wwPDB X-ray Structure Validation Summary Report (i)

Aug 7, 2026 – 07:55 AM JST

PDB ID	:	8IJN / pdb_00008ijn
Title	:	Bovine Heart Cytochrome c Oxidase in the Nitric Oxide-Bound Fully Reduced State at 100 K
Authors	:	Tsukihara, T.; Shimada, A.; Muramoto, K.
Deposited on	:	2023-02-27
Resolution	:	1.80 Å(reported)

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

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

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

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

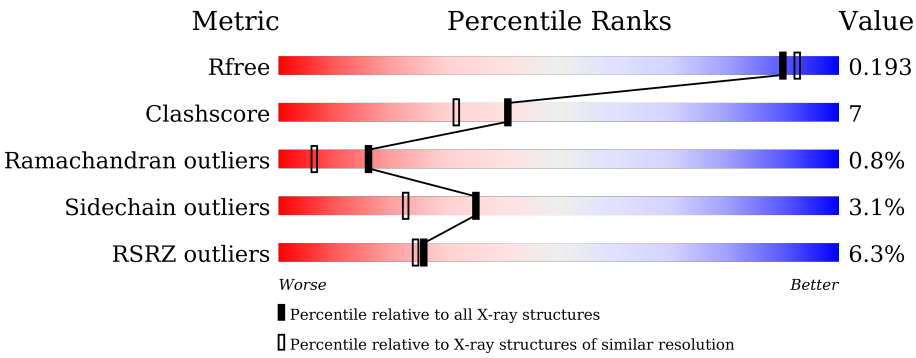
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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

Mol	Chain	Length	Quality of chain
1	A	514	.% 89% 9% •
1	N	514	.% 90% 9% •
2	B	227	5% 83% 15% •
2	O	227	6% 78% 20% •
3	C	261	2% 90% 10% •
3	P	261	.% 89% 11% •

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Mol	Chain	Length	Quality of chain
4	D	147	4% 88% 9%
4	Q	147	12% 90% 8%
5	E	109	4% 91% 5%
5	R	109	4% 90% 5%
6	F	98	10% 87% 10%
6	S	98	9% 89% 7%
7	G	85	27% 76% 18%
7	T	85	24% 72% 16% 9%
8	H	85	15% 81% 8% 7%
8	U	85	18% 81% 8% 7%
9	I	73	11% 89% 10%
9	V	73	15% 86% 14%
10	J	59	8% 88% 10%
10	W	59	8% 90% 7%
11	K	56	7% 82% 5% 12%
11	X	56	12% 79% 7% 12%
12	L	47	6% 85% 13%
12	Y	47	9% 81% 13%
13	M	46	13% 72% 20% 7%
13	Z	46	15% 80% 9% 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
25	CDL	G	102	-	-	X	-

2 Entry composition (i)

There are 29 unique types of molecules in this entry. The entry contains 32780 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	4072	2716	631	687	38	0	10	0
1	N	514	4072	2717	631	686	38	0	9	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	1831	1191	281	341	18	0	2	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	2116	1415	336	351	14	0	3	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.

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	601	390	107	100	4	0	0	0
9	V	73	601	390	107	100	4	0	0	0

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

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

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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.

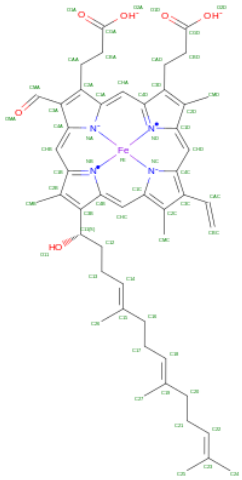
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	L	46	380	254	64	60	2	0	0	0
			Total	C	N	O	S			
12	Y	46	380	254	64	60	2	0	0	0

- 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 (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).

HEA



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
14	A	1	60	49	1	4	6	0	0
			Total	C	Fe	N	O		
14	A	1	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 NITRIC OXIDE (CCD ID: NO) (formula: NO).

NO

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

- Molecule 16 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

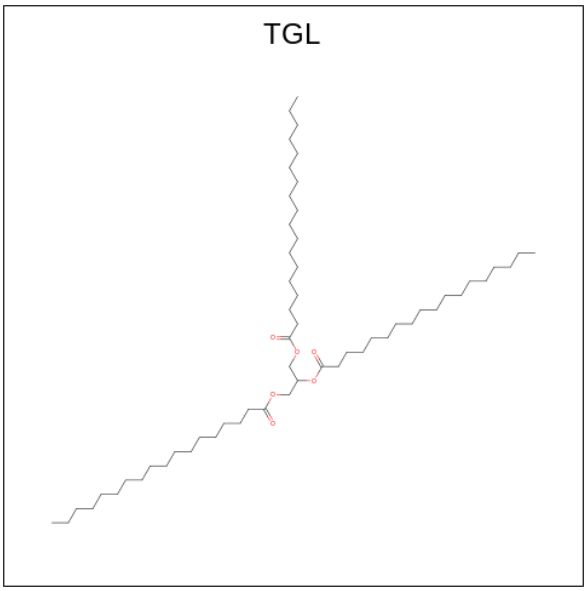
- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 18 is SODIUM ION (CCD ID: NA) (formula: Na).

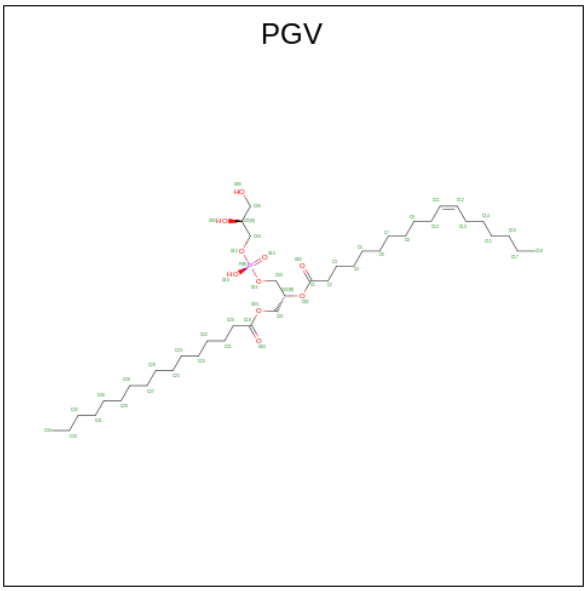
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
18	A	1	1	1	0	0
18	N	1	1	1	0	0

- Molecule 19 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: $C_{57}H_{110}O_6$).



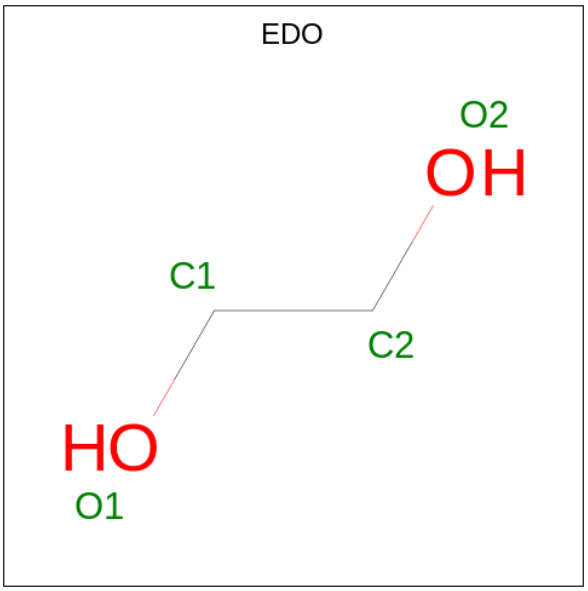
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
19	A	1	63	57	6	0	0
19	D	1	63	57	6	0	0
19	L	1	63	57	6	0	0
19	N	1	63	57	6	0	0
19	O	1	63	57	6	0	0
19	Q	1	63	57	6	0	0

- Molecule 20 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: 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	46	37	8	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 (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

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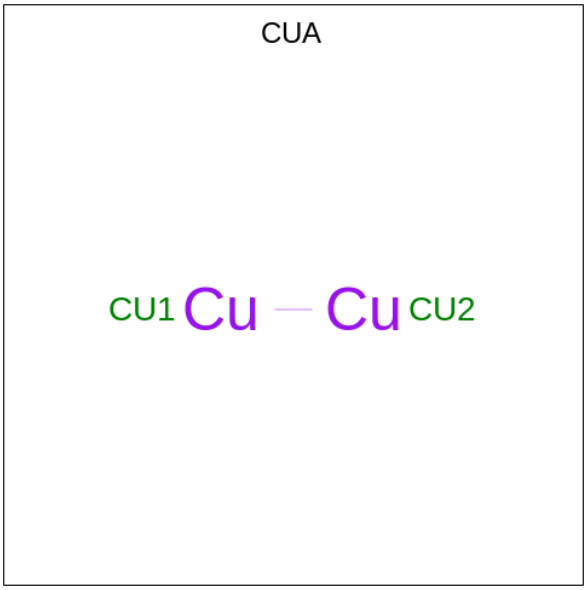
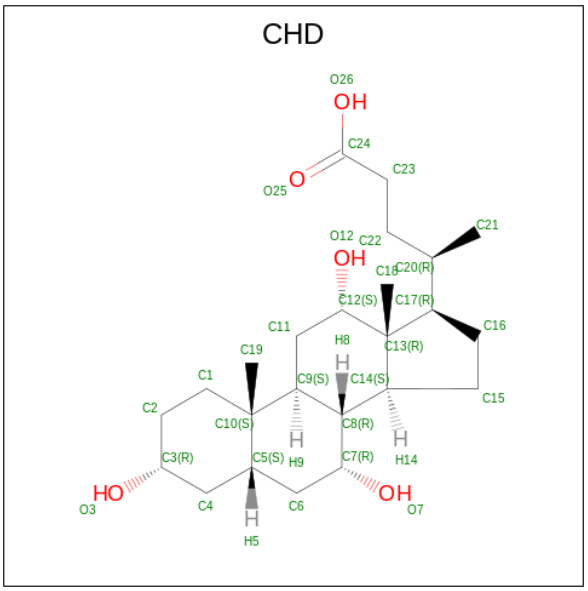
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
21	O	1	4	2	2	0	0
21	P	1	4	2	2	0	0
21	P	1	4	2	2	0	0
21	Q	1	4	2	2	0	0
21	Q	1	4	2	2	0	0
21	S	1	4	2	2	0	0
21	S	1	4	2	2	0	0
21	S	1	4	2	2	0	0

- Molecule 22 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu_2).



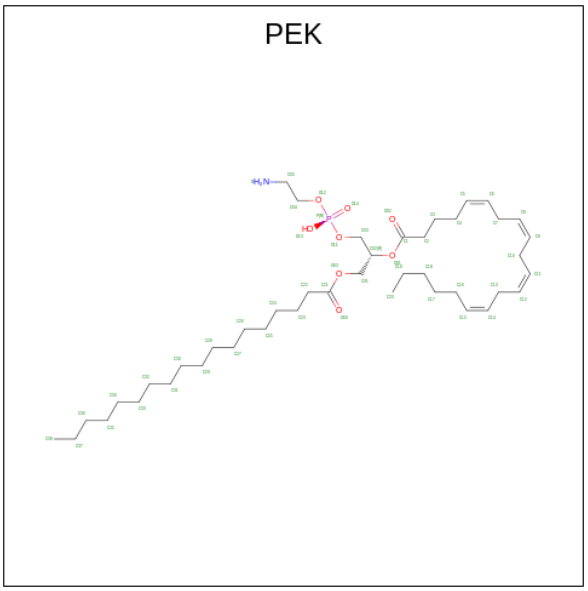
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cu		
22	B	1	2	2	0	0
22	O	1	2	2	0	0

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



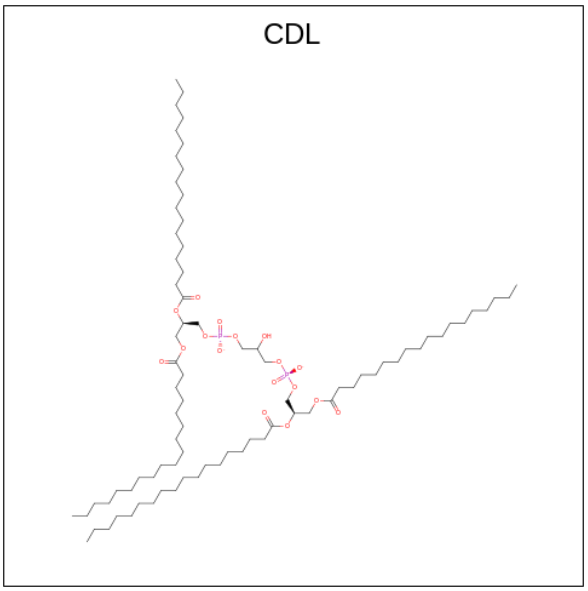
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
23	B	1	29	24	5		0	0
			Total	C	O			
23	C	1	29	24	5		0	0
			Total	C	O			
23	C	1	29	24	5		0	0
			Total	C	O			
23	J	1	29	24	5		0	0
			Total	C	O			
23	O	1	29	24	5		0	0
			Total	C	O			
23	P	1	29	24	5		0	0
			Total	C	O			
23	P	1	29	24	5		0	0
			Total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

- Molecule 24 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (CCD ID: PEK) (formula: $C_{43}H_{78}NO_8P$).



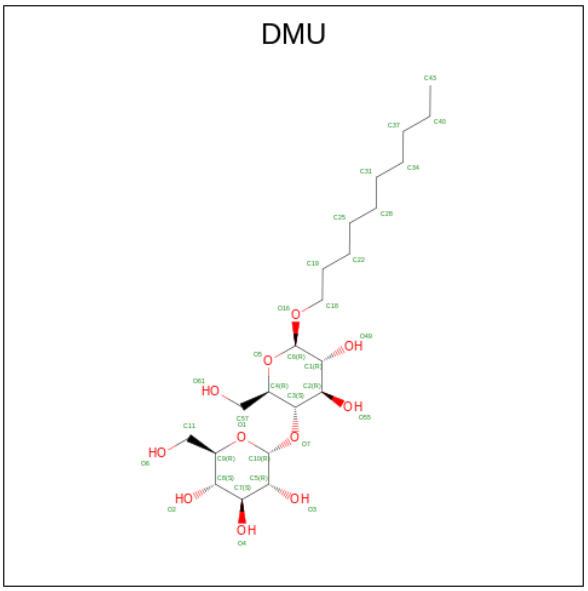
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	C	1	Total C N O P 53 43 1 8 1	0	0
24	G	1	Total C O P 50 41 8 1	0	0
24	G	1	Total C N O P 53 43 1 8 1	0	0
24	P	1	Total C N O P 53 43 1 8 1	0	0
24	T	1	Total C N O P 53 43 1 8 1	0	0
24	T	1	Total C N O P 53 43 1 8 1	0	0

- Molecule 25 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



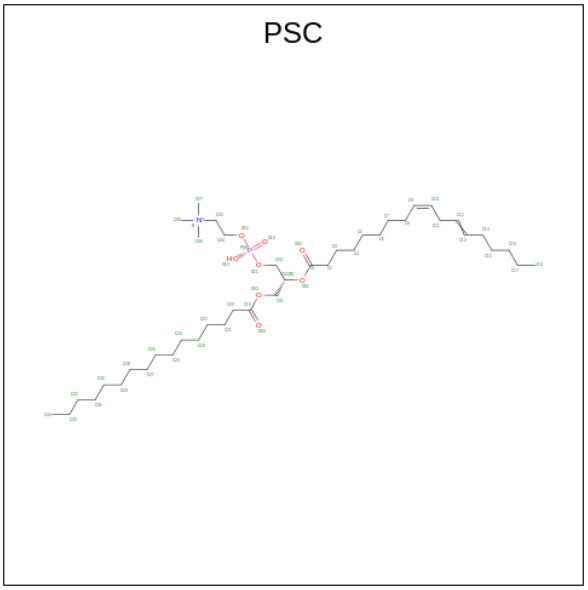
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	C	1	Total	C	O	P	0	0
			100	81	17	2		
25	G	1	Total	C	O	P	0	0
			100	81	17	2		
25	P	1	Total	C	O	P	0	0
			100	81	17	2		
25	T	1	Total	C	O	P	0	0
			100	81	17	2		

- Molecule 26 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: $C_{22}H_{42}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
26	C	1	33	22	11	0	0
			Total	C	O		
26	M	1	33	22	11	0	0
			Total	C	O		
26	O	1	22	16	6	0	0
			Total	C	O		
26	P	1	33	22	11	0	0
			Total	C	O		
26	W	1	32	21	11	0	0
			Total	C	O		
26	Z	1	33	22	11	0	0

- Molecule 27 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (CCD ID: PSC) (formula: $C_{42}H_{81}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
27	E	1	52	42	1	8	1	0	0
			Total	C	N	O	P		
27	R	1	52	42	1	8	1	0	0

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

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

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

- Molecule 29 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
29	A	229	229	229	0	0
29	B	148	149	149	0	1
29	C	120	120	120	0	0
29	D	79	79	79	0	0
29	E	48	48	48	0	0
29	F	68	68	68	0	0
29	G	48	48	48	0	0
29	H	51	51	51	0	0
29	I	39	39	39	0	0
29	J	26	26	26	0	0
29	K	30	30	30	0	0
29	L	23	23	23	0	0
29	M	24	24	24	0	0
29	N	231	231	231	0	0
29	O	146	146	146	0	2
29	P	106	106	106	0	0
29	Q	59	59	59	0	0
29	R	55	55	55	0	0

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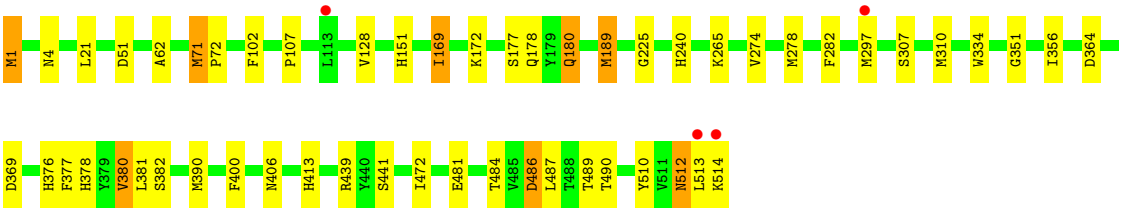
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
29	S	72	72	72	0	0
			Total	O		
29	T	51	51	51	0	0
			Total	O		
29	U	48	48	48	0	0
			Total	O		
29	V	29	29	29	0	0
			Total	O		
29	W	22	22	22	0	0
			Total	O		
29	X	22	22	22	0	0
			Total	O		
29	Y	17	17	17	0	0
			Total	O		
29	Z	17	17	17	0	0

3 Residue-property plots (i)

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

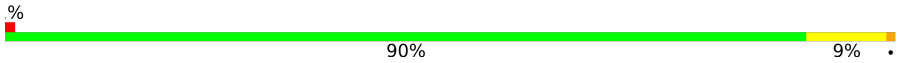
• Molecule 1: Cytochrome c oxidase subunit 1

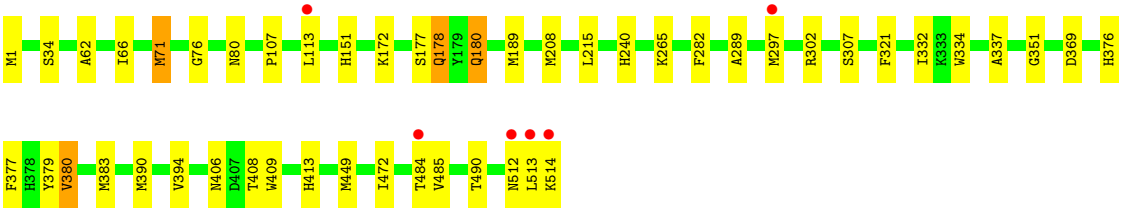
Chain A:



• Molecule 1: Cytochrome c oxidase subunit 1

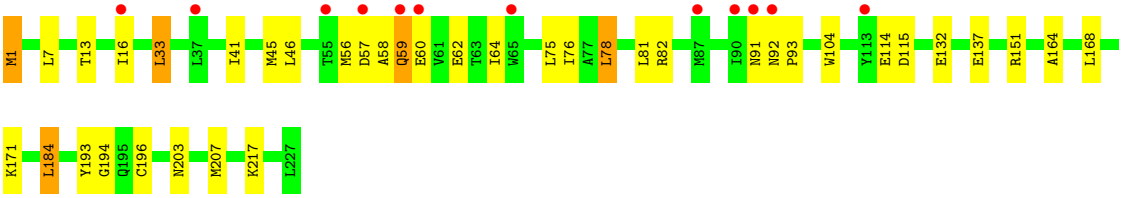
Chain N:





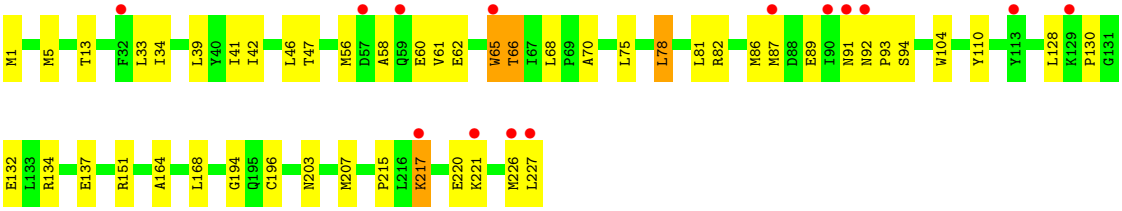
• Molecule 2: Cytochrome c oxidase subunit 2

Chain B:

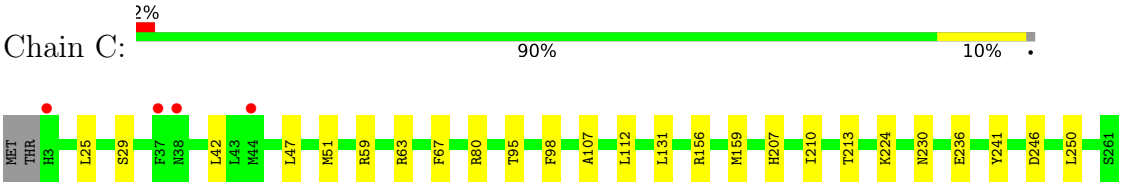


• Molecule 2: Cytochrome c oxidase subunit 2

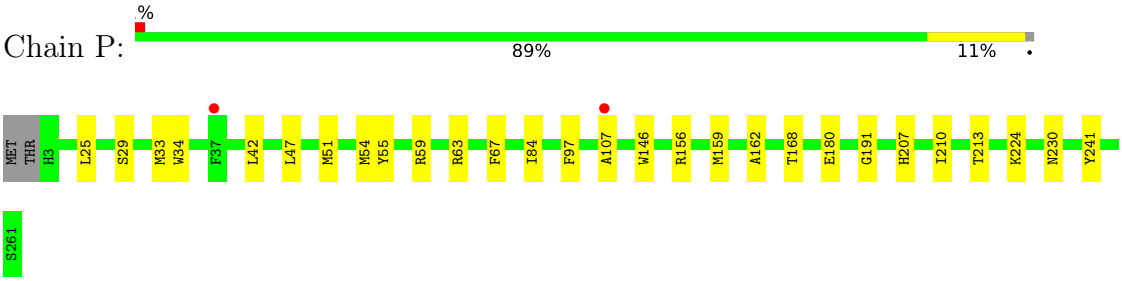
Chain O:



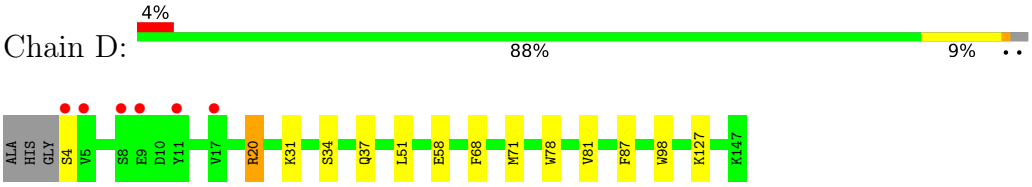
• Molecule 3: Cytochrome c oxidase subunit 3



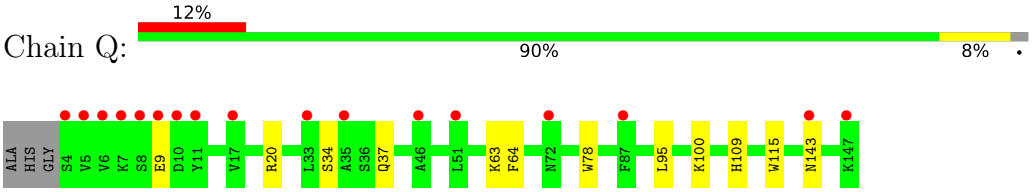
• Molecule 3: Cytochrome c oxidase subunit 3



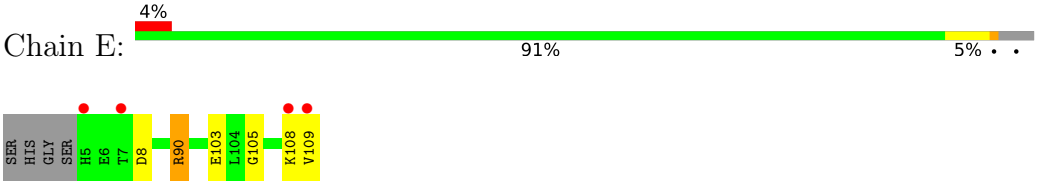
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



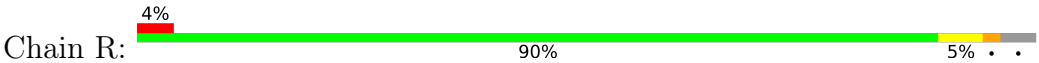
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

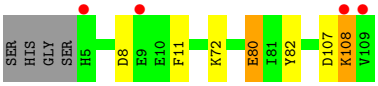


• Molecule 5: Cytochrome c oxidase subunit 5A



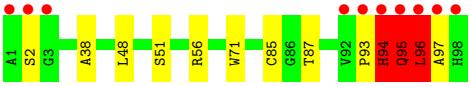
• Molecule 5: Cytochrome c oxidase subunit 5A





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

Chain F:

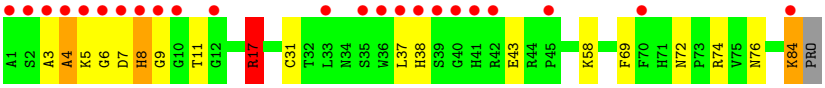


• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

Chain S:

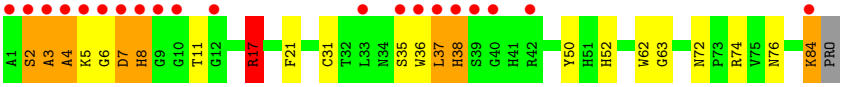
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain G:



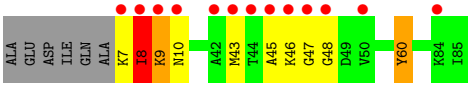
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain T:



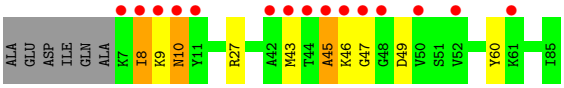
• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain H:



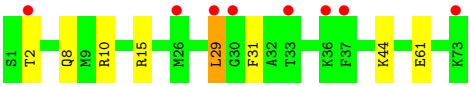
• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain U:



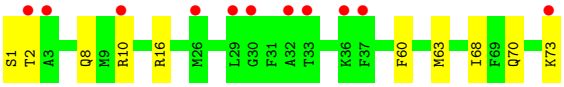
• Molecule 9: Cytochrome c oxidase subunit 6C

Chain I:



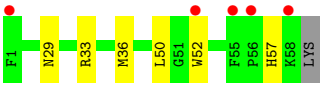
• Molecule 9: Cytochrome c oxidase subunit 6C

Chain V:



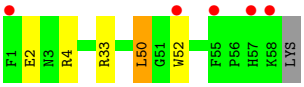
• Molecule 10: Cytochrome c oxidase subunit 7A1

Chain J:



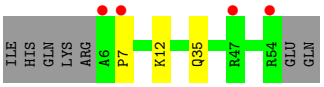
• Molecule 10: Cytochrome c oxidase subunit 7A1

Chain W:



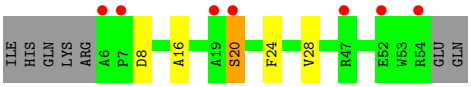
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

Chain K:



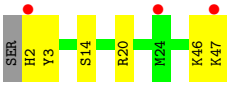
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

Chain X:



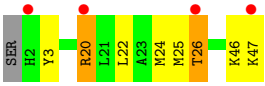
• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain L:



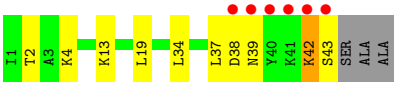
• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain Y:



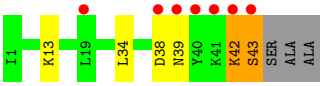
• Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

Chain M:



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

Chain Z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	182.29Å 208.36Å 177.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.37 – 1.80 35.37 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (35.37-1.80) 99.6 (35.37-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.29 (at 1.80Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.169 , 0.192 0.169 , 0.193	Depositor DCC
R_{free} test set	30652 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	28.1	Xtriage
Anisotropy	0.505	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 62.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.007 for l,-k,h	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	32780	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HEA, CU, NO, CUA, EDO, CHD, PGV, SAC, TGL, NA, TPO, PEK, DMU, CDL, ZN, MG, FME, PSC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	1.08	2/4230 (0.0%)	0.92	4/5775 (0.1%)
1	N	0.90	1/4224 (0.0%)	0.85	2/5767 (0.0%)
2	B	0.96	0/1878	0.96	5/2558 (0.2%)
2	O	0.74	0/1860	0.86	1/2534 (0.0%)
3	C	0.87	0/2219	0.79	0/3033
3	P	0.80	0/2197	0.75	0/3005
4	D	0.78	0/1229	0.77	0/1658
4	Q	0.56	0/1229	0.63	0/1658
5	E	0.74	0/871	0.72	0/1182
5	R	0.59	0/871	0.67	0/1182
6	F	0.84	1/765 (0.1%)	0.87	0/1038
6	S	0.69	0/765	0.83	2/1038 (0.2%)
7	G	0.81	0/690	0.87	2/937 (0.2%)
7	T	0.73	0/690	0.85	2/937 (0.2%)
8	H	0.73	0/682	0.77	0/921
8	U	0.60	0/682	0.76	0/921
9	I	0.62	0/605	0.69	0/802
9	V	0.56	0/605	0.70	0/802
10	J	0.68	0/471	0.66	0/636
10	W	0.53	0/471	0.62	0/636
11	K	0.72	0/398	0.77	0/546
11	X	0.46	0/398	0.54	0/546
12	L	0.83	0/393	0.86	0/526
12	Y	0.63	0/393	0.64	0/526
13	M	0.81	0/345	0.71	0/470
13	Z	0.54	0/345	0.57	0/470
All	All	0.83	4/29506 (0.0%)	0.81	18/40104 (0.0%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	F	0	1
6	S	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	189	MET	CB-CG	5.52	1.69	1.52
1	A	439	ARG	CD-NE	5.46	1.53	1.46
6	F	56	ARG	CZ-NH1	5.32	1.40	1.32
1	A	512	ASN	CB-CG	-5.02	1.39	1.52

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	71	MET	CG-SD-CE	-11.39	75.84	100.90
1	N	71	MET	CG-SD-CE	-9.19	80.68	100.90
1	A	189	MET	CG-SD-CE	-7.36	84.72	100.90
1	A	240	HIS	CA-CB-CG	-6.87	106.93	113.80
7	T	17	ARG	NE-CZ-NH1	6.56	128.06	121.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	F	93	PRO	Peptide
6	S	93	PRO	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4072	0	4041	45	0
1	N	4072	0	4044	47	0
2	B	1831	0	1839	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	O	1824	0	1833	34	0
3	C	2116	0	2034	26	0
3	P	2110	0	2027	33	0
4	D	1195	0	1183	11	0
4	Q	1195	0	1183	10	0
5	E	852	0	845	3	0
5	R	852	0	845	5	1
6	F	748	0	728	7	0
6	S	748	0	728	12	0
7	G	675	0	643	18	0
7	T	675	0	643	28	0
8	H	662	0	623	7	0
8	U	662	0	623	6	0
9	I	601	0	613	5	1
9	V	601	0	613	7	0
10	J	460	0	459	4	0
10	W	460	0	459	4	0
11	K	384	0	366	2	0
11	X	384	0	366	4	0
12	L	380	0	380	7	0
12	Y	380	0	380	8	0
13	M	335	0	352	6	0
13	Z	335	0	352	2	0
14	A	120	0	108	5	0
14	N	120	0	108	5	0
15	A	2	0	0	0	0
15	N	2	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	1	0	0	0	0
18	N	1	0	0	0	0
19	A	63	0	110	3	0
19	D	63	0	110	8	0
19	L	63	0	110	8	0
19	N	63	0	110	8	0
19	O	63	0	110	0	0
19	Q	63	0	110	9	0
20	A	102	0	152	4	0
20	C	102	0	152	9	0
20	N	97	0	145	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	P	102	0	152	6	0
21	A	16	0	24	1	0
21	B	4	0	6	0	0
21	C	4	0	6	0	0
21	F	4	0	6	0	0
21	N	24	0	36	2	0
21	O	8	0	12	0	0
21	P	8	0	12	1	0
21	Q	8	0	12	0	0
21	S	12	0	18	0	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	3	0
23	J	29	0	38	2	0
23	O	29	0	39	2	0
23	P	58	0	78	1	0
23	W	29	0	38	1	0
24	C	53	0	77	6	0
24	G	103	0	148	5	0
24	P	53	0	77	6	0
24	T	106	0	154	10	0
25	C	100	0	153	15	0
25	G	100	0	156	23	0
25	P	100	0	156	19	0
25	T	100	0	156	14	0
26	C	33	0	42	2	0
26	M	33	0	42	1	0
26	O	22	0	31	1	0
26	P	33	0	42	8	0
26	W	32	0	36	4	0
26	Z	33	0	42	1	0
27	E	52	0	80	12	0
27	R	52	0	80	10	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	A	229	0	0	2	0
29	B	149	0	0	3	0
29	C	120	0	0	1	0
29	D	79	0	0	1	0
29	E	48	0	0	0	0
29	F	68	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	G	48	0	0	1	0
29	H	51	0	0	0	0
29	I	39	0	0	2	0
29	J	26	0	0	0	0
29	K	30	0	0	1	0
29	L	23	0	0	0	0
29	M	24	0	0	0	0
29	N	231	0	0	4	0
29	O	146	0	0	1	0
29	P	106	0	0	2	0
29	Q	59	0	0	2	0
29	R	55	0	0	1	0
29	S	72	0	0	1	0
29	T	51	0	0	0	0
29	U	48	0	0	1	0
29	V	29	0	0	0	0
29	W	22	0	0	1	0
29	X	22	0	0	2	0
29	Y	17	0	0	1	0
29	Z	17	0	0	0	0
All	All	32780	0	31593	408	1

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 7.

The worst 5 of 408 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:94:HIS:CD2	6:S:95:GLN:H	1.72	1.05
21:N:614:EDO:O2	29:N:701:HOH:O	1.80	0.99
6:S:94:HIS:NE2	29:S:201:HOH:O	1.97	0.96
7:T:17:ARG:HH22	24:T:101:PEK:H041	1.27	0.96
6:S:94:HIS:HD2	6:S:95:GLN:H	1.09	0.89

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:2:THR:OG1	5:R:80:GLU:OE1[3_647]	2.17	0.03

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	522/514 (102%)	509 (98%)	13 (2%)	0	100	100
1	N	521/514 (101%)	509 (98%)	12 (2%)	0	100	100
2	B	227/227 (100%)	222 (98%)	4 (2%)	1 (0%)	30	19
2	O	225/227 (99%)	217 (96%)	6 (3%)	2 (1%)	14	5
3	C	260/261 (100%)	255 (98%)	5 (2%)	0	100	100
3	P	257/261 (98%)	252 (98%)	5 (2%)	0	100	100
4	D	142/147 (97%)	139 (98%)	3 (2%)	0	100	100
4	Q	142/147 (97%)	136 (96%)	6 (4%)	0	100	100
5	E	103/109 (94%)	103 (100%)	0	0	100	100
5	R	103/109 (94%)	103 (100%)	0	0	100	100
6	F	96/98 (98%)	90 (94%)	2 (2%)	4 (4%)	2	0
6	S	96/98 (98%)	90 (94%)	3 (3%)	3 (3%)	3	0
7	G	81/85 (95%)	69 (85%)	7 (9%)	5 (6%)	1	0
7	T	81/85 (95%)	69 (85%)	7 (9%)	5 (6%)	1	0
8	H	77/85 (91%)	70 (91%)	4 (5%)	3 (4%)	2	0
8	U	77/85 (91%)	70 (91%)	3 (4%)	4 (5%)	1	0
9	I	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
9	V	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	W	56/59 (95%)	56 (100%)	0	0	100	100
11	K	47/56 (84%)	47 (100%)	0	0	100	100
11	X	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
12	L	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
12	Y	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
13	M	41/46 (89%)	40 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	Z	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
All	All	3528/3614 (98%)	3410 (97%)	91 (3%)	27 (1%)	16	6

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	2	SER
6	F	94	HIS
6	F	95	GLN
7	G	4	ALA
7	G	7	ASP

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	435/426 (102%)	427 (98%)	8 (2%)	51	43
1	N	434/426 (102%)	426 (98%)	8 (2%)	51	43
2	B	212/210 (101%)	202 (95%)	10 (5%)	23	11
2	O	210/210 (100%)	200 (95%)	10 (5%)	23	11
3	C	227/226 (100%)	225 (99%)	2 (1%)	70	67
3	P	224/226 (99%)	221 (99%)	3 (1%)	61	54
4	D	128/129 (99%)	123 (96%)	5 (4%)	28	16
4	Q	128/129 (99%)	126 (98%)	2 (2%)	55	47
5	E	92/95 (97%)	90 (98%)	2 (2%)	45	34
5	R	92/95 (97%)	90 (98%)	2 (2%)	45	34
6	F	81/81 (100%)	77 (95%)	4 (5%)	22	10
6	S	81/81 (100%)	78 (96%)	3 (4%)	30	18
7	G	67/68 (98%)	63 (94%)	4 (6%)	17	7
7	T	67/68 (98%)	60 (90%)	7 (10%)	7	2
8	H	71/75 (95%)	69 (97%)	2 (3%)	38	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	U	71/75 (95%)	69 (97%)	2 (3%)	38	26
9	I	57/57 (100%)	53 (93%)	4 (7%)	14	4
9	V	57/57 (100%)	54 (95%)	3 (5%)	20	9
10	J	49/50 (98%)	48 (98%)	1 (2%)	48	38
10	W	49/50 (98%)	48 (98%)	1 (2%)	48	38
11	K	39/46 (85%)	39 (100%)	0	100	100
11	X	39/46 (85%)	38 (97%)	1 (3%)	40	28
12	L	39/40 (98%)	39 (100%)	0	100	100
12	Y	39/40 (98%)	37 (95%)	2 (5%)	21	9
13	M	37/38 (97%)	33 (89%)	4 (11%)	6	1
13	Z	37/38 (97%)	32 (86%)	5 (14%)	4	1
All	All	3062/3082 (99%)	2967 (97%)	95 (3%)	35	23

5 of 95 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	O	68	LEU
6	S	37	LYS
2	O	78	LEU
3	P	180	GLU
7	T	17	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
2	O	91	ASN
4	Q	37	GLN
2	O	181	GLN
3	P	76	GLN
4	Q	109	HIS

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	$\#\|Z\| > 2$
1	FME	A	1	1	8,9,10	0.55	0	7,9,11	1.84	1 (14%)
2	FME	O	1	2	8,9,10	1.25	2 (25%)	7,9,11	4.10	2 (28%)
2	FME	B	1	2	8,9,10	2.14	3 (37%)	7,9,11	3.73	4 (57%)
1	FME	N	1	1	8,9,10	0.48	0	7,9,11	1.29	0
7	TPO	T	11	7	8,10,11	1.61	2 (25%)	10,14,16	1.34	1 (10%)
9	SAC	I	1	9	7,8,9	0.57	0	8,9,11	0.76	0
9	SAC	V	1	9	7,8,9	0.61	0	8,9,11	1.81	2 (25%)
7	TPO	G	11	7	8,10,11	1.55	2 (25%)	10,14,16	1.37	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
1	FME	A	1	1	-	4/7/9/11	-
2	FME	O	1	2	-	2/7/9/11	-
2	FME	B	1	2	-	1/7/9/11	-
1	FME	N	1	1	-	5/7/9/11	-
7	TPO	T	11	7	-	3/9/11/13	-
9	SAC	I	1	9	-	4/7/8/10	-
9	SAC	V	1	9	-	6/7/8/10	-
7	TPO	G	11	7	-	3/9/11/13	-

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	CA-N	4.01	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	CN-N	3.66	1.45	1.33
7	T	11	TPO	P-O1P	2.94	1.60	1.50
7	G	11	TPO	P-O1P	2.94	1.60	1.50
2	O	1	FME	O1-CN	-2.54	1.15	1.22

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	O	1	FME	CA-N-CN	-10.11	107.27	122.82
2	B	1	FME	C-CA-N	7.67	123.58	109.73
2	B	1	FME	CA-N-CN	-3.91	116.80	122.82
7	G	11	TPO	CG2-CB-CA	3.73	120.52	113.16
2	B	1	FME	CG-CB-CA	-3.59	102.96	112.95

There are no chirality outliers.

5 of 28 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-CG2
7	G	11	TPO	N-CA-CB-OG1

There are no ring outliers.

3 monomers are involved in 4 short contacts:

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 78 ligands modelled in this entry, 8 are monoatomic - leaving 70 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
21	EDO	B	303	-	3,3,3	0.73	0	2,2,2	0.55	0
14	HEA	A	602	1,15	66,67,67	1.93	20 (30%)	78,103,103	2.09	31 (39%)
21	EDO	S	103	-	3,3,3	0.55	0	2,2,2	0.55	0
22	CUA	O	301	2	0,1,1	-	-	-		
23	CHD	B	302	-	32,32,32	0.92	1 (3%)	51,51,51	1.51	11 (21%)
26	DMU	O	304	-	22,22,34	0.74	0	27,27,45	1.73	6 (22%)
20	PGV	N	609	-	50,50,50	1.05	3 (6%)	53,56,56	1.12	4 (7%)
23	CHD	P	301	-	32,32,32	1.00	2 (6%)	51,51,51	1.38	7 (13%)
21	EDO	S	102	-	3,3,3	1.09	0	2,2,2	0.62	0
20	PGV	A	608	-	50,50,50	1.02	6 (12%)	53,56,56	1.23	5 (9%)
14	HEA	N	601	1	66,67,67	1.79	18 (27%)	78,103,103	1.88	25 (32%)
20	PGV	C	303	-	50,50,50	0.89	2 (4%)	53,56,56	1.11	5 (9%)
23	CHD	O	302	-	32,32,32	1.00	1 (3%)	51,51,51	1.48	6 (11%)
21	EDO	Q	203	-	3,3,3	0.17	0	2,2,2	0.81	0
25	CDL	C	305	3	99,99,99	1.35	13 (13%)	105,111,111	1.56	13 (12%)
14	HEA	N	602	1,15	66,67,67	1.78	22 (33%)	78,103,103	1.79	24 (30%)
26	DMU	P	307	-	34,34,34	0.87	1 (2%)	45,45,45	2.03	11 (24%)
21	EDO	Q	202	-	3,3,3	0.36	0	2,2,2	0.42	0
24	PEK	G	101	-	49,49,52	1.09	3 (6%)	53,54,57	1.32	4 (7%)
20	PGV	P	304	-	50,50,50	1.03	2 (4%)	53,56,56	1.44	6 (11%)
26	DMU	M	101	-	34,34,34	0.60	1 (2%)	45,45,45	0.96	2 (4%)
19	TGL	O	303	-	62,62,62	1.06	3 (4%)	65,65,65	1.16	4 (6%)
21	EDO	C	308	-	3,3,3	0.34	0	2,2,2	0.92	0
23	CHD	J	101	-	32,32,32	0.70	0	51,51,51	1.83	13 (25%)
26	DMU	Z	101	-	34,34,34	0.43	0	45,45,45	0.84	1 (2%)
24	PEK	P	302	-	52,52,52	0.74	1 (1%)	55,57,57	1.67	5 (9%)
24	PEK	G	103	-	52,52,52	1.03	2 (3%)	55,57,57	1.49	5 (9%)
20	PGV	P	303	-	50,50,50	0.71	1 (2%)	53,56,56	1.13	7 (13%)
19	TGL	N	607	-	62,62,62	1.14	3 (4%)	65,65,65	1.33	11 (16%)
21	EDO	N	612	-	3,3,3	0.47	0	2,2,2	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
25	CDL	G	102	-	99,99,99	1.35	12 (12%)	105,111,111	1.49	12 (11%)
26	DMU	C	307	-	34,34,34	0.77	1 (2%)	45,45,45	1.64	10 (22%)
15	NO	A	603	14,16	0,1,1	-	-	-		
26	DMU	W	102	-	33,33,34	0.86	1 (3%)	44,44,45	2.36	17 (38%)
19	TGL	Q	201	-	62,62,62	1.03	3 (4%)	65,65,65	0.98	3 (4%)
21	EDO	A	610	-	3,3,3	1.09	0	2,2,2	0.88	0
14	HEA	A	601	1	66,67,67	1.80	19 (28%)	78,103,103	2.00	20 (25%)
21	EDO	A	611	-	3,3,3	0.92	0	2,2,2	0.70	0
21	EDO	N	610	-	3,3,3	0.79	0	2,2,2	0.50	0
21	EDO	N	615	-	3,3,3	0.64	0	2,2,2	0.27	0
21	EDO	P	309	-	3,3,3	0.79	0	2,2,2	0.39	0
23	CHD	P	306	-	32,32,32	0.64	0	51,51,51	1.25	3 (5%)
25	CDL	P	305	-	99,99,99	1.36	13 (13%)	105,111,111	1.61	14 (13%)
25	CDL	T	103	-	99,99,99	1.31	12 (12%)	105,111,111	1.48	10 (9%)
21	EDO	A	613	-	3,3,3	0.48	0	2,2,2	0.30	0
15	NO	N	603	14,16	0,1,1	-	-	-		
20	PGV	C	304	-	50,50,50	1.00	2 (4%)	53,56,56	1.46	6 (11%)
21	EDO	O	305	-	3,3,3	0.90	0	2,2,2	0.25	0
21	EDO	N	614	-	3,3,3	0.71	0	2,2,2	0.47	0
27	PSC	E	201	-	51,51,51	1.08	3 (5%)	57,59,59	1.20	4 (7%)
21	EDO	O	306	-	3,3,3	0.53	0	2,2,2	0.13	0
21	EDO	A	612	-	3,3,3	0.64	0	2,2,2	0.27	0
21	EDO	S	104	-	3,3,3	0.66	0	2,2,2	0.36	0
19	TGL	L	101	-	62,62,62	1.16	3 (4%)	65,65,65	1.67	10 (15%)
19	TGL	D	201	-	62,62,62	1.11	4 (6%)	65,65,65	1.02	4 (6%)
23	CHD	C	301	-	32,32,32	0.96	2 (6%)	51,51,51	1.61	11 (21%)
24	PEK	C	302	-	52,52,52	0.83	3 (5%)	55,57,57	1.47	10 (18%)
21	EDO	N	613	-	3,3,3	0.46	0	2,2,2	0.59	0
21	EDO	N	611	-	3,3,3	0.73	0	2,2,2	0.83	0
19	TGL	A	607	-	62,62,62	1.06	3 (4%)	65,65,65	1.14	6 (9%)
24	PEK	T	101	-	52,52,52	1.06	2 (3%)	55,57,57	1.30	5 (9%)
27	PSC	R	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.20	5 (8%)
24	PEK	T	102	-	52,52,52	1.02	2 (3%)	55,57,57	1.67	6 (10%)
20	PGV	N	608	-	45,45,50	1.06	2 (4%)	49,50,56	1.53	9 (18%)
23	CHD	C	306	-	32,32,32	0.63	0	51,51,51	1.18	6 (11%)
23	CHD	W	101	-	32,32,32	0.69	0	51,51,51	1.98	14 (27%)
21	EDO	F	102	-	3,3,3	0.99	0	2,2,2	0.65	0
22	CUA	B	301	2	0,1,1	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
20	PGV	A	609	-	50,50,50	1.00	2 (4%)	53,56,56	1.23	6 (11%)
21	EDO	P	308	-	3,3,3	0.48	0	2,2,2	0.69	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	EDO	B	303	-	-	0/1/1/1	-
14	HEA	A	602	1,15	-	5/36/76/76	-
21	EDO	S	103	-	-	0/1/1/1	-
23	CHD	B	302	-	-	2/9/74/74	0/4/4/4
26	DMU	O	304	-	-	6/13/33/59	0/1/1/2
20	PGV	N	609	-	-	8/55/55/55	-
23	CHD	P	301	-	-	2/9/74/74	0/4/4/4
21	EDO	S	102	-	-	0/1/1/1	-
20	PGV	A	608	-	-	8/55/55/55	-
14	HEA	N	601	1	-	7/36/76/76	-
20	PGV	C	303	-	-	6/55/55/55	-
23	CHD	O	302	-	-	2/9/74/74	0/4/4/4
21	EDO	Q	203	-	-	0/1/1/1	-
25	CDL	C	305	3	-	48/110/110/110	-
14	HEA	N	602	1,15	-	5/36/76/76	-
26	DMU	P	307	-	-	10/19/59/59	0/2/2/2
21	EDO	Q	202	-	-	1/1/1/1	-
24	PEK	G	101	-	-	25/51/51/56	-
20	PGV	P	304	-	-	18/55/55/55	-
26	DMU	M	101	-	-	6/19/59/59	0/2/2/2
19	TGL	O	303	-	-	33/65/65/65	-
21	EDO	C	308	-	-	1/1/1/1	-
23	CHD	J	101	-	-	5/9/74/74	0/4/4/4
26	DMU	Z	101	-	-	5/19/59/59	0/2/2/2
24	PEK	P	302	-	-	19/56/56/56	-
24	PEK	G	103	-	-	24/56/56/56	-
20	PGV	P	303	-	-	9/55/55/55	-
19	TGL	N	607	-	-	33/65/65/65	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	EDO	N	612	-	-	0/1/1/1	-
25	CDL	G	102	-	-	50/110/110/110	-
26	DMU	C	307	-	-	7/19/59/59	0/2/2/2
26	DMU	W	102	-	-	5/18/58/59	0/2/2/2
19	TGL	Q	201	-	-	26/65/65/65	-
21	EDO	A	610	-	-	0/1/1/1	-
14	HEA	A	601	1	-	7/36/76/76	-
21	EDO	A	611	-	-	0/1/1/1	-
21	EDO	N	610	-	-	0/1/1/1	-
21	EDO	N	615	-	-	0/1/1/1	-
21	EDO	P	309	-	-	0/1/1/1	-
23	CHD	P	306	-	-	2/9/74/74	0/4/4/4
25	CDL	P	305	-	-	58/110/110/110	-
25	CDL	T	103	-	-	48/110/110/110	-
21	EDO	A	613	-	-	0/1/1/1	-
20	PGV	C	304	-	-	15/55/55/55	-
21	EDO	O	305	-	-	0/1/1/1	-
21	EDO	N	614	-	-	1/1/1/1	-
27	PSC	E	201	-	-	32/55/55/55	-
21	EDO	O	306	-	-	0/1/1/1	-
21	EDO	A	612	-	-	0/1/1/1	-
21	EDO	S	104	-	-	0/1/1/1	-
19	TGL	L	101	-	-	29/65/65/65	-
19	TGL	D	201	-	-	30/65/65/65	-
23	CHD	C	301	-	-	1/9/74/74	0/4/4/4
24	PEK	C	302	-	-	15/56/56/56	-
21	EDO	N	613	-	-	0/1/1/1	-
21	EDO	N	611	-	-	0/1/1/1	-
19	TGL	A	607	-	-	33/65/65/65	-
24	PEK	T	101	-	-	36/56/56/56	-
27	PSC	R	201	-	-	23/55/55/55	-
24	PEK	T	102	-	-	25/56/56/56	-
20	PGV	N	608	-	-	20/47/47/55	-
23	CHD	C	306	-	-	4/9/74/74	0/4/4/4
23	CHD	W	101	-	-	6/9/74/74	0/4/4/4
21	EDO	F	102	-	-	0/1/1/1	-
20	PGV	A	609	-	-	19/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	EDO	P	308	-	-	1/1/1/1	-

The worst 5 of 197 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	N	607	TGL	OG2-CB1	5.33	1.49	1.34
19	L	101	TGL	OG2-CB1	5.22	1.49	1.34
24	T	101	PEK	O03-C21	5.15	1.48	1.33
20	P	304	PGV	O01-C1	5.11	1.48	1.34
14	N	601	HEA	CHA-C1A	5.07	1.48	1.38

The worst 5 of 397 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	P	302	PEK	C2-C3-C4	9.28	129.78	113.23
26	P	307	DMU	C18-O16-C6	8.01	127.12	113.84
14	A	601	HEA	C13-C12-C11	-7.40	103.24	114.35
25	C	305	CDL	CB4-OB6-CB5	-6.83	100.98	117.79
25	P	305	CDL	CB4-OB6-CB5	-6.70	101.29	117.79

There are no chirality outliers.

5 of 781 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	N	601	HEA	C2A-C3A-CMA-OMA
19	A	607	TGL	OG1-CG1-CG2-OG2
19	N	607	TGL	CB2-CB1-OG2-CG2
20	A	609	PGV	C03-O11-P-O13
20	A	609	PGV	C04-O12-P-O11

There are no ring outliers.

44 monomers are involved in 216 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	602	HEA	2	0
23	B	302	CHD	1	0
26	O	304	DMU	1	0
14	N	601	HEA	3	0
20	C	303	PGV	5	0
23	O	302	CHD	2	0
25	C	305	CDL	15	0

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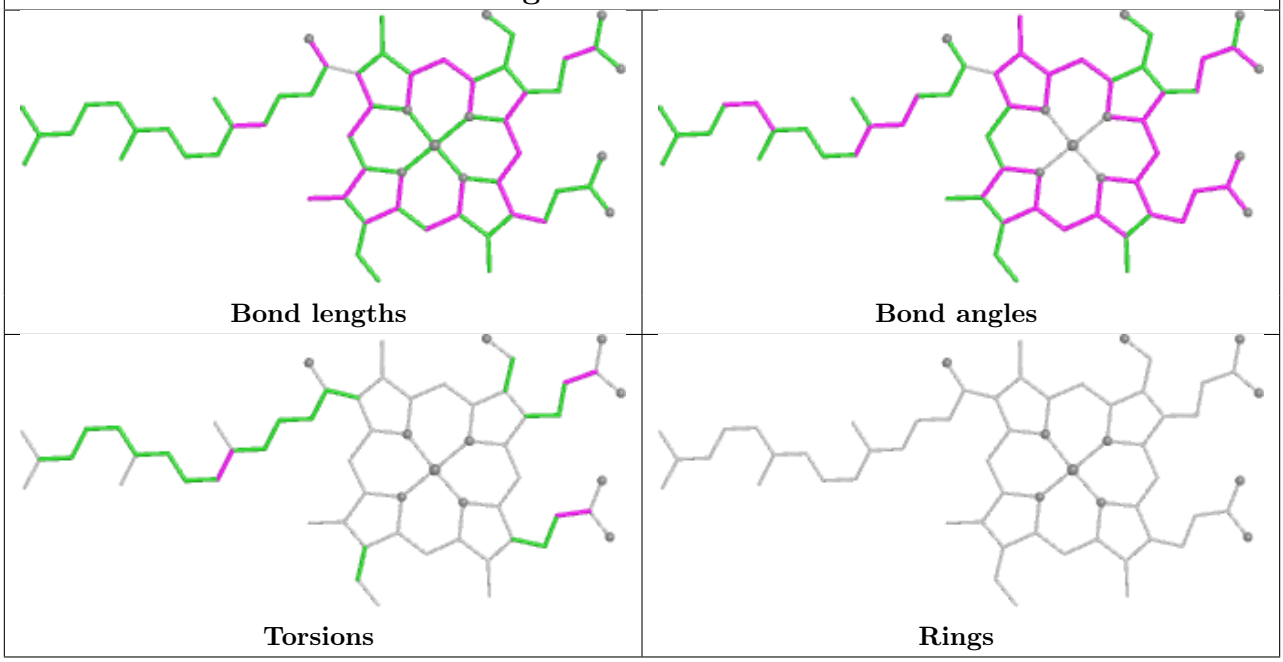
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	N	602	HEA	2	0
26	P	307	DMU	8	0
24	G	101	PEK	1	0
20	P	304	PGV	3	0
26	M	101	DMU	1	0
23	J	101	CHD	2	0
26	Z	101	DMU	1	0
24	P	302	PEK	6	0
24	G	103	PEK	4	0
20	P	303	PGV	3	0
19	N	607	TGL	8	0
25	G	102	CDL	23	0
26	C	307	DMU	2	0
26	W	102	DMU	4	0
19	Q	201	TGL	9	0
14	A	601	HEA	3	0
21	N	615	EDO	1	0
23	P	306	CHD	1	0
25	P	305	CDL	19	0
25	T	103	CDL	14	0
21	A	613	EDO	1	0
20	C	304	PGV	4	0
21	N	614	EDO	1	0
27	E	201	PSC	12	0
19	L	101	TGL	8	0
19	D	201	TGL	8	0
23	C	301	CHD	1	0
24	C	302	PEK	6	0
19	A	607	TGL	3	0
24	T	101	PEK	4	0
27	R	201	PSC	10	0
24	T	102	PEK	6	0
20	N	608	PGV	5	0
23	C	306	CHD	2	0
23	W	101	CHD	1	0
20	A	609	PGV	4	0
21	P	308	EDO	1	0

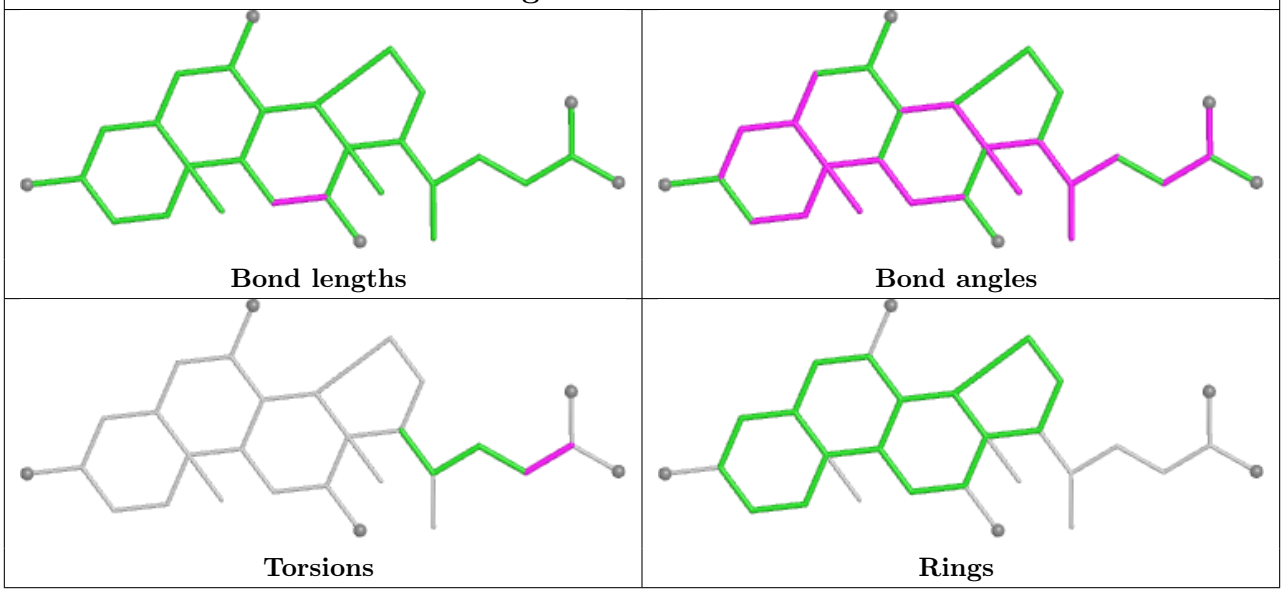
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

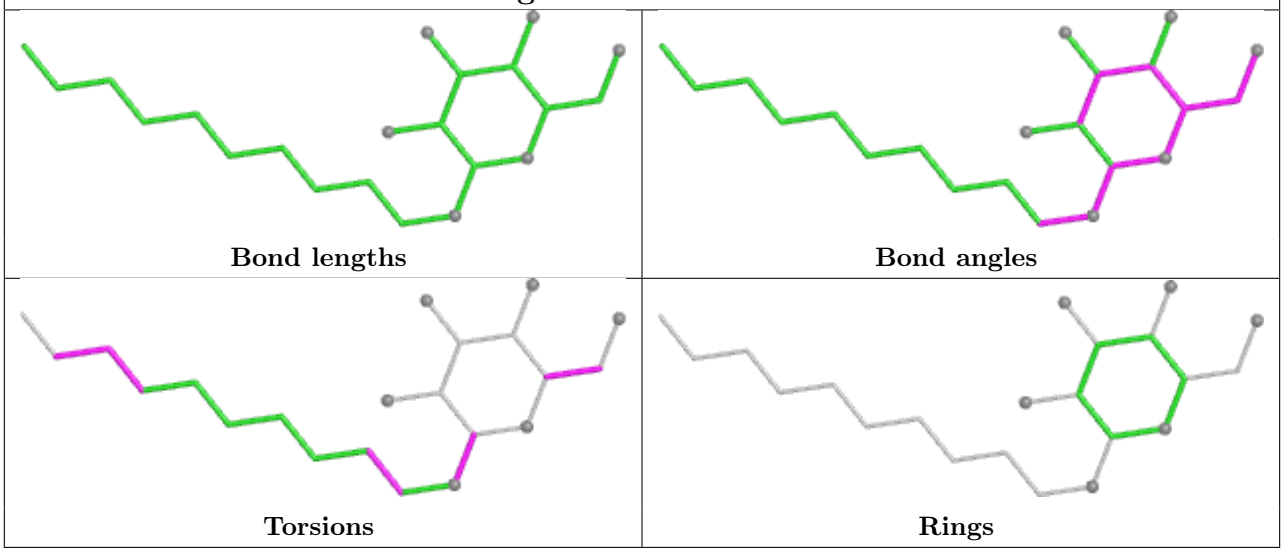
Ligand HEA A 602



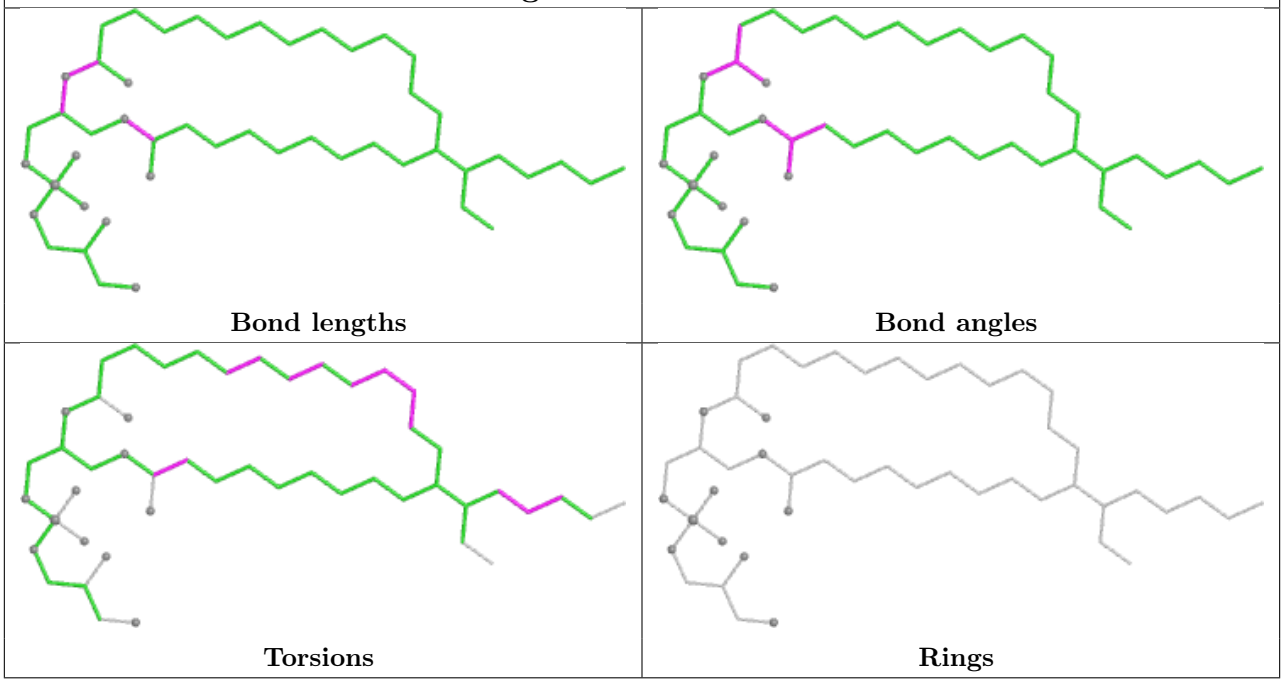
Ligand CHD B 302



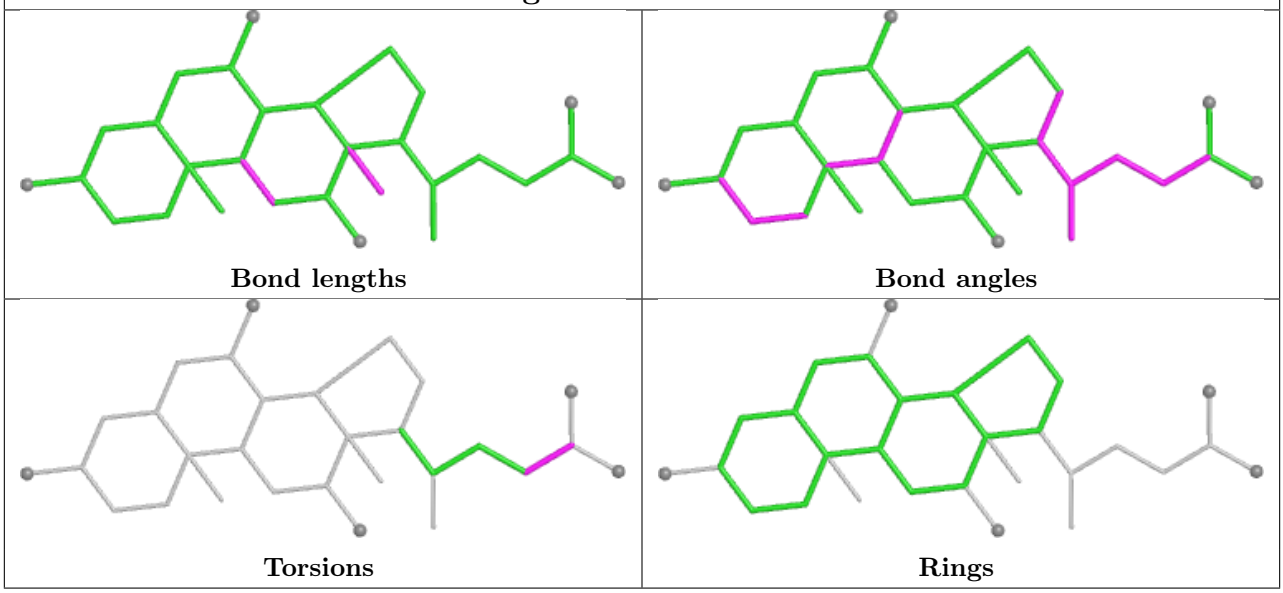
Ligand DMU O 304



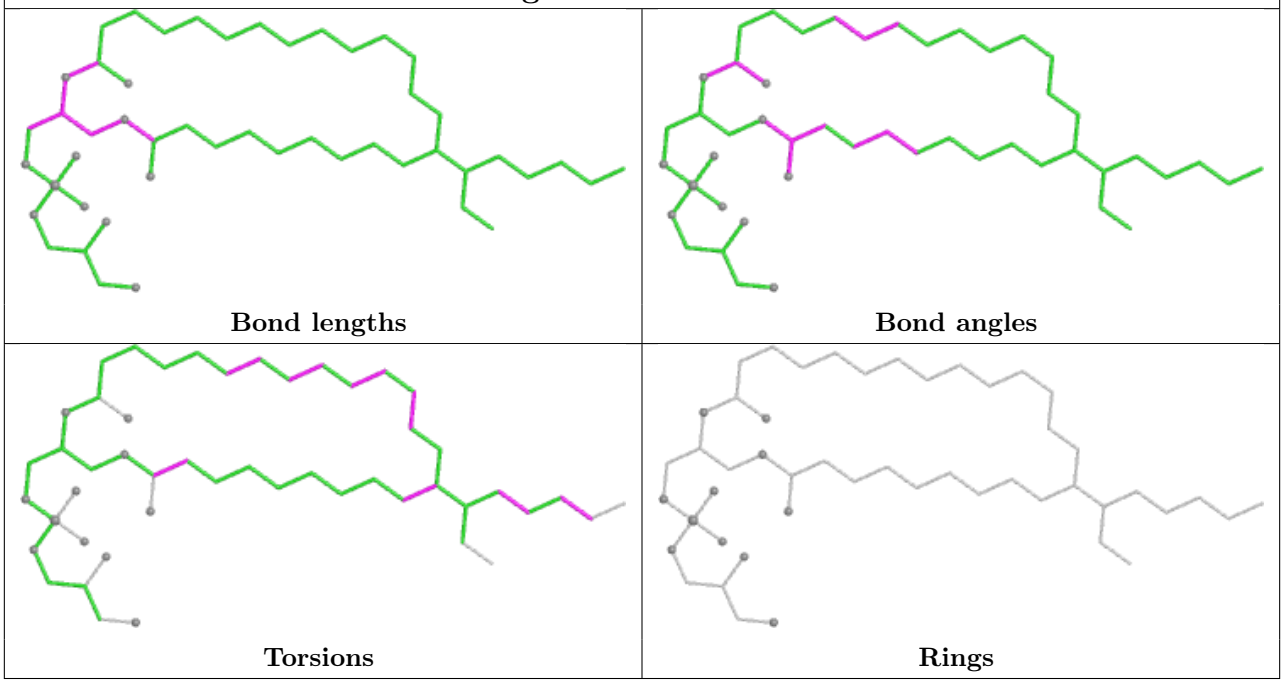
Ligand PGV N 609



Ligand CHD P 301



Ligand PGV A 608



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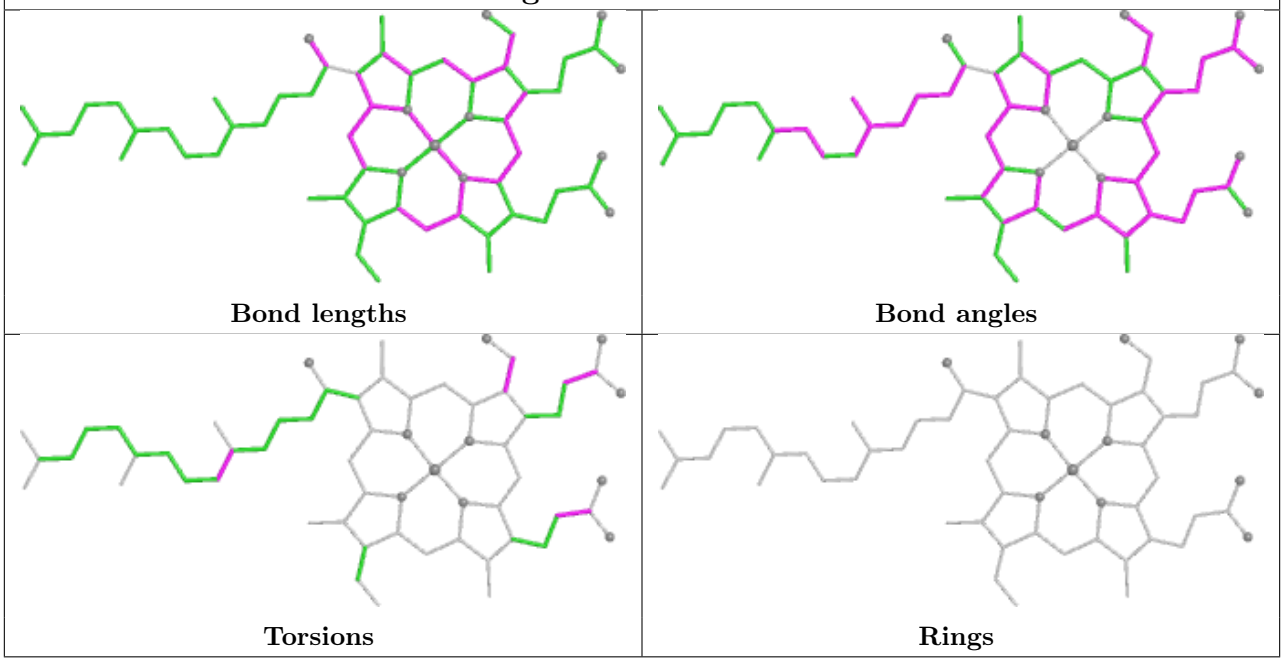

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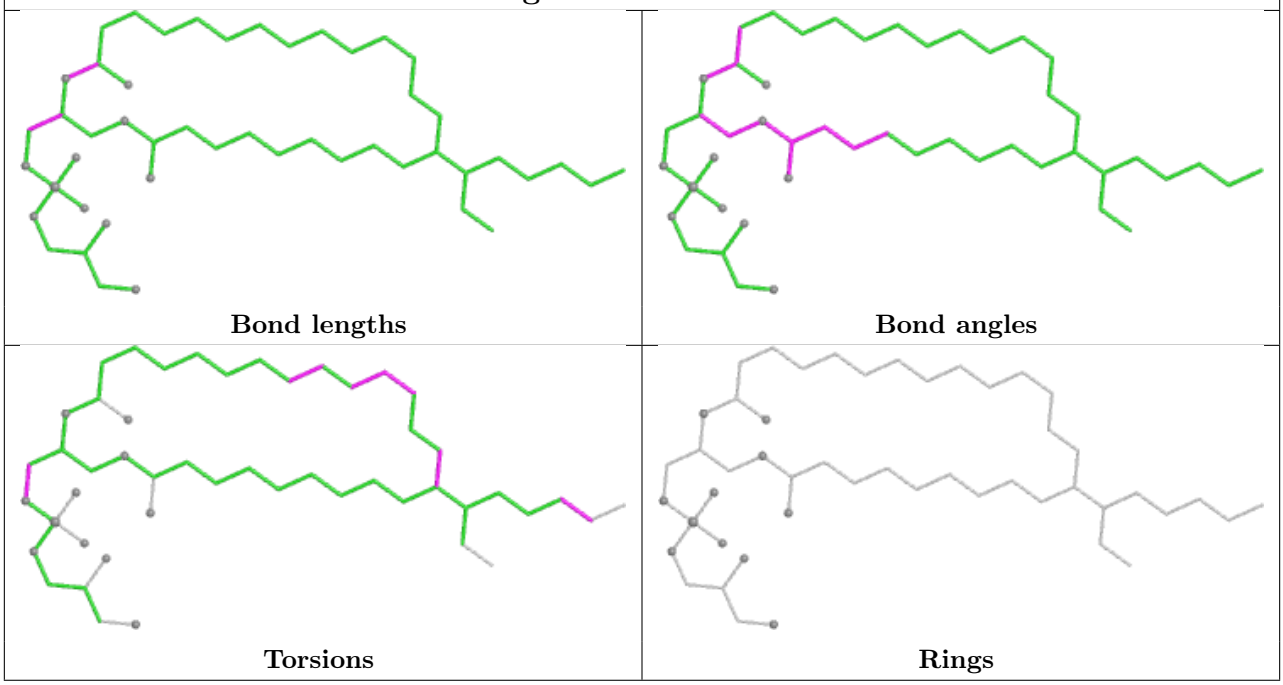

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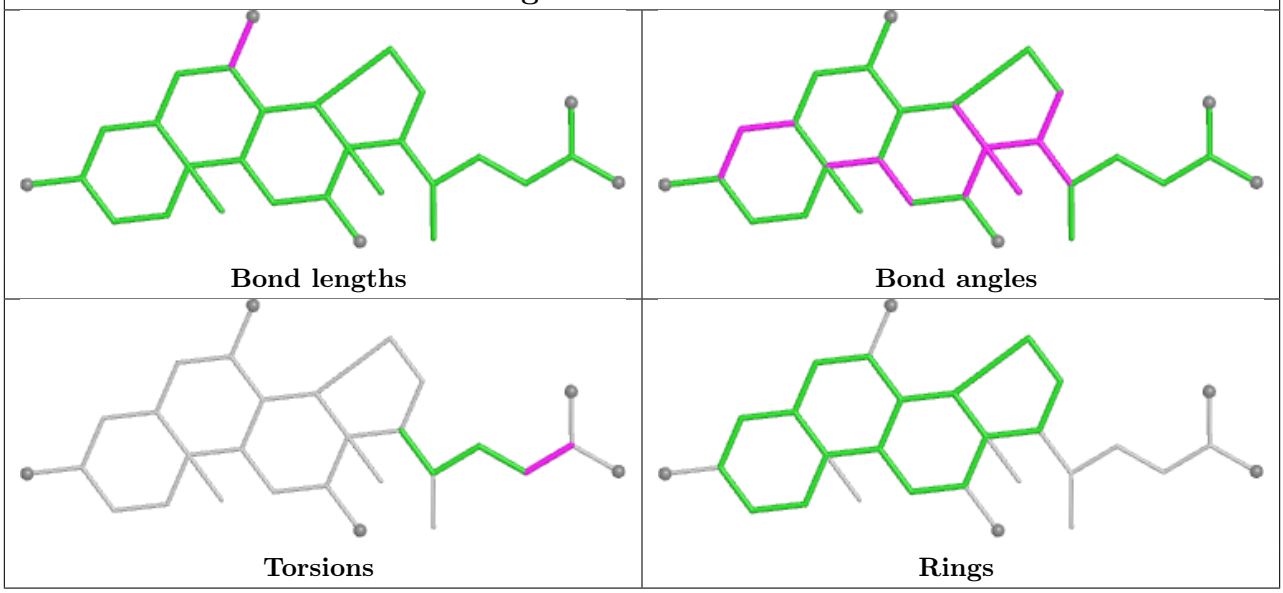

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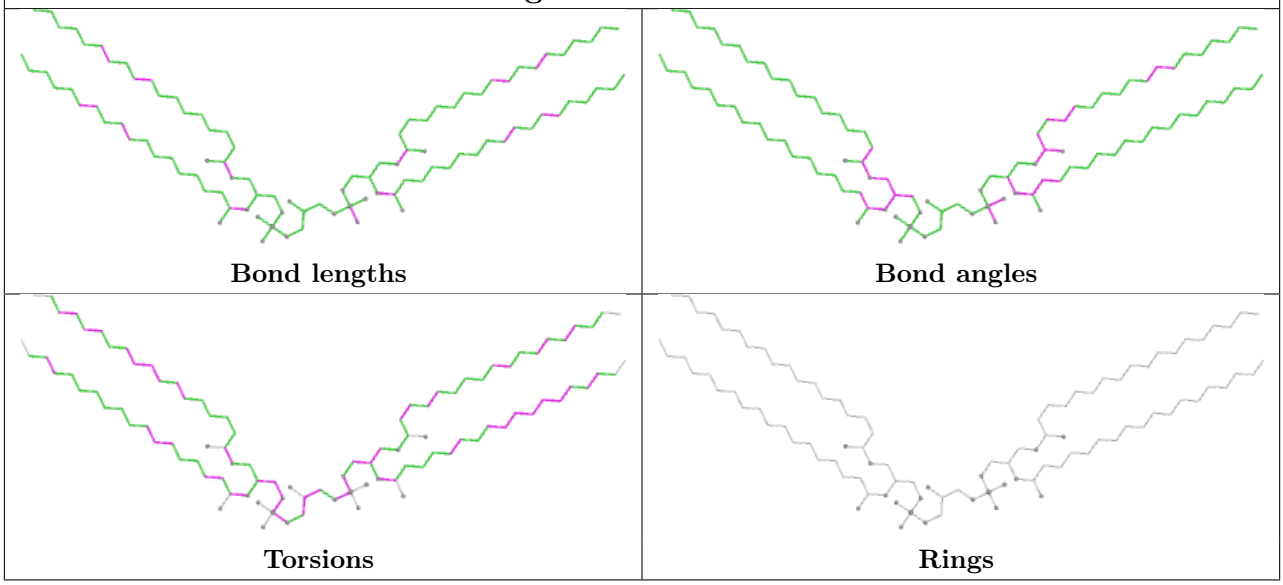

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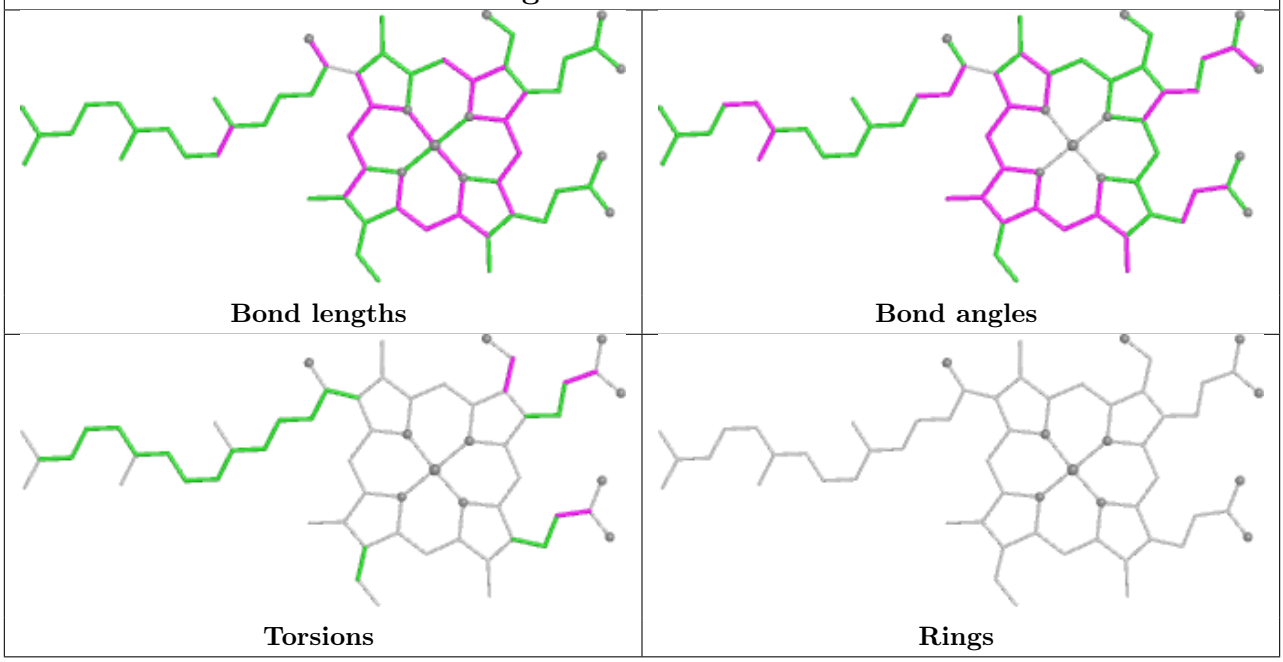
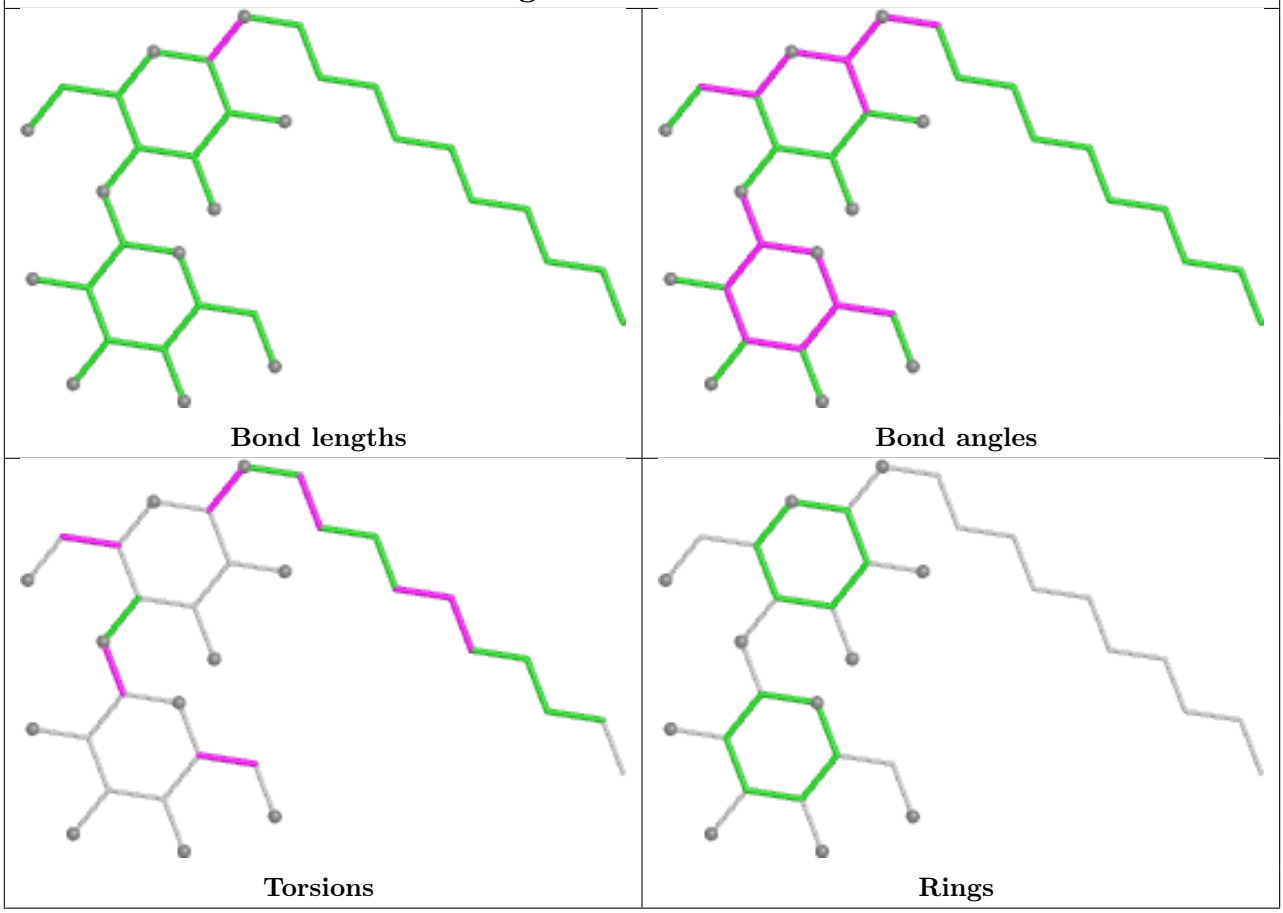
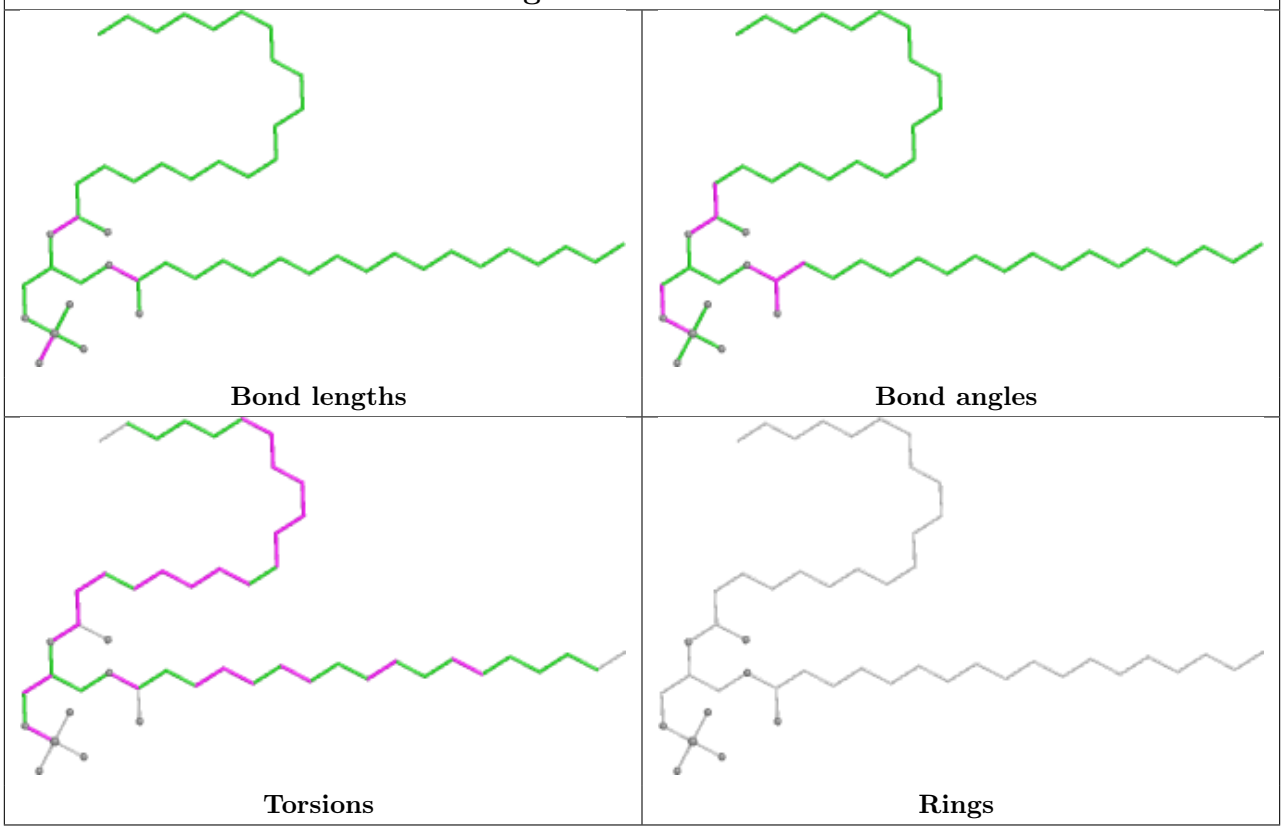


Ligand DMU P 307



Ligand PEK G 101



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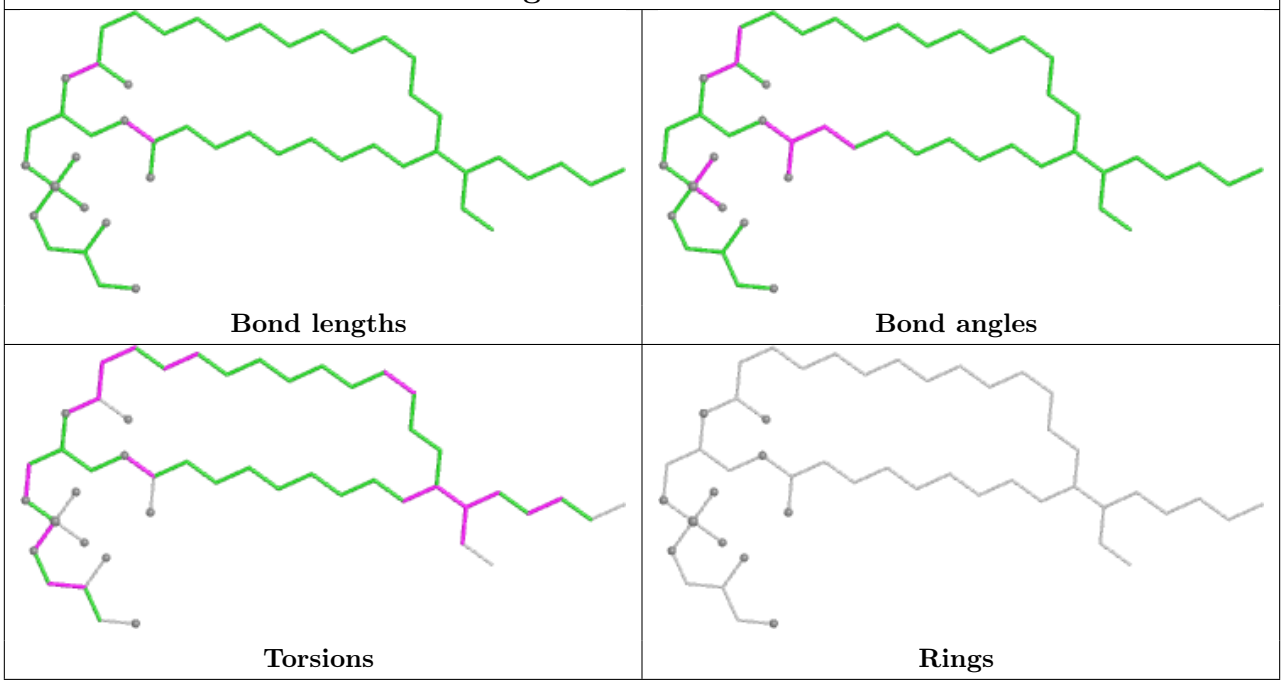

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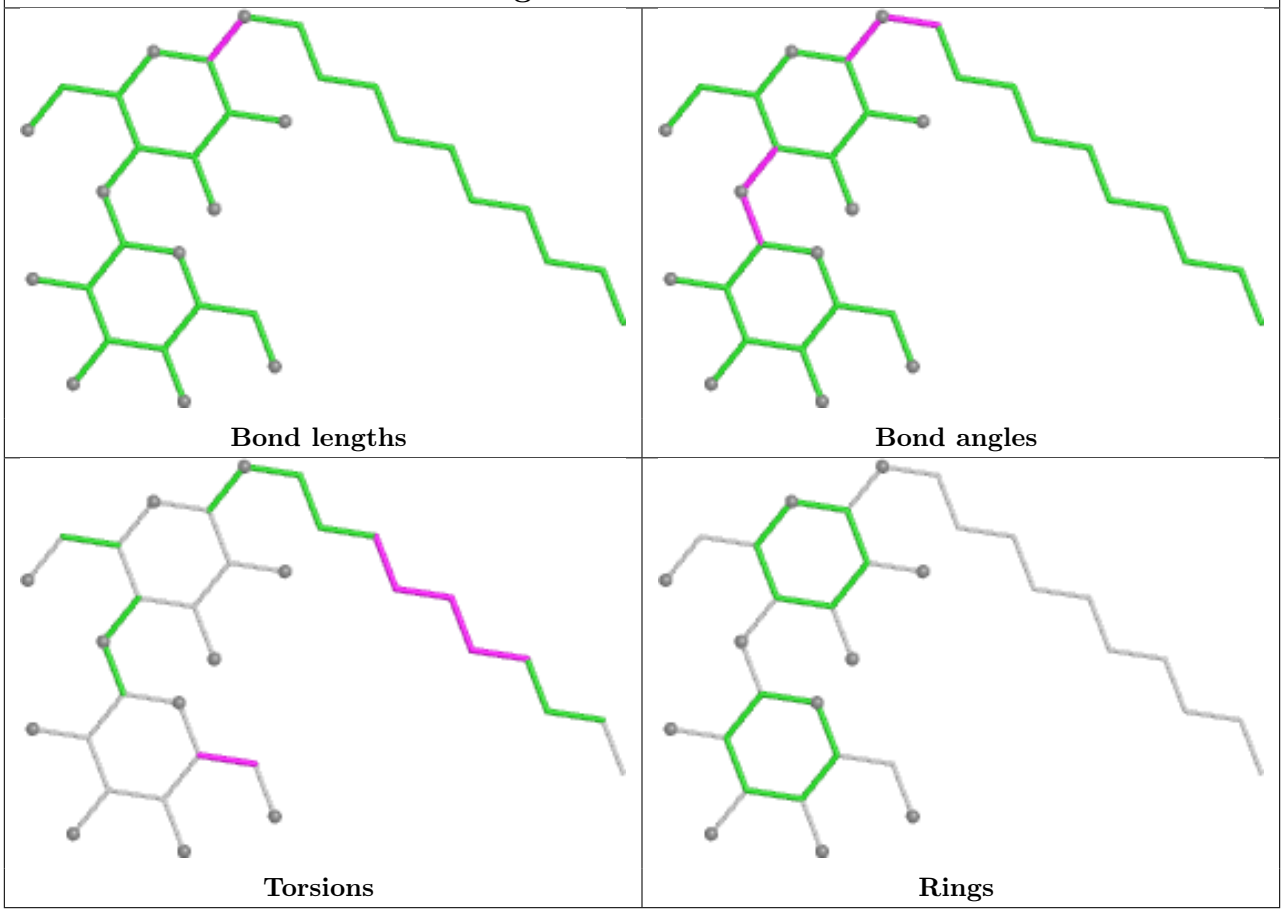

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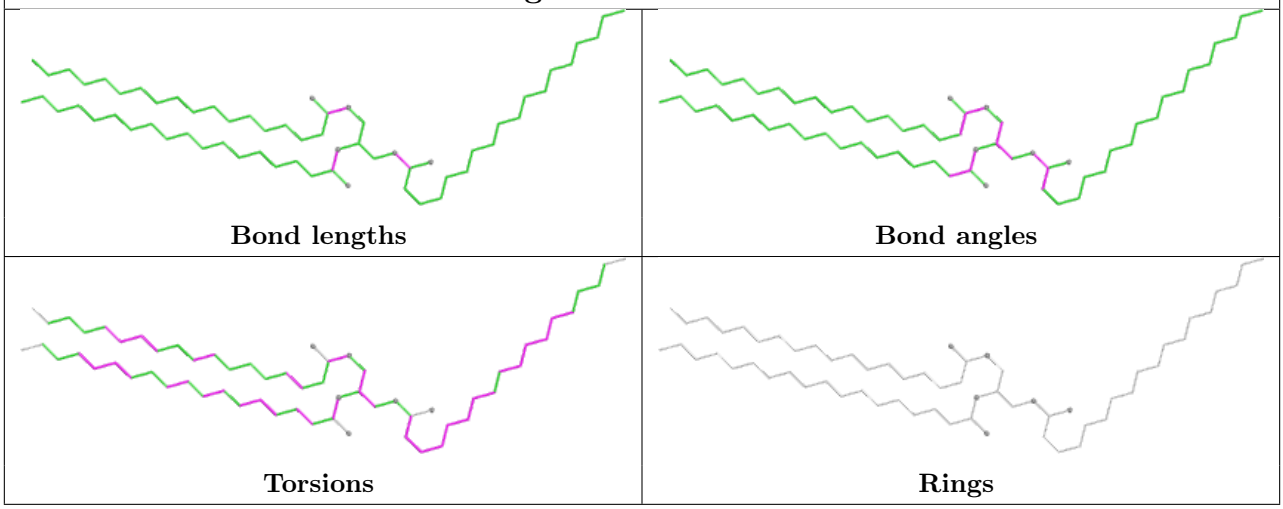

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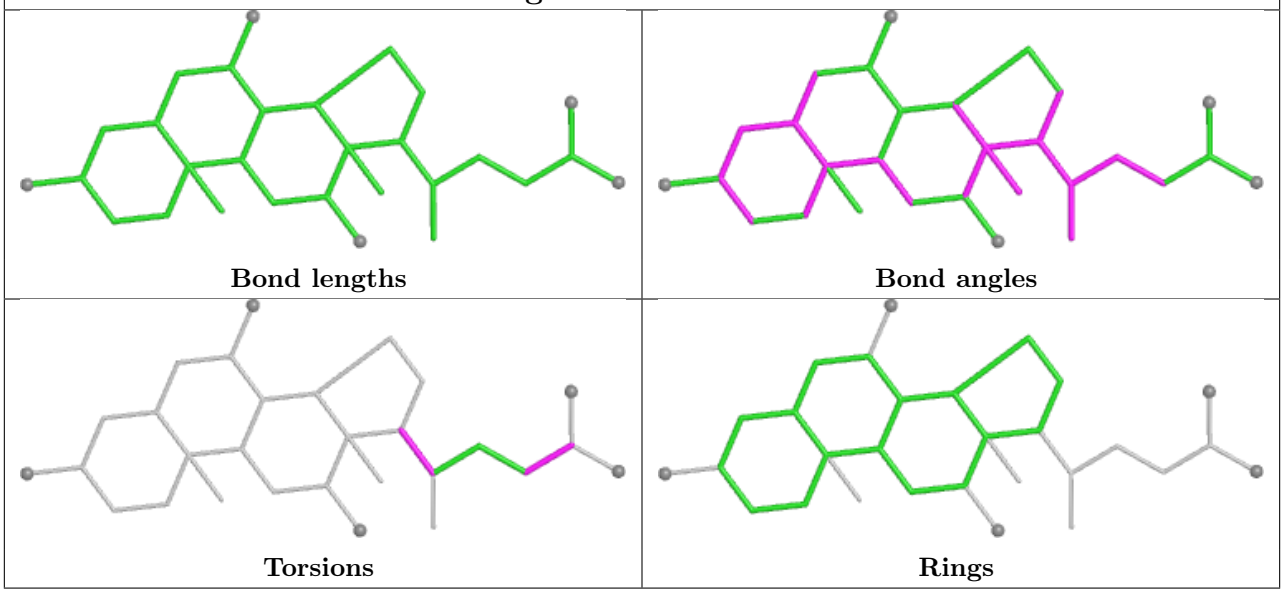

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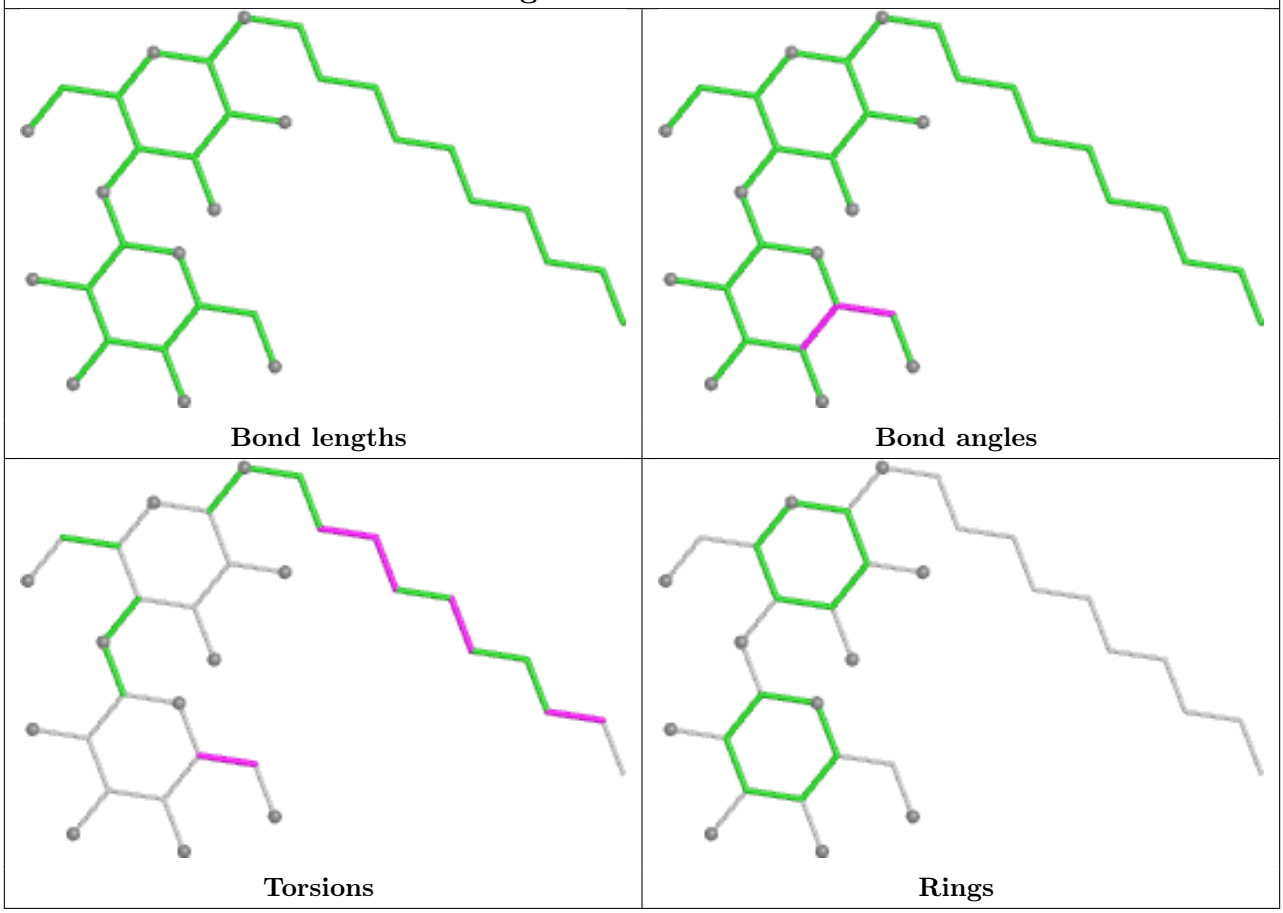

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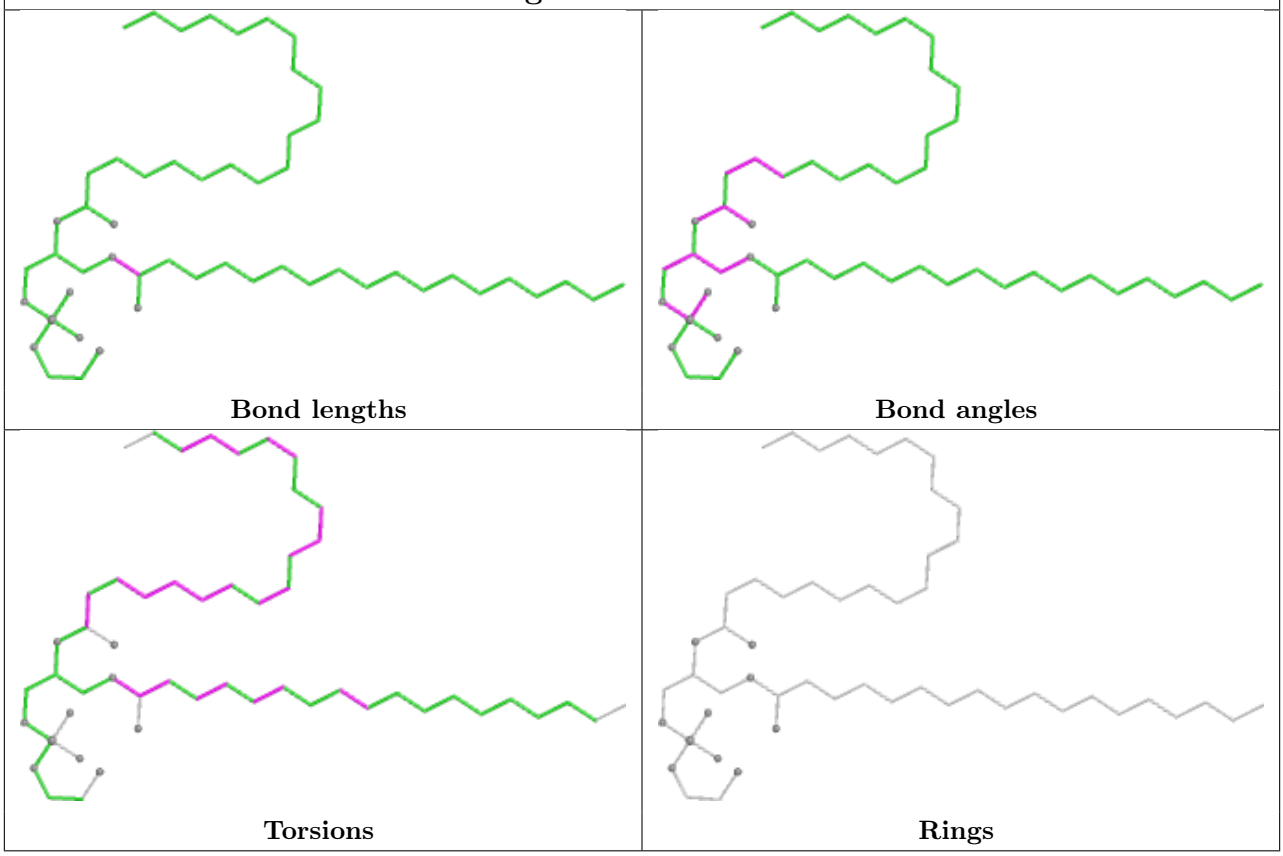

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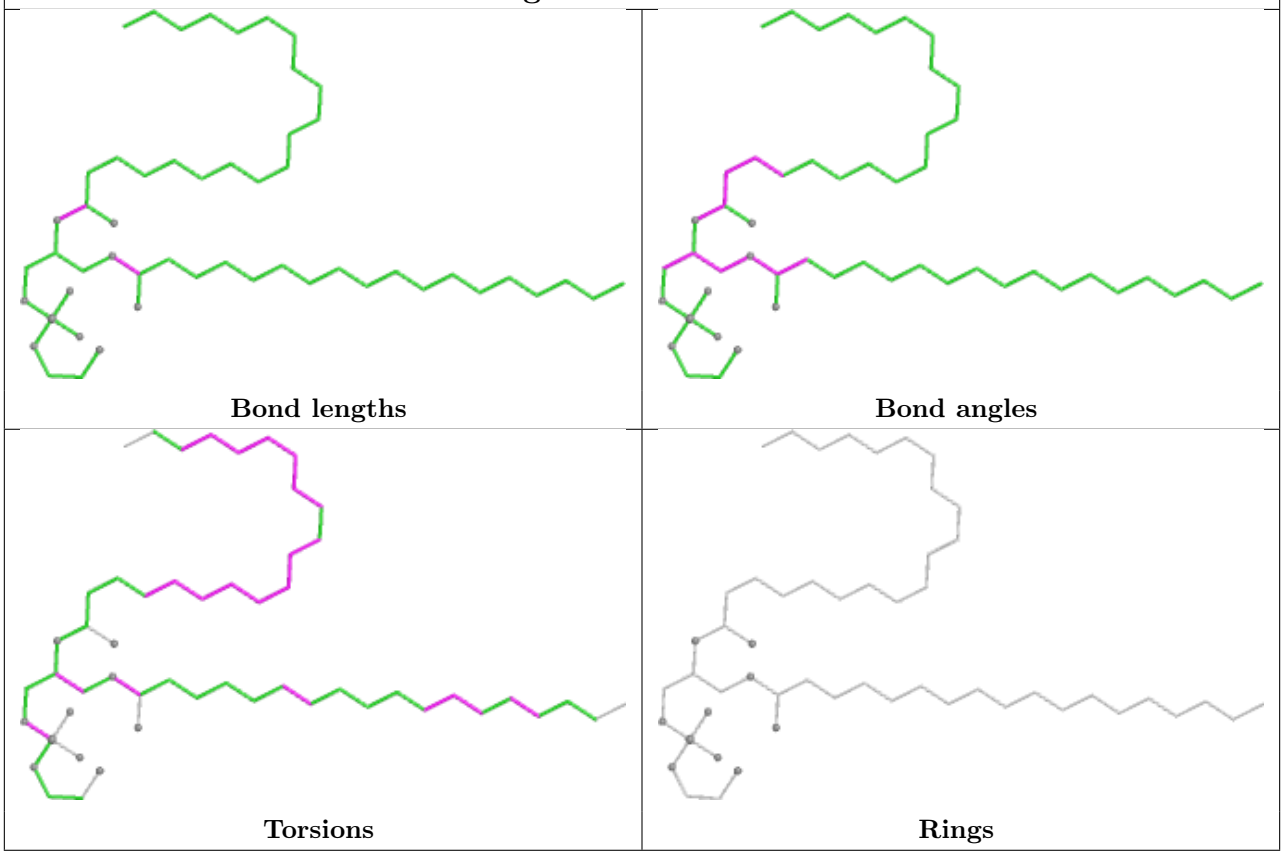

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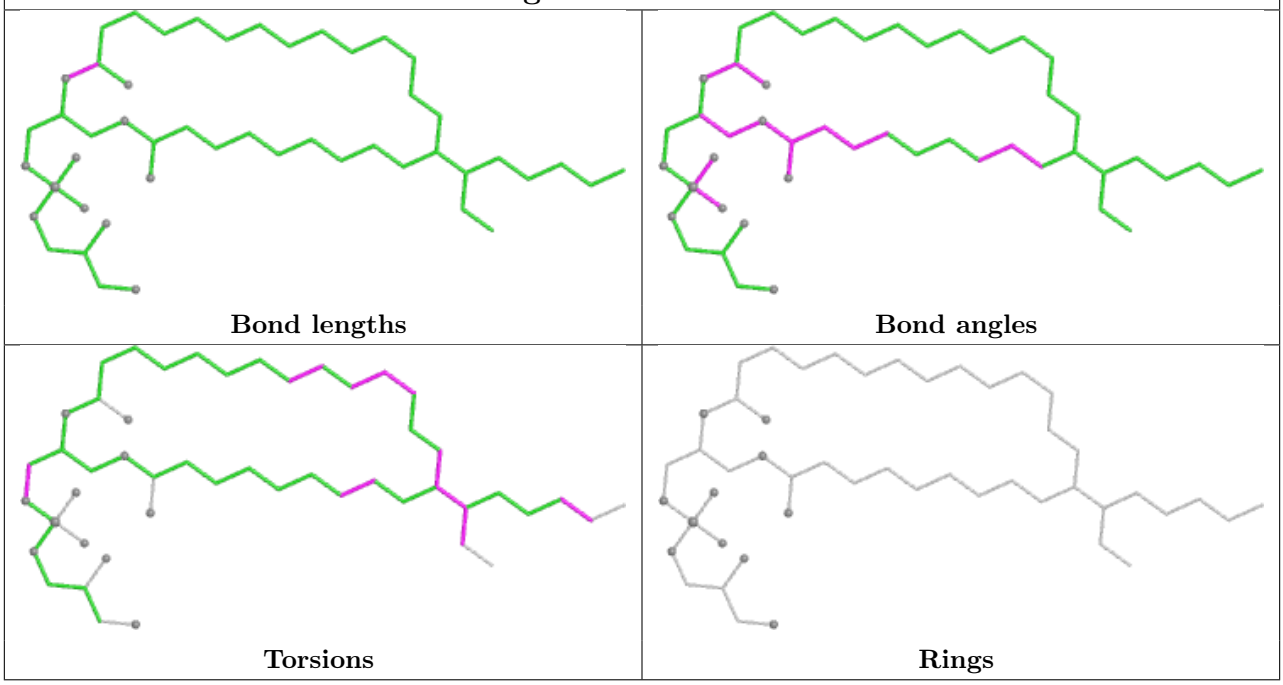

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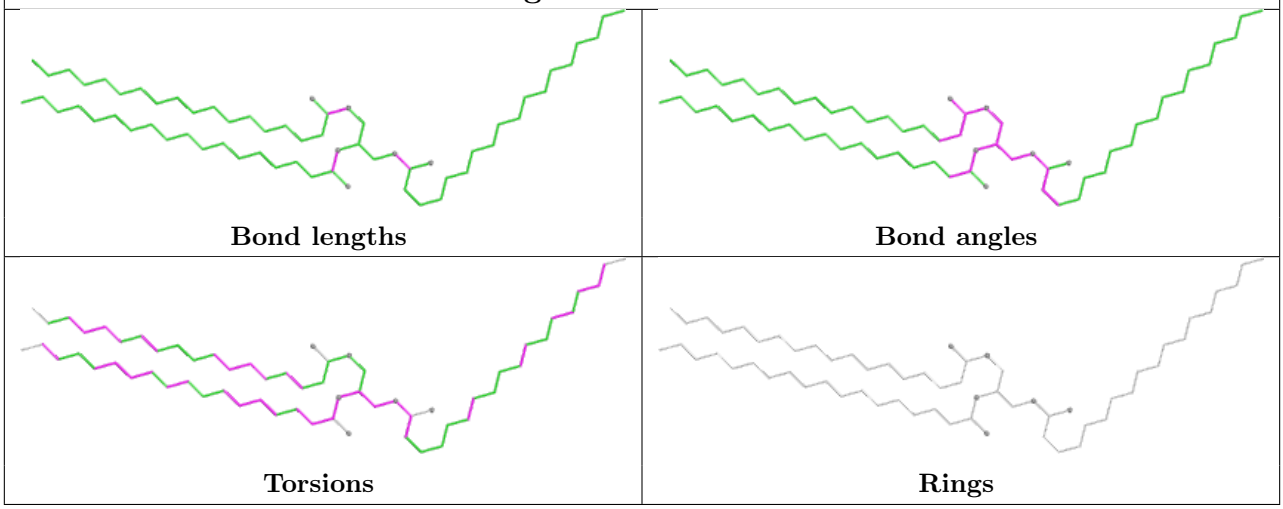

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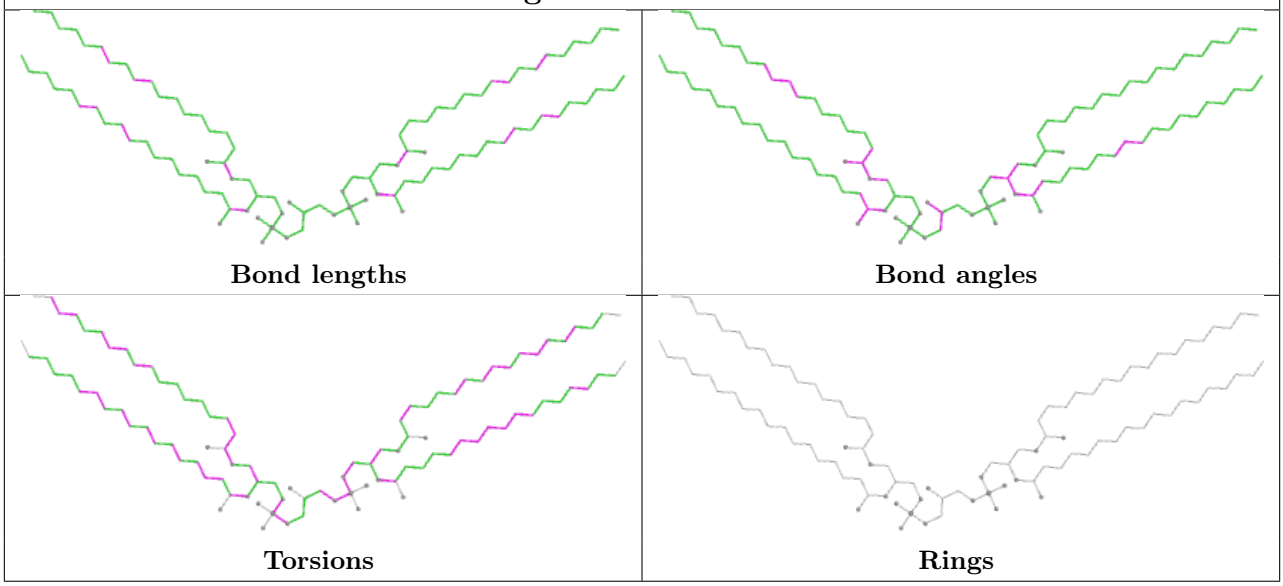

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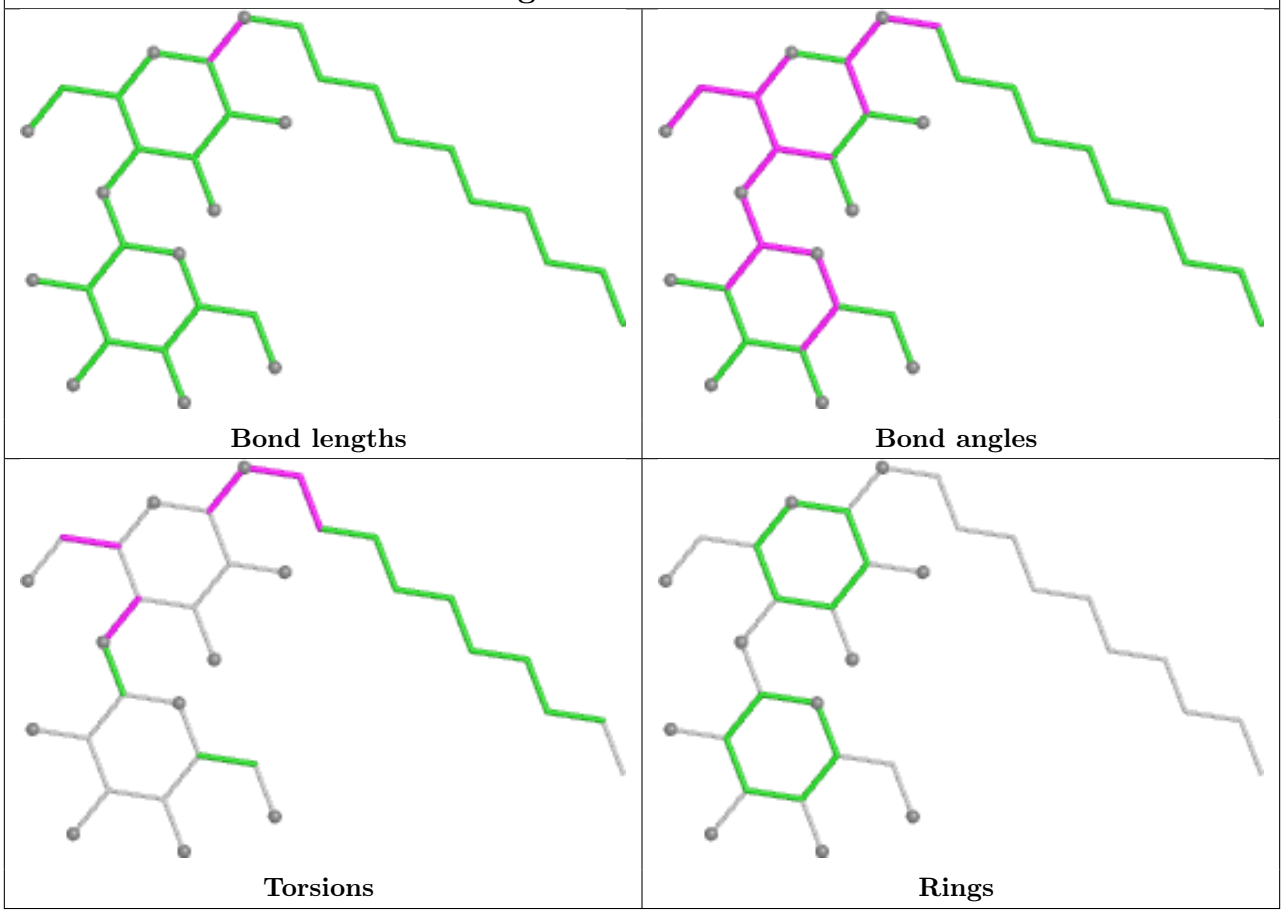

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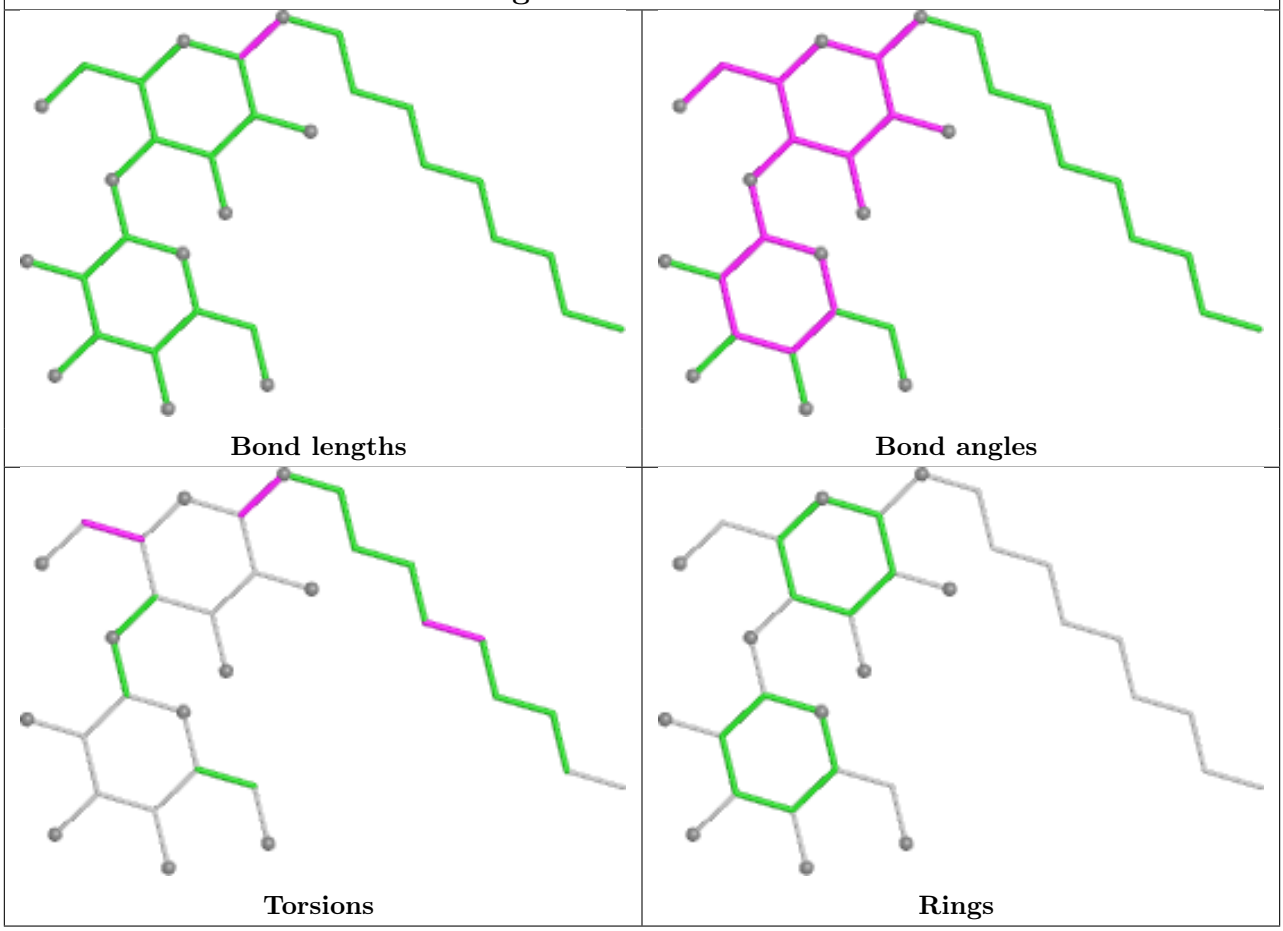

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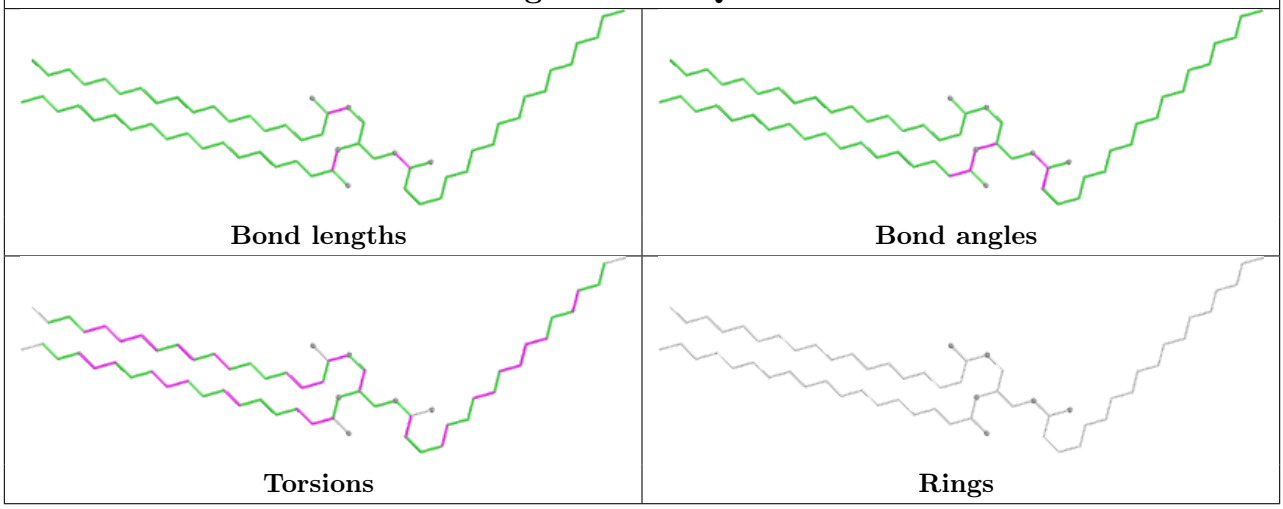
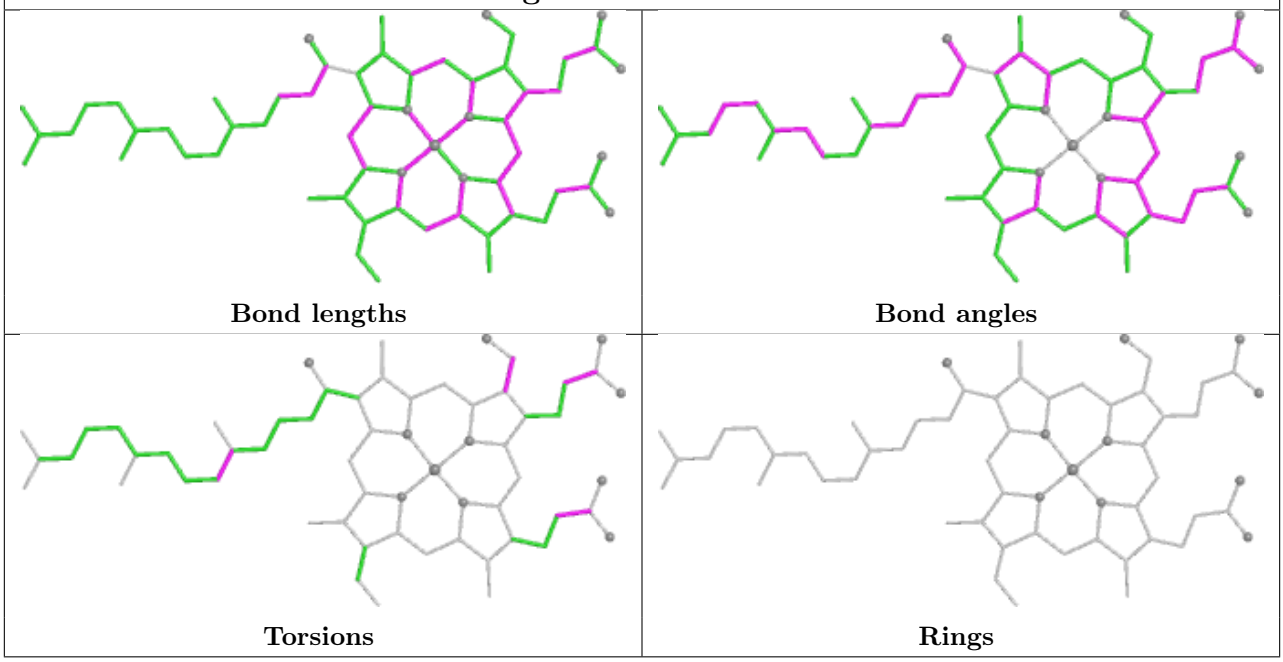
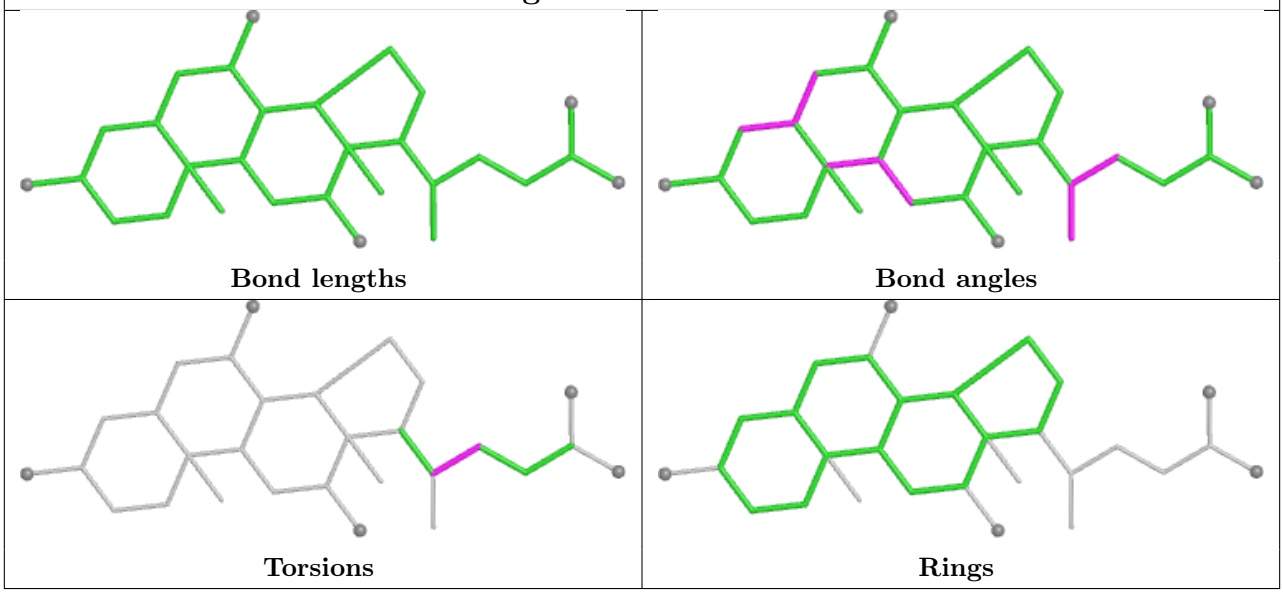


Ligand HEA A 601



Ligand CHD P 306



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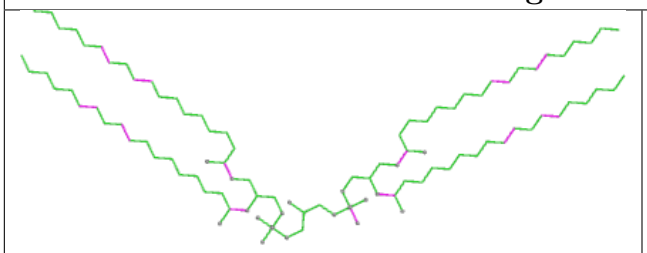
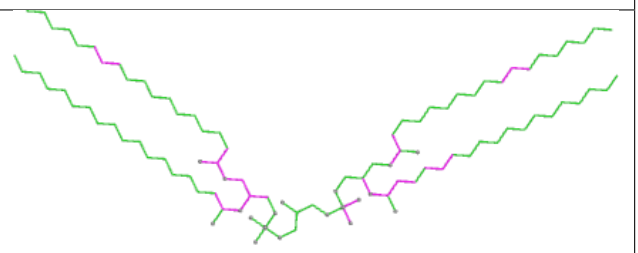
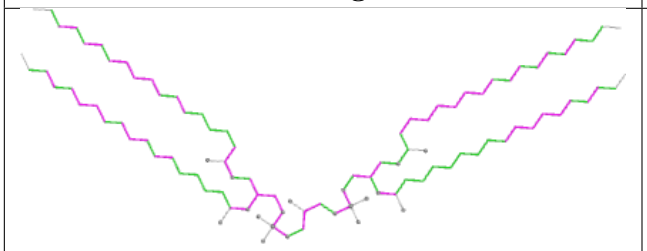


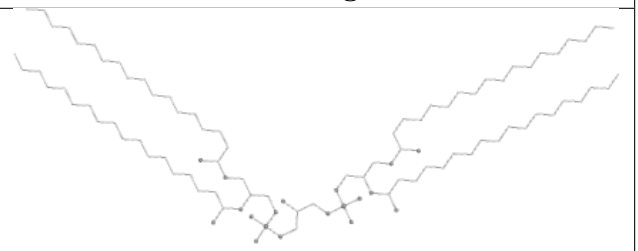
Bond lengths



Bond angles

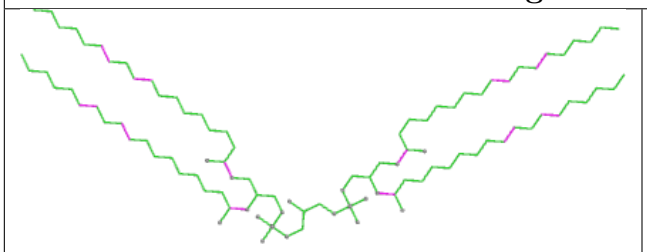


Torsions



Rings

Ligand CDL T 103



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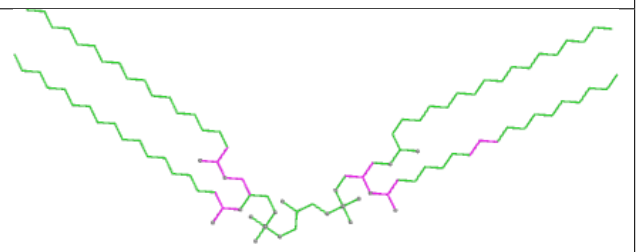
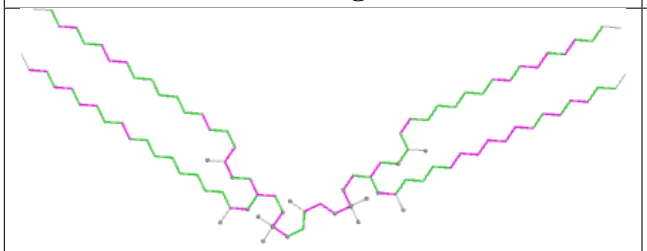
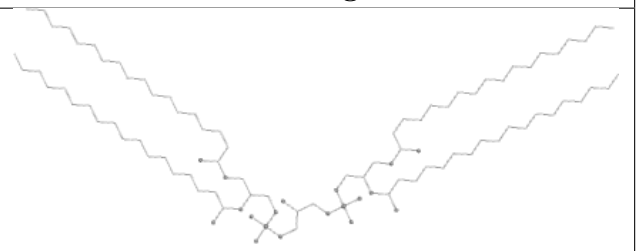


Bond angles

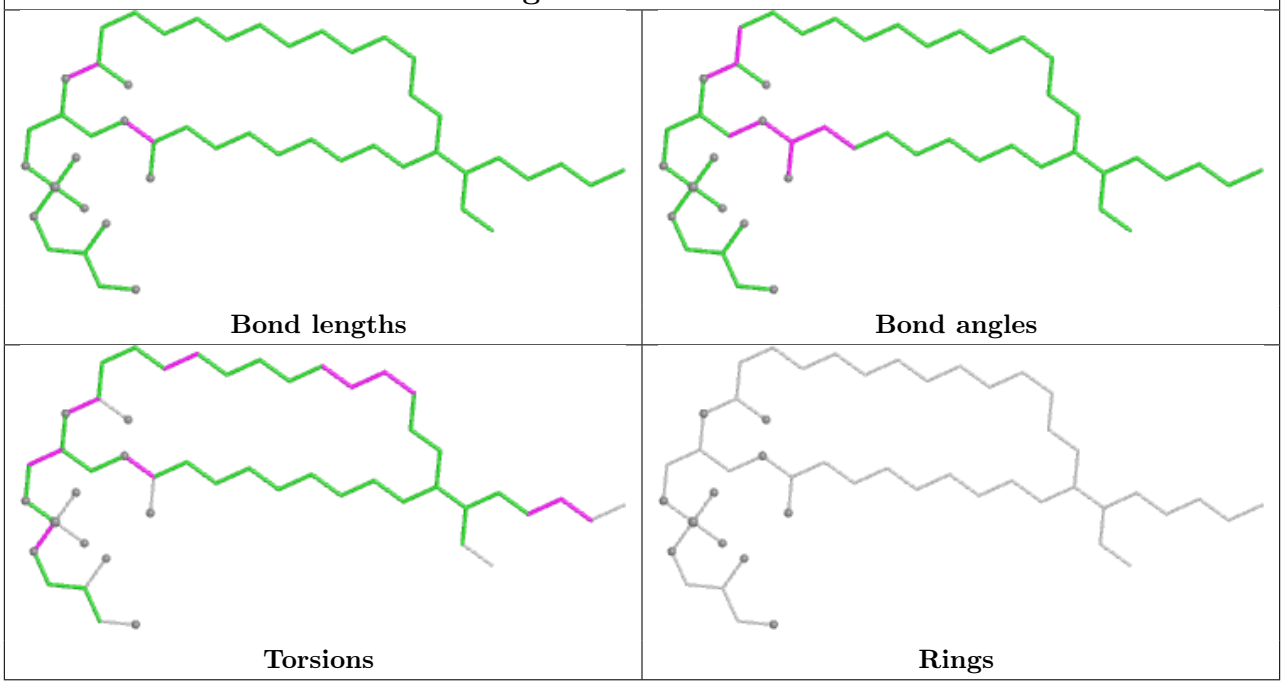


Torsions

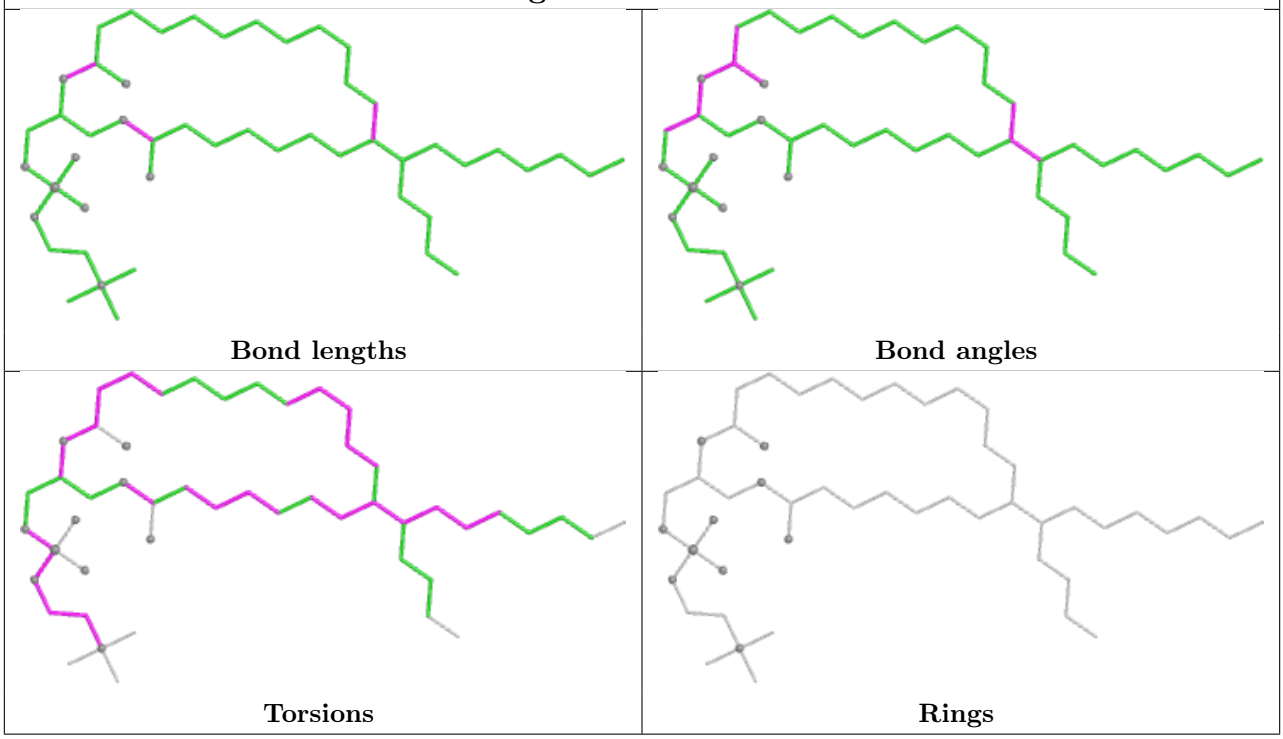


Rings

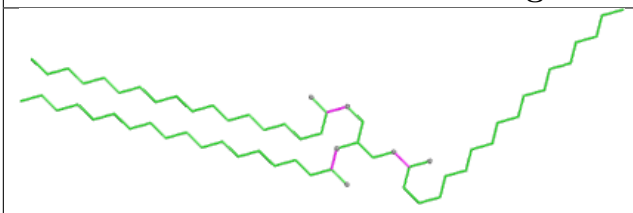
Ligand PGV C 304



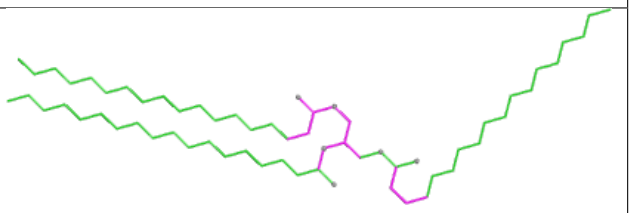
Ligand PSC E 201



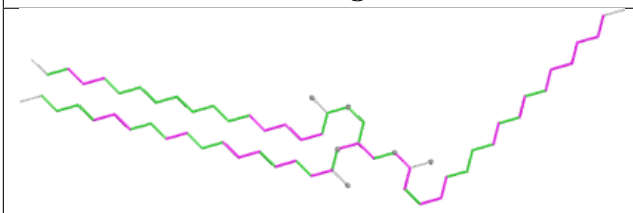
Ligand TGL L 101



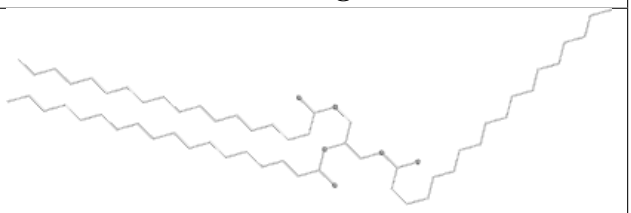
Bond lengths



Bond angles

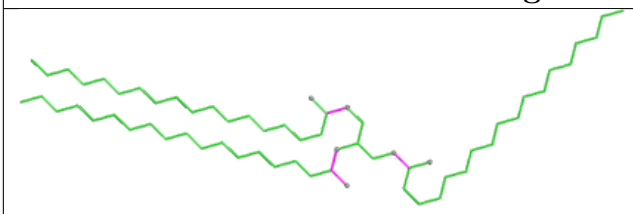


Torsions

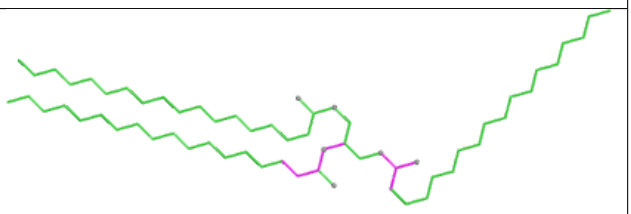


Rings

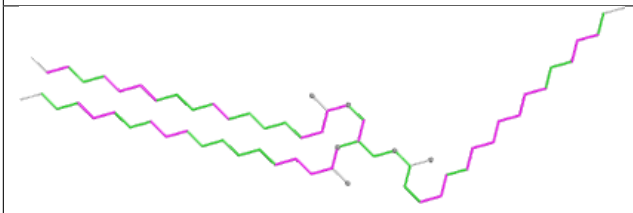
Ligand TGL D 201



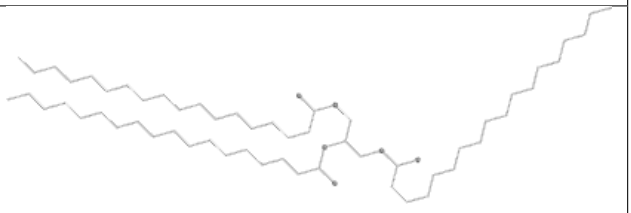
Bond lengths



Bond angles

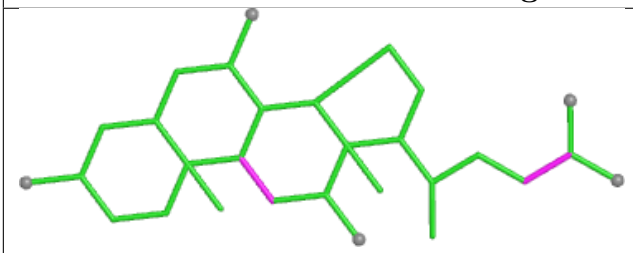


Torsions

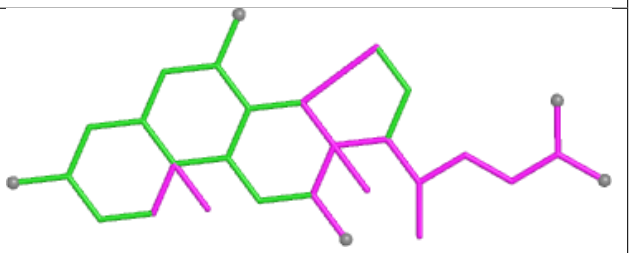


Rings

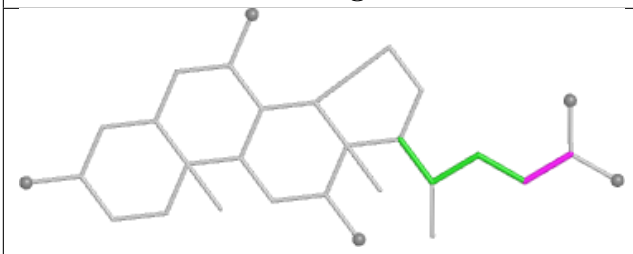
Ligand CHD C 301



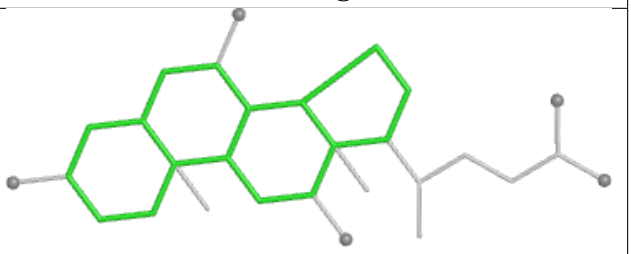
Bond lengths



Bond angles

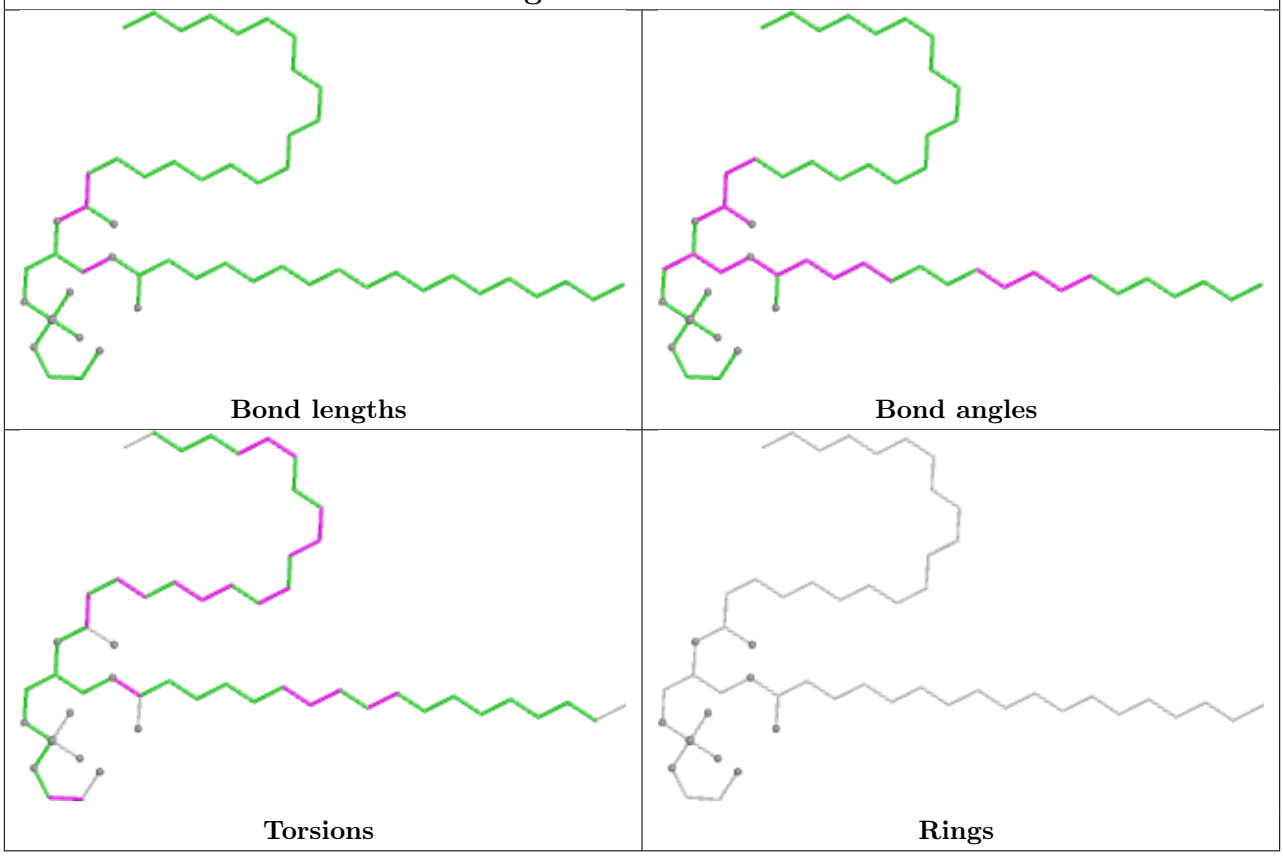


Torsions

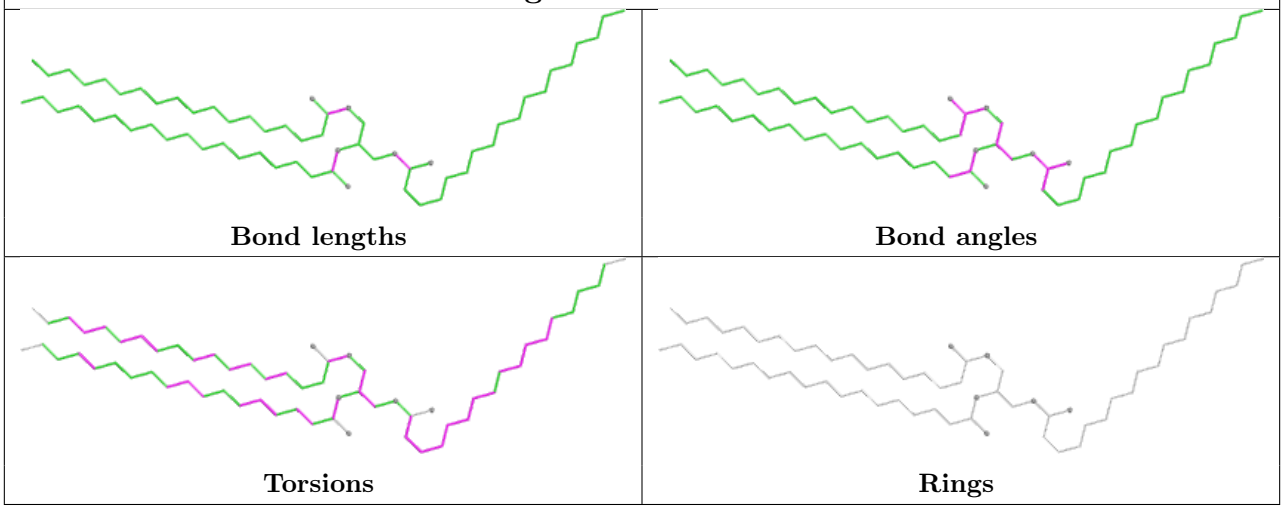


Rings

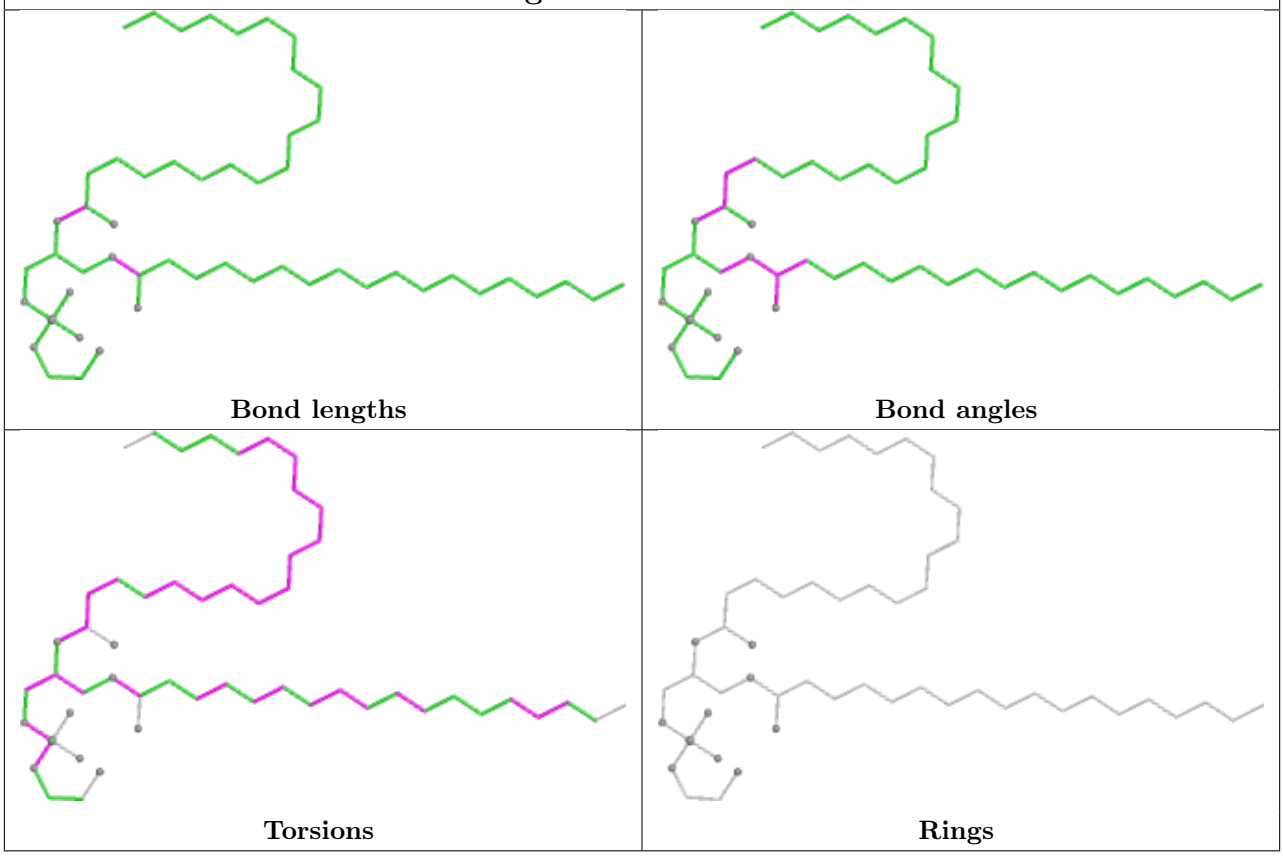
Ligand PEK C 302



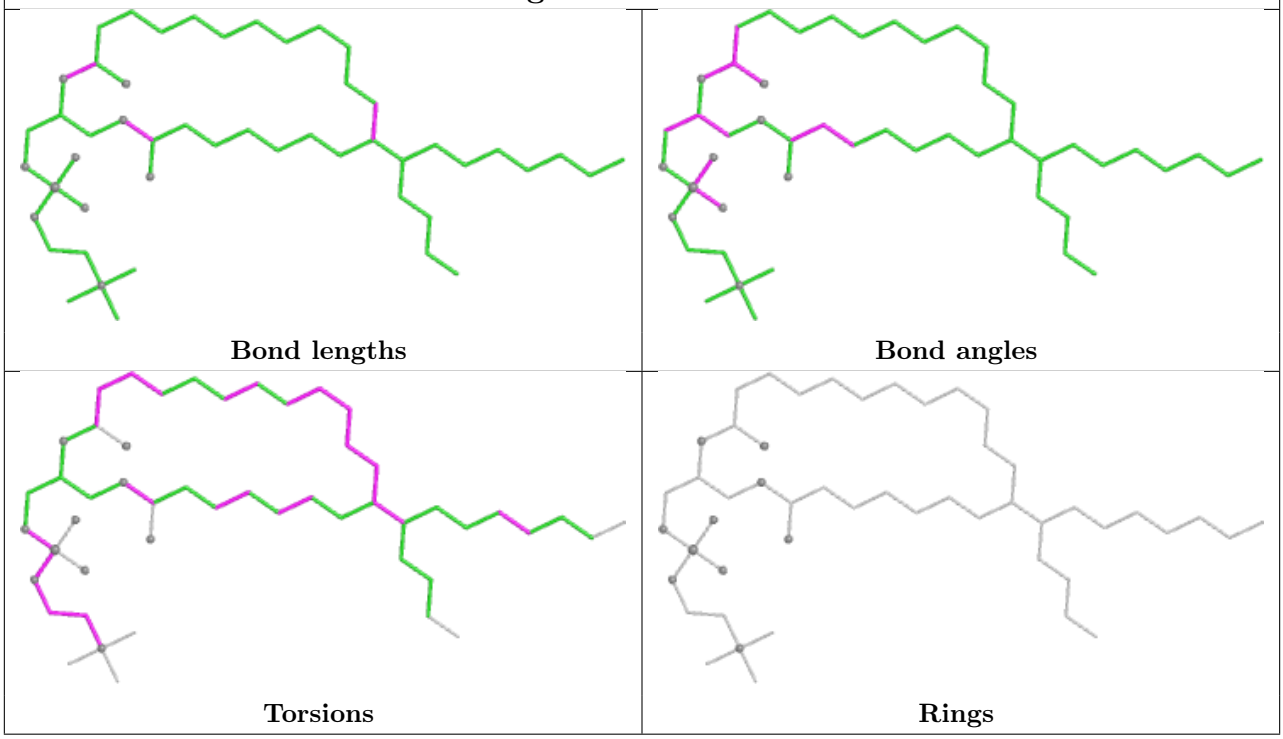
Ligand TGL A 607



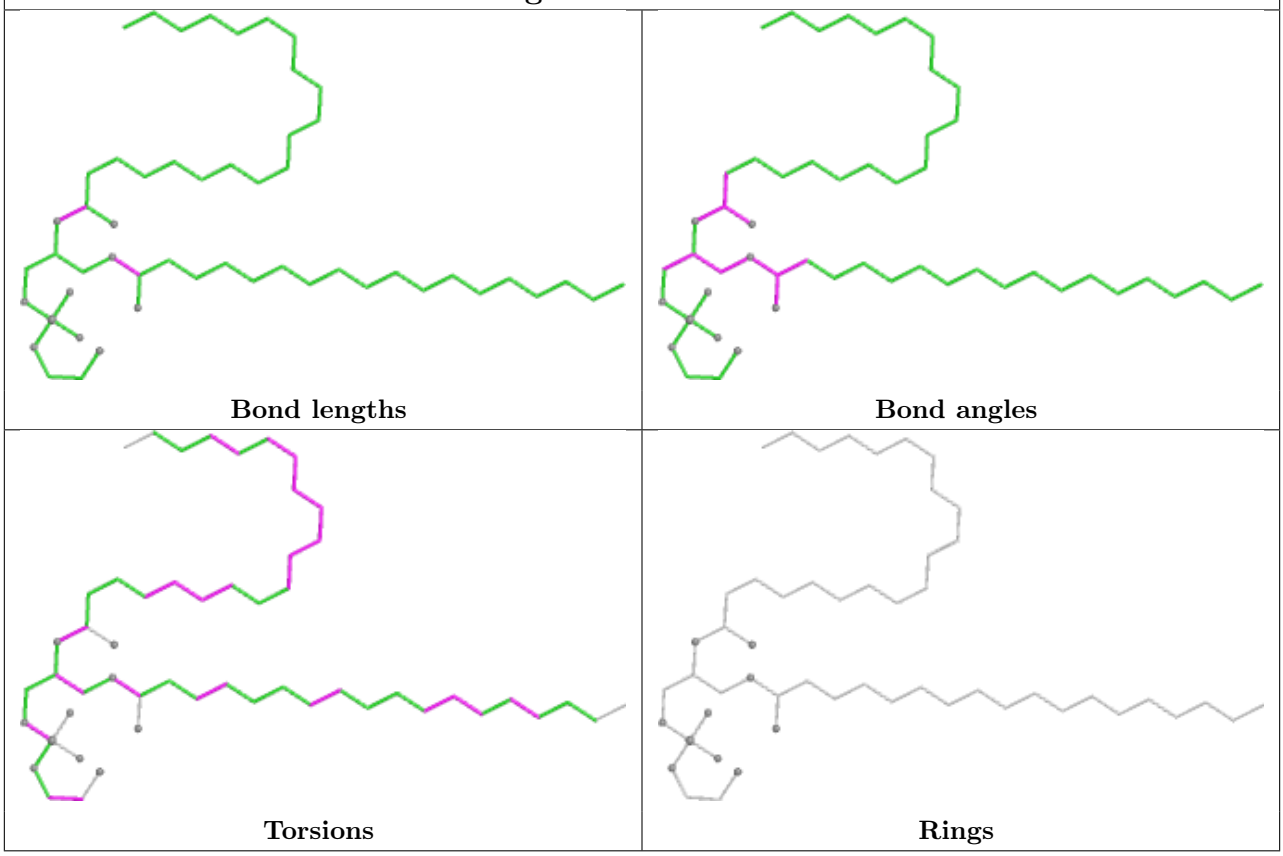
Ligand PEK T 101



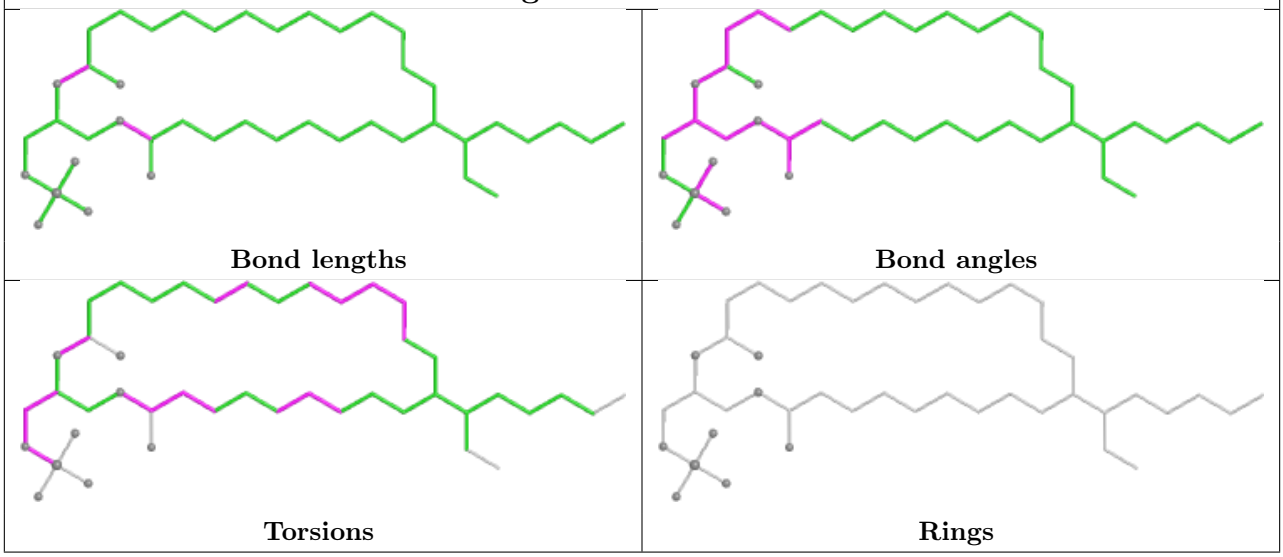
Ligand PSC R 201



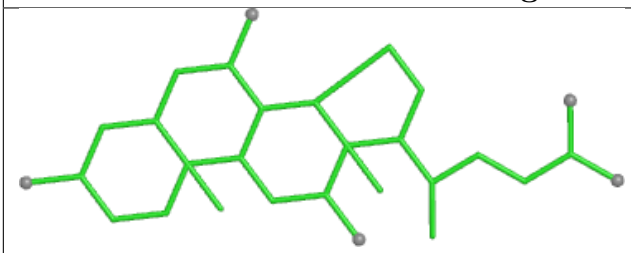
Ligand PEK T 102



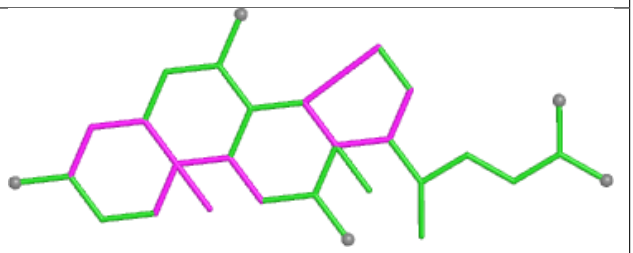
Ligand PGV N 608



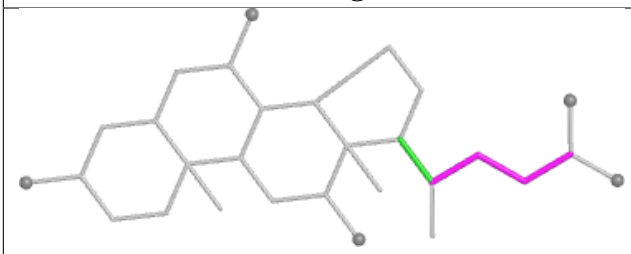
Ligand CHD C 306



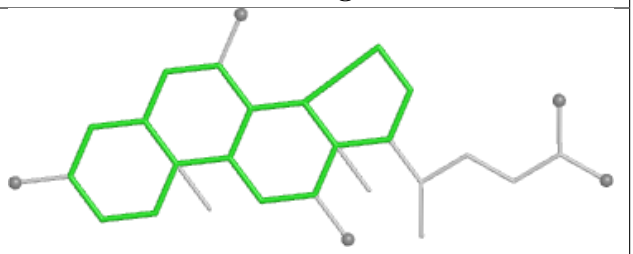
Bond lengths



Bond angles

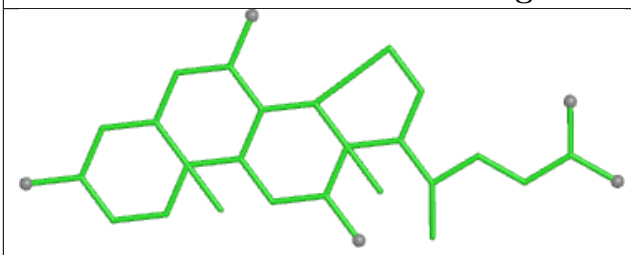


Torsions

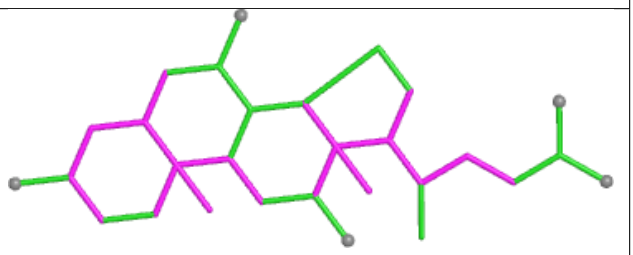


Rings

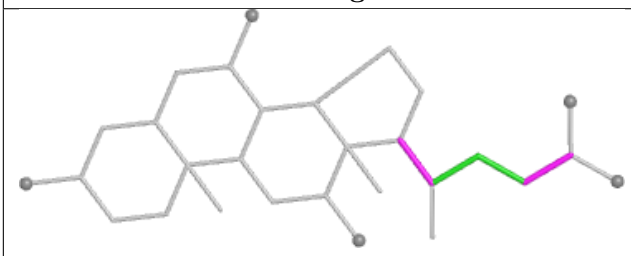
Ligand CHD W 101



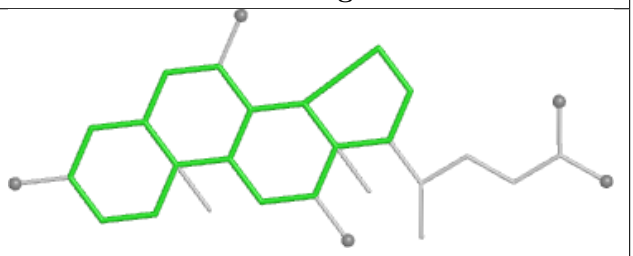
Bond lengths



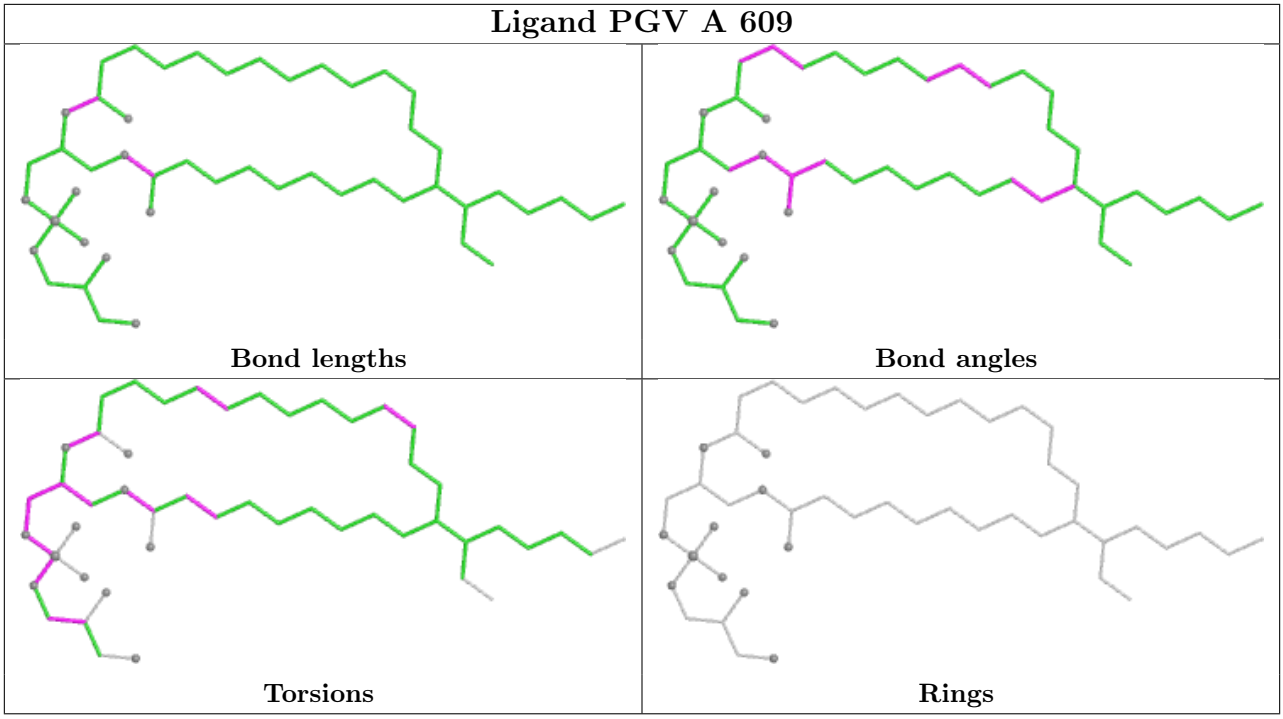
Bond angles



Torsions



Rings



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%)	-0.59	4 (0%)	82	83	11, 25, 34, 79	10 (1%)
1	N	513/514 (99%)	-0.43	6 (1%)	76	77	14, 30, 40, 78	9 (1%)
2	B	226/227 (99%)	-0.03	12 (5%)	32	31	22, 32, 55, 85	2 (0%)
2	O	226/227 (99%)	0.29	14 (6%)	26	25	27, 38, 72, 110	0
3	C	259/261 (99%)	-0.31	4 (1%)	72	72	22, 29, 42, 77	3 (1%)
3	P	259/261 (99%)	-0.25	2 (0%)	82	83	25, 31, 47, 70	0
4	D	144/147 (97%)	0.32	6 (4%)	40	40	29, 39, 57, 86	0
4	Q	144/147 (97%)	0.88	17 (11%)	9	7	35, 48, 83, 162	0
5	E	105/109 (96%)	0.10	4 (3%)	44	44	32, 39, 69, 134	0
5	R	105/109 (96%)	0.30	4 (3%)	44	44	34, 46, 73, 145	0
6	F	98/98 (100%)	0.61	10 (10%)	12	10	26, 37, 120, 152	0
6	S	98/98 (100%)	0.79	9 (9%)	14	12	26, 39, 118, 159	0
7	G	83/85 (97%)	1.20	23 (27%)	1	1	26, 37, 109, 152	0
7	T	83/85 (97%)	1.21	20 (24%)	2	1	27, 41, 112, 149	0
8	H	79/85 (92%)	0.77	13 (16%)	4	3	28, 40, 91, 135	0
8	U	79/85 (92%)	1.05	15 (18%)	3	2	33, 44, 115, 144	0
9	I	72/73 (98%)	0.71	8 (11%)	10	8	32, 45, 68, 77	0
9	V	72/73 (98%)	1.06	11 (15%)	5	4	33, 51, 74, 128	0
10	J	58/59 (98%)	0.41	5 (8%)	16	14	29, 38, 68, 127	0
10	W	58/59 (98%)	0.57	5 (8%)	16	14	33, 44, 76, 146	0
11	K	49/56 (87%)	0.57	4 (8%)	17	15	32, 41, 62, 71	0
11	X	49/56 (87%)	0.90	7 (14%)	6	5	40, 51, 75, 93	0
12	L	46/47 (97%)	0.12	3 (6%)	25	23	26, 32, 54, 94	0
12	Y	46/47 (97%)	0.44	4 (8%)	16	14	33, 41, 68, 125	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
13	M	43/46 (93%)	0.51	6 (13%)	6	5	29, 34, 76, 123	0
13	Z	43/46 (93%)	0.81	7 (16%)	4	3	37, 45, 98, 153	0
All	All	3550/3614 (98%)	0.12	223 (6%)	26	24	11, 34, 70, 162	24 (0%)

The worst 5 of 223 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	S	1	ALA	22.1
6	S	97	ALA	11.4
4	Q	6	VAL	11.0
6	F	1	ALA	10.2
7	T	3	ALA	9.4

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	0.31	0.23	147,152,161,162	0
7	TPO	G	11	11/12	0.57	0.38	90,120,150,166	0
7	TPO	T	11	11/12	0.65	0.30	103,113,156,158	0
9	SAC	I	1	9/10	0.68	0.23	65,84,106,118	0
1	FME	N	1	10/11	0.91	0.14	40,54,91,104	0
1	FME	A	1	10/11	0.94	0.12	36,39,76,103	0
2	FME	B	1	10/11	0.97	0.10	17,34,75,76	0
2	FME	O	1	10/11	0.97	0.09	30,39,45,76	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column

labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	PEK	G	103	53/53	0.71	0.26	46,95,133,145	0
26	DMU	P	307	33/33	0.71	0.21	60,110,126,129	0
20	PGV	P	304	51/51	0.72	0.24	43,78,120,149	0
23	CHD	J	101	29/29	0.72	0.23	73,104,110,113	0
24	PEK	T	102	53/53	0.73	0.25	47,94,128,138	0
23	CHD	W	101	29/29	0.73	0.22	81,107,119,120	0
26	DMU	C	307	33/33	0.74	0.21	58,102,122,124	0
25	CDL	T	103	100/100	0.74	0.23	52,88,125,150	0
20	PGV	N	608	46/51	0.75	0.25	40,83,127,143	0
24	PEK	T	101	53/53	0.75	0.24	40,80,124,154	0
24	PEK	G	101	50/53	0.75	0.24	46,82,118,145	0
26	DMU	W	102	32/33	0.75	0.21	50,80,104,115	0
19	TGL	D	201	63/63	0.76	0.24	41,71,103,117	0
19	TGL	Q	201	63/63	0.76	0.25	49,77,107,112	0
25	CDL	G	102	100/100	0.77	0.23	46,88,122,152	0
20	PGV	C	304	51/51	0.78	0.25	44,88,114,150	0
20	PGV	A	609	51/51	0.78	0.25	43,77,132,157	0
27	PSC	R	201	52/52	0.78	0.27	44,94,141,175	0
25	CDL	P	305	100/100	0.79	0.24	41,90,124,138	0
19	TGL	A	607	63/63	0.79	0.23	47,73,96,105	0
25	CDL	C	305	100/100	0.80	0.23	41,86,116,128	0
19	TGL	O	303	63/63	0.80	0.21	52,76,99,106	0
19	TGL	L	101	63/63	0.80	0.23	33,63,97,113	0
19	TGL	N	607	63/63	0.80	0.25	45,69,101,121	0
21	EDO	N	615	4/4	0.81	0.24	46,68,84,87	0
27	PSC	E	201	52/52	0.81	0.27	42,95,144,175	0
21	EDO	S	103	4/4	0.81	0.26	40,50,56,68	0
21	EDO	Q	203	4/4	0.82	0.22	41,46,57,69	0
21	EDO	P	308	4/4	0.84	0.18	53,62,69,87	0
26	DMU	O	304	22/33	0.86	0.15	43,69,95,113	0
21	EDO	N	610	4/4	0.87	0.20	39,45,49,55	0
23	CHD	C	306	29/29	0.87	0.13	42,54,66,104	0
26	DMU	Z	101	33/33	0.89	0.14	46,58,88,96	0
21	EDO	Q	202	4/4	0.90	0.14	35,43,43,59	0
23	CHD	P	306	29/29	0.90	0.12	46,57,72,86	0
21	EDO	A	613	4/4	0.90	0.15	34,42,61,62	0
21	EDO	O	306	4/4	0.91	0.16	43,43,53,53	0
26	DMU	M	101	33/33	0.92	0.11	36,48,66,80	0
21	EDO	A	611	4/4	0.93	0.13	29,30,33,47	0
21	EDO	N	613	4/4	0.93	0.12	40,47,52,58	0
21	EDO	N	612	4/4	0.94	0.14	33,47,64,72	0
24	PEK	P	302	53/53	0.94	0.15	31,53,96,104	0

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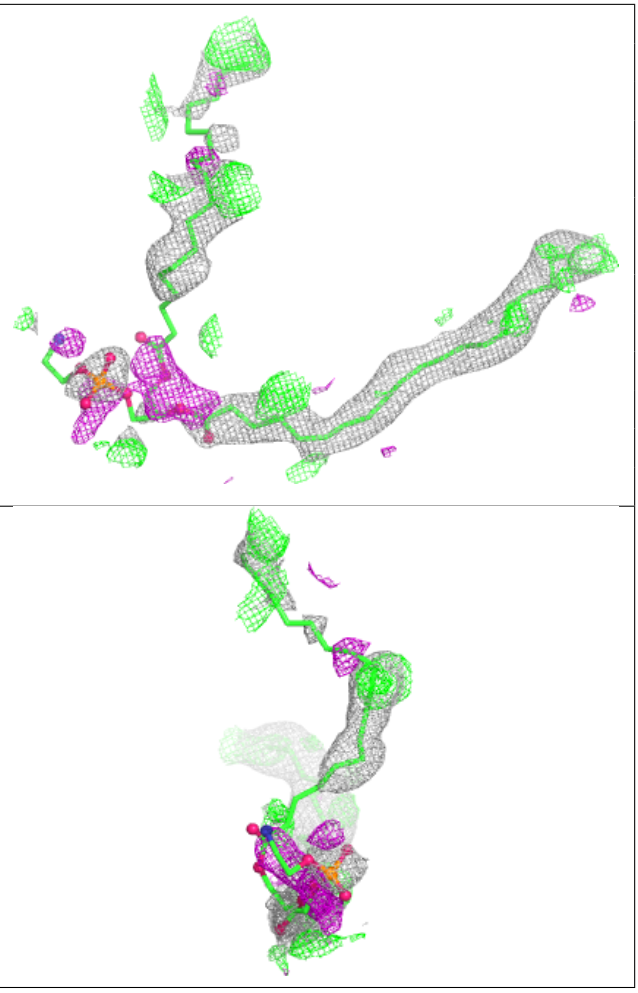
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	PEK	C	302	53/53	0.94	0.13	26,46,92,97	0
21	EDO	P	309	4/4	0.94	0.12	37,41,42,53	0
20	PGV	P	303	51/51	0.95	0.12	24,36,88,99	0
20	PGV	N	609	51/51	0.96	0.11	23,35,75,81	0
21	EDO	A	612	4/4	0.96	0.14	31,38,51,57	0
21	EDO	N	611	4/4	0.96	0.08	31,32,32,40	0
21	EDO	O	305	4/4	0.96	0.08	32,33,36,36	0
21	EDO	N	614	4/4	0.97	0.07	26,33,35,37	0
21	EDO	S	104	4/4	0.97	0.08	40,40,47,58	0
23	CHD	C	301	29/29	0.97	0.06	24,29,35,38	0
20	PGV	C	303	51/51	0.97	0.10	20,33,83,93	0
21	EDO	C	308	4/4	0.97	0.09	34,40,48,56	0
23	CHD	O	302	29/29	0.97	0.06	24,28,36,41	0
23	CHD	P	301	29/29	0.97	0.06	24,31,35,37	0
20	PGV	A	608	51/51	0.97	0.10	20,31,73,85	0
21	EDO	S	102	4/4	0.97	0.07	26,27,29,30	0
18	NA	N	606	1/1	0.98	0.09	34,34,34,34	0
14	HEA	N	601	60/60	0.98	0.06	21,27,44,47	0
21	EDO	B	303	4/4	0.98	0.05	27,27,29,31	0
15	NO	A	603	2/2	0.98	0.06	20,20,20,25	0
21	EDO	F	102	4/4	0.98	0.05	25,25,26,27	0
21	EDO	A	610	4/4	0.98	0.07	24,24,26,29	0
23	CHD	B	302	29/29	0.98	0.05	24,28,35,40	0
18	NA	A	606	1/1	0.98	0.10	29,29,29,29	0
14	HEA	A	601	60/60	0.99	0.05	16,22,37,41	0
14	HEA	N	602	60/60	0.99	0.05	21,25,31,37	0
14	HEA	A	602	60/60	0.99	0.05	17,21,28,34	0
15	NO	N	603	2/2	0.99	0.04	26,26,26,27	0
16	CU	A	604	1/1	1.00	0.01	22,22,22,22	0
16	CU	N	604	1/1	1.00	0.01	24,24,24,24	0
22	CUA	B	301	2/2	1.00	0.01	23,23,23,23	0
22	CUA	O	301	2/2	1.00	0.02	28,28,28,28	0
17	MG	A	605	1/1	1.00	0.05	19,19,19,19	0
17	MG	N	605	1/1	1.00	0.07	24,24,24,24	0
28	ZN	F	101	1/1	1.00	0.04	29,29,29,29	0
28	ZN	S	101	1/1	1.00	0.03	31,31,31,31	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.

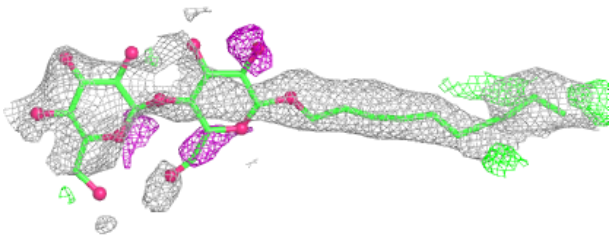
Electron density around PEK G 103:

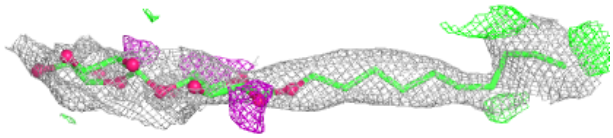
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

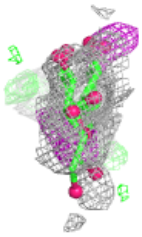


Electron density around DMU P 307:

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

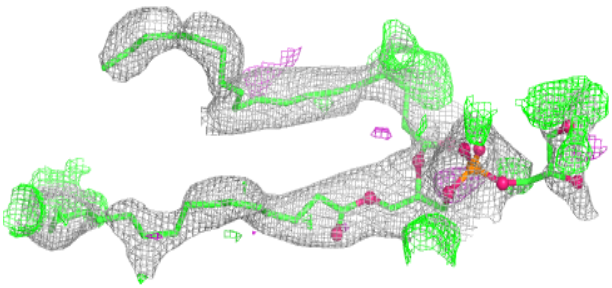


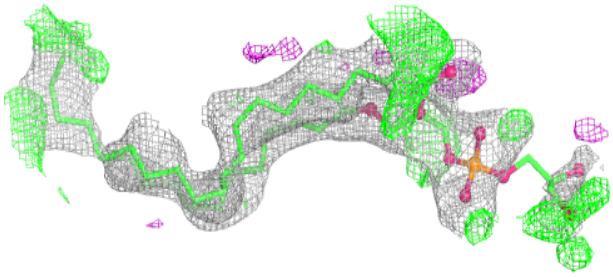


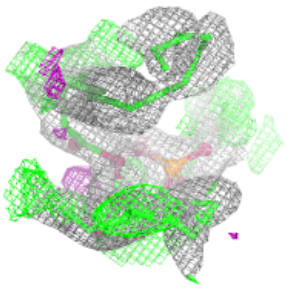


Electron density around PGV P 304:

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

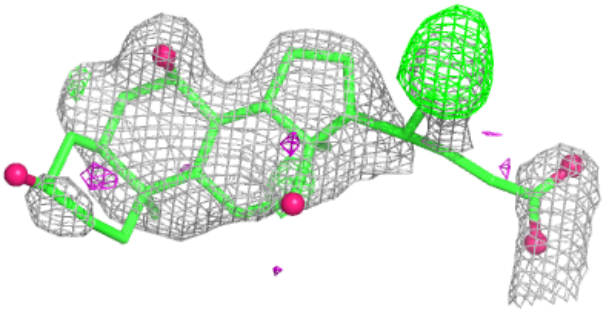


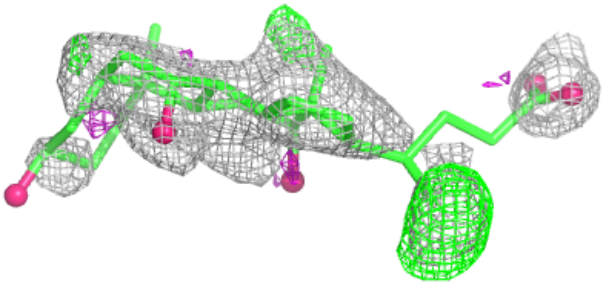


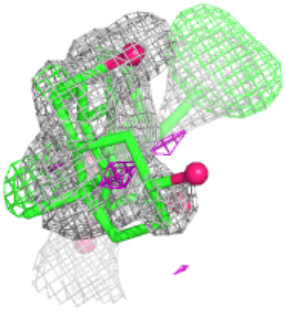


Electron density around CHD J 101:

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

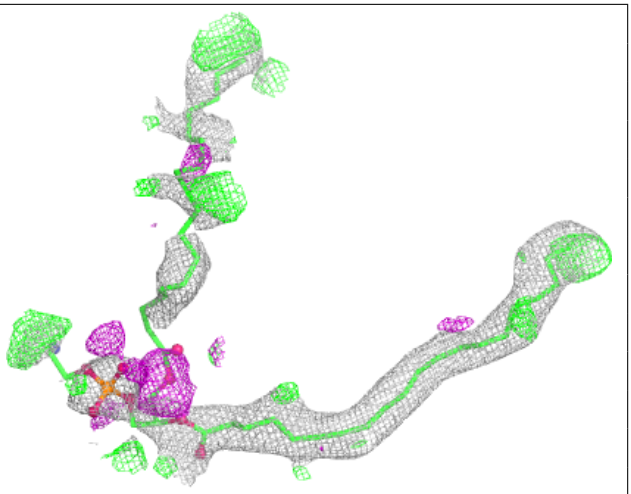


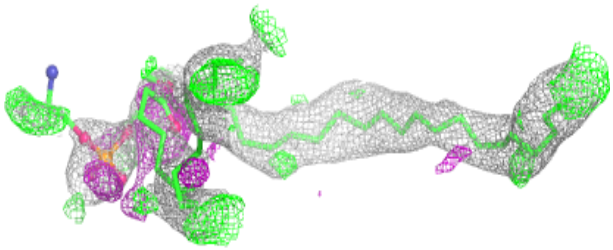


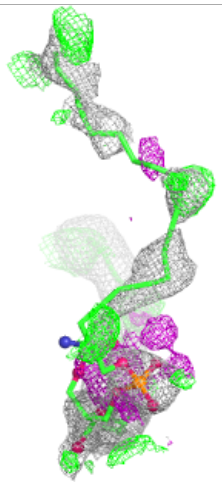


Electron density around PEK T 102:

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

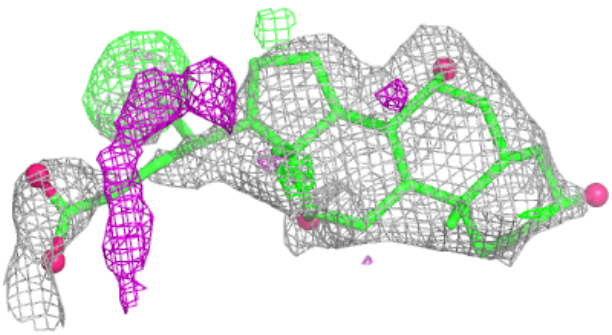


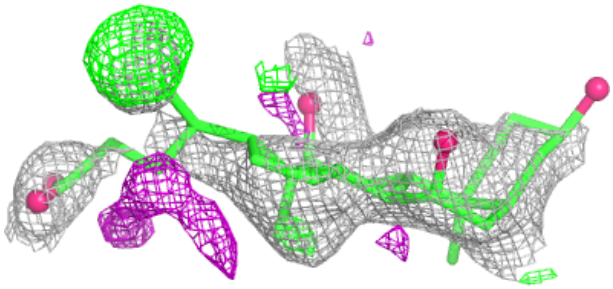


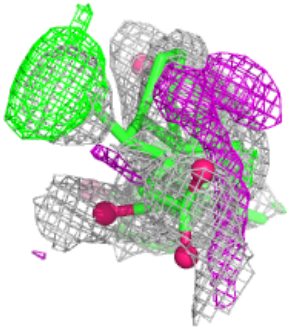


Electron density around CHD W 101:

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

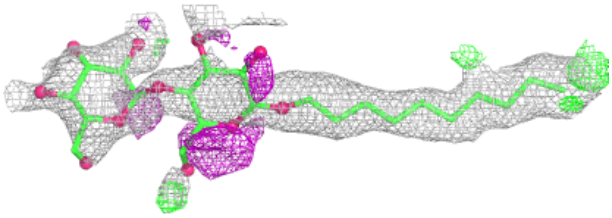


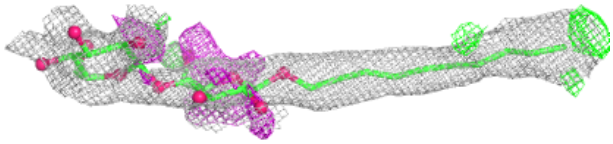


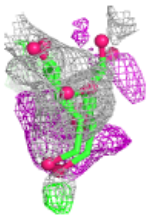


Electron density around DMU C 307:

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

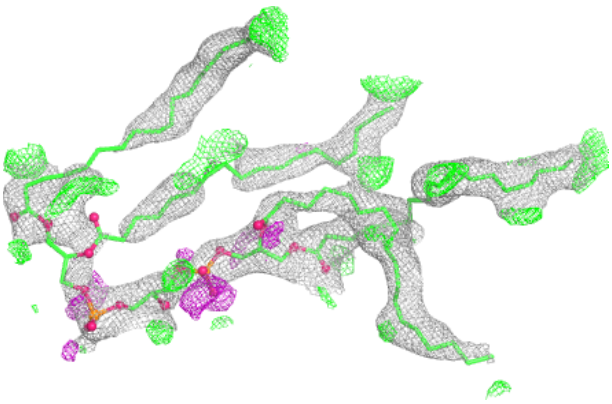


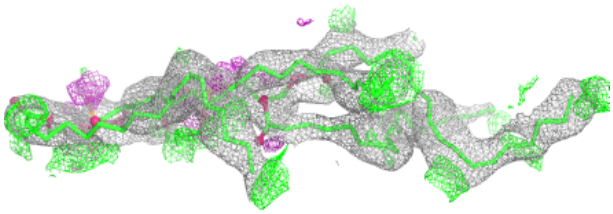


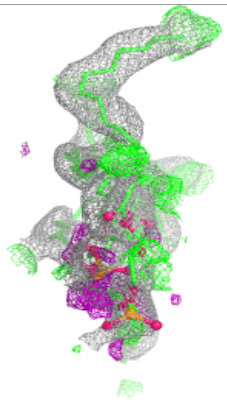


Electron density around CDL T 103:

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

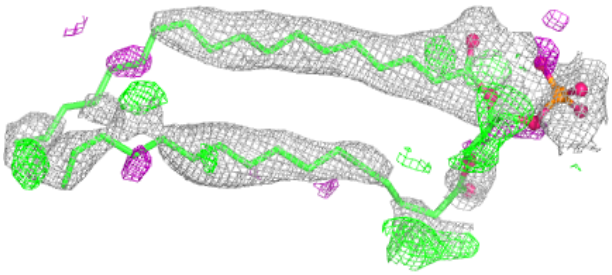


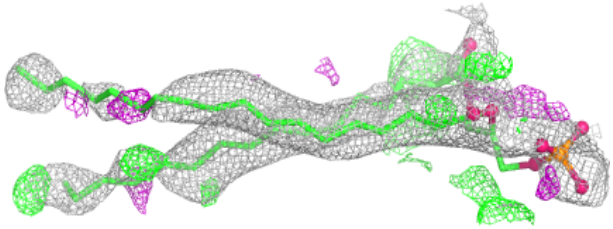


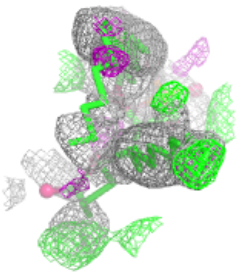


Electron density around PGV N 608:

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

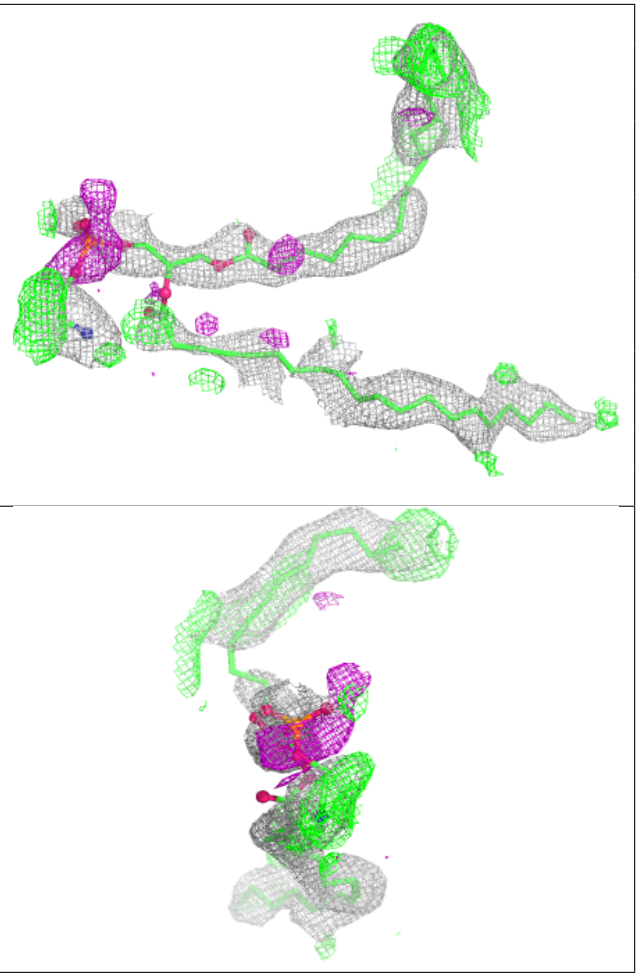






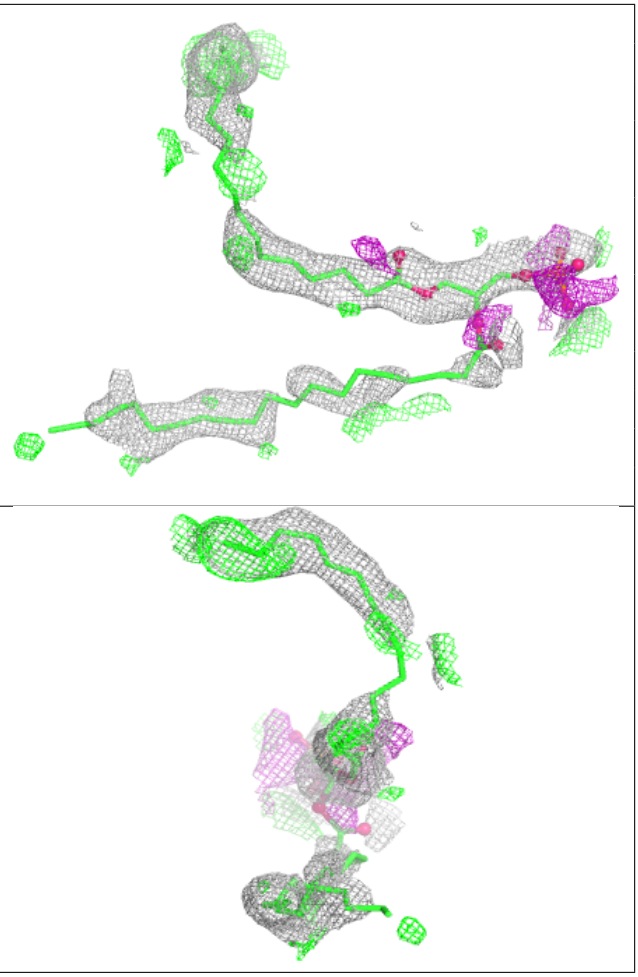
Electron density around PEK T 101:

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



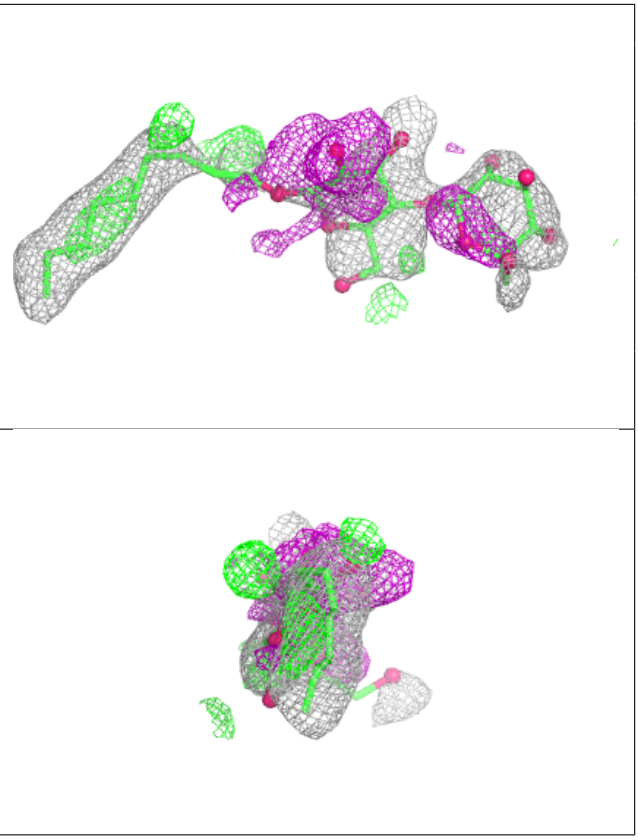
Electron density around PEK G 101:

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



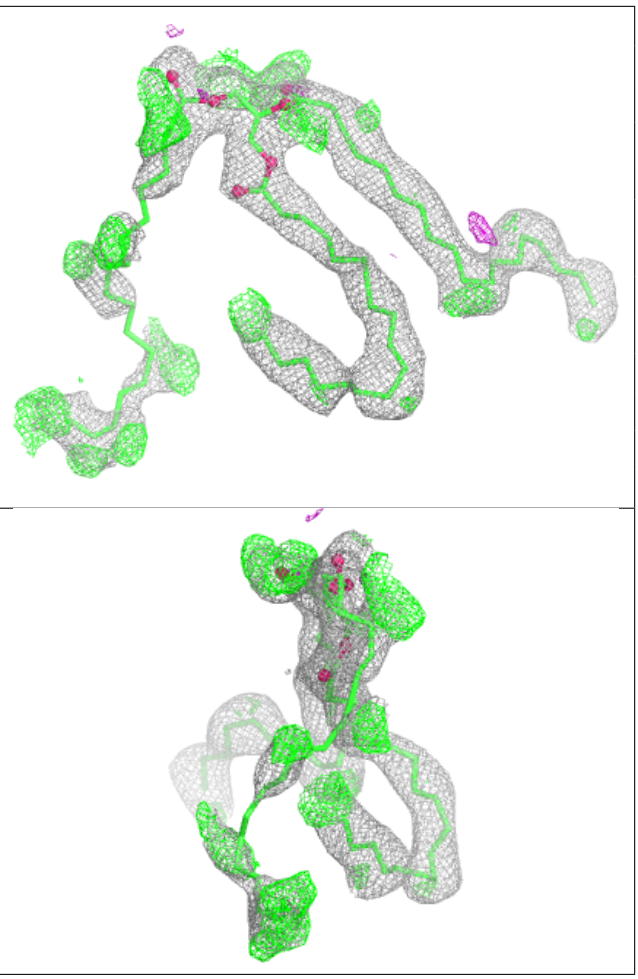
Electron density around DMU W 102:

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



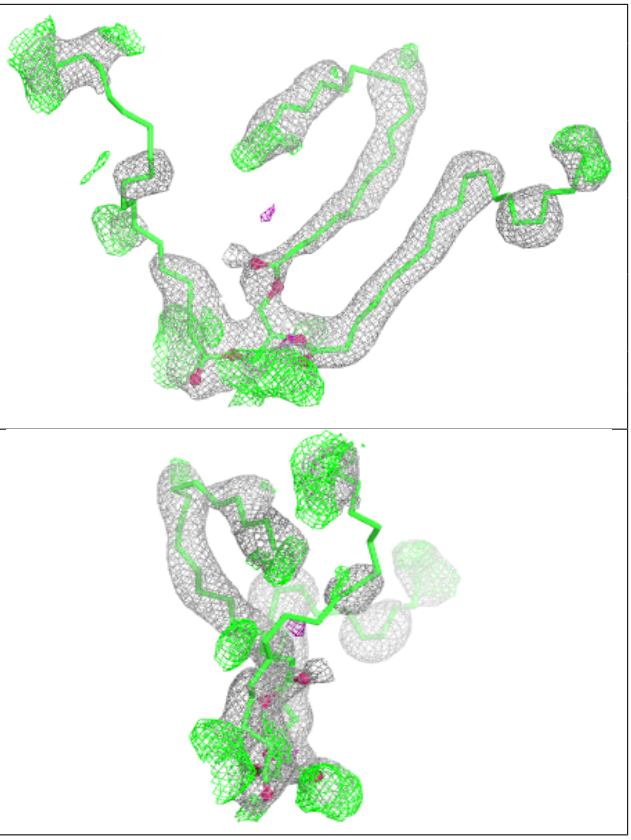
Electron density around TGL D 201:

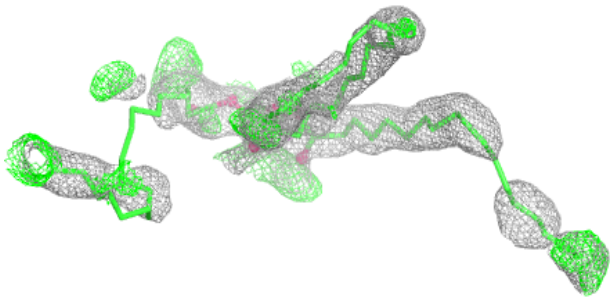
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around TGL Q 201:

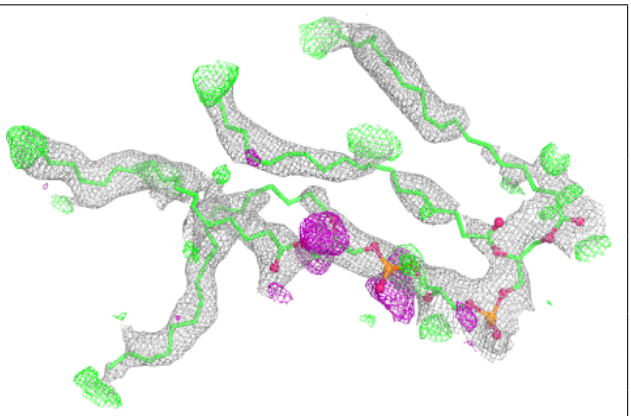
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

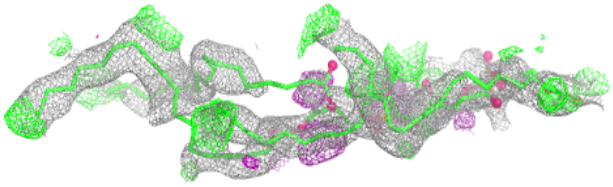


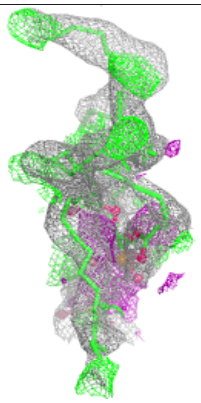


Electron density around CDL G 102:

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

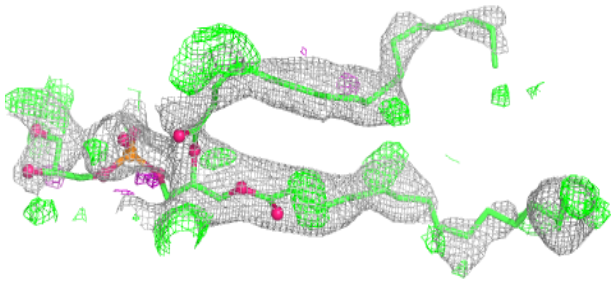


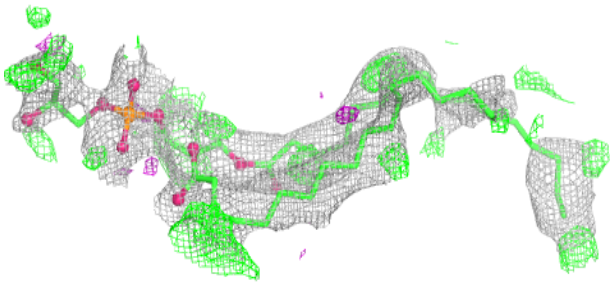


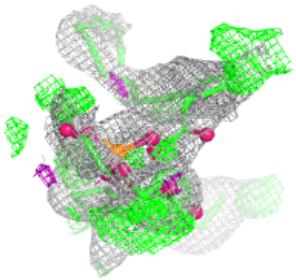


Electron density around PGV C 304:

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

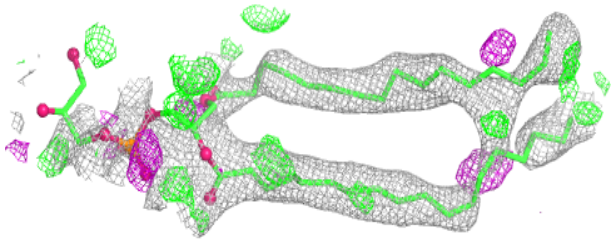


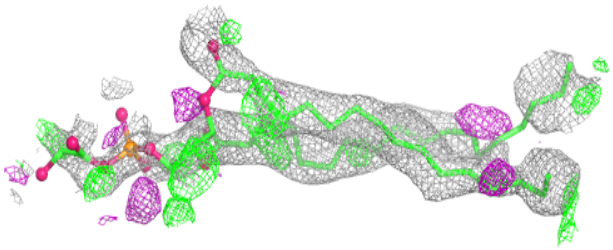


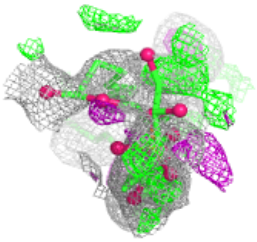


Electron density around PGV A 609:

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

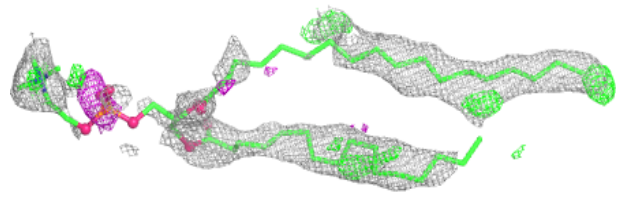


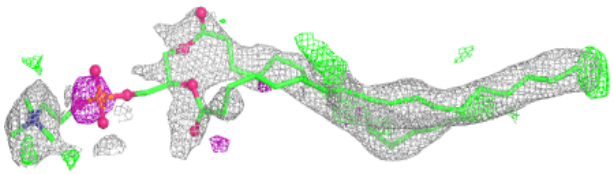


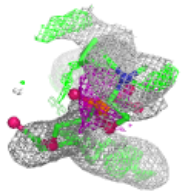


Electron density around PSC R 201:

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

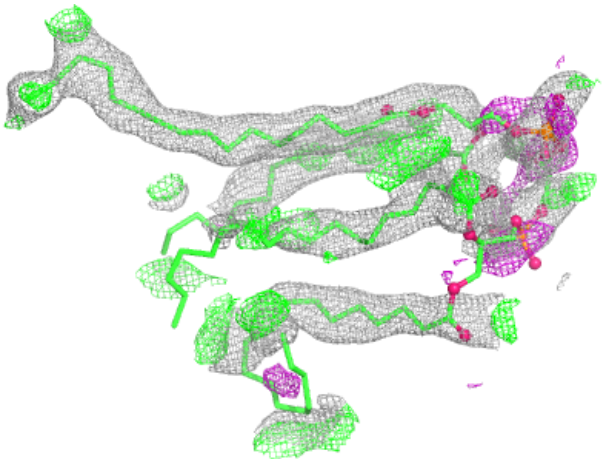


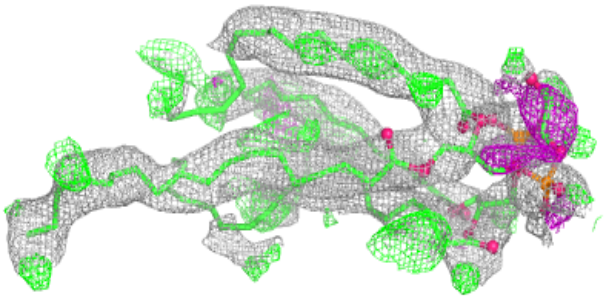


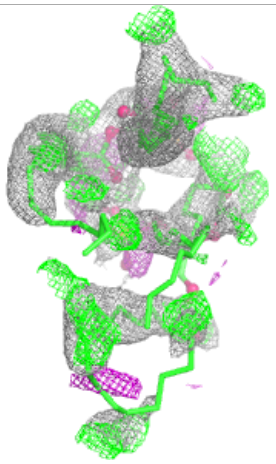


Electron density around CDL P 305:

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

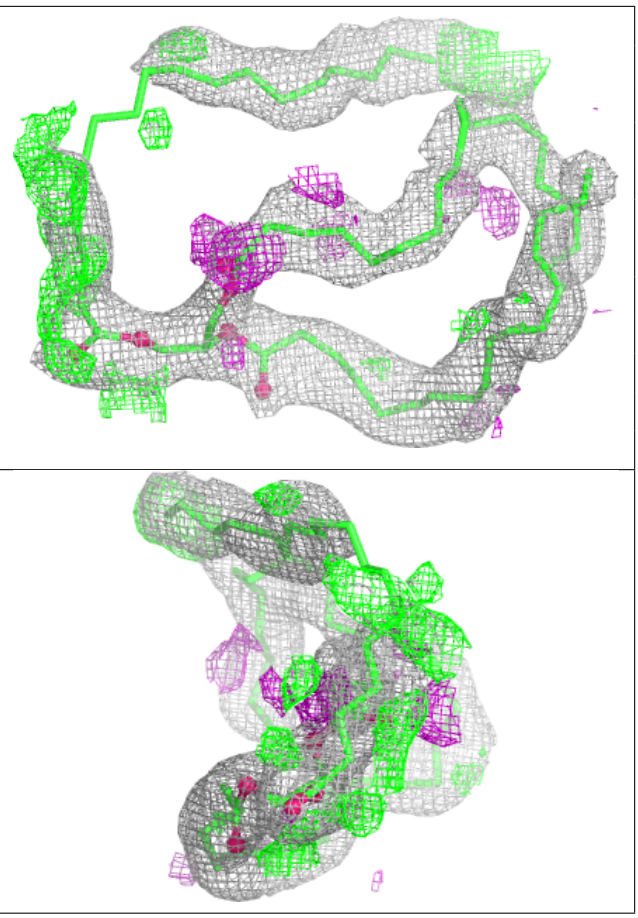






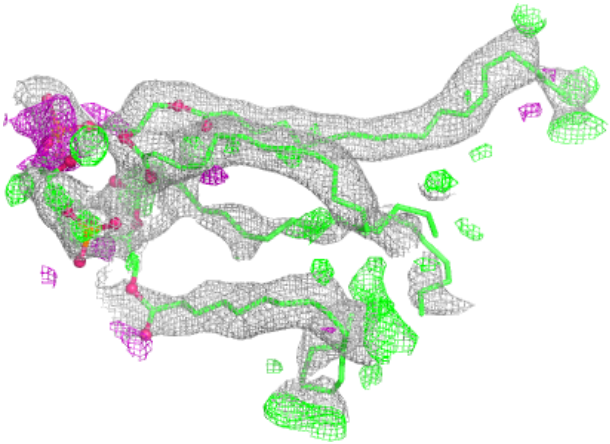
Electron density around TGL A 607:

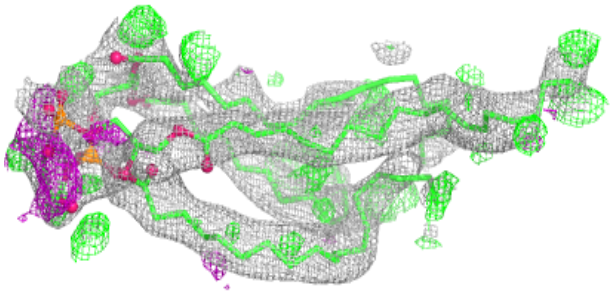
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

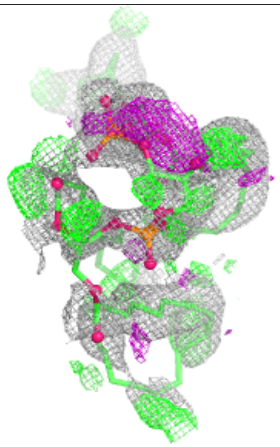


Electron density around CDL C 305:

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

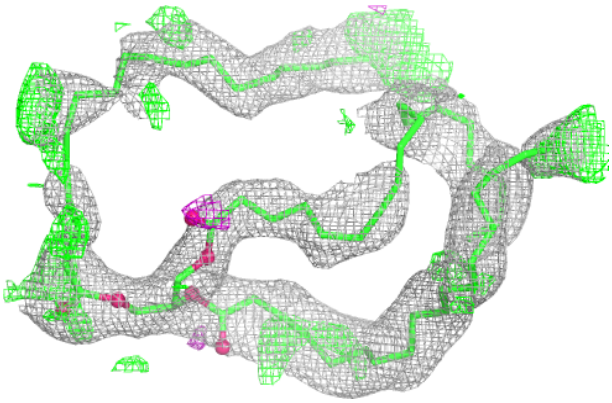


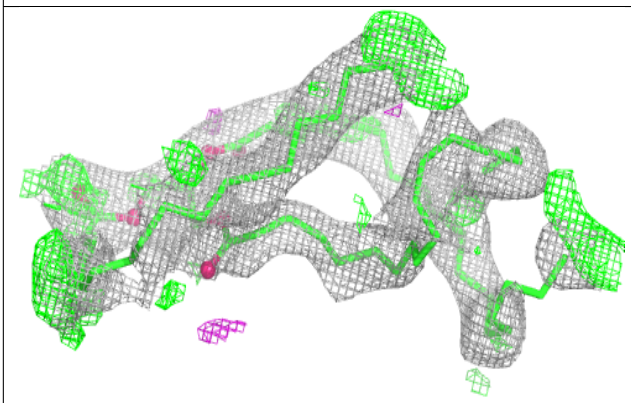


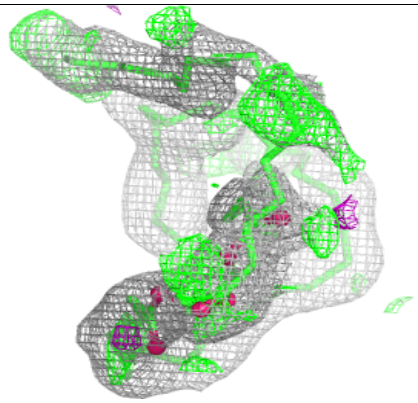


Electron density around TGL O 303:

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

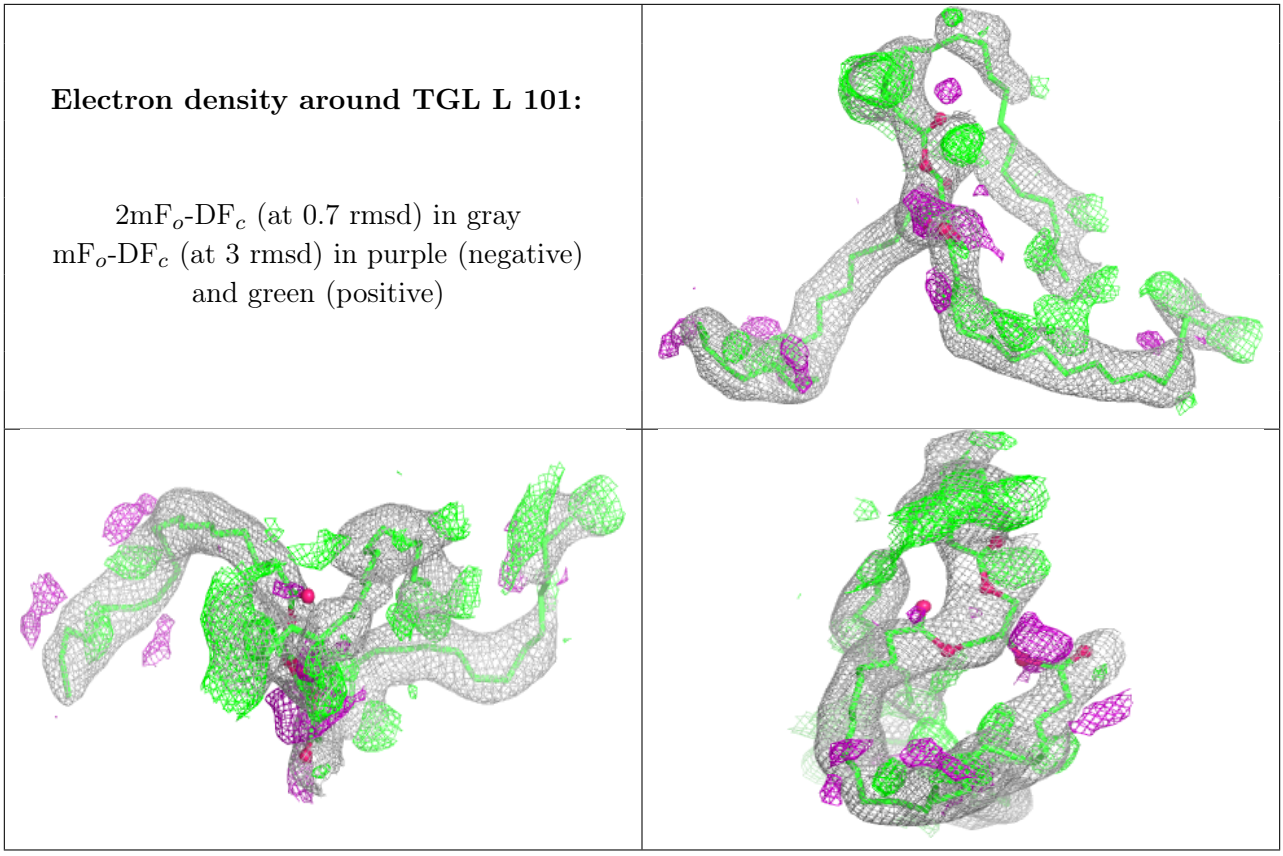






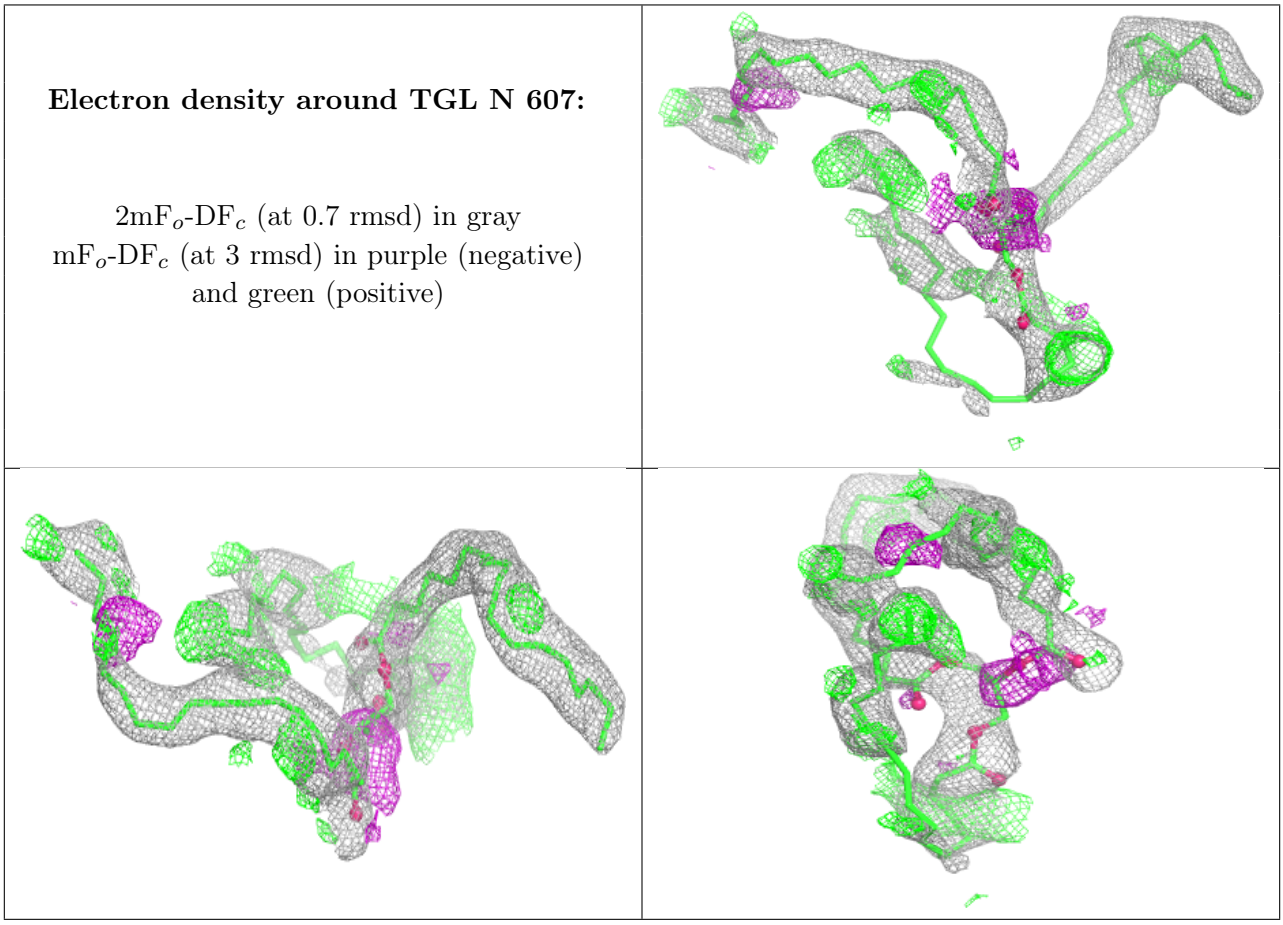
Electron density around TGL L 101:

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



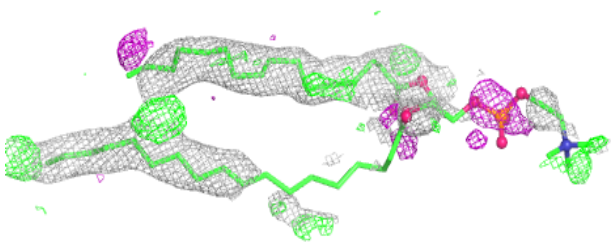
Electron density around TGL N 607:

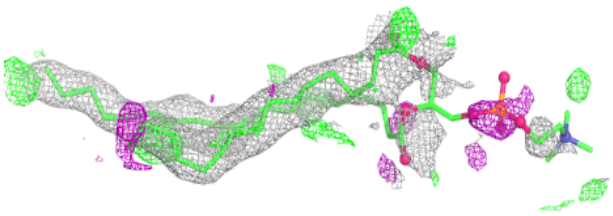
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

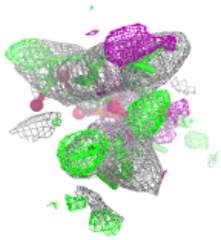


Electron density around PSC E 201:

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

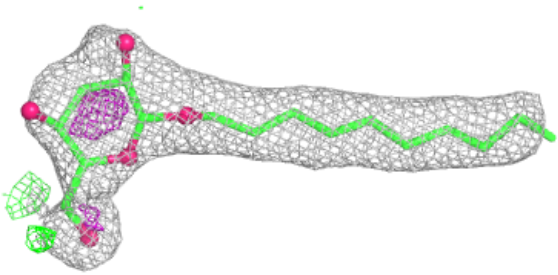


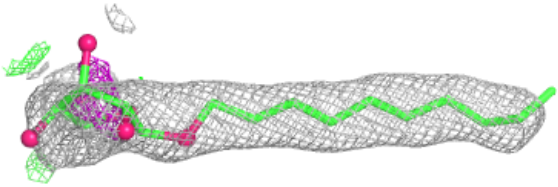


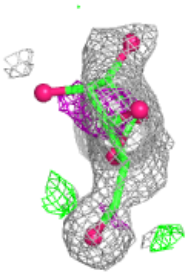


Electron density around DMU O 304:

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

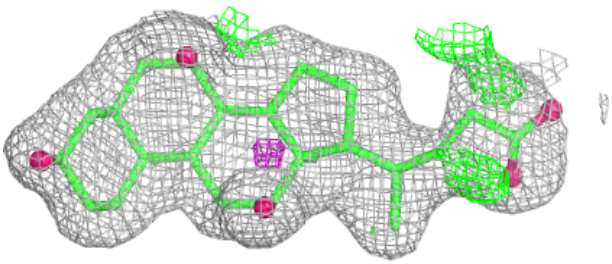


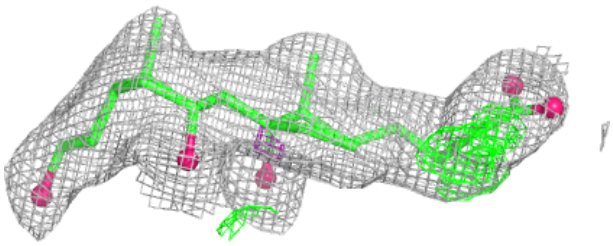


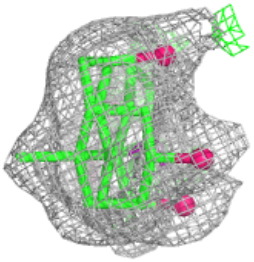


Electron density around CHD C 306:

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

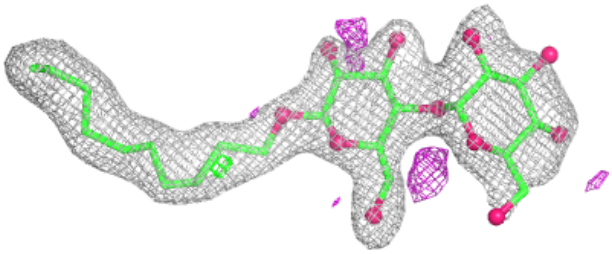


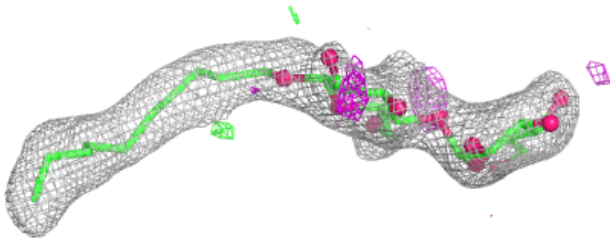


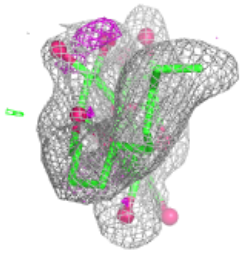


Electron density around DMU Z 101:

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

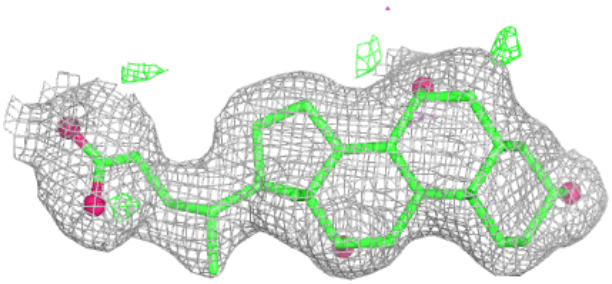


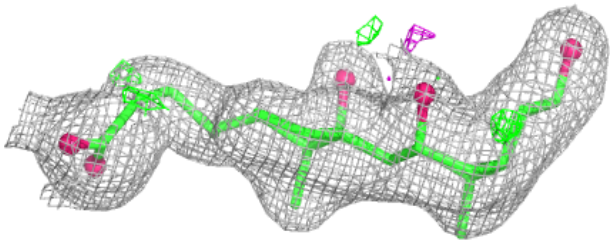


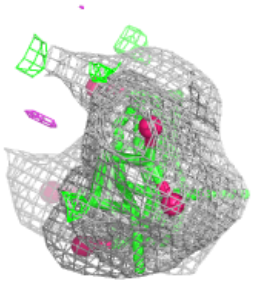


Electron density around CHD P 306:

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

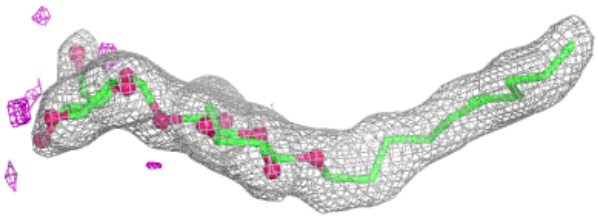


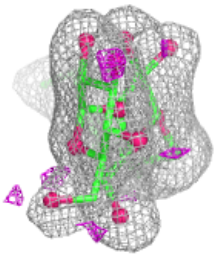




Electron density around DMU M 101:

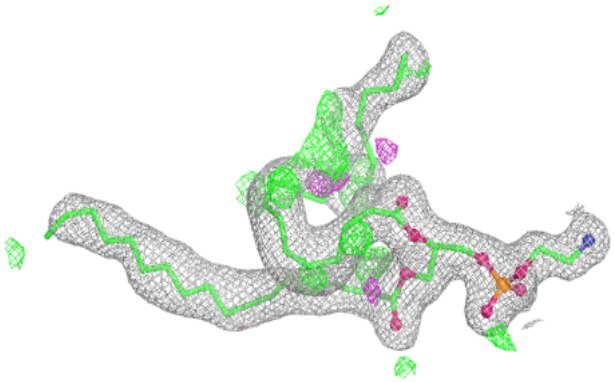
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

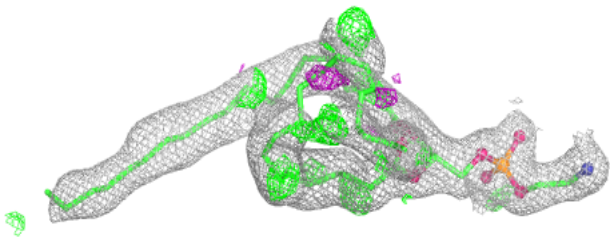


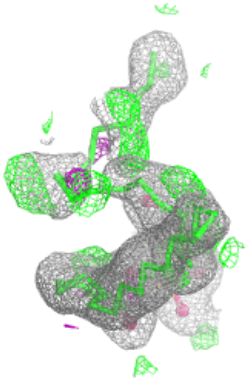


Electron density around PEK P 302:

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

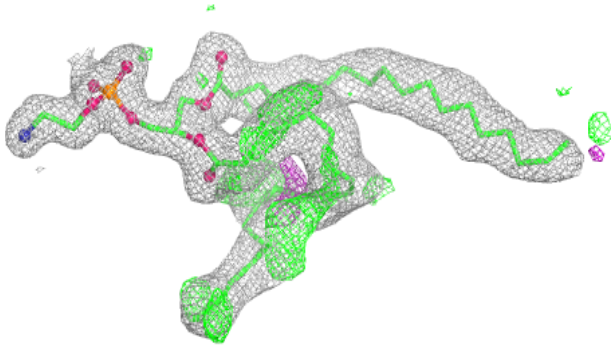


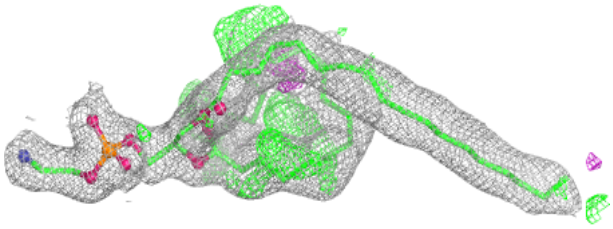




Electron density around PEK C 302:

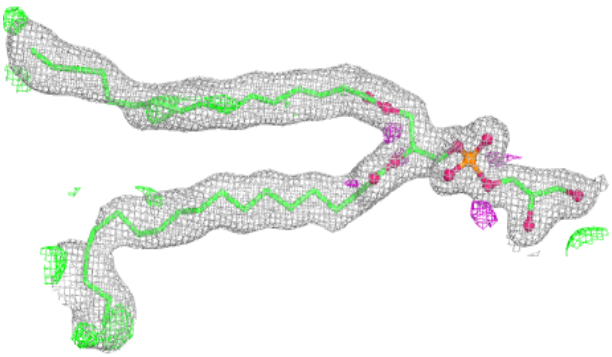
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

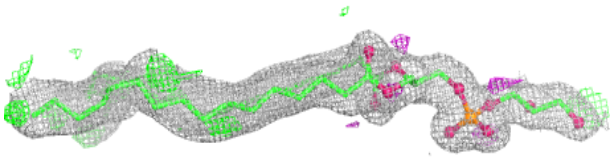


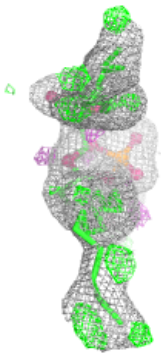


Electron density around PGV P 303:

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

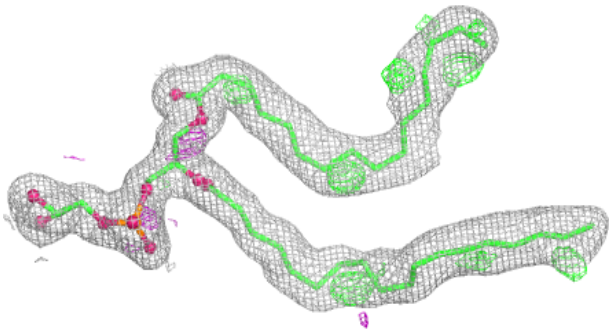


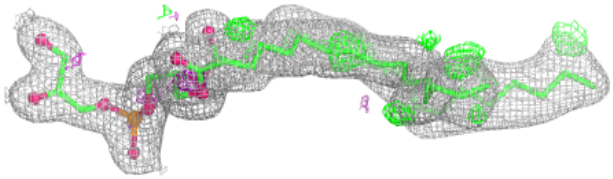


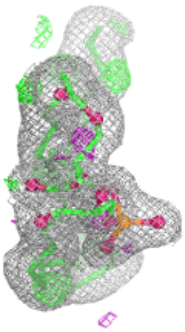


Electron density around PGV N 609:

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

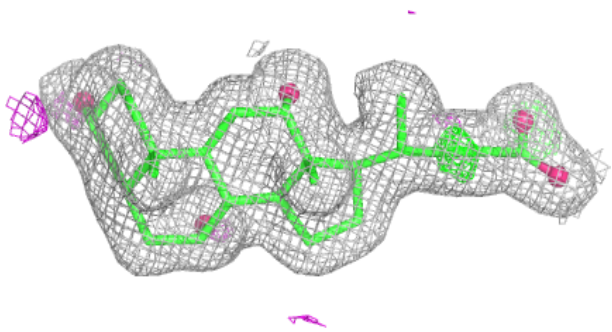


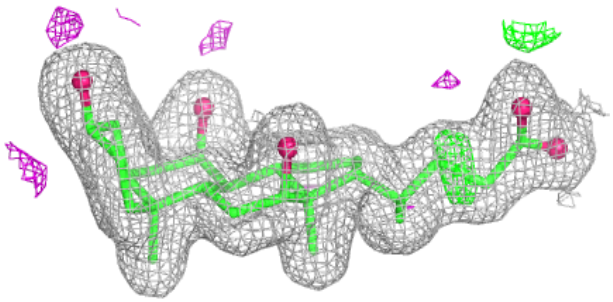


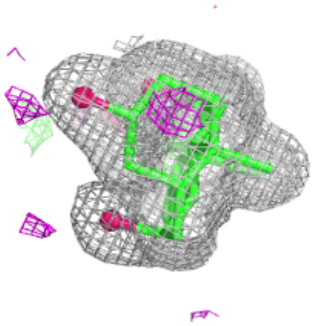


Electron density around CHD C 301:

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

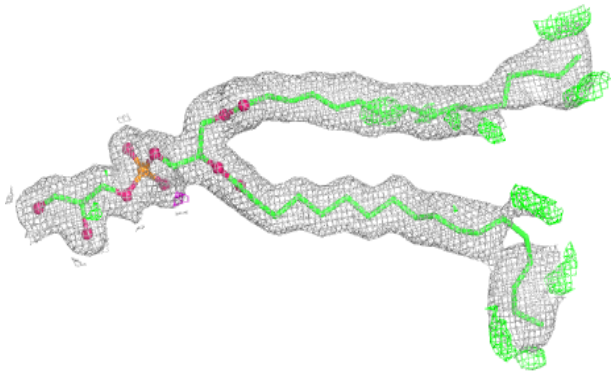


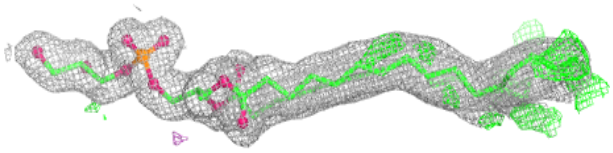


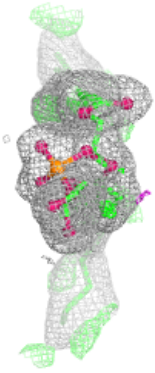


Electron density around PGV C 303:

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

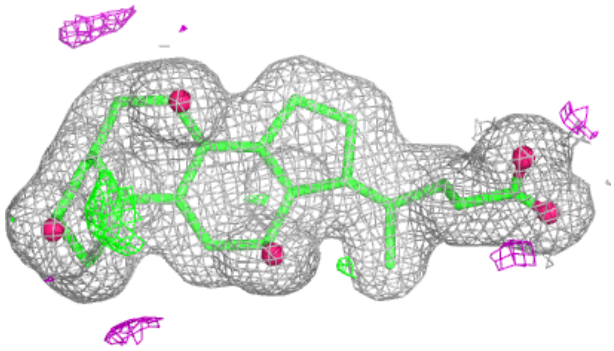


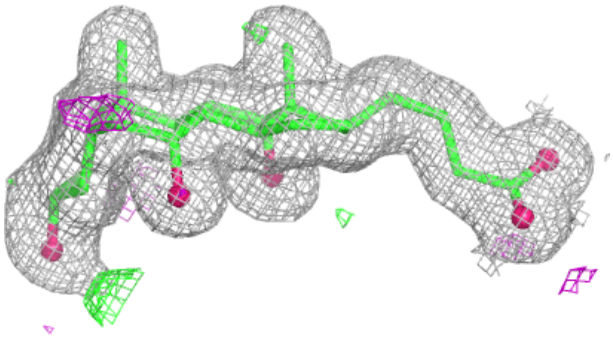


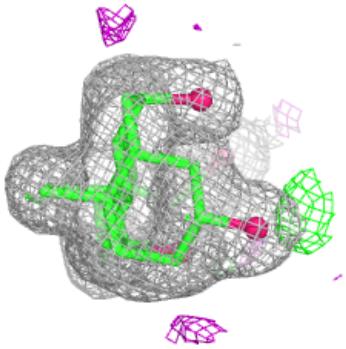


Electron density around CHD O 302:

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

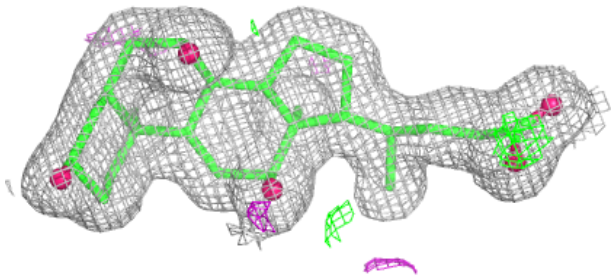


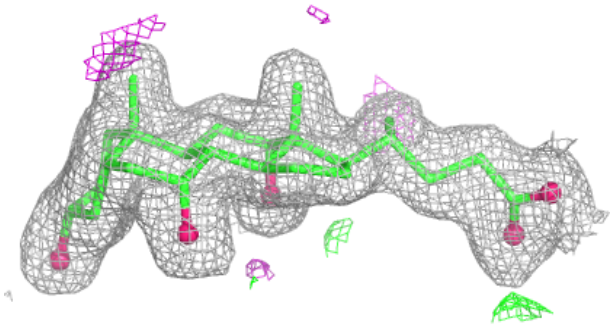


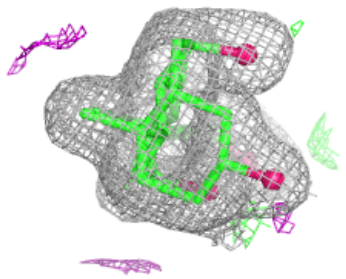


Electron density around CHD P 301:

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

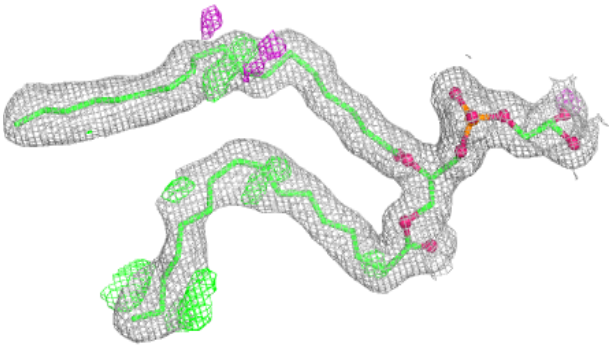


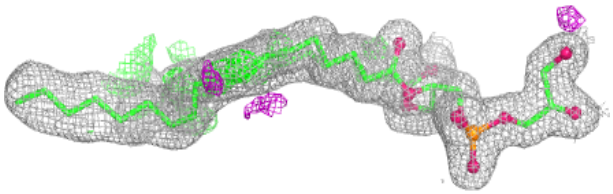


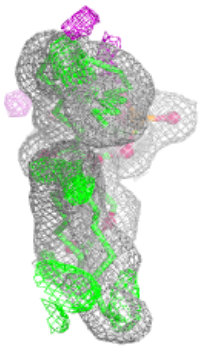


Electron density around PGV A 608:

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

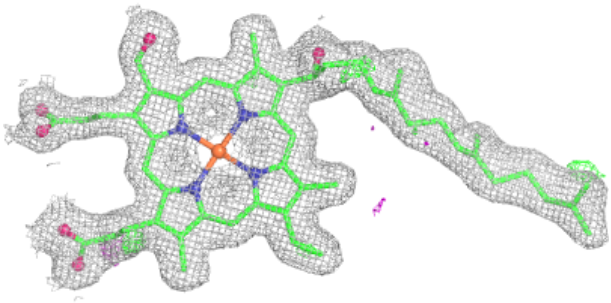


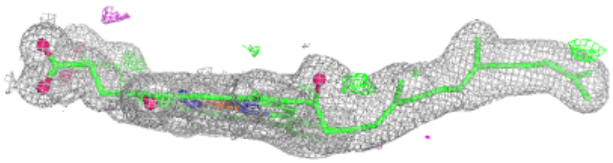


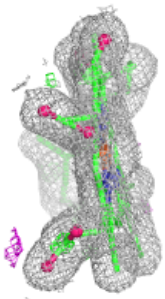


Electron density around HEA N 601:

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

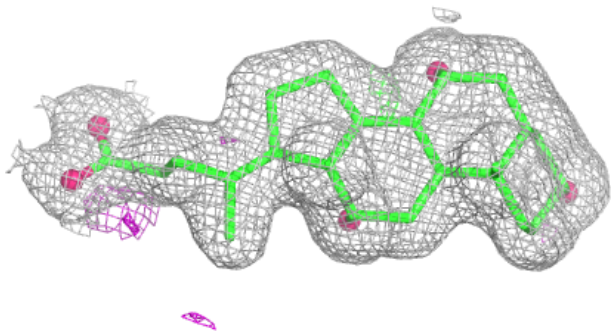


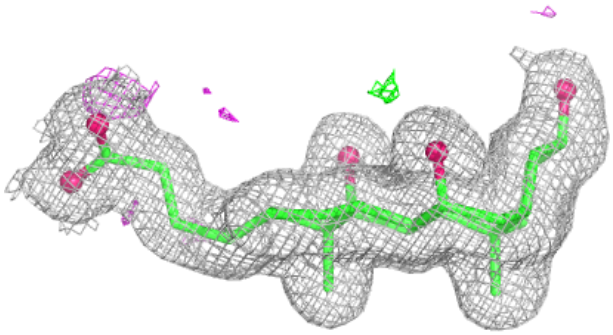


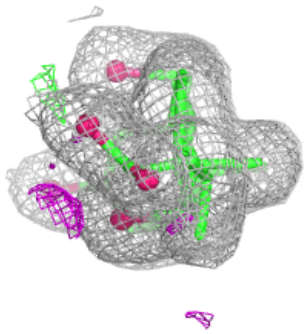


Electron density around CHD B 302:

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

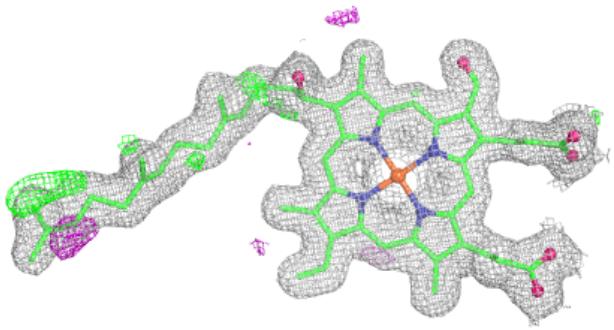


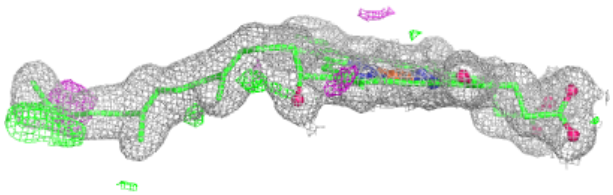


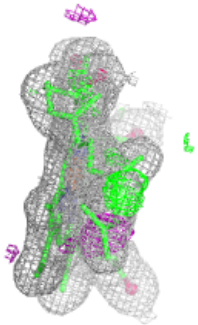


Electron density around HEA A 601:

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

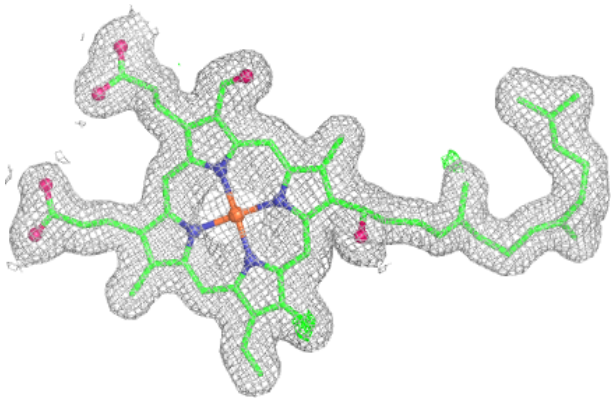


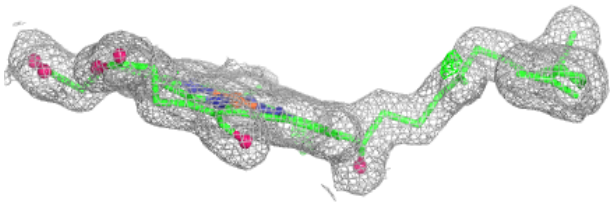


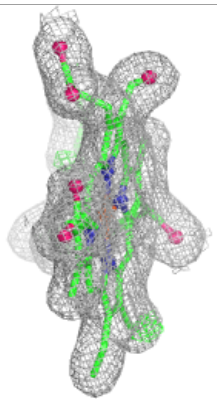


Electron density around HEA N 602:

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

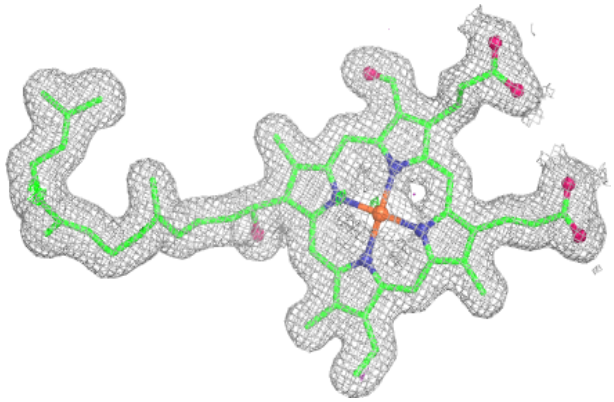


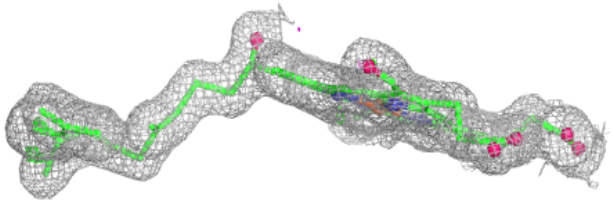


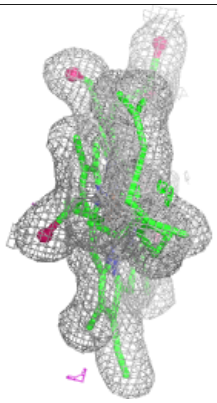


Electron density around HEA A 602:

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







6.5 Other polymers (i)

There are no such residues in this entry.