wwPDB X-ray Structure Validation Summary Report (i)

Nov 13, 2023 – 12:10 PM JST

PDB ID	:	5X19
Title	:	CO bound cytochrome c oxidase at 100 micro sec after pump laser irradiation to release CO from O2 reduction center
Authors	:	Shimada, A.; Kubo, M.; Baba, S.; Yamashita, K.; Hirata, K.; Ueno, G.; Nomura, T.; Kimura, T.; Shinzawa-Itoh, K.; Baba, J.; Hatano, K.; Eto, Y.; Miyamoto, A.; Murakami, H.; Kumasaka, T.; Owada, S.; Tono, K.; Yabashi, M.; Yamaguchi, Y.; Yanagisawa, S.; Sakaguchi, M.; Ogura, T.; Komiya, R.; Yan, J.; Yamashita, E.; Yamamoto, M.; Ago, H.; Yoshikawa, S.; Tsukihara, T.
Deposited on	:	2017-01-25
Resolution	:	2.20 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:

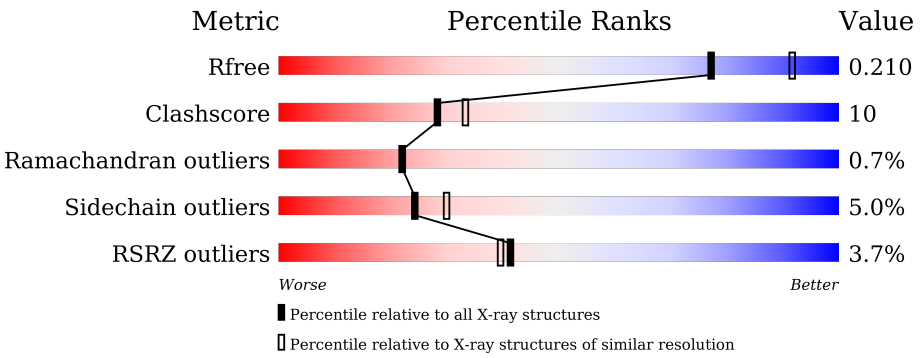
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)

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 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	85% 14% •
1	N	514	% 81% 18% •
2	B	227	% 77% 22% •

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Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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Mol	Chain	Length	Quality of chain
2	O	227	3% 74% 22%
3	C	261	84% 15%
3	P	261	2% 88% 11%
4	D	147	% 84% 12%
4	Q	147	11% 79% 17%
5	E	109	2% 85% 11%
5	R	109	6% 73% 19%
6	F	98	10% 67% 24% 5%
6	S	98	6% 76% 20%
7	G	85	18% 66% 26% 5%
7	T	85	12% 62% 28% 8%
8	H	85	5% 71% 18% 7%
8	U	85	6% 76% 15% 7%
9	I	73	4% 81% 14% 5%
9	V	73	7% 79% 19%
10	J	59	8% 88% 7%
10	W	59	5% 76% 19%
11	K	56	9% 68% 20% 12%
11	X	56	14% 70% 16% 12%
12	L	47	66% 28%
12	Y	47	6% 72% 23%
13	M	46	2% 74% 17% 7%
13	Z	46	9% 72% 22% 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	CMO	N	606	-	-	X	-
21	EDO	A	612	-	-	X	-
21	EDO	A	613	-	-	X	-
21	EDO	C	310	-	-	-	X
21	EDO	N	610	-	-	-	X
21	EDO	T	105	-	-	X	-
25	UNX	P	302	-	-	-	X
26	CDL	T	104	-	-	X	-
27	PEK	G	103	-	-	-	X
27	PEK	T	102	-	-	-	X
9	SAC	V	1	-	-	-	X

2 Entry composition (i)

There are 30 unique types of molecules in this entry. The entry contains 32242 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	4068	2718	628	686	36	0	7	0
1	N	514	4027	2691	623	678	35	0	0	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	1824	1185	281	340	18	0	0	0
2	O	227	1824	1185	281	340	18	0	0	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	2110	1412	336	350	12	0	0	0
3	P	259	2110	1412	336	350	12	0	0	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	1195	777	196	218	4	0	0	0
4	Q	144	1195	777	196	218	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	105	852	544	144	162	2	0	0	0
5	R	105	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	748	464	134	145	5	0	0	0
6	S	98	748	464	134	145	5	0	0	0

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
7	G	84	675	431	129	113	1	1	0	0	0
7	T	84	675	431	129	113	1	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	79	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	73	609	398	107	100	4	0	1	0
9	V	73	617	406	107	100	4	0	2	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	J	58	460	297	78	82	3	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	W	58	460	297	78	82	3	0	0	0

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

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

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

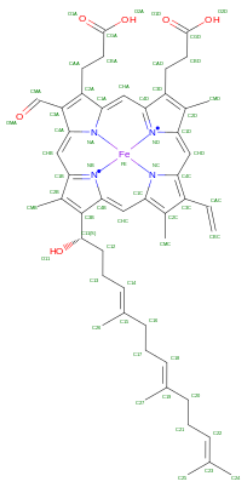
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	L	46	380	254	64	60	2	0	0	0
			Total	C	N	O	S			
12	Y	46	380	254	64	60	2	0	0	0

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

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

- Molecule 14 is HEME-A (three-letter code: 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	60	49	1	4	6	0	0
			Total	C	Fe	N	O		
14	N	1	60	49	1	4	6	0	0
			Total	C	Fe	N	O		
14	N	1	60	49	1	4	6	0	0

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

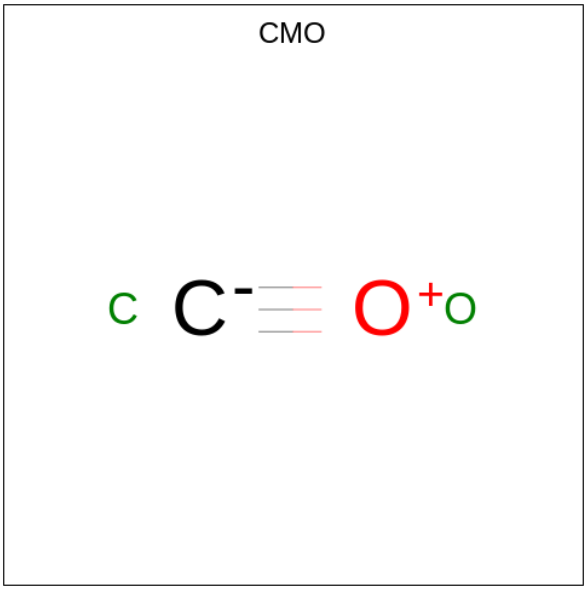
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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 (three-letter code: NA) (formula: Na).

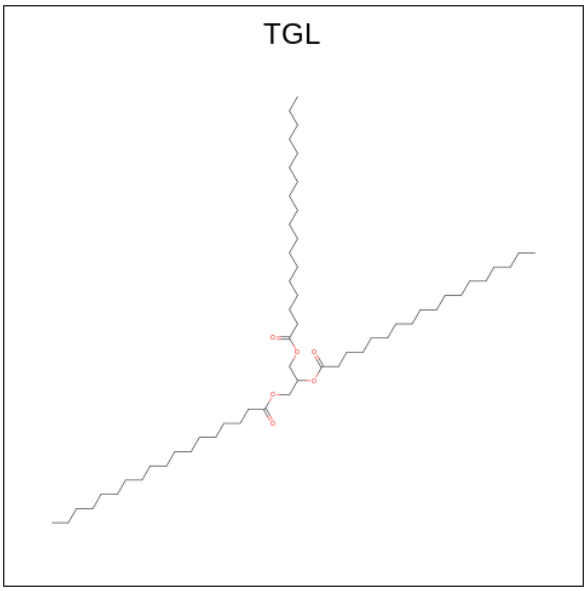
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
17	A	1	1	1	0	0
			Total	Na		
17	N	1	1	1	0	0

- Molecule 18 is CARBON MONOXIDE (three-letter code: CMO) (formula: CO).



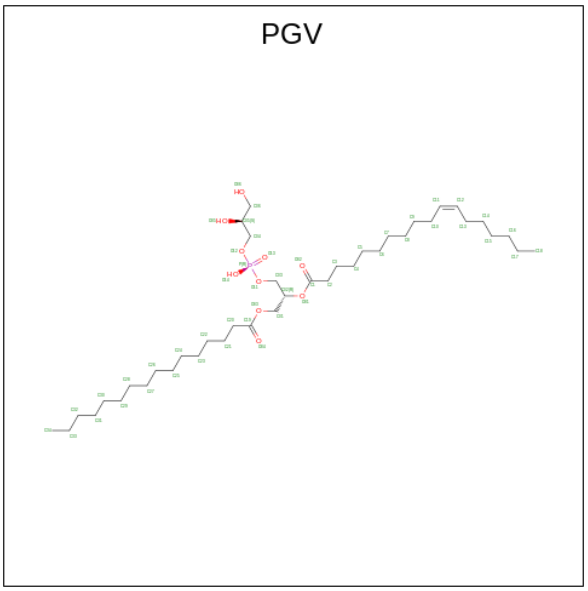
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
18	A	1	2	1	1	0	0
			Total	C	O		
18	N	1	2	1	1	0	0

- Molecule 19 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: $C_{57}H_{110}O_6$).



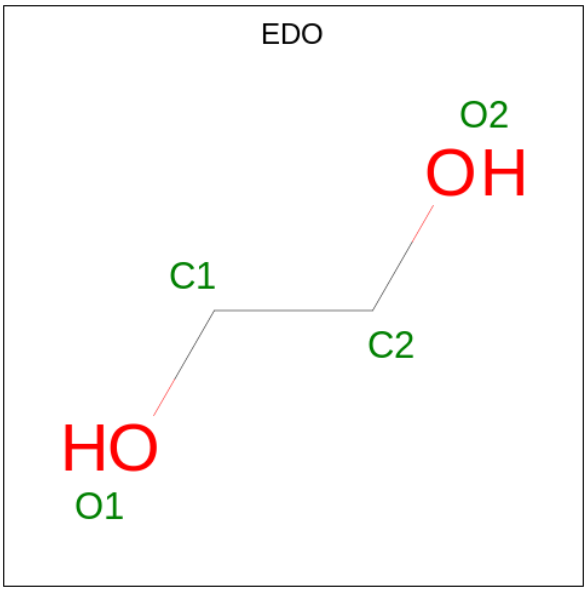
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
19	A	1	63	57	6	0	0
19	D	1	63	57	6	0	0
19	L	1	63	57	6	0	0
19	O	1	63	57	6	0	0
19	Q	1	63	57	6	0	0
19	Y	1	63	57	6	0	0

- Molecule 20 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: $C_{40}H_{77}O_{10}P$).



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

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



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

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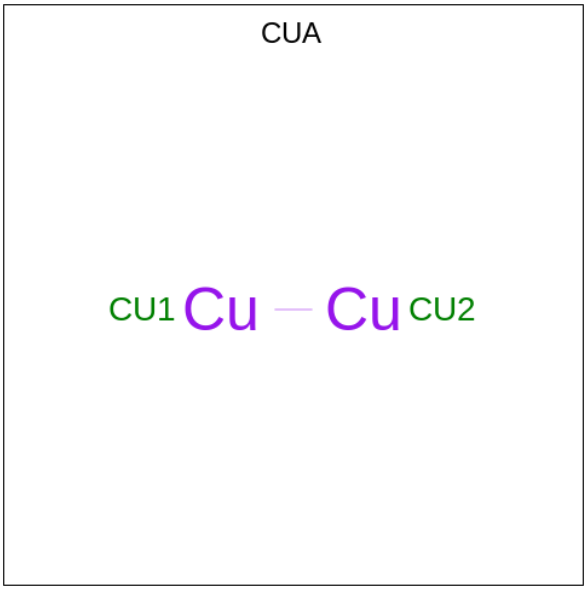
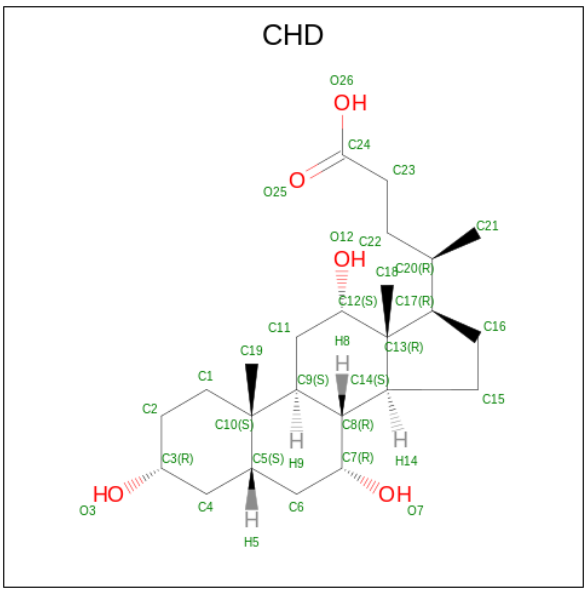
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
21	K	1	4	2	2	0	0
			Total	C	O		
21	K	1	4	2	2	0	0
			Total	C	O		
21	L	1	4	2	2	0	0
			Total	C	O		
21	N	1	4	2	2	0	0
			Total	C	O		
21	N	1	4	2	2	0	0
			Total	C	O		
21	O	1	4	2	2	0	0
			Total	C	O		
21	P	1	4	2	2	0	0
			Total	C	O		
21	P	1	4	2	2	0	0
	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

- Molecule 22 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).



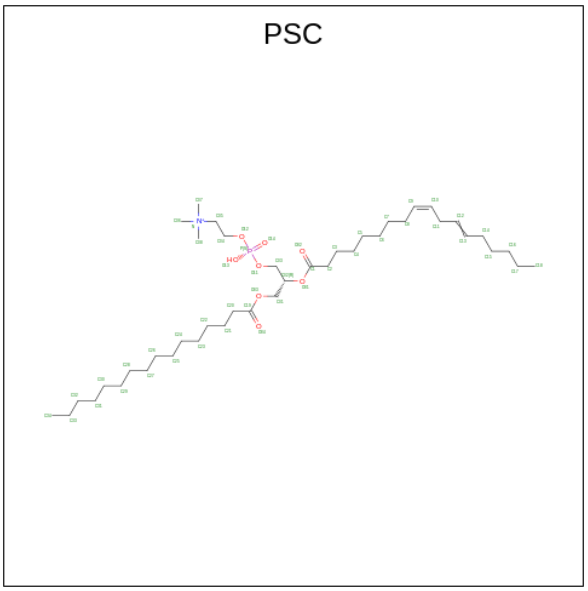
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cu		
22	B	1	2	2	0	0
			Total	Cu		
22	O	1	2	2	0	0

- Molecule 23 is CHOLIC ACID (three-letter code: CHD) (formula: $C_{24}H_{40}O_5$).



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

- 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 (three-letter code: PSC) (formula: $C_{42}H_{81}NO_8P$).

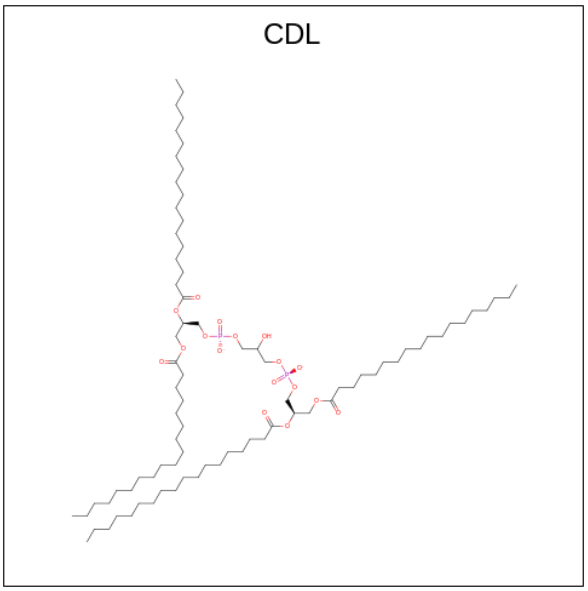


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
24	B	1	52	42	1	8	1	0	0
			Total	C	N	O	P		
24	O	1	52	42	1	8	1	0	0

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

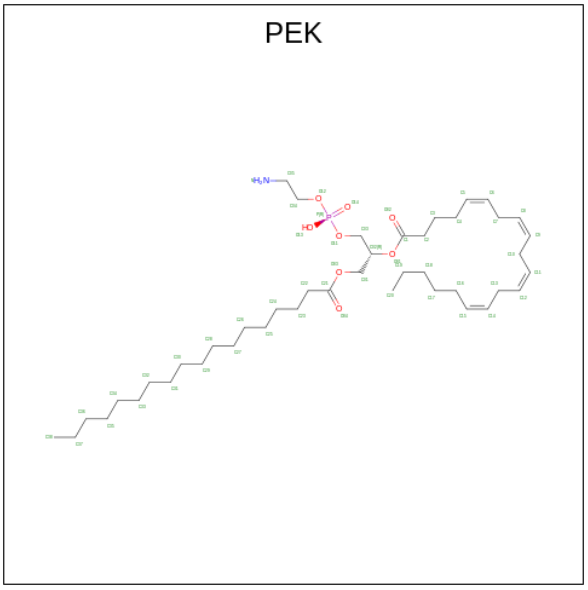
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	X		
25	C	1	1	1	0	0
			Total	X		
25	P	1	1	1	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	C	1	Total	C	O	P	0	0
			100	81	17	2		
26	G	1	Total	C	O	P	0	0
			100	81	17	2		
26	P	1	Total	C	O	P	0	0
			100	81	17	2		
26	T	1	Total	C	O	P	0	0
			100	81	17	2		

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

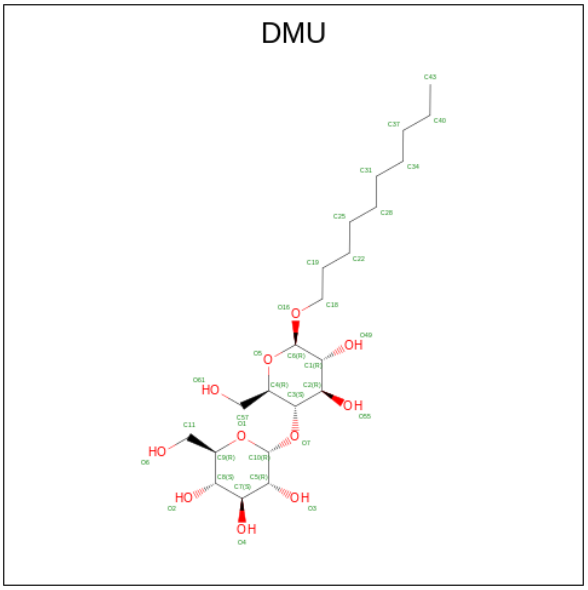


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
27	C	1	53	43	1	8	1	0	0
27	G	1	53	43	1	8	1	0	0
27	G	1	53	43	1	8	1	0	0
27	T	1	53	43	1	8	1	0	0
27	T	1	53	43	1	8	1	0	0
27	T	1	53	43	1	8	1	0	0

- Molecule 28 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 29 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
29	M	1	33	22	11	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
29	Z	1	33	22	11	0	0

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
30	A	191	191	191	0	0
30	B	120	121	121	0	1
30	C	83	83	83	0	0
30	D	89	89	89	0	0
30	E	45	45	45	0	0
30	F	49	49	49	0	0
30	G	40	40	40	0	0
30	H	37	37	37	0	0
30	I	19	19	19	0	0
30	J	19	19	19	0	0
30	K	27	27	27	0	0
30	L	27	27	27	0	0
30	M	18	18	18	0	0
30	N	169	169	169	0	0
30	O	100	101	101	0	1
30	P	91	91	91	0	0
30	Q	38	38	38	0	0
30	R	40	40	40	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
30	S	55	55	55	0	0
			Total	O		
30	T	45	45	45	0	0
			Total	O		
30	U	27	27	27	0	0
			Total	O		
30	V	23	23	23	0	0
			Total	O		
30	W	23	23	23	0	0
			Total	O		
30	X	16	16	16	0	0
			Total	O		
30	Y	18	18	18	0	0
			Total	O		
30	Z	4	4	4	0	0

3 Residue-property plots (i)

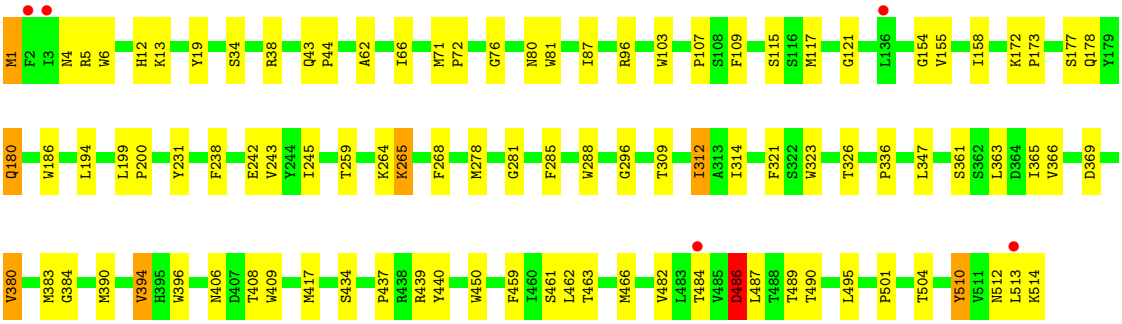
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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:

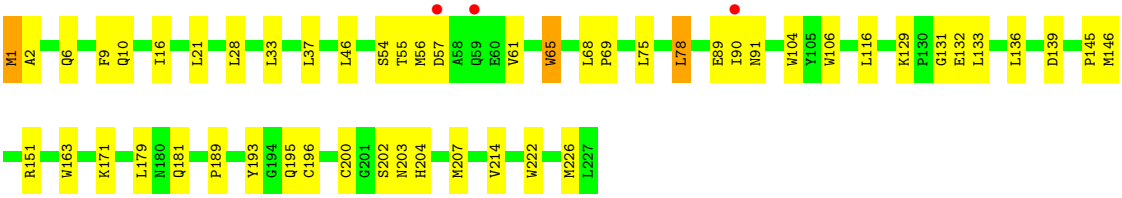
• Molecule 1: Cytochrome c oxidase subunit 1

Chain N:



• Molecule 2: Cytochrome c oxidase subunit 2

Chain B:



• Molecule 2: Cytochrome c oxidase subunit 2

Chain O: 3% 74% 22%

M1 A2 Q6 D11 A12 T13 S14 P15 I16 D25 L33 I42 L46 T47 L50 Q59 E60 W65 L68 P69 L75 I76 A77 L78 R82 M86 M87 D88 E89 I90 N91 N92 P93 H102 Q103 W104 Y105 W106 Y113 E114 D115 L116 Y121

G131 E132 E137 V138 D139 N140 M146 R151 E157 H161 A164 L168 Q181 T182 T183 L184 M185 G194 Q195 C196 C200 N203 H204 M207 L211 E212 L213 K221 M226 L227

- Molecule 3: Cytochrome c oxidase subunit 3

Chain C: 84% 15%

MET THR H3 V11 N12 P13 P17 A21 L22 S23 S29 N38 S39 M40 T41 L42 L43 M44 L47 M51 M54 W58 F67 L85 W99 S105 P110 E111 W116 N125 P126 L127 E128 W146 G154 K157 H158 M159 L160 Q177

T187 F214 L223 H226 H231 W240 D246 W249 W259 G260 S261

- Molecule 3: Cytochrome c oxidase subunit 3

Chain P: 2% 88% 11%

MET THR H3 L22 L25 G30 M33 F37 N38 S39 M40 T41 L42 Y55 Q56 W57 R63 F67 H103 L106 T109 L112 W116 L127 E128 V129 W146 K157 H158 M159 L160 E180 G194 T213 F244 V245 D246 W249

W258 W259 G260 S261

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

Chain D: % 84% 12%

ALA HIS GLY S4 S8 L13 D21 N32 L33 S34 Q37 K45 W48 L51 E58 W78 W98 E114 W115 Q119 T120 K121 V128 A129 W138 W145 K146 K147

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

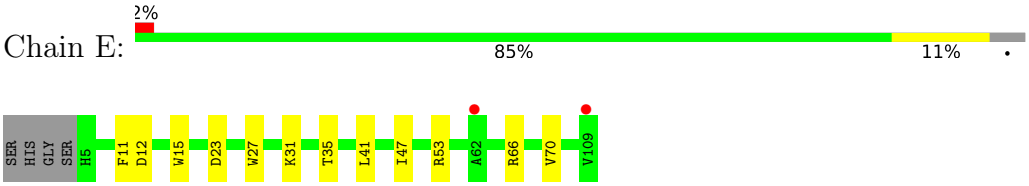
Chain Q: 11% 79% 17%

ALA HIS GLY S4 V5 V6 K7 S8 E9 A12 R20 N32 L33 S34 A35 S36 Q37 K43 E44 S49 S52 E55 R73 E77 W78 K79 M86 T92 A93 I97 W98 Y102 V103 Y104 P108 H109 V116 A117 K118 Q119 T120 K121 W138 D139

Y140 D141 K142 W145 K146 K147

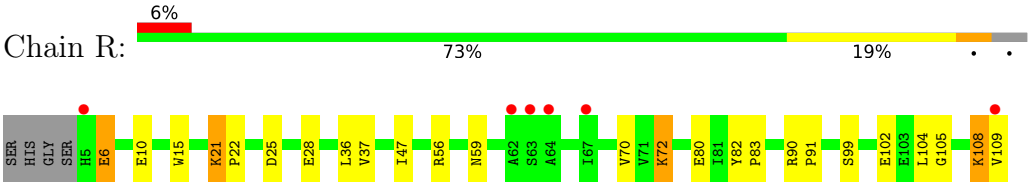
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

Chain E:



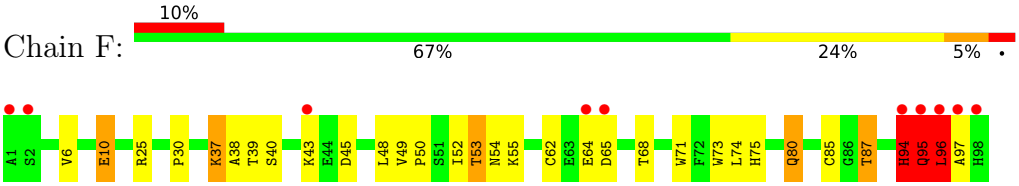
• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

Chain R:



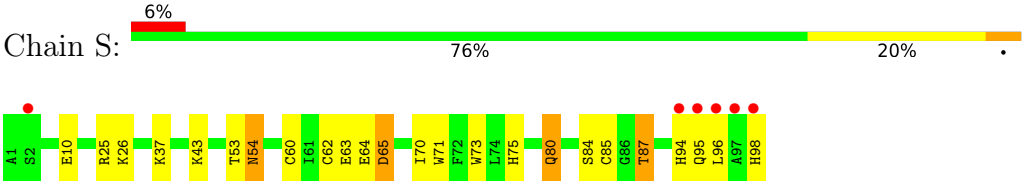
• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

Chain F:



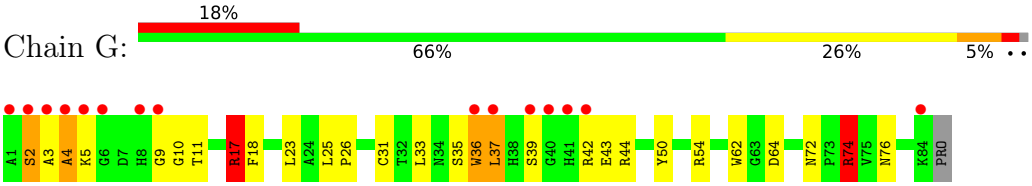
• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

Chain S:



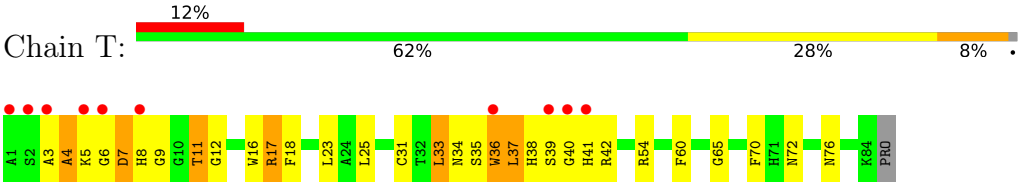
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain G:



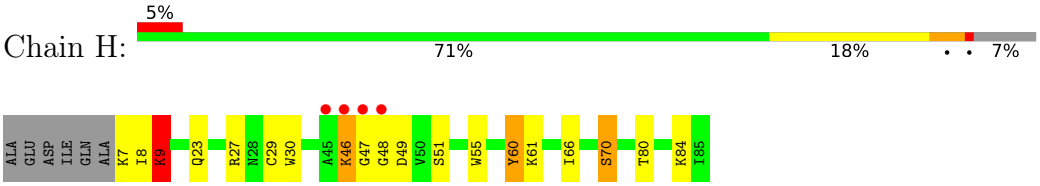
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain T:



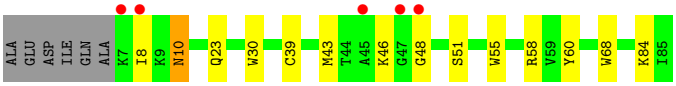
• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain H:



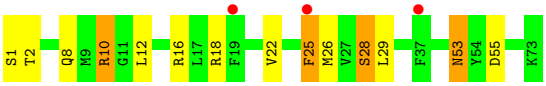
• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain U:



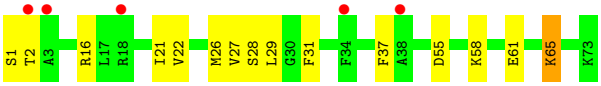
• Molecule 9: Cytochrome c oxidase subunit 6C

Chain I:



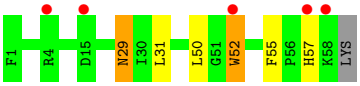
• Molecule 9: Cytochrome c oxidase subunit 6C

Chain V:



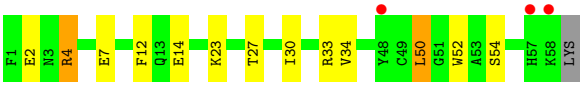
• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial

Chain J:



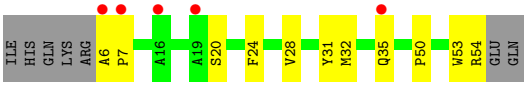
• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial

Chain W:



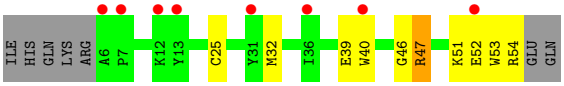
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

Chain K:



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

Chain X:

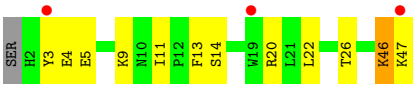


• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain L:

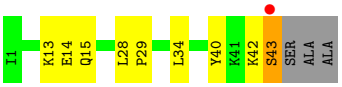
• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain Y:



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

Chain M:



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

Chain Z:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	185.03Å 208.85Å 178.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.20 24.99 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.8 (25.00-2.20) 96.9 (24.99-2.20)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.35 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.8.0048	Depositor
R, R_{free}	0.173 , 0.210 0.173 , 0.210	Depositor DCC
R_{free} test set	17156 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	51.4	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 63.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.028 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	32242	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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	1.05	12/4205 (0.3%)	0.95	5/5744 (0.1%)
1	N	1.02	9/4156 (0.2%)	0.92	4/5678 (0.1%)
2	B	0.94	3/1860 (0.2%)	0.96	4/2534 (0.2%)
2	O	0.83	2/1860 (0.1%)	0.91	2/2534 (0.1%)
3	C	1.06	5/2197 (0.2%)	0.92	1/3005 (0.0%)
3	P	1.01	4/2197 (0.2%)	0.87	1/3005 (0.0%)
4	D	0.94	5/1229 (0.4%)	0.88	2/1658 (0.1%)
4	Q	0.78	3/1229 (0.2%)	0.80	2/1658 (0.1%)
5	E	0.82	2/871 (0.2%)	0.94	2/1182 (0.2%)
5	R	0.72	1/871 (0.1%)	0.79	0/1182
6	F	0.86	2/765 (0.3%)	0.89	0/1038
6	S	0.80	0/765	0.89	1/1038 (0.1%)
7	G	0.97	2/690 (0.3%)	0.99	5/937 (0.5%)
7	T	0.90	1/690 (0.1%)	0.86	0/937
8	H	0.88	1/682 (0.1%)	0.88	0/921
8	U	0.84	3/682 (0.4%)	0.81	0/921
9	I	0.76	0/617	0.93	2/818 (0.2%)
9	V	0.70	0/629	0.83	1/834 (0.1%)
10	J	0.80	1/471 (0.2%)	0.84	0/636
10	W	0.71	1/471 (0.2%)	0.75	0/636
11	K	0.93	1/398 (0.3%)	0.75	0/546
11	X	0.85	2/398 (0.5%)	0.80	0/546
12	L	0.88	0/393	0.84	0/526
12	Y	0.77	0/393	0.76	0/526
13	M	0.85	0/345	0.82	0/470
13	Z	0.76	0/345	0.74	0/470
All	All	0.93	60/29409 (0.2%)	0.89	32/39980 (0.1%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
8	H	0	1

The worst 5 of 60 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	81	TRP	CD2-CE2	7.66	1.50	1.41
2	B	65	TRP	CD2-CE2	7.41	1.50	1.41
1	N	323	TRP	CD2-CE2	7.36	1.50	1.41
3	C	240	TRP	CD2-CE2	7.11	1.49	1.41
1	N	81	TRP	CD2-CE2	7.05	1.49	1.41

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	246	ASP	CB-CG-OD1	-8.98	110.22	118.30
9	I	10	ARG	NE-CZ-NH2	-8.12	116.24	120.30
1	A	71	MET	CG-SD-CE	-7.57	88.08	100.20
1	N	96	ARG	NE-CZ-NH2	-7.12	116.74	120.30
5	E	53	ARG	NE-CZ-NH1	6.43	123.52	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	H	9	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	4068	0	4048	86	0
1	N	4027	0	4001	90	0
2	B	1824	0	1833	34	0
2	O	1824	0	1833	48	0
3	C	2110	0	2027	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	P	2110	0	2027	18	0
4	D	1195	0	1183	12	0
4	Q	1195	0	1183	28	0
5	E	852	0	845	4	0
5	R	852	0	845	13	0
6	F	748	0	728	24	0
6	S	748	0	728	17	0
7	G	675	0	643	23	0
7	T	675	0	643	29	0
8	H	662	0	623	9	0
8	U	662	0	623	7	0
9	I	609	0	622	11	0
9	V	617	0	631	7	0
10	J	460	0	459	3	0
10	W	460	0	459	13	0
11	K	384	0	366	5	0
11	X	384	0	366	7	0
12	L	380	0	380	20	0
12	Y	380	0	380	9	0
13	M	335	0	352	7	0
13	Z	335	0	352	8	0
14	A	120	0	108	13	0
14	N	120	0	108	11	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	2	0	0	1	0
18	N	2	0	0	2	0
19	A	63	0	110	3	0
19	D	63	0	110	5	0
19	L	63	0	110	9	0
19	O	63	0	110	7	0
19	Q	63	0	110	5	0
19	Y	63	0	110	3	0
20	A	102	0	152	5	0
20	C	102	0	152	4	0
20	N	102	0	152	6	0
20	P	102	0	152	3	0
21	A	16	0	24	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	B	8	0	12	1	0
21	C	16	0	24	2	0
21	F	8	0	12	2	0
21	G	4	0	6	0	0
21	H	4	0	6	2	0
21	K	8	0	12	0	0
21	L	4	0	6	0	0
21	N	8	0	12	3	0
21	O	4	0	6	0	0
21	P	8	0	12	0	0
21	T	4	0	6	4	0
22	B	2	0	0	0	0
22	O	2	0	0	0	0
23	B	29	0	39	1	0
23	C	58	0	78	5	0
23	G	29	0	39	1	0
23	J	29	0	38	0	0
23	P	58	0	78	6	0
23	W	29	0	38	9	0
24	B	52	0	80	4	0
24	O	52	0	80	5	0
25	C	1	0	0	0	0
25	P	1	0	0	0	0
26	C	100	0	156	6	0
26	G	100	0	156	6	0
26	P	100	0	156	7	0
26	T	100	0	156	21	0
27	C	53	0	77	3	0
27	G	106	0	154	6	0
27	T	159	0	231	13	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	M	33	0	42	0	0
29	Z	33	0	42	2	0
30	A	191	0	0	17	0
30	B	121	0	0	5	0
30	C	83	0	0	16	0
30	D	89	0	0	1	0
30	E	45	0	0	2	0
30	F	49	0	0	2	0
30	G	40	0	0	6	0
30	H	37	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	I	19	0	0	0	0
30	J	19	0	0	1	0
30	K	27	0	0	1	0
30	L	27	0	0	6	0
30	M	18	0	0	0	0
30	N	169	0	0	22	0
30	O	101	0	0	21	0
30	P	91	0	0	7	0
30	Q	38	0	0	8	0
30	R	40	0	0	0	0
30	S	55	0	0	5	0
30	T	45	0	0	3	0
30	U	27	0	0	0	0
30	V	23	0	0	1	0
30	W	23	0	0	4	0
30	X	16	0	0	1	0
30	Y	18	0	0	3	0
30	Z	4	0	0	0	0
All	All	32242	0	31442	611	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 10.

The worst 5 of 611 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:PHE:HE1	30:A:867:HOH:O	1.15	1.25
1:N:312:ILE:HB	30:N:844:HOH:O	1.31	1.23
7:G:50:TYR:HA	30:G:208:HOH:O	1.07	1.23
30:A:704:HOH:O	3:C:17:PRO:HB3	1.34	1.21
3:P:246:ASP:HB2	30:P:464:HOH:O	1.35	1.20

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	519/514 (101%)	503 (97%)	16 (3%)	0	100	100
1	N	512/514 (100%)	493 (96%)	19 (4%)	0	100	100
2	B	225/227 (99%)	215 (96%)	10 (4%)	0	100	100
2	O	225/227 (99%)	217 (96%)	6 (3%)	2 (1%)	17	16
3	C	257/261 (98%)	251 (98%)	5 (2%)	1 (0%)	34	37
3	P	257/261 (98%)	253 (98%)	4 (2%)	0	100	100
4	D	142/147 (97%)	139 (98%)	3 (2%)	0	100	100
4	Q	142/147 (97%)	137 (96%)	4 (3%)	1 (1%)	22	22
5	E	103/109 (94%)	101 (98%)	2 (2%)	0	100	100
5	R	103/109 (94%)	101 (98%)	2 (2%)	0	100	100
6	F	96/98 (98%)	89 (93%)	4 (4%)	3 (3%)	4	2
6	S	96/98 (98%)	88 (92%)	8 (8%)	0	100	100
7	G	81/85 (95%)	69 (85%)	9 (11%)	3 (4%)	3	1
7	T	81/85 (95%)	69 (85%)	5 (6%)	7 (9%)	1	0
8	H	77/85 (91%)	71 (92%)	4 (5%)	2 (3%)	5	3
8	U	77/85 (91%)	70 (91%)	4 (5%)	3 (4%)	3	1
9	I	72/73 (99%)	71 (99%)	1 (1%)	0	100	100
9	V	73/73 (100%)	71 (97%)	1 (1%)	1 (1%)	11	8
10	J	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
10	W	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
11	K	47/56 (84%)	47 (100%)	0	0	100	100
11	X	47/56 (84%)	42 (89%)	5 (11%)	0	100	100
12	L	44/47 (94%)	44 (100%)	0	0	100	100
12	Y	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
13	M	41/46 (89%)	41 (100%)	0	0	100	100
13	Z	41/46 (89%)	41 (100%)	0	0	100	100
All	All	3514/3614 (97%)	3374 (96%)	117 (3%)	23 (1%)	22	22

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	94	HIS
6	F	96	LEU
7	G	4	ALA
7	G	39	SER
7	T	4	ALA

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	432/426 (101%)	423 (98%)	9 (2%)	53	67
1	N	426/426 (100%)	413 (97%)	13 (3%)	40	51
2	B	210/210 (100%)	204 (97%)	6 (3%)	42	54
2	O	210/210 (100%)	199 (95%)	11 (5%)	23	28
3	C	224/226 (99%)	218 (97%)	6 (3%)	44	57
3	P	224/226 (99%)	219 (98%)	5 (2%)	52	65
4	D	128/129 (99%)	122 (95%)	6 (5%)	26	33
4	Q	128/129 (99%)	124 (97%)	4 (3%)	40	51
5	E	92/95 (97%)	90 (98%)	2 (2%)	52	65
5	R	92/95 (97%)	87 (95%)	5 (5%)	22	26
6	F	81/81 (100%)	71 (88%)	10 (12%)	4	4
6	S	81/81 (100%)	72 (89%)	9 (11%)	6	5
7	G	67/68 (98%)	58 (87%)	9 (13%)	4	3
7	T	67/68 (98%)	60 (90%)	7 (10%)	7	6
8	H	71/75 (95%)	61 (86%)	10 (14%)	3	2
8	U	71/75 (95%)	67 (94%)	4 (6%)	21	25
9	I	58/57 (102%)	51 (88%)	7 (12%)	5	4
9	V	59/57 (104%)	53 (90%)	6 (10%)	7	6
10	J	49/50 (98%)	46 (94%)	3 (6%)	18	21
10	W	49/50 (98%)	46 (94%)	3 (6%)	18	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	39/46 (85%)	36 (92%)	3 (8%)	13	13
11	X	39/46 (85%)	36 (92%)	3 (8%)	13	13
12	L	39/40 (98%)	36 (92%)	3 (8%)	13	13
12	Y	39/40 (98%)	38 (97%)	1 (3%)	46	58
13	M	37/38 (97%)	33 (89%)	4 (11%)	6	6
13	Z	37/38 (97%)	33 (89%)	4 (11%)	6	6
All	All	3049/3082 (99%)	2896 (95%)	153 (5%)	24	30

5 of 153 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	R	109	VAL
10	W	27	THR
6	S	54	ASN
7	T	42	ARG
13	Z	34	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
1	N	512	ASN
4	Q	29	HIS
2	O	10	GLN
2	O	181	GLN
5	R	94	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)

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FME	B	1	2	8,9,10	1.12	0	7,9,11	5.86	2 (28%)
1	FME	N	1	1	8,9,10	0.47	0	7,9,11	3.11	3 (42%)
1	FME	A	1	1	8,9,10	0.97	0	7,9,11	5.70	4 (57%)
9	SAC	V	1	9	7,8,9	1.74	1 (14%)	8,9,11	1.68	2 (25%)
9	SAC	I	1	9	7,8,9	1.54	1 (14%)	8,9,11	1.05	0
2	FME	O	1	2	8,9,10	1.07	1 (12%)	7,9,11	4.24	3 (42%)
7	TPO	G	11	7	8,10,11	1.72	2 (25%)	10,14,16	0.94	0
7	TPO	T	11	7	8,10,11	1.53	2 (25%)	10,14,16	1.10	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	B	1	2	-	3/7/9/11	-
1	FME	N	1	1	-	4/7/9/11	-
1	FME	A	1	1	-	4/7/9/11	-
9	SAC	V	1	9	-	6/7/8/10	-
9	SAC	I	1	9	-	4/7/8/10	-
2	FME	O	1	2	-	2/7/9/11	-
7	TPO	G	11	7	-	3/9/11/13	-
7	TPO	T	11	7	-	3/9/11/13	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	V	1	SAC	CA-N	4.34	1.52	1.46
9	I	1	SAC	CA-N	3.81	1.51	1.46
7	G	11	TPO	P-O1P	2.85	1.59	1.50
7	T	11	TPO	P-O1P	2.78	1.59	1.50
7	G	11	TPO	P-OG1	2.52	1.64	1.59

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	FME	CA-N-CN	-14.94	99.85	122.82
1	A	1	FME	CA-N-CN	-13.87	101.50	122.82
2	O	1	FME	CA-N-CN	-10.10	107.28	122.82
1	N	1	FME	CA-N-CN	-7.45	111.36	122.82
2	O	1	FME	C-CA-N	3.84	116.67	109.73

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O1-CN-N-CA
1	A	1	FME	N-CA-CB-CG
2	B	1	FME	O1-CN-N-CA
7	G	11	TPO	N-CA-CB-OG1
7	G	11	TPO	CG2-CB-OG1-P

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	FME	3	0
1	N	1	FME	1	0
7	T	11	TPO	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 77 ligands modelled in this entry, 8 are monoatomic and 2 are unknown - leaving 67 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	$\#\|Z\| > 2$
23	CHD	B	302	-	32,32,32	0.75	0	51,51,51	1.45	11 (21%)
19	TGL	Q	201	-	62,62,62	1.14	3 (4%)	65,65,65	1.05	5 (7%)
21	EDO	F	102	-	3,3,3	0.54	0	2,2,2	0.12	0
27	PEK	T	102	-	52,52,52	1.12	2 (3%)	55,57,57	0.98	5 (9%)
14	HEA	A	602	1	57,67,67	1.56	10 (17%)	61,103,103	1.98	18 (29%)
21	EDO	C	309	-	3,3,3	0.52	0	2,2,2	0.22	0
20	PGV	A	608	-	50,50,50	0.87	2 (4%)	53,56,56	1.45	4 (7%)
21	EDO	G	105	-	3,3,3	0.42	0	2,2,2	0.56	0
23	CHD	G	104	-	32,32,32	1.16	2 (6%)	51,51,51	1.51	10 (19%)
21	EDO	A	611	-	3,3,3	0.39	0	2,2,2	1.09	0
26	CDL	C	303	-	99,99,99	1.39	12 (12%)	105,111,111	1.23	9 (8%)
21	EDO	C	310	-	3,3,3	0.57	0	2,2,2	0.35	0
21	EDO	K	102	-	3,3,3	0.47	0	2,2,2	0.30	0
20	PGV	N	607	-	50,50,50	1.04	2 (4%)	53,56,56	1.11	5 (9%)
21	EDO	K	101	-	3,3,3	0.52	0	2,2,2	0.29	0
14	HEA	A	601	1	57,67,67	1.63	12 (21%)	61,103,103	1.61	11 (18%)
21	EDO	C	311	-	3,3,3	0.73	0	2,2,2	0.41	0
18	CMO	N	606	-	0,1,1	-	-	-		
23	CHD	J	101	-	32,32,32	0.79	0	51,51,51	1.86	9 (17%)
26	CDL	T	104	-	99,99,99	1.37	12 (12%)	105,111,111	1.16	5 (4%)
21	EDO	O	304	-	3,3,3	0.40	0	2,2,2	0.69	0
19	TGL	L	101	-	62,62,62	1.19	3 (4%)	65,65,65	1.43	8 (12%)
23	CHD	W	101	-	32,32,32	0.89	0	51,51,51	4.04	25 (49%)
23	CHD	C	305	-	32,32,32	0.87	1 (3%)	51,51,51	1.66	11 (21%)
22	CUA	B	301	2	0,1,1	-	-	-		
24	PSC	B	303	-	51,51,51	1.20	3 (5%)	57,59,59	1.13	4 (7%)
21	EDO	A	613	-	3,3,3	0.57	0	2,2,2	0.07	0
21	EDO	N	610	-	3,3,3	0.41	0	2,2,2	0.19	0
20	PGV	C	302	-	50,50,50	0.88	2 (4%)	53,56,56	0.95	4 (7%)
21	EDO	P	307	-	3,3,3	0.54	0	2,2,2	0.17	0
21	EDO	T	105	-	3,3,3	0.48	0	2,2,2	0.25	0
18	CMO	A	606	15	0,1,1	-	-	-		
19	TGL	D	201	-	62,62,62	1.30	3 (4%)	65,65,65	1.07	6 (9%)
20	PGV	P	303	-	50,50,50	0.86	3 (6%)	53,56,56	1.17	7 (13%)
23	CHD	P	306	-	32,32,32	0.83	0	51,51,51	1.61	11 (21%)
19	TGL	A	607	-	62,62,62	1.19	4 (6%)	65,65,65	1.69	8 (12%)
29	DMU	Z	101	-	34,34,34	0.49	0	45,45,45	0.85	2 (4%)
21	EDO	A	612	-	3,3,3	0.47	0	2,2,2	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
29	DMU	M	101	-	34,34,34	0.46	0	45,45,45	0.94	1 (2%)
20	PGV	P	301	-	50,50,50	1.07	2 (4%)	53,56,56	1.11	4 (7%)
19	TGL	Y	101	-	62,62,62	1.14	3 (4%)	65,65,65	1.24	6 (9%)
21	EDO	C	308	-	3,3,3	0.41	0	2,2,2	0.38	0
21	EDO	H	101	-	3,3,3	0.53	0	2,2,2	0.20	0
27	PEK	T	101	-	52,52,52	0.90	3 (5%)	55,57,57	1.01	3 (5%)
26	CDL	P	304	-	99,99,99	1.42	12 (12%)	105,111,111	1.27	7 (6%)
14	HEA	N	602	1	57,67,67	1.61	14 (24%)	61,103,103	1.88	16 (26%)
21	EDO	A	610	-	3,3,3	0.49	0	2,2,2	0.29	0
21	EDO	N	609	-	3,3,3	0.41	0	2,2,2	0.65	0
24	PSC	O	303	-	51,51,51	1.19	3 (5%)	57,59,59	1.05	4 (7%)
26	CDL	G	102	-	99,99,99	1.43	12 (12%)	105,111,111	1.21	9 (8%)
21	EDO	B	304	-	3,3,3	0.35	0	2,2,2	0.63	0
20	PGV	N	608	-	50,50,50	0.87	2 (4%)	53,56,56	1.08	4 (7%)
23	CHD	C	304	-	32,32,32	0.56	0	51,51,51	1.94	16 (31%)
20	PGV	A	609	-	50,50,50	1.04	2 (4%)	53,56,56	1.17	7 (13%)
23	CHD	P	305	-	32,32,32	0.60	0	51,51,51	1.73	13 (25%)
21	EDO	P	308	-	3,3,3	0.59	0	2,2,2	0.16	0
27	PEK	C	306	-	52,52,52	1.18	3 (5%)	55,57,57	1.17	5 (9%)
21	EDO	F	103	-	3,3,3	0.53	0	2,2,2	0.41	0
27	PEK	G	103	-	52,52,52	1.17	2 (3%)	55,57,57	1.07	5 (9%)
21	EDO	B	305	-	3,3,3	0.52	0	2,2,2	0.85	0
14	HEA	N	601	1	57,67,67	1.58	12 (21%)	61,103,103	1.32	8 (13%)
19	TGL	O	302	-	62,62,62	1.12	3 (4%)	65,65,65	1.24	7 (10%)
20	PGV	C	307	-	50,50,50	1.04	2 (4%)	53,56,56	0.92	3 (5%)
21	EDO	L	102	-	3,3,3	0.41	0	2,2,2	0.31	0
27	PEK	T	103	-	52,52,52	1.13	2 (3%)	55,57,57	0.94	2 (3%)
22	CUA	O	301	2,30	0,1,1	-	-	-		
27	PEK	G	101	-	52,52,52	0.87	3 (5%)	55,57,57	1.37	4 (7%)

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
23	CHD	B	302	-	-	3/9/74/74	0/4/4/4
19	TGL	Q	201	-	-	35/65/65/65	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	EDO	F	102	-	-	0/1/1/1	-
27	PEK	T	102	-	-	29/56/56/56	-
14	HEA	A	602	1	-	2/32/76/76	-
21	EDO	C	309	-	-	0/1/1/1	-
20	PGV	A	608	-	-	15/55/55/55	-
21	EDO	G	105	-	-	0/1/1/1	-
23	CHD	G	104	-	-	3/9/74/74	0/4/4/4
21	EDO	A	611	-	-	1/1/1/1	-
26	CDL	C	303	-	-	58/110/110/110	-
21	EDO	C	310	-	-	0/1/1/1	-
21	EDO	K	102	-	-	1/1/1/1	-
20	PGV	N	607	-	-	28/55/55/55	-
21	EDO	K	101	-	-	1/1/1/1	-
14	HEA	A	601	1	-	3/32/76/76	-
21	EDO	C	311	-	-	0/1/1/1	-
23	CHD	J	101	-	-	8/9/74/74	0/4/4/4
26	CDL	T	104	-	-	61/110/110/110	-
21	EDO	O	304	-	-	1/1/1/1	-
19	TGL	L	101	-	-	39/65/65/65	-
23	CHD	W	101	-	-	7/9/74/74	0/4/4/4
23	CHD	C	305	-	-	2/9/74/74	0/4/4/4
24	PSC	B	303	-	-	38/55/55/55	-
21	EDO	A	613	-	-	1/1/1/1	-
21	EDO	N	610	-	-	0/1/1/1	-
20	PGV	C	302	-	-	10/55/55/55	-
21	EDO	P	307	-	-	0/1/1/1	-
21	EDO	T	105	-	-	1/1/1/1	-
19	TGL	D	201	-	-	37/65/65/65	-
20	PGV	P	303	-	-	20/55/55/55	-
23	CHD	P	306	-	-	1/9/74/74	0/4/4/4
19	TGL	A	607	-	-	42/65/65/65	-
29	DMU	Z	101	-	-	5/19/59/59	0/2/2/2
21	EDO	A	612	-	-	1/1/1/1	-
29	DMU	M	101	-	-	7/19/59/59	0/2/2/2
20	PGV	P	301	-	-	25/55/55/55	-
19	TGL	Y	101	-	-	43/65/65/65	-
21	EDO	C	308	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	EDO	H	101	-	-	0/1/1/1	-
27	PEK	T	101	-	-	23/56/56/56	-
26	CDL	P	304	-	-	64/110/110/110	-
14	HEA	N	602	1	-	7/32/76/76	-
21	EDO	A	610	-	-	0/1/1/1	-
21	EDO	N	609	-	-	0/1/1/1	-
24	PSC	O	303	-	-	34/55/55/55	-
26	CDL	G	102	-	-	66/110/110/110	-
21	EDO	B	304	-	-	1/1/1/1	-
20	PGV	N	608	-	-	14/55/55/55	-
23	CHD	C	304	-	-	2/9/74/74	0/4/4/4
20	PGV	A	609	-	-	38/55/55/55	-
23	CHD	P	305	-	-	2/9/74/74	1/4/4/4
21	EDO	P	308	-	-	1/1/1/1	-
27	PEK	C	306	-	-	30/56/56/56	-
21	EDO	F	103	-	-	0/1/1/1	-
27	PEK	G	103	-	-	28/56/56/56	-
21	EDO	B	305	-	-	1/1/1/1	-
14	HEA	N	601	1	-	4/32/76/76	-
19	TGL	O	302	-	-	36/65/65/65	-
20	PGV	C	307	-	-	28/55/55/55	-
21	EDO	L	102	-	-	1/1/1/1	-
27	PEK	T	103	-	-	31/56/56/56	-
27	PEK	G	101	-	-	19/56/56/56	-

The worst 5 of 156 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	L	101	TGL	OG2-CB1	5.61	1.50	1.34
19	D	201	TGL	OG2-CB1	5.59	1.50	1.34
26	P	304	CDL	OA6-CA5	5.57	1.50	1.34
19	A	607	TGL	OG2-CB1	5.52	1.49	1.34
26	G	102	CDL	OB8-CB7	5.49	1.49	1.33

The worst 5 of 302 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	W	101	CHD	C14-C8-C9	-13.54	91.13	109.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	W	101	CHD	C18-C13-C12	-9.16	99.74	109.07
23	W	101	CHD	C14-C13-C12	9.14	115.91	107.40
23	W	101	CHD	C10-C9-C8	8.27	120.70	111.82
19	A	607	TGL	OG2-CB1-CB2	8.22	129.22	111.50

There are no chirality outliers.

5 of 959 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	D	201	TGL	CB2-CB1-OG2-CG2
19	D	201	TGL	OB1-CB1-OG2-CG2
19	L	101	TGL	CB2-CB1-OG2-CG2
19	L	101	TGL	OB1-CB1-OG2-CG2
19	Q	201	TGL	CC2-CC1-OG3-CG3

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	P	305	CHD	C1-C10-C2-C3-C4-C5

48 monomers are involved in 198 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	302	CHD	1	0
19	Q	201	TGL	5	0
21	F	102	EDO	1	0
27	T	102	PEK	8	0
14	A	602	HEA	8	0
20	A	608	PGV	1	0
23	G	104	CHD	1	0
26	C	303	CDL	6	0
20	N	607	PGV	5	0
14	A	601	HEA	5	0
21	C	311	EDO	2	0
18	N	606	CMO	2	0
26	T	104	CDL	21	0
19	L	101	TGL	9	0
23	W	101	CHD	9	0
23	C	305	CHD	1	0
24	B	303	PSC	4	0
21	A	613	EDO	7	0
21	N	610	EDO	3	0

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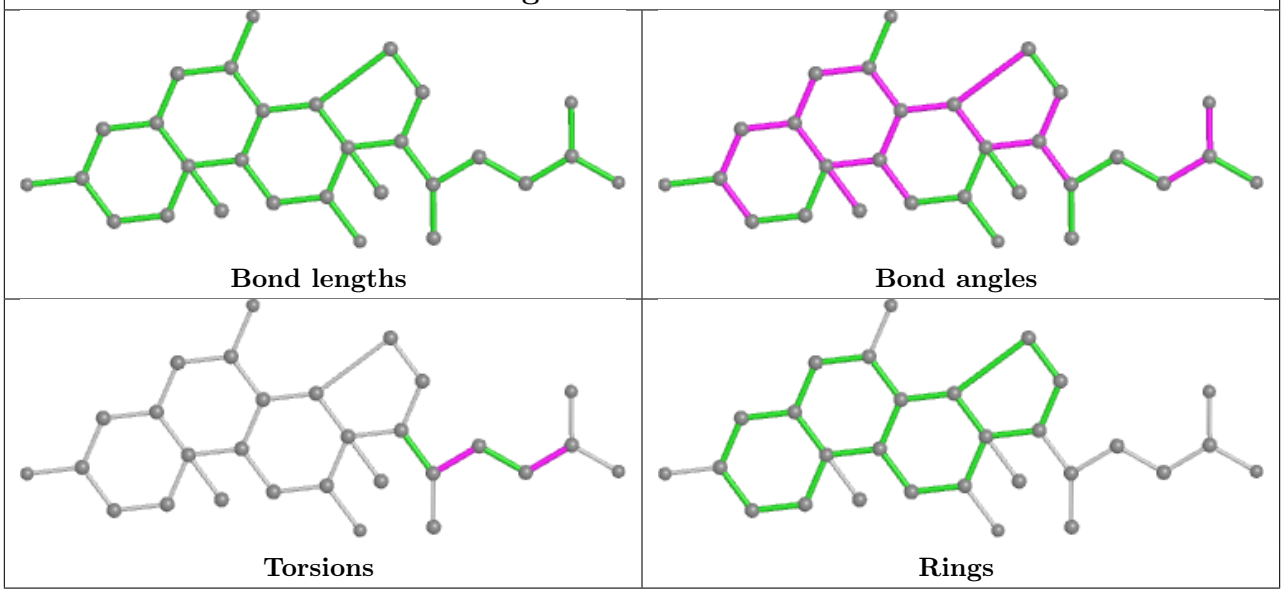
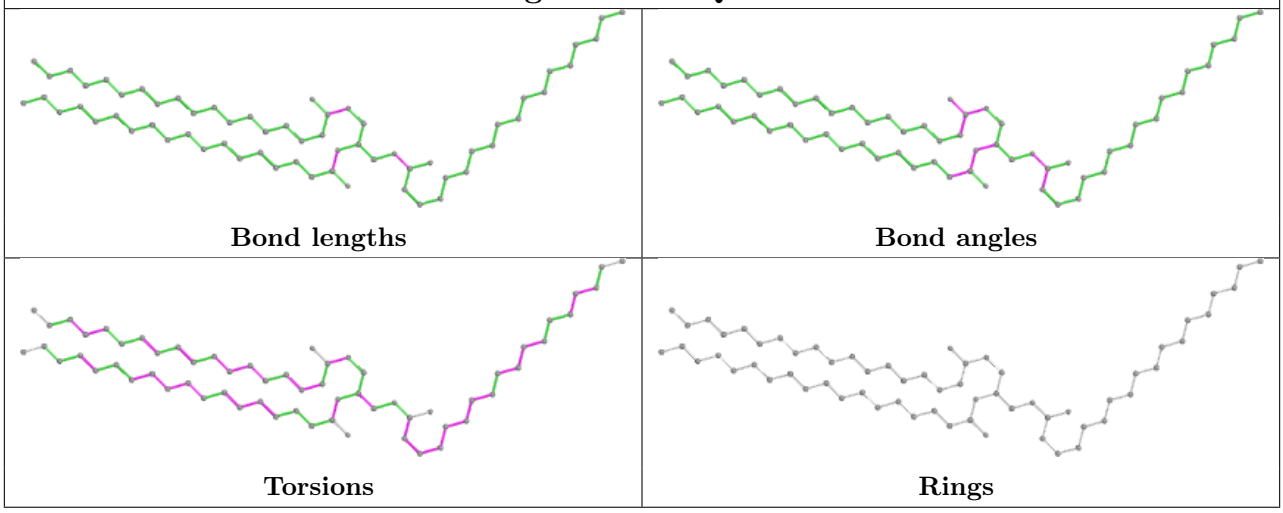
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	T	105	EDO	4	0
18	A	606	CMO	1	0
19	D	201	TGL	5	0
20	P	303	PGV	1	0
23	P	306	CHD	3	0
19	A	607	TGL	3	0
29	Z	101	DMU	2	0
21	A	612	EDO	12	0
20	P	301	PGV	2	0
19	Y	101	TGL	3	0
21	H	101	EDO	2	0
27	T	101	PEK	3	0
26	P	304	CDL	7	0
14	N	602	HEA	5	0
24	O	303	PSC	5	0
26	G	102	CDL	6	0
21	B	304	EDO	1	0
20	N	608	PGV	1	0
23	C	304	CHD	4	0
20	A	609	PGV	4	0
23	P	305	CHD	3	0
27	C	306	PEK	3	0
21	F	103	EDO	1	0
27	G	103	PEK	3	0
14	N	601	HEA	6	0
19	O	302	TGL	7	0
20	C	307	PGV	4	0
27	T	103	PEK	2	0
27	G	101	PEK	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.

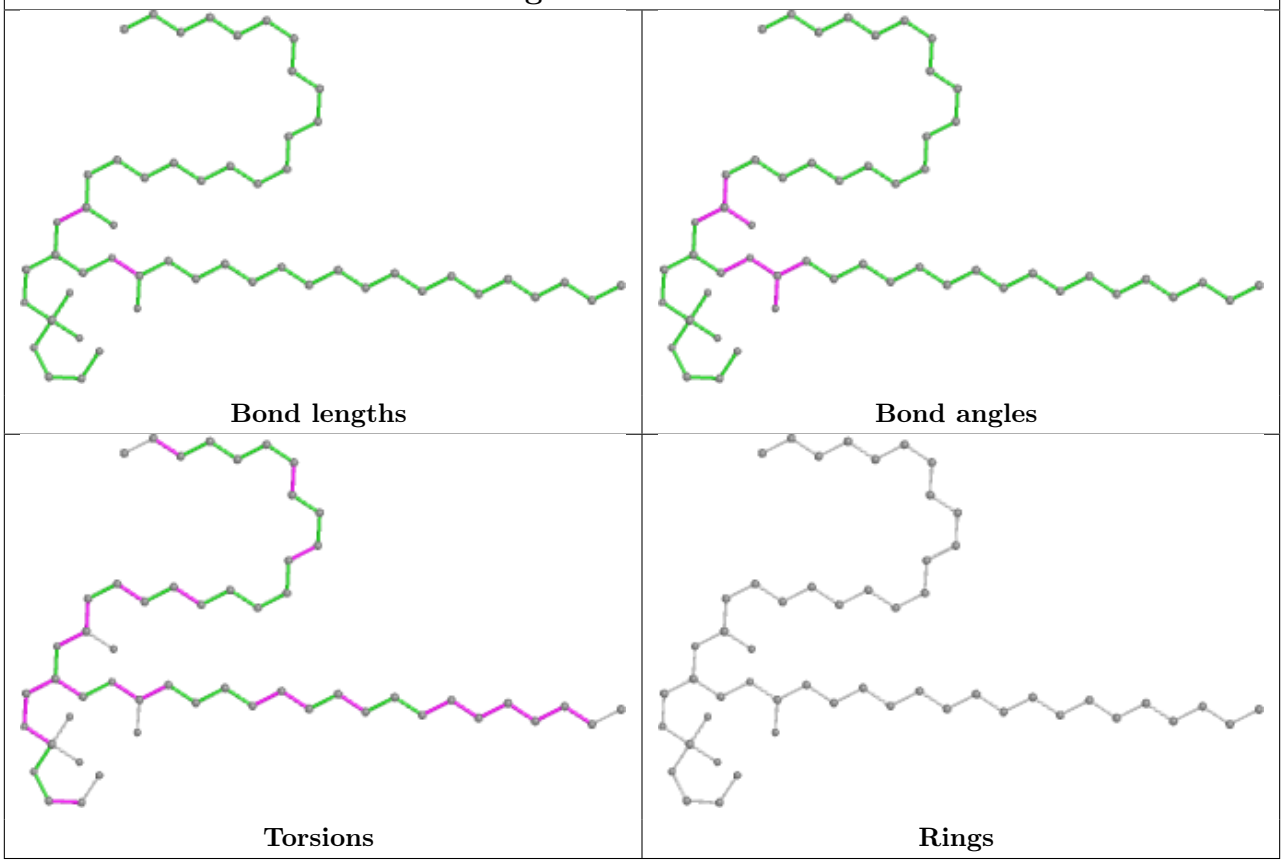
Ligand CHD B 302



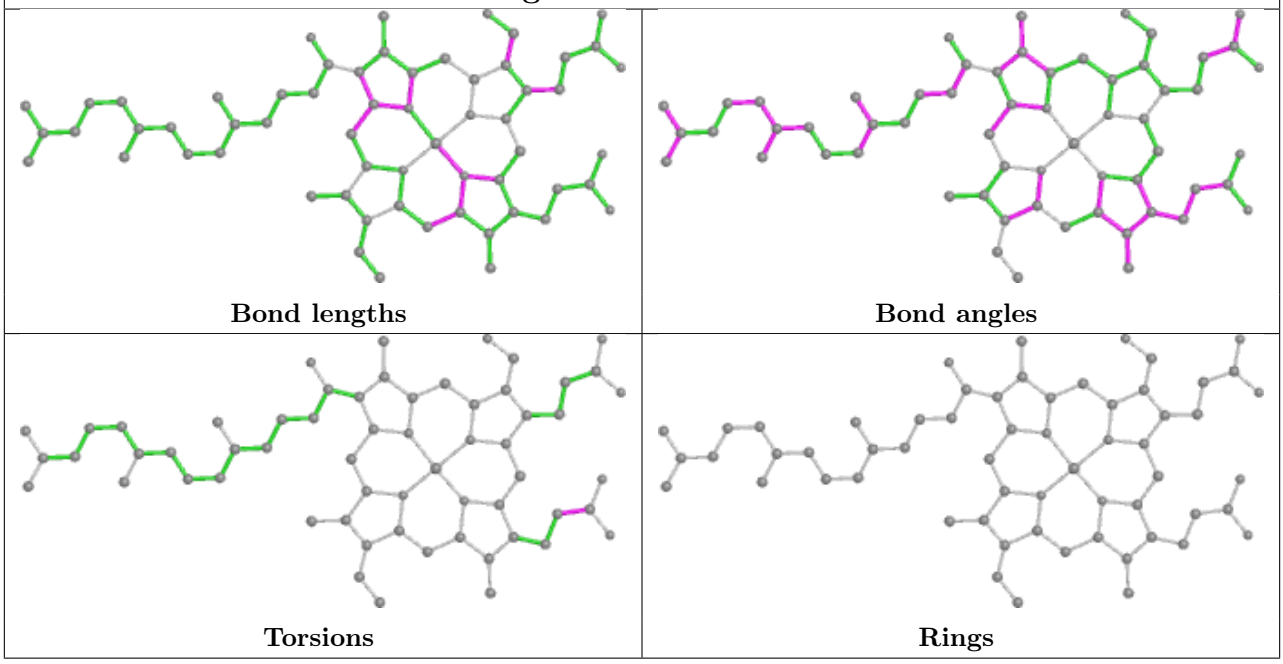
Ligand TGL Q 201



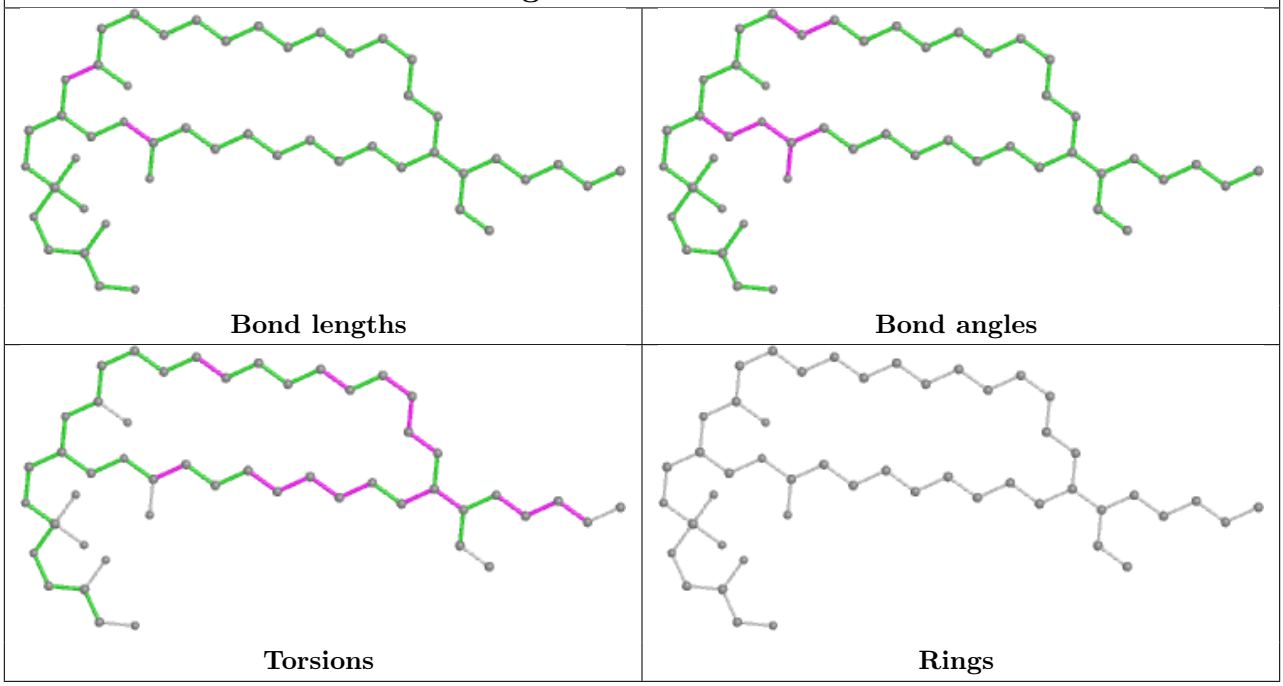
Ligand PEK T 102



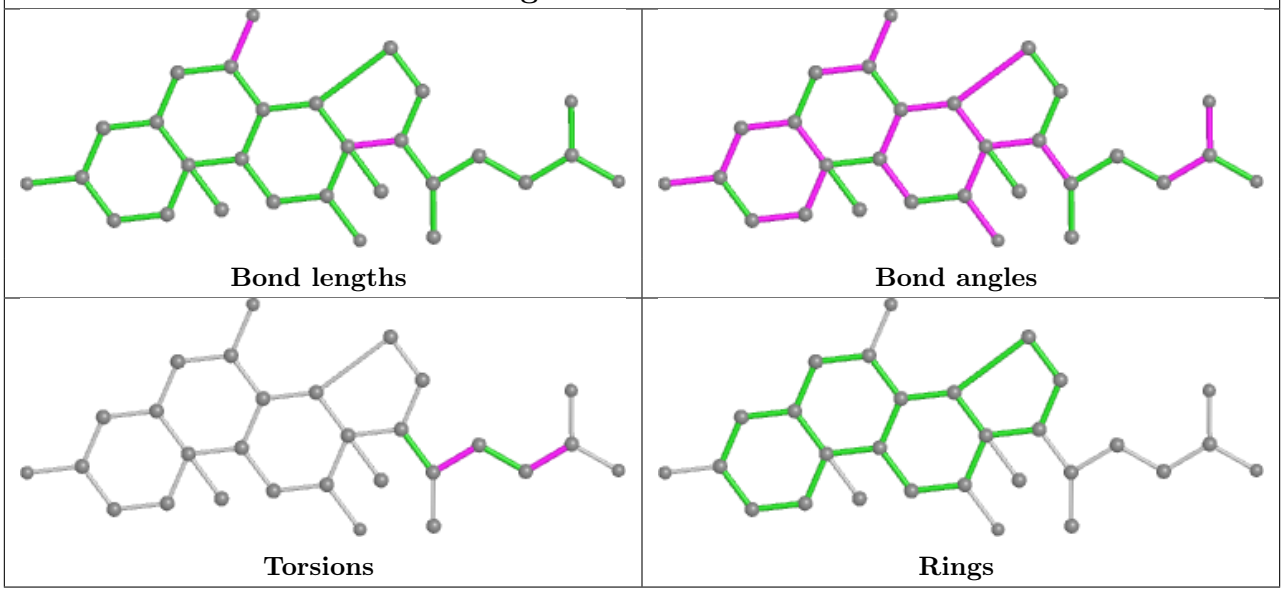
Ligand HEA A 602



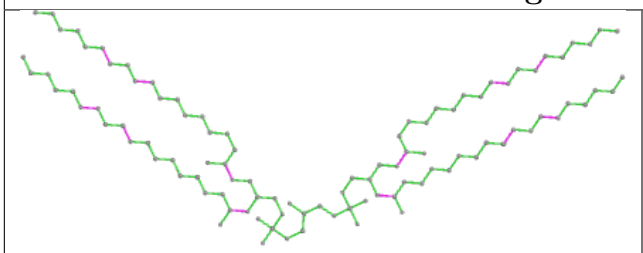
Ligand PGV A 608



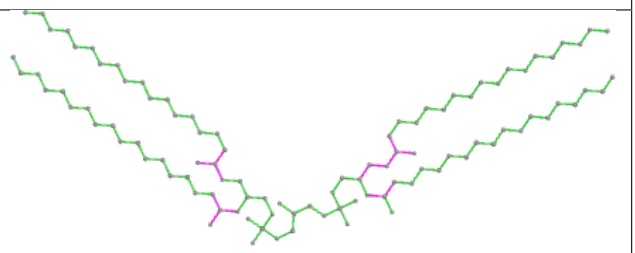
Ligand CHD G 104



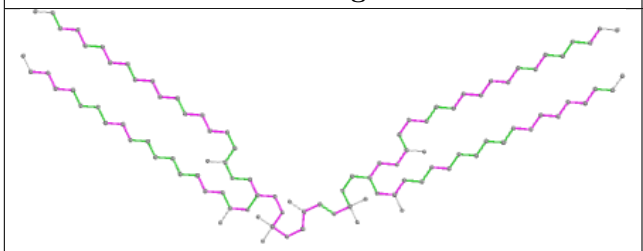
Ligand CDL C 303



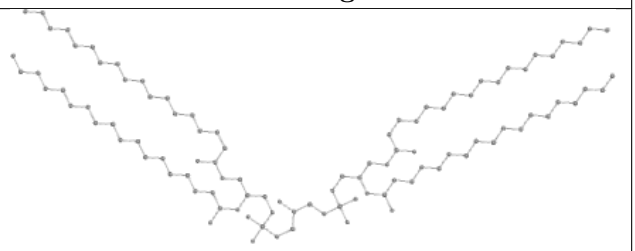
Bond lengths



Bond angles

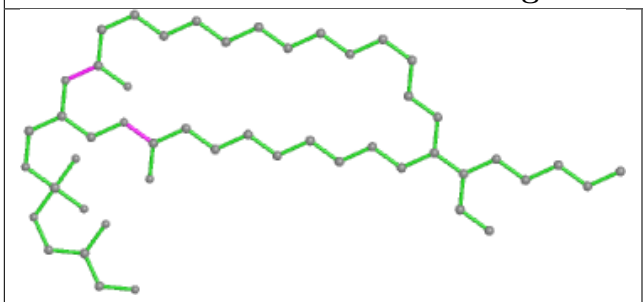


Torsions

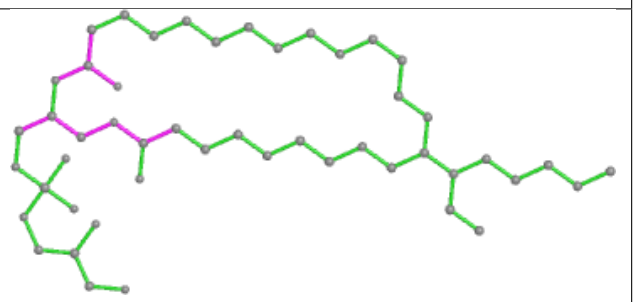


Rings

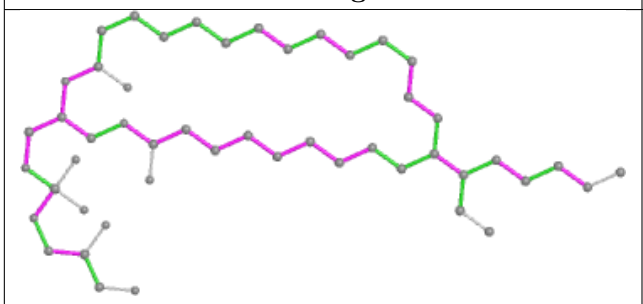
Ligand PGV N 607



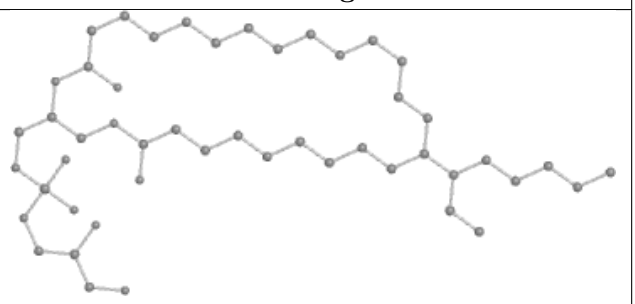
Bond lengths



Bond angles

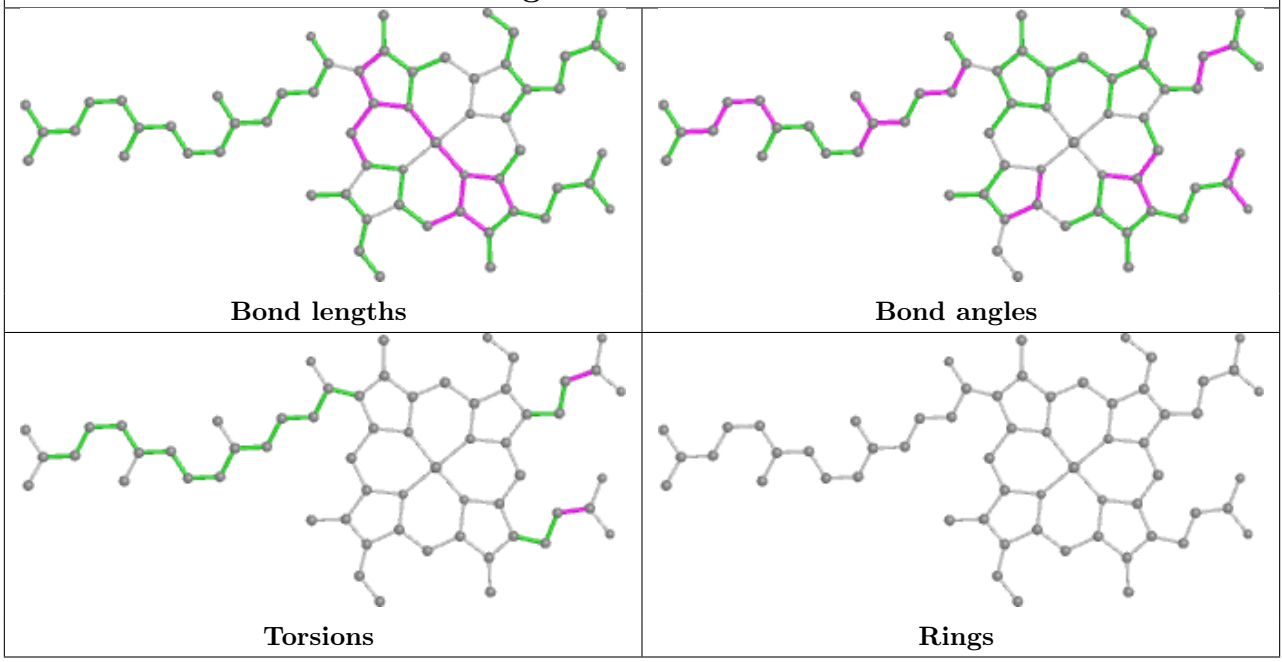


Torsions

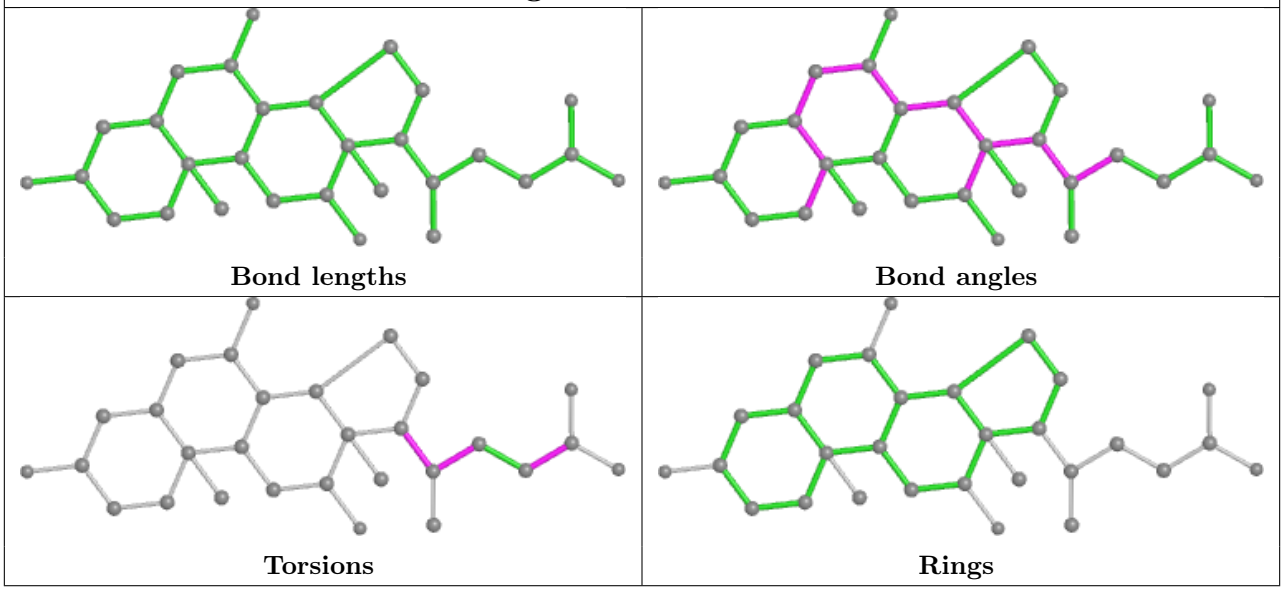


Rings

Ligand HEA A 601



Ligand CHD J 101



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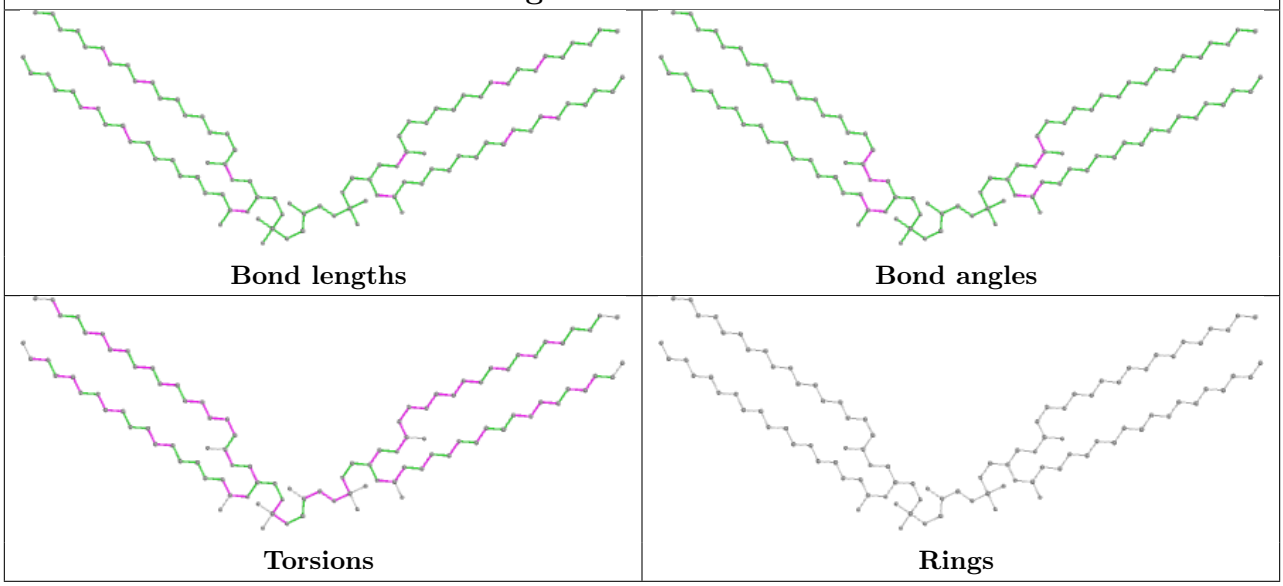

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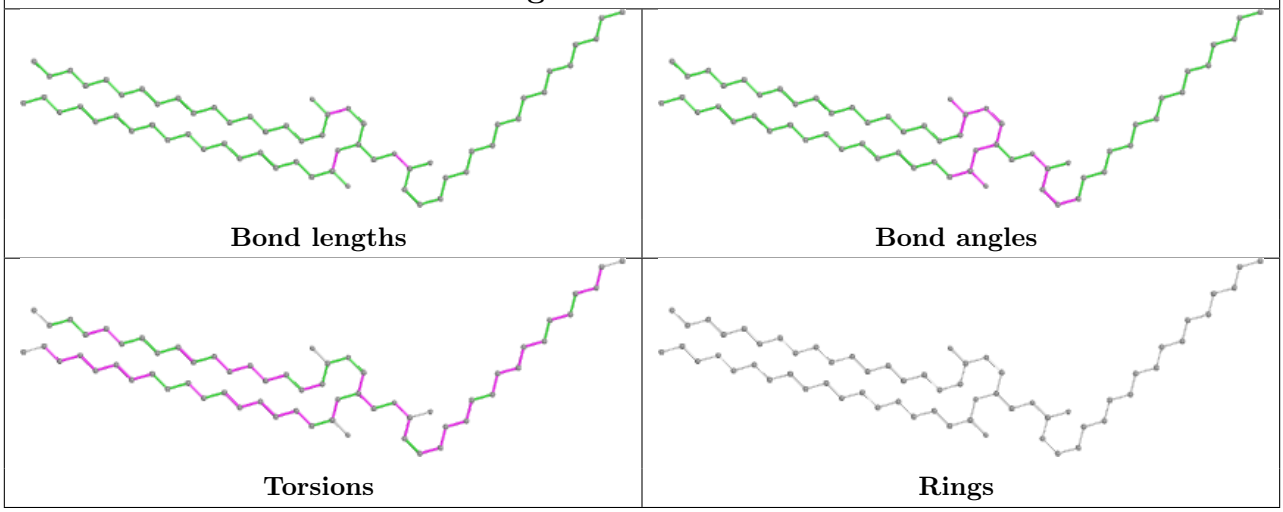

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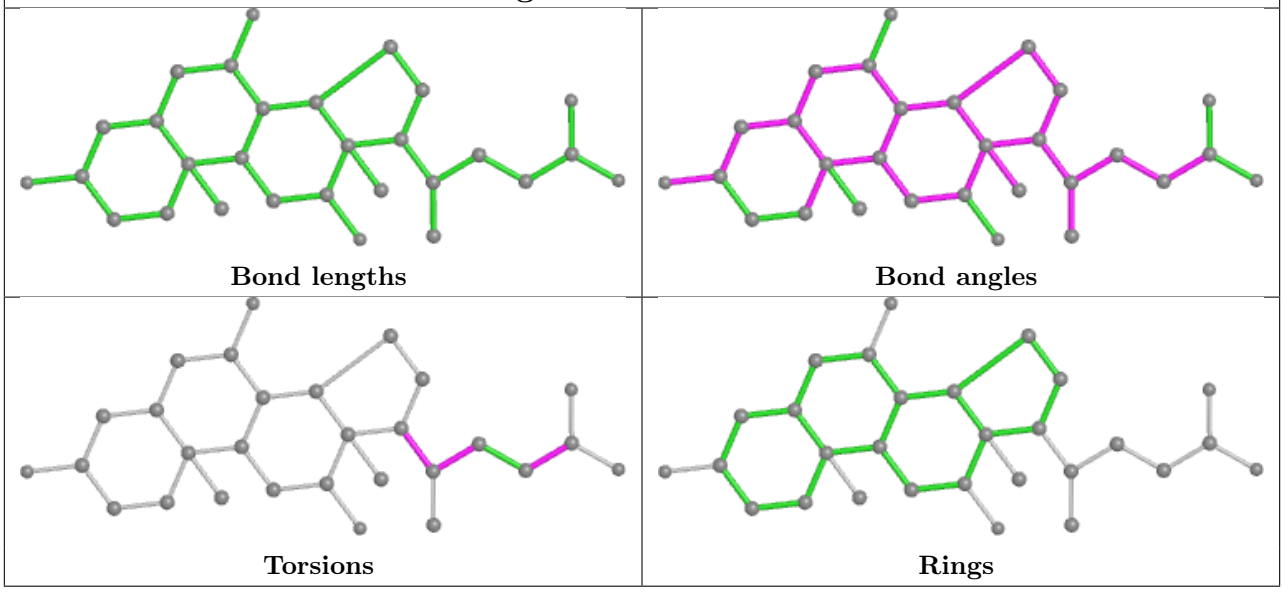

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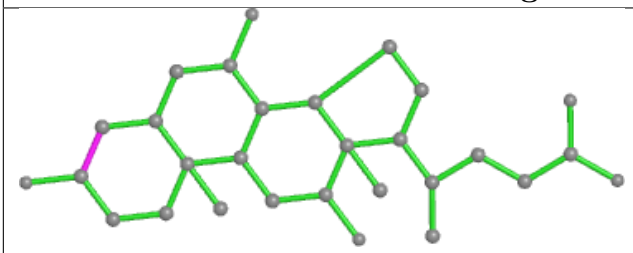
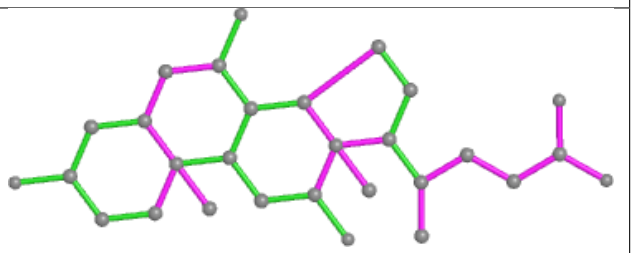
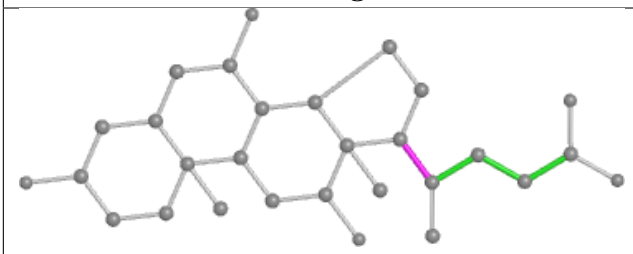


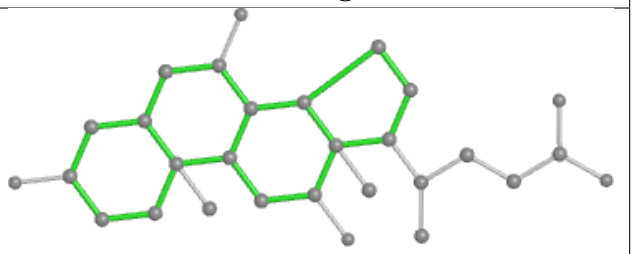
Bond lengths



Bond angles

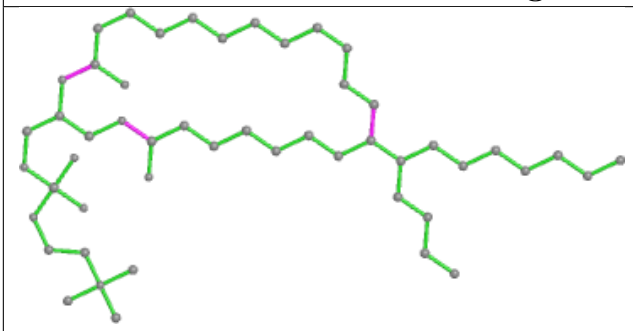


Torsions



Rings

Ligand PSC B 303



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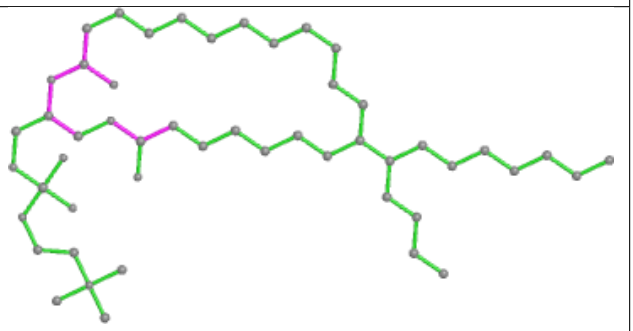

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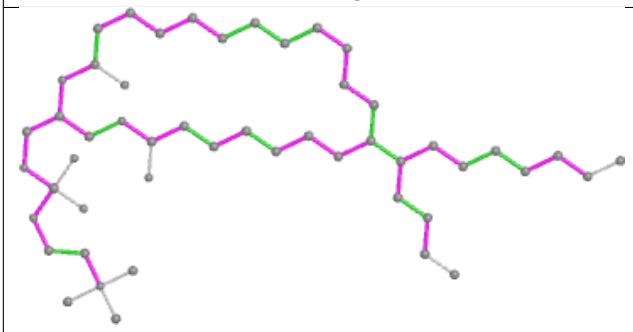

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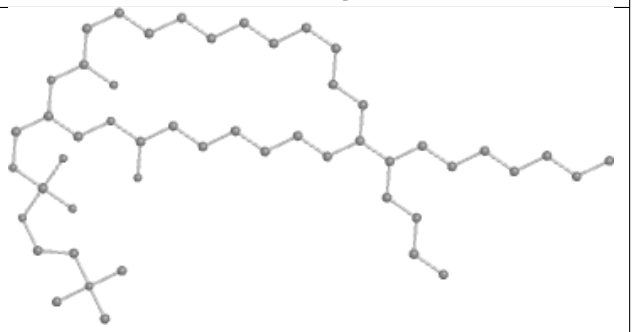
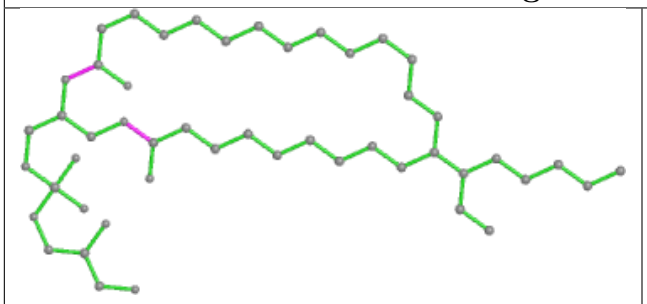


Rings

Ligand PGV C 302



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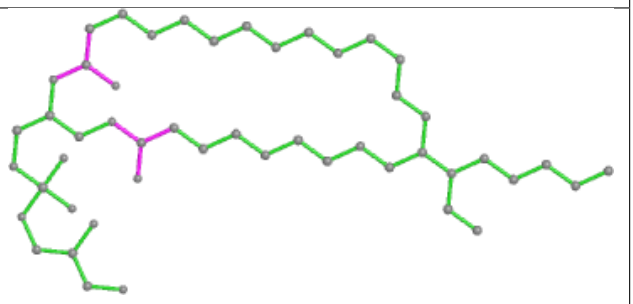
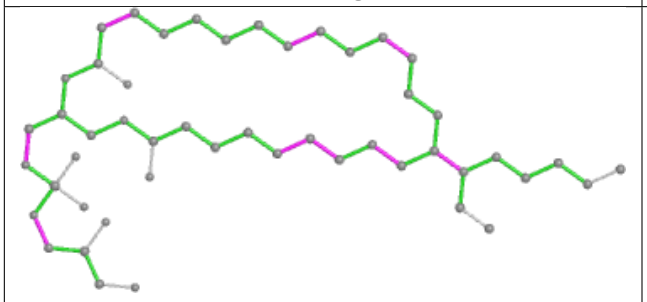


Bond angles



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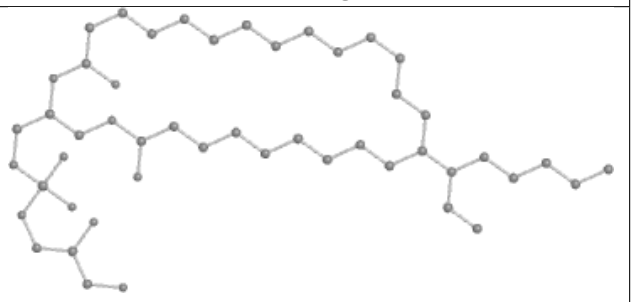
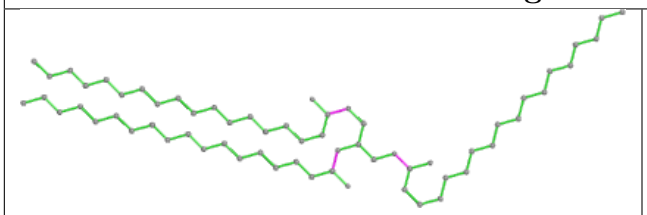
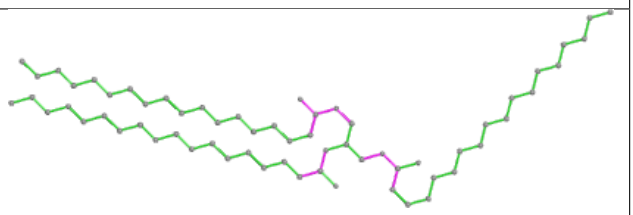


Rings

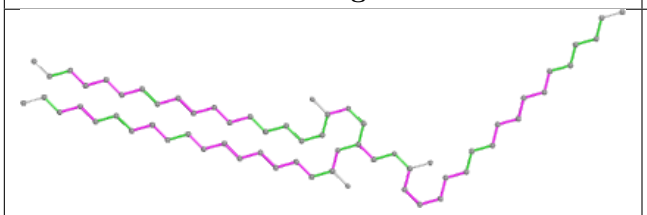
Ligand TGL D 201



Bond lengths



Bond angles



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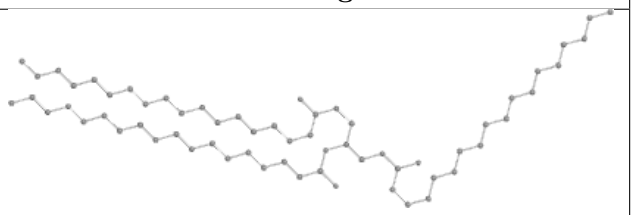
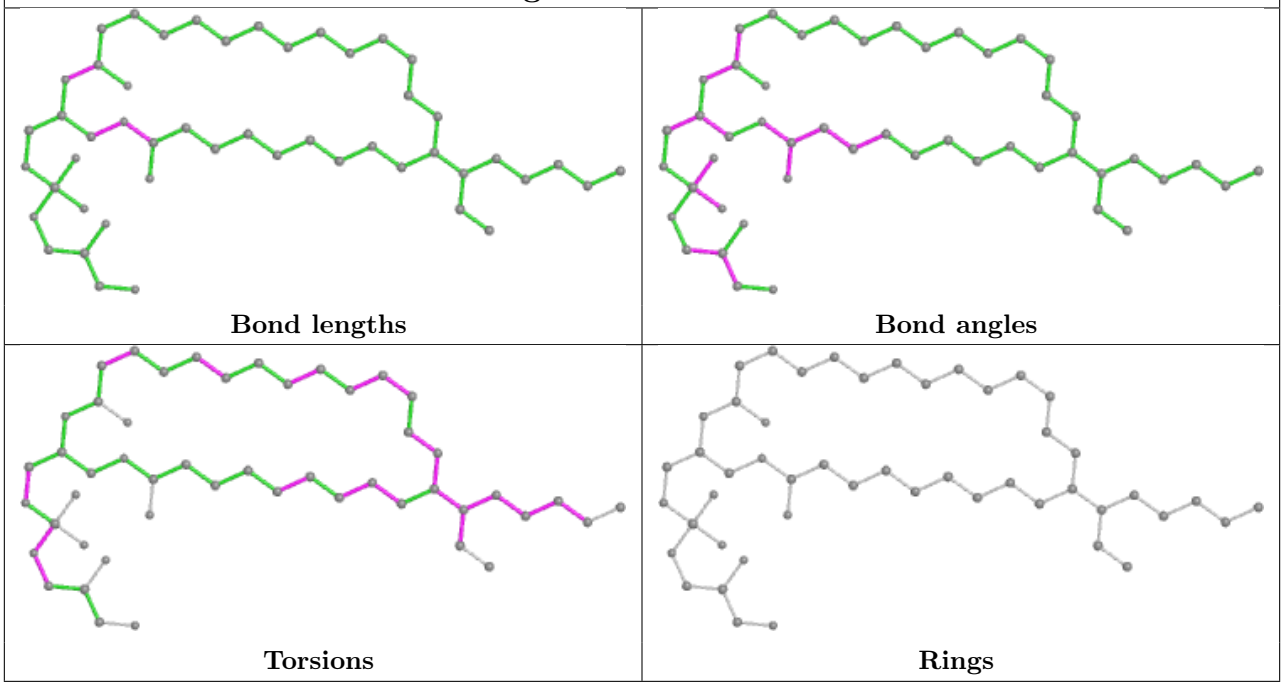


Rings

Ligand PGV P 303



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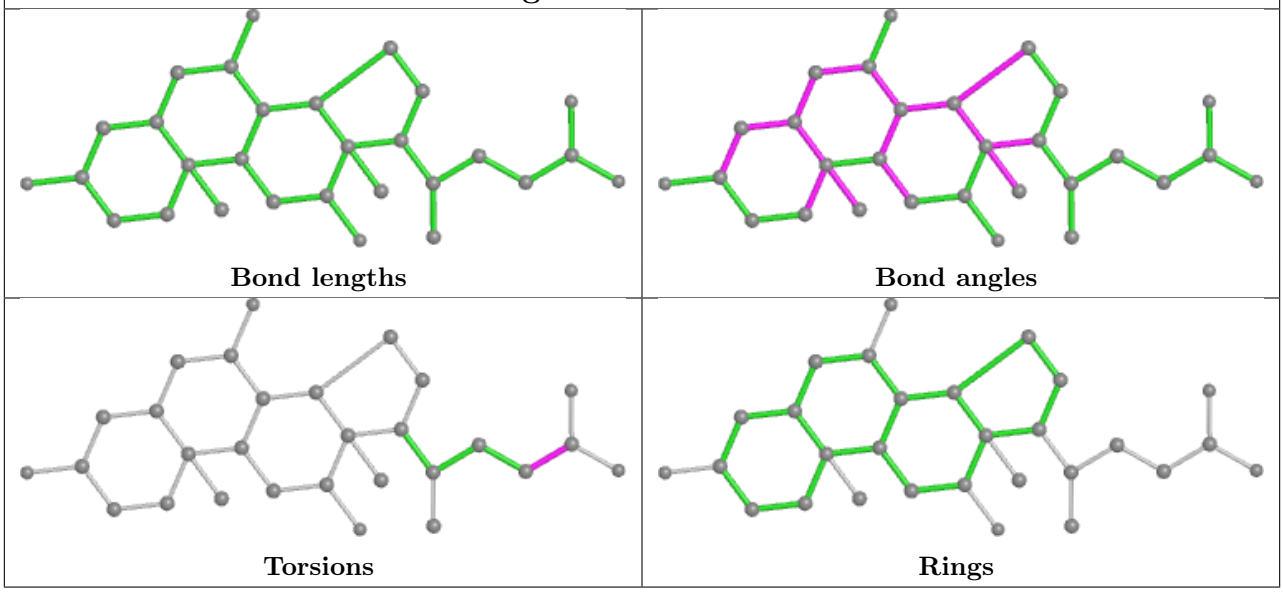
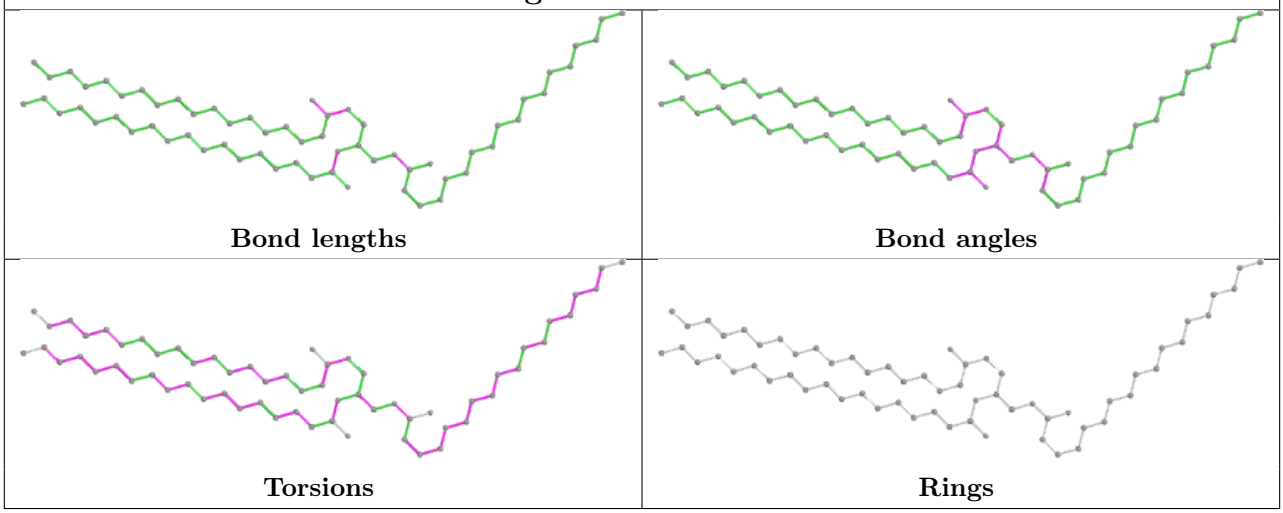
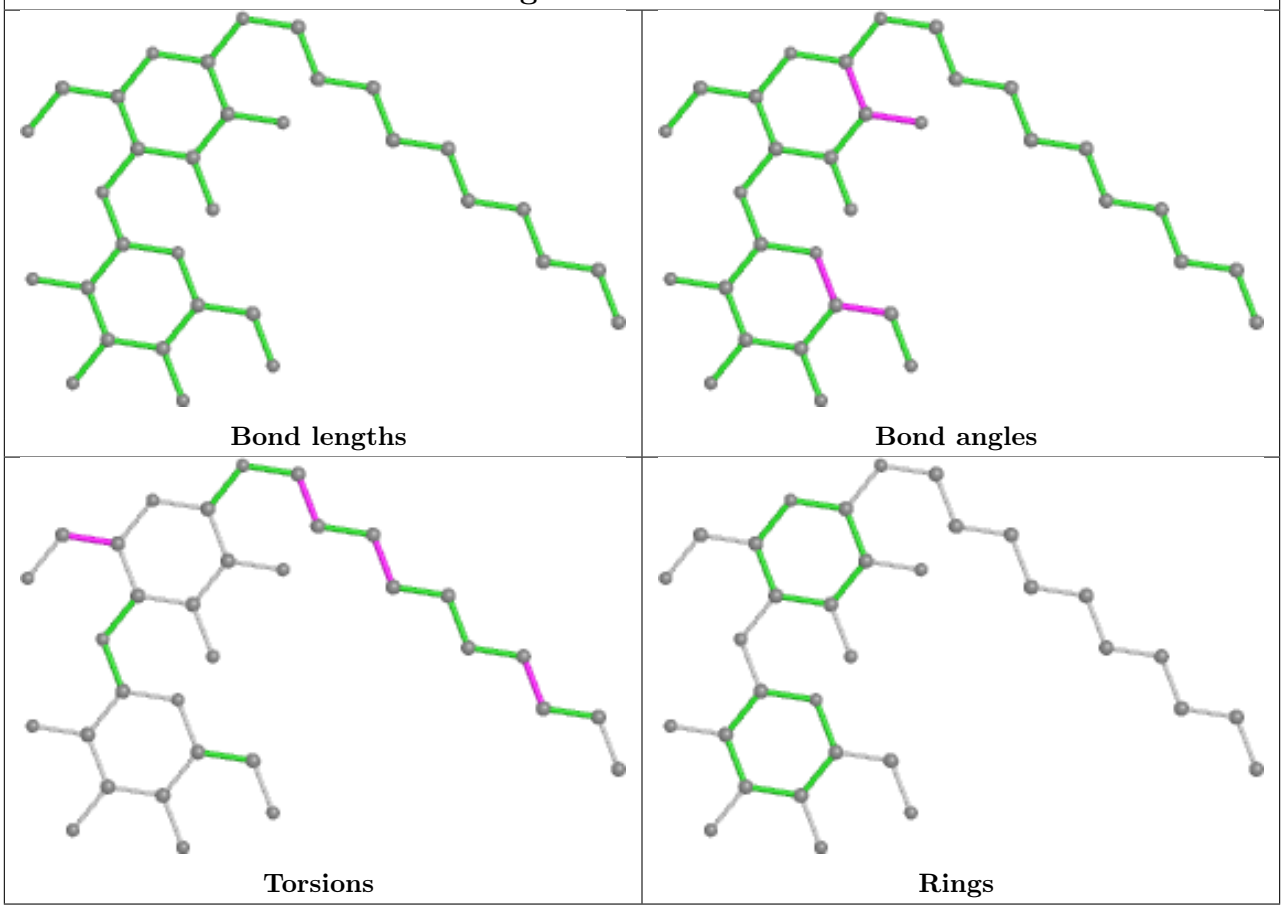


Ligand TGL A 607



Ligand DMU Z 101



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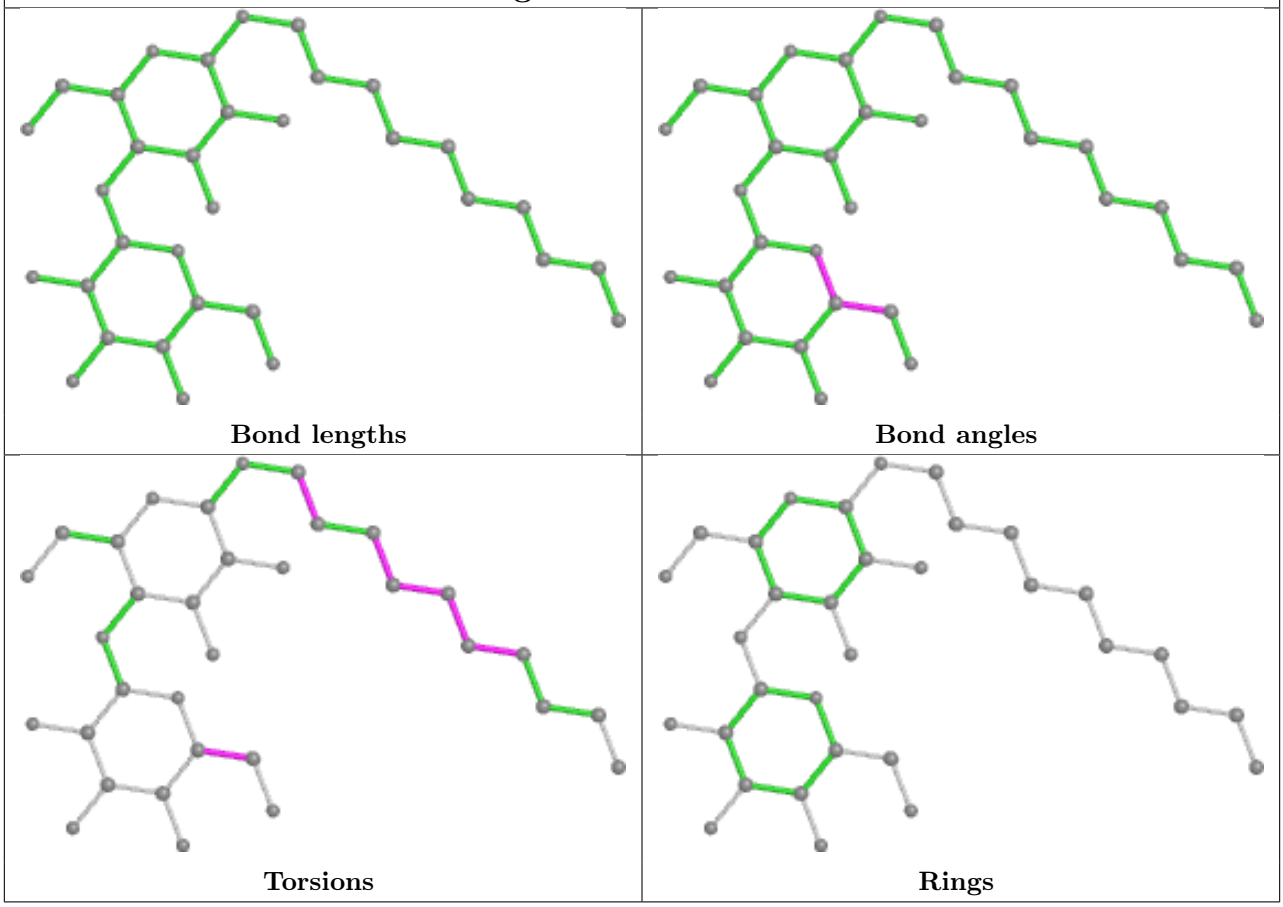

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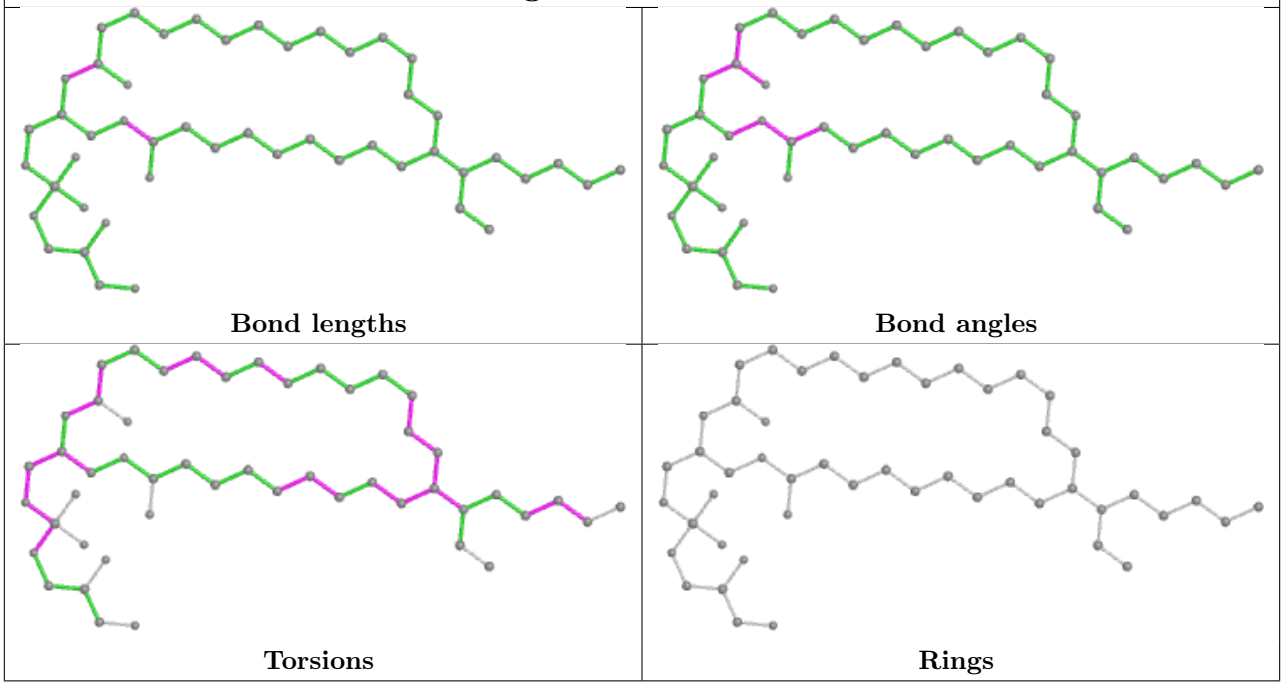
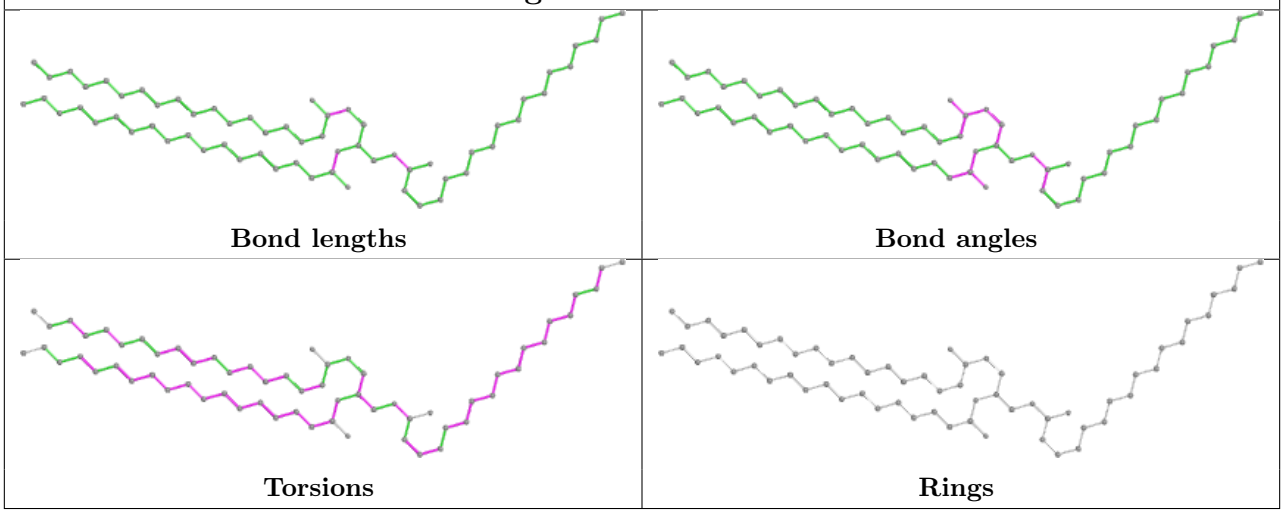
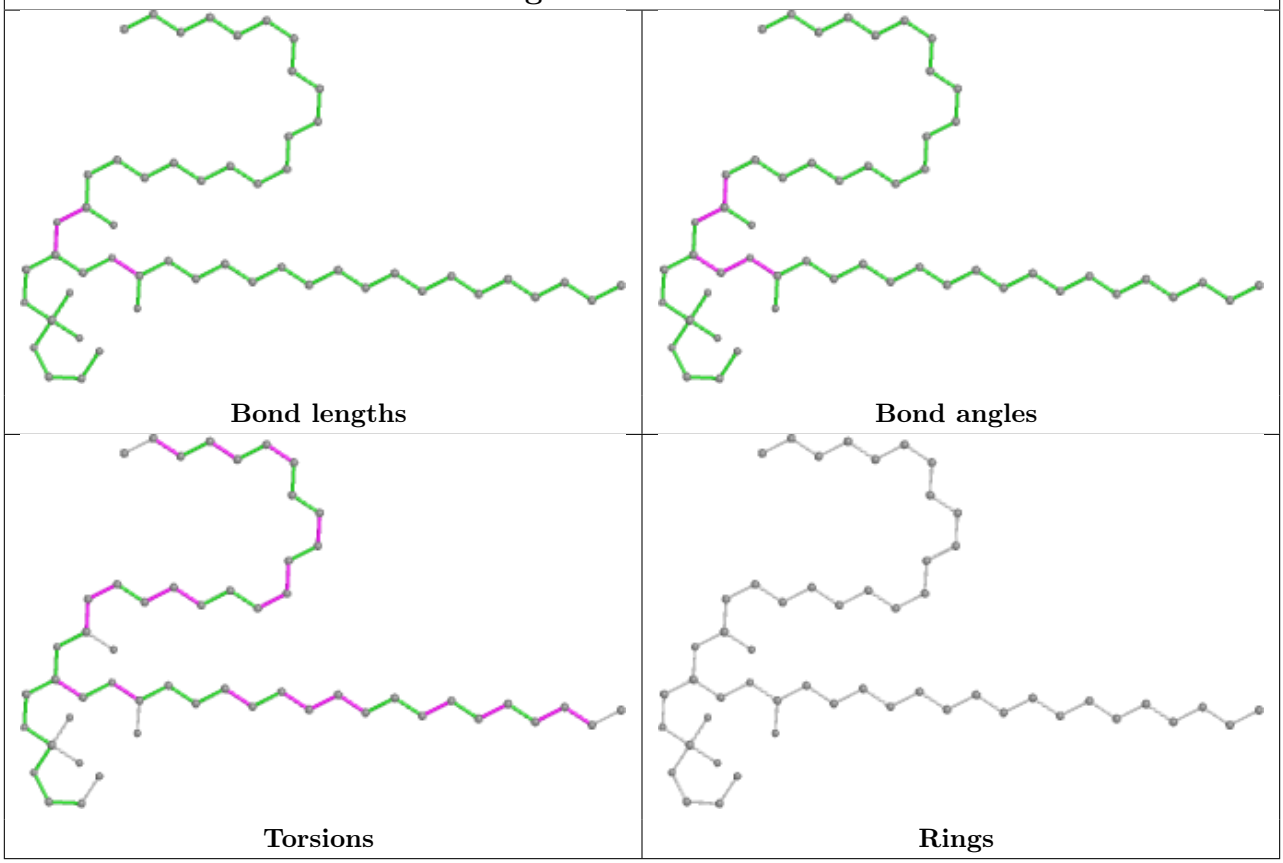


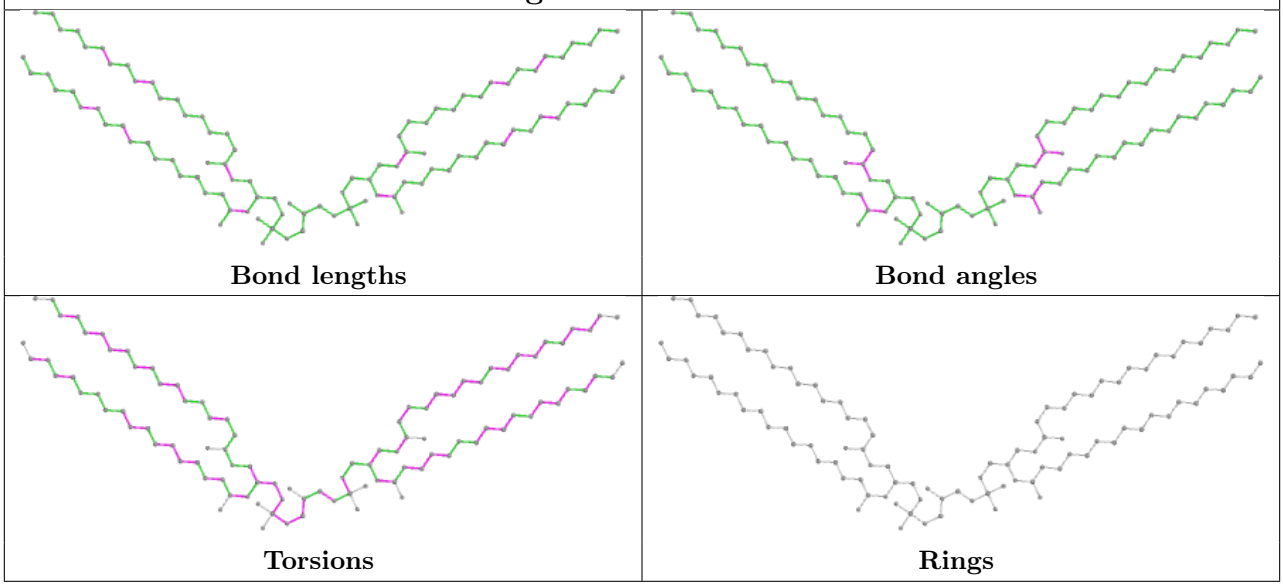
Ligand TGL Y 101



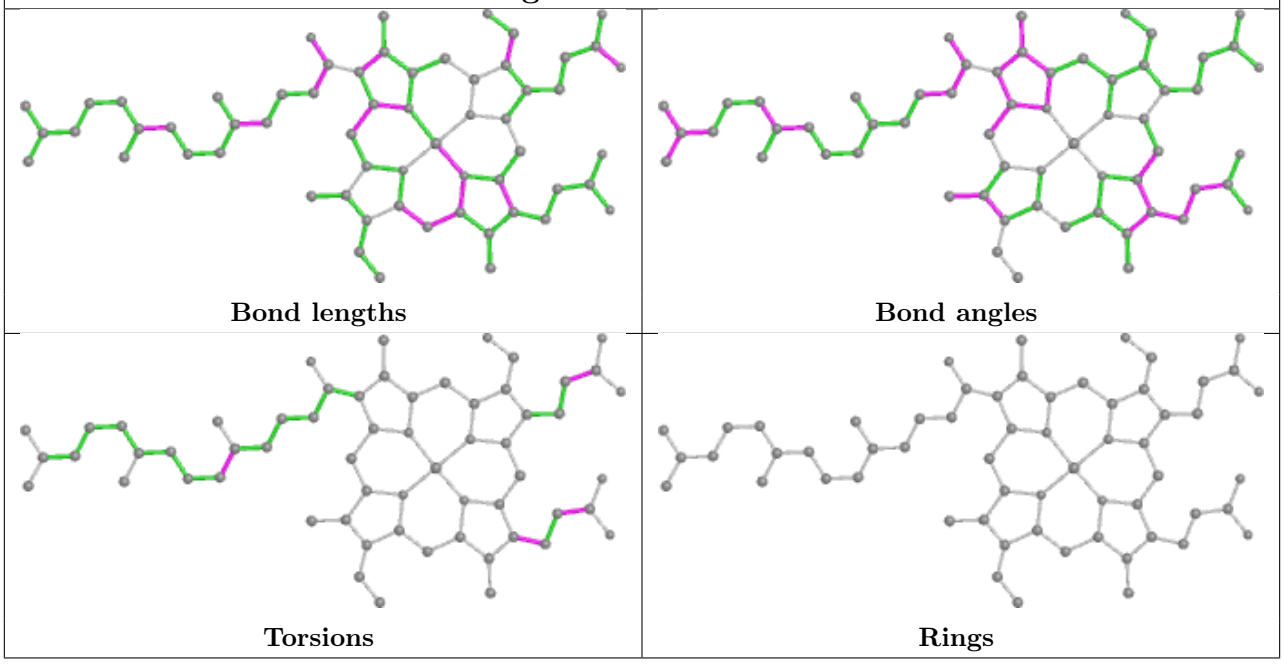
Ligand PEK T 101



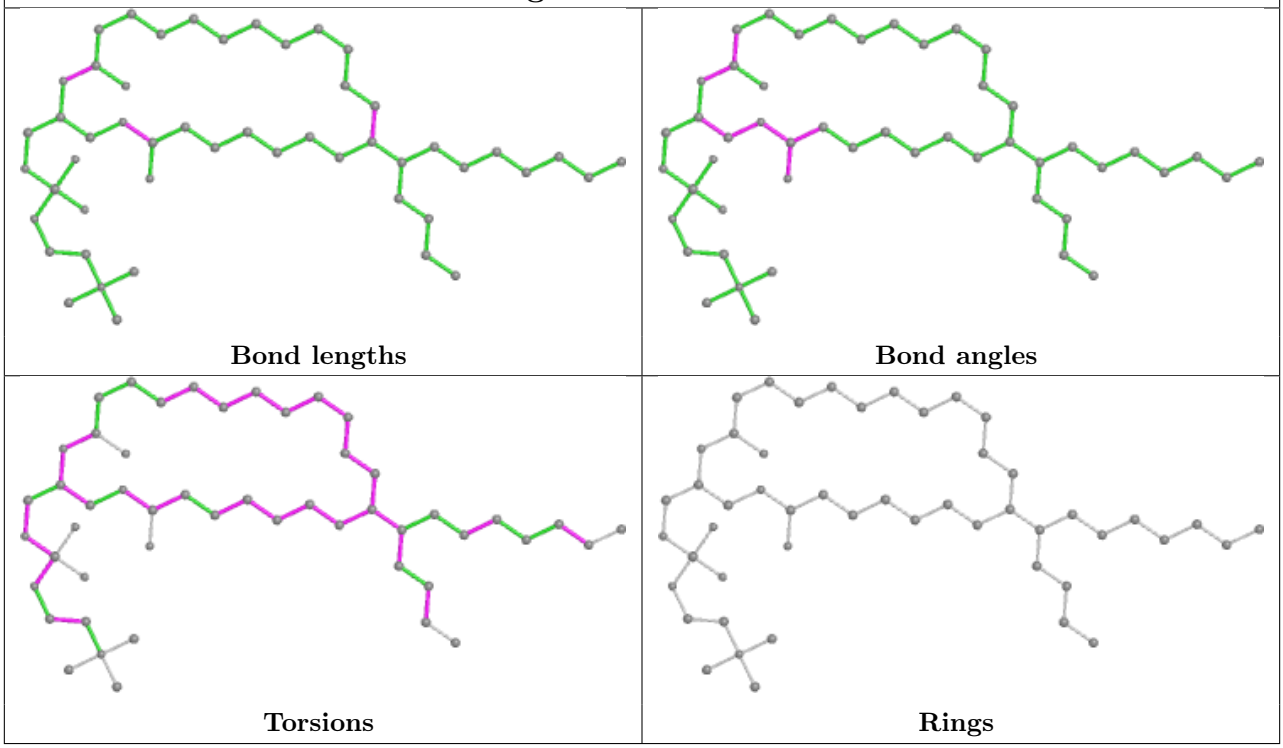
Ligand CDL P 304



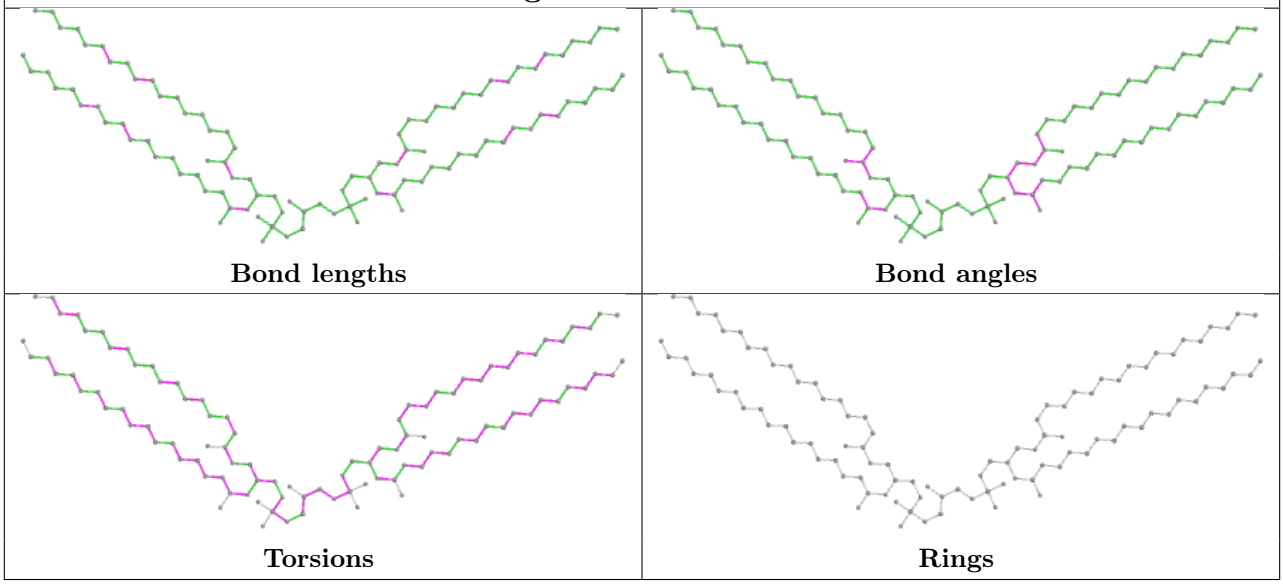
Ligand HEA N 602



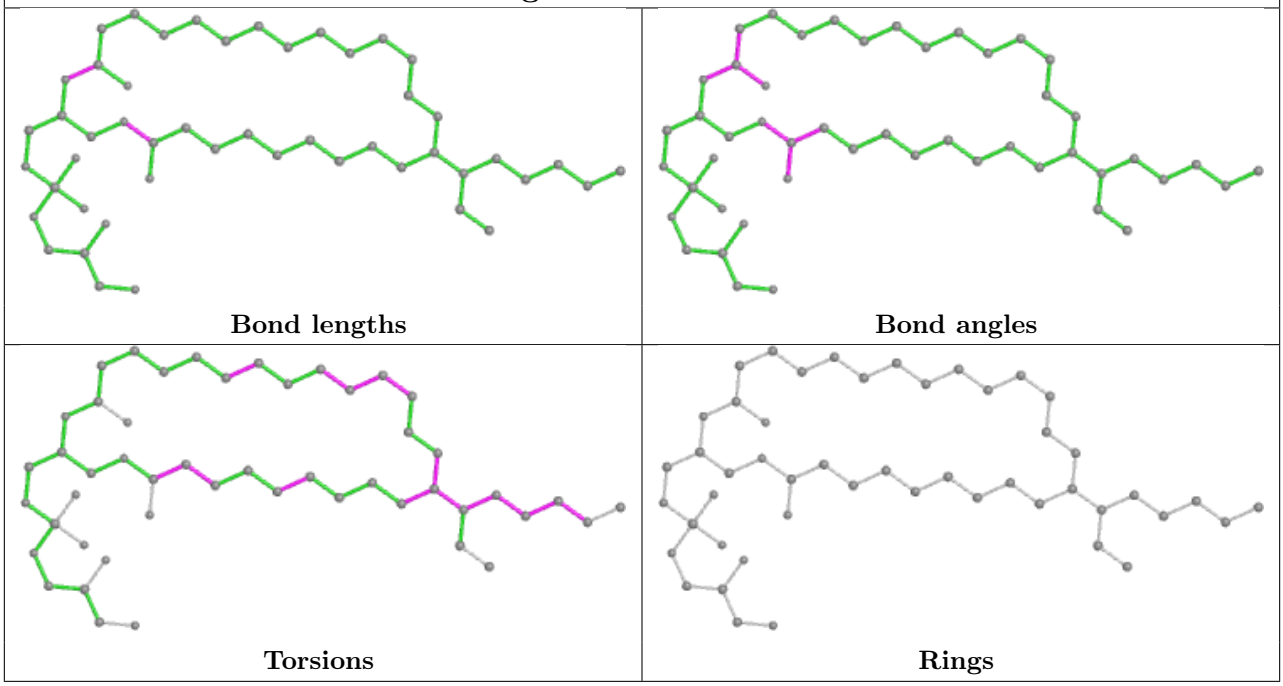
Ligand PSC O 303



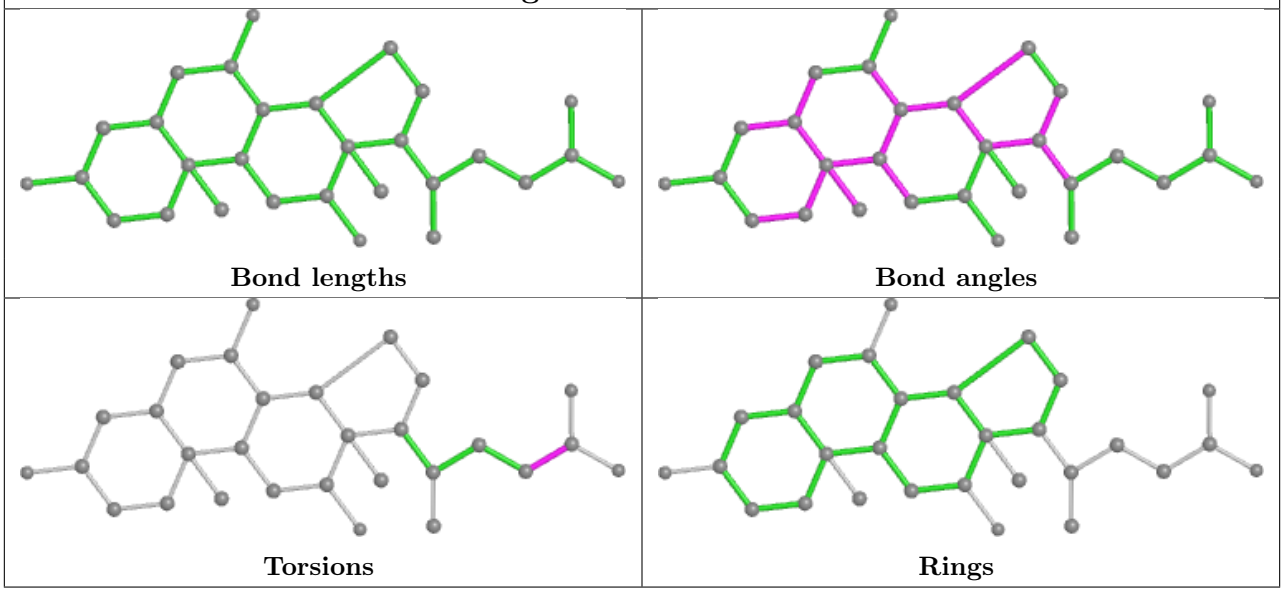
Ligand CDL G 102



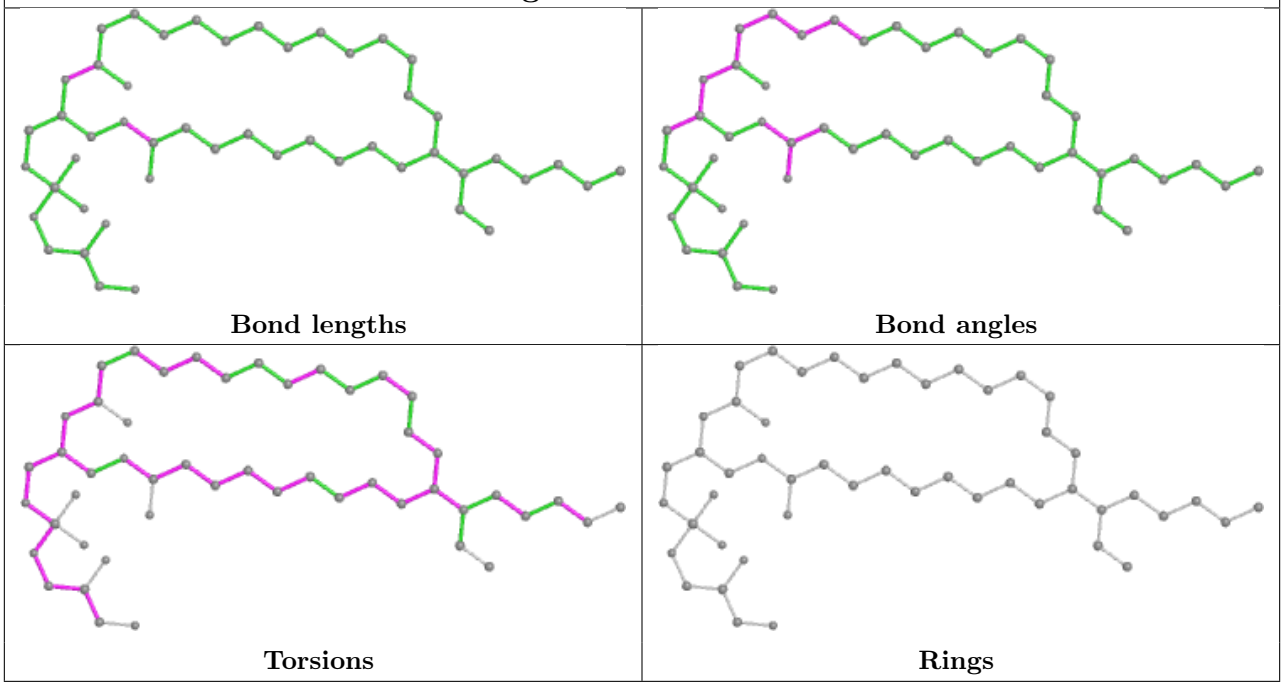
Ligand PGV N 608



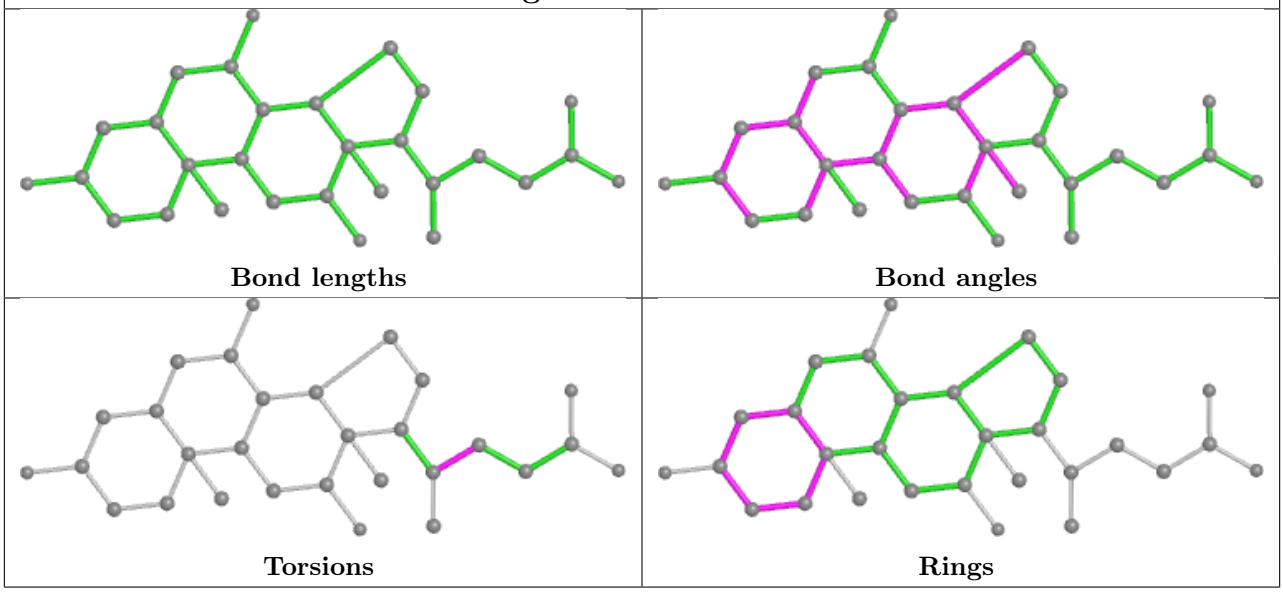
Ligand CHD C 304



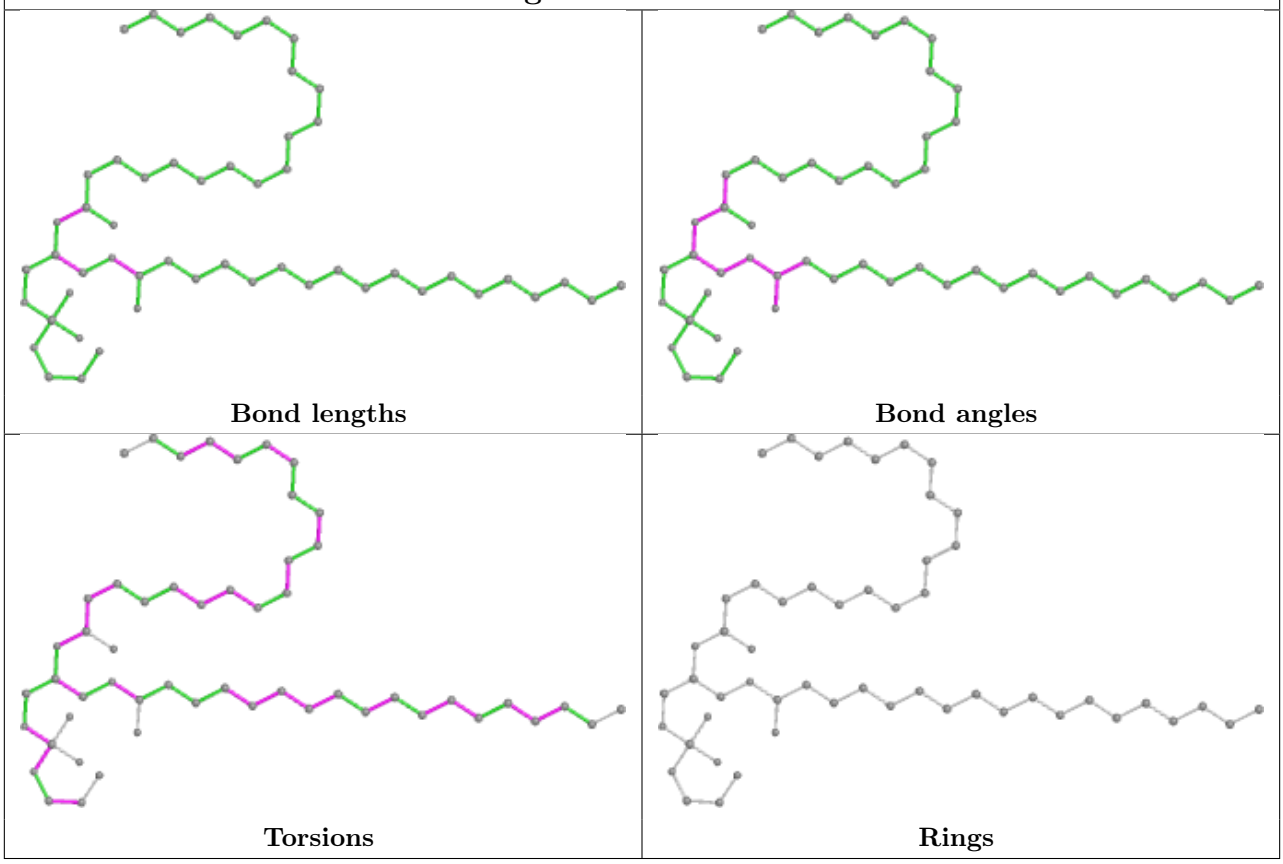
Ligand PGV A 609



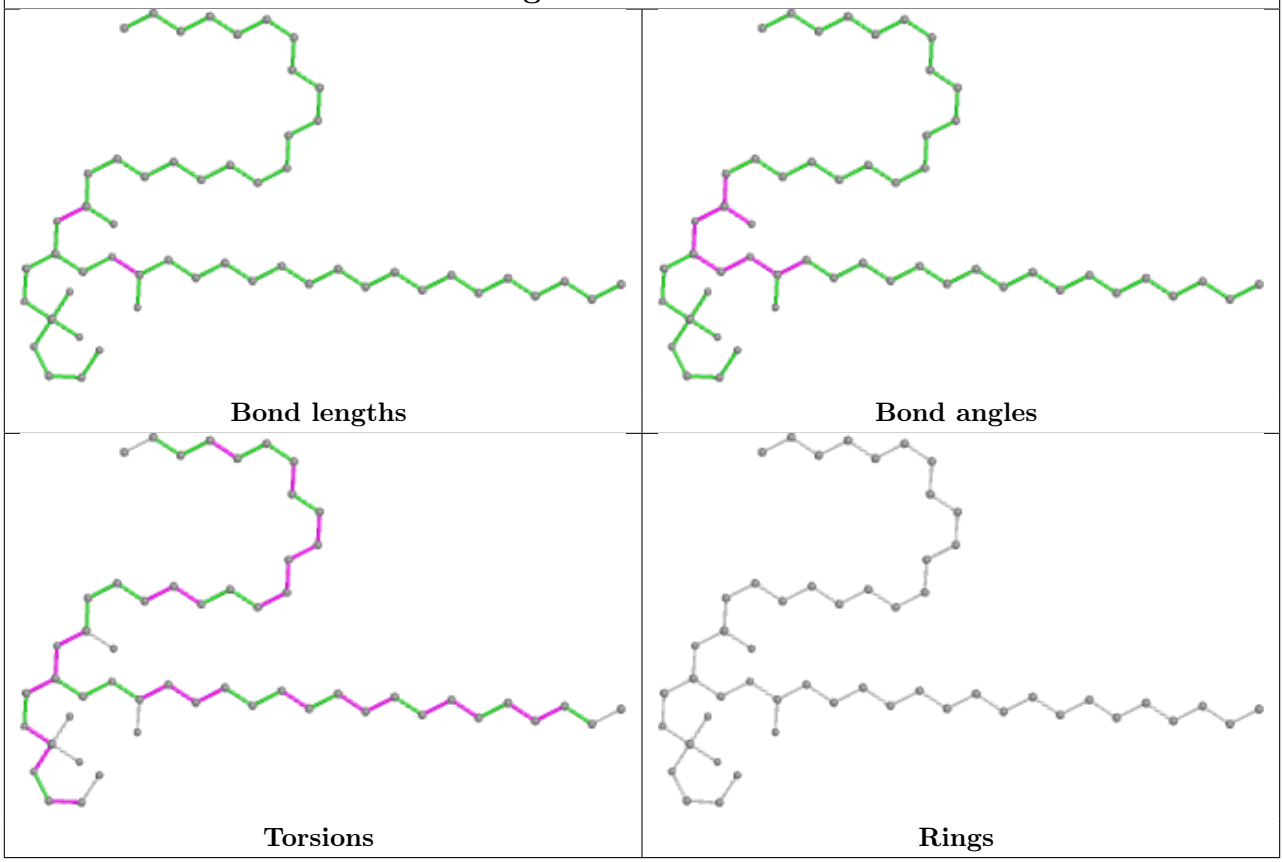
Ligand CHD P 305



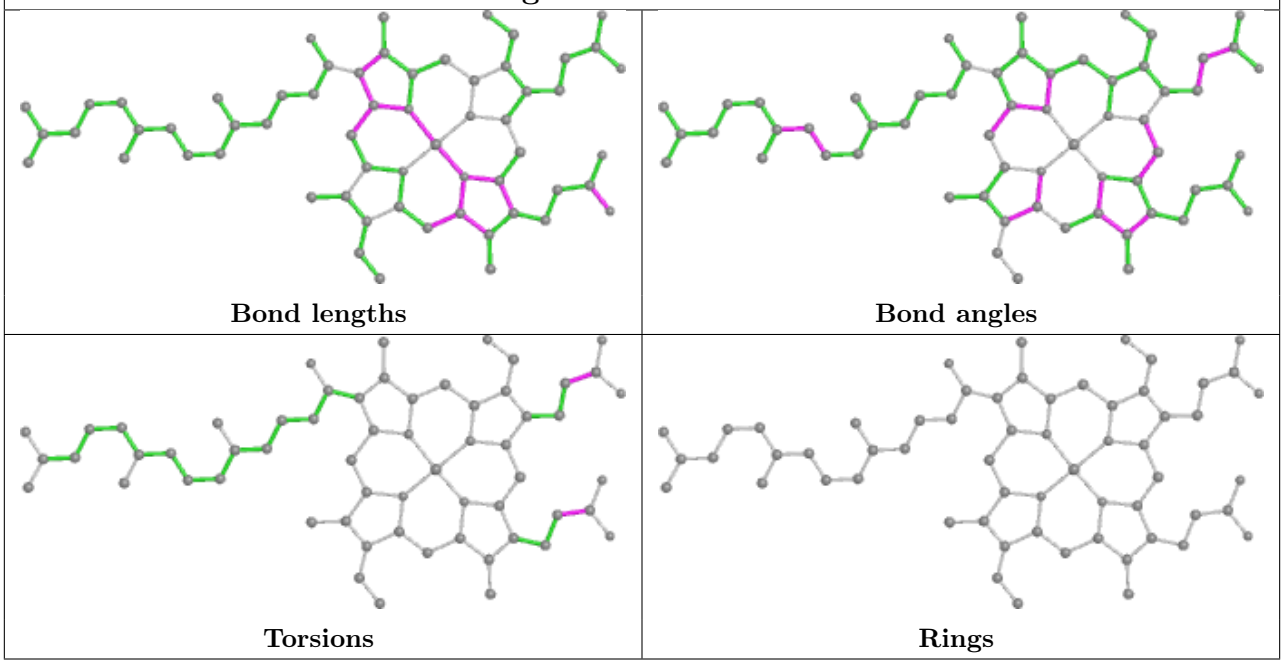
Ligand PEK C 306



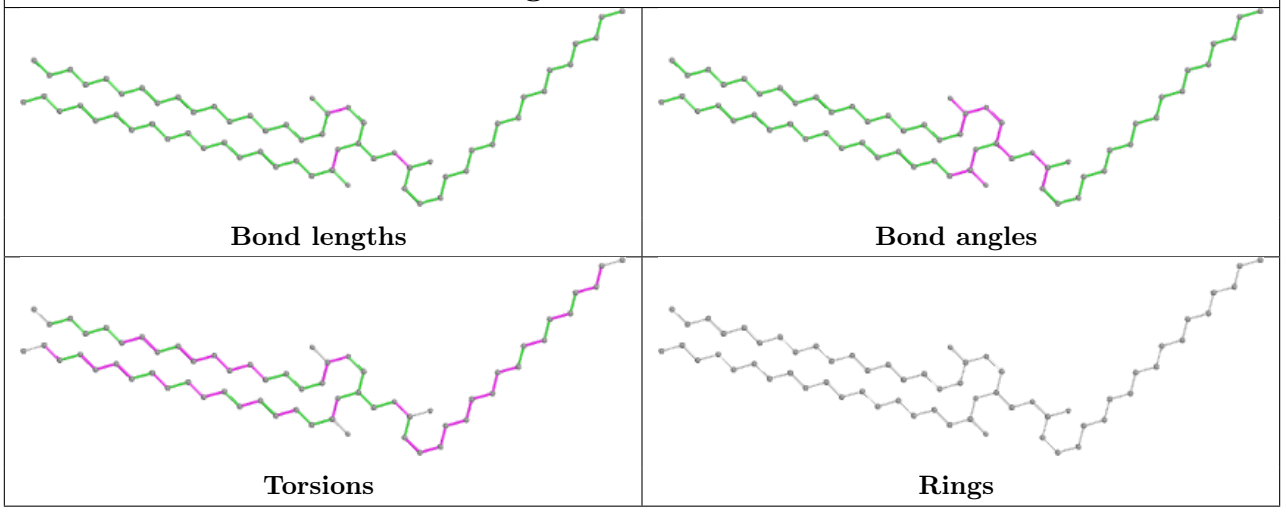
Ligand PEK G 103



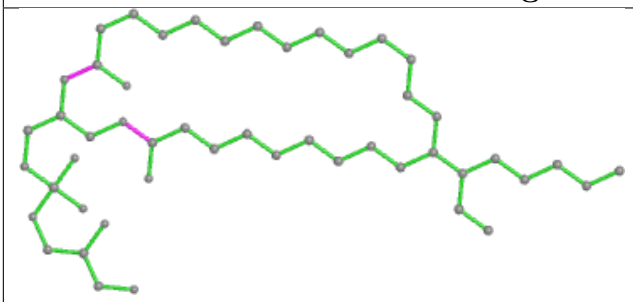
Ligand HEA N 601



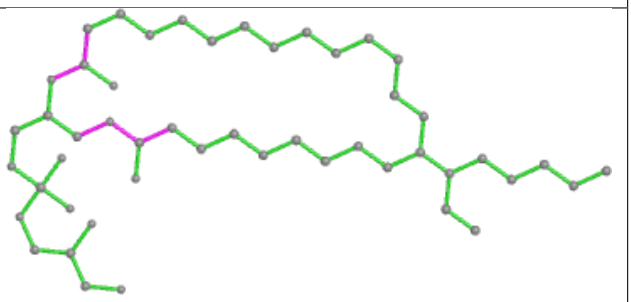
Ligand TGL O 302



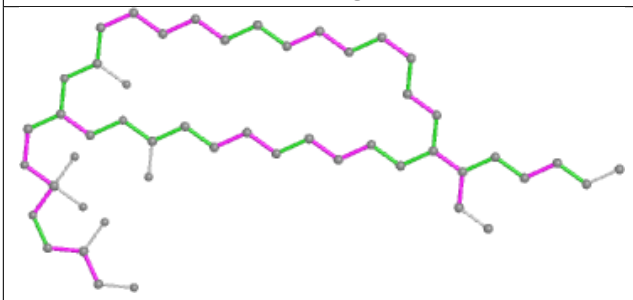
Ligand PGV C 307



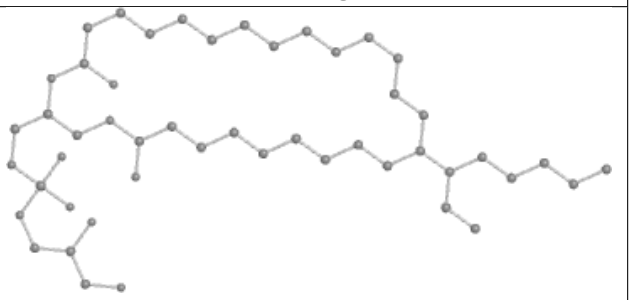
Bond lengths



Bond angles

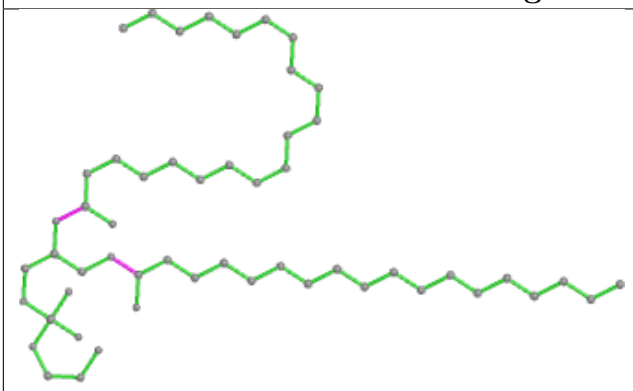


Torsions

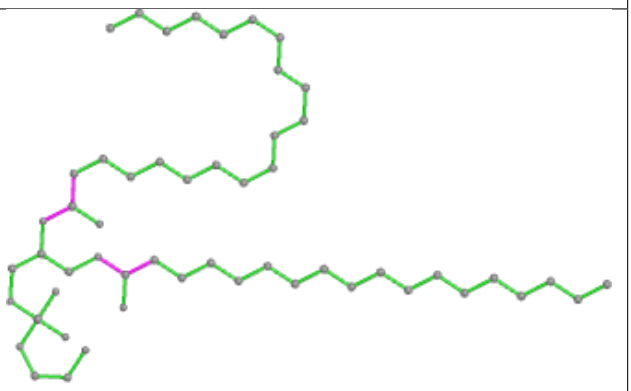


Rings

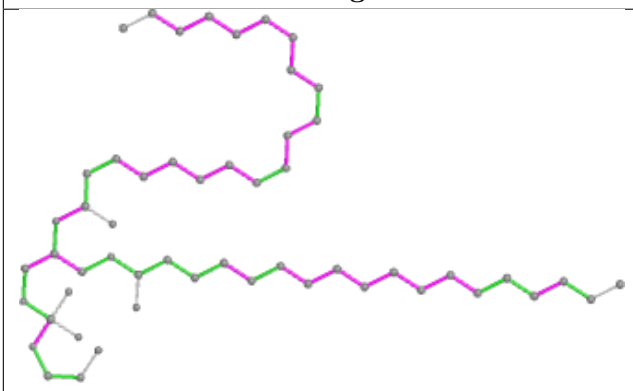
Ligand PEK T 103



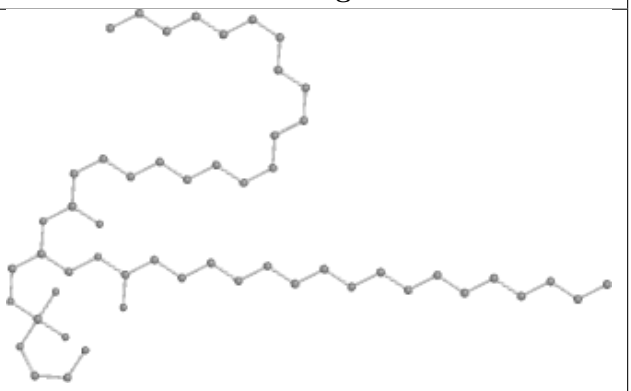
Bond lengths



Bond angles

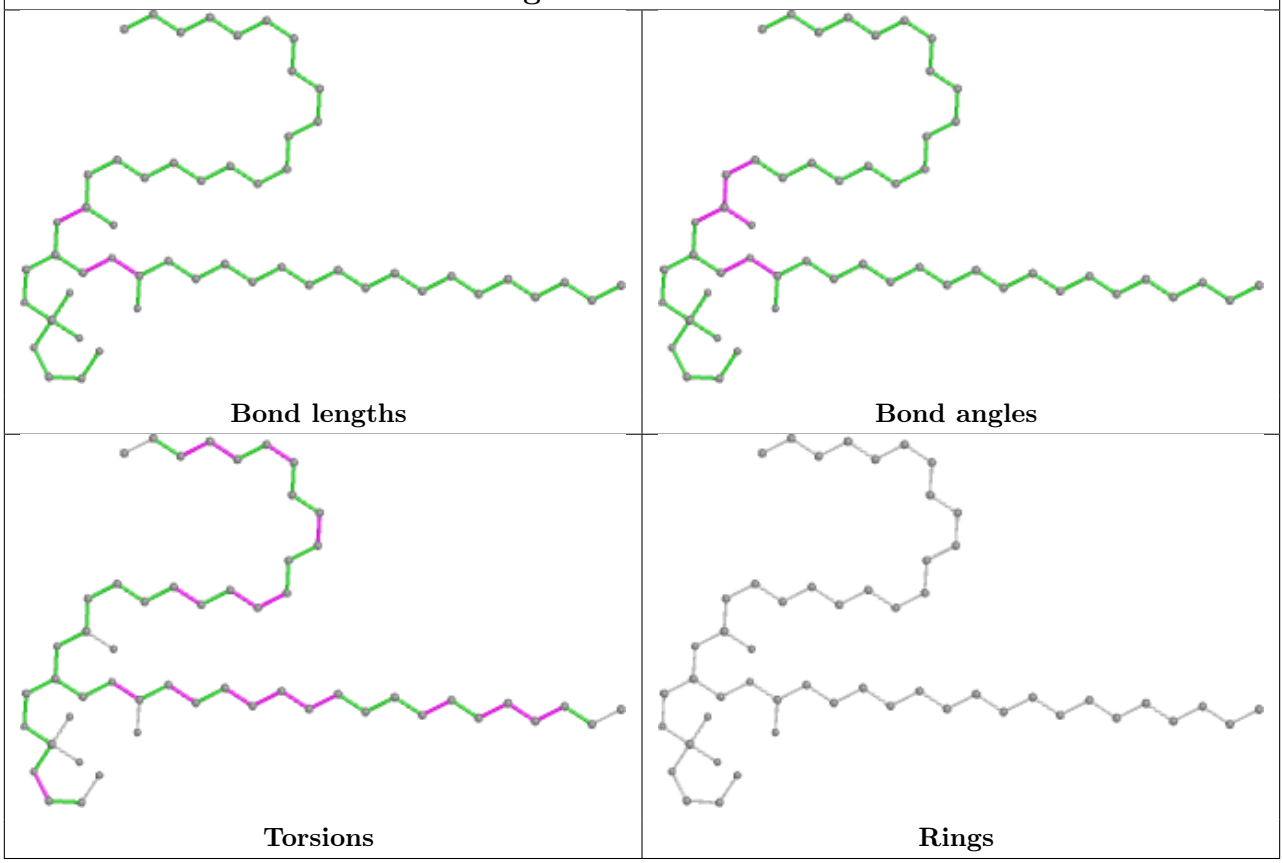


Torsions



Rings

Ligand PEK G 101



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%)	-0.71	0	100	100	39, 47, 59, 90	0
1	N	513/514 (99%)	-0.71	5 (0%)	82	81	43, 55, 71, 103	0
2	B	226/227 (99%)	-0.74	3 (1%)	77	75	43, 54, 82, 118	0
2	O	226/227 (99%)	-0.48	6 (2%)	54	52	51, 64, 98, 140	0
3	C	259/261 (99%)	-0.55	0	100	100	44, 51, 69, 123	0
3	P	259/261 (99%)	-0.41	6 (2%)	60	58	46, 56, 75, 129	0
4	D	144/147 (97%)	-0.52	1 (0%)	87	86	49, 59, 87, 126	0
4	Q	144/147 (97%)	0.43	16 (11%)	5	4	60, 81, 126, 157	0
5	E	105/109 (96%)	-0.31	2 (1%)	66	65	49, 59, 88, 147	0
5	R	105/109 (96%)	-0.00	6 (5%)	23	22	56, 73, 104, 142	0
6	F	98/98 (100%)	-0.27	10 (10%)	6	6	47, 61, 138, 155	0
6	S	98/98 (100%)	-0.06	6 (6%)	21	20	51, 70, 140, 158	0
7	G	83/85 (97%)	0.62	15 (18%)	1	1	49, 62, 150, 157	0
7	T	83/85 (97%)	0.54	10 (12%)	4	3	49, 68, 143, 154	0
8	H	79/85 (92%)	-0.16	4 (5%)	28	26	49, 64, 129, 144	0
8	U	79/85 (92%)	-0.14	5 (6%)	20	19	56, 71, 143, 153	0
9	I	72/73 (98%)	-0.39	3 (4%)	36	34	53, 66, 96, 118	0
9	V	72/73 (98%)	-0.31	5 (6%)	16	15	50, 77, 105, 140	0
10	J	58/59 (98%)	0.06	5 (8%)	10	9	52, 64, 98, 150	0
10	W	58/59 (98%)	-0.17	3 (5%)	27	26	59, 76, 110, 157	0
11	K	49/56 (87%)	-0.08	5 (10%)	6	6	57, 67, 88, 105	0
11	X	49/56 (87%)	0.33	8 (16%)	1	1	69, 80, 109, 122	0
12	L	46/47 (97%)	-0.84	0	100	100	47, 55, 75, 109	0
12	Y	46/47 (97%)	-0.35	3 (6%)	18	17	57, 72, 98, 140	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	43/46 (93%)	-0.41	1 (2%) 60 58	51, 57, 89, 130	0
13	Z	43/46 (93%)	-0.13	4 (9%) 8 7	66, 78, 113, 150	0
All	All	3550/3614 (98%)	-0.39	132 (3%) 41 39	39, 59, 103, 158	0

The worst 5 of 132 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	S	97	ALA	16.4
7	T	3	ALA	12.1
7	G	1	ALA	11.1
7	G	2	SER	10.3
4	Q	6	VAL	9.9

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	SAC	V	1	9/10	0.58	0.59	134,154,162,162	0
9	SAC	I	1	9/10	0.73	0.27	108,138,147,149	0
7	TPO	G	11	11/12	0.74	0.13	105,144,154,158	0
7	TPO	T	11	11/12	0.77	0.24	100,127,155,158	0
1	FME	A	1	10/11	0.96	0.28	58,69,114,141	0
2	FME	O	1	10/11	0.98	0.15	62,65,74,76	0
2	FME	B	1	10/11	0.98	0.08	51,56,62,76	0
1	FME	N	1	10/11	0.98	0.48	77,90,144,145	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
27	PEK	T	102	53/53	0.50	0.51	74,133,150,150	0
21	EDO	C	310	4/4	0.57	0.84	146,146,149,149	0
25	UNX	P	302	1/1	0.58	0.71	20,20,20,20	1
23	CHD	W	101	29/29	0.61	0.35	108,149,150,150	0
27	PEK	C	306	53/53	0.61	0.30	68,138,150,150	0
24	PSC	O	303	52/52	0.61	0.33	72,134,150,150	0
26	CDL	G	102	100/100	0.63	0.37	99,145,150,150	0
26	CDL	T	104	100/100	0.63	0.33	83,136,150,150	0
26	CDL	P	304	100/100	0.67	0.27	70,139,150,150	0
19	TGL	Y	101	63/63	0.68	0.35	78,127,150,150	0
19	TGL	D	201	63/63	0.68	0.29	68,117,150,150	0
21	EDO	P	307	4/4	0.68	0.30	92,96,107,115	0
21	EDO	P	308	4/4	0.68	0.22	89,95,98,99	0
21	EDO	K	101	4/4	0.69	0.16	87,91,96,105	0
27	PEK	G	103	53/53	0.70	0.47	84,136,150,150	0
24	PSC	B	303	52/52	0.70	0.27	73,142,150,150	0
20	PGV	A	609	51/51	0.72	0.30	62,112,152,160	0
19	TGL	Q	201	63/63	0.75	0.23	76,124,150,150	0
20	PGV	N	607	51/51	0.75	0.39	66,140,150,150	0
21	EDO	N	610	4/4	0.75	0.91	125,132,135,138	0
26	CDL	C	303	100/100	0.77	0.24	56,121,153,157	0
27	PEK	T	103	53/53	0.77	0.26	67,132,150,150	0
19	TGL	A	607	63/63	0.78	0.24	50,96,139,151	0
21	EDO	H	101	4/4	0.78	0.33	111,112,118,127	0
19	TGL	O	302	63/63	0.78	0.21	67,115,150,150	0
19	TGL	L	101	63/63	0.79	0.26	67,106,149,150	0
20	PGV	C	307	51/51	0.80	0.26	61,126,150,150	0
20	PGV	P	301	51/51	0.81	0.21	73,119,150,150	0
21	EDO	F	103	4/4	0.82	0.55	71,125,128,147	0
21	EDO	B	305	4/4	0.82	0.32	84,86,91,94	0
29	DMU	Z	101	33/33	0.83	0.30	95,106,138,147	0
23	CHD	J	101	29/29	0.84	0.33	90,142,150,150	0
21	EDO	A	611	4/4	0.84	0.16	81,82,106,109	0
25	UNX	C	301	1/1	0.85	0.75	17,17,17,17	1
21	EDO	G	105	4/4	0.87	0.17	74,78,88,97	0
21	EDO	A	613	4/4	0.88	0.47	96,116,120,122	0
18	CMO	N	606	2/2	0.89	0.12	47,47,47,50	2
23	CHD	P	305	29/29	0.89	0.21	82,131,147,148	0
21	EDO	C	309	4/4	0.89	0.25	80,86,89,95	0
29	DMU	M	101	33/33	0.89	0.23	61,78,111,115	0
23	CHD	C	304	29/29	0.89	0.27	89,104,112,113	0
21	EDO	C	308	4/4	0.91	0.22	89,93,96,106	0

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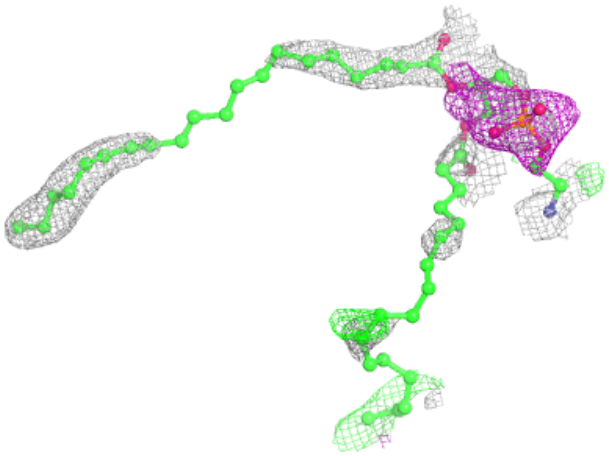
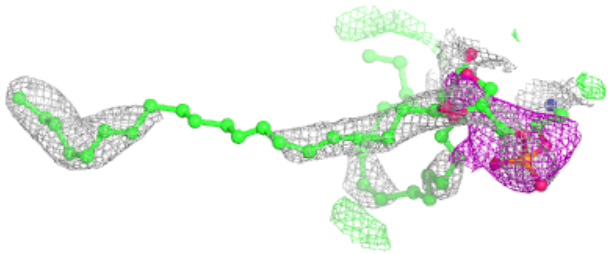
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
21	EDO	T	105	4/4	0.91	0.22	121,130,135,136	0
21	EDO	F	102	4/4	0.92	0.17	82,82,101,101	0
21	EDO	K	102	4/4	0.92	0.60	89,96,101,112	0
21	EDO	L	102	4/4	0.93	0.16	83,86,90,95	0
21	EDO	N	609	4/4	0.93	0.09	88,91,100,108	0
21	EDO	A	612	4/4	0.94	0.28	62,76,80,93	0
20	PGV	P	303	51/51	0.94	0.22	53,65,143,148	0
21	EDO	C	311	4/4	0.95	0.12	60,77,78,84	0
27	PEK	T	101	53/53	0.95	0.18	62,77,149,150	0
21	EDO	O	304	4/4	0.96	0.18	68,70,73,77	0
27	PEK	G	101	53/53	0.96	0.15	50,67,123,137	0
23	CHD	P	306	29/29	0.97	0.10	52,60,64,66	0
20	PGV	C	302	51/51	0.97	0.13	46,57,107,115	0
23	CHD	C	305	29/29	0.97	0.09	48,56,63,68	0
23	CHD	G	104	29/29	0.97	0.11	42,51,59,66	0
20	PGV	A	608	51/51	0.97	0.12	43,65,86,105	0
21	EDO	B	304	4/4	0.97	0.14	64,66,67,75	0
18	CMO	A	606	2/2	0.98	0.25	33,33,33,35	2
20	PGV	N	608	51/51	0.98	0.13	50,71,101,113	0
14	HEA	A	601	60/60	0.98	0.09	38,44,59,72	0
23	CHD	B	302	29/29	0.98	0.09	49,57,63,73	0
14	HEA	A	602	60/60	0.98	0.08	37,44,53,64	0
21	EDO	A	610	4/4	0.98	0.08	54,63,68,71	0
14	HEA	N	601	60/60	0.98	0.11	48,57,76,84	0
16	MG	N	604	1/1	0.98	0.03	52,52,52,52	0
17	NA	N	605	1/1	0.98	0.05	65,65,65,65	0
14	HEA	N	602	60/60	0.99	0.08	40,49,58,65	0
28	ZN	S	101	1/1	0.99	0.03	64,64,64,64	0
22	CUA	B	301	2/2	0.99	0.07	48,48,48,50	0
22	CUA	O	301	2/2	0.99	0.03	56,56,56,59	0
17	NA	A	605	1/1	1.00	0.10	53,53,53,53	0
28	ZN	F	101	1/1	1.00	0.05	57,57,57,57	0
15	CU	N	603	1/1	1.00	0.05	51,51,51,51	0
16	MG	A	604	1/1	1.00	0.02	41,41,41,41	0
15	CU	A	603	1/1	1.00	0.04	45,45,45,45	0

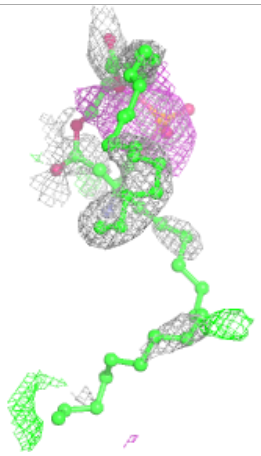
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PEK T 102:

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

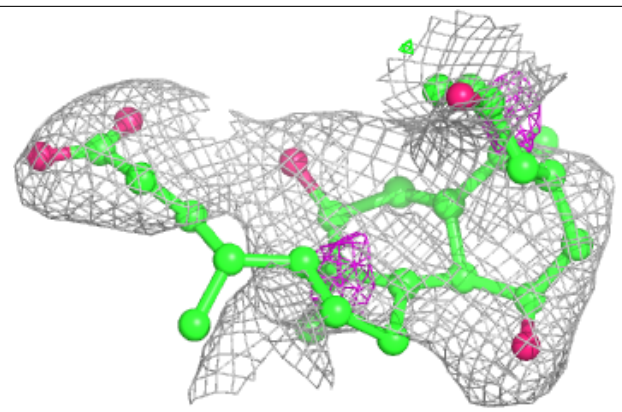


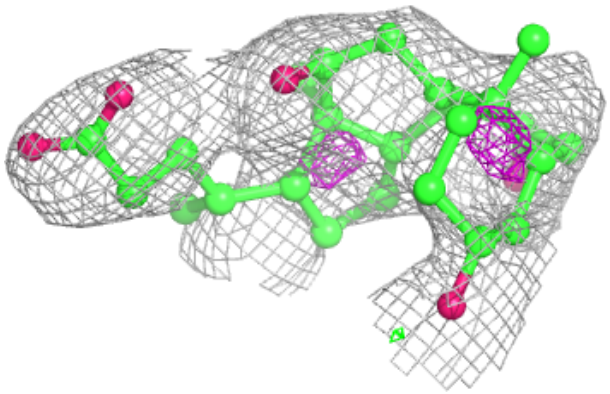


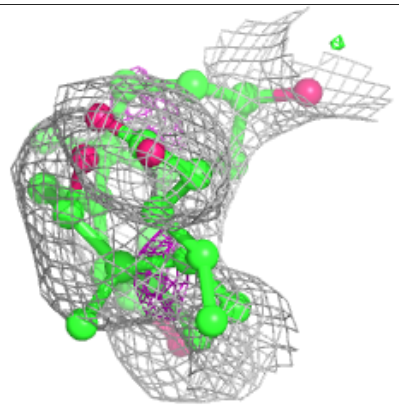


Electron density around CHD W 101:

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

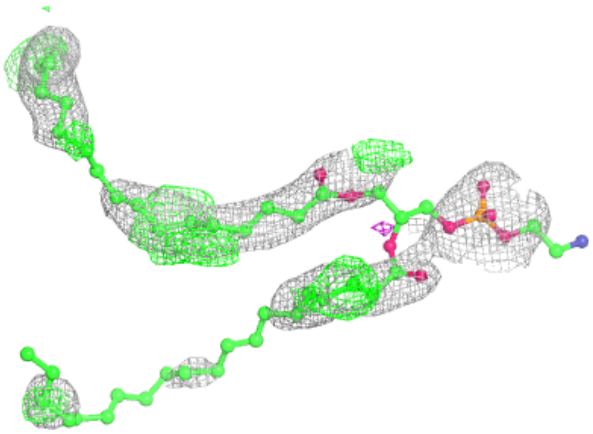


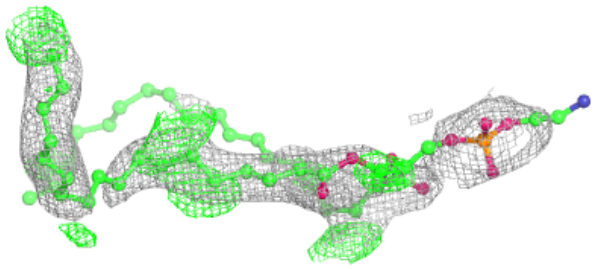


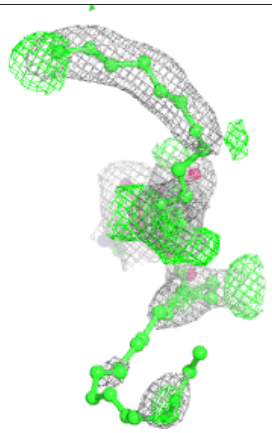


Electron density around PEK C 306:

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

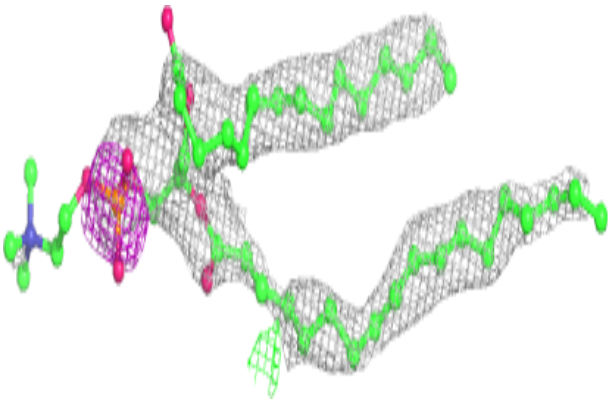


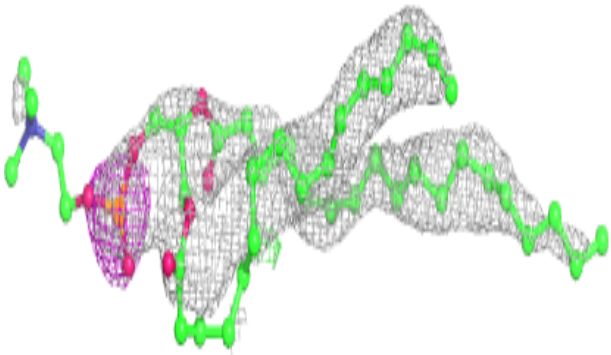


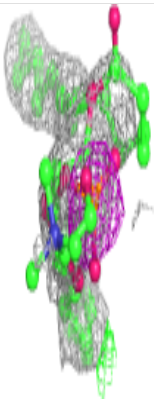


Electron density around PSC O 303:

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

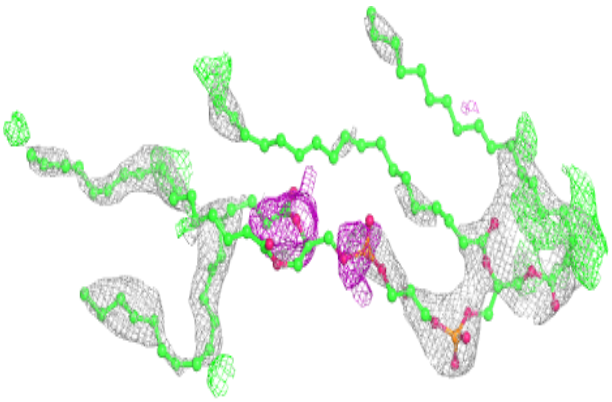


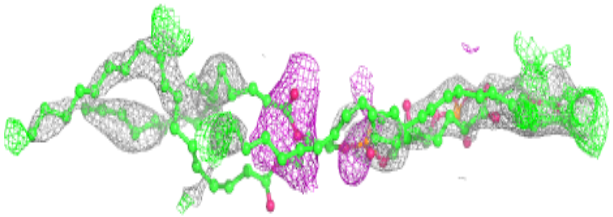


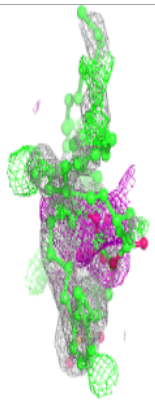


Electron density around CDL G 102:

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

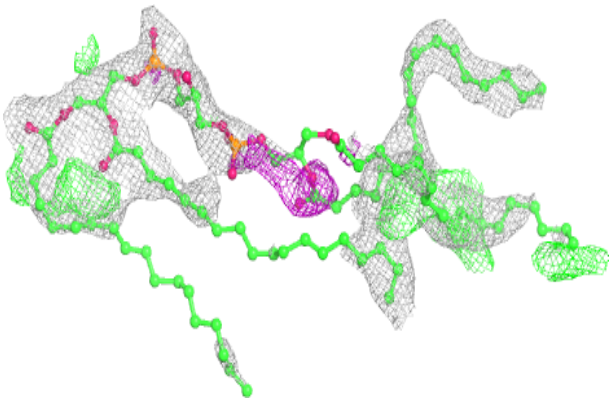


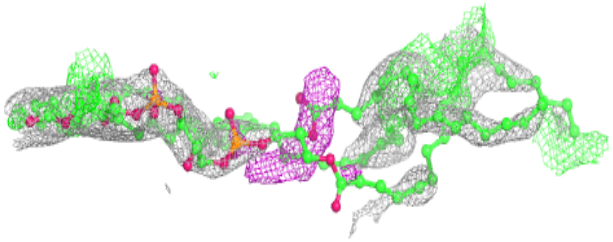


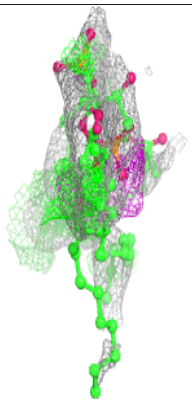


Electron density around CDL T 104:

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

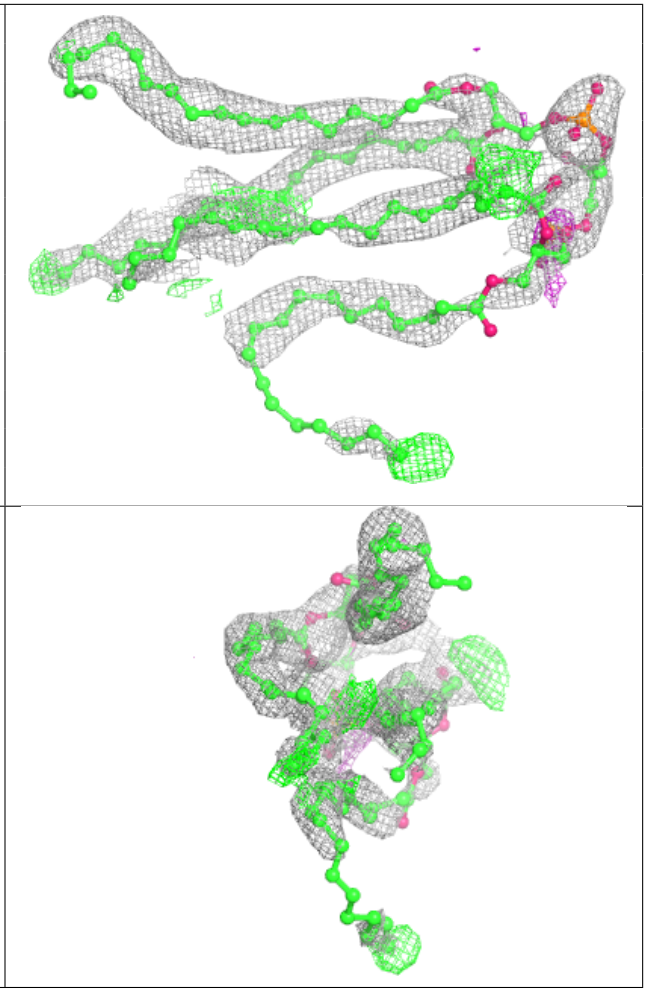






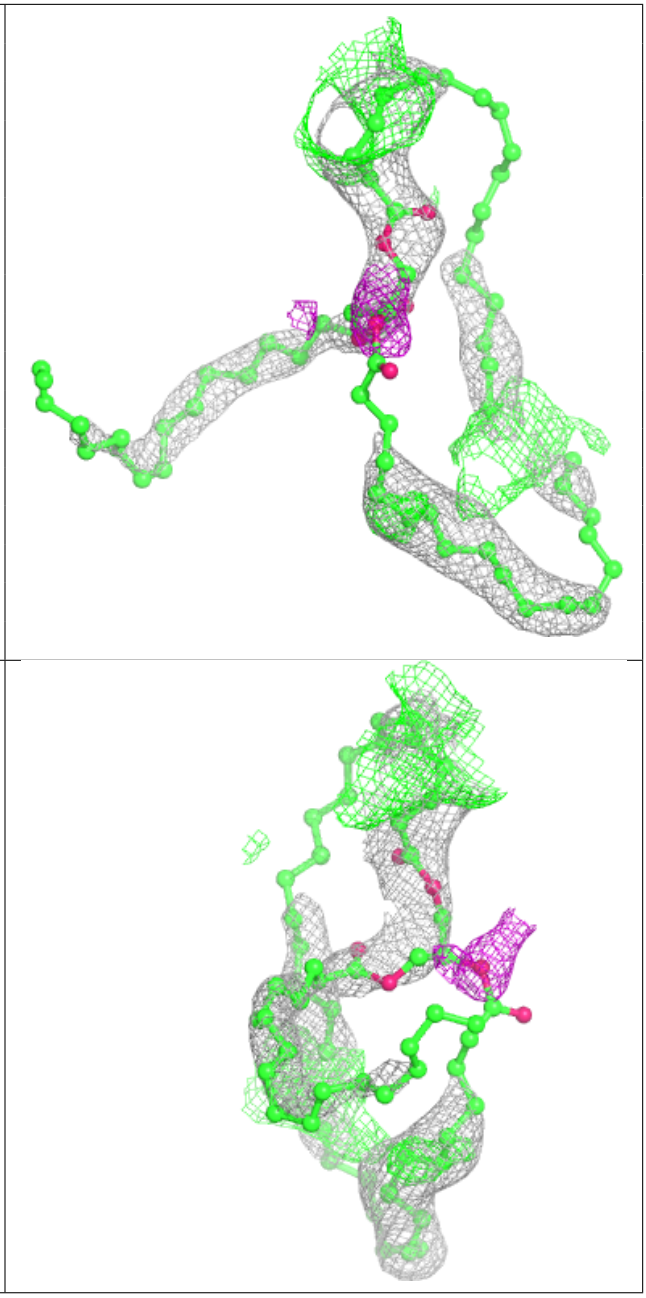
Electron density around CDL P 304:

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



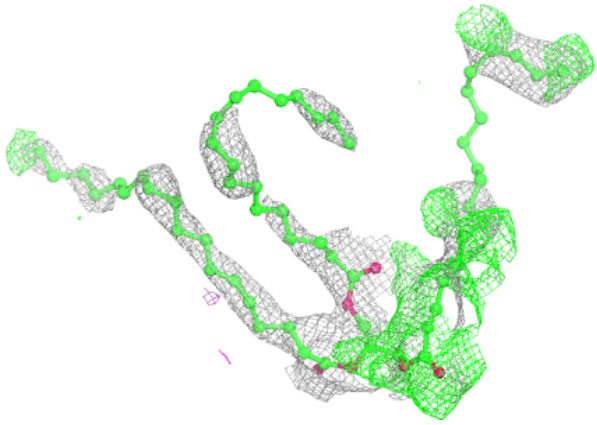
Electron density around TGL Y 101:

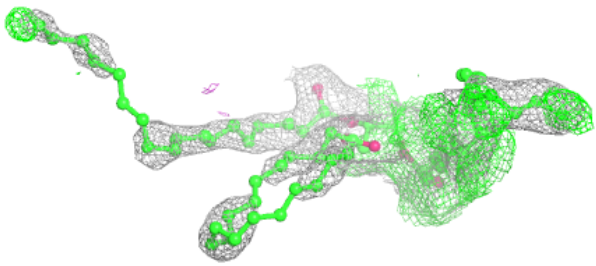
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

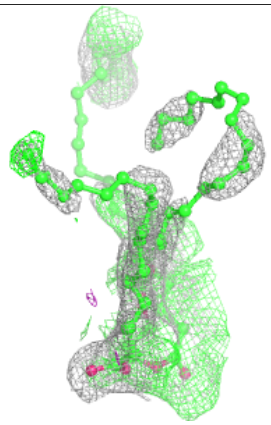


Electron density around TGL D 201:

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

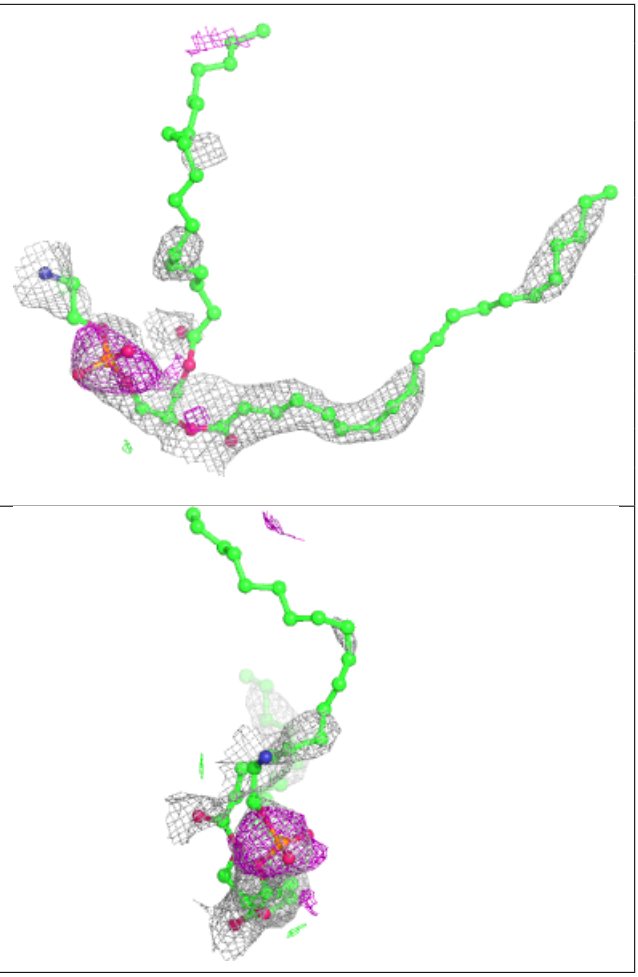






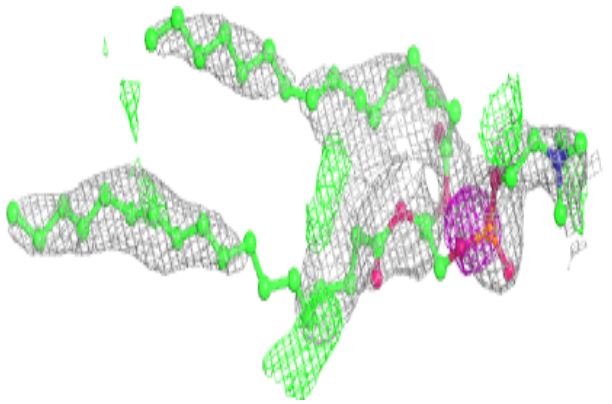
Electron density around PEK G 103:

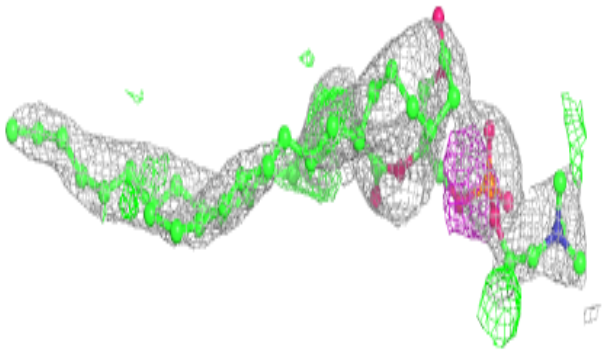
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

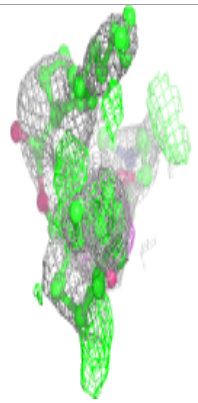


Electron density around PSC B 303:

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

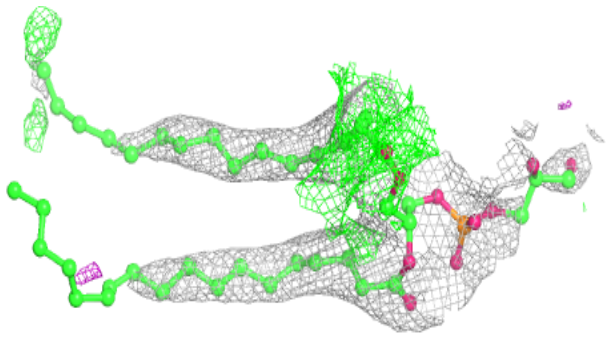


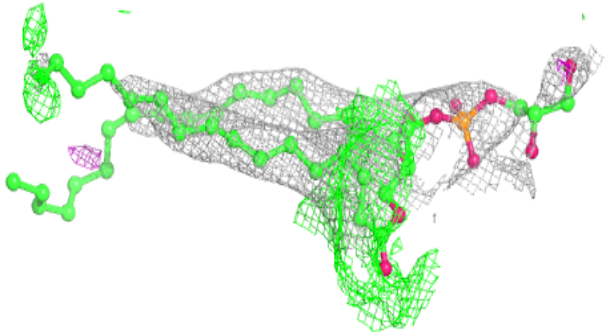


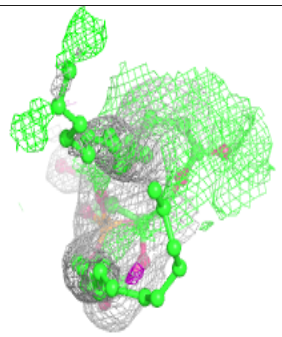


Electron density around PGV A 609:

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

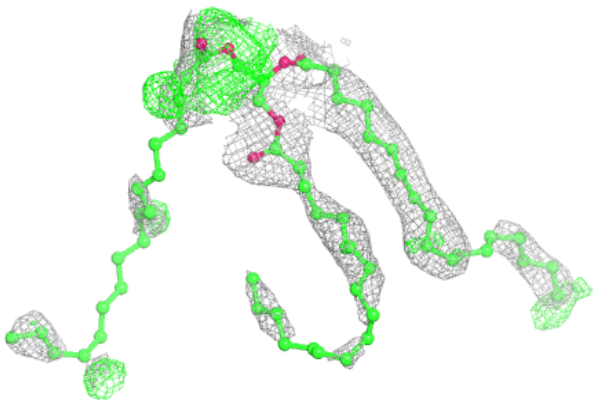


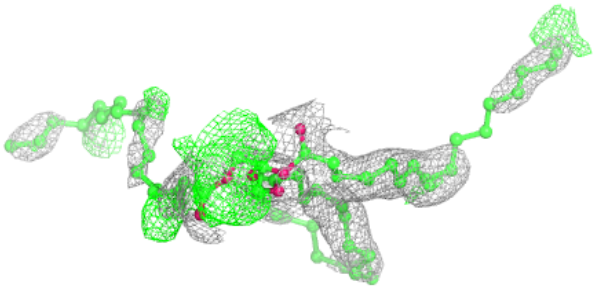


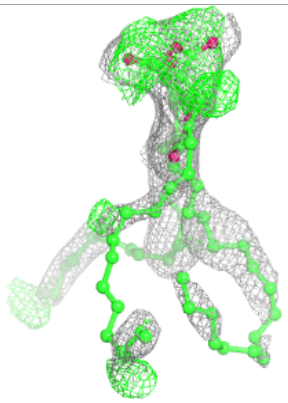


Electron density around TGL Q 201:

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

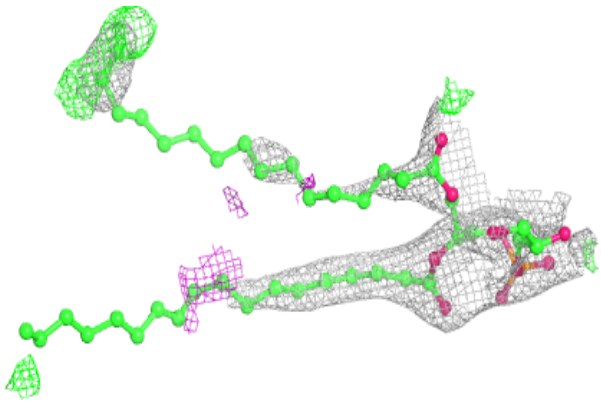


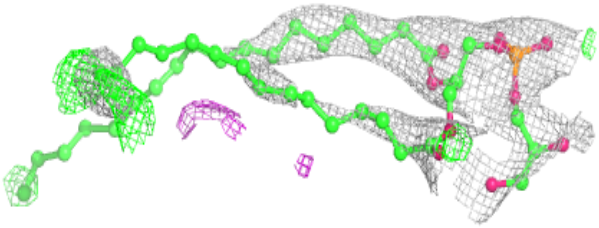


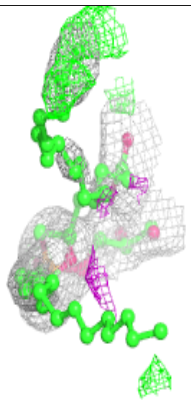


Electron density around PGV N 607:

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

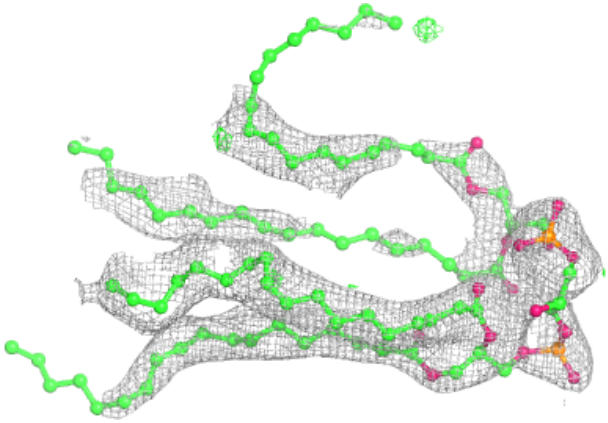


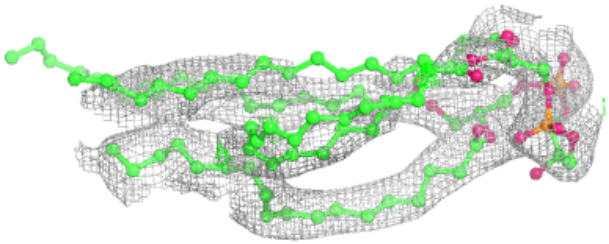


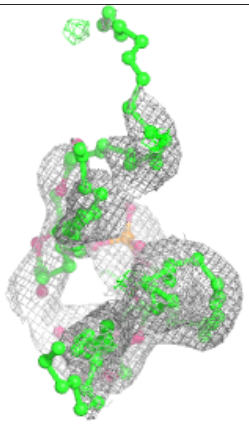


Electron density around CDL C 303:

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

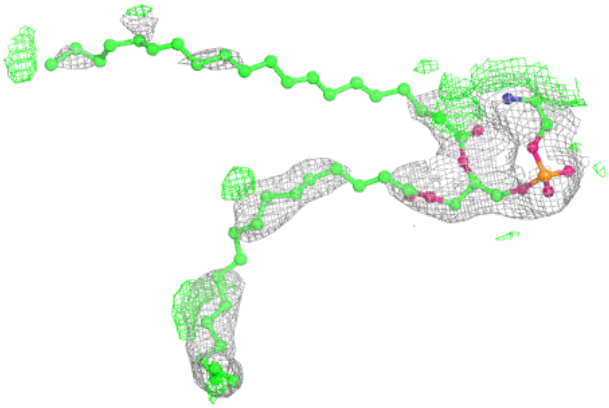


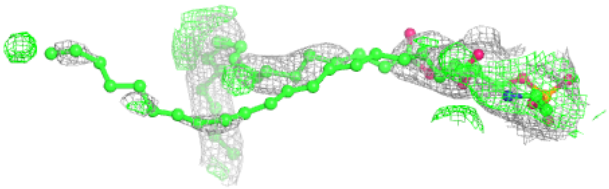


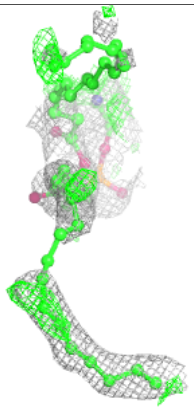


Electron density around PEK T 103:

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

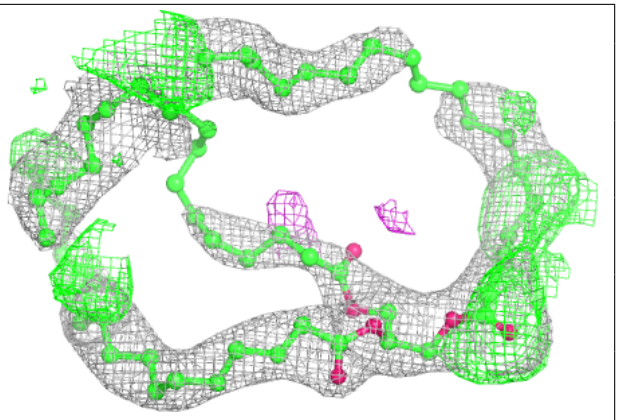


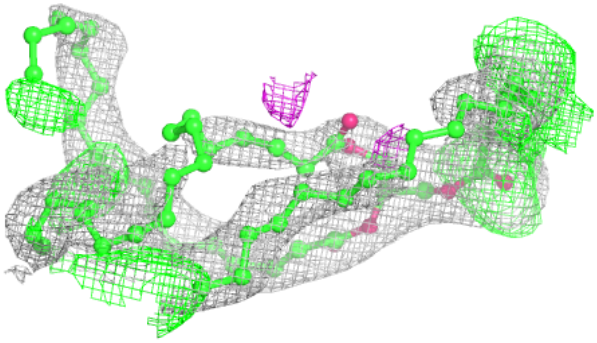


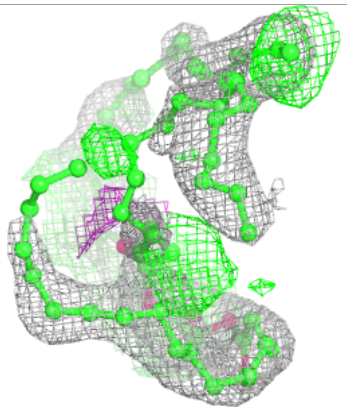


Electron density around TGL A 607:

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

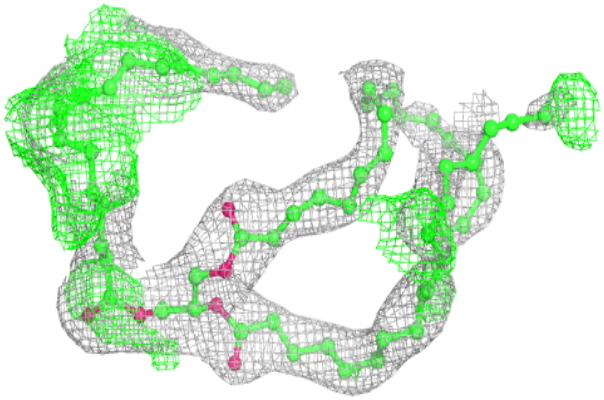


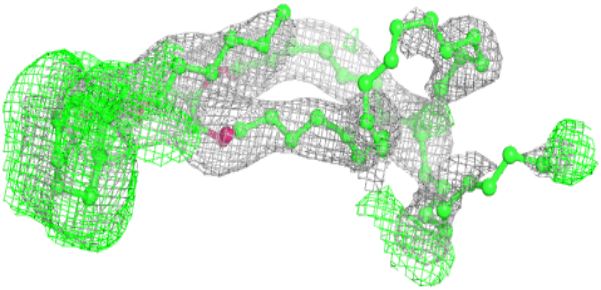


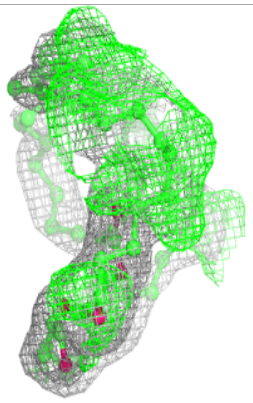


Electron density around TGL O 302:

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

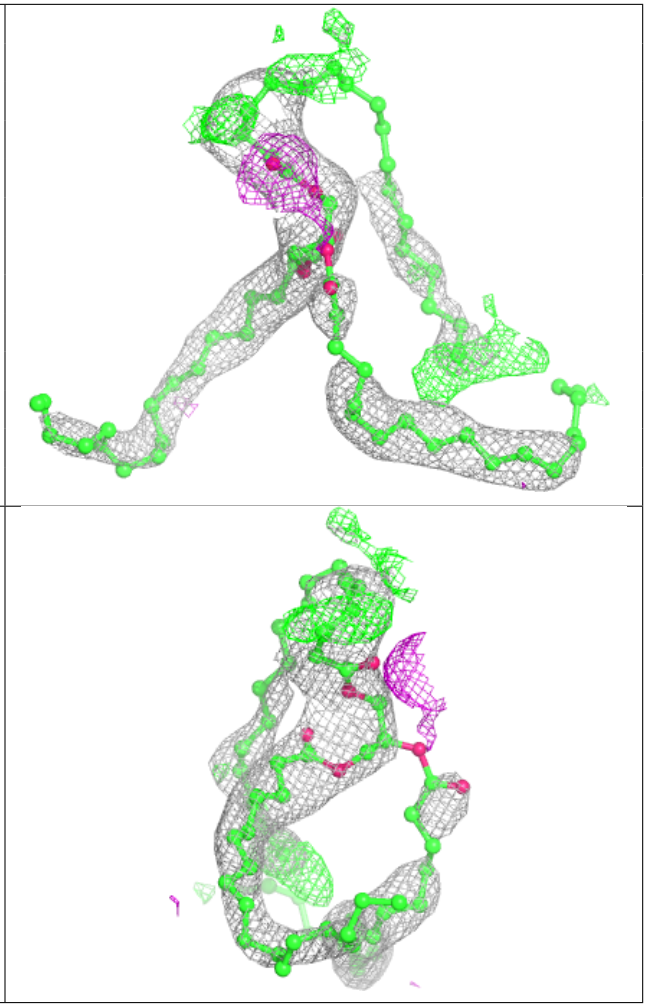






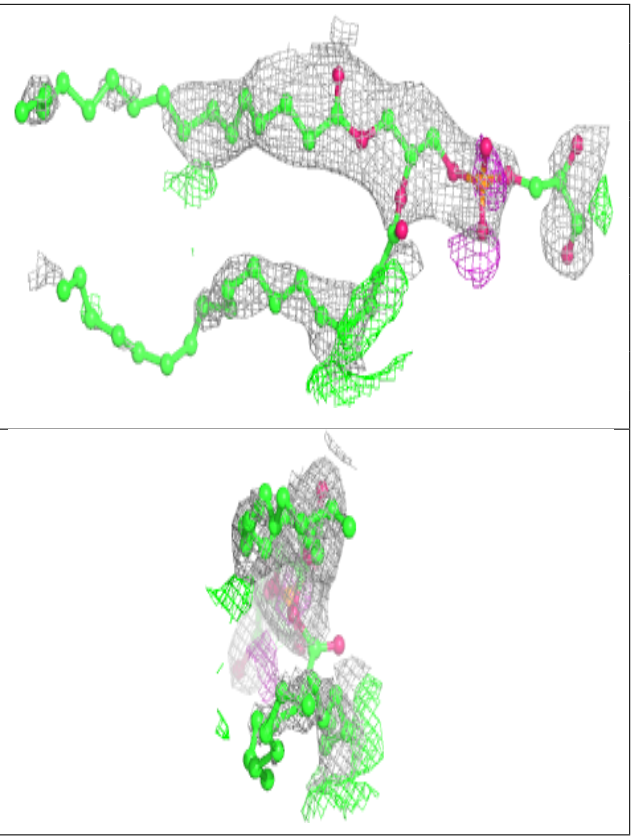
Electron density around TGL L 101:

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



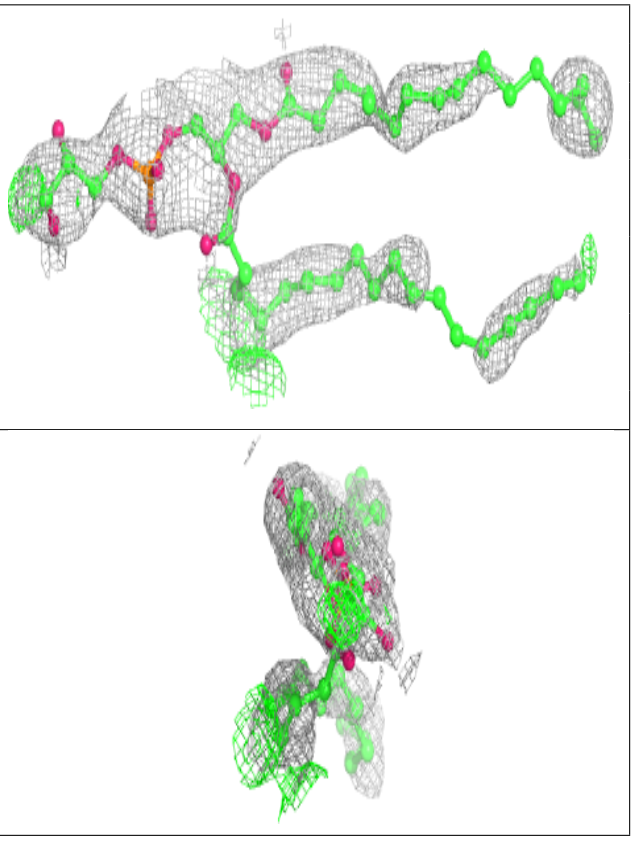
Electron density around PGV C 307:

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



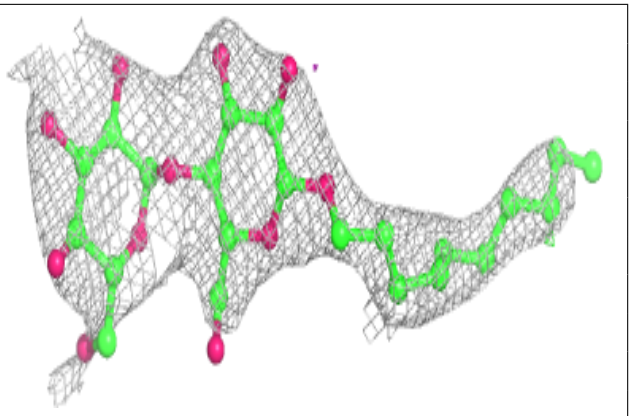
Electron density around PGV P 301:

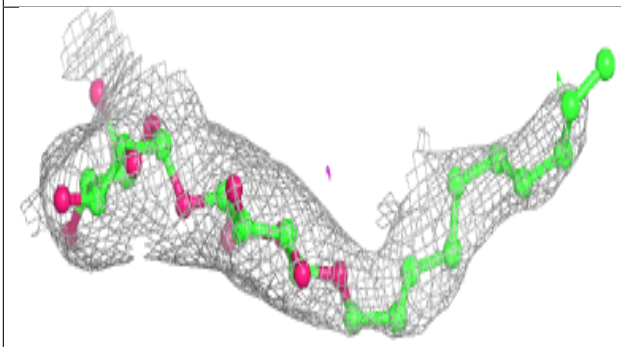
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

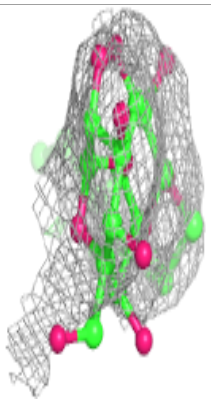


Electron density around DMU Z 101:

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

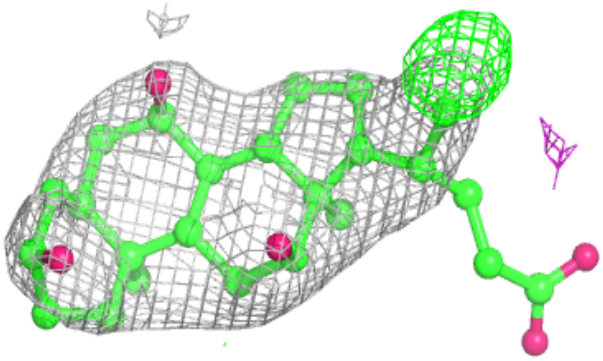


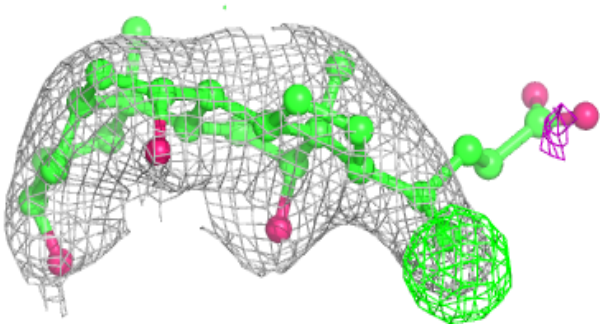


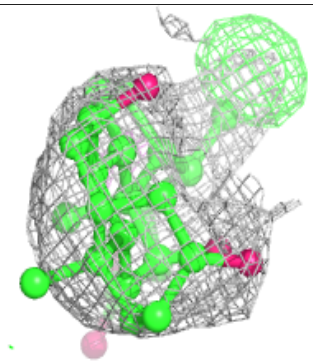


Electron density around CHD J 101:

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

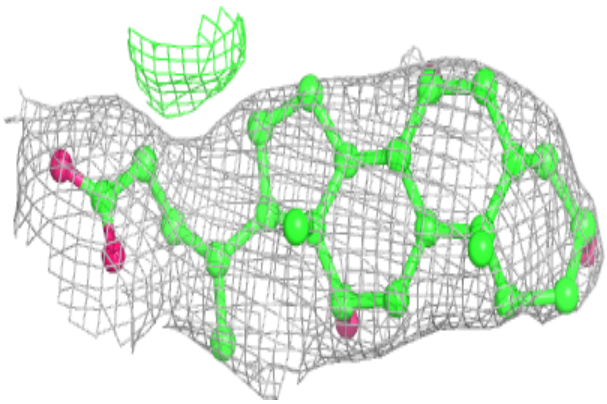


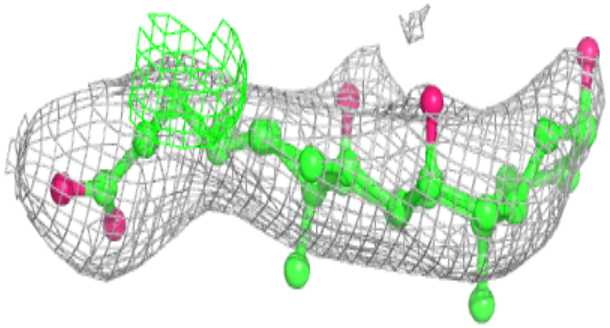


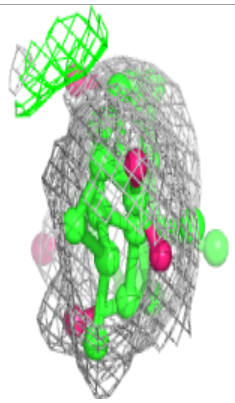


Electron density around CHD P 305:

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

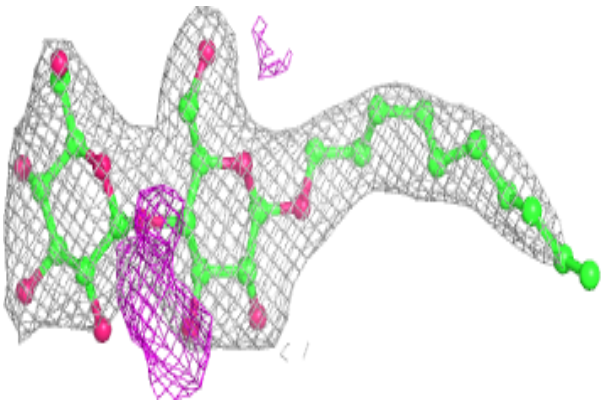


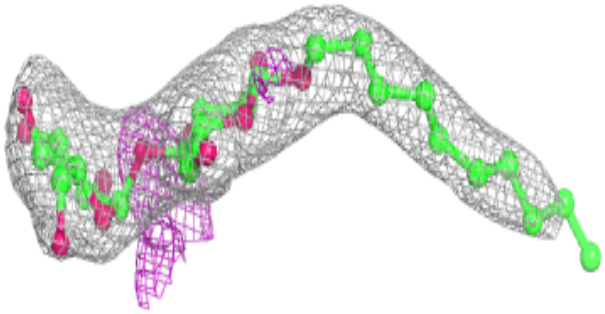


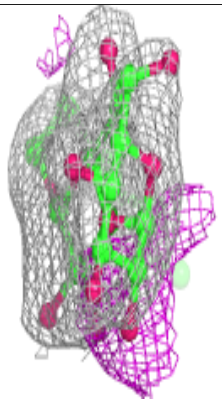


Electron density around DMU M 101:

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

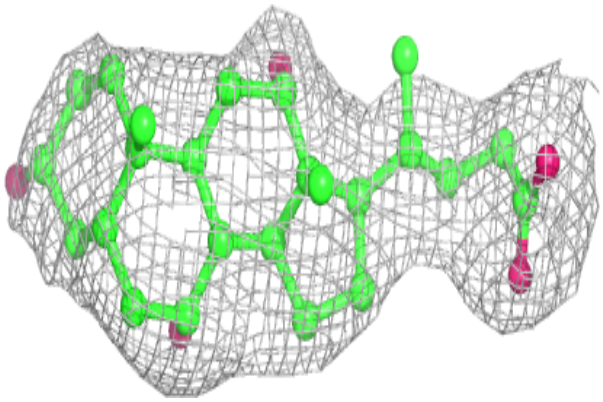


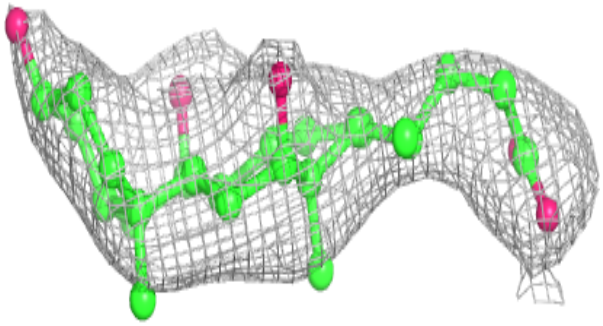


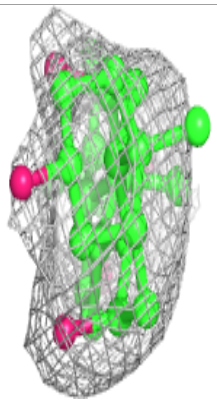


Electron density around CHD C 304:

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

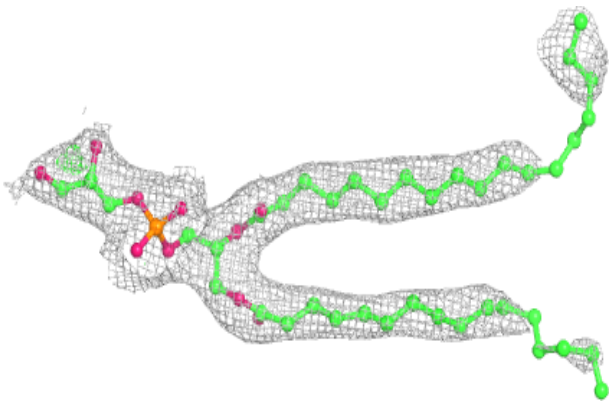


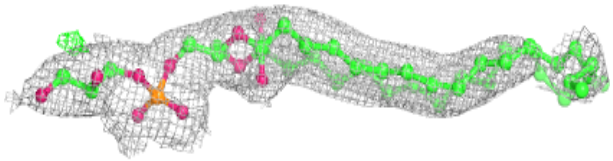


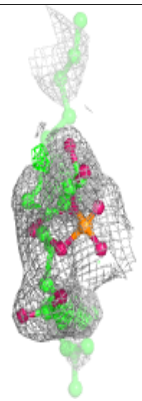


Electron density around PGV P 303:

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

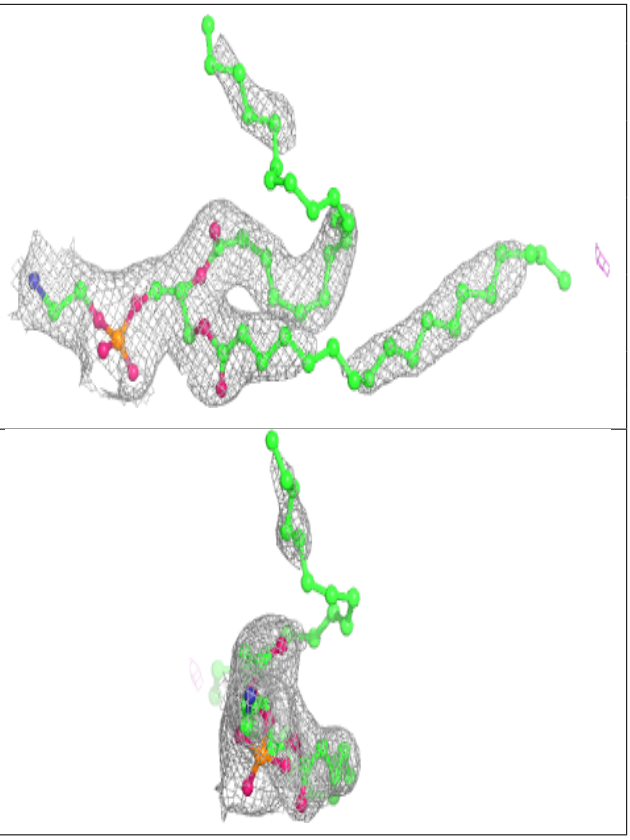


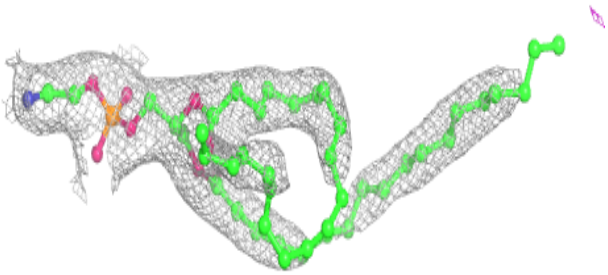




Electron density around PEK T 101:

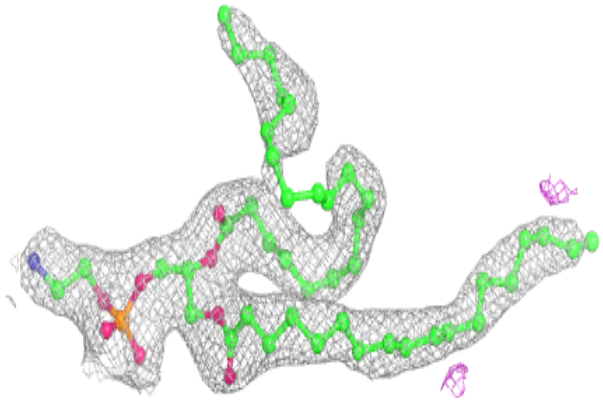
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

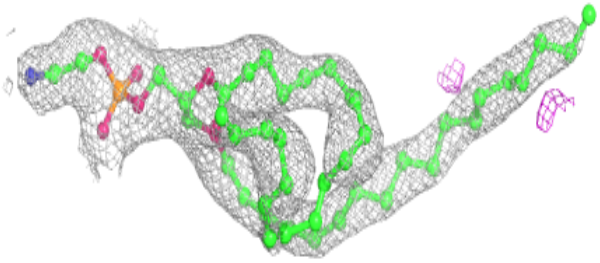


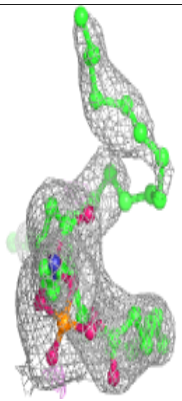


Electron density around PEK G 101:

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

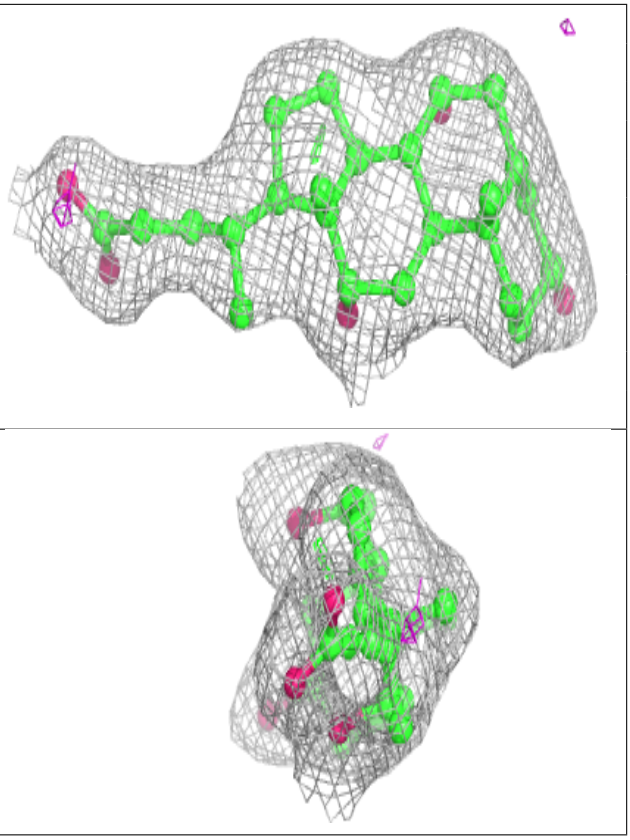






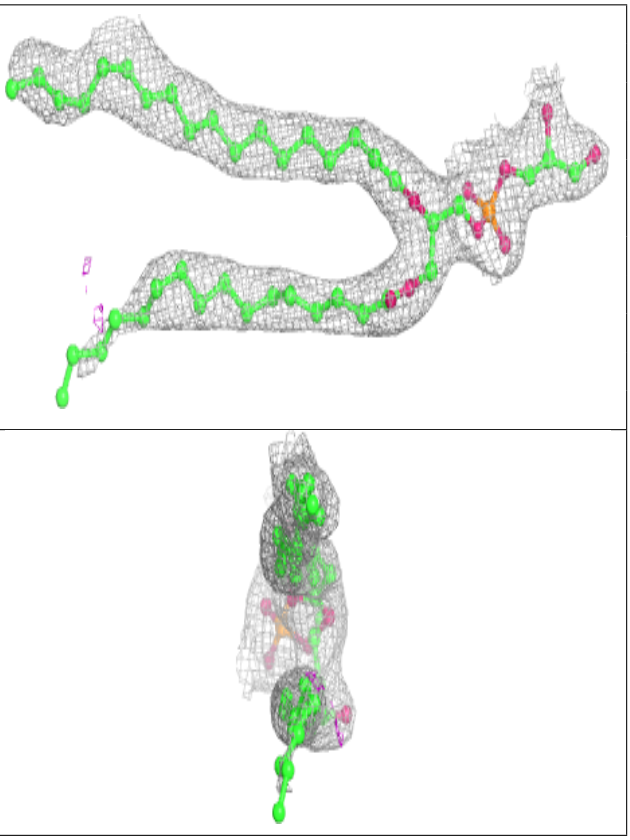
Electron density around CHD P 306:

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



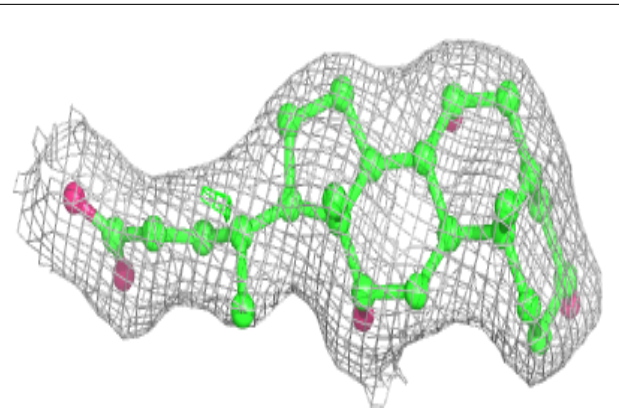
Electron density around PGV C 302:

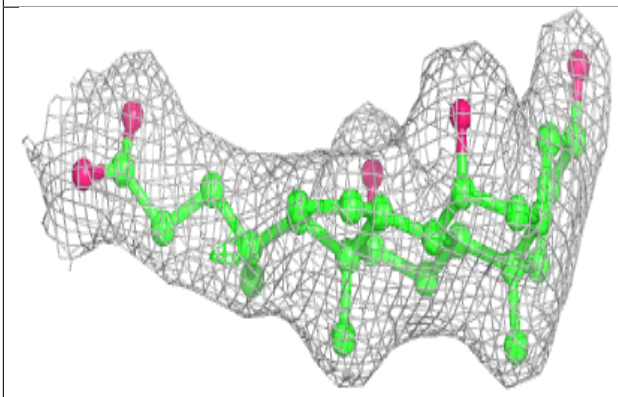
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

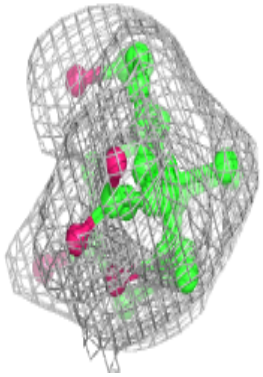


Electron density around CHD C 305:

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

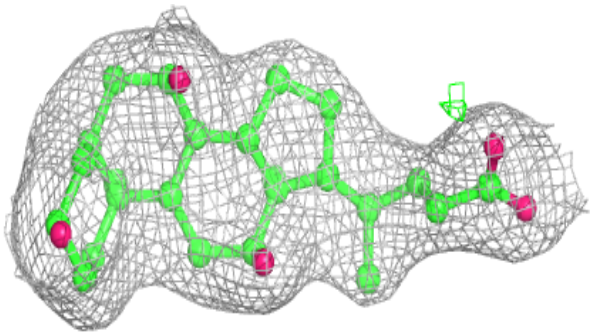


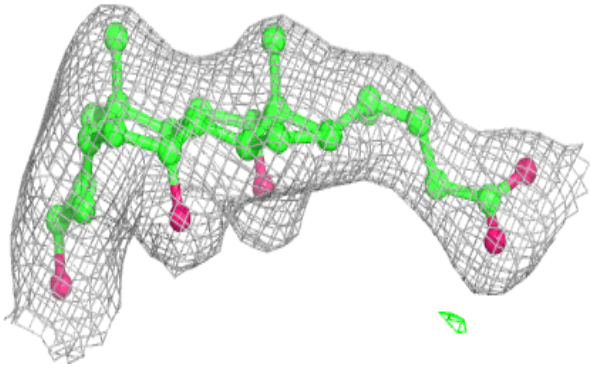


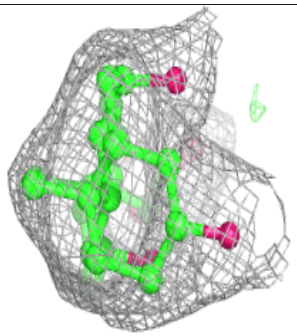


Electron density around CHD G 104:

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

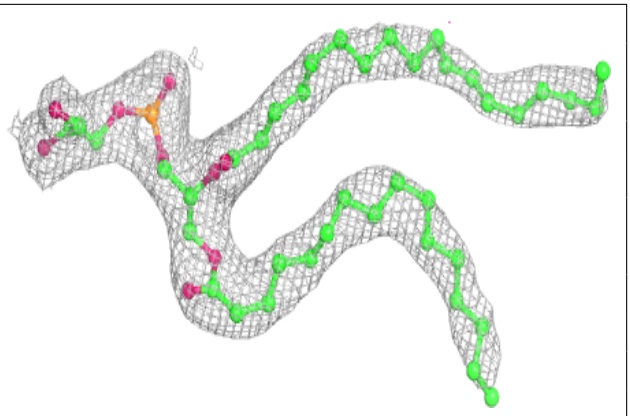


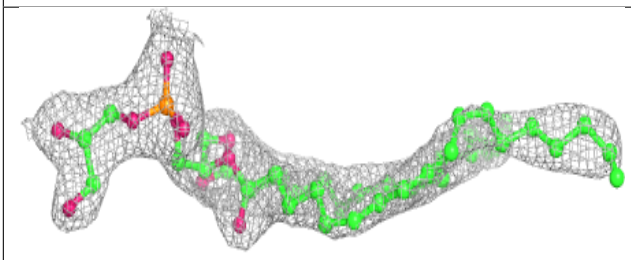


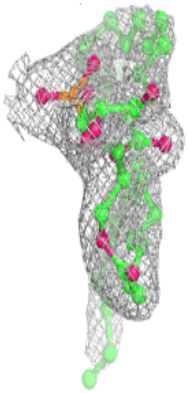


Electron density around PGV A 608:

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

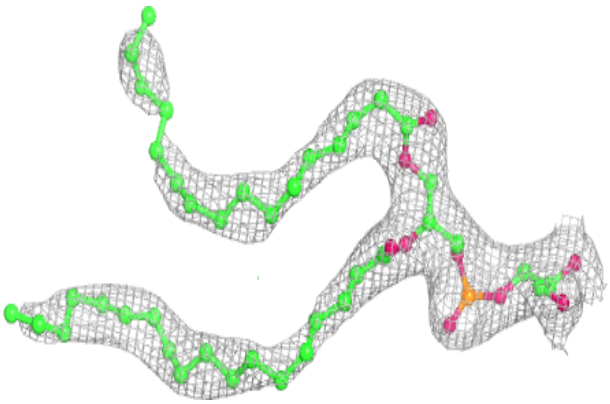


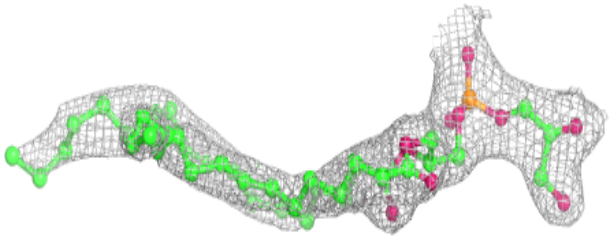


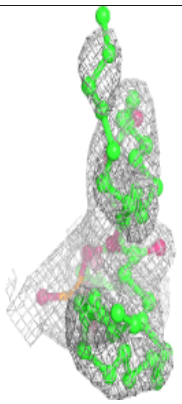


Electron density around PGV N 608:

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

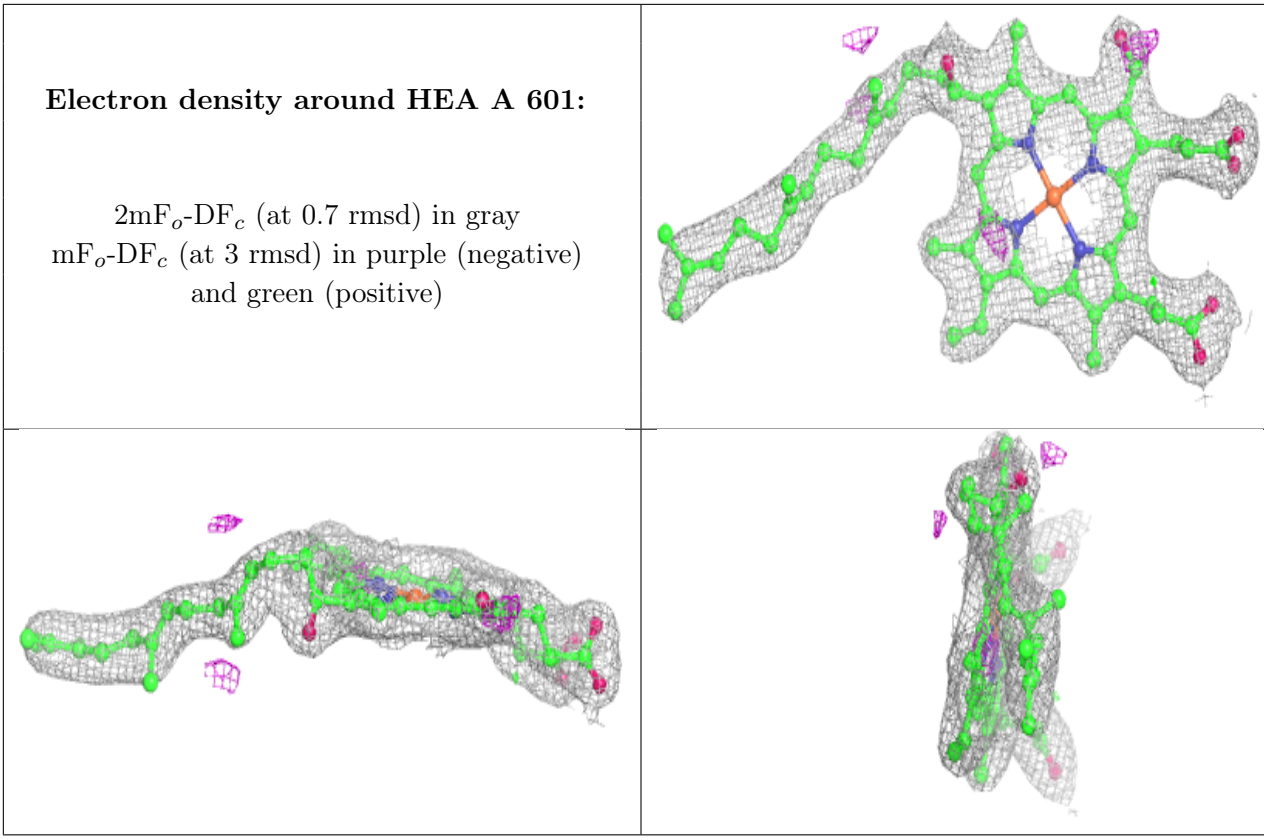






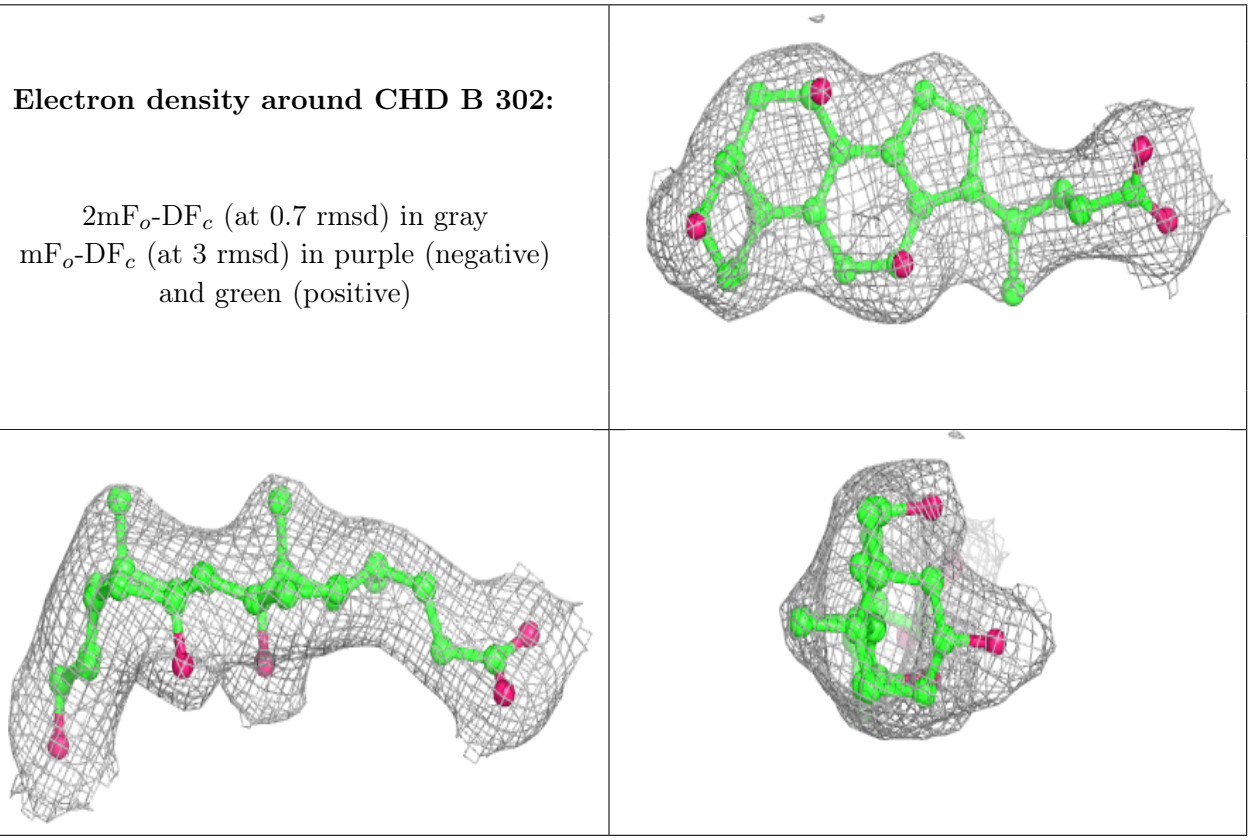
Electron density around HEA A 601:

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



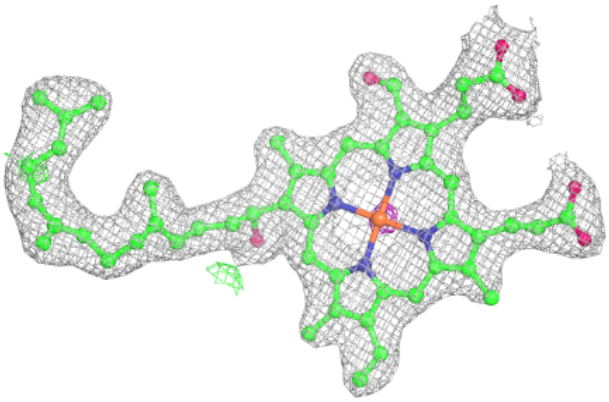
Electron density around CHD B 302:

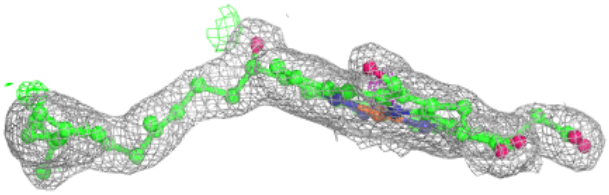
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

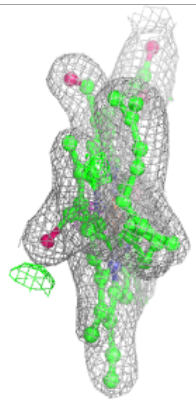


Electron density around HEA A 602:

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

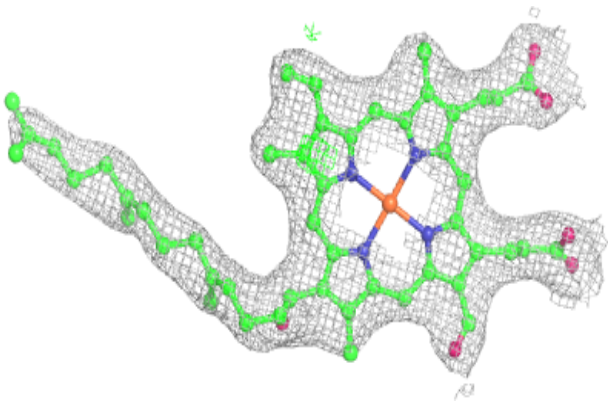


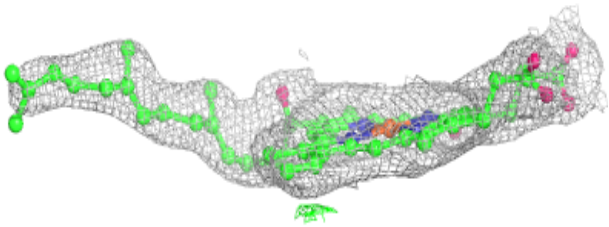


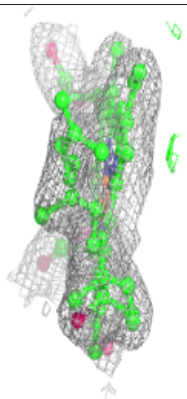


Electron density around HEA N 601:

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

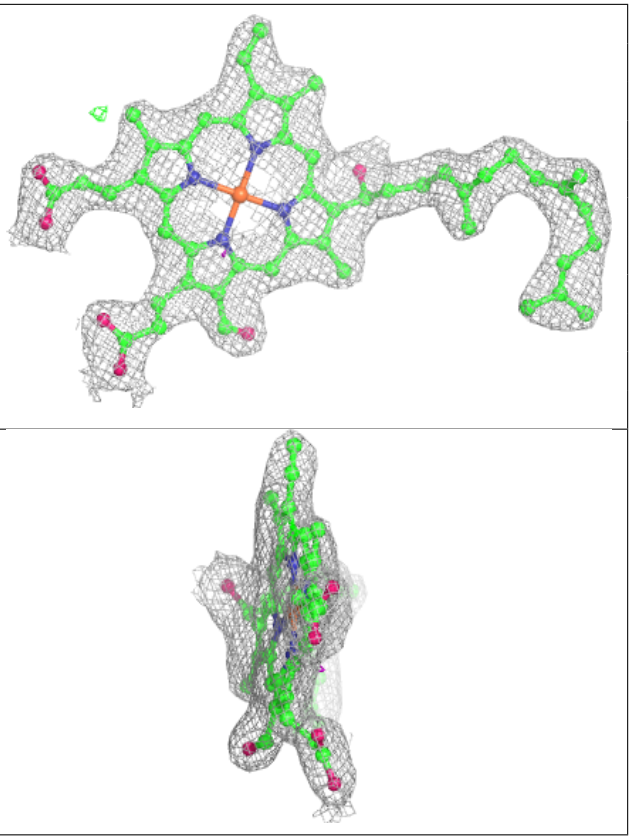






Electron density around HEA N 602:

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



6.5 Other polymers (i)

There are no such residues in this entry.