wwPDB X-ray Structure Validation Summary Report (i)

Oct 15, 2023 – 05:07 PM EDT

PDB ID	:	2DYR
Title	:	Bovine heart cytochrome C oxidase at the fully oxidized state
Authors	:	Shinzawa-Itoh, K.; Aoyama, H.; Muramoto, K.; Kurauchi, T.; Mizushima, T.; Yamashita, E.; Tsukihara, T.; Yoshikawa, S.
Deposited on	:	2006-09-16
Resolution	:	1.80 Å(reported)

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

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

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

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

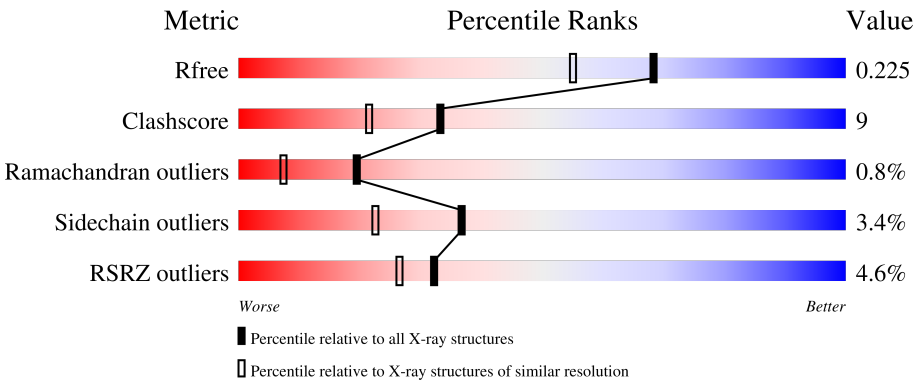
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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

Mol	Chain	Length	Quality of chain
1	A	514	87% 13% •
1	N	514	84% 16% •
2	B	227	% 81% 17% •
2	O	227	4% 75% 22% •
3	C	261	90% 10% •

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Mol	Chain	Length	Quality of chain
3	P	261	%, 88%, 11%
4	D	147	2%, 88%, 10%
4	Q	147	12%, 82%, 16%
5	E	109	2%, 84%, 11%
5	R	109	11%, 73%, 21%
6	F	98	8%, 81%, 14%, 5%
6	S	98	8%, 83%, 13%
7	G	85	20%, 69%, 21%, 8%
7	T	85	20%, 74%, 16%, 8%
8	H	85	13%, 85%, 6%, 7%
8	U	85	12%, 73%, 19%, 7%
9	I	73	7%, 85%, 14%
9	V	73	10%, 81%, 19%
10	J	59	8%, 86%, 10%
10	W	59	14%, 92%, 5%
11	K	56	2%, 80%, 7%, 12%
11	X	56	9%, 80%, 5%, 12%
12	L	47	4%, 83%, 15%
12	Y	47	2%, 81%, 15%
13	M	46	9%, 74%, 17%, 7%
13	Z	46	11%, 67%, 24%, 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
20	TGL	L	522	-	-	X	-
22	CHD	C	271	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CHD	J	60	X	-	-	-
22	CHD	P	1271	X	-	-	-
22	CHD	W	1060	X	-	-	-
23	DMU	C	272	X	-	-	-
23	DMU	M	526	X	-	-	-
23	DMU	P	1272	X	-	-	-
23	DMU	Z	1526	X	-	-	-
26	CDL	G	269	-	-	X	-
26	CDL	T	1269	-	-	X	-
9	SAC	V	1	-	X	-	X

2 Entry composition (i)

There are 28 unique types of molecules in this entry. The entry contains 32735 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 polypeptide Va.

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 polypeptide Vb.

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 polypeptide VIa-heart.

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 VIb isoform 1.

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 polypeptide VIc.

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 VIIa-heart.

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 polypeptide VIIb.

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 polypeptide VIIc.

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 polypeptide VIII-heart.

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 COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

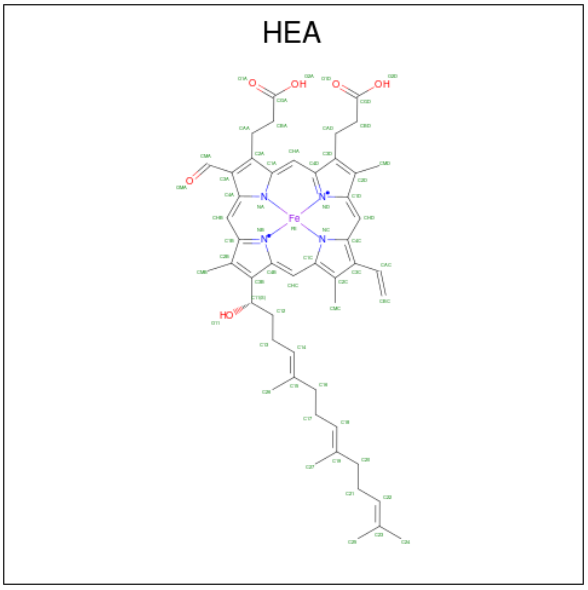
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 16 is SODIUM ION (three-letter code: NA) (formula: Na).

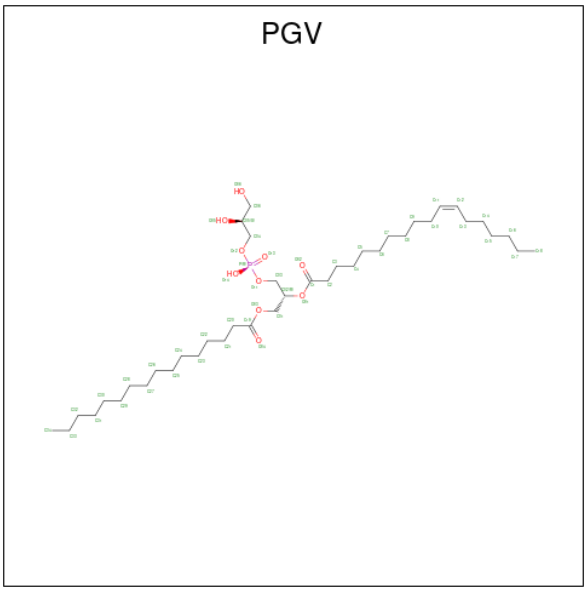
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
16	A	1	1	1	0	0
			Total	Na		
16	N	1	1	1	0	0

- Molecule 17 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



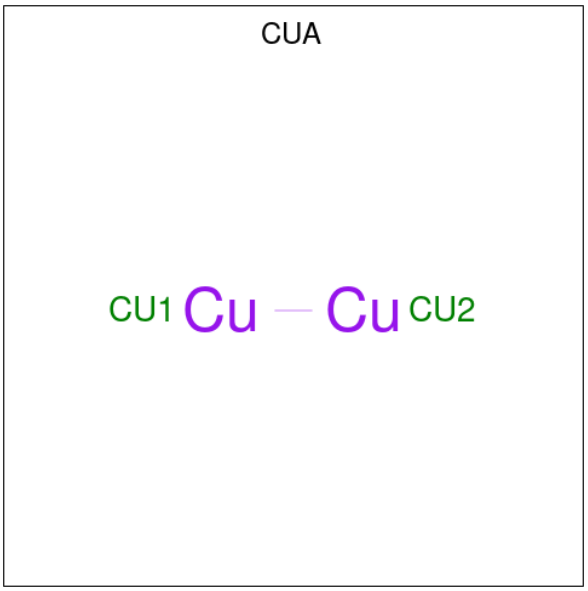
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
17	A	1	60	49	1	4	6	0	0
			Total	C	Fe	N	O		
17	A	1	60	49	1	4	6	0	0
			Total	C	Fe	N	O		
17	N	1	60	49	1	4	6	0	0
			Total	C	Fe	N	O		
17	N	1	60	49	1	4	6	0	0

- Molecule 18 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: $C_{40}H_{77}O_{10}P$).



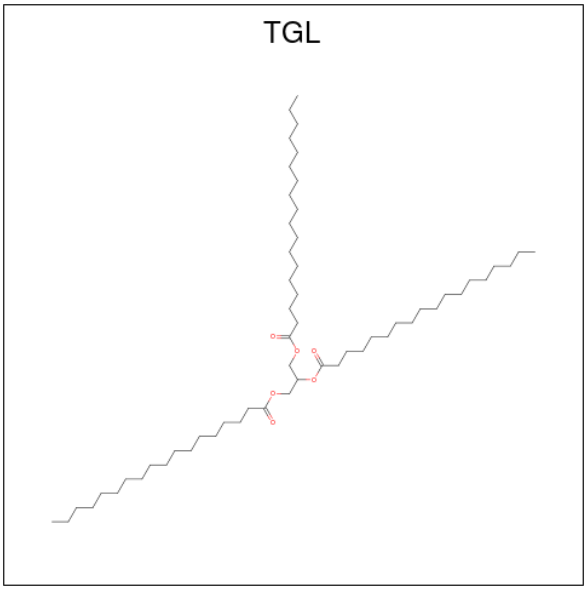
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
18	A	1	51	40	10	1	0	0
			Total	C	O	P		
18	A	1	51	40	10	1	0	0
			Total	C	O	P		
18	C	1	51	40	10	1	0	0
			Total	C	O	P		
18	C	1	51	40	10	1	0	0
			Total	C	O	P		
18	N	1	51	40	10	1	0	0
			Total	C	O	P		
18	P	1	51	40	10	1	0	0
			Total	C	O	P		
18	P	1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

- Molecule 19 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).



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

- Molecule 20 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: $C_{57}H_{110}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
20	B	1	63	57	6	0	0
			Total	C	O		
20	D	1	63	57	6	0	0

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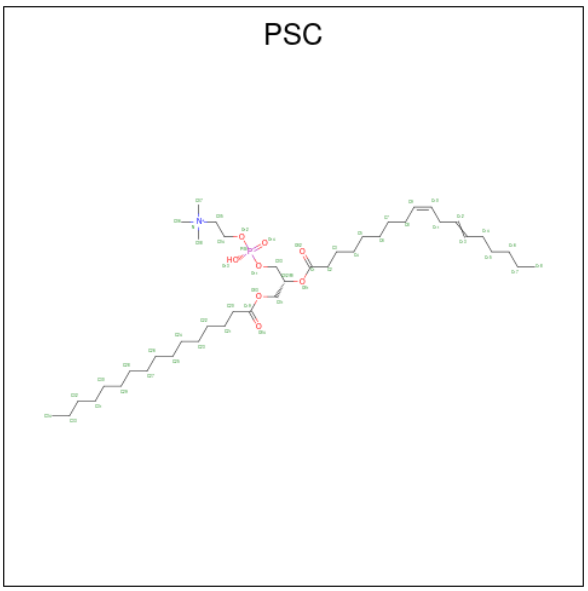
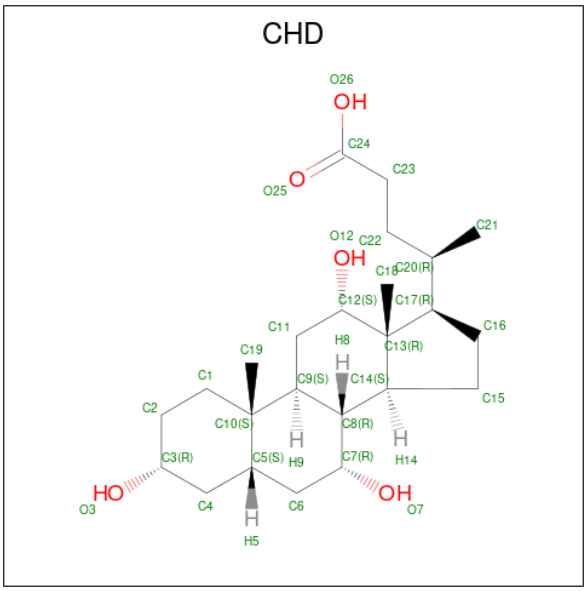
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
20	L	1	63	57	6	0	0
			Total	C	O		
20	N	1	63	57	6	0	0
			Total	C	O		
20	N	1	63	57	6	0	0
			Total	C	O		
20	Q	1	63	57	6	0	0

- Molecule 21 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: $C_{42}H_{81}NO_8P$).



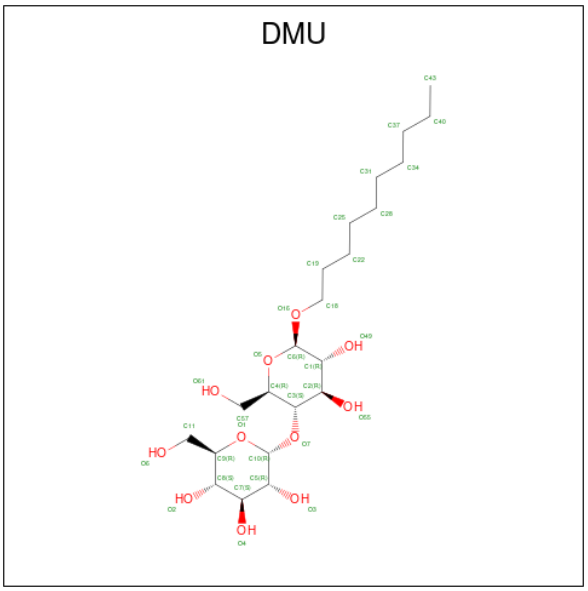
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
21	B	1	52	42	1	8	1	0	0
			Total	C	N	O	P		
21	O	1	52	42	1	8	1	0	0

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



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

- Molecule 23 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).

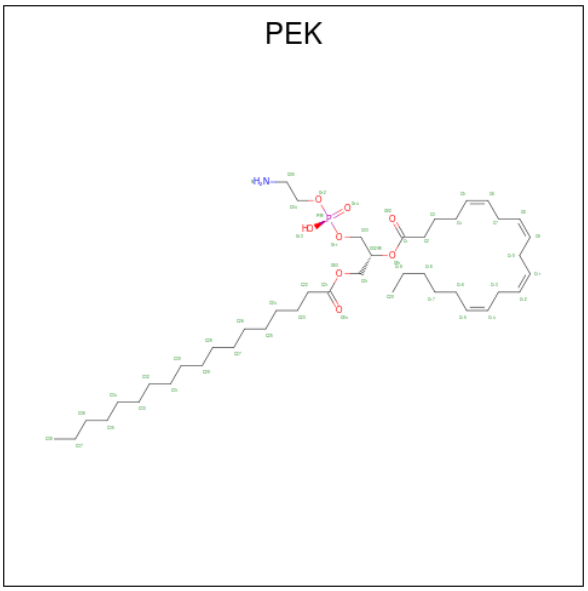


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
23	C	1	33	22	11	0	0
			Total	C	O		
23	M	1	33	22	11	0	0
			Total	C	O		
23	P	1	33	22	11	0	0
			Total	C	O		
23	Z	1	33	22	11	0	0

- Molecule 24 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

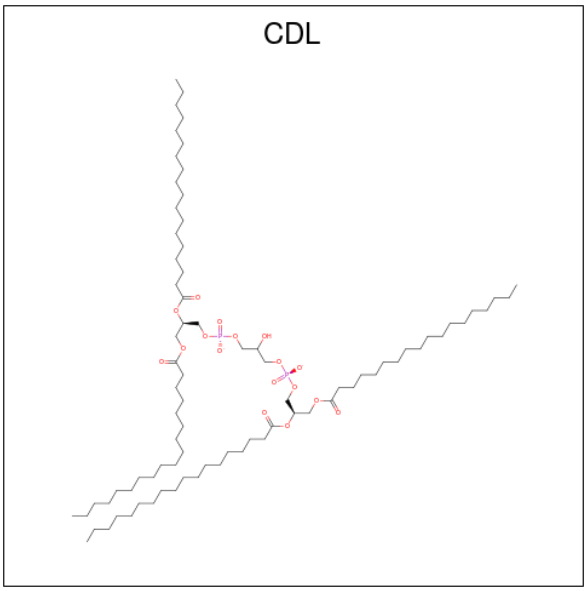
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	X		
24	C	1	1	1	0	0
			Total	X		
24	P	1	1	1	0	0

- Molecule 25 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula: $C_{43}H_{78}NO_8P$).



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

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



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

- Molecule 27 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 28 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	243	Total	O	0	0
			243	243		
28	B	186	Total	O	0	0
			186	186		
28	C	127	Total	O	0	0
			127	127		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
28	D	109	109	109	0	0
			Total	O		
28	E	67	67	67	0	0
			Total	O		
28	F	85	85	85	0	0
			Total	O		
28	G	57	57	57	0	0
			Total	O		
28	H	66	66	66	0	0
			Total	O		
28	I	58	58	58	0	0
			Total	O		
28	J	21	21	21	0	0
			Total	O		
28	K	38	38	38	0	0
			Total	O		
28	L	22	22	22	0	0
			Total	O		
28	M	27	27	27	0	0
			Total	O		
28	N	212	212	212	0	0
			Total	O		
28	O	152	152	152	0	0
			Total	O		
28	P	120	120	120	0	0
			Total	O		
28	Q	75	75	75	0	0
			Total	O		
28	R	32	32	32	0	0
			Total	O		
28	S	53	53	53	0	0
			Total	O		
28	T	59	59	59	0	0
			Total	O		
28	U	62	62	62	0	0
			Total	O		
28	V	33	33	33	0	0
			Total	O		
28	W	18	18	18	0	0
			Total	O		
28	X	29	29	29	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	Y	31	Total O 31 31	0	0
28	Z	21	Total O 21 21	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

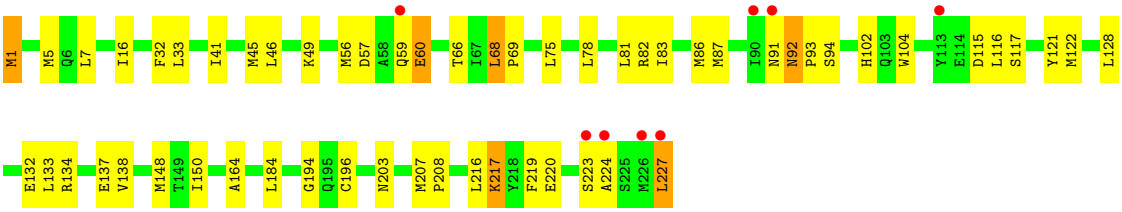
Chain N:

• Molecule 2: Cytochrome c oxidase subunit 2

Chain B:

• Molecule 2: Cytochrome c oxidase subunit 2

Chain O:

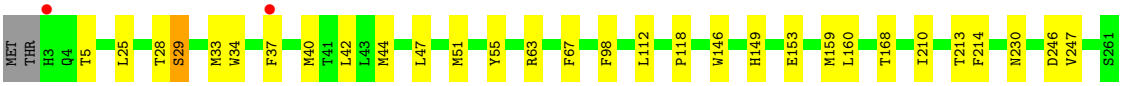


- Molecule 3: Cytochrome c oxidase subunit 3

Chain C:

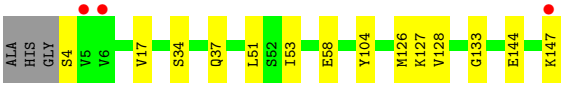
- Molecule 3: Cytochrome c oxidase subunit 3

Chain P:



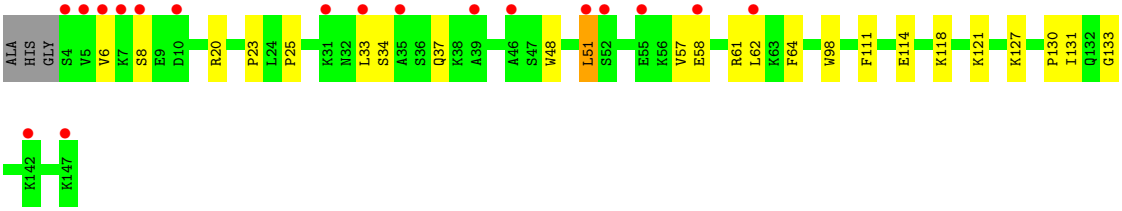
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain D:



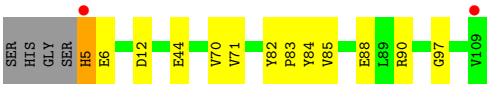
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain Q:



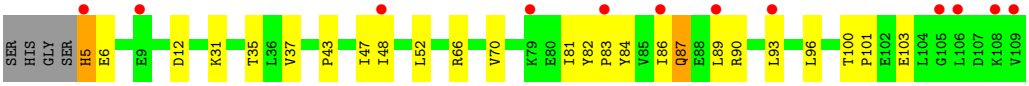
- Molecule 5: Cytochrome c oxidase polypeptide Va

Chain E:



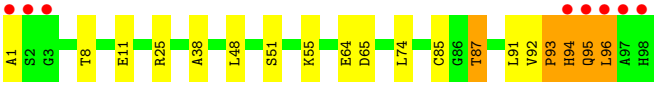
• Molecule 5: Cytochrome c oxidase polypeptide Va

Chain R:



• Molecule 6: Cytochrome c oxidase polypeptide Vb

Chain F:

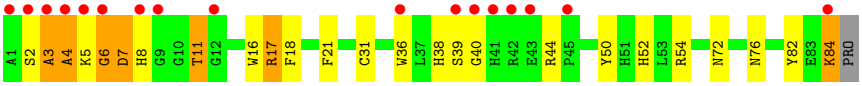


• Molecule 6: Cytochrome c oxidase polypeptide Vb

Chain S:

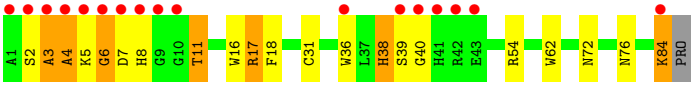
• Molecule 7: Cytochrome c oxidase polypeptide VIa-heart

Chain G:



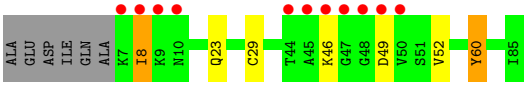
• Molecule 7: Cytochrome c oxidase polypeptide VIa-heart

Chain T:



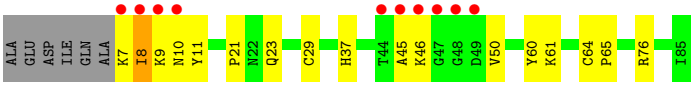
• Molecule 8: Cytochrome c oxidase subunit VIb isoform 1

Chain H:



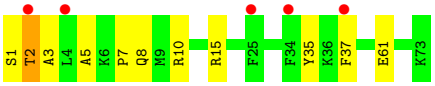
• Molecule 8: Cytochrome c oxidase subunit VIb isoform 1

Chain U:



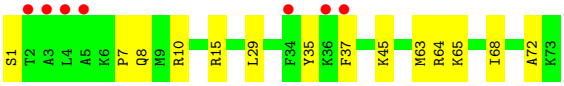
• Molecule 9: Cytochrome c oxidase polypeptide VIc

Chain I:



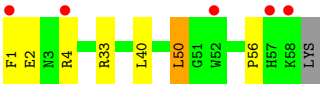
• Molecule 9: Cytochrome c oxidase polypeptide VIc

Chain V:



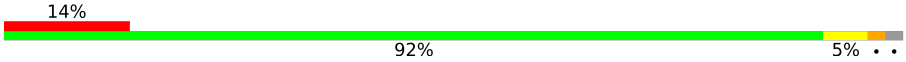
• Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart

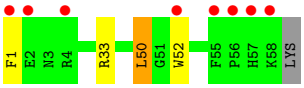
Chain J:



• Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart

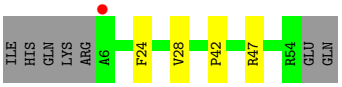
Chain W:





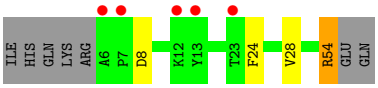
• Molecule 11: Cytochrome c oxidase polypeptide VIIb

Chain K:



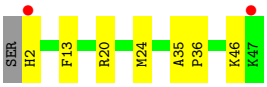
• Molecule 11: Cytochrome c oxidase polypeptide VIIb

Chain X:



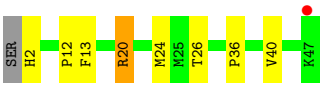
• Molecule 12: Cytochrome c oxidase polypeptide VIIc

Chain L:



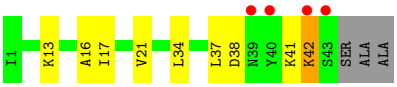
• Molecule 12: Cytochrome c oxidase polypeptide VIIc

Chain Y:



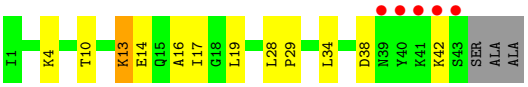
• Molecule 13: Cytochrome c oxidase polypeptide VIII-heart

Chain M:



• Molecule 13: Cytochrome c oxidase polypeptide VIII-heart

Chain Z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	182.59Å 205.14Å 178.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.80 68.19 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-1.80) 98.9 (68.19-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.09 (at 1.80Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.202 , 0.227 0.203 , 0.225	Depositor DCC
R_{free} test set	22992 reflections (3.78%)	wwPDB-VP
Wilson B-factor (Å^2)	25.2	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 64.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.009 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	32735	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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: CUA, TGL, HEA, ZN, PSC, NA, CHD, FME, MG, CU, SAC, PEK, PGV, TPO, UNX, DMU, CDL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.49	0/4156	0.67	0/5678
1	N	0.48	0/4156	0.65	0/5678
2	B	0.48	0/1860	0.76	0/2534
2	O	0.50	0/1860	0.79	1/2534 (0.0%)
3	C	0.51	0/2197	0.58	0/3005
3	P	0.48	0/2197	0.61	0/3005
4	D	0.47	0/1229	0.66	1/1658 (0.1%)
4	Q	0.50	0/1229	0.65	1/1658 (0.1%)
5	E	0.50	0/871	0.66	0/1182
5	R	0.48	0/871	0.68	0/1182
6	F	0.47	0/765	0.83	3/1038 (0.3%)
6	S	0.47	0/765	0.87	3/1038 (0.3%)
7	G	0.51	0/690	0.70	1/937 (0.1%)
7	T	0.53	0/690	0.70	1/937 (0.1%)
8	H	0.47	0/682	0.68	0/921
8	U	0.48	0/682	0.67	0/921
9	I	0.52	0/605	0.59	0/802
9	V	0.51	0/605	0.62	0/802
10	J	0.45	0/471	0.60	0/636
10	W	0.46	0/471	0.63	0/636
11	K	0.48	0/398	0.66	0/546
11	X	0.47	0/398	0.65	0/546
12	L	0.48	0/393	0.55	0/526
12	Y	0.53	0/393	0.57	0/526
13	M	0.46	0/345	0.62	0/470
13	Z	0.45	0/345	0.62	0/470
All	All	0.49	0/29324	0.67	11/39866 (0.0%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	N	0	1
8	U	0	1
All	All	0	3

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	S	94	HIS	N-CA-C	7.74	131.91	111.00
6	F	94	HIS	N-CA-C	7.14	130.29	111.00
4	D	133	GLY	N-CA-C	5.67	127.28	113.10
2	O	227	LEU	CA-CB-CG	5.64	128.28	115.30
4	Q	133	GLY	N-CA-C	5.61	127.12	113.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	N	240	HIS	Sidechain
8	U	11	TYR	Sidechain

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	63	0
1	N	4027	0	4001	74	0
2	B	1824	0	1833	28	0
2	O	1824	0	1833	39	0
3	C	2110	0	2027	24	0
3	P	2110	0	2027	29	0
4	D	1195	0	1183	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Q	1195	0	1183	18	0
5	E	852	0	845	6	0
5	R	852	0	845	15	0
6	F	748	0	728	12	0
6	S	748	0	728	15	0
7	G	675	0	644	26	0
7	T	675	0	644	28	0
8	H	662	0	623	4	0
8	U	662	0	623	9	0
9	I	601	0	613	6	0
9	V	601	0	613	9	0
10	J	460	0	459	6	0
10	W	460	0	459	4	0
11	K	384	0	366	3	0
11	X	384	0	366	6	0
12	L	380	0	380	14	0
12	Y	380	0	380	9	0
13	M	335	0	352	6	0
13	Z	335	0	352	6	0
14	A	1	0	0	0	0
14	N	1	0	0	0	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	120	0	108	3	0
17	N	120	0	108	4	0
18	A	102	0	152	7	0
18	C	102	0	152	7	0
18	N	51	0	76	2	0
18	P	102	0	152	8	0
18	Z	51	0	76	4	0
19	B	2	0	0	0	0
19	O	2	0	0	0	0
20	B	63	0	110	10	0
20	D	63	0	110	5	0
20	L	63	0	110	23	0
20	N	126	0	220	30	0
20	Q	63	0	110	6	0
21	B	52	0	80	13	0
21	O	52	0	80	12	0
22	B	29	0	39	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	C	58	0	78	2	0
22	J	29	0	39	2	0
22	O	29	0	39	1	0
22	P	58	0	78	2	0
22	W	29	0	39	2	0
23	C	33	0	36	2	0
23	M	33	0	36	0	0
23	P	33	0	36	7	0
23	Z	33	0	36	1	0
24	C	1	0	0	0	0
24	P	1	0	0	0	0
25	C	106	0	154	11	0
25	G	53	0	77	7	0
25	P	106	0	154	12	0
25	T	53	0	77	8	0
26	C	100	0	156	16	0
26	G	100	0	156	21	0
26	P	100	0	156	13	0
26	T	100	0	156	21	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	A	243	0	0	4	0
28	B	186	0	0	4	0
28	C	127	0	0	2	0
28	D	109	0	0	4	0
28	E	67	0	0	0	0
28	F	85	0	0	1	0
28	G	57	0	0	2	0
28	H	66	0	0	1	0
28	I	58	0	0	3	0
28	J	21	0	0	1	0
28	K	38	0	0	0	0
28	L	22	0	0	2	0
28	M	27	0	0	2	0
28	N	212	0	0	3	0
28	O	152	0	0	2	0
28	P	120	0	0	3	0
28	Q	75	0	0	3	0
28	R	32	0	0	0	0
28	S	53	0	0	1	0
28	T	59	0	0	2	0
28	U	62	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	V	33	0	0	2	0
28	W	18	0	0	0	0
28	X	29	0	0	1	0
28	Y	31	0	0	2	0
28	Z	21	0	0	2	0
All	All	32735	0	31294	534	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 9.

The worst 5 of 534 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)
7:G:84:LYS:H	7:G:84:LYS:HD2	1.17	1.05
7:T:84:LYS:HD2	7:T:84:LYS:H	1.19	1.02
3:C:63:ARG:HE	26:C:270:CDL:HA22	1.24	1.01
21:O:1230:PSC:H142	21:O:1230:PSC:H343	1.42	1.01
21:B:230:PSC:H343	21:B:230:PSC:H142	1.42	1.01

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%)	497 (97%)	15 (3%)	0	100 100
1	N	512/514 (100%)	497 (97%)	15 (3%)	0	100 100
2	B	225/227 (99%)	211 (94%)	12 (5%)	2 (1%)	17 6
2	O	225/227 (99%)	208 (92%)	15 (7%)	2 (1%)	17 6
3	C	257/261 (98%)	252 (98%)	5 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	P	257/261 (98%)	251 (98%)	6 (2%)	0	100	100
4	D	142/147 (97%)	138 (97%)	4 (3%)	0	100	100
4	Q	142/147 (97%)	138 (97%)	4 (3%)	0	100	100
5	E	103/109 (94%)	103 (100%)	0	0	100	100
5	R	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
6	F	96/98 (98%)	89 (93%)	5 (5%)	2 (2%)	7	1
6	S	96/98 (98%)	90 (94%)	3 (3%)	3 (3%)	4	0
7	G	81/85 (95%)	67 (83%)	7 (9%)	7 (9%)	1	0
7	T	81/85 (95%)	65 (80%)	9 (11%)	7 (9%)	1	0
8	H	77/85 (91%)	70 (91%)	5 (6%)	2 (3%)	5	1
8	U	77/85 (91%)	70 (91%)	5 (6%)	2 (3%)	5	1
9	I	71/73 (97%)	67 (94%)	4 (6%)	0	100	100
9	V	71/73 (97%)	66 (93%)	5 (7%)	0	100	100
10	J	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
10	W	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
11	K	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
11	X	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
12	L	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
12	Y	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
13	M	41/46 (89%)	41 (100%)	0	0	100	100
13	Z	41/46 (89%)	41 (100%)	0	0	100	100
All	All	3504/3614 (97%)	3350 (96%)	127 (4%)	27 (1%)	19	7

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	4	ALA
7	G	7	ASP
7	G	8	HIS
7	G	39	SER
6	S	94	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%)	417 (98%)	9 (2%)	53	42
1	N	426/426 (100%)	414 (97%)	12 (3%)	43	30
2	B	210/210 (100%)	201 (96%)	9 (4%)	29	14
2	O	210/210 (100%)	199 (95%)	11 (5%)	23	10
3	C	224/226 (99%)	220 (98%)	4 (2%)	59	48
3	P	224/226 (99%)	219 (98%)	5 (2%)	52	39
4	D	128/129 (99%)	126 (98%)	2 (2%)	62	54
4	Q	128/129 (99%)	125 (98%)	3 (2%)	50	37
5	E	92/95 (97%)	89 (97%)	3 (3%)	38	23
5	R	92/95 (97%)	89 (97%)	3 (3%)	38	23
6	F	81/81 (100%)	79 (98%)	2 (2%)	47	34
6	S	81/81 (100%)	78 (96%)	3 (4%)	34	19
7	G	67/68 (98%)	62 (92%)	5 (8%)	13	4
7	T	67/68 (98%)	61 (91%)	6 (9%)	9	2
8	H	71/75 (95%)	68 (96%)	3 (4%)	30	15
8	U	71/75 (95%)	68 (96%)	3 (4%)	30	15
9	I	57/57 (100%)	52 (91%)	5 (9%)	10	3
9	V	57/57 (100%)	55 (96%)	2 (4%)	36	21
10	J	49/50 (98%)	48 (98%)	1 (2%)	55	44
10	W	49/50 (98%)	48 (98%)	1 (2%)	55	44
11	K	39/46 (85%)	39 (100%)	0	100	100
11	X	39/46 (85%)	38 (97%)	1 (3%)	46	32
12	L	39/40 (98%)	38 (97%)	1 (3%)	46	32
12	Y	39/40 (98%)	37 (95%)	2 (5%)	24	10
13	M	37/38 (97%)	33 (89%)	4 (11%)	6	1
13	Z	37/38 (97%)	33 (89%)	4 (11%)	6	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3040/3082 (99%)	2936 (97%)	104 (3%)	37 22

5 of 104 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	484	THR
3	P	29	SER
12	Y	26	THR
1	N	513	LEU
2	O	78	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	N	178	GLN
2	O	10	GLN
7	T	76	ASN
1	N	512	ASN
2	O	52	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FME	O	1	2	8,9,10	0.67	0	7,9,11	1.81	2 (28%)
1	FME	N	1	1	8,9,10	0.75	0	7,9,11	1.68	2 (28%)

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	2.75	2 (28%)	8,9,11	3.18	5 (62%)
2	FME	B	1	2	8,9,10	0.85	0	7,9,11	2.43	2 (28%)
1	FME	A	1	1	8,9,10	0.66	0	7,9,11	1.20	1 (14%)
7	TPO	G	11	7	8,10,11	1.53	1 (12%)	10,14,16	1.03	0
7	TPO	T	11	7	8,10,11	1.30	1 (12%)	10,14,16	1.05	0
9	SAC	I	1	9	7,8,9	2.55	2 (28%)	8,9,11	2.99	4 (50%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FME	O	1	2	-	1/7/9/11	-
1	FME	N	1	1	-	4/7/9/11	-
9	SAC	V	1	9	-	3/7/8/10	-
2	FME	B	1	2	-	1/7/9/11	-
1	FME	A	1	1	-	3/7/9/11	-
7	TPO	G	11	7	-	5/9/11/13	-
7	TPO	T	11	7	-	4/9/11/13	-
9	SAC	I	1	9	-	3/7/8/10	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	V	1	SAC	OAC-C1A	5.27	1.35	1.23
9	I	1	SAC	OAC-C1A	5.12	1.34	1.23
9	V	1	SAC	CA-N	4.56	1.52	1.46
9	I	1	SAC	CA-N	4.11	1.52	1.46
7	G	11	TPO	CB-CA	2.94	1.60	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	V	1	SAC	CA-N-C1A	-6.81	110.59	123.15
9	I	1	SAC	CA-N-C1A	-6.06	111.98	123.15
2	B	1	FME	C-CA-N	4.41	117.69	109.73
2	B	1	FME	CA-N-CN	-4.41	116.05	122.82
1	N	1	FME	CA-N-CN	-3.73	117.09	122.82

There are no chirality outliers.

5 of 24 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.

5 monomers are involved in 9 short contacts:

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 54 ligands modelled in this entry, 8 are monoatomic and 2 are unknown - leaving 44 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	$\#\|Z\| > 2$
17	HEA	N	515	1	57,67,67	1.14	3 (5%)	61,103,103	1.26	8 (13%)
17	HEA	N	516	1	57,67,67	1.12	1 (1%)	61,103,103	1.35	10 (16%)
18	PGV	C	268	-	50,50,50	1.22	3 (6%)	53,56,56	0.81	1 (1%)
18	PGV	Z	1524	-	50,50,50	1.04	3 (6%)	53,56,56	0.90	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	CHD	C	525	-	32,32,32	0.85	1 (3%)	51,51,51	1.65	12 (23%)
22	CHD	O	229	-	32,32,32	0.84	0	51,51,51	1.84	13 (25%)
21	PSC	O	1230	-	51,51,51	1.13	3 (5%)	57,59,59	0.87	1 (1%)
25	PEK	G	1263	-	52,52,52	1.81	11 (21%)	55,57,57	1.19	4 (7%)
23	DMU	C	272	-	34,34,34	3.01	8 (23%)	45,45,45	4.01	19 (42%)
18	PGV	C	267	-	50,50,50	0.82	1 (2%)	53,56,56	0.84	2 (3%)
25	PEK	C	265	-	52,52,52	1.59	10 (19%)	55,57,57	1.10	6 (10%)
25	PEK	P	1265	-	52,52,52	1.63	11 (21%)	55,57,57	1.08	6 (10%)
23	DMU	Z	1526	-	34,34,34	3.18	8 (23%)	45,45,45	4.18	19 (42%)
18	PGV	A	525	-	50,50,50	0.88	2 (4%)	53,56,56	0.74	2 (3%)
22	CHD	W	1060	-	32,32,32	0.96	2 (6%)	51,51,51	3.19	26 (50%)
17	HEA	A	516	1	57,67,67	1.17	4 (7%)	61,103,103	1.33	7 (11%)
23	DMU	P	1272	-	34,34,34	3.01	9 (26%)	45,45,45	4.00	19 (42%)
20	TGL	Q	1523	-	62,62,62	0.80	2 (3%)	65,65,65	1.26	9 (13%)
17	HEA	A	515	1	57,67,67	1.07	4 (7%)	61,103,103	1.26	7 (11%)
22	CHD	B	1086	-	32,32,32	0.73	0	51,51,51	1.79	15 (29%)
20	TGL	N	1521	-	62,62,62	0.71	1 (1%)	65,65,65	1.40	10 (15%)
22	CHD	P	1271	-	32,32,32	0.79	0	51,51,51	3.54	22 (43%)
21	PSC	B	230	-	51,51,51	1.16	3 (5%)	57,59,59	0.86	1 (1%)
22	CHD	C	271	-	32,32,32	0.82	0	51,51,51	3.60	21 (41%)
18	PGV	A	524	-	50,50,50	1.07	3 (6%)	53,56,56	0.93	2 (3%)
20	TGL	N	1522	-	62,62,62	1.15	4 (6%)	65,65,65	1.70	13 (20%)
22	CHD	P	1525	-	32,32,32	0.86	0	51,51,51	1.59	8 (15%)
22	CHD	J	60	-	32,32,32	0.89	1 (3%)	51,51,51	3.20	25 (49%)
25	PEK	C	264	-	52,52,52	1.40	4 (7%)	55,57,57	1.02	3 (5%)
25	PEK	P	1264	-	52,52,52	1.39	4 (7%)	55,57,57	1.05	3 (5%)
23	DMU	M	526	-	34,34,34	3.22	8 (23%)	45,45,45	4.23	19 (42%)
25	PEK	T	263	-	52,52,52	1.83	12 (23%)	55,57,57	1.20	4 (7%)
19	CUA	B	228	2	0,1,1	-	-	-		
19	CUA	O	228	2	0,1,1	-	-	-		
26	CDL	G	269	-	99,99,99	0.91	5 (5%)	105,111,111	0.96	7 (6%)
20	TGL	L	522	-	62,62,62	1.11	4 (6%)	65,65,65	1.72	13 (20%)
26	CDL	P	1270	-	99,99,99	0.81	3 (3%)	105,111,111	0.95	6 (5%)
20	TGL	D	523	-	62,62,62	0.76	1 (1%)	65,65,65	1.28	9 (13%)
18	PGV	P	1267	-	50,50,50	0.84	1 (2%)	53,56,56	0.82	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
26	CDL	C	270	-	99,99,99	0.78	3 (3%)	105,111,111	0.97	6 (5%)
18	PGV	N	1266	-	50,50,50	0.92	2 (4%)	53,56,56	0.77	3 (5%)
18	PGV	P	1268	-	50,50,50	1.25	4 (8%)	53,56,56	0.83	1 (1%)
20	TGL	B	521	-	62,62,62	0.67	0	65,65,65	1.41	11 (16%)
26	CDL	T	1269	-	99,99,99	0.88	5 (5%)	105,111,111	0.97	7 (6%)

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
17	HEA	N	515	1	-	7/32/76/76	-
17	HEA	N	516	1	-	6/32/76/76	-
18	PGV	C	268	-	-	34/55/55/55	-
18	PGV	Z	1524	-	-	32/55/55/55	-
22	CHD	C	525	-	-	2/9/74/74	0/4/4/4
22	CHD	O	229	-	-	2/9/74/74	0/4/4/4
21	PSC	O	1230	-	-	40/55/55/55	-
25	PEK	G	1263	-	-	27/56/56/56	-
23	DMU	C	272	-	6/6/10/10	8/19/59/59	0/2/2/2
18	PGV	C	267	-	-	17/55/55/55	-
25	PEK	C	265	-	-	22/56/56/56	-
25	PEK	P	1265	-	-	23/56/56/56	-
23	DMU	Z	1526	-	5/5/10/10	8/19/59/59	0/2/2/2
22	CHD	W	1060	-	5/5/12/12	8/9/74/74	0/4/4/4
18	PGV	A	525	-	-	13/55/55/55	-
17	HEA	A	516	1	-	5/32/76/76	-
23	DMU	P	1272	-	6/6/10/10	8/19/59/59	0/2/2/2
20	TGL	Q	1523	-	-	14/65/65/65	-
17	HEA	A	515	1	-	8/32/76/76	-
22	CHD	B	1086	-	-	2/9/74/74	0/4/4/4
22	CHD	P	1271	-	5/5/12/12	8/9/74/74	0/4/4/4
20	TGL	N	1521	-	-	14/65/65/65	-
21	PSC	B	230	-	-	40/55/55/55	-
22	CHD	C	271	-	5/5/12/12	8/9/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	PGV	A	524	-	-	33/55/55/55	-
20	TGL	N	1522	-	-	16/65/65/65	-
22	CHD	P	1525	-	-	2/9/74/74	0/4/4/4
22	CHD	J	60	-	5/5/12/12	8/9/74/74	0/4/4/4
25	PEK	C	264	-	-	21/56/56/56	-
25	PEK	P	1264	-	-	21/56/56/56	-
23	DMU	M	526	-	5/5/10/10	8/19/59/59	0/2/2/2
25	PEK	T	263	-	-	27/56/56/56	-
26	CDL	G	269	-	-	62/110/110/110	-
20	TGL	L	522	-	-	16/65/65/65	-
26	CDL	P	1270	-	-	69/110/110/110	-
20	TGL	D	523	-	-	14/65/65/65	-
18	PGV	P	1267	-	-	17/55/55/55	-
26	CDL	C	270	-	-	70/110/110/110	-
18	PGV	N	1266	-	-	14/55/55/55	-
18	PGV	P	1268	-	-	35/55/55/55	-
20	TGL	B	521	-	-	14/65/65/65	-
26	CDL	T	1269	-	-	62/110/110/110	-

The worst 5 of 154 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	Z	1526	DMU	O7-C3	-8.03	1.23	1.43
23	M	526	DMU	O7-C3	-7.98	1.23	1.43
23	M	526	DMU	O16-C6	-7.34	1.27	1.40
23	Z	1526	DMU	O16-C6	-7.27	1.27	1.40
23	M	526	DMU	O1-C9	-7.23	1.26	1.44

The worst 5 of 382 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	271	CHD	C17-C13-C14	10.46	110.64	100.09
22	P	1271	CHD	C10-C9-C8	10.23	122.80	111.82
23	C	272	DMU	C1-C2-C3	10.05	132.62	109.68
22	P	1271	CHD	C17-C13-C14	9.94	110.12	100.09
23	P	1272	DMU	C1-C2-C3	9.93	132.34	109.68

5 of 42 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	C	271	CHD	C12
22	C	271	CHD	C3
22	C	271	CHD	C8
22	C	271	CHD	C14
22	C	271	CHD	C9

5 of 865 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	524	PGV	C04-O12-P-O11
18	A	524	PGV	C04-O12-P-O13
18	A	524	PGV	C04-O12-P-O14
18	A	524	PGV	C02-C03-O11-P
18	A	524	PGV	C05-C04-O12-P

There are no ring outliers.

37 monomers are involved in 249 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	N	515	HEA	4	0
18	C	268	PGV	1	0
18	Z	1524	PGV	4	0
22	O	229	CHD	1	0
21	O	1230	PSC	12	0
25	G	1263	PEK	7	0
23	C	272	DMU	2	0
18	C	267	PGV	6	0
25	C	265	PEK	6	0
25	P	1265	PEK	6	0
23	Z	1526	DMU	1	0
18	A	525	PGV	1	0
22	W	1060	CHD	2	0
17	A	516	HEA	1	0
23	P	1272	DMU	7	0
20	Q	1523	TGL	6	0
17	A	515	HEA	2	0
20	N	1521	TGL	14	0
22	P	1271	CHD	2	0
21	B	230	PSC	13	0
22	C	271	CHD	2	0
18	A	524	PGV	6	0
20	N	1522	TGL	16	0
22	J	60	CHD	2	0

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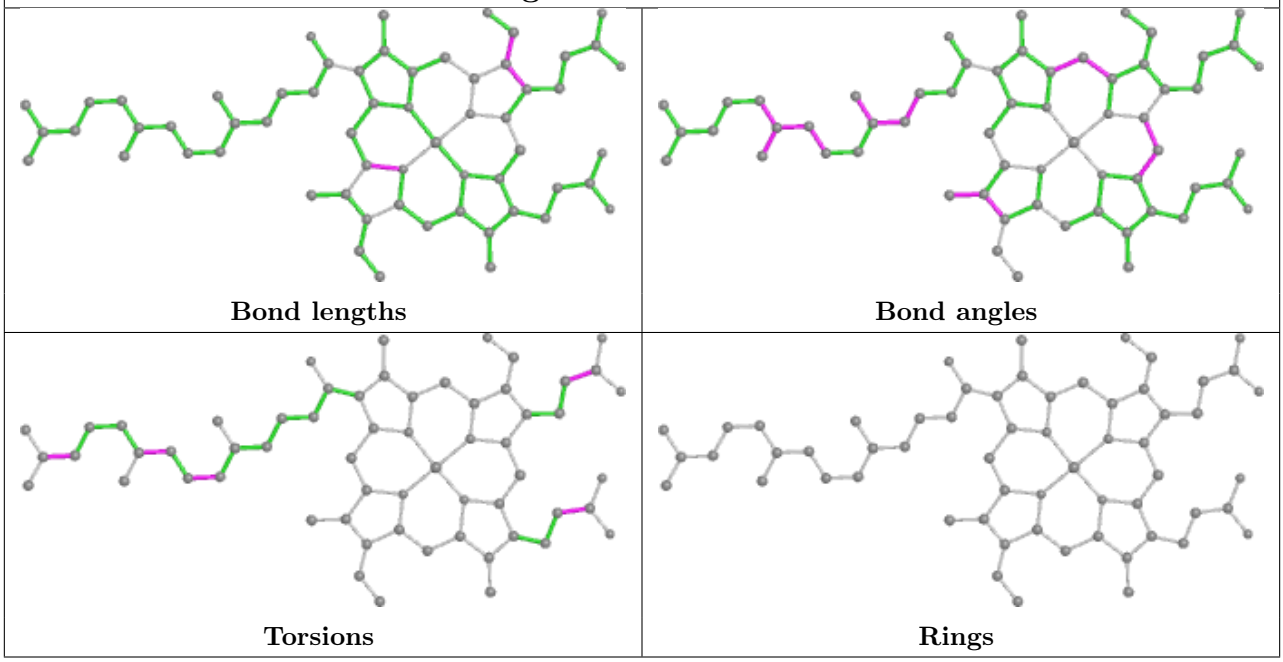
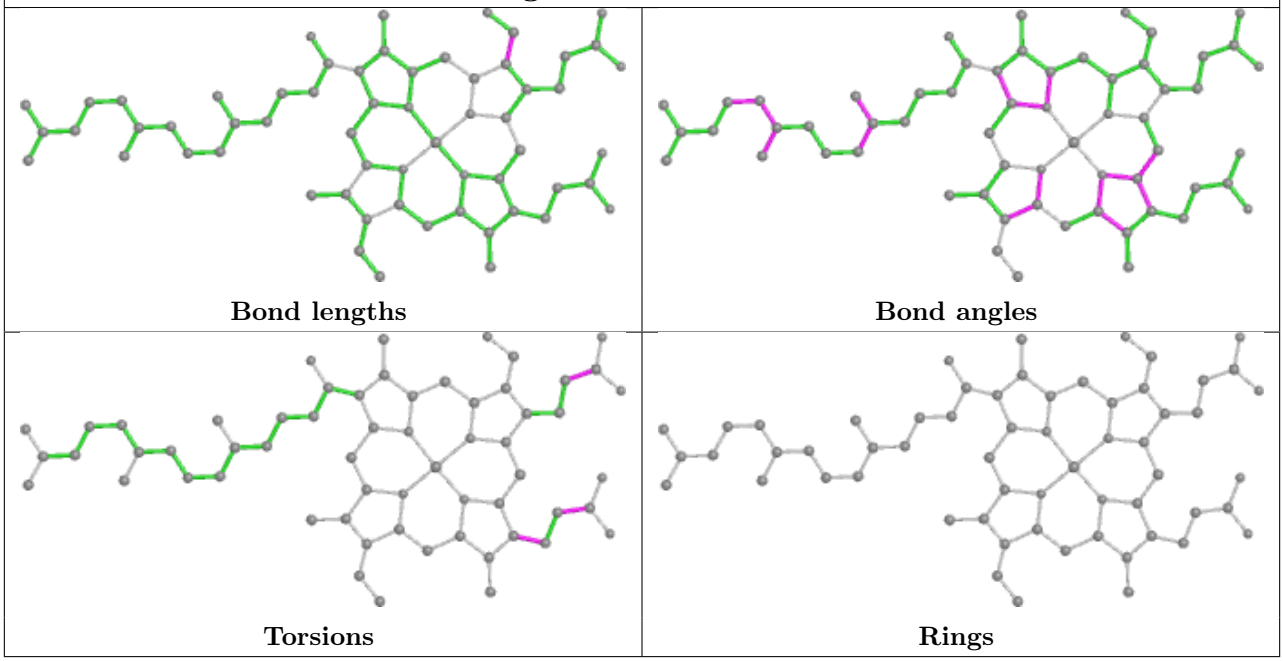
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	C	264	PEK	5	0
25	P	1264	PEK	6	0
25	T	263	PEK	8	0
26	G	269	CDL	21	0
20	L	522	TGL	23	0
26	P	1270	CDL	13	0
20	D	523	TGL	5	0
18	P	1267	PGV	5	0
26	C	270	CDL	16	0
18	N	1266	PGV	2	0
18	P	1268	PGV	3	0
20	B	521	TGL	10	0
26	T	1269	CDL	21	0

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

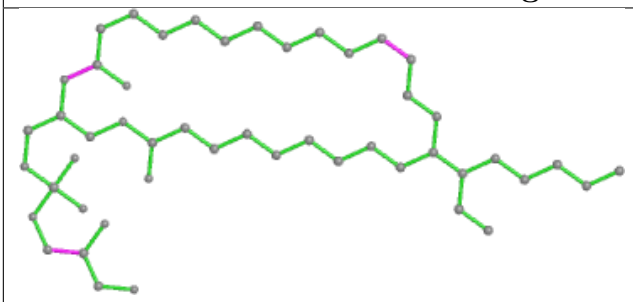
Ligand HEA N 515



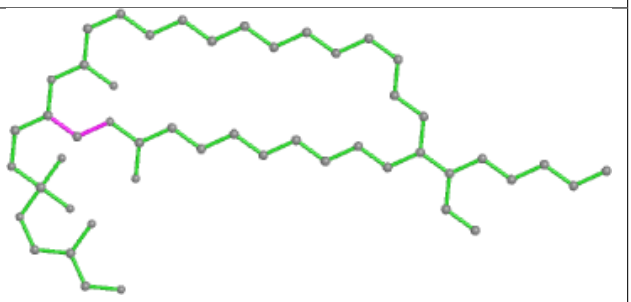
Ligand HEA N 516



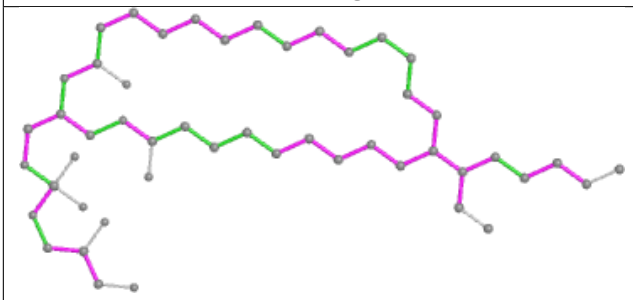
Ligand PGV C 268



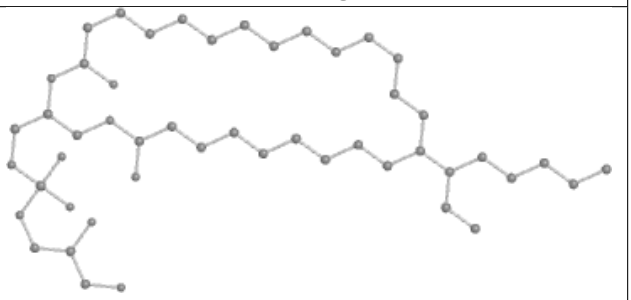
Bond lengths



Bond angles

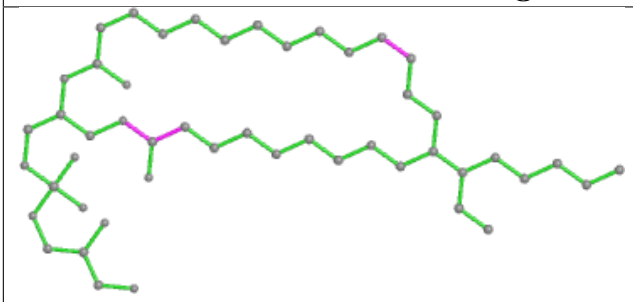


Torsions

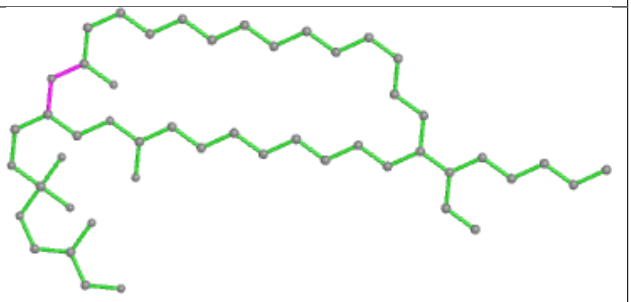


Rings

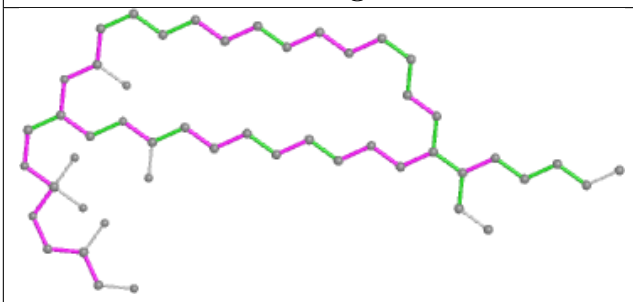
Ligand PGV Z 1524



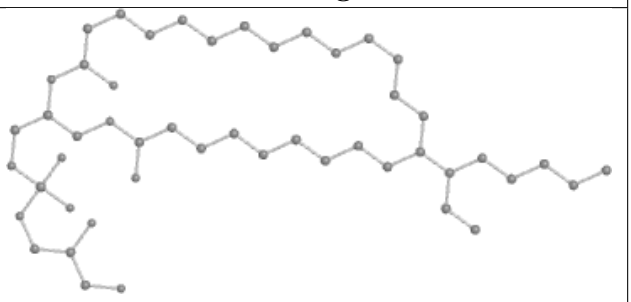
Bond lengths



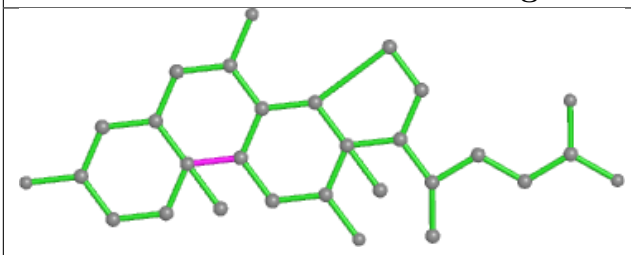
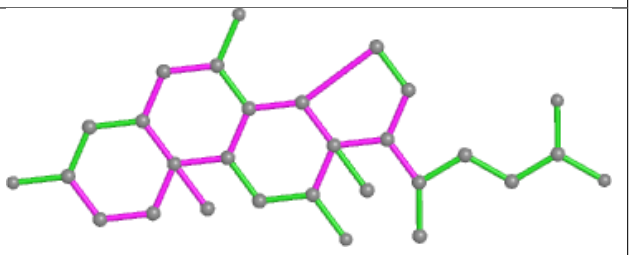
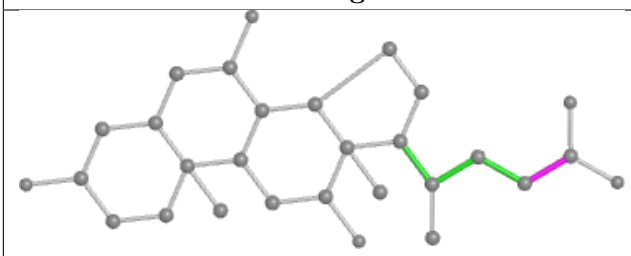
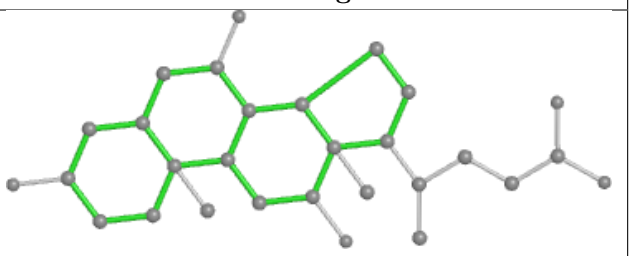
Bond angles

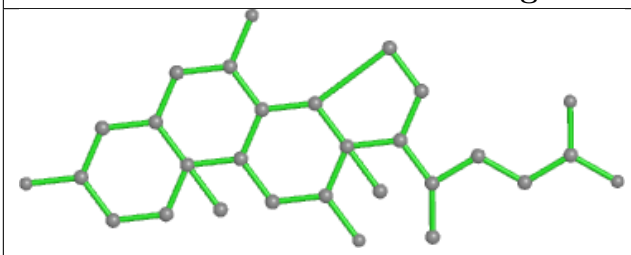
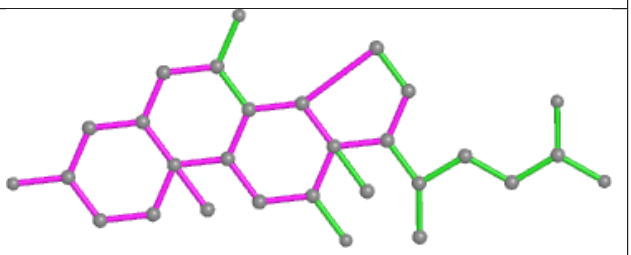
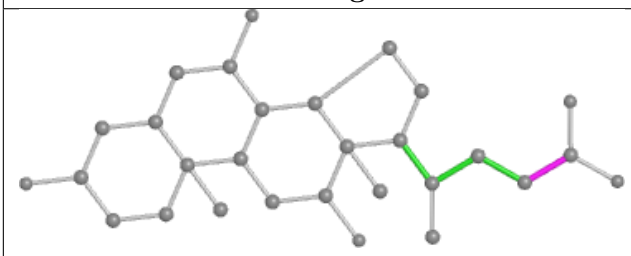
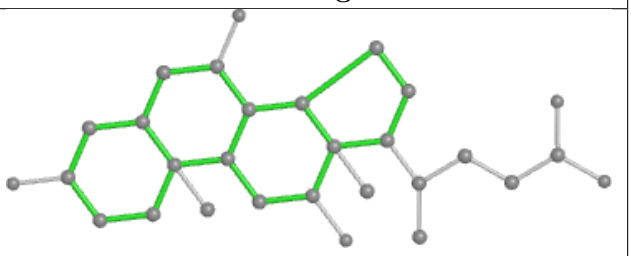


Torsions

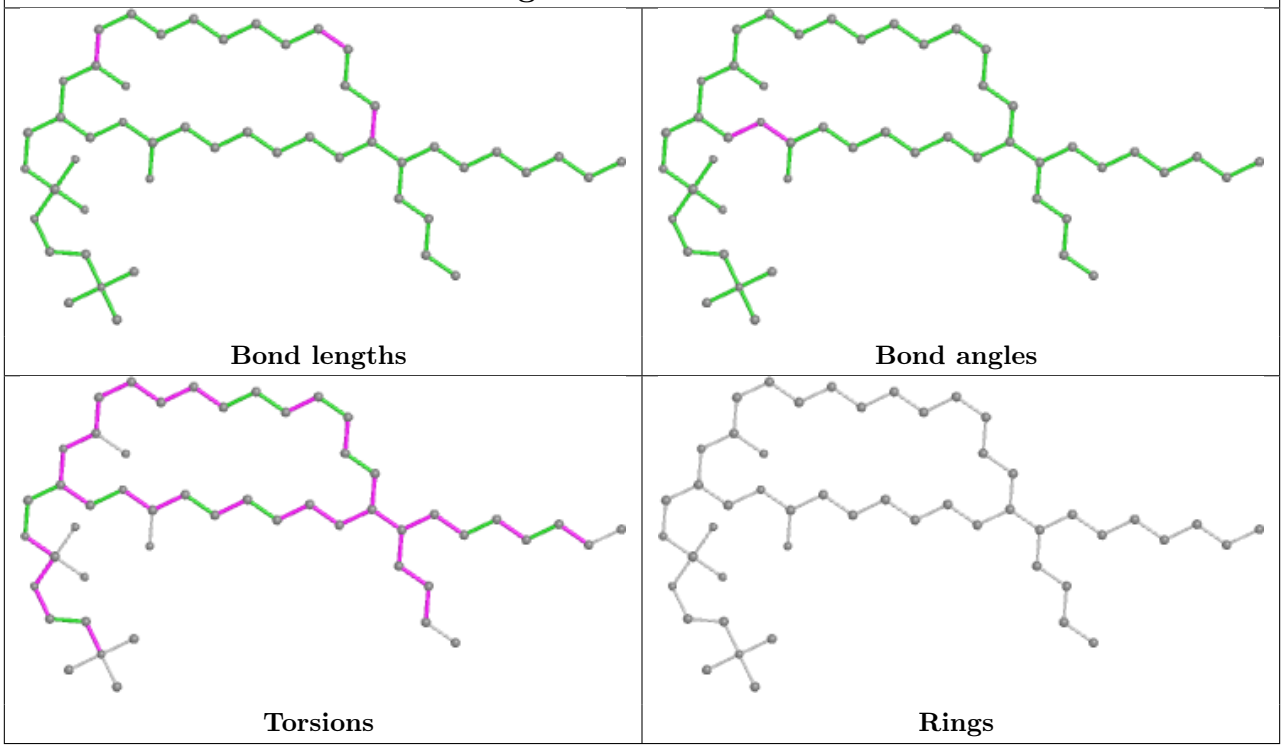


Rings

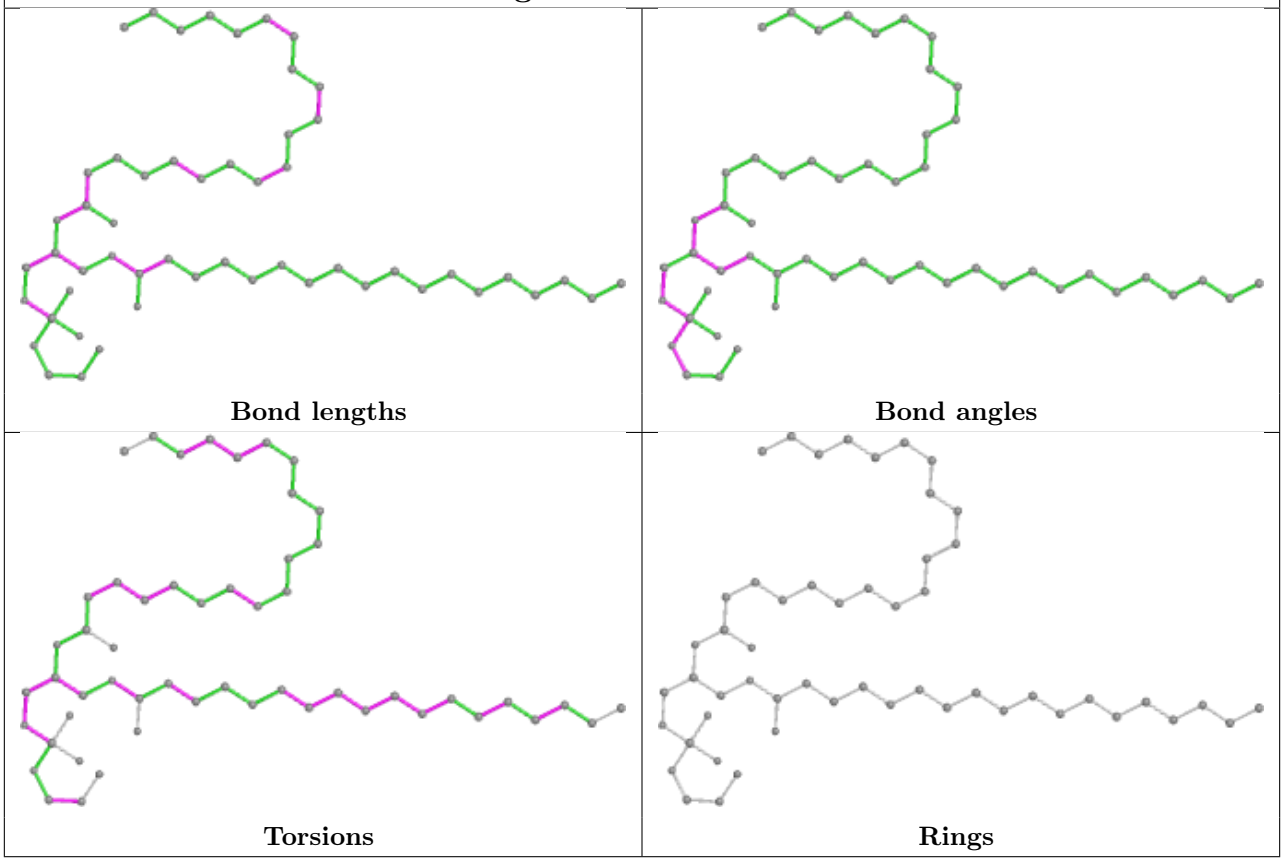
Ligand CHD C 525	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHD O 229	
 Bond lengths	 Bond angles
 Torsions	 Rings

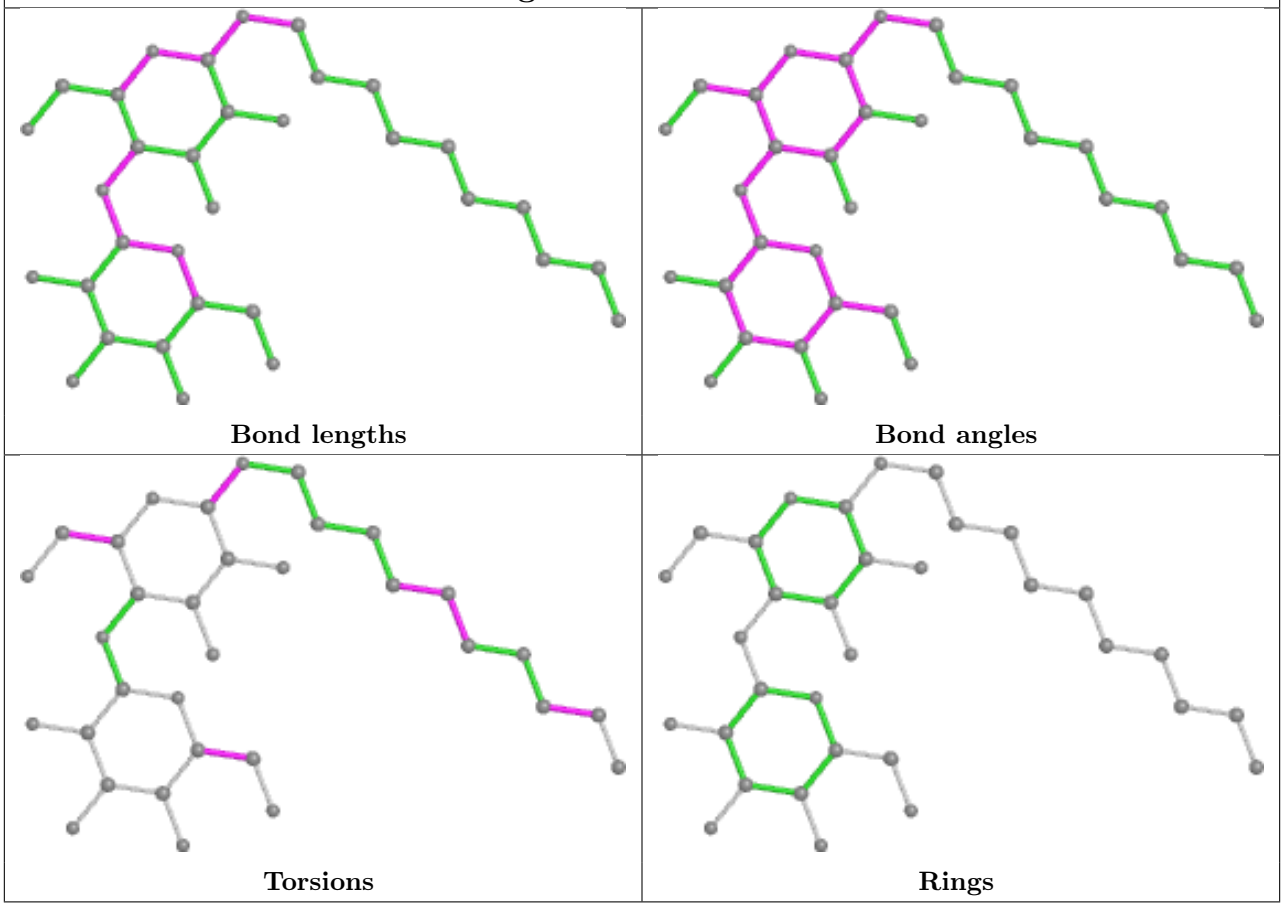
Ligand PSC O 1230



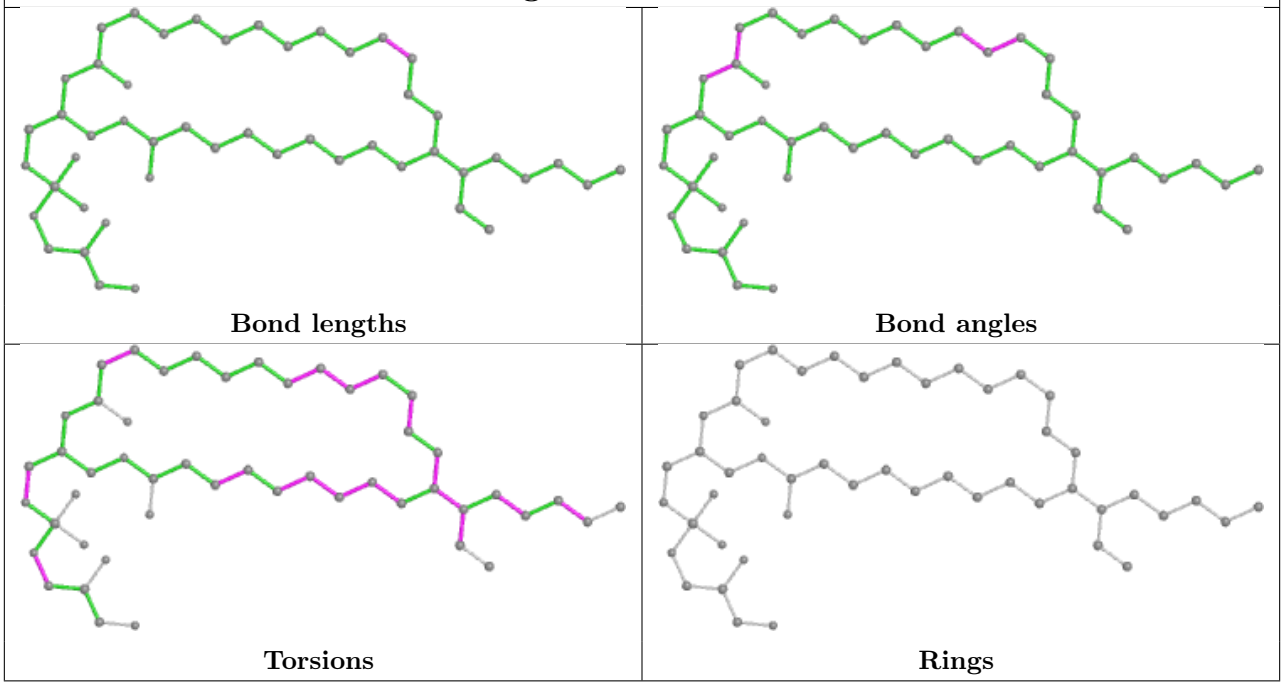
Ligand PEK G 1263



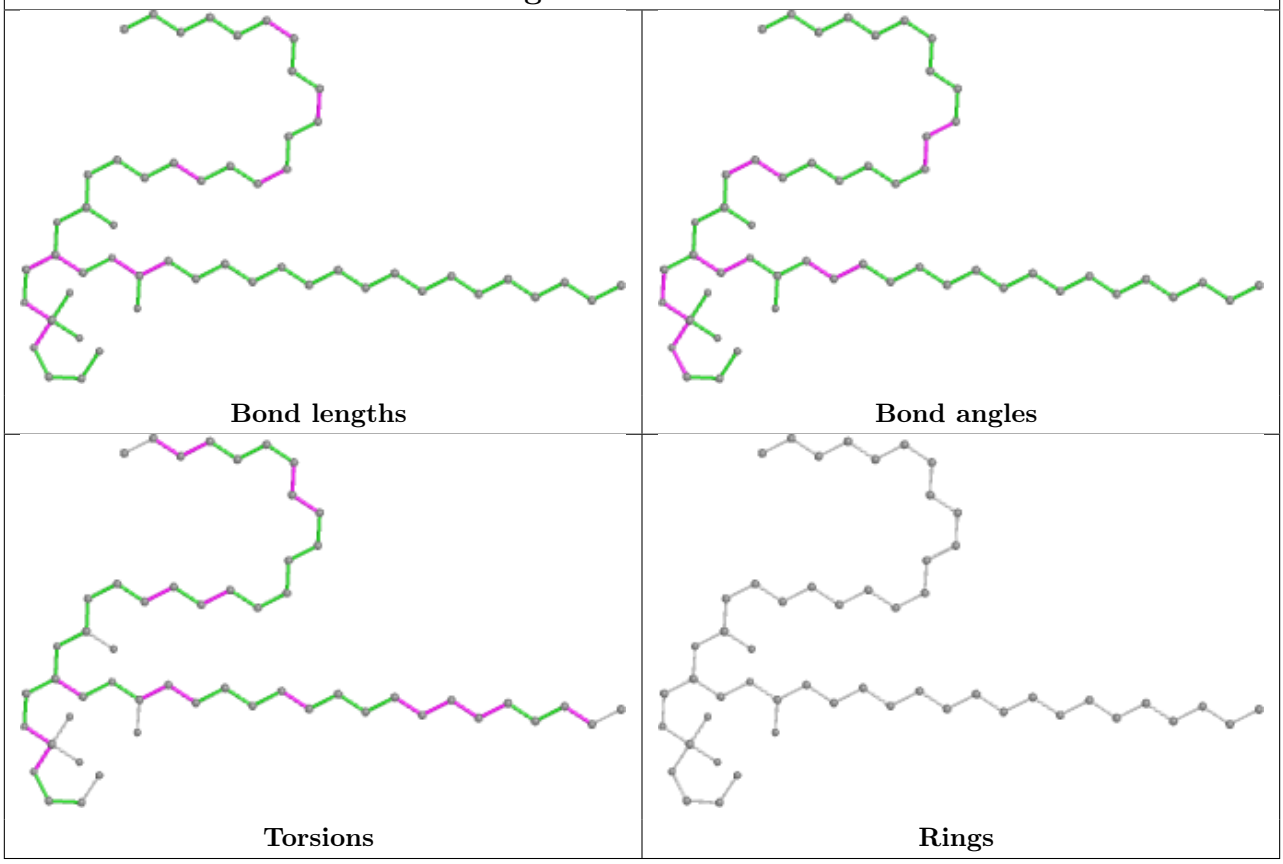
Ligand DMU C 272



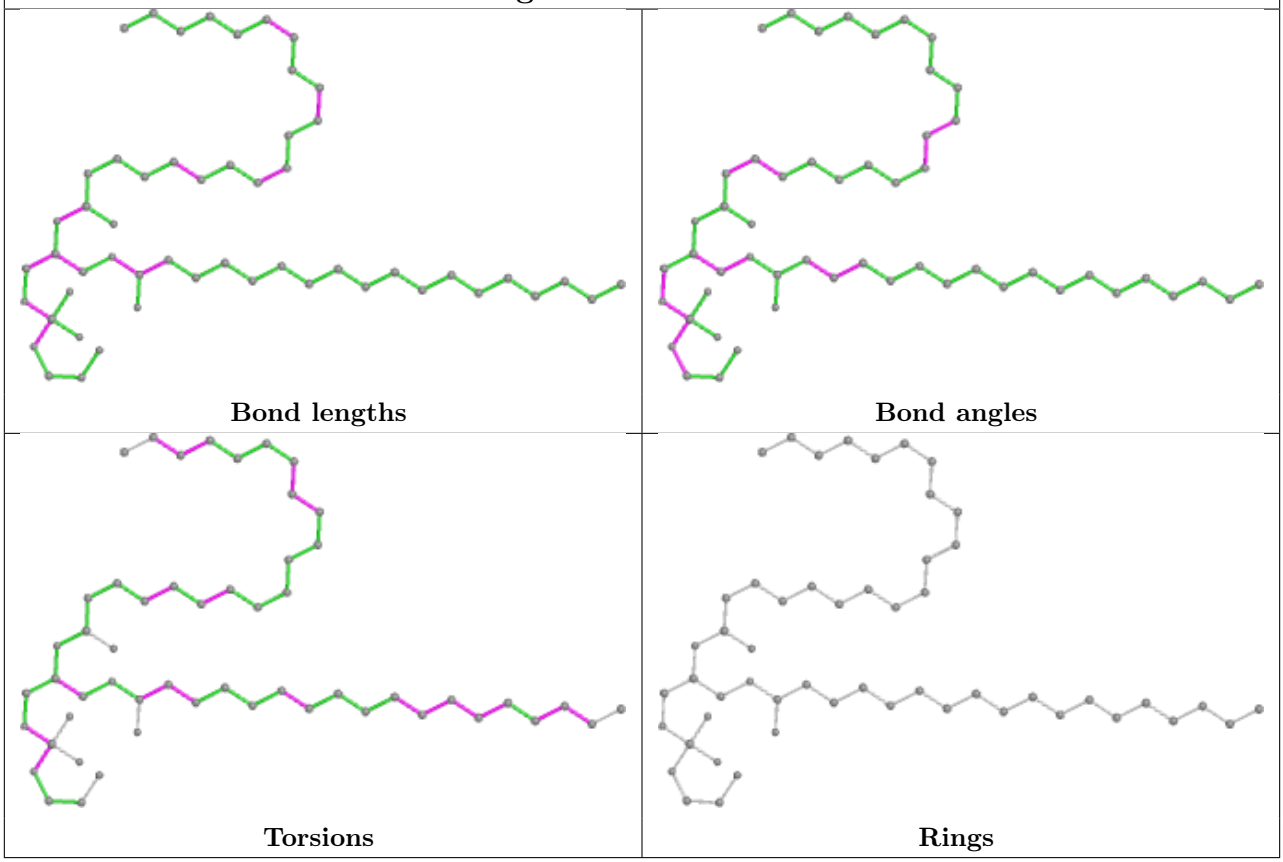
Ligand PGV C 267



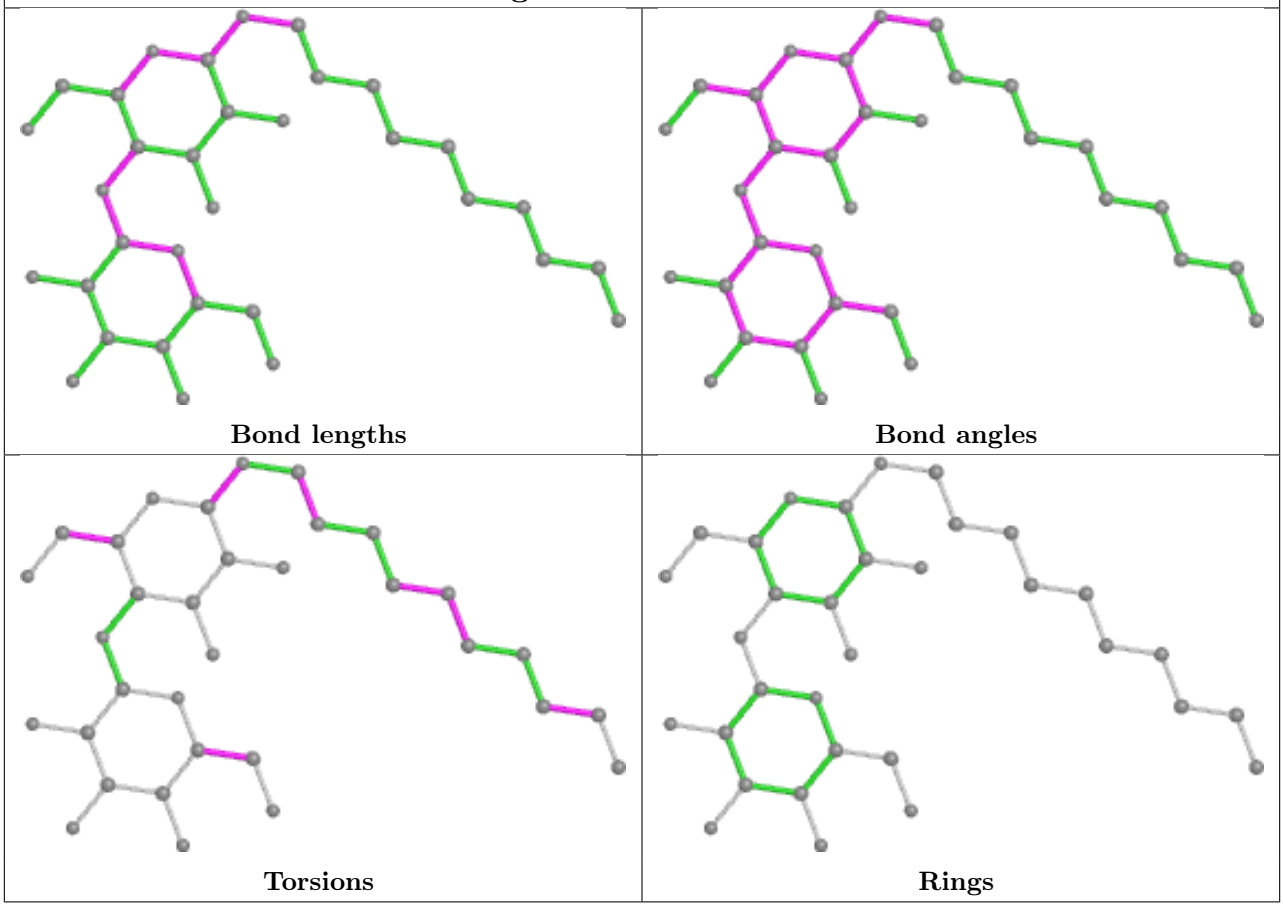
Ligand PEK C 265



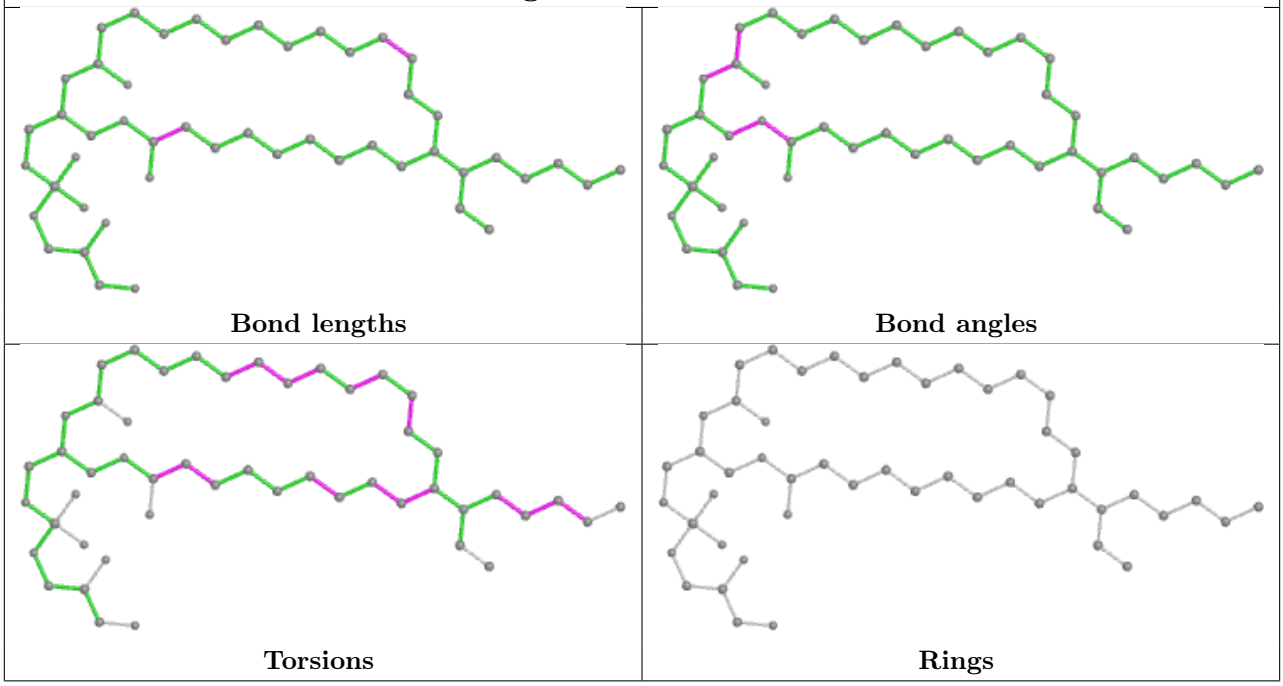
Ligand PEK P 1265



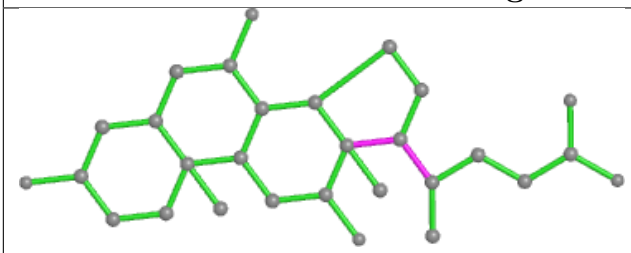
Ligand DMU Z 1526



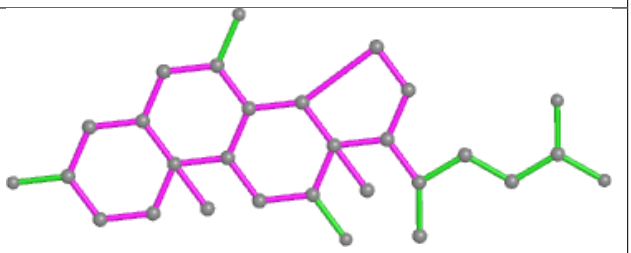
Ligand PGV A 525



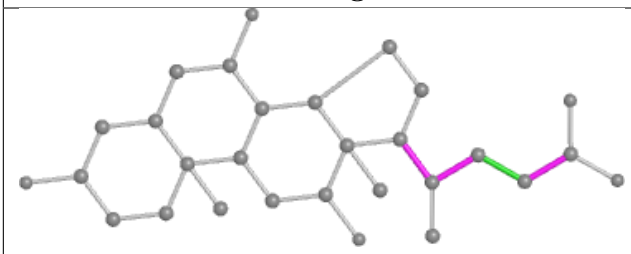
Ligand CHD W 1060



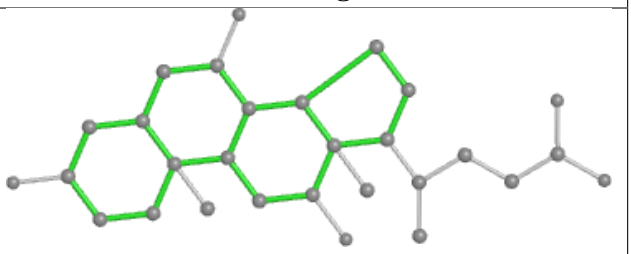
Bond lengths



Bond angles

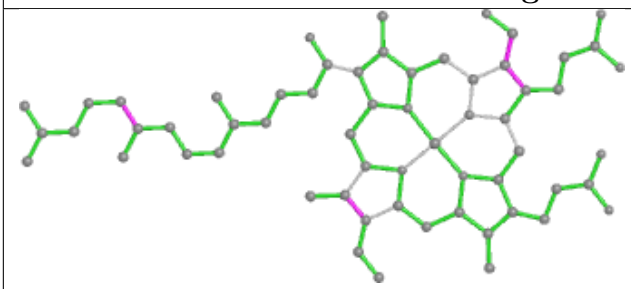


Torsions

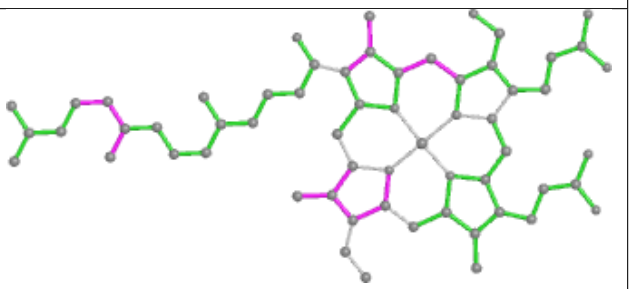


Rings

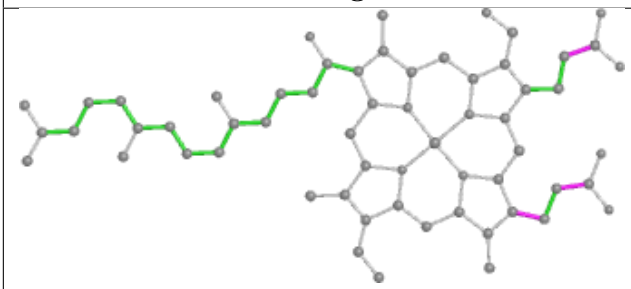
Ligand HEA A 516



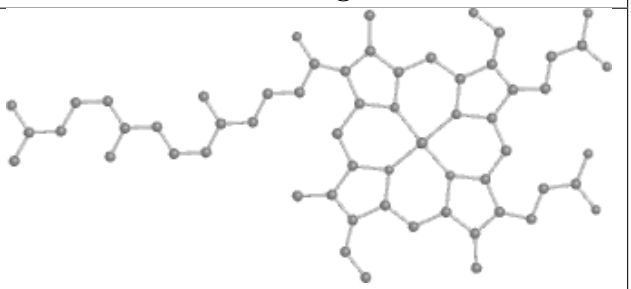
Bond lengths



Bond angles

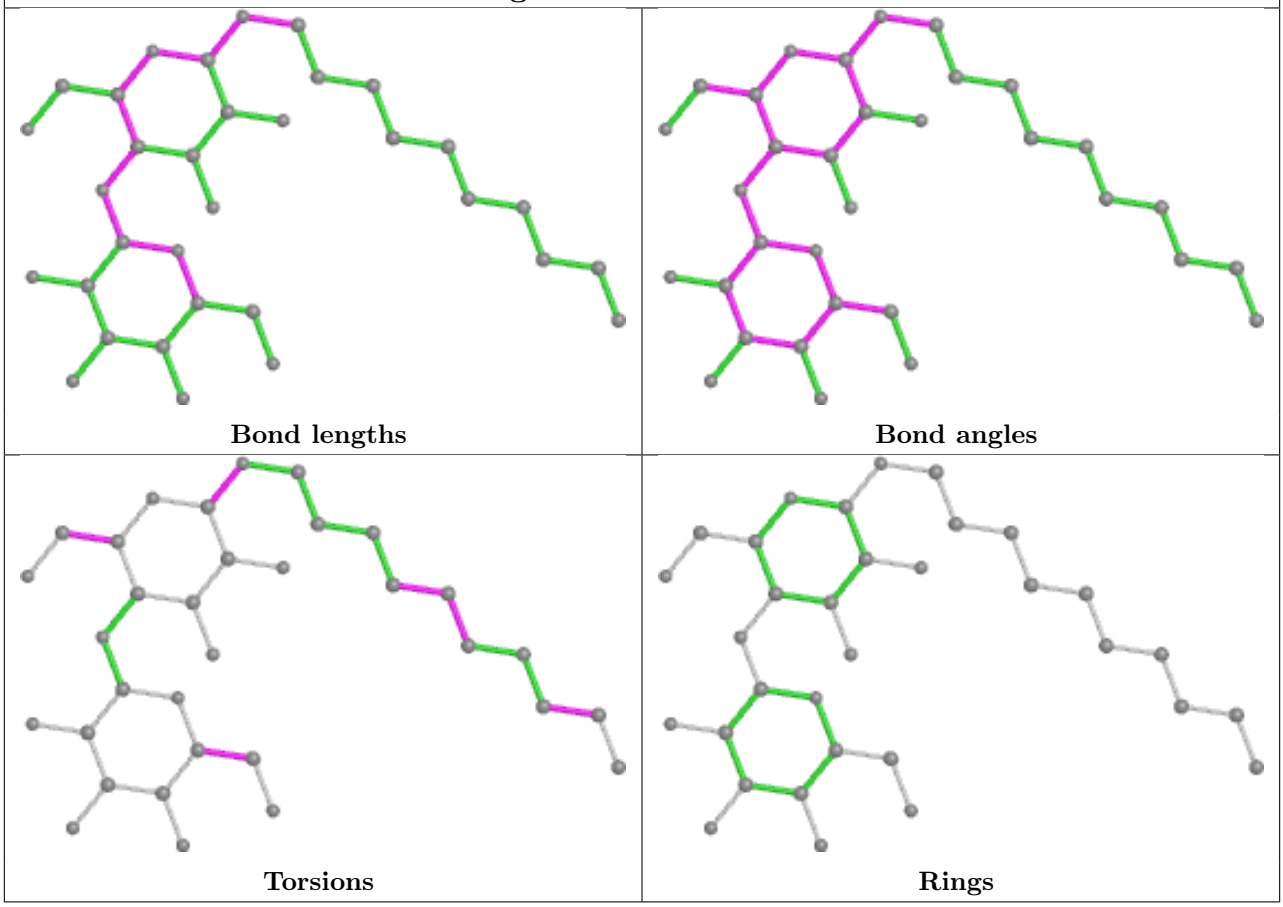


Torsions

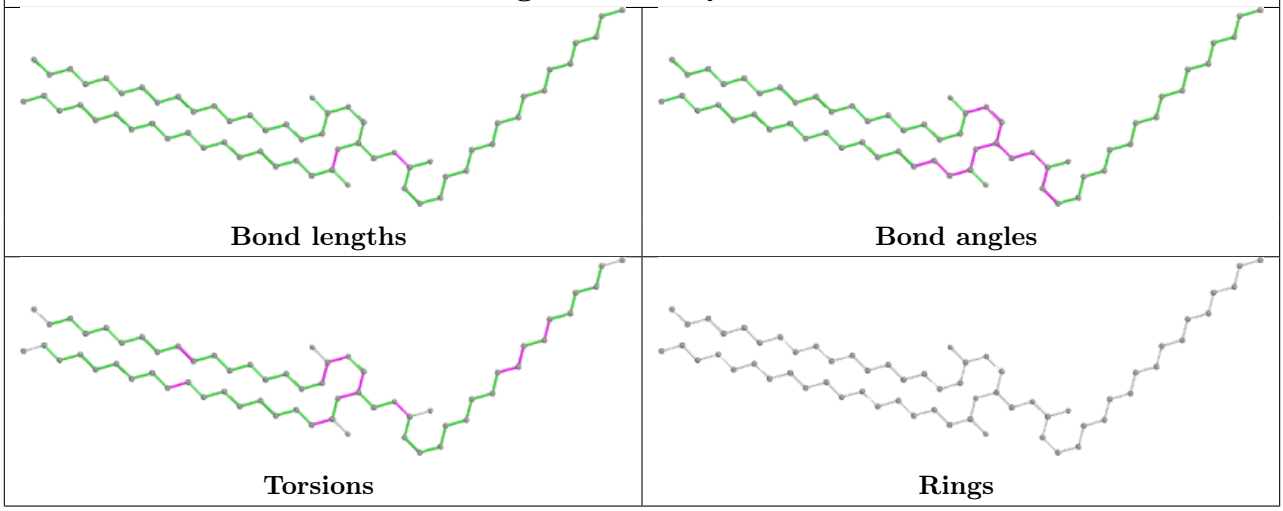


Rings

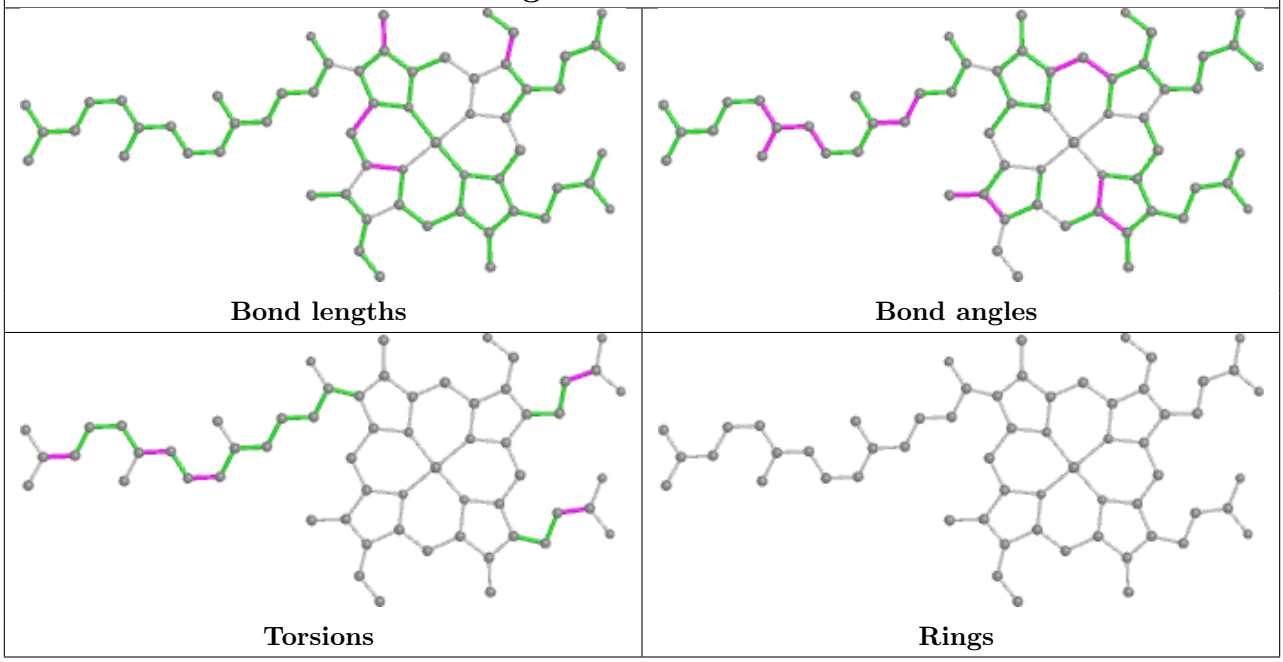
Ligand DMU P 1272



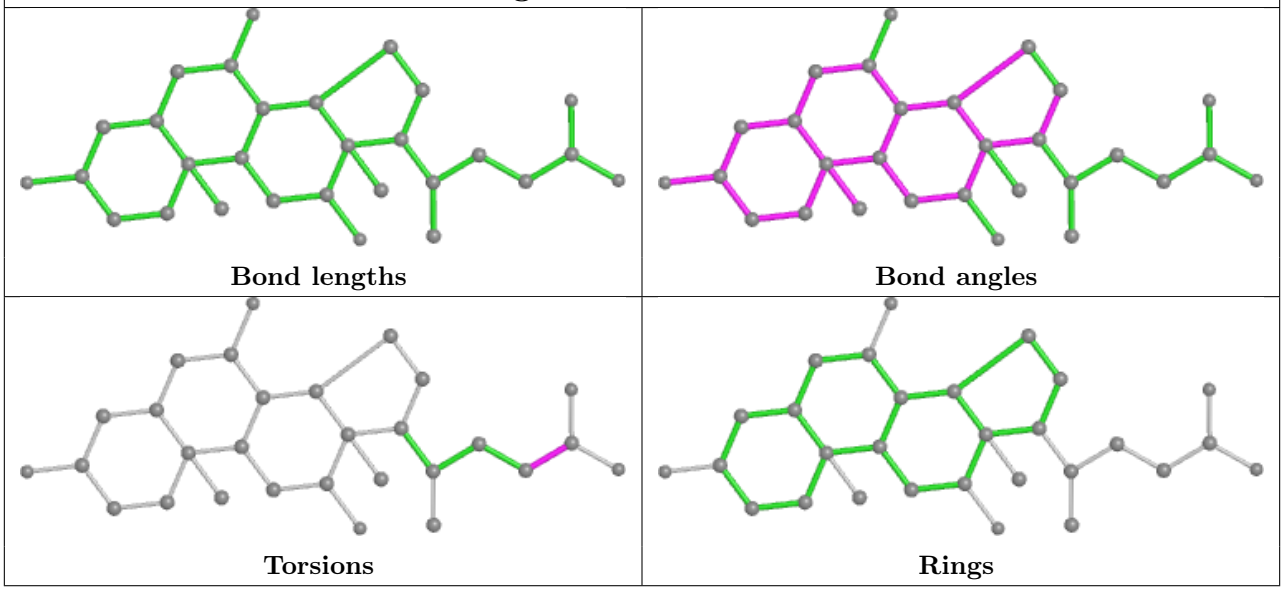
Ligand TGL Q 1523



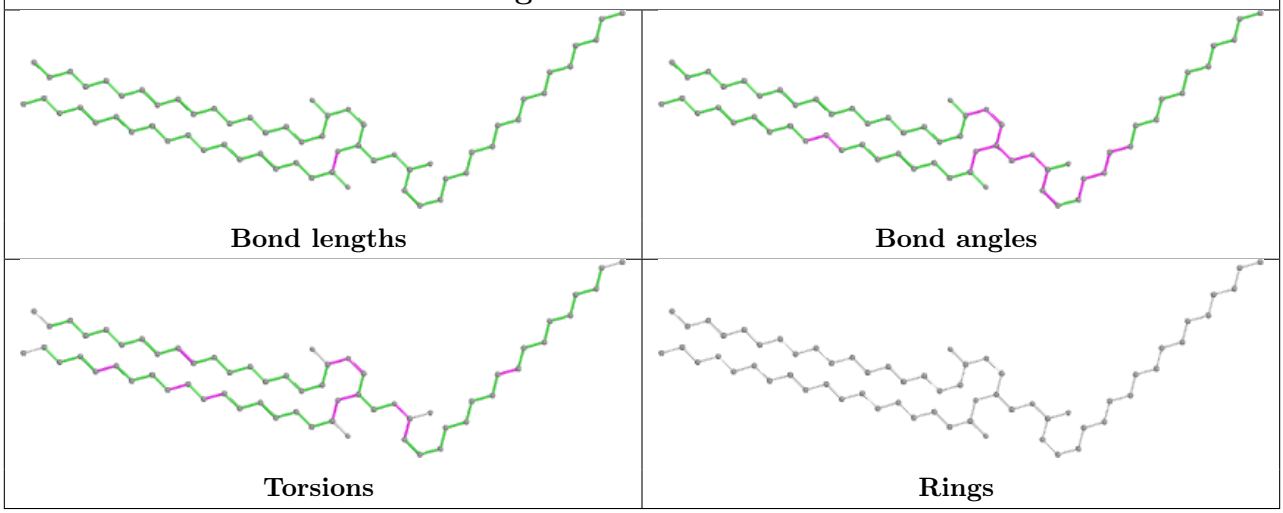
Ligand HEA A 515



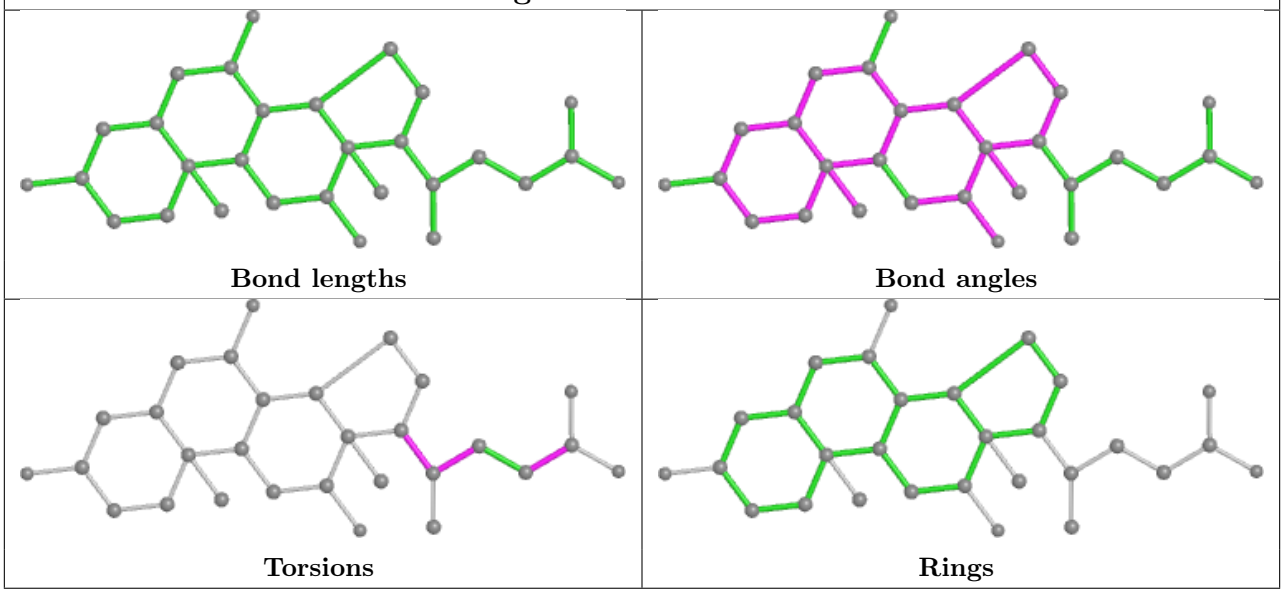
Ligand CHD B 1086



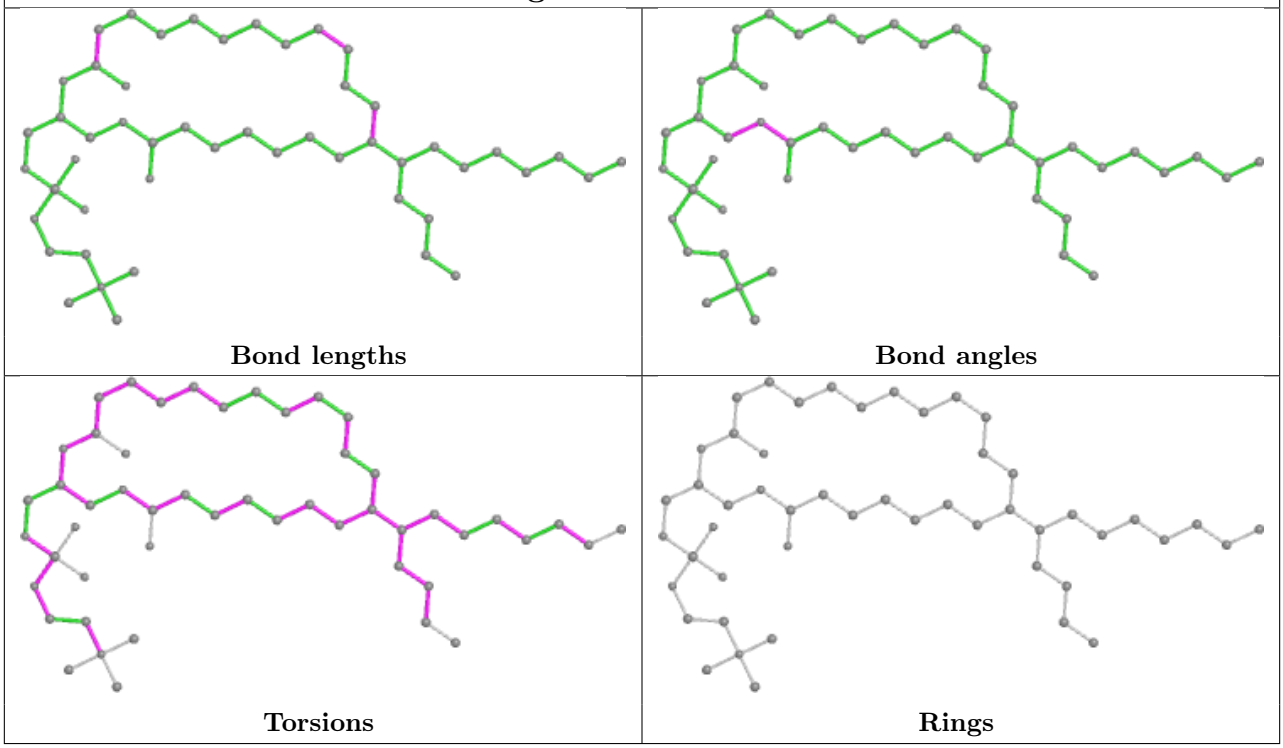
Ligand TGL N 1521



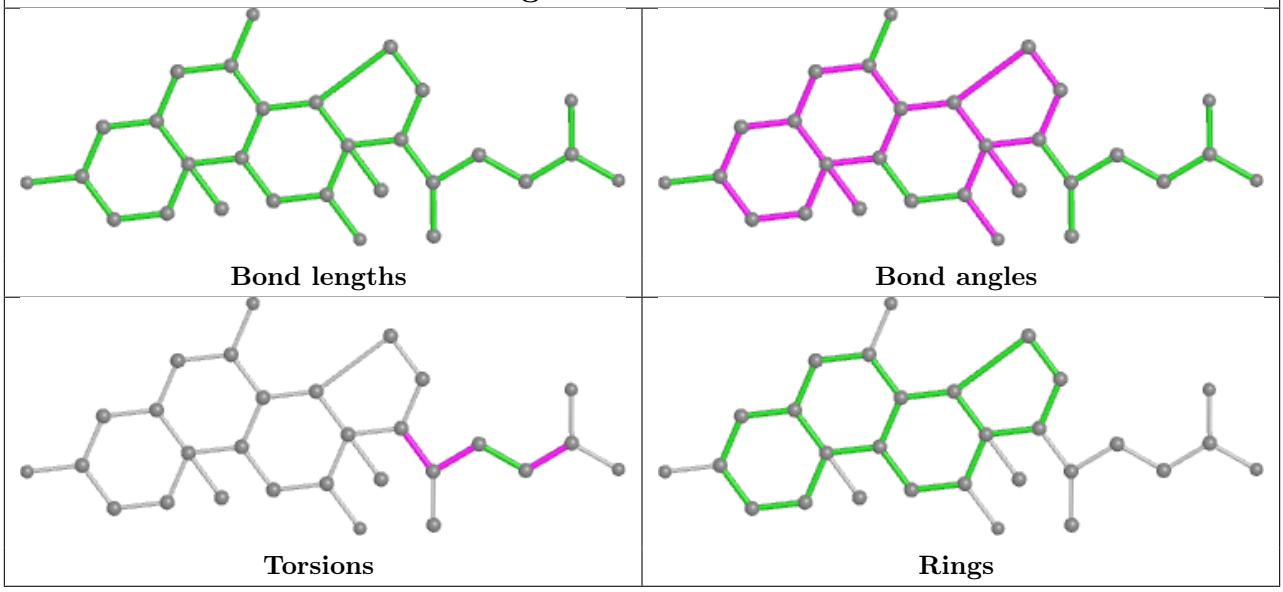
Ligand CHD P 1271



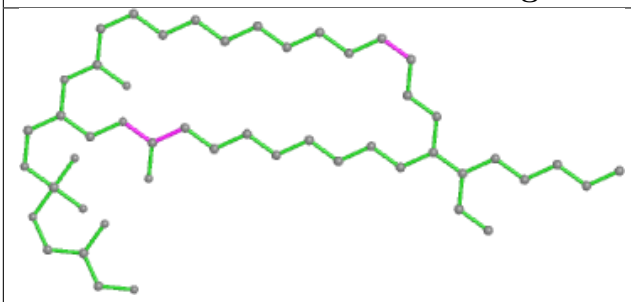
Ligand PSC B 230



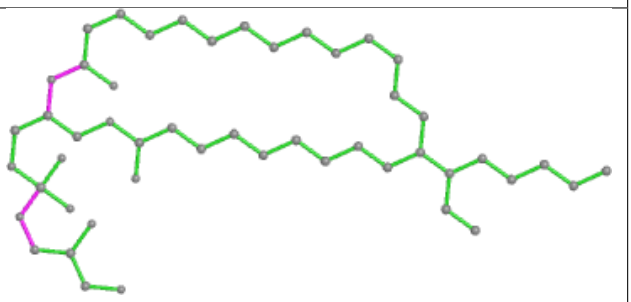
Ligand CHD C 271



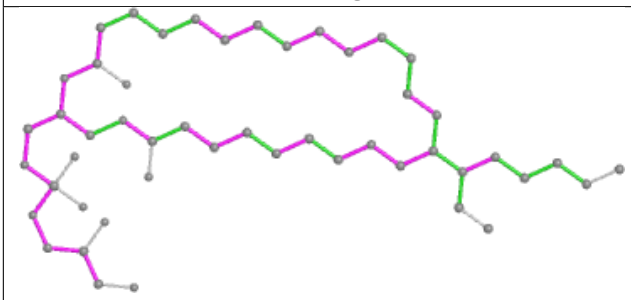
Ligand PGV A 524



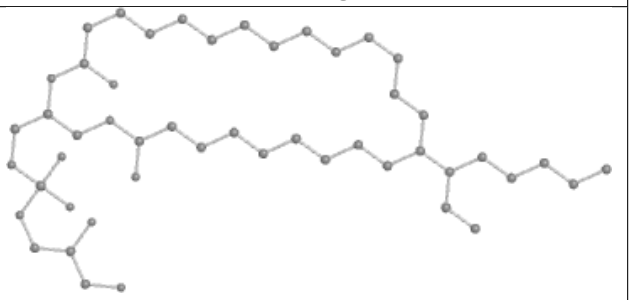
Bond lengths



Bond angles

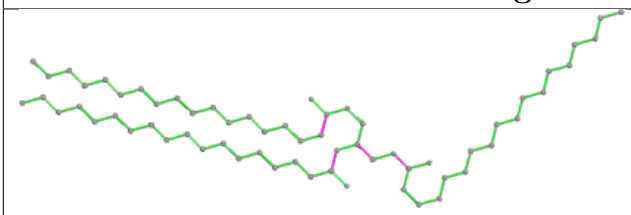


Torsions

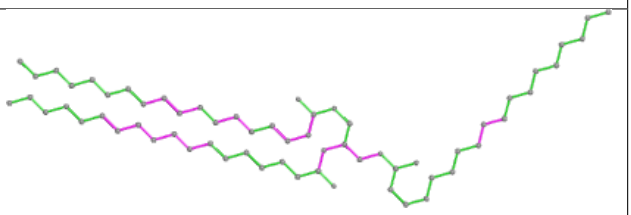


Rings

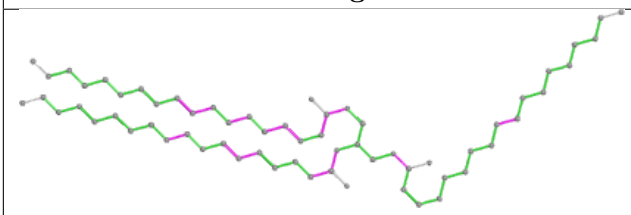
Ligand TGL N 1522



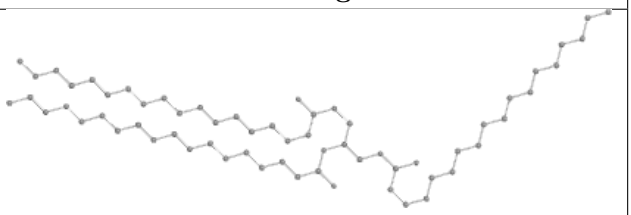
Bond lengths



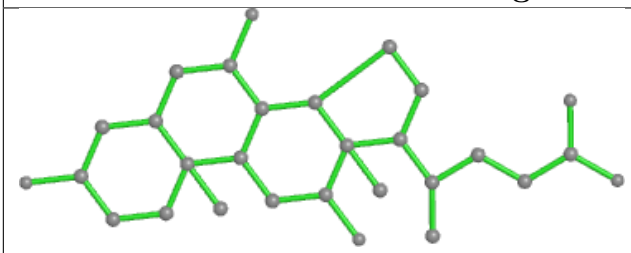
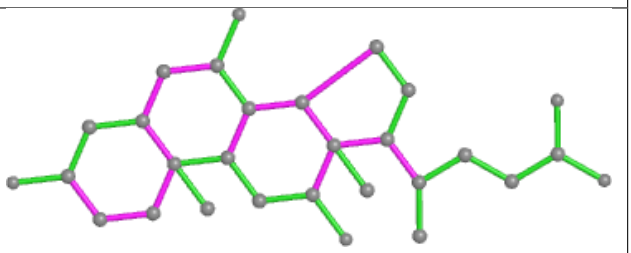
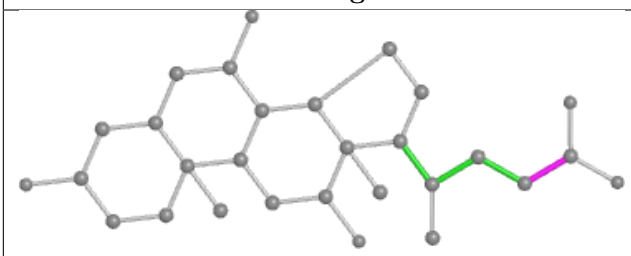
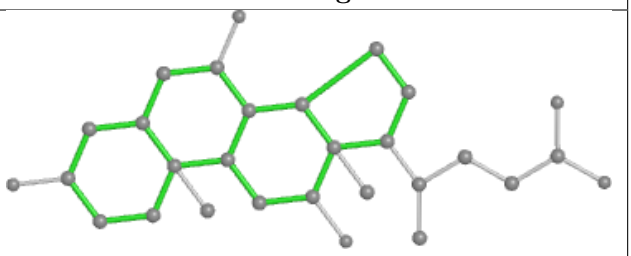
Bond angles

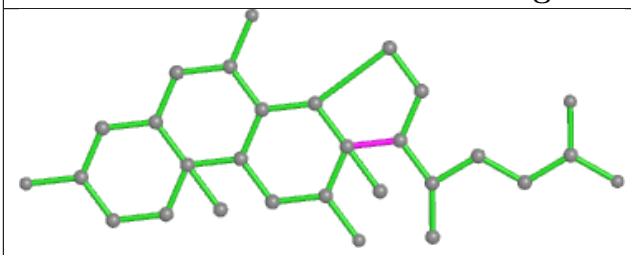
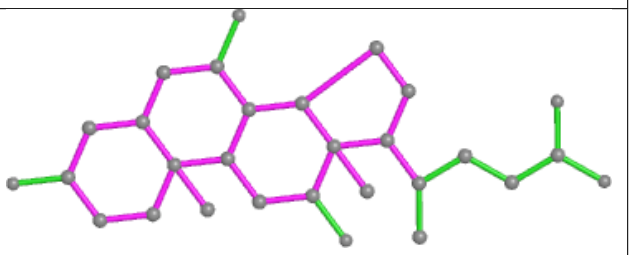
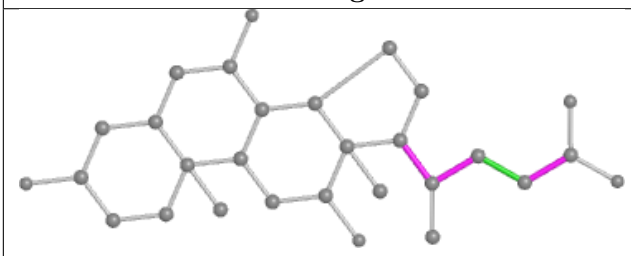
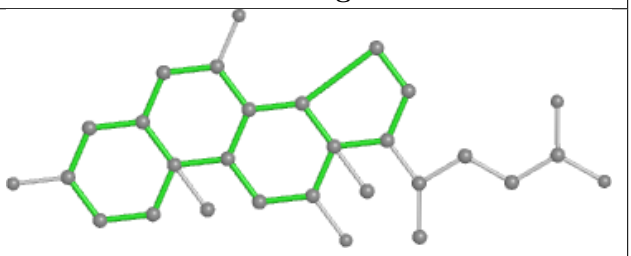


Torsions

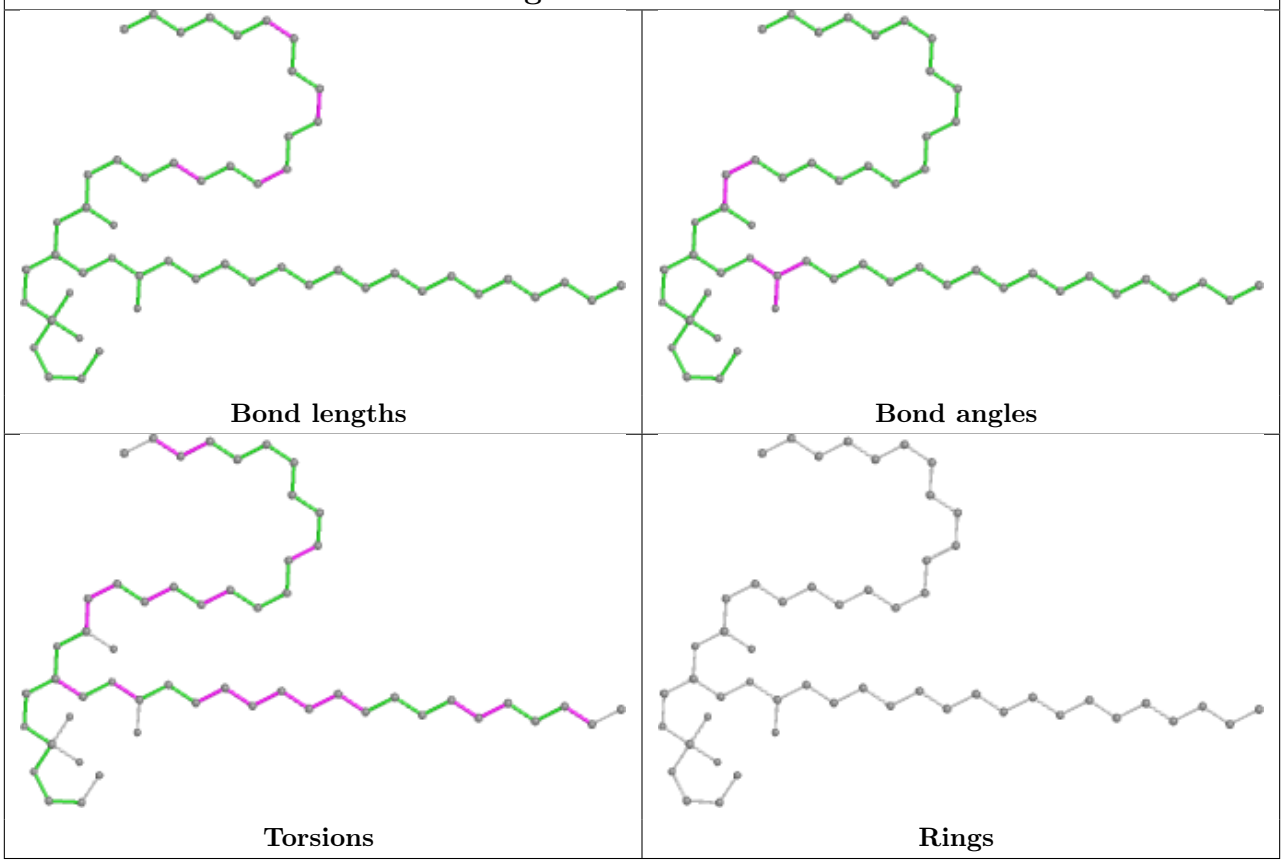


Rings

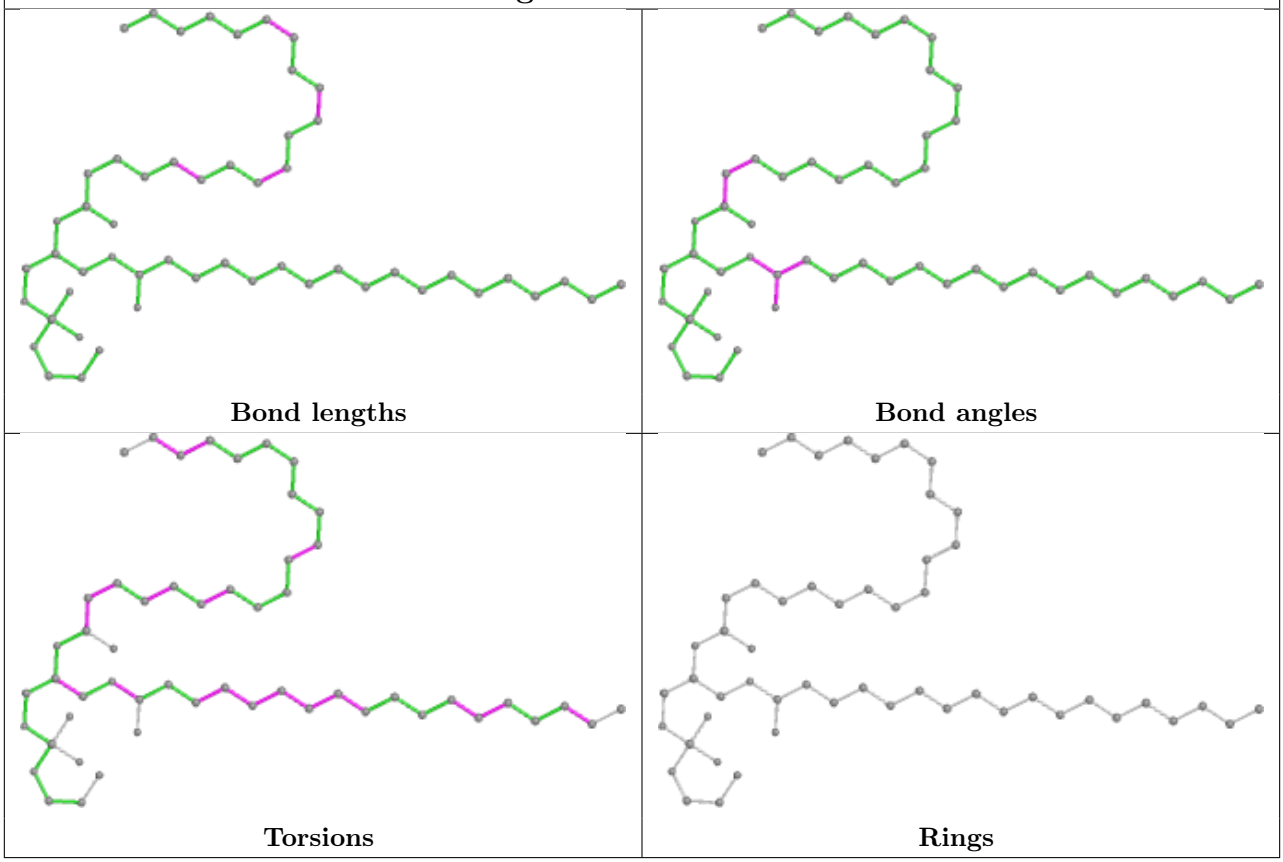
Ligand CHD P 1525	
 Bond lengths	 Bond angles
 Torsions	 Rings

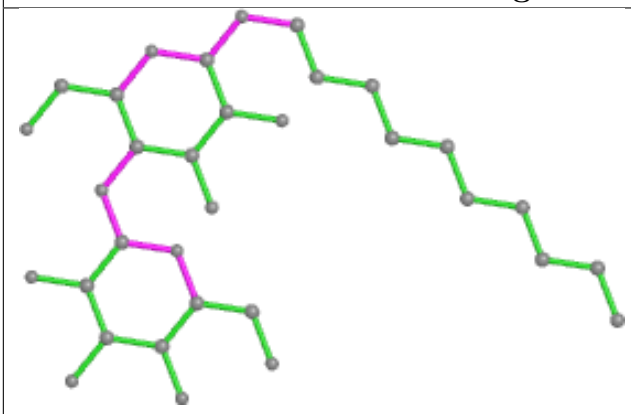
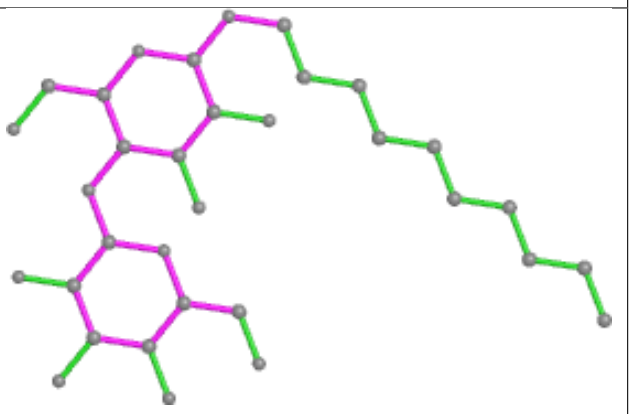
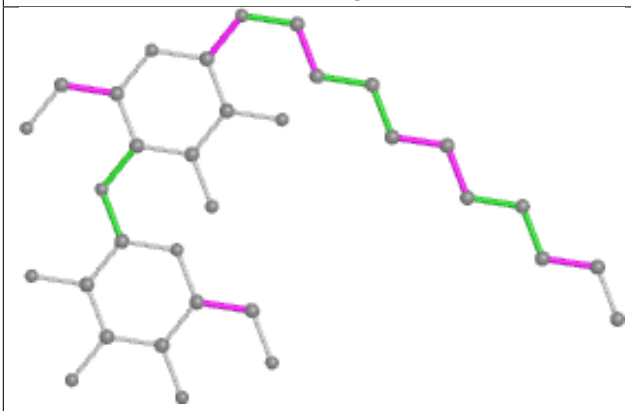
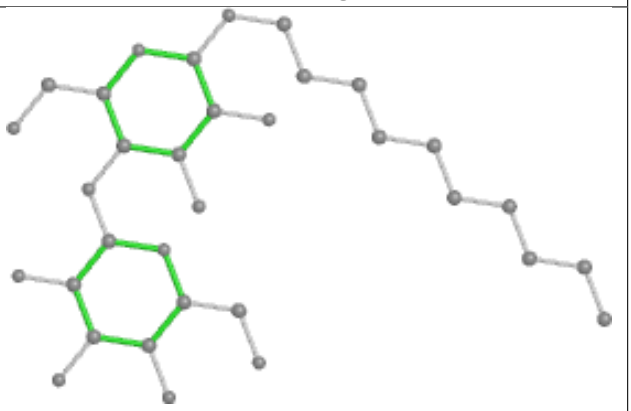
Ligand CHD J 60	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PEK C 264

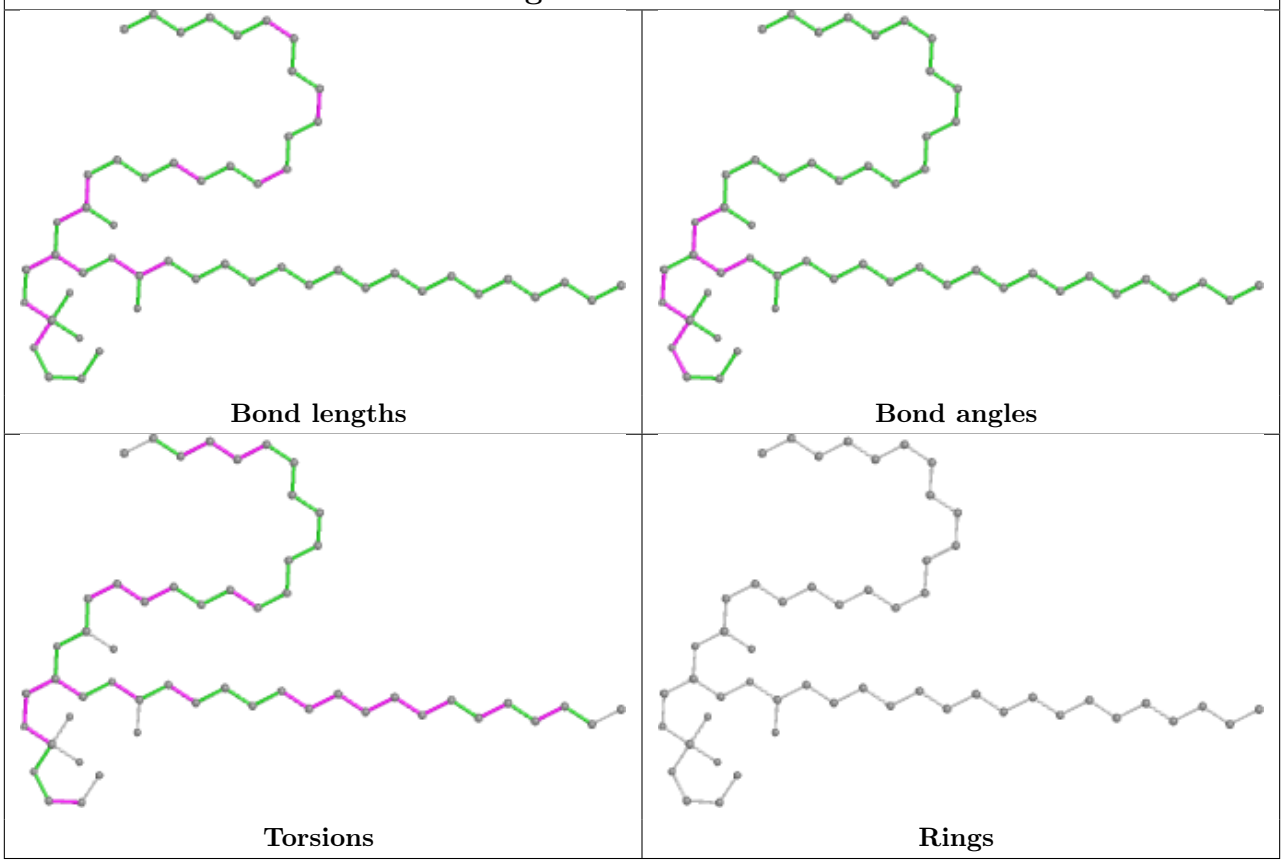


Ligand PEK P 1264

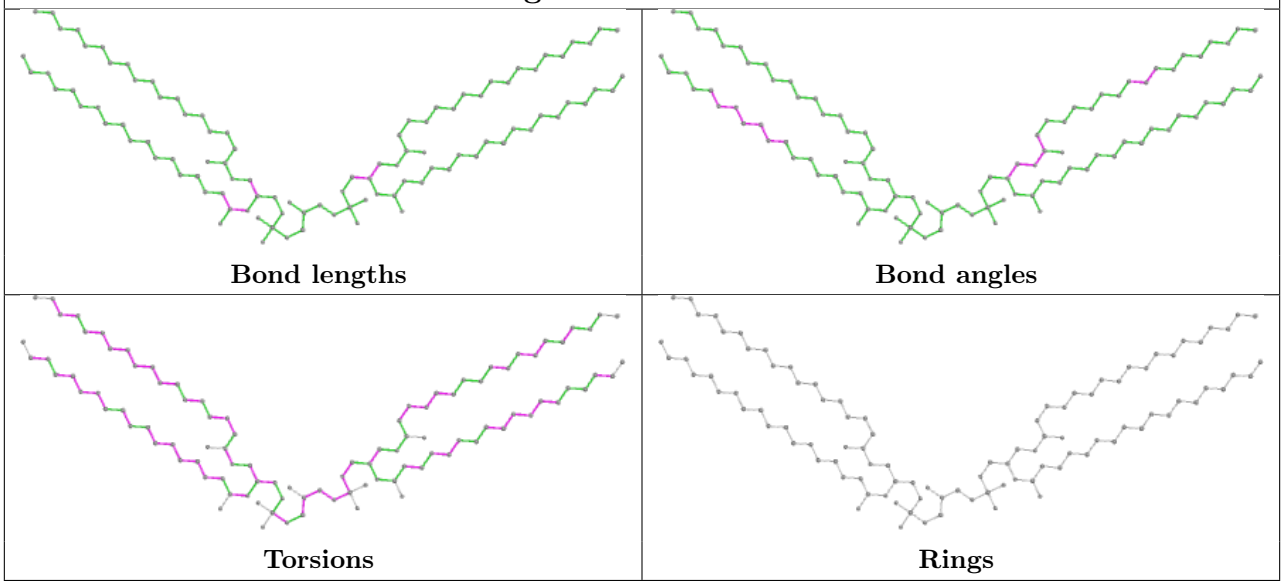


Ligand DMU M 526	
 Bond lengths	 Bond angles
 Torsions	 Rings

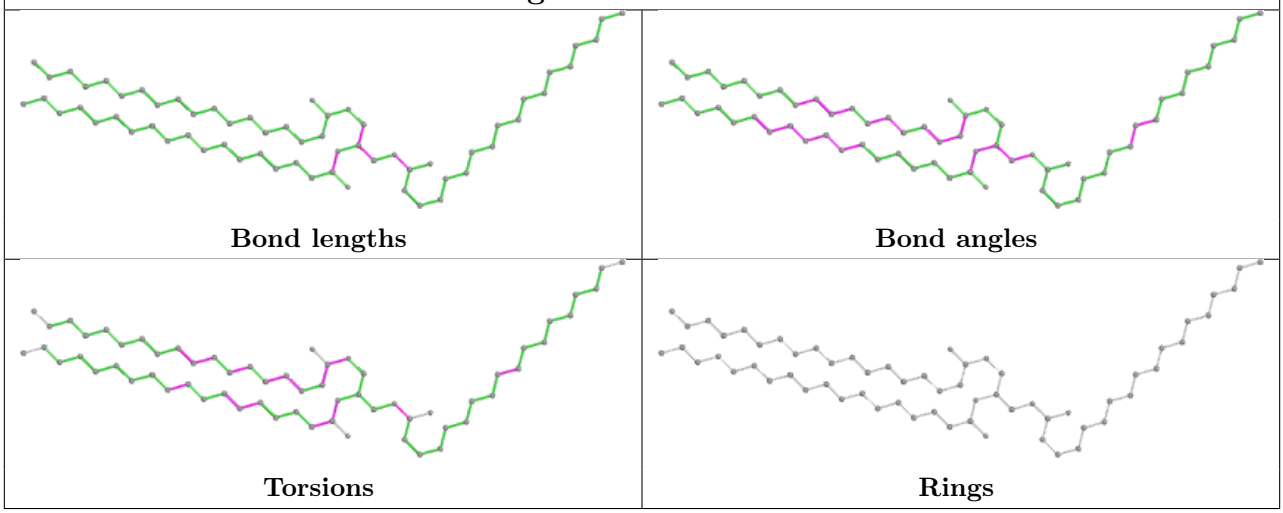
Ligand PEK T 263



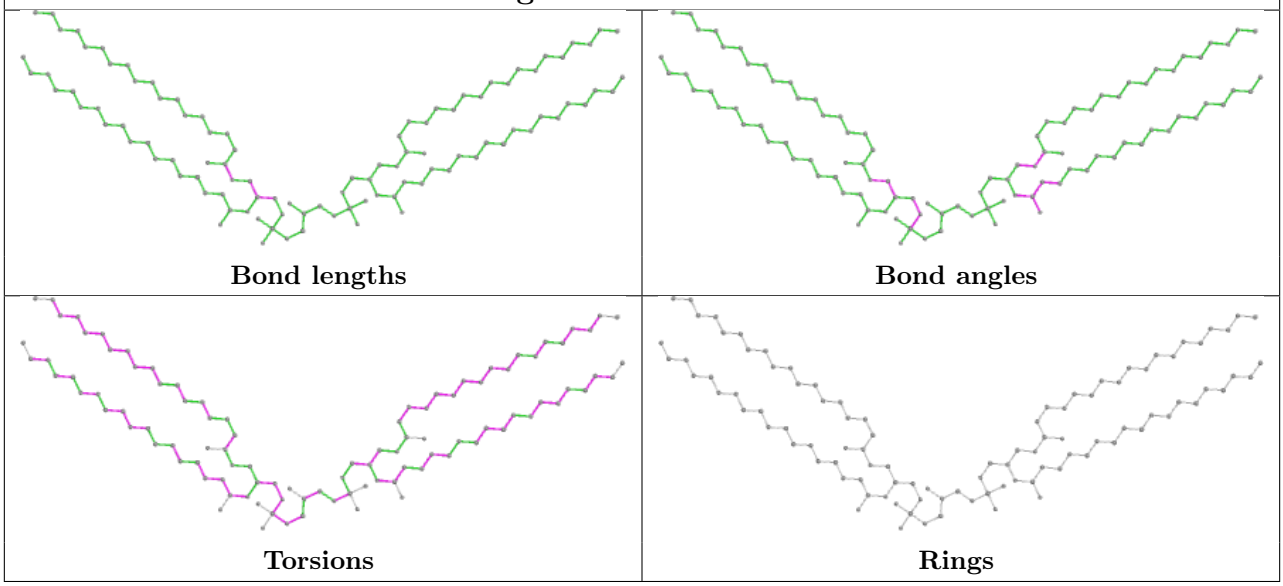
Ligand CDL G 269



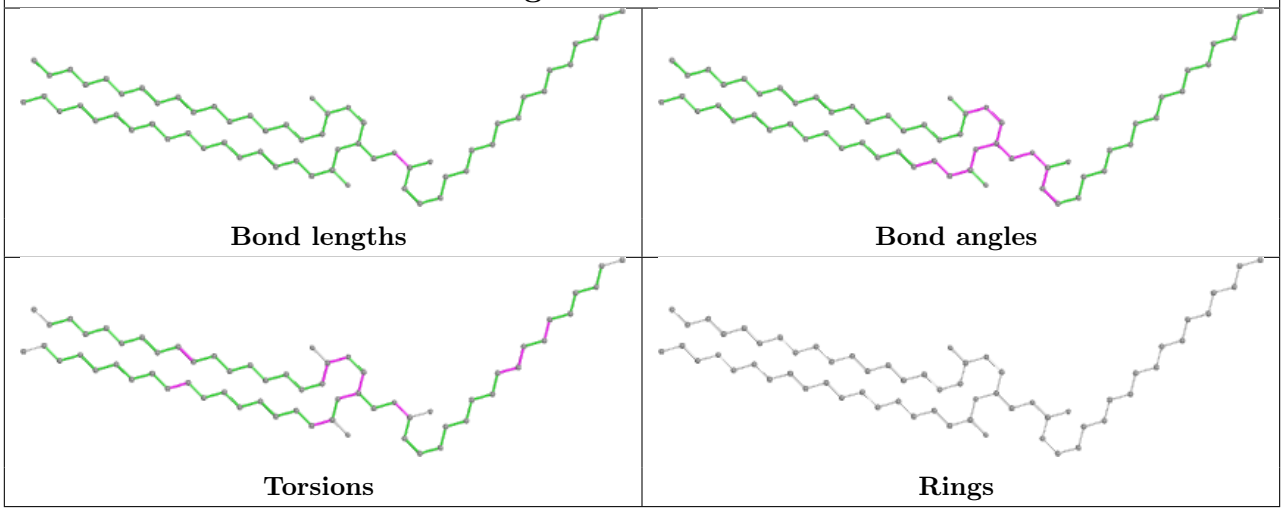
Ligand TGL L 522



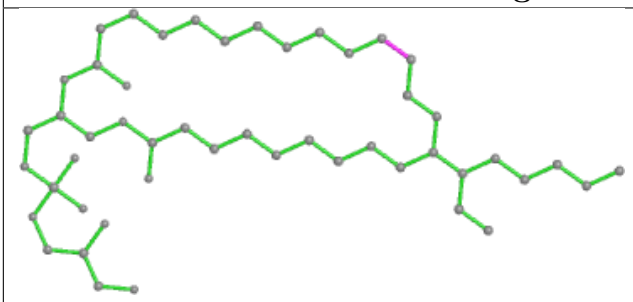
Ligand CDL P 1270



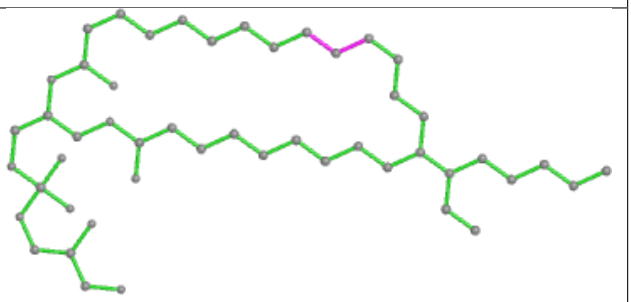
Ligand TGL D 523



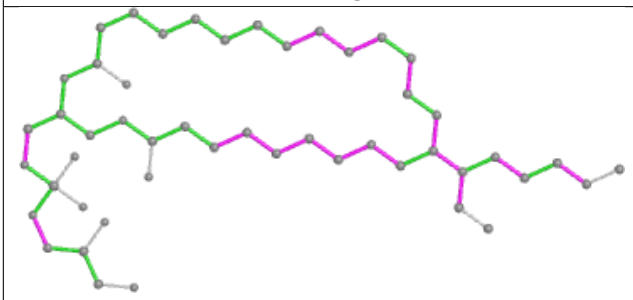
Ligand PGV P 1267



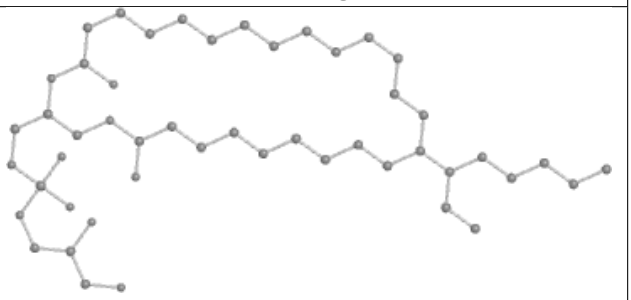
Bond lengths



Bond angles

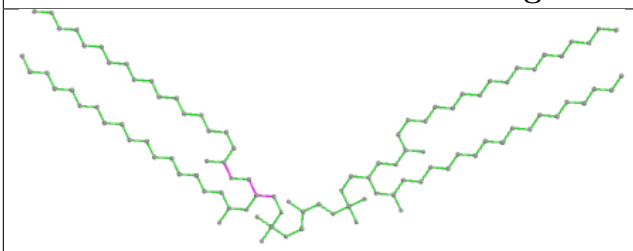


Torsions



Rings

Ligand CDL C 270



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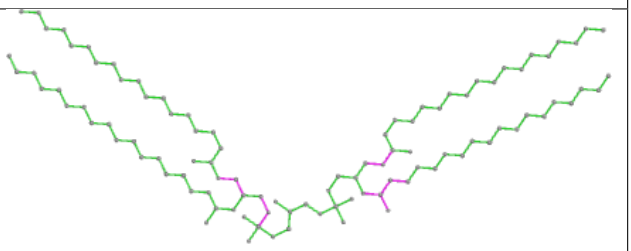
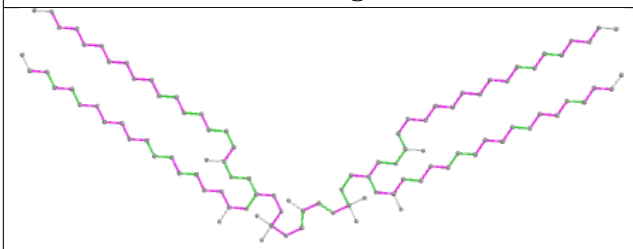
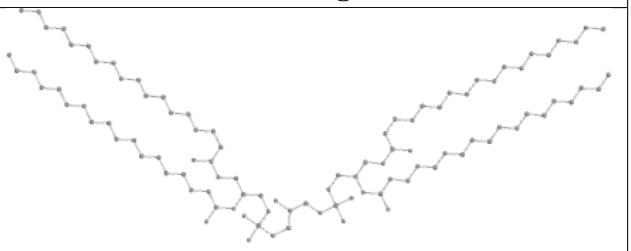


Bond angles

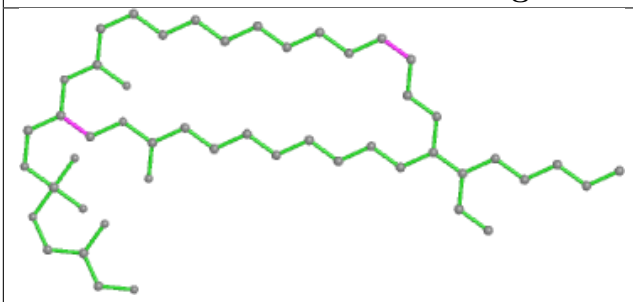


Torsions

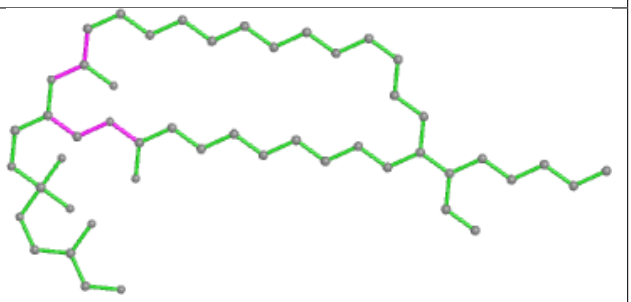


Rings

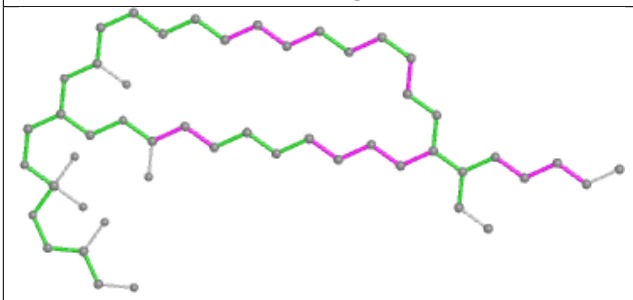
Ligand PGV N 1266



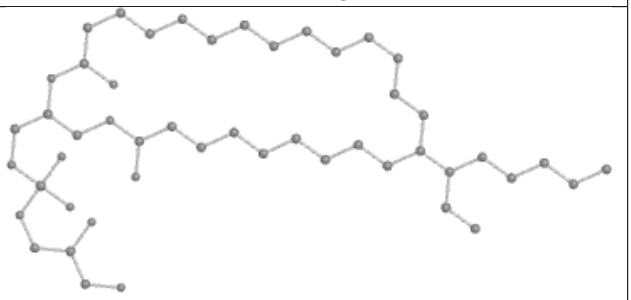
Bond lengths



Bond angles

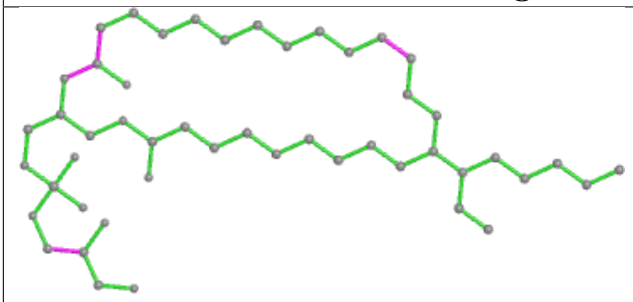


Torsions

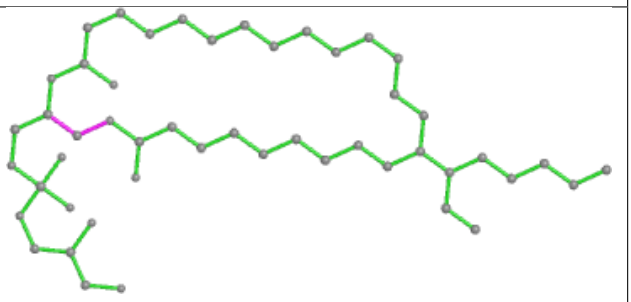


Rings

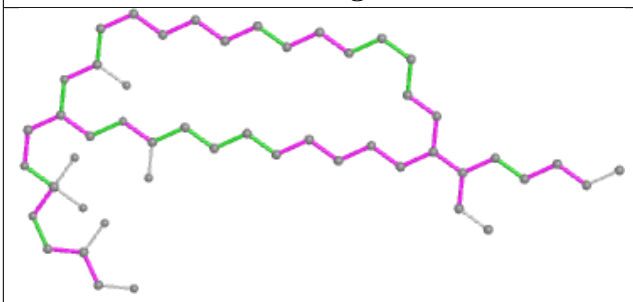
Ligand PGV P 1268



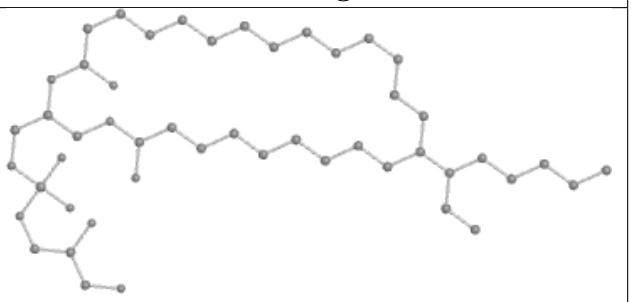
Bond lengths



Bond angles

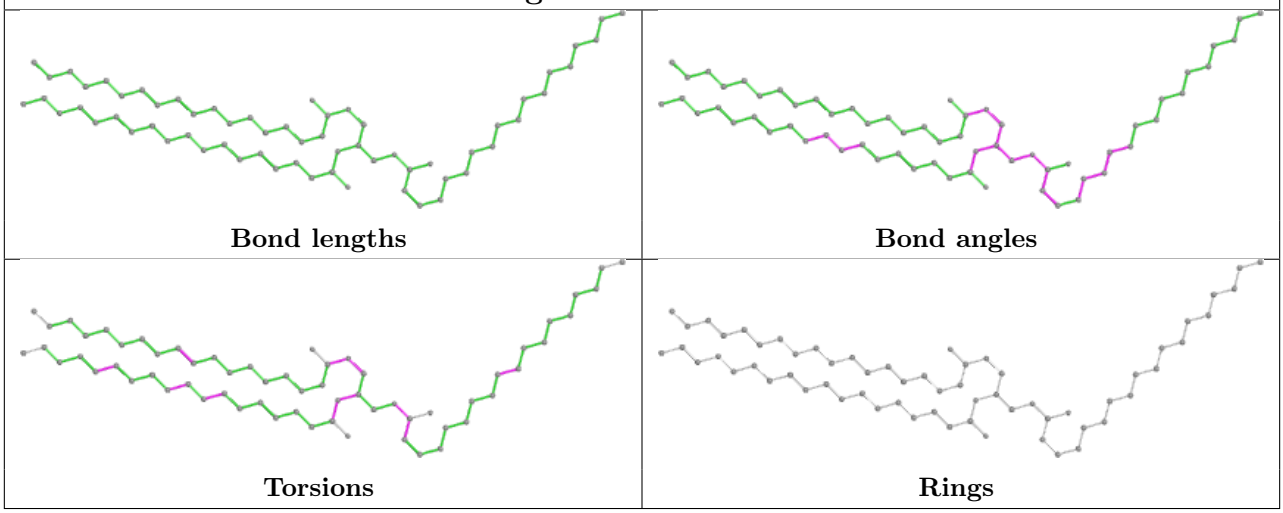


Torsions

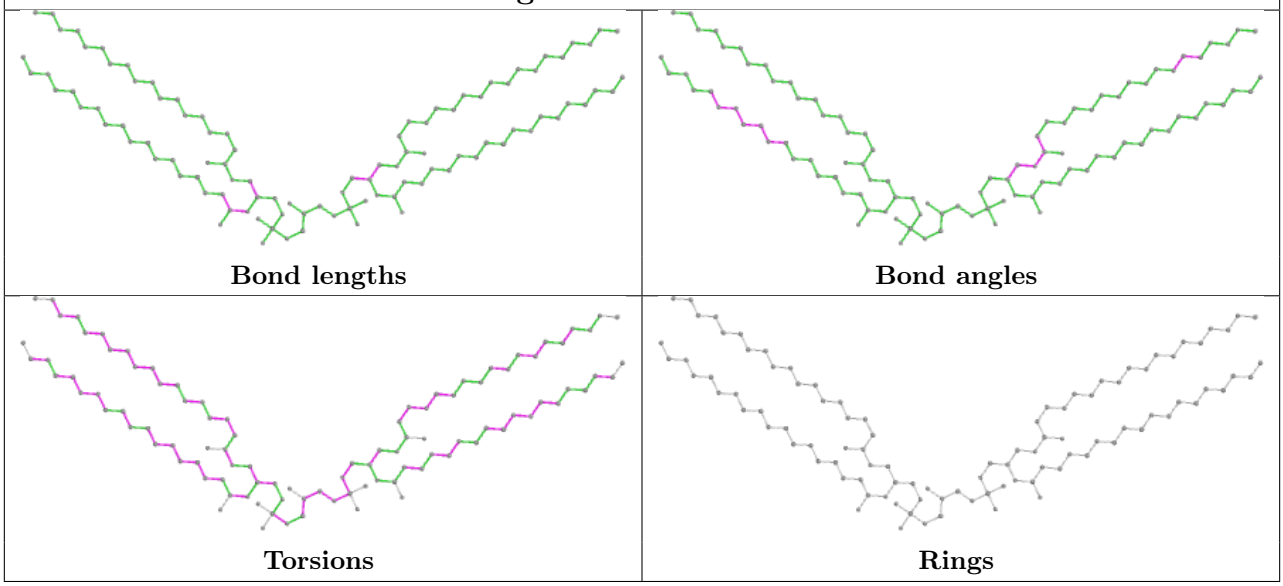


Rings

Ligand TGL B 521



Ligand CDL T 1269



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%)	-0.23	0	100	100	16, 22, 31, 72	0
1	N	513/514 (99%)	-0.27	1 (0%)	95	93	17, 24, 34, 66	0
2	B	226/227 (99%)	-0.50	3 (1%)	77	74	18, 29, 52, 90	0
2	O	226/227 (99%)	-0.22	8 (3%)	44	38	22, 32, 61, 84	0
3	C	259/261 (99%)	-0.53	1 (0%)	92	90	19, 25, 39, 70	0
3	P	259/261 (99%)	-0.47	2 (0%)	86	84	19, 26, 40, 74	0
4	D	144/147 (97%)	-0.33	3 (2%)	63	59	21, 31, 57, 86	0
4	Q	144/147 (97%)	1.00	18 (12%)	3	2	28, 42, 65, 100	0
5	E	105/109 (96%)	-0.05	2 (1%)	66	63	22, 31, 59, 101	0
5	R	105/109 (96%)	0.76	12 (11%)	5	3	25, 39, 71, 102	0
6	F	98/98 (100%)	0.23	8 (8%)	11	9	20, 32, 88, 110	0
6	S	98/98 (100%)	0.23	8 (8%)	11	9	20, 31, 93, 106	0
7	G	83/85 (97%)	0.78	17 (20%)	1	0	23, 34, 99, 107	0
7	T	83/85 (97%)	0.84	17 (20%)	1	0	23, 36, 102, 109	0
8	H	79/85 (92%)	0.22	11 (13%)	2	2	23, 35, 90, 108	0
8	U	79/85 (92%)	0.39	10 (12%)	3	2	27, 39, 91, 110	0
9	I	72/73 (98%)	0.31	5 (6%)	16	13	25, 44, 65, 85	0
9	V	72/73 (98%)	0.62	7 (9%)	7	6	24, 49, 68, 94	0
10	J	58/59 (98%)	0.34	5 (8%)	10	8	26, 36, 72, 99	0
10	W	58/59 (98%)	0.44	8 (13%)	2	2	26, 38, 75, 106	0
11	K	49/56 (87%)	-0.16	1 (2%)	65	61	26, 36, 50, 66	0
11	X	49/56 (87%)	0.79	5 (10%)	6	5	35, 41, 60, 76	0
12	L	46/47 (97%)	-0.39	2 (4%)	35	29	22, 28, 52, 87	0
12	Y	46/47 (97%)	-0.31	1 (2%)	62	57	26, 34, 65, 88	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	M	43/46 (93%)	-0.10	4 (9%)	8	6	23, 28, 75, 103	0
13	Z	43/46 (93%)	0.31	5 (11%)	4	3	31, 36, 80, 106	0
All	All	3550/3614 (98%)	-0.04	164 (4%)	32	26	16, 29, 64, 110	0

The worst 5 of 164 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	5	VAL	25.6
4	Q	6	VAL	24.6
4	Q	4	SER	19.0
6	S	97	ALA	16.9
6	F	98	HIS	12.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	TPO	G	11	11/12	0.38	0.37	77,85,107,108	0
9	SAC	V	1	9/10	0.51	0.49	99,100,104,104	0
7	TPO	T	11	11/12	0.53	0.31	76,84,110,112	0
9	SAC	I	1	9/10	0.69	0.39	93,97,99,99	0
1	FME	A	1	10/11	0.83	0.15	40,45,66,72	0
1	FME	N	1	10/11	0.90	0.16	39,43,65,69	0
2	FME	B	1	10/11	0.93	0.14	23,31,39,50	0
2	FME	O	1	10/11	0.93	0.15	37,38,47,53	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	PEK	T	263	53/53	0.50	0.40	45,83,100,103	0
25	PEK	P	1265	53/53	0.52	0.33	46,89,107,109	0
25	PEK	C	265	53/53	0.52	0.29	44,88,103,104	0
23	DMU	P	1272	33/33	0.56	0.39	73,96,104,105	0
23	DMU	C	272	33/33	0.58	0.39	71,97,102,104	0
21	PSC	O	1230	52/52	0.59	0.34	48,80,111,116	0
26	CDL	G	269	100/100	0.59	0.32	61,83,101,105	0
26	CDL	T	1269	100/100	0.59	0.32	54,84,97,105	0
21	PSC	B	230	52/52	0.61	0.35	48,84,113,116	0
25	PEK	G	1263	53/53	0.61	0.39	46,83,99,101	0
18	PGV	C	268	51/51	0.62	0.39	65,84,103,106	0
20	TGL	N	1522	63/63	0.63	0.32	42,67,79,82	0
22	CHD	W	1060	29/29	0.64	0.40	98,104,106,108	0
26	CDL	P	1270	100/100	0.67	0.37	42,88,101,105	0
20	TGL	Q	1523	63/63	0.67	0.23	45,70,80,84	0
18	PGV	P	1268	51/51	0.69	0.37	65,84,104,106	0
20	TGL	L	522	63/63	0.71	0.30	34,65,79,81	0
22	CHD	J	60	29/29	0.73	0.37	98,104,107,109	0
20	TGL	D	523	63/63	0.73	0.23	47,65,79,82	0
26	CDL	C	270	100/100	0.73	0.38	44,87,100,106	0
18	PGV	A	524	51/51	0.74	0.26	35,71,101,104	0
22	CHD	C	271	29/29	0.76	0.26	87,95,96,97	0
22	CHD	P	1271	29/29	0.78	0.28	89,95,98,101	0
18	PGV	Z	1524	51/51	0.78	0.27	38,71,101,104	0
20	TGL	N	1521	63/63	0.78	0.24	49,67,84,86	0
20	TGL	B	521	63/63	0.80	0.23	49,64,85,90	0
24	UNX	C	262	1/1	0.86	0.27	47,47,47,47	0
23	DMU	Z	1526	33/33	0.89	0.19	40,49,61,64	0
24	UNX	P	1262	1/1	0.90	0.44	43,43,43,43	0
23	DMU	M	526	33/33	0.92	0.12	32,42,55,58	0
16	NA	N	1519	1/1	0.93	0.07	30,30,30,30	0
25	PEK	P	1264	53/53	0.95	0.13	25,44,68,72	0
25	PEK	C	264	53/53	0.96	0.12	10,44,70,73	0
16	NA	A	519	1/1	0.96	0.06	27,27,27,27	0
15	MG	N	1518	1/1	0.96	0.10	26,26,26,26	0
18	PGV	P	1267	51/51	0.96	0.12	23,34,59,61	0
22	CHD	P	1525	29/29	0.96	0.10	20,27,31,34	0
18	PGV	C	267	51/51	0.97	0.10	20,34,58,62	0
18	PGV	A	525	51/51	0.97	0.11	21,36,56,63	0
22	CHD	B	1086	29/29	0.97	0.07	20,24,30,37	0
22	CHD	C	525	29/29	0.97	0.12	21,27,30,33	0
18	PGV	N	1266	51/51	0.97	0.11	20,38,55,64	0

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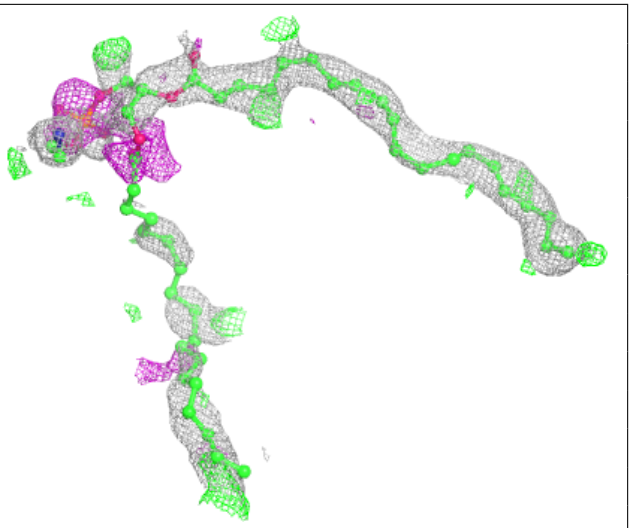
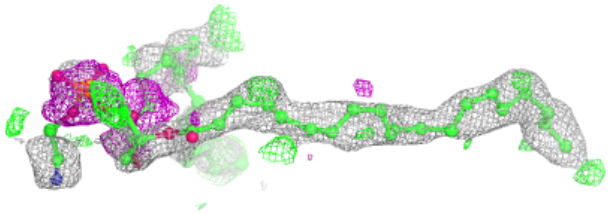
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
19	CUA	O	228	2/2	0.98	0.08	26,26,26,27	0
22	CHD	O	229	29/29	0.98	0.07	19,22,28,32	0
17	HEA	N	515	60/60	0.98	0.11	18,24,41,43	0
17	HEA	N	516	60/60	0.99	0.10	17,20,29,31	0
19	CUA	B	228	2/2	0.99	0.08	19,19,19,22	0
17	HEA	A	515	60/60	0.99	0.11	12,20,44,45	0
17	HEA	A	516	60/60	0.99	0.10	15,18,29,29	0
15	MG	A	518	1/1	0.99	0.10	20,20,20,20	0
27	ZN	F	99	1/1	0.99	0.06	25,25,25,25	0
27	ZN	S	99	1/1	0.99	0.06	27,27,27,27	0
14	CU	A	517	1/1	1.00	0.09	20,20,20,20	0
14	CU	N	517	1/1	1.00	0.09	21,21,21,21	0

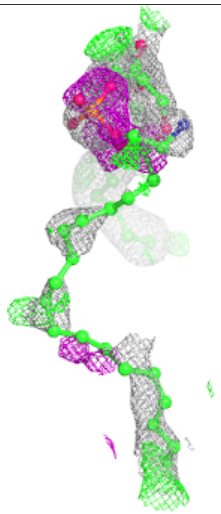
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

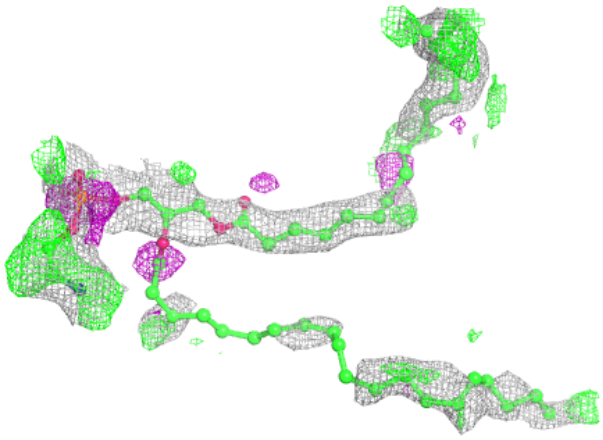


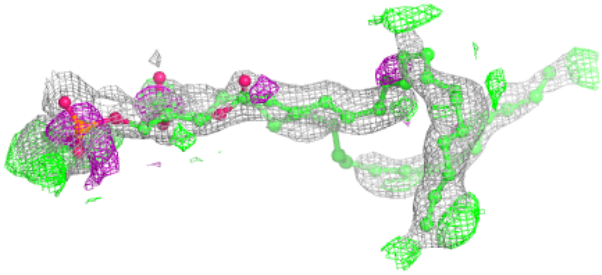




Electron density around PEK P 1265:

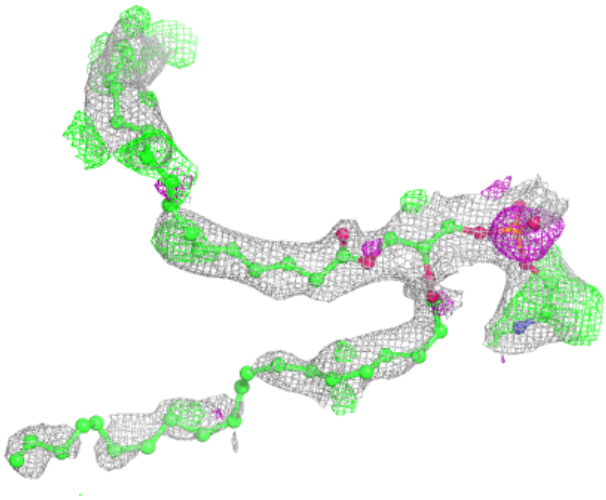
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

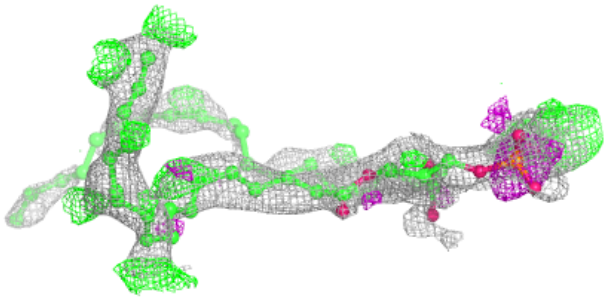


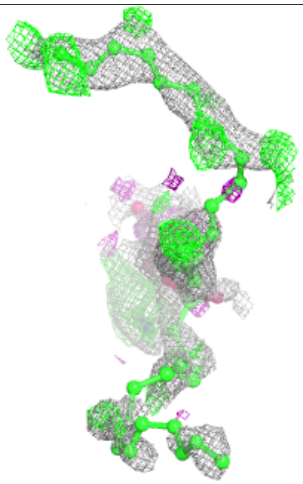


Electron density around PEK C 265:

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

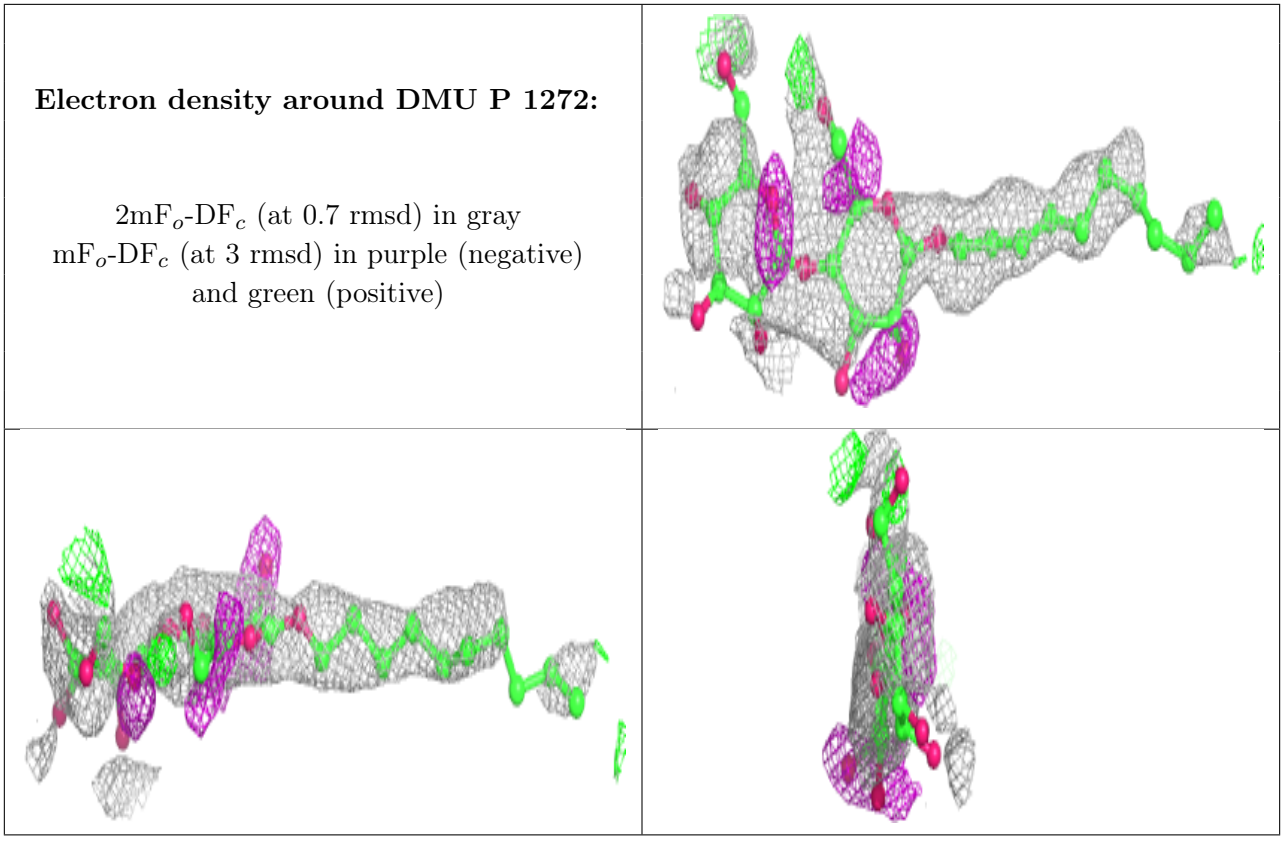






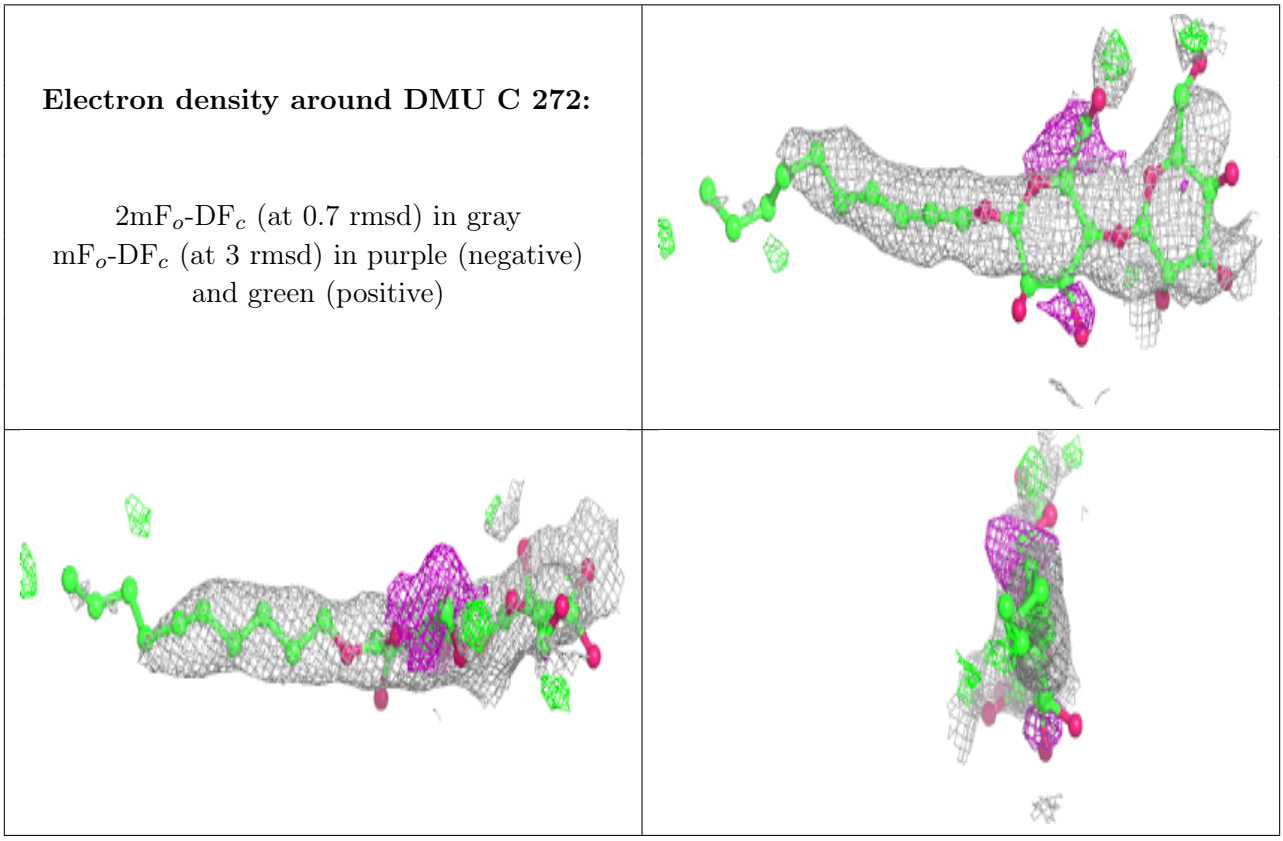
Electron density around DMU P 1272:

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



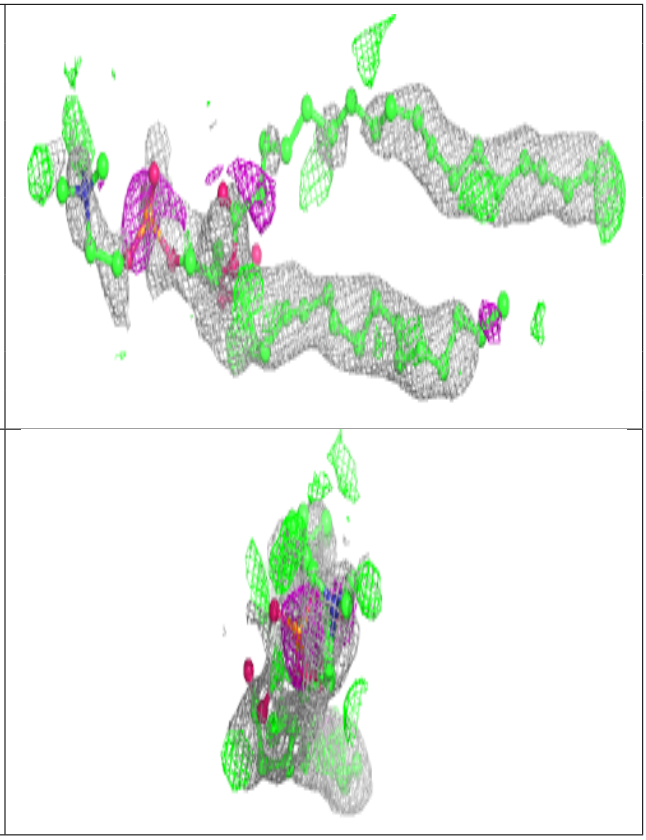
Electron density around DMU C 272:

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



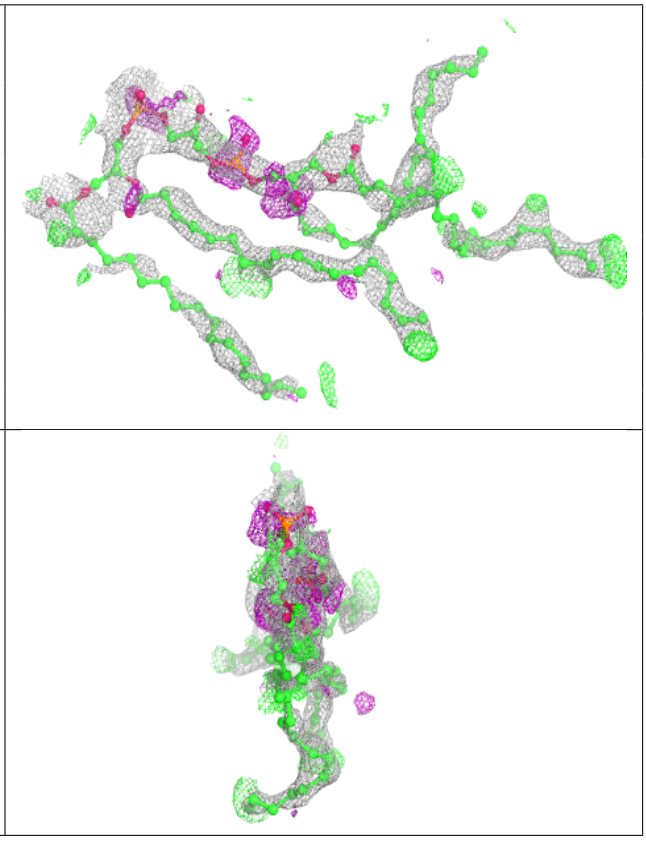
Electron density around PSC O 1230:

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



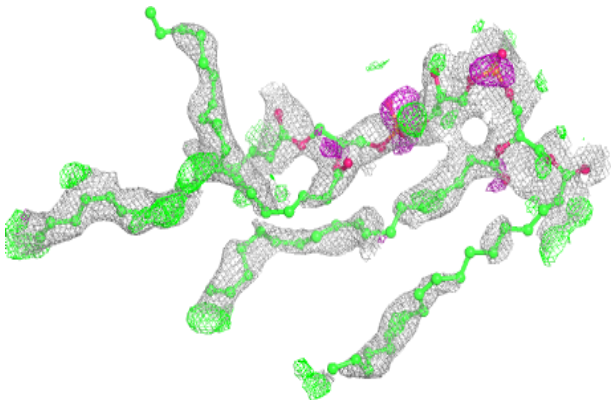
Electron density around CDL G 269:

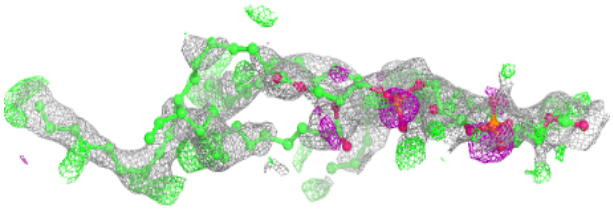
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

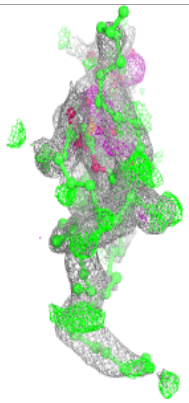


Electron density around CDL T 1269:

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

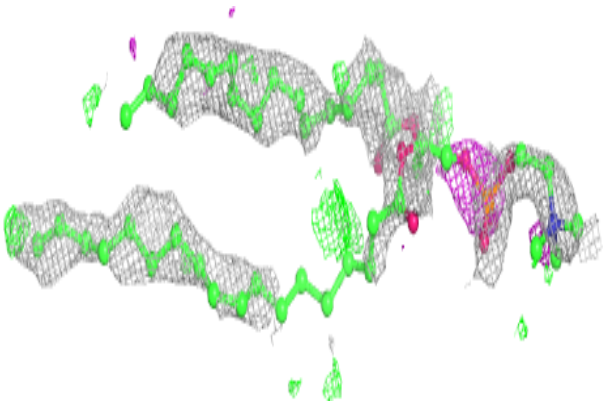


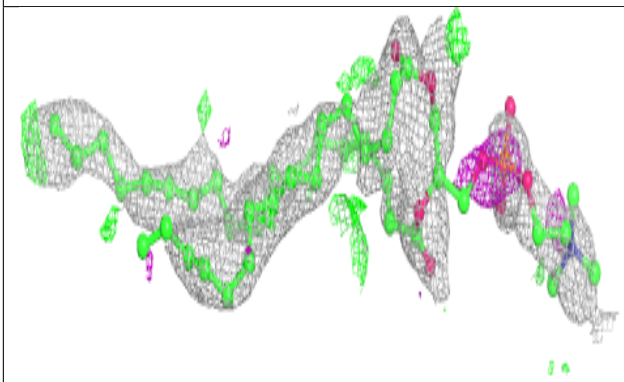


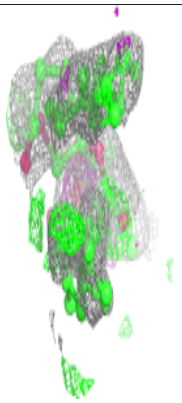


Electron density around PSC B 230:

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

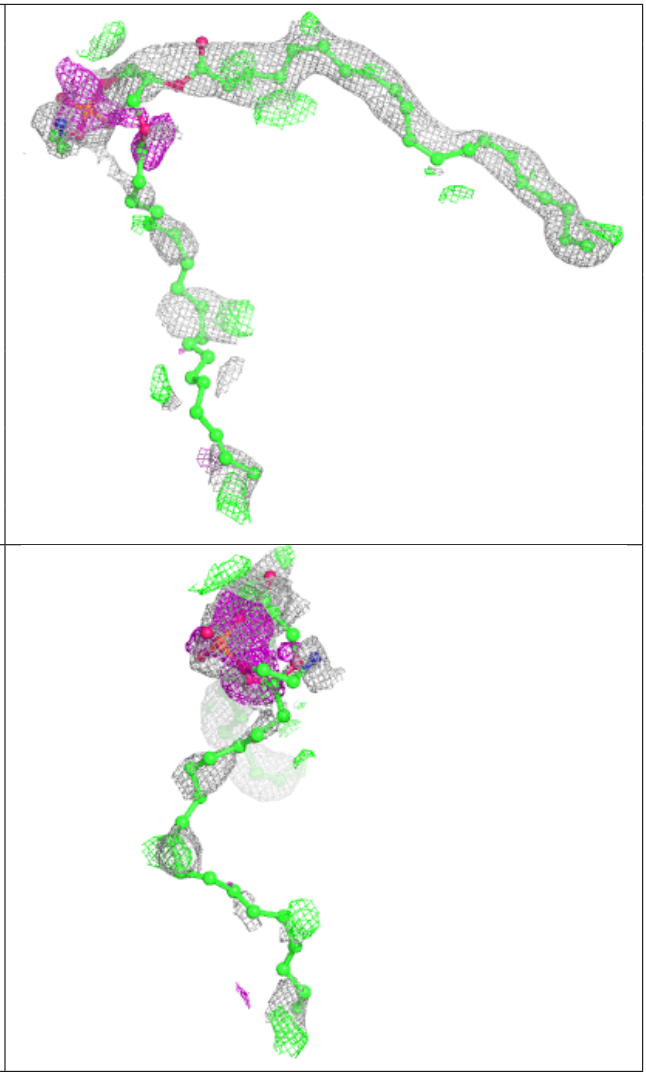






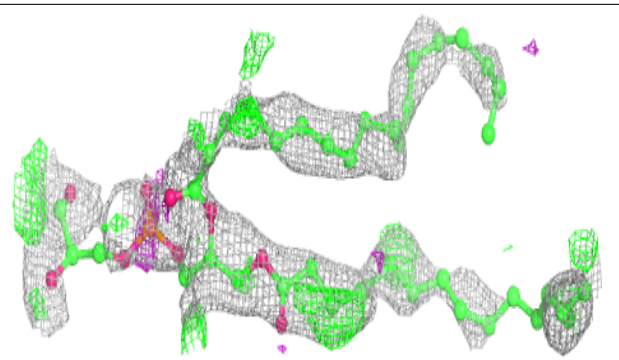
Electron density around PEK G 1263:

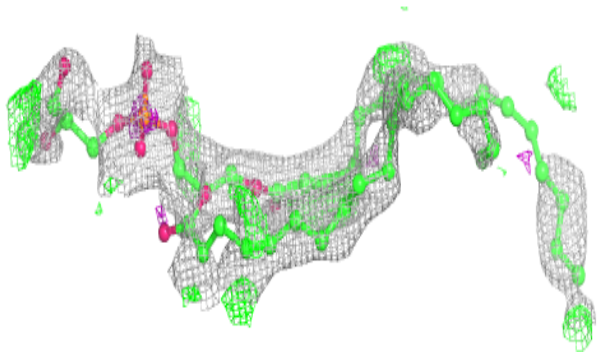
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

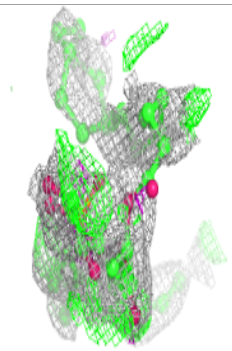


Electron density around PGV C 268:

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

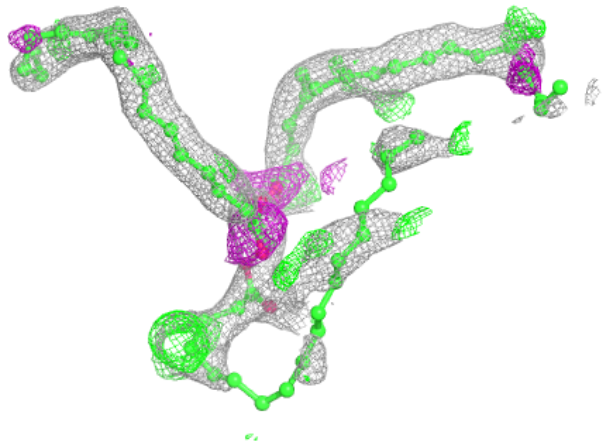


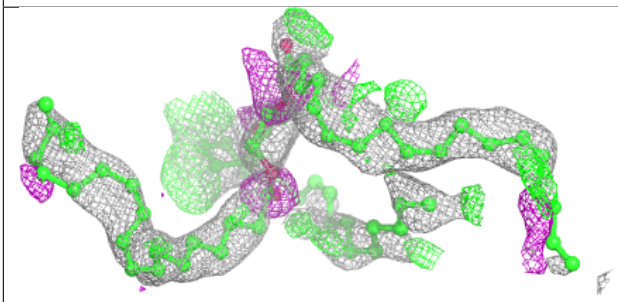


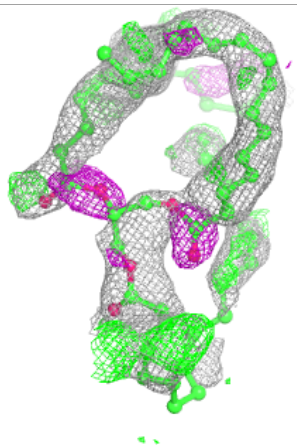


Electron density around TGL N 1522:

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

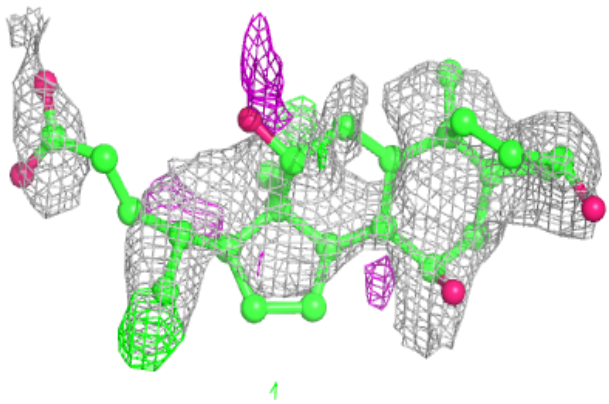


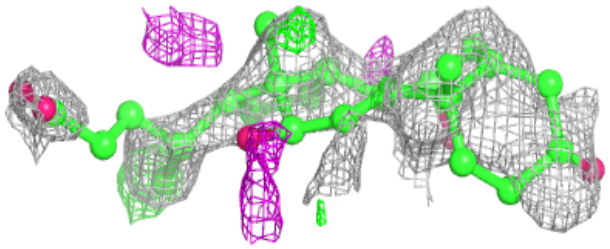


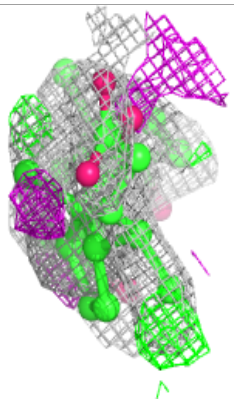


Electron density around CHD W 1060:

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

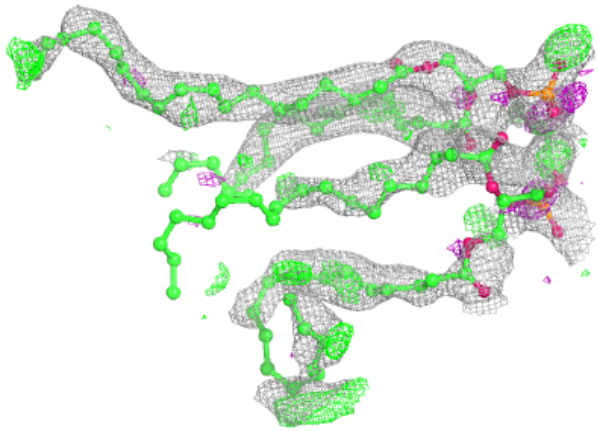


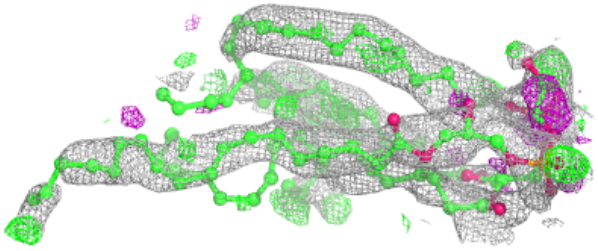


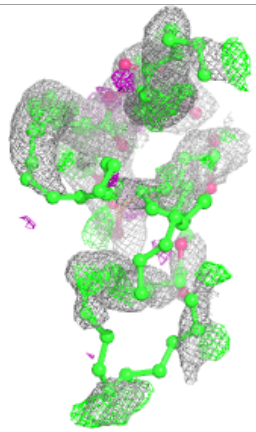


Electron density around CDL P 1270:

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

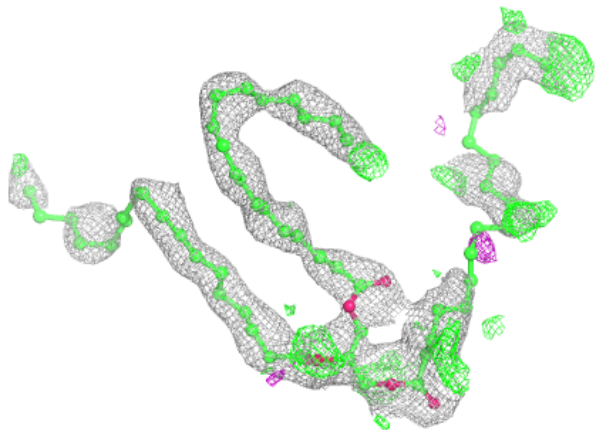


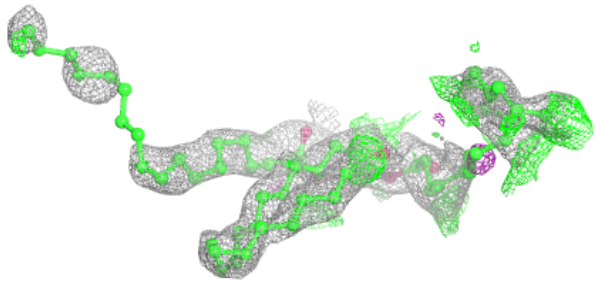


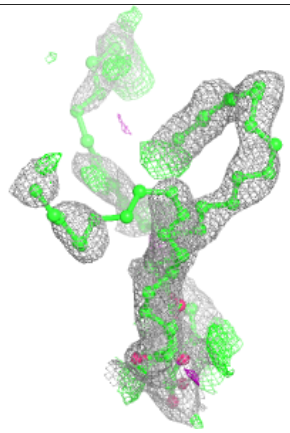


Electron density around TGL Q 1523:

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

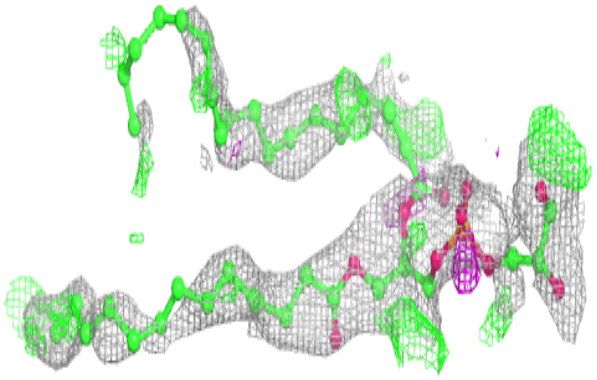


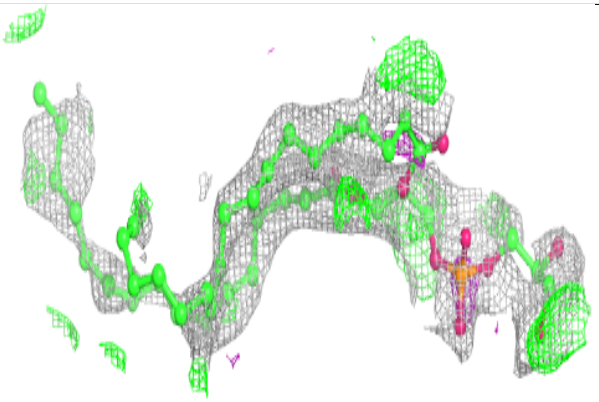


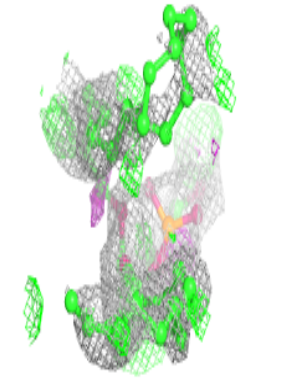


Electron density around PGV P 1268:

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

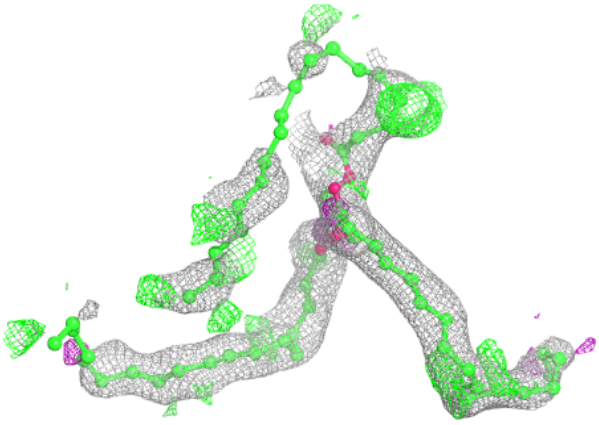


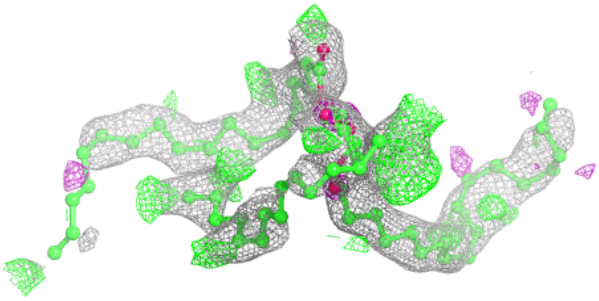


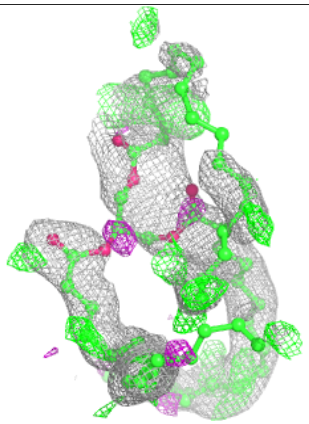


Electron density around TGL L 522:

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

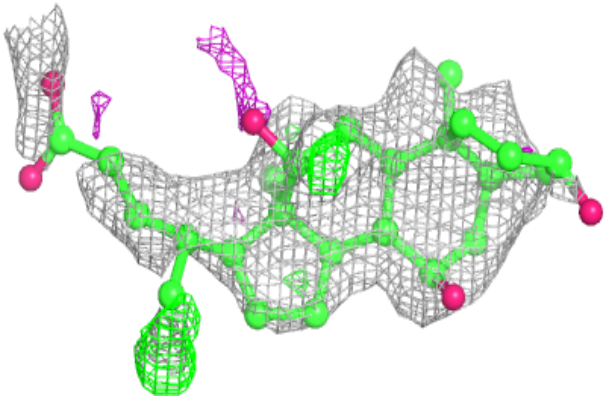


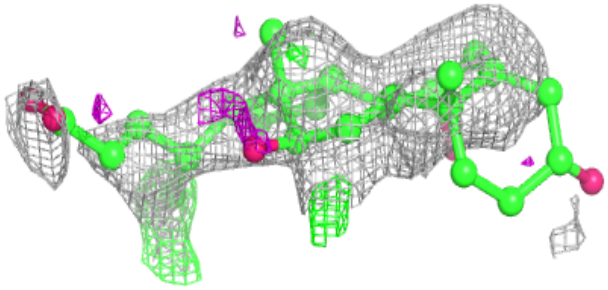


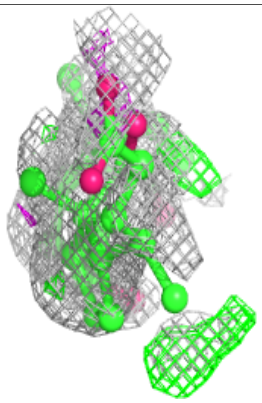


Electron density around CHD J 60:

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

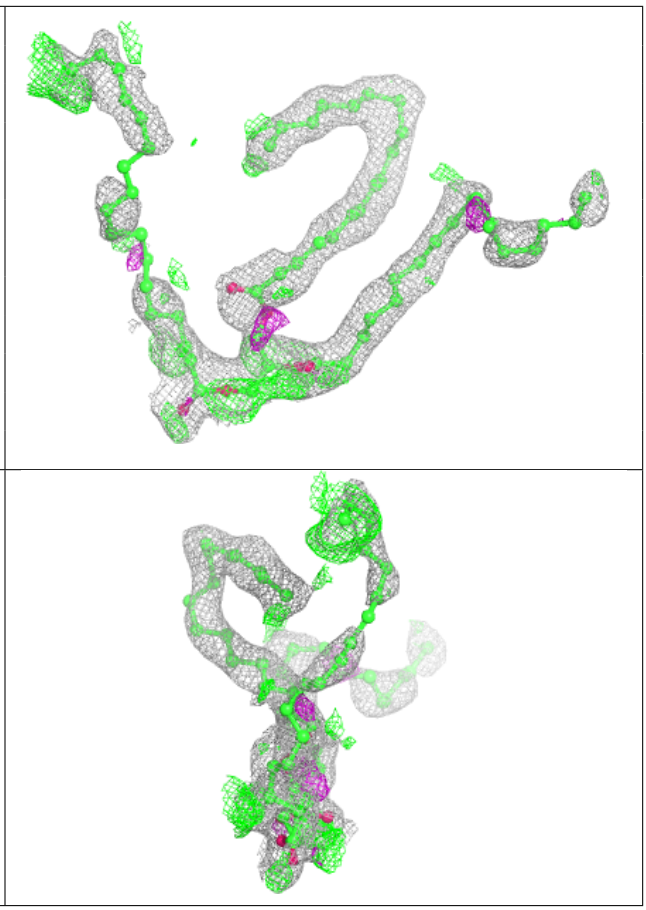


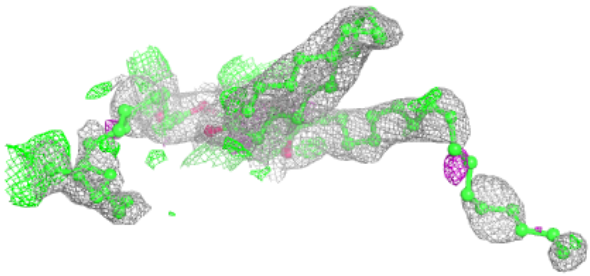




Electron density around TGL D 523:

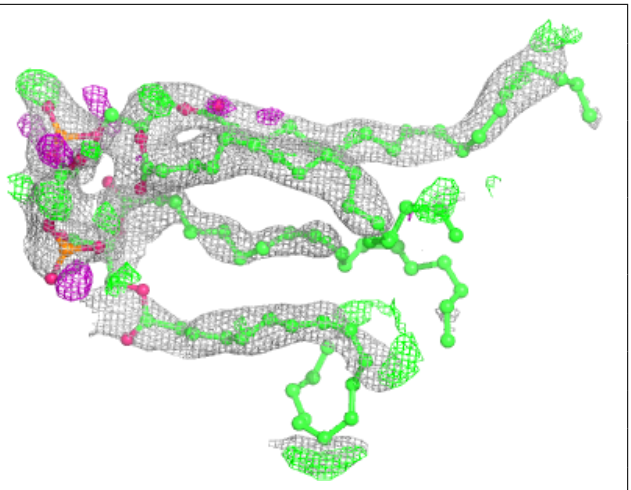
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

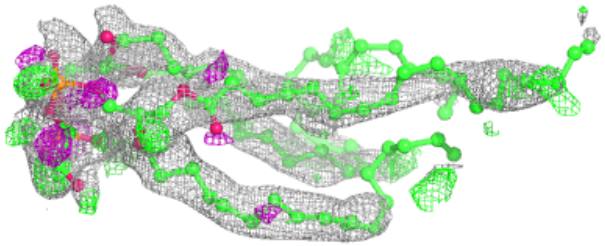


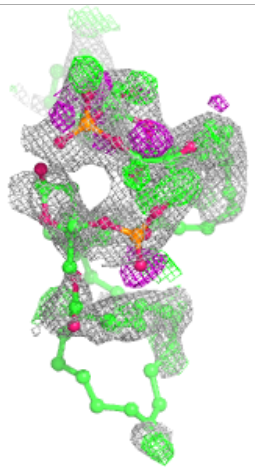


Electron density around CDL C 270:

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

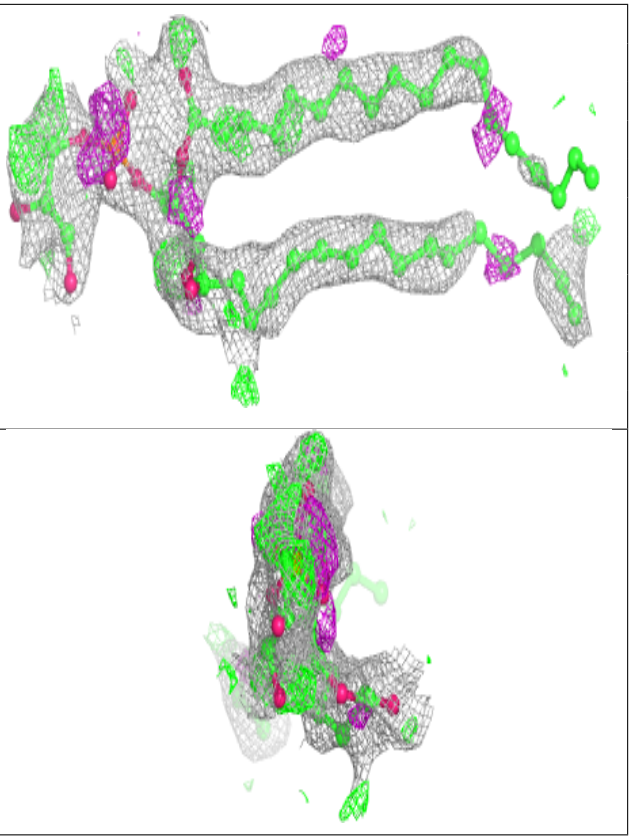






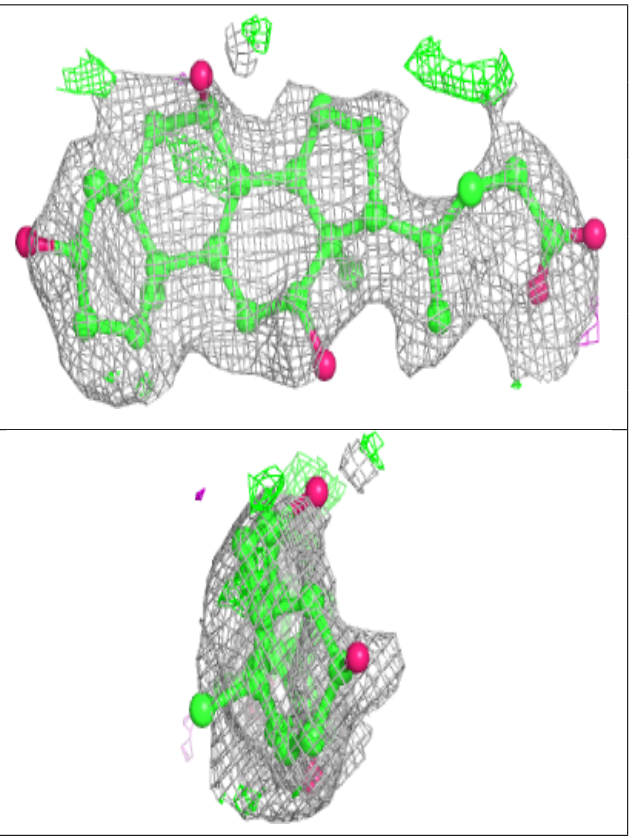
Electron density around PGV A 524:

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



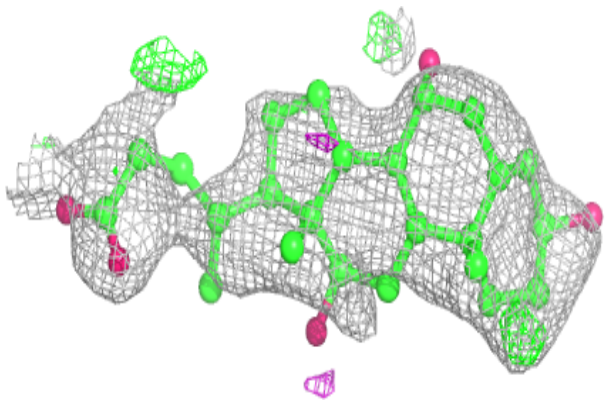
Electron density around CHD C 271:

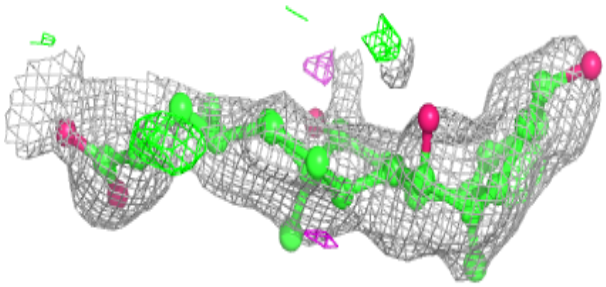
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

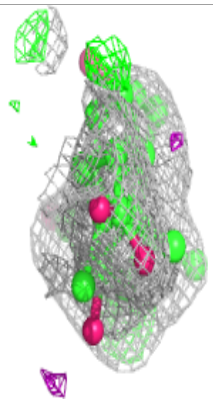


Electron density around CHD P 1271:

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

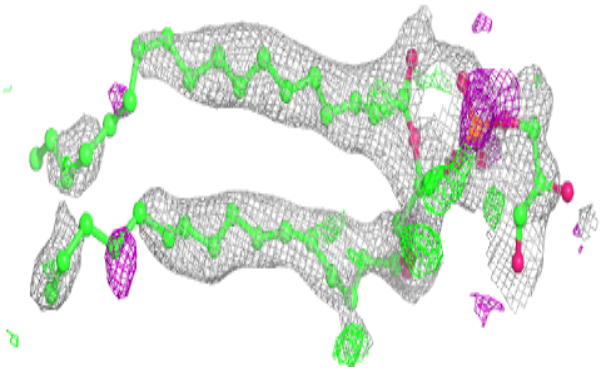


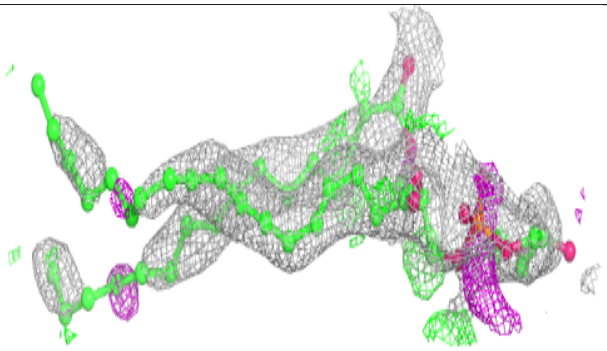


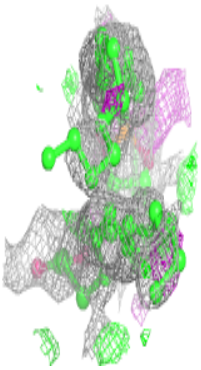


Electron density around PGV Z 1524:

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

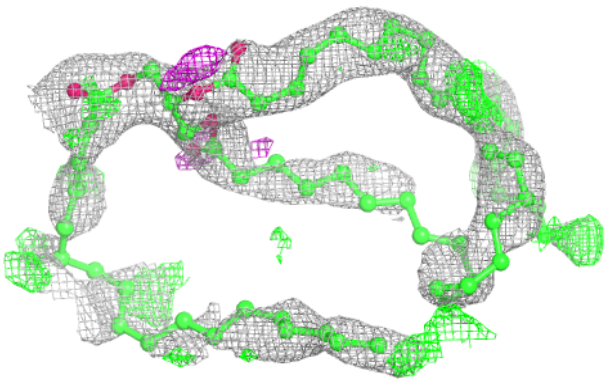


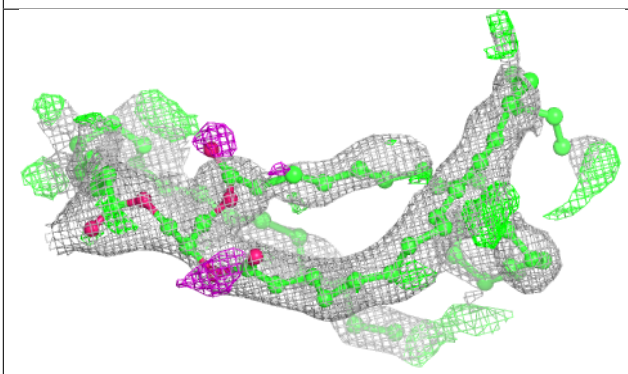


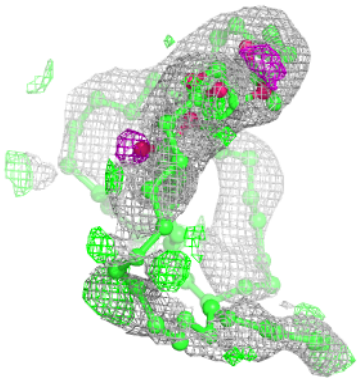


Electron density around TGL N 1521:

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

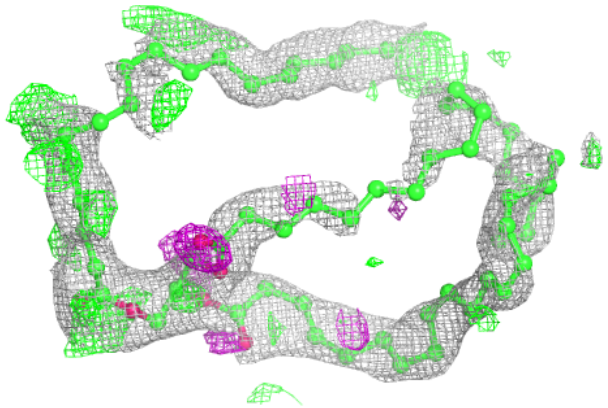


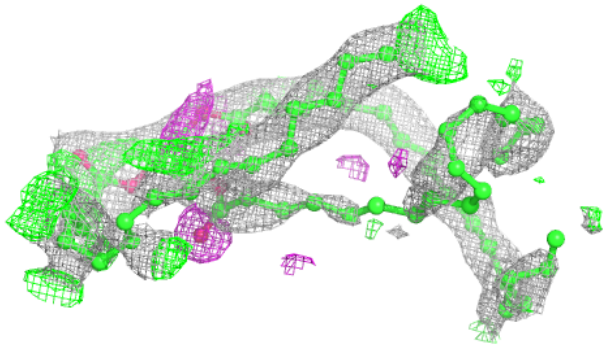


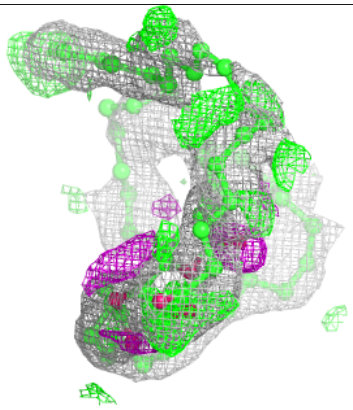


Electron density around TGL B 521:

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

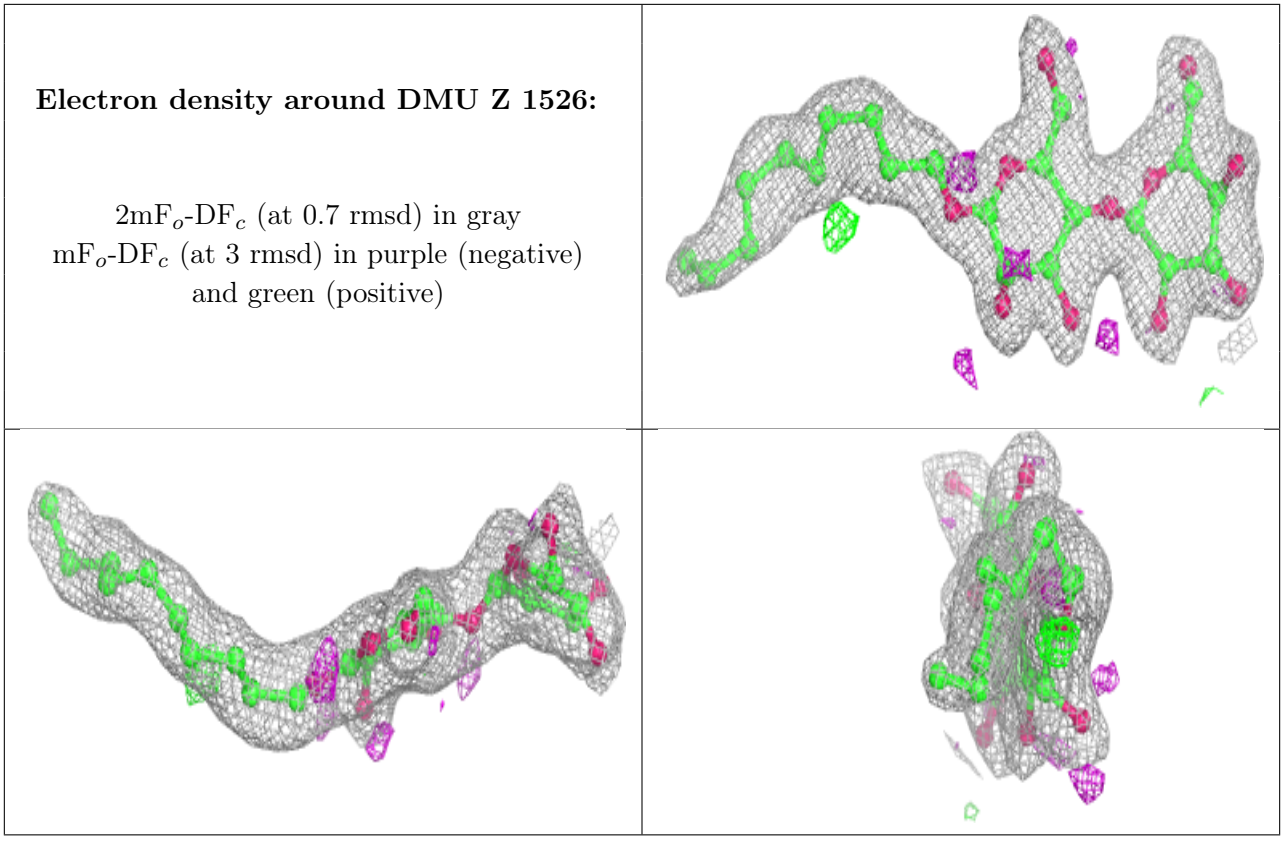






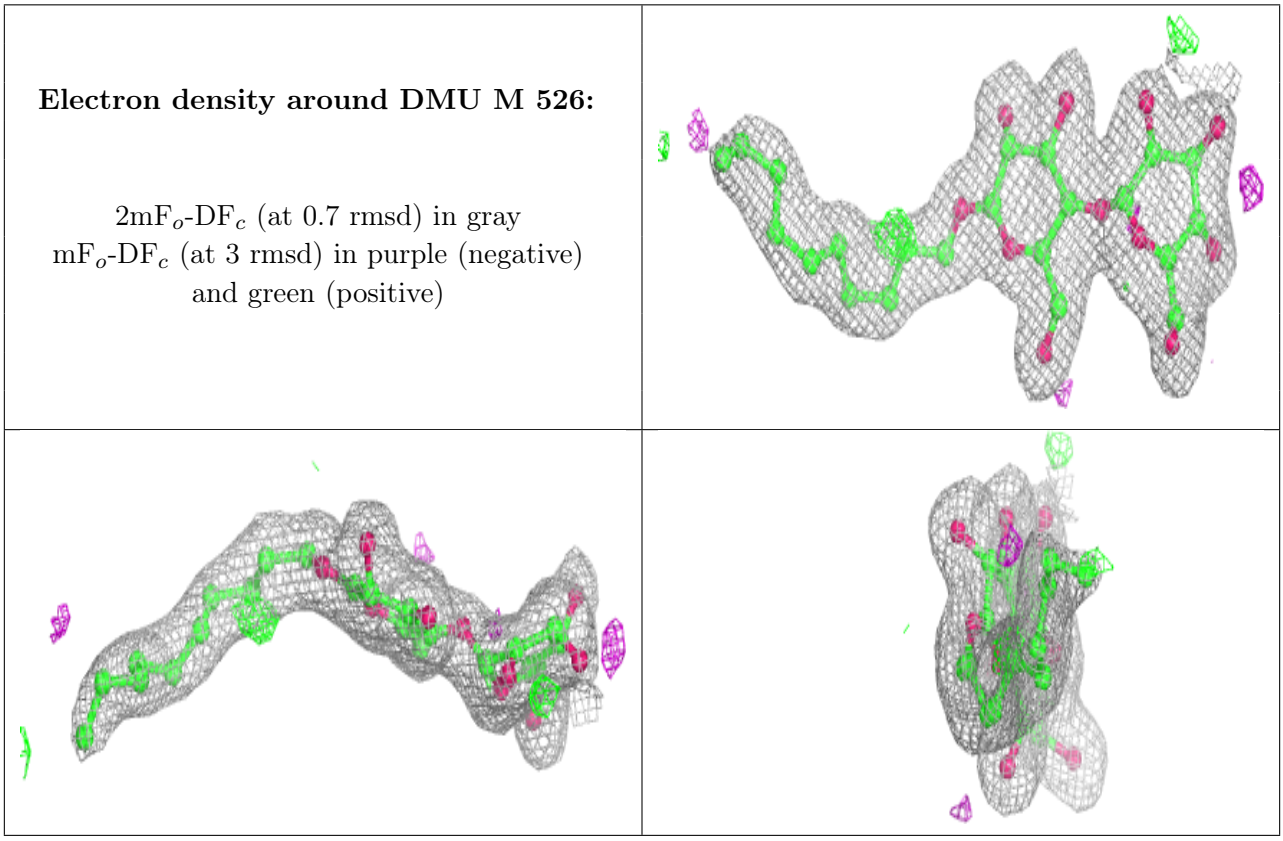
Electron density around DMU Z 1526:

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



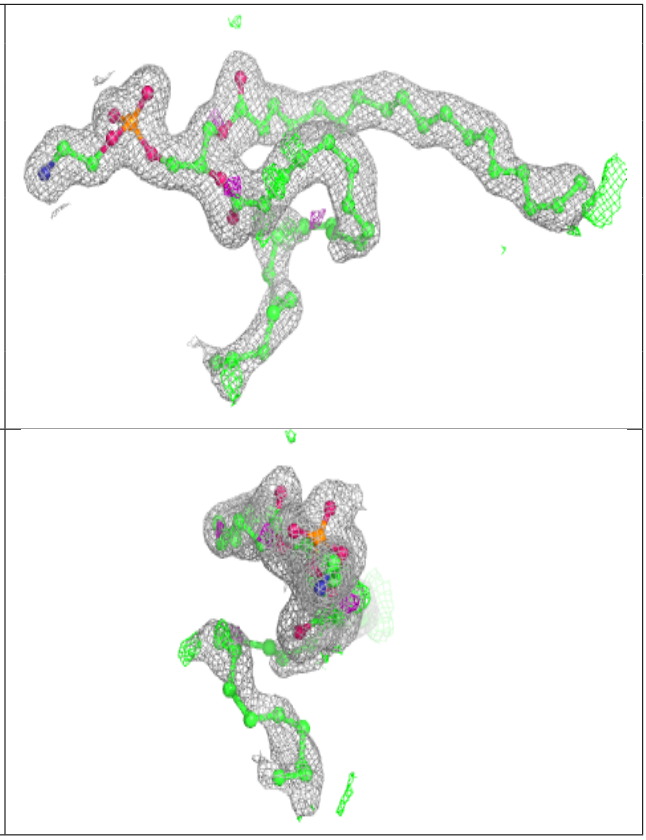
Electron density around DMU M 526:

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



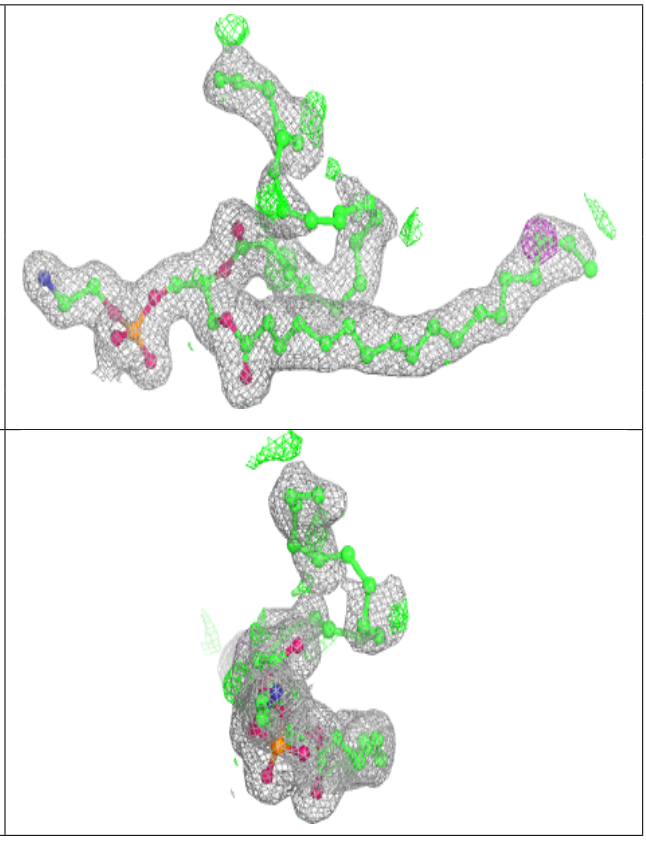
Electron density around PEK P 1264:

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



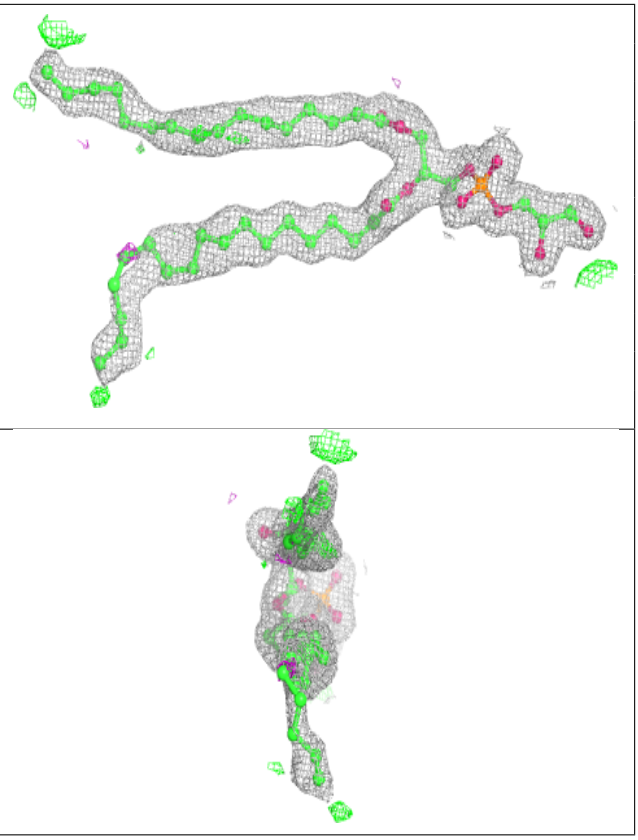
Electron density around PEK C 264:

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



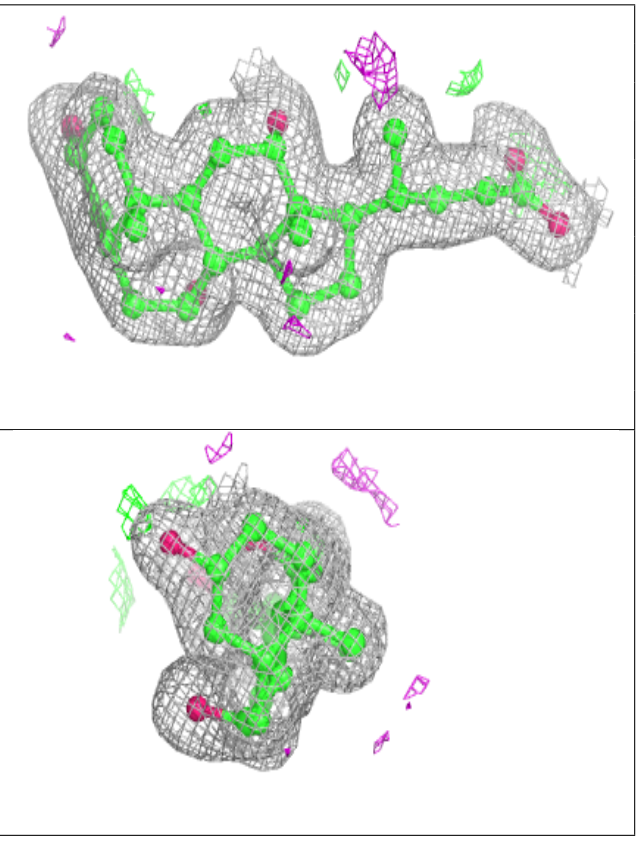
Electron density around PGV P 1267:

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



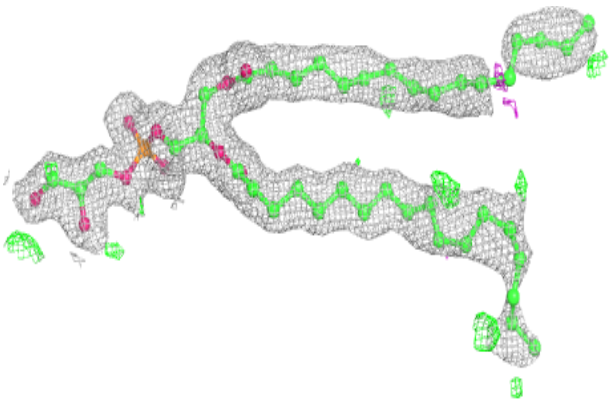
Electron density around CHD P 1525:

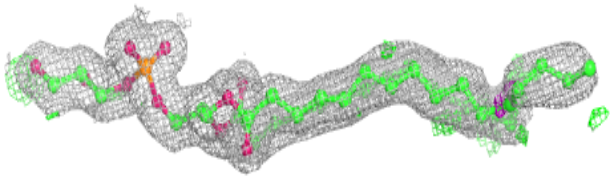
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

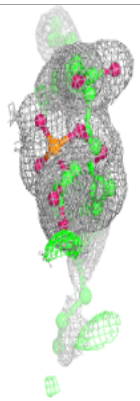


Electron density around PGV C 267:

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

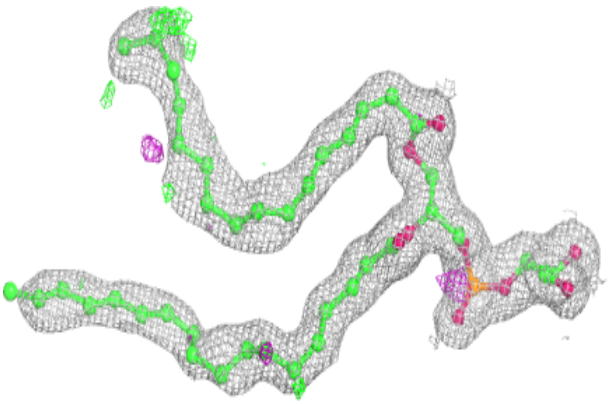


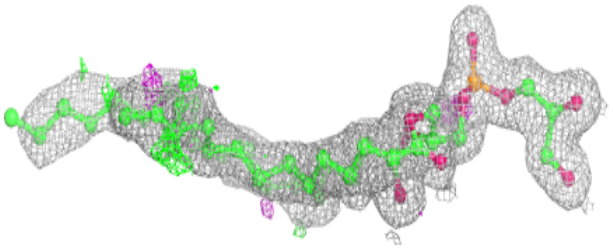


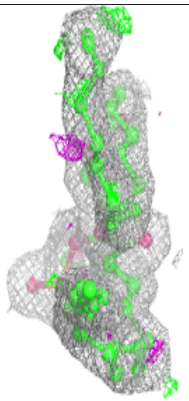


Electron density around PGV A 525:

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

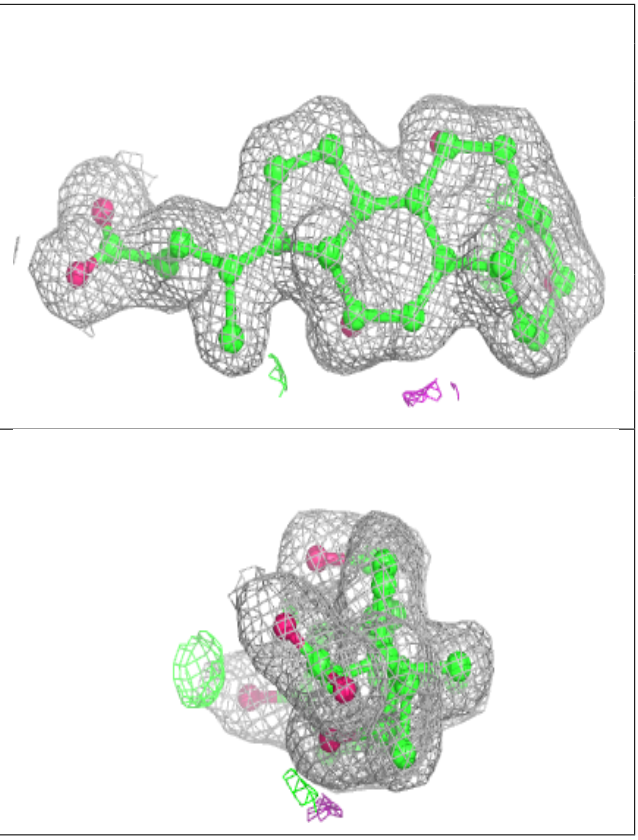






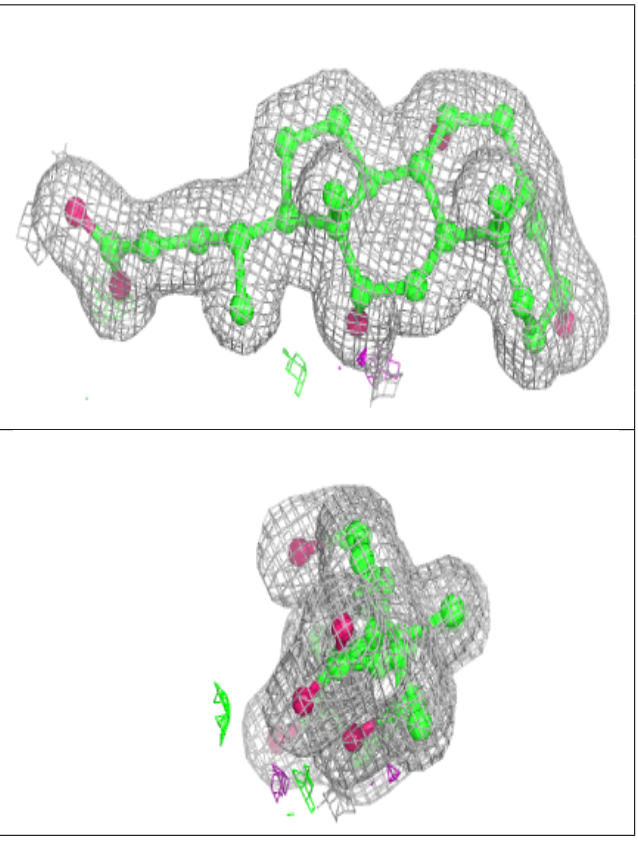
Electron density around CHD B 1086:

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



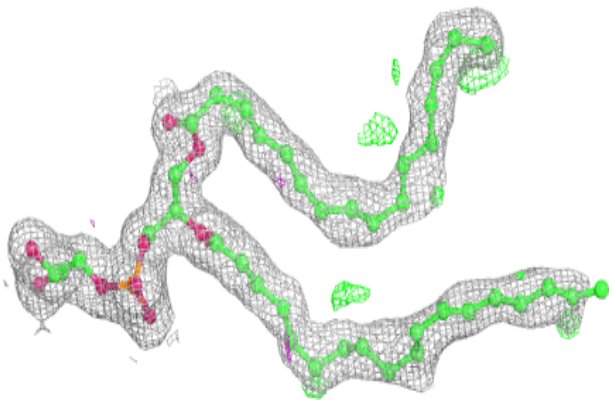
Electron density around CHD C 525:

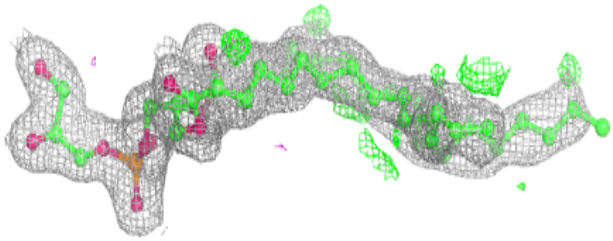
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

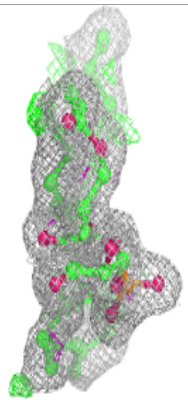


Electron density around PGV N 1266:

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

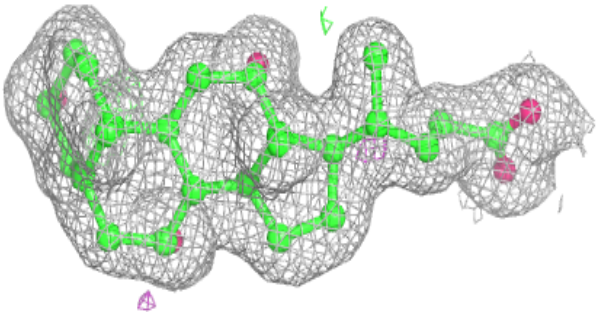


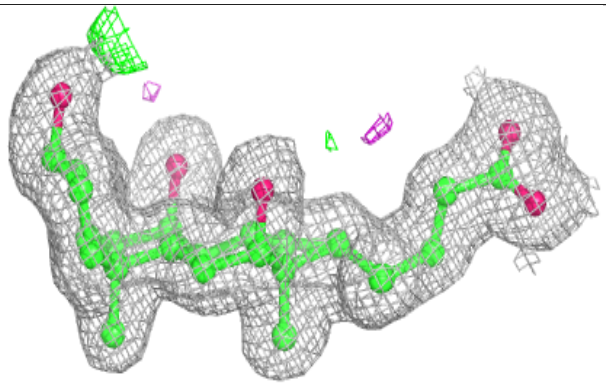


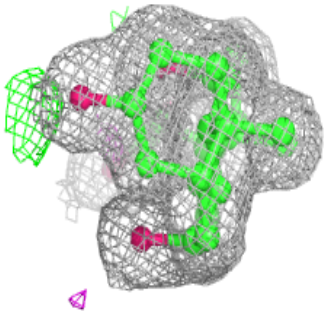


Electron density around CHD O 229:

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

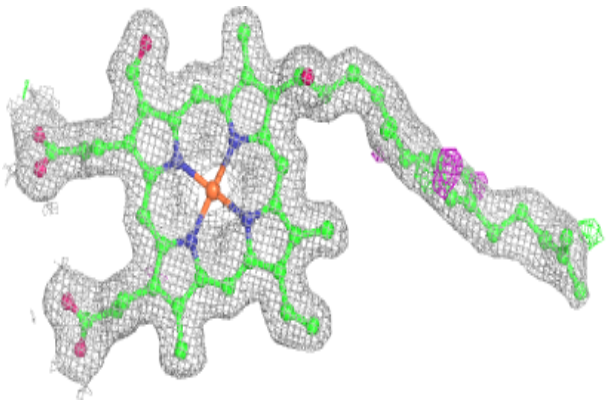


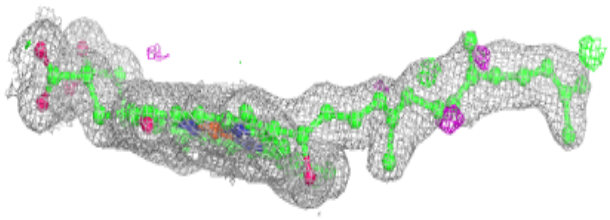


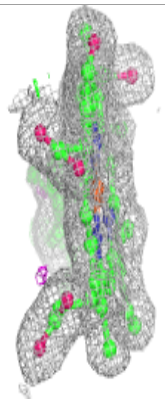


Electron density around HEA N 515:

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

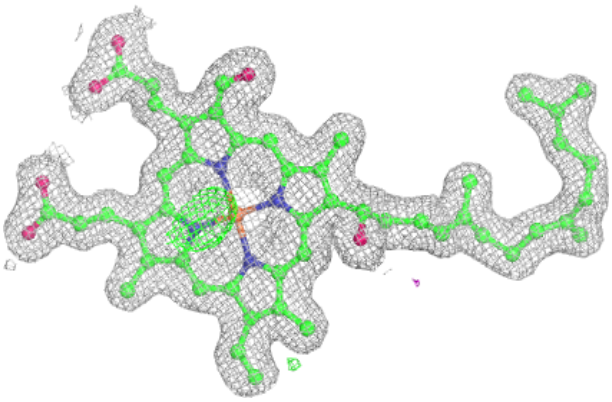


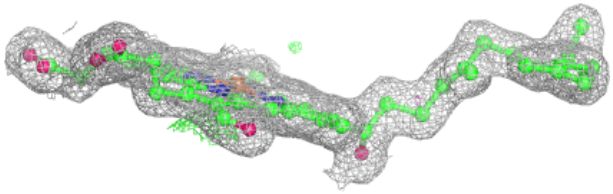


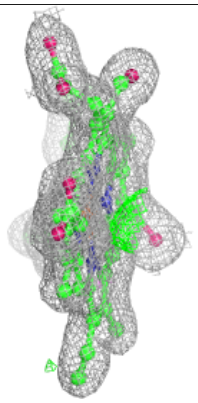


Electron density around HEA N 516:

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

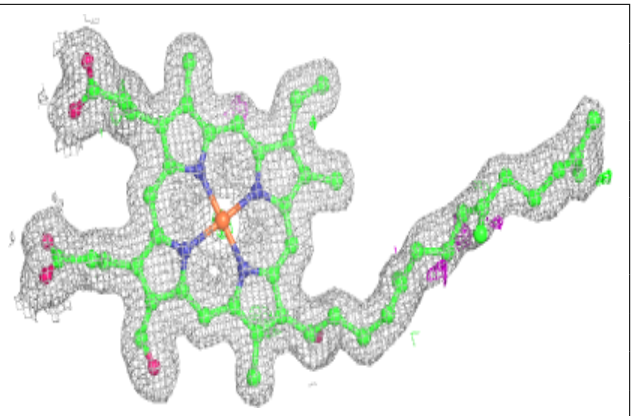


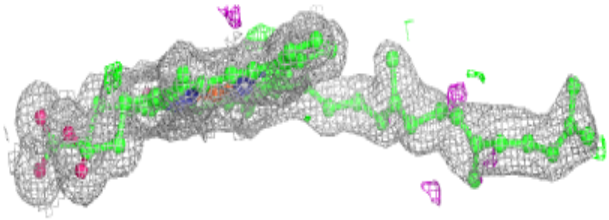


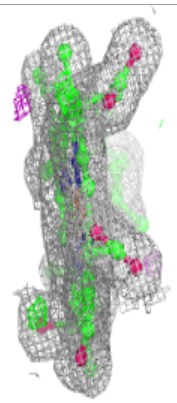


Electron density around HEA A 515:

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

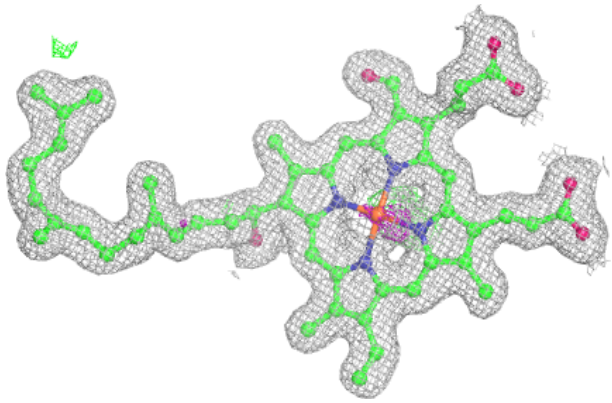


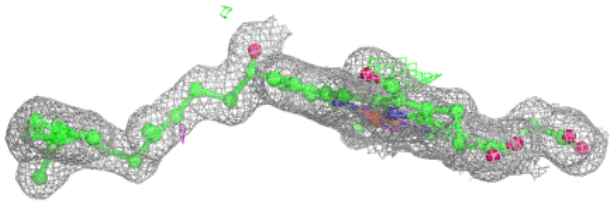


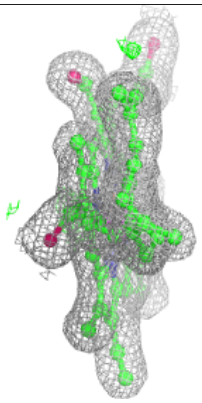


Electron density around HEA A 516:

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







6.5 Other polymers (i)

There are no such residues in this entry.