wwPDB X-ray Structure Validation Summary Report (i)

Aug 7, 2026 – 06:45 AM JST

PDB ID	:	8GVM / pdb_00008gvm
Title	:	The structure of azide-bound cytochrome C oxidase determined using the crystals exposed to 20 mm azide solution for 4 days
Authors	:	Tsukihara, T.; Shimada, A.
Deposited on	:	2022-09-15
Resolution	:	1.85 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:

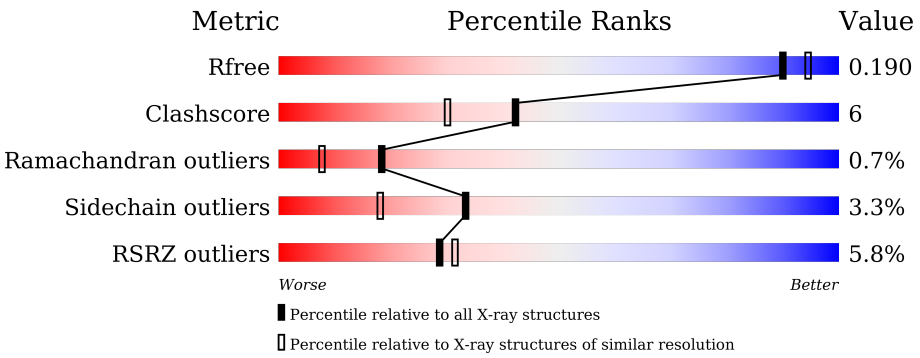
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
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 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	.% 89% 10% •
1	N	514	.% 89% 10% •
2	B	227	6% 86% 13% •
2	O	227	4% 80% 18% •
3	C	261	2% 90% 9% •
3	P	261	2% 89% 10% •

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Mol	Chain	Length	Quality of chain
4	D	147	3% 89% 8%
4	Q	147	8% 87% 10%
5	E	109	4% 86% 9%
5	R	109	3% 90% 6%
6	F	98	8% 81% 16%
6	S	98	11% 88% 9%
7	G	85	24% 79% 11% 6%
7	T	85	22% 81% 13% 5%
8	H	85	14% 79% 9% 5% 7%
8	U	85	14% 80% 8% 5% 7%
9	I	74	16% 82% 18%
9	V	74	16% 81% 18%
10	J	59	12% 90% 7%
10	W	59	14% 88% 8%
11	K	56	5% 80% 7% 12%
11	X	56	11% 82% 5% 12%
12	L	47	4% 77% 21%
12	Y	47	4% 77% 21%
13	M	46	7% 80% 9% 7%
13	Z	46	7% 85% 7% 7%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	AZI	A	607[A]	-	-	X	-
18	AZI	A	607[B]	-	-	X	-
18	AZI	N	608[A]	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	EDO	S	101	-	-	X	-

2 Entry composition (i)

There are 29 unique types of molecules in this entry. The entry contains 33558 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	4125	2753	637	694	41	0	20	0
1	N	514	4122	2753	634	694	41	0	18	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	1996	1304	304	368	20	0	23	0
2	O	227	1975	1289	301	365	20	0	20	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	2152	1437	345	356	14	0	8	0
3	P	259	2173	1449	348	361	15	0	9	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	1198	779	197	218	4	0	2	0
4	Q	144	1213	791	198	220	4	0	2	0

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

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	852	544	144	162	2	0	0	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	98	773	478	138	151	6	0	4	0
6	S	98	763	473	136	148	6	0	2	0

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
7	G	84	675	431	129	113	1	1	0	0	0
7	T	84	681	438	129	112	1	1	0	1	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	662	417	121	119	5	0	0	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	74	601	390	107	100	4	0	0	0
9	V	74	601	390	107	100	4	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	0	ACE	-	acetylation	UNP P04038
V	0	ACE	-	acetylation	UNP P04038

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	J	58	460	297	78	82	3	0	0	0
10	W	58	469	302	79	85	3	0	1	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	384	250	65	67	2	0	0	0
11	X	49	391	255	66	68	2	0	1	0

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

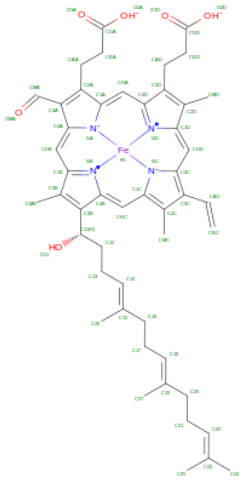
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	L	46	383	256	64	60	3	0	1	0
12	Y	46	383	256	64	60	3	0	1	0

- 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	335	223	53	59	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	60	49	1	4	6	0	0
			Total	C	Fe	N	O		
14	A	1	120	98	2	8	12	0	1
			Total	C	Fe	N	O		
14	N	1	60	49	1	4	6	0	0
			Total	C	Fe	N	O		
14	N	1	120	98	2	8	12	0	1

- 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

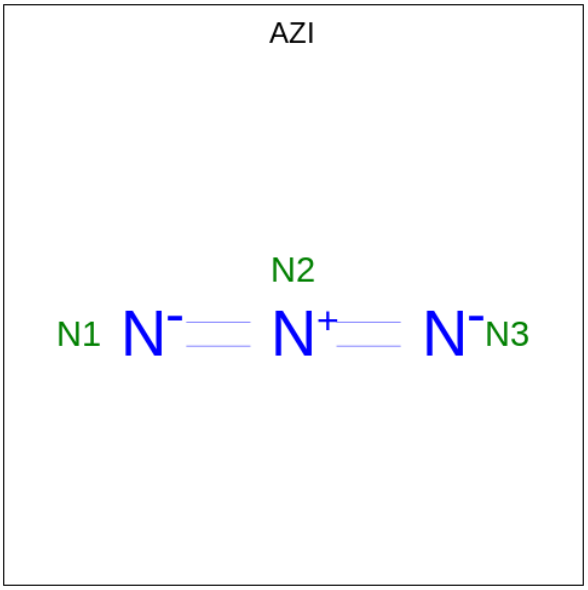
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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).

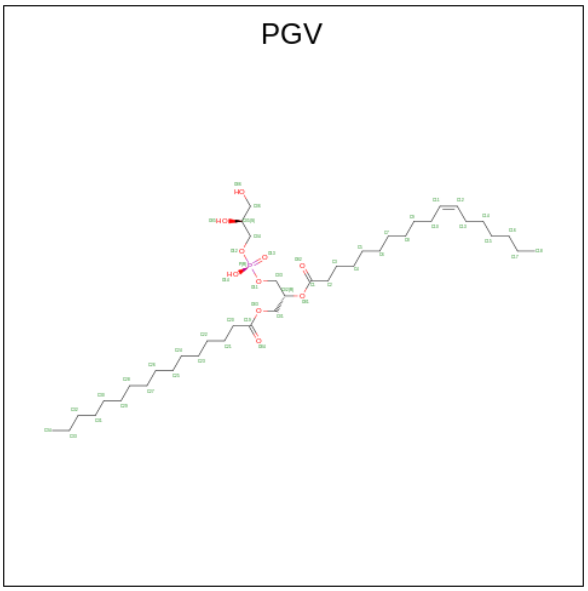
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
17	A	1	1	1	0	0
			Total	Na		
17	C	1	1	1	0	0
			Total	Na		
17	N	1	1	1	0	0
			Total	Na		
17	P	1	1	1	0	0

- Molecule 18 is AZIDE ION (CCD ID: AZI) (formula: N_3).



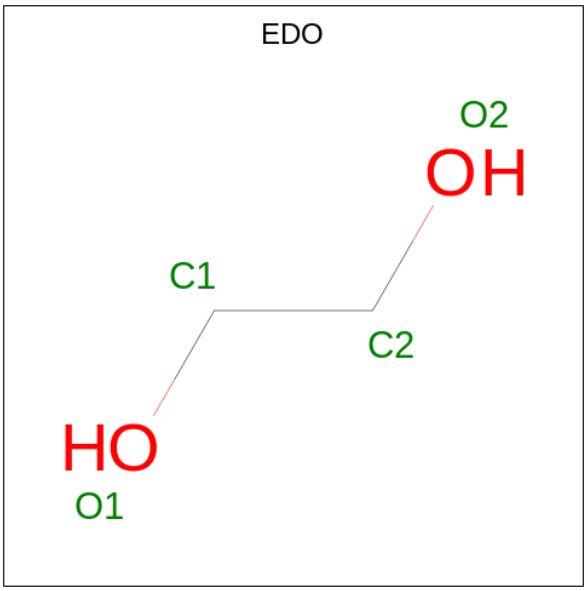
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	N		
18	A	1	3	3	0	1
			Total	N		
18	A	1	6	6	0	1
			Total	N		
18	N	1	3	3	0	1
			Total	N		
18	N	1	6	6	0	1

- Molecule 19 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
			Total	C	O	P		
19	A	1	51	40	10	1	0	0
			Total	C	O	P		
19	A	1	51	40	10	1	0	0
			Total	C	O	P		
19	C	1	51	40	10	1	0	0
			Total	C	O	P		
19	C	1	49	39	9	1	0	0
			Total	C	O	P		
19	G	1	51	40	10	1	0	0
			Total	C	O	P		
19	N	1	51	40	10	1	0	0
			Total	C	O	P		
19	N	1	51	40	10	1	0	0
			Total	C	O	P		
19	P	1	51	40	10	1	0	0

- Molecule 20 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
20	G	1	4	2	2	0	0
20	H	1	4	2	2	0	0
20	H	1	4	2	2	0	0
20	L	1	4	2	2	0	0
20	N	1	4	2	2	0	0
20	N	1	4	2	2	0	0
20	N	1	4	2	2	0	0
20	N	1	4	2	2	0	0
20	N	1	4	2	2	0	0
20	N	1	4	2	2	0	0
20	N	1	4	2	2	0	0
20	N	1	4	2	2	0	0
20	O	1	4	2	2	0	0
20	O	1	4	2	2	0	0
20	O	1	4	2	2	0	0
20	P	1	4	2	2	0	0
20	P	1	4	2	2	0	0
20	P	1	4	2	2	0	0
20	Q	1	4	2	2	0	0
20	Q	1	4	2	2	0	0
20	R	1	4	2	2	0	0

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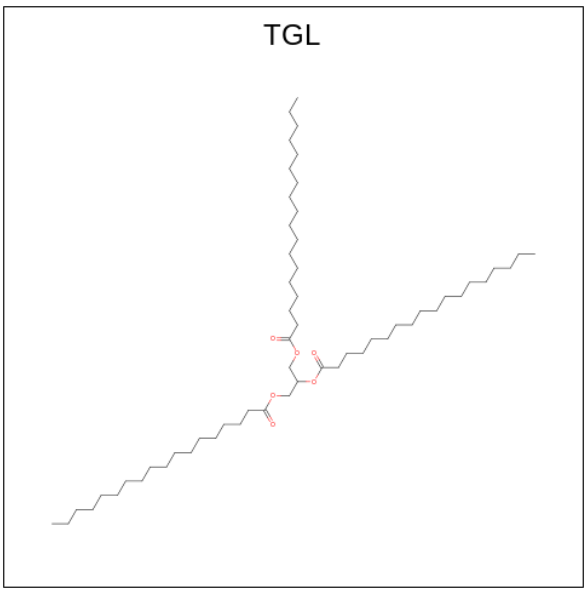
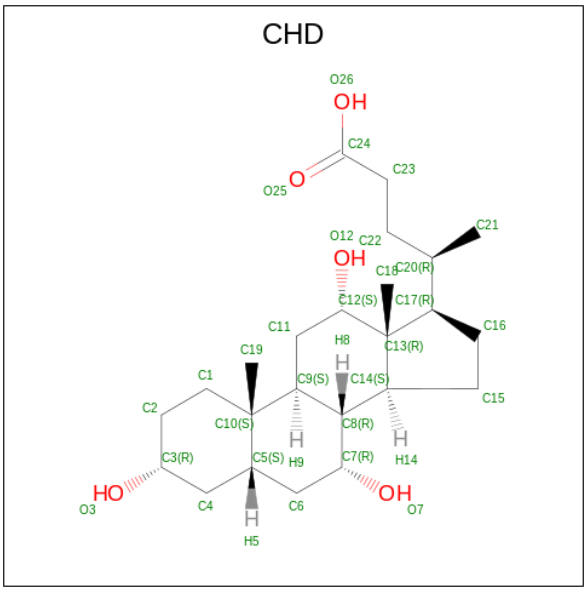
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
20	R	1	4	2	2	0	0
			Total	C	O		
20	R	1	4	2	2	0	0
			Total	C	O		
20	R	1	4	2	2	0	0
			Total	C	O		
20	R	1	4	2	2	0	0
			Total	C	O		
20	R	1	4	2	2	0	0
			Total	C	O		
20	S	1	4	2	2	0	0
			Total	C	O		
20	S	1	4	2	2	0	0
			Total	C	O		
20	S	1	4	2	2	0	0
			Total	C	O		
20	T	1	4	2	2	0	0
			Total	C	O		
20	U	1	4	2	2	0	0
			Total	C	O		
20	V	1	4	2	2	0	0

- Molecule 21 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: $C_{57}H_{110}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
21	B	1	63	57	6	0	0
21	D	1	63	57	6	0	0
21	L	1	63	57	6	0	0
21	N	1	61	55	6	0	0
21	Q	1	63	57	6	0	0
21	Y	1	63	57	6	0	0

- Molecule 22 is CHOLIC ACID (CCD ID: CHD) (formula: $C_{24}H_{40}O_5$).



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

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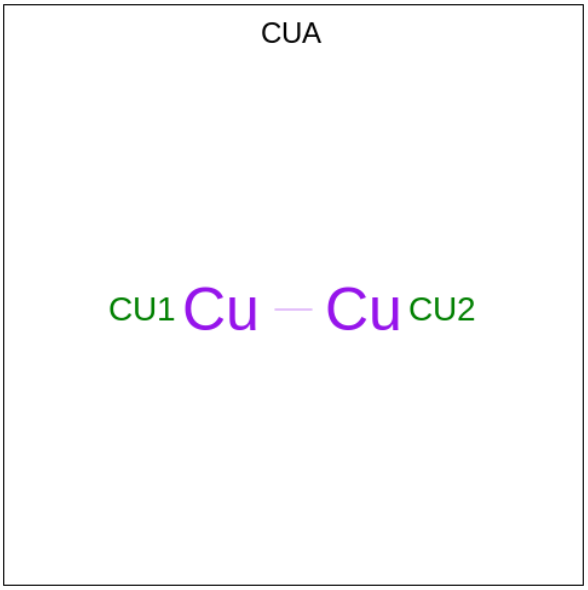
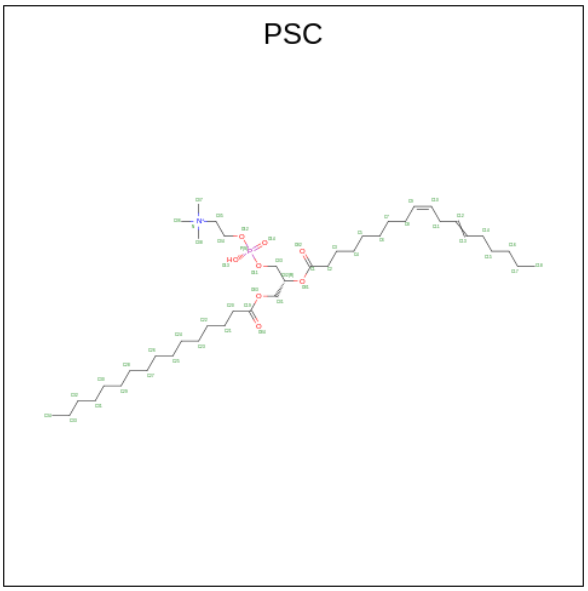
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
22	P	1	29	24	5	0	0
			Total	C	O		
22	W	1	29	24	5	0	0

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



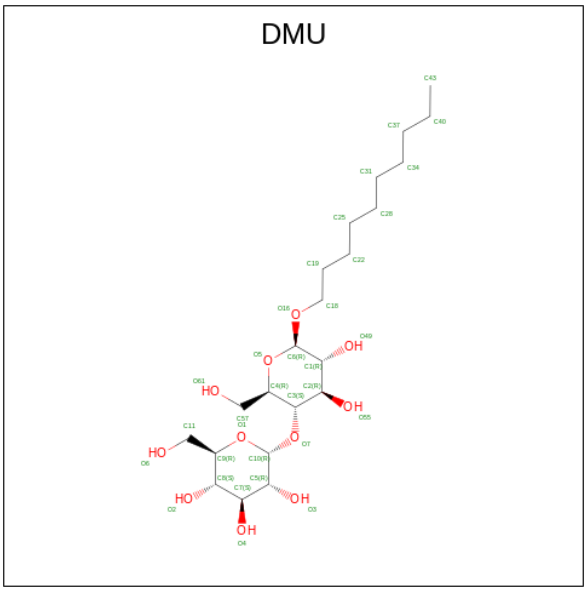
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cu		
23	B	1	2	2	0	0
			Total	Cu		
23	O	1	2	2	0	0

- Molecule 24 is (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	N	O	P		
24	B	1	50	40	1	8	1	0	0
			Total	C	N	O	P		
24	O	1	51	41	1	8	1	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
			Total	C	O		
25	C	1	33	22	11	0	0

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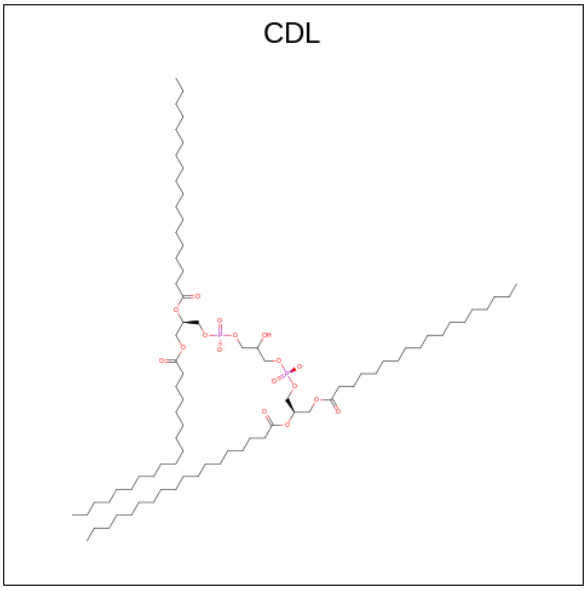
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
25	C	1	33	22	11		0	0
			Total	C	O			
25	C	1	22	16	6		0	0
			Total	C	O			
25	L	1	30	19	11		0	0
			Total	C	O			
25	M	1	33	22	11		0	0
			Total	C	O			
25	P	1	33	22	11		0	0
			Total	C	O			
25	P	1	33	22	11		0	0
			Total	C	O			
25	P	1	33	22	11		0	0
			Total	C	O			
25	Z	1	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
			Total	C	O	P		
26	C	1	89	71	16	2	0	0
			Total	C	O	P		
26	N	1	96	77	17	2	0	0
			Total	C	O	P		
26	P	1	80	62	16	2	0	0

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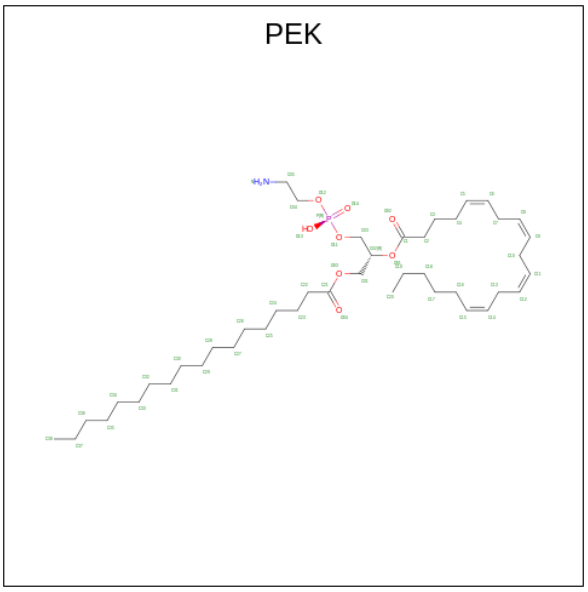
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
26	T	1	97	78	17	2	0	0

- 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	N	O	P		
27	C	1	53	43	1	8	1	0	0
			Total	C	N	O	P		
27	C	1	44	34	1	8	1	0	0
			Total	C	N	O	P		
27	G	1	53	43	1	8	1	0	0
			Total	C	O	P			
27	G	1	44	35	8	1		0	0
			Total	C	N	O	P		
27	P	1	53	43	1	8	1	0	0
			Total	C	O	P			
27	T	1	50	41	8	1		0	0

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

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

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

- Molecule 29 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
29	A	222	222	222	0	1
			Total	O		
29	B	133	134	134	0	2
			Total	O		
29	C	99	99	99	0	0
			Total	O		
29	D	108	108	108	0	0
			Total	O		
29	E	82	82	82	0	0
			Total	O		
29	F	79	79	79	0	0
			Total	O		
29	G	52	52	52	0	0
			Total	O		
29	H	44	44	44	0	0
			Total	O		
29	I	27	27	27	0	0
			Total	O		
29	J	27	27	27	0	0
			Total	O		
29	K	20	20	20	0	0
			Total	O		
29	L	26	26	26	0	0
			Total	O		
29	M	24	24	24	0	0
			Total	O		
29	N	209	209	209	0	1
			Total	O		
29	O	111	112	112	0	1
			Total	O		
29	P	90	90	90	0	0
			Total	O		
29	Q	38	38	38	0	0
			Total	O		
29	R	39	39	39	0	0

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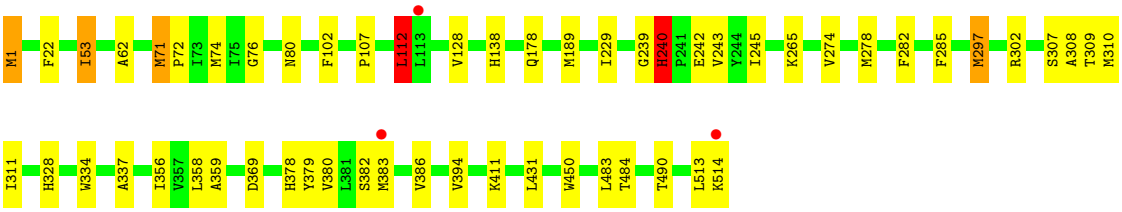
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
29	S	59	59	59	0	0
			Total	O		
29	T	35	35	35	0	0
			Total	O		
29	U	33	33	33	0	0
			Total	O		
29	V	14	14	14	0	0
			Total	O		
29	W	12	12	12	0	0
			Total	O		
29	X	11	11	11	0	0
			Total	O		
29	Y	13	13	13	0	0
			Total	O		
29	Z	16	16	16	0	0

3 Residue-property plots (i)

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

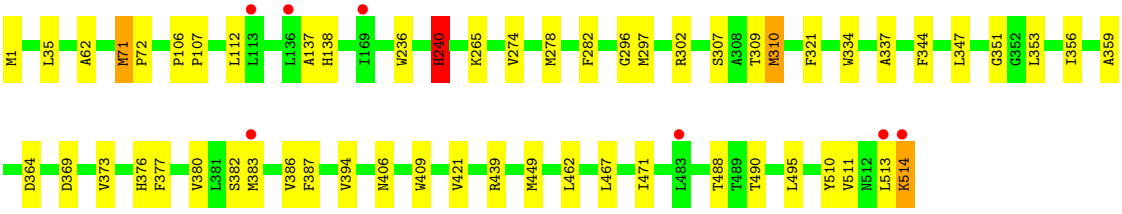
• Molecule 1: Cytochrome c oxidase subunit 1

Chain A:



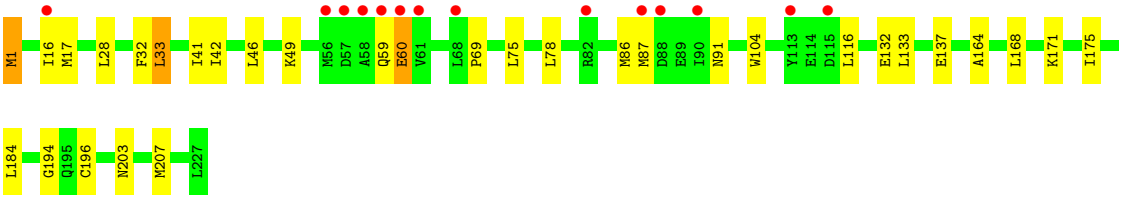
• Molecule 1: Cytochrome c oxidase subunit 1

Chain N:



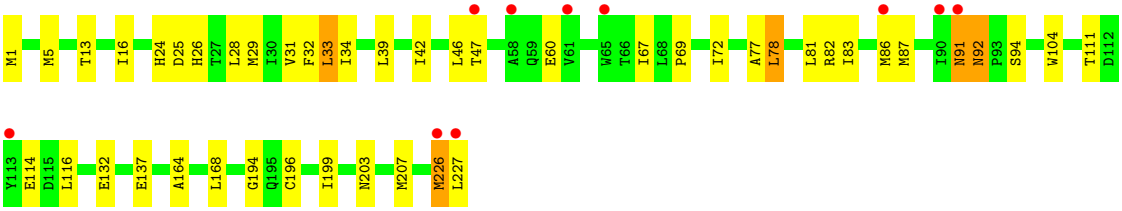
• Molecule 2: Cytochrome c oxidase subunit 2

Chain B:



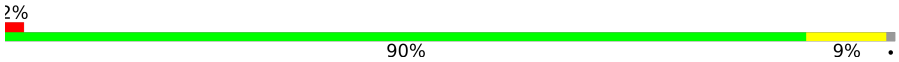
• Molecule 2: Cytochrome c oxidase subunit 2

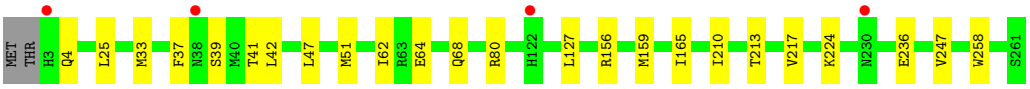
Chain O:



• Molecule 3: Cytochrome c oxidase subunit 3

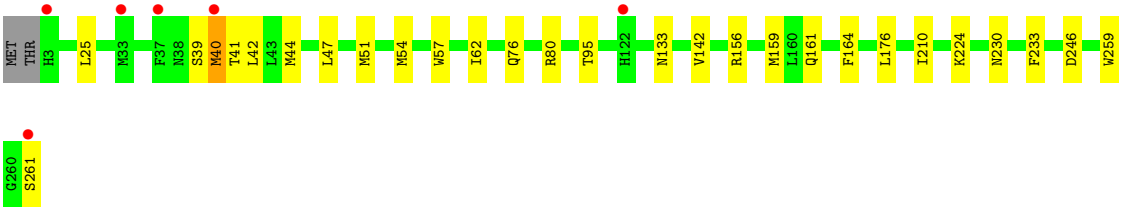
Chain C:





• Molecule 3: Cytochrome c oxidase subunit 3

Chain P:

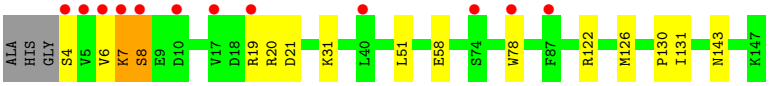


• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain D:

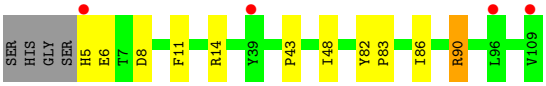
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain Q:



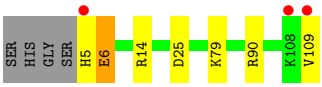
• Molecule 5: Cytochrome c oxidase subunit 5A

Chain E:



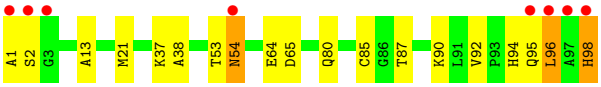
• Molecule 5: Cytochrome c oxidase subunit 5A

Chain R:



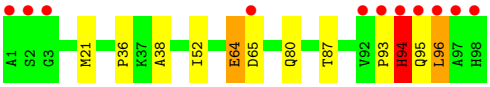
• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

Chain F:



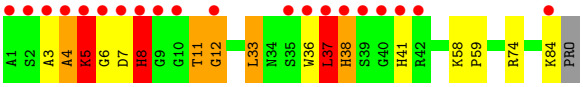
• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

Chain S:



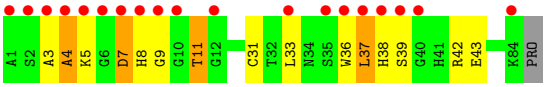
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain G:



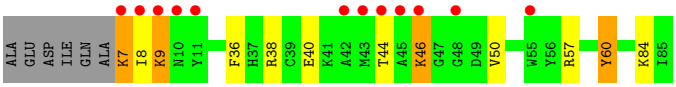
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain T:



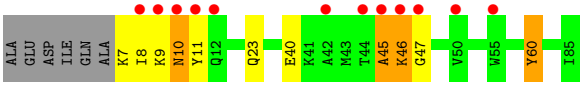
• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain H:



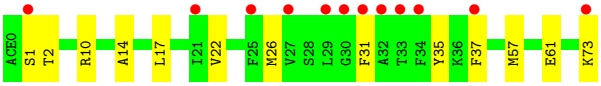
• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain U:



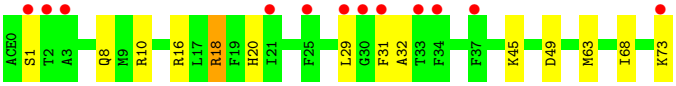
- Molecule 9: Cytochrome c oxidase subunit 6C

Chain I:



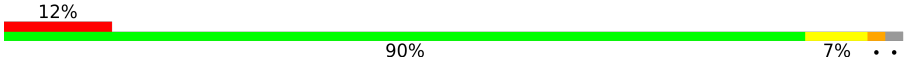
- Molecule 9: Cytochrome c oxidase subunit 6C

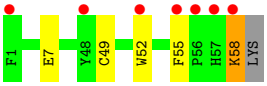
Chain V:



- Molecule 10: Cytochrome c oxidase subunit 7A1

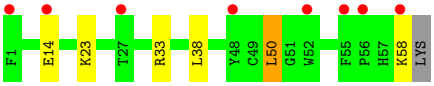
Chain J:





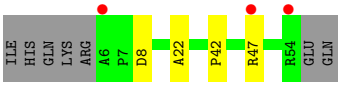
- Molecule 10: Cytochrome c oxidase subunit 7A1

Chain W:



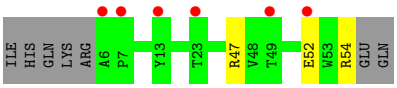
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

Chain K:



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

Chain X:

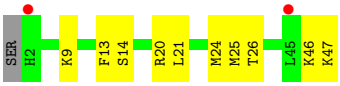


- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain L:

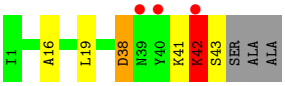
• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain Y:



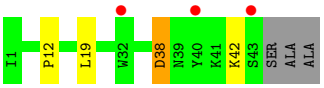
• Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

Chain M:



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

Chain Z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	183.41Å 206.27Å 177.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.97 – 1.85 39.97 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.4 (39.97-1.85) 99.4 (39.97-1.85)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.42 (at 1.86Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.164 , 0.188 0.166 , 0.190	Depositor DCC
R_{free} test set	28371 reflections (2.24%)	wwPDB-VP
Wilson B-factor (Å^2)	32.1	Xtriage
Anisotropy	0.601	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 48.8	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	33558	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% 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: CU, CDL, PGV, TPO, PEK, PSC, NA, MG, HEA, EDO, ACE, ZN, CHD, TGL, DMU, CUA, FME, AZI

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	1.06	3/4308 (0.1%)	0.94	8/5878 (0.1%)
1	N	0.85	1/4288 (0.0%)	0.85	2/5852 (0.0%)
2	B	0.83	0/2047	0.89	2/2790 (0.1%)
2	O	0.62	0/2024	0.77	0/2757
3	C	0.84	0/2263	0.76	0/3090
3	P	0.78	0/2272	0.74	0/3102
4	D	0.83	0/1245	0.82	1/1679 (0.1%)
4	Q	0.49	0/1248	0.62	0/1684
5	E	0.78	0/871	0.71	0/1182
5	R	0.60	0/871	0.71	0/1182
6	F	0.80	0/795	0.84	0/1079
6	S	0.69	0/780	0.86	1/1058 (0.1%)
7	G	0.79	0/690	0.89	1/937 (0.1%)
7	T	0.73	0/701	0.88	1/951 (0.1%)
8	H	0.77	0/682	0.80	0/921
8	U	0.61	0/682	0.71	0/921
9	I	0.69	0/612	0.75	0/812
9	V	0.49	0/612	0.71	0/812
10	J	0.61	0/471	0.70	0/636
10	W	0.54	0/480	0.62	0/648
11	K	0.74	0/398	0.72	0/546
11	X	0.42	0/405	0.53	0/556
12	L	0.78	0/401	0.78	0/536
12	Y	0.55	0/401	0.66	0/536
13	M	0.80	0/345	0.76	0/470
13	Z	0.48	0/345	0.57	0/470
All	All	0.80	4/30237 (0.0%)	0.81	16/41085 (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
12	Y	0	1
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	310	MET	SD-CE	-7.65	1.60	1.79
1	N	310	MET	SD-CE	-7.64	1.60	1.79
1	A	74	MET	CB-CG	6.17	1.71	1.52
1	A	74	MET	CG-SD	-5.59	1.66	1.80

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	71	MET	CG-SD-CE	-8.49	82.22	100.90
1	A	240	HIS	CA-CB-CG	-7.68	106.12	113.80
1	N	240	HIS	CA-CB-CG	-7.62	106.17	113.80
1	N	71	MET	CG-SD-CE	-7.38	84.67	100.90
6	S	94	HIS	N-CA-C	6.05	123.68	110.80

There are no chirality outliers.

All (4) 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
12	Y	46	LYS	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	4125	0	4107	45	0
1	N	4122	0	4101	54	0
2	B	1996	0	2031	24	0
2	O	1975	0	2000	37	0
3	C	2152	0	2068	27	0
3	P	2173	0	2081	24	0
4	D	1198	0	1179	9	0
4	Q	1213	0	1199	7	0
5	E	852	0	845	7	0
5	R	852	0	845	3	0
6	F	773	0	751	14	0
6	S	763	0	742	8	0
7	G	675	0	643	12	0
7	T	681	0	648	10	0
8	H	662	0	623	8	0
8	U	662	0	623	6	0
9	I	601	0	613	9	0
9	V	601	0	613	13	0
10	J	460	0	459	7	0
10	W	469	0	463	8	0
11	K	384	0	366	3	0
11	X	391	0	374	1	0
12	L	383	0	385	7	0
12	Y	383	0	385	7	0
13	M	335	0	352	4	0
13	Z	335	0	352	3	0
14	A	180	0	162	14	0
14	N	180	0	162	17	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	9	0	0	7	0
18	N	9	0	0	6	0
19	A	102	0	152	6	0
19	C	100	0	148	4	0
19	G	51	0	76	4	0
19	N	102	0	152	9	0
19	P	51	0	76	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	A	40	0	60	3	0
20	B	8	0	12	0	0
20	C	32	0	48	2	0
20	D	16	0	24	1	0
20	E	20	0	30	0	0
20	F	20	0	30	0	0
20	G	8	0	12	2	0
20	H	8	0	12	2	0
20	L	4	0	6	0	0
20	N	32	0	48	1	0
20	O	12	0	18	1	0
20	P	12	0	18	0	0
20	Q	8	0	12	0	0
20	R	24	0	36	2	0
20	S	12	0	18	5	0
20	T	4	0	6	0	0
20	U	4	0	6	0	0
20	V	4	0	6	0	0
21	B	63	0	110	7	0
21	D	63	0	110	11	0
21	L	63	0	110	4	0
21	N	61	0	102	0	0
21	Q	63	0	110	7	0
21	Y	63	0	110	8	0
22	B	29	0	39	0	0
22	C	58	0	78	4	0
22	G	29	0	39	1	0
22	J	29	0	39	1	0
22	P	58	0	78	3	0
22	W	29	0	37	4	0
23	B	2	0	0	0	0
23	O	2	0	0	0	0
24	B	50	0	72	10	0
24	O	51	0	75	6	0
25	C	88	0	115	10	0
25	L	30	0	33	4	0
25	M	33	0	42	1	0
25	P	99	0	126	9	0
25	Z	33	0	42	1	0
26	C	89	0	133	13	0
26	N	96	0	140	10	0
26	P	80	0	106	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	T	97	0	146	11	0
27	C	97	0	133	4	0
27	G	97	0	131	3	0
27	P	53	0	77	1	0
27	T	50	0	71	4	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	A	222	0	0	2	0
29	B	134	0	0	2	0
29	C	99	0	0	0	0
29	D	108	0	0	2	0
29	E	82	0	0	1	0
29	F	79	0	0	2	0
29	G	52	0	0	1	0
29	H	44	0	0	0	0
29	I	27	0	0	2	0
29	J	27	0	0	1	0
29	K	20	0	0	1	0
29	L	26	0	0	0	0
29	M	24	0	0	0	0
29	N	209	0	0	0	0
29	O	112	0	0	0	0
29	P	90	0	0	1	0
29	Q	38	0	0	1	0
29	R	39	0	0	0	0
29	S	59	0	0	1	0
29	T	35	0	0	0	0
29	U	33	0	0	0	0
29	V	14	0	0	0	0
29	W	12	0	0	0	0
29	X	11	0	0	0	0
29	Y	13	0	0	0	0
29	Z	16	0	0	1	0
All	All	33558	0	32582	410	0

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

The worst 5 of 410 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)
6:F:85:CYS:SG	6:F:87[B]:THR:HG23	2.09	0.93
4:D:78:TRP:HB3	21:D:201:TGL:HB22	1.61	0.82
26:N:601:CDL:H371	2:O:78:LEU:HD12	1.63	0.79
7:T:7:ASP:O	7:T:9:GLY:N	2.17	0.78
3:P:161[A]:GLN:HE22	27:T:101:PEK:H22	1.49	0.77

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	532/514 (104%)	514 (97%)	18 (3%)	0	100	100
1	N	530/514 (103%)	517 (98%)	13 (2%)	0	100	100
2	B	248/227 (109%)	242 (98%)	6 (2%)	0	100	100
2	O	245/227 (108%)	239 (98%)	5 (2%)	1 (0%)	30	17
3	C	265/261 (102%)	260 (98%)	5 (2%)	0	100	100
3	P	266/261 (102%)	261 (98%)	5 (2%)	0	100	100
4	D	144/147 (98%)	139 (96%)	5 (4%)	0	100	100
4	Q	144/147 (98%)	138 (96%)	4 (3%)	2 (1%)	9	2
5	E	103/109 (94%)	103 (100%)	0	0	100	100
5	R	103/109 (94%)	102 (99%)	0	1 (1%)	12	4
6	F	100/98 (102%)	96 (96%)	2 (2%)	2 (2%)	6	1
6	S	98/98 (100%)	92 (94%)	3 (3%)	3 (3%)	3	0
7	G	81/85 (95%)	70 (86%)	5 (6%)	6 (7%)	1	0
7	T	82/85 (96%)	68 (83%)	10 (12%)	4 (5%)	1	0
8	H	77/85 (91%)	72 (94%)	5 (6%)	0	100	100
8	U	77/85 (91%)	72 (94%)	2 (3%)	3 (4%)	2	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	72/74 (97%)	70 (97%)	2 (3%)	0	100	100
9	V	72/74 (97%)	71 (99%)	1 (1%)	0	100	100
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	W	57/59 (97%)	56 (98%)	1 (2%)	0	100	100
11	K	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
11	X	48/56 (86%)	47 (98%)	1 (2%)	0	100	100
12	L	45/47 (96%)	42 (93%)	2 (4%)	1 (2%)	5	1
12	Y	45/47 (96%)	44 (98%)	1 (2%)	0	100	100
13	M	41/46 (89%)	39 (95%)	1 (2%)	1 (2%)	4	1
13	Z	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
All	All	3619/3616 (100%)	3496 (97%)	99 (3%)	24 (1%)	18	8

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	4	ALA
7	G	8	HIS
13	M	42	LYS
4	Q	7	LYS
4	Q	8	SER

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	445/426 (104%)	438 (98%)	7 (2%)	55	44
1	N	443/426 (104%)	438 (99%)	5 (1%)	65	57
2	B	233/210 (111%)	223 (96%)	10 (4%)	26	11
2	O	230/210 (110%)	223 (97%)	7 (3%)	36	21
3	C	232/226 (103%)	230 (99%)	2 (1%)	70	64
3	P	233/226 (103%)	229 (98%)	4 (2%)	53	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	130/129 (101%)	126 (97%)	4 (3%)	35	20
4	Q	130/129 (101%)	122 (94%)	8 (6%)	16	5
5	E	92/95 (97%)	90 (98%)	2 (2%)	45	32
5	R	92/95 (97%)	89 (97%)	3 (3%)	33	18
6	F	85/81 (105%)	80 (94%)	5 (6%)	18	5
6	S	83/81 (102%)	77 (93%)	6 (7%)	13	3
7	G	67/68 (98%)	60 (90%)	7 (10%)	7	1
7	T	68/68 (100%)	63 (93%)	5 (7%)	13	3
8	H	71/75 (95%)	65 (92%)	6 (8%)	10	2
8	U	71/75 (95%)	66 (93%)	5 (7%)	14	3
9	I	58/58 (100%)	54 (93%)	4 (7%)	14	3
9	V	58/58 (100%)	53 (91%)	5 (9%)	10	2
10	J	49/50 (98%)	48 (98%)	1 (2%)	48	36
10	W	50/50 (100%)	49 (98%)	1 (2%)	48	36
11	K	39/46 (85%)	39 (100%)	0	100	100
11	X	40/46 (87%)	38 (95%)	2 (5%)	22	8
12	L	40/40 (100%)	39 (98%)	1 (2%)	42	27
12	Y	40/40 (100%)	37 (92%)	3 (8%)	12	3
13	M	37/38 (97%)	35 (95%)	2 (5%)	20	7
13	Z	37/38 (97%)	35 (95%)	2 (5%)	20	7
All	All	3153/3084 (102%)	3046 (97%)	107 (3%)	33	17

5 of 107 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	O	33[C]	LEU
4	Q	31	LYS
10	W	50	LEU
2	O	78	LEU
3	P	159	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	N	422	ASN
11	X	35	GLN
4	Q	101	HIS
8	U	31	GLN
3	P	133	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	O	1	2	8,9,10	0.59	0	7,9,11	1.44	2 (28%)
2	FME	B	1	2	8,9,10	0.85	0	7,9,11	1.97	2 (28%)
7	TPO	G	11	7	8,10,11	1.62	2 (25%)	10,14,16	1.13	1 (10%)
1	FME	A	1	1	8,9,10	0.56	0	7,9,11	1.79	1 (14%)
1	FME	N	1	1	8,9,10	0.43	0	7,9,11	1.42	1 (14%)
7	TPO	T	11	7	8,10,11	1.47	1 (12%)	10,14,16	1.35	1 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FME	O	1	2	-	0/7/9/11	-
2	FME	B	1	2	-	1/7/9/11	-
7	TPO	G	11	7	-	5/9/11/13	-
1	FME	A	1	1	-	3/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	N	1	1	-	3/7/9/11	-
7	TPO	T	11	7	-	5/9/11/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	11	TPO	P-O1P	2.88	1.59	1.50
7	G	11	TPO	P-O1P	2.84	1.59	1.50
7	G	11	TPO	P-OG1	2.61	1.64	1.59

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	FME	CG-CB-CA	-4.15	101.42	112.95
7	T	11	TPO	CG2-CB-CA	3.02	119.12	113.16
1	A	1	FME	C-CA-N	2.91	114.99	109.73
2	O	1	FME	CG-CB-CA	-2.70	105.45	112.95
1	N	1	FME	O-C-CA	-2.61	117.94	124.78

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	N-CA-CB-CG
7	G	11	TPO	N-CA-CB-CG2
7	G	11	TPO	N-CA-CB-OG1
7	G	11	TPO	C-CA-CB-CG2
7	G	11	TPO	O-C-CA-CB

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	FME	1	0
7	G	11	TPO	2	0
1	A	1	FME	1	0
7	T	11	TPO	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 134 ligands modelled in this entry, 10 are monoatomic - leaving 124 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	$\#\|Z\| > 2$
18	AZI	A	607[B]	15,14	0,2,2	-	-	0,1,1	-	-
25	DMU	Z	101	-	34,34,34	0.44	0	45,45,45	0.86	1 (2%)
20	EDO	F	105	-	3,3,3	0.36	0	2,2,2	0.77	0
27	PEK	C	319	-	43,43,52	1.15	2 (4%)	46,48,57	1.67	8 (17%)
25	DMU	C	302	-	34,34,34	0.69	0	45,45,45	1.66	8 (17%)
20	EDO	A	618	-	3,3,3	0.35	0	2,2,2	0.46	0
19	PGV	A	609	-	50,50,50	1.25	4 (8%)	53,56,56	1.64	10 (18%)
27	PEK	G	101	-	52,52,52	0.85	4 (7%)	55,57,57	1.13	5 (9%)
20	EDO	P	309	-	3,3,3	0.51	0	2,2,2	0.70	0
18	AZI	N	607[A]	15	0,2,2	-	-	0,1,1	-	-
20	EDO	F	103	-	3,3,3	0.59	0	2,2,2	0.49	0
20	EDO	E	204	-	3,3,3	0.74	0	2,2,2	0.11	0
21	TGL	Q	201	-	62,62,62	1.06	4 (6%)	65,65,65	0.90	5 (7%)
19	PGV	P	303	-	50,50,50	0.70	2 (4%)	53,56,56	1.08	5 (9%)
19	PGV	C	304	-	50,50,50	0.87	3 (6%)	53,56,56	1.13	7 (13%)
19	PGV	N	609	-	50,50,50	0.94	3 (6%)	53,56,56	1.38	7 (13%)
21	TGL	Y	101	-	62,62,62	1.18	3 (4%)	65,65,65	1.45	11 (16%)
22	CHD	P	301	-	32,32,32	0.83	0	51,51,51	1.45	7 (13%)
20	EDO	A	616	-	3,3,3	0.99	0	2,2,2	0.89	0
20	EDO	C	315	-	3,3,3	0.53	0	2,2,2	0.18	0
20	EDO	R	201	-	3,3,3	0.69	0	2,2,2	0.52	0
18	AZI	A	606[A]	15	0,2,2	-	-	0,1,1	-	-
27	PEK	G	103	-	43,43,52	1.09	2 (4%)	46,48,57	1.59	9 (19%)
20	EDO	F	102	-	3,3,3	0.83	0	2,2,2	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
20	EDO	Q	203	-	3,3,3	0.55	0	2,2,2	0.18	0
20	EDO	C	314	-	3,3,3	0.48	0	2,2,2	0.56	0
18	AZI	N	608[B]	15,14	0,2,2	-	-	0,1,1	-	-
25	DMU	P	307	-	34,34,34	0.63	0	45,45,45	1.94	10 (22%)
26	CDL	P	304	-	77,77,99	1.48	10 (12%)	84,85,111	1.68	13 (15%)
20	EDO	A	611	-	3,3,3	0.57	0	2,2,2	0.64	0
20	EDO	N	617	-	3,3,3	0.57	0	2,2,2	0.22	0
27	PEK	C	307	-	52,52,52	1.08	2 (3%)	55,57,57	1.57	10 (18%)
20	EDO	N	612	-	3,3,3	0.49	0	2,2,2	0.24	0
20	EDO	D	203	-	3,3,3	0.39	0	2,2,2	0.30	0
25	DMU	C	310	-	22,22,34	0.46	0	27,27,45	0.97	1 (3%)
20	EDO	C	313	-	3,3,3	0.53	0	2,2,2	0.36	0
22	CHD	C	306	-	32,32,32	0.93	0	51,51,51	2.14	16 (31%)
20	EDO	Q	202	-	3,3,3	0.45	0	2,2,2	0.60	0
22	CHD	J	101	-	32,32,32	0.79	1 (3%)	51,51,51	1.27	5 (9%)
25	DMU	P	308	-	34,34,34	0.65	1 (2%)	45,45,45	0.98	1 (2%)
25	DMU	M	101	-	34,34,34	0.45	0	45,45,45	1.35	4 (8%)
22	CHD	W	101	10	32,32,32	0.82	1 (3%)	51,51,51	2.51	19 (37%)
20	EDO	E	201	-	3,3,3	0.73	0	2,2,2	0.24	0
23	CUA	B	303	2	0,1,1	-	-	-		
20	EDO	H	102	-	3,3,3	0.45	0	2,2,2	0.58	0
20	EDO	P	311	-	3,3,3	0.58	0	2,2,2	0.46	0
25	DMU	L	102	-	31,31,34	0.91	0	42,42,45	1.83	12 (28%)
20	EDO	O	303	-	3,3,3	0.59	0	2,2,2	0.94	0
20	EDO	A	615	-	3,3,3	0.80	0	2,2,2	0.71	0
20	EDO	O	304	-	3,3,3	0.49	0	2,2,2	0.48	0
20	EDO	A	614	-	3,3,3	0.92	0	2,2,2	0.27	0
26	CDL	C	305	-	87,87,99	1.48	14 (16%)	95,97,111	1.73	22 (23%)
20	EDO	E	205	-	3,3,3	0.48	0	2,2,2	0.44	0
19	PGV	C	308	-	48,48,50	1.22	3 (6%)	51,53,56	1.33	4 (7%)
20	EDO	S	103	-	3,3,3	0.96	0	2,2,2	0.48	0
20	EDO	B	305	-	3,3,3	0.61	0	2,2,2	0.14	0
23	CUA	O	301	2	0,1,1	-	-	-		
20	EDO	R	203	-	3,3,3	0.49	0	2,2,2	0.41	0
24	PSC	O	302	-	50,50,51	1.16	3 (6%)	56,58,59	1.31	5 (8%)
20	EDO	A	613	-	3,3,3	0.95	0	2,2,2	0.59	0
19	PGV	N	619	-	50,50,50	1.04	2 (4%)	53,56,56	1.22	6 (11%)
20	EDO	R	205	-	3,3,3	0.45	0	2,2,2	0.59	0
27	PEK	T	101	-	49,49,52	1.13	3 (6%)	53,54,57	1.58	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
20	EDO	S	104	-	3,3,3	0.70	0	2,2,2	0.54	0
21	TGL	D	201	-	62,62,62	1.24	4 (6%)	65,65,65	1.21	5 (7%)
20	EDO	C	317	-	3,3,3	0.57	0	2,2,2	0.34	0
20	EDO	A	610	-	3,3,3	0.36	0	2,2,2	0.77	0
20	EDO	N	615	-	3,3,3	0.51	0	2,2,2	0.66	0
21	TGL	N	610	-	59,59,62	1.14	3 (5%)	61,61,65	1.39	7 (11%)
20	EDO	C	312	-	3,3,3	0.48	0	2,2,2	0.42	0
14	HEA	N	603[A]	1,18	66,67,67	1.90	25 (37%)	78,103,103	1.98	27 (34%)
27	PEK	P	312	-	52,52,52	0.86	3 (5%)	55,57,57	2.31	9 (16%)
22	CHD	P	305	-	32,32,32	0.77	0	51,51,51	1.89	11 (21%)
20	EDO	C	318	-	3,3,3	0.67	0	2,2,2	0.79	0
22	CHD	B	302	-	32,32,32	1.15	2 (6%)	51,51,51	1.46	9 (17%)
20	EDO	F	106	-	3,3,3	0.42	0	2,2,2	0.71	0
20	EDO	A	617	-	3,3,3	0.68	0	2,2,2	0.47	0
20	EDO	N	613	-	3,3,3	0.61	0	2,2,2	0.44	0
19	PGV	A	608	-	50,50,50	1.03	3 (6%)	53,56,56	0.93	3 (5%)
25	DMU	C	309	-	34,34,34	0.69	1 (2%)	45,45,45	1.66	8 (17%)
20	EDO	L	103	-	3,3,3	0.41	0	2,2,2	0.49	0
22	CHD	G	102	-	32,32,32	0.83	0	51,51,51	1.29	7 (13%)
20	EDO	C	316	-	3,3,3	0.55	0	2,2,2	0.32	0
24	PSC	B	304	-	48,48,51	1.31	4 (8%)	53,55,59	1.28	4 (7%)
14	HEA	A	602[A]	1,18	66,67,67	1.94	25 (37%)	78,103,103	2.17	27 (34%)
20	EDO	H	101	-	3,3,3	0.32	0	2,2,2	0.86	0
20	EDO	U	101	-	3,3,3	0.49	0	2,2,2	0.22	0
20	EDO	G	105	-	3,3,3	0.55	0	2,2,2	0.18	0
20	EDO	N	614	-	3,3,3	1.22	0	2,2,2	0.59	0
20	EDO	C	311	-	3,3,3	0.76	0	2,2,2	0.33	0
20	EDO	D	202	-	3,3,3	0.45	0	2,2,2	0.79	0
20	EDO	A	612	-	3,3,3	1.13	0	2,2,2	0.87	0
22	CHD	C	301	-	32,32,32	1.01	2 (6%)	51,51,51	1.77	12 (23%)
20	EDO	A	619	-	3,3,3	0.47	0	2,2,2	0.40	0
20	EDO	B	306	-	3,3,3	1.03	0	2,2,2	0.27	0
20	EDO	G	106	-	3,3,3	0.67	0	2,2,2	0.38	0
18	AZI	A	607[A]	14	0,2,2	-	-	0,1,1	-	-
20	EDO	F	104	-	3,3,3	0.38	0	2,2,2	0.48	0
20	EDO	D	204	-	3,3,3	0.36	0	2,2,2	0.64	0
20	EDO	O	305	-	3,3,3	0.55	0	2,2,2	0.18	0
20	EDO	D	205	-	3,3,3	0.58	0	2,2,2	0.36	0
21	TGL	L	101	-	62,62,62	1.60	5 (8%)	65,65,65	1.99	15 (23%)
20	EDO	S	101	-	3,3,3	0.55	0	2,2,2	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	HEA	N	603[B]	1,18	66,67,67	1.95	22 (33%)	78,103,103	1.93	24 (30%)
26	CDL	T	102	-	95,95,99	1.40	12 (12%)	100,106,111	1.48	13 (13%)
20	EDO	E	203	-	3,3,3	0.42	0	2,2,2	0.46	0
20	EDO	N	611	-	3,3,3	0.38	0	2,2,2	0.54	0
20	EDO	R	206	-	3,3,3	0.63	0	2,2,2	0.25	0
20	EDO	T	103	-	3,3,3	0.93	0	2,2,2	0.59	0
20	EDO	V	101	-	3,3,3	0.46	0	2,2,2	0.54	0
14	HEA	N	602	1	66,67,67	1.70	18 (27%)	78,103,103	2.18	29 (37%)
20	EDO	E	202	-	3,3,3	0.49	0	2,2,2	0.57	0
20	EDO	P	310	-	3,3,3	0.58	0	2,2,2	0.32	0
14	HEA	A	602[B]	1,18	66,67,67	1.86	22 (33%)	78,103,103	1.99	22 (28%)
20	EDO	N	616	-	3,3,3	0.77	0	2,2,2	0.09	0
26	CDL	N	601	-	93,93,99	1.43	12 (12%)	97,103,111	1.19	11 (11%)
19	PGV	G	104	-	50,50,50	1.08	2 (4%)	53,56,56	1.54	10 (18%)
18	AZI	N	608[A]	14	0,2,2	-	-	0,1,1	-	-
20	EDO	R	204	-	3,3,3	0.68	0	2,2,2	0.41	0
20	EDO	R	202	-	3,3,3	0.36	0	2,2,2	0.51	0
25	DMU	P	306	-	34,34,34	0.67	1 (2%)	45,45,45	0.88	2 (4%)
20	EDO	N	618	-	3,3,3	0.44	0	2,2,2	0.39	0
21	TGL	B	301	-	62,62,62	1.20	3 (4%)	65,65,65	1.38	6 (9%)
14	HEA	A	601	1	66,67,67	1.81	22 (33%)	78,103,103	2.25	29 (37%)

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
25	DMU	Z	101	-	-	5/19/59/59	0/2/2/2
20	EDO	F	105	-	-	1/1/1/1	-
27	PEK	C	319	-	-	28/47/47/56	-
25	DMU	C	302	-	-	5/19/59/59	0/2/2/2
20	EDO	A	618	-	-	1/1/1/1	-
19	PGV	A	609	-	-	21/55/55/55	-
27	PEK	G	101	-	-	10/56/56/56	-
20	EDO	P	309	-	-	1/1/1/1	-
20	EDO	F	103	-	-	0/1/1/1	-
20	EDO	E	204	-	-	1/1/1/1	-
21	TGL	Q	201	-	-	30/65/65/65	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	PGV	P	303	-	-	7/55/55/55	-
19	PGV	C	304	-	-	12/55/55/55	-
19	PGV	N	609	-	-	9/55/55/55	-
21	TGL	Y	101	-	-	30/65/65/65	-
22	CHD	P	301	-	-	2/9/74/74	0/4/4/4
20	EDO	A	616	-	-	0/1/1/1	-
20	EDO	C	315	-	-	1/1/1/1	-
20	EDO	R	201	-	-	0/1/1/1	-
27	PEK	G	103	-	-	23/47/47/56	-
20	EDO	F	102	-	-	0/1/1/1	-
20	EDO	Q	203	-	-	0/1/1/1	-
20	EDO	C	314	-	-	0/1/1/1	-
25	DMU	P	307	-	-	8/19/59/59	0/2/2/2
26	CDL	P	304	-	-	25/75/77/110	-
20	EDO	A	611	-	-	1/1/1/1	-
20	EDO	N	617	-	-	0/1/1/1	-
27	PEK	C	307	-	-	27/56/56/56	-
20	EDO	N	612	-	-	1/1/1/1	-
20	EDO	D	203	-	-	1/1/1/1	-
25	DMU	C	310	-	-	4/13/33/59	0/1/1/2
20	EDO	C	313	-	-	0/1/1/1	-
22	CHD	C	306	-	-	6/9/74/74	0/4/4/4
20	EDO	Q	202	-	-	0/1/1/1	-
22	CHD	J	101	-	-	4/9/74/74	0/4/4/4
25	DMU	P	308	-	-	6/19/59/59	0/2/2/2
25	DMU	M	101	-	-	3/19/59/59	0/2/2/2
22	CHD	W	101	10	-	8/9/74/74	0/4/4/4
20	EDO	E	201	-	-	0/1/1/1	-
20	EDO	H	102	-	-	0/1/1/1	-
20	EDO	P	311	-	-	0/1/1/1	-
25	DMU	L	102	-	-	10/16/56/59	0/2/2/2
20	EDO	O	303	-	-	0/1/1/1	-
20	EDO	A	615	-	-	1/1/1/1	-
20	EDO	O	304	-	-	1/1/1/1	-
20	EDO	A	614	-	-	0/1/1/1	-
26	CDL	C	305	-	-	51/91/91/110	-
20	EDO	E	205	-	-	0/1/1/1	-
19	PGV	C	308	-	-	21/52/52/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	S	103	-	-	0/1/1/1	-
20	EDO	B	305	-	-	0/1/1/1	-
20	EDO	R	203	-	-	0/1/1/1	-
24	PSC	O	302	-	-	30/54/54/55	-
20	EDO	A	613	-	-	0/1/1/1	-
19	PGV	N	619	-	-	23/55/55/55	-
20	EDO	R	205	-	-	0/1/1/1	-
27	PEK	T	101	-	-	21/51/51/56	-
20	EDO	S	104	-	-	0/1/1/1	-
21	TGL	D	201	-	-	36/65/65/65	-
20	EDO	C	317	-	-	1/1/1/1	-
20	EDO	A	610	-	-	1/1/1/1	-
20	EDO	N	615	-	-	0/1/1/1	-
21	TGL	N	610	-	-	29/60/60/65	-
20	EDO	C	312	-	-	1/1/1/1	-
14	HEA	N	603[A]	1,18	-	8/36/76/76	-
27	PEK	P	312	-	-	19/56/56/56	-
22	CHD	P	305	-	-	5/9/74/74	0/4/4/4
20	EDO	C	318	-	-	1/1/1/1	-
22	CHD	B	302	-	-	2/9/74/74	0/4/4/4
20	EDO	F	106	-	-	0/1/1/1	-
20	EDO	A	617	-	-	0/1/1/1	-
20	EDO	N	613	-	-	1/1/1/1	-
19	PGV	A	608	-	-	7/55/55/55	-
25	DMU	C	309	-	-	8/19/59/59	0/2/2/2
20	EDO	L	103	-	-	0/1/1/1	-
22	CHD	G	102	-	-	3/9/74/74	0/4/4/4
20	EDO	C	316	-	-	1/1/1/1	-
24	PSC	B	304	-	-	21/50/50/55	-
14	HEA	A	602[A]	1,18	-	8/36/76/76	-
20	EDO	H	101	-	-	1/1/1/1	-
20	EDO	U	101	-	-	1/1/1/1	-
20	EDO	G	105	-	-	1/1/1/1	-
20	EDO	N	614	-	-	0/1/1/1	-
20	EDO	C	311	-	-	0/1/1/1	-
20	EDO	D	202	-	-	1/1/1/1	-
20	EDO	A	612	-	-	0/1/1/1	-
22	CHD	C	301	-	-	3/9/74/74	0/4/4/4
20	EDO	A	619	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	B	306	-	-	1/1/1/1	-
20	EDO	G	106	-	-	1/1/1/1	-
20	EDO	F	104	-	-	1/1/1/1	-
20	EDO	D	204	-	-	1/1/1/1	-
20	EDO	O	305	-	-	0/1/1/1	-
20	EDO	D	205	-	-	0/1/1/1	-
21	TGL	L	101	-	-	37/65/65/65	-
20	EDO	S	101	-	-	1/1/1/1	-
14	HEA	N	603[B]	1,18	-	7/36/76/76	-
26	CDL	T	102	-	-	52/104/104/110	-
20	EDO	E	203	-	-	0/1/1/1	-
20	EDO	N	611	-	-	1/1/1/1	-
20	EDO	R	206	-	-	1/1/1/1	-
20	EDO	T	103	-	-	0/1/1/1	-
20	EDO	V	101	-	-	0/1/1/1	-
14	HEA	N	602	1	-	7/36/76/76	-
20	EDO	E	202	-	-	0/1/1/1	-
20	EDO	P	310	-	-	0/1/1/1	-
14	HEA	A	602[B]	1,18	-	7/36/76/76	-
20	EDO	N	616	-	-	0/1/1/1	-
26	CDL	N	601	-	-	47/100/100/110	-
19	PGV	G	104	-	-	28/55/55/55	-
20	EDO	R	204	-	-	0/1/1/1	-
20	EDO	R	202	-	-	1/1/1/1	-
25	DMU	P	306	-	-	7/19/59/59	0/2/2/2
20	EDO	N	618	-	-	0/1/1/1	-
21	TGL	B	301	-	-	30/65/65/65	-
14	HEA	A	601	1	-	6/36/76/76	-

The worst 5 of 258 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	L	101	TGL	OG3-CC1	7.63	1.55	1.33
21	L	101	TGL	OG2-CB1	7.07	1.54	1.34
14	N	603[B]	HEA	FE-ND	5.64	2.12	1.94
21	B	301	TGL	OG2-CB1	5.54	1.49	1.34
19	C	308	PGV	O03-C19	5.51	1.49	1.33

The worst 5 of 510 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	P	312	PEK	C2-C3-C4	11.86	134.37	113.23
21	L	101	TGL	OG2-CB1-CB2	8.28	129.34	111.50
22	C	306	CHD	C23-C22-C20	-7.67	100.50	114.52
27	P	312	PEK	O01-C1-O02	-7.62	105.29	123.70
21	B	301	TGL	OG2-CB1-CB2	7.06	126.72	111.50

There are no chirality outliers.

5 of 834 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	601	HEA	C2A-C3A-CMA-OMA
14	A	602[A]	HEA	C2A-C3A-CMA-OMA
14	A	602[A]	HEA	C4A-C3A-CMA-OMA
14	A	602[B]	HEA	C2A-C3A-CMA-OMA
14	A	602[B]	HEA	C4D-C3D-CAD-CBD

There are no ring outliers.

62 monomers are involved in 223 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	607[B]	AZI	2	0
25	Z	101	DMU	1	0
27	C	319	PEK	1	0
25	C	302	DMU	8	0
19	A	609	PGV	4	0
27	G	101	PEK	2	0
18	N	607[A]	AZI	1	0
21	Q	201	TGL	7	0
19	P	303	PGV	2	0
19	C	304	PGV	2	0
19	N	609	PGV	2	0
21	Y	101	TGL	8	0
20	A	616	EDO	2	0
18	A	606[A]	AZI	1	0
27	G	103	PEK	1	0
20	C	314	EDO	1	0
25	P	307	DMU	3	0
26	P	304	CDL	8	0
27	C	307	PEK	3	0
22	C	306	CHD	4	0
22	J	101	CHD	1	0
25	P	308	DMU	1	0

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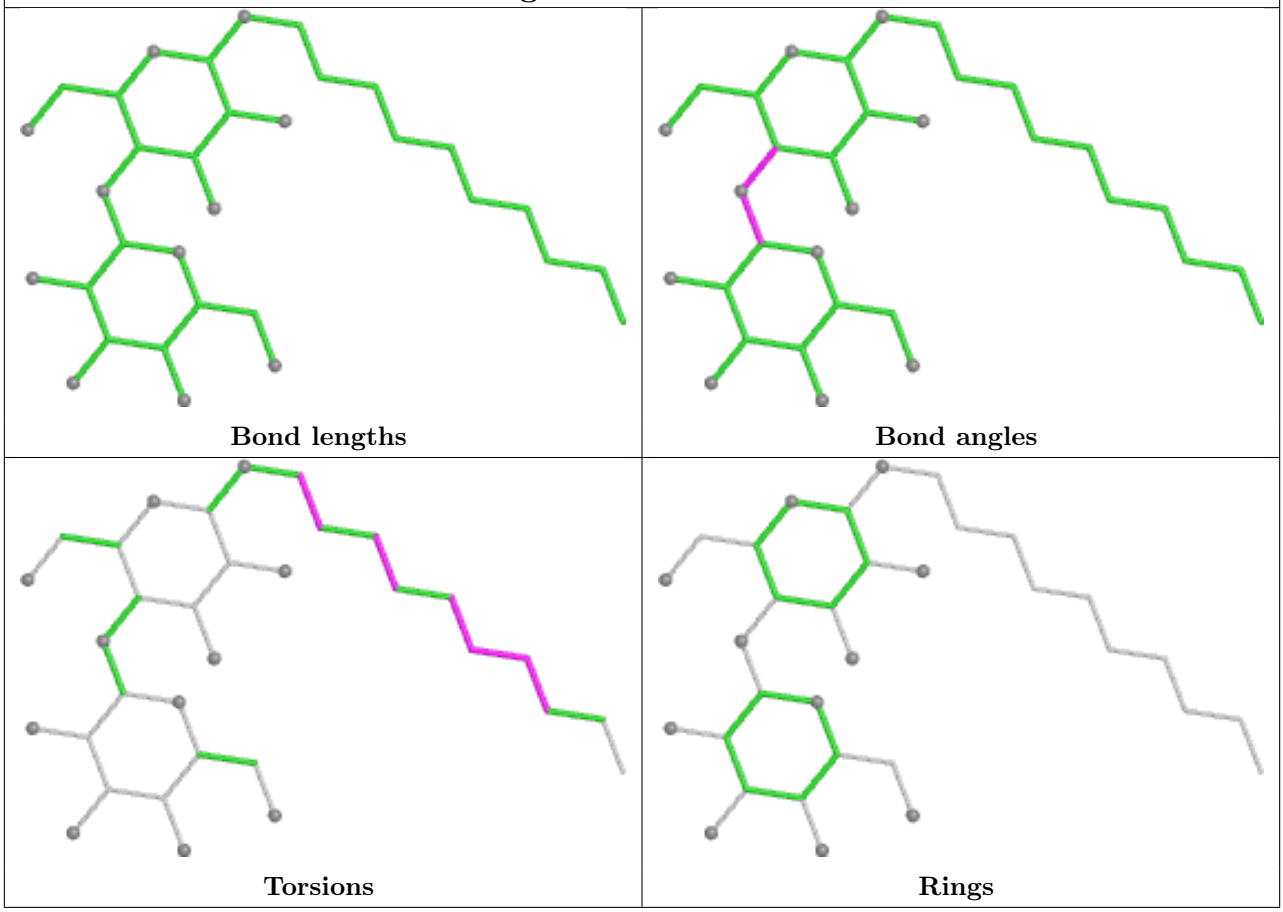
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	M	101	DMU	1	0
22	W	101	CHD	4	0
20	H	102	EDO	1	0
25	L	102	DMU	4	0
26	C	305	CDL	13	0
19	C	308	PGV	2	0
24	O	302	PSC	6	0
19	N	619	PGV	7	0
20	R	205	EDO	1	0
27	T	101	PEK	4	0
21	D	201	TGL	11	0
20	A	610	EDO	1	0
14	N	603[A]	HEA	7	0
27	P	312	PEK	1	0
22	P	305	CHD	3	0
20	C	318	EDO	1	0
20	N	613	EDO	1	0
19	A	608	PGV	2	0
25	C	309	DMU	2	0
22	G	102	CHD	1	0
24	B	304	PSC	10	0
14	A	602[A]	HEA	5	0
20	H	101	EDO	1	0
20	G	105	EDO	2	0
18	A	607[A]	AZI	5	0
20	D	204	EDO	1	0
20	O	305	EDO	1	0
21	L	101	TGL	4	0
20	S	101	EDO	5	0
14	N	603[B]	HEA	6	0
26	T	102	CDL	11	0
14	N	602	HEA	4	0
14	A	602[B]	HEA	6	0
26	N	601	CDL	10	0
19	G	104	PGV	4	0
18	N	608[A]	AZI	6	0
20	R	202	EDO	1	0
25	P	306	DMU	5	0
21	B	301	TGL	7	0
14	A	601	HEA	3	0

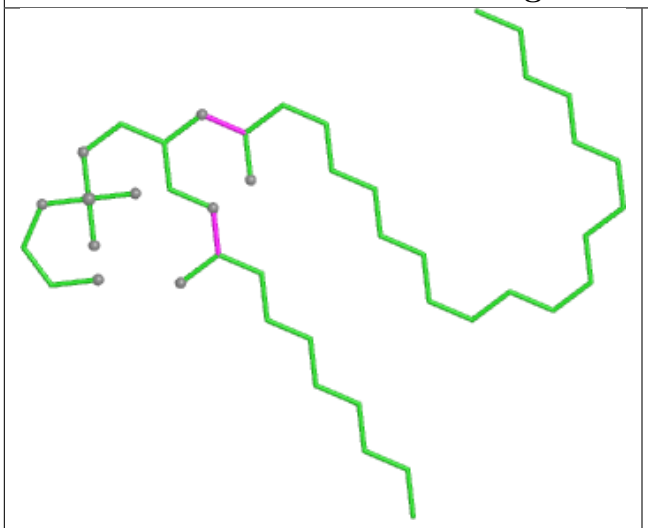
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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

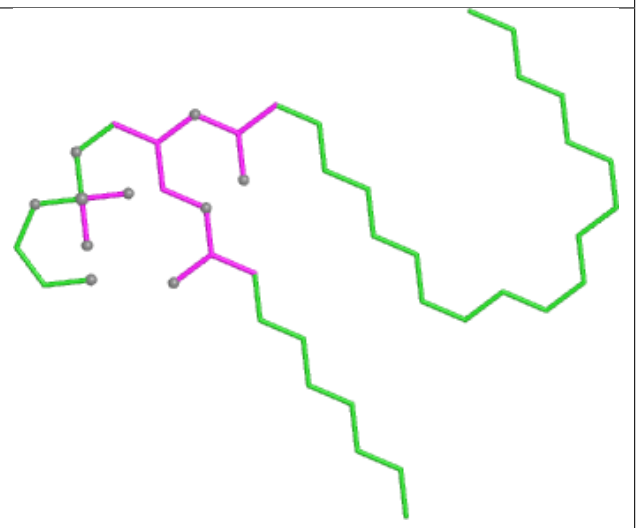
Ligand DMU Z 101



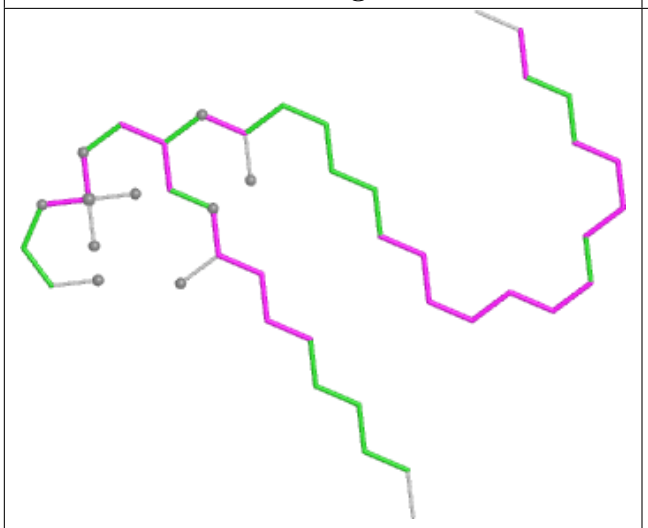
Ligand PEK C 319



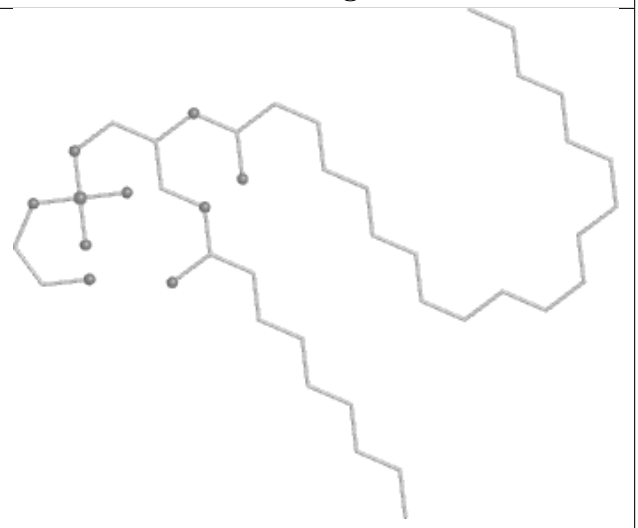
Bond lengths



Bond angles

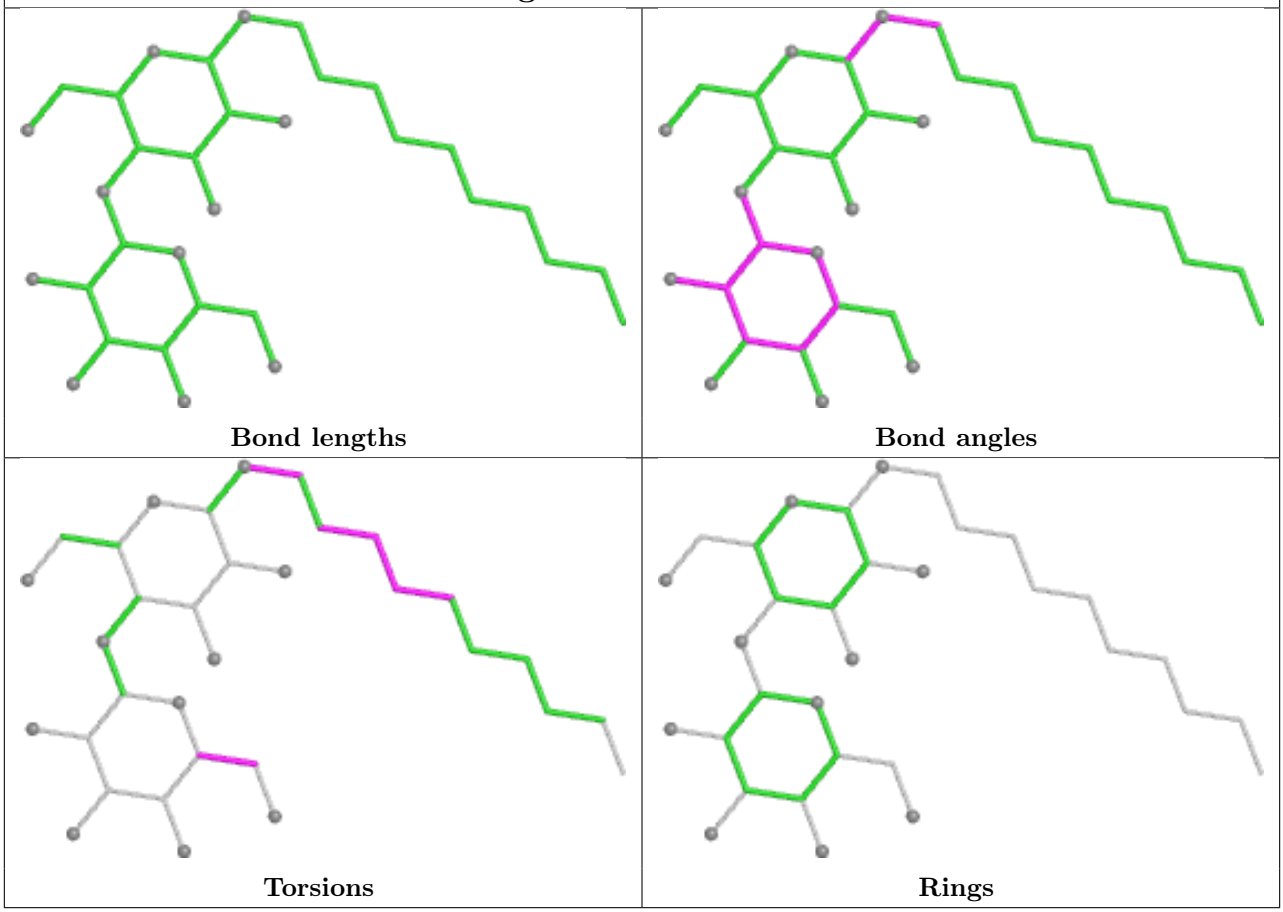


Torsions

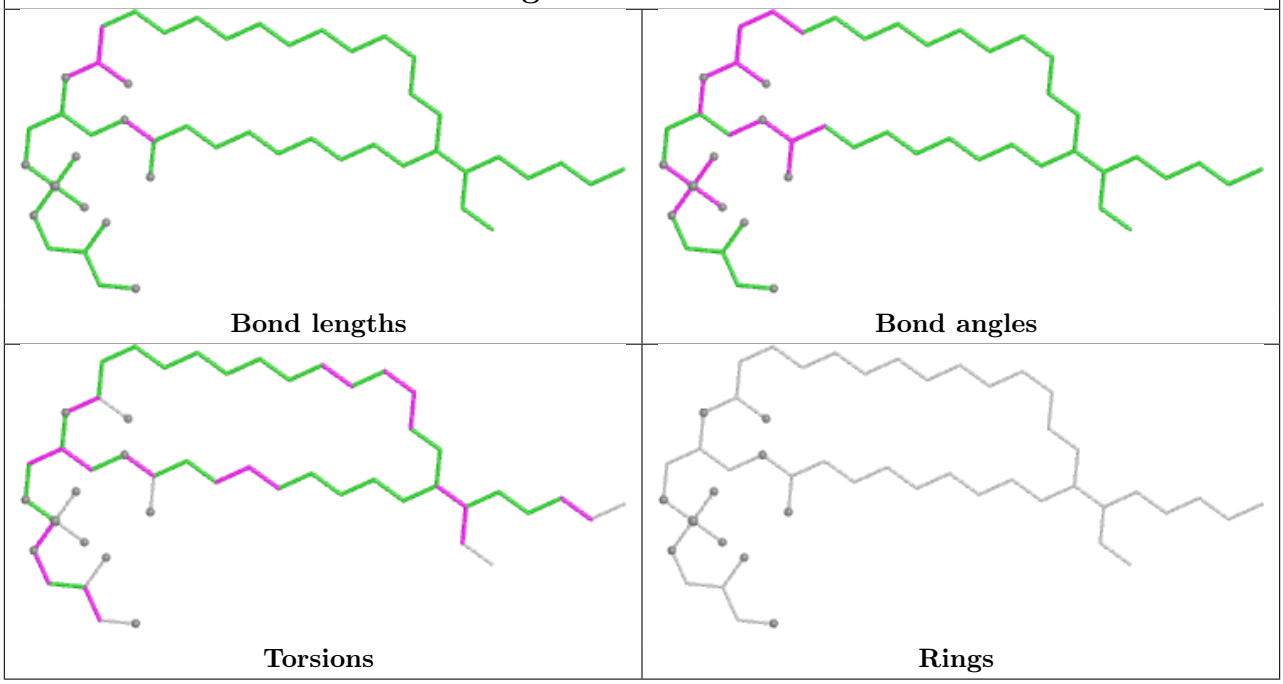


Rings

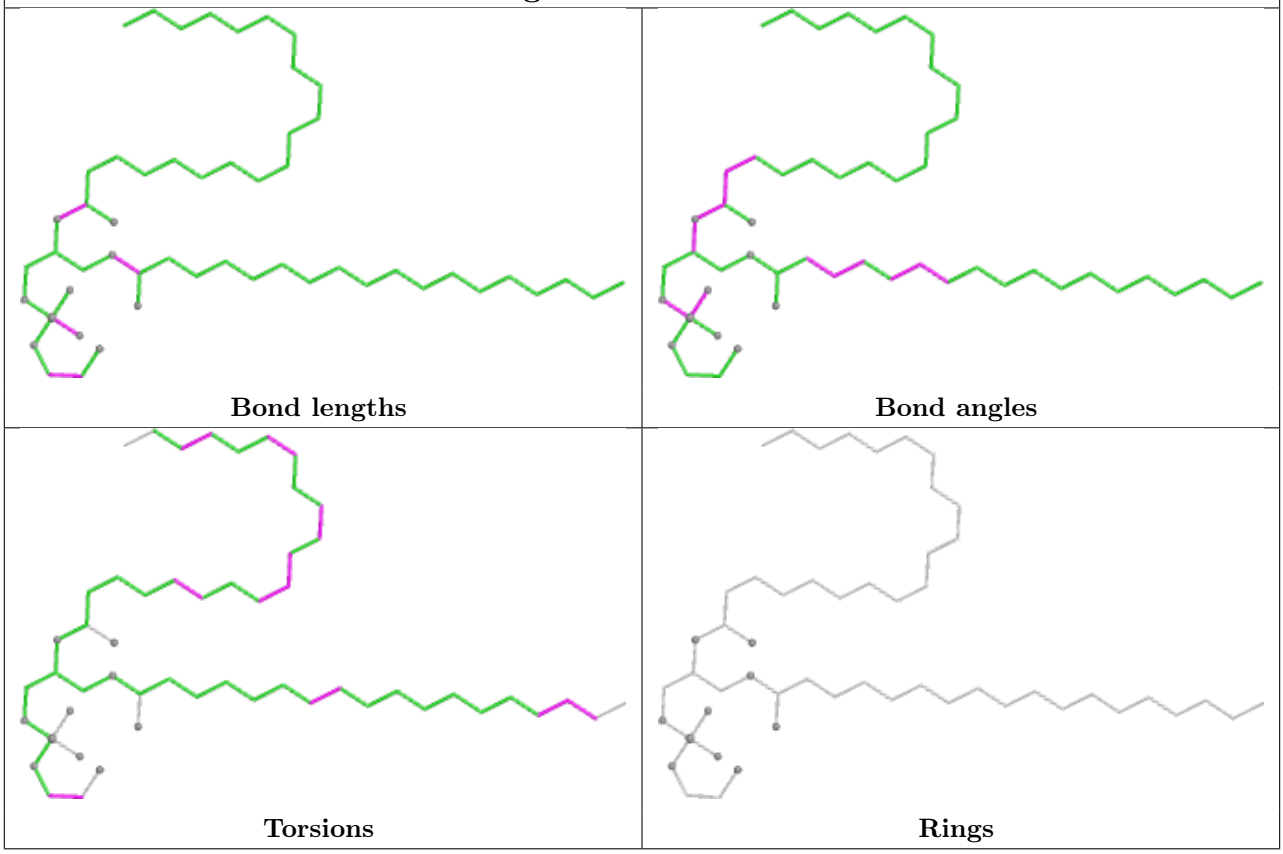
Ligand DMU C 302



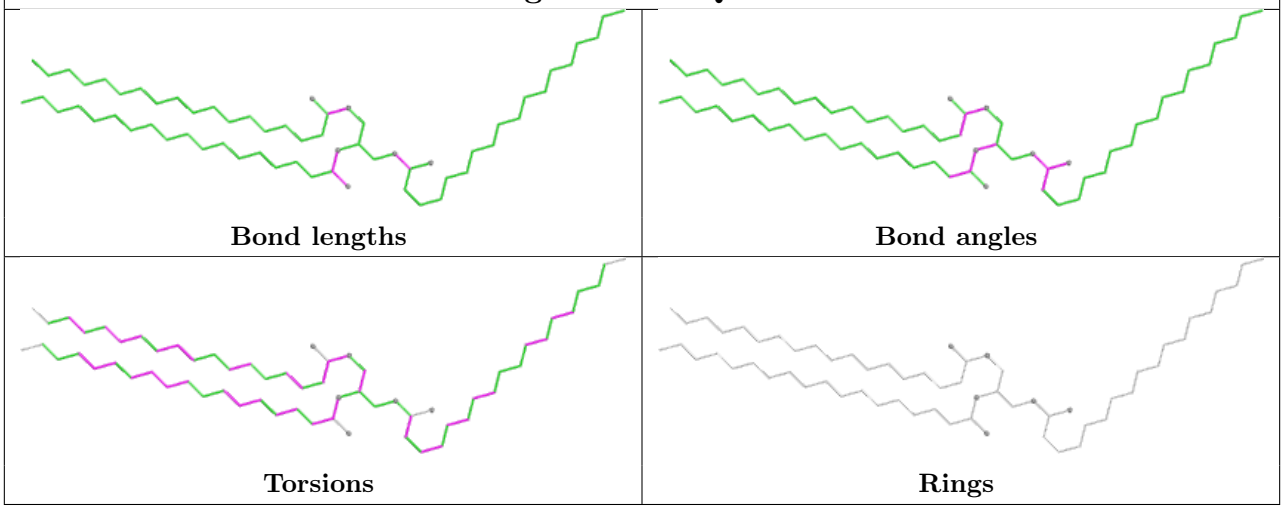
Ligand PGV A 609



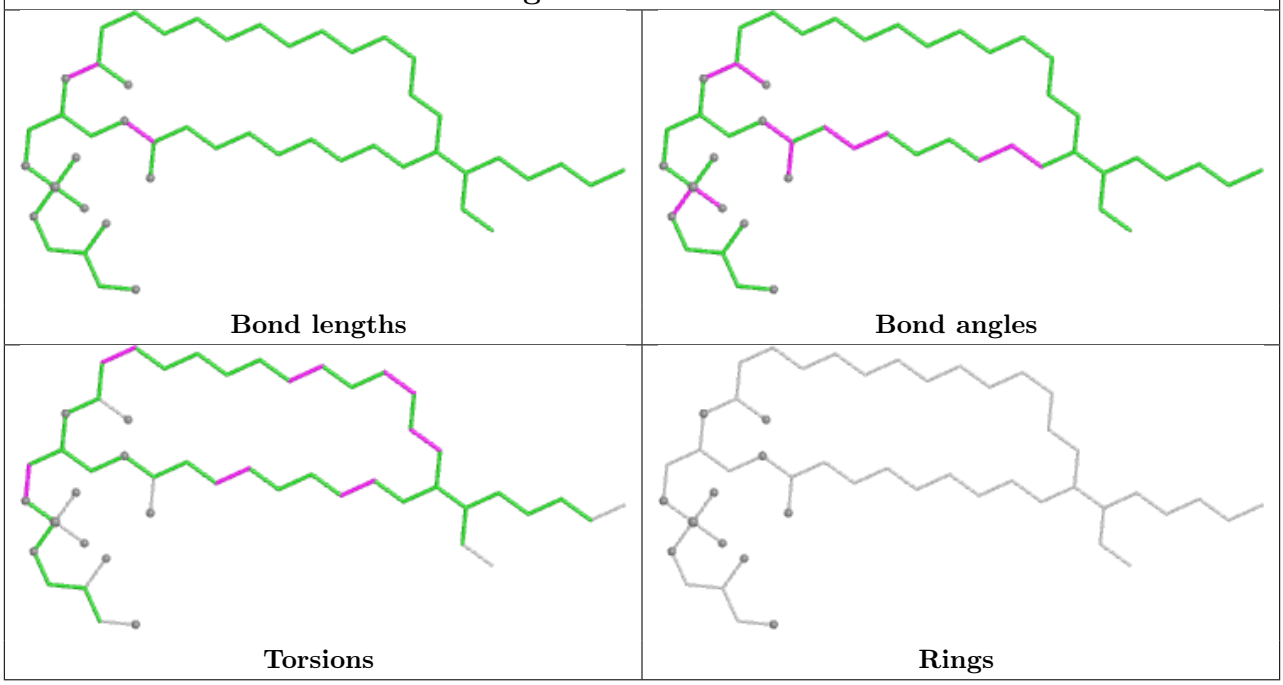
Ligand PEK G 101



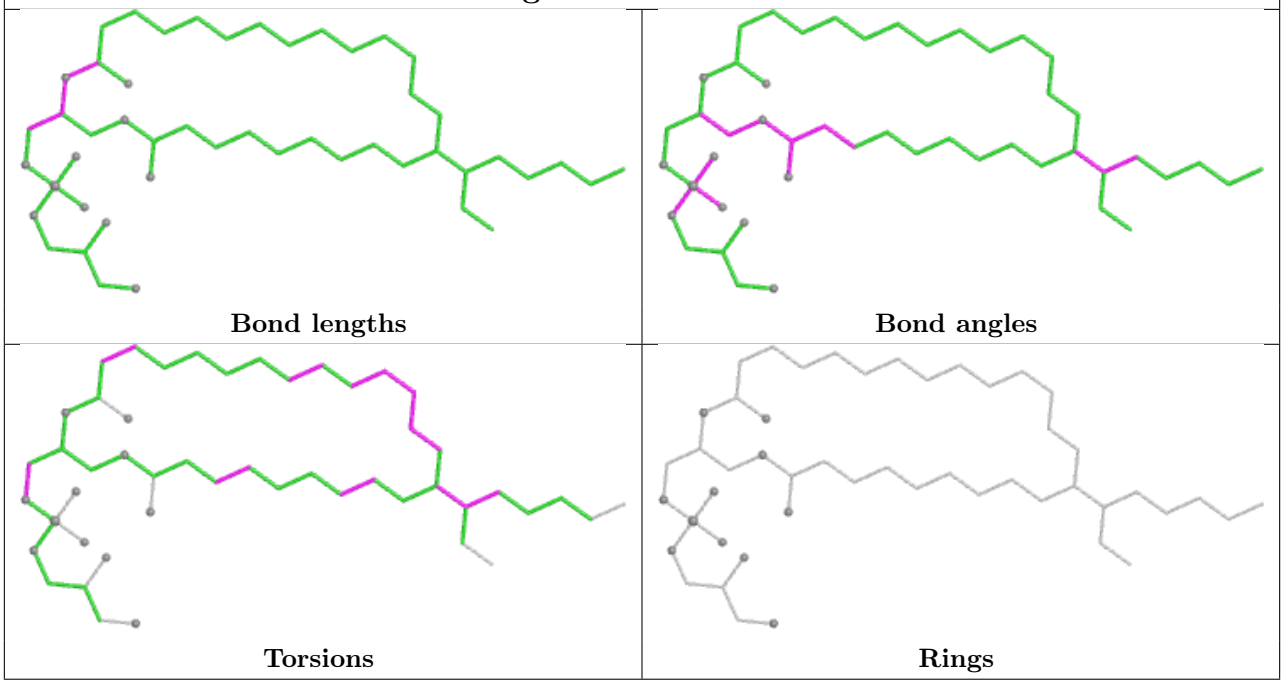
Ligand TGL Q 201



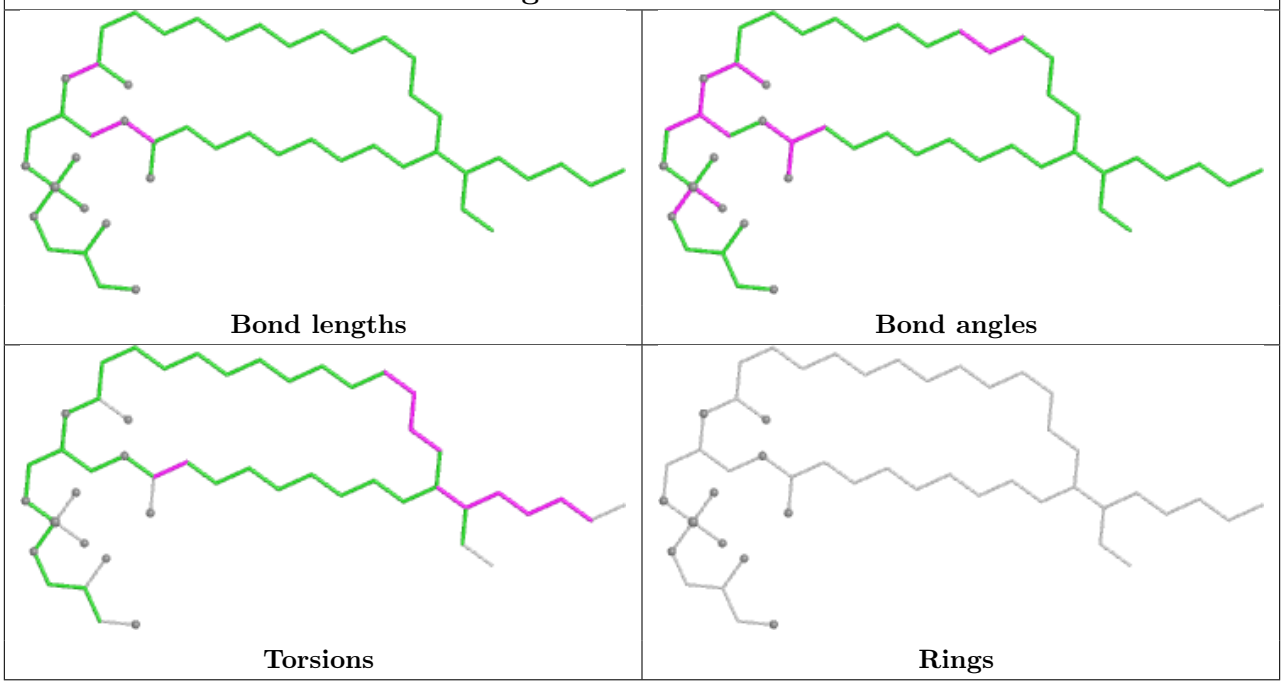
Ligand PGV P 303



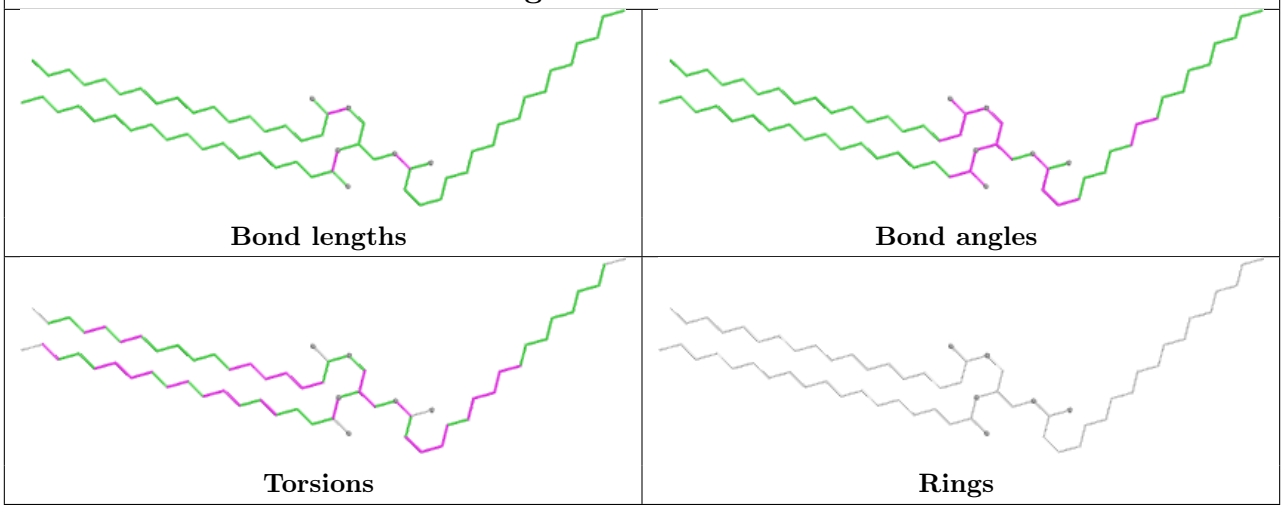
Ligand PGV C 304

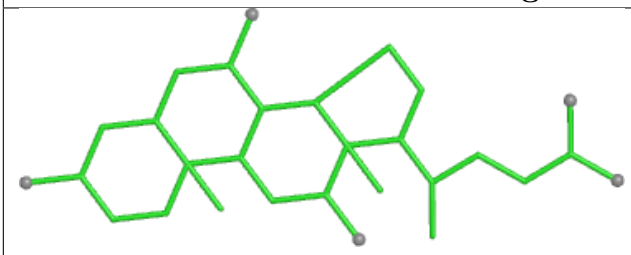
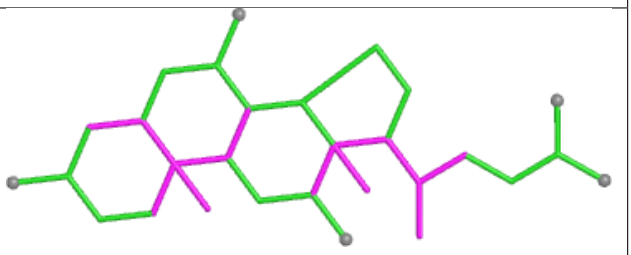
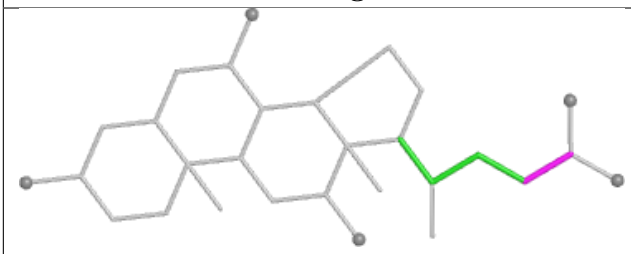
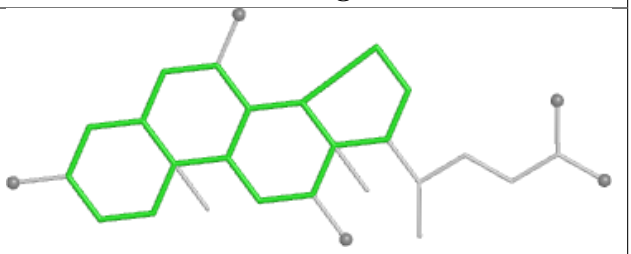


Ligand PGV N 609

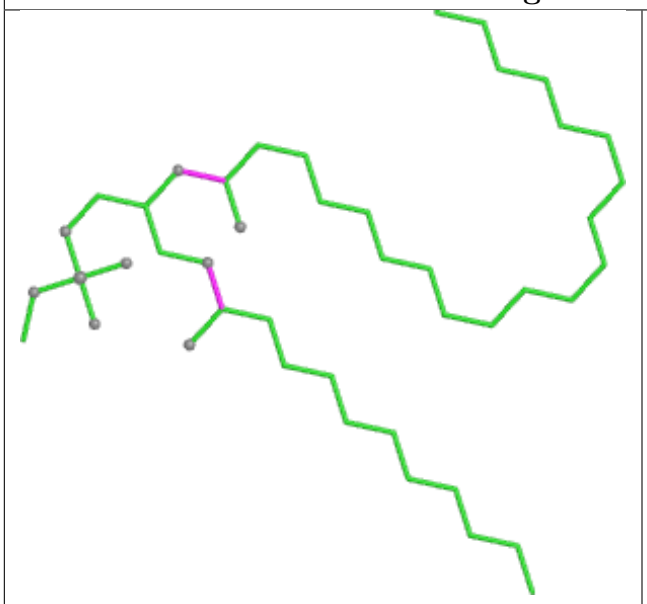


Ligand TGL Y 101

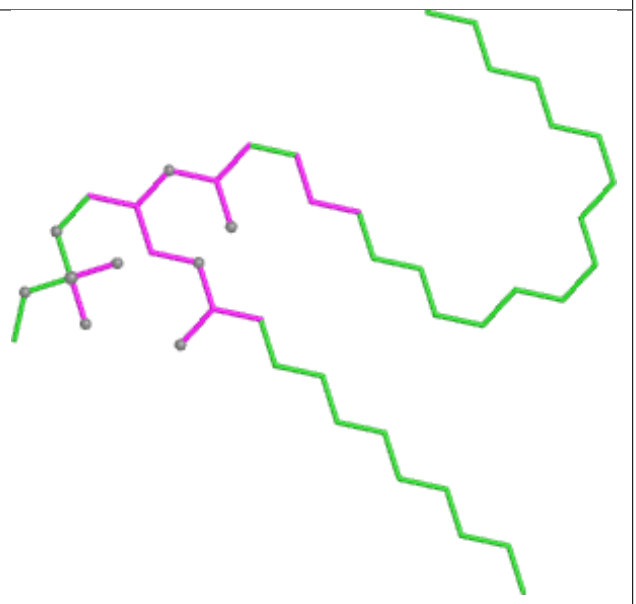


Ligand CHD P 301	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

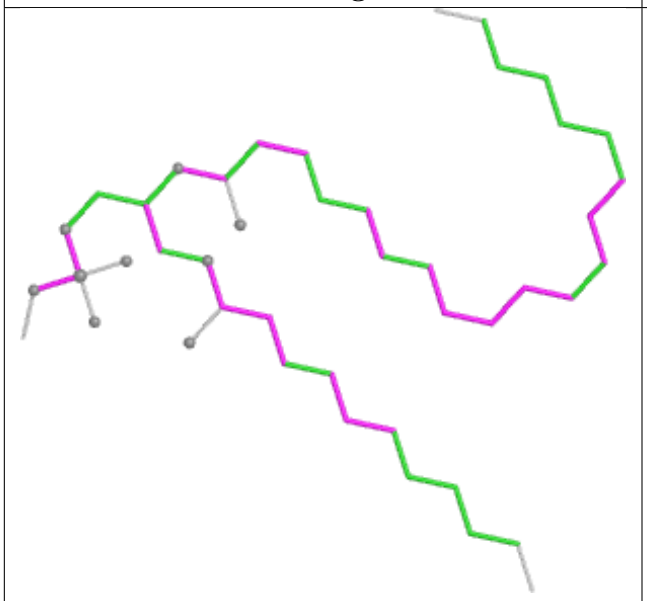
Ligand PEK G 103



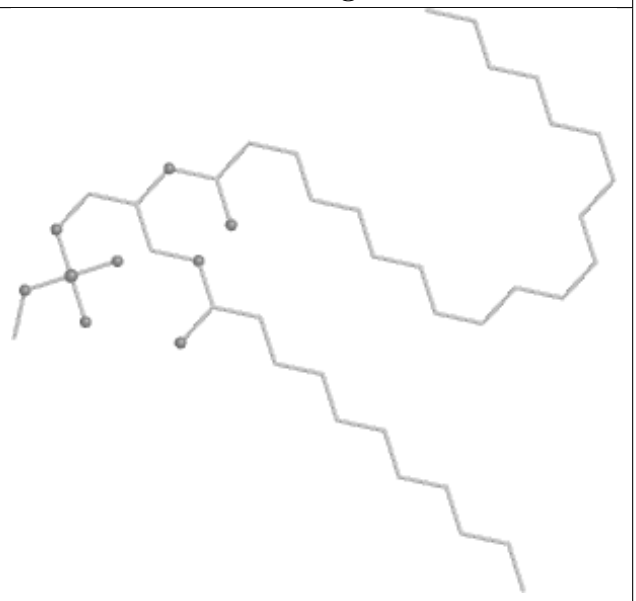
Bond lengths



Bond angles

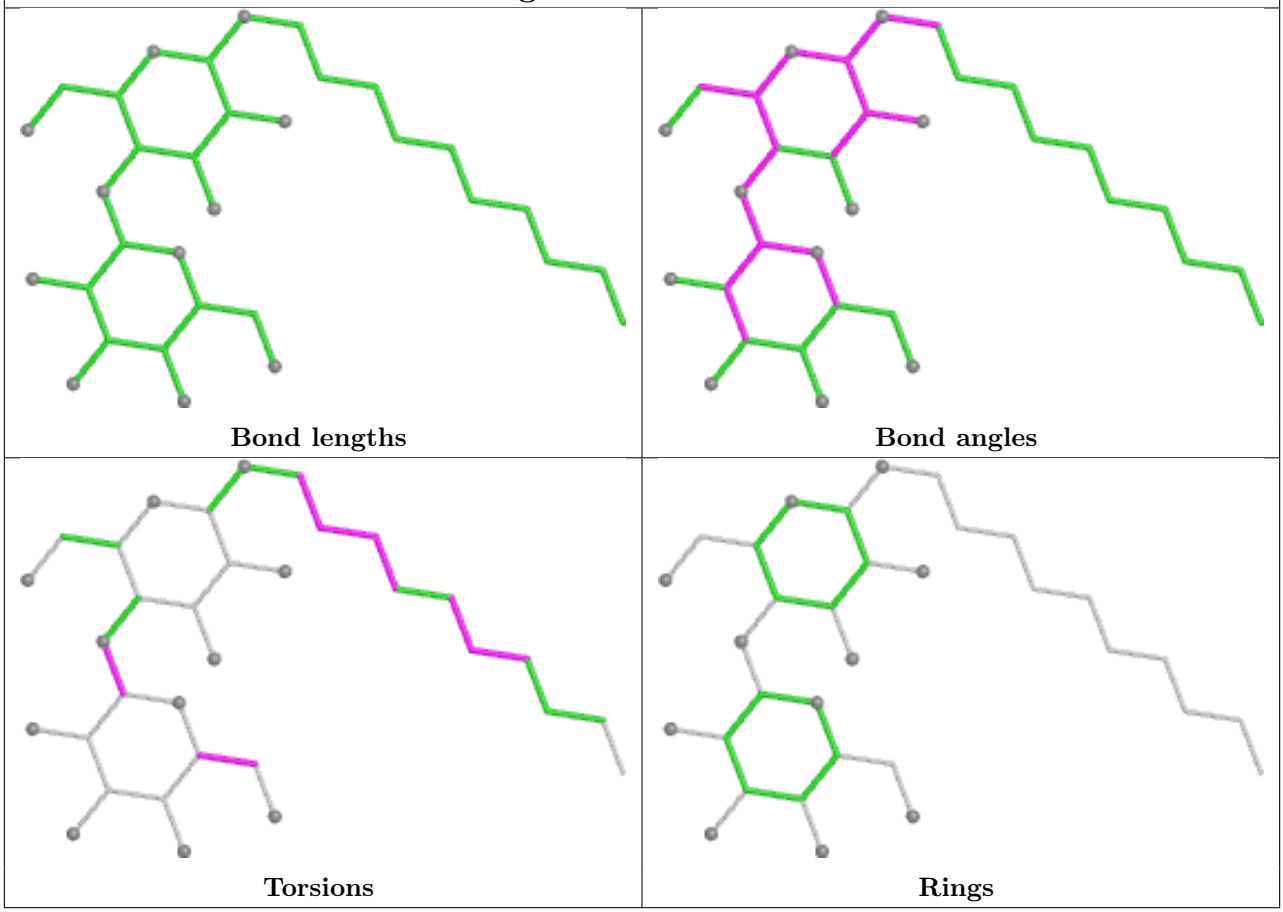


Torsions

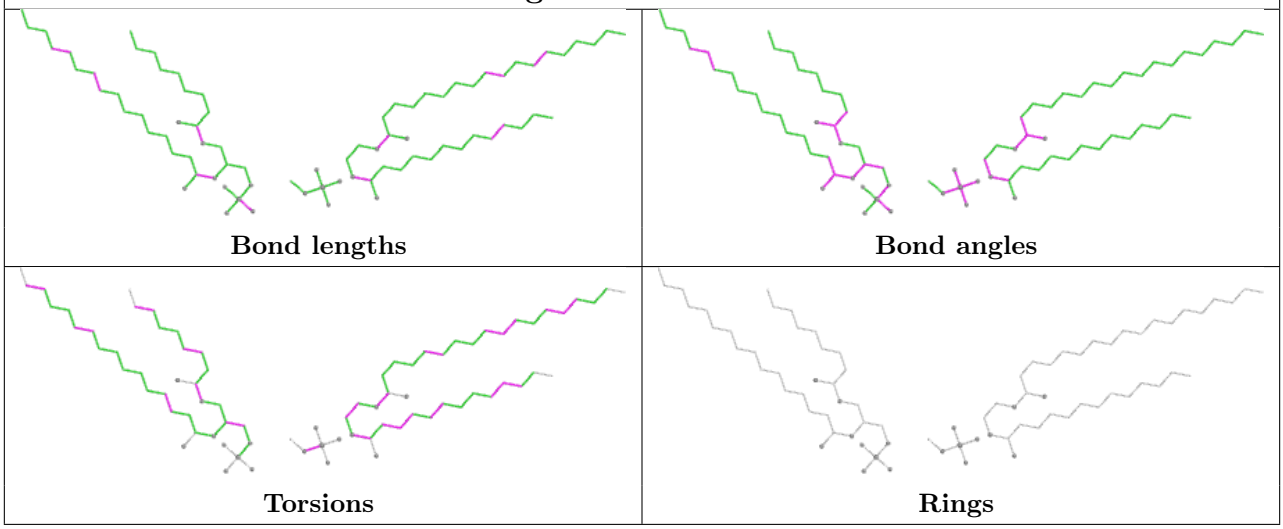


Rings

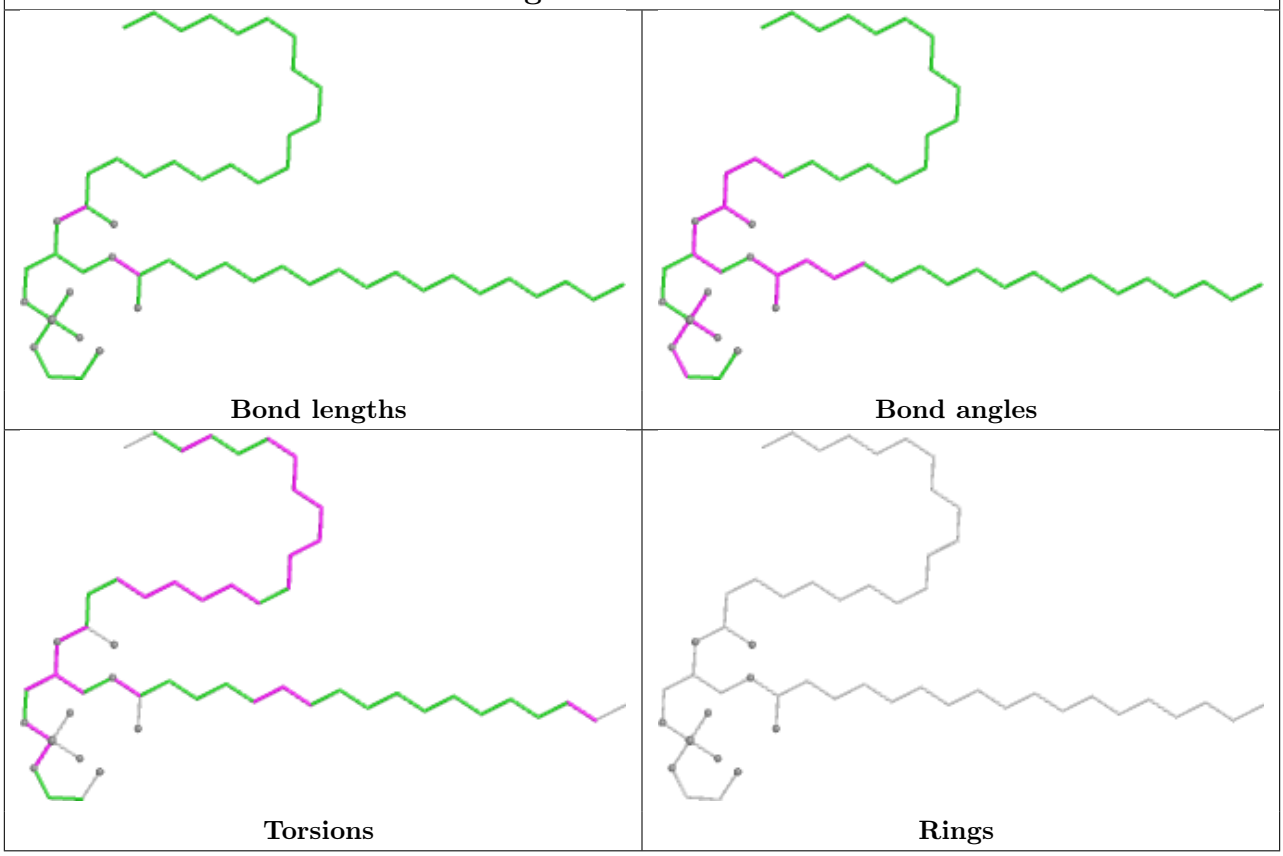
Ligand DMU P 307



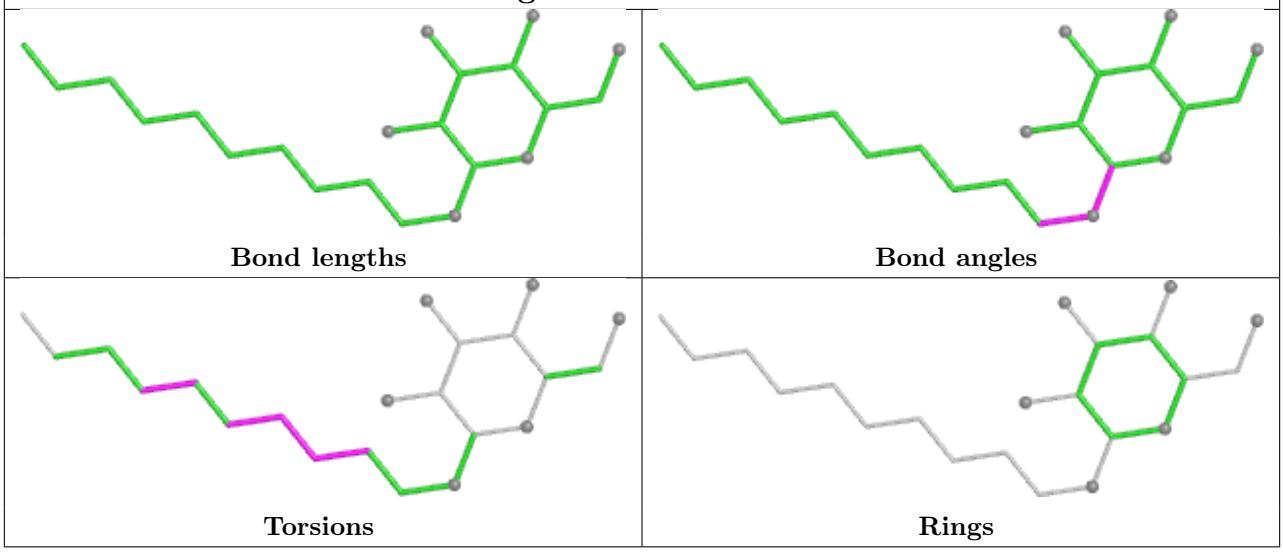
Ligand CDL P 304



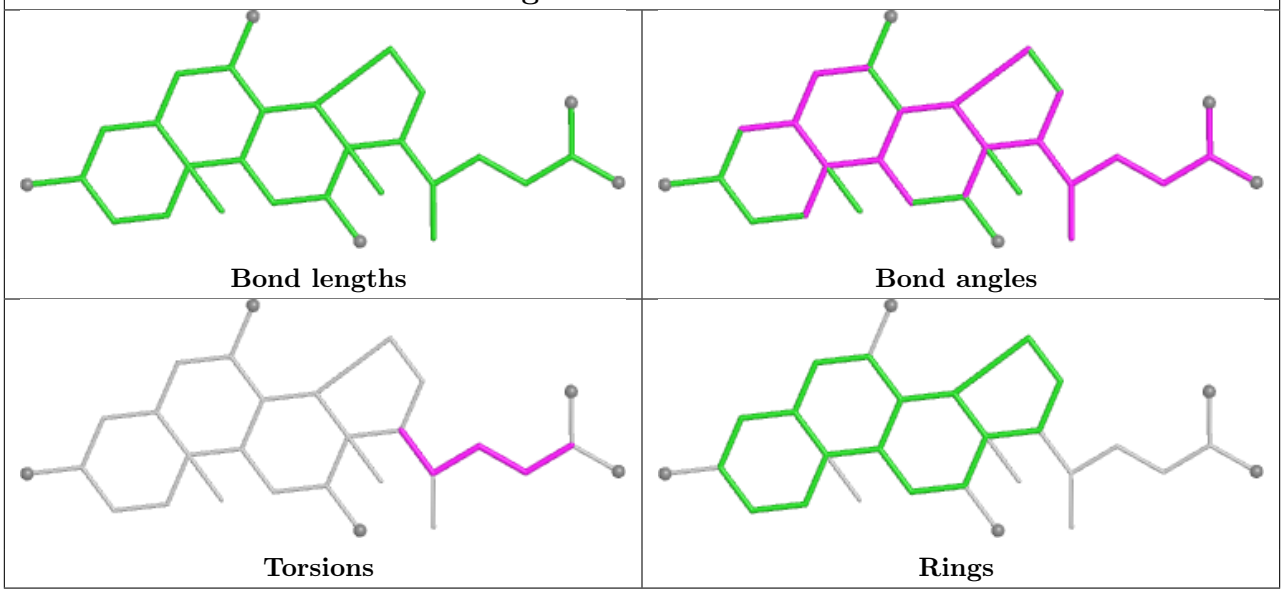
Ligand PEK C 307



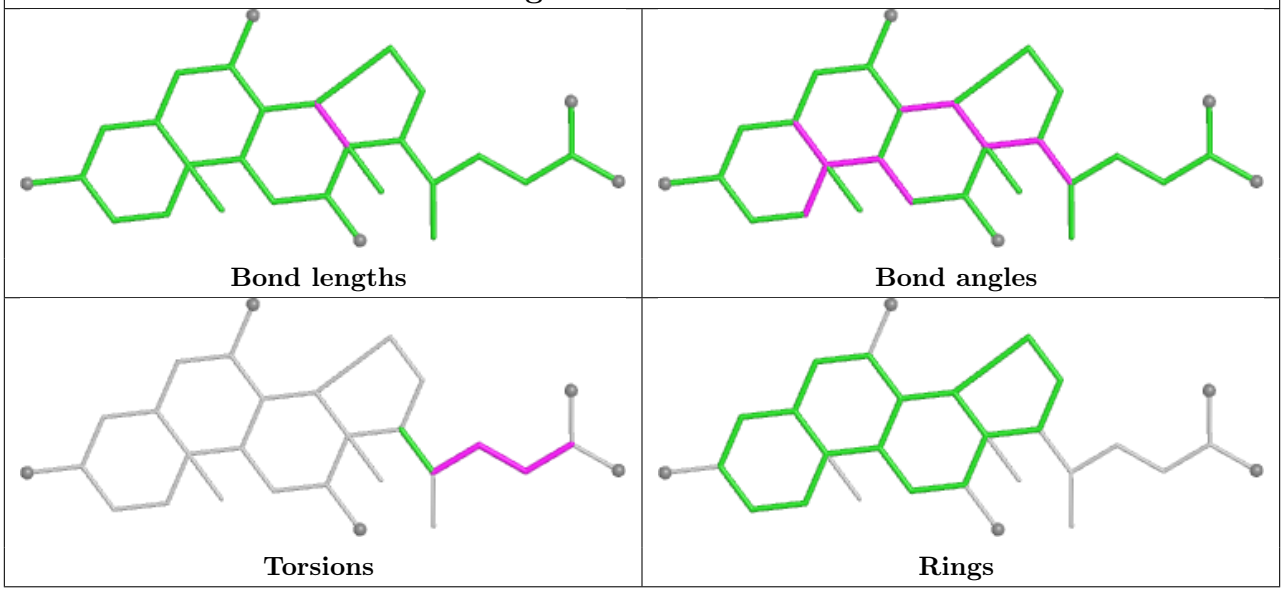
Ligand DMU C 310



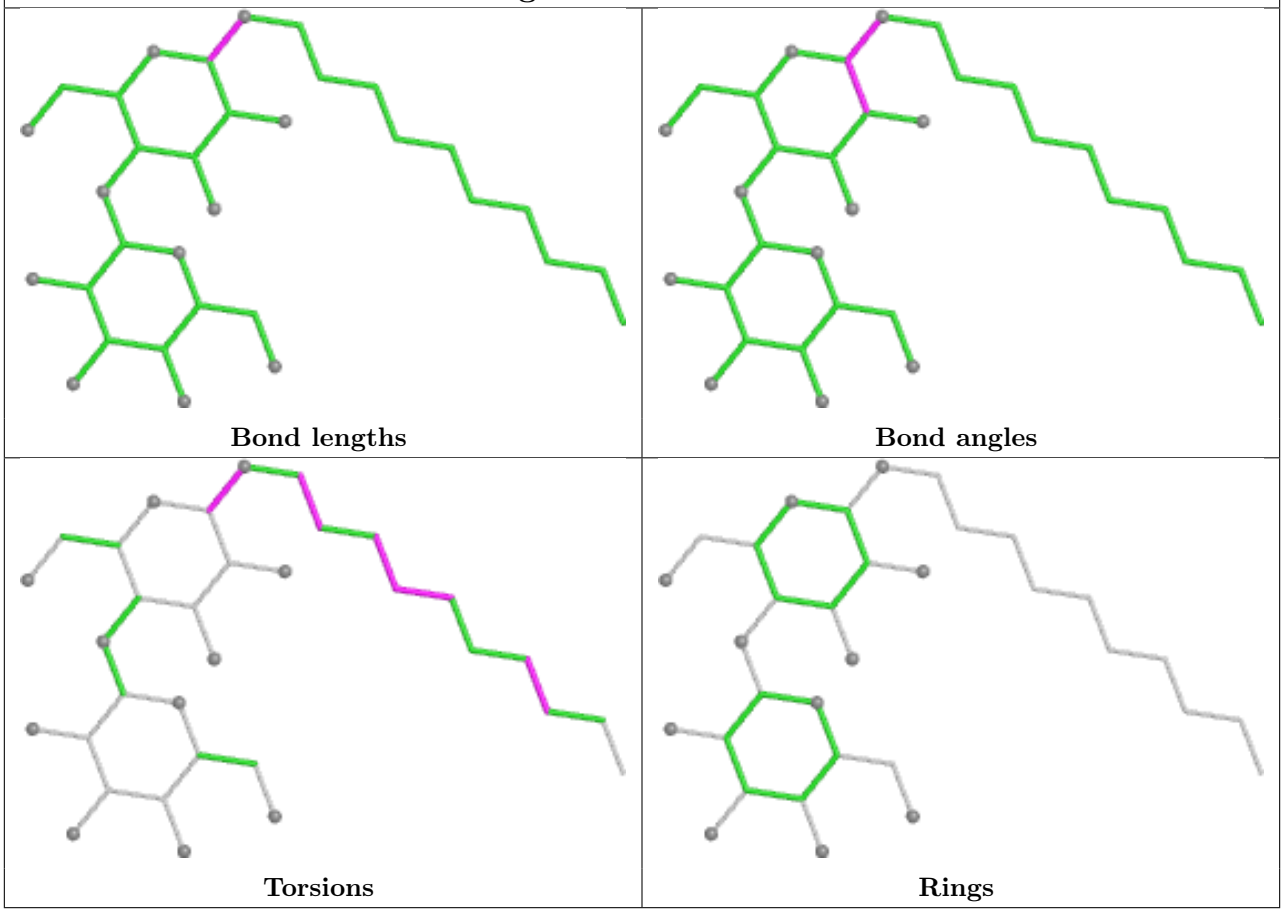
Ligand CHD C 306



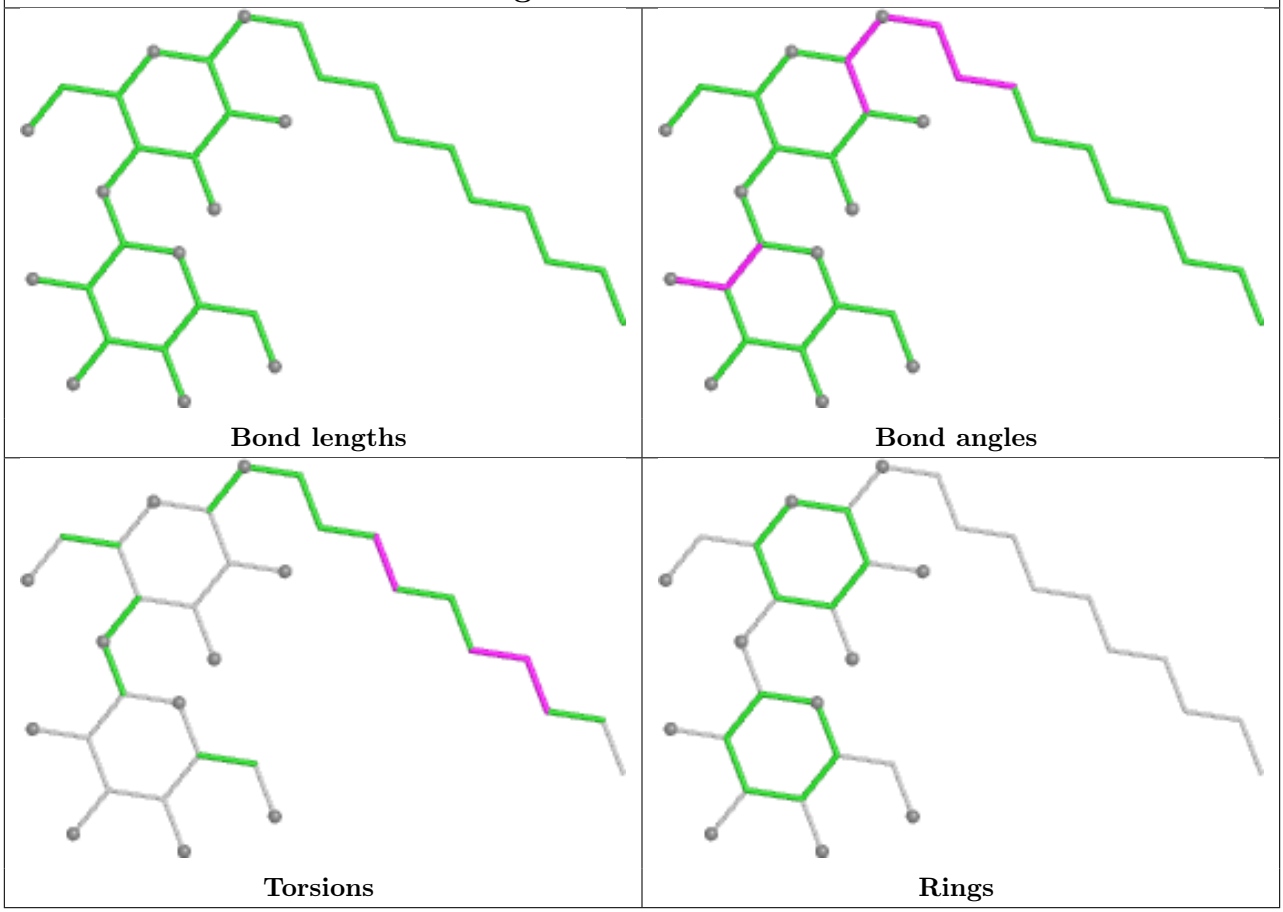
Ligand CHD J 101



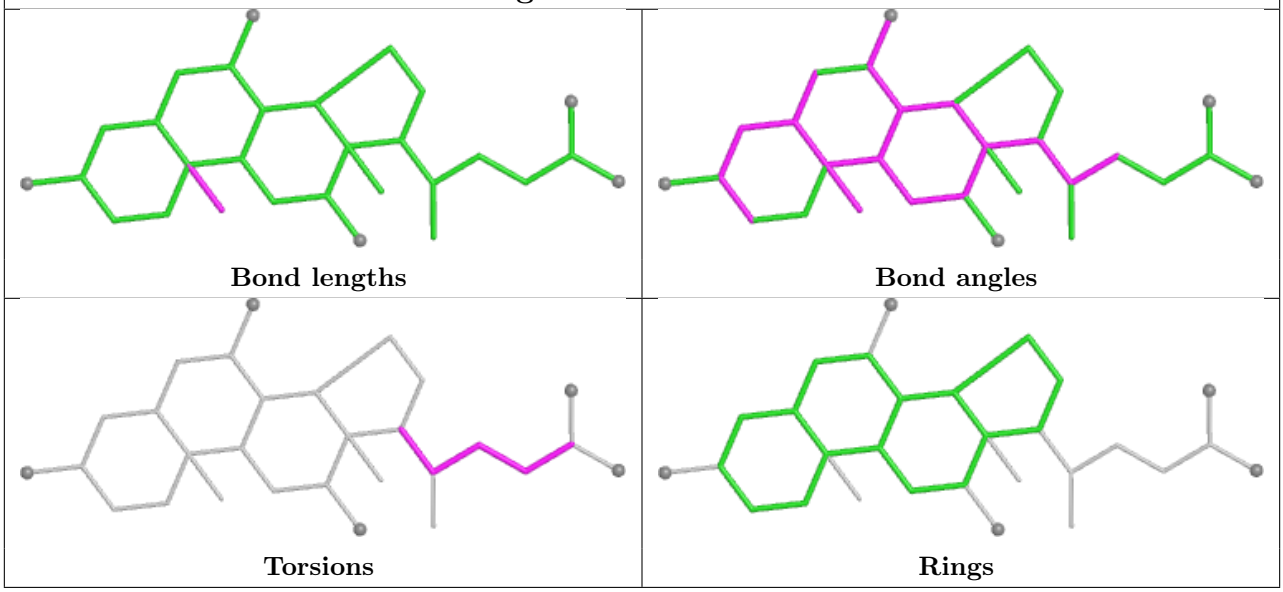
Ligand DMU P 308



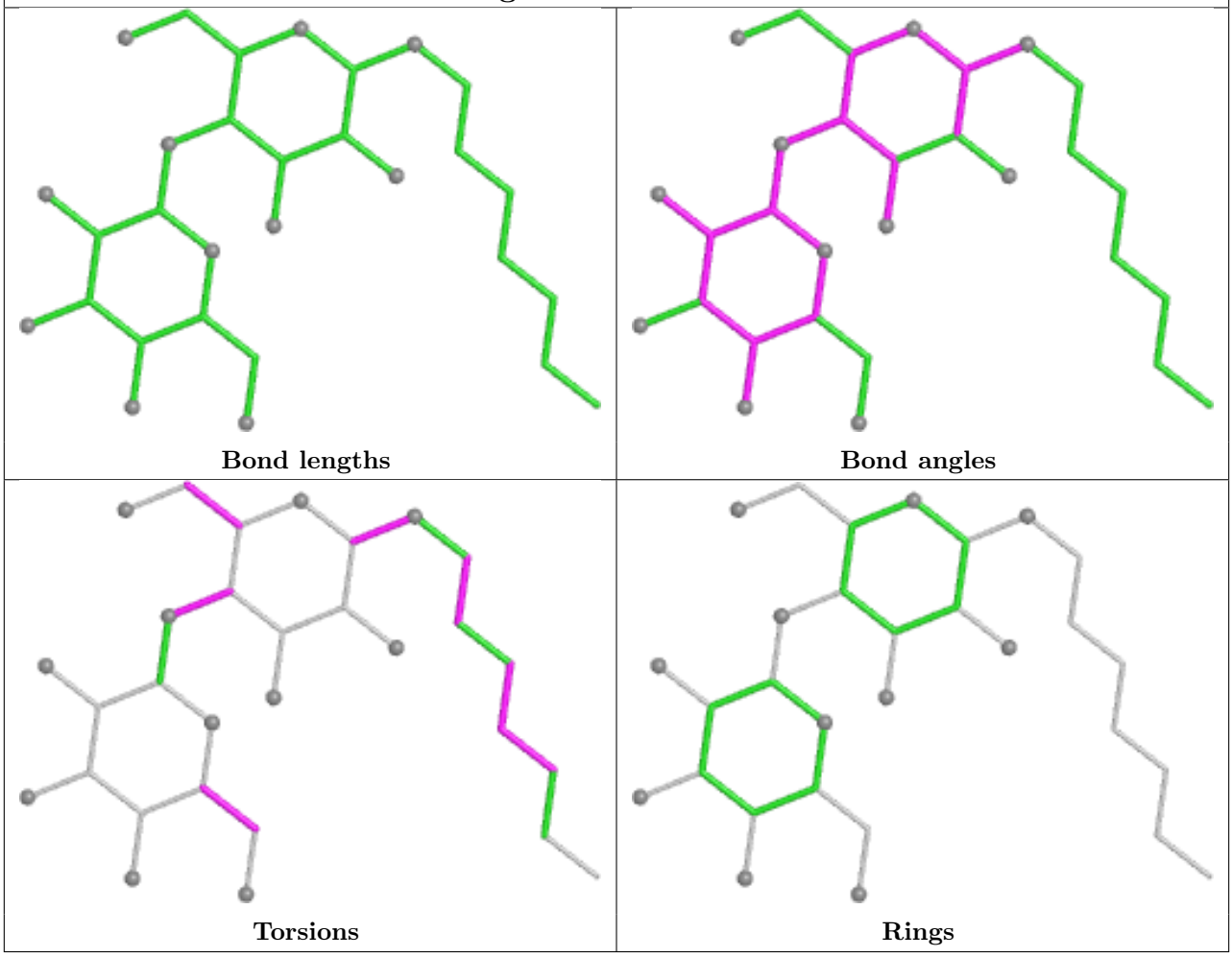
Ligand DMU M 101



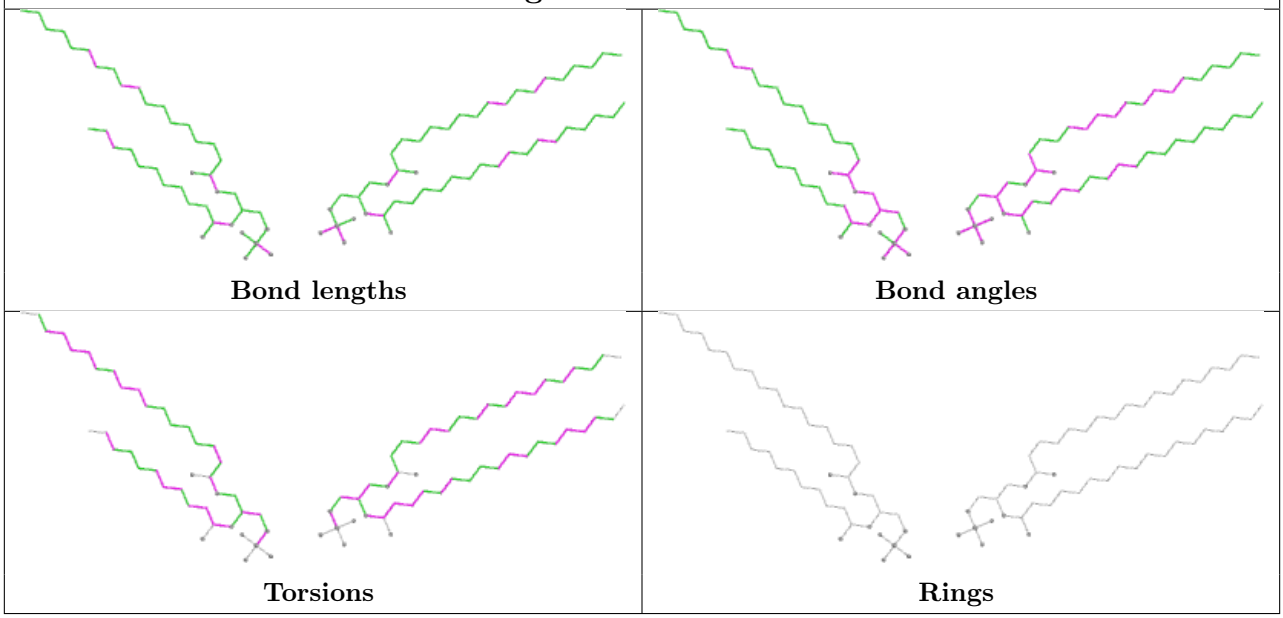
Ligand CHD W 101



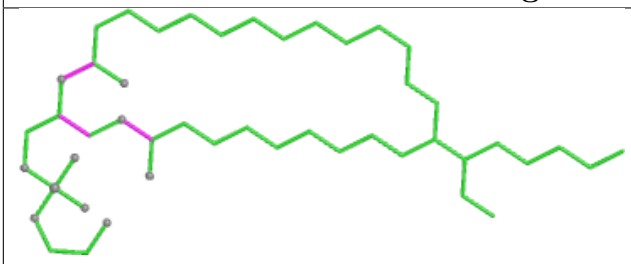
Ligand DMU L 102



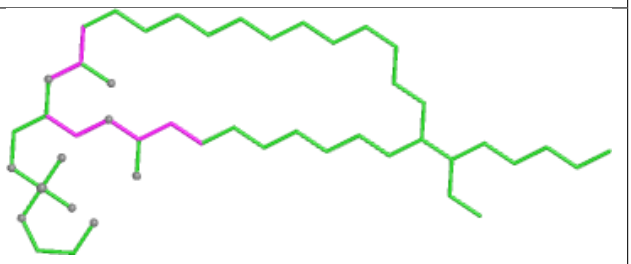
Ligand CDL C 305



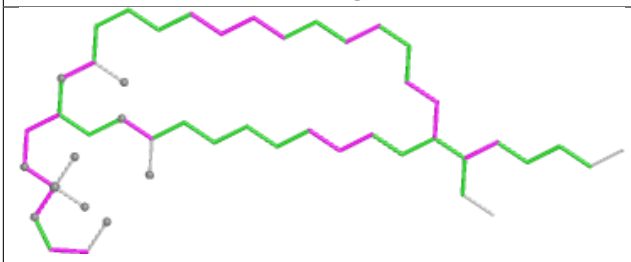
Ligand PGV C 308



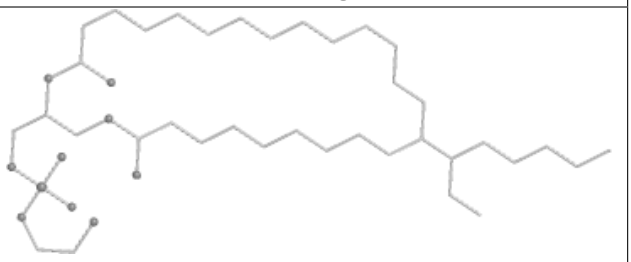
Bond lengths



Bond angles

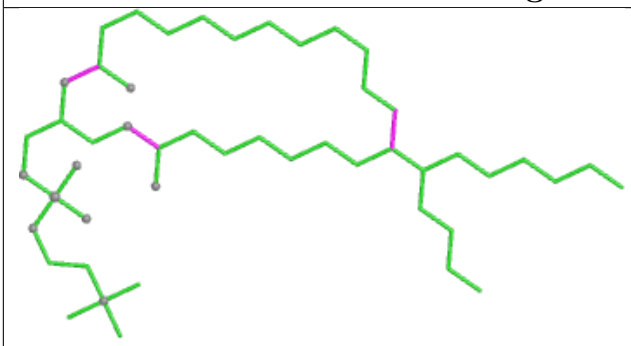


Torsions

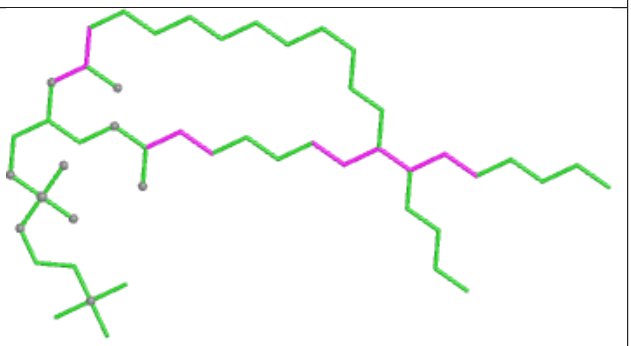


Rings

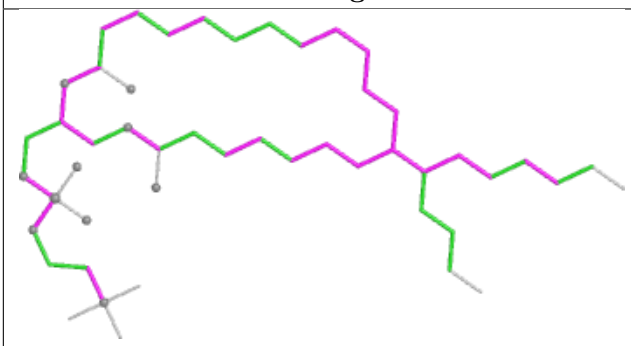
Ligand PSC O 302



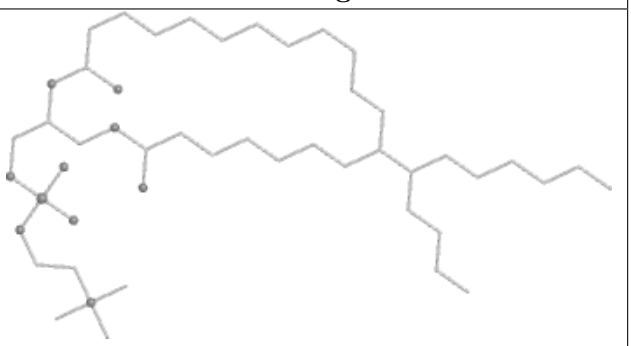
Bond lengths



Bond angles

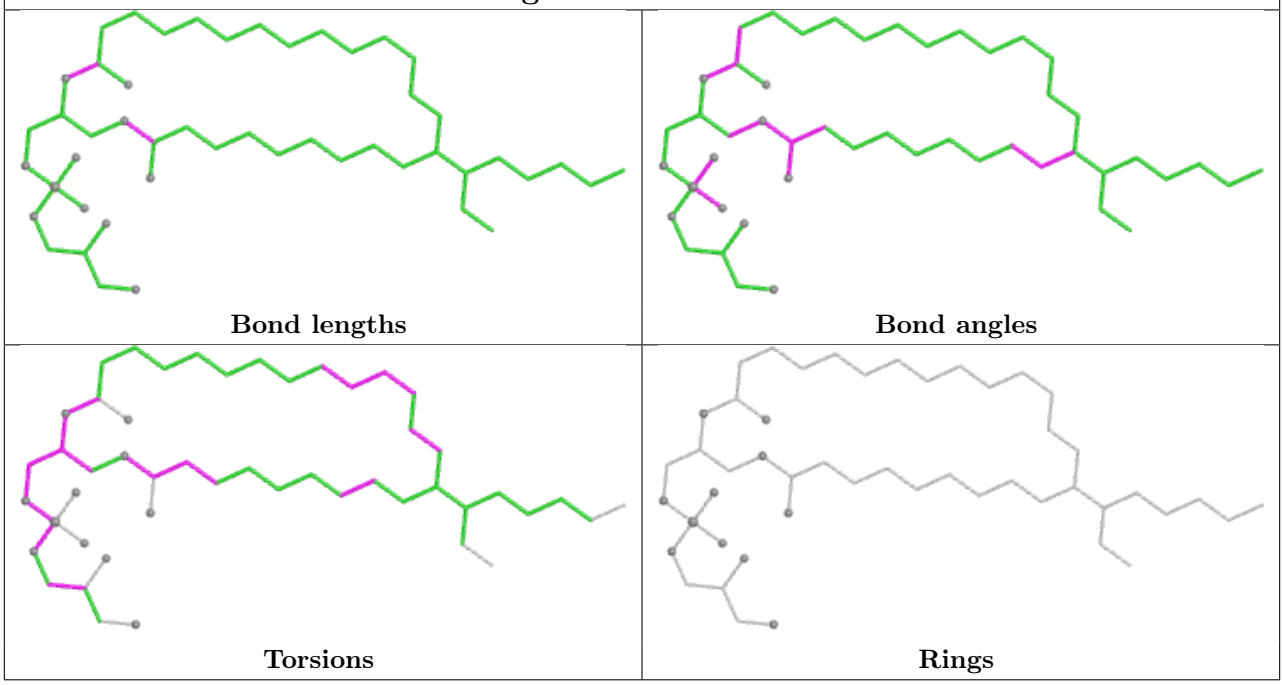


Torsions

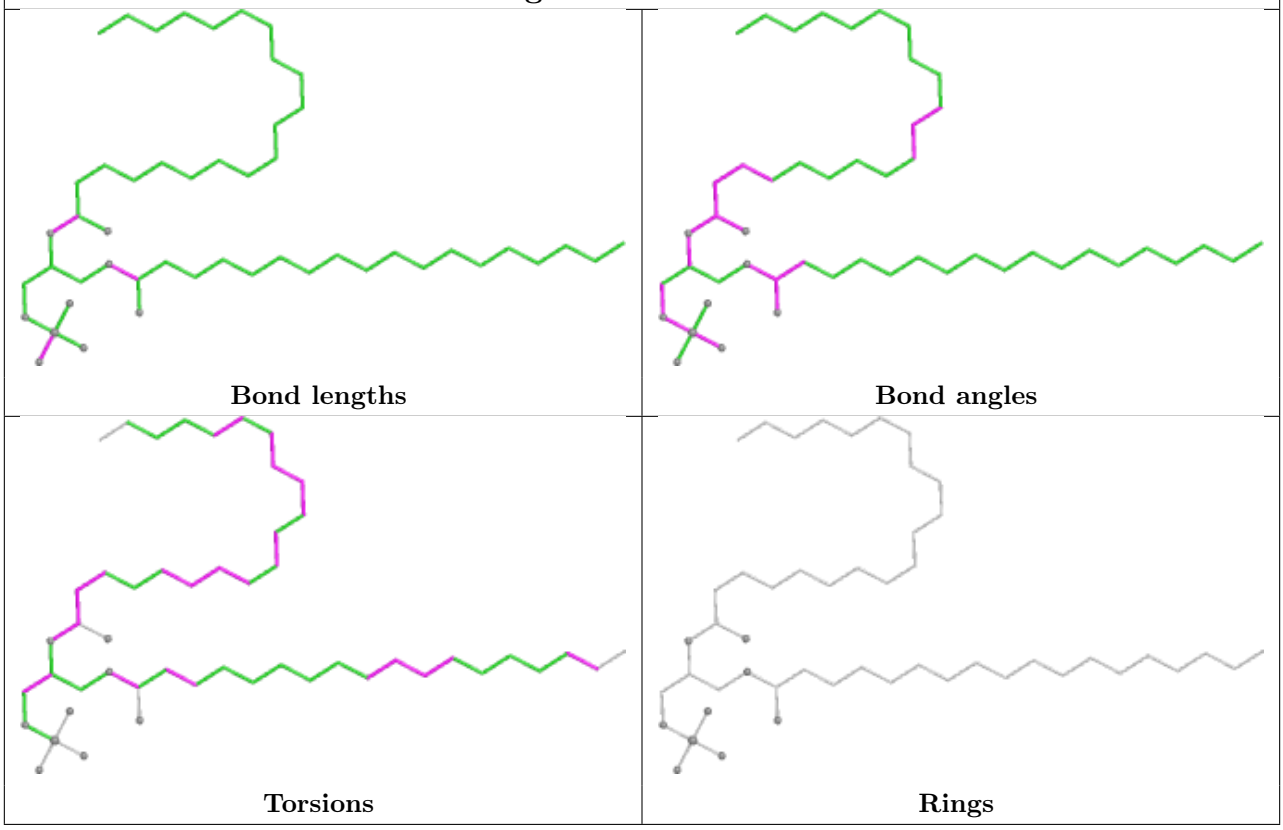


Rings

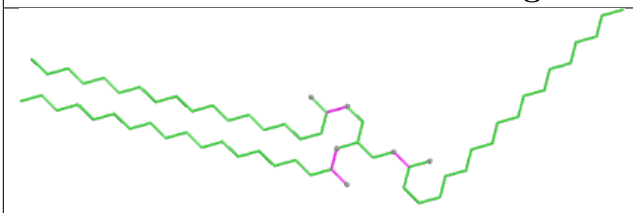
Ligand PGV N 619



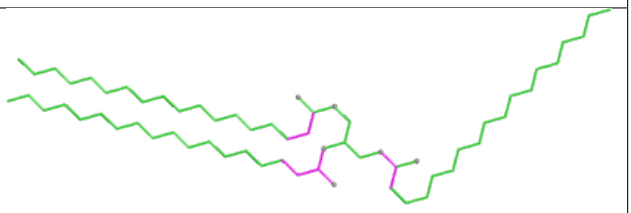
Ligand PEK T 101



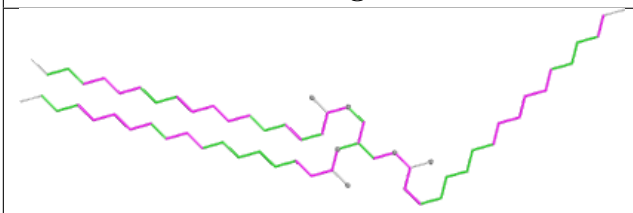
Ligand TGL D 201



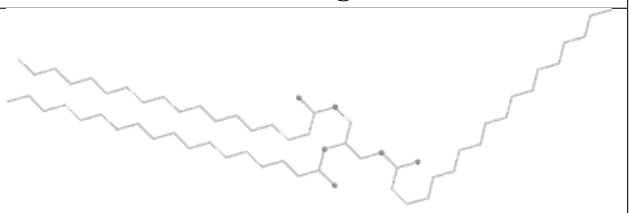
Bond lengths



Bond angles

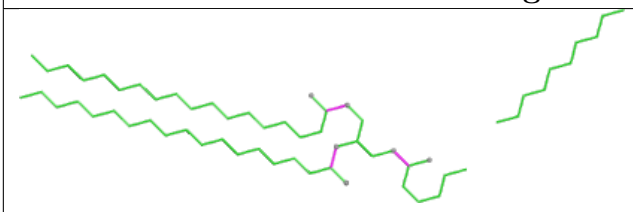


Torsions

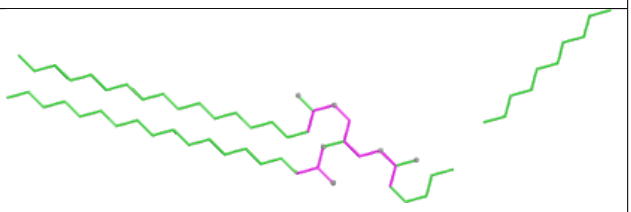


Rings

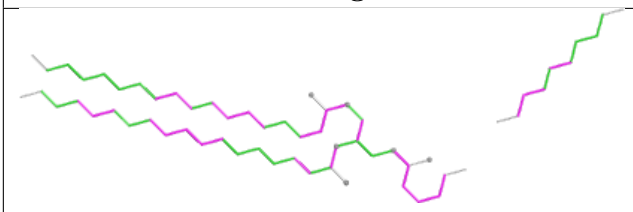
Ligand TGL N 610



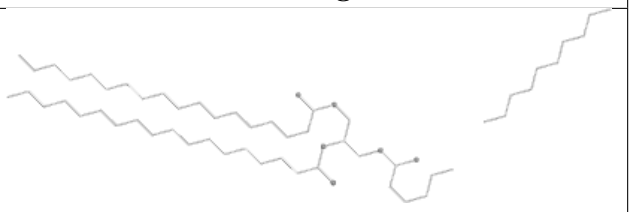
Bond lengths



Bond angles

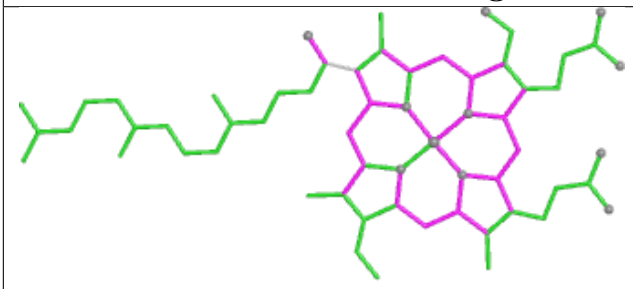


Torsions

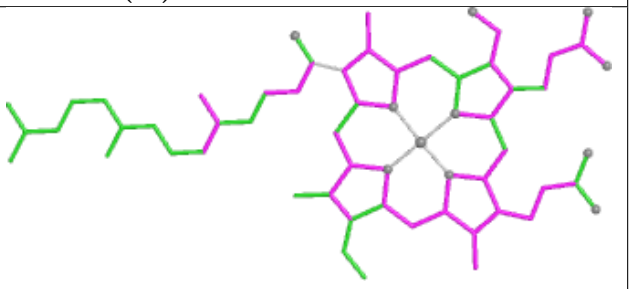


Rings

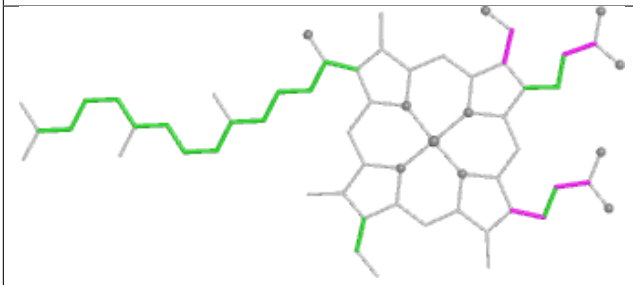
Ligand HEA N 603 (A)



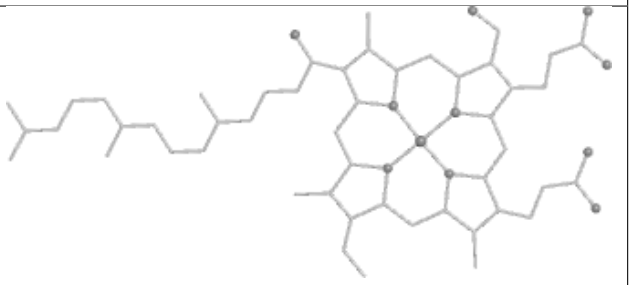
Bond lengths



Bond angles

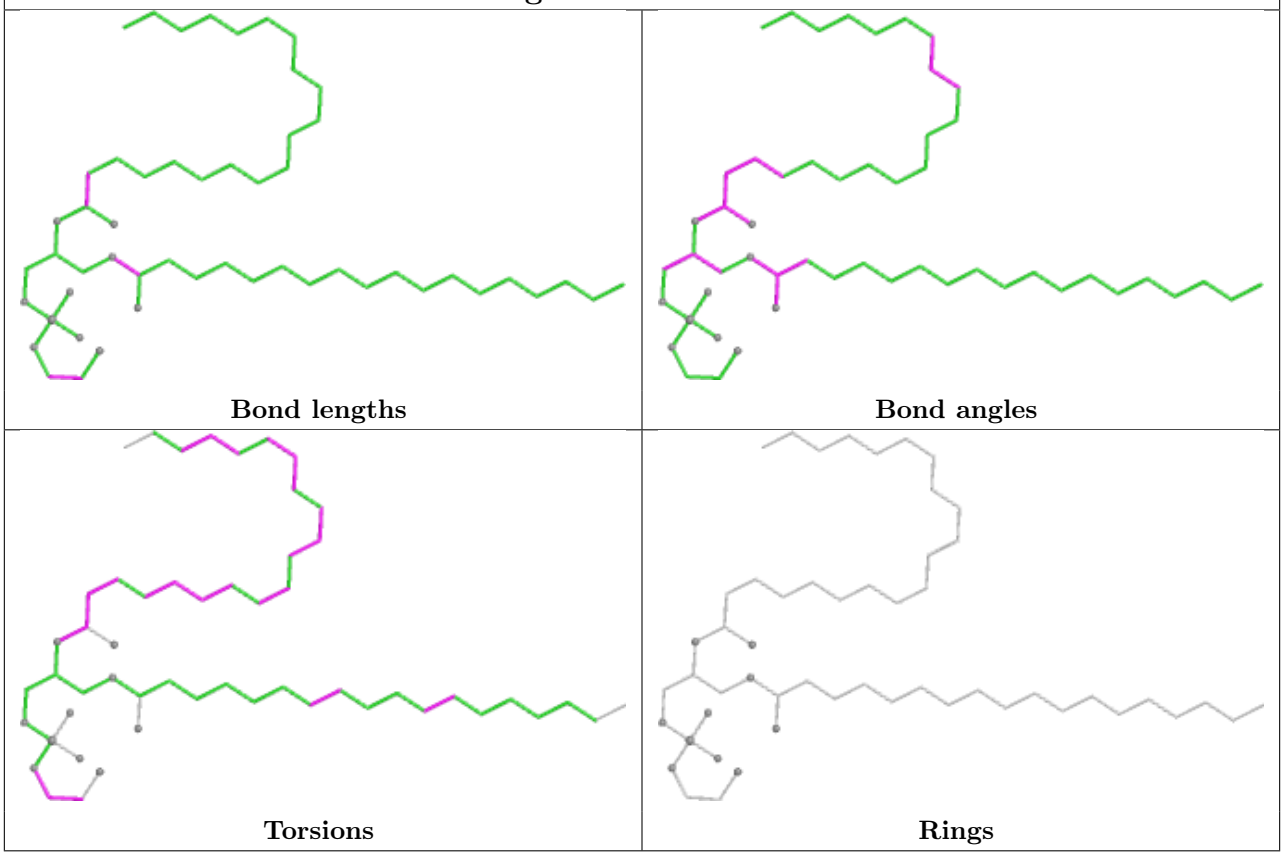


Torsions

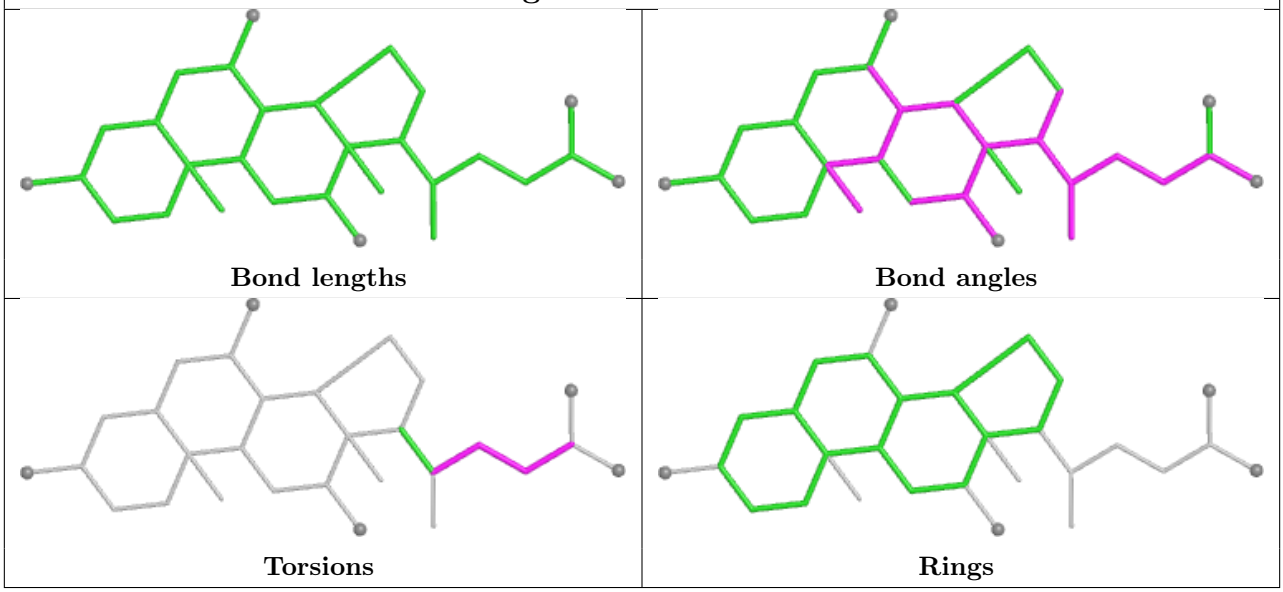


Rings

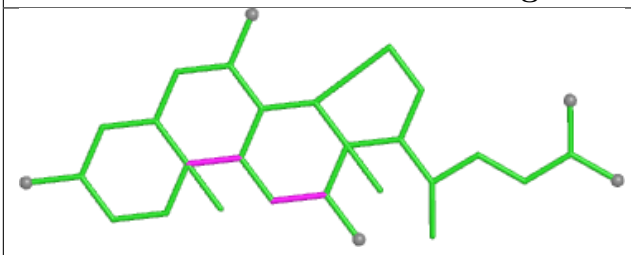
Ligand PEK P 312



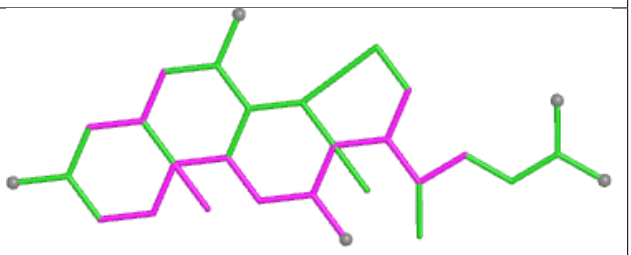
Ligand CHD P 305



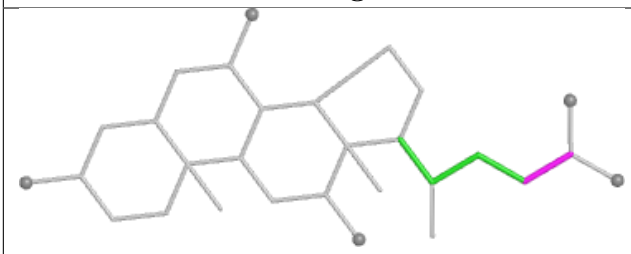
Ligand CHD B 302



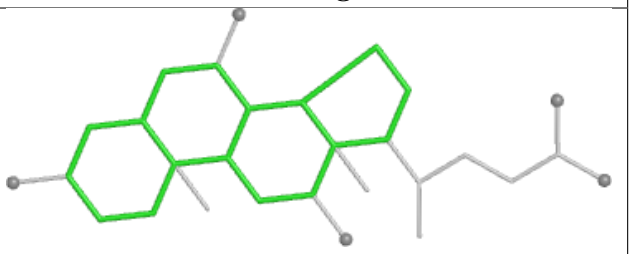
Bond lengths



Bond angles

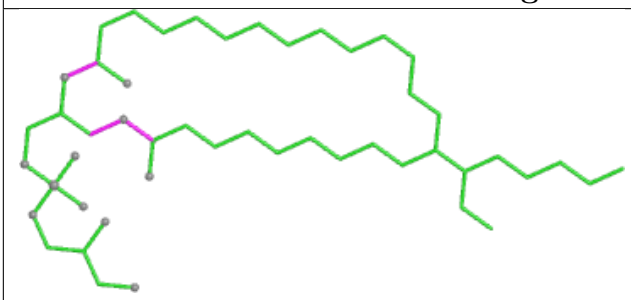


Torsions

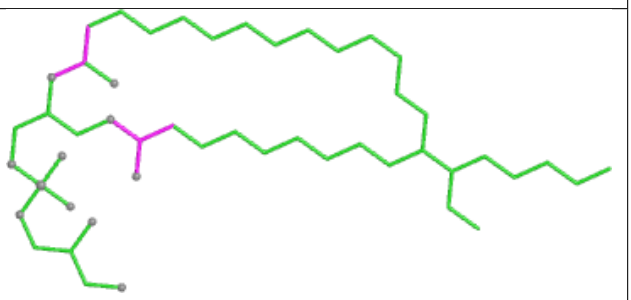


Rings

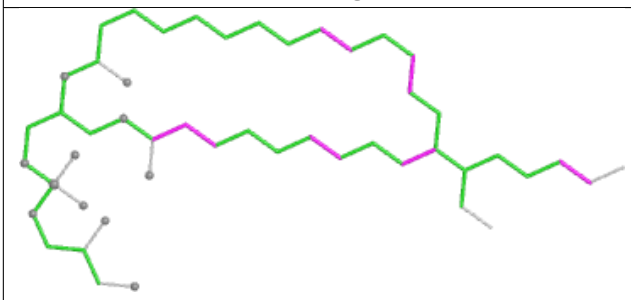
Ligand PGV A 608



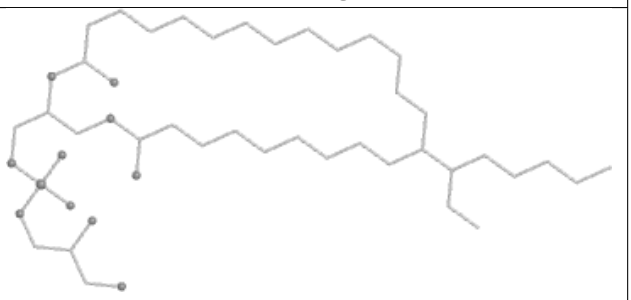
Bond lengths



Bond angles

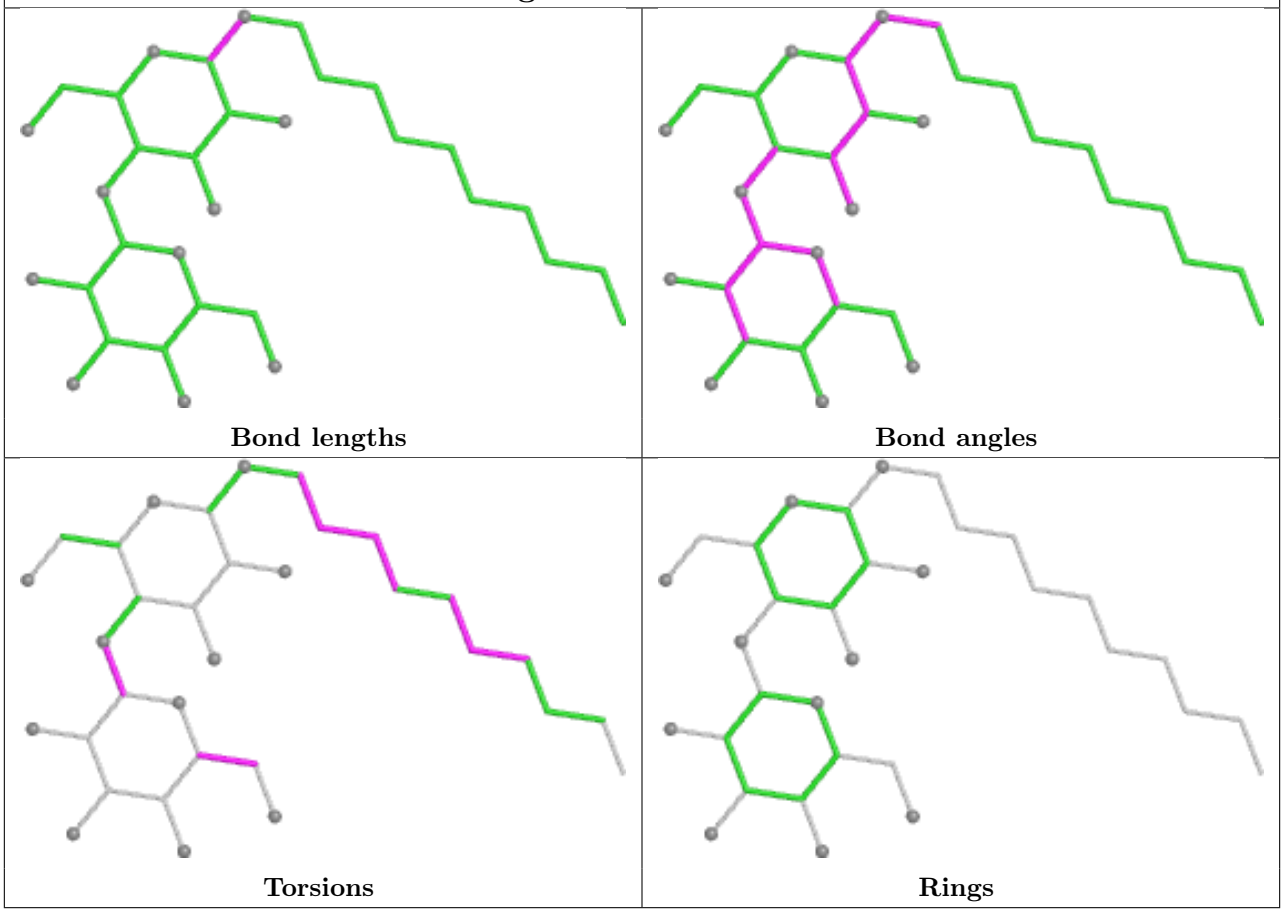


Torsions

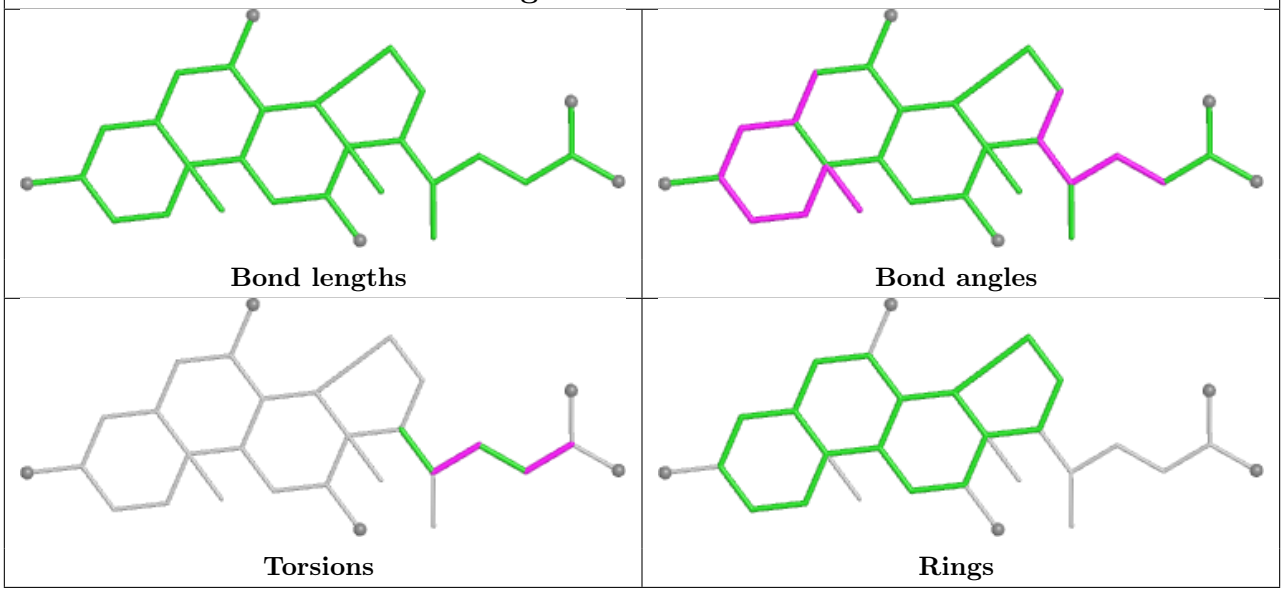


Rings

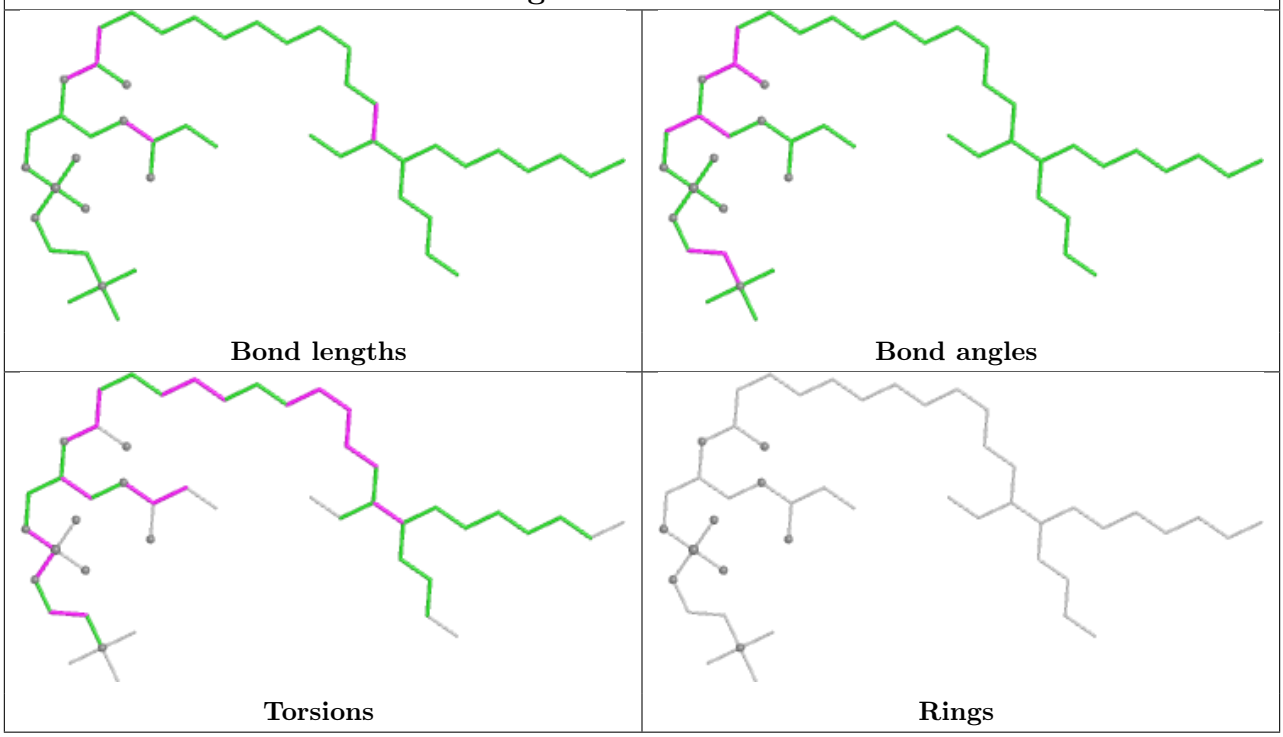
Ligand DMU C 309



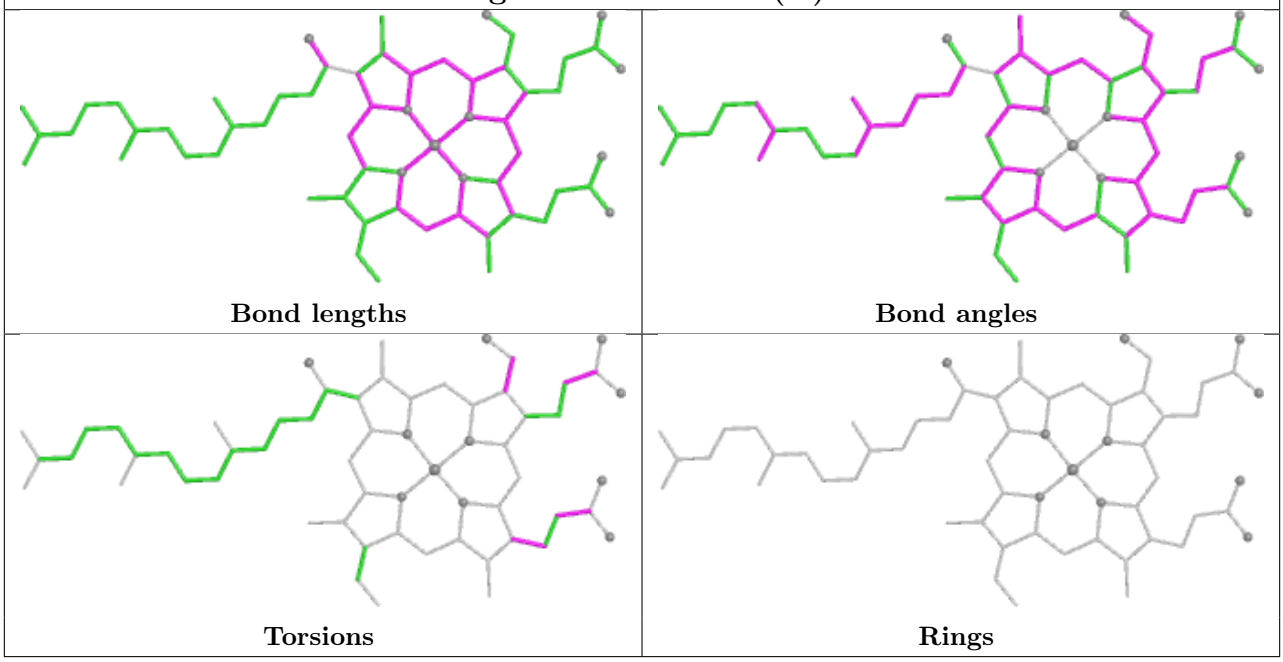
Ligand CHD G 102



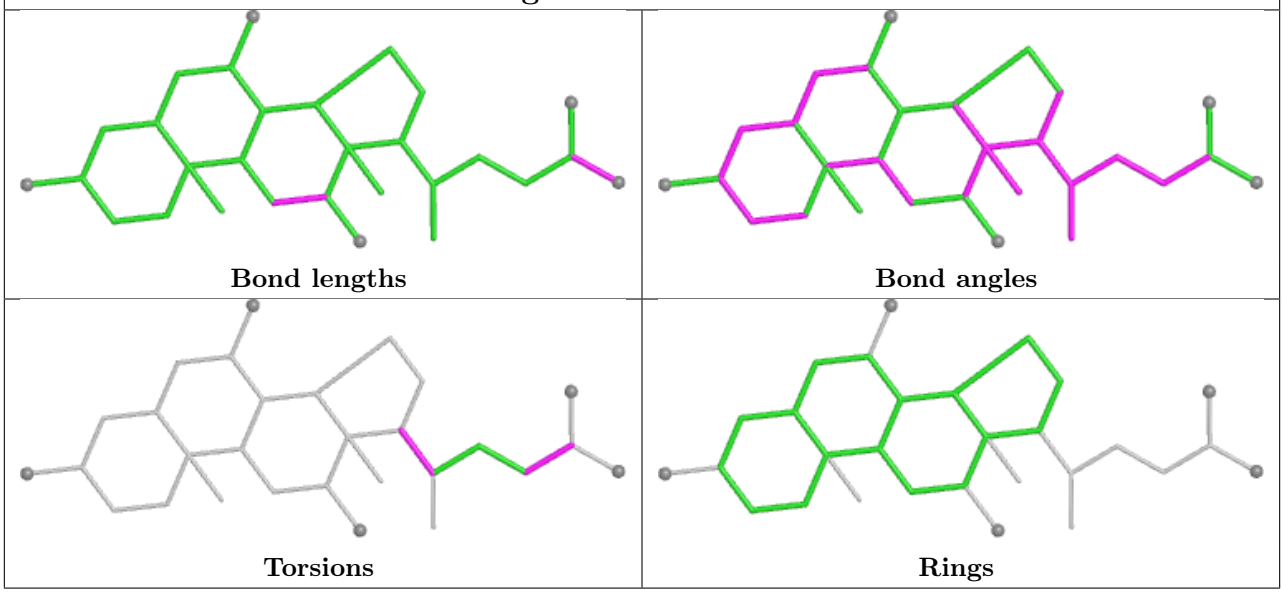
Ligand PSC B 304



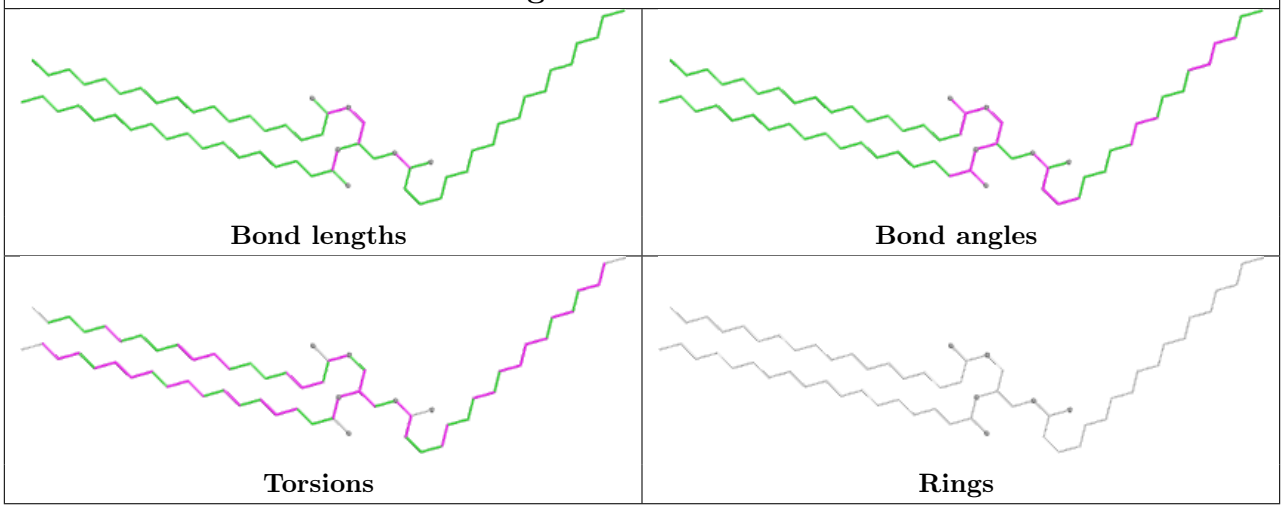
Ligand HEA A 602 (A)



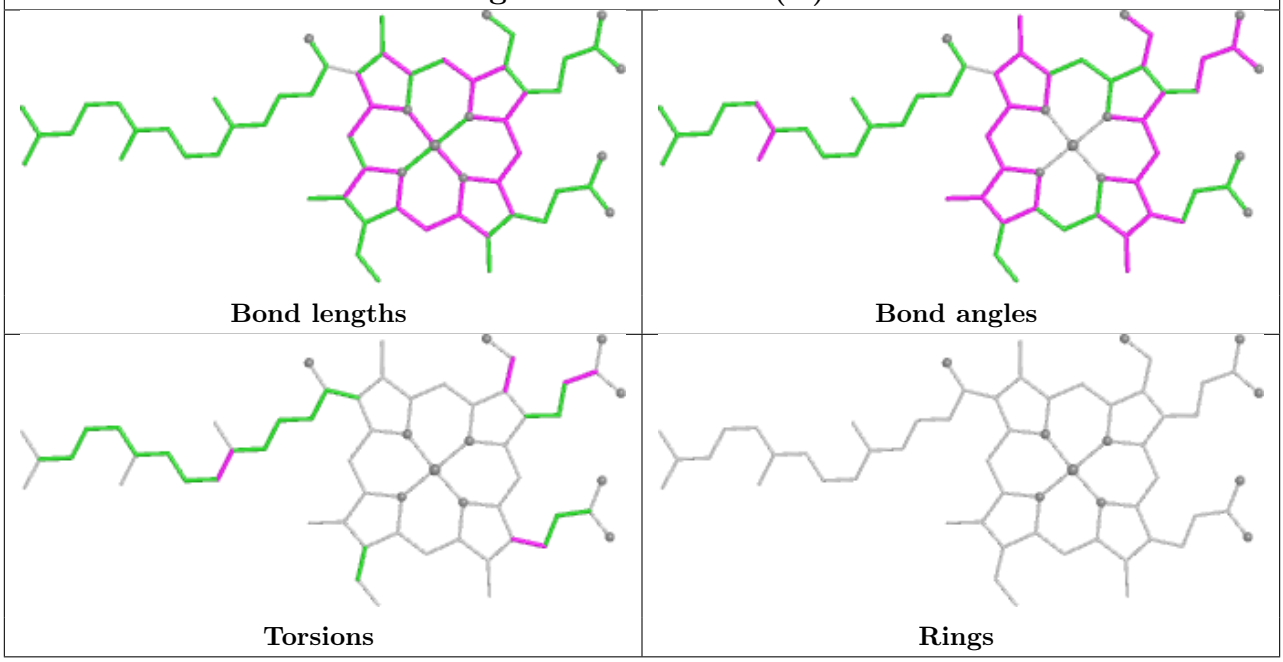
Ligand CHD C 301



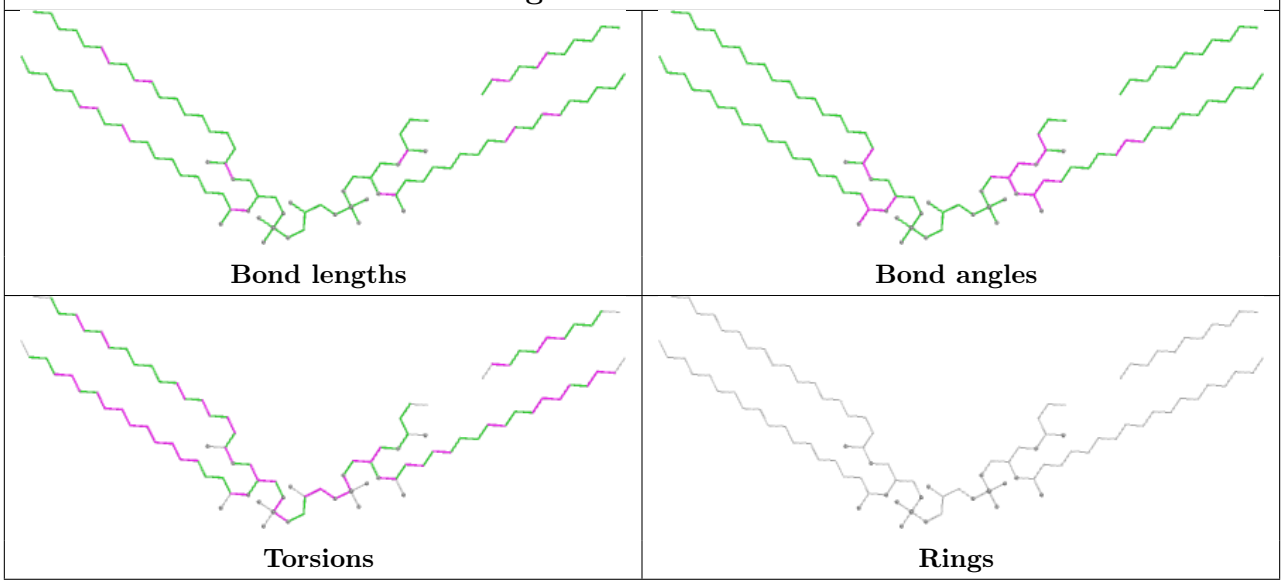
Ligand TGL L 101



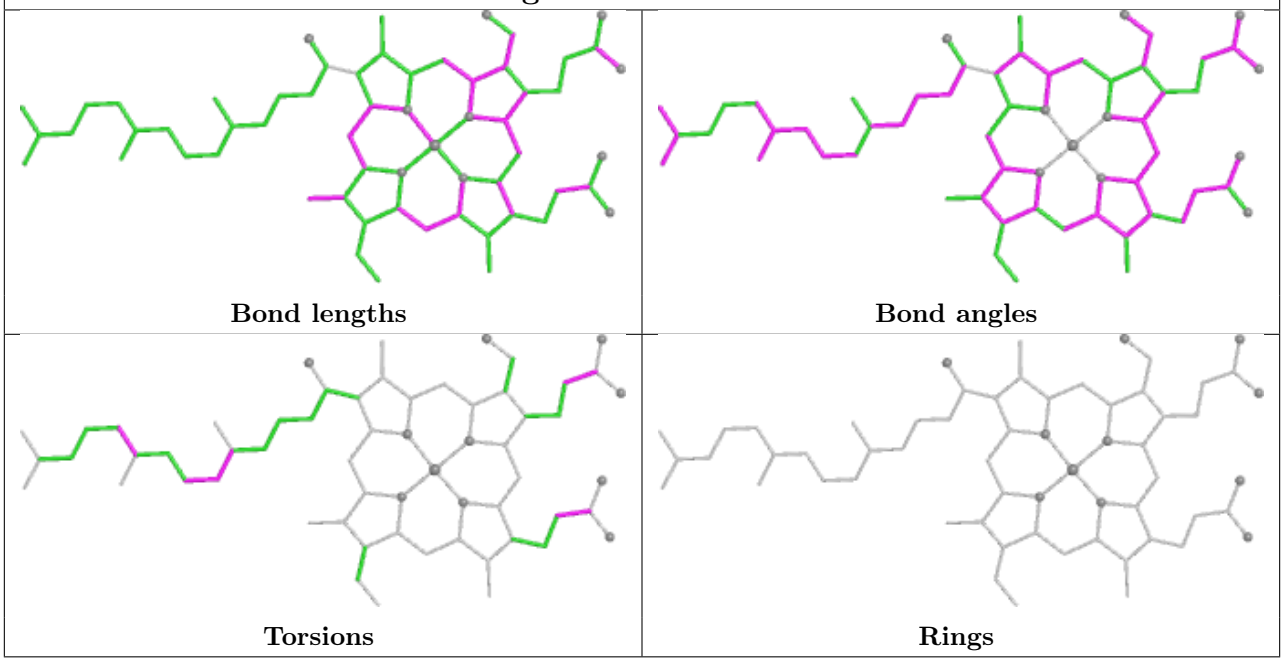
Ligand HEA N 603 (B)



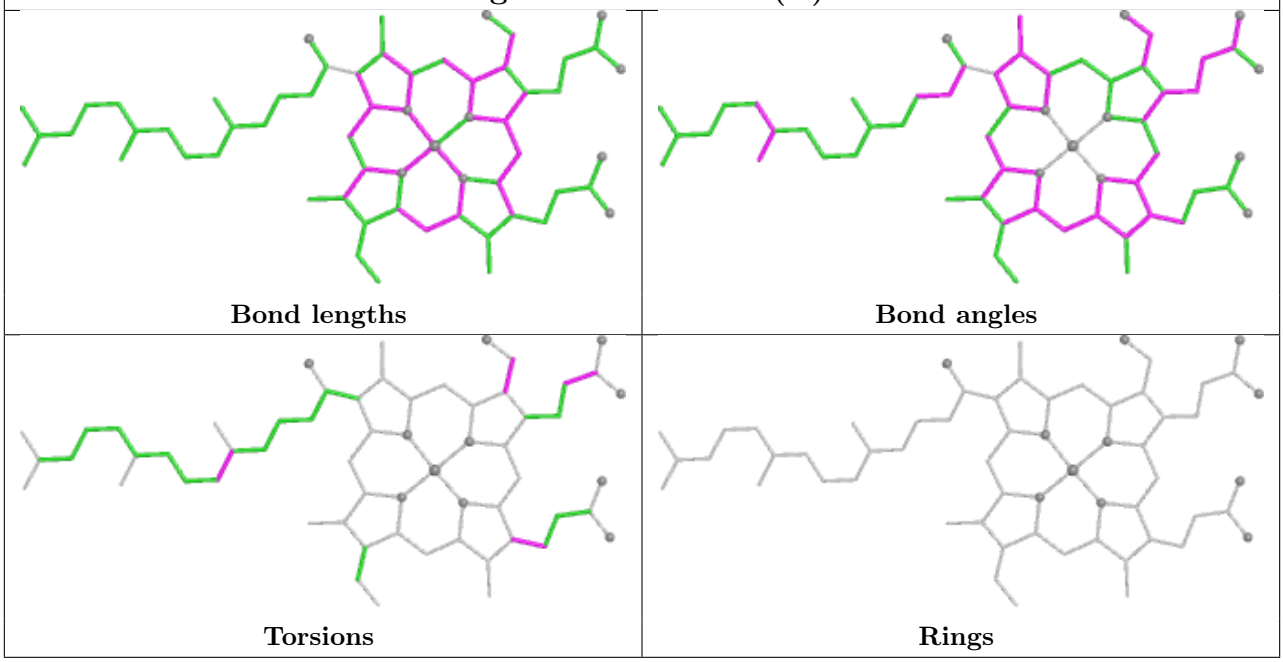
Ligand CDL T 102



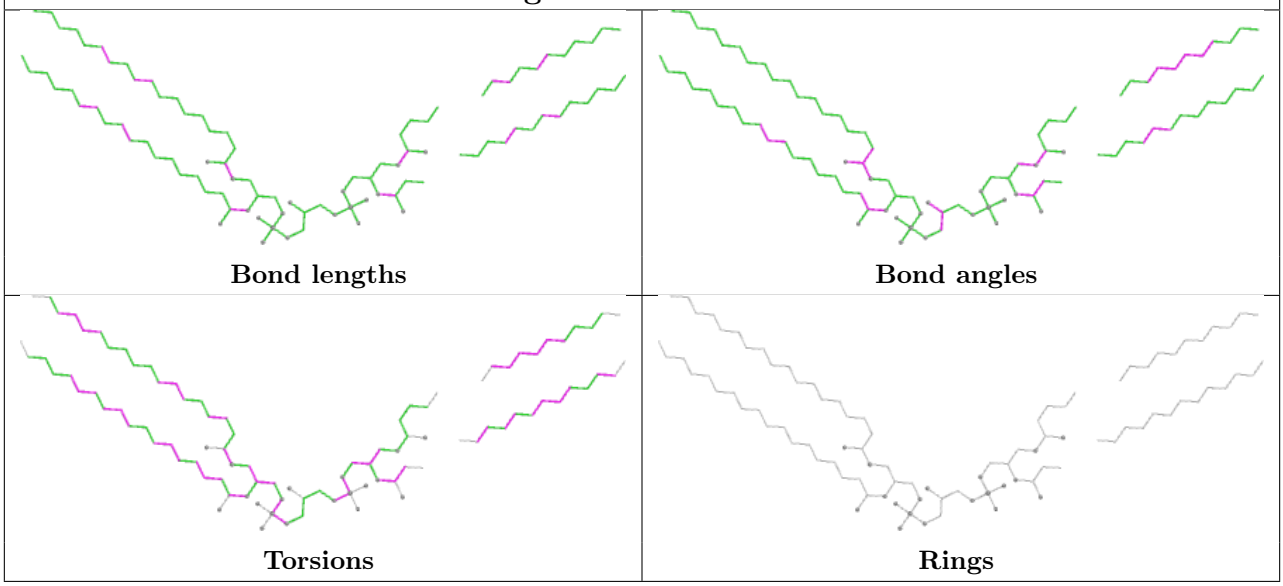
Ligand HEA N 602



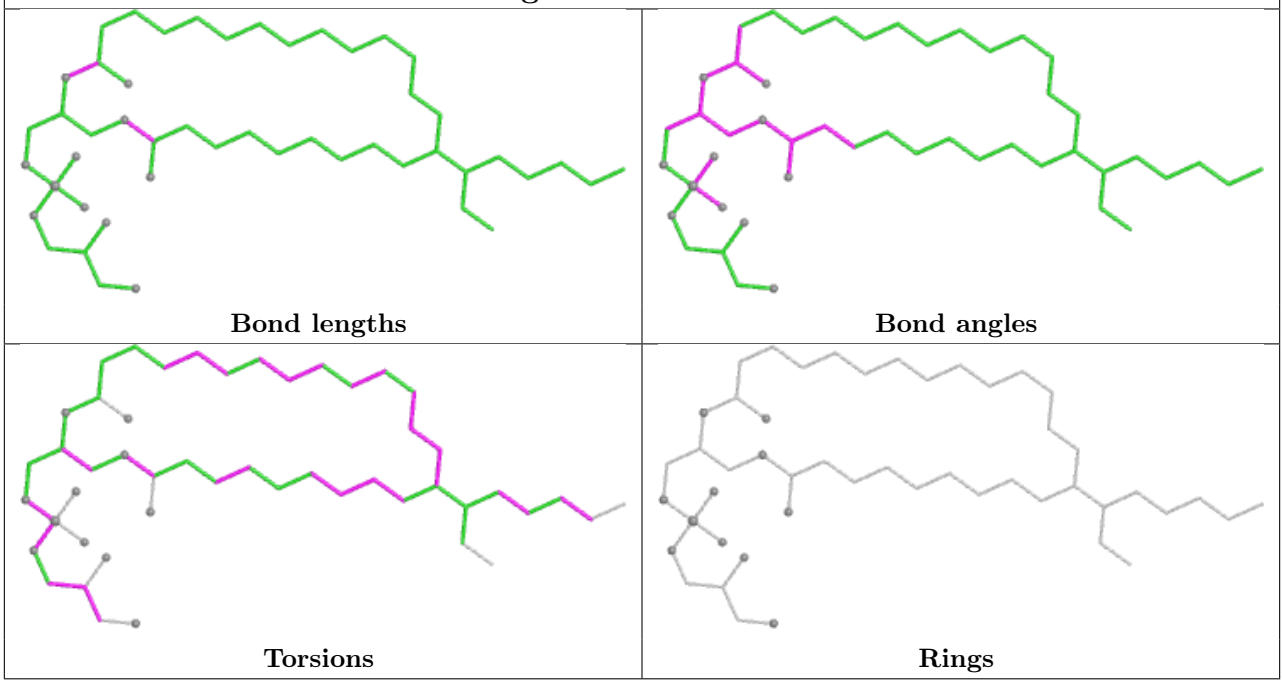
Ligand HEA A 602 (B)



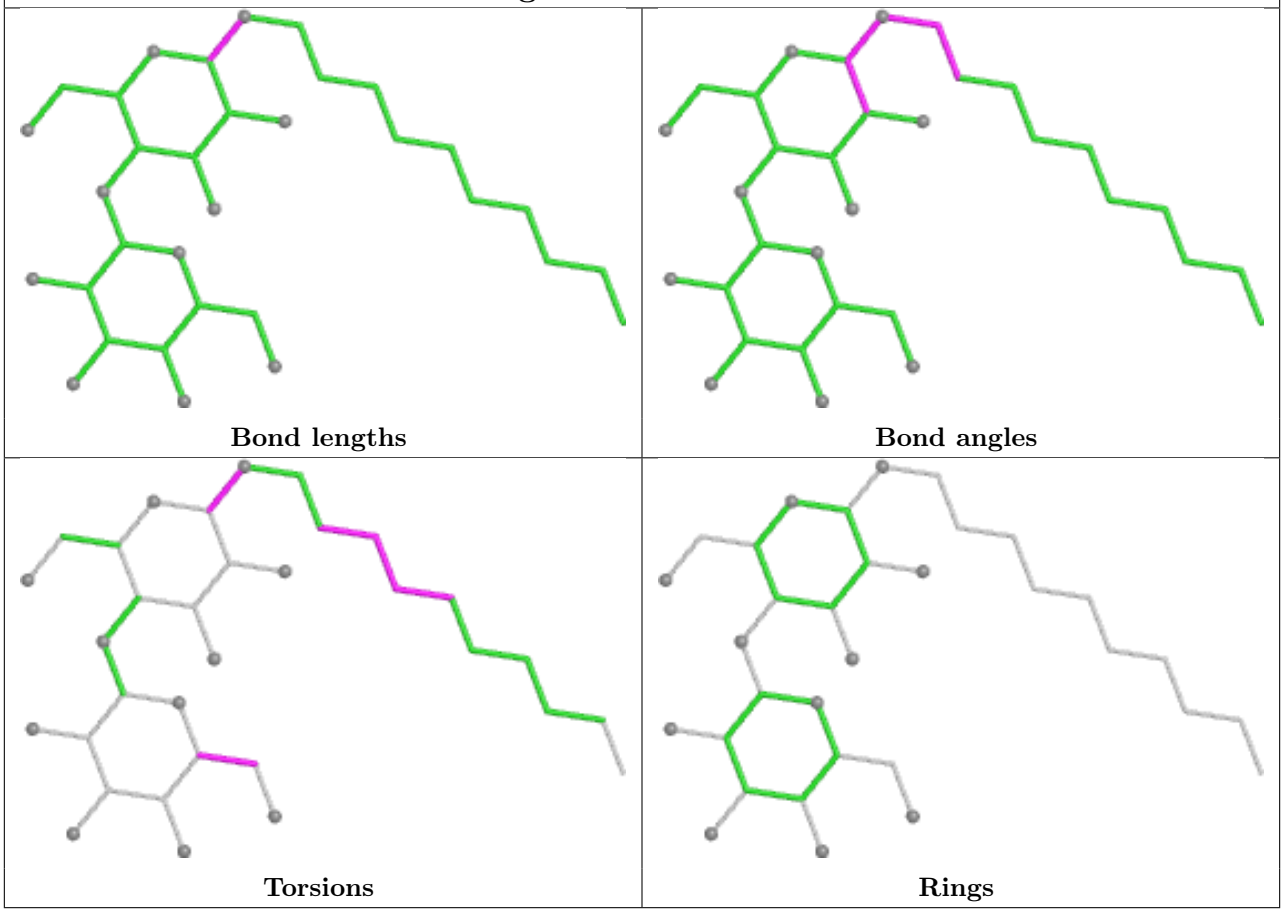
Ligand CDL N 601



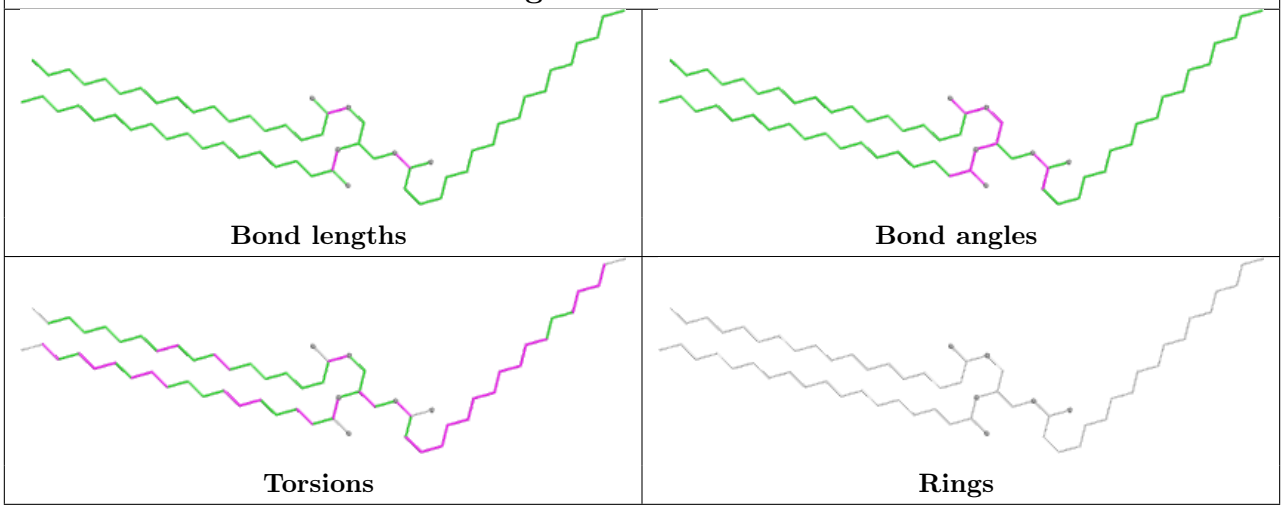
Ligand PGV G 104

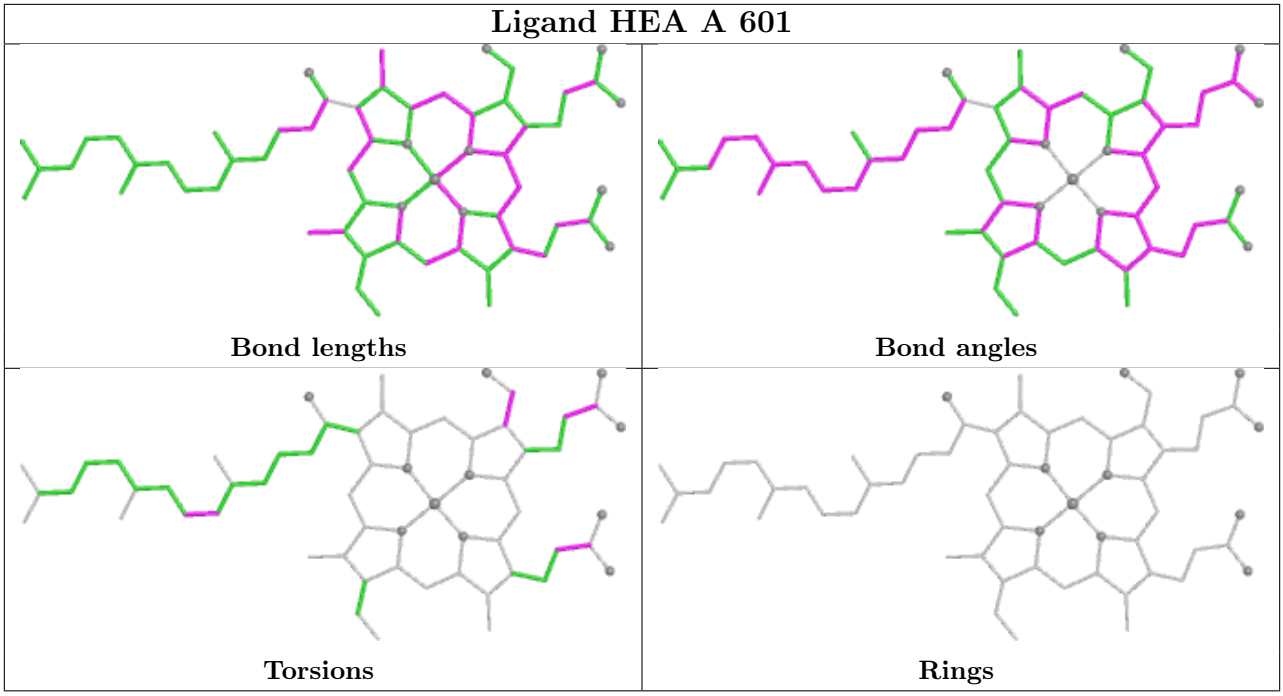


Ligand DMU P 306



Ligand TGL B 301





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%)	-0.47	3 (0%)	85	88	13, 29, 38, 83	20 (3%)
1	N	513/514 (99%)	-0.21	7 (1%)	73	77	16, 35, 46, 84	18 (3%)
2	B	226/227 (99%)	0.16	14 (6%)	26	29	16, 37, 58, 83	23 (10%)
2	O	226/227 (99%)	0.39	10 (4%)	39	42	19, 44, 75, 104	20 (8%)
3	C	259/261 (99%)	-0.19	4 (1%)	72	76	15, 33, 46, 97	8 (3%)
3	P	259/261 (99%)	-0.16	6 (2%)	61	64	14, 35, 48, 84	9 (3%)
4	D	144/147 (97%)	0.19	4 (2%)	55	58	29, 41, 67, 89	1 (0%)
4	Q	144/147 (97%)	0.94	12 (8%)	17	18	24, 57, 90, 177	2 (1%)
5	E	105/109 (96%)	0.17	4 (3%)	44	48	33, 40, 66, 127	0
5	R	105/109 (96%)	0.29	3 (2%)	53	57	38, 49, 73, 133	0
6	F	98/98 (100%)	0.50	8 (8%)	17	18	19, 40, 114, 163	4 (4%)
6	S	98/98 (100%)	0.87	11 (11%)	10	9	22, 43, 117, 165	2 (2%)
7	G	83/85 (97%)	1.21	20 (24%)	2	1	32, 42, 124, 144	0
7	T	83/85 (97%)	1.17	19 (22%)	2	2	26, 44, 113, 143	1 (1%)
8	H	79/85 (92%)	0.69	12 (15%)	5	5	34, 46, 103, 121	0
8	U	79/85 (92%)	0.81	12 (15%)	5	5	39, 51, 118, 143	0
9	I	73/74 (98%)	0.95	12 (16%)	4	4	35, 51, 88, 101	0
9	V	73/74 (98%)	1.08	12 (16%)	4	4	38, 64, 90, 159	0
10	J	58/59 (98%)	0.58	7 (12%)	8	8	34, 44, 77, 122	0
10	W	58/59 (98%)	0.65	8 (13%)	6	6	28, 51, 80, 148	1 (1%)
11	K	49/56 (87%)	0.48	3 (6%)	27	29	35, 44, 60, 69	0
11	X	49/56 (87%)	0.86	6 (12%)	8	8	27, 59, 87, 96	1 (2%)
12	L	46/47 (97%)	0.16	2 (4%)	40	43	30, 35, 59, 93	1 (2%)
12	Y	46/47 (97%)	0.48	2 (4%)	40	43	39, 46, 78, 132	1 (2%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	M	43/46 (93%)	0.25	3 (6%)	22	24	32, 37, 74, 118	0
13	Z	43/46 (93%)	0.57	3 (6%)	22	24	45, 53, 95, 174	0
All	All	3552/3616 (98%)	0.20	207 (5%)	29	31	13, 38, 78, 177	112 (3%)

The worst 5 of 207 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	F	1	ALA	11.7
6	S	97	ALA	9.8
4	Q	6	VAL	9.5
4	Q	5	VAL	8.5
6	S	93	PRO	7.7

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
7	TPO	T	11	11/12	0.64	0.22	115,127,158,161	0
7	TPO	G	11	11/12	0.70	0.27	98,137,157,162	0
1	FME	N	1	10/11	0.92	0.13	44,59,81,83	0
1	FME	A	1	10/11	0.93	0.12	40,51,92,92	0
2	FME	O	1	10/11	0.96	0.10	38,44,54,89	0
2	FME	B	1	10/11	0.97	0.09	29,34,46,89	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	CHD	W	101	29/29	0.70	0.24	54,125,146,153	0
25	DMU	L	102	30/33	0.71	0.20	45,95,141,147	0
20	EDO	D	202	4/4	0.72	0.30	66,77,81,95	0
27	PEK	C	319	44/53	0.73	0.22	50,80,155,168	0
27	PEK	G	103	44/53	0.73	0.23	45,84,153,164	0
20	EDO	C	317	4/4	0.74	0.18	75,93,107,109	0
26	CDL	T	102	97/100	0.74	0.28	41,86,149,173	0
26	CDL	N	601	96/100	0.75	0.29	50,90,144,168	0
25	DMU	C	309	33/33	0.75	0.17	53,79,115,123	0
22	CHD	J	101	29/29	0.76	0.21	88,129,148,149	0
25	DMU	C	302	33/33	0.76	0.19	32,85,116,134	0
27	PEK	T	101	50/53	0.76	0.23	40,82,132,162	0
25	DMU	P	306	33/33	0.77	0.17	45,83,118,130	0
19	PGV	G	104	51/51	0.77	0.24	47,82,123,155	0
20	EDO	N	611	4/4	0.78	0.24	65,65,72,81	0
22	CHD	P	305	29/29	0.78	0.16	54,67,81,93	0
27	PEK	C	307	53/53	0.78	0.22	43,78,143,155	0
20	EDO	R	205	4/4	0.78	0.18	54,57,60,80	0
24	PSC	B	304	50/52	0.78	0.25	35,80,154,170	0
25	DMU	P	307	33/33	0.78	0.16	50,76,108,114	0
26	CDL	P	304	80/100	0.79	0.27	44,84,125,140	0
19	PGV	C	308	49/51	0.79	0.24	42,76,127,157	0
20	EDO	A	616	4/4	0.79	0.21	45,53,54,102	0
20	EDO	C	314	4/4	0.79	0.25	58,79,79,82	0
20	EDO	C	316	4/4	0.79	0.24	56,80,96,103	0
21	TGL	N	610	61/63	0.79	0.26	52,82,106,121	0
21	TGL	Q	201	63/63	0.80	0.25	46,77,102,118	0
22	CHD	C	306	29/29	0.80	0.15	48,66,79,86	0
21	TGL	B	301	63/63	0.80	0.24	35,76,108,120	0
20	EDO	A	611	4/4	0.80	0.22	51,54,64,72	0
25	DMU	C	310	22/33	0.80	0.20	59,73,96,117	0
19	PGV	N	619	51/51	0.81	0.23	45,84,139,154	0
20	EDO	V	101	4/4	0.81	0.20	56,66,74,78	0
25	DMU	P	308	33/33	0.81	0.14	57,85,106,118	0
21	TGL	Y	101	63/63	0.81	0.26	45,74,117,149	0
19	PGV	A	609	51/51	0.81	0.23	34,68,120,156	0
21	TGL	D	201	63/63	0.82	0.23	36,68,97,114	0
26	CDL	C	305	89/100	0.82	0.20	46,79,109,126	0
24	PSC	O	302	51/52	0.82	0.24	46,87,162,170	0
20	EDO	H	101	4/4	0.83	0.21	53,54,73,76	0
20	EDO	Q	203	4/4	0.83	0.20	78,79,90,92	0
20	EDO	N	613	4/4	0.84	0.20	54,58,68,70	0
20	EDO	C	312	4/4	0.84	0.15	68,81,88,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
21	TGL	L	101	63/63	0.84	0.26	29,65,102,125	0
20	EDO	N	617	4/4	0.85	0.19	48,49,54,58	0
20	EDO	D	204	4/4	0.85	0.25	50,62,68,74	0
20	EDO	R	201	4/4	0.85	0.21	64,66,69,82	0
20	EDO	H	102	4/4	0.85	0.17	66,67,78,83	0
20	EDO	G	105	4/4	0.87	0.19	55,66,73,94	0
20	EDO	L	103	4/4	0.87	0.21	67,72,75,104	0
17	NA	C	303	1/1	0.89	0.11	41,41,41,41	0
20	EDO	A	614	4/4	0.89	0.14	39,45,47,50	0
20	EDO	U	101	4/4	0.89	0.17	67,68,73,85	0
25	DMU	Z	101	33/33	0.89	0.13	51,63,80,84	0
20	EDO	A	615	4/4	0.89	0.17	48,58,59,63	0
20	EDO	C	315	4/4	0.89	0.17	62,74,76,83	0
20	EDO	N	612	4/4	0.90	0.17	40,50,54,55	0
20	EDO	F	104	4/4	0.90	0.17	45,51,62,72	0
20	EDO	R	203	4/4	0.90	0.14	48,64,68,73	0
17	NA	P	302	1/1	0.90	0.11	43,43,43,43	0
20	EDO	R	206	4/4	0.90	0.15	47,50,60,71	0
20	EDO	S	101	4/4	0.90	0.16	44,52,59,64	0
20	EDO	E	203	4/4	0.91	0.12	46,49,59,75	0
20	EDO	N	616	4/4	0.91	0.15	48,50,53,60	0
20	EDO	A	619	4/4	0.91	0.15	52,52,61,67	0
20	EDO	C	313	4/4	0.91	0.13	57,64,65,88	0
20	EDO	S	104	4/4	0.91	0.16	42,47,81,88	0
20	EDO	E	201	4/4	0.91	0.13	43,49,54,66	0
20	EDO	R	202	4/4	0.91	0.16	56,67,69,85	0
20	EDO	A	617	4/4	0.92	0.14	59,62,68,72	0
25	DMU	M	101	33/33	0.92	0.11	38,50,65,78	0
20	EDO	A	612	4/4	0.92	0.13	32,33,35,39	0
20	EDO	D	205	4/4	0.92	0.16	61,62,70,72	0
20	EDO	F	105	4/4	0.92	0.16	49,57,71,82	0
20	EDO	P	309	4/4	0.92	0.17	34,43,47,60	0
20	EDO	F	106	4/4	0.92	0.17	42,54,65,68	0
20	EDO	Q	202	4/4	0.93	0.16	62,64,67,73	0
20	EDO	E	205	4/4	0.93	0.14	58,58,71,77	0
20	EDO	O	305	4/4	0.93	0.10	71,75,78,79	0
20	EDO	C	318	4/4	0.93	0.17	38,40,47,70	0
20	EDO	P	311	4/4	0.93	0.14	45,61,76,77	0
20	EDO	E	204	4/4	0.94	0.09	39,41,41,49	0
20	EDO	B	306	4/4	0.94	0.14	32,40,50,61	0
20	EDO	O	304	4/4	0.94	0.12	55,67,68,82	0
20	EDO	T	103	4/4	0.94	0.12	39,39,40,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
27	PEK	P	312	53/53	0.94	0.15	32,52,90,108	0
20	EDO	N	614	4/4	0.94	0.15	36,37,37,46	0
18	AZI	N	608[A]	3/3	0.95	0.10	38,38,40,42	0
20	EDO	P	310	4/4	0.95	0.10	44,44,45,51	0
18	AZI	N	608[B]	3/3	0.95	0.10	29,29,38,39	3
20	EDO	F	103	4/4	0.95	0.12	36,37,41,41	0
20	EDO	C	311	4/4	0.95	0.13	40,42,44,46	0
27	PEK	G	101	53/53	0.95	0.14	31,48,87,113	0
18	AZI	A	607[A]	3/3	0.95	0.15	30,30,32,34	3
18	AZI	A	607[B]	3/3	0.95	0.15	21,21,29,42	3
22	CHD	C	301	29/29	0.95	0.08	30,33,39,43	0
20	EDO	N	618	4/4	0.96	0.11	44,57,61,71	0
20	EDO	O	303	4/4	0.96	0.10	36,39,40,41	0
19	PGV	C	304	51/51	0.96	0.11	26,35,94,112	0
20	EDO	N	615	4/4	0.96	0.08	30,36,39,41	0
22	CHD	P	301	29/29	0.96	0.07	31,37,46,47	0
20	EDO	A	610	4/4	0.96	0.15	34,41,45,77	0
19	PGV	N	609	51/51	0.96	0.11	26,38,74,82	0
19	PGV	A	608	51/51	0.97	0.10	25,34,74,81	0
22	CHD	B	302	29/29	0.97	0.07	28,33,37,48	0
16	MG	N	605	1/1	0.97	0.09	29,29,29,29	0
20	EDO	E	202	4/4	0.97	0.08	44,45,46,47	0
22	CHD	G	102	29/29	0.97	0.06	30,35,41,47	0
20	EDO	S	103	4/4	0.97	0.12	33,33,35,37	0
19	PGV	P	303	51/51	0.97	0.10	29,39,75,93	0
18	AZI	N	607[A]	3/3	0.97	0.11	34,34,34,39	0
20	EDO	A	618	4/4	0.97	0.12	35,42,67,70	0
18	AZI	A	606[A]	3/3	0.97	0.10	27,27,30,33	3
20	EDO	B	305	4/4	0.97	0.08	29,30,34,38	0
17	NA	N	606	1/1	0.97	0.07	38,38,38,38	0
20	EDO	D	203	4/4	0.97	0.09	40,43,57,69	0
20	EDO	A	613	4/4	0.97	0.07	28,29,32,37	0
20	EDO	R	204	4/4	0.97	0.09	41,48,49,52	0
14	HEA	N	603[B]	60/60	0.98	0.07	19,31,50,59	60
14	HEA	A	601	60/60	0.98	0.06	21,27,49,67	0
14	HEA	A	602[A]	60/60	0.98	0.06	16,26,35,51	60
14	HEA	A	602[B]	60/60	0.98	0.06	15,26,36,40	60
14	HEA	N	602	60/60	0.98	0.08	27,34,58,61	0
20	EDO	G	106	4/4	0.98	0.07	33,36,41,45	0
14	HEA	N	603[A]	60/60	0.98	0.07	16,27,36,40	60
20	EDO	F	102	4/4	0.98	0.06	27,30,31,32	0
17	NA	A	605	1/1	0.99	0.03	30,30,30,30	0

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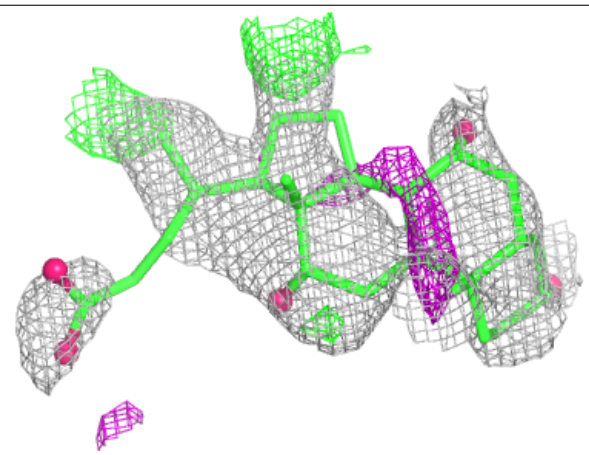
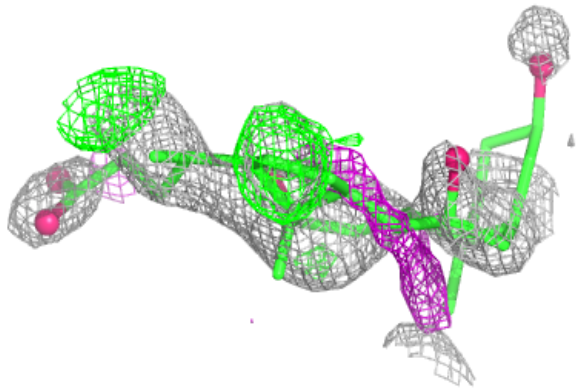
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
16	MG	A	604	1/1	1.00	0.05	25,25,25,25	0
15	CU	A	603	1/1	1.00	0.02	28,28,28,28	0
23	CUA	B	303	2/2	1.00	0.01	28,28,28,29	0
23	CUA	O	301	2/2	1.00	0.02	34,34,34,34	0
15	CU	N	604	1/1	1.00	0.02	31,31,31,31	0
28	ZN	F	101	1/1	1.00	0.03	33,33,33,33	0
28	ZN	S	102	1/1	1.00	0.04	35,35,35,35	0

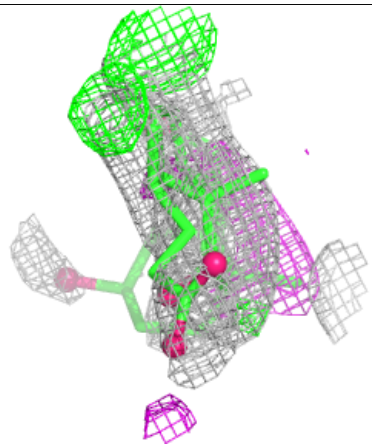
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CHD 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)

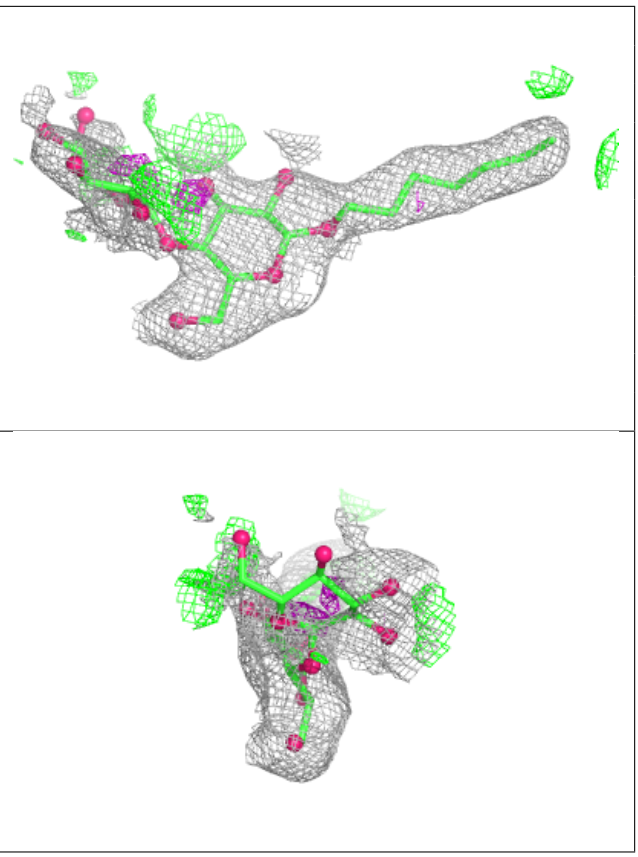






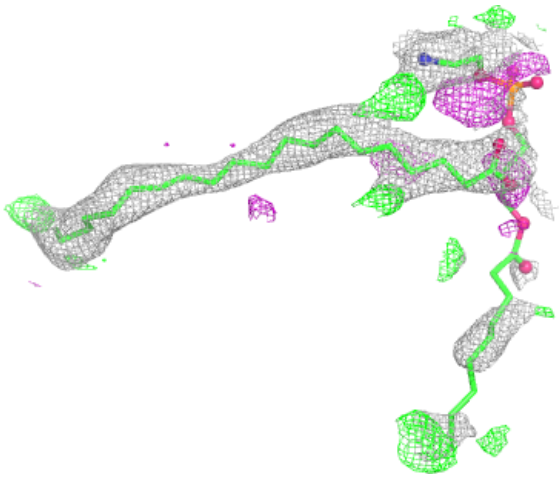
Electron density around DMU L 102:

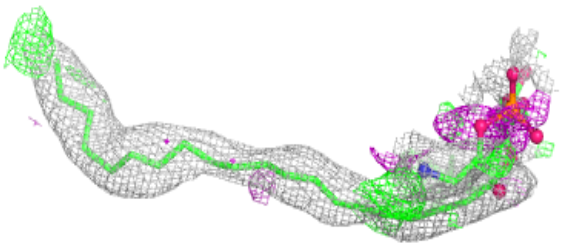
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

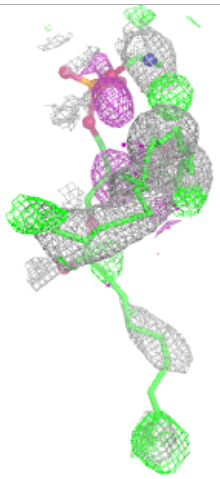


Electron density around PEK C 319:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

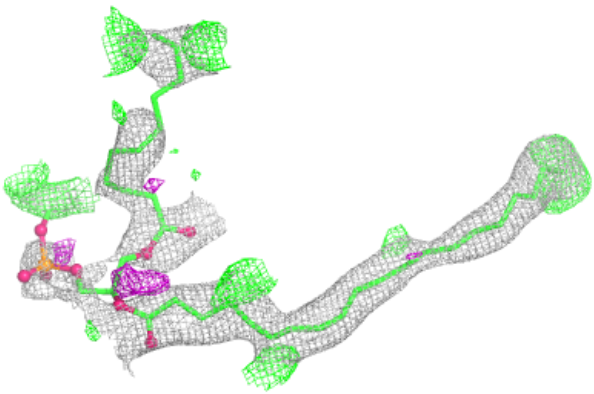


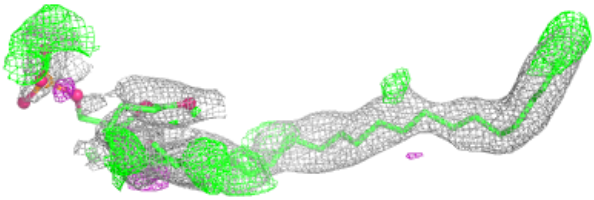


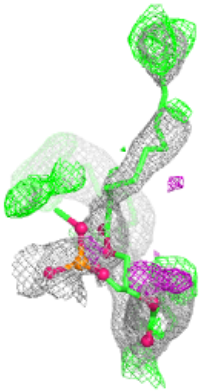


Electron density around PEK G 103:

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

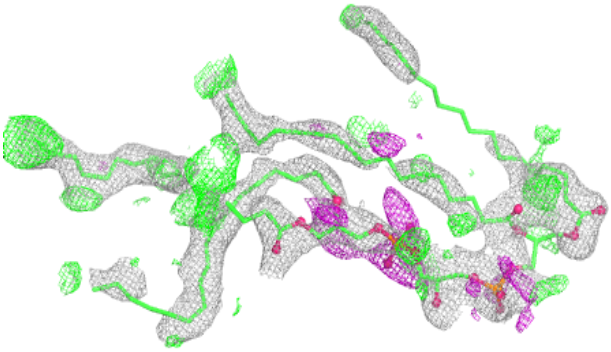


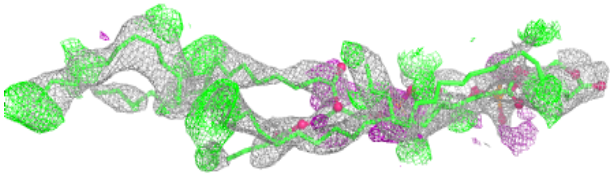


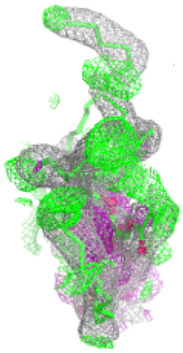


Electron density around CDL T 102:

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

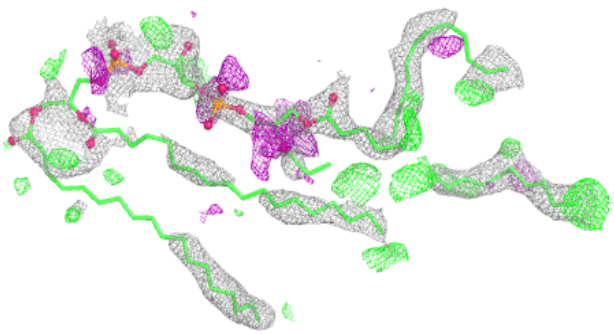


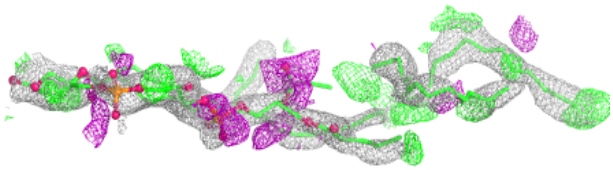




Electron density around CDL N 601:

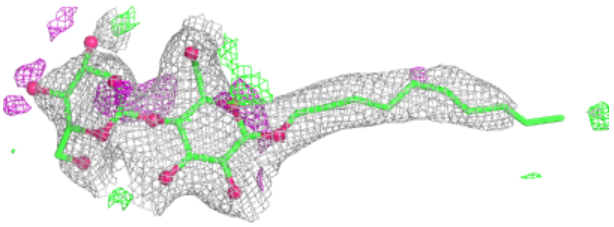
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

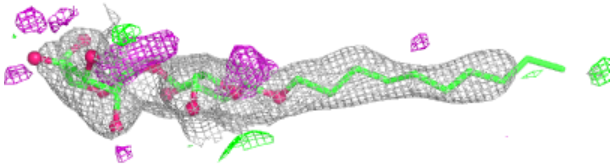


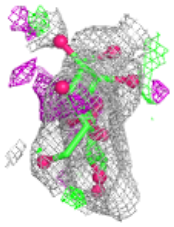


Electron density around DMU C 309:

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

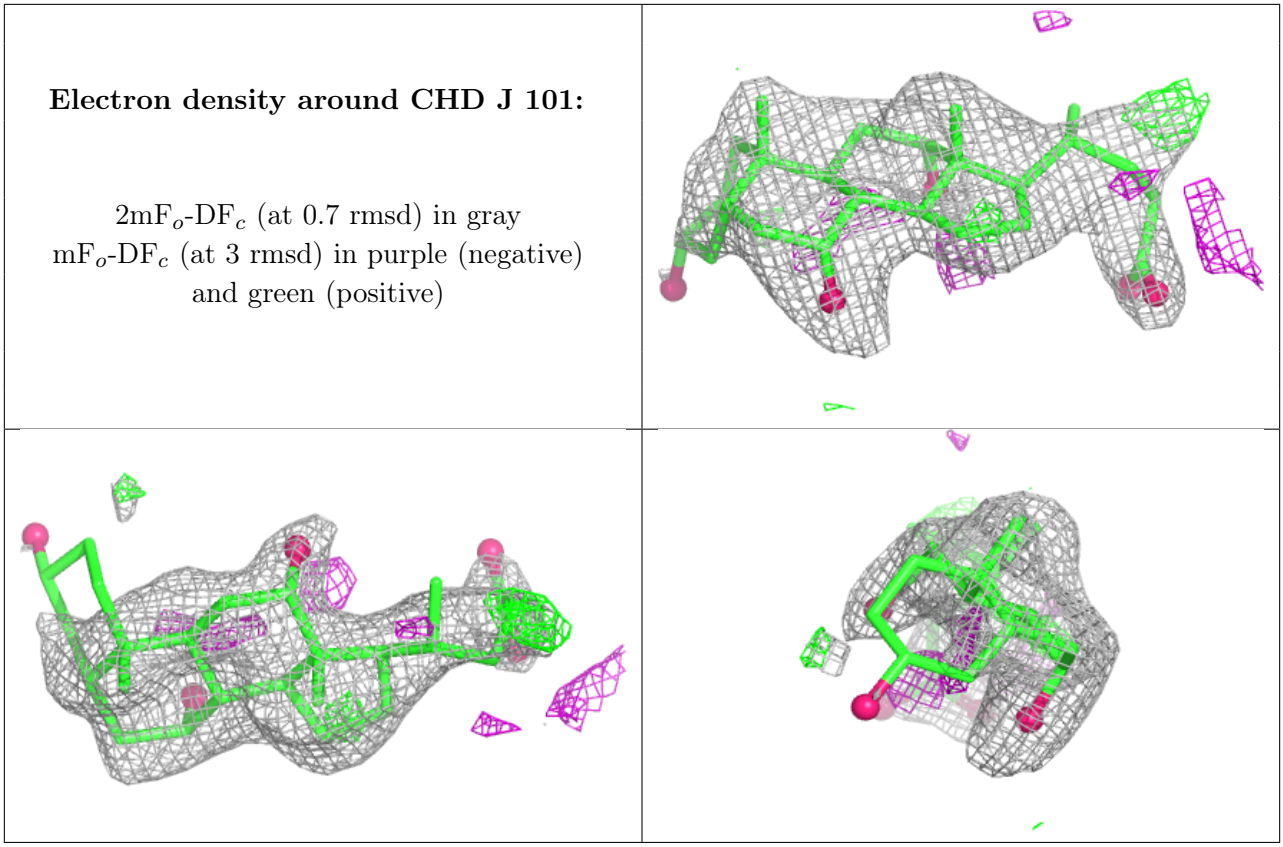






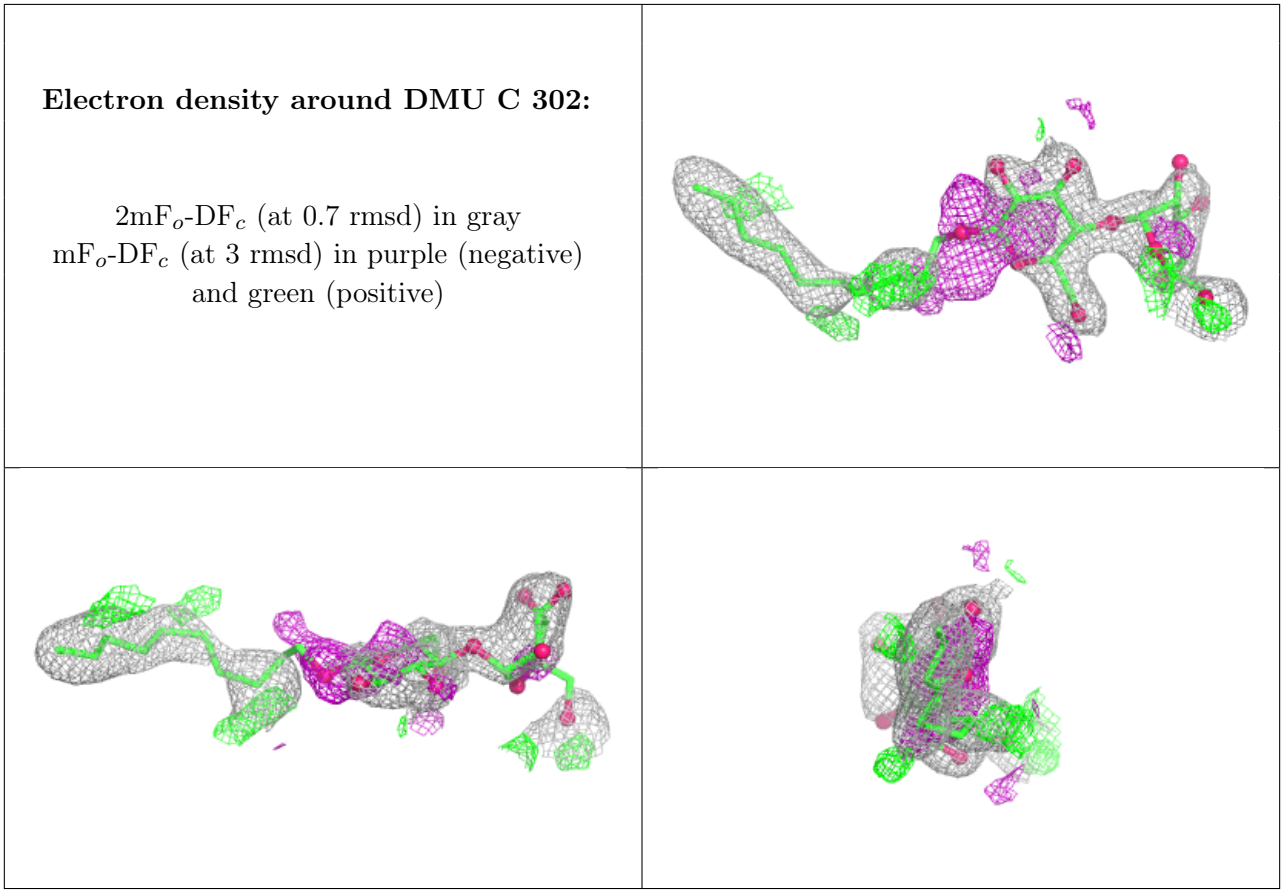
Electron density around CHD J 101:

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



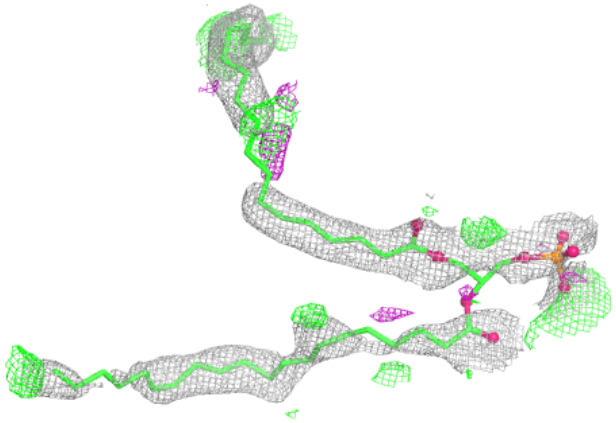
Electron density around DMU C 302:

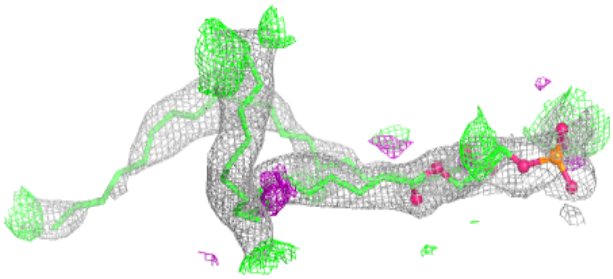
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

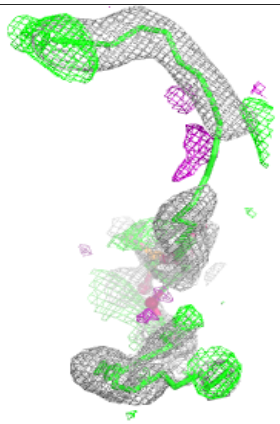


Electron density around PEK T 101:

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

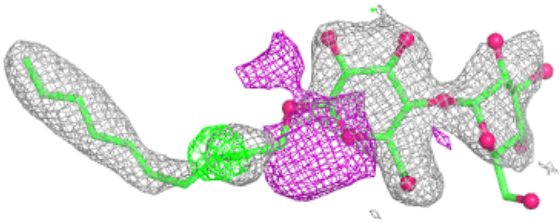


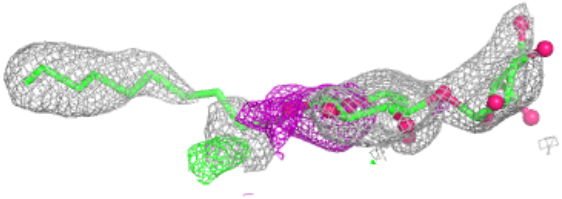


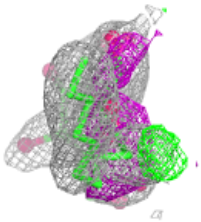


Electron density around DMU P 306:

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

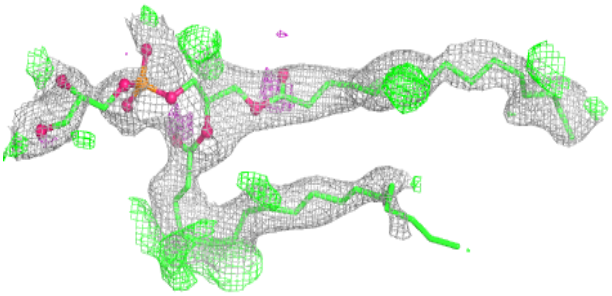


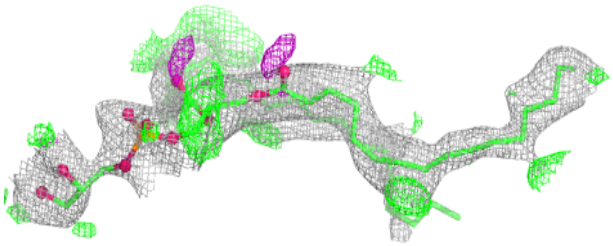


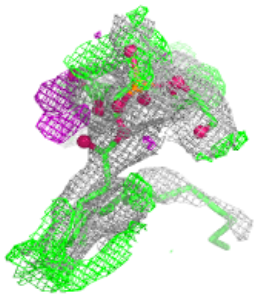


Electron density around PGV G 104:

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

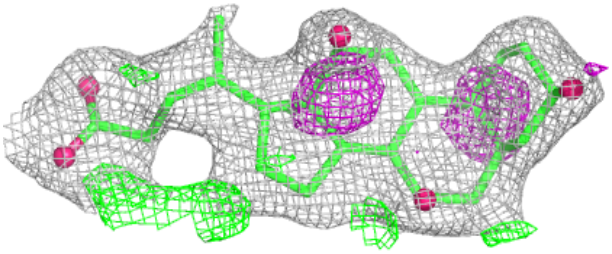


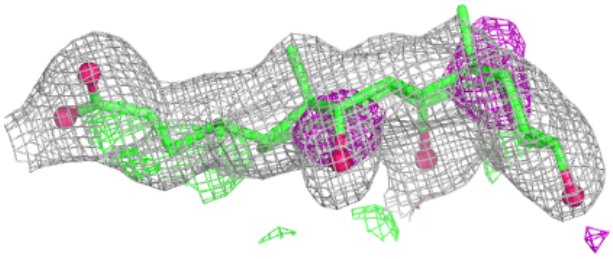


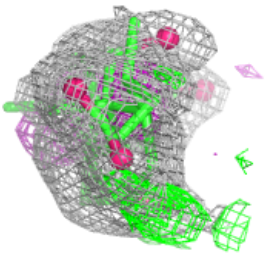


Electron density around CHD P 305:

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

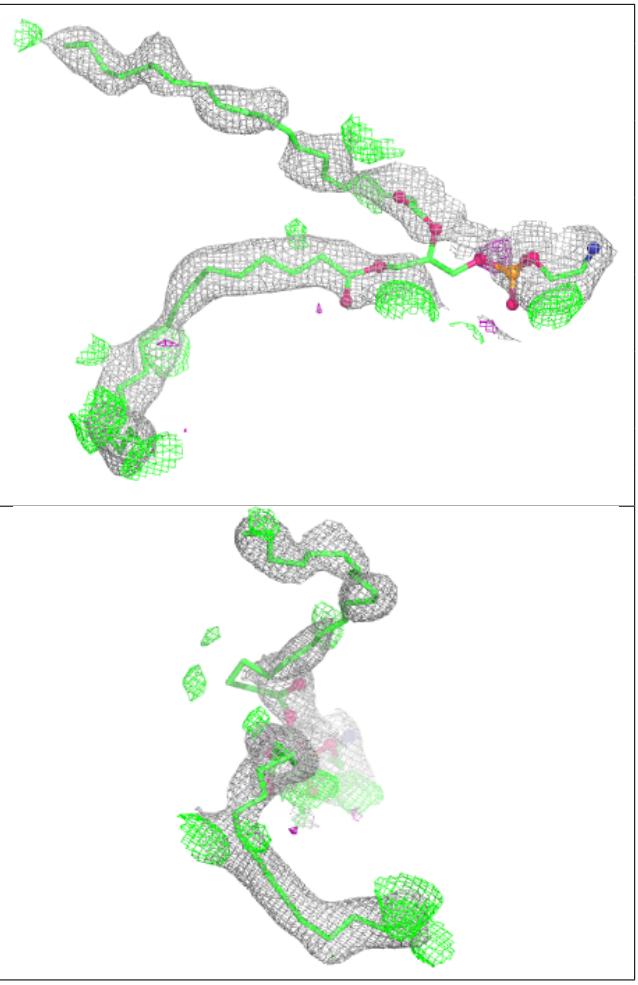






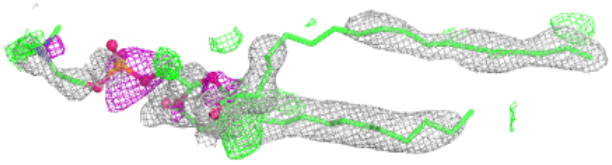
Electron density around PEK C 307:

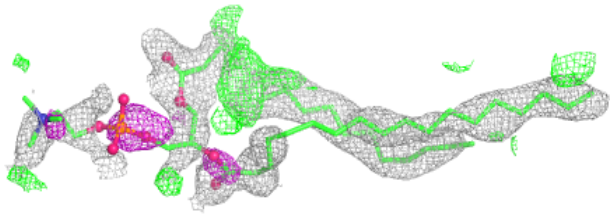
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

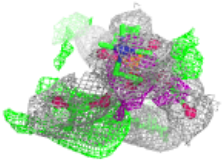


Electron density around PSC B 304:

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

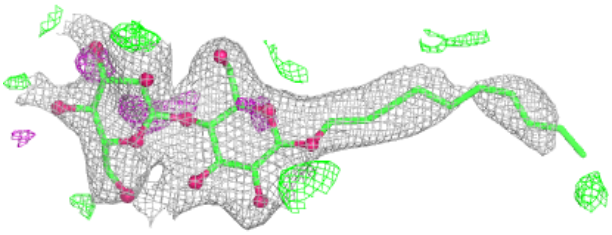


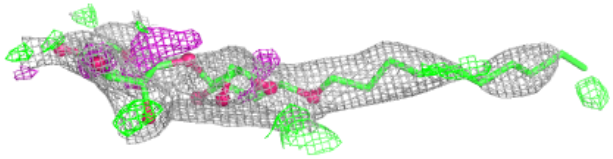


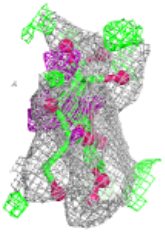


Electron density around DMU P 307:

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

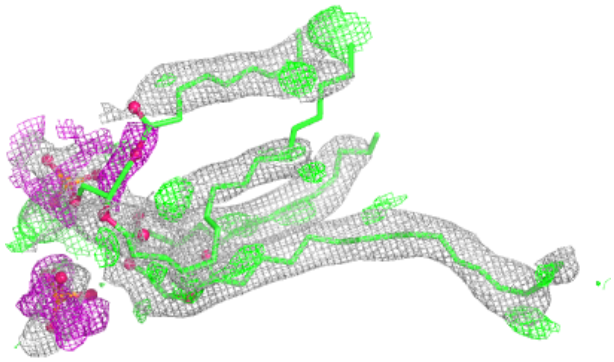


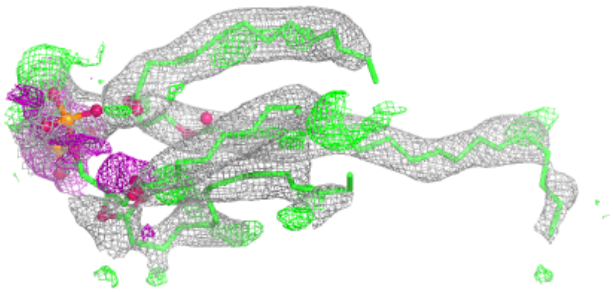


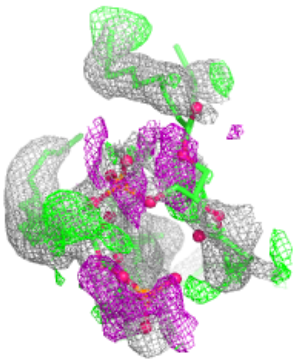


Electron density around CDL P 304:

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

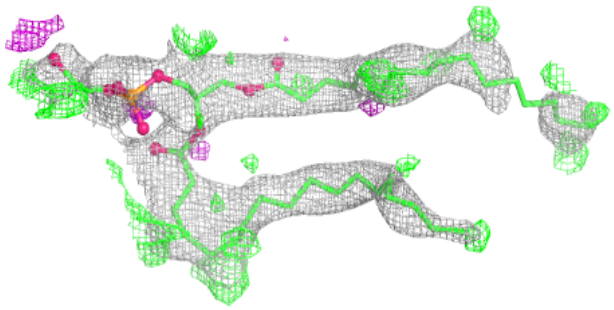


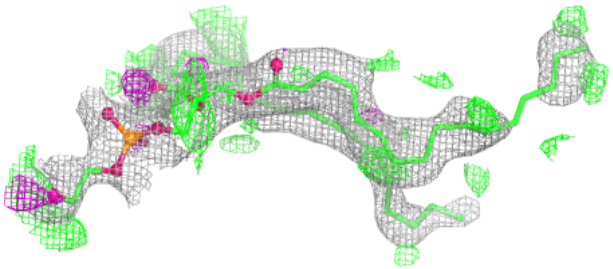


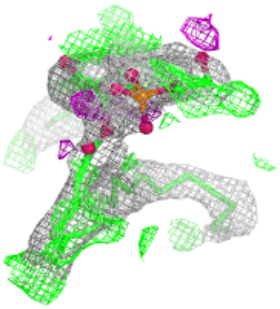


Electron density around PGV C 308:

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

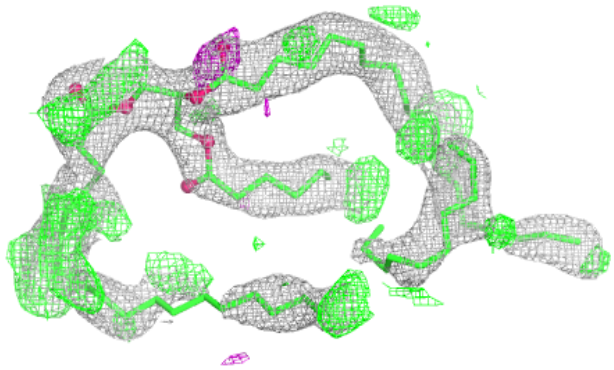


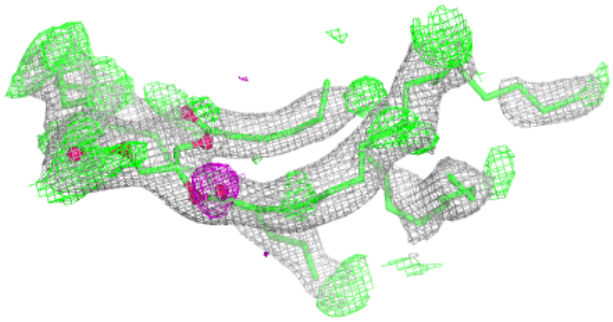


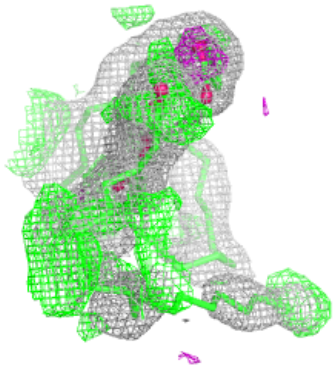


Electron density around TGL N 610:

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

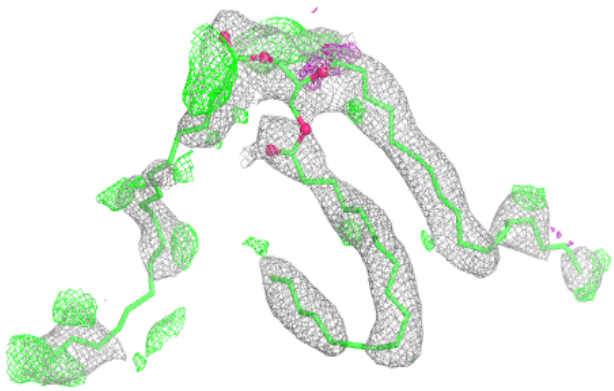


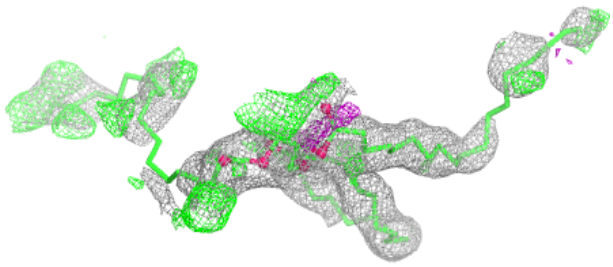


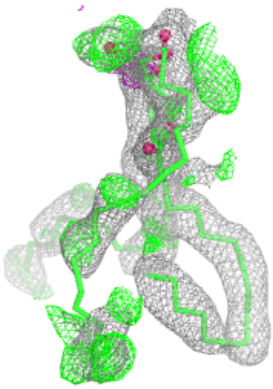


Electron density around TGL Q 201:

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

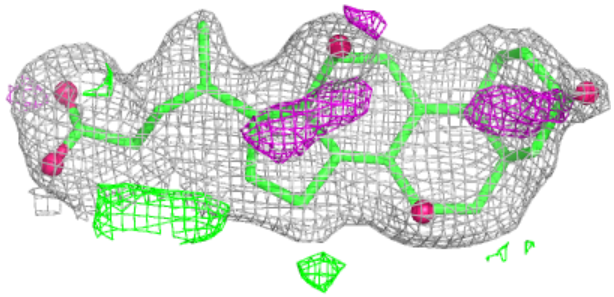


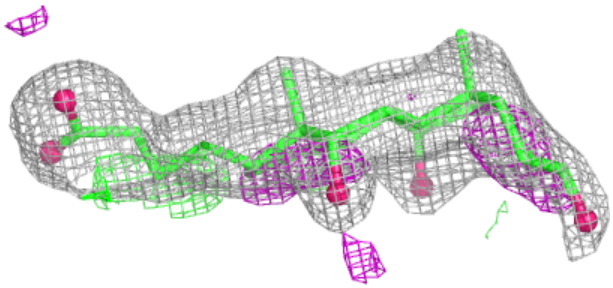


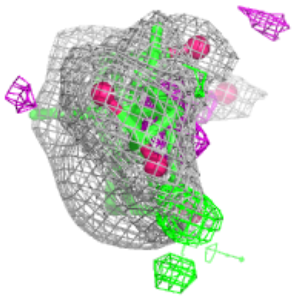


Electron density around CHD C 306:

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

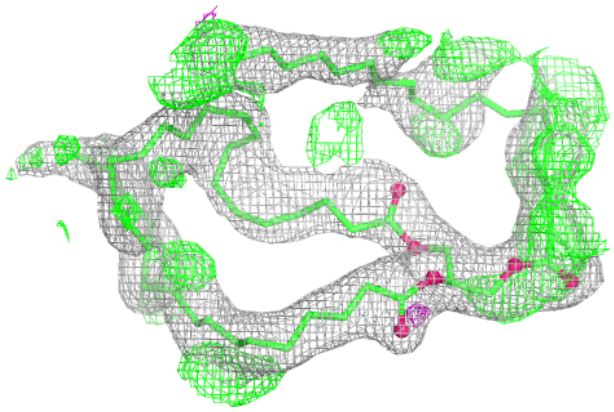


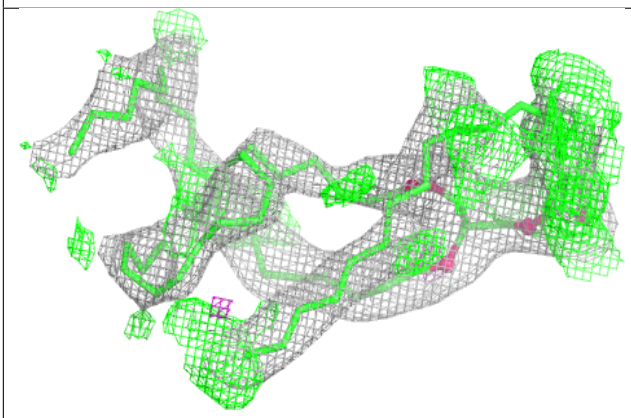


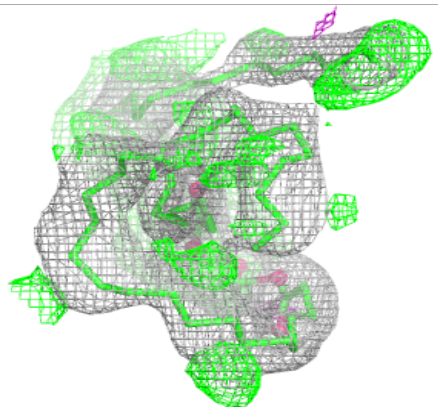


Electron density around TGL B 301:

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

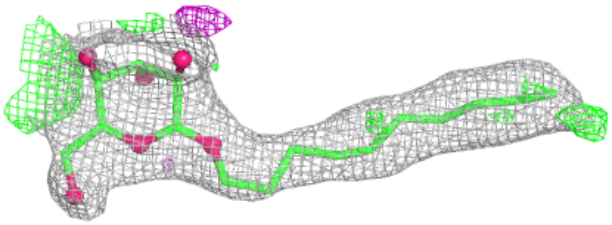


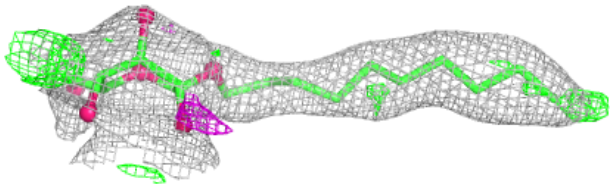


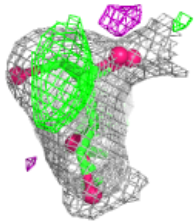


Electron density around DMU C 310:

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

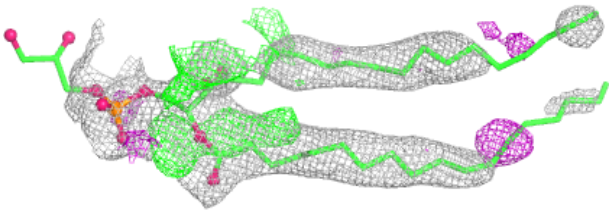


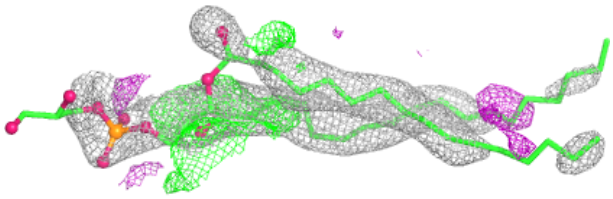


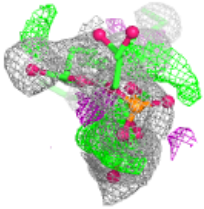


Electron density around PGV N 619:

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

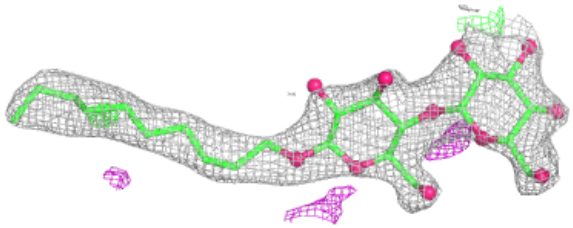


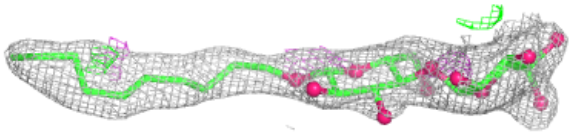




Electron density around DMU P 308:

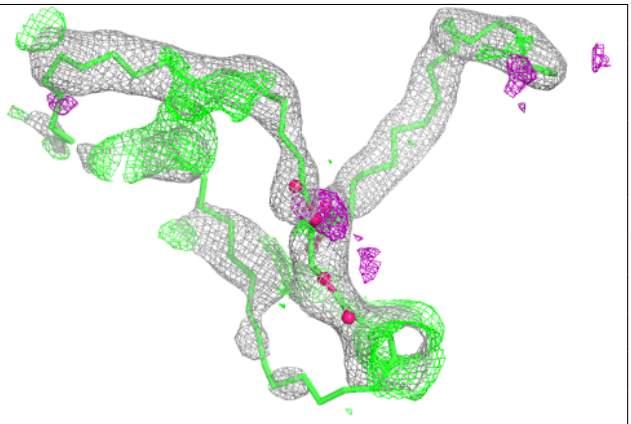
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

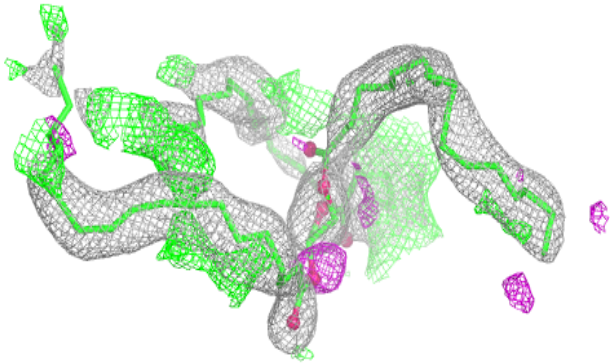


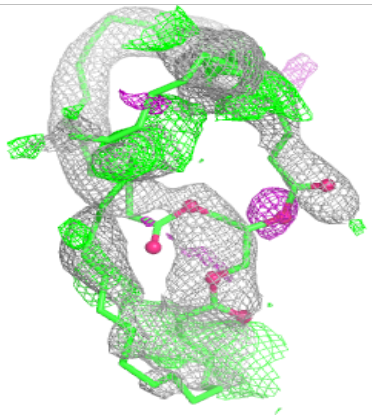


Electron density around TGL Y 101:

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

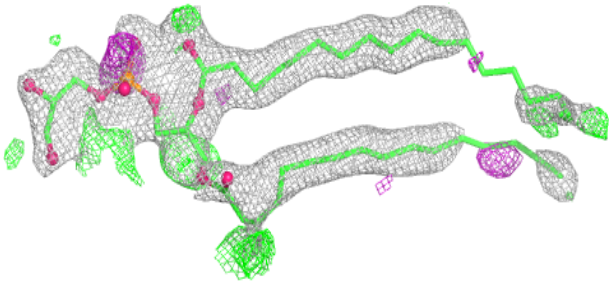


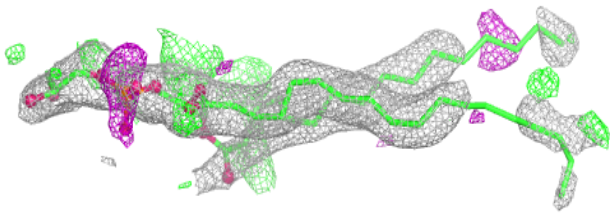


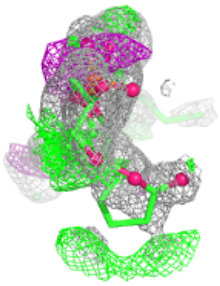


Electron density around PGV A 609:

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

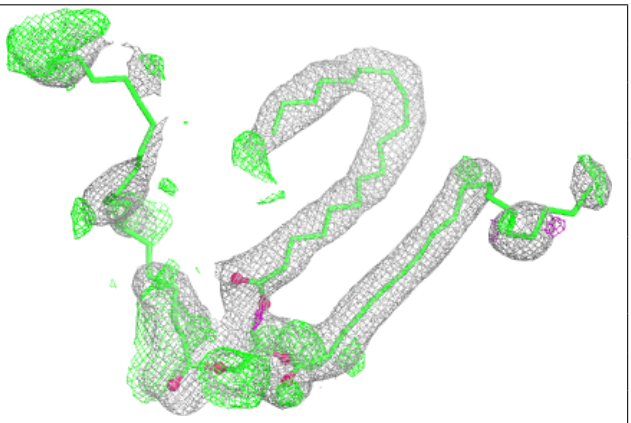


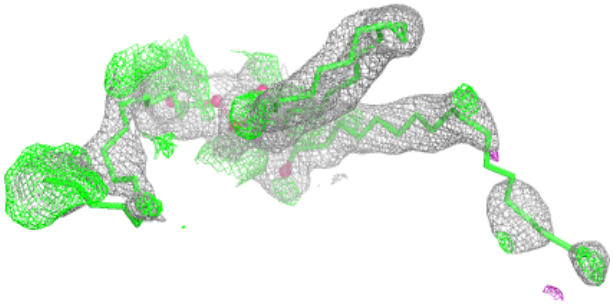


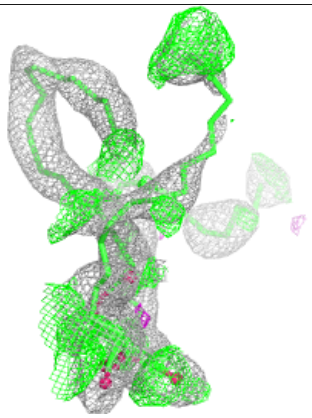


Electron density around TGL D 201:

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

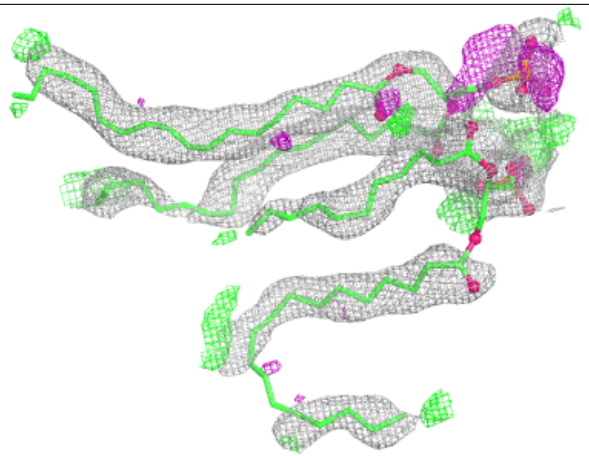


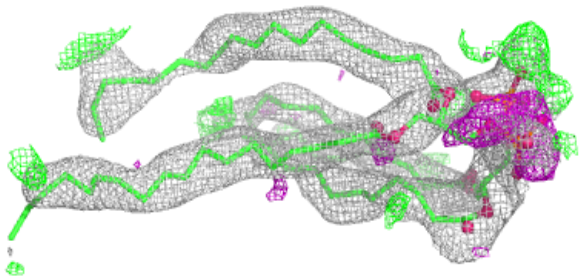


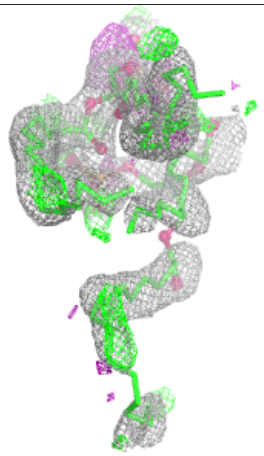


Electron density around CDL C 305:

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

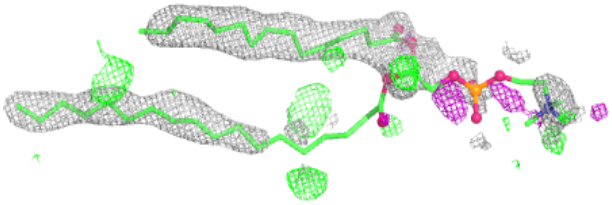


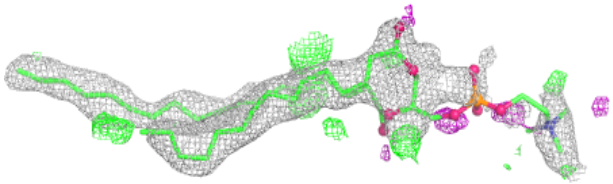


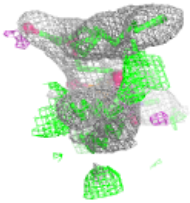


Electron density around PSC O 302:

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

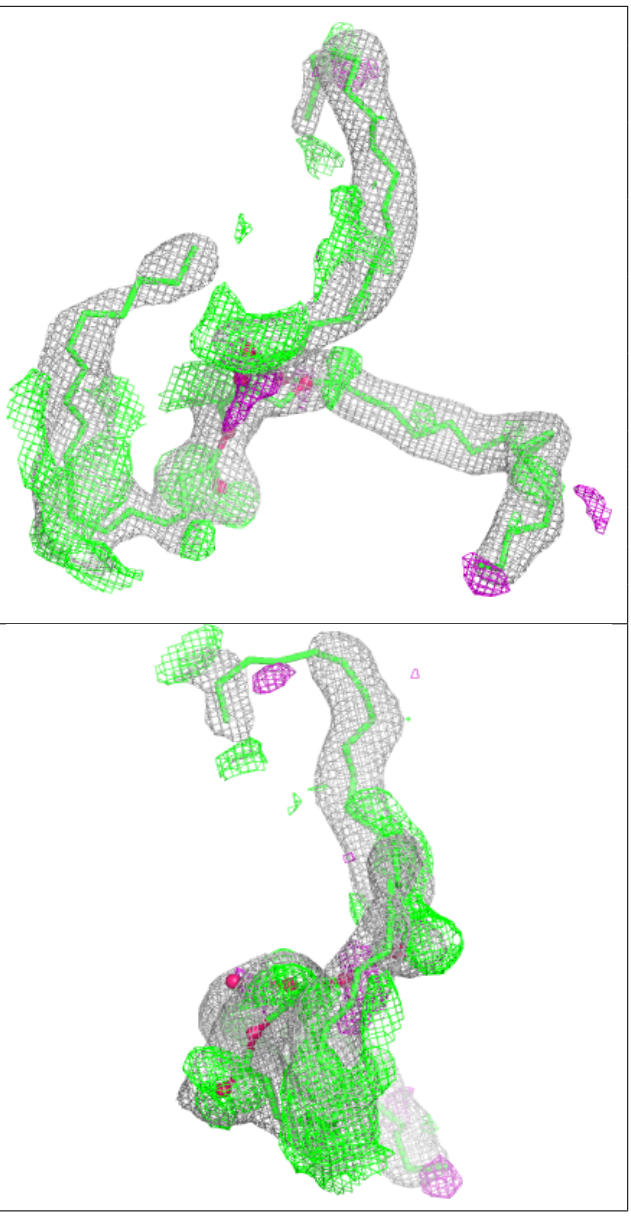






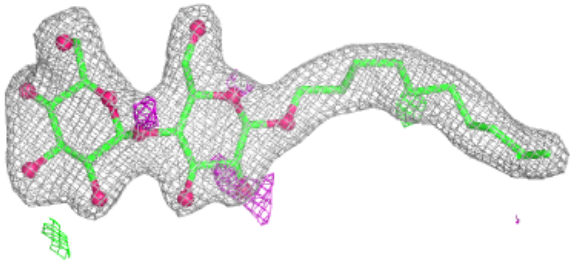
Electron density around TGL L 101:

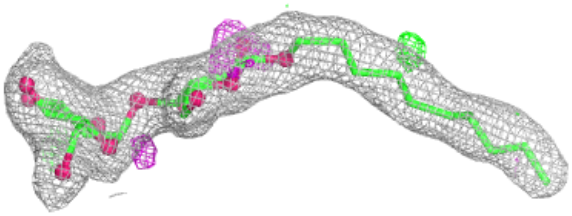
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

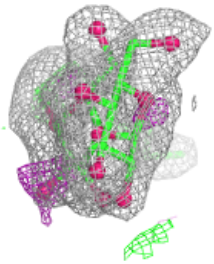


Electron density around DMU Z 101:

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

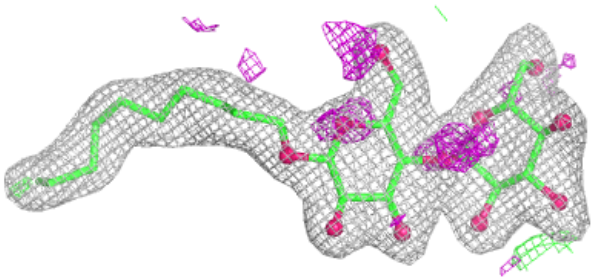


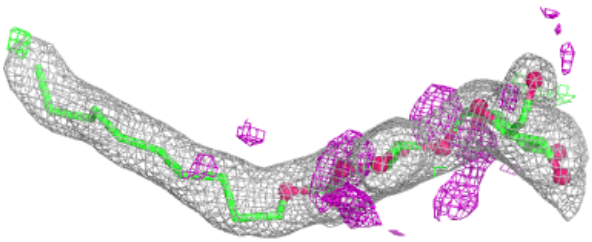


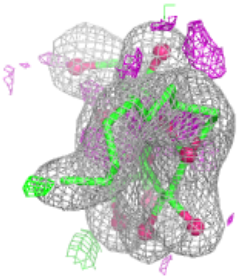


Electron density around DMU M 101:

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

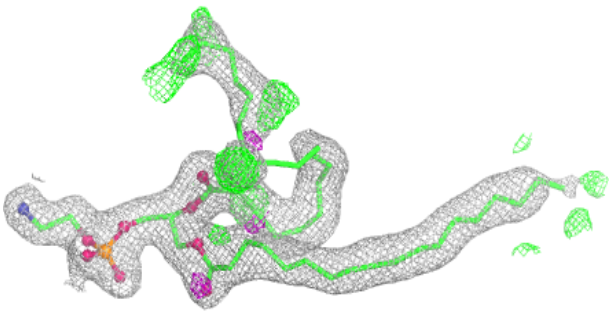


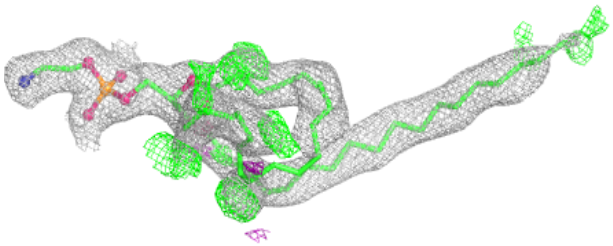


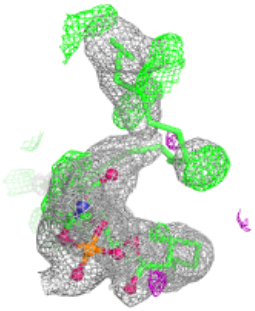


Electron density around PEK P 312:

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

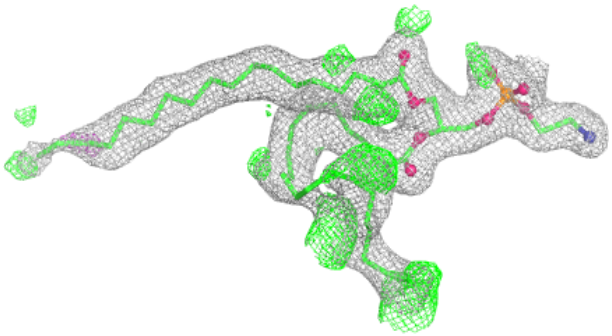


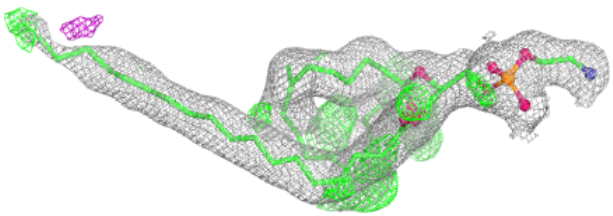


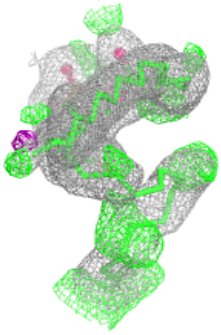


Electron density around PEK G 101:

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

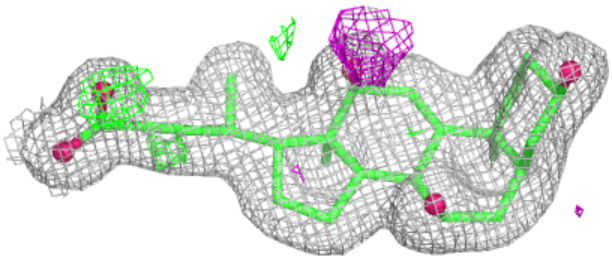


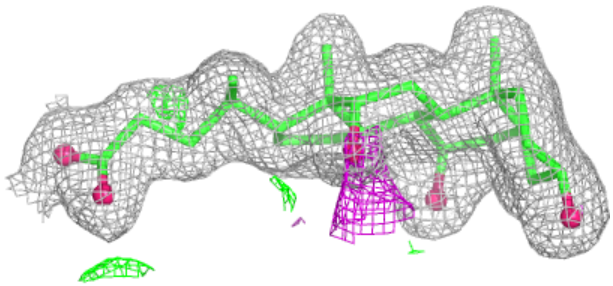


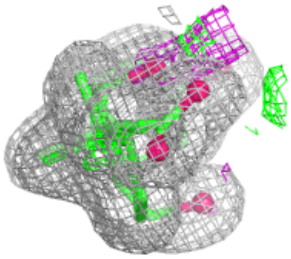


Electron density around CHD C 301:

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

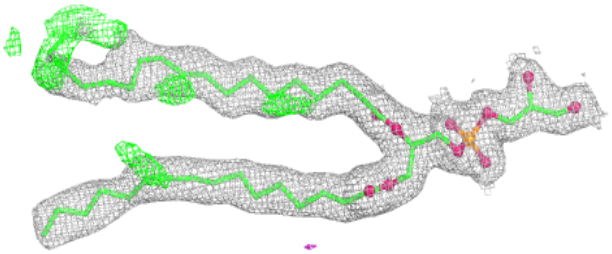


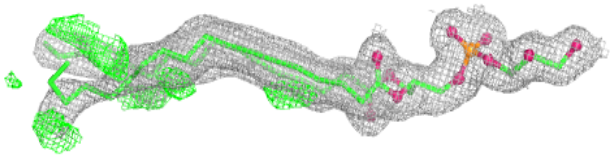


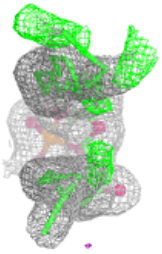


Electron density around PGV C 304:

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

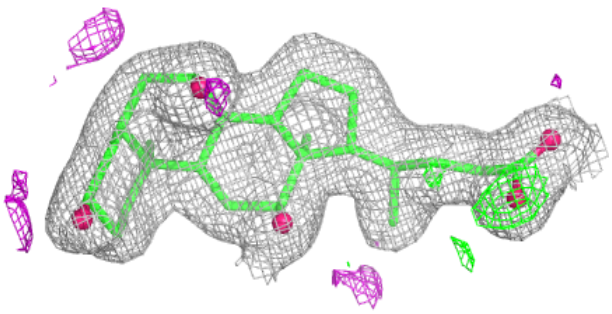


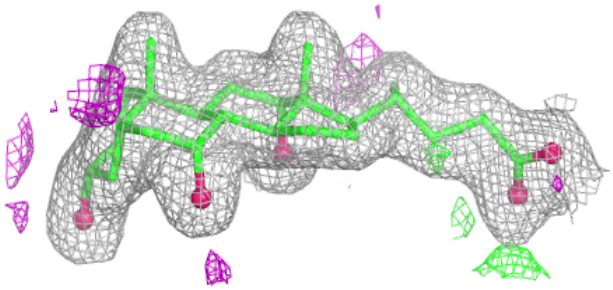


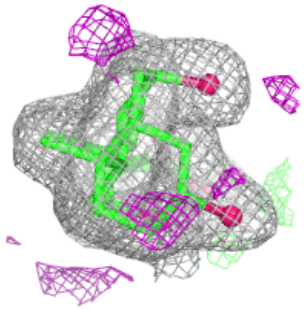


Electron density around CHD P 301:

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

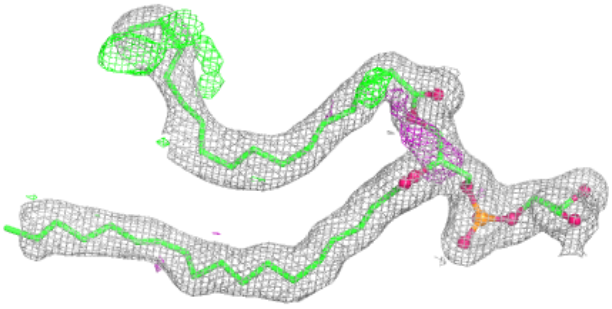


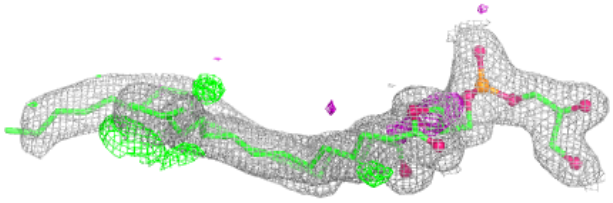




Electron density around PGV N 609:

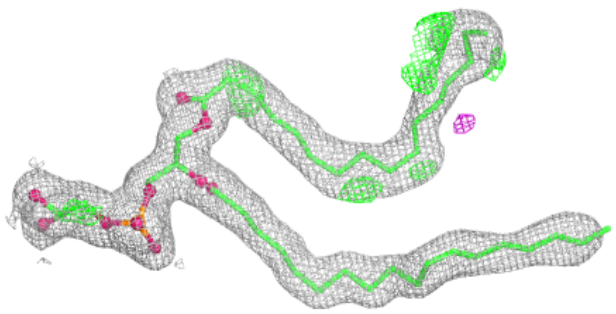
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

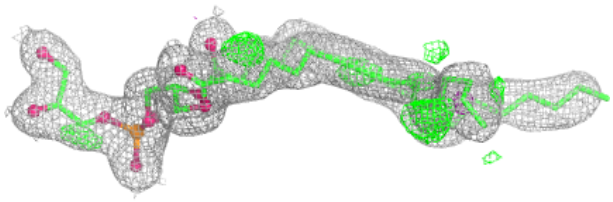


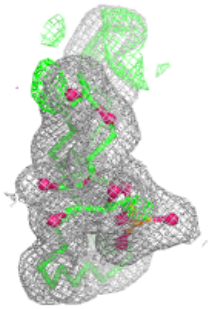


Electron density around PGV A 608:

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

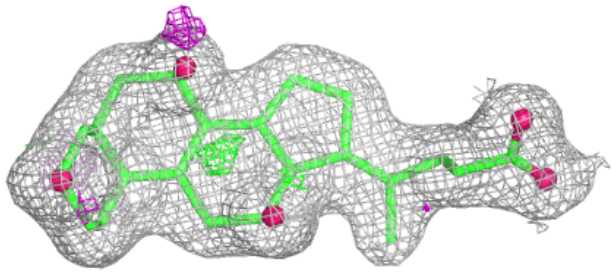


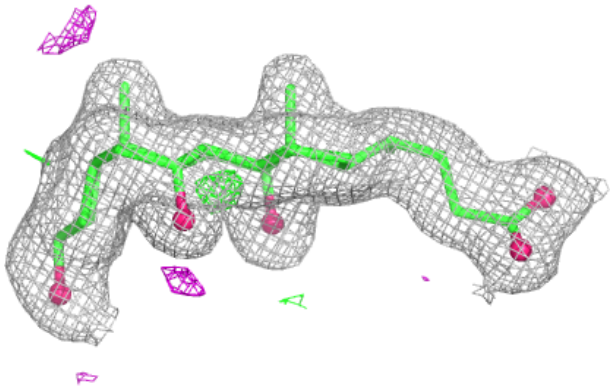


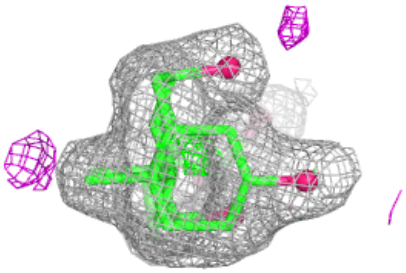


Electron density around CHD B 302:

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

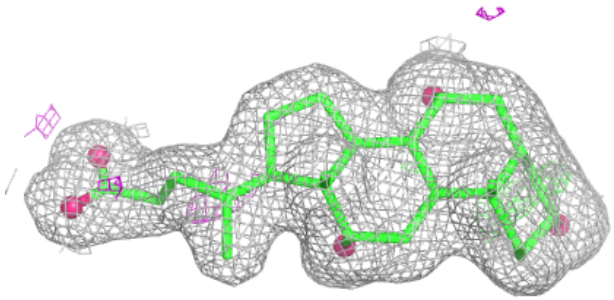


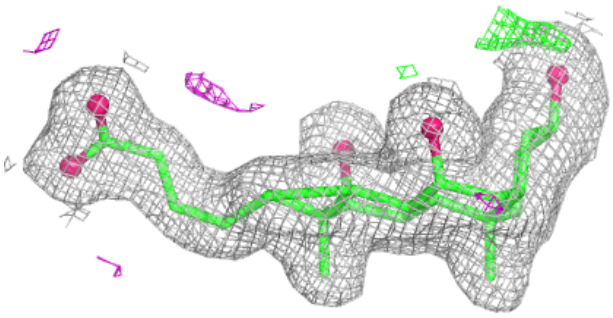


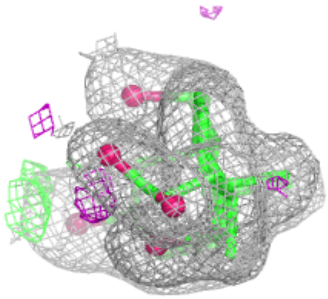


Electron density around CHD G 102:

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

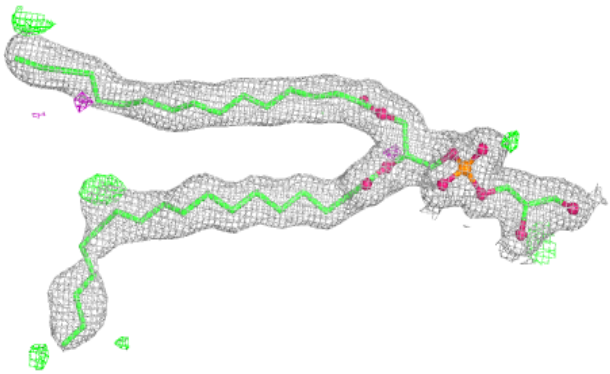


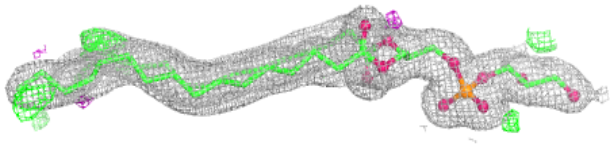


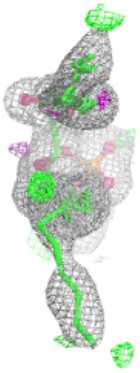


Electron density around PGV P 303:

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

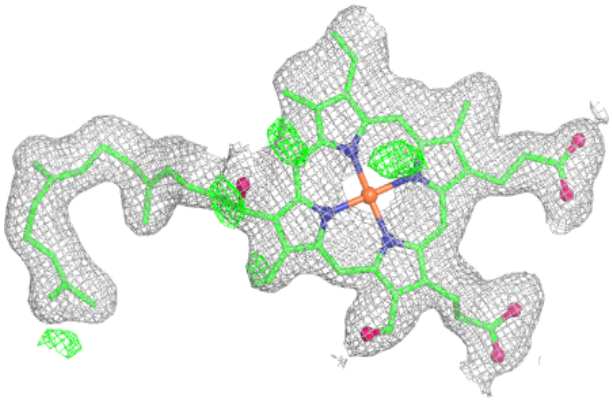


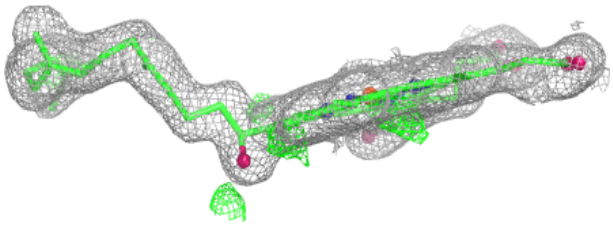


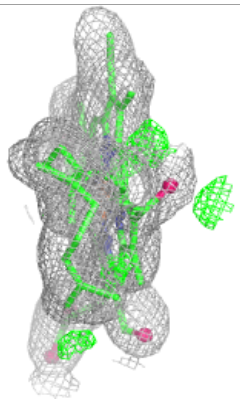


Electron density around HEA N 603 (B):

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

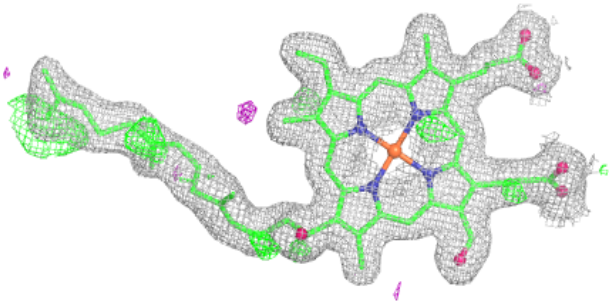


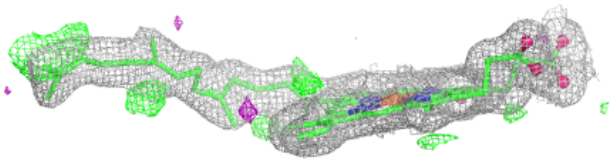


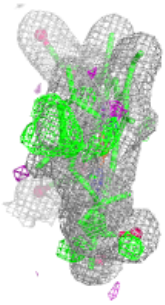


Electron density around HEA A 601:

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

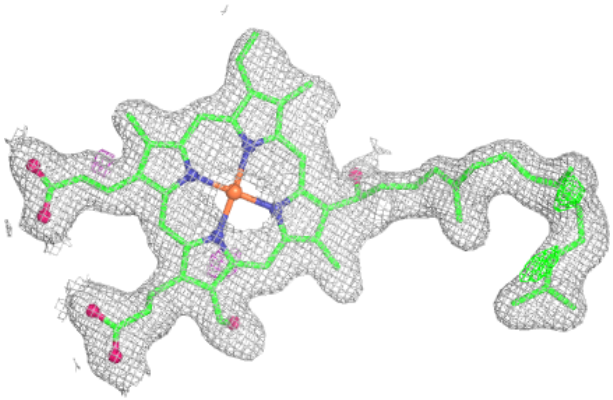


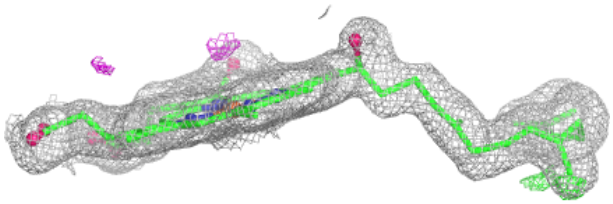


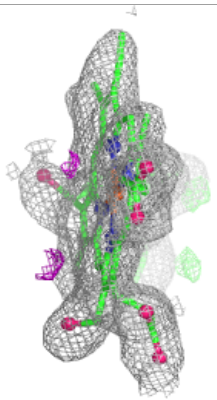


Electron density around HEA A 602 (A):

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

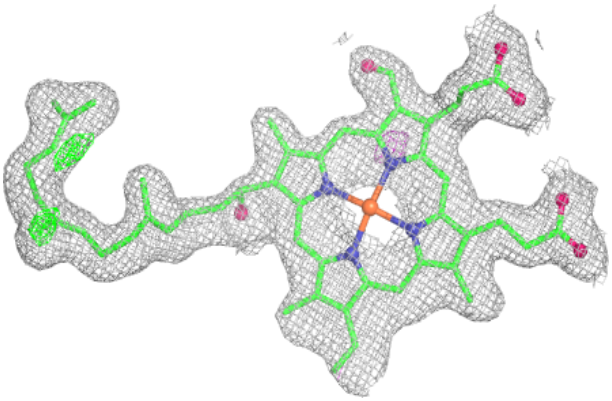


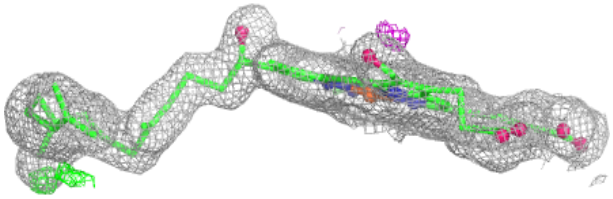




Electron density around HEA A 602 (B):

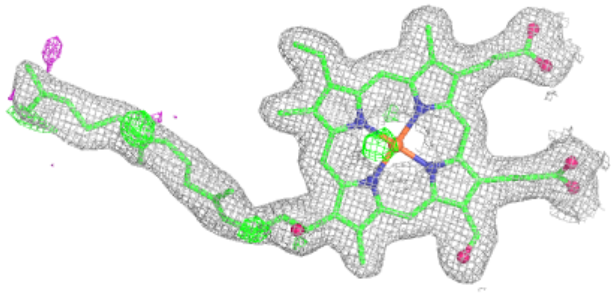
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

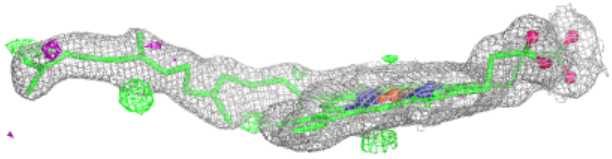


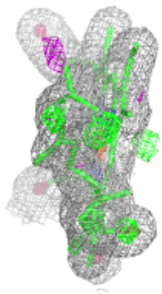


Electron density around HEA N 602:

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

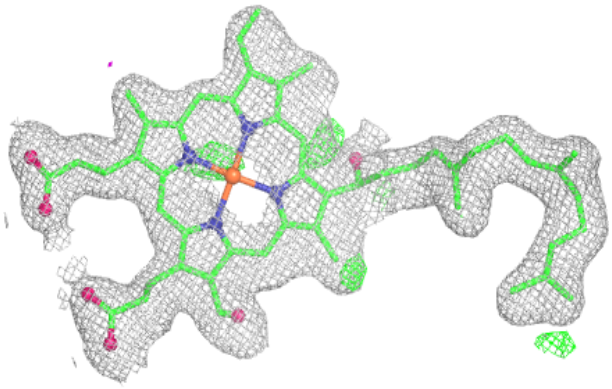


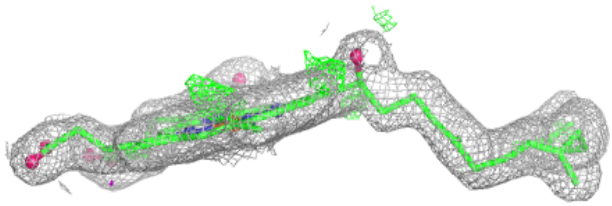


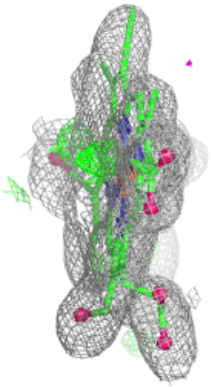


Electron density around HEA N 603 (A):

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







6.5 Other polymers (i)

There are no such residues in this entry.