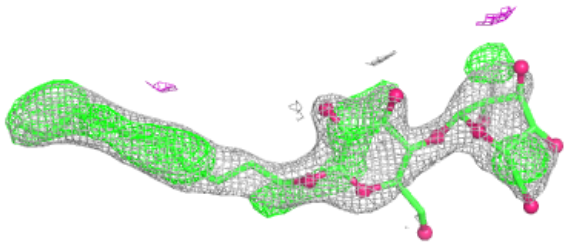


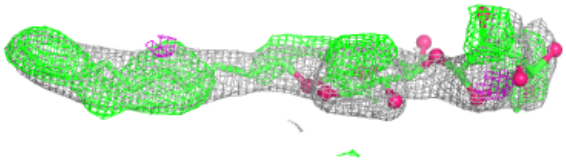


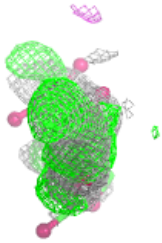


Electron density around DMU C 319:

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

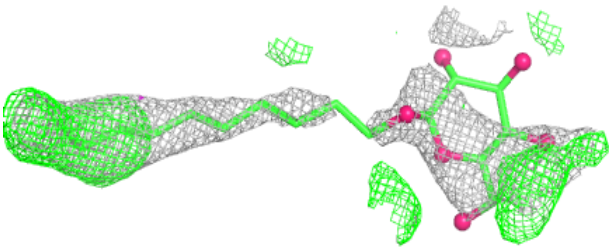


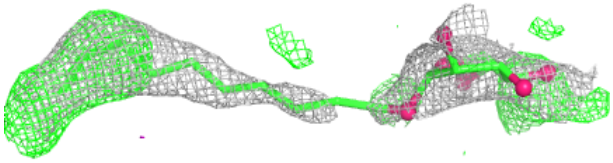


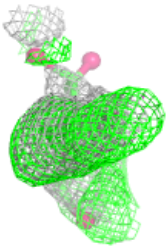


Electron density around DMU O 304:

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

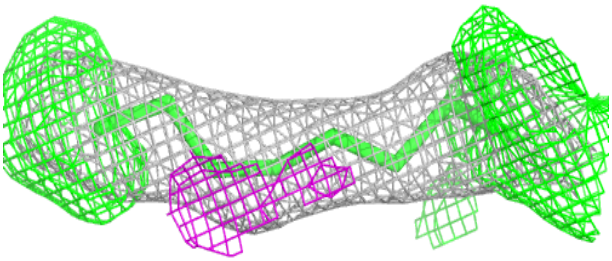


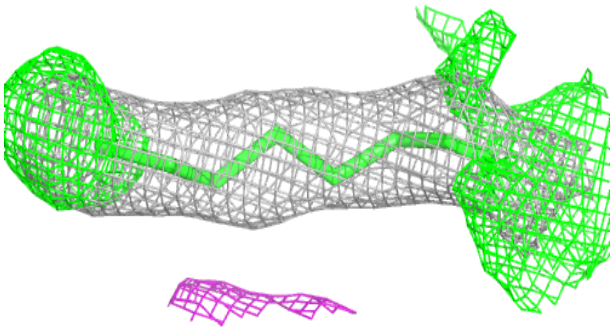


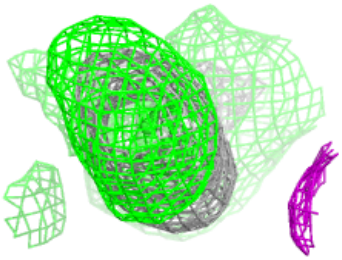


Electron density around DMU M 102:

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

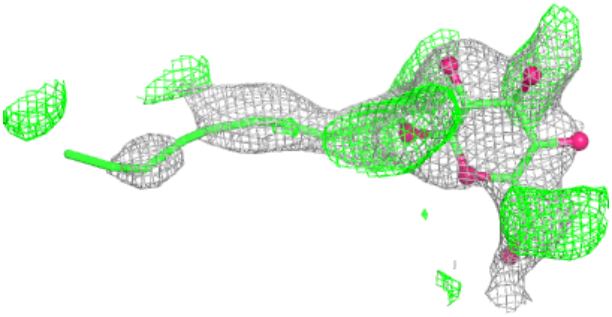


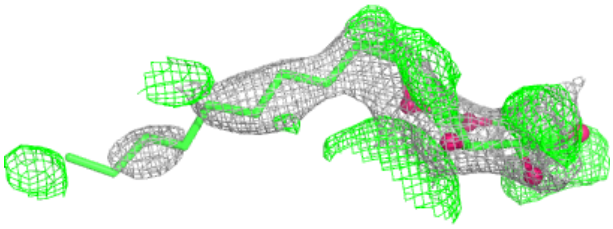


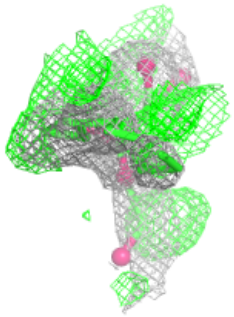


Electron density around DMU T 105:

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

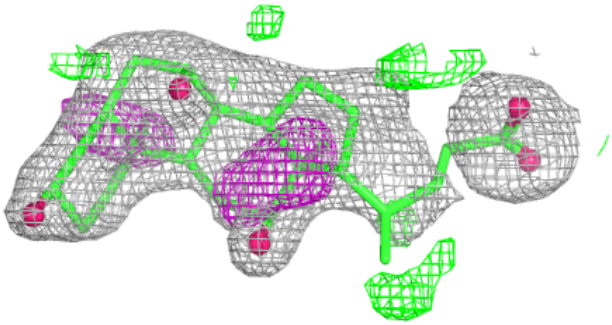


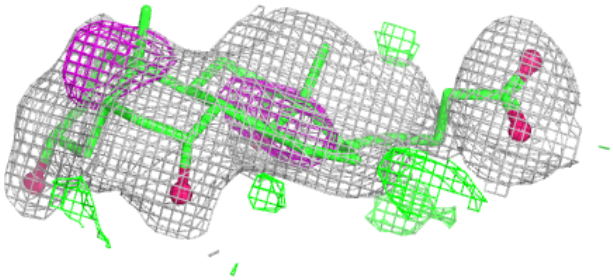


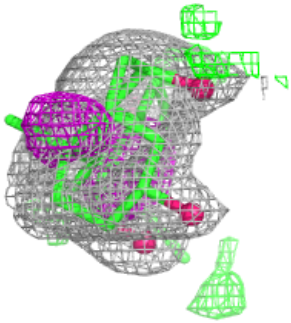


Electron density around CHD P 305:

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

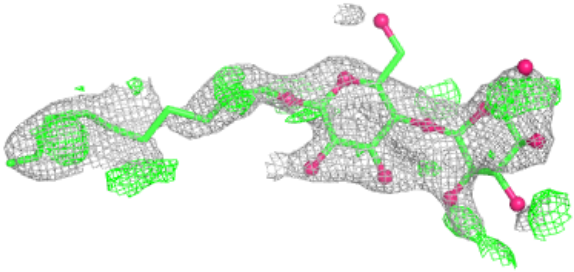


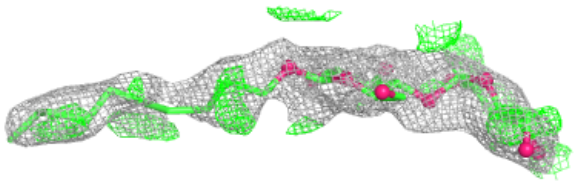


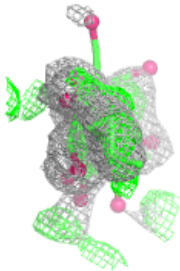


Electron density around DMU C 320:

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

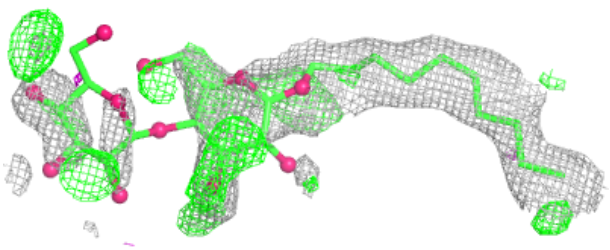


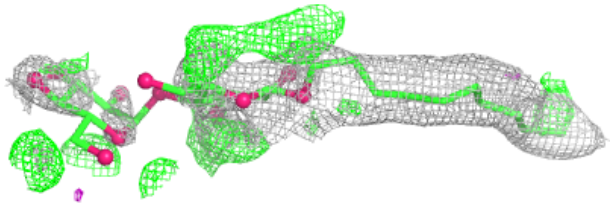


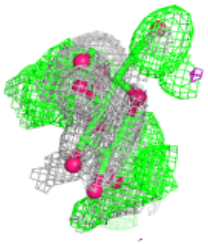


Electron density around DMU H 101:

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

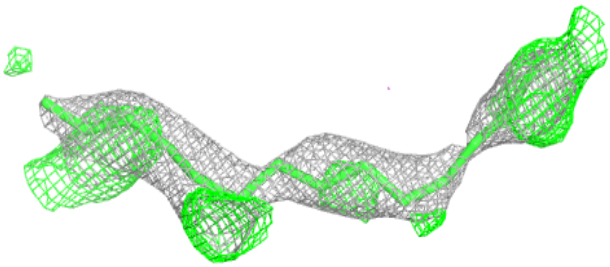


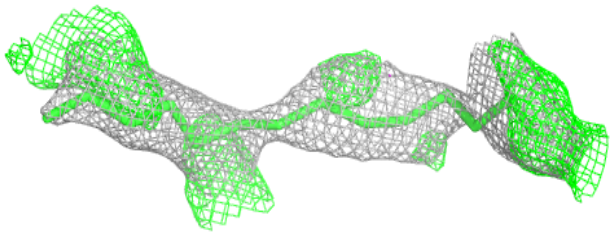


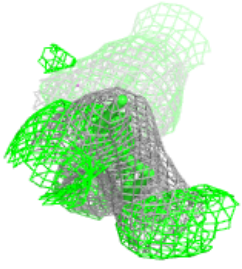


Electron density around LFA C 312:

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

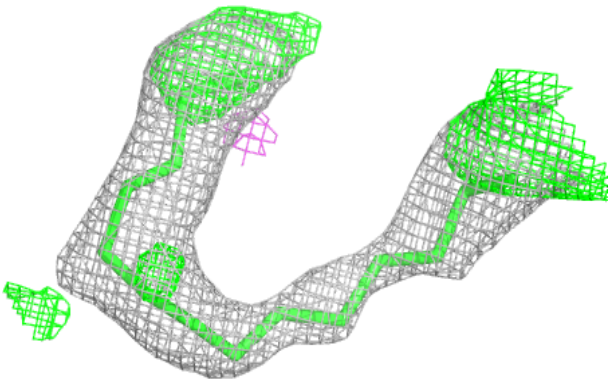


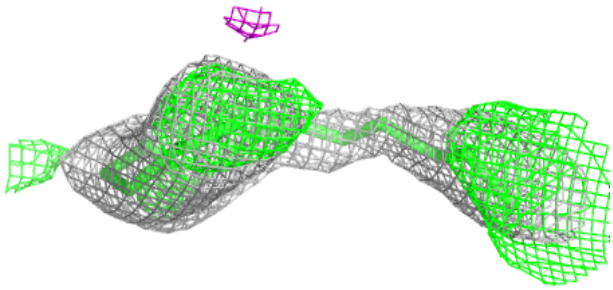


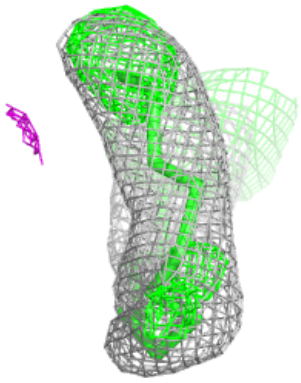


Electron density around LFA T 101:

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

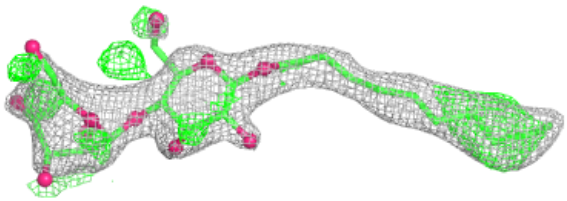


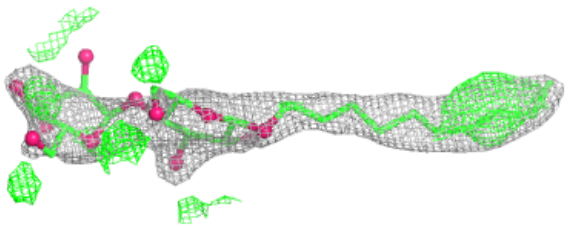


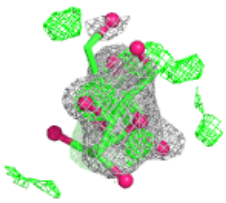


Electron density around DMU P 317:

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

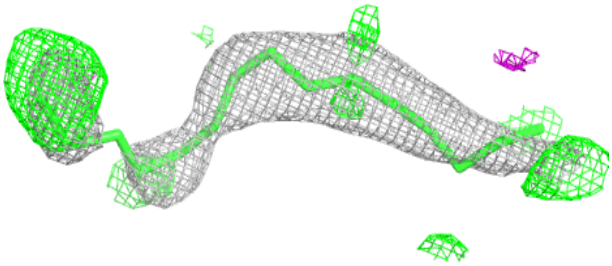


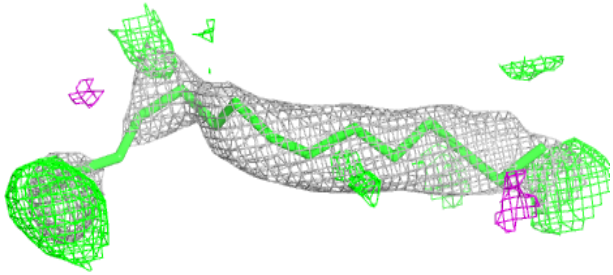


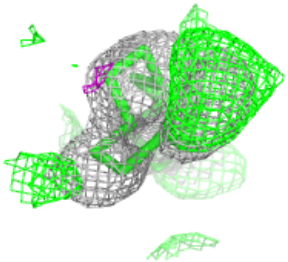


Electron density around LFA C 310:

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

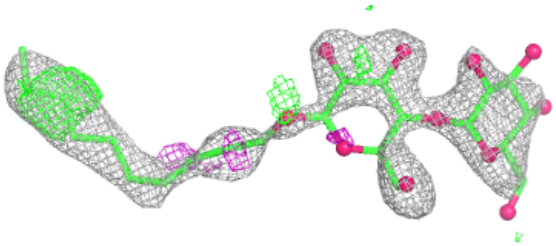


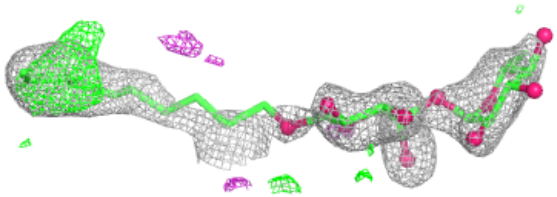


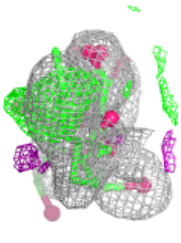


Electron density around DMU C 324:

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

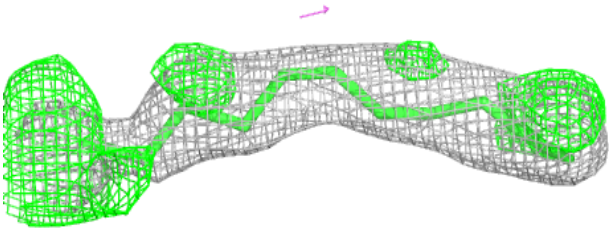


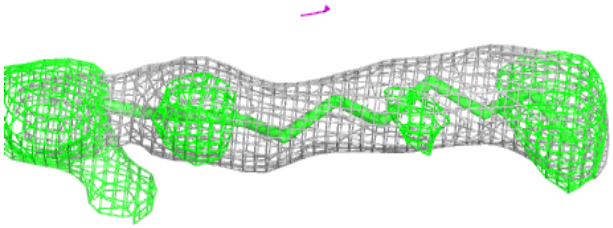


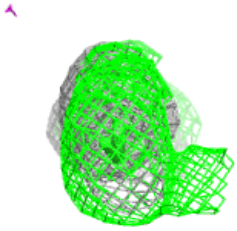


Electron density around LFA T 104:

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

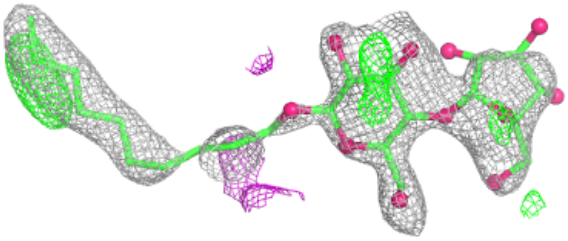


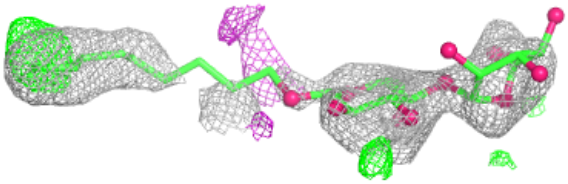


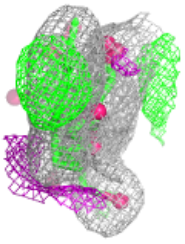


Electron density around DMU P 322:

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

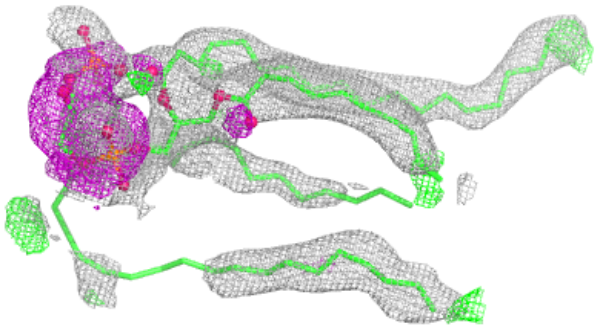


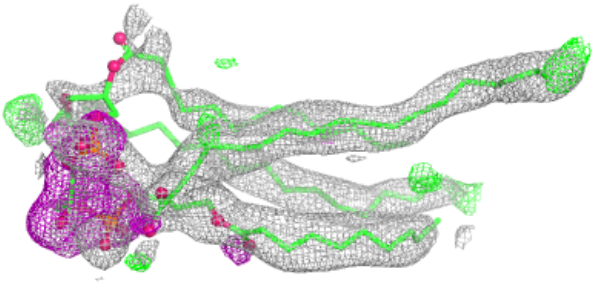




Electron density around CDL P 304:

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

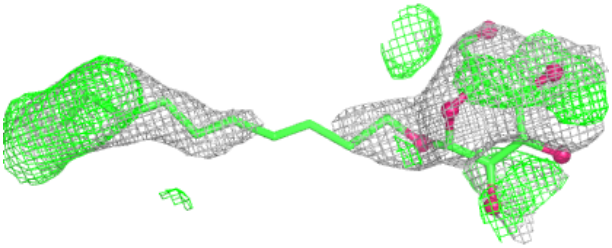


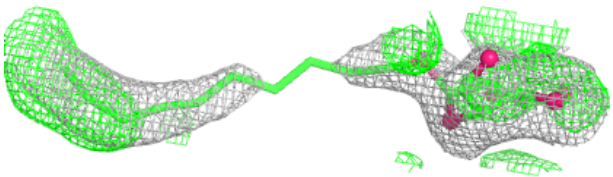


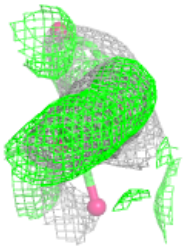


Electron density around DMU B 308:

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

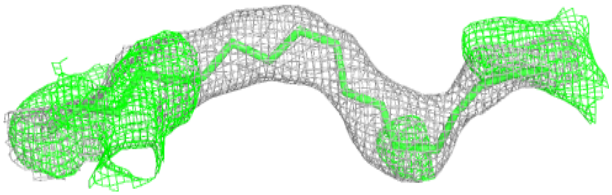


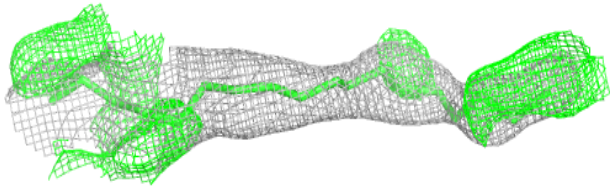


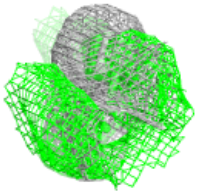


Electron density around LFA P 309:

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

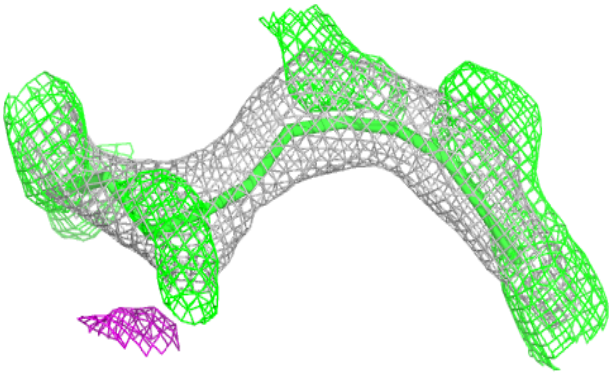


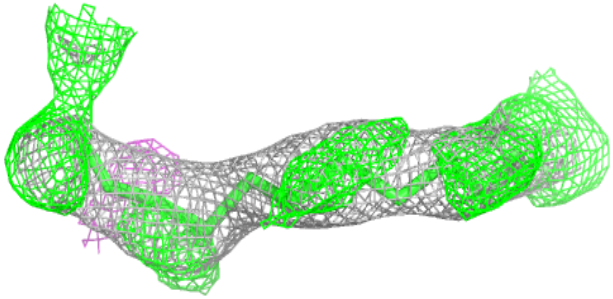


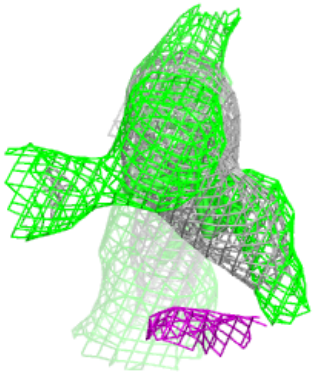


Electron density around LFA C 307:

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

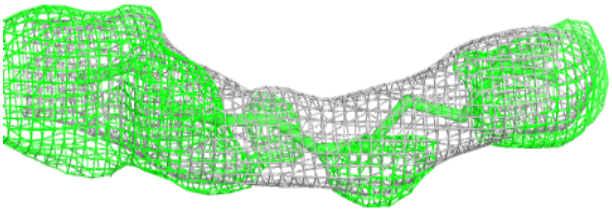


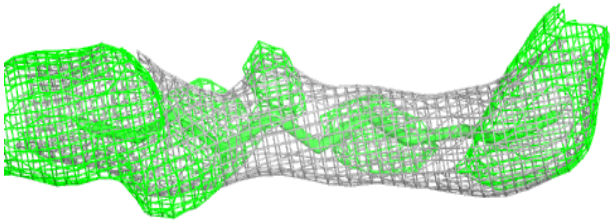


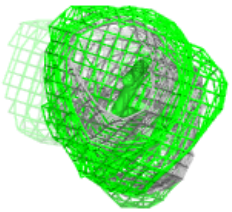


Electron density around LFA O 303:

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

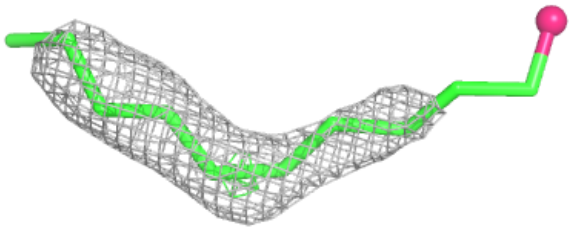


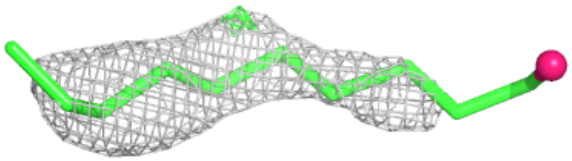


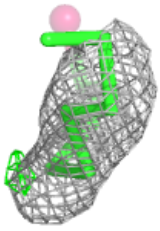


Electron density around DMU W 101:

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

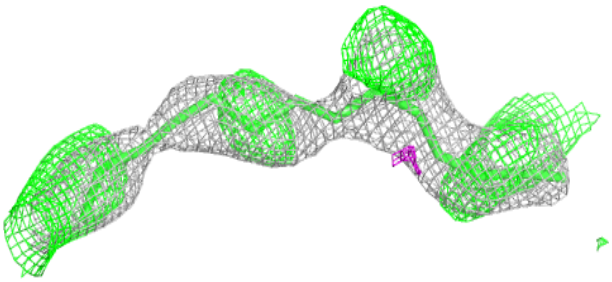


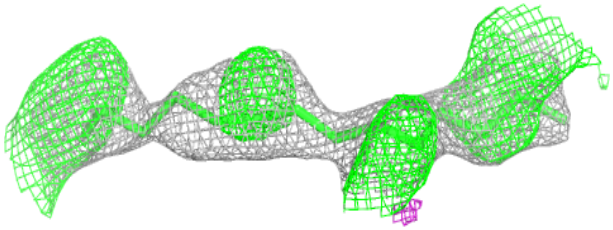


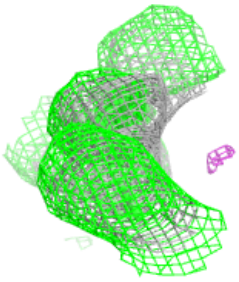


Electron density around LFA T 103:

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

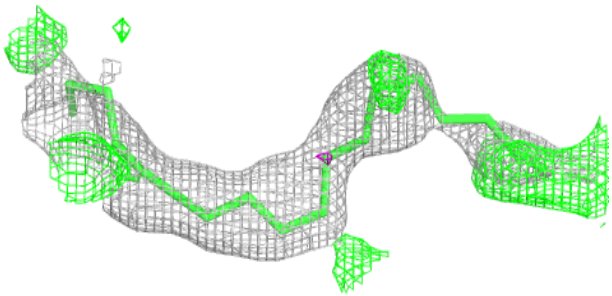


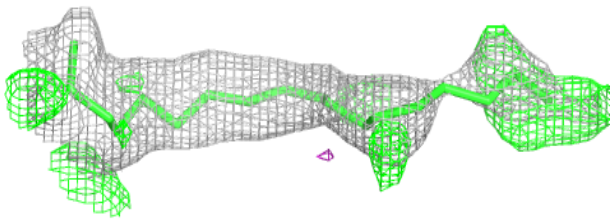


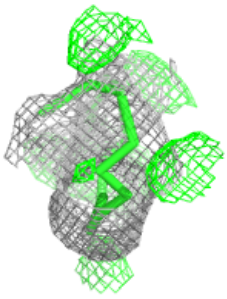


Electron density around LFA C 309:

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

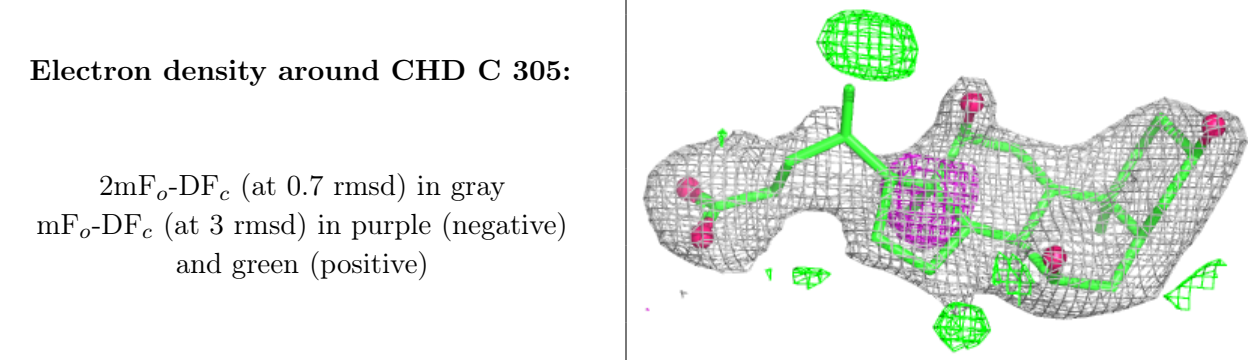


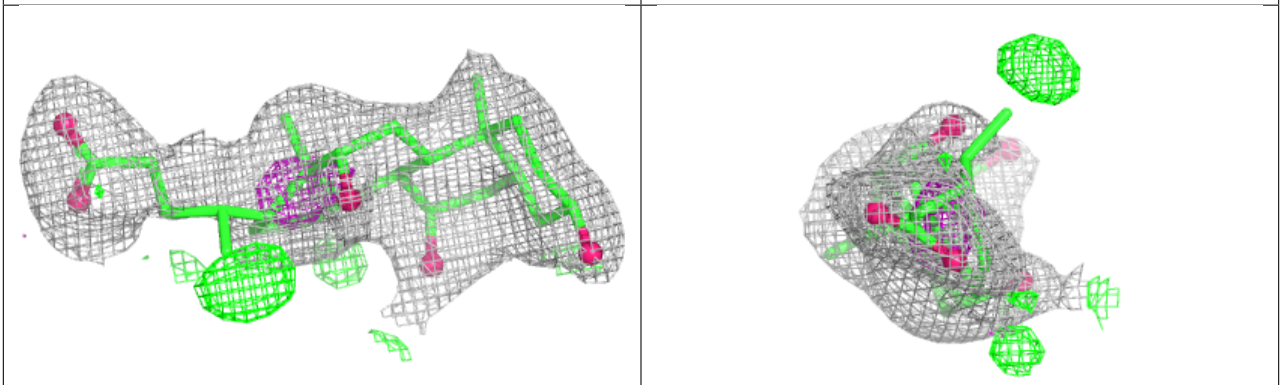




Electron density around CHD C 305:

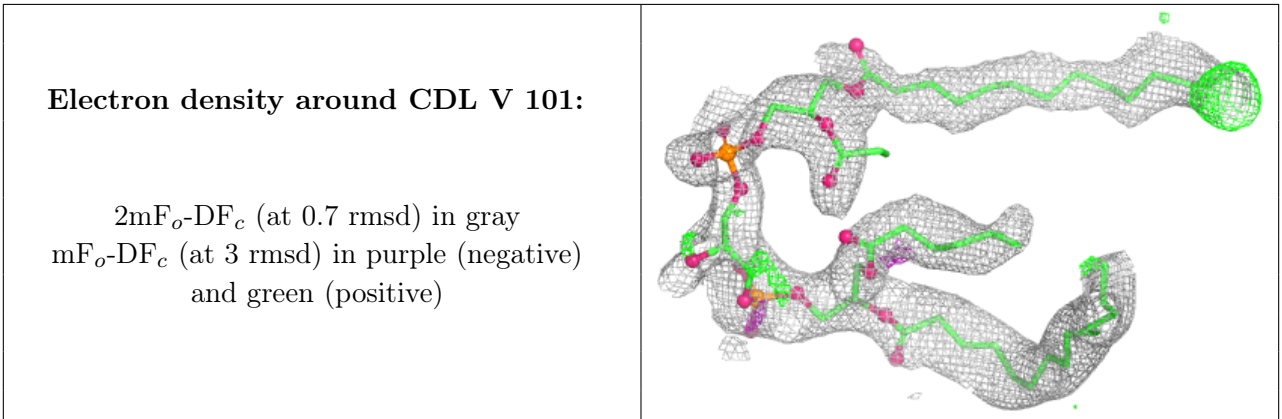
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

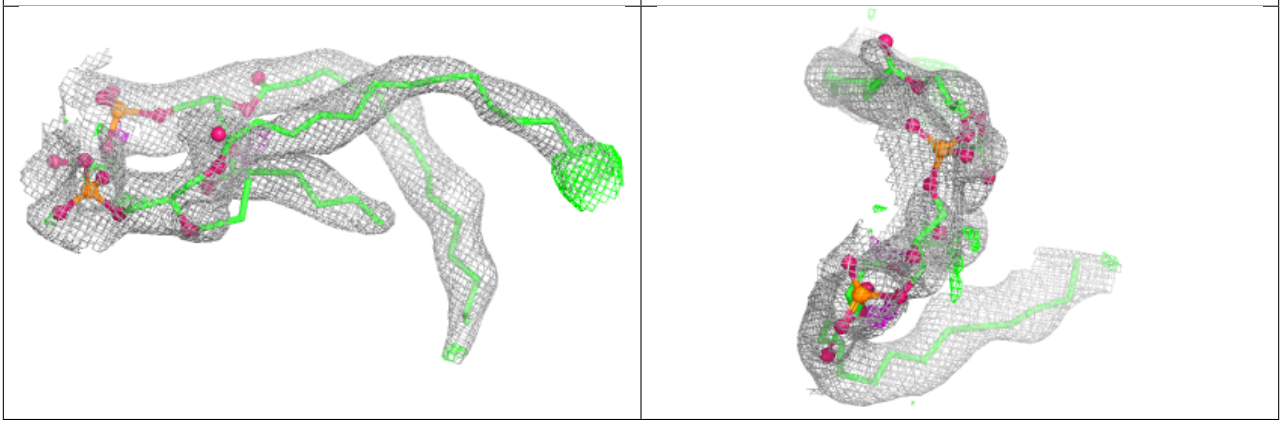




Electron density around CDL V 101:

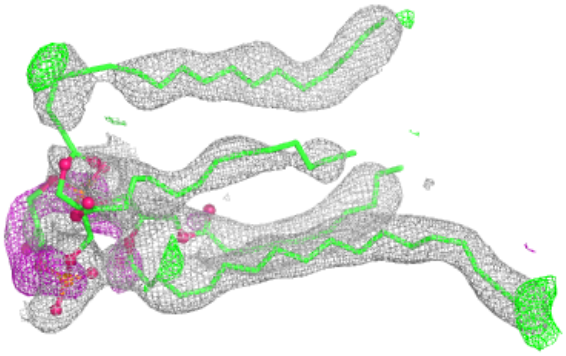
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

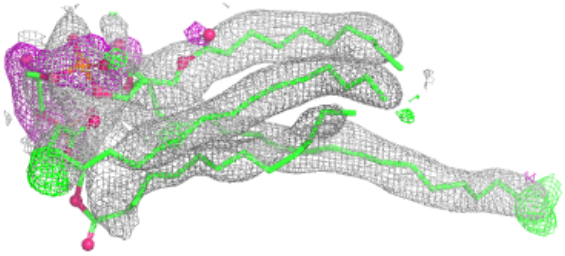


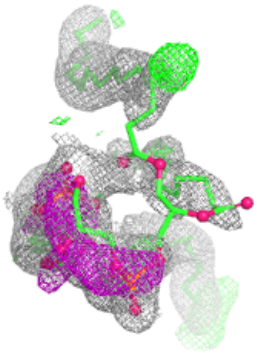


Electron density around CDL C 304:

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

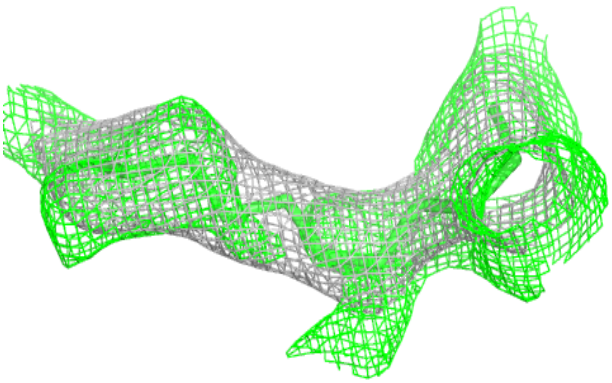


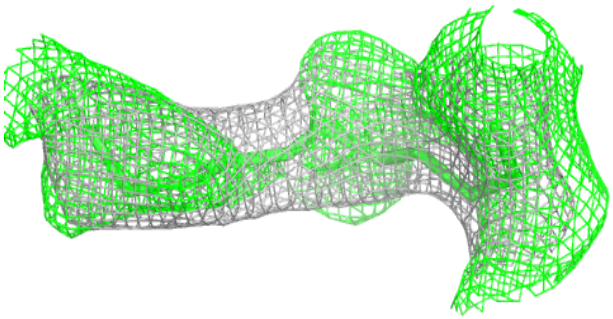


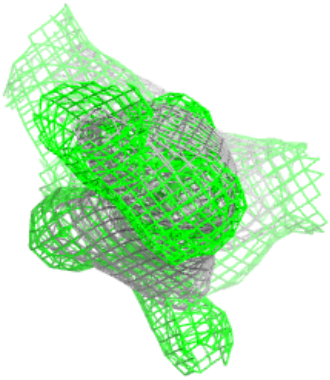


Electron density around LFA C 313:

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

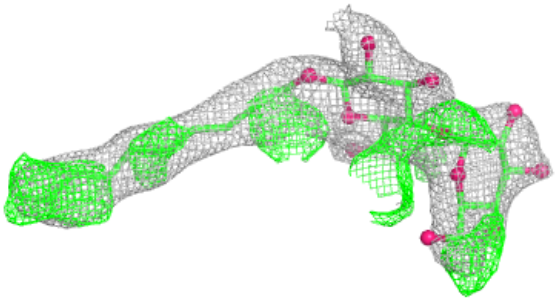


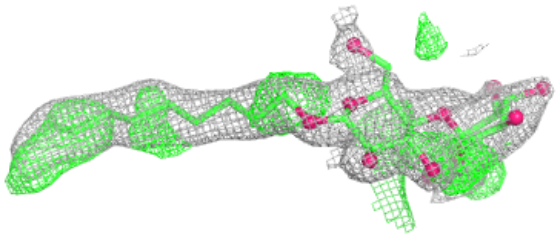


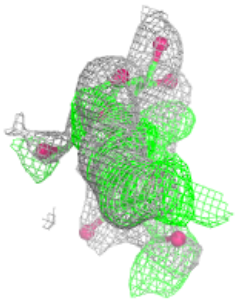


Electron density around DMU Q 201:

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

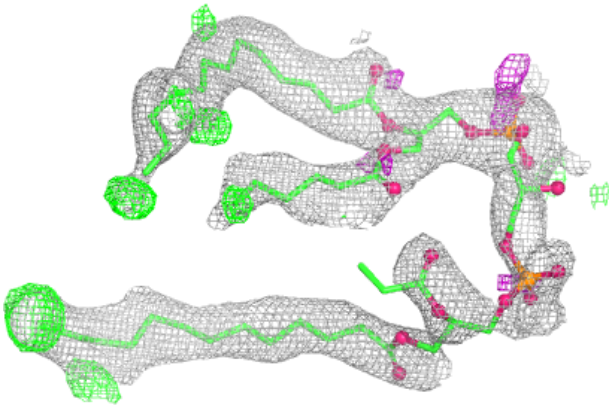


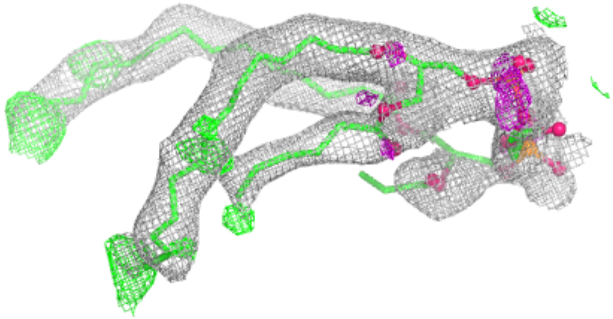


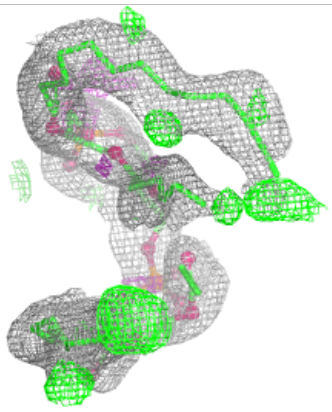


Electron density around CDL A 606:

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

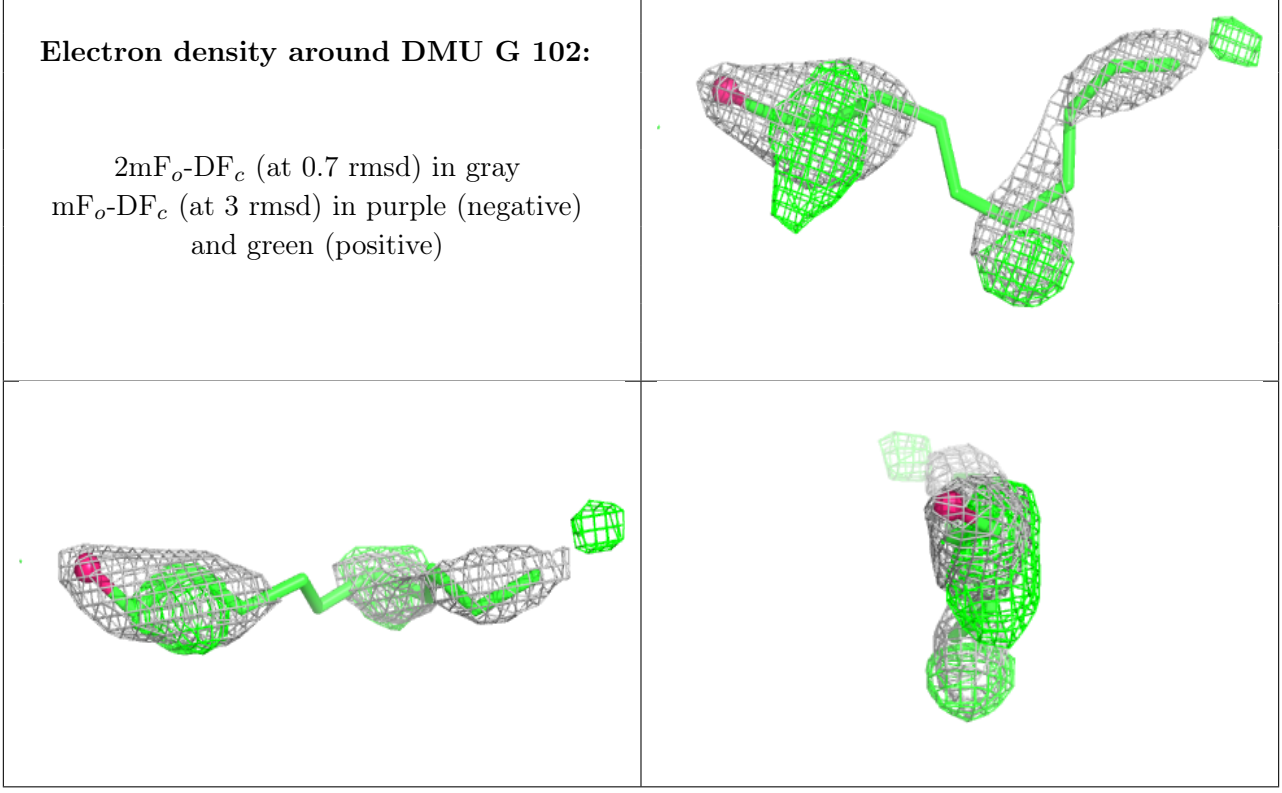






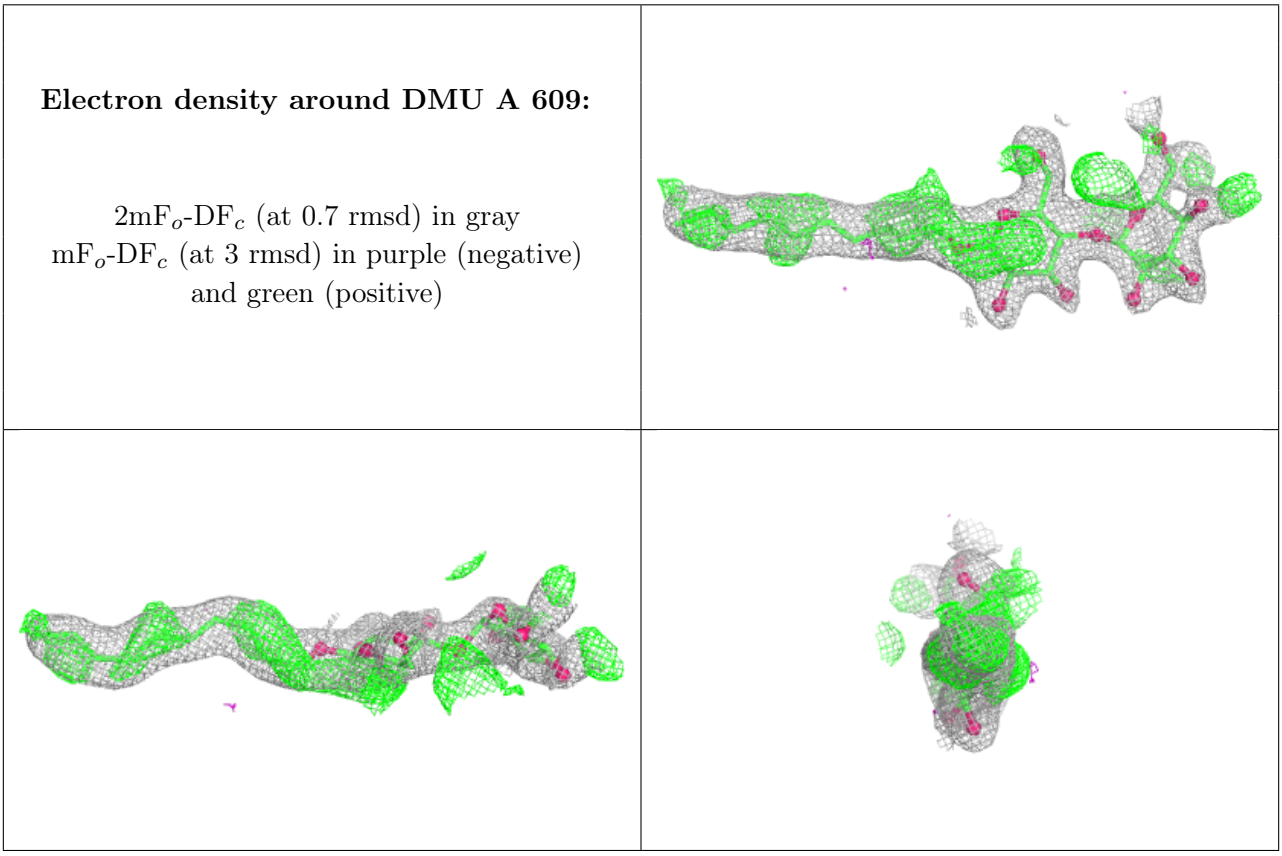
Electron density around DMU G 102:

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



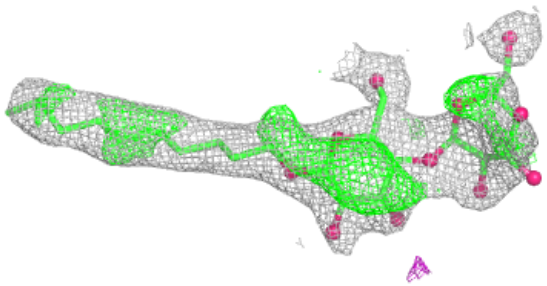
Electron density around DMU A 609:

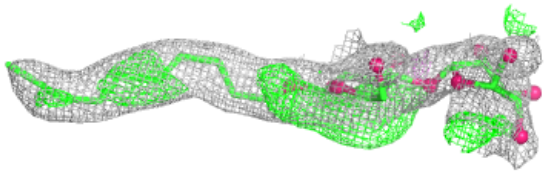
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

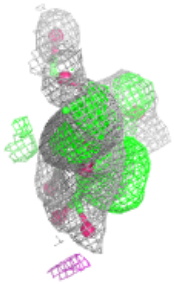


Electron density around DMU N 609:

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

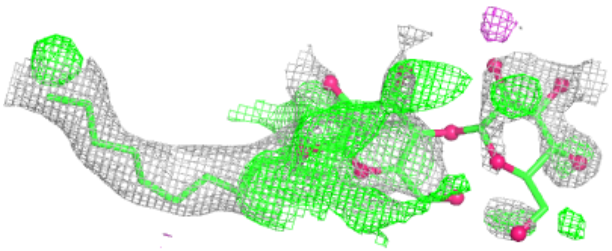


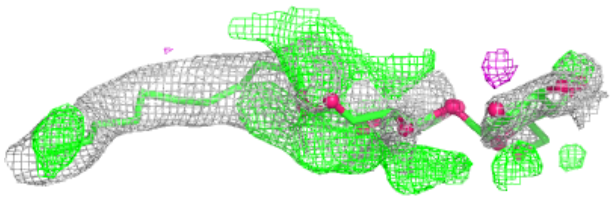


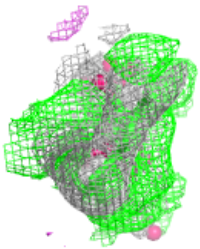


Electron density around DMU N 616:

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

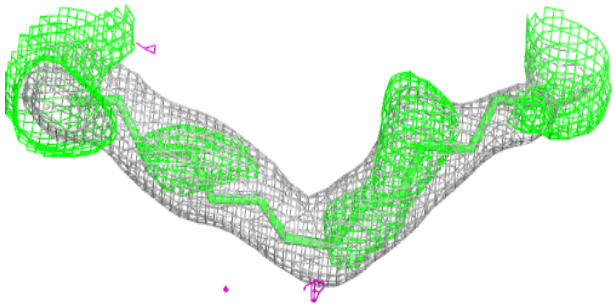


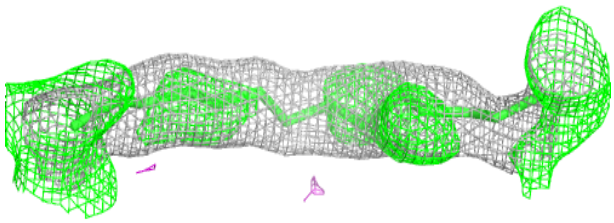


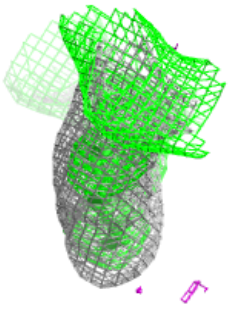


Electron density around LFA A 607:

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

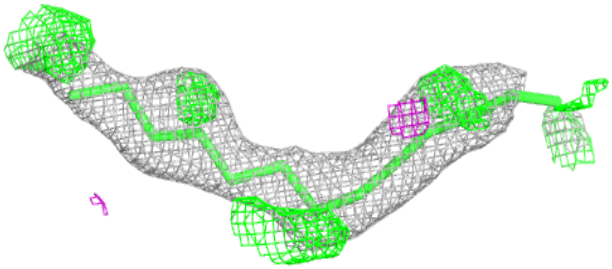


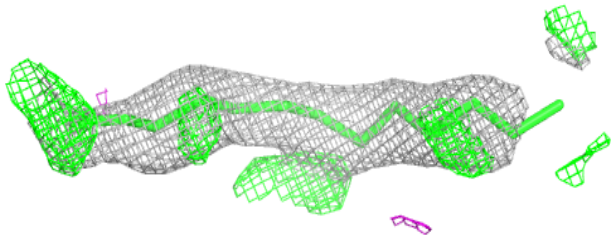


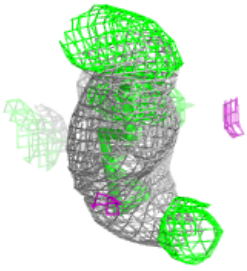


Electron density around LFA C 315:

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

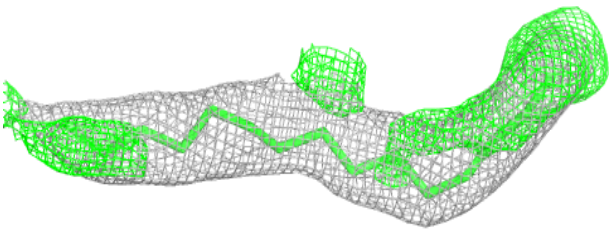


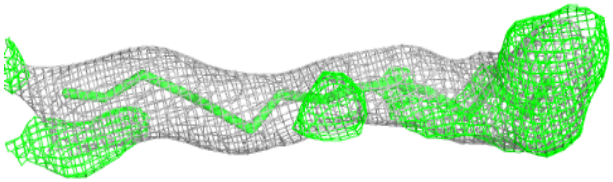


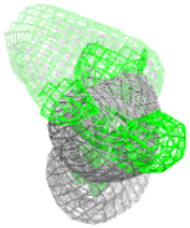


Electron density around LFA P 312:

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

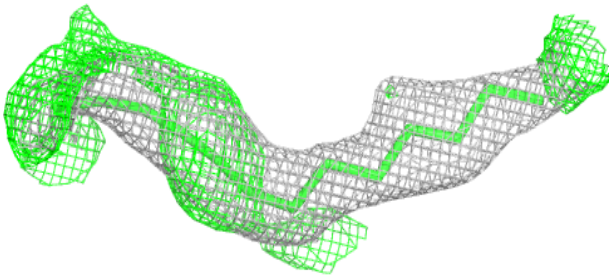


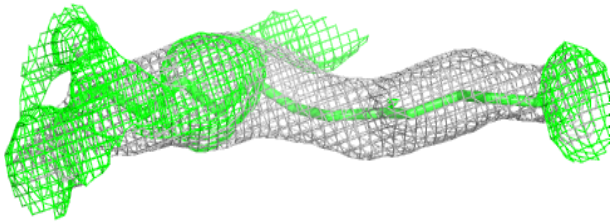


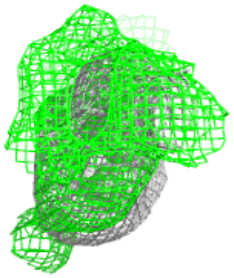


Electron density around LFA P 313:

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

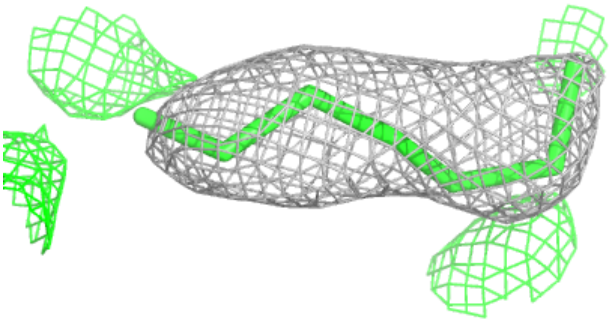


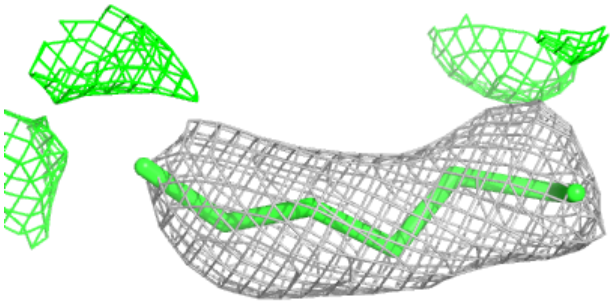


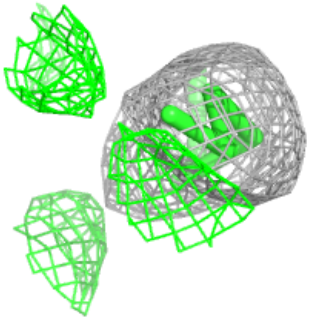


Electron density around DMU C 317:

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

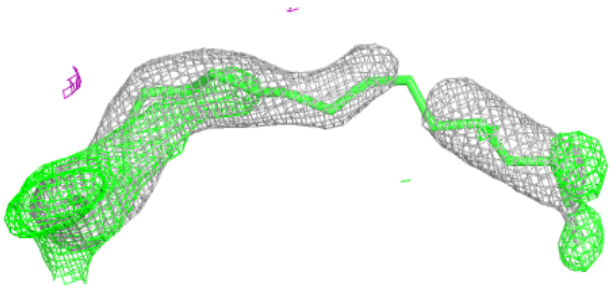


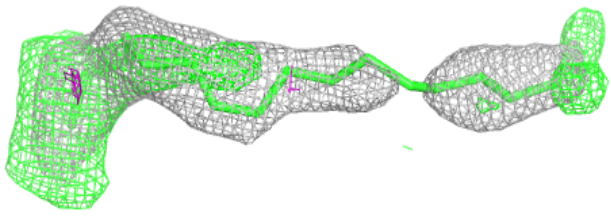


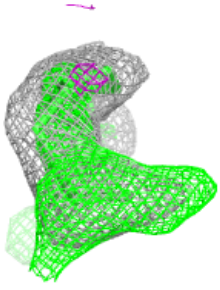


Electron density around LFA B 307:

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

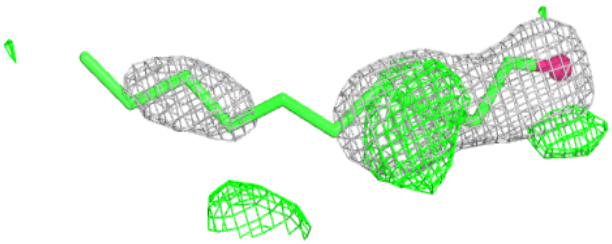


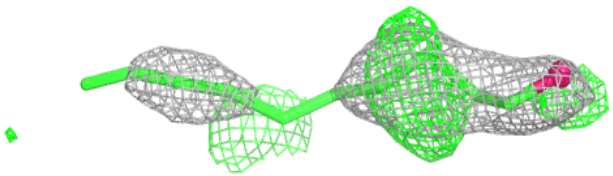


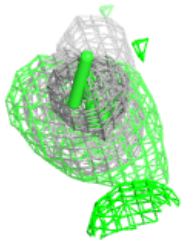


Electron density around DMU A 615:

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

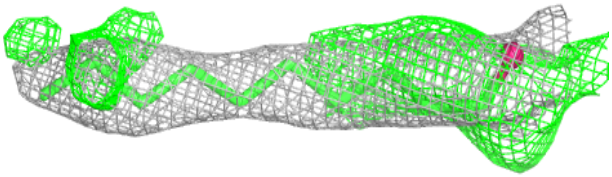


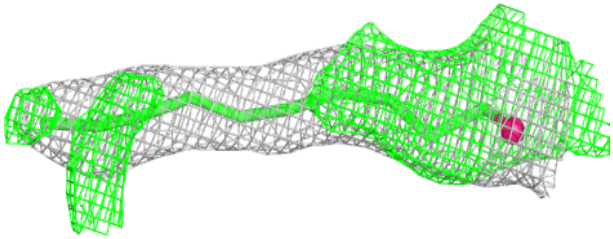


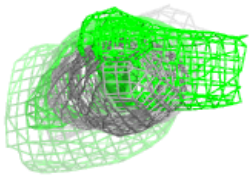


Electron density around DMU B 302:

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

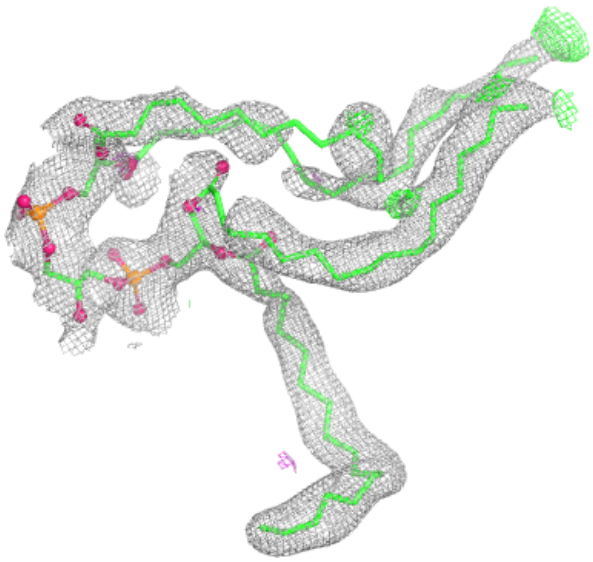


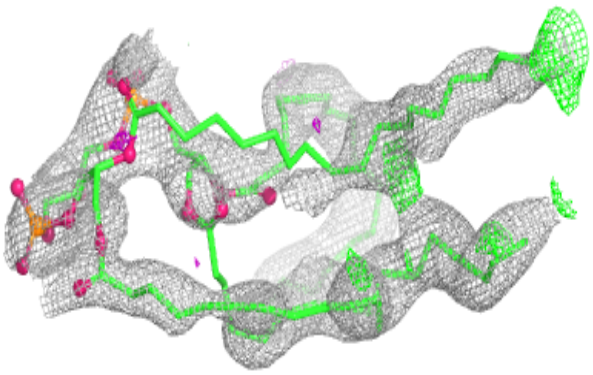


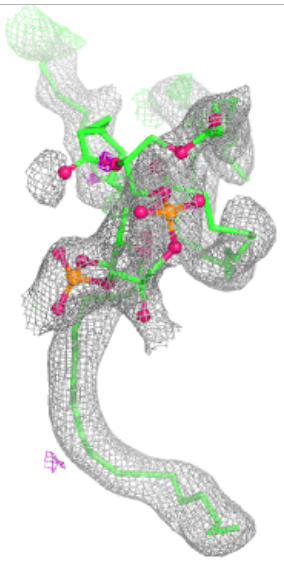


Electron density around CDL Y 101:

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

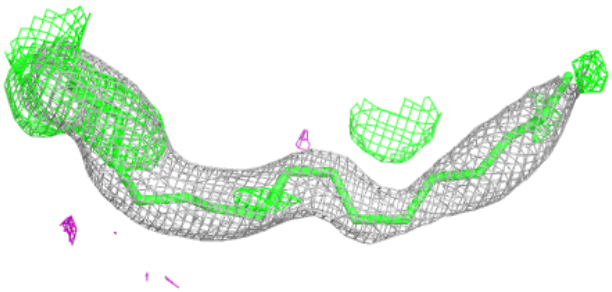


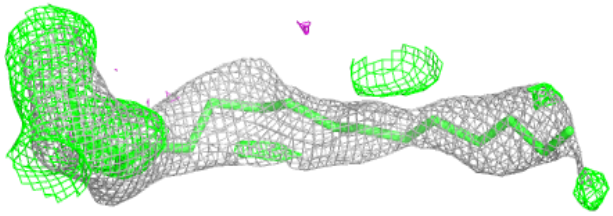


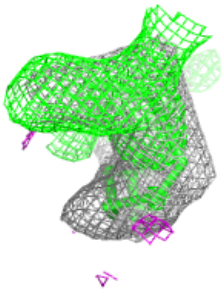


Electron density around LFA O 302:

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

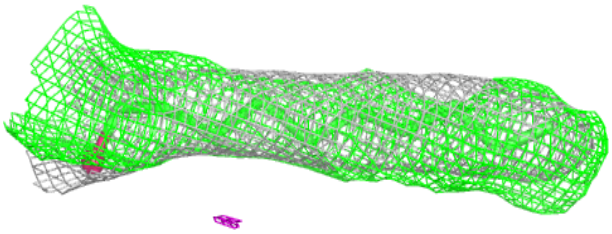


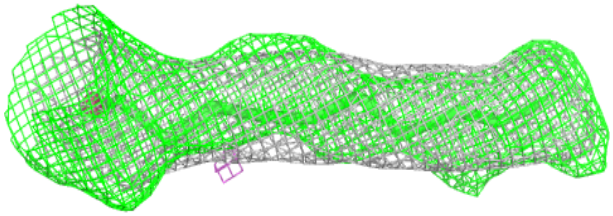


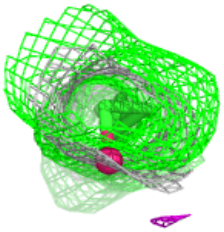


Electron density around DMU O 306:

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

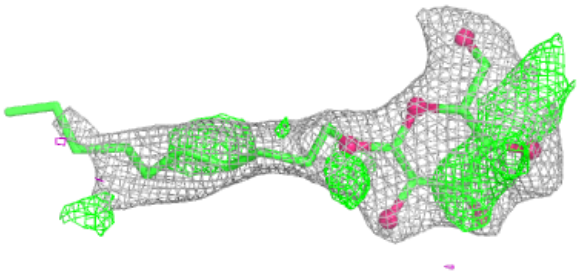


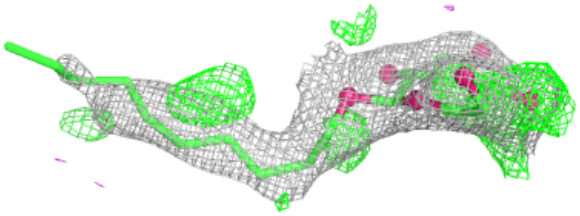


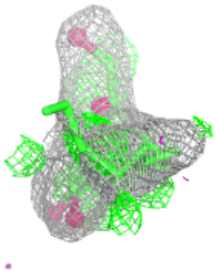


Electron density around DMU G 103:

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

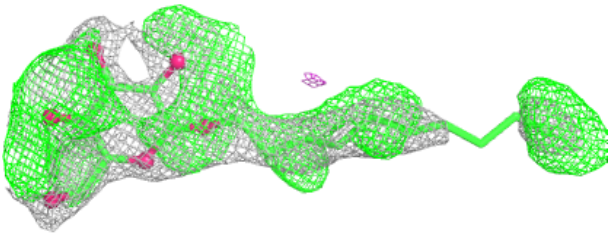


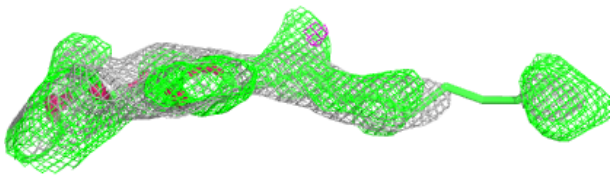


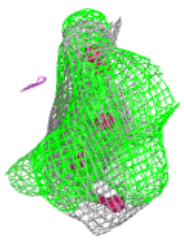


Electron density around DMU Y 102:

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

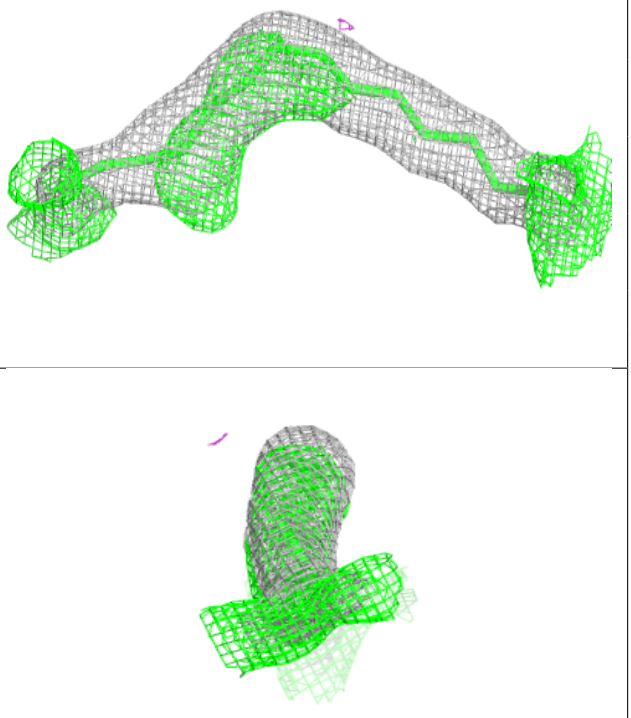


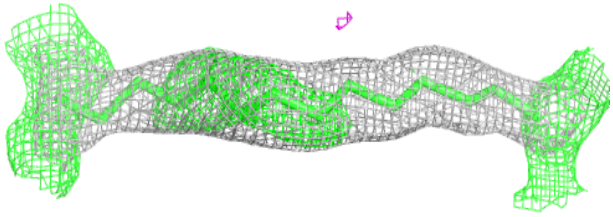




Electron density around LFA N 606:

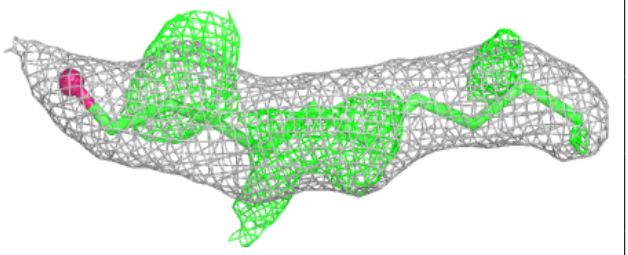
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

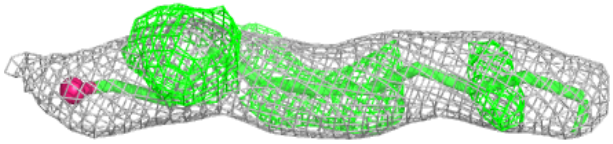


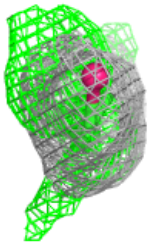


Electron density around DMU B 303:

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

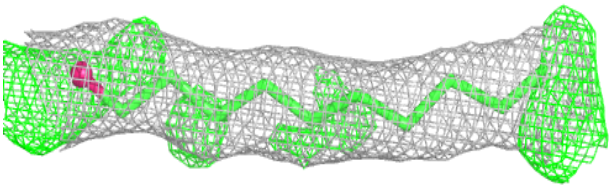


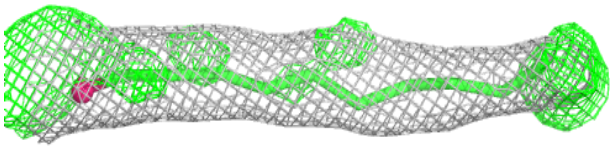


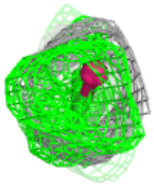


Electron density around DMU C 306:

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

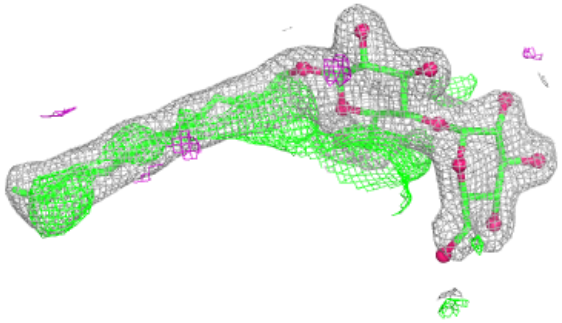


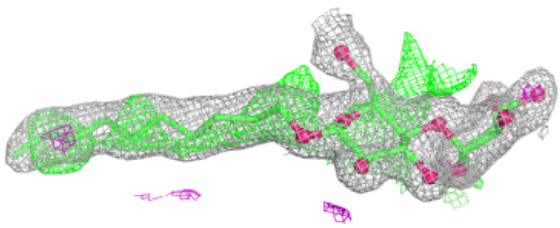


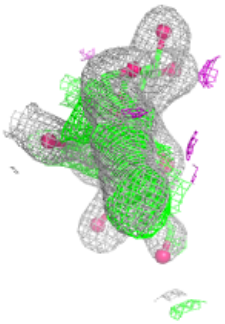


Electron density around DMU D 201:

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

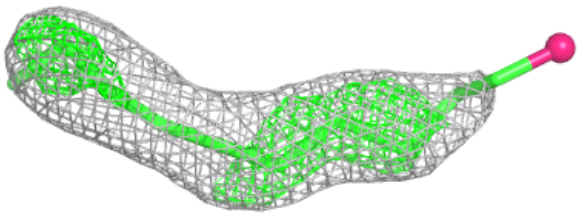


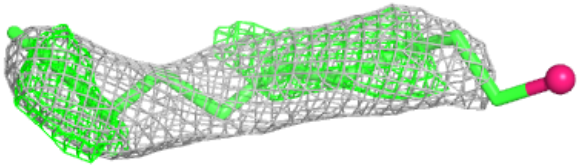


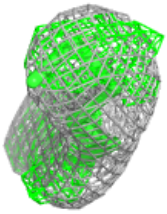


Electron density around DMU J 101:

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

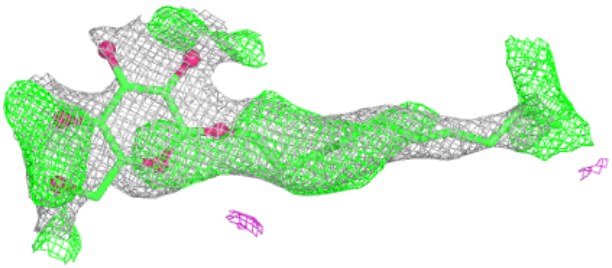


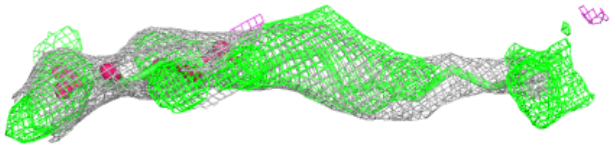


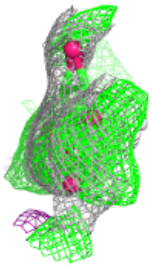


Electron density around DMU L 102:

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

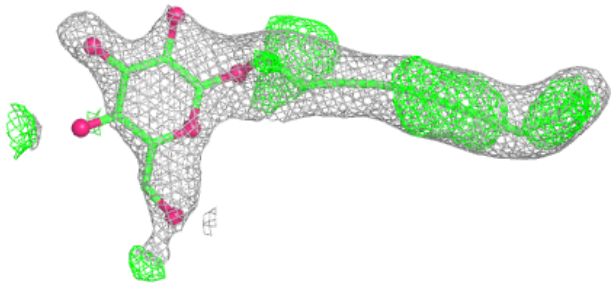


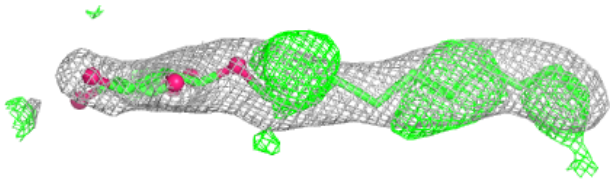


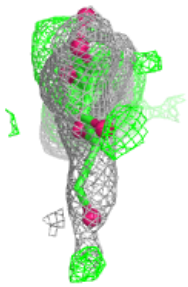


Electron density around DMU B 304:

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

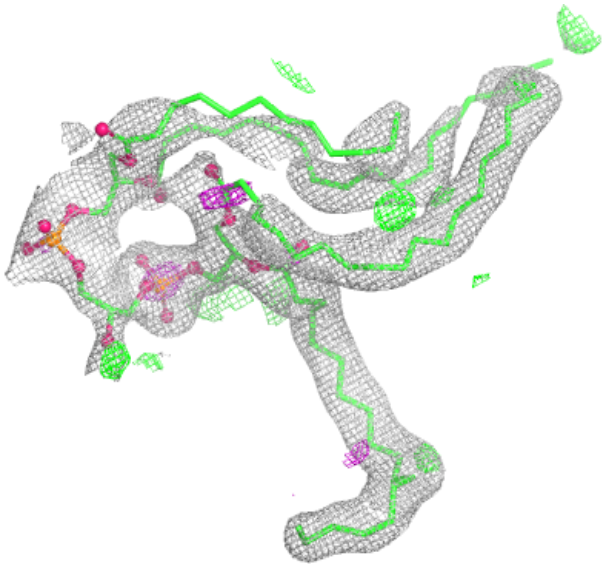


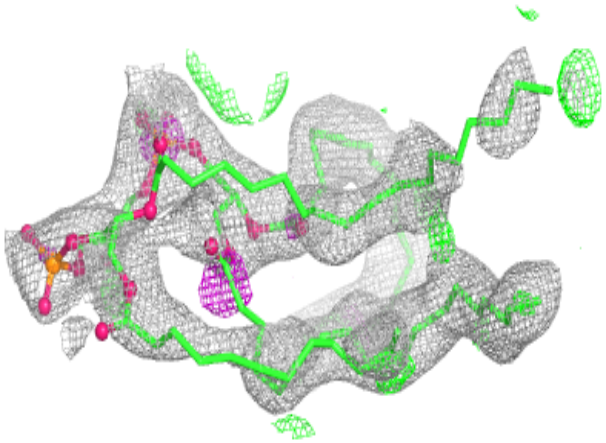


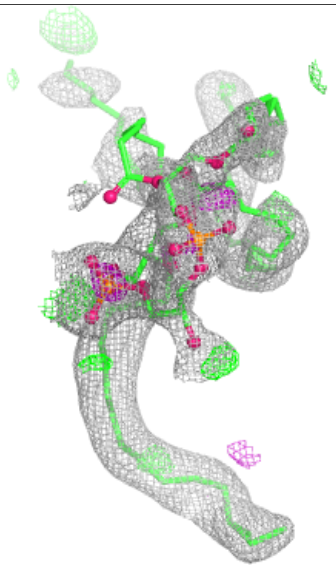


Electron density around CDL L 101:

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

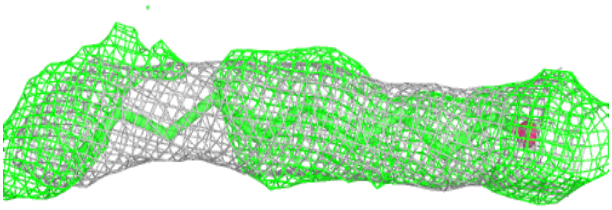


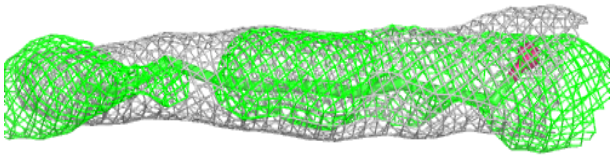


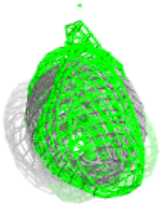


Electron density around DMU P 306:

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

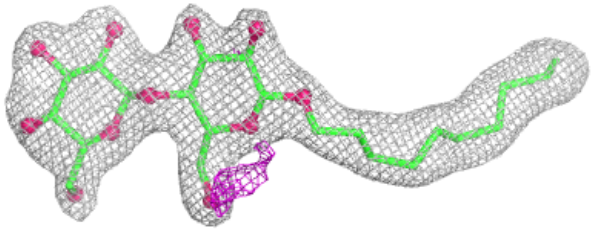


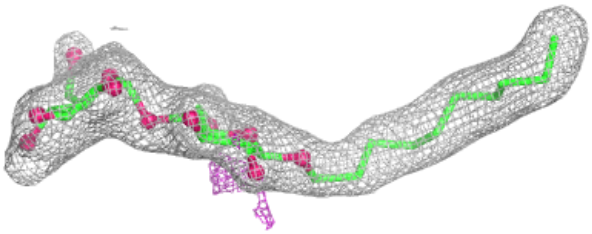


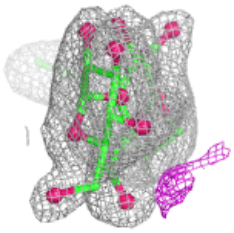


Electron density around DMU Z 101:

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

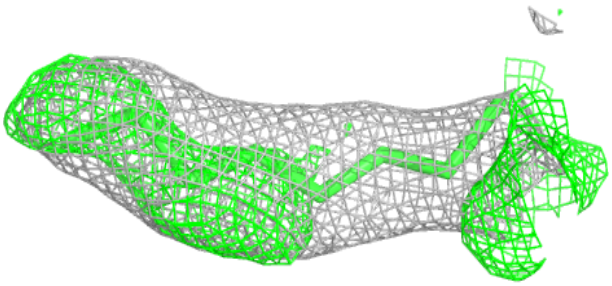


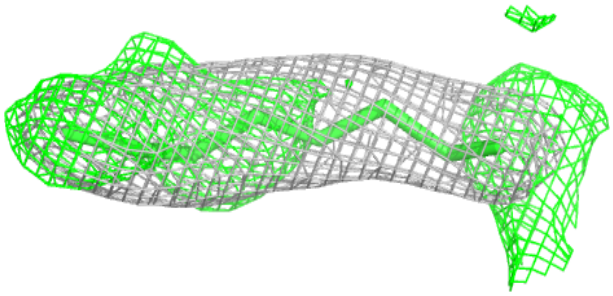


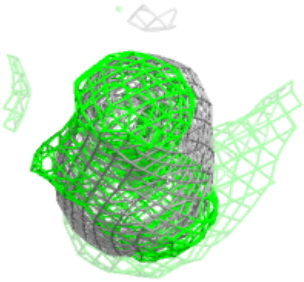


Electron density around DMU Z 102:

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

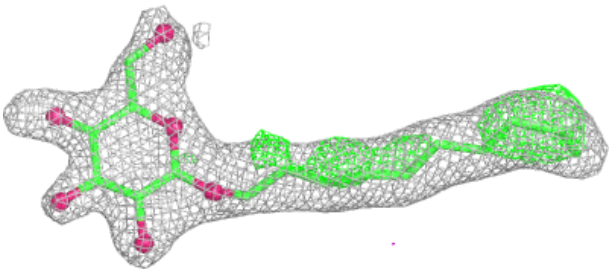


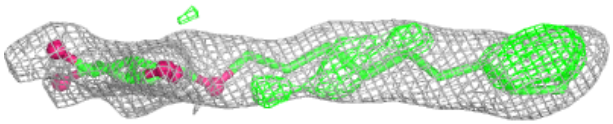


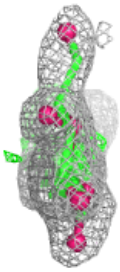


Electron density around DMU O 308:

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

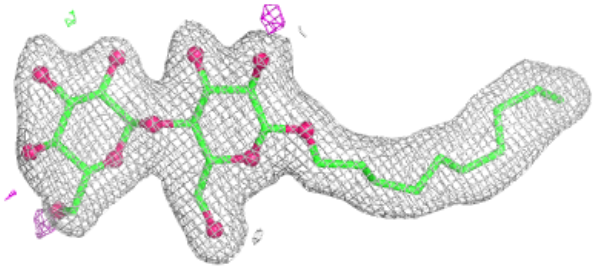


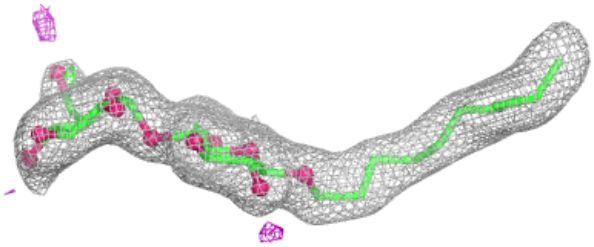


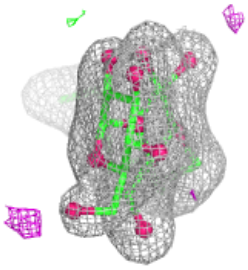


Electron density around DMU M 101:

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

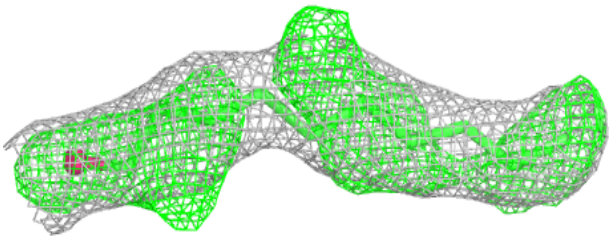


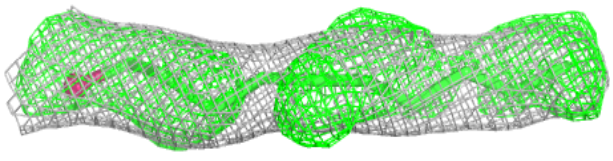


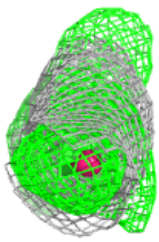


Electron density around DMU O 307:

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

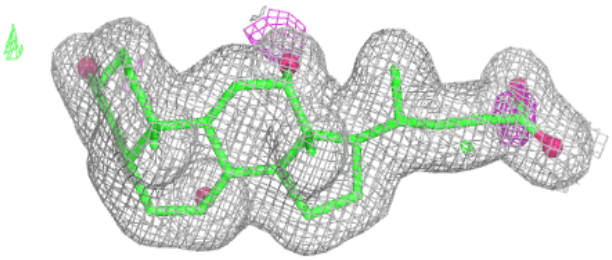


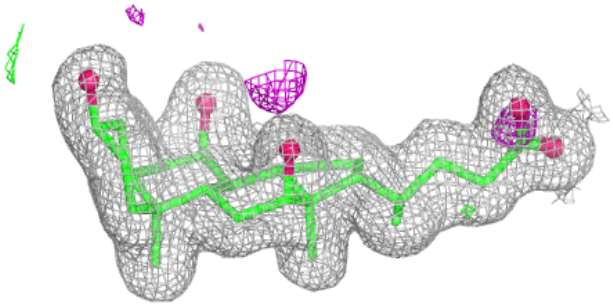


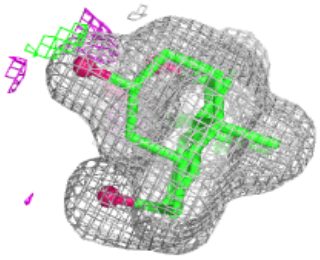


Electron density around CHD C 301:

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

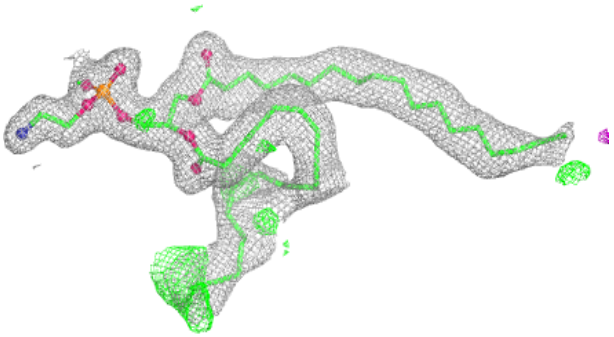


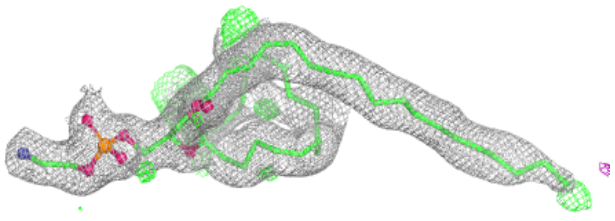


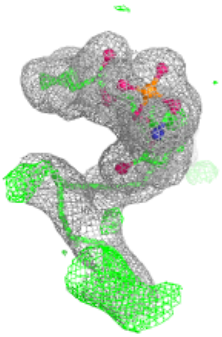


Electron density around PEK G 101:

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

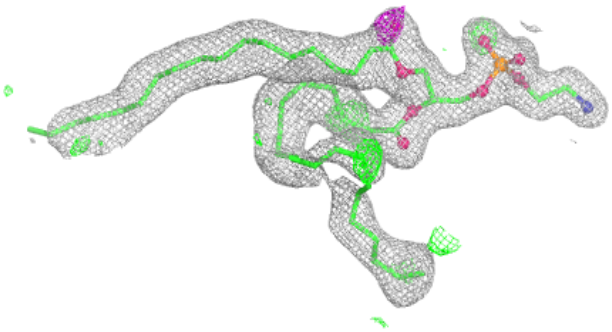


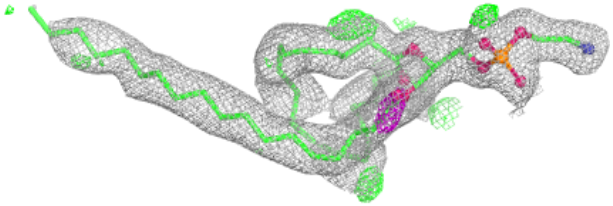


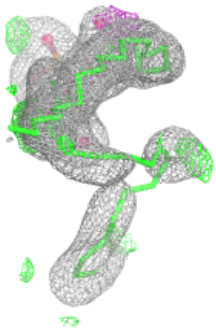


Electron density around PEK T 102:

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

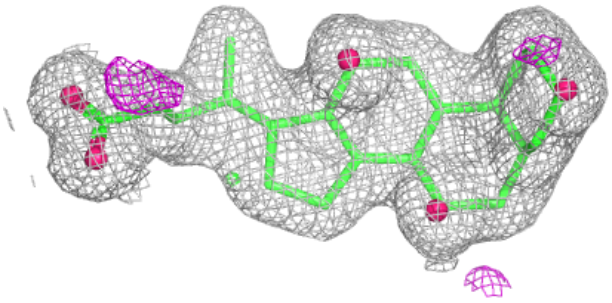


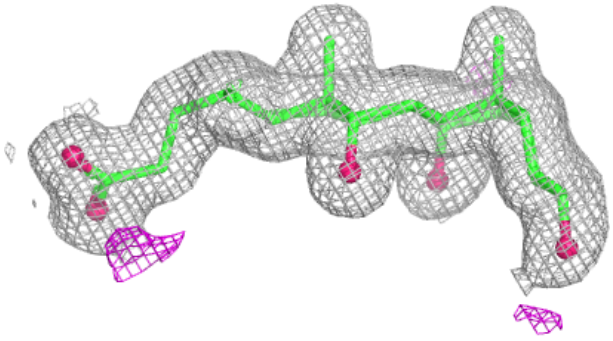


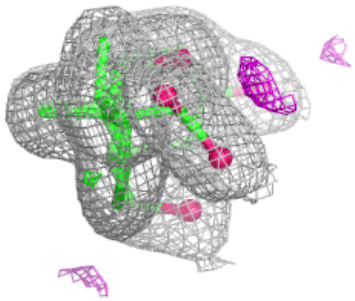


Electron density around CHD O 301:

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

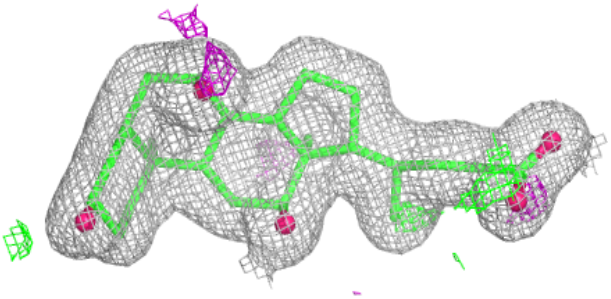


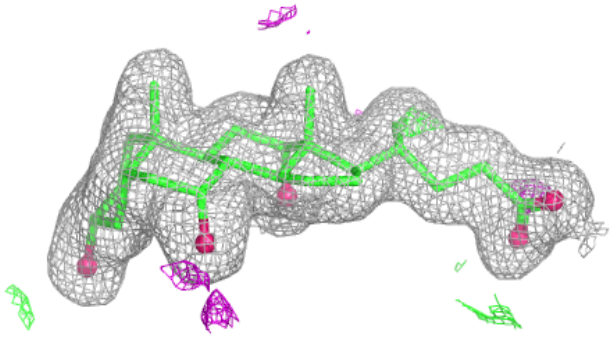


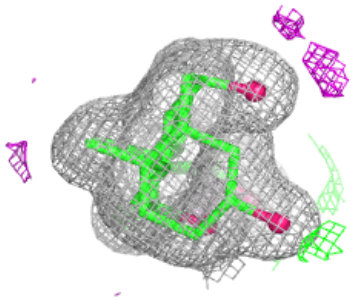


Electron density around CHD P 301:

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

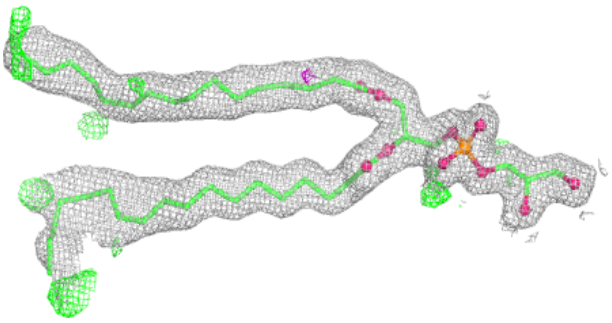


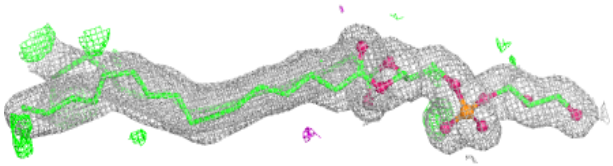


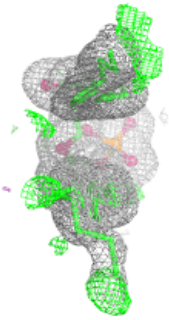


Electron density around PGV C 303:

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

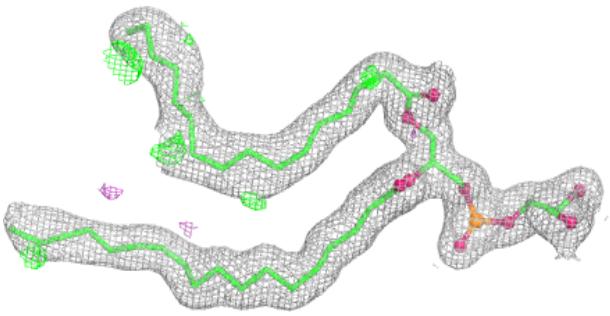


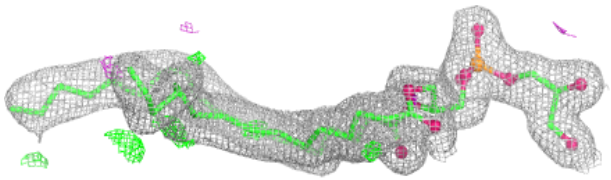


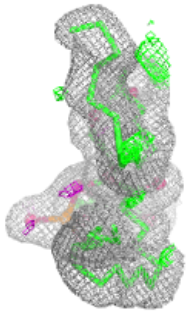


Electron density around PGV N 615:

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

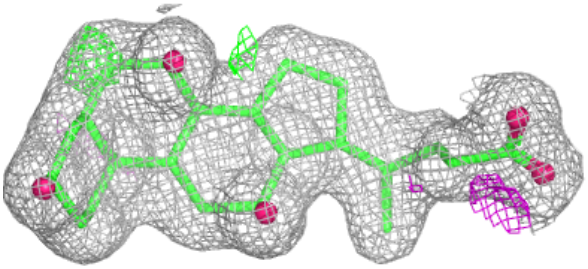


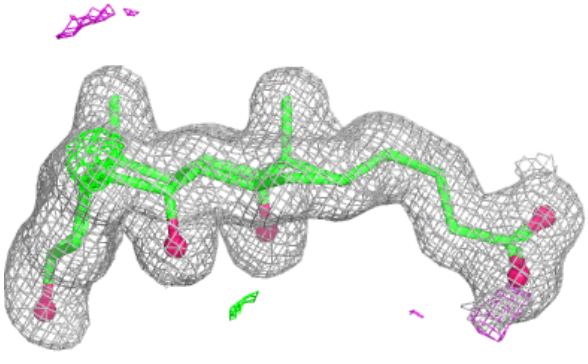


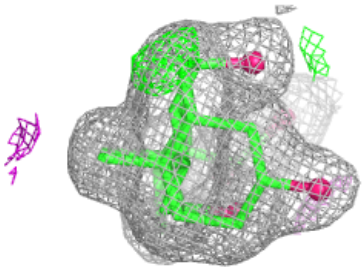


Electron density around CHD B 306:

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

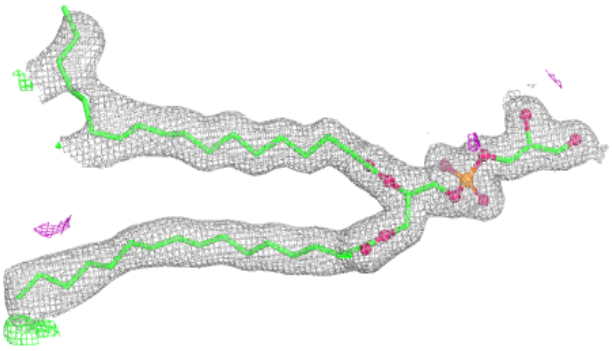


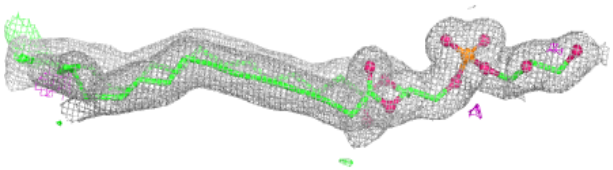


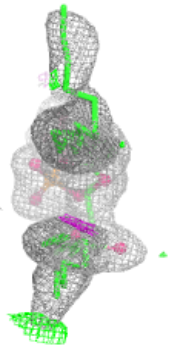


Electron density around PGV P 303:

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

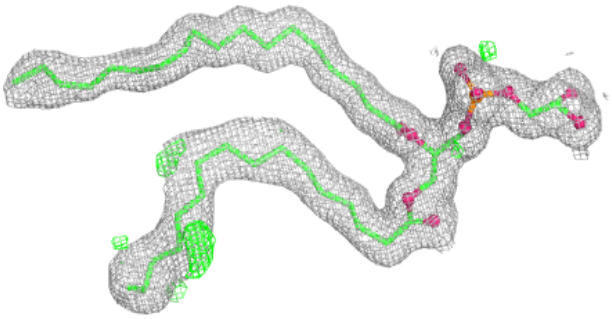


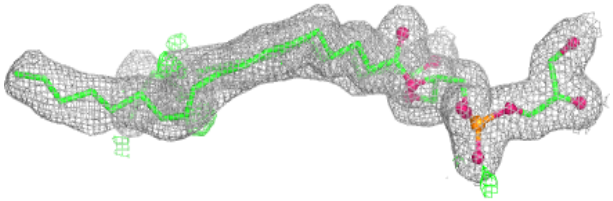


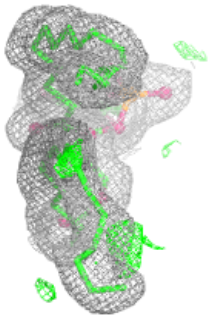


Electron density around PGV A 614:

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

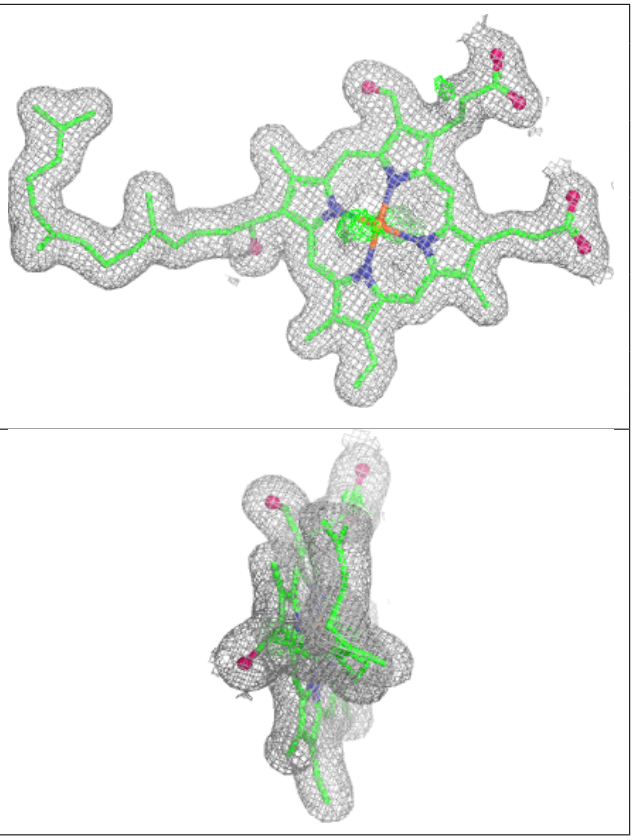


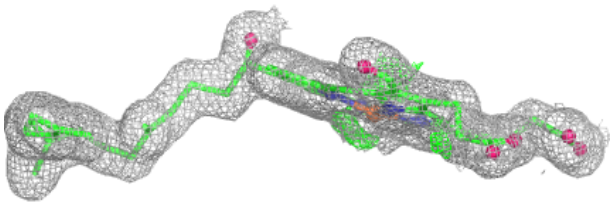




Electron density around HEA N 602:

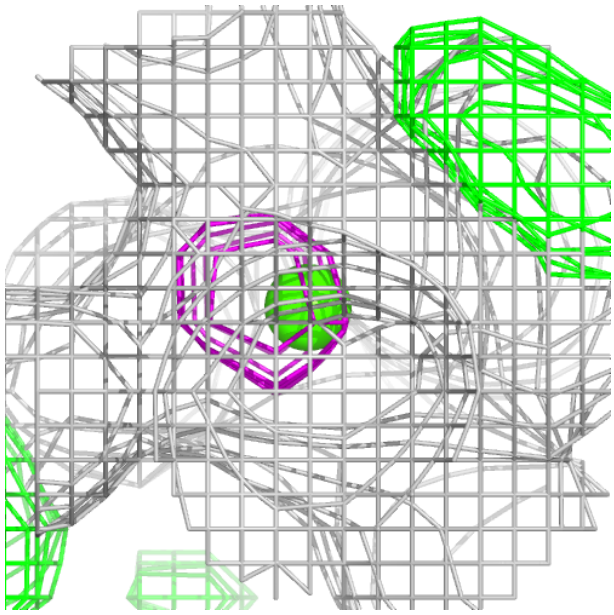
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

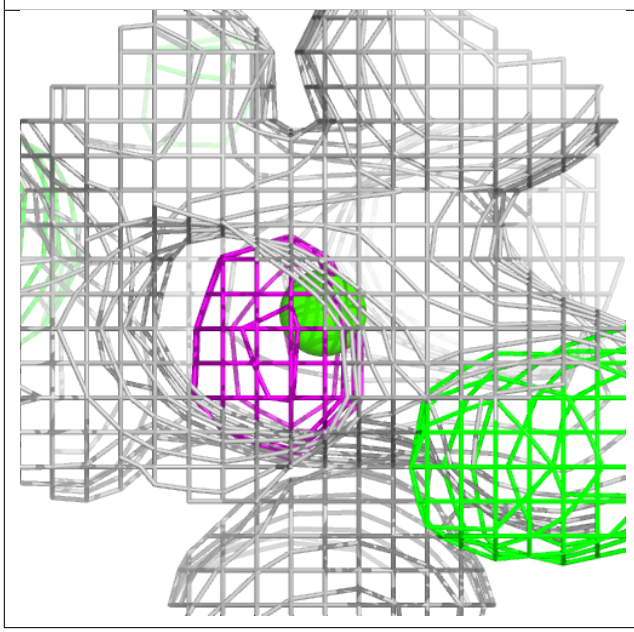


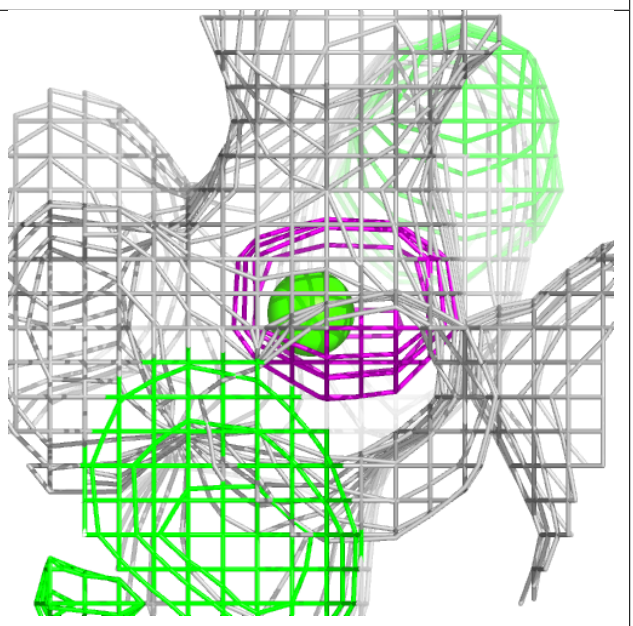


Electron density around CA A 605:

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

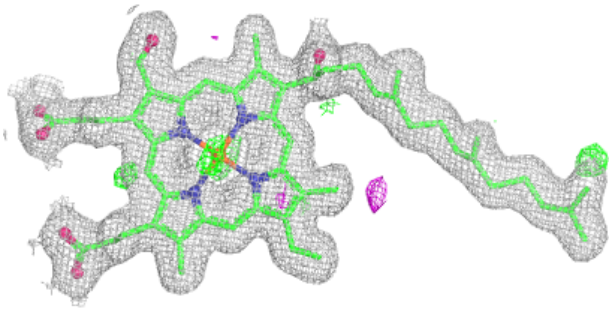


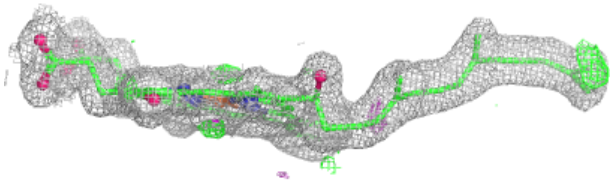


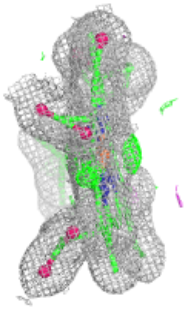


Electron density around HEA A 601:

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

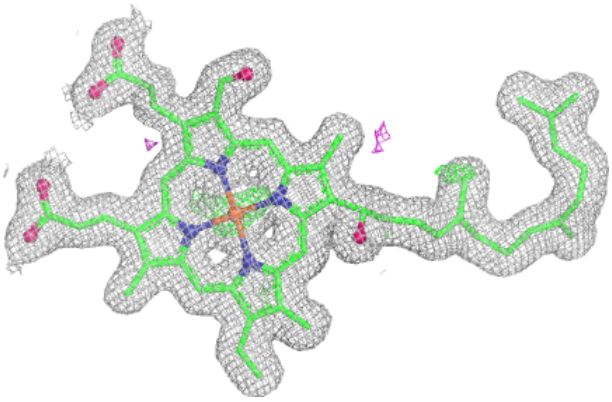


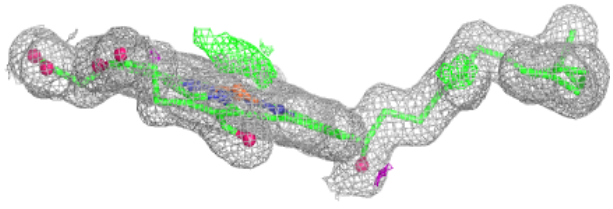


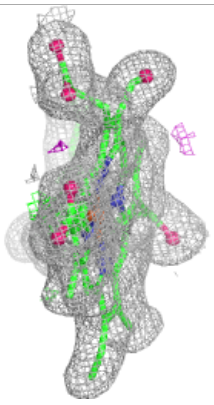


Electron density around HEA A 602:

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

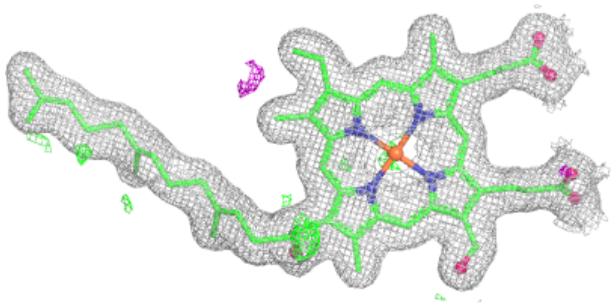


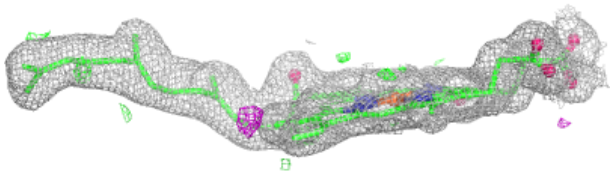


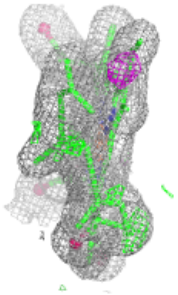


Electron density around HEA N 601:

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

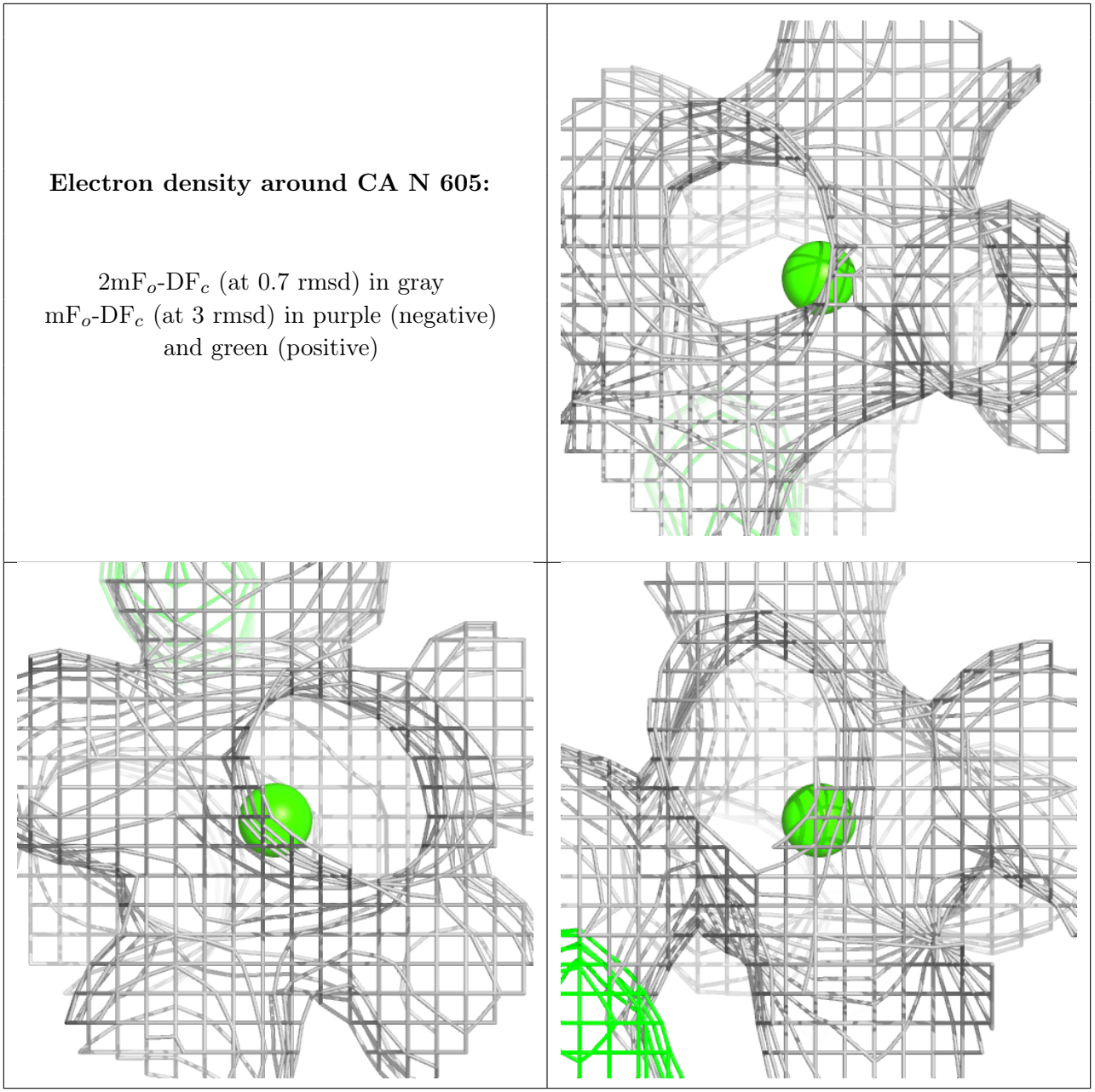






Electron density around CA N 605:

$2mF_o$-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.