wwPDB X-ray Structure Validation Summary Report (i)

Aug 5, 2026 – 10:42 AM EDT

PDB ID	:	3AG4 / pdb_00003ag4
Title	:	Bovine Heart Cytochrome c Oxidase in the Cyanide Ion-bound Fully Reduced State at 100 K
Authors	:	Muramoto, K.; Ohta, K.; Shinzawa-Itoh, K.; Kanda, K.; Taniguchi, M.; Nabekura, H.; Yamashita, E.; Tsukihara, T.; Yoshikawa, S.
Deposited on	:	2010-03-19
Resolution	:	2.05 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 (1)) were used in the production of this report:

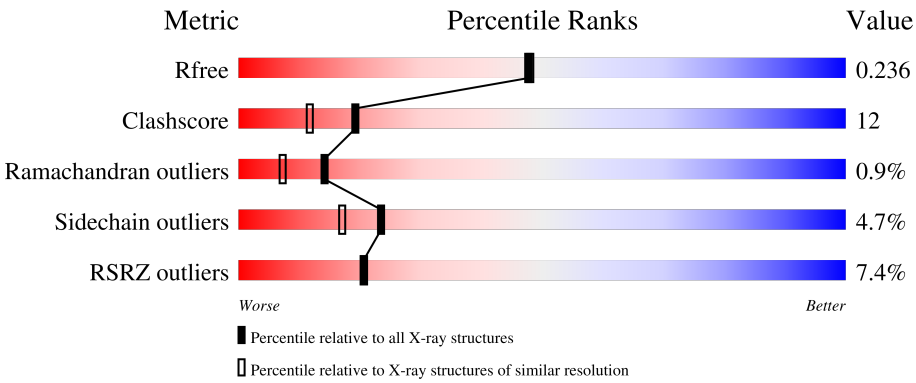
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.05 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	% 65% 31% •
1	N	514	3% 70% 25% •
2	B	227	7% 72% 22% 5% •
2	O	227	12% 68% 26% 5% •

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Mol	Chain	Length	Quality of chain
3	C	261	% 75% 21%
3	P	261	3% 74% 23%
4	D	147	3% 77% 18%
4	Q	147	18% 78% 18%
5	E	109	2% 78% 17%
5	R	109	5% 72% 20%
6	F	98	9% 71% 22%
6	S	98	12% 68% 21% 8%
7	G	85	24% 61% 27% 8%
7	T	85	22% 56% 25% 15%
8	H	85	15% 71% 18% 5% 7%
8	U	85	13% 67% 22% 7%
9	I	73	18% 79% 21%
9	V	73	21% 67% 29%
10	J	59	7% 80% 17%
10	W	59	10% 83% 10% 5%
11	K	56	4% 73% 14% 12%
11	X	56	16% 79% 7% 12%
12	L	47	4% 60% 36%
12	Y	47	6% 57% 26% 13%
13	M	46	9% 59% 26% 9% 7%
13	Z	46	13% 65% 28% 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
15	CYN	N	520	-	-	X	-
22	CHD	C	271	X	-	-	-
22	CHD	J	60	X	-	-	-
22	CHD	P	1271	X	-	-	-
22	CHD	W	1059	X	-	-	-
23	UNX	C	262	-	-	-	X
23	UNX	P	262	-	-	-	X
25	CDL	C	270	-	-	X	-
25	CDL	G	269	-	-	X	-
25	CDL	T	1269	-	-	X	-
28	DMU	G	272	X	-	-	-
28	DMU	M	526	X	-	-	-
28	DMU	P	1272	X	-	-	-
28	DMU	Z	1526	X	-	-	-

2 Entry composition (i)

There are 29 unique types of molecules in this entry. The entry contains 32324 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	4027	2691	623	678	35	0	0	0
1	N	514	4027	2691	623	678	35	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	227	1824	1185	281	340	18	0	0	0
2	O	227	1824	1185	281	340	18	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	259	2110	1412	336	350	12	0	0	0
3	P	259	2110	1412	336	350	12	0	0	0

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

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.

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.

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 polypeptide 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.

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

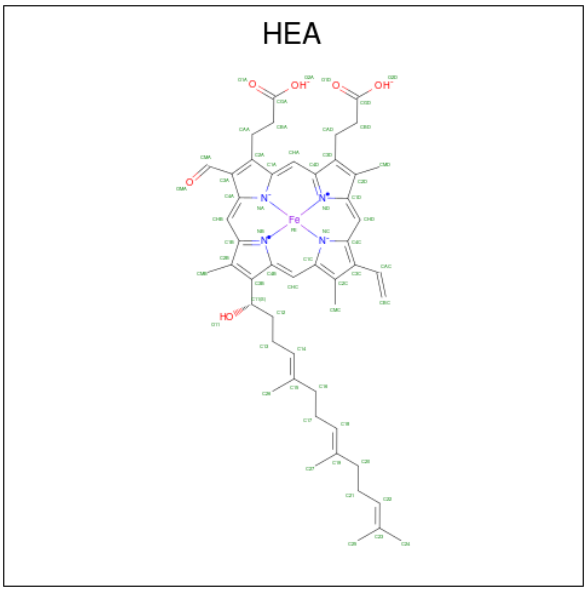
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C.

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.

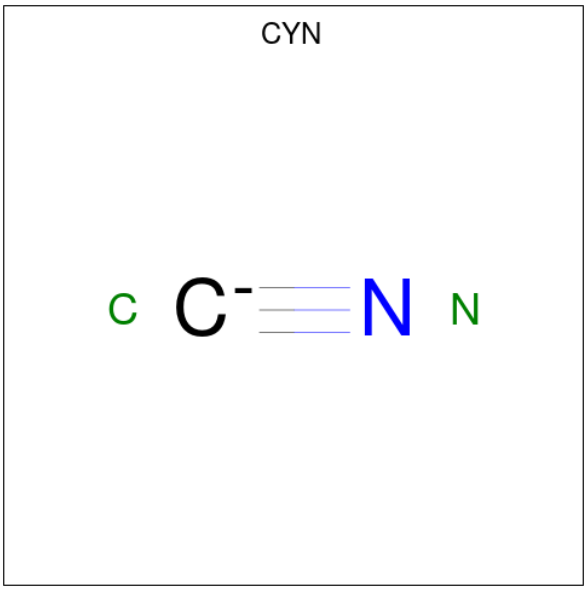
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
13	M	43	335	223	53	59	0	0	0
			Total	C	N	O			
13	Z	43	335	223	53	59	0	0	0

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



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 CYANIDE ION (CCD ID: CYN) (formula: CN).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
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

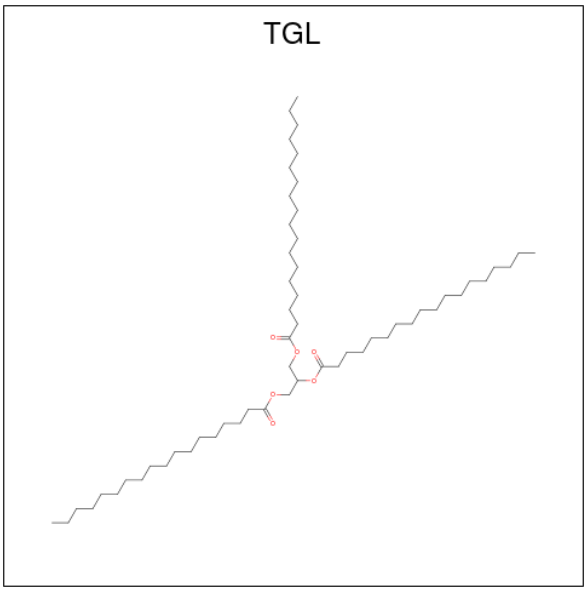
- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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).

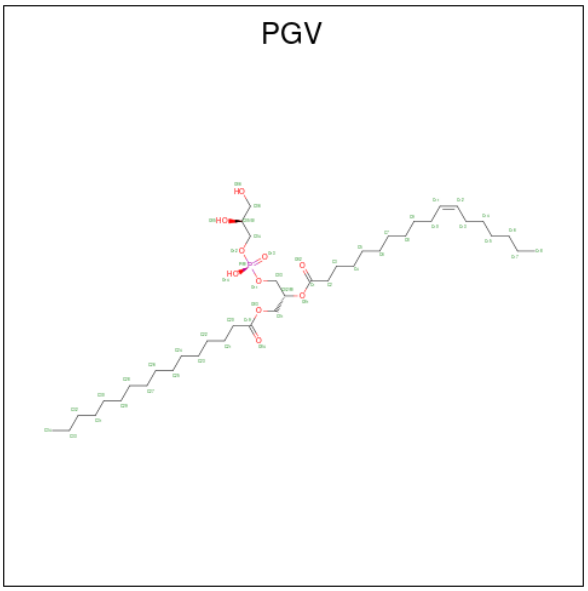
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
18	A	1	1	1	0	0
18	N	1	1	1	0	0

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



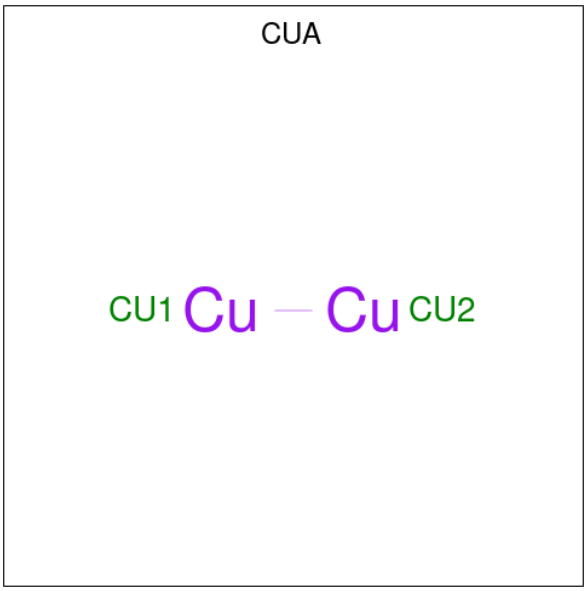
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
19	A	1	63	57	6	0	0
19	D	1	63	57	6	0	0
19	L	1	63	57	6	0	0
19	N	1	63	57	6	0	0
19	N	1	63	57	6	0	0
19	Q	1	63	57	6	0	0

- 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: $C_{40}H_{77}O_{10}P$).



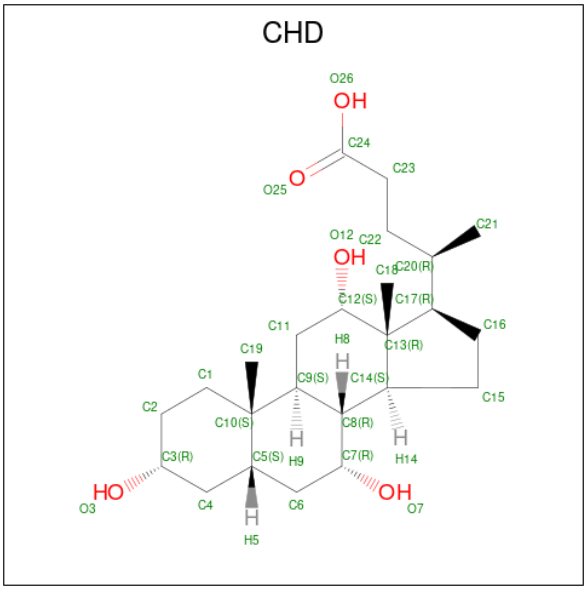
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
20	A	1	51	40	10	1	0	0
			Total	C	O	P		
20	A	1	51	40	10	1	0	0
			Total	C	O	P		
20	C	1	51	40	10	1	0	0
			Total	C	O	P		
20	C	1	51	40	10	1	0	0
			Total	C	O	P		
20	N	1	51	40	10	1	0	0
			Total	C	O	P		
20	N	1	51	40	10	1	0	0
			Total	C	O	P		
20	P	1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

- Molecule 21 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu_2).



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

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



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

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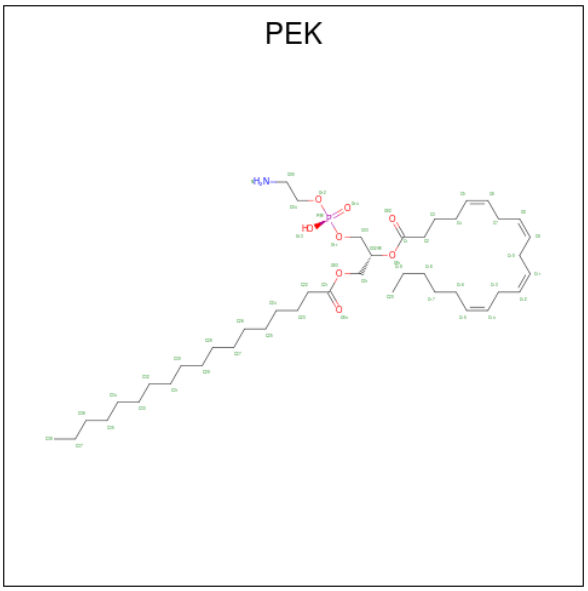
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
22	C	1	29	24	5	0	0
22	J	1	29	24	5	0	0
22	O	1	29	24	5	0	0
22	P	1	29	24	5	0	0
22	P	1	29	24	5	0	0
22	W	1	29	24	5	0	0

- Molecule 23 is UNKNOWN LIGAND (CCD ID: UNX) (formula: X).

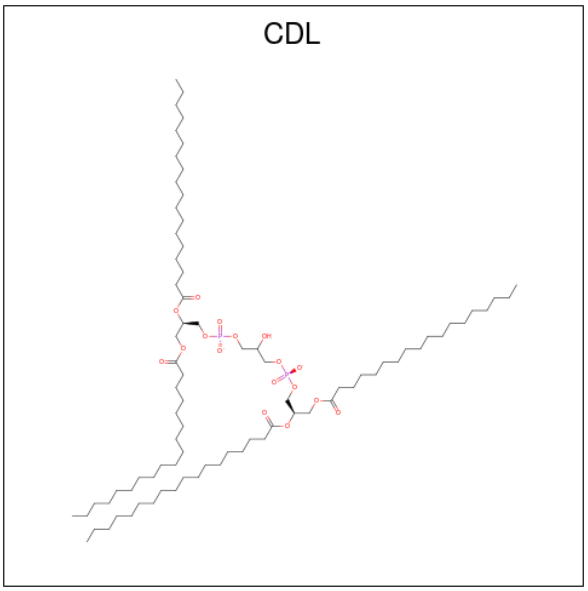
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	X		
23	C	1	1	1	0	0
23	P	1	Total	X	0	0
			1	1		

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



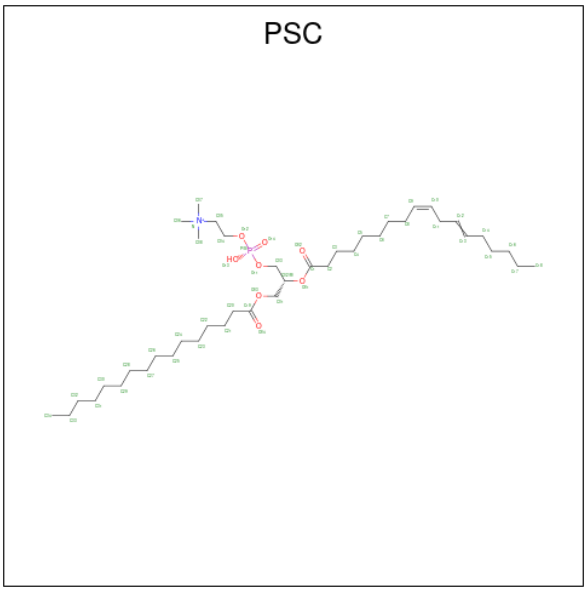
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
24	C	1	53	43	1	8	1	0	0
24	G	1	53	43	1	8	1	0	0
24	G	1	53	43	1	8	1	0	0
24	S	1	53	43	1	8	1	0	0
24	T	1	53	43	1	8	1	0	0
24	T	1	53	43	1	8	1	0	0

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



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

- Molecule 26 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: $C_{42}H_{81}NO_8P$).

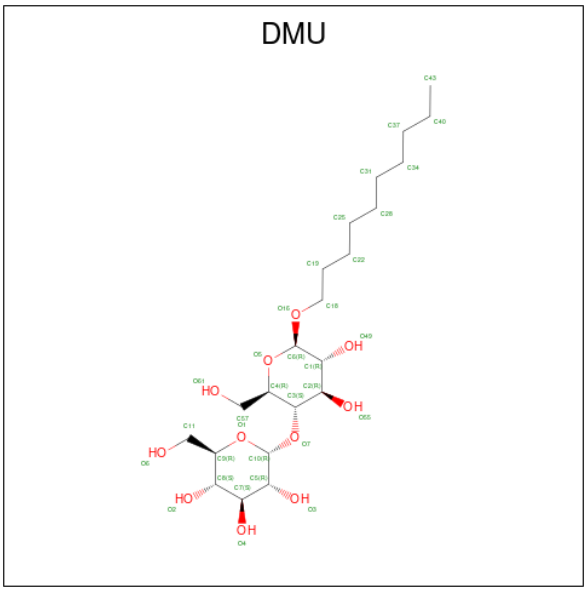


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
26	E	1	52	42	1	8	1	0	0
			Total	C	N	O	P		
26	R	1	52	42	1	8	1	0	0

- Molecule 27 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 28 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: $C_{22}H_{42}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
28	G	1	33	22	11	0	0
			Total	C	O		
28	M	1	33	22	11	0	0
			Total	C	O		
28	P	1	33	22	11	0	0
			Total	C	O		
28	Z	1	33	22	11	0	0

- Molecule 29 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
29	A	225	225	225	0	0
			Total	O		
29	B	125	125	125	0	0
			Total	O		
29	C	106	106	106	0	0
			Total	O		
29	D	91	91	91	0	0
			Total	O		
29	E	62	62	62	0	0
			Total	O		
29	F	75	75	75	0	0
			Total	O		
29	G	41	41	41	0	0
			Total	O		
29	H	47	47	47	0	0

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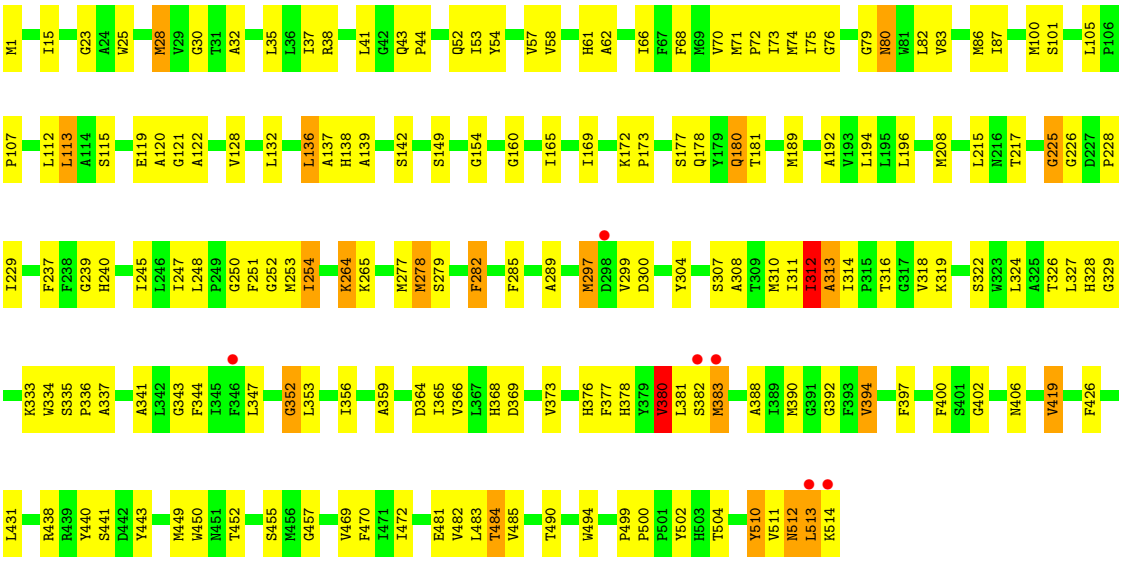
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	I	38	Total O 38 38	0	0
29	J	20	Total O 20 20	0	0
29	K	20	Total O 20 20	0	0
29	L	22	Total O 22 22	0	0
29	M	15	Total O 15 15	0	0
29	N	199	Total O 199 199	0	0
29	O	107	Total O 107 107	0	0
29	P	100	Total O 100 100	0	0
29	Q	55	Total O 55 55	0	0
29	R	40	Total O 40 40	0	0
29	S	56	Total O 56 56	0	0
29	T	36	Total O 36 36	0	0
29	U	41	Total O 41 41	0	0
29	V	18	Total O 18 18	0	0
29	W	12	Total O 12 12	0	0
29	X	14	Total O 14 14	0	0
29	Y	12	Total O 12 12	0	0
29	Z	11	Total O 11 11	0	0

3 Residue-property plots (i)

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

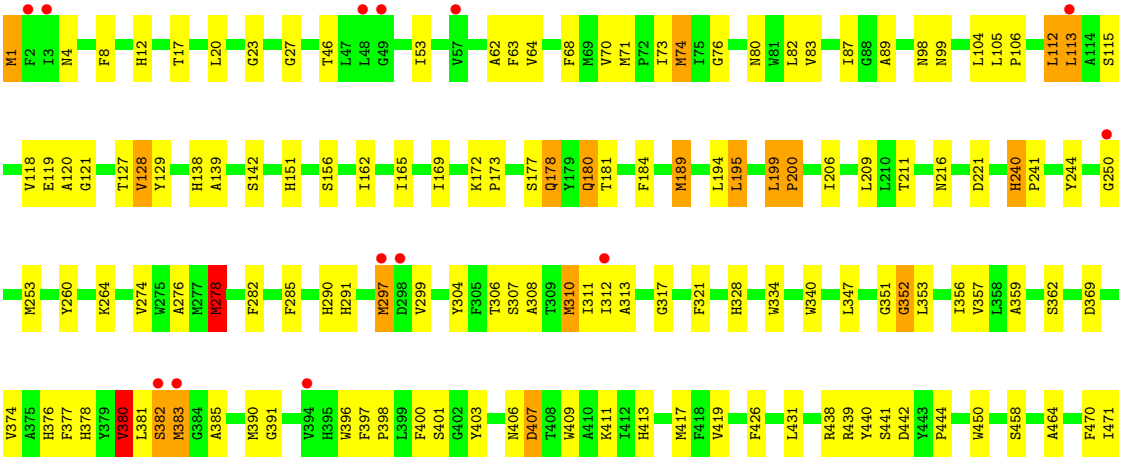
• Molecule 1: Cytochrome c oxidase subunit 1

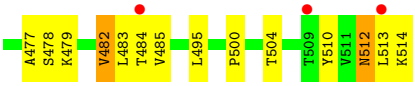
Chain A:



• Molecule 1: Cytochrome c oxidase subunit 1

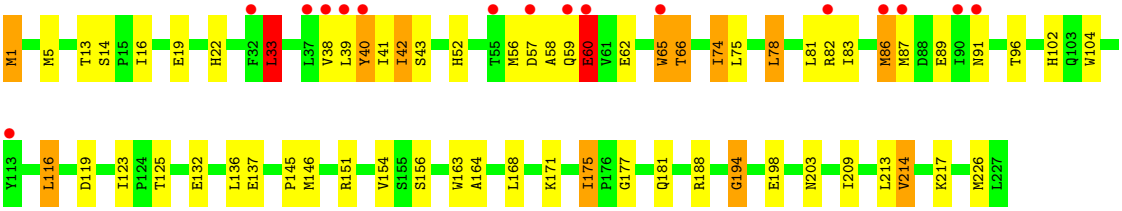
Chain N:





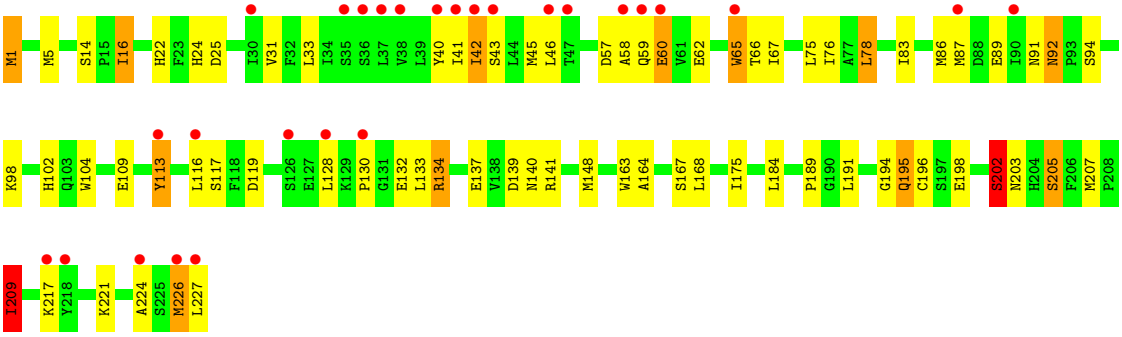
• Molecule 2: Cytochrome c oxidase subunit 2

Chain B:



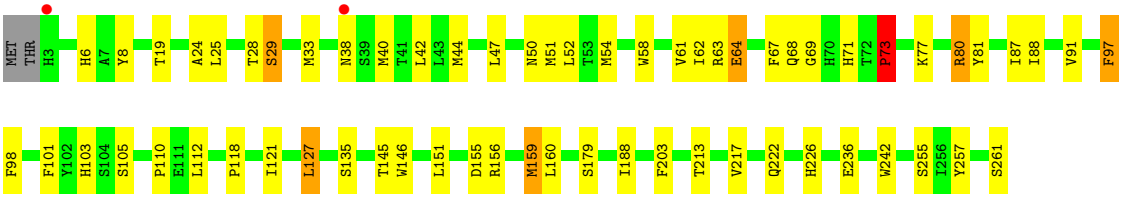
• Molecule 2: Cytochrome c oxidase subunit 2

Chain O:



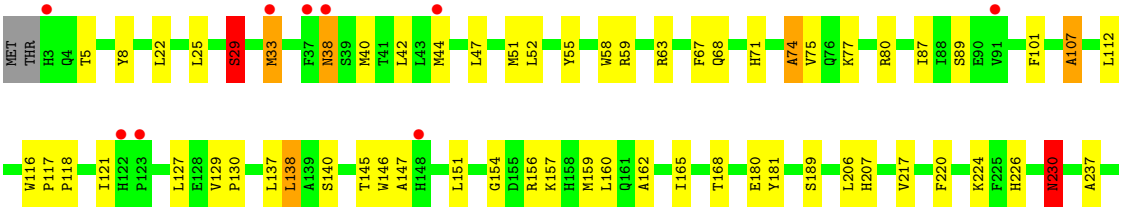
• Molecule 3: Cytochrome c oxidase subunit 3

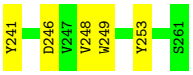
Chain C:



• Molecule 3: Cytochrome c oxidase subunit 3

Chain P:



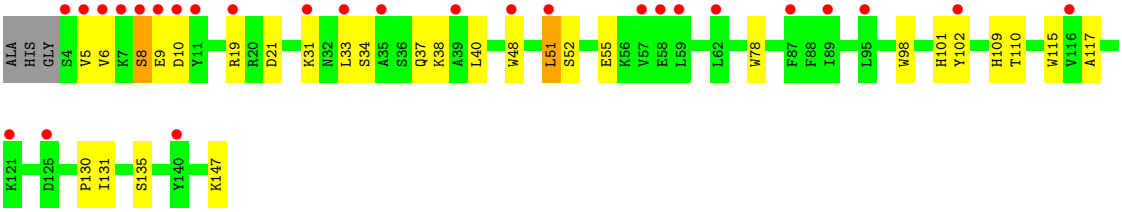


• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain D:

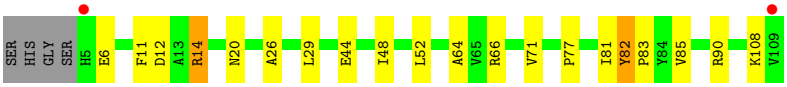
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain Q:



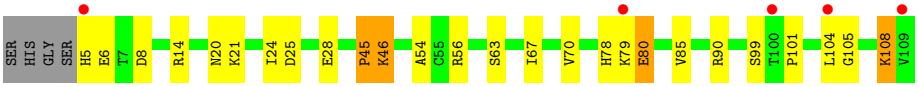
• Molecule 5: Cytochrome c oxidase subunit 5A

Chain E:



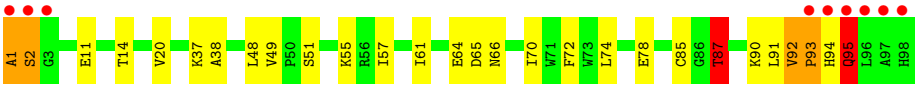
• Molecule 5: Cytochrome c oxidase subunit 5A

Chain R:



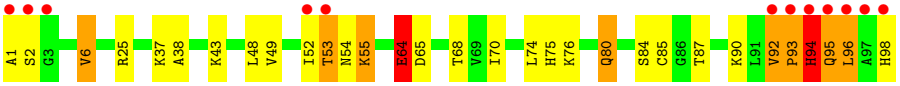
• Molecule 6: Cytochrome c oxidase subunit 5B

Chain F:



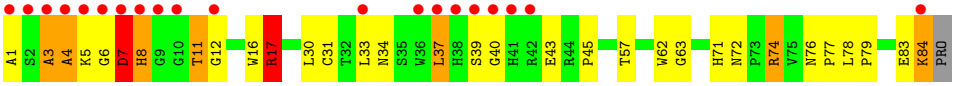
• Molecule 6: Cytochrome c oxidase subunit 5B

Chain S:



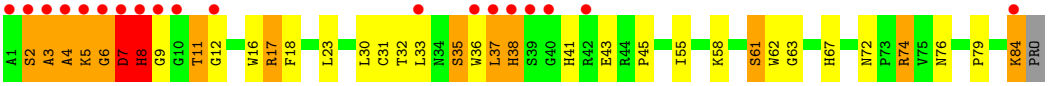
• Molecule 7: Cytochrome c oxidase subunit 6A2

Chain G:



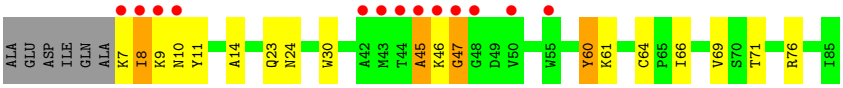
• Molecule 7: Cytochrome c oxidase subunit 6A2

Chain T:



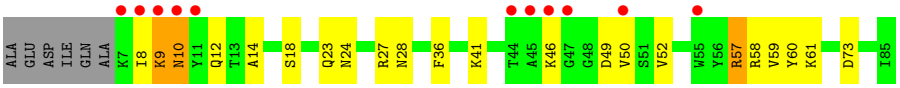
• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain H:



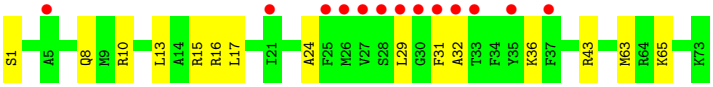
• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain U:



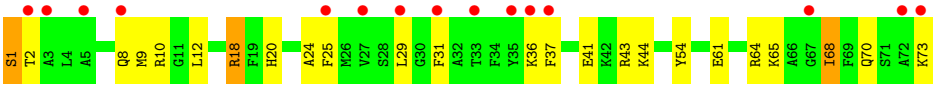
• Molecule 9: Cytochrome c oxidase subunit 6C

Chain I:



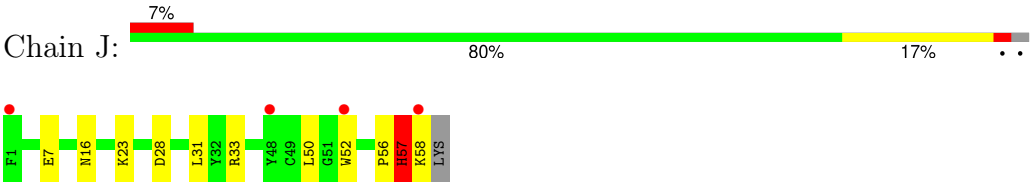
• Molecule 9: Cytochrome c oxidase subunit 6C

Chain V:



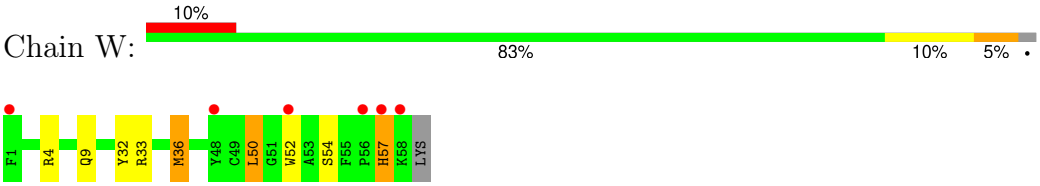
• Molecule 10: Cytochrome c oxidase polypeptide 7A1

Chain J:



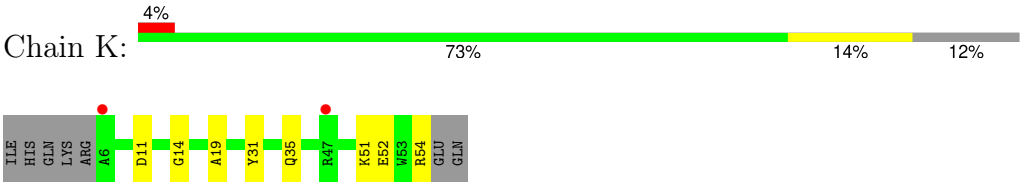
• Molecule 10: Cytochrome c oxidase polypeptide 7A1

Chain W:



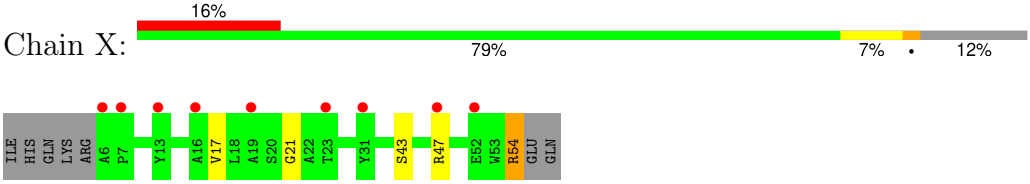
• Molecule 11: Cytochrome c oxidase subunit 7B

Chain K:



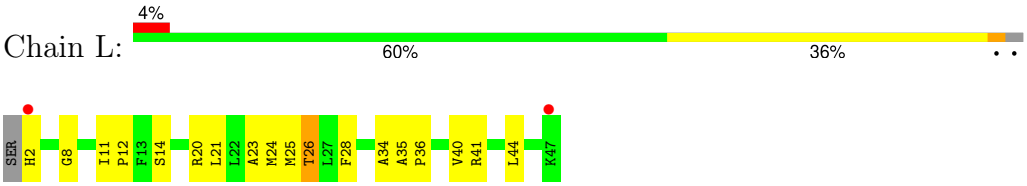
• Molecule 11: Cytochrome c oxidase subunit 7B

Chain X:



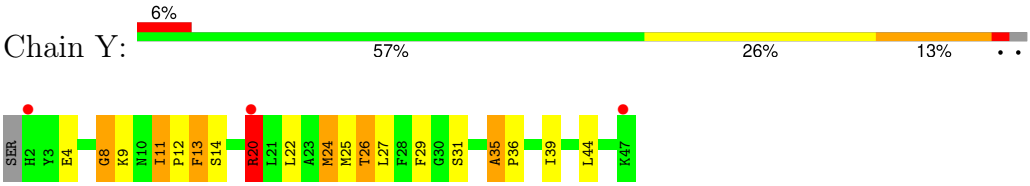
• Molecule 12: Cytochrome c oxidase subunit 7C

Chain L:



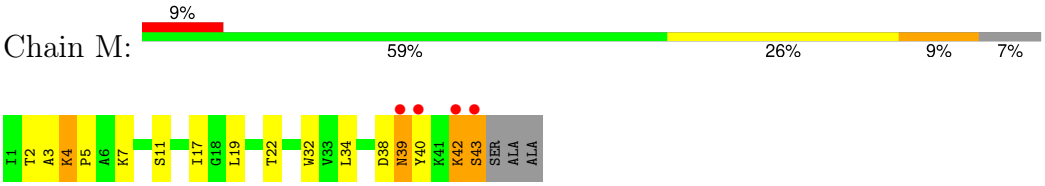
• Molecule 12: Cytochrome c oxidase subunit 7C

Chain Y:



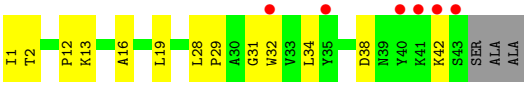
• Molecule 13: Cytochrome c oxidase subunit 8B

Chain M:



• Molecule 13: Cytochrome c oxidase subunit 8B

Chain Z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	183.36Å 206.65Å 178.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.05 40.00 – 2.05	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.05) 99.8 (40.00-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.60 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.3	Depositor
R, R_{free}	0.186 , 0.219 0.204 , 0.236	Depositor DCC
R_{free} test set	21002 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	34.5	Xtriage
Anisotropy	0.525	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 47.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.006 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	32324	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% 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: ZN, TPO, NA, HEA, SAC, PSC, TGL, FME, CDL, CUA, CYN, PEK, CU, UNX, CHD, PGV, DMU, MG

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	2.03	97/4156 (2.3%)	1.56	59/5678 (1.0%)
1	N	1.80	49/4156 (1.2%)	1.45	45/5678 (0.8%)
2	B	1.83	18/1860 (1.0%)	1.48	14/2534 (0.6%)
2	O	1.52	9/1860 (0.5%)	1.34	8/2534 (0.3%)
3	C	1.75	20/2197 (0.9%)	1.33	10/3005 (0.3%)
3	P	1.70	12/2197 (0.5%)	1.34	14/3005 (0.5%)
4	D	1.74	16/1229 (1.3%)	1.36	11/1658 (0.7%)
4	Q	1.32	5/1229 (0.4%)	1.22	2/1658 (0.1%)
5	E	1.74	9/871 (1.0%)	1.25	2/1182 (0.2%)
5	R	1.39	3/871 (0.3%)	1.20	0/1182
6	F	1.86	12/765 (1.6%)	1.49	7/1038 (0.7%)
6	S	1.60	6/765 (0.8%)	1.58	14/1038 (1.3%)
7	G	1.60	2/690 (0.3%)	1.34	4/937 (0.4%)
7	T	1.56	7/690 (1.0%)	1.46	6/937 (0.6%)
8	H	1.62	6/682 (0.9%)	1.38	3/921 (0.3%)
8	U	1.34	3/682 (0.4%)	1.32	5/921 (0.5%)
9	I	1.47	2/605 (0.3%)	1.36	3/802 (0.4%)
9	V	1.29	0/605	1.26	3/802 (0.4%)
10	J	1.45	0/471	1.29	2/636 (0.3%)
10	W	1.34	1/471 (0.2%)	1.20	1/636 (0.2%)
11	K	1.60	2/398 (0.5%)	1.40	4/546 (0.7%)
11	X	1.31	1/398 (0.3%)	1.31	3/546 (0.5%)
12	L	1.80	7/393 (1.8%)	1.44	4/526 (0.8%)
12	Y	1.56	2/393 (0.5%)	1.48	6/526 (1.1%)
13	M	1.80	6/345 (1.7%)	1.43	0/470
13	Z	1.43	0/345	1.29	0/470
All	All	1.70	295/29324 (1.0%)	1.40	230/39866 (0.6%)

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
10	J	0	1
10	W	0	1
12	L	0	1
All	All	0	5

The worst 5 of 295 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	198	GLU	C-O	12.55	1.37	1.23
1	A	388	ALA	CA-CB	11.34	1.71	1.53
2	B	198	GLU	C-O	11.09	1.37	1.23
1	N	139	ALA	CA-CB	10.72	1.70	1.53
1	A	419	VAL	CA-CB	9.76	1.65	1.54

The worst 5 of 230 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	240	HIS	N-CA-CB	11.78	121.58	110.39
1	A	310	MET	CG-SD-CE	-11.08	76.53	100.90
1	A	278	MET	CG-SD-CE	-10.50	77.80	100.90
1	N	278	MET	CG-SD-CE	-9.74	79.47	100.90
6	S	53	THR	CA-C-N	9.69	135.04	120.31

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	F	93	PRO	Peptide
10	J	57	HIS	Peptide
12	L	2	HIS	Peptide
6	S	93	PRO	Peptide
10	W	57	HIS	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	4027	0	4001	74	0
1	N	4027	0	4001	89	0
2	B	1824	0	1833	38	0
2	O	1824	0	1833	61	0
3	C	2110	0	2027	37	0
3	P	2110	0	2027	46	0
4	D	1195	0	1183	18	0
4	Q	1195	0	1183	21	0
5	E	852	0	845	5	0
5	R	852	0	845	13	0
6	F	748	0	728	17	0
6	S	748	0	728	27	0
7	G	675	0	643	37	0
7	T	675	0	643	50	0
8	H	662	0	623	6	0
8	U	662	0	623	11	0
9	I	601	0	613	10	0
9	V	601	0	613	19	0
10	J	460	0	459	7	0
10	W	460	0	459	8	0
11	K	384	0	366	2	0
11	X	384	0	366	4	0
12	L	380	0	380	12	0
12	Y	380	0	380	15	0
13	M	335	0	352	9	0
13	Z	335	0	352	9	0
14	A	120	0	108	10	0
14	N	120	0	108	13	0
15	A	2	0	0	0	0
15	N	2	0	0	2	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	7	0
19	D	63	0	110	13	0
19	L	63	0	110	16	0
19	N	126	0	220	22	0
19	Q	63	0	110	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	A	102	0	152	11	0
20	C	102	0	152	6	0
20	N	102	0	152	7	0
20	P	102	0	152	5	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	29	0	36	3	0
22	C	58	0	70	4	0
22	J	29	0	36	2	0
22	O	29	0	36	1	0
22	P	58	0	73	5	0
22	W	29	0	35	6	0
23	C	1	0	0	0	0
23	P	1	0	0	0	0
24	C	53	0	77	3	0
24	G	106	0	154	23	0
24	S	53	0	77	17	0
24	T	106	0	154	28	0
25	C	100	0	156	21	0
25	G	100	0	156	28	0
25	P	100	0	156	19	0
25	T	100	0	156	35	0
26	E	52	0	80	16	0
26	R	52	0	80	14	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	G	33	0	38	3	0
28	M	33	0	38	1	0
28	P	33	0	38	5	0
28	Z	33	0	39	3	0
29	A	225	0	0	8	0
29	B	125	0	0	4	0
29	C	106	0	0	2	0
29	D	91	0	0	1	0
29	E	62	0	0	0	0
29	F	75	0	0	2	0
29	G	41	0	0	3	0
29	H	47	0	0	2	0
29	I	38	0	0	1	0
29	J	20	0	0	1	0
29	K	20	0	0	1	0
29	L	22	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	M	15	0	0	1	0
29	N	199	0	0	6	0
29	O	107	0	0	4	0
29	P	100	0	0	3	0
29	Q	55	0	0	2	0
29	R	40	0	0	1	0
29	S	56	0	0	5	0
29	T	36	0	0	4	0
29	U	41	0	0	4	0
29	V	18	0	0	1	0
29	W	12	0	0	0	0
29	X	14	0	0	0	0
29	Y	12	0	0	1	0
29	Z	11	0	0	0	0
All	All	32324	0	31275	725	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

The worst 5 of 725 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:74:MET:CB	1:N:74:MET:CG	1.76	1.56
1:A:312:ILE:CG1	1:A:312:ILE:CD1	1.78	1.54
4:D:100:LYS:CE	4:D:100:LYS:NZ	1.69	1.51
3:C:73:PRO:CG	3:C:73:PRO:CB	1.75	1.48
14:A:516:HEA:O11	14:A:516:HEA:C11	1.64	1.45

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	512/514 (100%)	495 (97%)	17 (3%)	0	100	100
1	N	512/514 (100%)	495 (97%)	16 (3%)	1 (0%)	43	37
2	B	225/227 (99%)	212 (94%)	11 (5%)	2 (1%)	14	7
2	O	225/227 (99%)	211 (94%)	12 (5%)	2 (1%)	14	7
3	C	257/261 (98%)	251 (98%)	6 (2%)	0	100	100
3	P	257/261 (98%)	251 (98%)	5 (2%)	1 (0%)	30	22
4	D	142/147 (97%)	137 (96%)	5 (4%)	0	100	100
4	Q	142/147 (97%)	137 (96%)	5 (4%)	0	100	100
5	E	103/109 (94%)	97 (94%)	6 (6%)	0	100	100
5	R	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
6	F	96/98 (98%)	91 (95%)	3 (3%)	2 (2%)	5	1
6	S	96/98 (98%)	89 (93%)	4 (4%)	3 (3%)	3	0
7	G	81/85 (95%)	66 (82%)	7 (9%)	8 (10%)	0	0
7	T	81/85 (95%)	67 (83%)	9 (11%)	5 (6%)	1	0
8	H	77/85 (91%)	67 (87%)	4 (5%)	6 (8%)	1	0
8	U	77/85 (91%)	70 (91%)	5 (6%)	2 (3%)	4	0
9	I	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
9	V	71/73 (97%)	66 (93%)	5 (7%)	0	100	100
10	J	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
10	W	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
11	K	47/56 (84%)	46 (98%)	0	1 (2%)	5	1
11	X	47/56 (84%)	44 (94%)	3 (6%)	0	100	100
12	L	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
12	Y	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
13	M	41/46 (89%)	41 (100%)	0	0	100	100
13	Z	41/46 (89%)	38 (93%)	3 (7%)	0	100	100
All	All	3504/3614 (97%)	3336 (95%)	135 (4%)	33 (1%)	14	7

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	60	GLU
6	F	95	GLN
7	G	4	ALA

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Mol	Chain	Res	Type
7	G	7	ASP
7	G	8	HIS

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	426/426 (100%)	414 (97%)	12 (3%)	38	34
1	N	426/426 (100%)	413 (97%)	13 (3%)	35	30
2	B	210/210 (100%)	201 (96%)	9 (4%)	26	20
2	O	210/210 (100%)	195 (93%)	15 (7%)	13	7
3	C	224/226 (99%)	218 (97%)	6 (3%)	39	36
3	P	224/226 (99%)	219 (98%)	5 (2%)	45	44
4	D	128/129 (99%)	124 (97%)	4 (3%)	35	30
4	Q	128/129 (99%)	123 (96%)	5 (4%)	28	23
5	E	92/95 (97%)	90 (98%)	2 (2%)	45	44
5	R	92/95 (97%)	84 (91%)	8 (9%)	9	4
6	F	81/81 (100%)	76 (94%)	5 (6%)	16	9
6	S	81/81 (100%)	73 (90%)	8 (10%)	7	3
7	G	67/68 (98%)	62 (92%)	5 (8%)	12	6
7	T	67/68 (98%)	57 (85%)	10 (15%)	3	0
8	H	71/75 (95%)	67 (94%)	4 (6%)	19	12
8	U	71/75 (95%)	67 (94%)	4 (6%)	19	12
9	I	57/57 (100%)	53 (93%)	4 (7%)	14	7
9	V	57/57 (100%)	53 (93%)	4 (7%)	14	7
10	J	49/50 (98%)	48 (98%)	1 (2%)	48	48
10	W	49/50 (98%)	47 (96%)	2 (4%)	27	21
11	K	39/46 (85%)	38 (97%)	1 (3%)	40	37
11	X	39/46 (85%)	37 (95%)	2 (5%)	21	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	39/40 (98%)	38 (97%)	1 (3%)	40	37
12	Y	39/40 (98%)	37 (95%)	2 (5%)	21	14
13	M	37/38 (97%)	31 (84%)	6 (16%)	2	0
13	Z	37/38 (97%)	33 (89%)	4 (11%)	6	2
All	All	3040/3082 (99%)	2898 (95%)	142 (5%)	23	17

5 of 142 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	T	33	LEU
7	T	38	HIS
9	V	18	ARG
9	I	15	ARG
9	I	8	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
2	O	59	GLN
13	Z	39	ASN
3	P	76	GLN
10	W	57	HIS
6	S	95	GLN

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	$\#\|Z\| > 2$
9	SAC	V	1	9	7,8,9	3.08	2 (28%)	7,9,11	1.97	2 (28%)
9	SAC	I	1	9	7,8,9	2.30	2 (28%)	7,9,11	1.29	1 (14%)
7	TPO	G	11	7	8,10,11	2.49	4 (50%)	10,14,16	1.88	3 (30%)
2	FME	O	1	2	8,9,10	1.00	0	8,9,11	5.80	3 (37%)
1	FME	N	1	1	8,9,10	1.24	1 (12%)	8,9,11	5.31	4 (50%)
7	TPO	T	11	7	8,10,11	2.32	5 (62%)	10,14,16	2.18	2 (20%)
2	FME	B	1	2	8,9,10	1.67	1 (12%)	8,9,11	6.22	4 (50%)
1	FME	A	1	1	8,9,10	0.77	0	8,9,11	5.42	5 (62%)

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
9	SAC	V	1	9	-	3/7/8/10	-
9	SAC	I	1	9	-	2/7/8/10	-
7	TPO	G	11	7	-	5/9/11/13	-
2	FME	O	1	2	-	1/7/9/11	-
1	FME	N	1	1	-	4/7/9/11	-
7	TPO	T	11	7	-	3/9/11/13	-
2	FME	B	1	2	-	1/7/9/11	-
1	FME	A	1	1	-	3/7/9/11	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	V	1	SAC	OAC-C1A	5.58	1.35	1.23
9	V	1	SAC	CA-N	5.48	1.54	1.46
9	I	1	SAC	OAC-C1A	4.31	1.32	1.23
7	G	11	TPO	P-OG1	4.29	1.67	1.59
7	G	11	TPO	P-O1P	4.04	1.63	1.50

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	FME	CA-N-CN	-16.27	97.80	122.82
2	O	1	FME	CA-N-CN	-15.72	98.64	122.82
1	A	1	FME	CA-N-CN	-14.12	101.11	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	1	FME	CA-N-CN	-13.38	102.24	122.82
7	T	11	TPO	CG2-CB-CA	5.82	124.59	113.26

There are no chirality outliers.

5 of 22 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.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	V	1	SAC	1	0
7	G	11	TPO	1	0
2	O	1	FME	1	0
1	N	1	FME	1	0
7	T	11	TPO	1	0
2	B	1	FME	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 56 ligands modelled in this entry, 8 are monoatomic and 2 are unknown - leaving 46 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	$\#\|Z\| > 2$
20	PGV	C	268	-	50,50,50	1.31	3 (6%)	53,56,56	1.48	6 (11%)
21	CUA	B	228	2	0,1,1	-	-	-		
21	CUA	O	228	2	0,1,1	-	-	-		
25	CDL	G	269	-	99,99,99	1.58	14 (14%)	105,111,111	1.52	17 (16%)
14	HEA	N	515	1	67,67,67	1.87	16 (23%)	81,103,103	2.06	21 (25%)
19	TGL	A	521	-	62,62,62	1.51	7 (11%)	65,65,65	2.41	17 (26%)
20	PGV	N	1524	-	50,50,50	1.23	2 (4%)	53,56,56	1.29	6 (11%)
14	HEA	N	516	15,1	67,67,67	2.26	24 (35%)	81,103,103	3.04	40 (49%)
22	CHD	W	1059	-	32,32,32	1.16	2 (6%)	51,51,51	5.10	34 (66%)
20	PGV	C	267	-	50,50,50	0.90	3 (6%)	53,56,56	1.37	5 (9%)
15	CYN	A	520	16,14	1,1,1	0.25	0	-		
19	TGL	L	522	-	62,62,62	1.64	8 (12%)	65,65,65	1.85	16 (24%)
26	PSC	R	1229	-	51,51,51	1.23	3 (5%)	57,59,59	1.03	5 (8%)
14	HEA	A	516	15,1	67,67,67	2.55	27 (40%)	81,103,103	3.52	39 (48%)
25	CDL	P	1270	-	99,99,99	1.47	12 (12%)	105,111,111	1.40	14 (13%)
25	CDL	C	270	-	99,99,99	1.46	12 (12%)	105,111,111	1.44	15 (14%)
20	PGV	A	524	-	50,50,50	1.20	2 (4%)	53,56,56	1.35	6 (11%)
19	TGL	N	1522	-	62,62,62	1.64	7 (11%)	65,65,65	1.63	15 (23%)
28	DMU	G	272	-	34,34,34	1.29	4 (11%)	45,45,45	3.30	23 (51%)
22	CHD	P	1525	-	32,32,32	1.55	6 (18%)	51,51,51	5.14	43 (84%)
25	CDL	T	1269	-	99,99,99	1.47	12 (12%)	105,111,111	1.43	17 (16%)
24	PEK	G	1263	-	52,52,52	1.19	2 (3%)	55,57,57	1.19	6 (10%)
20	PGV	N	1266	-	50,50,50	0.94	1 (2%)	53,56,56	1.38	6 (11%)
24	PEK	T	263	-	52,52,52	1.23	2 (3%)	55,57,57	1.19	5 (9%)
20	PGV	P	1268	-	50,50,50	1.29	3 (6%)	53,56,56	1.53	7 (13%)
26	PSC	E	229	-	51,51,51	1.29	3 (5%)	57,59,59	1.37	7 (12%)
19	TGL	Q	1523	-	62,62,62	1.42	6 (9%)	65,65,65	1.26	9 (13%)
22	CHD	C	525	-	32,32,32	1.88	7 (21%)	51,51,51	5.40	34 (66%)
20	PGV	P	1267	-	50,50,50	0.87	2 (4%)	53,56,56	1.43	9 (16%)
20	PGV	A	522	-	50,50,50	0.99	2 (4%)	53,56,56	1.30	6 (11%)
24	PEK	T	1264	-	52,52,52	0.95	2 (3%)	55,57,57	1.77	9 (16%)
22	CHD	C	271	-	32,32,32	0.96	2 (6%)	51,51,51	5.05	35 (68%)
19	TGL	D	523	-	62,62,62	1.66	7 (11%)	65,65,65	1.53	12 (18%)
15	CYN	N	520	16,14	1,1,1	0.25	0	-		
22	CHD	J	60	-	32,32,32	0.81	0	51,51,51	4.87	39 (76%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	PEK	S	1265	-	52,52,52	1.35	3 (5%)	55,57,57	1.32	5 (9%)
14	HEA	A	515	1	67,67,67	2.16	20 (29%)	81,103,103	1.93	17 (20%)
22	CHD	O	229	-	32,32,32	1.27	2 (6%)	51,51,51	5.56	35 (68%)
24	PEK	C	264	-	52,52,52	0.91	2 (3%)	55,57,57	1.70	12 (21%)
19	TGL	N	1521	-	62,62,62	1.39	6 (9%)	65,65,65	1.50	12 (18%)
22	CHD	P	1271	-	32,32,32	0.82	1 (3%)	51,51,51	4.86	37 (72%)
24	PEK	G	265	-	52,52,52	1.22	4 (7%)	55,57,57	1.26	3 (5%)
28	DMU	Z	1526	-	34,34,34	0.96	2 (5%)	45,45,45	3.19	21 (46%)
28	DMU	P	1272	-	34,34,34	1.24	1 (2%)	45,45,45	3.24	23 (51%)
28	DMU	M	526	-	34,34,34	0.84	1 (2%)	45,45,45	3.46	26 (57%)
22	CHD	B	1085	-	32,32,32	1.56	6 (18%)	51,51,51	5.66	37 (72%)

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
20	PGV	C	268	-	-	32/55/55/55	-
25	CDL	G	269	-	-	63/110/110/110	-
14	HEA	N	515	1	-	8/36/76/76	-
19	TGL	A	521	-	-	35/65/65/65	-
20	PGV	N	1524	-	-	35/55/55/55	-
14	HEA	N	516	15,1	-	12/36/76/76	-
22	CHD	W	1059	-	2/2/12/12	7/9/74/74	0/4/4/4
20	PGV	C	267	-	-	14/55/55/55	-
28	DMU	G	272	-	6/6/10/10	12/19/59/59	0/2/2/2
19	TGL	L	522	-	-	35/65/65/65	-
26	PSC	R	1229	-	-	39/55/55/55	-
14	HEA	A	516	15,1	-	8/36/76/76	-
25	CDL	P	1270	-	-	68/110/110/110	-
25	CDL	C	270	-	-	73/110/110/110	-
19	TGL	N	1522	-	-	39/65/65/65	-
20	PGV	A	524	-	-	32/55/55/55	-
22	CHD	P	1525	-	-	2/9/74/74	0/4/4/4
25	CDL	T	1269	-	-	64/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PEK	G	1263	-	-	27/56/56/56	-
20	PGV	N	1266	-	-	13/55/55/55	-
24	PEK	T	263	-	-	32/56/56/56	-
20	PGV	P	1268	-	-	28/55/55/55	-
26	PSC	E	229	-	-	34/55/55/55	-
19	TGL	Q	1523	-	-	36/65/65/65	-
22	CHD	C	525	-	-	2/9/74/74	0/4/4/4
20	PGV	P	1267	-	-	14/55/55/55	-
20	PGV	A	522	-	-	14/55/55/55	-
24	PEK	T	1264	-	-	22/56/56/56	-
22	CHD	C	271	-	1/1/12/12	4/9/74/74	0/4/4/4
19	TGL	D	523	-	-	37/65/65/65	-
22	CHD	J	60	-	2/2/12/12	6/9/74/74	0/4/4/4
24	PEK	S	1265	-	-	24/56/56/56	-
14	HEA	A	515	1	-	6/36/76/76	-
22	CHD	O	229	-	-	2/9/74/74	0/4/4/4
24	PEK	C	264	-	-	21/56/56/56	-
19	TGL	N	1521	-	-	42/65/65/65	-
22	CHD	P	1271	-	1/1/12/12	7/9/74/74	0/4/4/4
24	PEK	G	265	-	-	26/56/56/56	-
28	DMU	Z	1526	-	5/5/10/10	9/19/59/59	0/2/2/2
28	DMU	P	1272	-	6/6/10/10	10/19/59/59	0/2/2/2
28	DMU	M	526	-	4/4/10/10	10/19/59/59	0/2/2/2
22	CHD	B	1085	-	-	2/9/74/74	0/4/4/4

The worst 5 of 251 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	516	HEA	O11-C11	9.70	1.64	1.42
14	A	516	HEA	C11-C3B	7.86	1.61	1.51
14	N	516	HEA	O11-C11	7.34	1.59	1.42
19	N	1522	TGL	OG2-CB1	6.84	1.53	1.34
14	A	515	HEA	FE-NA	6.45	2.16	1.95

The worst 5 of 751 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	1085	CHD	C18-C13-C12	-16.72	92.32	109.06
22	P	1271	CHD	C10-C9-C8	13.71	127.12	111.84
22	C	271	CHD	C10-C9-C8	13.17	126.52	111.84
22	B	1085	CHD	C1-C10-C5	12.87	126.22	107.75
22	C	525	CHD	C1-C10-C5	12.75	126.05	107.75

5 of 27 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	C	271	CHD	C9
22	J	60	CHD	C9
22	J	60	CHD	C17
22	P	1271	CHD	C9
22	W	1059	CHD	C9

5 of 1006 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	516	HEA	C2A-C3A-CMA-OMA
14	A	516	HEA	C4A-C3A-CMA-OMA
14	A	516	HEA	C2D-C3D-CAD-CBD
14	N	515	HEA	C2A-C3A-CMA-OMA
14	N	515	HEA	C4A-C3A-CMA-OMA

There are no ring outliers.

42 monomers are involved in 342 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	C	268	PGV	3	0
25	G	269	CDL	28	0
14	N	515	HEA	3	0
19	A	521	TGL	7	0
20	N	1524	PGV	7	0
14	N	516	HEA	10	0
22	W	1059	CHD	6	0
20	C	267	PGV	3	0
19	L	522	TGL	16	0
26	R	1229	PSC	14	0
14	A	516	HEA	4	0
25	P	1270	CDL	19	0
25	C	270	CDL	21	0
20	A	524	PGV	8	0
19	N	1522	TGL	15	0

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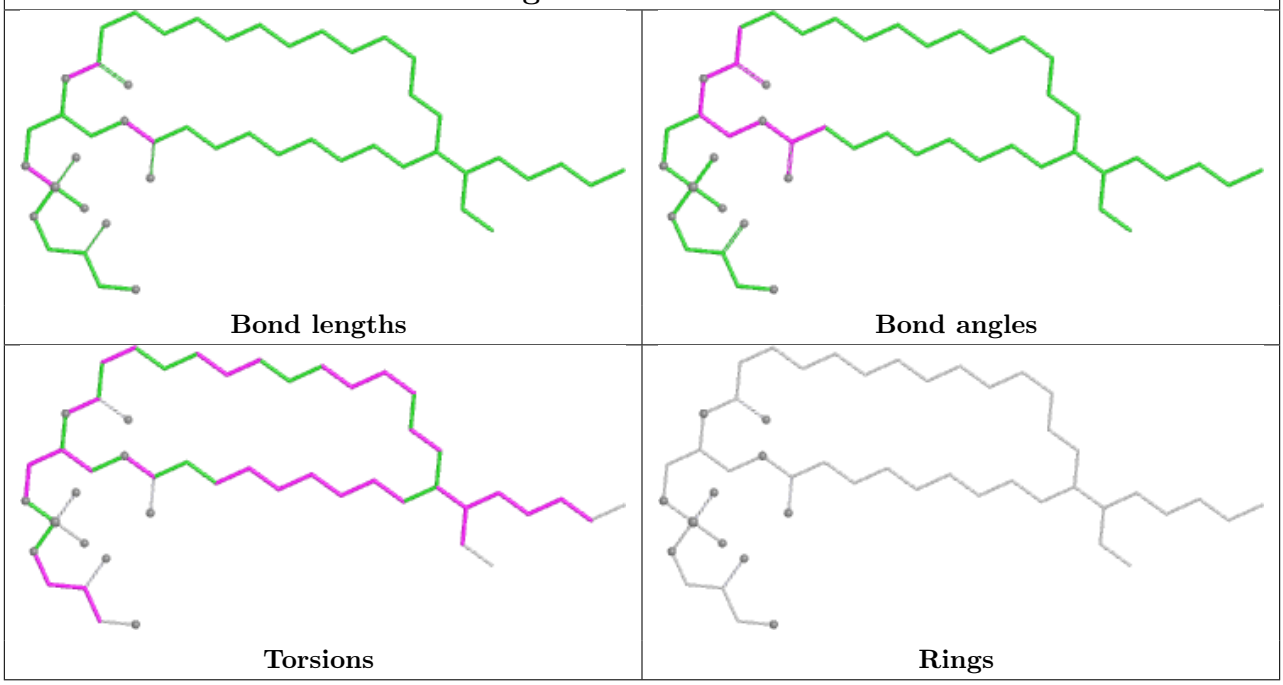
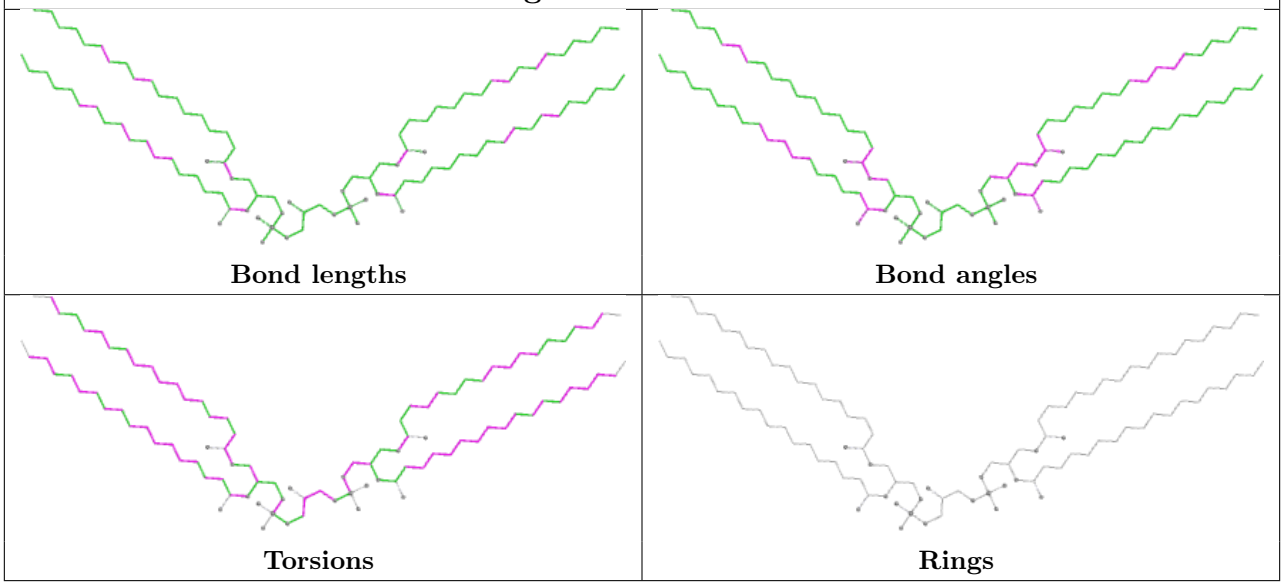
Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	G	272	DMU	3	0
22	P	1525	CHD	1	0
25	T	1269	CDL	35	0
24	G	1263	PEK	10	0
24	T	263	PEK	19	0
20	P	1268	PGV	2	0
26	E	229	PSC	16	0
19	Q	1523	TGL	10	0
22	C	525	CHD	1	0
20	P	1267	PGV	3	0
20	A	522	PGV	3	0
24	T	1264	PEK	9	0
22	C	271	CHD	3	0
19	D	523	TGL	13	0
15	N	520	CYN	2	0
22	J	60	CHD	2	0
24	S	1265	PEK	17	0
14	A	515	HEA	6	0
22	O	229	CHD	1	0
24	C	264	PEK	3	0
19	N	1521	TGL	7	0
22	P	1271	CHD	4	0
24	G	265	PEK	13	0
28	Z	1526	DMU	3	0
28	P	1272	DMU	5	0
28	M	526	DMU	1	0
22	B	1085	CHD	3	0

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

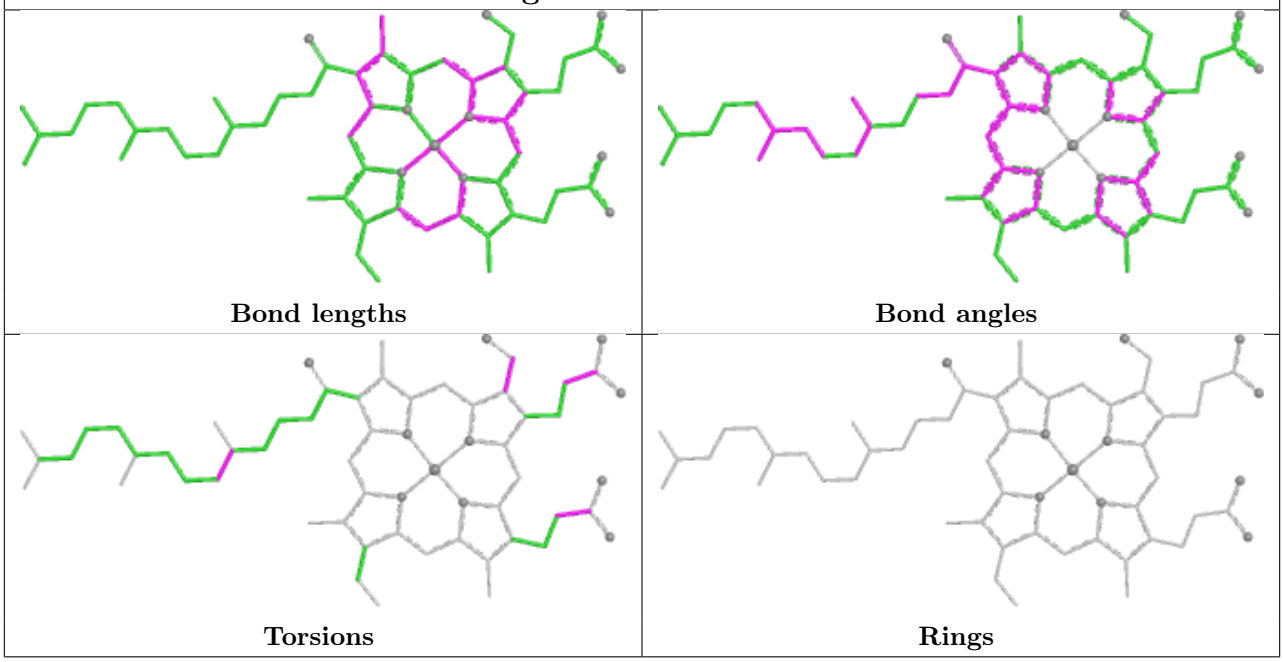
Ligand PGV C 268



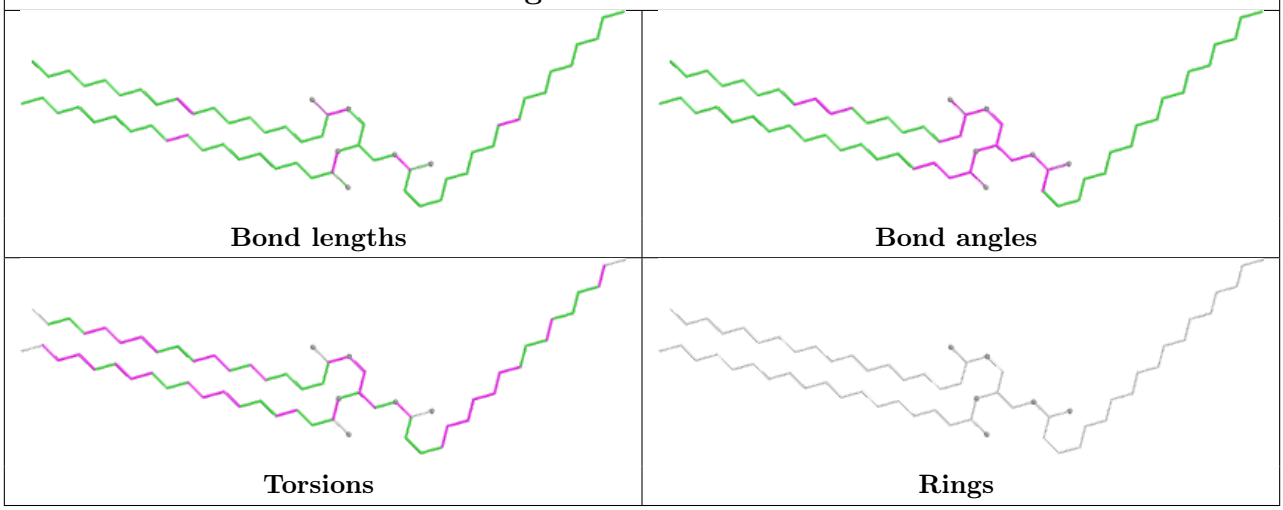
Ligand CDL G 269



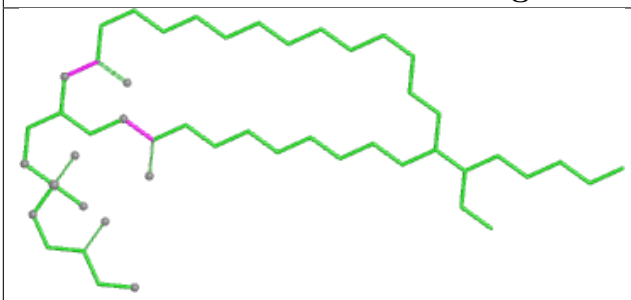
Ligand HEA N 515



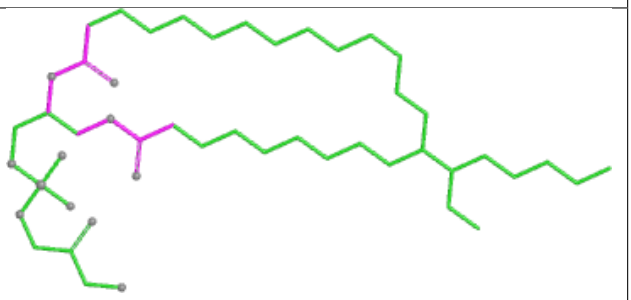
Ligand TGL A 521



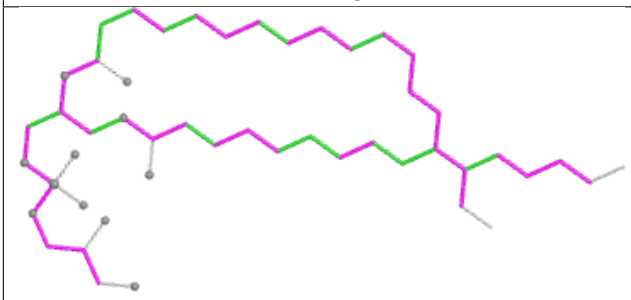
Ligand PGV N 1524



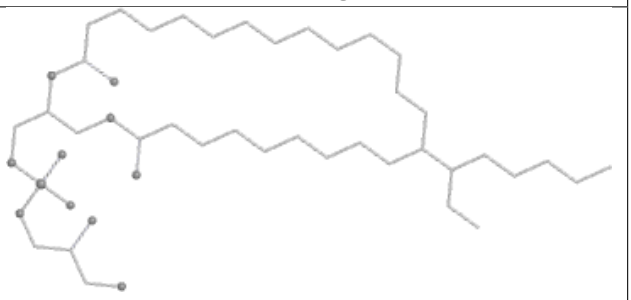
Bond lengths



Bond angles

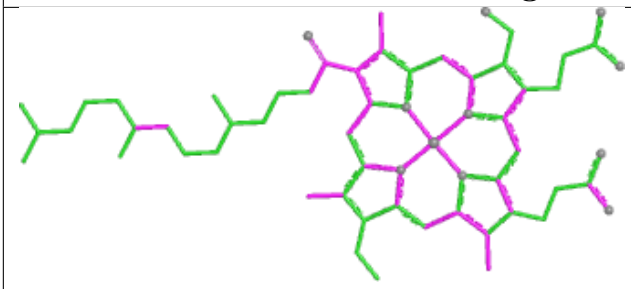


Torsions

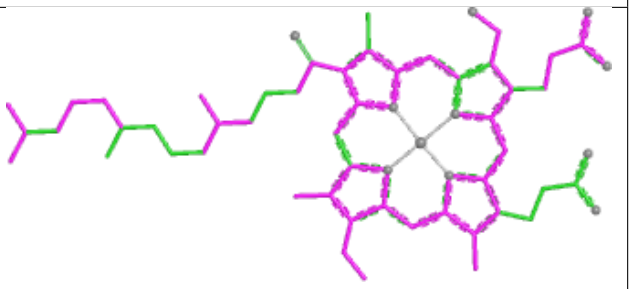


Rings

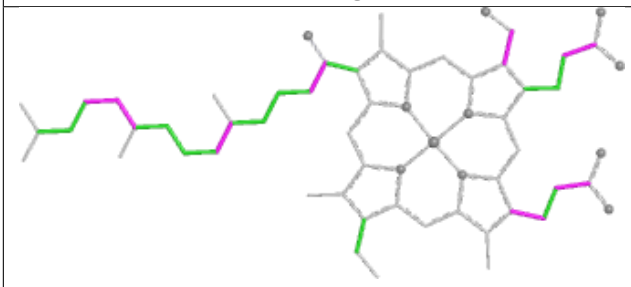
Ligand HEA N 516



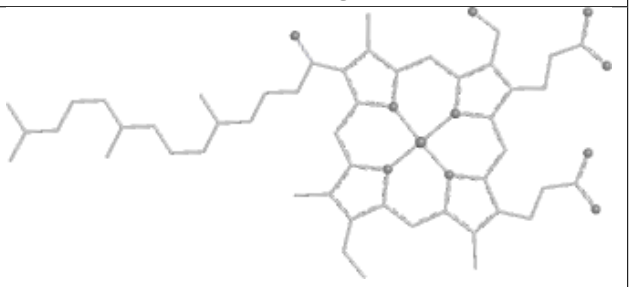
Bond lengths



Bond angles

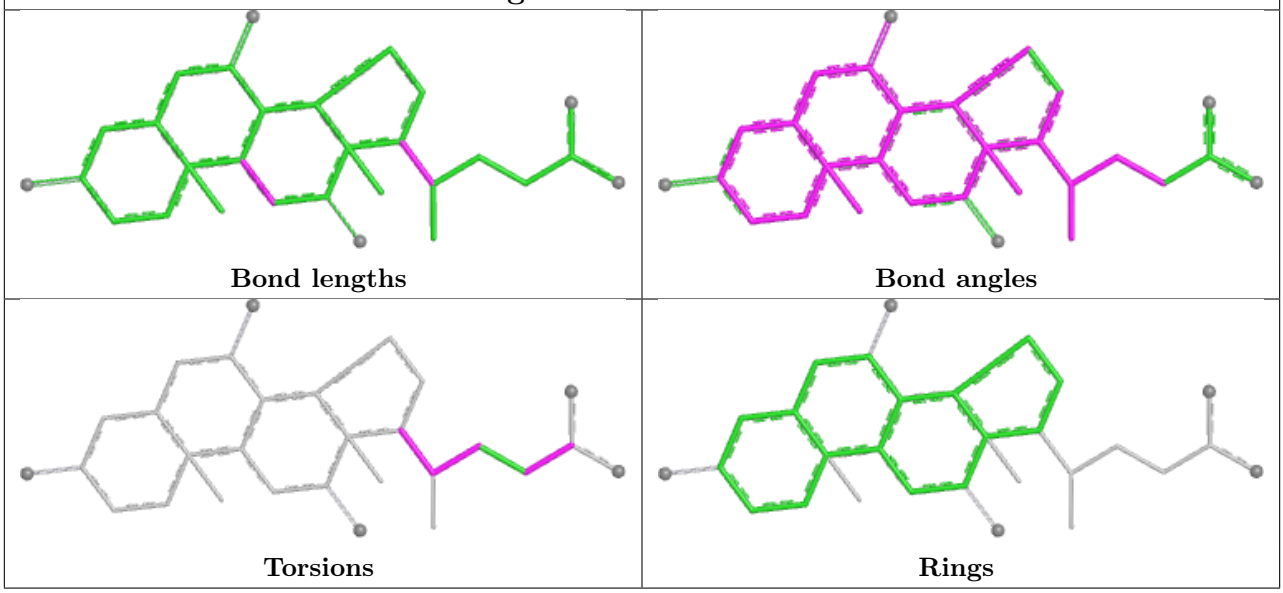


Torsions

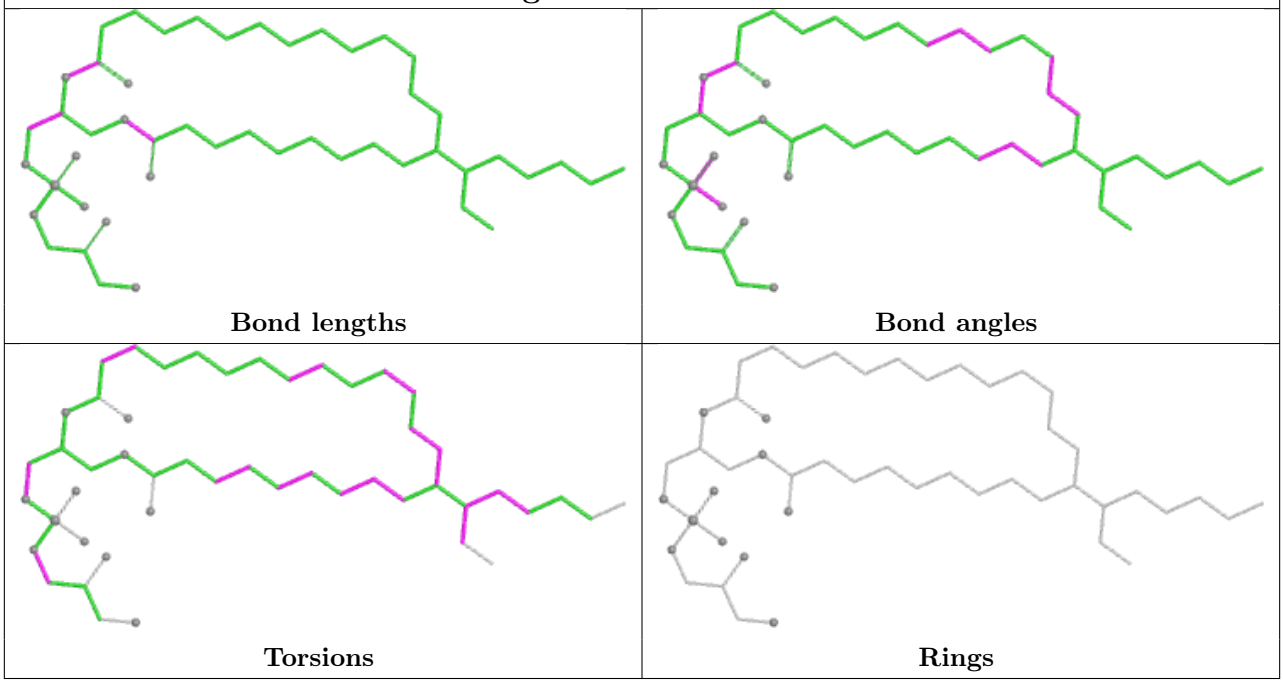


Rings

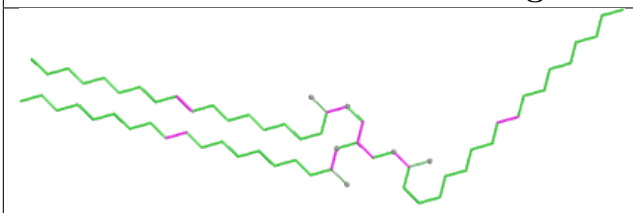
Ligand CHD W 1059



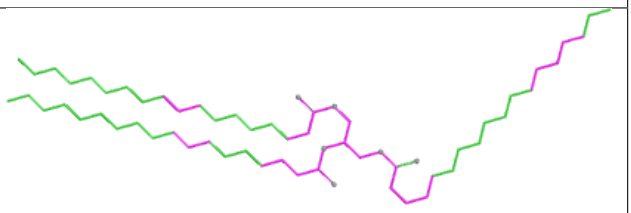
Ligand PGV C 267



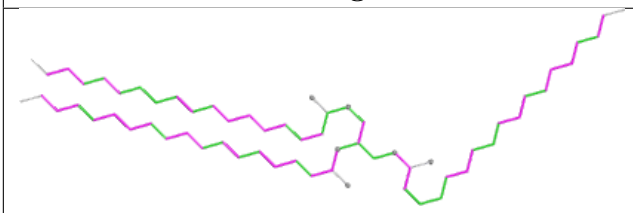
Ligand TGL L 522



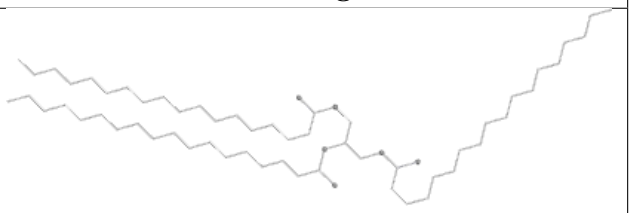
Bond lengths



Bond angles

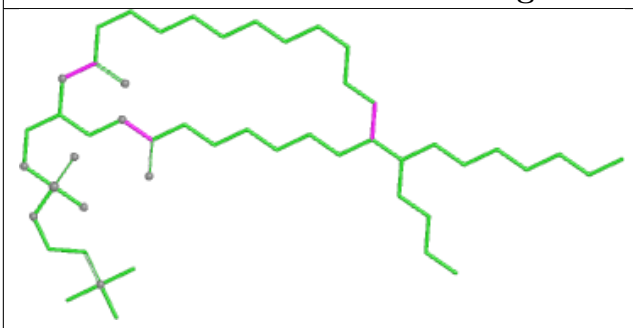


Torsions



Rings

Ligand PSC R 1229



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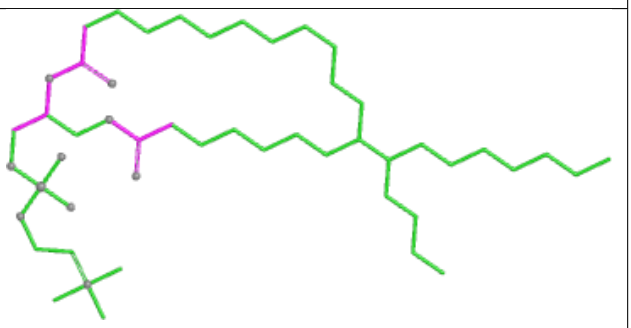
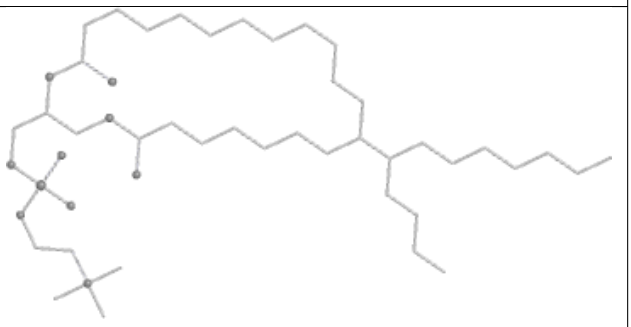


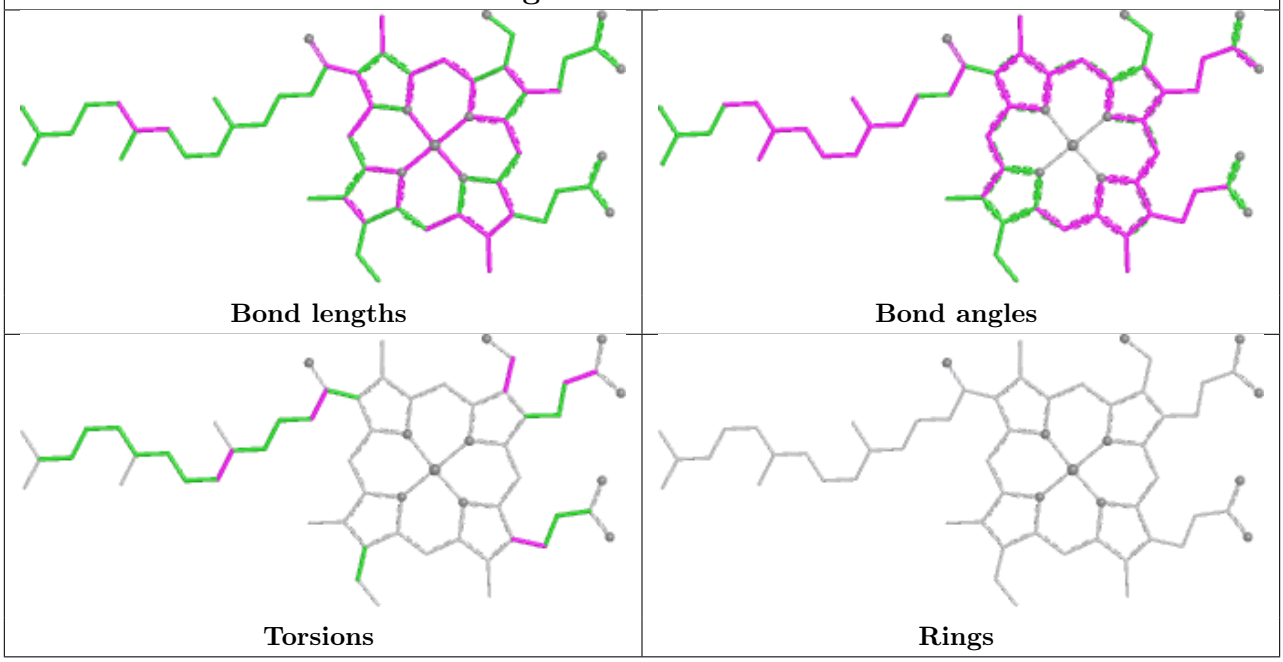
Bond angles

Torsions

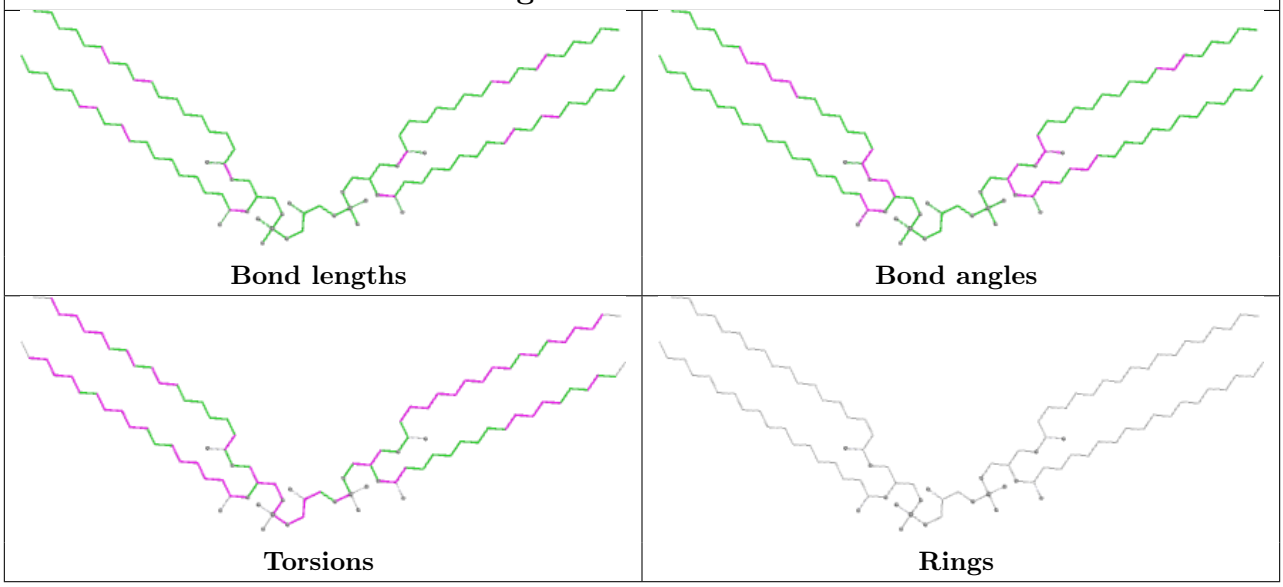


Rings

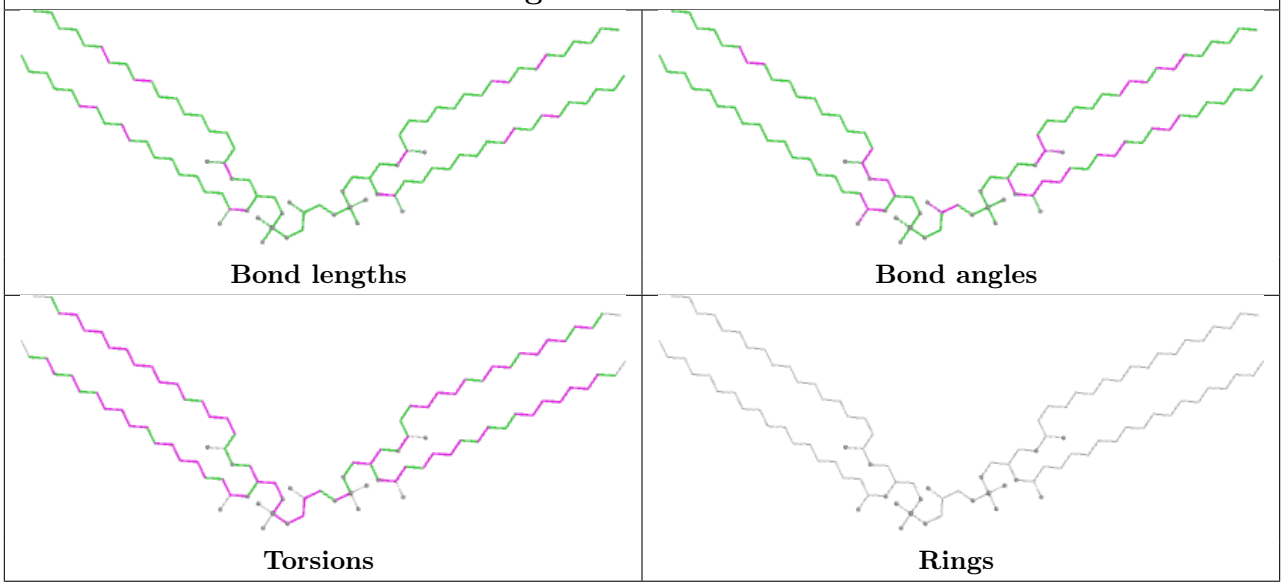
Ligand HEA A 516



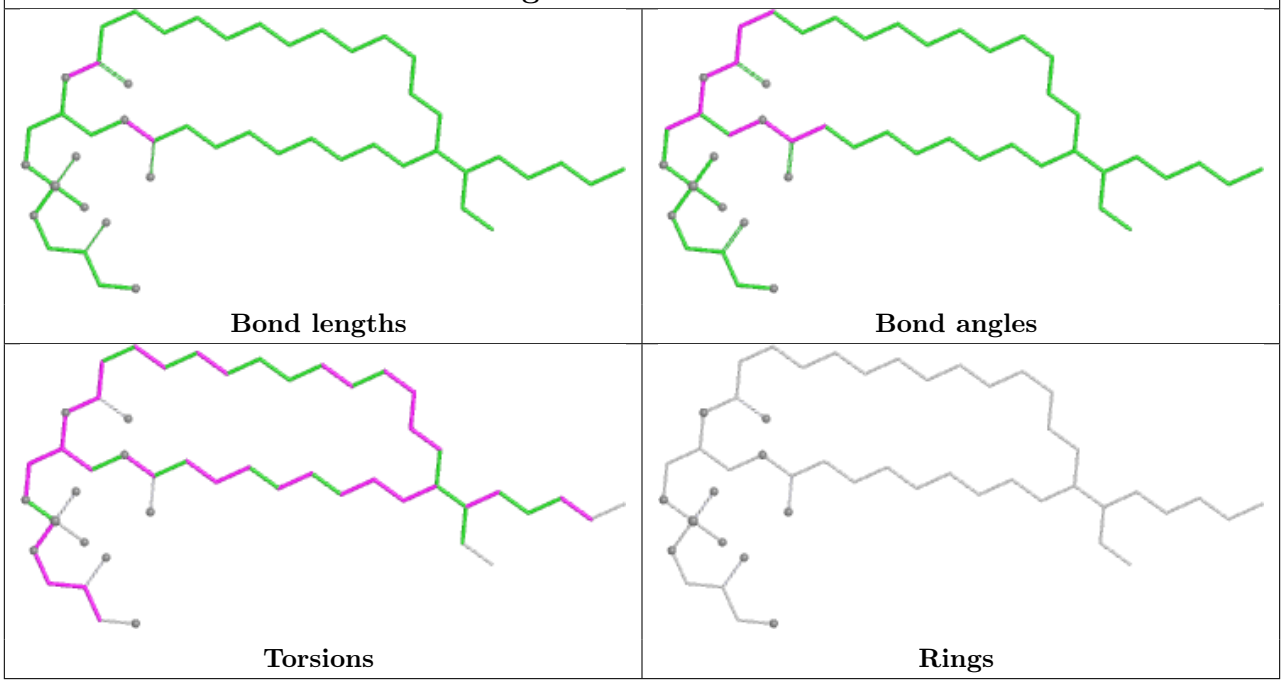
Ligand CDL P 1270



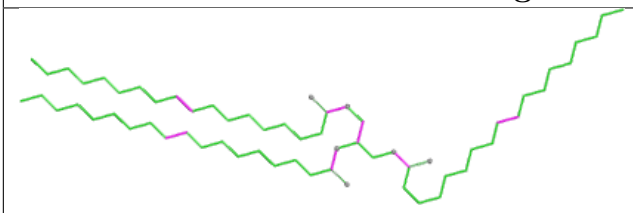
Ligand CDL C 270



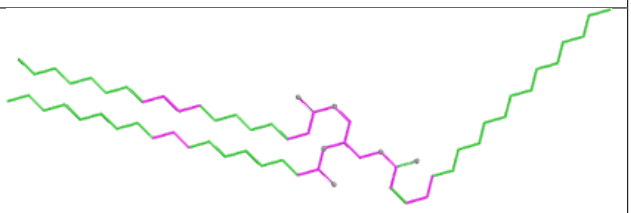
Ligand PGV A 524



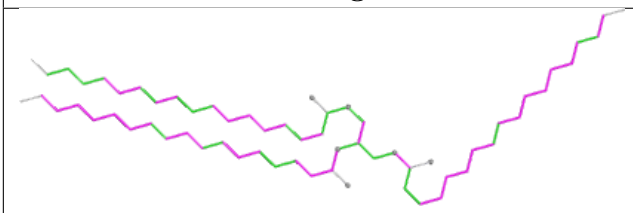
Ligand TGL N 1522



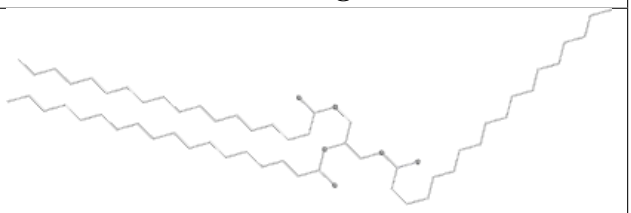
Bond lengths



Bond angles

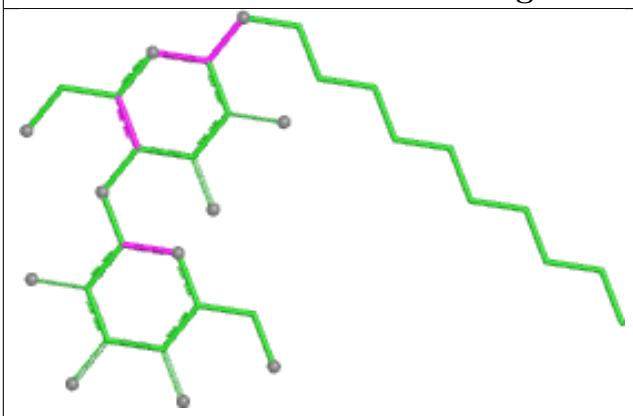


Torsions

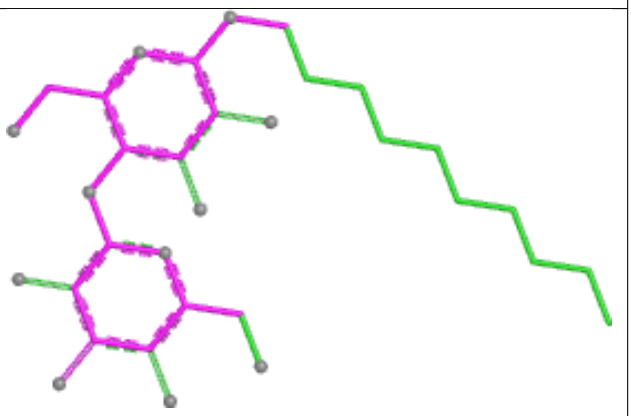


Rings

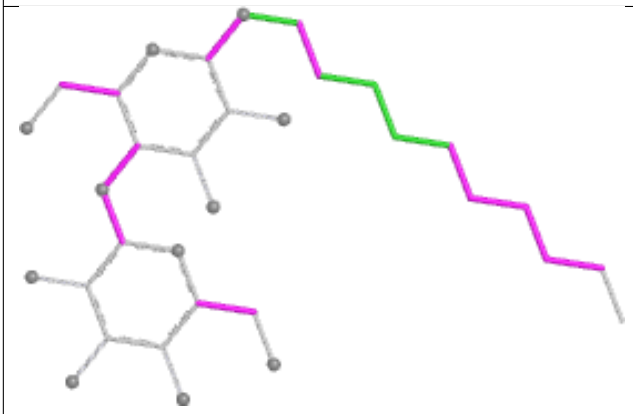
Ligand DMU G 272



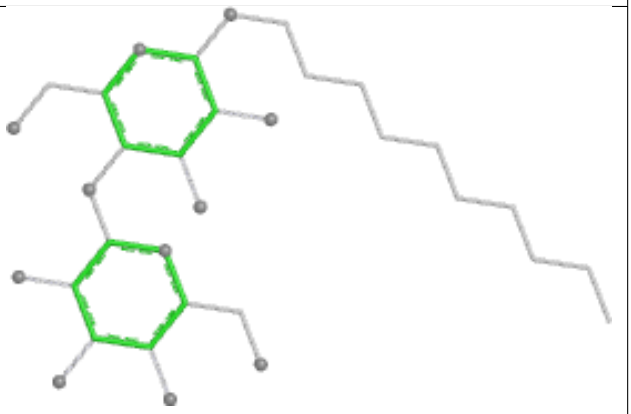
Bond lengths



Bond angles

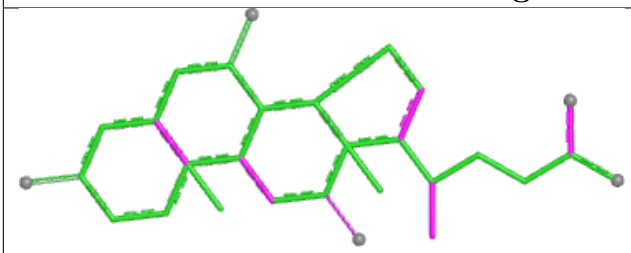


Torsions

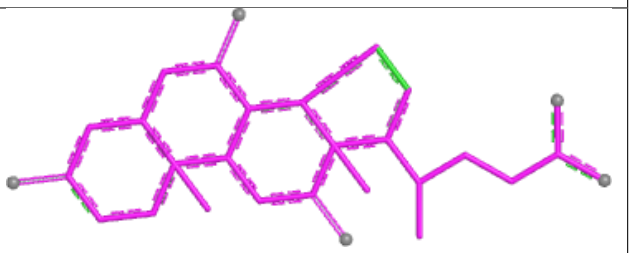


Rings

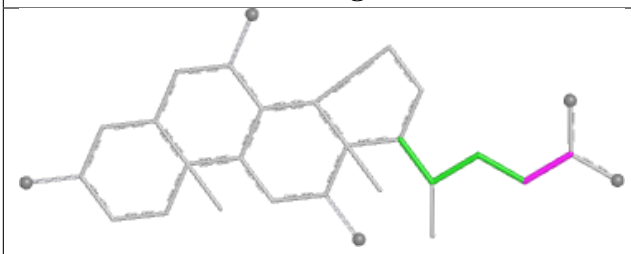
Ligand CHD P 1525



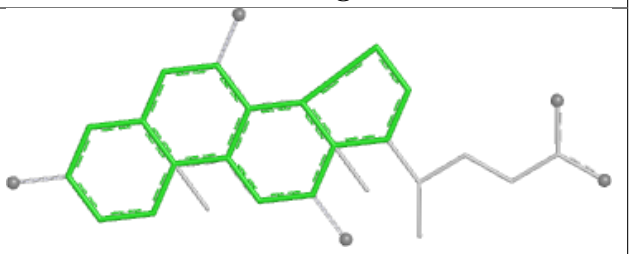
Bond lengths



Bond angles

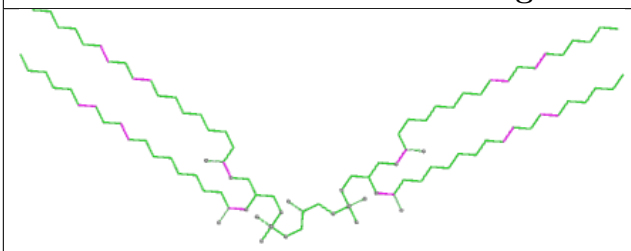


Torsions

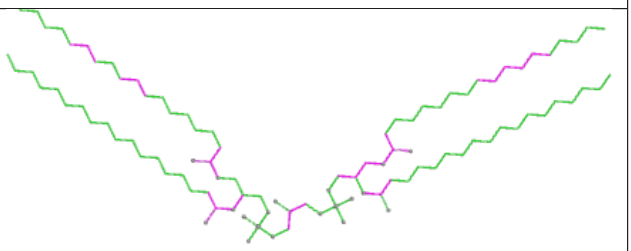


Rings

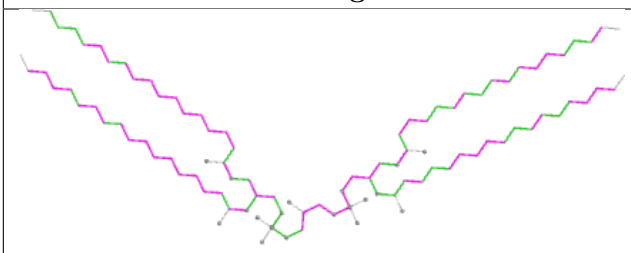
Ligand CDL T 1269



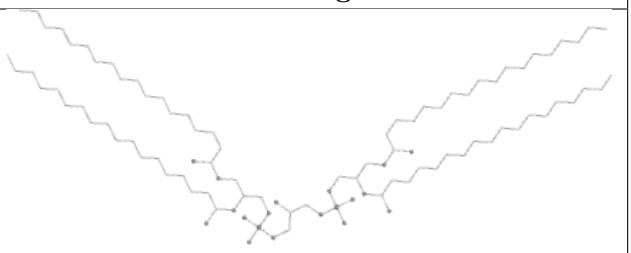
Bond lengths



Bond angles

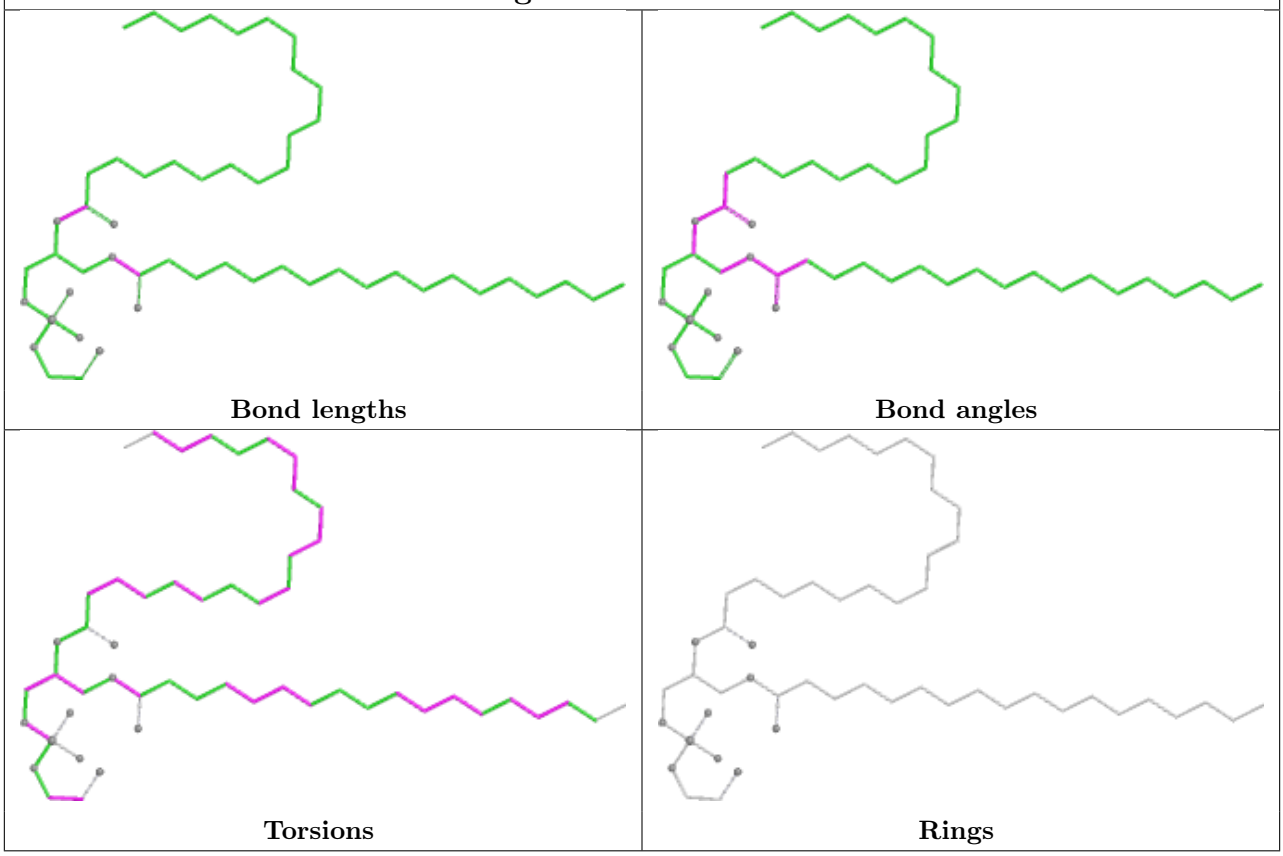


Torsions

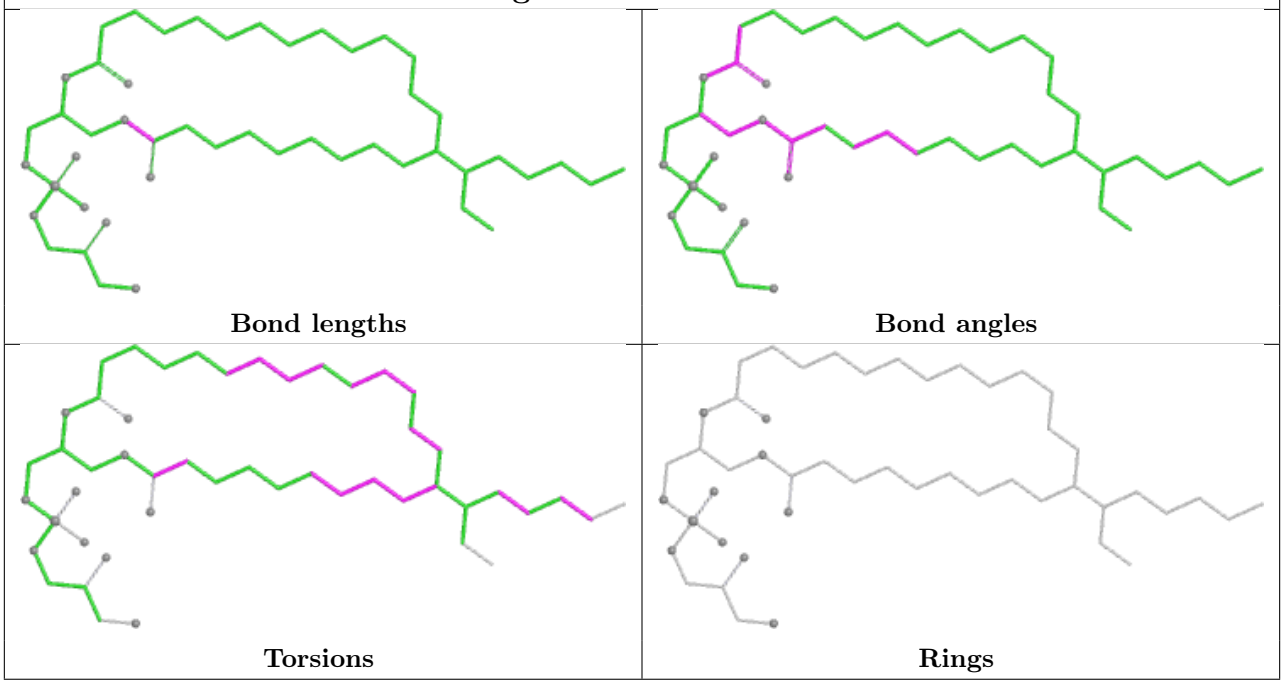


Rings

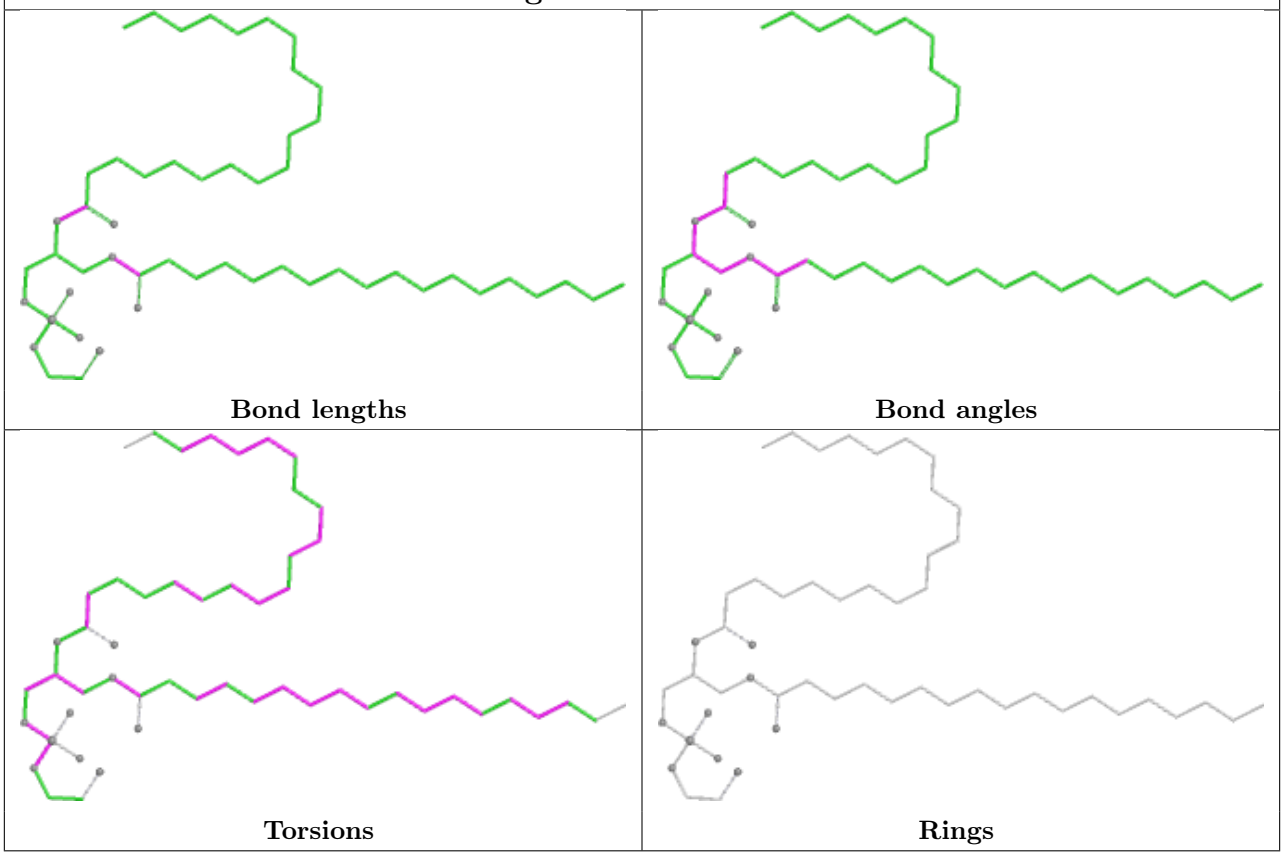
Ligand PEK G 1263



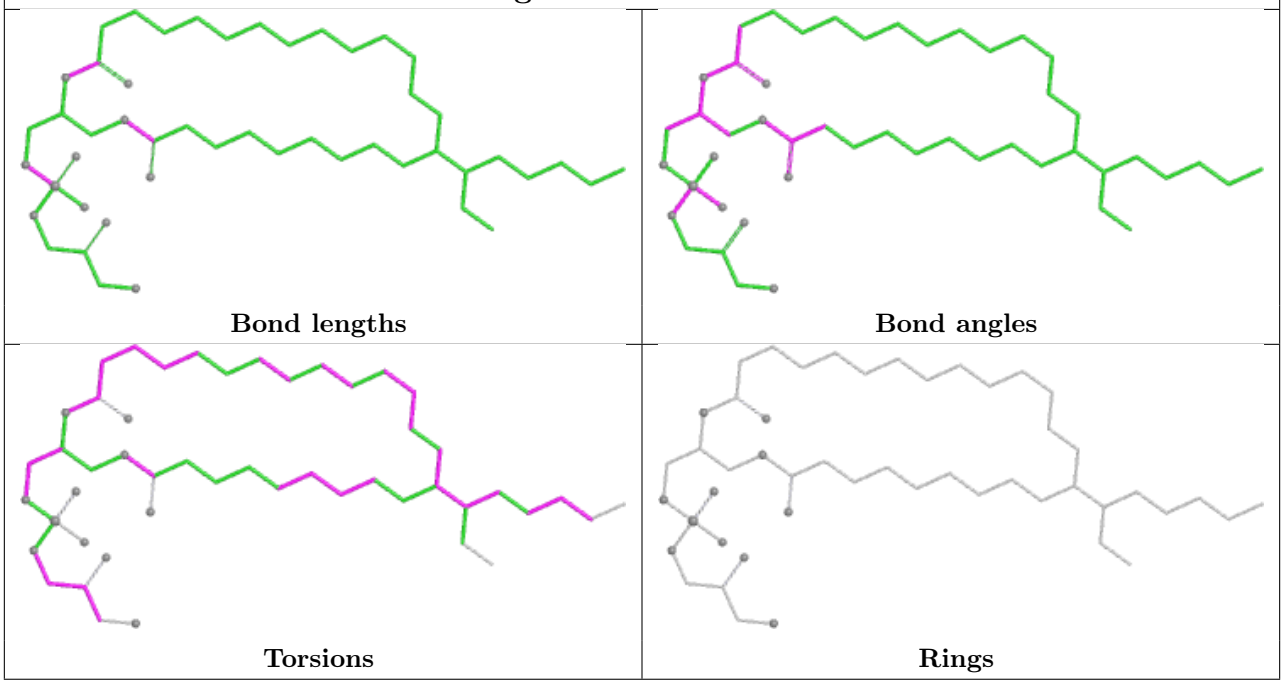
Ligand PGV N 1266



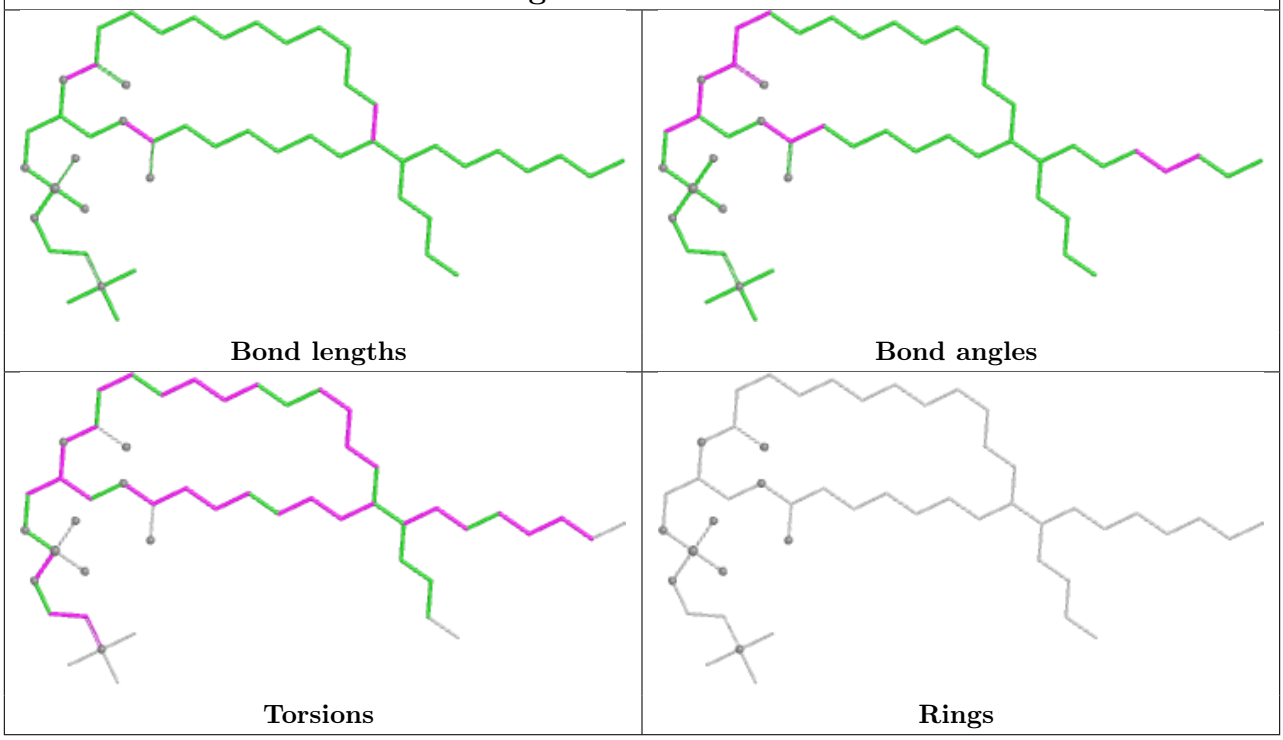
Ligand PEK T 263



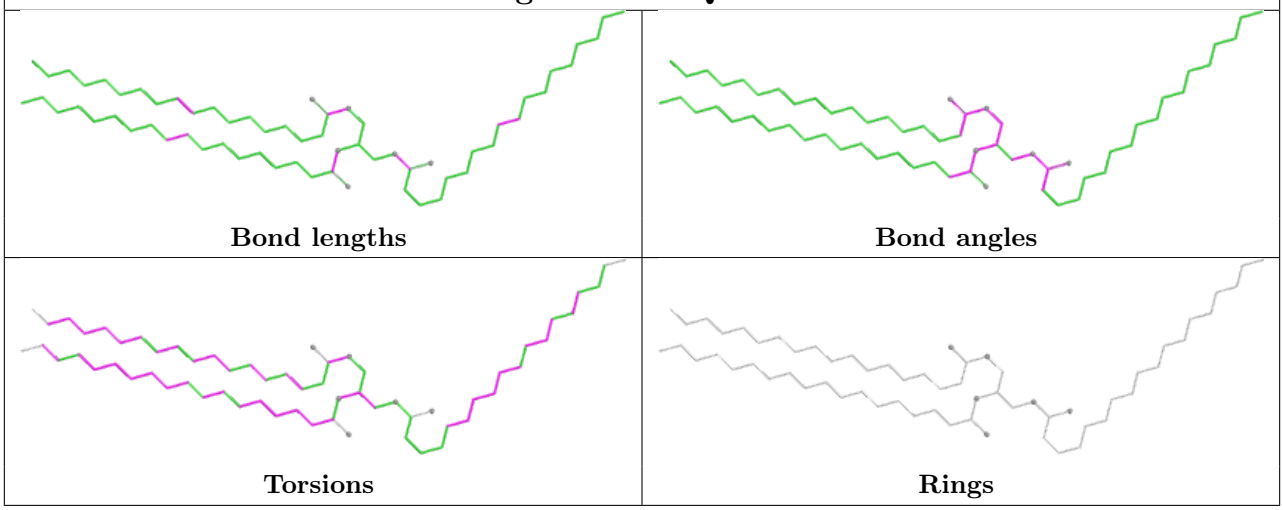
Ligand PGV P 1268



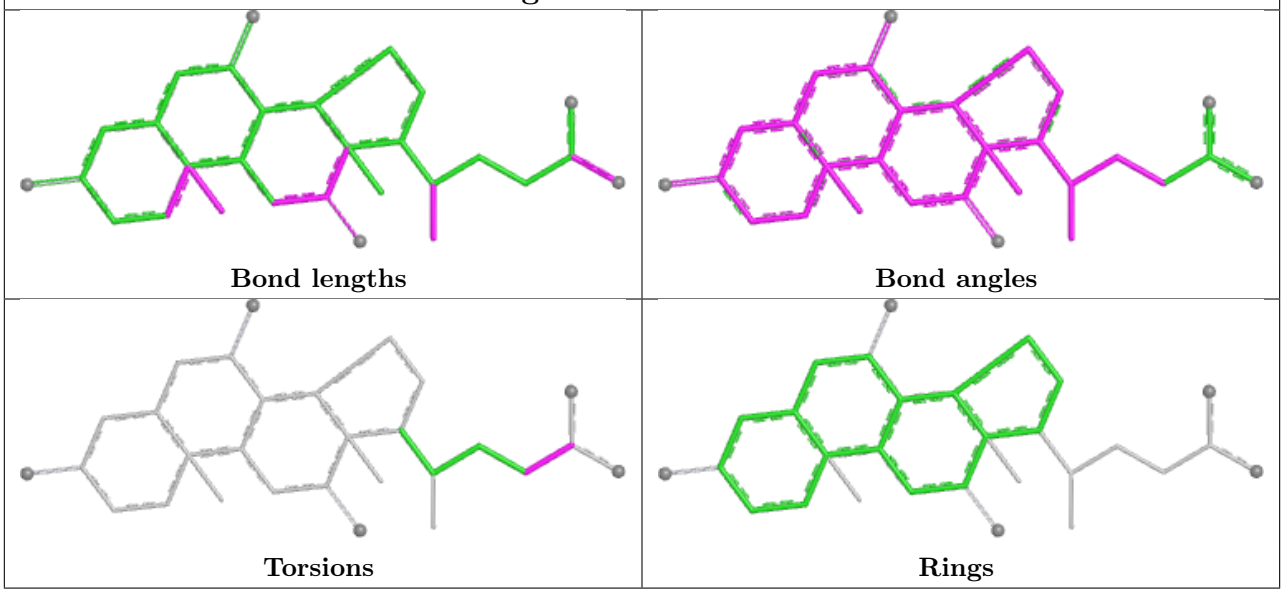
Ligand PSC E 229



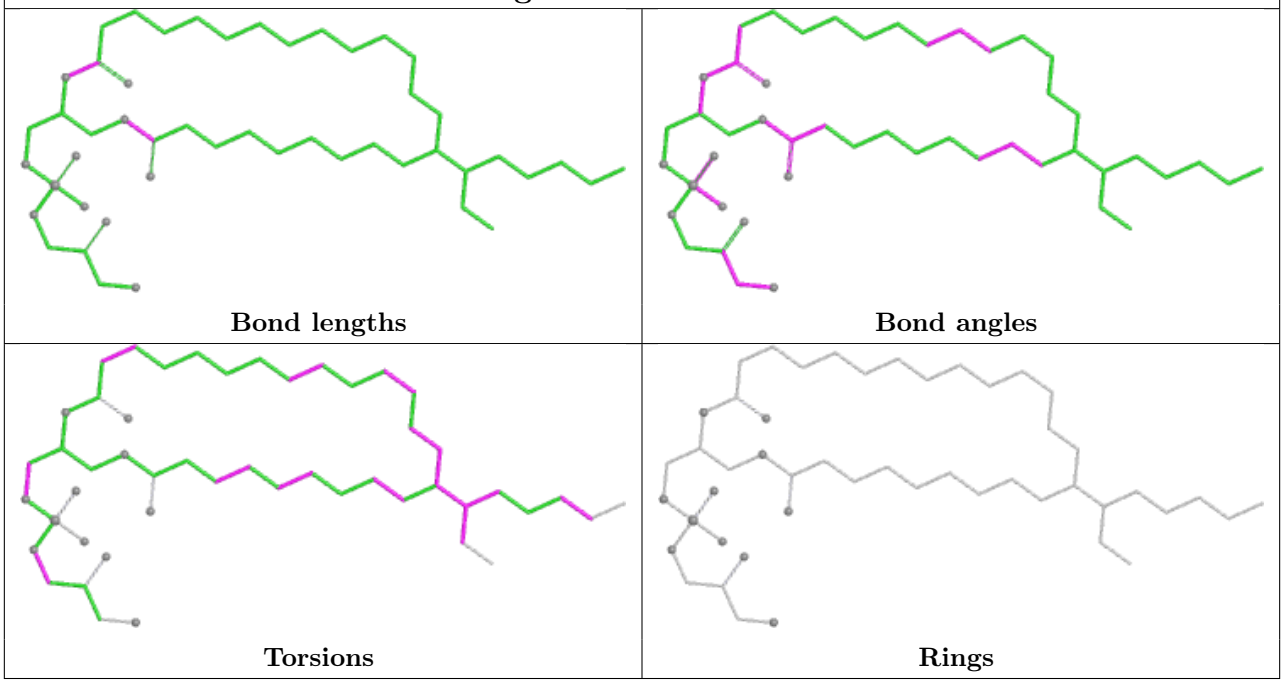
Ligand TGL Q 1523



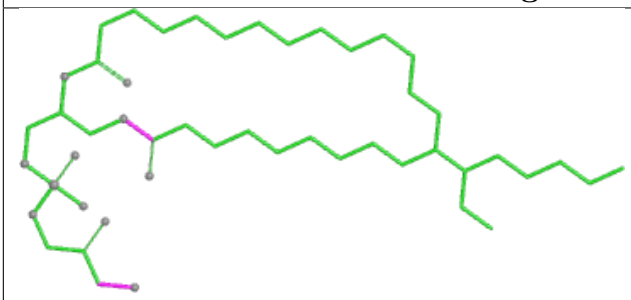
Ligand CHD C 525



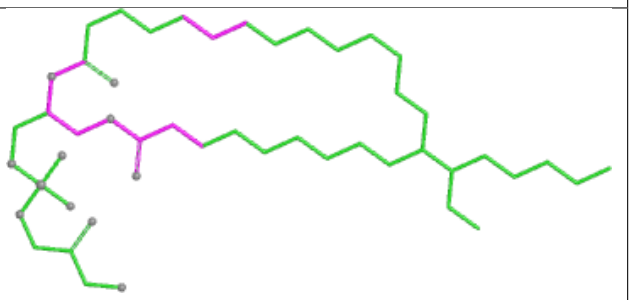
Ligand PGV P 1267



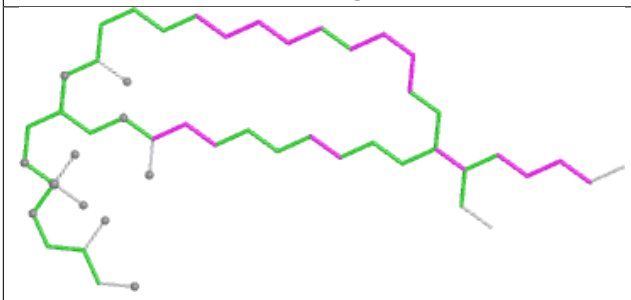
Ligand PGV A 522



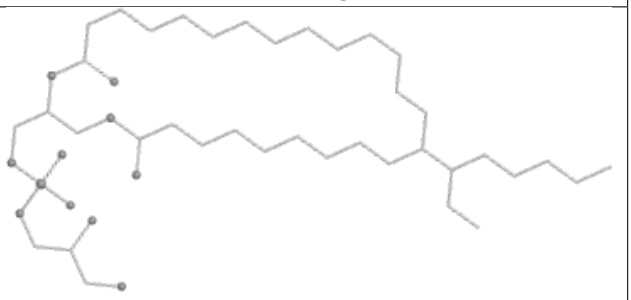
Bond lengths



Bond angles

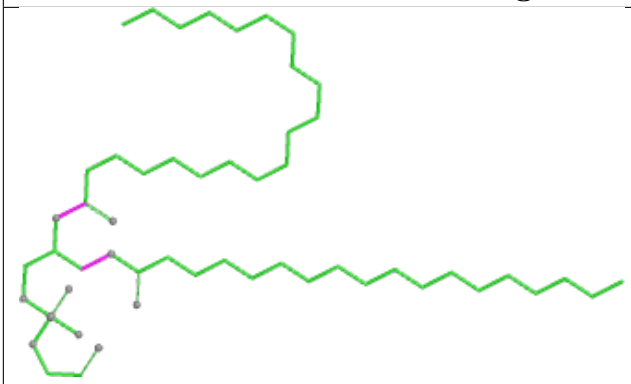


Torsions

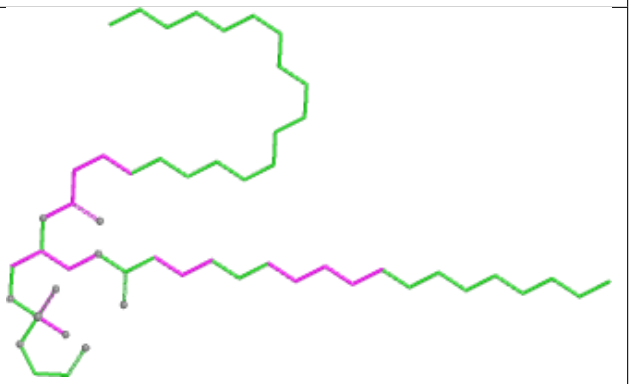


Rings

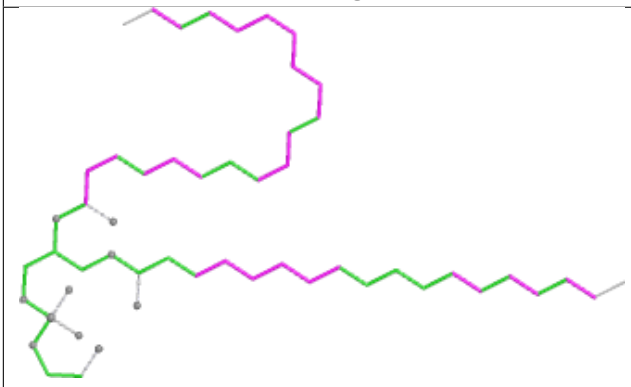
Ligand PEK T 1264



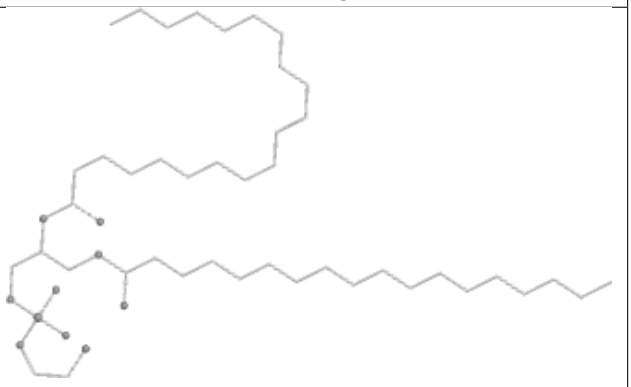
Bond lengths



Bond angles

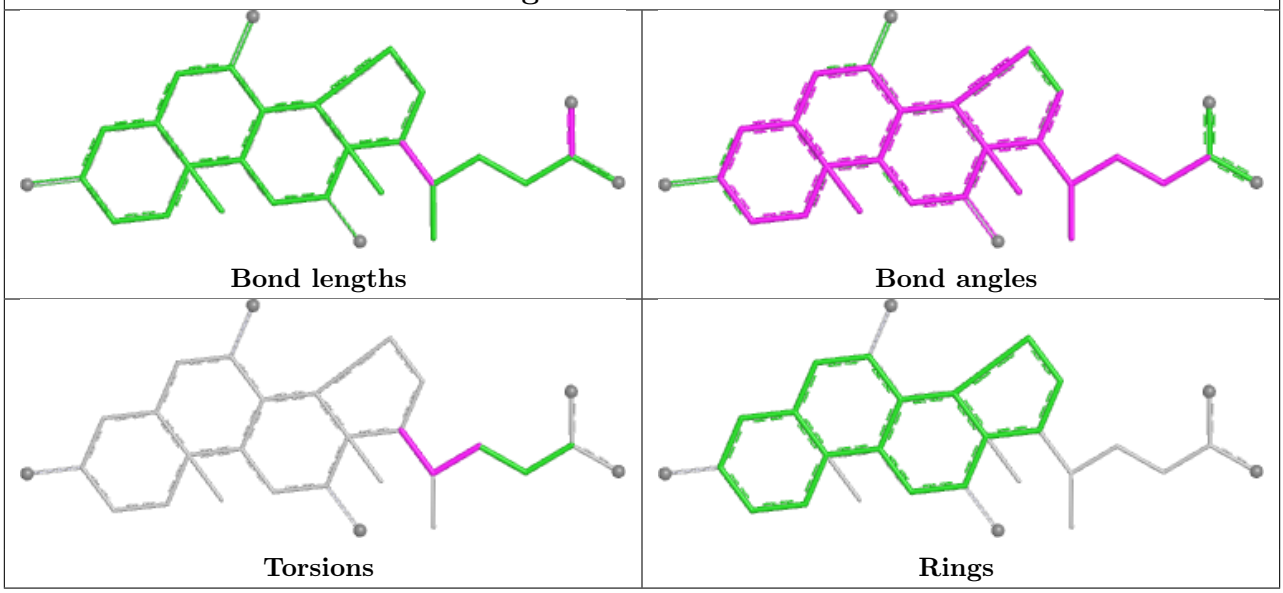


Torsions

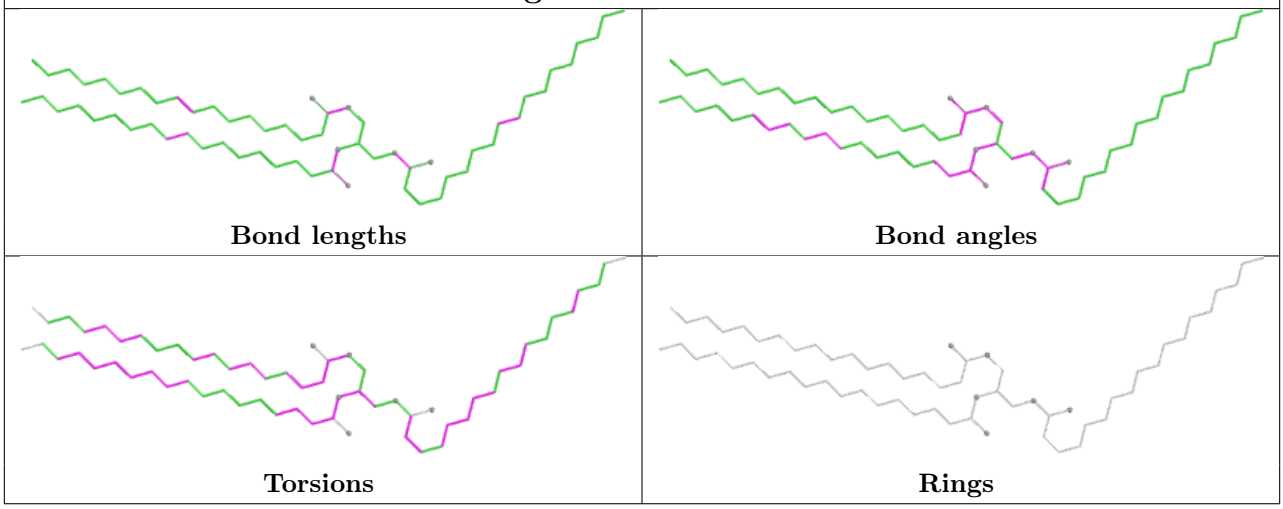


Rings

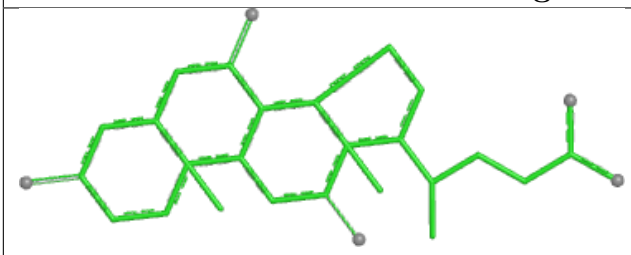
Ligand CHD C 271



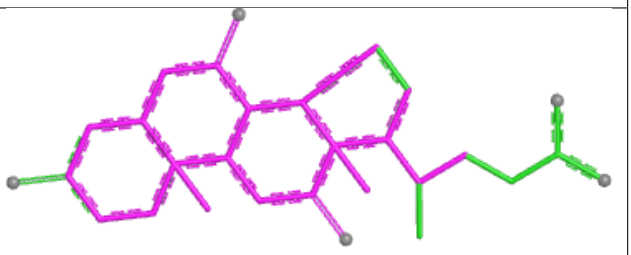
Ligand TGL D 523



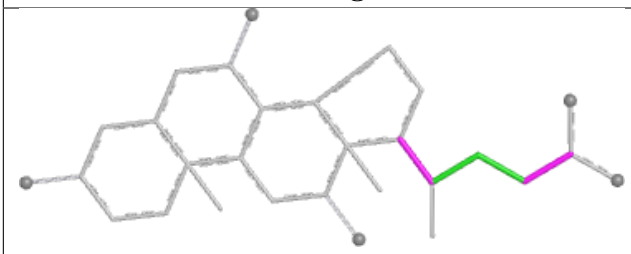
Ligand CHD J 60



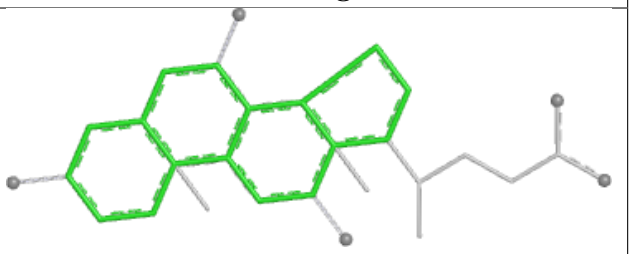
Bond lengths



Bond angles

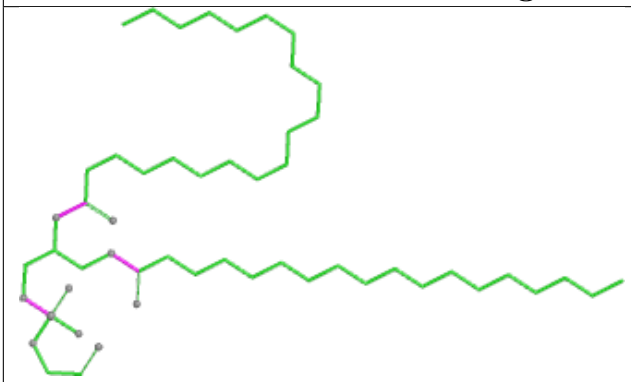


Torsions

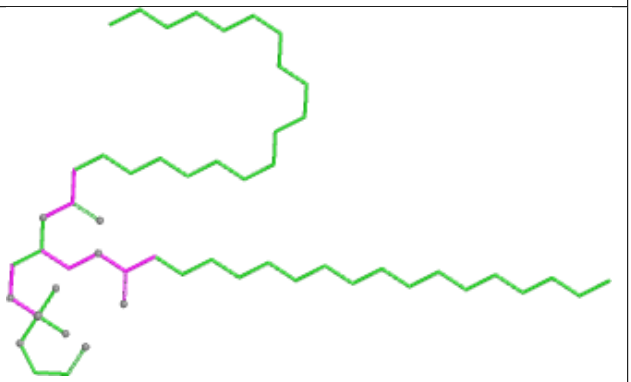


Rings

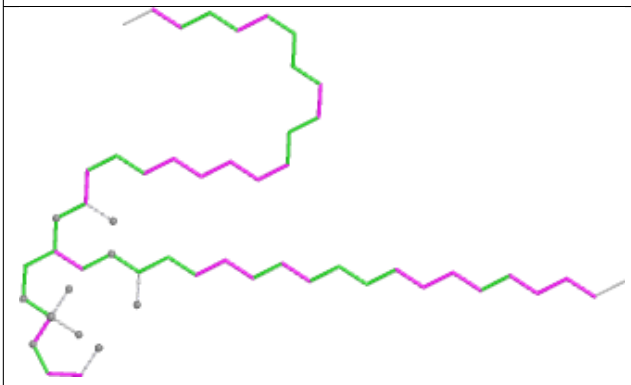
Ligand PEK S 1265



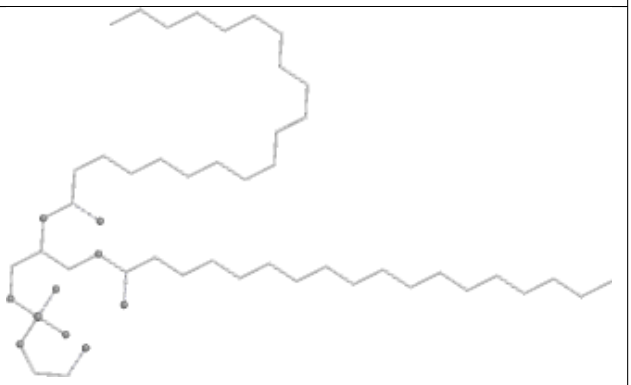
Bond lengths



Bond angles

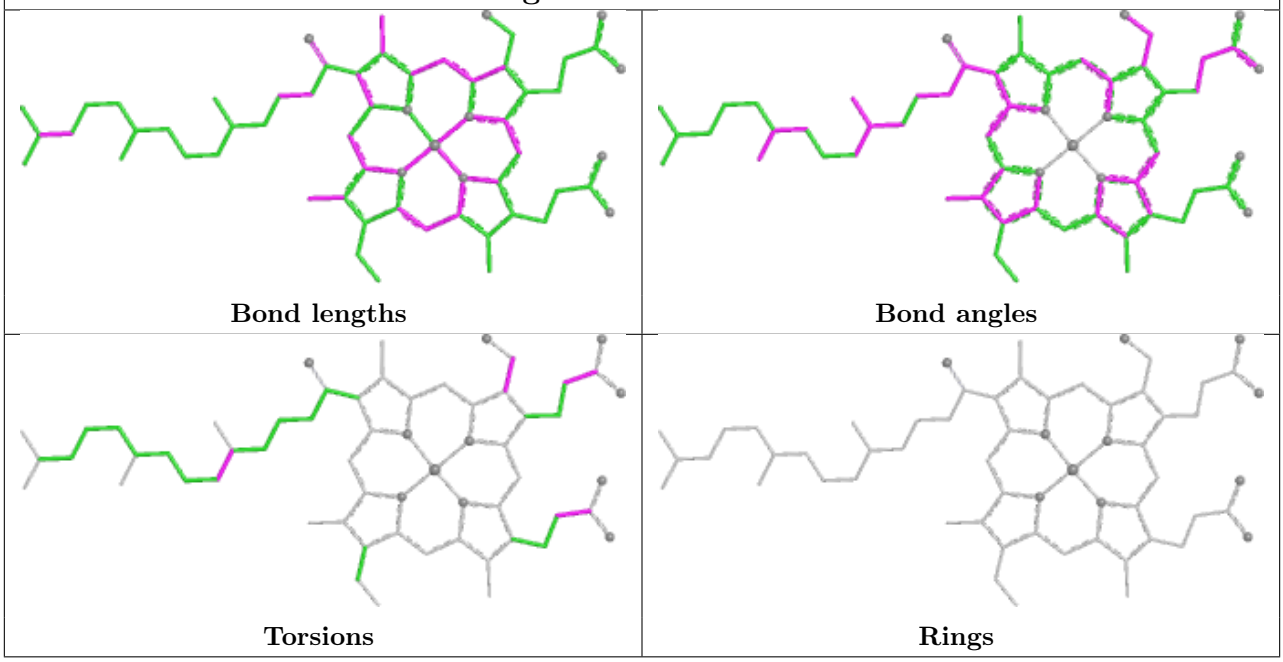


Torsions

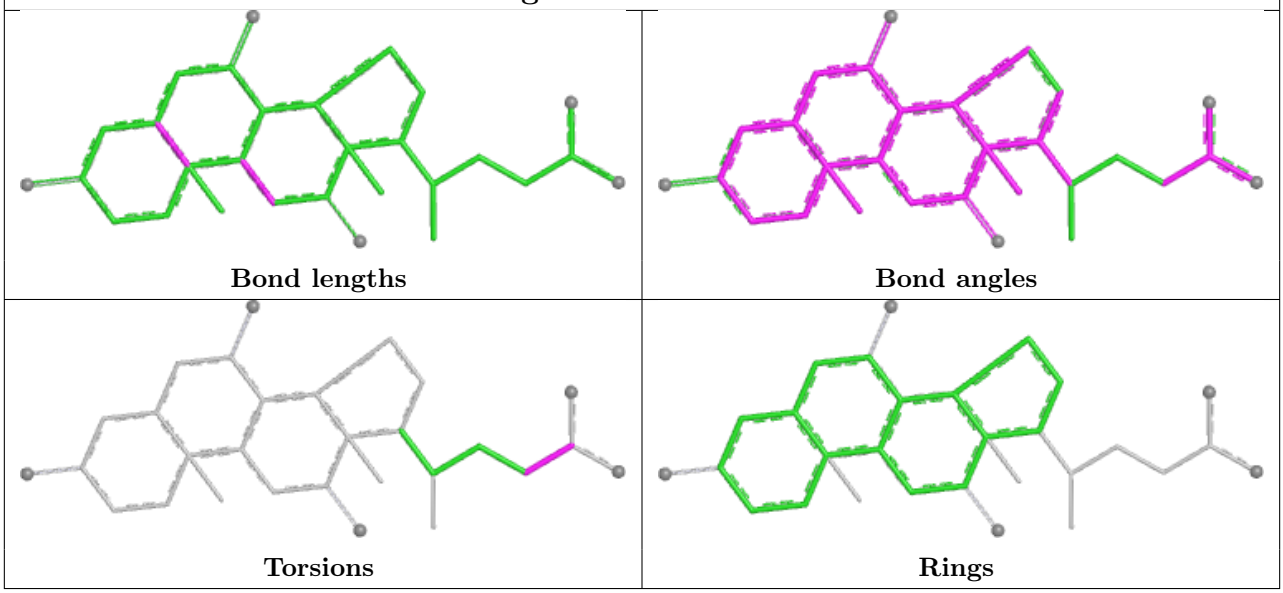


Rings

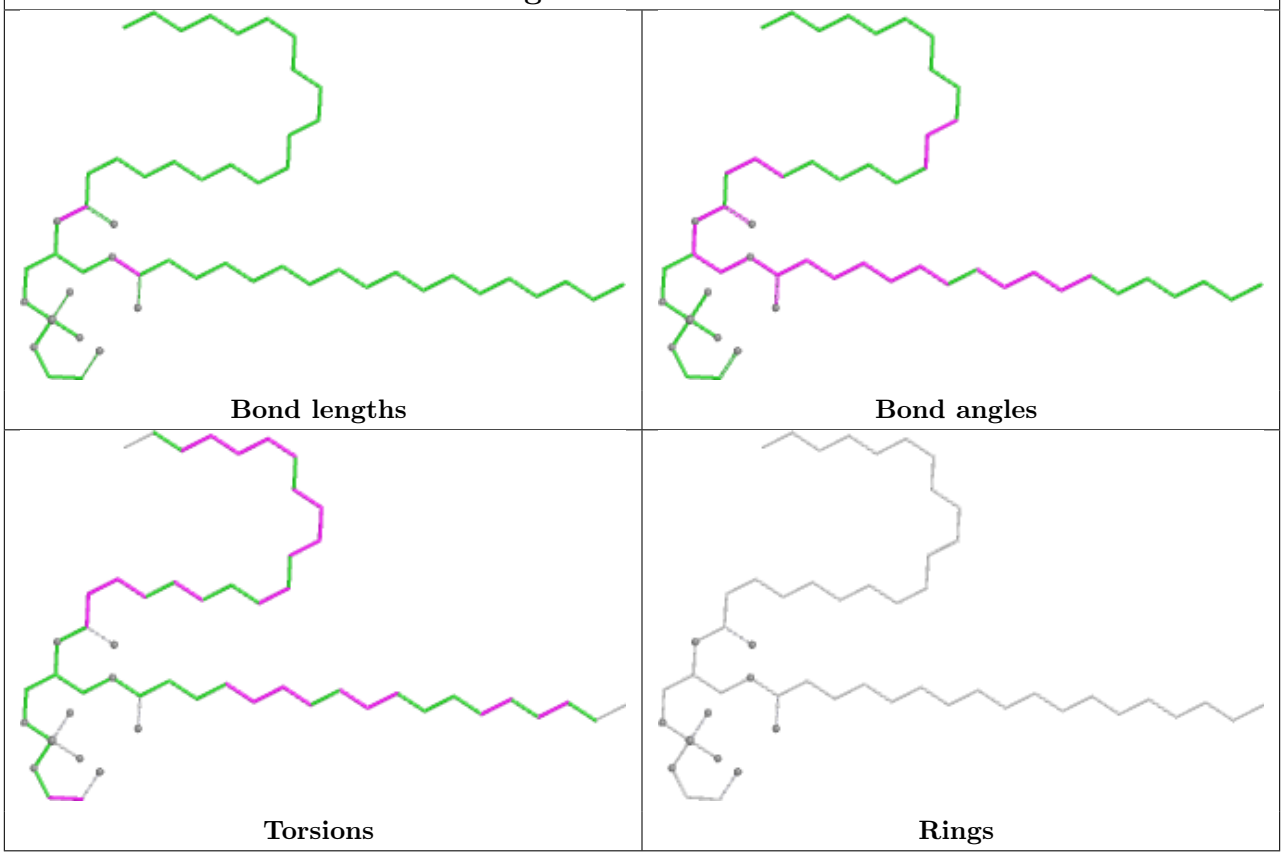
Ligand HEA A 515



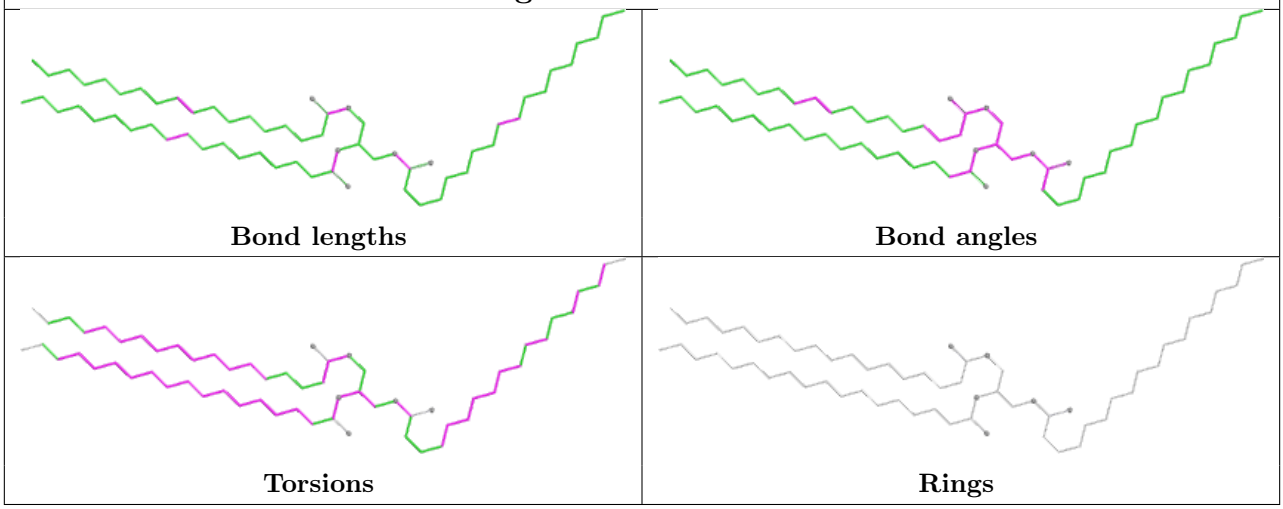
Ligand CHD O 229



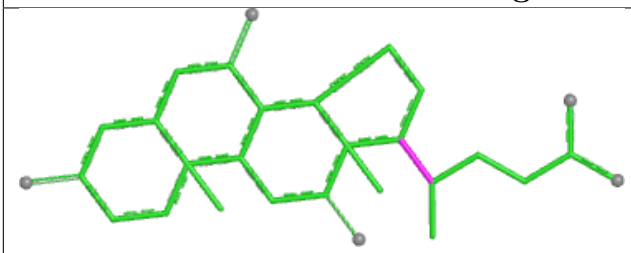
Ligand PEK C 264



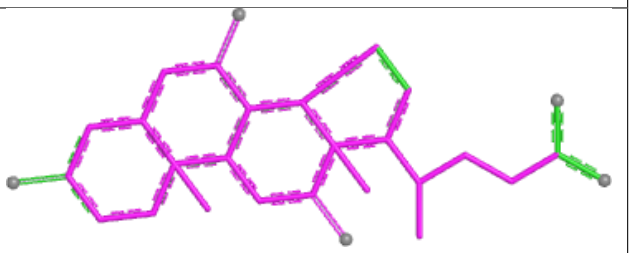
Ligand TGL N 1521



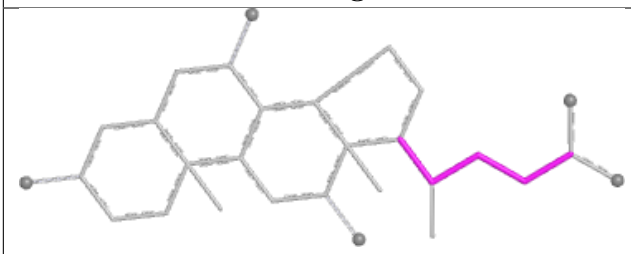
Ligand CHD P 1271



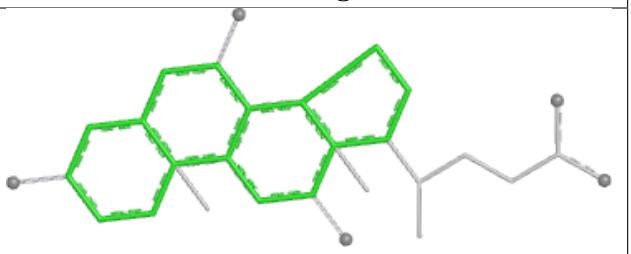
Bond lengths



Bond angles

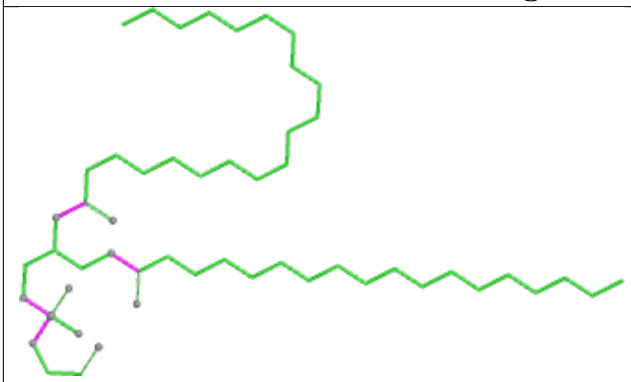


Torsions

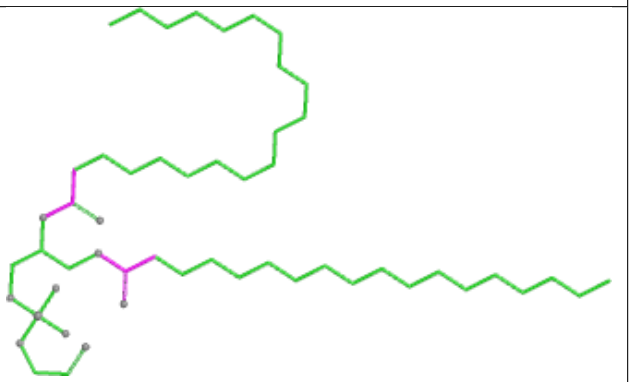


Rings

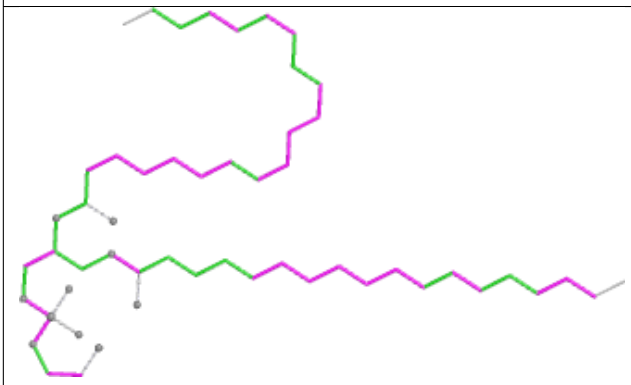
Ligand PEK G 265



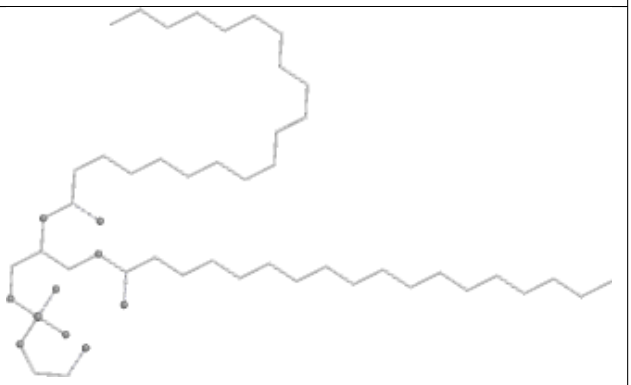
Bond lengths



Bond angles

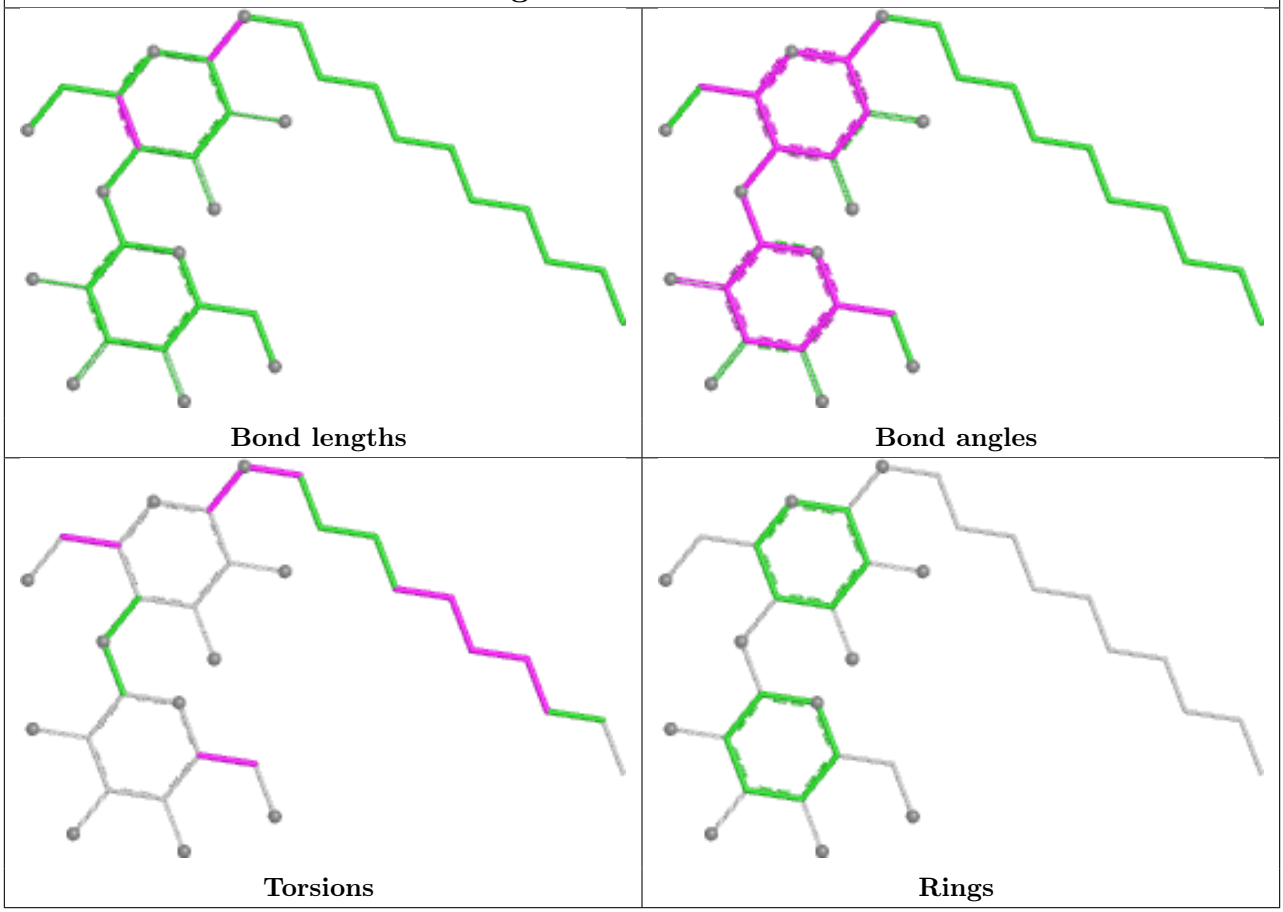


Torsions

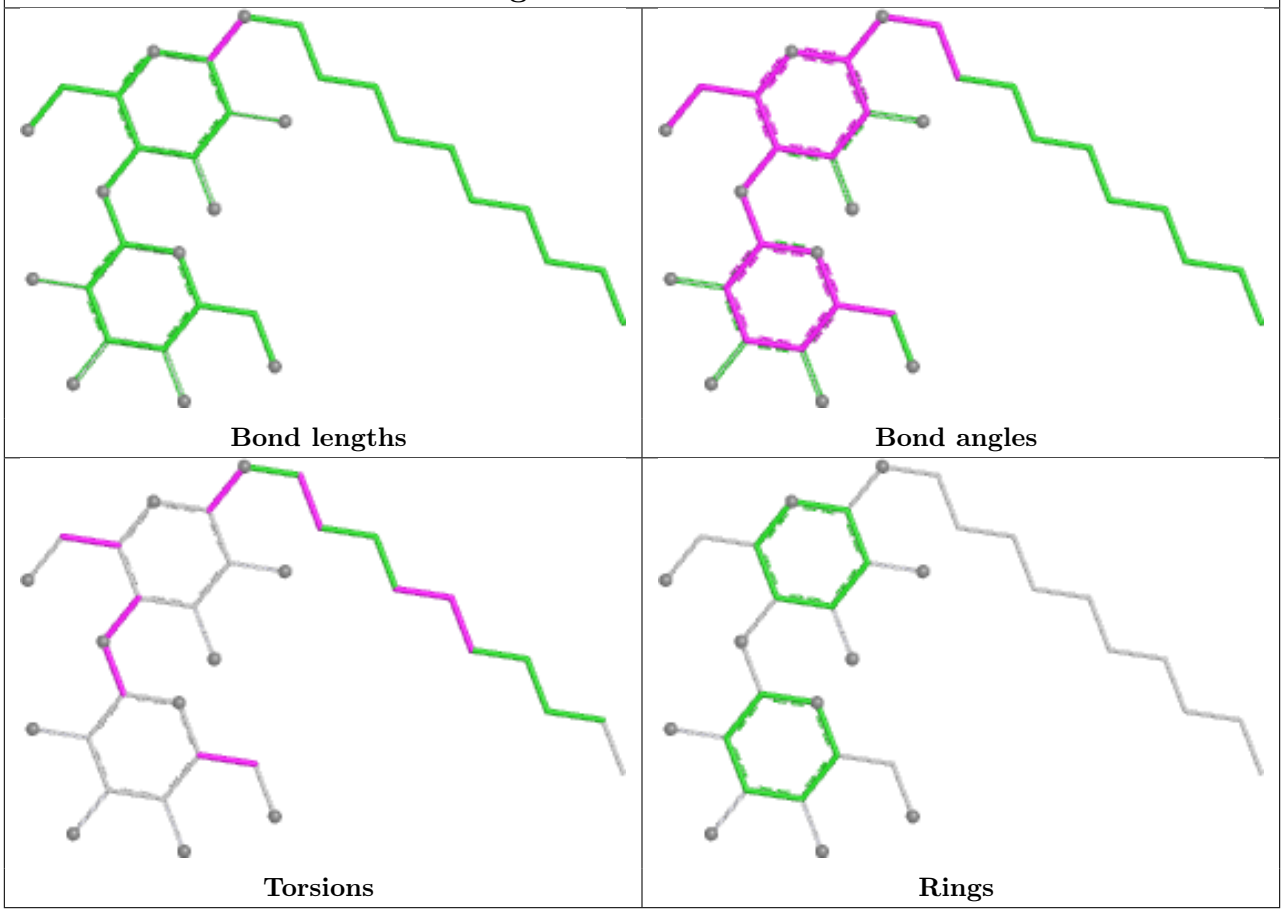


Rings

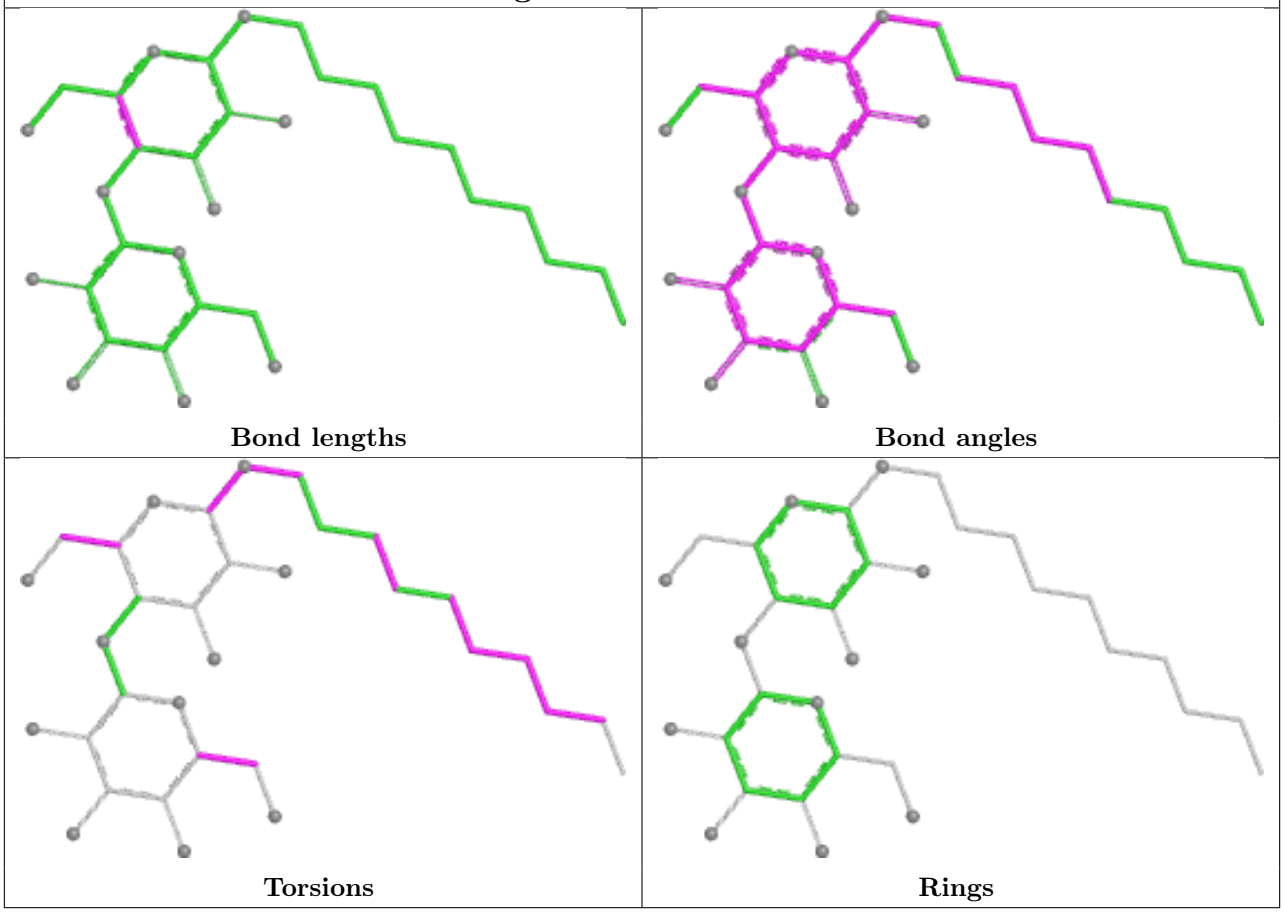
Ligand DMU Z 1526



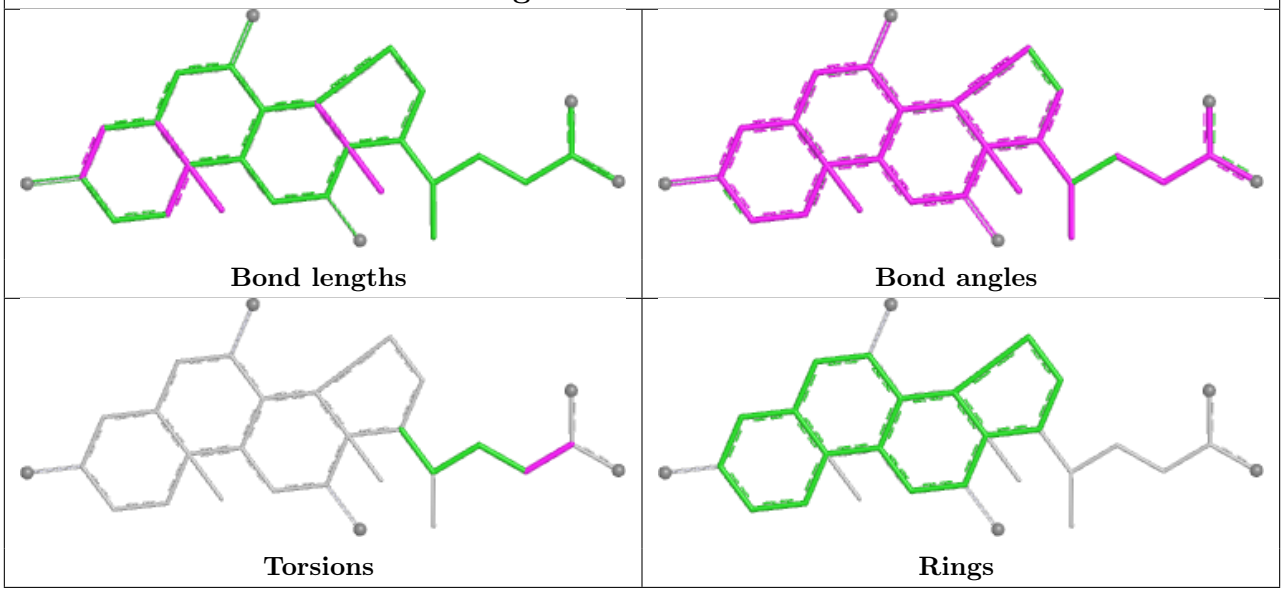
Ligand DMU P 1272



Ligand DMU M 526



Ligand CHD B 1085



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%)	-0.28	6 (1%)	76	78	23, 29, 40, 63	0
1	N	513/514 (99%)	0.36	16 (3%)	51	52	30, 36, 47, 68	0
2	B	226/227 (99%)	0.26	16 (7%)	22	22	24, 35, 59, 78	0
2	O	226/227 (99%)	0.87	27 (11%)	9	8	33, 45, 70, 88	0
3	C	259/261 (99%)	-0.09	2 (0%)	82	84	26, 32, 43, 62	0
3	P	259/261 (99%)	0.30	9 (3%)	47	48	29, 36, 47, 67	0
4	D	144/147 (97%)	0.19	4 (2%)	55	57	30, 37, 56, 70	0
4	Q	144/147 (97%)	1.44	27 (18%)	3	2	39, 52, 76, 118	0
5	E	105/109 (96%)	0.25	2 (1%)	66	68	31, 38, 63, 99	0
5	R	105/109 (96%)	0.84	5 (4%)	35	36	36, 43, 68, 103	0
6	F	98/98 (100%)	0.58	9 (9%)	14	14	29, 39, 80, 127	0
6	S	98/98 (100%)	1.12	12 (12%)	8	7	34, 43, 86, 123	0
7	G	83/85 (97%)	1.30	20 (24%)	2	1	29, 39, 110, 113	0
7	T	83/85 (97%)	1.33	19 (22%)	2	1	29, 42, 102, 110	0
8	H	79/85 (92%)	0.75	13 (16%)	4	4	30, 41, 90, 112	0
8	U	79/85 (92%)	0.97	11 (13%)	6	6	37, 48, 94, 113	0
9	I	72/73 (98%)	0.83	13 (18%)	3	3	34, 46, 80, 83	0
9	V	72/73 (98%)	1.37	15 (20%)	2	2	39, 55, 82, 85	0
10	J	58/59 (98%)	0.60	4 (6%)	23	23	31, 41, 65, 96	0
10	W	58/59 (98%)	0.95	6 (10%)	12	11	34, 45, 69, 107	0
11	K	49/56 (87%)	0.49	2 (4%)	41	41	33, 41, 52, 62	0
11	X	49/56 (87%)	1.36	9 (18%)	3	2	44, 51, 64, 76	0
12	L	46/47 (97%)	0.19	2 (4%)	40	40	29, 34, 50, 79	0
12	Y	46/47 (97%)	0.96	3 (6%)	25	24	34, 45, 61, 81	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	43/46 (93%)	0.31	4 (9%) 14 14	30, 34, 71, 101	0
13	Z	43/46 (93%)	1.29	6 (13%) 6 5	41, 46, 90, 112	0
All	All	3550/3614 (98%)	0.47	262 (7%) 20 21	23, 38, 69, 127	0

The worst 5 of 262 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	6	VAL	11.5
6	S	1	ALA	10.8
4	Q	5	VAL	10.2
6	F	1	ALA	9.9
6	S	97	ALA	9.9

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	SAC	V	1	9/10	0.03	0.23	88,90,92,93	0
7	TPO	T	11	11/12	0.52	0.24	75,82,101,102	0
7	TPO	G	11	11/12	0.52	0.29	74,82,105,105	0
9	SAC	I	1	9/10	0.70	0.18	77,82,84,85	0
1	FME	N	1	10/11	0.81	0.24	50,54,74,77	0
1	FME	A	1	10/11	0.85	0.15	46,51,63,76	0
2	FME	O	1	10/11	0.94	0.12	41,42,49,55	0
2	FME	B	1	10/11	0.96	0.09	31,33,40,56	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
23	UNX	C	262	1/1	0.68	0.58	49,49,49,49	0
24	PEK	T	263	53/53	0.68	0.31	54,103,127,128	0
23	UNX	P	262	1/1	0.71	0.58	49,49,49,49	0
22	CHD	W	1059	29/29	0.72	0.25	107,115,119,120	0
24	PEK	G	265	53/53	0.73	0.27	51,91,109,114	0
28	DMU	P	1272	33/33	0.73	0.25	104,118,124,125	0
24	PEK	G	1263	53/53	0.74	0.32	59,107,131,132	0
19	TGL	N	1522	63/63	0.74	0.29	54,76,92,95	0
20	PGV	N	1524	51/51	0.74	0.26	54,81,117,119	0
20	PGV	P	1268	51/51	0.76	0.29	64,100,119,121	0
24	PEK	S	1265	53/53	0.76	0.27	50,87,111,114	0
26	PSC	R	1229	52/52	0.77	0.28	53,109,133,136	0
25	CDL	G	269	100/100	0.77	0.28	72,99,122,124	0
25	CDL	T	1269	100/100	0.78	0.28	66,96,122,126	0
26	PSC	E	229	52/52	0.78	0.26	53,106,131,133	0
19	TGL	Q	1523	63/63	0.78	0.28	67,83,98,100	0
22	CHD	J	60	29/29	0.78	0.21	105,109,113,114	0
19	TGL	A	521	63/63	0.79	0.25	49,82,106,110	0
28	DMU	G	272	33/33	0.79	0.23	85,116,119,121	0
25	CDL	P	1270	100/100	0.79	0.28	46,100,119,122	0
20	PGV	C	268	51/51	0.80	0.28	60,91,117,117	0
19	TGL	D	523	63/63	0.80	0.27	48,70,93,94	0
20	PGV	A	524	51/51	0.80	0.26	45,75,117,118	0
19	TGL	N	1521	63/63	0.81	0.26	71,92,105,109	0
19	TGL	L	522	63/63	0.81	0.26	43,68,84,87	0
25	CDL	C	270	100/100	0.82	0.23	49,96,120,122	0
28	DMU	Z	1526	33/33	0.82	0.15	44,59,75,75	0
22	CHD	C	271	29/29	0.83	0.19	72,84,87,90	0
15	CYN	N	520	2/2	0.87	0.16	42,42,42,43	0
22	CHD	P	1271	29/29	0.87	0.17	68,86,90,91	0
28	DMU	M	526	33/33	0.91	0.11	36,51,69,71	0
24	PEK	T	1264	53/53	0.93	0.16	30,54,83,85	0
22	CHD	P	1525	29/29	0.94	0.09	28,38,43,51	0
22	CHD	O	229	29/29	0.94	0.08	27,34,42,45	0
20	PGV	N	1266	51/51	0.95	0.12	28,43,70,75	0
18	NA	N	519	1/1	0.95	0.10	40,40,40,40	0
24	PEK	C	264	53/53	0.95	0.14	27,50,76,79	0
22	CHD	B	1085	29/29	0.95	0.08	29,34,40,50	0
22	CHD	C	525	29/29	0.95	0.08	25,35,39,46	0
14	HEA	N	516	60/60	0.95	0.12	32,40,54,57	0
17	MG	N	518	1/1	0.96	0.05	33,33,33,33	0
20	PGV	A	522	51/51	0.96	0.11	25,36,68,72	0

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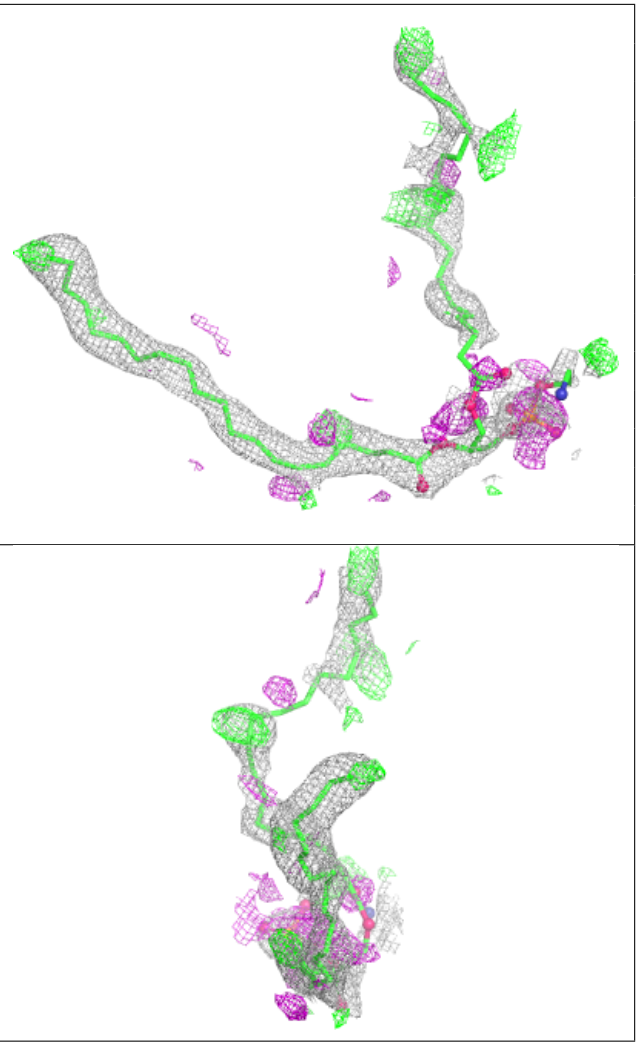
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	PGV	P	1267	51/51	0.96	0.12	29,40,77,85	0
20	PGV	C	267	51/51	0.96	0.12	23,36,72,75	0
15	CYN	A	520	2/2	0.96	0.08	31,31,31,31	0
21	CUA	O	228	2/2	0.97	0.04	36,36,36,37	0
18	NA	A	519	1/1	0.97	0.05	30,30,30,30	0
14	HEA	A	516	60/60	0.97	0.10	23,35,51,52	0
14	HEA	N	515	60/60	0.98	0.08	30,36,50,52	0
14	HEA	A	515	60/60	0.98	0.06	18,27,40,45	0
27	ZN	F	99	1/1	0.99	0.02	35,35,35,35	0
27	ZN	S	99	1/1	0.99	0.02	38,38,38,38	0
21	CUA	B	228	2/2	0.99	0.03	28,28,28,28	0
17	MG	A	518	1/1	0.99	0.03	25,25,25,25	0
16	CU	A	517	1/1	0.99	0.04	31,31,31,31	0
16	CU	N	517	1/1	0.99	0.04	37,37,37,37	0

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

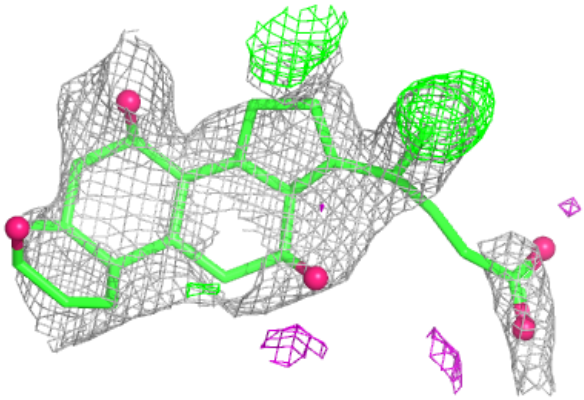
Electron density around PEK T 263:

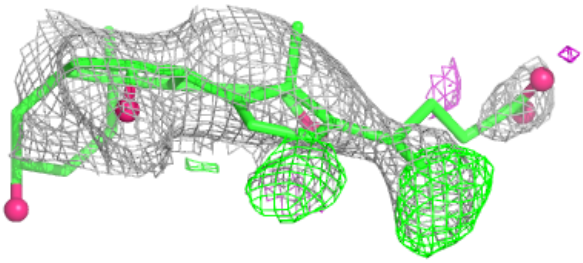
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

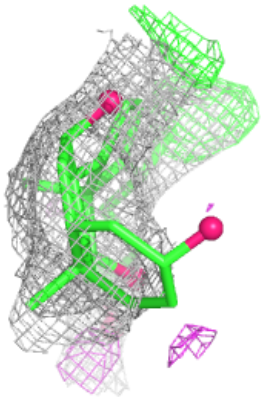


Electron density around CHD W 1059:

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

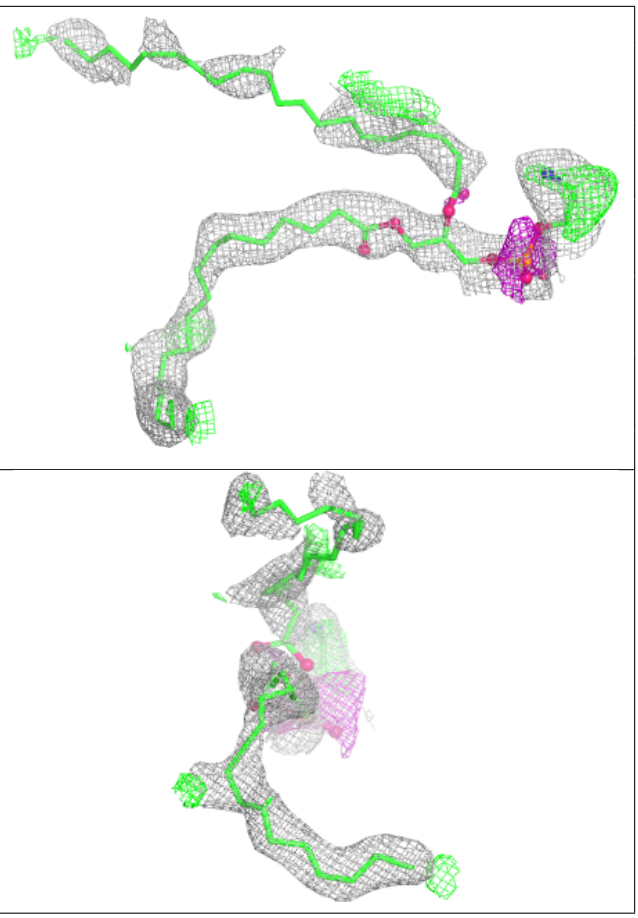






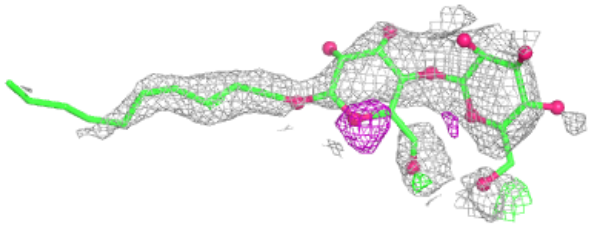
Electron density around PEK G 265:

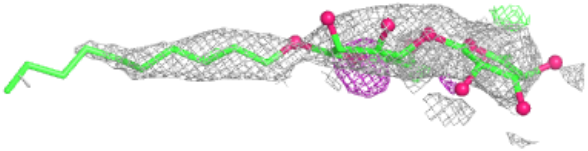
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

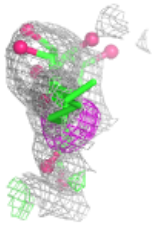


Electron density around DMU P 1272:

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

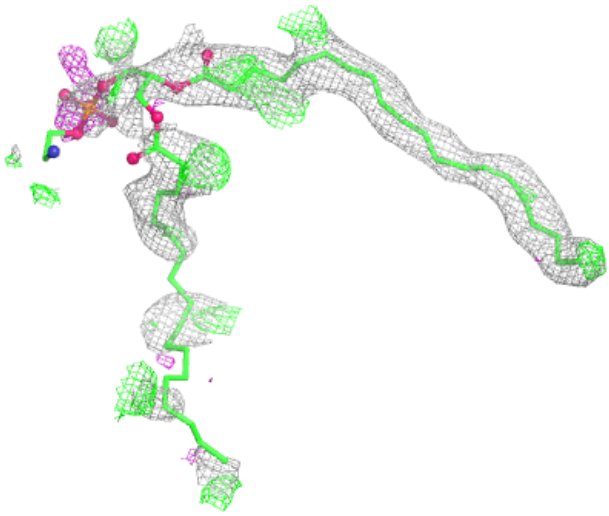


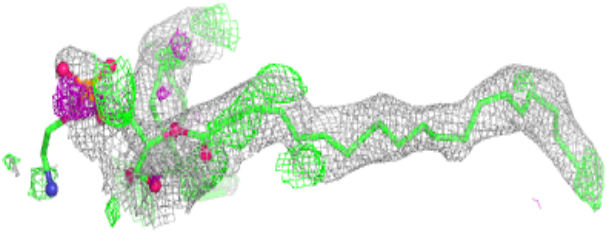


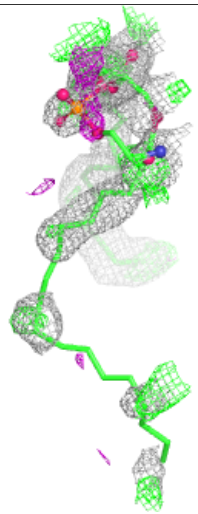


Electron density around PEK G 1263:

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

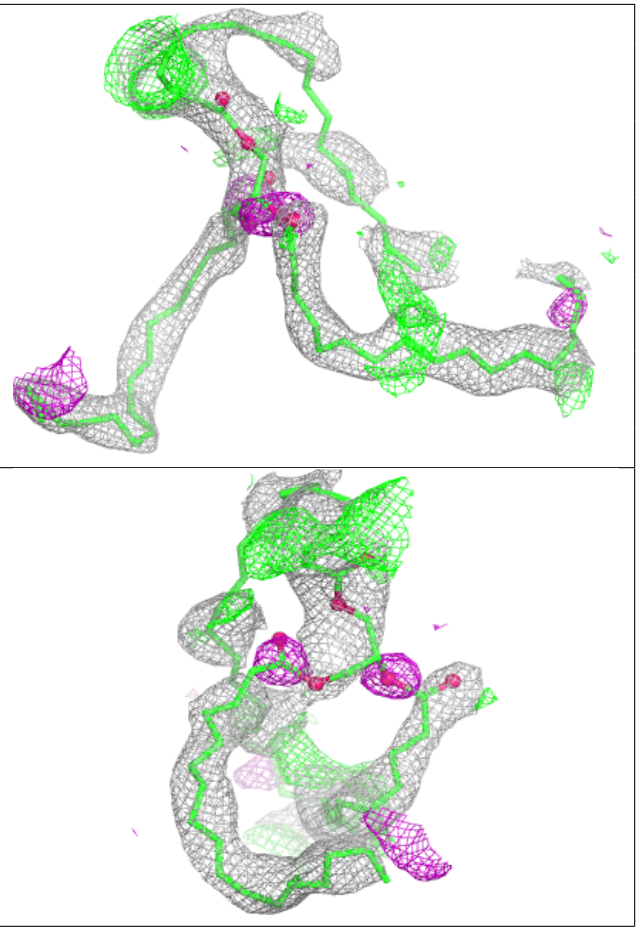






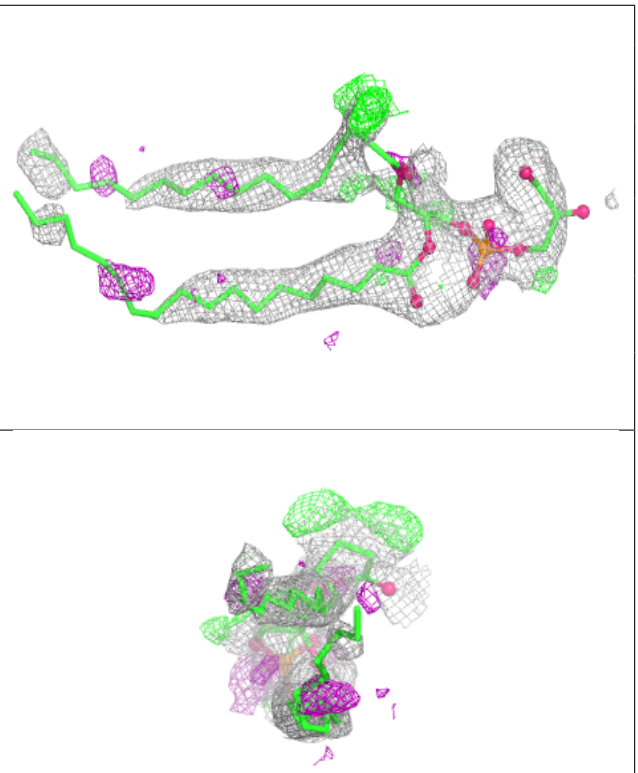
Electron density around TGL N 1522:

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



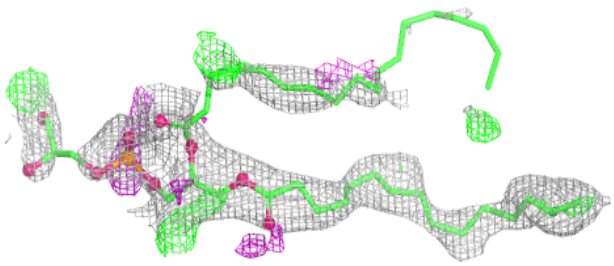
Electron density around PGV N 1524:

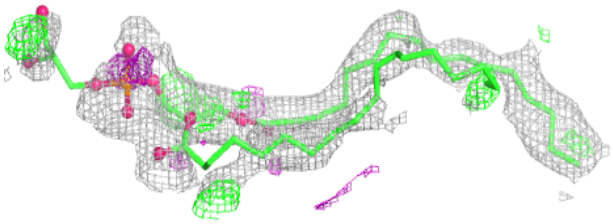
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

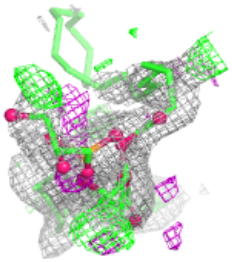


Electron density around PGV P 1268:

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

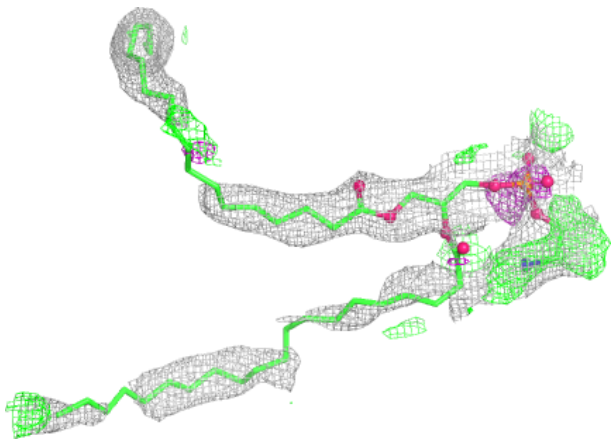


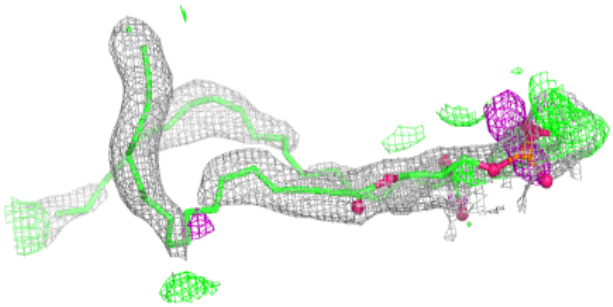


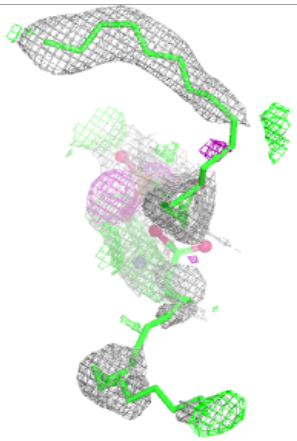


Electron density around PEK S 1265:

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

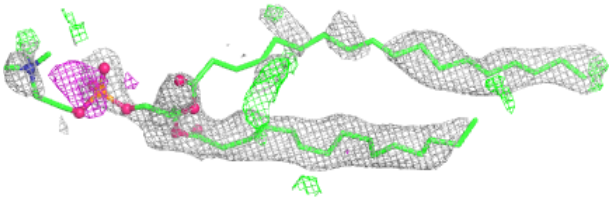


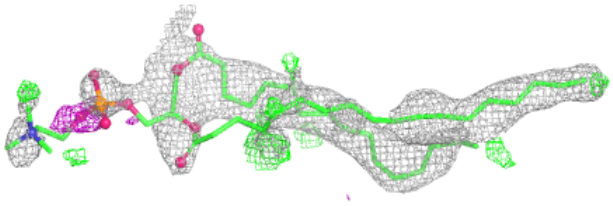


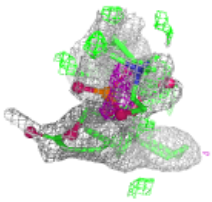


Electron density around PSC R 1229:

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

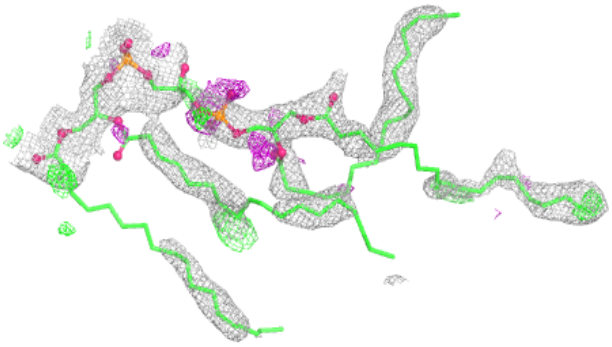


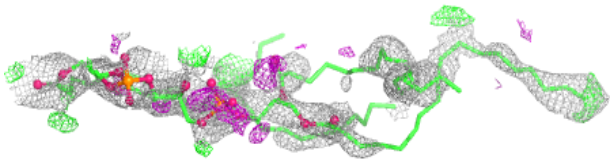


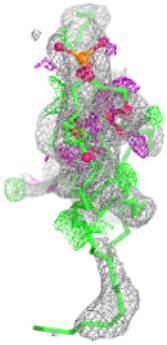


Electron density around CDL G 269:

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

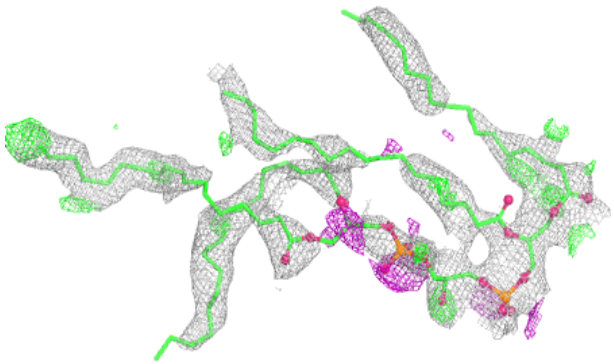


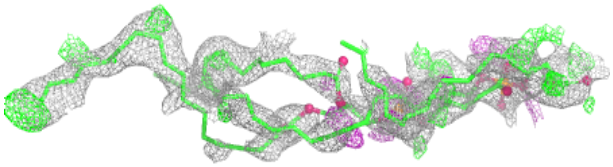


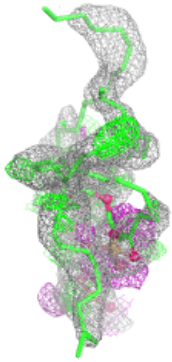


Electron density around CDL T 1269:

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

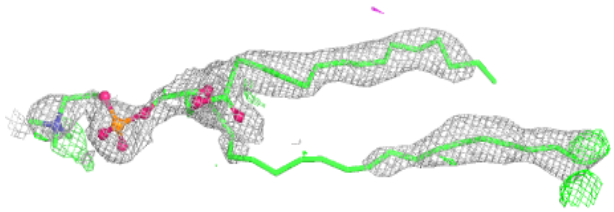


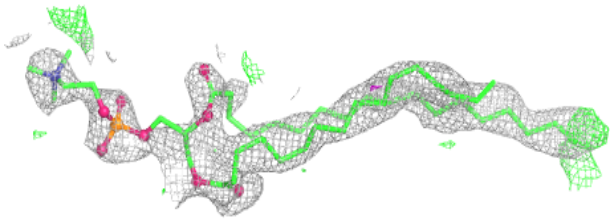


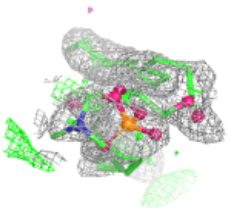


Electron density around PSC E 229:

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

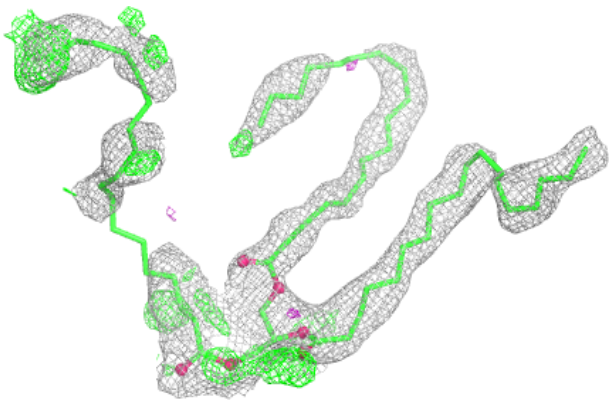


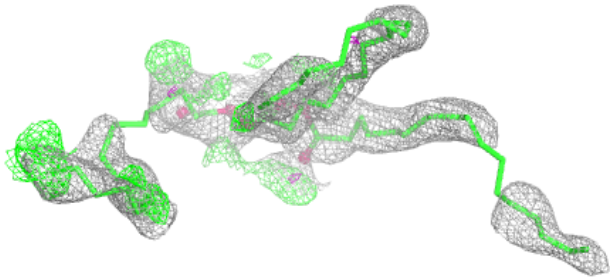


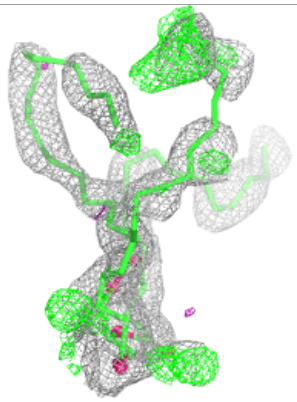


Electron density around TGL Q 1523:

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

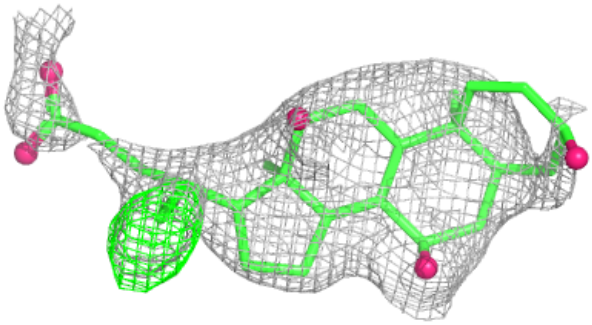


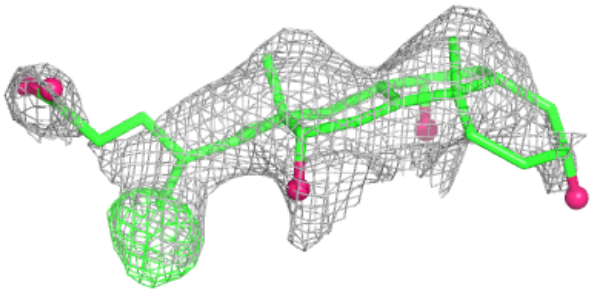


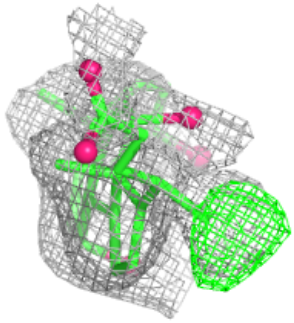


Electron density around CHD J 60:

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

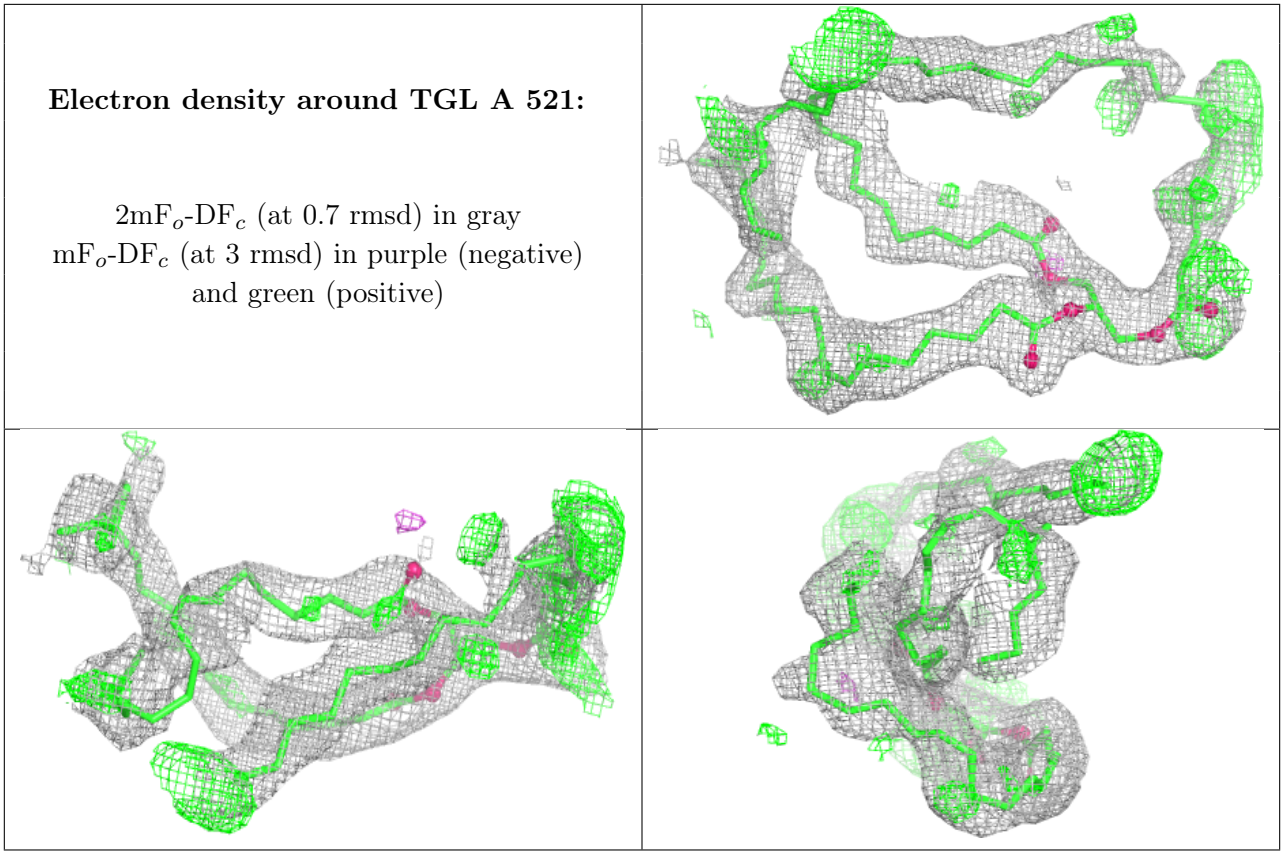






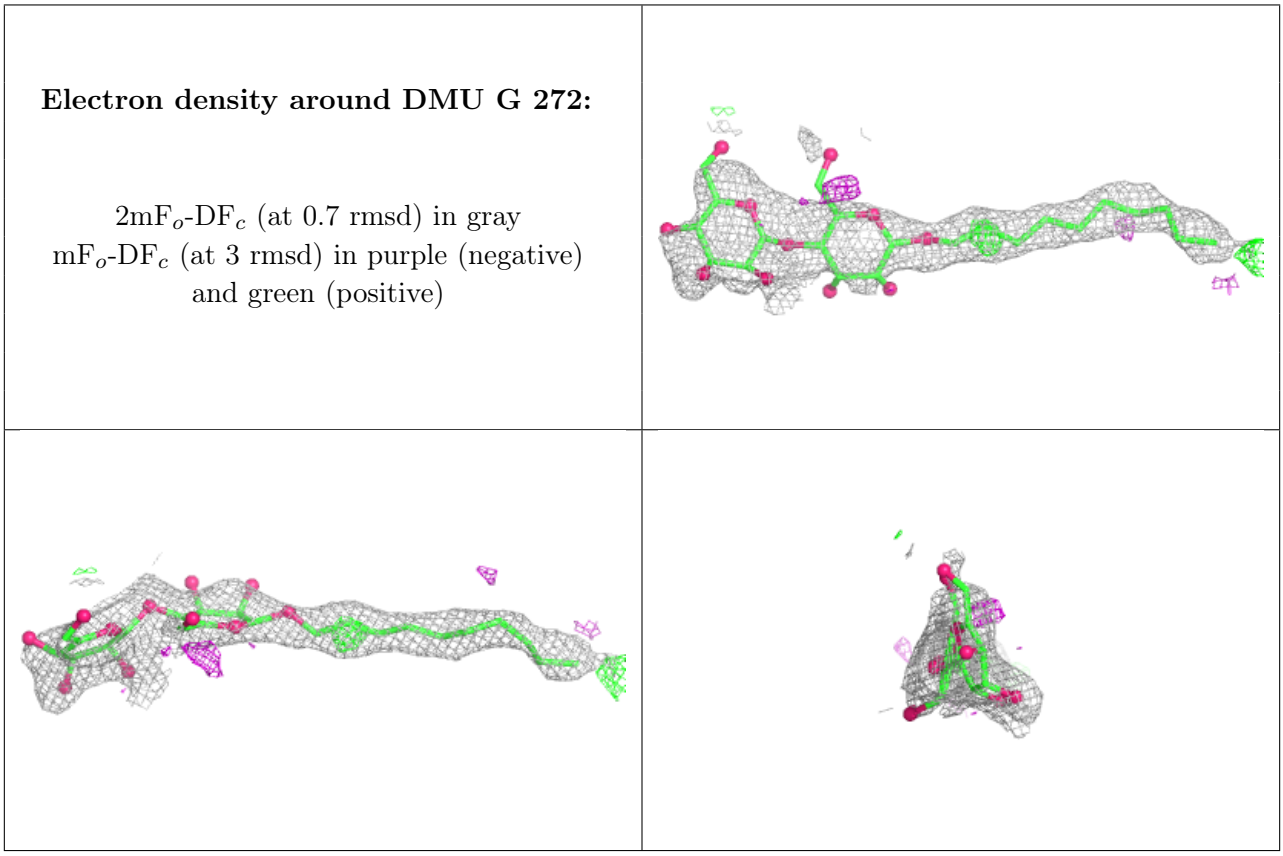
Electron density around TGL A 521:

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



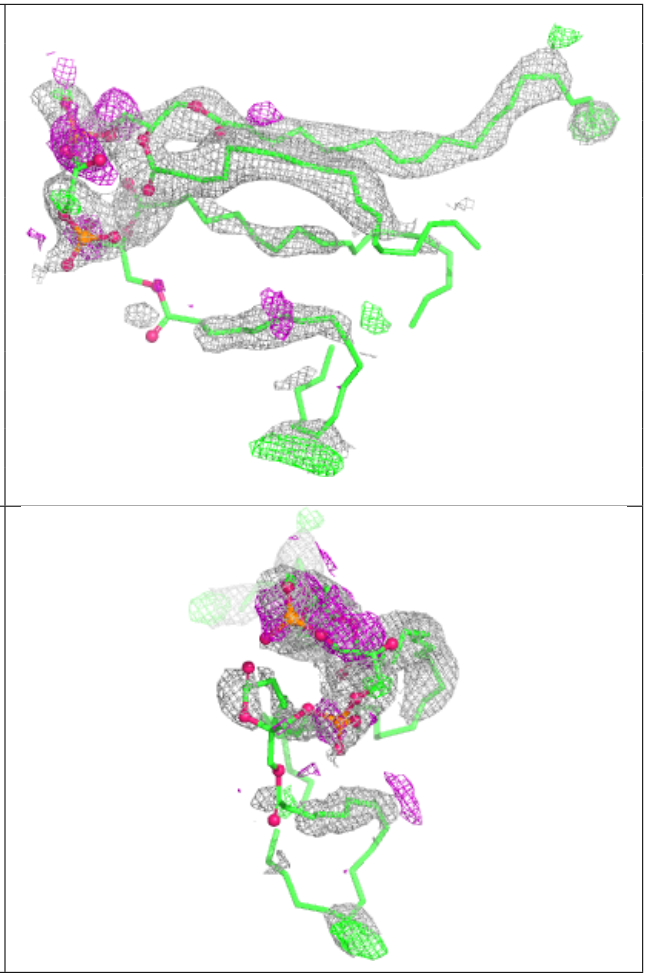
Electron density around DMU G 272:

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



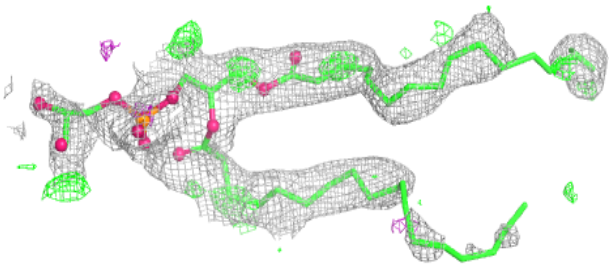
Electron density around CDL P 1270:

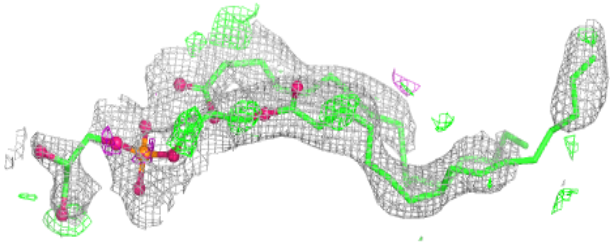
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

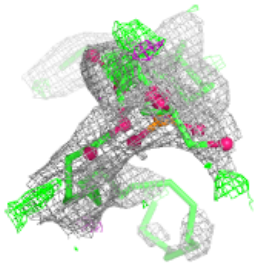


Electron density around PGV C 268:

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

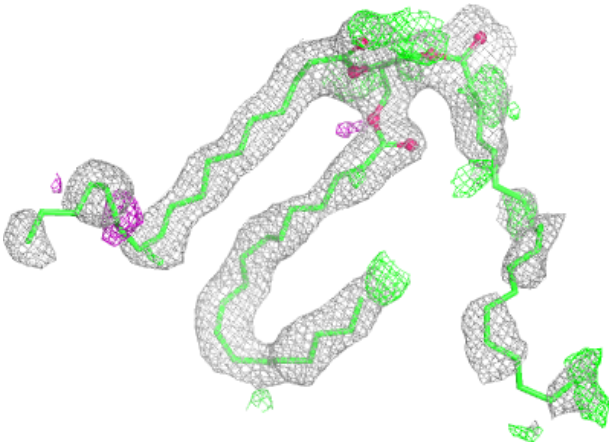


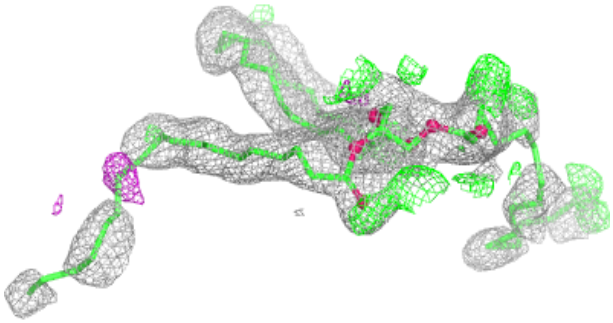




Electron density around TGL D 523:

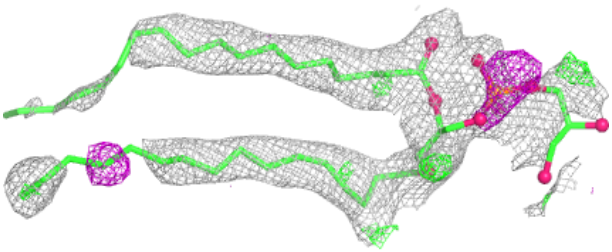
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

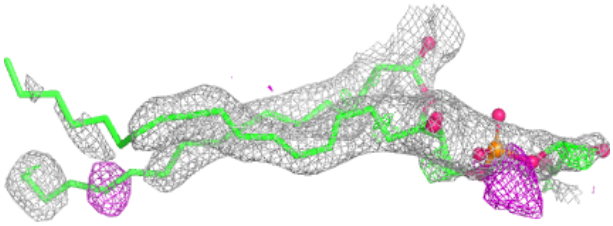


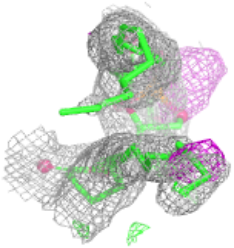


Electron density around PGV A 524:

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

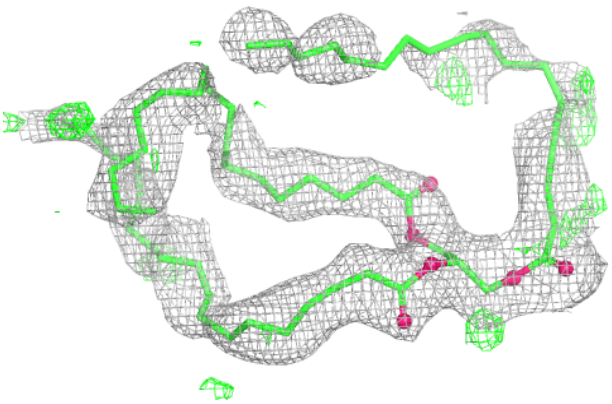


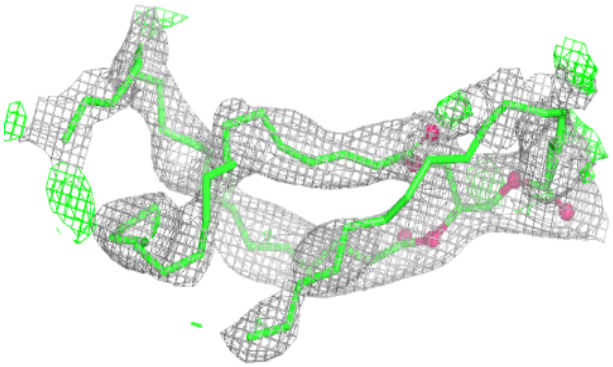


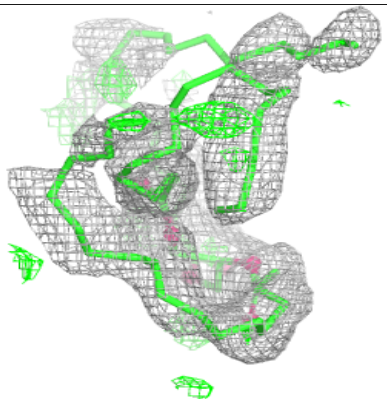


Electron density around TGL N 1521:

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

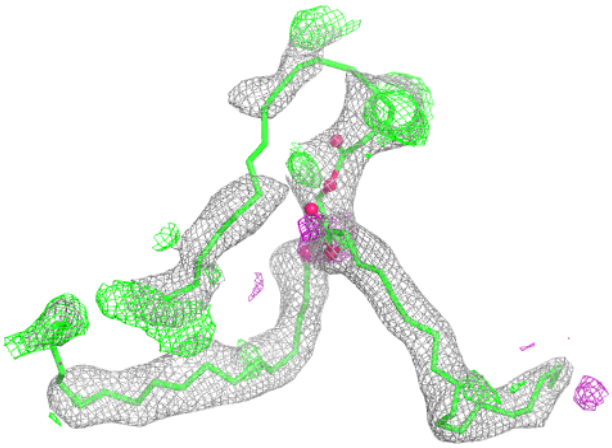


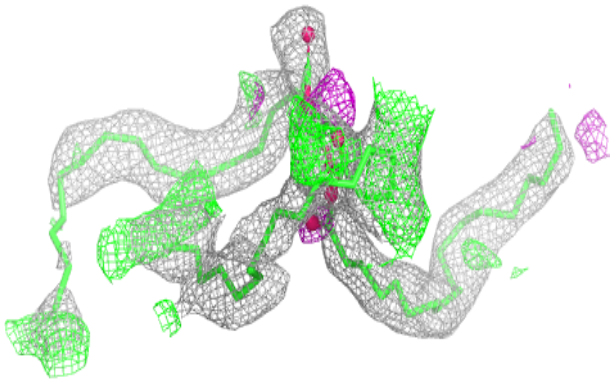


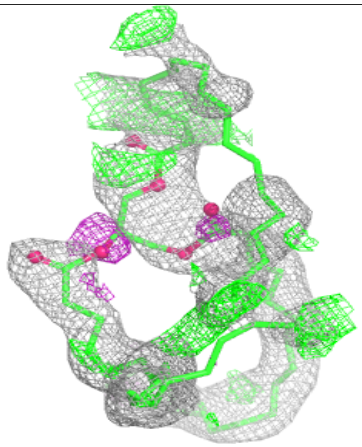


Electron density around TGL L 522:

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

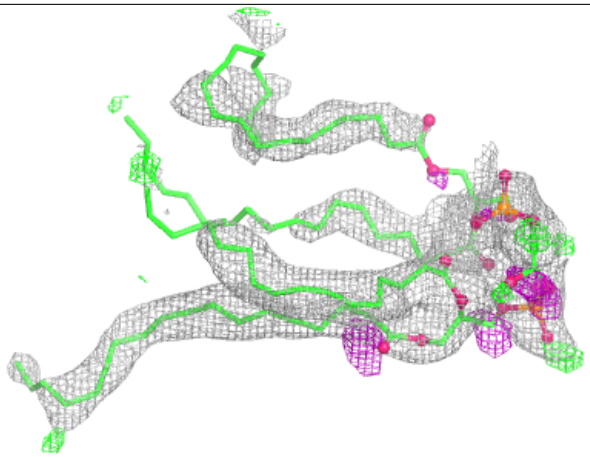


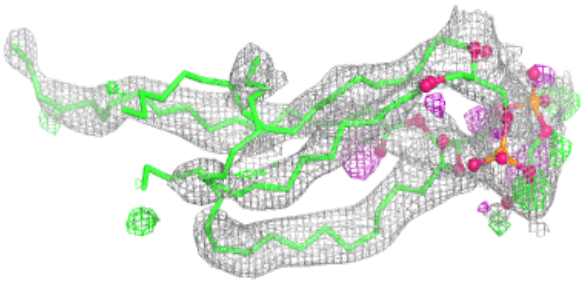


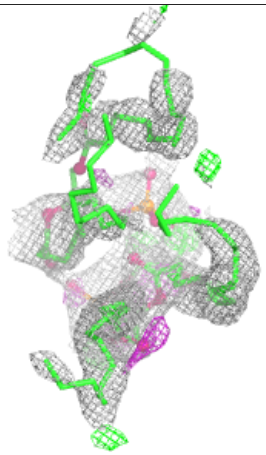


Electron density around CDL C 270:

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

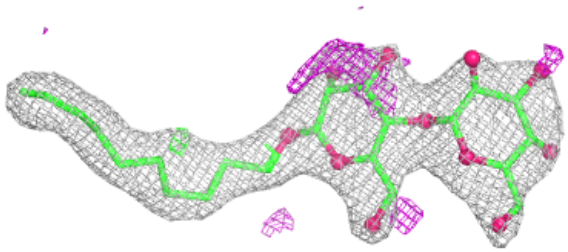


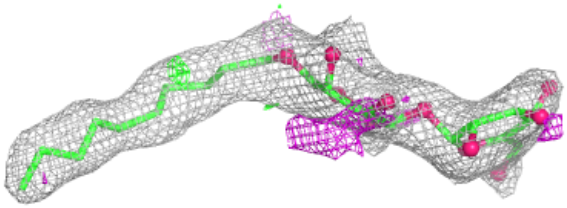


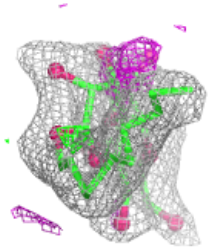


Electron density around DMU Z 1526:

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

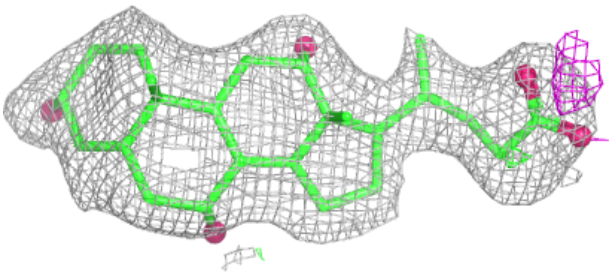


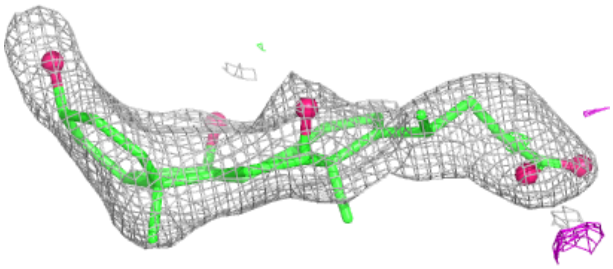


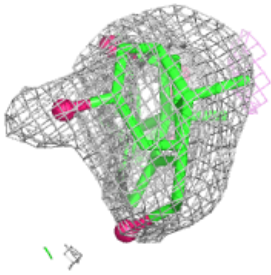


Electron density around CHD C 271:

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

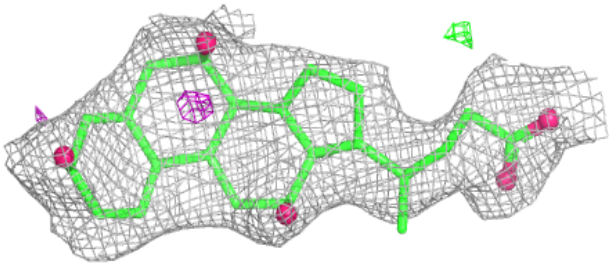


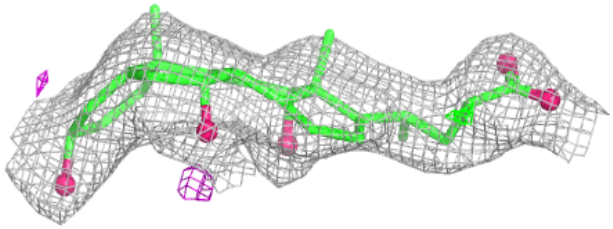


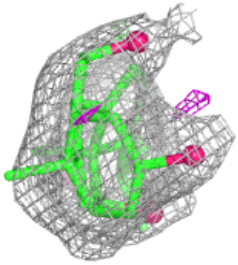


Electron density around CHD P 1271:

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

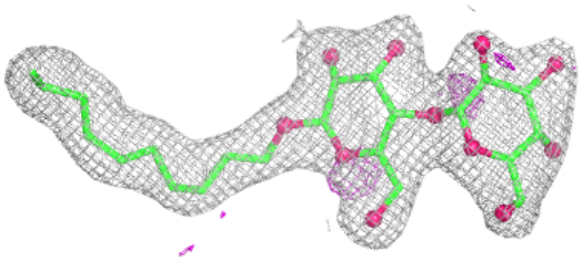


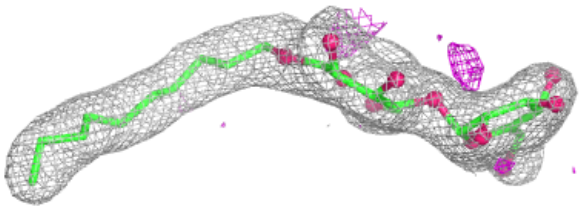


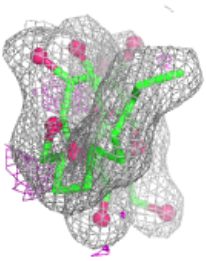


Electron density around DMU M 526:

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

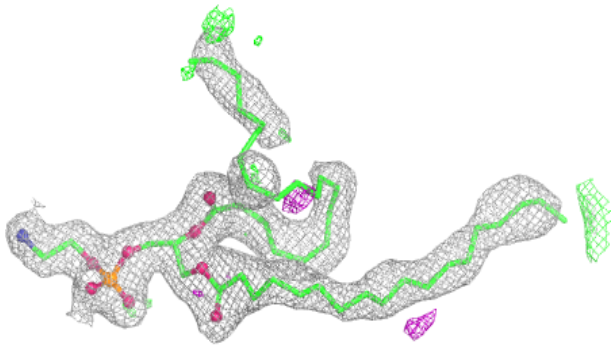


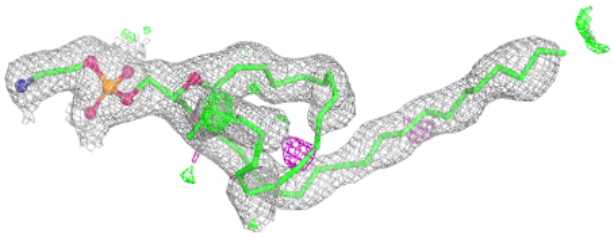


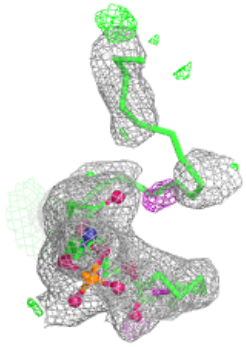


Electron density around PEK T 1264:

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

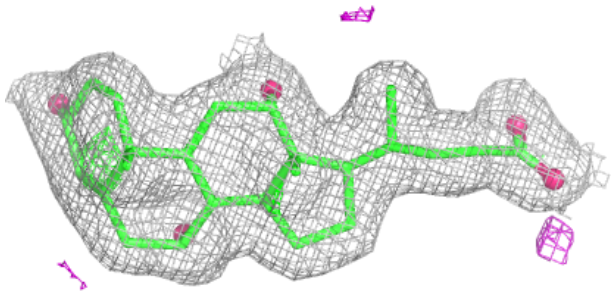


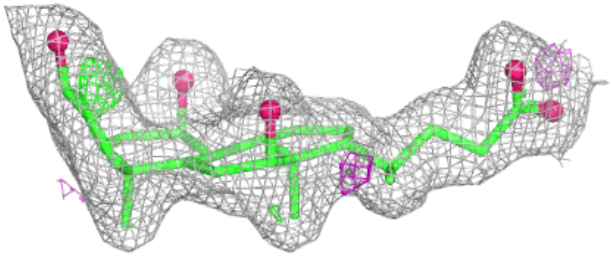


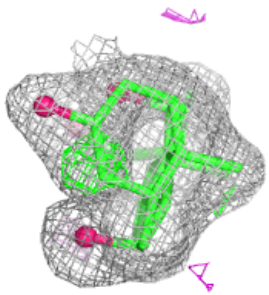


Electron density around CHD P 1525:

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

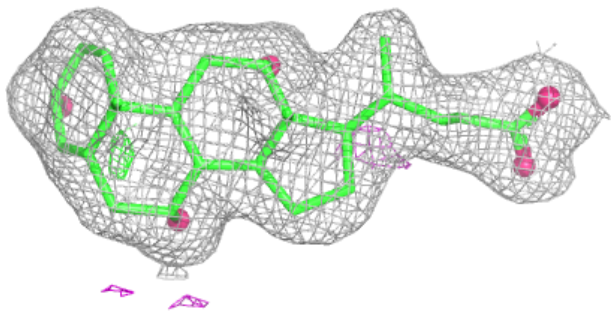


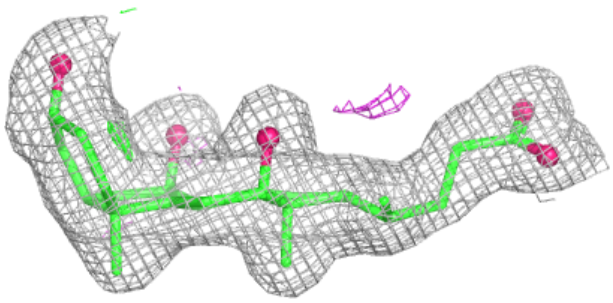


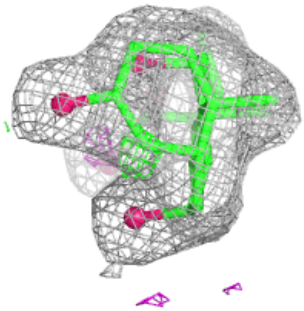


Electron density around CHD O 229:

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

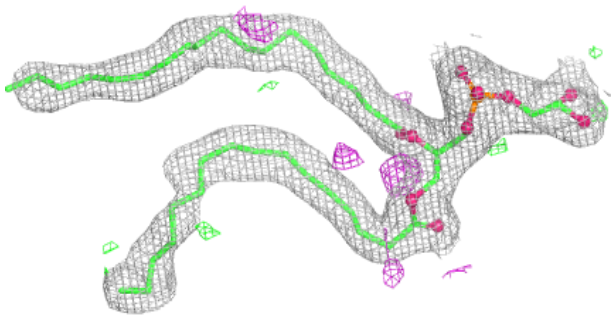


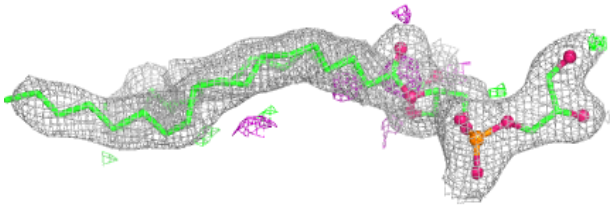


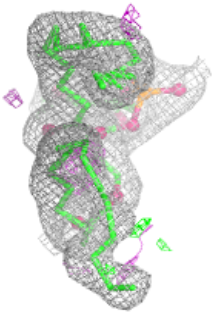


Electron density around PGV N 1266:

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

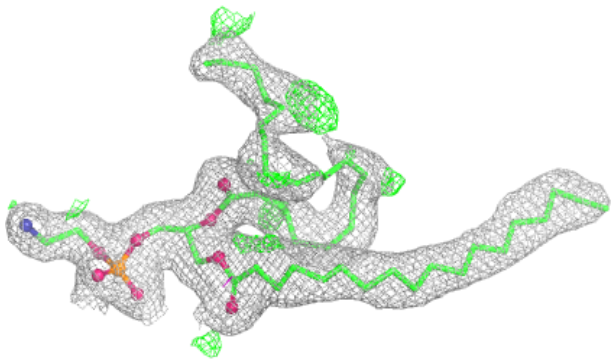


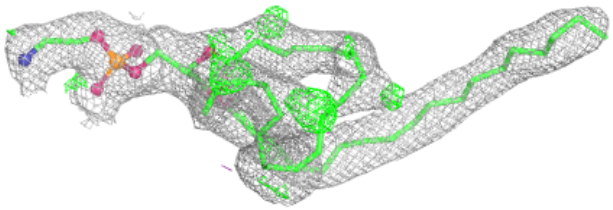


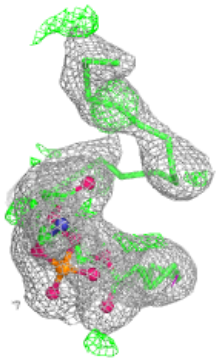


Electron density around PEK C 264:

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

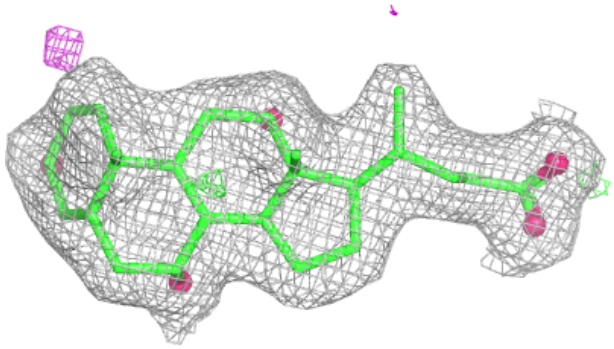


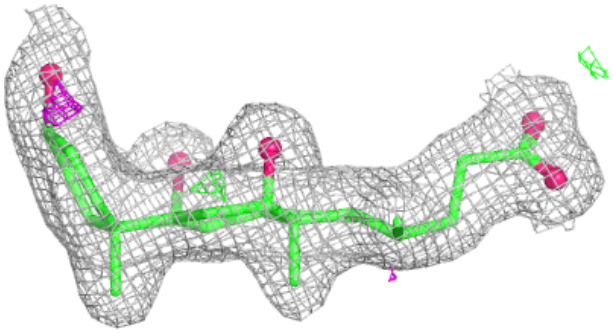


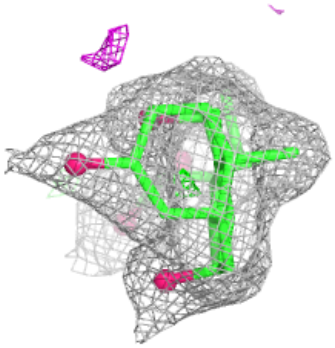


Electron density around CHD B 1085:

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

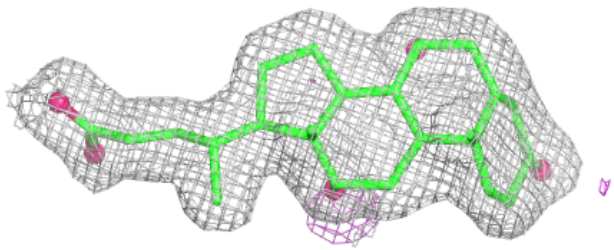


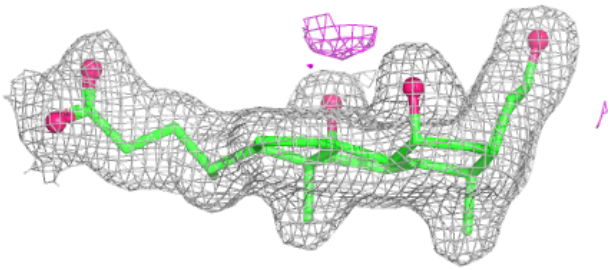


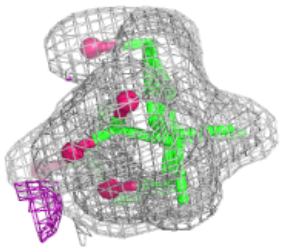


Electron density around CHD C 525:

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

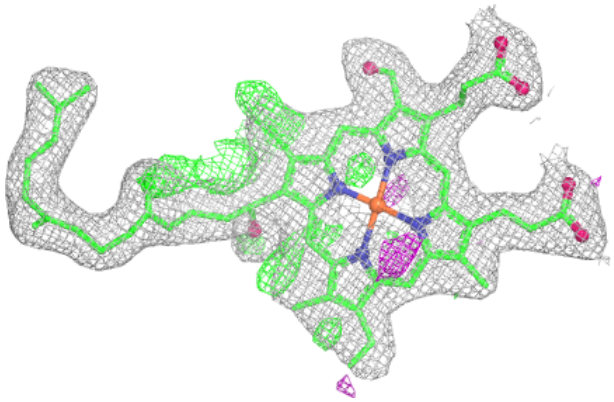


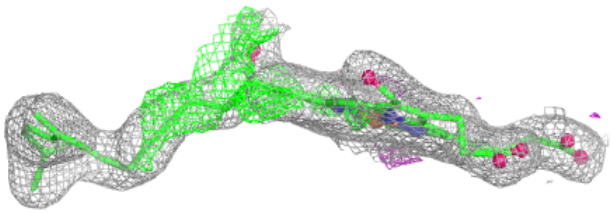


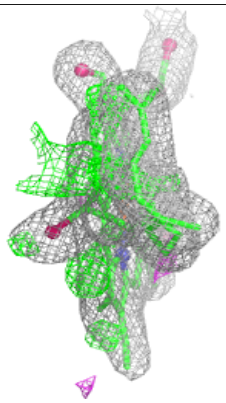


Electron density around HEA N 516:

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

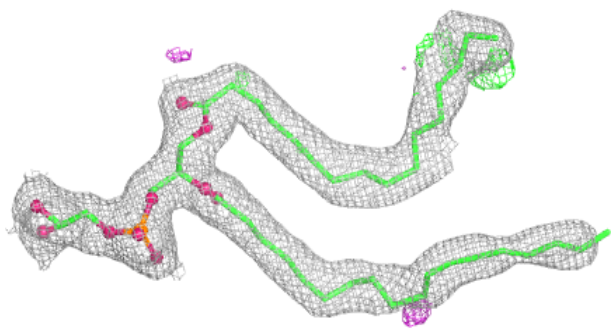


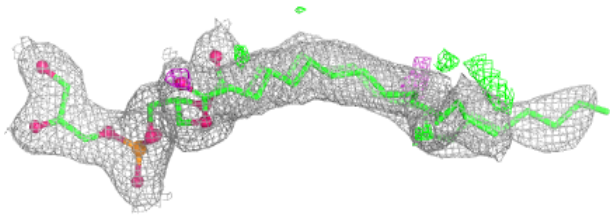


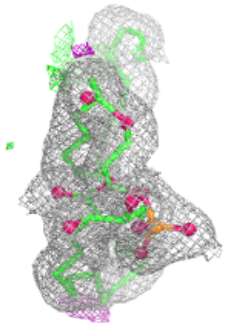


Electron density around PGV A 522:

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

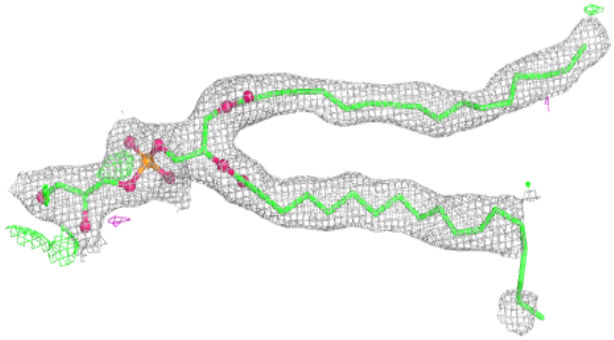


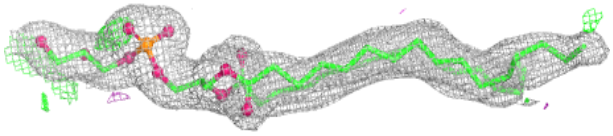


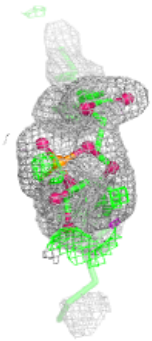


Electron density around PGV P 1267:

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

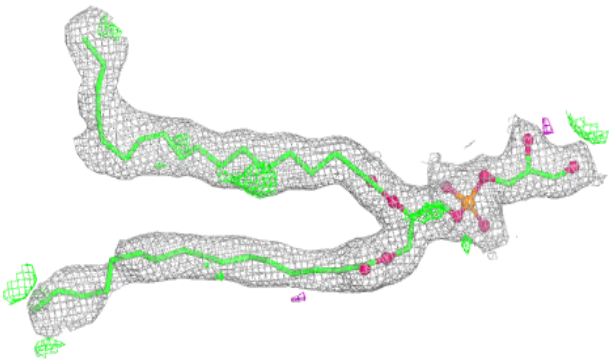


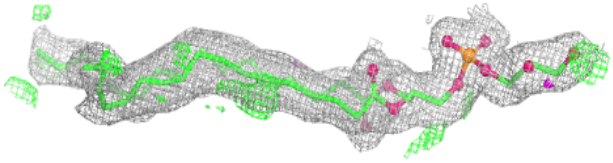


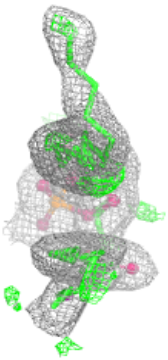


Electron density around PGV C 267:

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

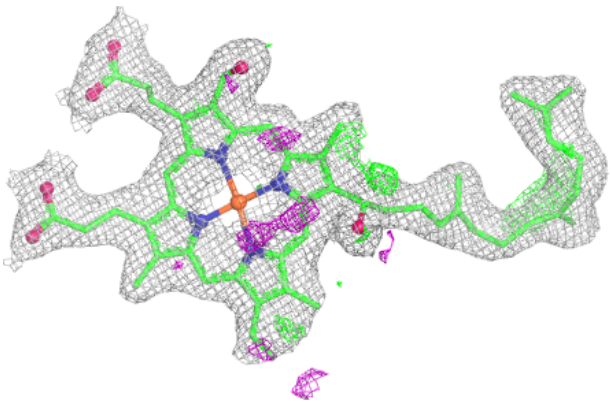


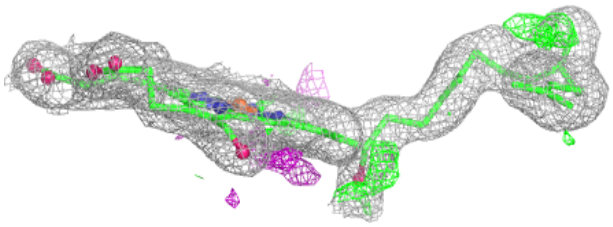


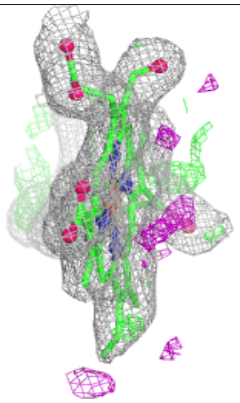


Electron density around HEA A 516:

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

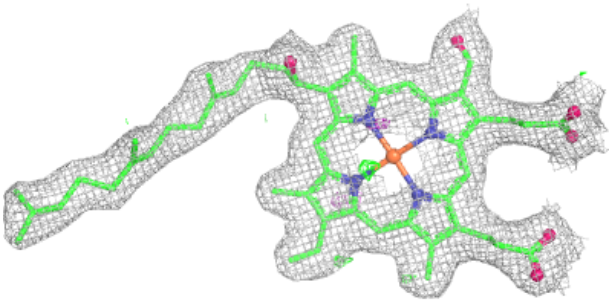


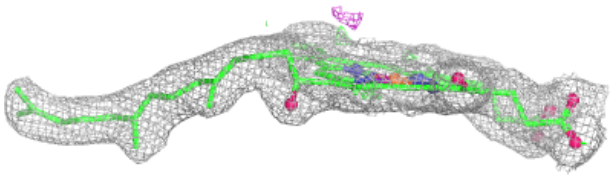


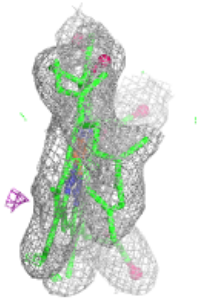


Electron density around HEA N 515:

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

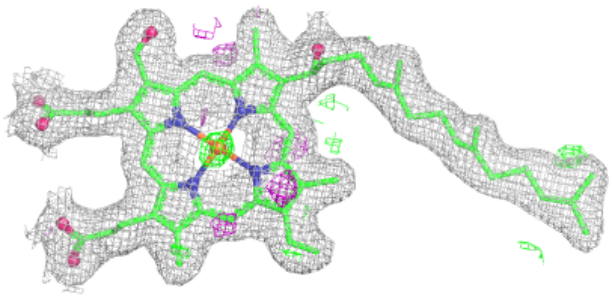


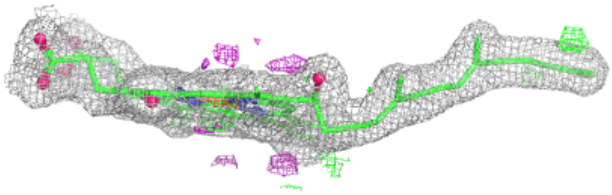


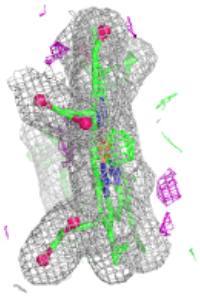


Electron density around HEA A 515:

$2mF_o$-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.