wwPDB X-ray Structure Validation Summary Report (i)

Aug 5, 2026 – 06:46 PM JST

PDB ID	:	7CP5 / pdb_00007cp5
Title	:	Bovine heart cytochrome c oxidase in a catalytic intermediate of E at 1.76 angstrom resolution
Authors	:	Tsukihara, T.; Shimada, A.
Deposited on	:	2020-08-06
Resolution	:	1.76 Å(reported)

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

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

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

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

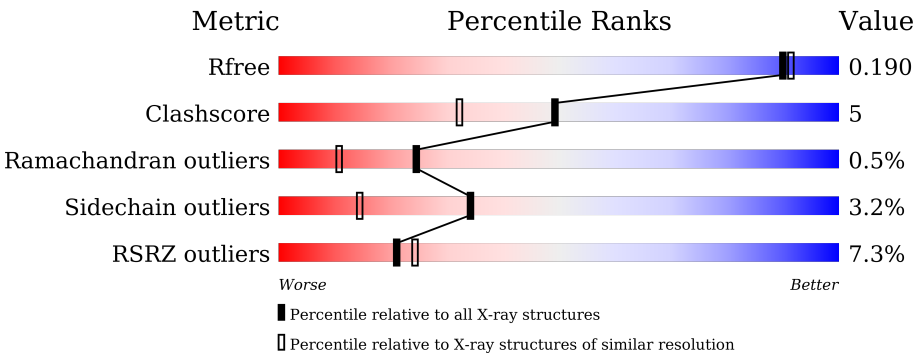
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.76 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	514	%, 90%, 9%, •
1	N	514	91%, 9%
2	B	227	6%, 84%, 15%
2	O	227	7%, 78%, 20%, •
3	C	259	2%, 92%, 8%
3	P	259	3%, 87%, 13%

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Mol	Chain	Length	Quality of chain
4	D	144	4% 91% 9%
4	Q	144	15% 88% 10%
5	E	105	4% 93% 6%
5	R	105	8% 95% 5%
6	F	94	6% 86% 13%
6	S	94	11% 91% 7%
7	G	84	27% 83% 11% 6%
7	T	84	26% 85% 14%
8	H	79	14% 77% 18%
8	U	79	20% 81% 14% 5%
9	I	73	15% 90% 7%
9	V	73	38% 88% 11%
10	J	58	12% 90% 10%
10	W	58	14% 91% 5%
11	K	49	4% 90% 8%
11	X	49	24% 96%
12	L	46	7% 76% 22%
12	Y	46	9% 89% 9%
13	M	43	9% 93% 7%
13	Z	43	14% 91% 9%

2 Entry composition (i)

There are 30 unique types of molecules in this entry. The entry contains 34258 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
			Total	C	N	O	S			
1	A	514	4190	2796	644	711	39	0	31	0
1	N	514	4213	2816	642	713	42	0	35	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	227	1862	1214	281	347	20	0	7	0
2	O	227	1882	1229	287	345	21	0	11	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	259	2167	1451	341	360	15	0	12	0
3	P	259	2161	1448	341	357	15	0	12	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	144	1211	790	199	218	4	0	3	0
4	Q	144	1199	781	196	218	4	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	105	852	544	144	162	2	0	0	0
5	R	105	860	549	147	162	2	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	94	736	458	128	144	6	0	5	0
6	S	94	716	444	127	140	5	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	G	84	692	448	129	114	1	0	4	0
7	T	84	672	431	129	111	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	79	667	420	122	120	5	0	1	0
8	U	79	662	417	121	119	5	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	I	73	604	391	107	102	4	0	1	0
9	V	73	601	390	107	100	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	J	58	464	299	78	84	3	0	1	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	W	58	461	297	78	83	3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	K	49	395	260	65	68	2	0	3	0
11	X	49	385	250	65	68	2	0	0	0

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

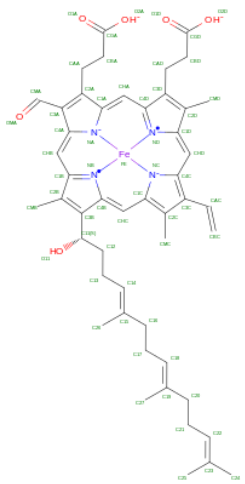
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	L	46	384	258	64	60	2	0	1	0
12	Y	46	380	254	64	60	2	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
13	M	43	336	223	53	60	0	0	0
13	Z	43	335	223	53	59	0	0	0

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

HEA



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
14	A	1	78	66	1	4	7	0	1
			Total	C	Fe	N	O		
14	A	1	60	49	1	4	6	0	0
			Total	C	Fe	N	O		
14	N	1	78	66	1	4	7	0	1
			Total	C	Fe	N	O		
14	N	1	60	49	1	4	6	0	0

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

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

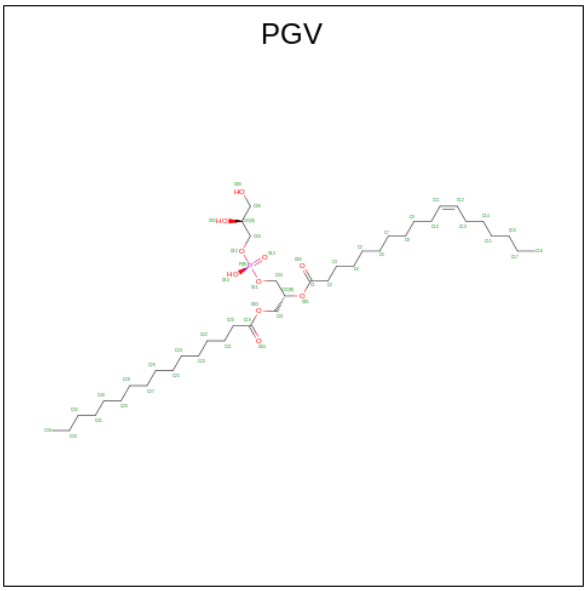
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

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

- Molecule 18 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
18	A	1	Total C O 22 21 1	0	0
18	C	1	Total C O P 51 40 10 1	0	0
18	C	1	Total C O P 48 37 10 1	0	0
18	C	1	Total C O 28 26 2	0	0
18	G	1	Total C O 32 30 2	0	0
18	N	1	Total C 24 24	0	0
18	N	1	Total C O P 51 40 10 1	0	0

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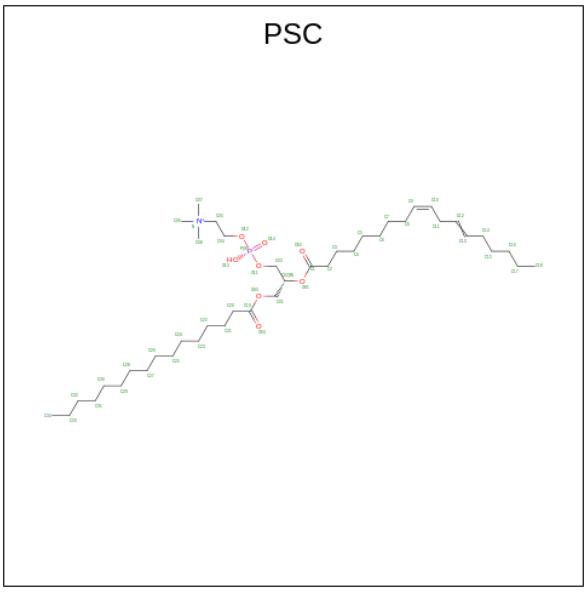
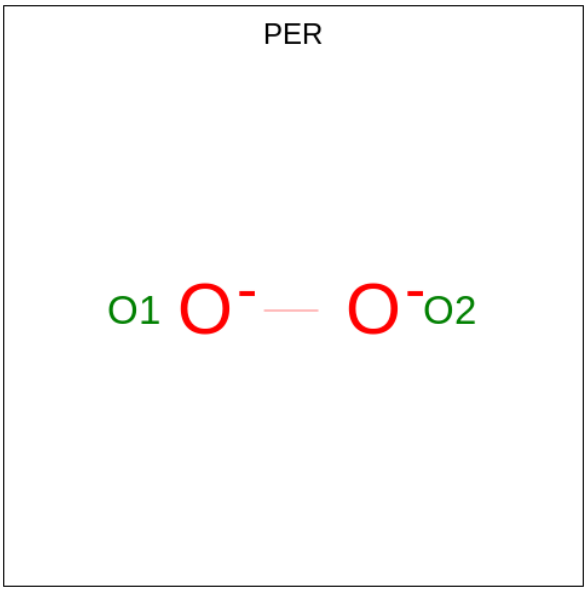
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
18	P	1	51	40	10	1	0	0

- Molecule 19 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (CCD ID: PSC) (formula: $C_{42}H_{81}NO_8P$).



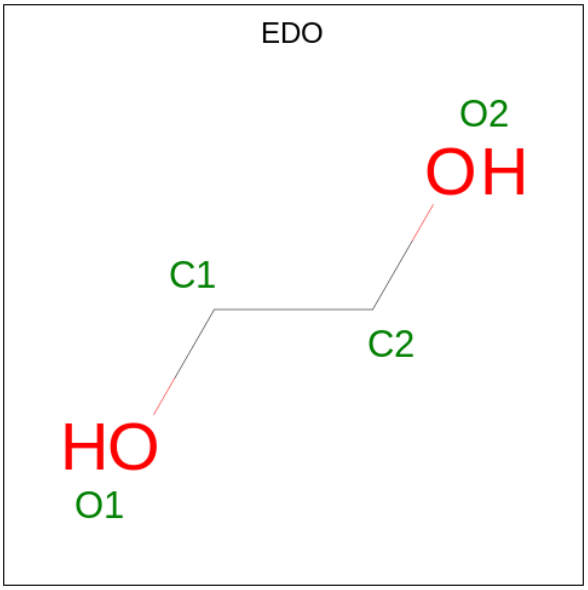
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C				
19	A	1	27	27			0	0
			Total	C	O			
19	O	1	30	28	2		0	0

- Molecule 20 is PEROXIDE ION (CCD ID: PER) (formula: O_2).



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

- 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 4 2 2	0	0
21	A	1	Total C O 4 2 2	0	0

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
21	D	1	4	2	2	0	0
21	D	1	4	2	2	0	0
21	D	1	4	2	2	0	0
21	E	1	4	2	2	0	0
21	E	1	4	2	2	0	0
21	E	1	4	2	2	0	0
21	F	1	4	2	2	0	0
21	F	1	4	2	2	0	0
21	F	1	4	2	2	0	0
21	F	1	4	2	2	0	0
21	F	1	4	2	2	0	0
21	G	1	4	2	2	0	0
21	G	1	4	2	2	0	0
21	J	1	4	2	2	0	0
21	J	1	4	2	2	0	0
21	L	1	4	2	2	0	0
21	N	1	4	2	2	0	0
21	N	1	4	2	2	0	0
21	N	1	4	2	2	0	0
21	N	1	4	2	2	0	0
21	N	1	4	2	2	0	0

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

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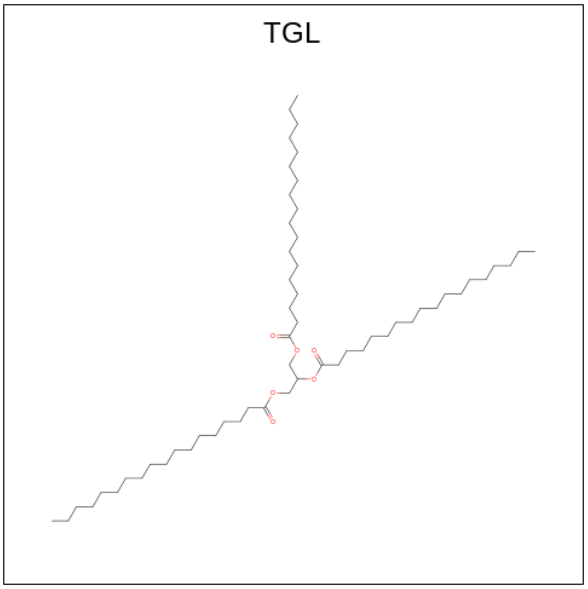
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	T	1	Total C O 4 2 2	0	0
21	T	1	Total C O 4 2 2	0	0
21	T	1	Total C O 4 2 2	0	0
21	W	1	Total C O 4 2 2	0	0
21	Y	1	Total C O 4 2 2	0	0
21	Y	1	Total C O 4 2 2	0	0

- Molecule 22 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: $C_{57}H_{110}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	B	1	Total C O 49 43 6	0	0
22	D	1	Total C O 57 51 6	0	0
22	L	1	Total C O 56 52 4	0	0
22	N	1	Total C O 63 57 6	0	0
22	N	1	Total C 48 48	0	0

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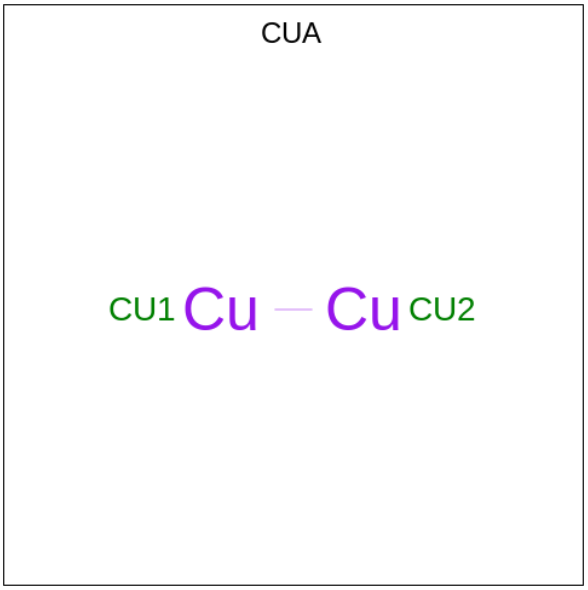
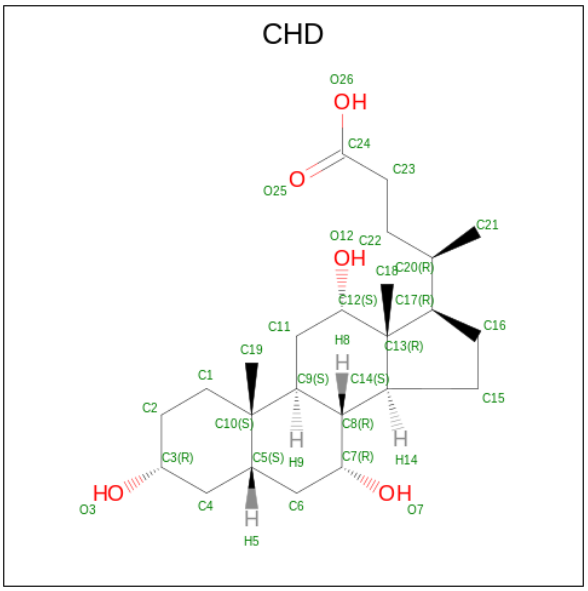
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
22	N	1	44	39	5	0	0

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



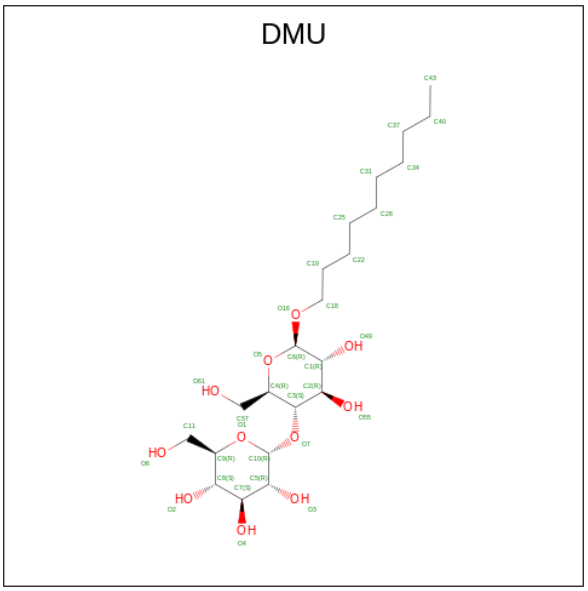
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cu		
23	B	1	2	2	0	0
			Total	Cu		
23	O	1	2	2	0	0

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



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

- Molecule 25 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: $C_{22}H_{42}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	C	1	Total C O 13 11 2	0	0
25	C	1	Total C O 21 16 5	0	0
25	D	1	Total C O 11 10 1	0	0
25	D	1	Total C O 11 10 1	0	0
25	J	1	Total C O 11 10 1	0	0
25	K	1	Total C 9 9	0	0
25	K	1	Total C 10 10	0	0
25	K	1	Total C O 11 10 1	0	0
25	K	1	Total C 9 9	0	0
25	K	1	Total C 9 9	0	0
25	K	1	Total C 10 10	0	0
25	L	1	Total C O 21 16 5	0	0
25	M	1	Total C O 33 22 11	0	0
25	O	1	Total C O 11 10 1	0	0

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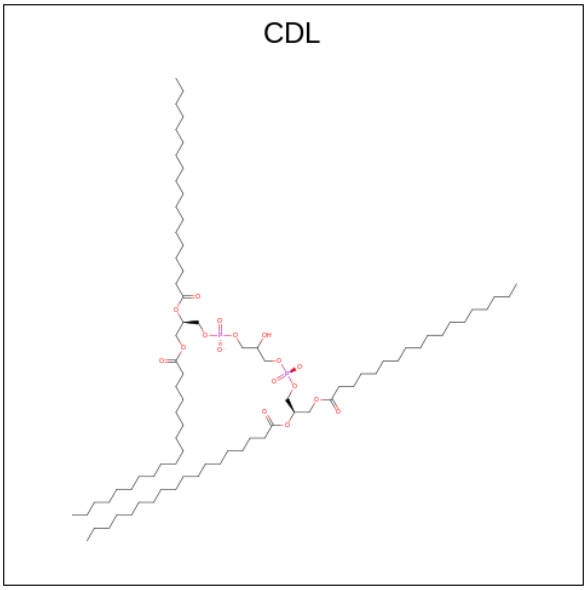
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	P	1	Total C O 13 11 2	0	0
25	P	1	Total C O 11 10 1	0	0
25	Q	1	Total C 10 10	0	0
25	W	1	Total C O 11 10 1	0	0
25	X	1	Total C O 11 10 1	0	0
25	X	1	Total C 10 10	0	0
25	X	1	Total C 9 9	0	0
25	X	1	Total C 10 10	0	0
25	Z	1	Total C O 33 22 11	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	C	1	Total C O 58 56 2	0	0
26	N	1	Total C O 55 54 1	0	0

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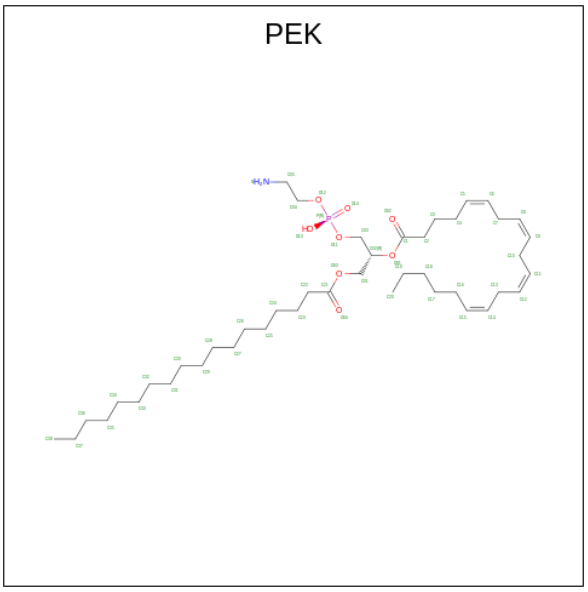
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
26	P	1	61	58	3	0	0
			Total	C	O		
26	T	1	57	54	3	0	0

- 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: $C_{43}H_{78}NO_8P$).

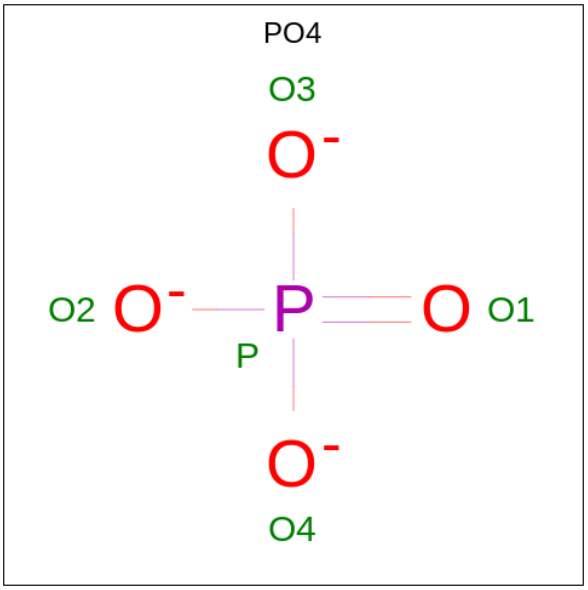


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C					
27	C	1	25	25				0	0
			Total	C	N	O	P		
27	C	1	53	43	1	8	1	0	0
			Total	C					
27	C	1	36	36				0	0
			Total	C					
27	P	1	20	20				0	0
			Total	C	N	O	P		
27	P	1	53	43	1	8	1	0	0
			Total	C					
27	P	1	34	34				0	0

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

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

- Molecule 29 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	H	1	Total O P 5 4 1	0	0
29	U	1	Total O P 5 4 1	0	0

- Molecule 30 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	A	273	Total O 273 273	0	14
30	B	223	Total O 223 223	0	2
30	C	142	Total O 142 142	0	2
30	D	213	Total O 213 213	0	0
30	E	160	Total O 160 160	0	0
30	F	162	Total O 162 162	0	3

Continued on next page...

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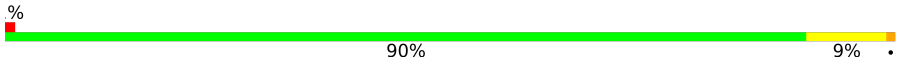
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	G	89	Total O 89 89	0	0
30	H	94	Total O 94 94	0	0
30	I	70	Total O 70 70	0	0
30	J	58	Total O 58 58	0	0
30	K	44	Total O 44 44	0	0
30	L	38	Total O 38 38	0	1
30	M	39	Total O 39 39	0	0
30	N	273	Total O 273 273	0	12
30	O	205	Total O 205 205	0	2
30	P	147	Total O 147 147	0	0
30	Q	114	Total O 114 114	0	0
30	R	117	Total O 117 117	0	0
30	S	141	Total O 141 141	0	0
30	T	66	Total O 66 66	0	0
30	U	94	Total O 94 94	0	0
30	V	72	Total O 72 72	0	0
30	W	43	Total O 43 43	0	0
30	X	31	Total O 31 31	0	0
30	Y	31	Total O 31 31	0	0
30	Z	29	Total O 29 29	0	0

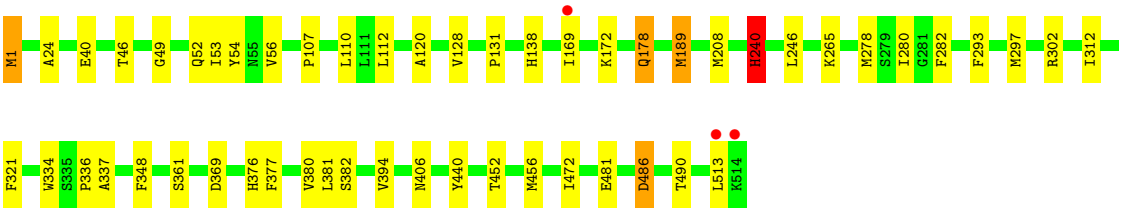
3 Residue-property plots (i)

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

• Molecule 1: Cytochrome c oxidase subunit 1

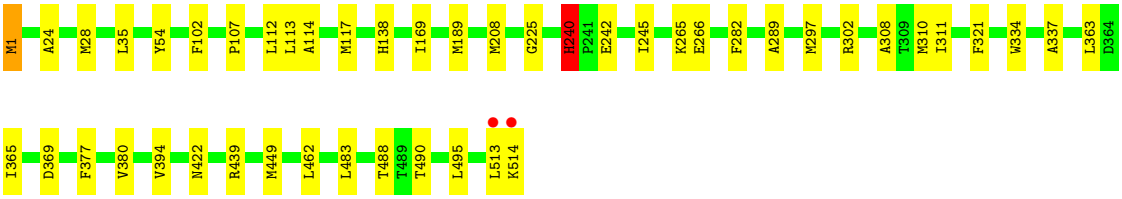
Chain A:





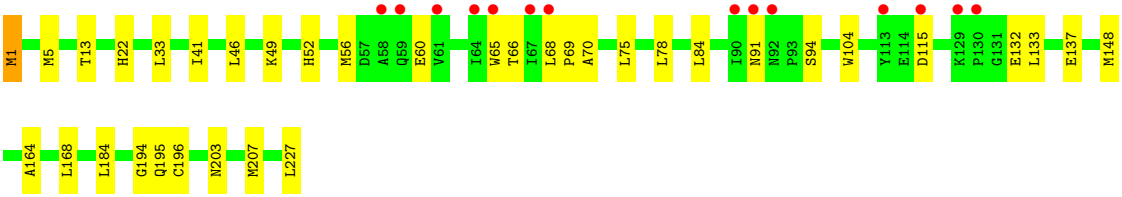
• Molecule 1: Cytochrome c oxidase subunit 1

Chain N:



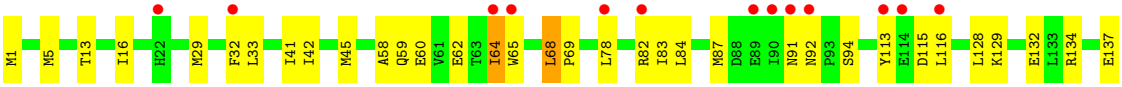
• Molecule 2: Cytochrome c oxidase subunit 2

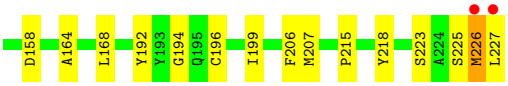
Chain B:



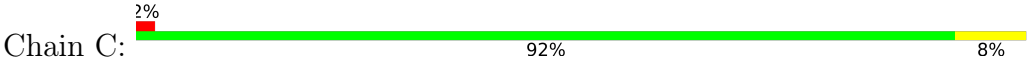
• Molecule 2: Cytochrome c oxidase subunit 2

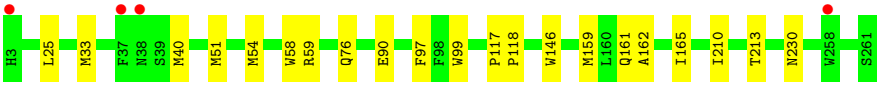
Chain O:



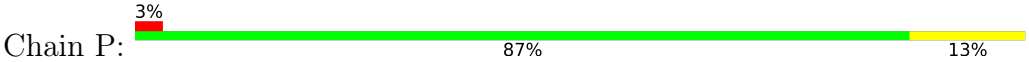


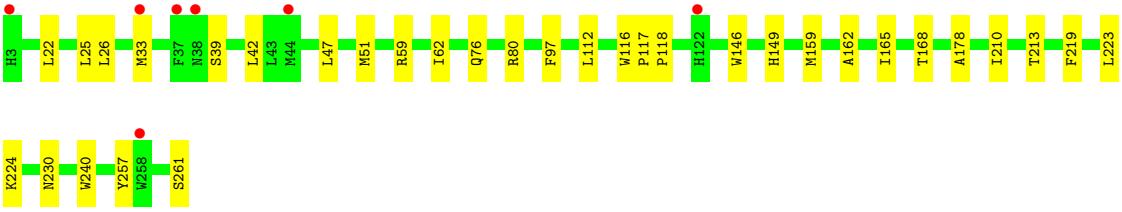
• Molecule 3: Cytochrome c oxidase subunit 3



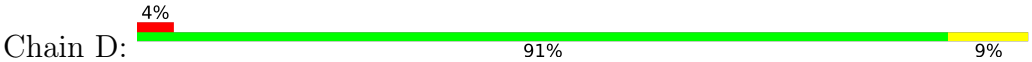


• Molecule 3: Cytochrome c oxidase subunit 3

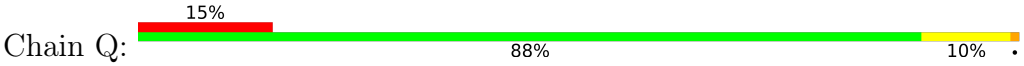


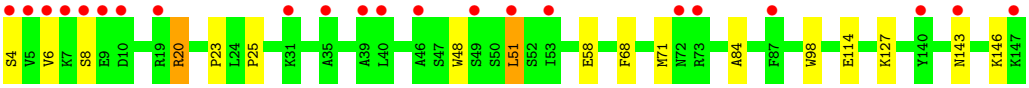


• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

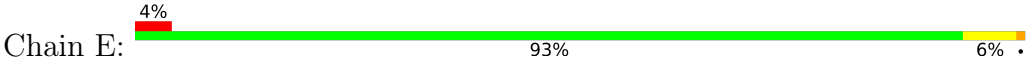


• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

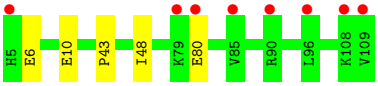




• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

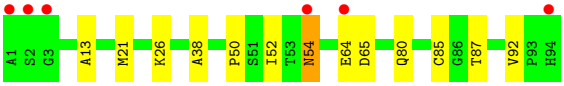


• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



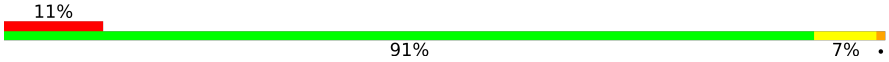
• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

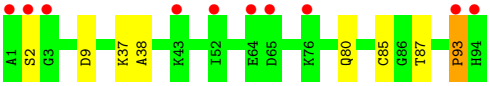
Chain F:



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

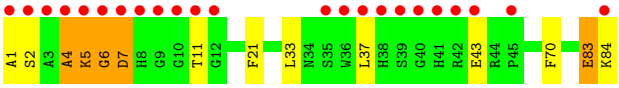
Chain S:





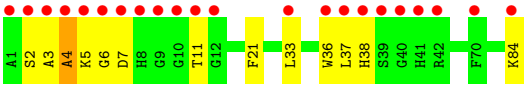
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain G:



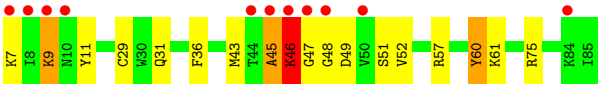
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain T:



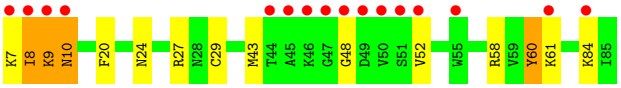
• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain H:



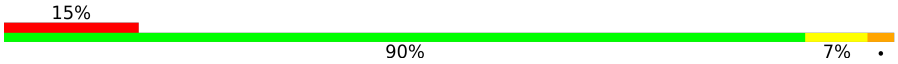
• Molecule 8: Cytochrome c oxidase subunit 6B1

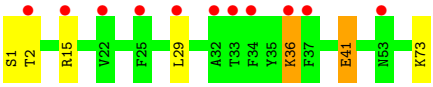
Chain U:



• Molecule 9: Cytochrome c oxidase subunit 6C

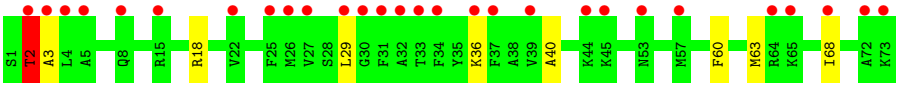
Chain I:





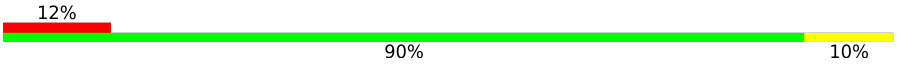
• Molecule 9: Cytochrome c oxidase subunit 6C

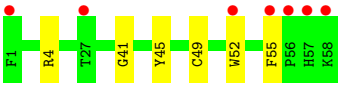
Chain V:



• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial

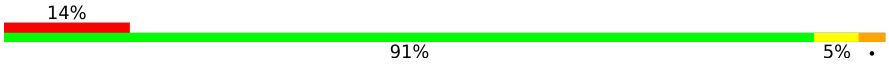
Chain J:

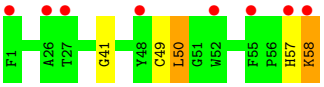




• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial

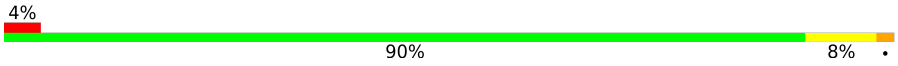
Chain W:

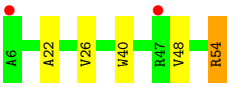




• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

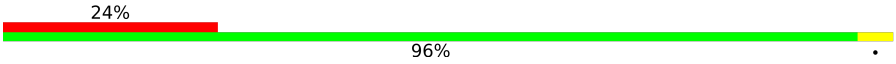
Chain K:

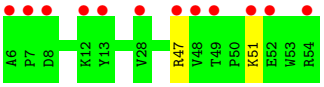




• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

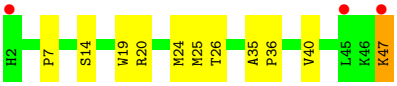
Chain X:





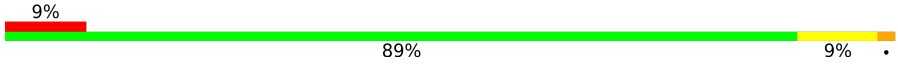
• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

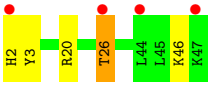
Chain L:



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

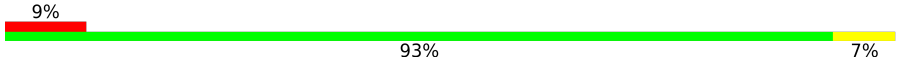
Chain Y:

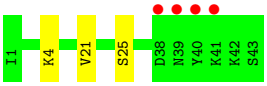




• Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

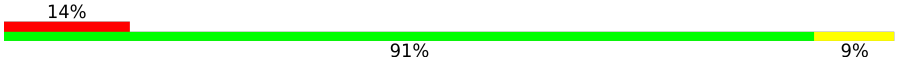
Chain M:

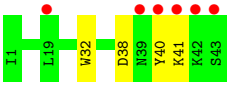




• Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

Chain Z:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	181.59Å 203.22Å 177.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.91 – 1.76 39.91 – 1.76	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.91-1.76) 99.8 (39.91-1.76)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.52 (at 1.76Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.160 , 0.189 0.162 , 0.190	Depositor DCC
R_{free} test set	32242 reflections (2.54%)	wwPDB-VP
Wilson B-factor (Å^2)	24.9	Xtriage
Anisotropy	0.782	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 74.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.004 for l,-k,h	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	34258	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SAC, EDO, NA, CU, PEK, PGV, ZN, CDL, CUA, PER, DMU, HEA, CHD, TGL, PO4, MG, FME, PSC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.87	1/4411 (0.0%)	0.88	6/6016 (0.1%)
1	N	0.78	1/4434 (0.0%)	0.84	3/6051 (0.0%)
2	B	0.79	0/1920	0.92	0/2613
2	O	0.71	0/1966	0.84	1/2675 (0.0%)
3	C	0.73	0/2296	0.73	0/3136
3	P	0.71	0/2295	0.75	0/3134
4	D	0.75	0/1259	0.79	0/1698
4	Q	0.54	0/1236	0.66	0/1668
5	E	0.71	0/871	0.72	0/1182
5	R	0.59	0/882	0.69	0/1196
6	F	0.74	0/771	0.81	0/1047
6	S	0.73	0/732	0.81	0/993
7	G	0.68	0/734	0.86	1/997 (0.1%)
7	T	0.63	0/699	0.82	0/950
8	H	0.70	0/690	0.82	1/932 (0.1%)
8	U	0.63	0/682	0.73	0/921
9	I	0.62	0/614	0.70	0/814
9	V	0.53	0/605	0.69	0/802
10	J	0.55	0/478	0.67	0/644
10	W	0.50	0/472	0.71	0/636
11	K	0.66	0/420	0.70	0/576
11	X	0.53	0/399	0.61	0/546
12	L	0.79	0/401	0.83	0/537
12	Y	0.67	0/393	0.74	0/526
13	M	0.74	0/346	0.76	0/470
13	Z	0.55	0/345	0.71	0/470
All	All	0.73	2/30351 (0.0%)	0.80	12/41230 (0.0%)

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

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	278	MET	CG-SD	-5.93	1.66	1.80
1	N	310	MET	SD-CE	-5.19	1.66	1.79

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	278	MET	CG-SD-CE	-7.85	83.64	100.90
1	N	240	HIS	CA-CB-CG	-6.96	106.84	113.80
1	A	189	MET	CG-SD-CE	-6.81	85.93	100.90
1	A	240	HIS	CA-CB-CG	-6.43	107.37	113.80
1	A	376	HIS	CA-C-N	-5.36	111.77	121.14

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	N	240	HIS	Sidechain
6	S	93	PRO	Peptide

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	4190	0	4166	51	0
1	N	4213	0	4222	44	0
2	B	1862	0	1881	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	O	1882	0	1903	32	0
3	C	2167	0	2104	16	0
3	P	2161	0	2106	29	0
4	D	1211	0	1202	14	0
4	Q	1199	0	1192	11	0
5	E	852	0	845	6	0
5	R	860	0	858	3	0
6	F	736	0	726	12	0
6	S	716	0	697	6	0
7	G	692	0	672	7	0
7	T	672	0	645	4	0
8	H	667	0	629	9	0
8	U	662	0	623	9	0
9	I	604	0	611	3	0
9	V	601	0	613	4	0
10	J	464	0	464	6	0
10	W	461	0	459	4	0
11	K	395	0	389	7	0
11	X	385	0	366	1	0
12	L	384	0	391	14	0
12	Y	380	0	380	2	0
13	M	336	0	352	4	0
13	Z	335	0	352	2	0
14	A	138	0	111	6	0
14	N	138	0	111	5	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	C	1	0	0	0	0
17	N	1	0	0	0	0
17	P	1	0	0	0	0
18	A	22	0	33	2	0
18	C	127	0	181	6	0
18	G	32	0	51	2	0
18	N	75	0	114	4	0
18	P	51	0	76	2	0
19	A	27	0	48	4	0
19	O	30	0	47	4	0
20	A	2	0	0	1	0
20	N	2	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	A	40	0	60	2	0
21	B	16	0	24	0	0
21	C	36	0	54	1	0
21	D	12	0	18	0	0
21	E	12	0	18	0	0
21	F	20	0	29	0	0
21	G	8	0	12	0	0
21	J	8	0	12	1	0
21	L	4	0	6	0	0
21	N	36	0	54	0	0
21	O	12	0	18	3	0
21	P	32	0	48	1	0
21	Q	4	0	6	0	0
21	S	20	0	30	1	0
21	T	12	0	18	0	0
21	W	4	0	6	1	0
21	Y	8	0	12	0	0
22	B	49	0	77	1	0
22	D	57	0	95	9	0
22	L	56	0	94	9	0
22	N	155	0	275	14	0
23	B	2	0	0	0	0
23	O	2	0	0	0	0
24	B	29	0	39	0	0
24	C	29	0	39	0	0
24	G	29	0	39	1	0
24	L	29	0	39	4	0
24	P	29	0	39	0	0
24	Y	29	0	39	1	0
25	C	34	0	51	5	0
25	D	22	0	40	2	0
25	J	11	0	21	2	0
25	K	58	0	110	4	0
25	L	21	0	30	1	0
25	M	33	0	42	2	0
25	O	11	0	21	1	0
25	P	24	0	42	6	0
25	Q	10	0	19	1	0
25	W	11	0	21	1	0
25	X	40	0	74	0	0
25	Z	33	0	42	1	0
26	C	58	0	100	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	N	55	0	101	3	0
26	P	61	0	104	4	0
26	T	57	0	88	7	0
27	C	114	0	173	8	0
27	P	107	0	163	9	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	H	5	0	0	0	0
29	U	5	0	0	0	0
30	A	273	0	0	2	0
30	B	223	0	0	1	0
30	C	142	0	0	1	0
30	D	213	0	0	1	0
30	E	160	0	0	3	0
30	F	162	0	0	4	0
30	G	89	0	0	0	0
30	H	94	0	0	1	0
30	I	70	0	0	2	0
30	J	58	0	0	3	0
30	K	44	0	0	1	0
30	L	38	0	0	1	0
30	M	39	0	0	0	0
30	N	273	0	0	4	0
30	O	205	0	0	4	0
30	P	147	0	0	0	0
30	Q	114	0	0	2	0
30	R	117	0	0	0	0
30	S	141	0	0	3	0
30	T	66	0	0	0	0
30	U	94	0	0	0	0
30	V	72	0	0	1	0
30	W	43	0	0	1	0
30	X	31	0	0	0	0
30	Y	31	0	0	0	0
30	Z	29	0	0	2	0
All	All	34258	0	32062	342	0

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

The worst 5 of 342 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)
20:N:610[A]:PER:O2	20:N:610[A]:PER:O1	1.54	1.25
20:A:608[A]:PER:O2	20:A:608[A]:PER:O1	1.55	1.25
1:N:311[A]:ILE:HG22	26:N:601:CDL:H441	1.58	0.85
3:P:224[B]:LYS:HE2	26:P:304:CDL:H131	1.62	0.82
1:A:406:ASN:HD21	18:A:606:PGV:H22	1.47	0.79

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	545/514 (106%)	530 (97%)	15 (3%)	0	100	100
1	N	550/514 (107%)	538 (98%)	12 (2%)	0	100	100
2	B	232/227 (102%)	227 (98%)	5 (2%)	0	100	100
2	O	236/227 (104%)	229 (97%)	6 (2%)	1 (0%)	30	15
3	C	269/259 (104%)	264 (98%)	5 (2%)	0	100	100
3	P	269/259 (104%)	264 (98%)	5 (2%)	0	100	100
4	D	145/144 (101%)	142 (98%)	3 (2%)	0	100	100
4	Q	143/144 (99%)	138 (96%)	5 (4%)	0	100	100
5	E	103/105 (98%)	103 (100%)	0	0	100	100
5	R	104/105 (99%)	103 (99%)	1 (1%)	0	100	100
6	F	97/94 (103%)	95 (98%)	2 (2%)	0	100	100
6	S	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
7	G	86/84 (102%)	77 (90%)	4 (5%)	5 (6%)	1	0
7	T	82/84 (98%)	72 (88%)	5 (6%)	5 (6%)	1	0
8	H	78/79 (99%)	70 (90%)	5 (6%)	3 (4%)	2	0
8	U	77/79 (98%)	72 (94%)	4 (5%)	1 (1%)	9	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	72/73 (99%)	71 (99%)	1 (1%)	0	100	100
9	V	71/73 (97%)	68 (96%)	2 (3%)	1 (1%)	9	2
10	J	57/58 (98%)	56 (98%)	1 (2%)	0	100	100
10	W	56/58 (97%)	56 (100%)	0	0	100	100
11	K	50/49 (102%)	48 (96%)	2 (4%)	0	100	100
11	X	47/49 (96%)	46 (98%)	1 (2%)	0	100	100
12	L	45/46 (98%)	43 (96%)	2 (4%)	0	100	100
12	Y	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
13	M	41/43 (95%)	41 (100%)	0	0	100	100
13	Z	41/43 (95%)	40 (98%)	1 (2%)	0	100	100
All	All	3632/3550 (102%)	3525 (97%)	91 (2%)	16 (0%)	24	15

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	4	ALA
7	G	7	ASP
7	G	37	LEU
7	T	4	ALA
7	T	5	LYS

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	456/426 (107%)	447 (98%)	9 (2%)	48	29
1	N	460/426 (108%)	457 (99%)	3 (1%)	76	67
2	B	217/210 (103%)	209 (96%)	8 (4%)	30	11
2	O	221/210 (105%)	207 (94%)	14 (6%)	16	3
3	C	236/224 (105%)	232 (98%)	4 (2%)	53	36
3	P	236/224 (105%)	233 (99%)	3 (1%)	61	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	131/128 (102%)	129 (98%)	2 (2%)	57	41
4	Q	129/128 (101%)	124 (96%)	5 (4%)	28	9
5	E	92/92 (100%)	90 (98%)	2 (2%)	45	26
5	R	93/92 (101%)	93 (100%)	0	100	100
6	F	83/78 (106%)	79 (95%)	4 (5%)	23	6
6	S	78/78 (100%)	74 (95%)	4 (5%)	21	5
7	G	72/68 (106%)	63 (88%)	9 (12%)	4	0
7	T	68/68 (100%)	62 (91%)	6 (9%)	9	1
8	H	72/71 (101%)	65 (90%)	7 (10%)	8	1
8	U	71/71 (100%)	64 (90%)	7 (10%)	7	1
9	I	58/57 (102%)	53 (91%)	5 (9%)	10	1
9	V	57/57 (100%)	54 (95%)	3 (5%)	20	5
10	J	50/49 (102%)	50 (100%)	0	100	100
10	W	49/49 (100%)	47 (96%)	2 (4%)	27	8
11	K	42/39 (108%)	41 (98%)	1 (2%)	43	23
11	X	39/39 (100%)	38 (97%)	1 (3%)	40	20
12	L	40/39 (103%)	39 (98%)	1 (2%)	42	22
12	Y	39/39 (100%)	35 (90%)	4 (10%)	7	0
13	M	37/37 (100%)	37 (100%)	0	100	100
13	Z	37/37 (100%)	36 (97%)	1 (3%)	39	19
All	All	3163/3036 (104%)	3058 (97%)	105 (3%)	34	13

5 of 105 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	O	64[A]	ILE
3	P	230	ASN
11	X	47	ARG
2	O	68	LEU
2	O	223	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	N	422	ASN
4	Q	109	HIS
8	U	12	GLN
4	Q	143	ASN
4	D	76	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FME	B	1	2	8,9,10	1.01	1 (12%)	7,9,11	1.86	2 (28%)
2	FME	O	1	2	8,9,10	0.80	0	7,9,11	1.54	2 (28%)
9	SAC	I	1	9	7,8,9	0.68	0	8,9,11	1.42	1 (12%)
9	SAC	V	1	9	7,8,9	0.61	0	8,9,11	0.90	0
1	FME	N	1	1	8,9,10	0.56	0	7,9,11	1.47	1 (14%)
1	FME	A	1	1	8,9,10	0.47	0	7,9,11	1.26	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FME	B	1	2	-	0/7/9/11	-
2	FME	O	1	2	-	0/7/9/11	-
9	SAC	I	1	9	-	2/7/8/10	-
9	SAC	V	1	9	-	4/7/8/10	-

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	CG-SD	-2.03	1.70	1.81

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	FME	CG-CB-CA	-3.36	103.62	112.95
2	O	1	FME	CG-CB-CA	-2.67	105.52	112.95
1	N	1	FME	O-C-CA	-2.67	117.79	124.78
9	I	1	SAC	CA-N-C1A	-2.58	118.38	123.15
2	B	1	FME	C-CA-N	-2.46	105.29	109.73

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	N-CA-CB-CG
9	I	1	SAC	C-CA-CB-OG
1	N	1	FME	O1-CN-N-CA
1	N	1	FME	N-CA-CB-CG
9	V	1	SAC	C2A-C1A-N-CA

There are no ring outliers.

3 monomers are involved in 4 short contacts:

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 150 ligands modelled in this entry, 10 are monoatomic - leaving 140 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	P	313	-	3,3,3	0.80	0	2,2,2	0.15	0
21	EDO	C	314	-	3,3,3	0.84	0	2,2,2	0.40	0
21	EDO	P	315	-	3,3,3	0.40	0	2,2,2	1.15	0
22	TGL	B	301	-	47,47,62	1.16	3 (6%)	50,50,65	1.47	5 (10%)
21	EDO	N	617	-	3,3,3	0.51	0	2,2,2	0.36	0
18	PGV	A	606	-	20,20,50	0.51	0	18,18,56	0.78	0
25	DMU	W	101	-	10,10,34	0.38	0	9,9,45	0.54	0
22	TGL	N	611	-	45,45,62	0.36	0	42,42,65	0.44	0
29	PO4	H	101	-	4,4,4	0.77	0	6,6,6	0.66	0
25	DMU	O	302	-	10,10,34	0.20	0	9,9,45	0.72	0
18	PGV	C	308	-	47,47,50	0.84	1 (2%)	50,53,56	0.93	3 (6%)
21	EDO	A	618	-	3,3,3	0.70	0	2,2,2	0.78	0
25	DMU	X	103	-	8,8,34	0.40	0	7,7,45	0.53	0
25	DMU	P	309	-	10,10,34	0.33	0	9,9,45	0.55	0
14	HEA	A	602	1,20,30	66,67,67	1.79	20 (30%)	78,103,103	1.98	21 (26%)
25	DMU	C	303	-	12,12,34	0.54	0	10,11,45	0.35	0
18	PGV	C	301	-	50,50,50	0.94	4 (8%)	53,56,56	1.21	4 (7%)
21	EDO	C	319	-	3,3,3	0.60	0	2,2,2	0.16	0
21	EDO	P	316	-	3,3,3	0.58	0	2,2,2	0.42	0
21	EDO	Y	102	-	3,3,3	0.46	0	2,2,2	0.21	0
21	EDO	N	621	-	3,3,3	0.56	0	2,2,2	0.09	0
21	EDO	N	616	-	3,3,3	0.47	0	2,2,2	0.50	0
18	PGV	C	311	-	26,26,50	1.17	1 (3%)	25,25,56	2.06	5 (20%)
21	EDO	B	306	-	3,3,3	0.82	0	2,2,2	0.33	0
21	EDO	B	305	-	3,3,3	0.41	0	2,2,2	0.78	0
29	PO4	U	101	-	4,4,4	1.14	0	6,6,6	0.76	0
21	EDO	N	615	-	3,3,3	0.58	0	2,2,2	0.12	0
25	DMU	P	303	-	11,11,34	0.43	0	10,10,45	0.37	0
25	DMU	J	101	-	10,10,34	0.36	0	9,9,45	0.39	0
25	DMU	K	103	-	10,10,34	0.40	0	9,9,45	0.48	0
21	EDO	F	104	-	3,3,3	0.58	0	2,2,2	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
27	PEK	P	306	-	52,52,52	0.75	2 (3%)	55,57,57	1.09	4 (7%)
14	HEA	N	602[A]	-	66,67,67	1.64	15 (22%)	78,103,103	1.87	24 (30%)
24	CHD	G	101	-	32,32,32	0.90	0	51,51,51	1.30	7 (13%)
18	PGV	G	102	-	30,30,50	0.98	1 (3%)	28,29,56	1.48	3 (10%)
21	EDO	S	106	-	3,3,3	0.43	0	2,2,2	0.79	0
14	HEA	N	602[C]	-	66,58,67	3.25	15 (22%)	78,91,103	3.55	29 (37%)
24	CHD	P	301	-	32,32,32	0.78	0	51,51,51	1.52	8 (15%)
19	PSC	A	607	-	25,25,51	0.81	1 (4%)	22,23,59	0.93	0
21	EDO	W	102	-	3,3,3	0.34	0	2,2,2	0.24	0
24	CHD	Y	101	-	32,32,32	0.77	0	51,51,51	2.34	18 (35%)
21	EDO	T	102	-	3,3,3	0.65	0	2,2,2	0.77	0
25	DMU	C	310	-	21,21,34	0.88	1 (4%)	24,25,45	1.35	3 (12%)
21	EDO	S	104	-	3,3,3	0.50	0	2,2,2	0.23	0
21	EDO	P	314	-	3,3,3	0.44	0	2,2,2	0.87	0
25	DMU	K	106	-	9,9,34	0.28	0	8,8,45	0.32	0
26	CDL	P	304	-	57,57,99	1.22	7 (12%)	54,54,111	1.05	4 (7%)
20	PER	N	610[A]	14,15	1,1,1	1.17	0	-		
26	CDL	N	601	-	51,51,99	1.20	8 (15%)	47,47,111	0.88	1 (2%)
27	PEK	C	306	-	23,23,52	0.39	0	21,21,57	0.42	0
21	EDO	S	102	-	3,3,3	0.80	0	2,2,2	0.74	0
21	EDO	F	106	-	3,3,3	0.68	0	2,2,2	0.76	0
18	PGV	N	607	-	22,22,50	0.36	0	20,20,56	0.52	0
21	EDO	A	612	-	3,3,3	0.79	0	2,2,2	0.67	0
21	EDO	P	311	-	3,3,3	0.46	0	2,2,2	0.31	0
26	CDL	C	305	-	54,54,99	1.04	5 (9%)	50,50,111	1.12	5 (10%)
21	EDO	A	617	-	3,3,3	0.62	0	2,2,2	0.13	0
25	DMU	L	101	-	21,21,34	0.66	1 (4%)	24,25,45	2.46	6 (25%)
21	EDO	F	103	6	3,3,3	0.63	0	2,2,2	0.17	0
25	DMU	K	105	-	8,8,34	0.24	0	7,7,45	0.61	0
21	EDO	C	313	-	3,3,3	0.70	0	2,2,2	0.61	0
27	PEK	C	309	-	34,34,52	0.35	0	32,32,57	0.62	0
21	EDO	B	304	-	3,3,3	0.63	0	2,2,2	0.34	0
21	EDO	G	103	-	3,3,3	0.62	0	2,2,2	0.55	0
19	PSC	O	303	-	28,28,51	1.15	2 (7%)	27,27,59	1.08	3 (11%)
21	EDO	Q	202	-	3,3,3	0.46	0	2,2,2	0.64	0
22	TGL	N	612	-	43,43,62	1.18	2 (4%)	45,45,65	1.60	8 (17%)
22	TGL	N	609	-	62,62,62	1.13	3 (4%)	65,65,65	1.07	4 (6%)
21	EDO	N	618	-	3,3,3	0.50	0	2,2,2	0.36	0
21	EDO	D	206	-	3,3,3	0.56	0	2,2,2	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
18	PGV	P	307	-	50,50,50	0.69	2 (4%)	53,56,56	1.09	5 (9%)
21	EDO	O	304	-	3,3,3	0.66	0	2,2,2	0.30	0
25	DMU	Z	101	-	34,34,34	0.51	0	45,45,45	1.03	2 (4%)
21	EDO	C	312	-	3,3,3	0.47	0	2,2,2	0.14	0
21	EDO	C	320	-	3,3,3	0.68	0	2,2,2	0.53	0
21	EDO	D	204	-	3,3,3	0.57	0	2,2,2	0.13	0
27	PEK	P	308	-	32,32,52	0.43	0	29,30,57	0.57	0
27	PEK	C	307	-	52,52,52	0.84	2 (3%)	55,57,57	1.07	3 (5%)
21	EDO	C	315	-	3,3,3	0.39	0	2,2,2	1.06	0
24	CHD	C	304	-	32,32,32	0.90	1 (3%)	51,51,51	1.52	7 (13%)
21	EDO	A	609	-	3,3,3	0.57	0	2,2,2	0.60	0
21	EDO	A	610	-	3,3,3	0.49	0	2,2,2	0.28	0
21	EDO	P	317	-	3,3,3	0.55	0	2,2,2	0.17	0
21	EDO	F	105	-	3,3,3	0.58	0	2,2,2	0.36	0
22	TGL	D	202	-	56,56,62	1.17	3 (5%)	59,59,65	1.13	5 (8%)
25	DMU	M	101	-	34,34,34	0.57	0	45,45,45	1.28	4 (8%)
21	EDO	O	305	-	3,3,3	0.56	0	2,2,2	0.13	0
21	EDO	C	318	-	3,3,3	0.56	0	2,2,2	0.49	0
21	EDO	T	104	-	3,3,3	0.72	0	2,2,2	0.41	0
25	DMU	X	102	-	9,9,34	0.39	0	8,8,45	0.37	0
27	PEK	P	305	-	19,19,52	0.30	0	18,18,57	0.57	0
21	EDO	F	102	-	3,3,3	0.98	0	2,2,2	0.54	0
21	EDO	Y	103	-	3,3,3	0.50	0	2,2,2	0.71	0
21	EDO	E	203	-	3,3,3	0.57	0	2,2,2	0.27	0
25	DMU	K	104	-	8,8,34	0.53	0	7,7,45	0.25	0
24	CHD	B	303	-	32,32,32	0.96	1 (3%)	51,51,51	1.59	10 (19%)
21	EDO	A	611	-	3,3,3	0.81	0	2,2,2	0.53	0
21	EDO	S	105	-	3,3,3	0.78	0	2,2,2	0.53	0
21	EDO	N	619	-	3,3,3	0.74	0	2,2,2	0.18	0
25	DMU	K	101	-	8,8,34	0.28	0	7,7,45	0.59	0
21	EDO	N	614	-	3,3,3	0.79	0	2,2,2	0.35	0
25	DMU	D	203	-	9,9,34	0.36	0	8,8,45	0.55	0
25	DMU	K	102	-	9,9,34	0.27	0	8,8,45	0.46	0
18	PGV	N	608	-	50,50,50	0.90	4 (8%)	53,56,56	1.24	5 (9%)
21	EDO	T	103	-	3,3,3	0.49	0	2,2,2	0.34	0
25	DMU	X	104	-	9,9,34	0.46	0	8,8,45	0.18	0
24	CHD	L	102	-	32,32,32	0.75	0	51,51,51	2.79	20 (39%)
21	EDO	J	103	-	3,3,3	0.34	0	2,2,2	0.58	0
25	DMU	X	101	-	9,9,34	0.41	0	8,8,45	0.44	0
20	PER	A	608[A]	14,15	1,1,1	1.21	0	-		
21	EDO	O	306	-	3,3,3	0.49	0	2,2,2	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
23	CUA	B	302	2	0,1,1	-	-	-		
14	HEA	N	603	1,20,30	66,67,67	1.75	21 (31%)	78,103,103	1.73	18 (23%)
25	DMU	D	201	-	10,10,34	0.33	0	9,9,45	0.41	0
21	EDO	P	312	-	3,3,3	0.58	0	2,2,2	0.28	0
22	TGL	L	103	-	53,53,62	0.74	1 (1%)	51,51,65	1.08	3 (5%)
21	EDO	B	307	-	3,3,3	0.64	0	2,2,2	0.25	0
21	EDO	A	614	-	3,3,3	0.48	0	2,2,2	0.48	0
21	EDO	A	615	-	3,3,3	0.76	0	2,2,2	0.25	0
21	EDO	C	317	-	3,3,3	0.62	0	2,2,2	0.18	0
21	EDO	P	310	-	3,3,3	0.61	0	2,2,2	0.15	0
21	EDO	N	620	-	3,3,3	0.76	0	2,2,2	0.34	0
26	CDL	T	101	-	52,53,99	1.34	8 (15%)	49,51,111	1.21	4 (8%)
14	HEA	A	601[A]	-	66,67,67	1.77	19 (28%)	78,103,103	2.28	33 (42%)
21	EDO	C	316	-	3,3,3	0.40	0	2,2,2	0.36	0
25	DMU	Q	201	-	9,9,34	0.45	0	8,8,45	0.22	0
21	EDO	A	616	-	3,3,3	0.47	0	2,2,2	0.42	0
21	EDO	D	205	-	3,3,3	0.67	0	2,2,2	0.24	0
21	EDO	E	202	-	3,3,3	0.43	0	2,2,2	0.32	0
21	EDO	L	104	-	3,3,3	0.53	0	2,2,2	0.76	0
14	HEA	A	601[C]	-	66,58,67	1.82	20 (30%)	78,91,103	3.16	34 (43%)
23	CUA	O	301	2	0,1,1	-	-	-		
21	EDO	G	104	-	3,3,3	0.62	0	2,2,2	0.16	0
21	EDO	E	201	-	3,3,3	0.54	0	2,2,2	0.38	0
21	EDO	N	613	-	3,3,3	0.81	0	2,2,2	0.75	0
21	EDO	A	613	-	3,3,3	0.51	0	2,2,2	0.26	0
21	EDO	S	103	-	3,3,3	0.63	0	2,2,2	0.06	0
21	EDO	J	102	-	3,3,3	0.53	0	2,2,2	0.37	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	P	313	-	-	0/1/1/1	-
21	EDO	C	314	-	-	0/1/1/1	-
21	EDO	P	315	-	-	1/1/1/1	-
22	TGL	B	301	-	-	29/50/50/65	-
21	EDO	N	617	-	-	0/1/1/1	-
18	PGV	A	606	-	-	3/15/16/55	-
25	DMU	W	101	-	-	1/8/8/59	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	TGL	N	611	-	-	20/39/39/65	-
25	DMU	O	302	-	-	3/8/8/59	-
18	PGV	C	308	-	-	10/52/52/55	-
21	EDO	A	618	-	-	0/1/1/1	-
25	DMU	X	103	-	-	1/6/6/59	-
25	DMU	P	309	-	-	2/8/8/59	-
14	HEA	A	602	1,20,30	-	5/36/76/76	-
25	DMU	C	303	-	-	2/9/10/59	-
18	PGV	C	301	-	-	8/55/55/55	-
21	EDO	C	319	-	-	0/1/1/1	-
21	EDO	P	316	-	-	0/1/1/1	-
21	EDO	Y	102	-	-	0/1/1/1	-
21	EDO	N	621	-	-	0/1/1/1	-
21	EDO	N	616	-	-	0/1/1/1	-
18	PGV	C	311	-	-	10/23/23/55	-
21	EDO	B	306	-	-	0/1/1/1	-
21	EDO	B	305	-	-	0/1/1/1	-
21	EDO	N	615	-	-	0/1/1/1	-
25	DMU	P	303	-	-	4/9/9/59	-
25	DMU	J	101	-	-	6/8/8/59	-
25	DMU	K	103	-	-	6/8/8/59	-
21	EDO	F	104	-	-	0/1/1/1	-
27	PEK	P	306	-	-	14/56/56/56	-
14	HEA	N	602[A]	-	-	5/36/76/76	-
24	CHD	G	101	-	-	2/9/74/74	0/4/4/4
18	PGV	G	102	-	-	7/27/27/55	-
21	EDO	S	106	-	-	0/1/1/1	-
14	HEA	N	602[C]	-	-	13/36/60/76	-
24	CHD	P	301	-	-	1/9/74/74	0/4/4/4
19	PSC	A	607	-	-	10/21/21/55	-
21	EDO	W	102	-	-	1/1/1/1	-
24	CHD	Y	101	-	-	4/9/74/74	0/4/4/4
21	EDO	T	102	-	-	0/1/1/1	-
25	DMU	C	310	-	-	5/13/29/59	0/1/1/2
21	EDO	S	104	-	-	0/1/1/1	-
21	EDO	P	314	-	-	0/1/1/1	-
25	DMU	K	106	-	-	3/7/7/59	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CDL	P	304	-	-	17/49/50/110	-
26	CDL	N	601	-	-	17/42/43/110	-
27	PEK	C	306	-	-	9/19/19/56	-
21	EDO	S	102	-	-	0/1/1/1	-
21	EDO	F	106	-	-	0/1/1/1	-
18	PGV	N	607	-	-	5/18/18/55	-
21	EDO	A	612	-	-	0/1/1/1	-
21	EDO	P	311	-	-	1/1/1/1	-
26	CDL	C	305	-	-	14/45/46/110	-
21	EDO	A	617	-	-	0/1/1/1	-
25	DMU	L	101	-	-	4/13/29/59	0/1/1/2
21	EDO	F	103	6	-	0/1/1/1	-
25	DMU	K	105	-	-	4/6/6/59	-
21	EDO	C	313	-	-	0/1/1/1	-
27	PEK	C	309	-	-	15/30/30/56	-
21	EDO	B	304	-	-	0/1/1/1	-
21	EDO	G	103	-	-	0/1/1/1	-
19	PSC	O	303	-	-	9/24/24/55	-
21	EDO	Q	202	-	-	0/1/1/1	-
22	TGL	N	612	-	-	26/45/45/65	-
22	TGL	N	609	-	-	34/65/65/65	-
21	EDO	N	618	-	-	0/1/1/1	-
21	EDO	D	206	-	-	0/1/1/1	-
18	PGV	P	307	-	-	6/55/55/55	-
21	EDO	O	304	-	-	0/1/1/1	-
25	DMU	Z	101	-	-	6/19/59/59	0/2/2/2
21	EDO	C	312	-	-	0/1/1/1	-
21	EDO	C	320	-	-	1/1/1/1	-
21	EDO	D	204	-	-	0/1/1/1	-
27	PEK	P	308	-	-	12/28/28/56	-
27	PEK	C	307	-	-	15/56/56/56	-
21	EDO	C	315	-	-	0/1/1/1	-
24	CHD	C	304	-	-	2/9/74/74	0/4/4/4
21	EDO	A	609	-	-	0/1/1/1	-
21	EDO	A	610	-	-	1/1/1/1	-
21	EDO	P	317	-	-	0/1/1/1	-
21	EDO	F	105	-	-	0/1/1/1	-
22	TGL	D	202	-	-	32/59/59/65	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	DMU	M	101	-	-	3/19/59/59	0/2/2/2
21	EDO	O	305	-	-	1/1/1/1	-
21	EDO	C	318	-	-	0/1/1/1	-
21	EDO	T	104	-	-	1/1/1/1	-
25	DMU	X	102	-	-	2/7/7/59	-
27	PEK	P	305	-	-	10/17/17/56	-
21	EDO	F	102	-	-	0/1/1/1	-
21	EDO	Y	103	-	-	1/1/1/1	-
21	EDO	E	203	-	-	1/1/1/1	-
25	DMU	K	104	-	-	2/6/6/59	-
24	CHD	B	303	-	-	2/9/74/74	0/4/4/4
21	EDO	A	611	-	-	0/1/1/1	-
21	EDO	S	105	-	-	0/1/1/1	-
21	EDO	N	619	-	-	1/1/1/1	-
25	DMU	K	101	-	-	0/6/6/59	-
21	EDO	N	614	-	-	0/1/1/1	-
25	DMU	D	203	-	-	2/7/7/59	-
25	DMU	K	102	-	-	3/7/7/59	-
18	PGV	N	608	-	-	9/55/55/55	-
21	EDO	T	103	-	-	0/1/1/1	-
25	DMU	X	104	-	-	0/7/7/59	-
24	CHD	L	102	-	-	6/9/74/74	0/4/4/4
21	EDO	J	103	-	-	1/1/1/1	-
25	DMU	X	101	-	-	0/7/7/59	-
21	EDO	O	306	-	-	0/1/1/1	-
14	HEA	N	603	1,20,30	-	6/36/76/76	-
25	DMU	D	201	-	-	3/8/8/59	-
21	EDO	P	312	-	-	0/1/1/1	-
22	TGL	L	103	-	-	24/47/48/65	-
21	EDO	B	307	-	-	0/1/1/1	-
21	EDO	A	614	-	-	1/1/1/1	-
21	EDO	A	615	-	-	1/1/1/1	-
21	EDO	C	317	-	-	0/1/1/1	-
21	EDO	P	310	-	-	1/1/1/1	-
21	EDO	N	620	-	-	0/1/1/1	-
26	CDL	T	101	-	-	21/47/47/110	-
14	HEA	A	601[A]	-	-	7/36/76/76	-
21	EDO	C	316	-	-	0/1/1/1	-
25	DMU	Q	201	-	-	4/7/7/59	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	EDO	A	616	-	-	0/1/1/1	-
21	EDO	D	205	-	-	1/1/1/1	-
21	EDO	E	202	-	-	1/1/1/1	-
21	EDO	L	104	-	-	1/1/1/1	-
14	HEA	A	601[C]	-	-	11/36/60/76	-
21	EDO	G	104	-	-	1/1/1/1	-
21	EDO	E	201	-	-	0/1/1/1	-
21	EDO	N	613	-	-	0/1/1/1	-
21	EDO	A	613	-	-	1/1/1/1	-
21	EDO	S	103	-	-	0/1/1/1	-
21	EDO	J	102	-	-	1/1/1/1	-

The worst 5 of 174 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	602[C]	HEA	C18-C19	22.89	1.87	1.33
22	N	612	TGL	OG2-CB1	5.58	1.50	1.34
18	C	311	PGV	O03-C19	5.52	1.49	1.33
22	N	609	TGL	OG2-CB1	5.12	1.48	1.34
22	D	202	TGL	OG1-CA1	4.92	1.47	1.33

The worst 5 of 318 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	N	602[C]	HEA	C20-C19-C18	18.57	158.70	121.12
14	N	602[C]	HEA	C27-C19-C18	-17.43	78.95	123.68
14	A	601[C]	HEA	C20-C19-C18	13.27	147.98	121.12
14	A	601[C]	HEA	C27-C19-C18	-12.76	90.94	123.68
14	A	601[C]	HEA	C13-C12-C11	-9.41	100.21	114.35

There are no chirality outliers.

5 of 536 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	601[A]	HEA	C2A-C3A-CMA-OMA
14	A	601[C]	HEA	C2A-C3A-CMA-OMA
14	A	601[C]	HEA	C11-C12-C13-C14
14	N	602[C]	HEA	O11-C11-C3B-C2B
14	N	602[C]	HEA	C14-C15-C16-C17

There are no ring outliers.

62 monomers are involved in 141 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	301	TGL	1	0
18	A	606	PGV	2	0
25	W	101	DMU	1	0
22	N	611	TGL	5	0
25	O	302	DMU	1	0
18	C	308	PGV	3	0
25	P	309	DMU	5	0
14	A	602	HEA	2	0
25	C	303	DMU	1	0
18	C	301	PGV	1	0
18	C	311	PGV	2	0
25	P	303	DMU	1	0
25	J	101	DMU	2	0
25	K	103	DMU	1	0
27	P	306	PEK	5	0
14	N	602[A]	HEA	2	0
24	G	101	CHD	1	0
18	G	102	PGV	2	0
21	S	106	EDO	1	0
14	N	602[C]	HEA	1	0
19	A	607	PSC	4	0
21	W	102	EDO	1	0
24	Y	101	CHD	1	0
25	C	310	DMU	4	0
25	K	106	DMU	1	0
26	P	304	CDL	4	0
20	N	610[A]	PER	1	0
26	N	601	CDL	3	0
18	N	607	PGV	1	0
26	C	305	CDL	6	0
25	L	101	DMU	1	0
25	K	105	DMU	1	0
27	C	309	PEK	4	0
19	O	303	PSC	4	0
22	N	612	TGL	3	0
22	N	609	TGL	6	0
18	P	307	PGV	2	0
25	Z	101	DMU	1	0
21	C	320	EDO	1	0
27	P	308	PEK	4	0
27	C	307	PEK	4	0
22	D	202	TGL	9	0

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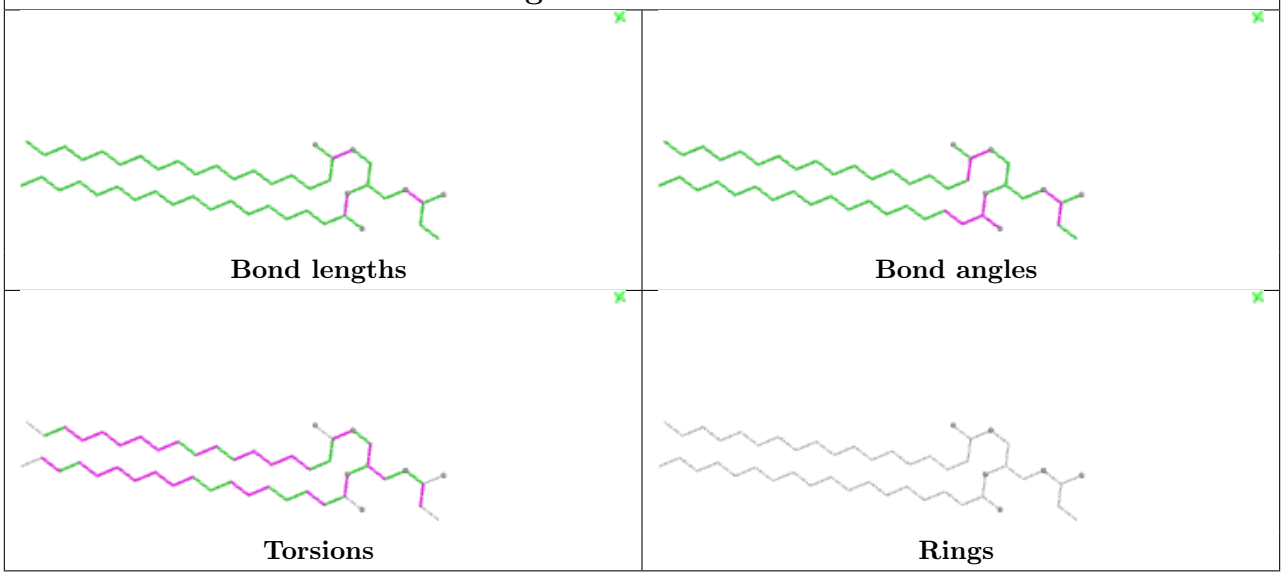
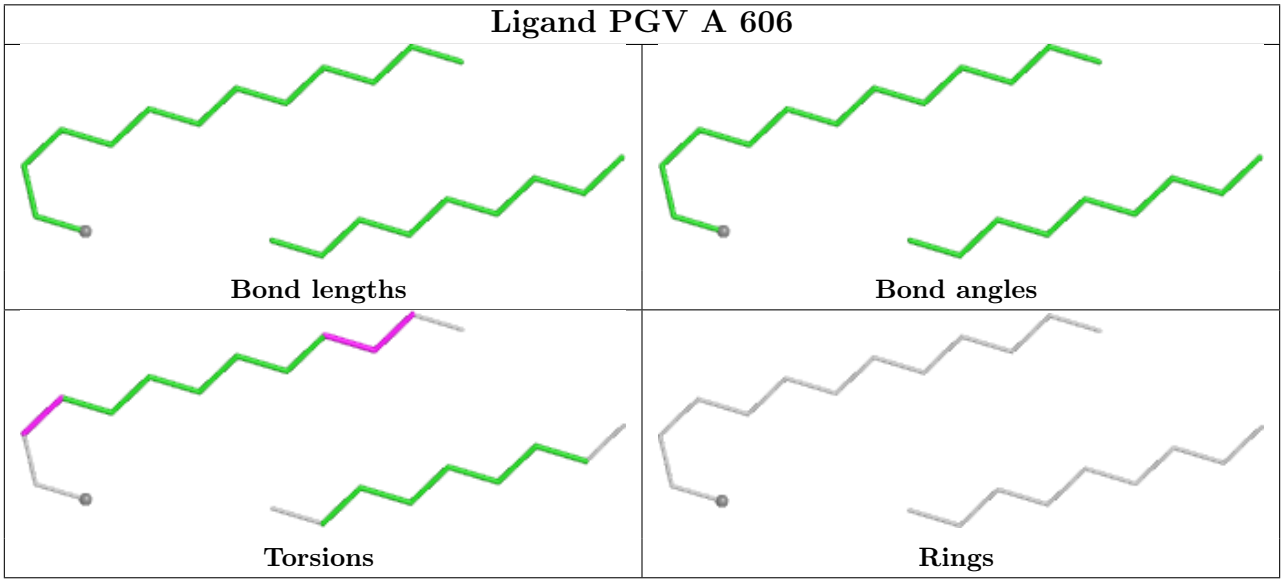
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	M	101	DMU	2	0
21	O	305	EDO	2	0
25	K	104	DMU	1	0
25	K	101	DMU	1	0
25	K	102	DMU	1	0
18	N	608	PGV	3	0
24	L	102	CHD	4	0
21	J	103	EDO	1	0
20	A	608[A]	PER	1	0
21	O	306	EDO	1	0
14	N	603	HEA	2	0
25	D	201	DMU	2	0
22	L	103	TGL	9	0
21	A	615	EDO	1	0
21	P	310	EDO	1	0
26	T	101	CDL	7	0
14	A	601[A]	HEA	2	0
25	Q	201	DMU	1	0
14	A	601[C]	HEA	1	0
21	A	613	EDO	1	0

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

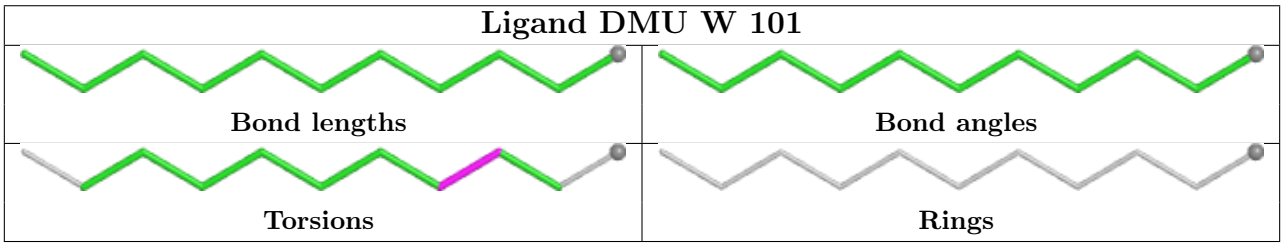
Ligand TGL B 301



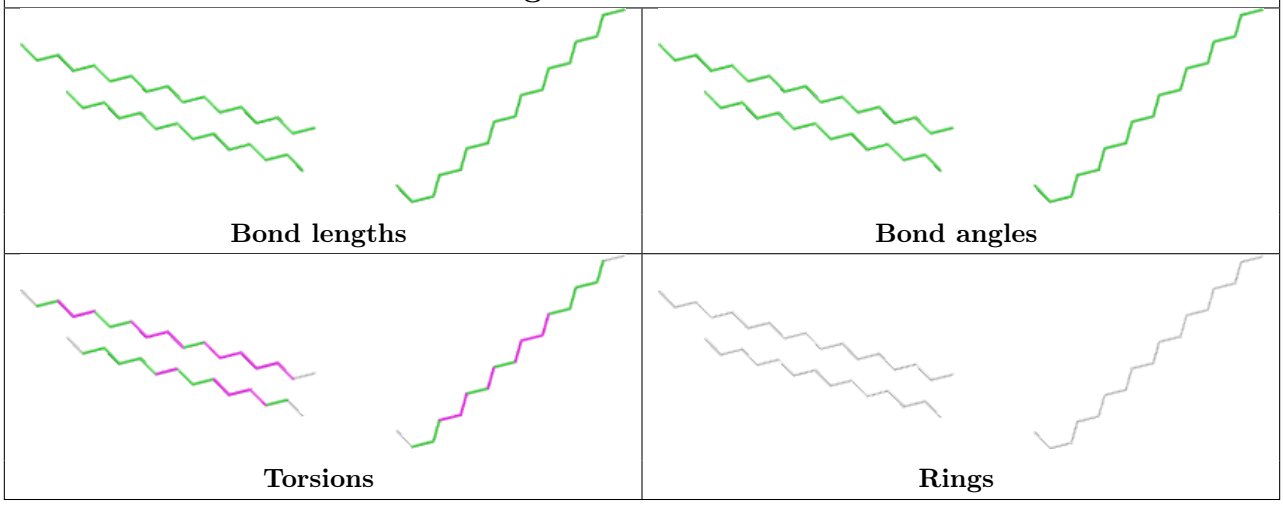
Ligand PGV A 606



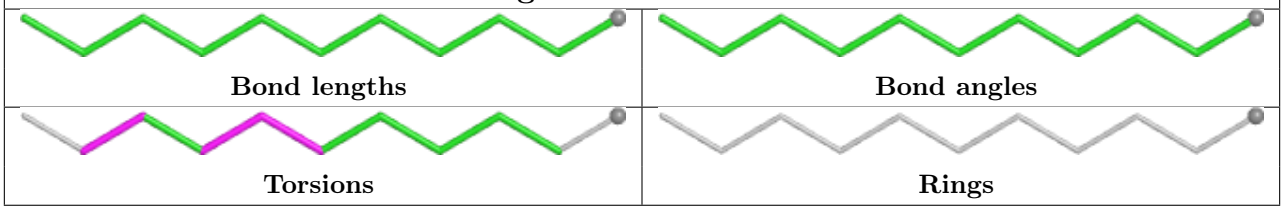
Ligand DMU W 101



Ligand TGL N 611



Ligand DMU O 302



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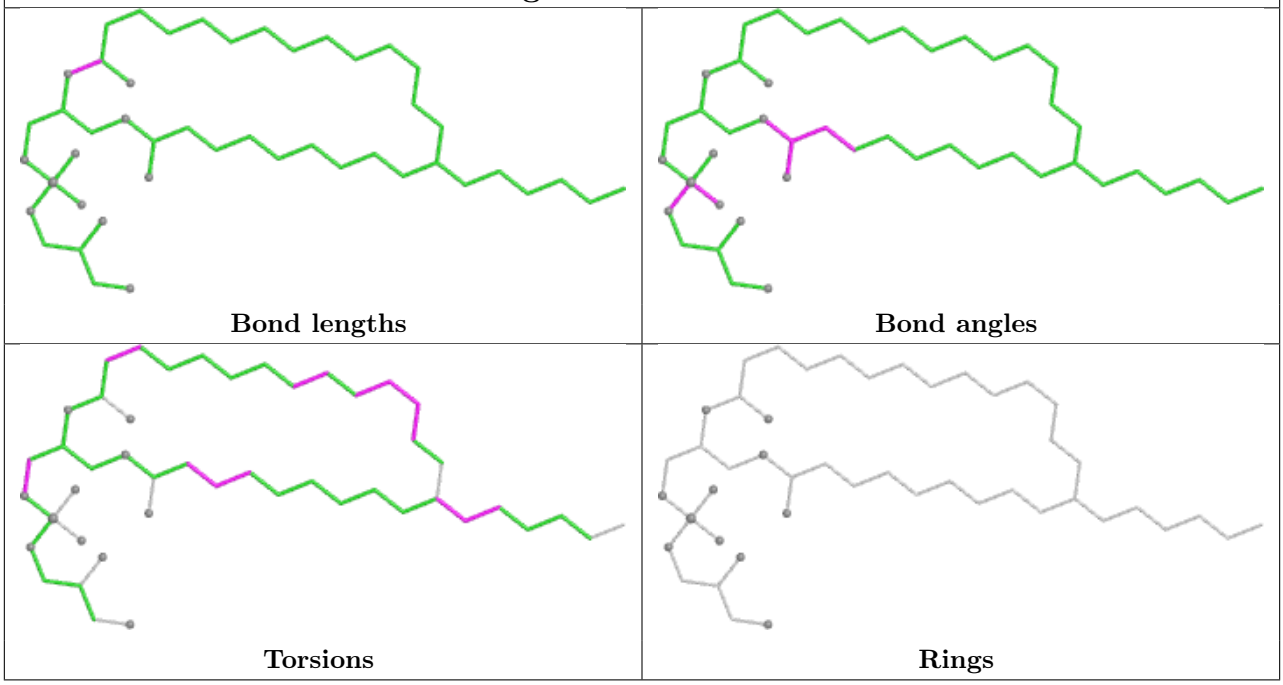

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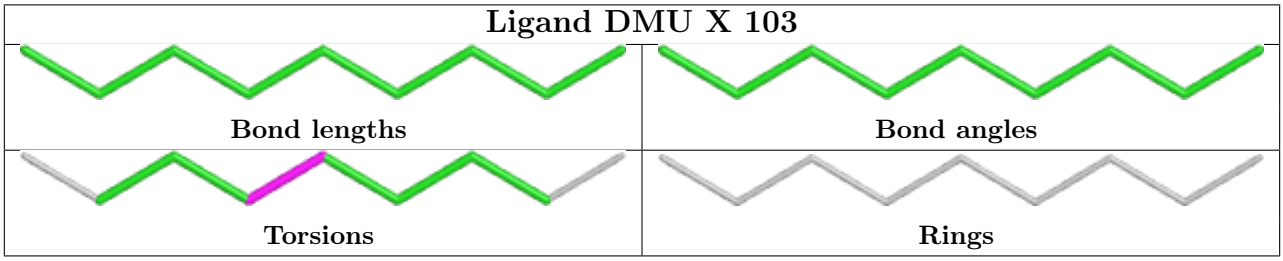
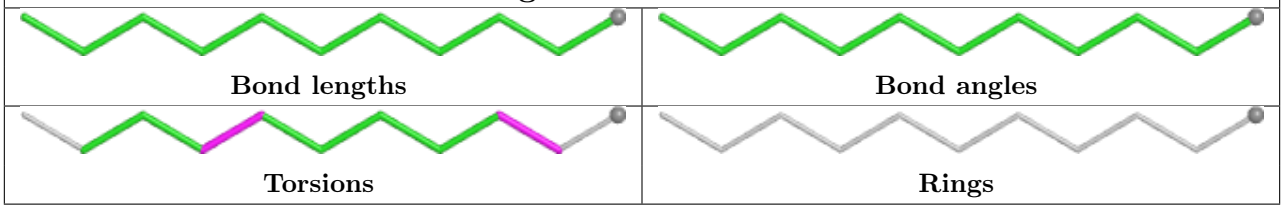
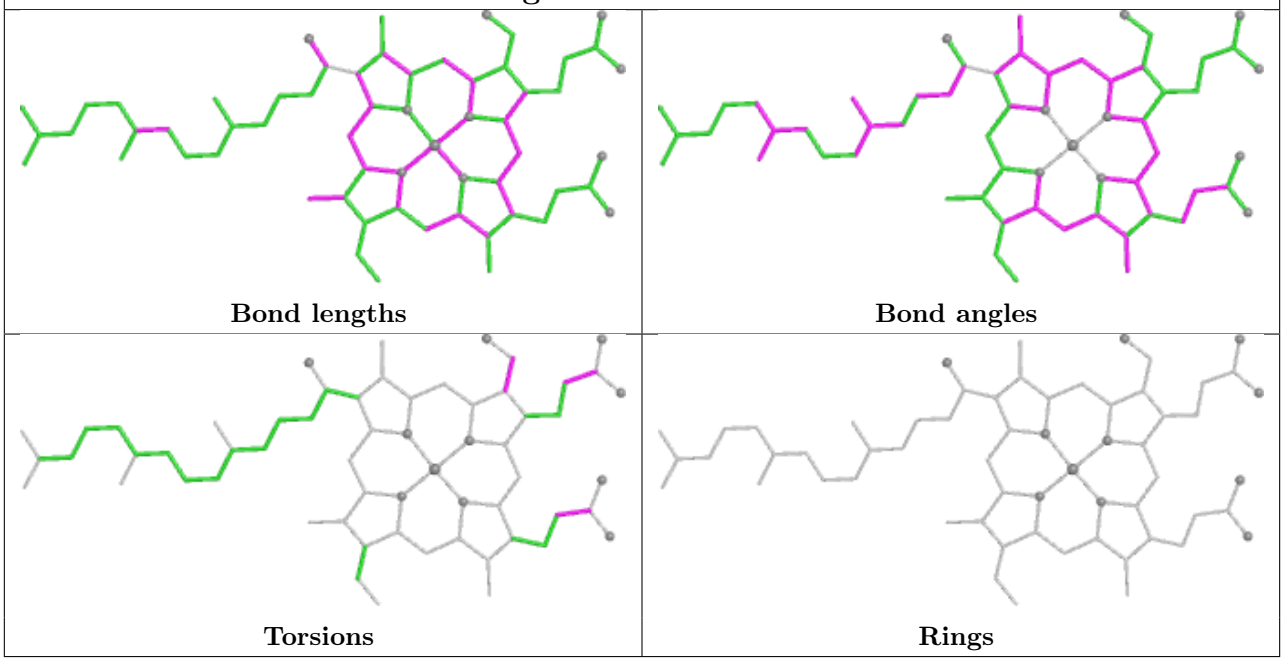


Ligand DMU P 309



Ligand HEA A 602



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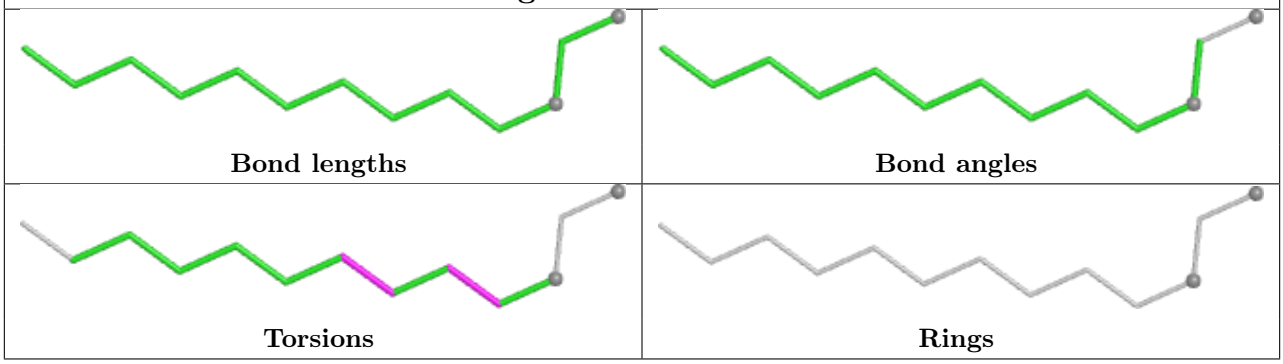
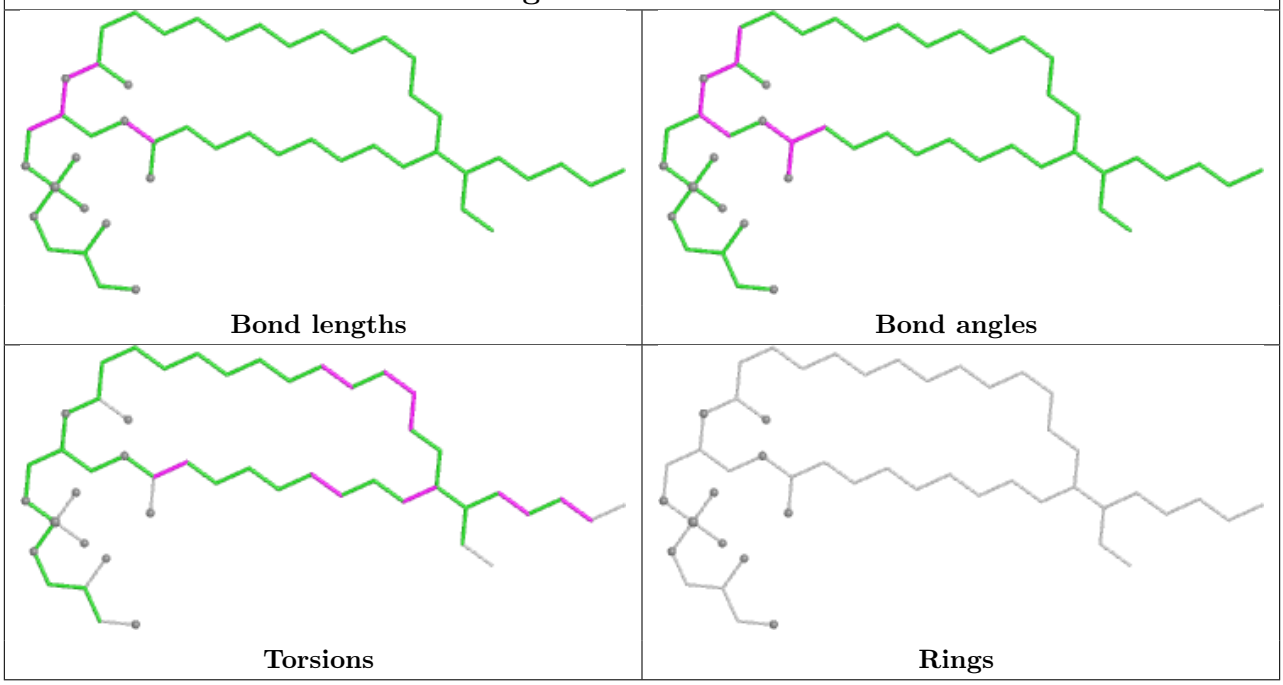


Ligand PGV C 301



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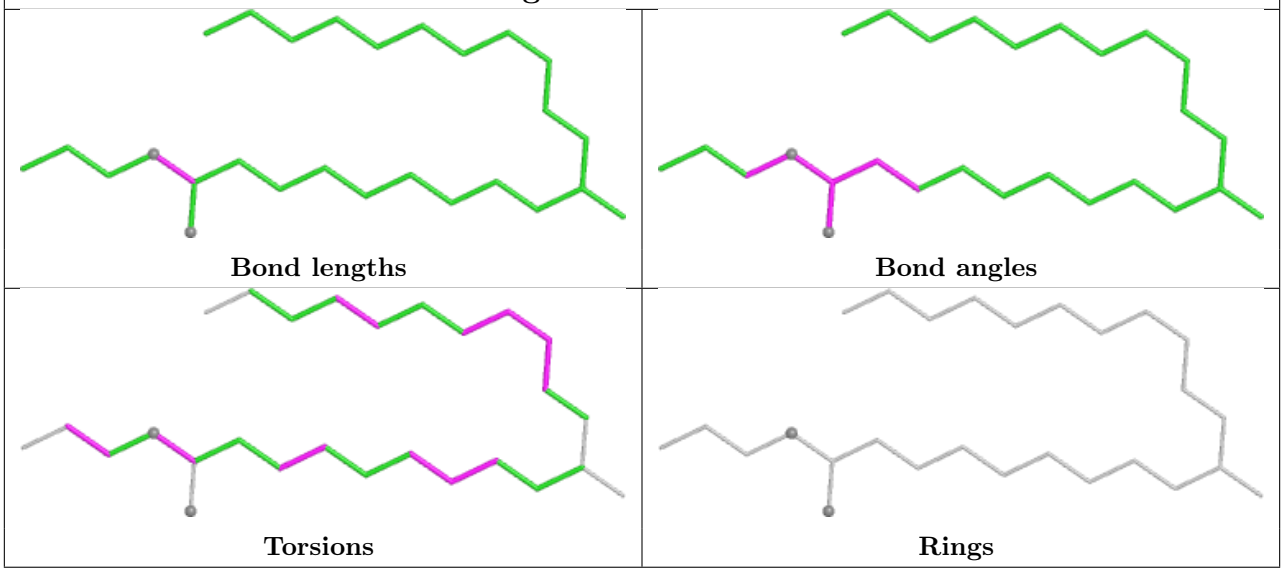

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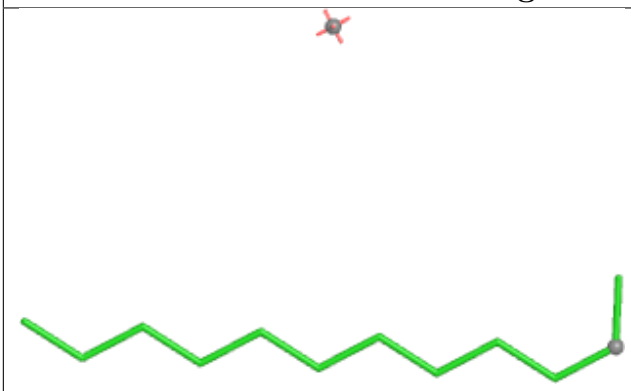
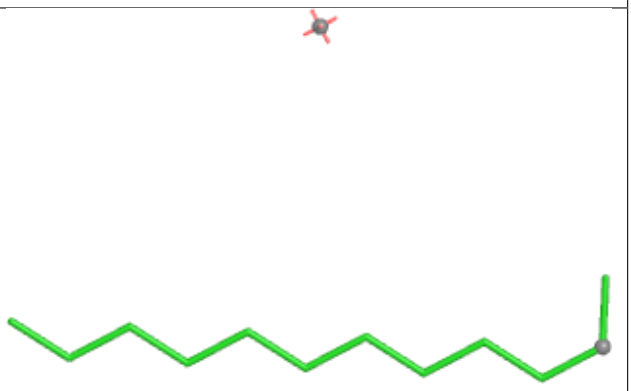
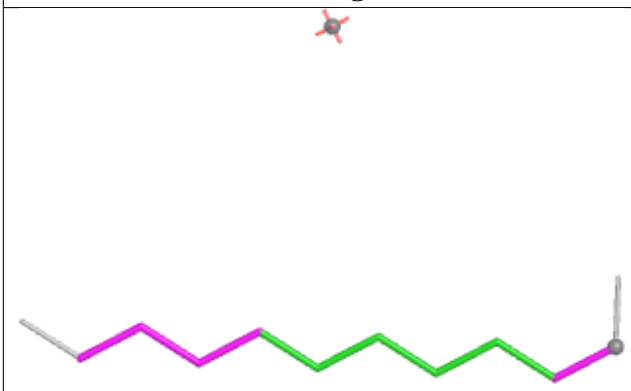


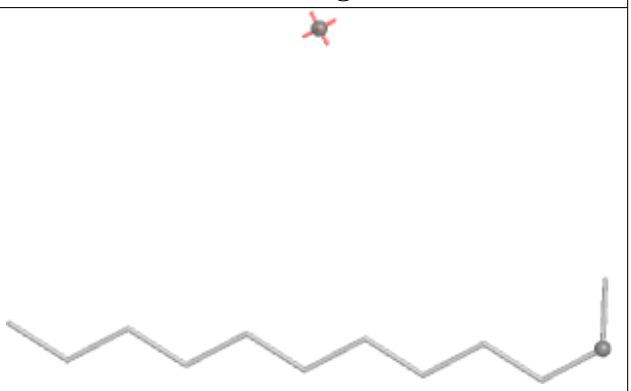
Bond lengths



Bond angles

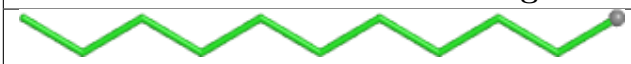


Torsions



Rings

Ligand DMU J 101



Bond lengths

Bond angles

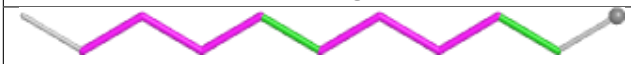
Torsions

Rings

Ligand DMU K 103

Bond lengths

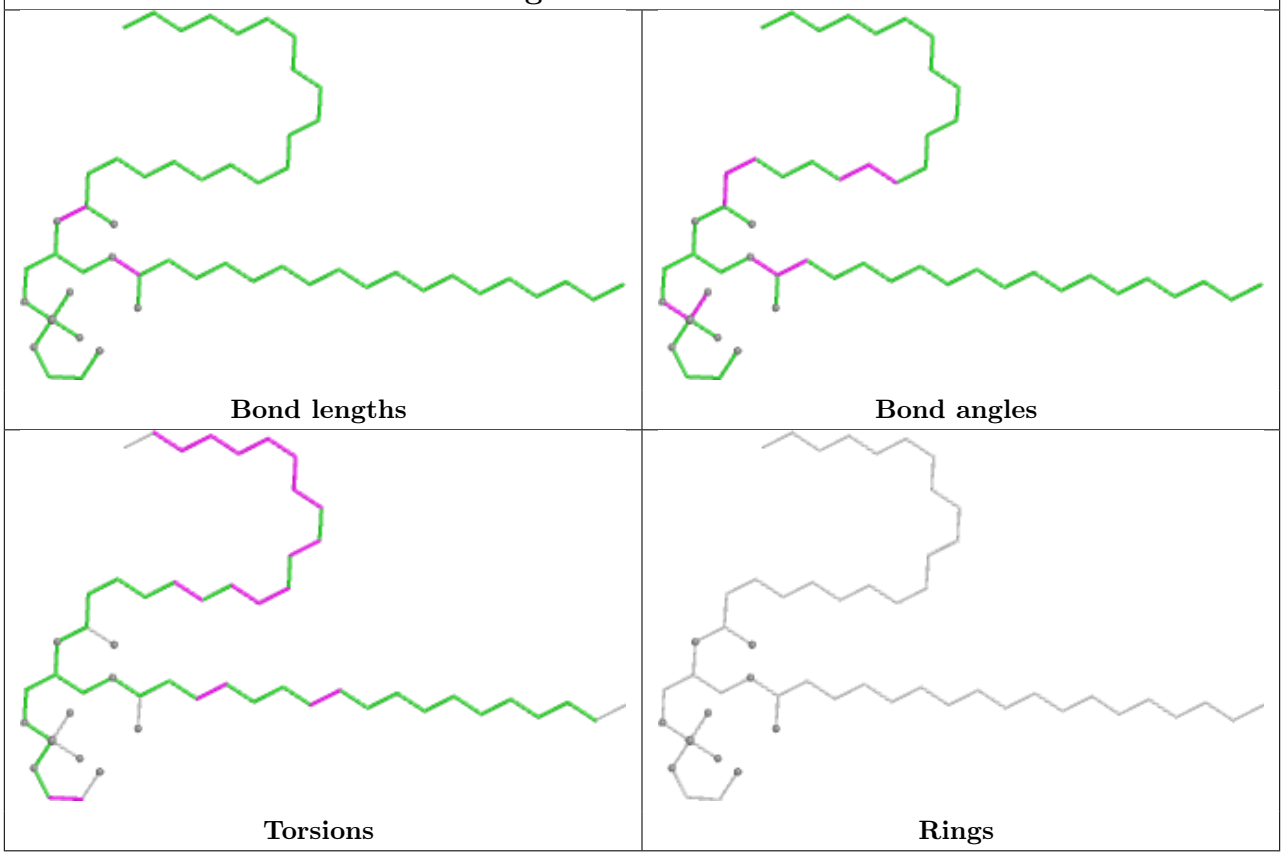
Bond angles



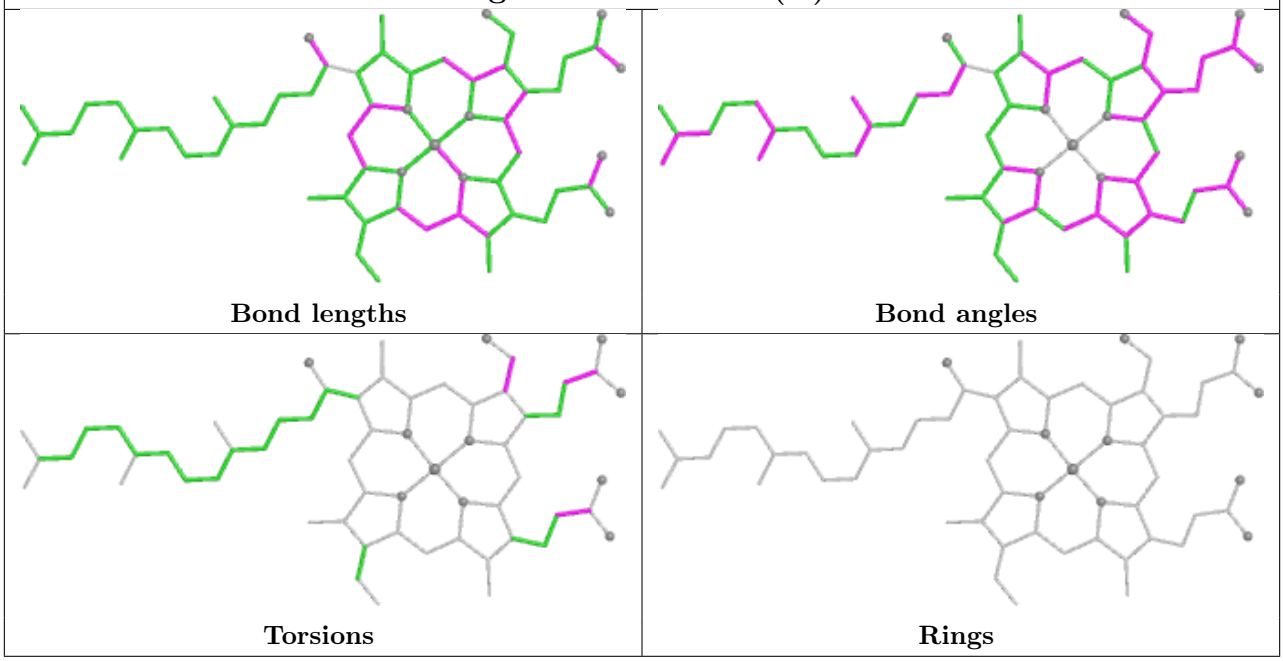
Torsions

Rings

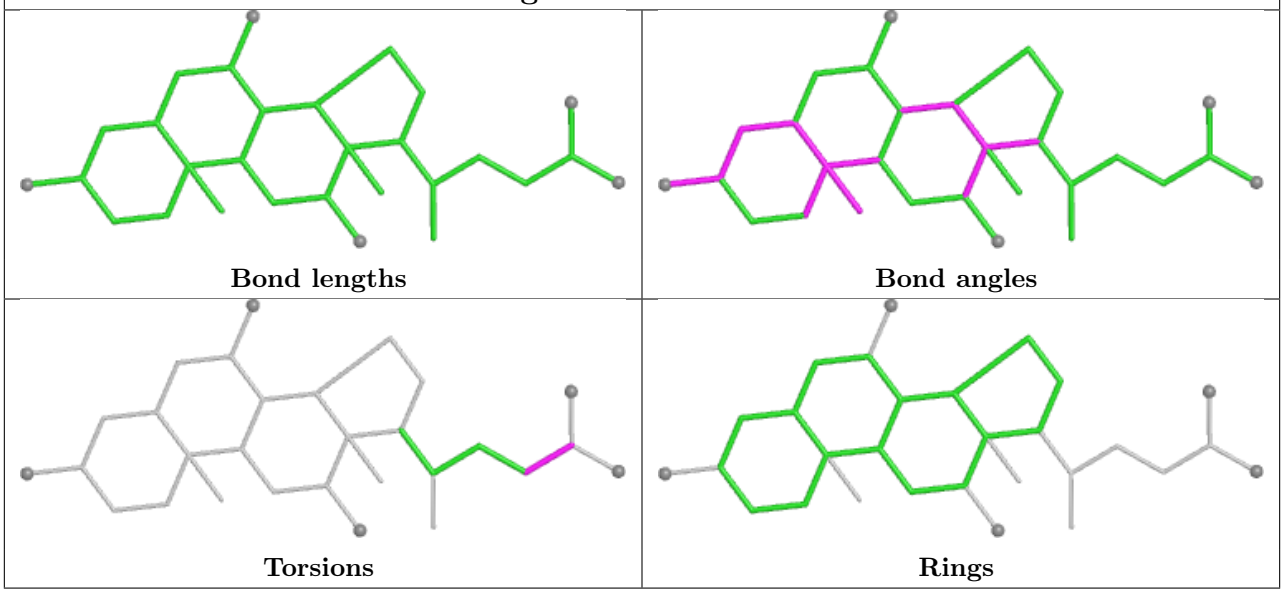
Ligand PEK P 306



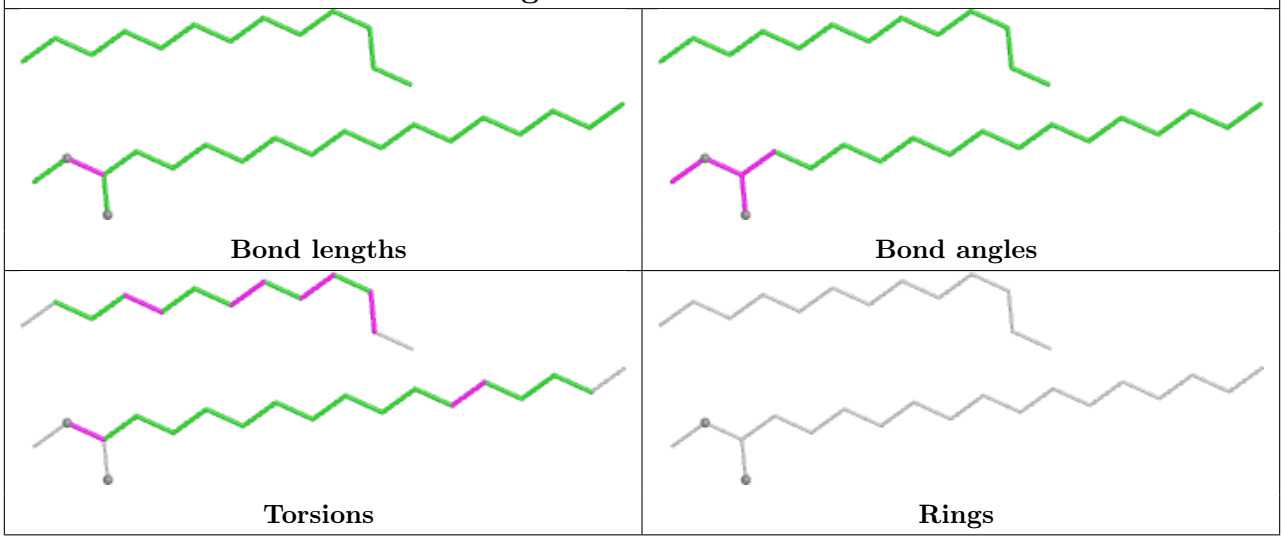
Ligand HEA N 602 (A)

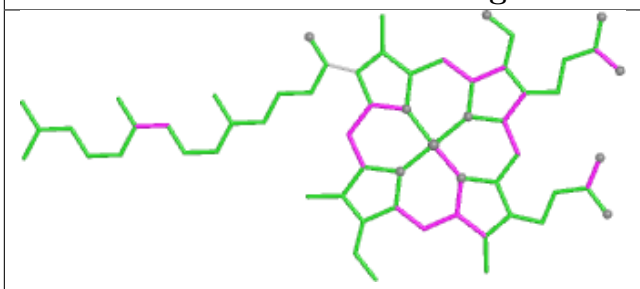
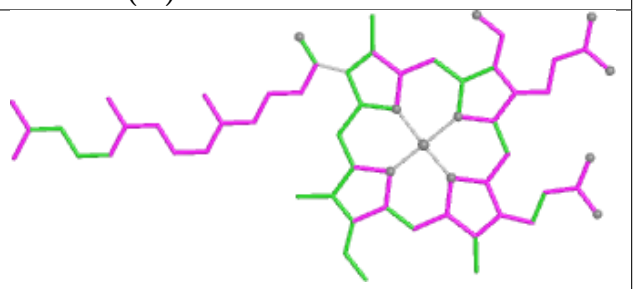
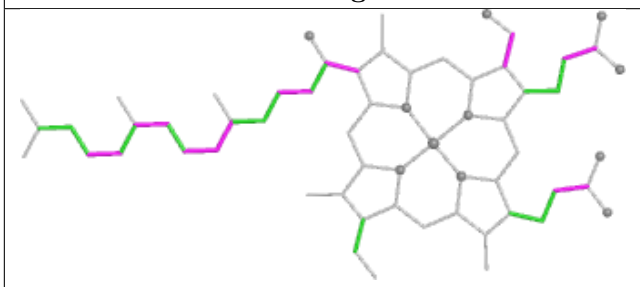
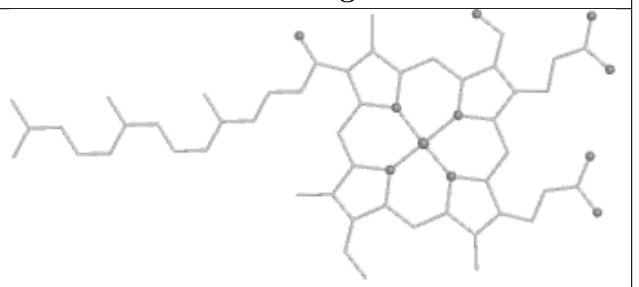


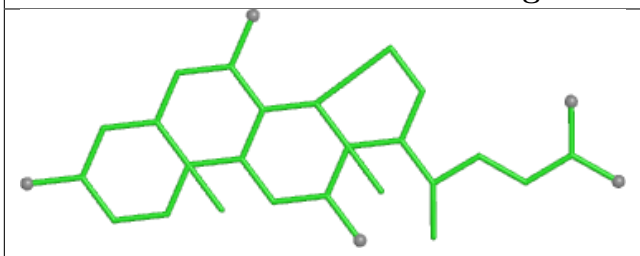
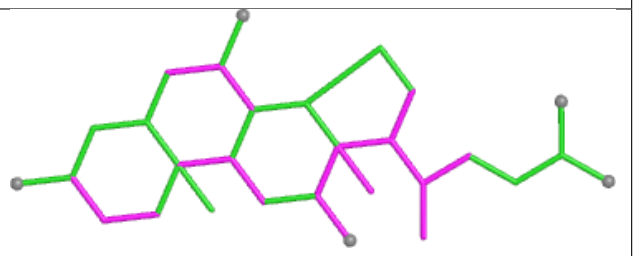
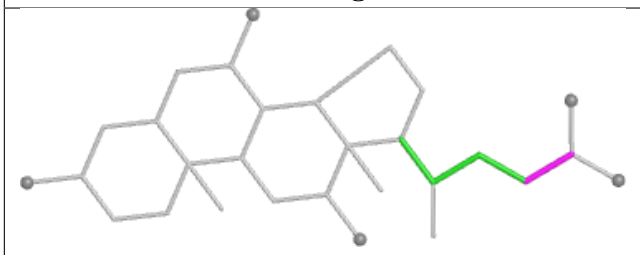
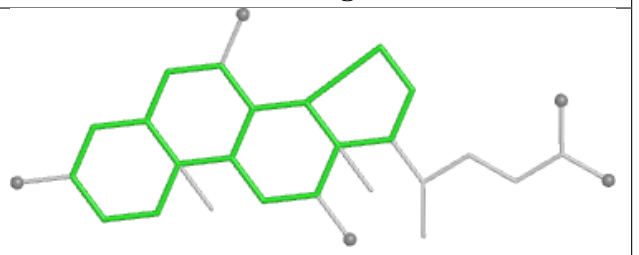
Ligand CHD G 101



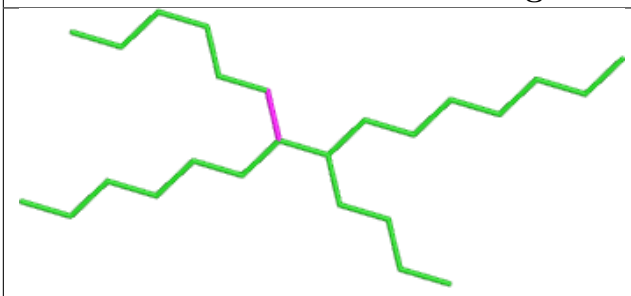
Ligand PGV G 102



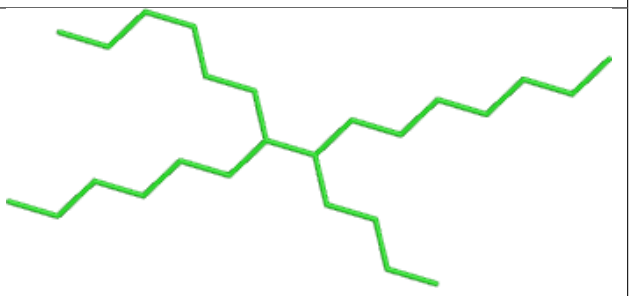
Ligand HEA N 602 (C)	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHD P 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

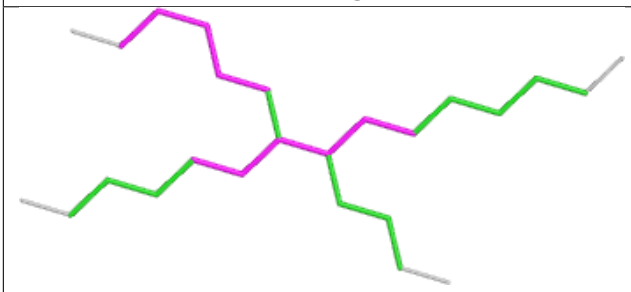
Ligand PSC A 607



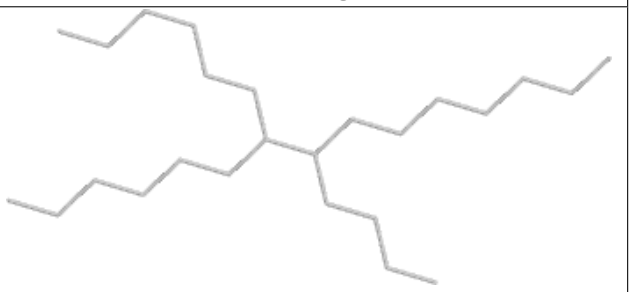
Bond lengths



Bond angles

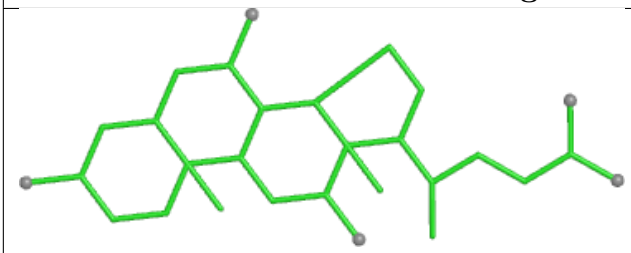


Torsions

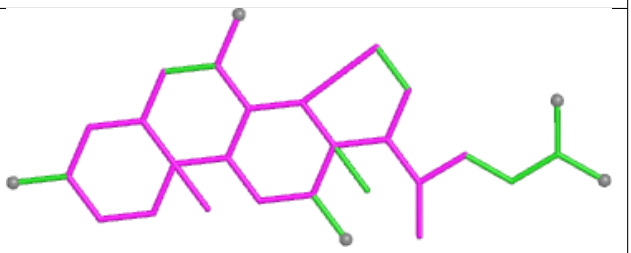


Rings

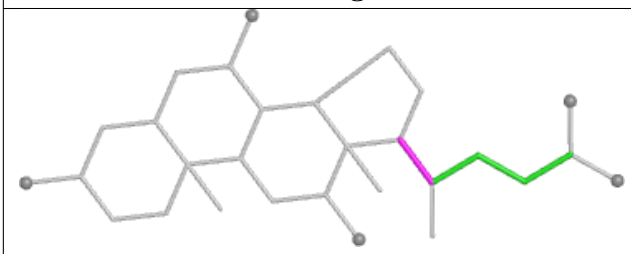
Ligand CHD Y 101



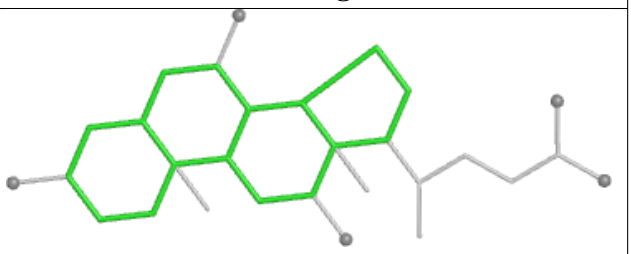
Bond lengths



Bond angles

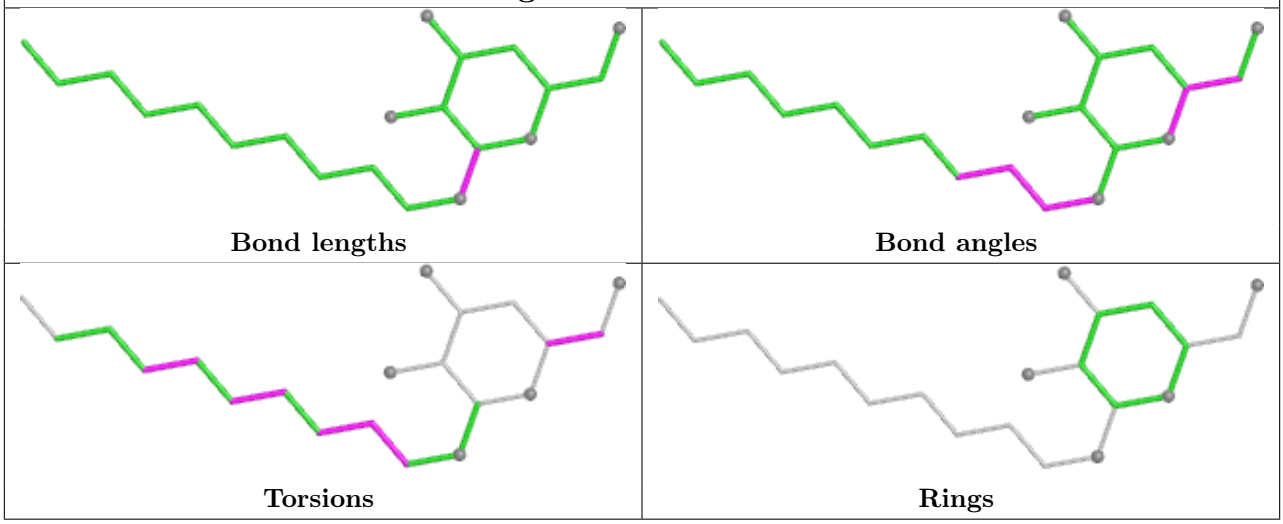


Torsions

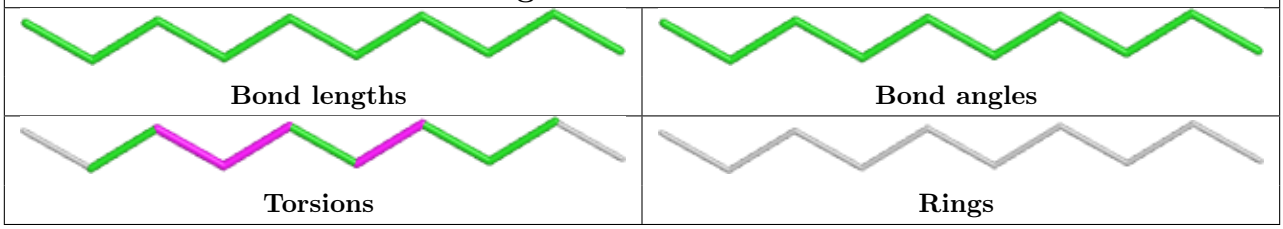


Rings

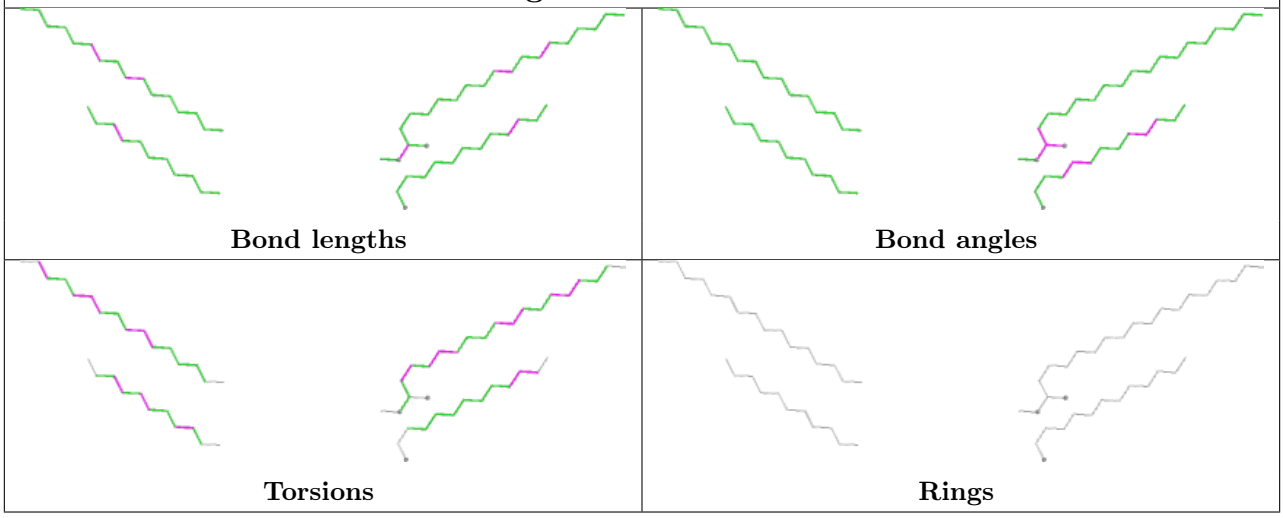
Ligand DMU C 310



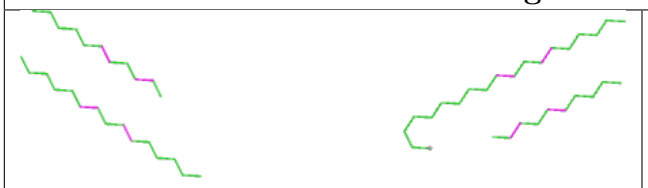
Ligand DMU K 106



Ligand CDL P 304



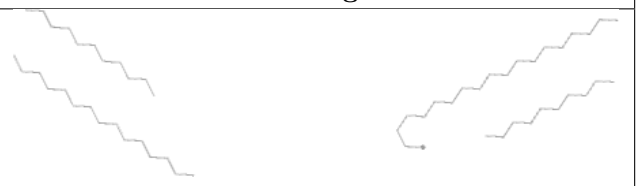
Ligand CDL N 601



Bond lengths

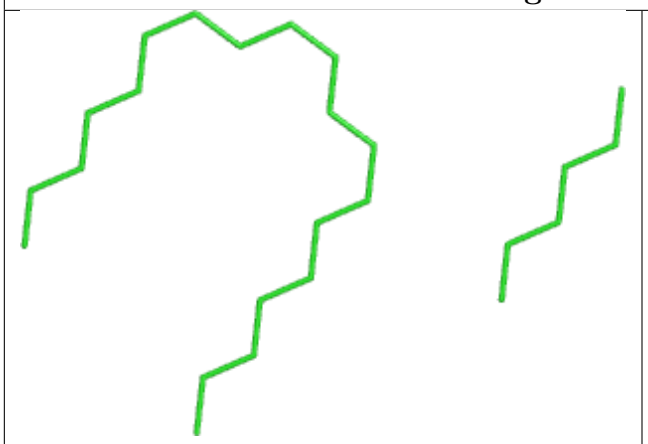
Bond angles

Torsions

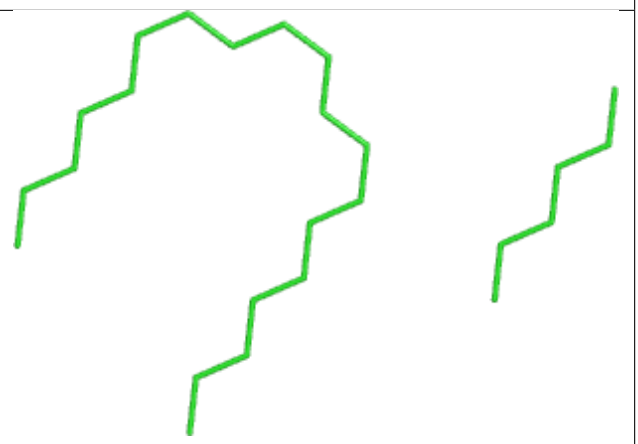


Rings

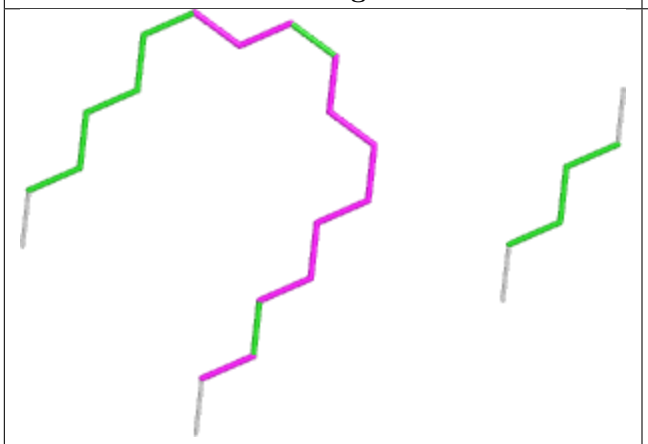
Ligand PEK C 306



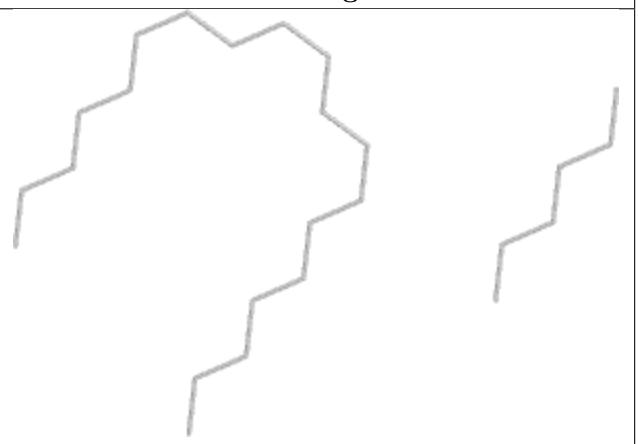
Bond lengths



Bond angles

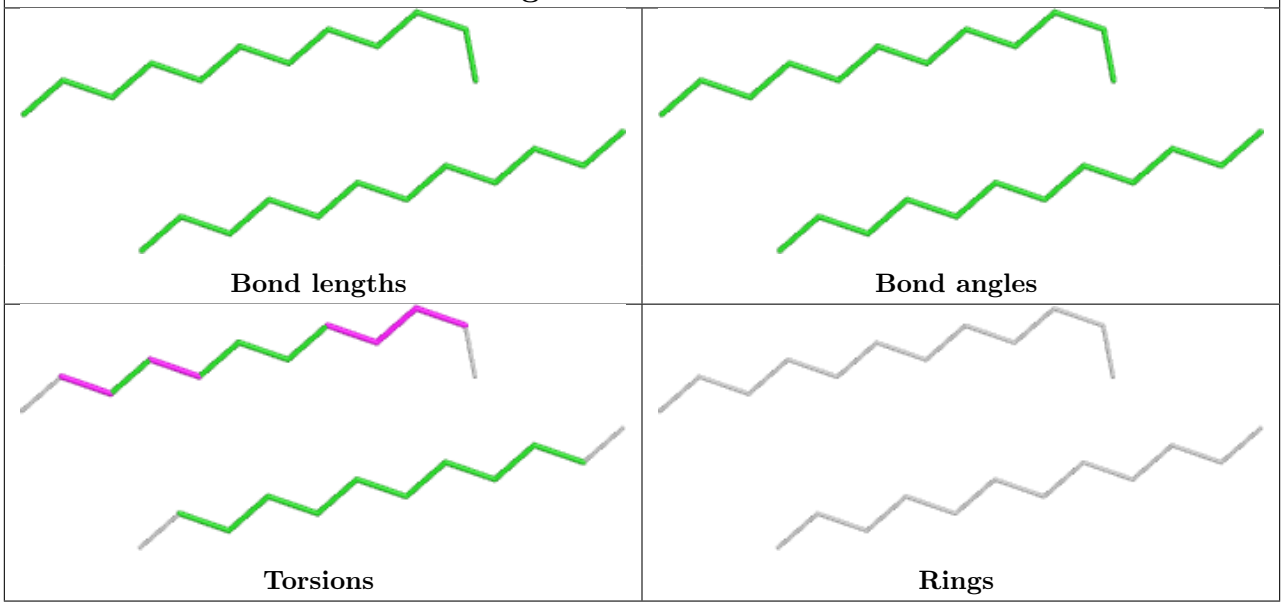


Torsions

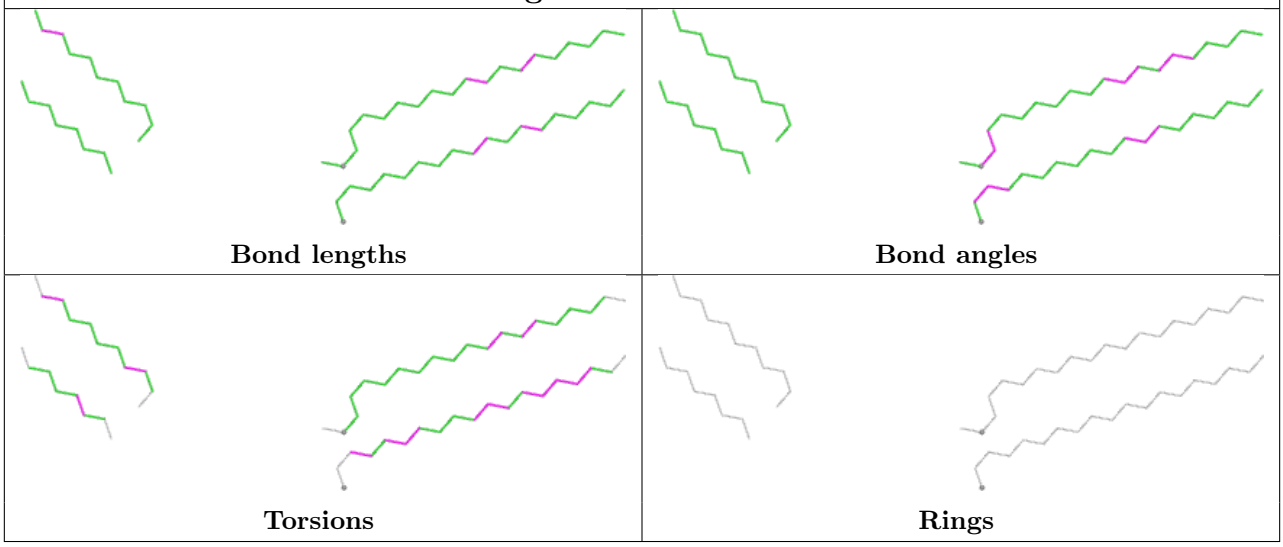


Rings

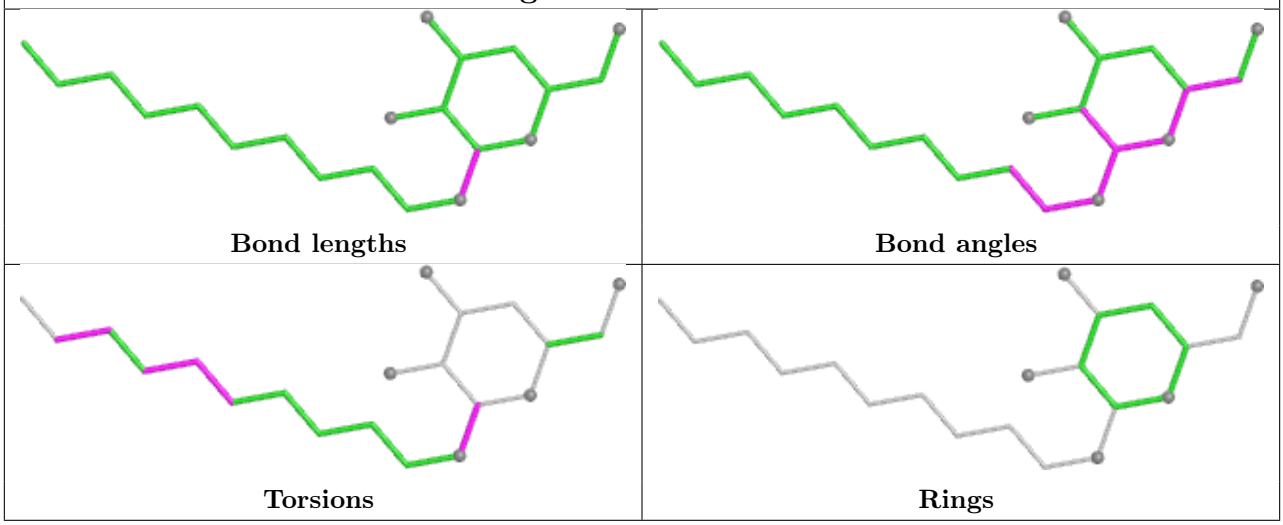
Ligand PGV N 607

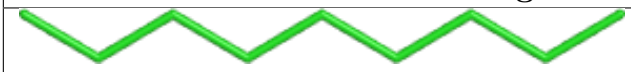
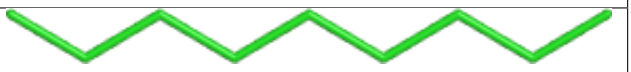


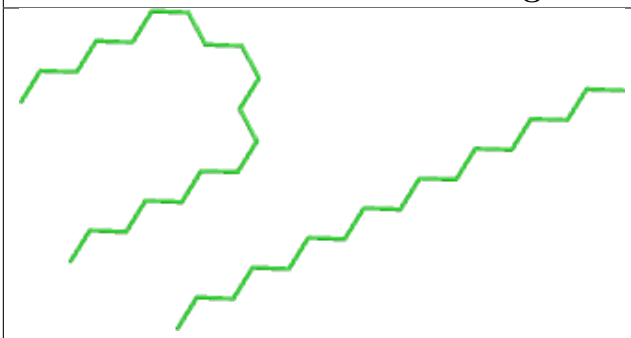
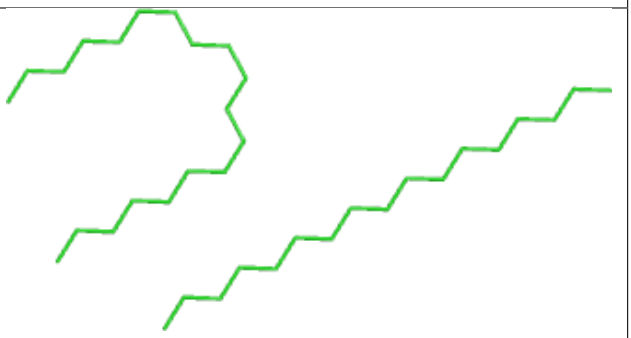
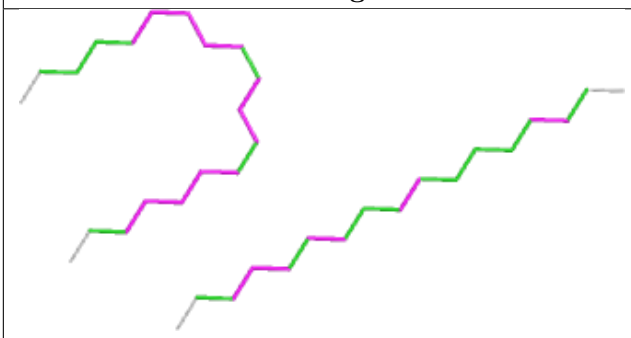
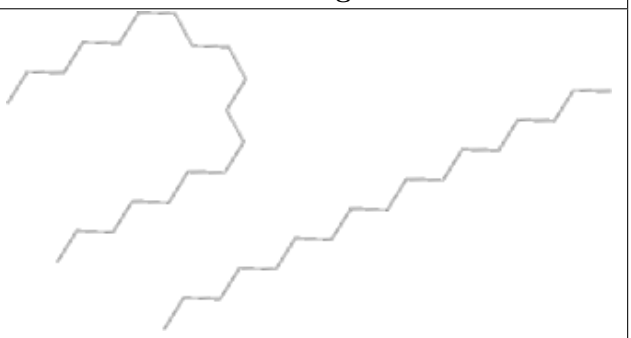
Ligand CDL C 305



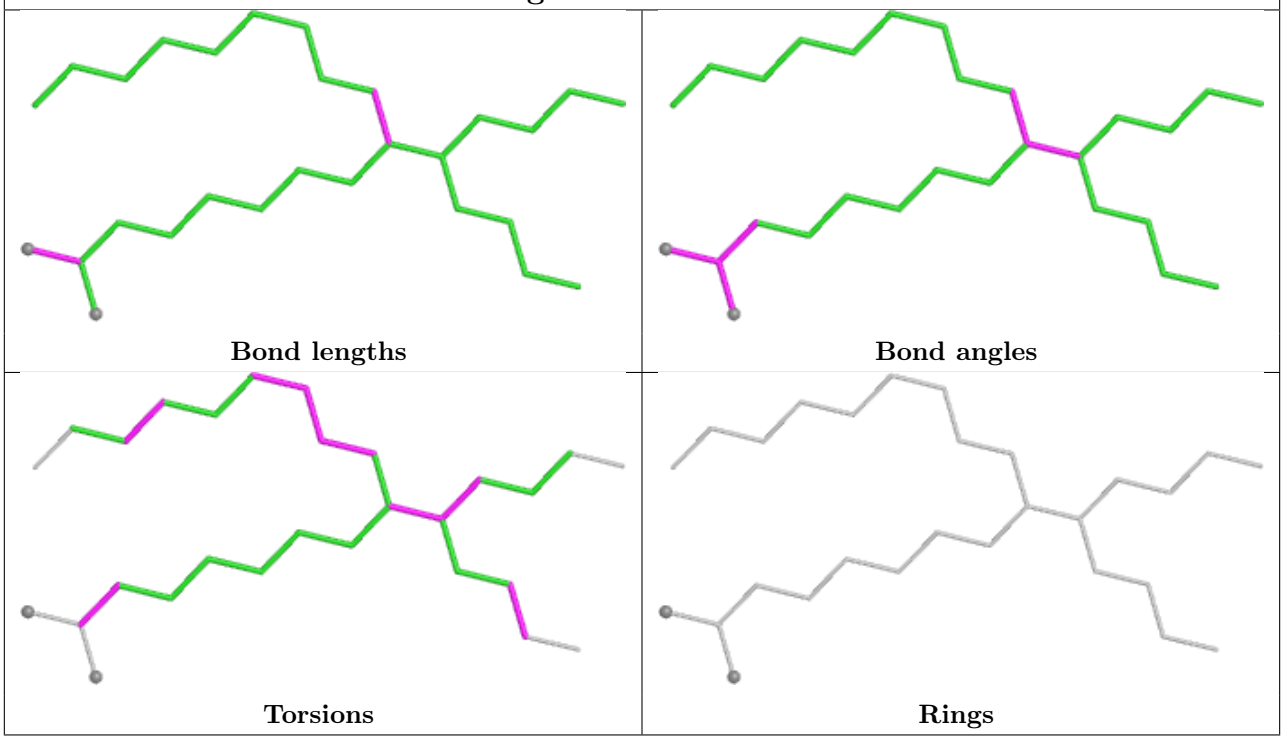
Ligand DMU L 101



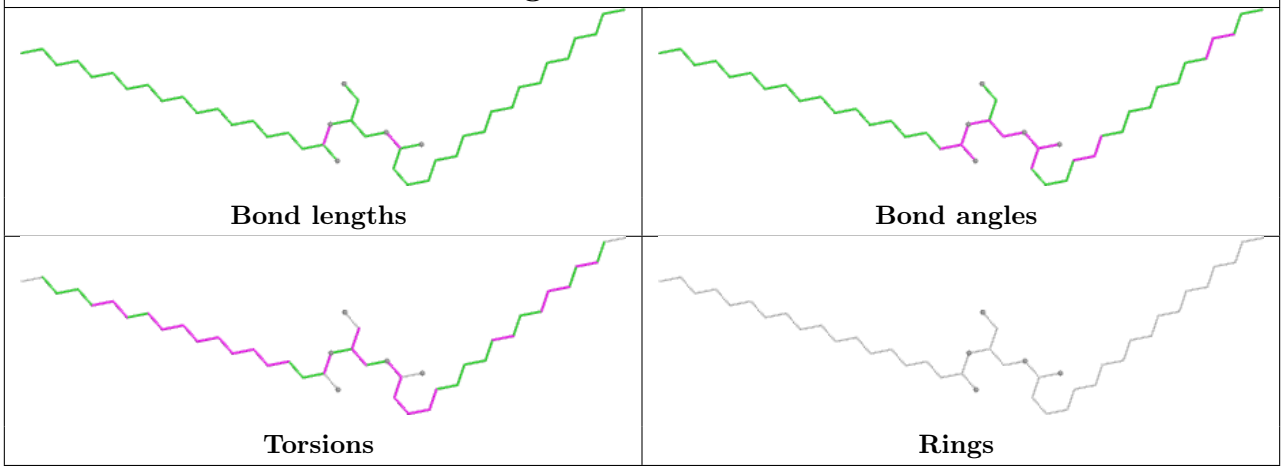
Ligand DMU K 105	
 Bond lengths	 Bond angles
Torsions	Rings

Ligand PEK C 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

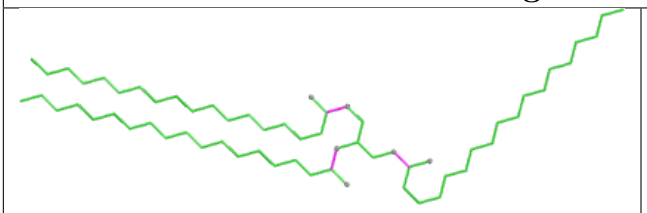
Ligand PSC O 303



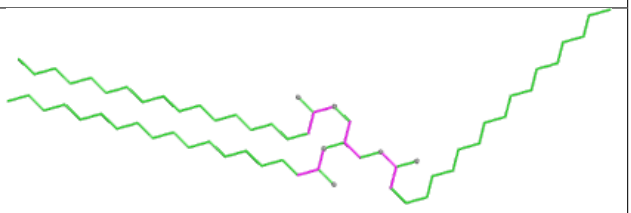
Ligand TGL N 612



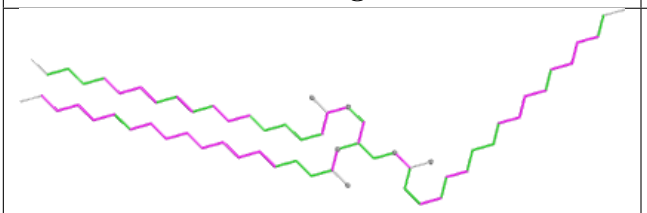
Ligand TGL N 609



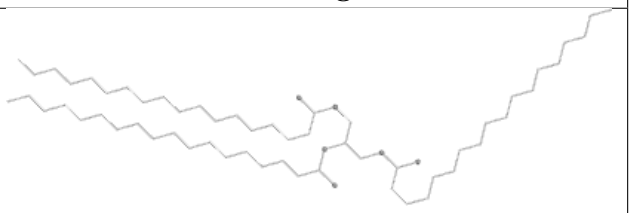
Bond lengths



Bond angles

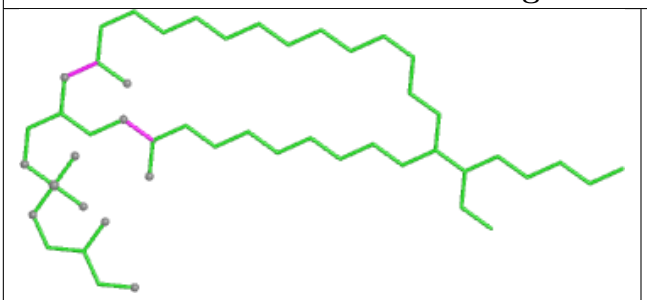


Torsions



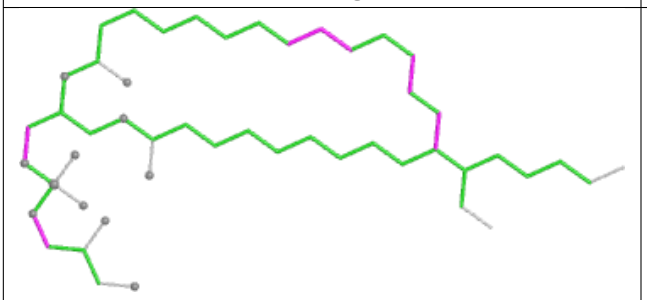
Rings

Ligand PGV P 307

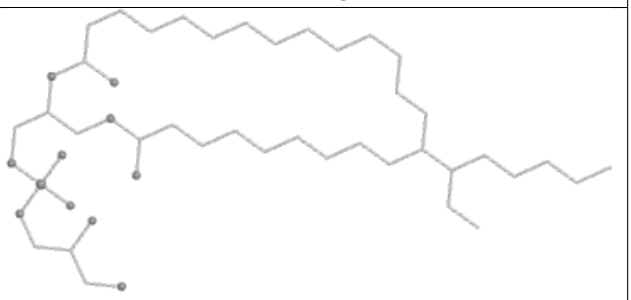


Bond lengths

Bond angles

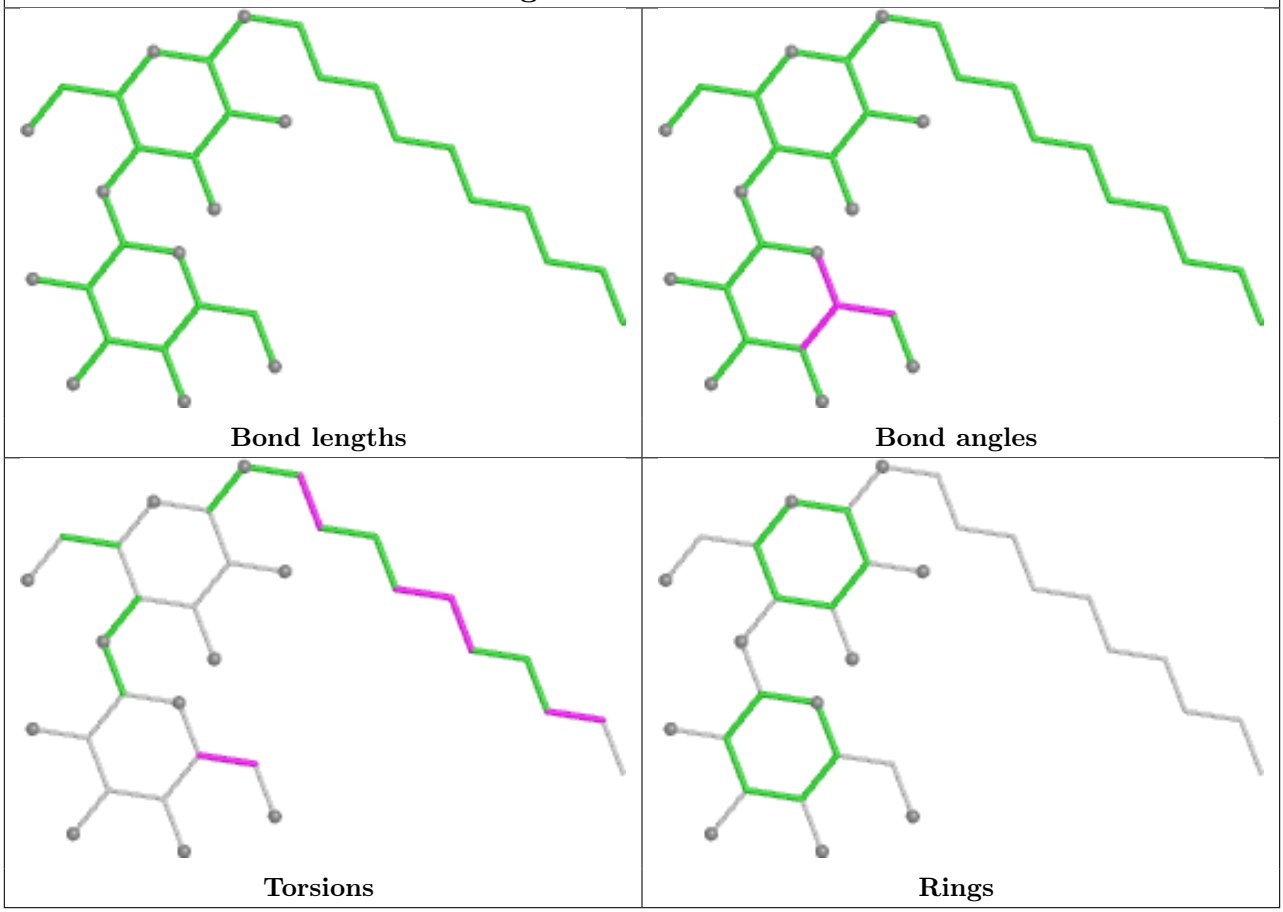


Torsions

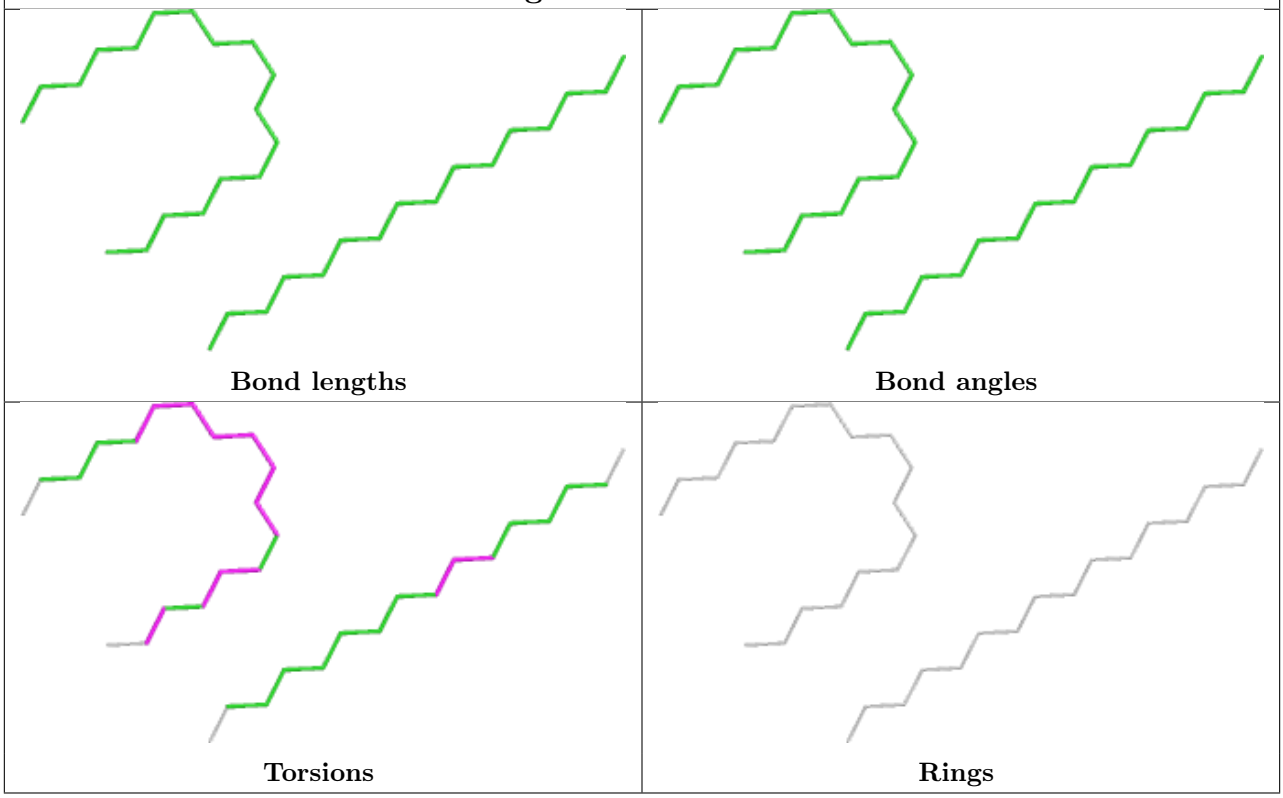


Rings

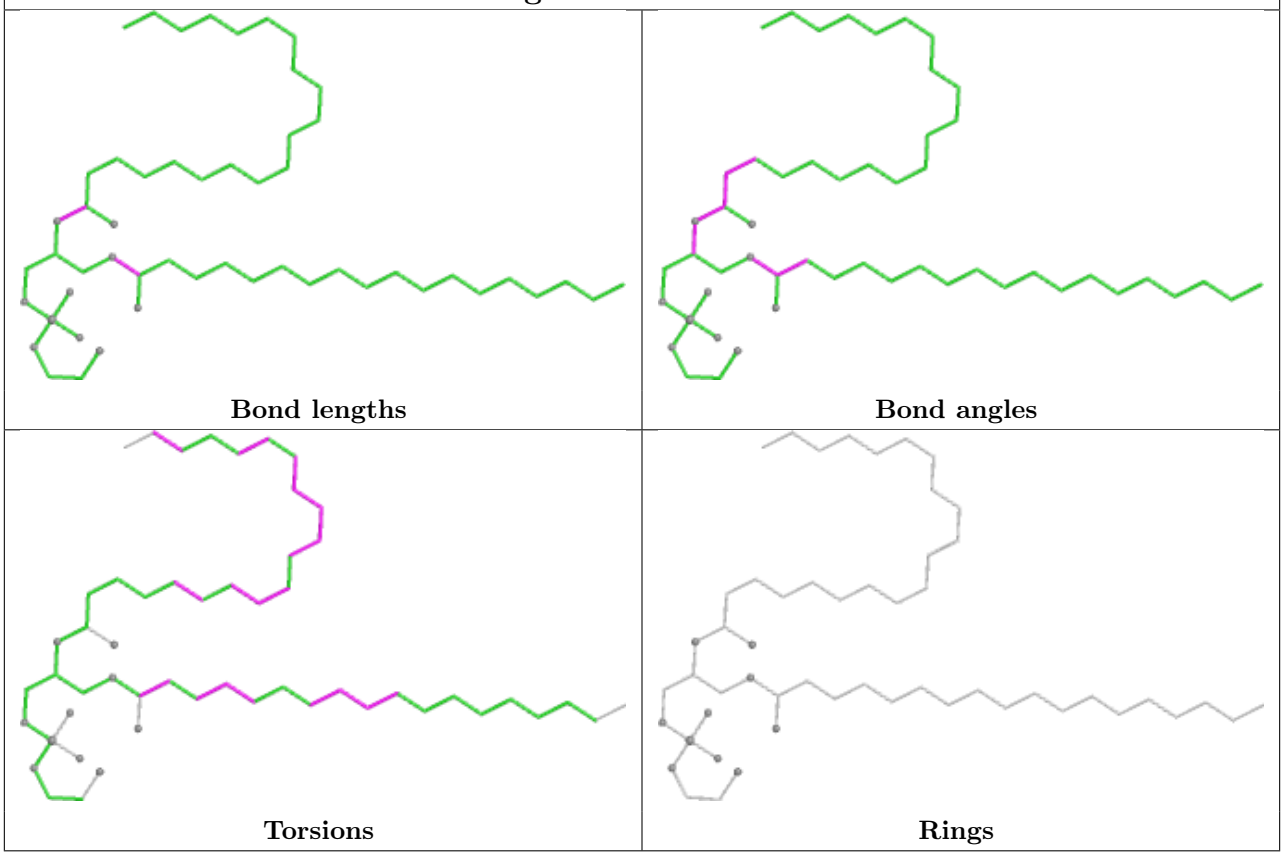
Ligand DMU Z 101



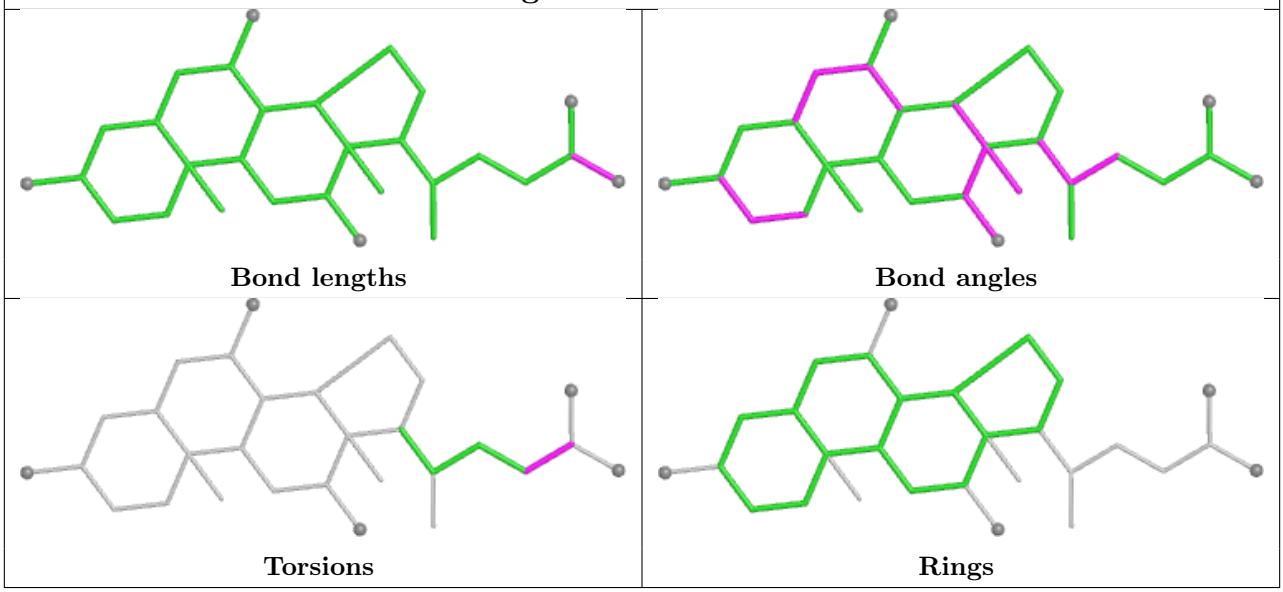
Ligand PEK P 308



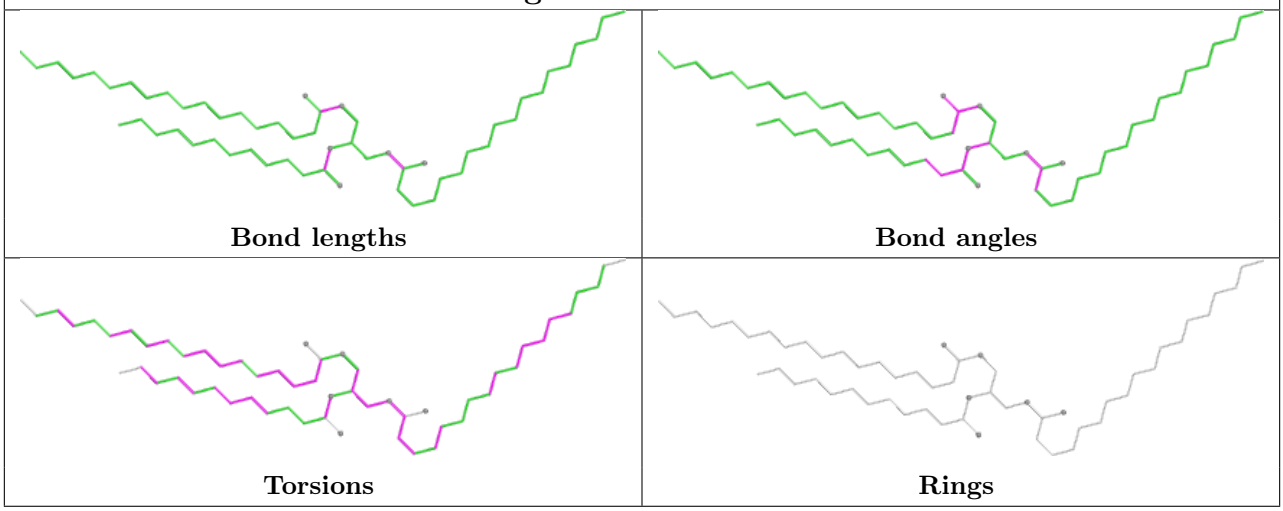
Ligand PEK C 307



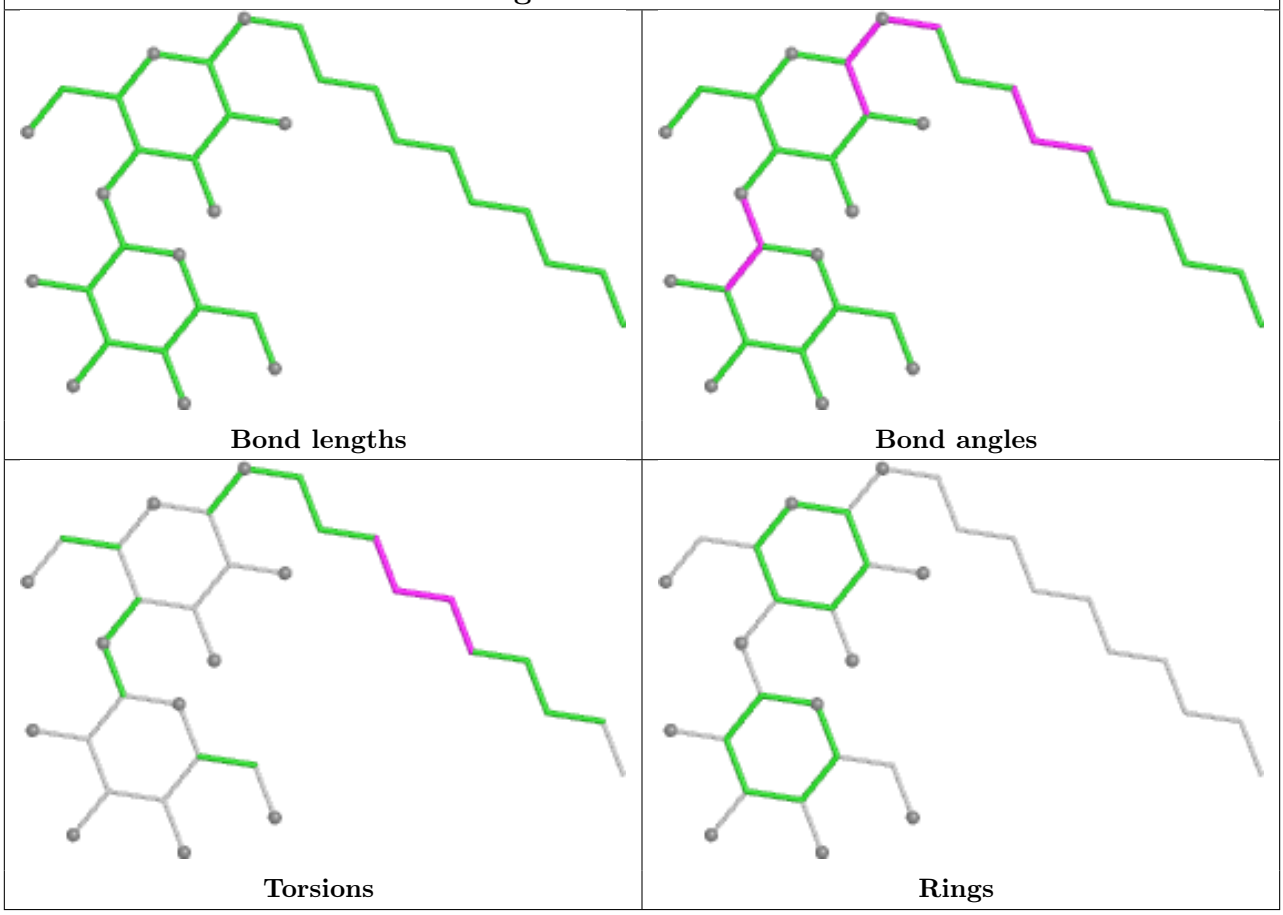
Ligand CHD C 304



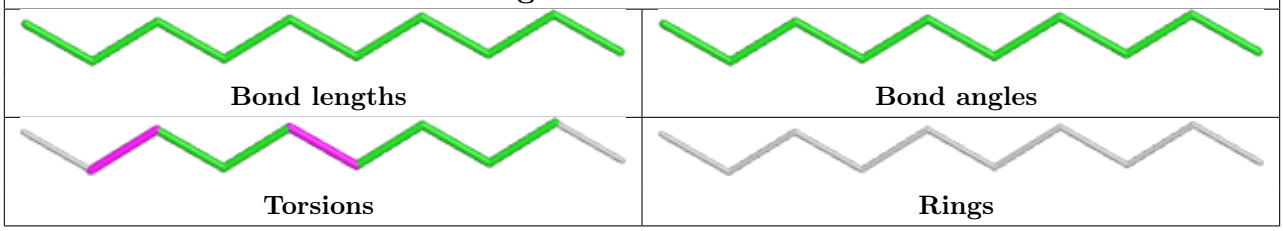
Ligand TGL D 202



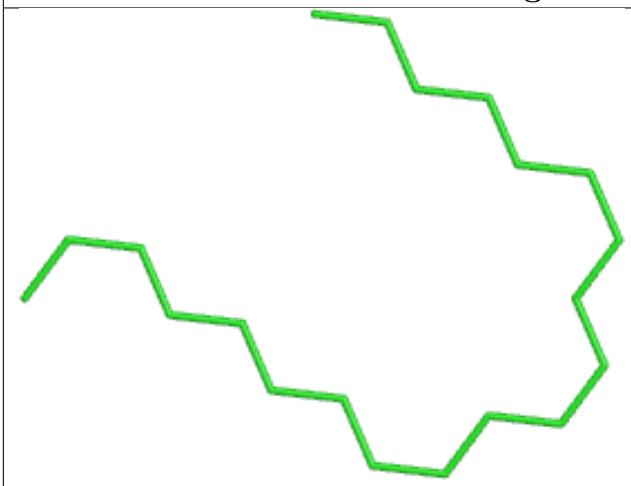
Ligand DMU M 101



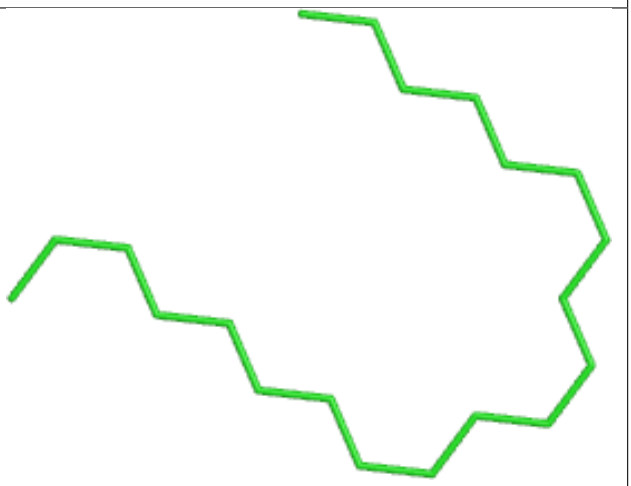
Ligand DMU X 102



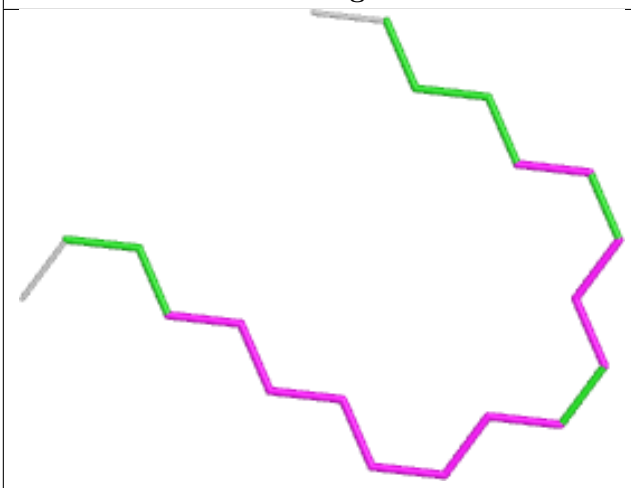
Ligand PEK P 305



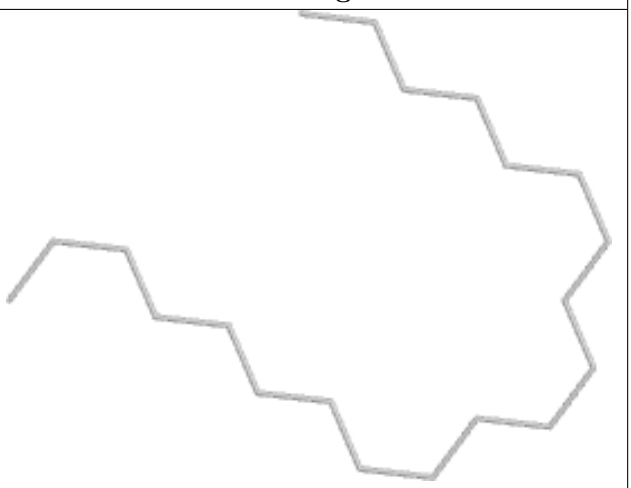
Bond lengths



Bond angles



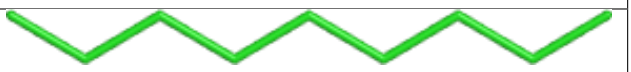
Torsions



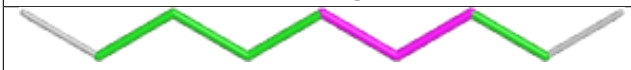
Rings

Ligand DMU K 104

Bond lengths



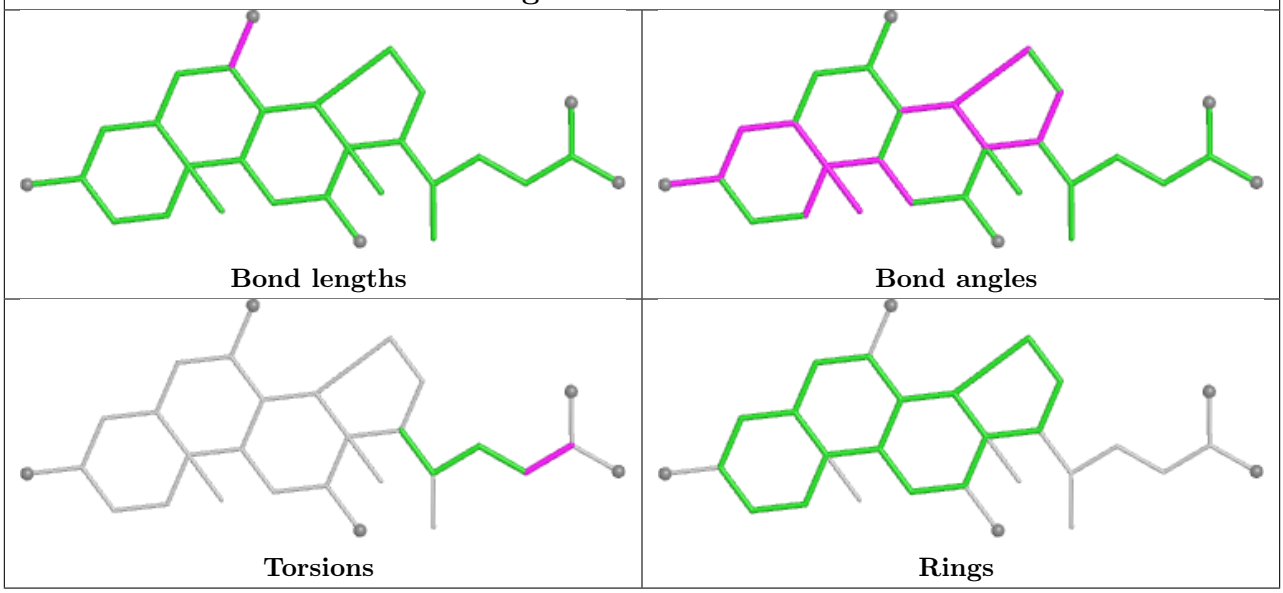
Bond angles



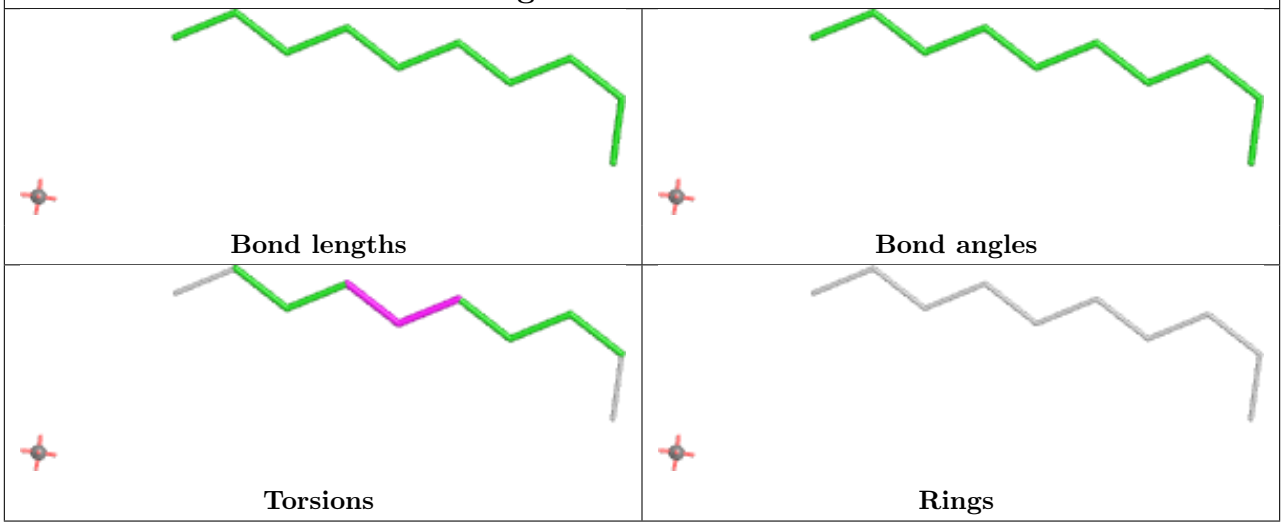
Torsions

Rings

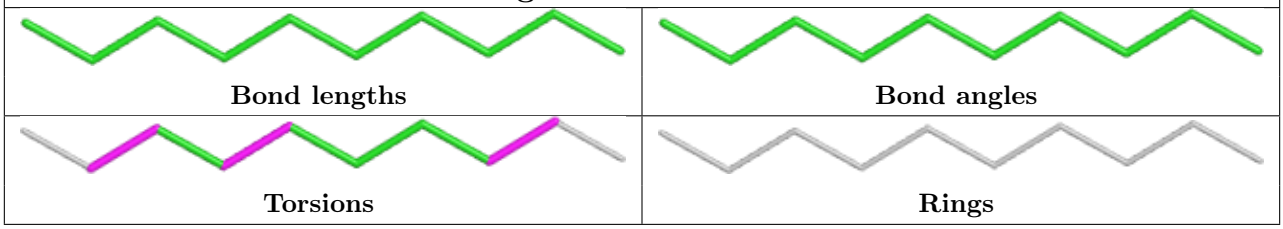
Ligand CHD B 303



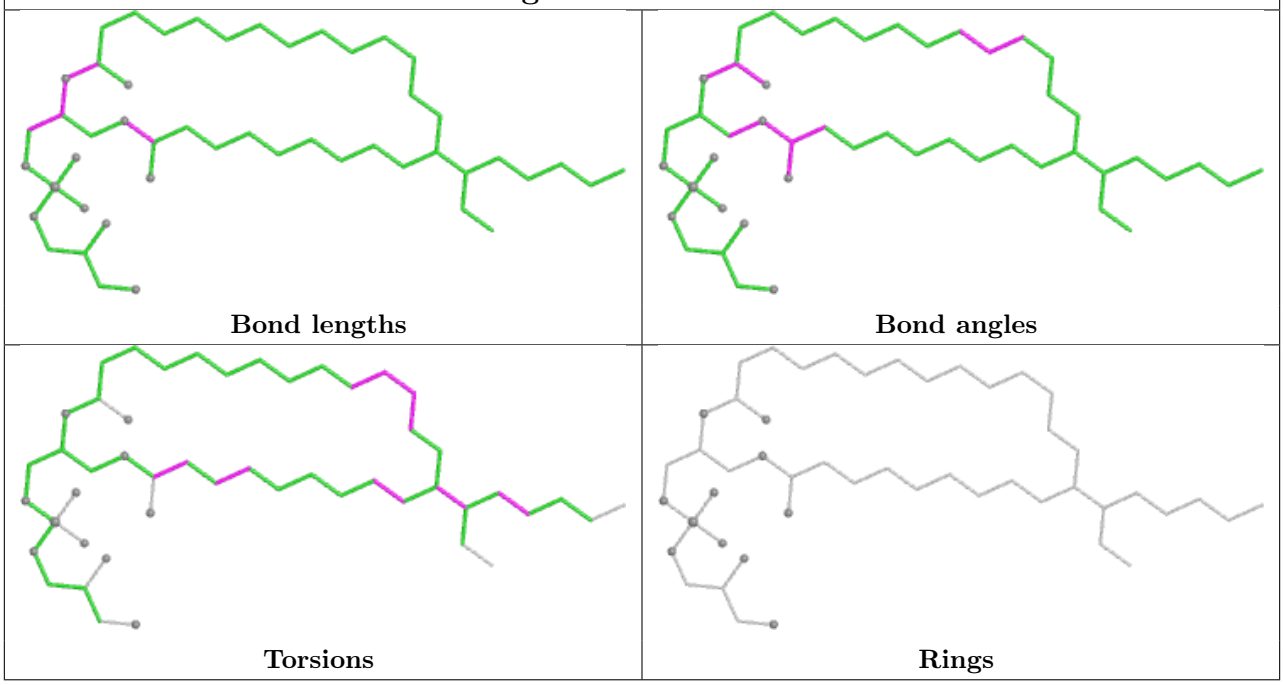
Ligand DMU D 203



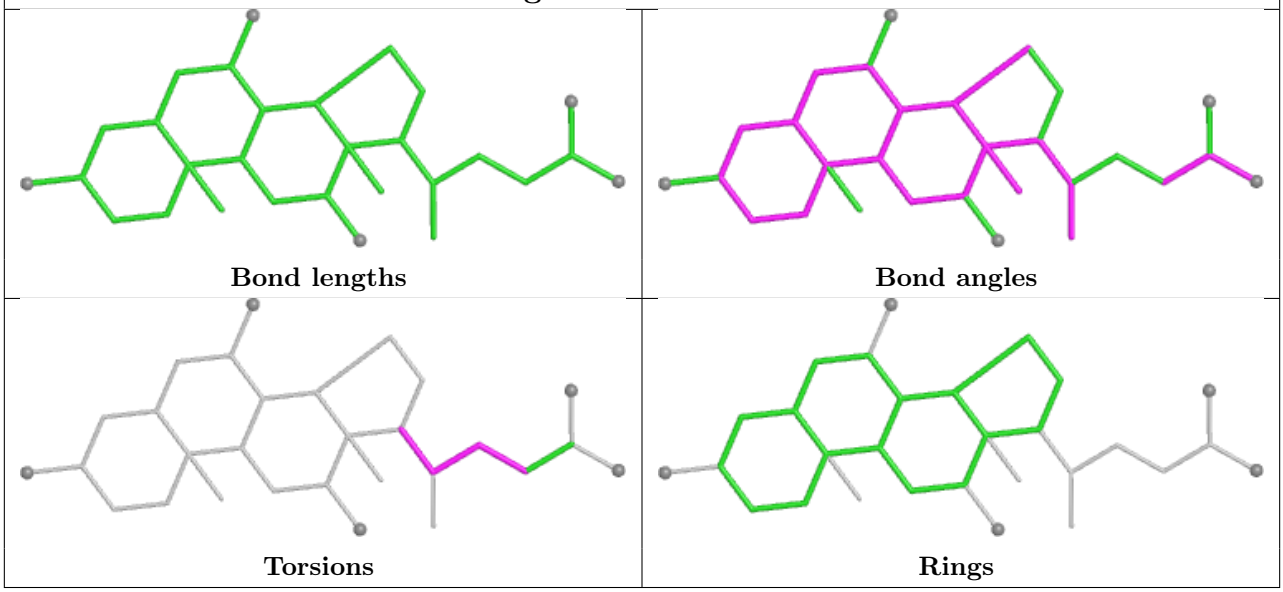
Ligand DMU K 102



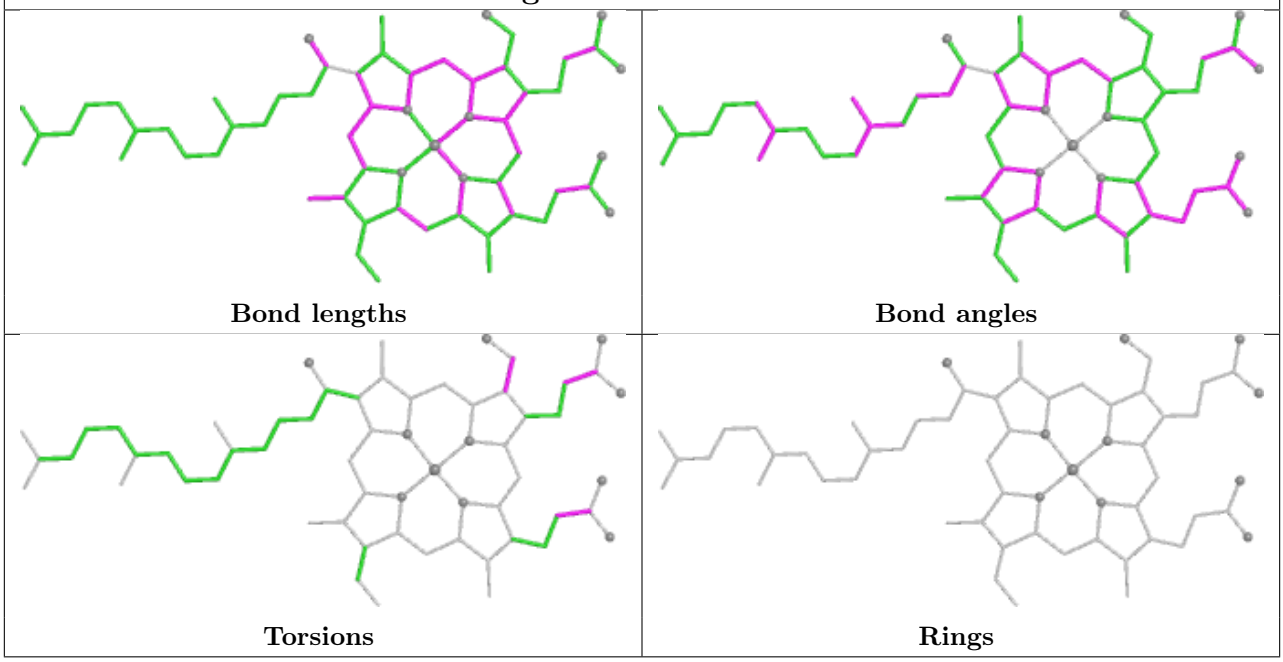
Ligand PGV N 608



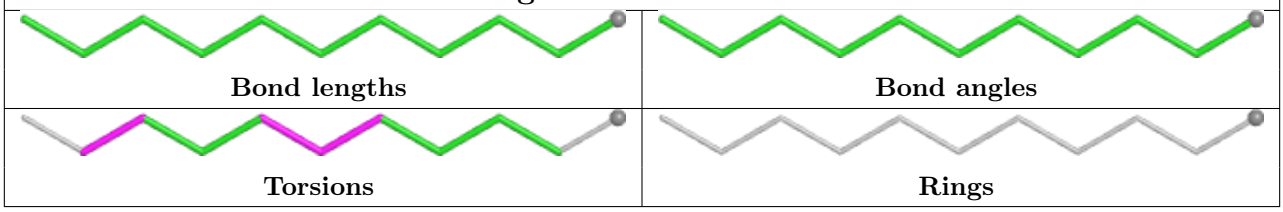
Ligand CHD L 102



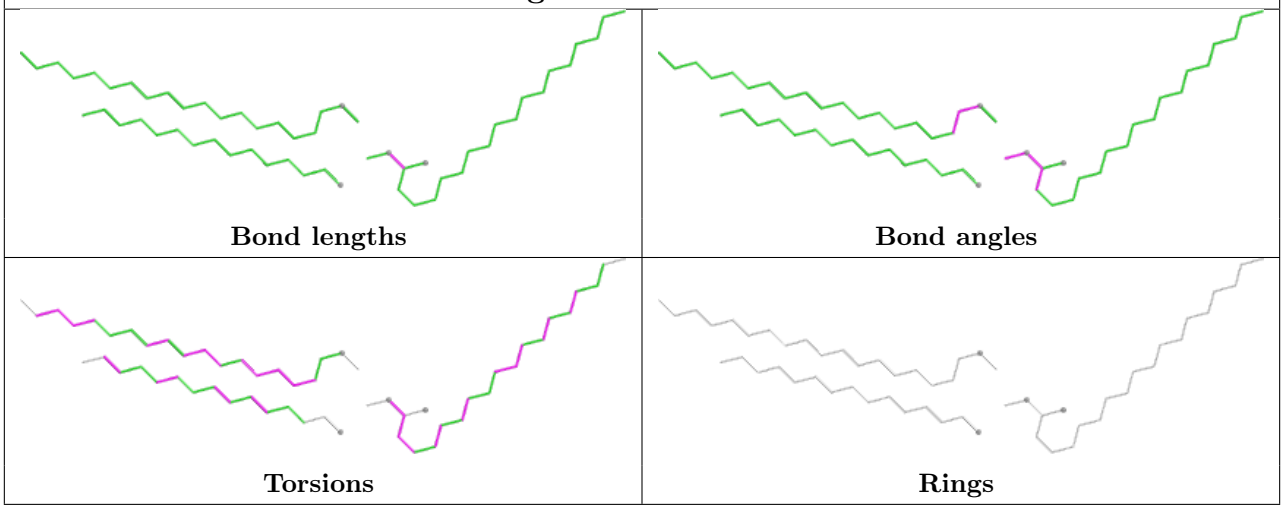
Ligand HEA N 603



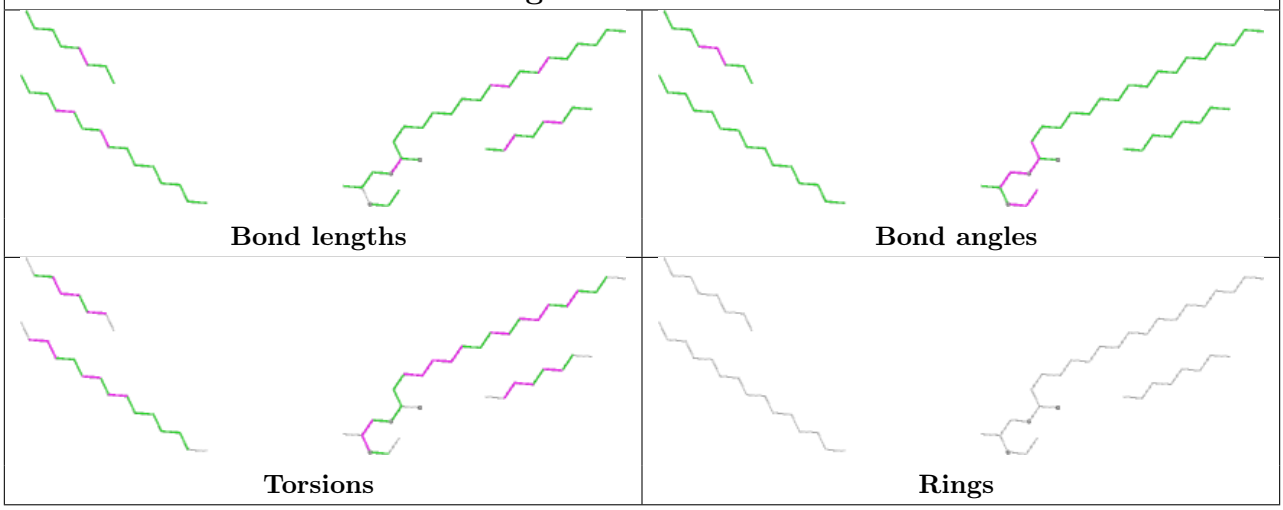
Ligand DMU D 201



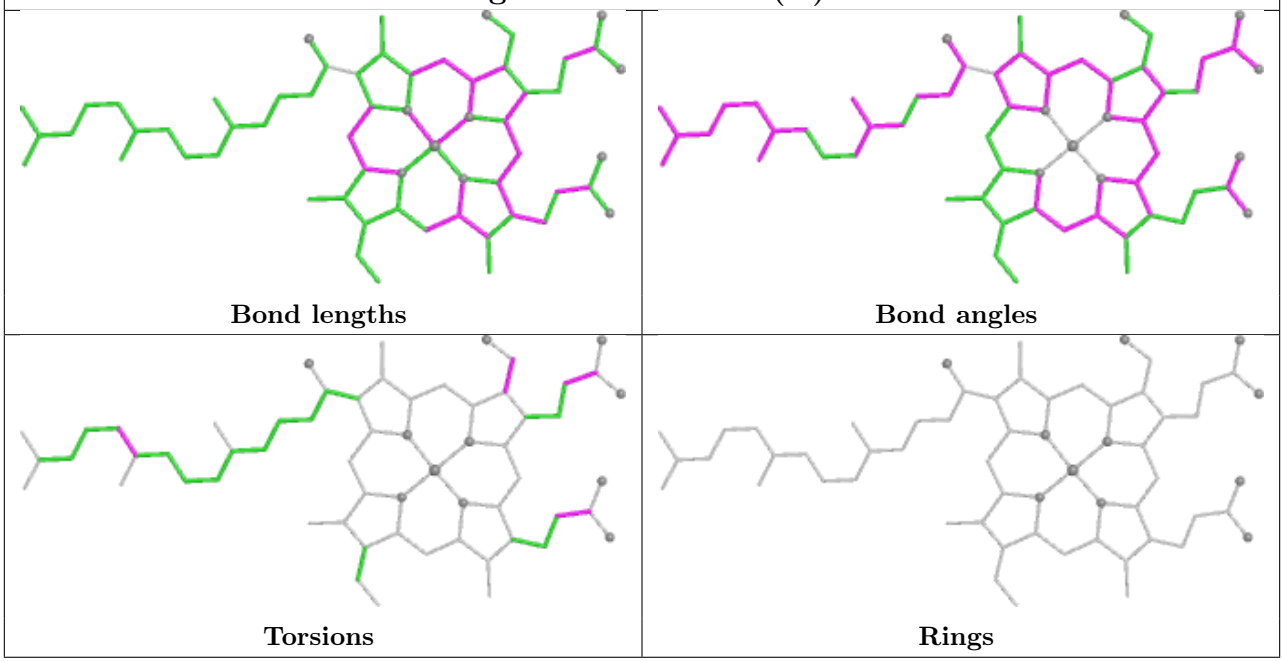
Ligand TGL L 103



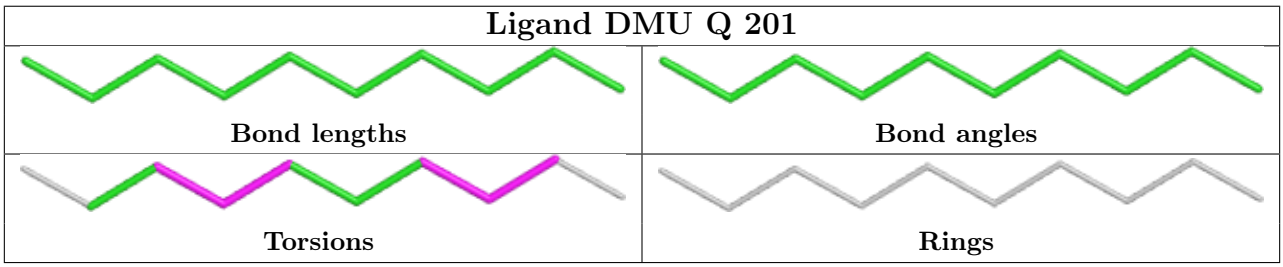
Ligand CDL T 101

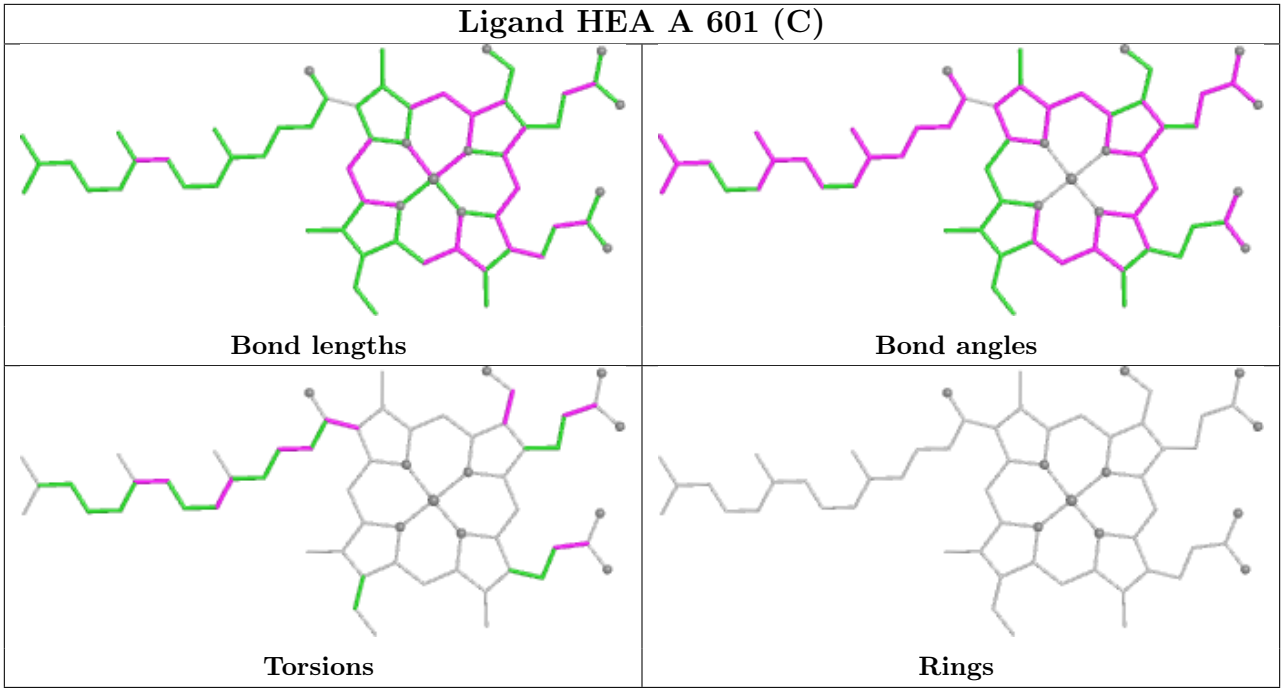


Ligand HEA A 601 (A)



Ligand DMU Q 201





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	513/514 (99%)	-0.30	3 (0%)	85	89	10, 24, 31, 73	31 (6%)
1	N	513/514 (99%)	-0.19	2 (0%)	88	91	11, 26, 35, 89	35 (6%)
2	B	226/227 (99%)	0.24	14 (6%)	26	30	17, 30, 59, 105	7 (3%)
2	O	226/227 (99%)	0.45	15 (6%)	24	28	22, 34, 75, 148	11 (4%)
3	C	259/259 (100%)	-0.03	4 (1%)	72	78	15, 27, 41, 105	12 (4%)
3	P	259/259 (100%)	0.12	7 (2%)	56	62	15, 28, 42, 111	12 (4%)
4	D	144/144 (100%)	0.14	6 (4%)	40	46	19, 31, 57, 97	3 (2%)
4	Q	144/144 (100%)	1.27	22 (15%)	5	5	27, 46, 101, 215	1 (0%)
5	E	105/105 (100%)	0.17	4 (3%)	44	50	25, 32, 66, 157	0
5	R	105/105 (100%)	0.72	8 (7%)	20	23	28, 40, 78, 155	1 (0%)
6	F	94/94 (100%)	0.33	6 (6%)	25	29	19, 31, 66, 148	5 (5%)
6	S	94/94 (100%)	0.61	10 (10%)	11	13	23, 32, 73, 159	0
7	G	84/84 (100%)	1.47	23 (27%)	1	1	20, 36, 137, 156	4 (4%)
7	T	84/84 (100%)	1.54	22 (26%)	1	1	25, 38, 137, 184	0
8	H	79/79 (100%)	0.87	11 (13%)	6	7	26, 36, 116, 171	1 (1%)
8	U	79/79 (100%)	1.02	16 (20%)	3	3	30, 40, 117, 216	0
9	I	72/73 (98%)	0.97	11 (15%)	5	5	27, 45, 77, 103	1 (1%)
9	V	72/73 (98%)	1.58	28 (38%)	1	1	30, 52, 96, 146	0
10	J	58/58 (100%)	0.80	7 (12%)	8	10	27, 38, 93, 172	1 (1%)
10	W	58/58 (100%)	0.92	8 (13%)	6	7	29, 42, 92, 152	0
11	K	49/49 (100%)	0.55	2 (4%)	41	47	21, 37, 59, 79	3 (6%)
11	X	49/49 (100%)	1.43	12 (24%)	2	2	36, 48, 98, 113	0
12	L	46/46 (100%)	0.23	3 (6%)	25	29	23, 29, 57, 111	1 (2%)
12	Y	46/46 (100%)	0.60	4 (8%)	16	19	29, 36, 85, 125	0

Continued on next page...

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	43/43 (100%)	0.32	4 (9%) 14 17	25, 29, 95, 126	0
13	Z	43/43 (100%)	0.98	6 (13%) 6 7	32, 37, 110, 225	0
All	All	3544/3550 (99%)	0.34	258 (7%) 21 24	10, 30, 78, 225	129 (3%)

The worst 5 of 258 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	6	VAL	12.2
6	S	1	ALA	10.7
7	T	3	ALA	10.0
7	T	6	GLY	9.7
4	Q	5	VAL	9.3

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	SAC	V	1	9/10	0.30	0.21	113,156,190,197	0
9	SAC	I	1	9/10	0.58	0.27	112,134,180,200	0
1	FME	N	1	10/11	0.91	0.17	38,42,98,131	0
1	FME	A	1	10/11	0.95	0.09	35,49,83,103	0
2	FME	O	1	10/11	0.96	0.11	31,34,42,112	0
2	FME	B	1	10/11	0.96	0.13	27,28,38,142	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	DMU	X	102	10/33	0.58	0.32	62,71,99,116	0
25	DMU	D	203	11/33	0.69	0.25	52,74,124,137	0
25	DMU	K	105	9/33	0.71	0.22	72,75,92,107	0
24	CHD	Y	101	29/29	0.71	0.25	56,95,143,158	0
25	DMU	X	103	9/33	0.72	0.23	55,62,94,101	0
21	EDO	L	104	4/4	0.73	0.34	50,51,77,148	0
25	DMU	K	104	9/33	0.74	0.32	49,70,113,125	0
21	EDO	P	310	4/4	0.74	0.19	46,60,67,75	0
26	CDL	T	101	57/100	0.75	0.28	42,72,104,149	0
24	CHD	L	102	29/29	0.77	0.23	51,100,145,177	0
25	DMU	X	104	10/33	0.77	0.26	62,84,90,92	0
22	TGL	N	611	48/63	0.77	0.27	48,68,120,134	0
18	PGV	C	311	28/51	0.78	0.30	41,66,117,126	0
27	PEK	P	308	34/53	0.78	0.28	37,70,117,134	0
25	DMU	X	101	11/33	0.79	0.21	43,59,104,225	0
25	DMU	P	303	13/33	0.79	0.23	53,62,94,101	0
27	PEK	C	309	36/53	0.80	0.25	42,75,110,130	0
18	PGV	G	102	32/51	0.80	0.25	39,72,108,130	0
26	CDL	N	601	55/100	0.81	0.25	51,69,104,118	0
21	EDO	G	104	4/4	0.81	0.30	33,77,87,92	0
25	DMU	Q	201	10/33	0.81	0.25	52,62,68,111	0
22	TGL	B	301	49/63	0.81	0.22	38,61,98,147	0
21	EDO	P	317	4/4	0.82	0.17	57,90,97,106	0
22	TGL	N	609	63/63	0.82	0.23	40,72,117,154	0
25	DMU	K	106	10/33	0.83	0.25	52,65,91,120	0
25	DMU	L	101	21/33	0.83	0.18	42,81,114,129	0
27	PEK	C	306	25/53	0.83	0.24	41,57,96,119	0
25	DMU	C	303	13/33	0.83	0.20	53,63,88,92	0
27	PEK	P	305	20/53	0.83	0.21	47,56,95,96	0
22	TGL	D	202	57/63	0.83	0.23	32,65,134,156	0
21	EDO	S	104	4/4	0.84	0.20	40,56,58,88	0
25	DMU	K	102	10/33	0.84	0.21	46,69,87,103	0
18	PGV	N	607	24/51	0.84	0.27	41,53,106,166	0
26	CDL	P	304	61/100	0.85	0.25	37,69,128,196	0
25	DMU	O	302	11/33	0.85	0.19	54,58,104,111	0
22	TGL	L	103	56/63	0.85	0.22	28,56,121,139	0
21	EDO	A	615	4/4	0.85	0.18	49,58,60,64	0
26	CDL	C	305	58/100	0.85	0.22	44,65,131,156	0
21	EDO	J	102	4/4	0.85	0.24	52,52,100,116	0
19	PSC	A	607	27/52	0.86	0.22	36,66,100,129	0
21	EDO	C	320	4/4	0.86	0.26	32,56,75,112	0
21	EDO	Q	202	4/4	0.86	0.15	43,50,52,56	0
21	EDO	F	103	4/4	0.86	0.19	50,61,64,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	DMU	K	103	11/33	0.86	0.22	50,70,100,120	0
21	EDO	N	619	4/4	0.86	0.24	51,52,54,67	0
21	EDO	T	104	4/4	0.87	0.17	39,49,54,71	0
21	EDO	P	312	4/4	0.87	0.16	67,72,73,77	0
21	EDO	P	316	4/4	0.87	0.17	39,56,66,82	0
18	PGV	A	606	22/51	0.87	0.19	31,45,70,94	0
21	EDO	C	314	4/4	0.87	0.14	32,39,42,44	0
21	EDO	A	609	4/4	0.87	0.25	34,38,47,146	0
22	TGL	N	612	44/63	0.87	0.23	41,59,127,197	0
21	EDO	T	103	4/4	0.87	0.21	43,65,78,97	0
21	EDO	F	106	4/4	0.88	0.21	35,38,76,104	0
25	DMU	P	309	11/33	0.88	0.24	42,58,101,104	0
19	PSC	O	303	30/52	0.88	0.20	37,59,103,106	0
21	EDO	P	311	4/4	0.89	0.16	62,62,65,73	0
21	EDO	D	205	4/4	0.89	0.17	44,45,46,101	0
21	EDO	W	102	4/4	0.89	0.22	47,57,68,111	0
21	EDO	J	103	4/4	0.89	0.17	51,52,72,74	0
25	DMU	C	310	21/33	0.89	0.16	29,58,111,142	0
21	EDO	A	614	4/4	0.89	0.13	55,66,70,75	0
21	EDO	C	319	4/4	0.89	0.20	43,53,61,115	0
25	DMU	W	101	11/33	0.89	0.20	51,59,82,111	0
21	EDO	A	610	4/4	0.89	0.17	39,48,53,70	0
21	EDO	S	106	4/4	0.89	0.23	39,47,67,81	0
25	DMU	K	101	9/33	0.90	0.16	41,52,77,94	0
21	EDO	E	203	4/4	0.90	0.18	42,45,54,117	0
25	DMU	D	201	11/33	0.90	0.17	44,69,79,88	0
21	EDO	C	312	4/4	0.90	0.15	48,71,72,75	0
21	EDO	D	204	4/4	0.91	0.21	37,47,79,85	0
21	EDO	P	315	4/4	0.91	0.15	53,58,63,73	0
25	DMU	J	101	11/33	0.91	0.17	49,58,81,102	0
29	PO4	H	101	5/5	0.91	0.10	56,61,94,161	0
29	PO4	U	101	5/5	0.91	0.12	47,54,128,200	0
21	EDO	O	306	4/4	0.92	0.18	48,63,79,92	0
21	EDO	Y	102	4/4	0.92	0.16	48,57,57,83	0
21	EDO	Y	103	4/4	0.92	0.14	46,59,90,134	0
21	EDO	B	307	4/4	0.92	0.13	34,45,46,48	0
21	EDO	C	316	4/4	0.92	0.12	53,56,61,69	0
21	EDO	N	620	4/4	0.92	0.21	33,34,66,104	0
21	EDO	N	616	4/4	0.93	0.14	33,41,44,71	0
21	EDO	C	313	4/4	0.93	0.15	30,32,33,94	0
21	EDO	B	306	4/4	0.93	0.12	29,35,41,55	0
25	DMU	Z	101	33/33	0.93	0.10	38,46,79,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
21	EDO	N	621	4/4	0.93	0.12	46,52,52,62	0
21	EDO	O	305	4/4	0.93	0.17	42,46,51,95	0
25	DMU	M	101	33/33	0.93	0.10	31,40,53,69	0
21	EDO	C	318	4/4	0.94	0.15	40,60,63,111	0
21	EDO	D	206	4/4	0.94	0.12	36,38,58,71	0
21	EDO	A	612	4/4	0.94	0.11	28,31,32,38	0
21	EDO	A	618	4/4	0.94	0.15	33,34,39,87	0
21	EDO	F	105	4/4	0.94	0.14	39,44,64,96	0
21	EDO	C	317	4/4	0.94	0.12	55,56,72,75	0
24	CHD	C	304	29/29	0.94	0.08	26,29,35,41	0
21	EDO	A	616	4/4	0.95	0.15	30,42,68,94	0
21	EDO	A	617	4/4	0.95	0.13	37,39,46,63	0
21	EDO	N	613	4/4	0.95	0.09	28,29,29,32	0
21	EDO	N	614	4/4	0.95	0.09	37,38,39,44	0
21	EDO	N	615	4/4	0.95	0.12	37,40,41,67	0
21	EDO	P	313	4/4	0.95	0.14	34,37,39,39	0
21	EDO	P	314	4/4	0.95	0.12	30,35,40,62	0
20	PER	N	610[A]	2/2	0.95	0.16	28,28,28,28	2
21	EDO	C	315	4/4	0.95	0.14	28,35,50,72	0
18	PGV	N	608	51/51	0.95	0.12	23,34,69,80	0
20	PER	A	608[A]	2/2	0.95	0.12	23,23,23,23	2
21	EDO	O	304	4/4	0.95	0.08	30,31,32,32	0
21	EDO	S	102	4/4	0.96	0.08	23,25,25,25	0
24	CHD	B	303	29/29	0.96	0.07	21,26,31,46	0
18	PGV	C	301	51/51	0.96	0.10	22,32,67,80	0
24	CHD	G	101	29/29	0.96	0.07	21,26,35,42	0
21	EDO	B	305	4/4	0.96	0.11	32,34,45,103	0
27	PEK	C	307	53/53	0.96	0.12	26,42,102,136	0
24	CHD	P	301	29/29	0.96	0.07	24,29,35,40	0
21	EDO	T	102	4/4	0.96	0.12	31,32,37,40	0
27	PEK	P	306	53/53	0.96	0.12	28,41,84,122	0
21	EDO	E	202	4/4	0.96	0.08	31,38,43,45	0
21	EDO	N	617	4/4	0.96	0.08	22,29,30,32	0
21	EDO	N	618	4/4	0.96	0.11	31,41,43,47	0
21	EDO	A	613	4/4	0.97	0.12	28,39,46,48	0
21	EDO	B	304	4/4	0.97	0.07	24,25,27,29	0
18	PGV	P	307	51/51	0.97	0.11	23,32,97,138	0
17	NA	P	302	1/1	0.97	0.05	30,30,30,30	0
21	EDO	G	103	4/4	0.97	0.07	30,31,35,35	0
18	PGV	C	308	48/51	0.97	0.10	22,29,71,88	0
21	EDO	E	201	4/4	0.97	0.08	37,38,38,39	0
17	NA	C	302	1/1	0.97	0.06	31,31,31,31	0

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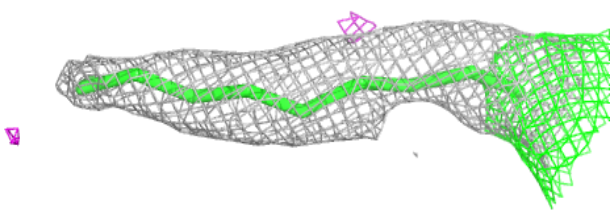
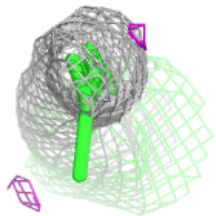
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
21	EDO	S	105	4/4	0.97	0.08	31,31,31,33	0
14	HEA	A	602	60/60	0.98	0.06	18,22,28,38	0
21	EDO	F	104	4/4	0.98	0.10	30,30,31,32	0
16	MG	A	604	1/1	0.98	0.07	19,19,19,19	0
21	EDO	S	103	4/4	0.98	0.07	32,33,38,41	0
21	EDO	F	102	4/4	0.98	0.06	24,25,26,27	0
14	HEA	A	601[A]	60/60	0.99	0.05	17,21,33,63	17
14	HEA	N	602[A]	60/60	0.99	0.06	20,25,38,46	17
14	HEA	N	602[B]	52/60	0.99	0.06	16,24,33,47	9
14	HEA	N	602[C]	52/60	0.99	0.06	20,24,40,52	9
14	HEA	N	603	60/60	0.99	0.06	19,23,29,38	0
21	EDO	A	611	4/4	0.99	0.07	22,24,27,28	0
14	HEA	A	601[B]	52/60	0.99	0.05	10,20,27,55	9
16	MG	N	605	1/1	0.99	0.07	21,21,21,21	0
17	NA	A	605	1/1	0.99	0.03	24,24,24,24	0
28	ZN	S	101	1/1	0.99	0.03	26,26,26,26	0
14	HEA	A	601[C]	52/60	0.99	0.05	17,21,31,57	9
17	NA	N	606	1/1	0.99	0.04	28,28,28,28	0
23	CUA	B	302	2/2	1.00	0.02	22,22,22,22	0
28	ZN	F	101	1/1	1.00	0.04	25,25,25,25	0
23	CUA	O	301	2/2	1.00	0.02	26,26,26,26	0
15	CU	N	604	1/1	1.00	0.02	24,24,24,24	0
15	CU	A	603	1/1	1.00	0.02	22,22,22,22	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 X 102:

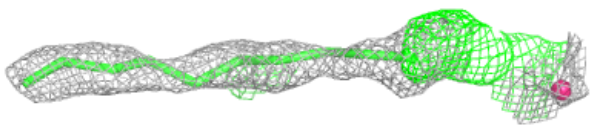
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

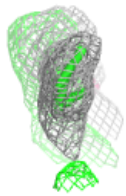




Electron density around DMU D 203:

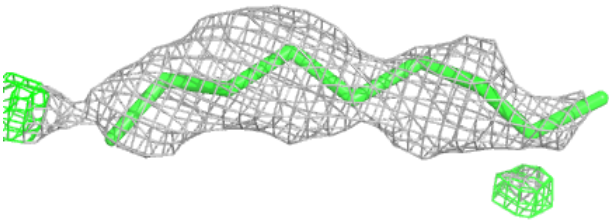
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

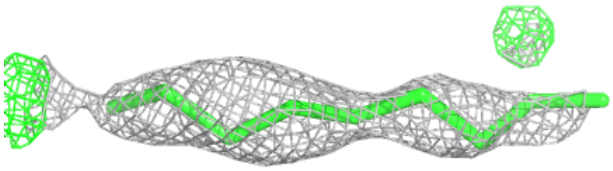


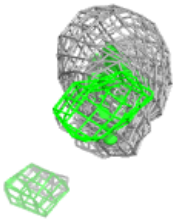


Electron density around DMU K 105:

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

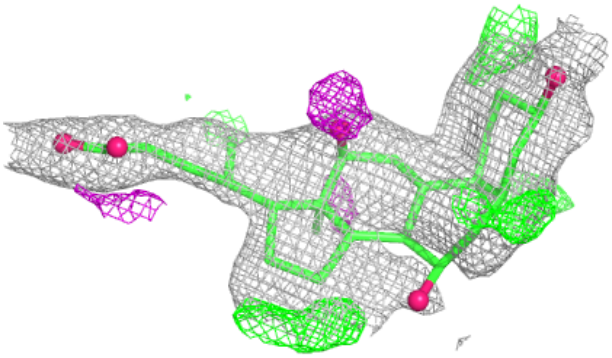


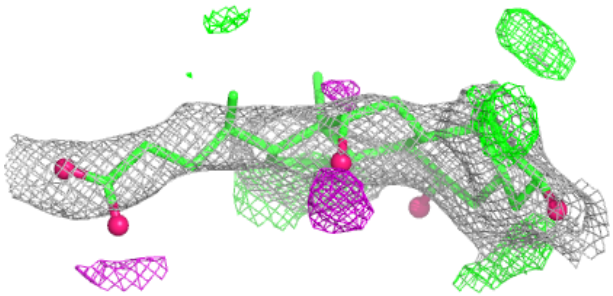


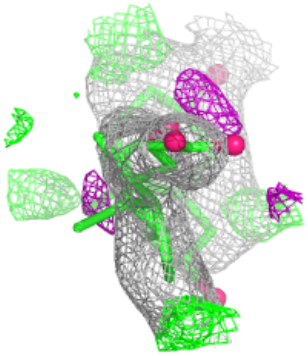


Electron density around CHD Y 101:

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

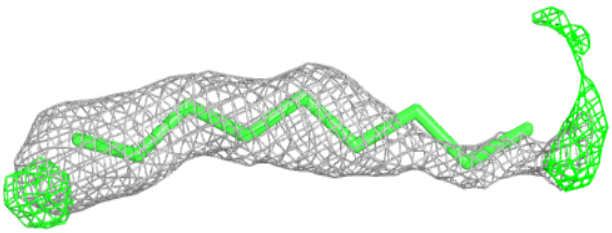


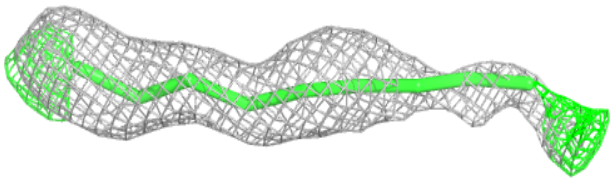


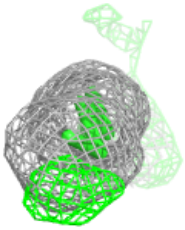


Electron density around DMU X 103:

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

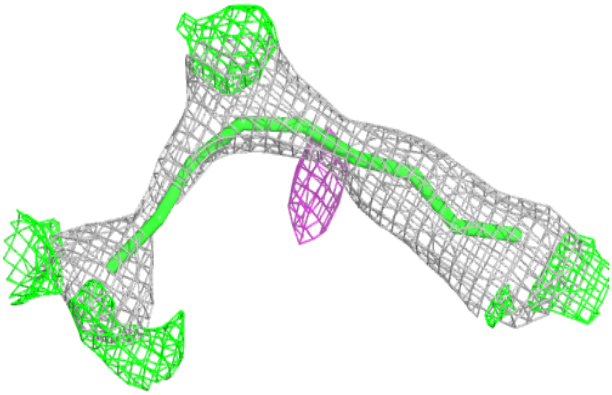


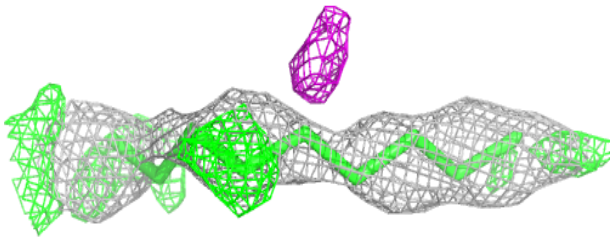


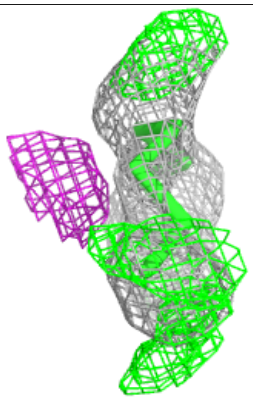


Electron density around DMU K 104:

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

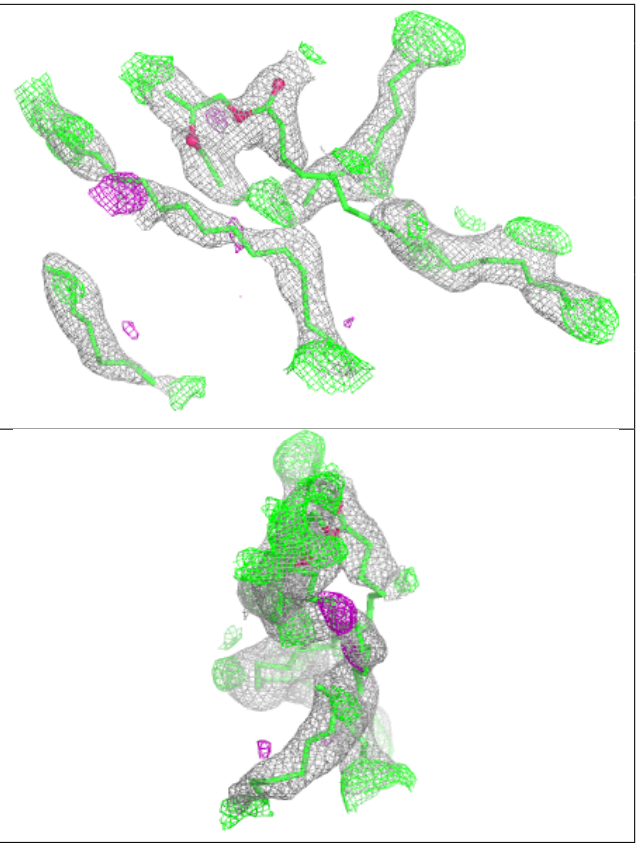






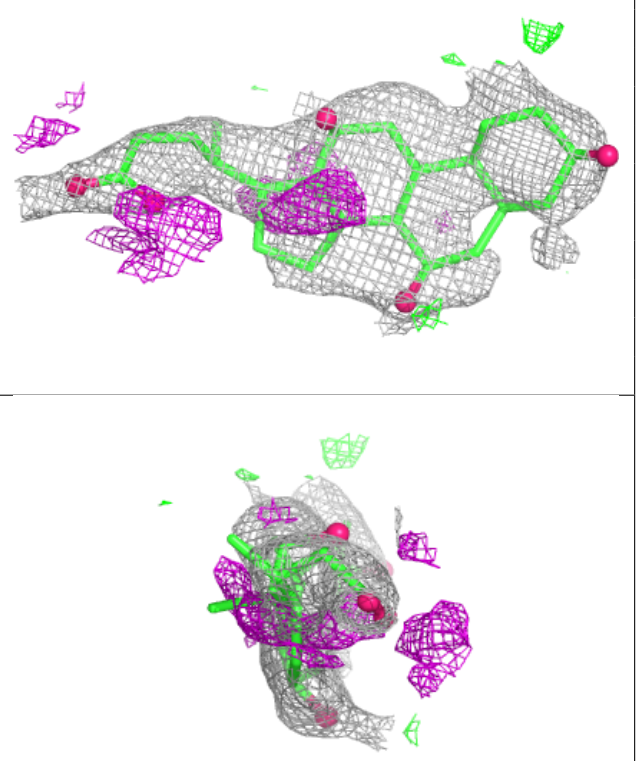
Electron density around CDL T 101:

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



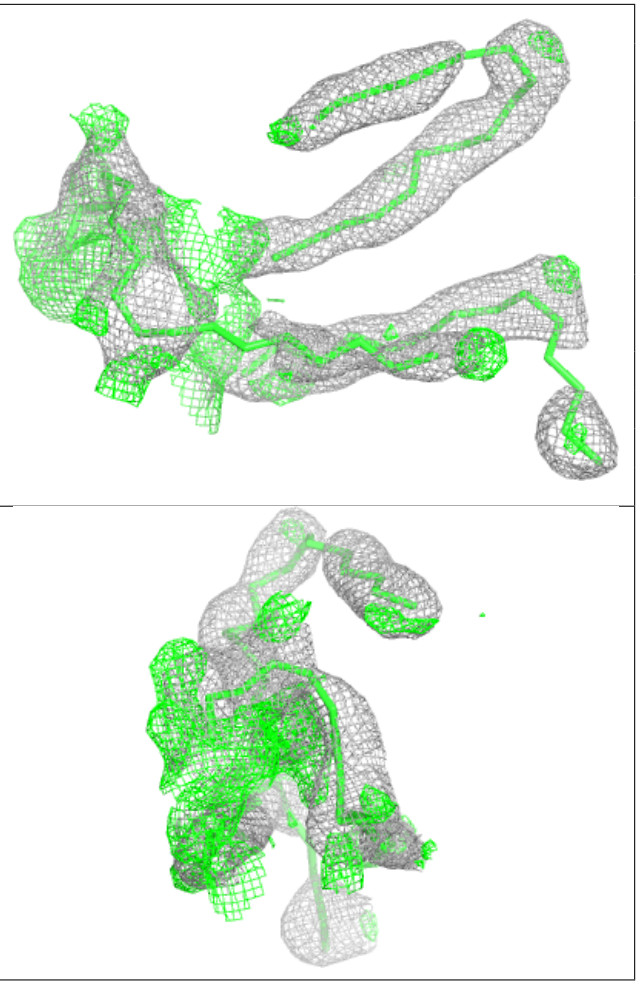
Electron density around CHD L 102:

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



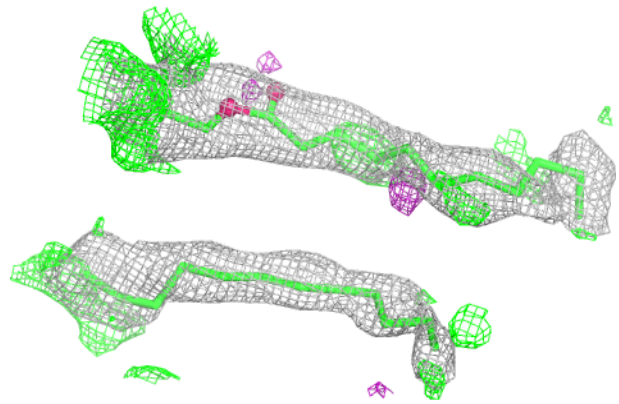
Electron density around TGL N 611:

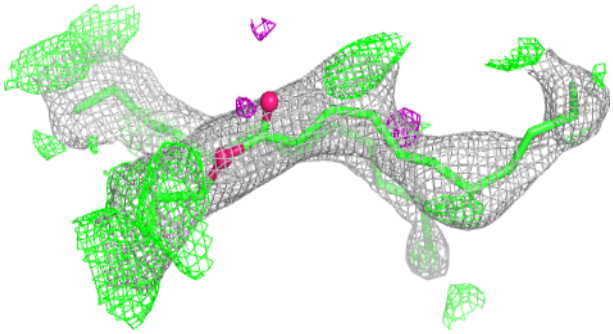
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

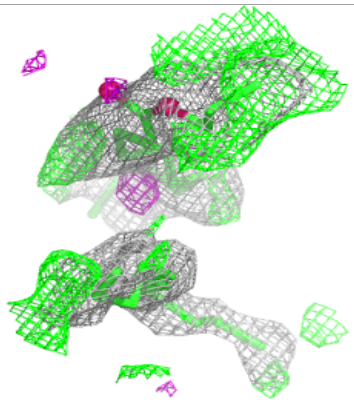


Electron density around PGV C 311:

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

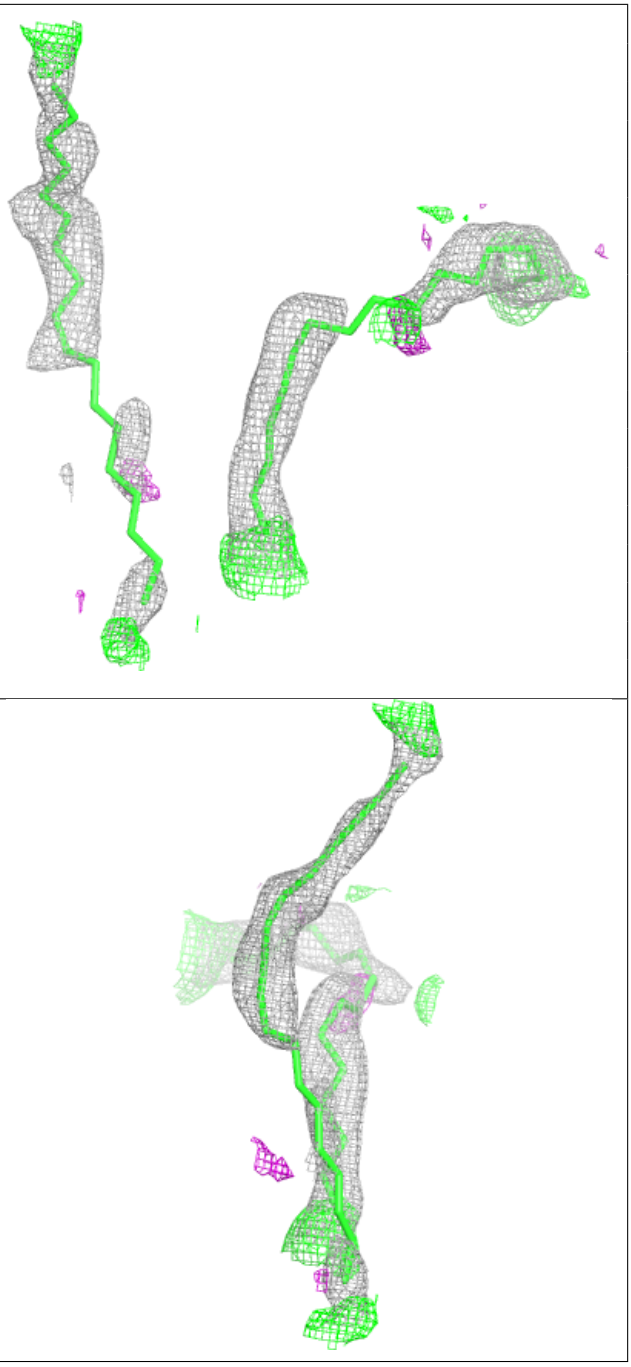






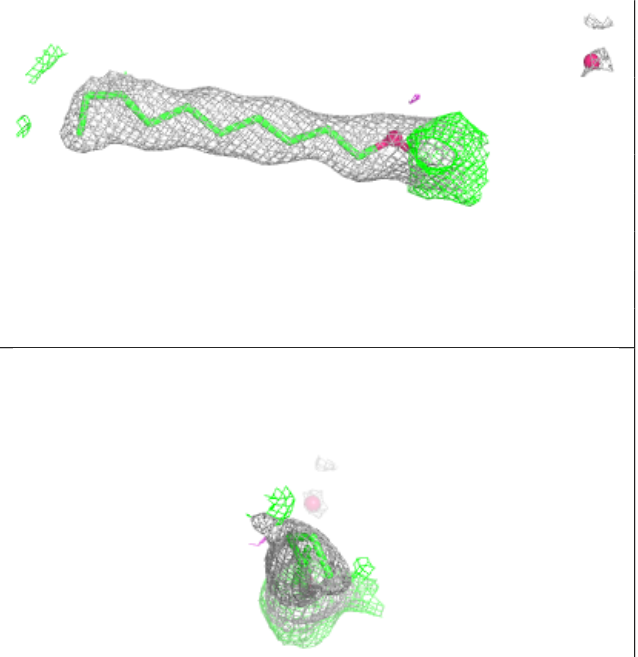
Electron density around PEK P 308:

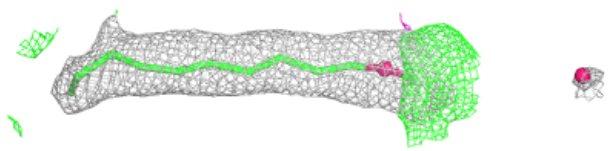
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around DMU P 303:

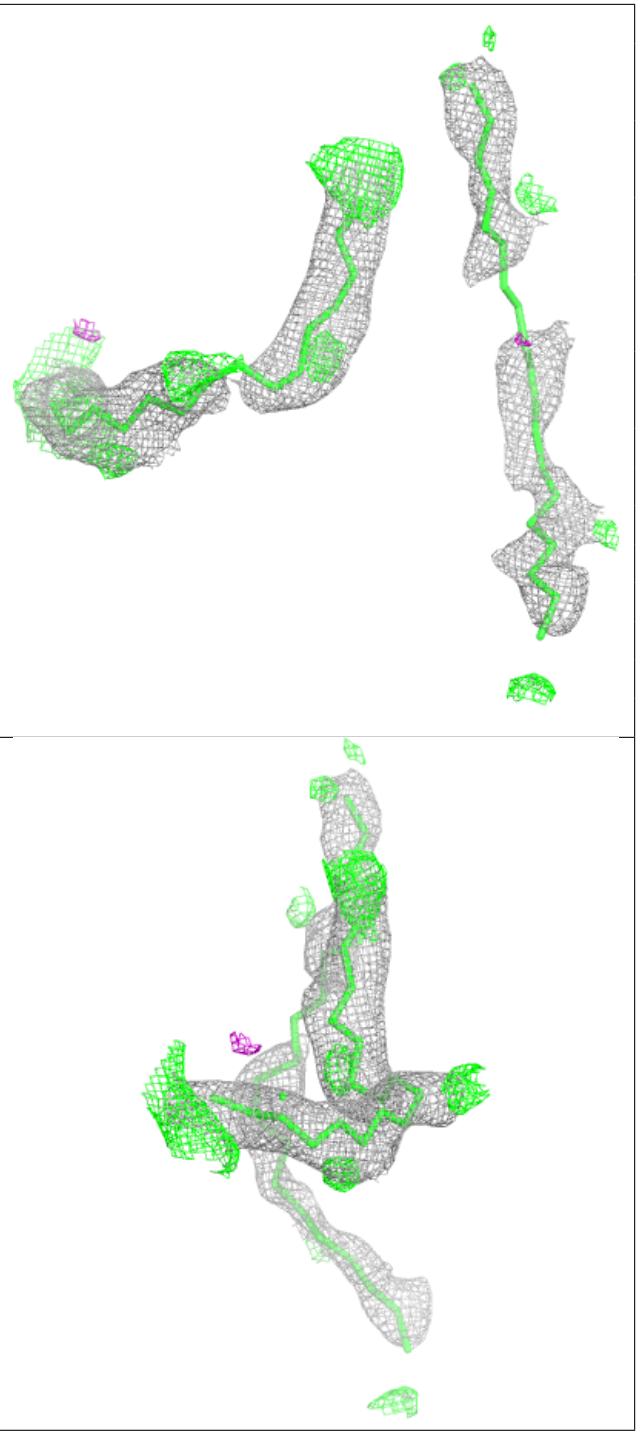
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





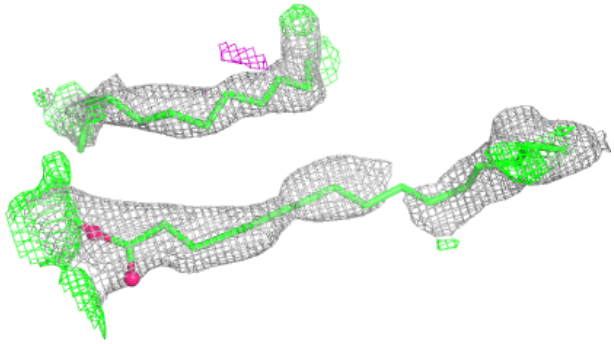
Electron density around PEK C 309:

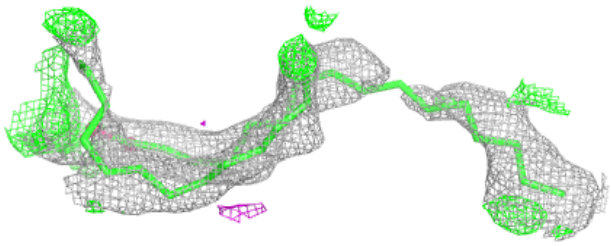
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

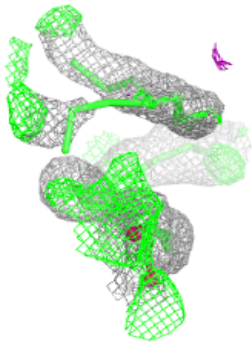


Electron density around PGV G 102:

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

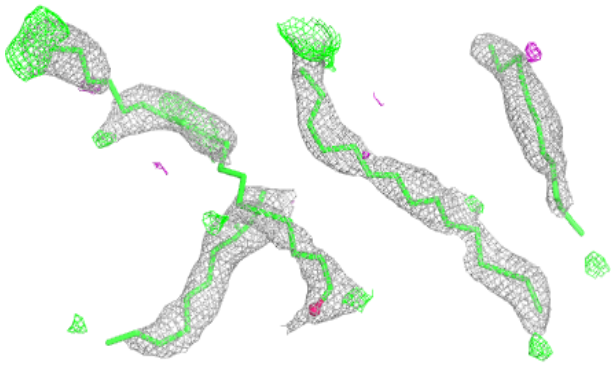


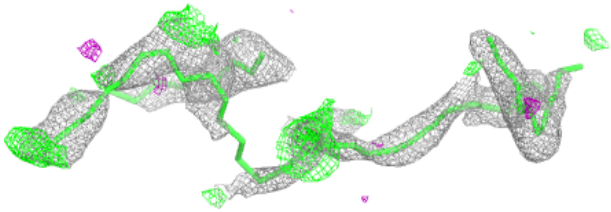


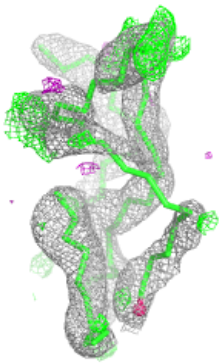


Electron density around CDL N 601:

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

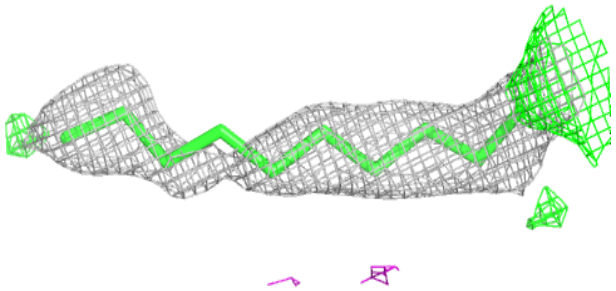


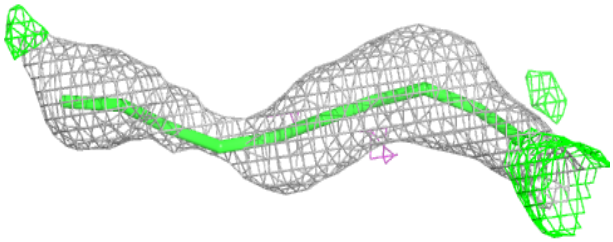


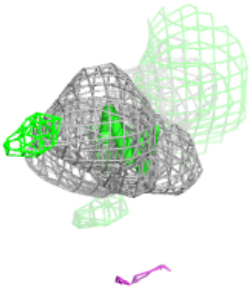


Electron density around DMU Q 201:

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

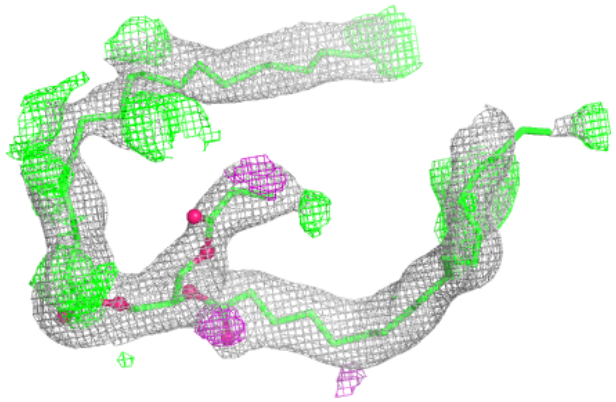


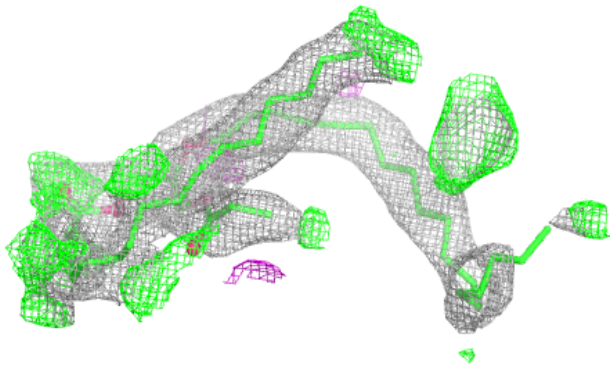


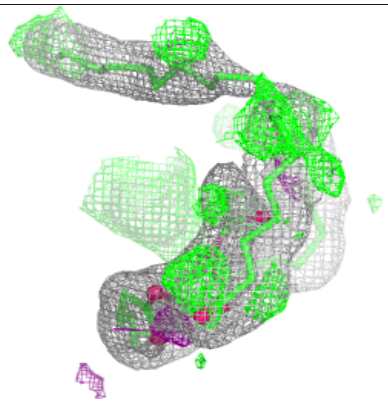


Electron density around TGL B 301:

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

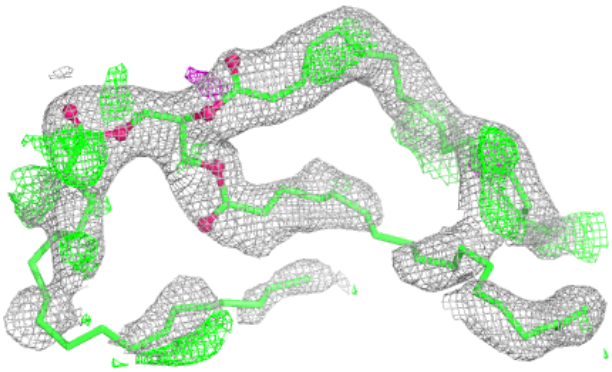


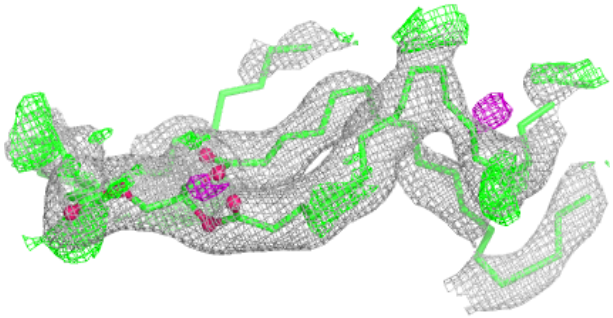


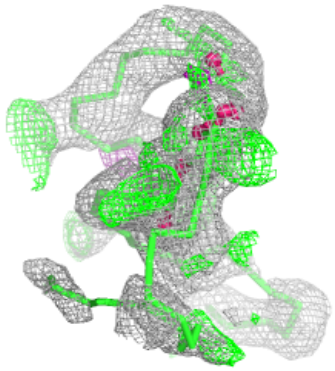


Electron density around TGL N 609:

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

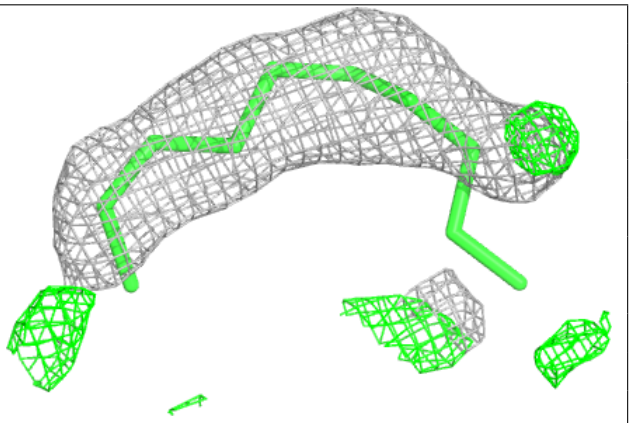


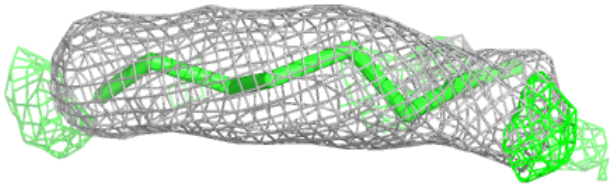


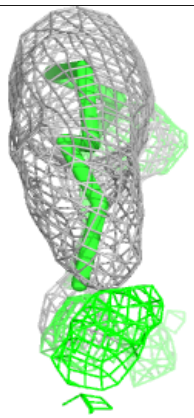


Electron density around DMU K 106:

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

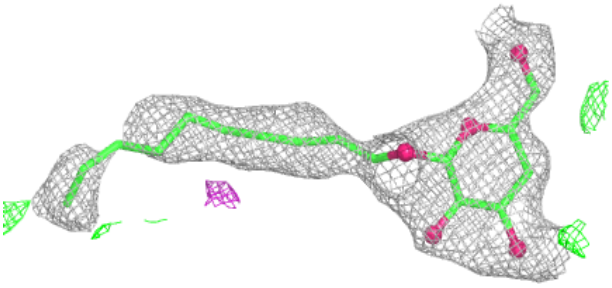


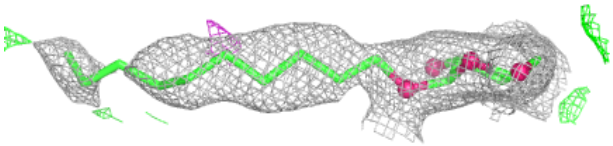


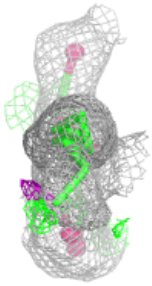


Electron density around DMU L 101:

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

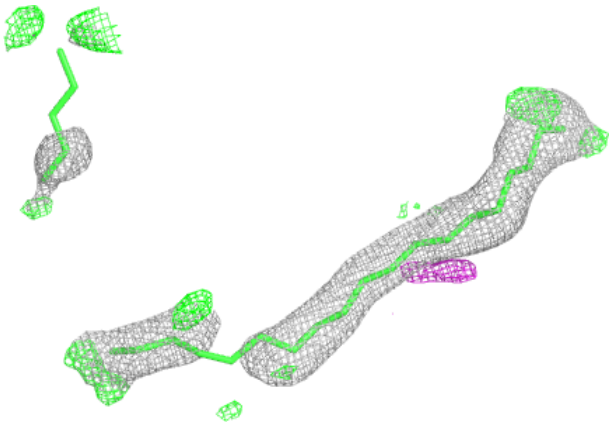


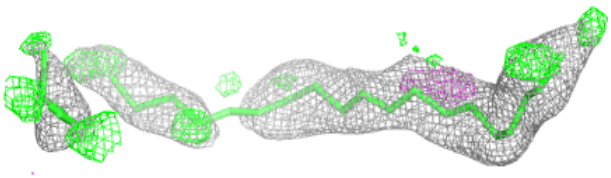


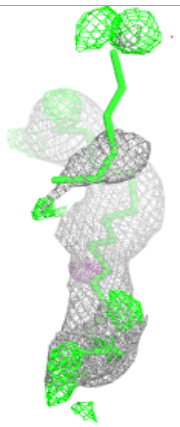


Electron density around PEK C 306:

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

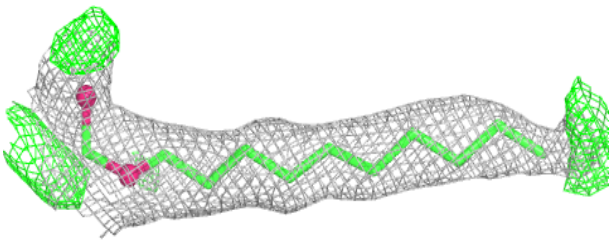


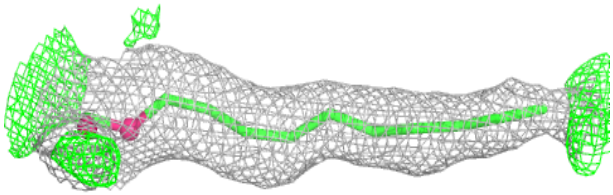


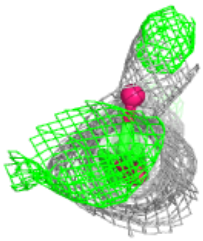


Electron density around DMU C 303:

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

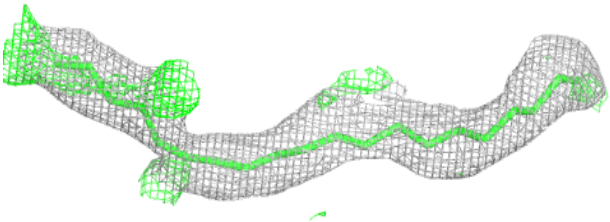


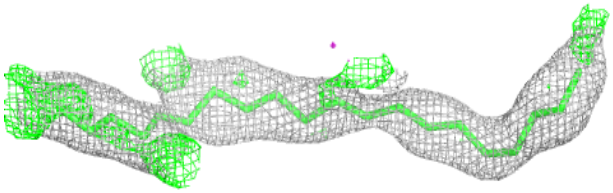


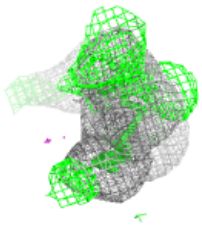


Electron density around PEK P 305:

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

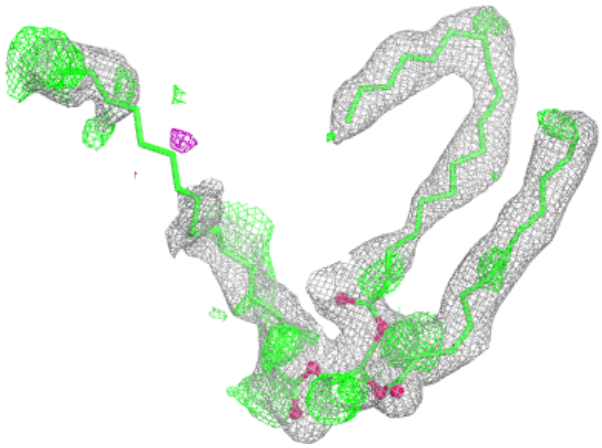


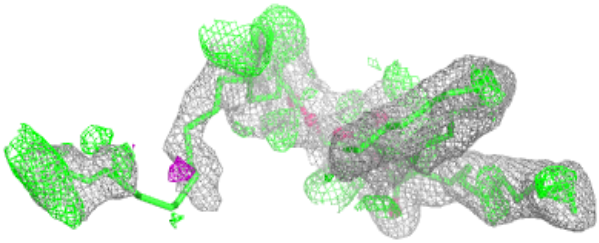




Electron density around TGL D 202:

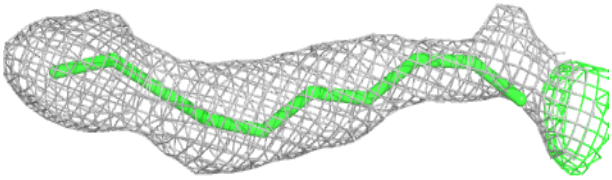
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

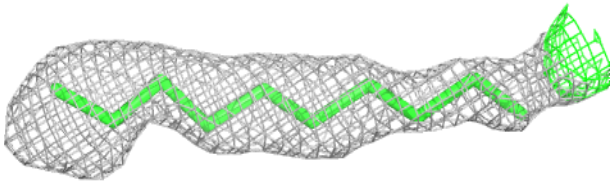


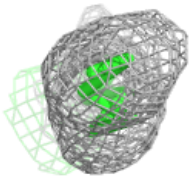


Electron density around DMU K 102:

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

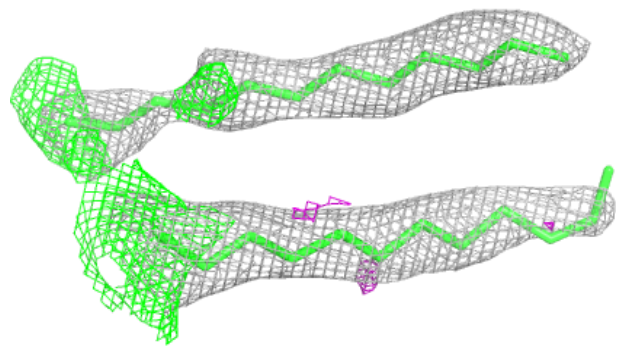


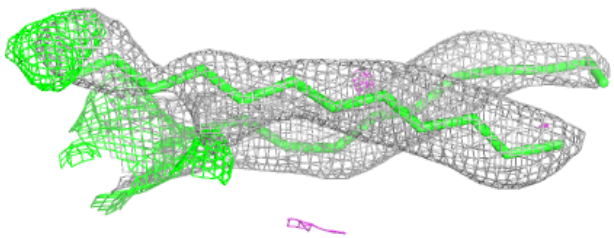


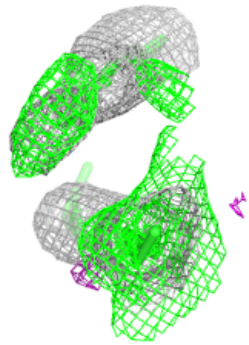


Electron density around PGV N 607:

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

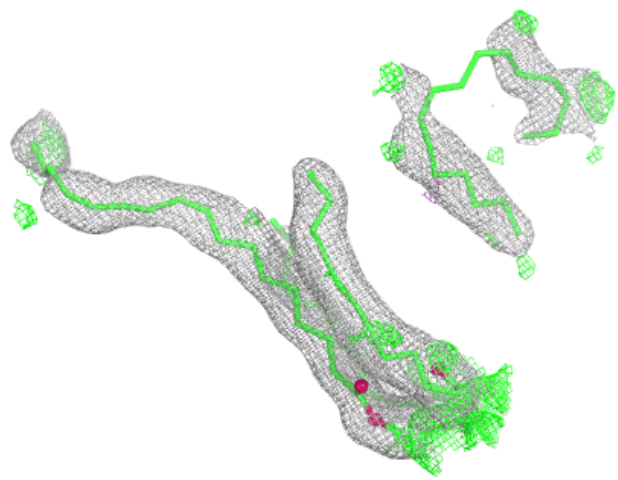


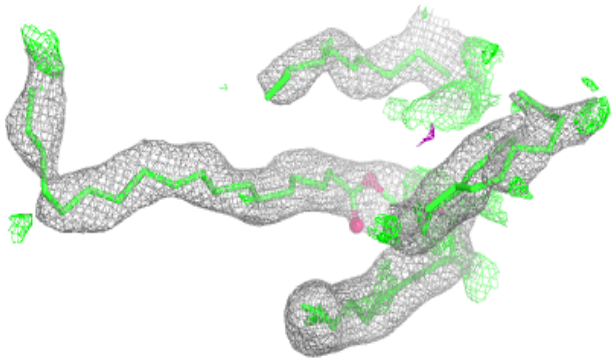


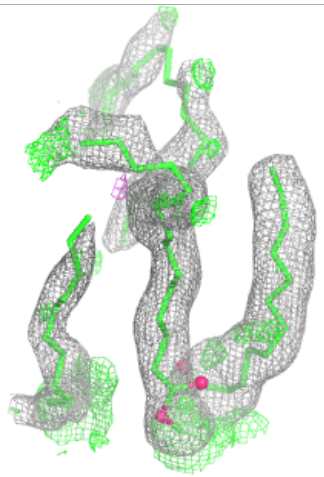


Electron density around CDL P 304:

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

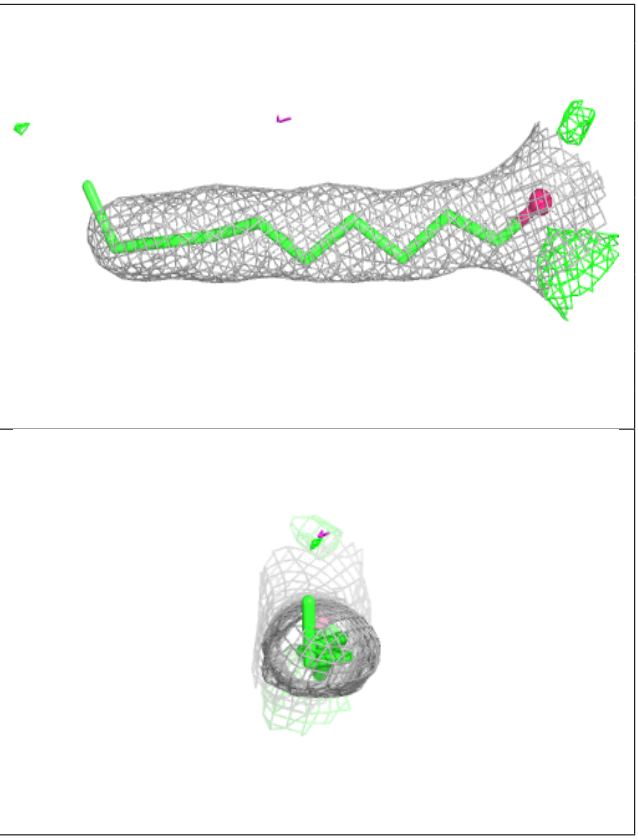






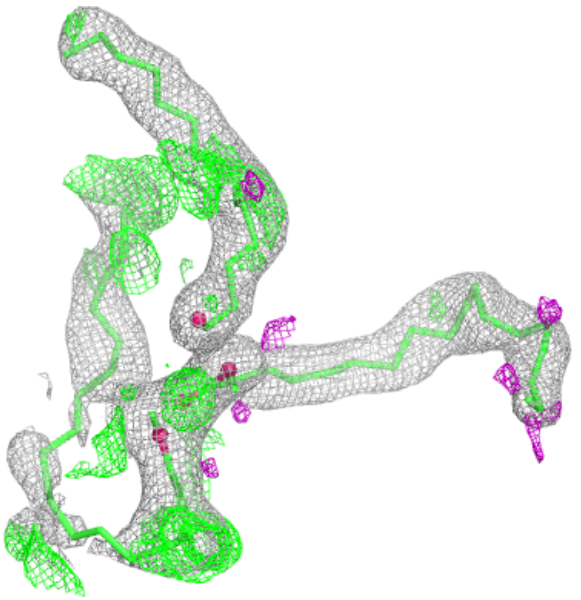
Electron density around DMU O 302:

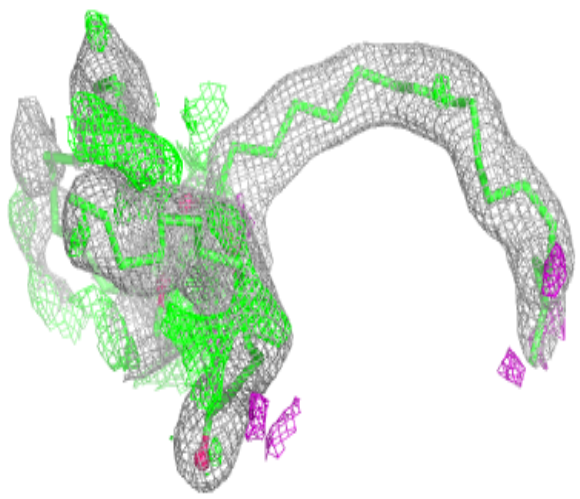
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

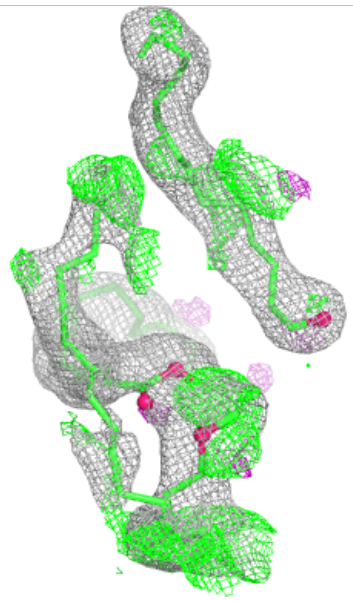


Electron density around TGL L 103:

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

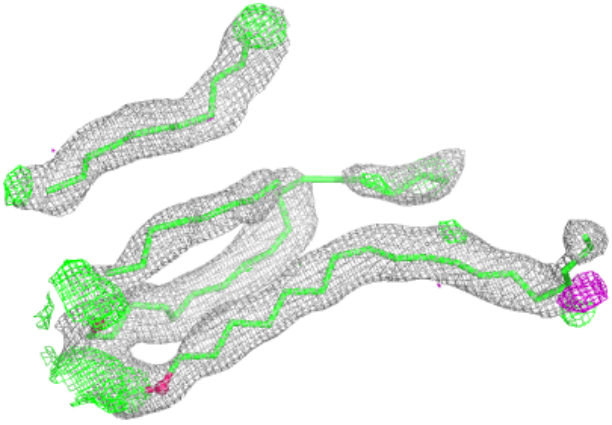


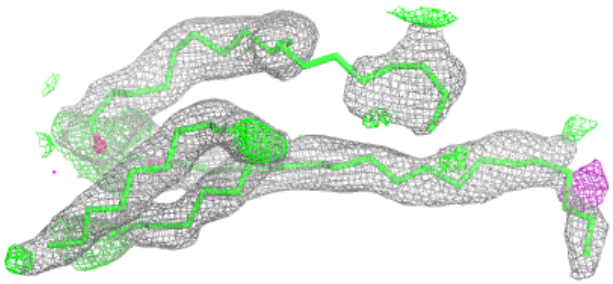


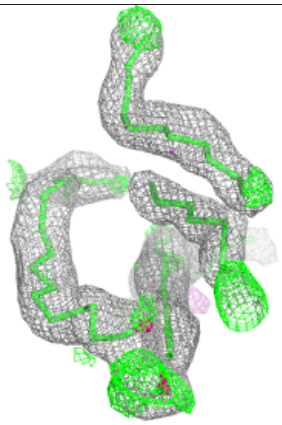


Electron density around CDL C 305:

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

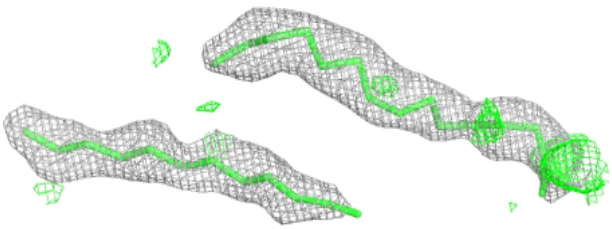


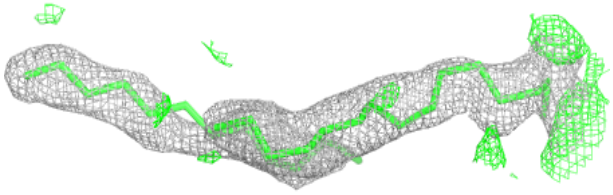


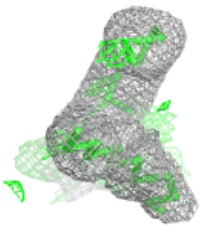


Electron density around PSC A 607:

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

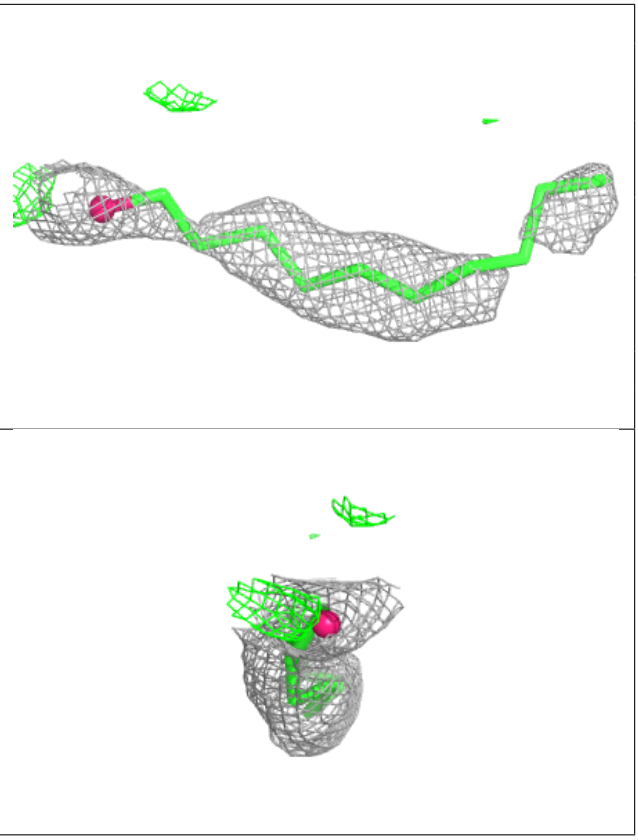






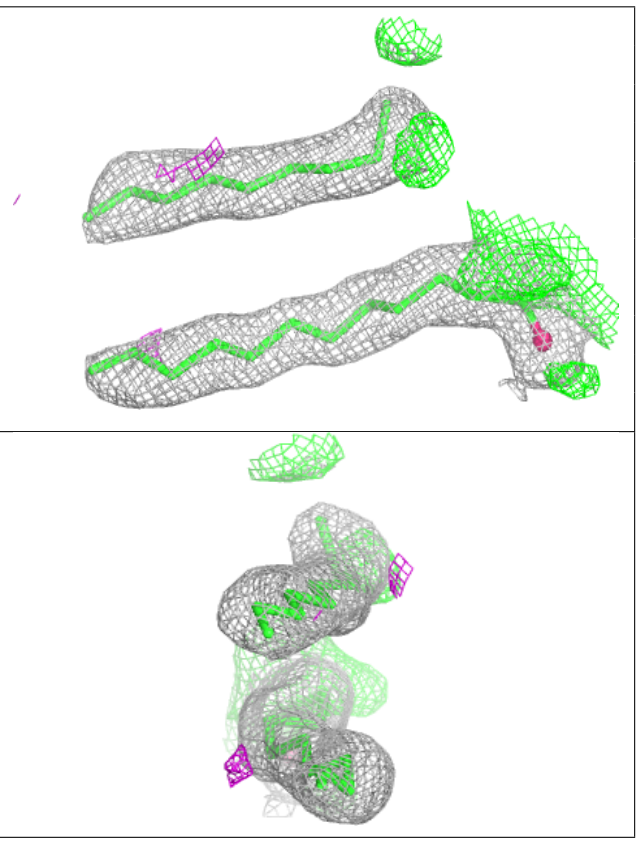
Electron density around DMU K 103:

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



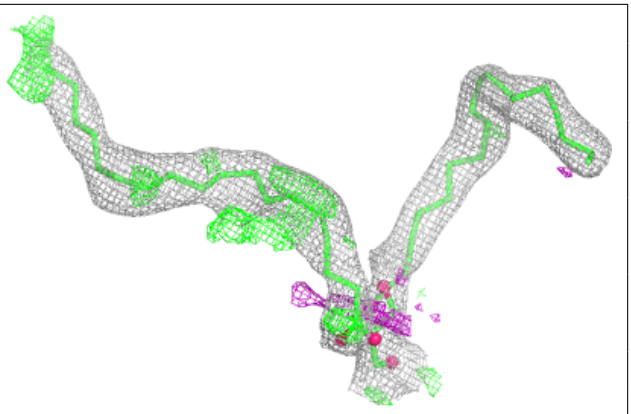
Electron density around PGV A 606:

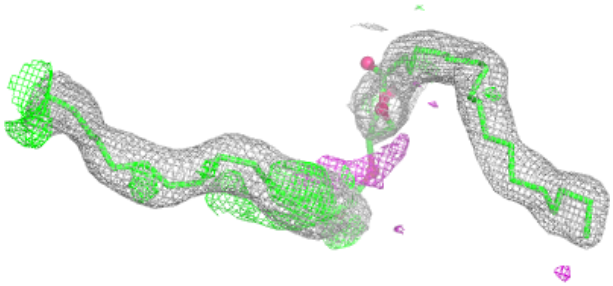
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

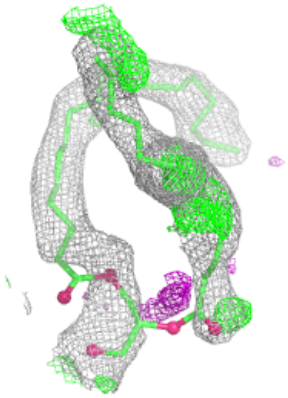


Electron density around TGL N 612:

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

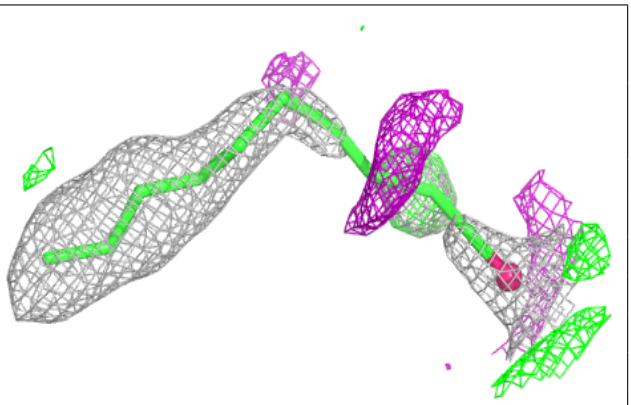


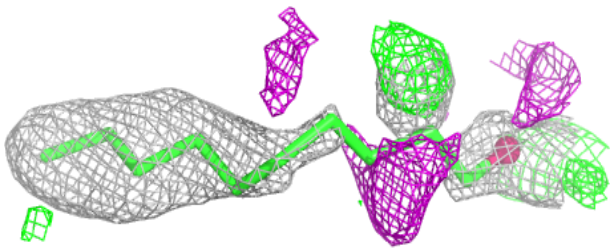


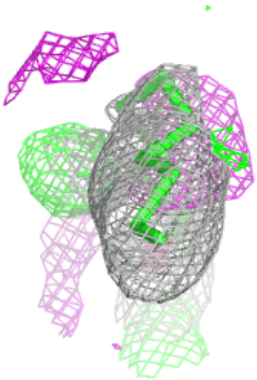


Electron density around DMU P 309:

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

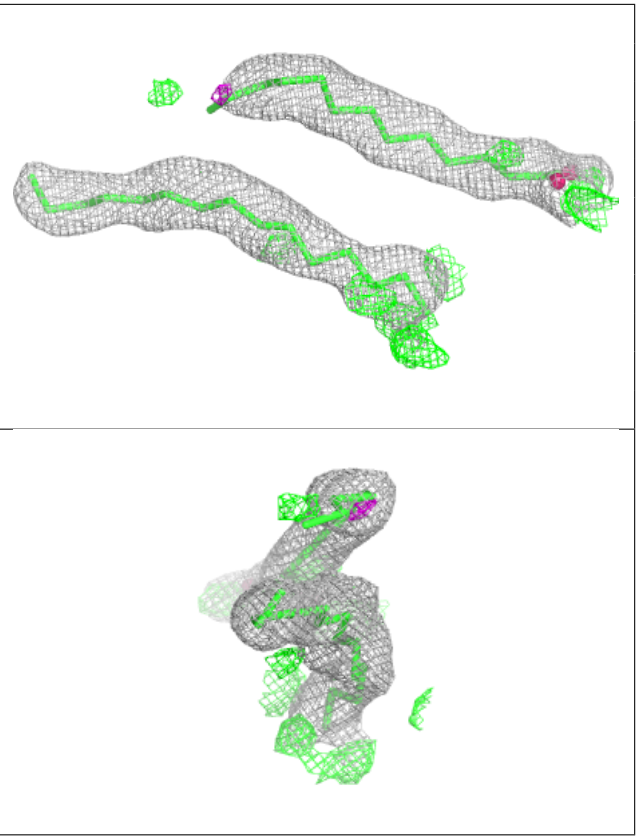






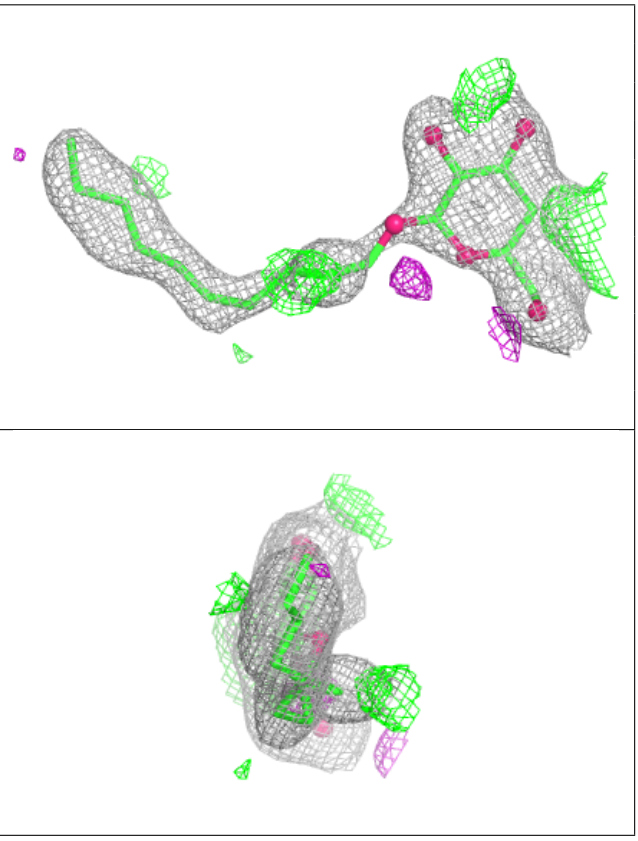
Electron density around PSC O 303:

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



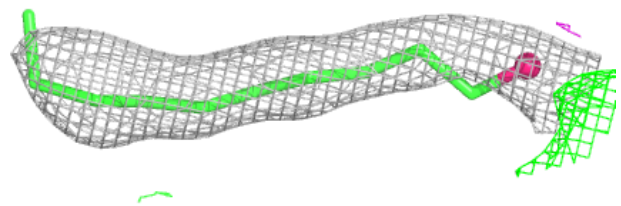
Electron density around DMU C 310:

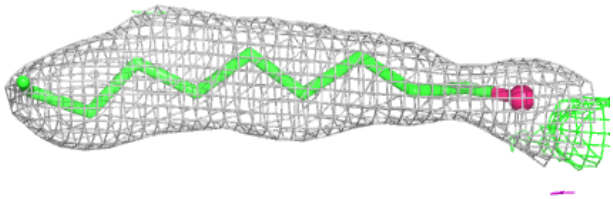
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

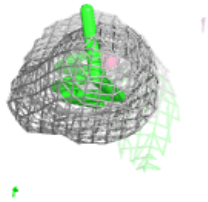


Electron density around DMU W 101:

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

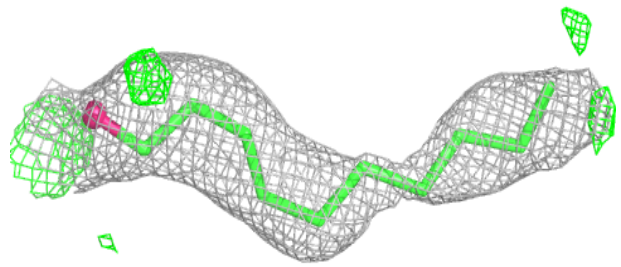


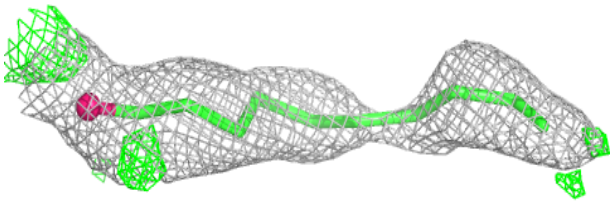


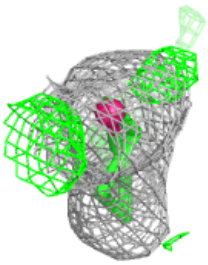


Electron density around DMU D 201:

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

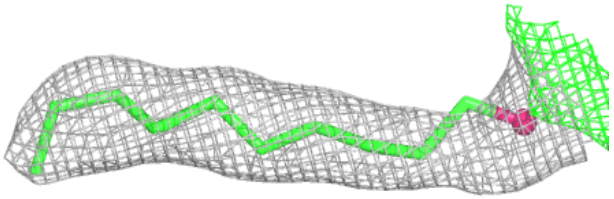


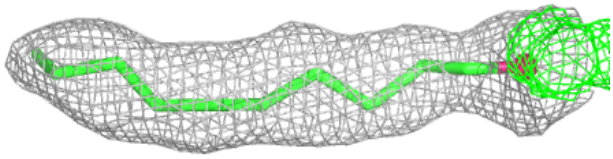


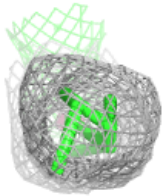


Electron density around DMU J 101:

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

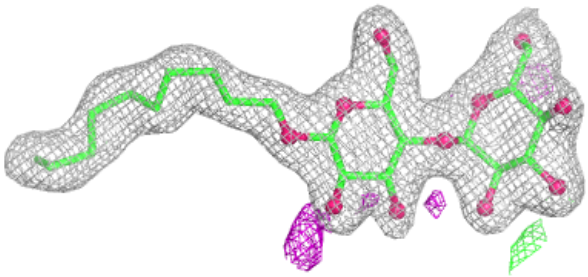


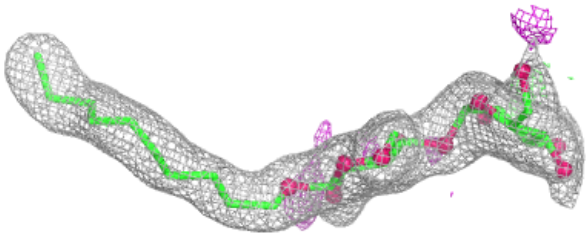


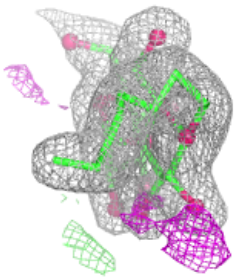


Electron density around DMU Z 101:

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

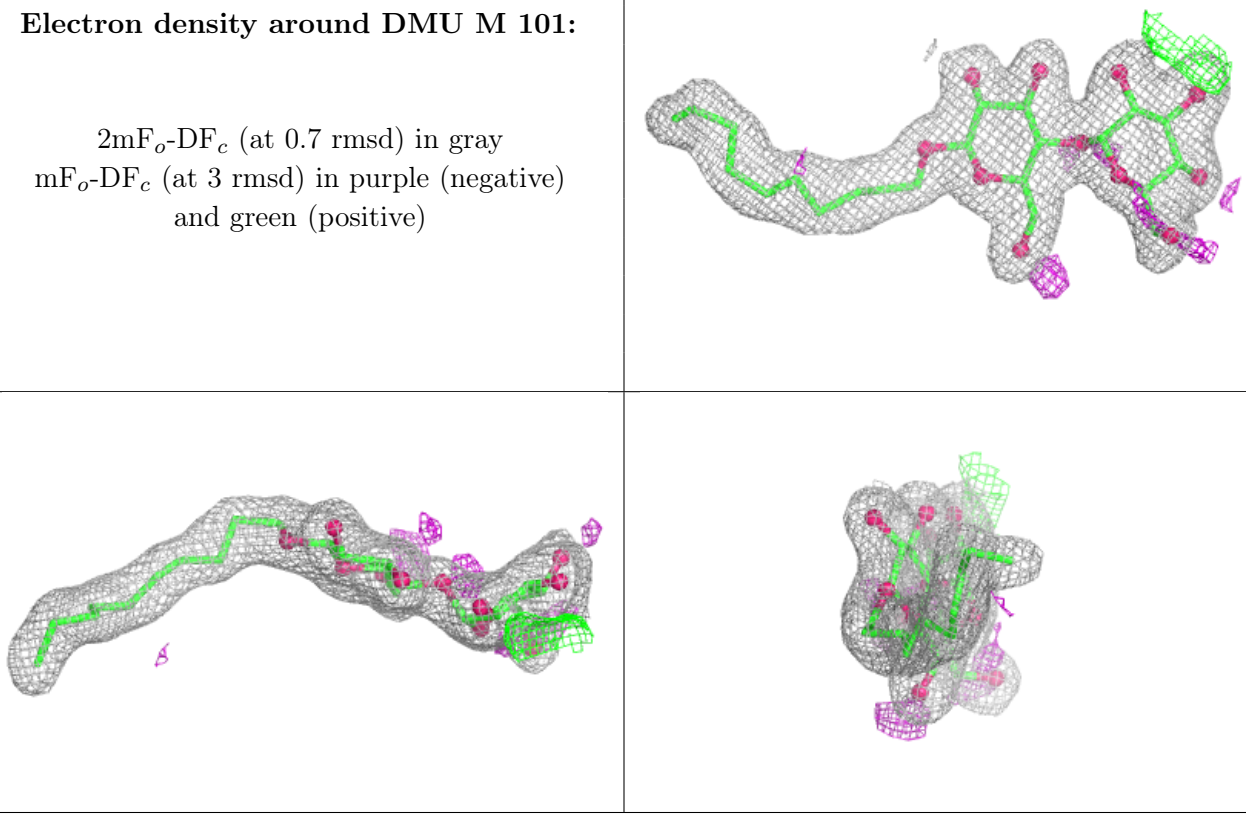






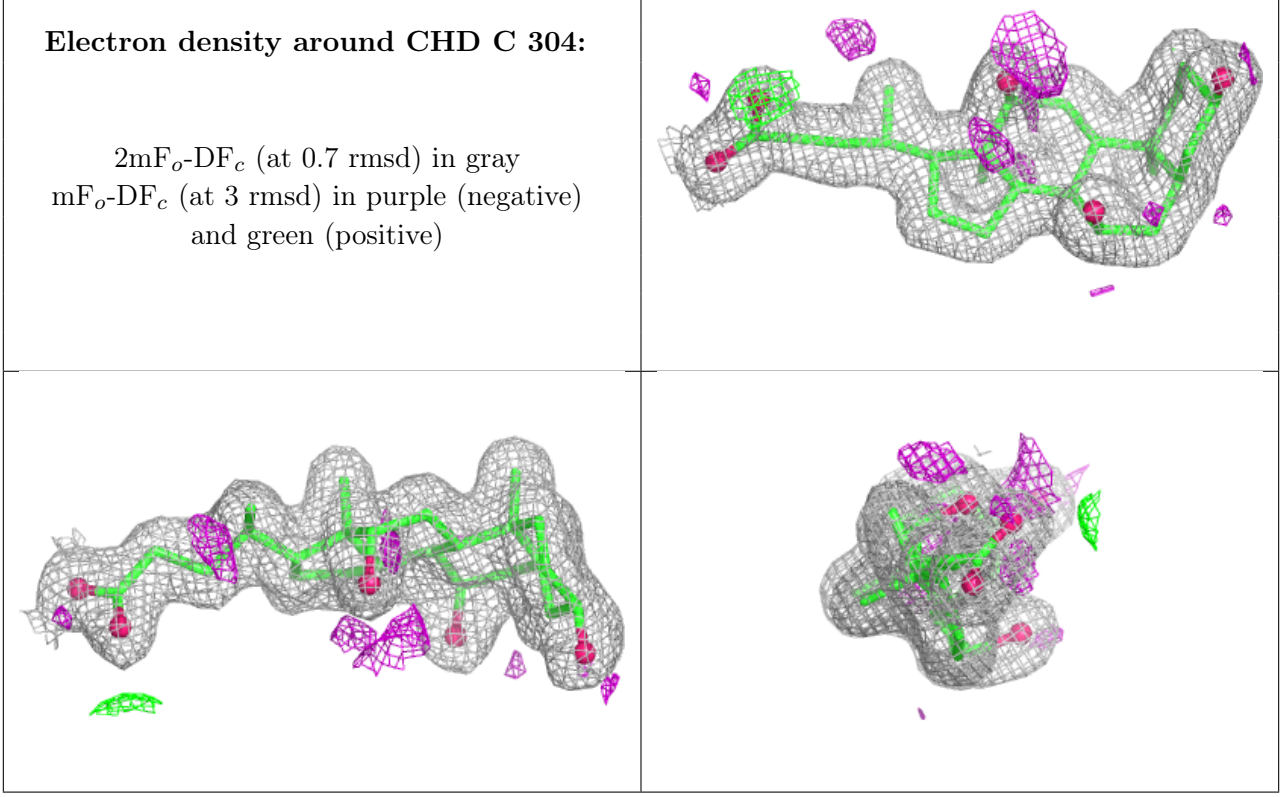
Electron density around DMU M 101:

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



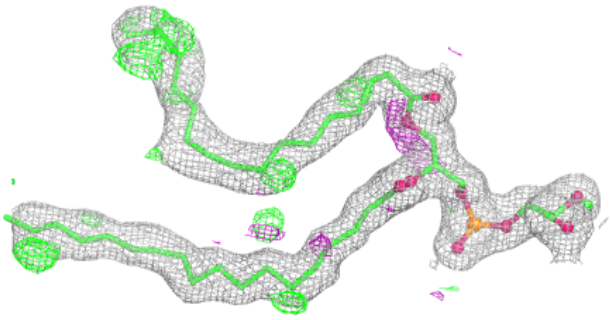
Electron density around CHD C 304:

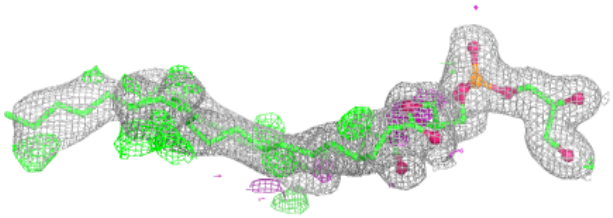
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

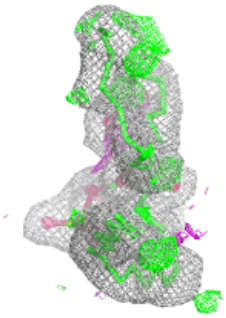


Electron density around PGV N 608:

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

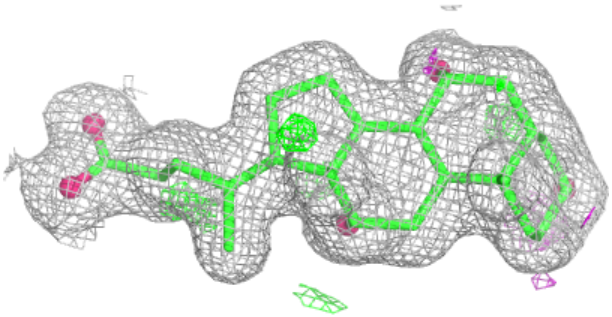


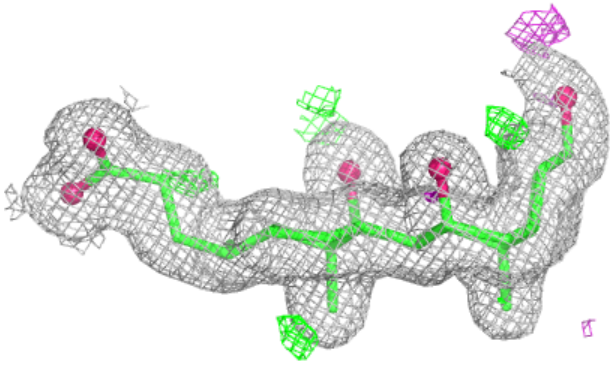


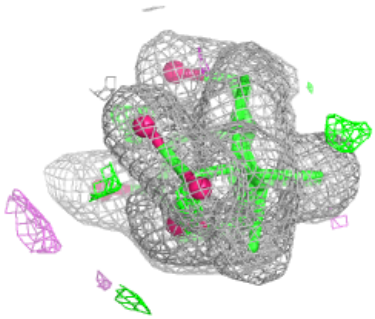


Electron density around CHD B 303:

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

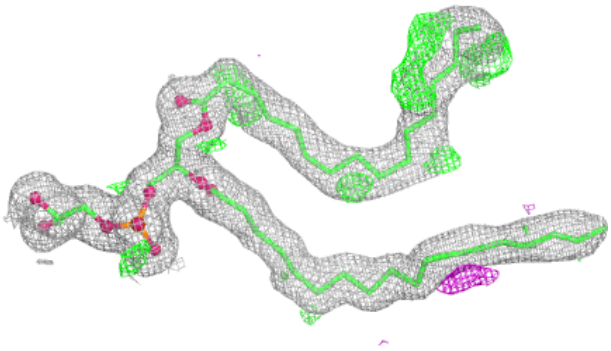


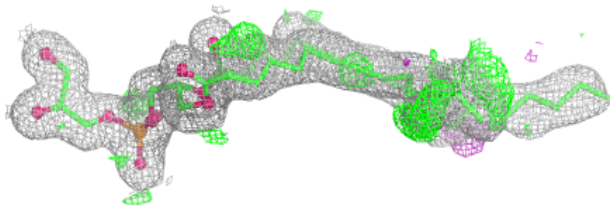


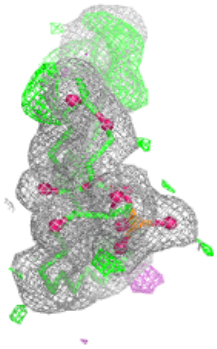


Electron density around PGV C 301:

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

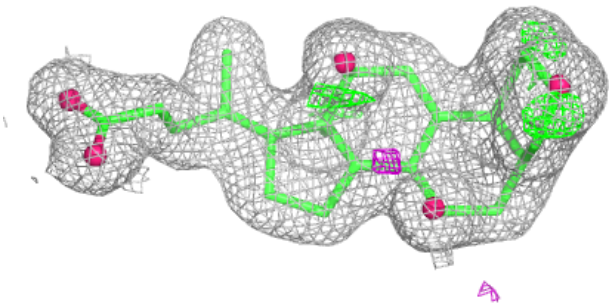


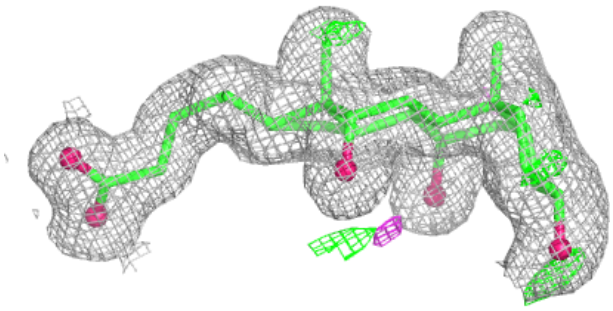


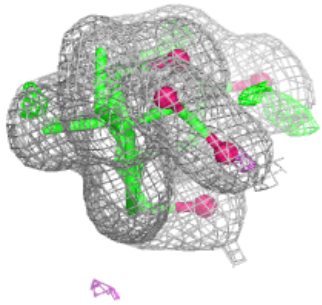


Electron density around CHD G 101:

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

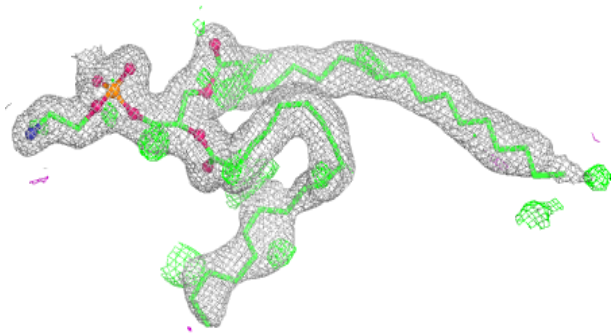


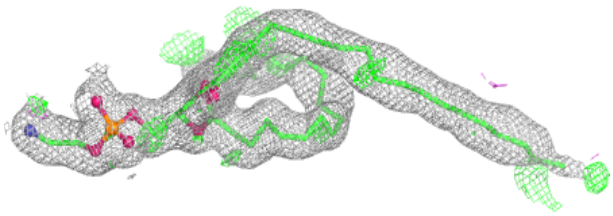


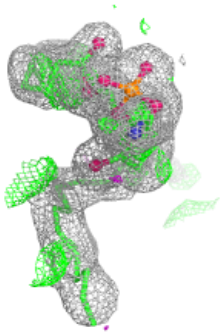


Electron density around PEK C 307:

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

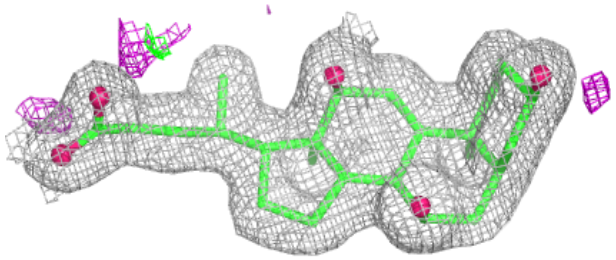


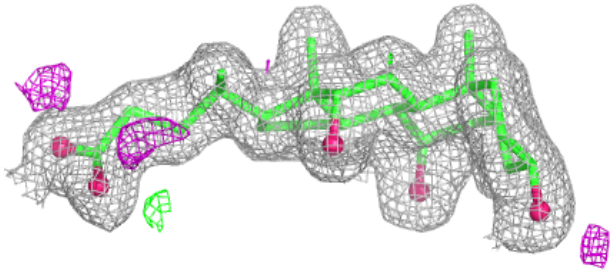


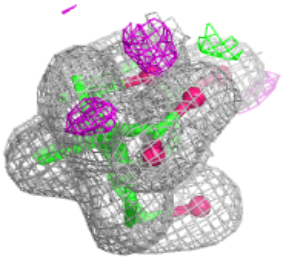


Electron density around CHD P 301:

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

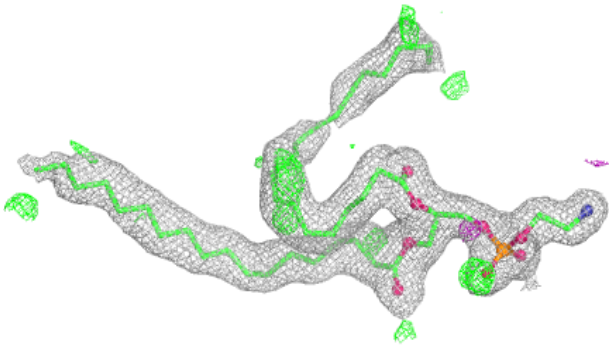


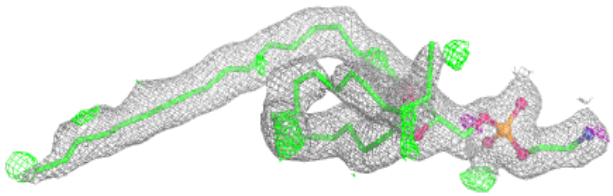


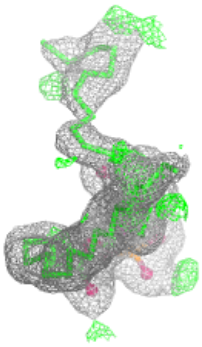


Electron density around PEK P 306:

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

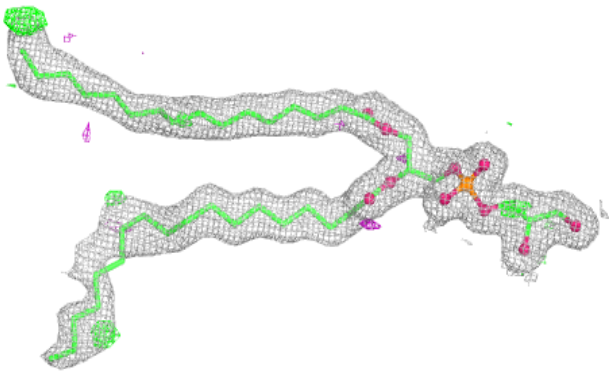


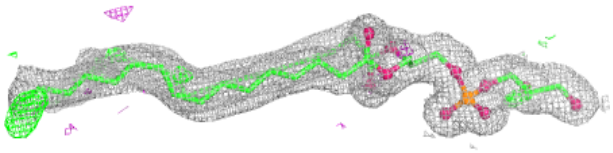


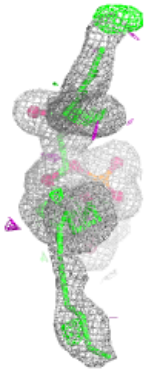


Electron density around PGV P 307:

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

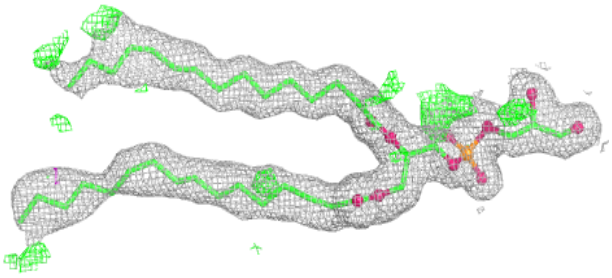


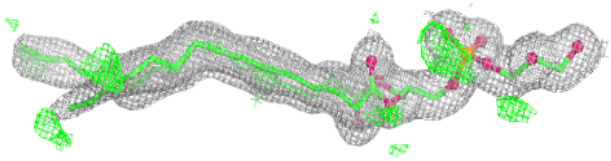


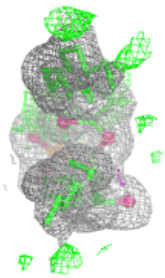


Electron density around PGV C 308:

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

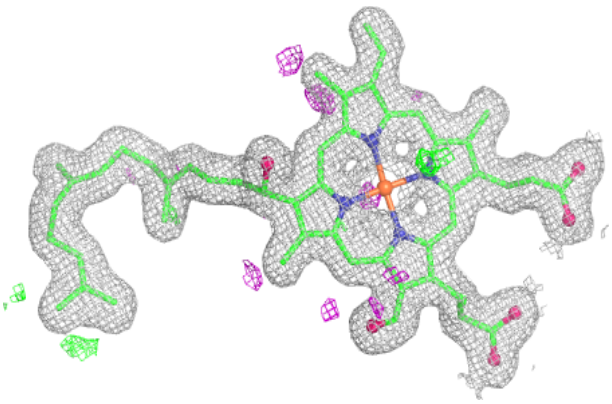


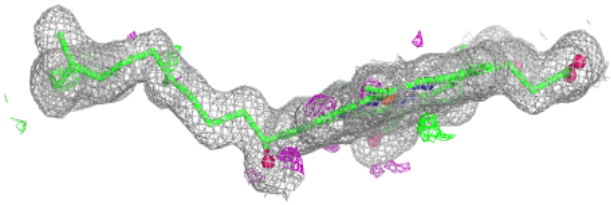


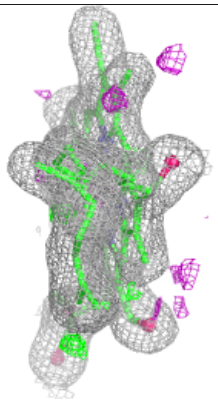


Electron density around HEA A 602:

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

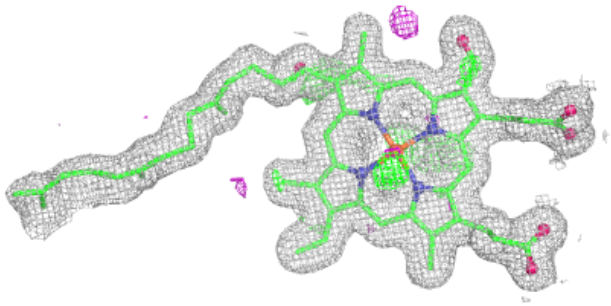


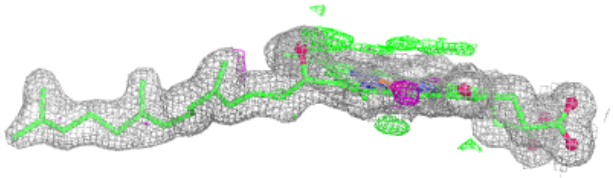


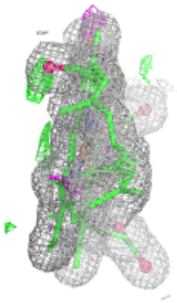


Electron density around HEA A 601 (A):

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

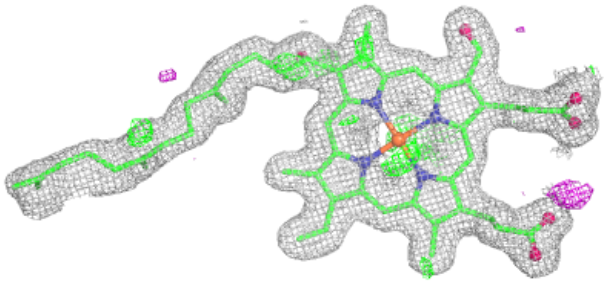


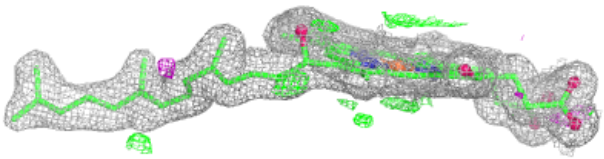


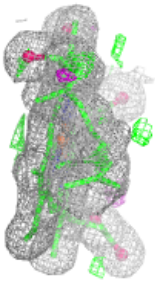


Electron density around HEA N 602 (A):

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

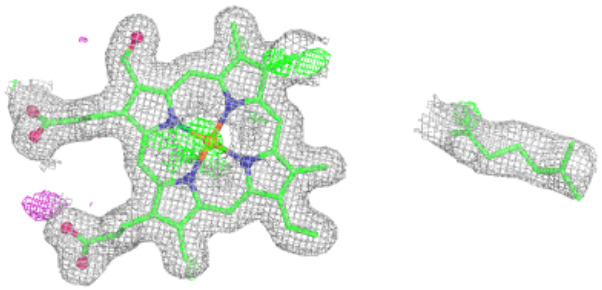


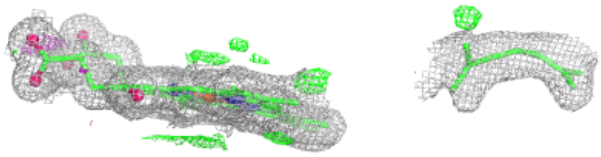


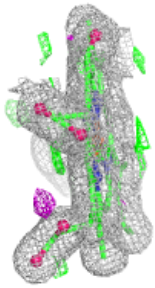


Electron density around HEA N 602 (C):

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

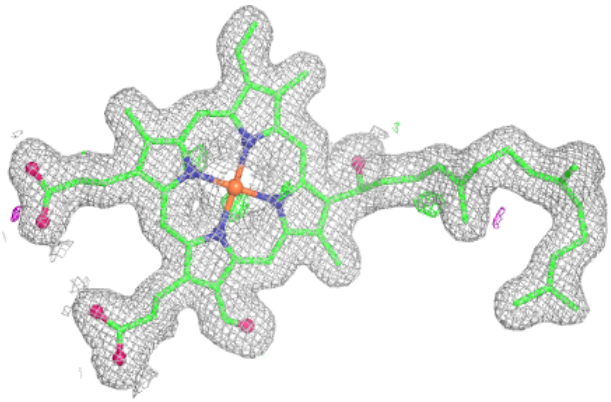


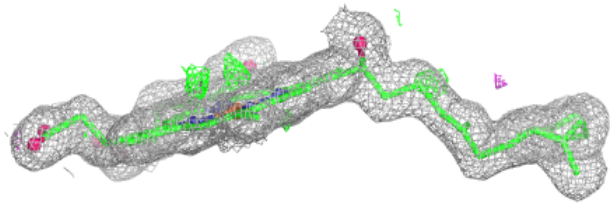


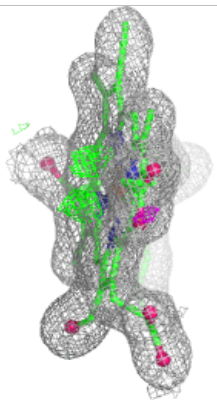


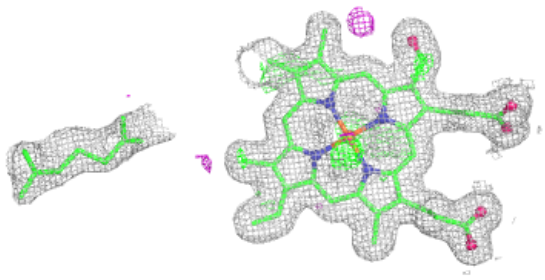
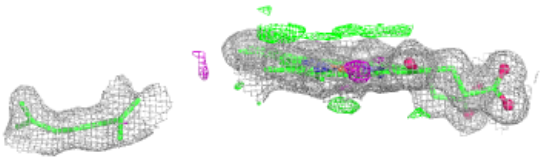
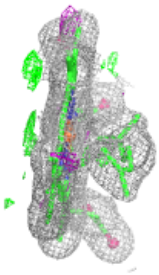
Electron density around HEA N 603:

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

6.5 Other polymers (i)

There are no such residues in this entry.