wwPDB X-ray Structure Validation Summary Report (i)

Nov 22, 2023 – 03:18 PM JST

PDB ID	:	7XMB
Title	:	Crystal structure of Bovine heart cytochrome c oxidase, the structure complexed with an allosteric inhibitor T113
Authors	:	Nishida, Y.; Shinzawa-Itoh, K.; Mizuno, N.; Kumasaka, T.; Yoshikawa, S.; Tsukihara, T.; Shintani, Y.; Takashima, S.
Deposited on	:	2022-04-25
Resolution	:	2.20 Å(reported)

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

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

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

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

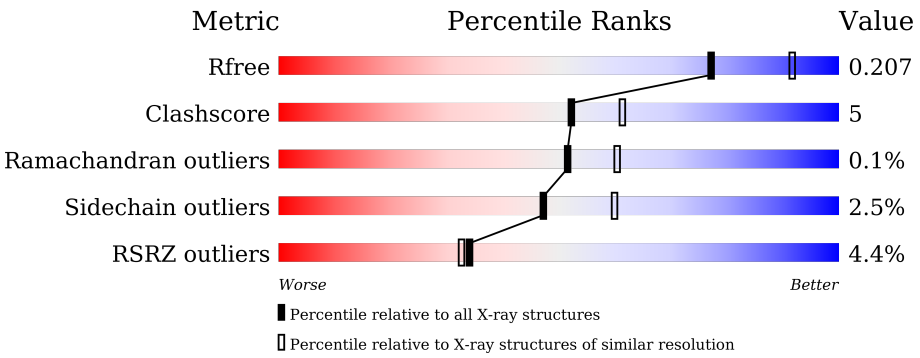
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.20 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	514	88% 12%
1	N	514	.% 87% 12% •
2	B	581	.% 32% 7% 61%
2	O	581	2% 32% 6% 61%
3	C	261	.% 89% 10% •

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Mol	Chain	Length	Quality of chain
3	P	261	%, 89%, 11%
4	D	147	%, 92%, 6%
4	Q	147	5%, 86%, 8%, 5%
5	E	109	3%, 92%, 5%
5	R	109	6%, 92%, 5%
6	F	98	5%, 89%, 6%, 5%
6	S	98	8%, 91%, 6%
7	G	84	20%, 76%, 19%
7	T	84	21%, 79%, 14%
8	H	85	11%, 82%, 11%, 7%
8	U	85	11%, 85%, 8%, 7%
9	I	73	10%, 97%
9	V	73	14%, 97%
10	J	59	8%, 92%, 5%
10	W	59	5%, 90%, 5%
11	K	56	5%, 88%, 9%
11	X	56	9%, 84%, 12%
12	L	47	2%, 89%, 9%
12	Y	47	81%, 11%
13	M	46	11%, 91%, 7%
13	Z	46	11%, 85%, 11%

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	J6X	A	608	-	-	-	X
22	CHD	C	304	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	PEK	C	309	-	-	-	X
7	TPO	G	11	-	-	-	X
7	TPO	T	11	-	-	-	X

2 Entry composition (i)

There are 29 unique types of molecules in this entry. The entry contains 33764 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	4194	2797	649	710	38	0	21	0
1	N	514	4208	2805	651	713	39	0	23	0

- Molecule 2 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	227	1861	1210	287	345	19	0	4	0
2	O	227	1878	1220	289	349	20	0	6	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	2166	1445	344	361	16	0	7	0
3	P	259	2157	1440	342	359	16	0	6	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	1213	791	198	220	4	0	2	0
4	Q	139	1178	769	192	213	4	0	2	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	105	863	550	148	163	2	0	1	0
5	R	105	863	550	148	163	2	0	1	0

- Molecule 6 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	93	729	452	130	141	6	0	2	0
6	S	96	740	460	131	143	6	0	1	0

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
7	G	82	678	436	129	111	1	1	0	1	0
7	T	82	678	436	129	111	1	1	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	79	662	417	121	119	5	0	0	0
8	U	79	662	417	121	119	5	0	0	0

- Molecule 9 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	I	72	592	385	106	97	4	0	0	0
9	V	72	592	385	106	97	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	J	57	451	291	76	81	3	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	W	57	460	296	77	84	3	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	K	51	402	260	68	72	2	0	0	0
			Total	C	N	O	S			
11	X	49	391	255	66	68	2	0	1	0

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

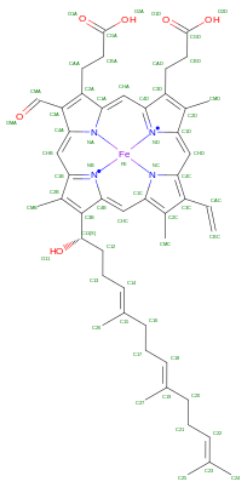
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	L	46	380	254	64	60	2	0	0	0
			Total	C	N	O	S			
12	Y	45	378	253	63	59	3	0	1	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
13	M	43	335	223	53	59	0	0	0
			Total	C	N	O			
13	Z	41	320	214	50	56	0	0	0

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

HEA



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
14	A	1	78	66	1	4	7	0	1
			Total	C	Fe	N	O		
14	A	1	60	49	1	4	6	0	0
			Total	C	Fe	N	O		
14	N	1	78	66	1	4	7	0	1
			Total	C	Fe	N	O		
14	N	1	60	49	1	4	6	0	0

- Molecule 15 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

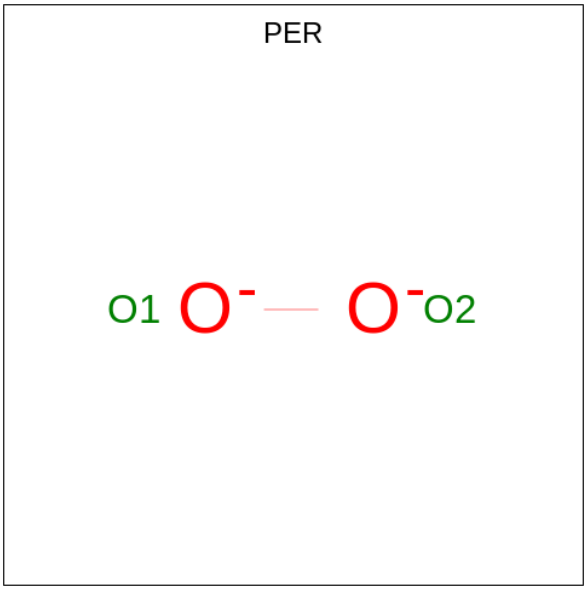
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 17 is SODIUM ION (three-letter code: NA) (formula: Na).

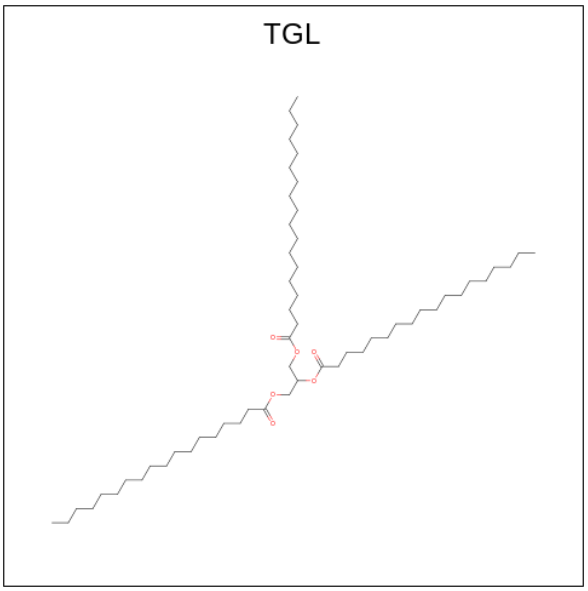
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
17	A	1	1	1	0	0
			Total	Na		
17	N	1	1	1	0	0

- Molecule 18 is PEROXIDE ION (three-letter code: PER) (formula: O_2).



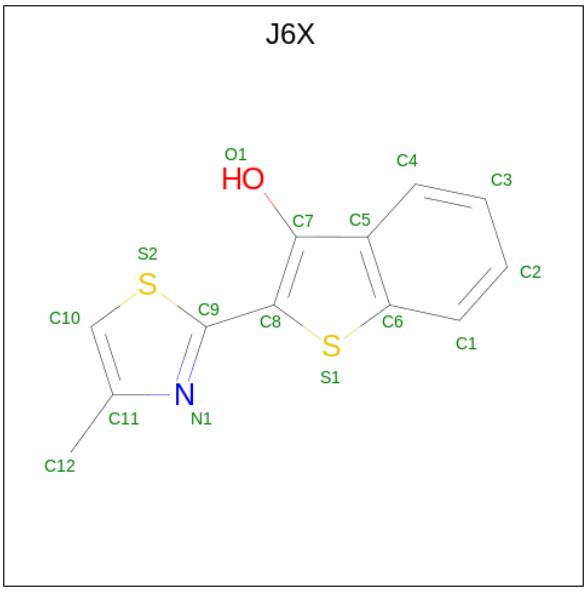
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
18	A	1	2	2	0	0
			Total	O		
18	N	1	2	2	0	0

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



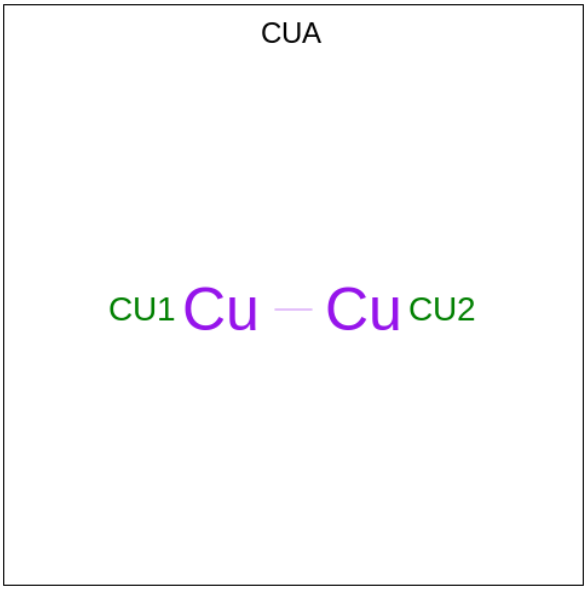
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
19	A	1	63	57	6	0	0
19	D	1	63	57	6	0	0
19	L	1	63	57	6	0	0
19	N	1	63	57	6	0	0
19	Q	1	63	57	6	0	0
19	Y	1	63	57	6	0	0

- Molecule 20 is 2-(4-methyl-1,3-thiazol-2-yl)-1-benzothiophen-3-ol (three-letter code: J6X) (formula: $C_{12}H_9NOS_2$) (labeled as "Ligand of Interest" by depositor).



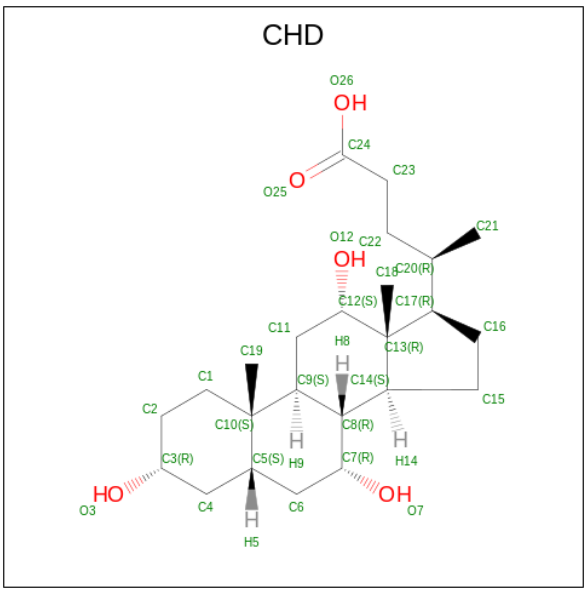
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
20	A	1	16	12	1	1	2	0	0
			Total	C	N	O	S		
20	N	1	16	12	1	1	2	0	0

- Molecule 21 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).



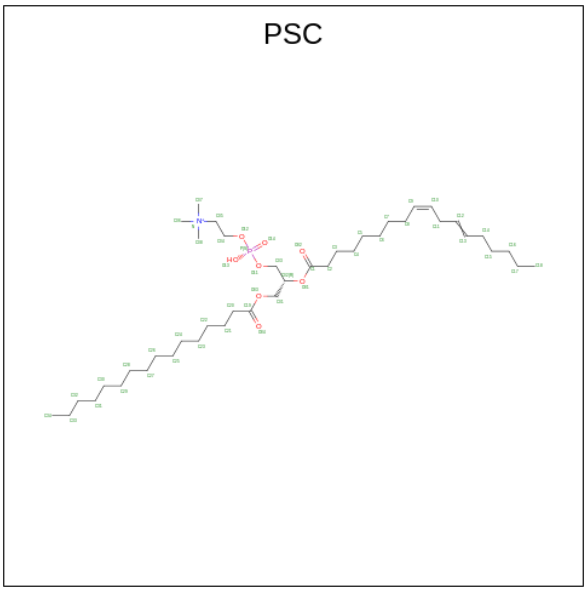
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cu		
21	B	1	2	2	0	0
			Total	Cu		
21	O	1	2	2	0	0

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



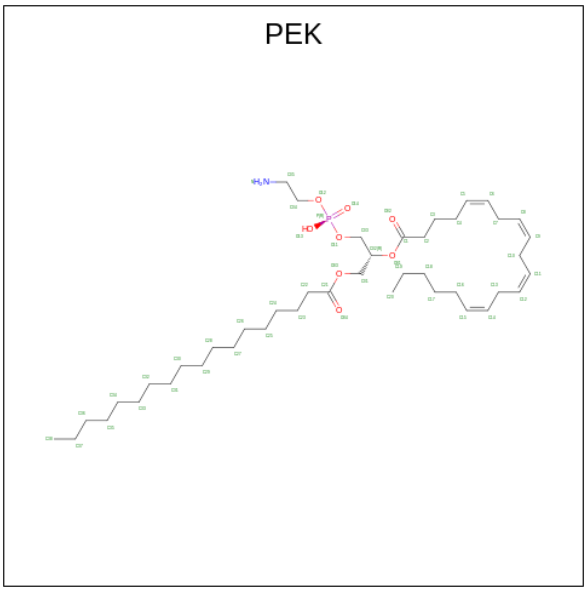
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
22	B	1	29	24	5	0	0
			Total	C	O		
22	C	1	29	24	5	0	0
			Total	C	O		
22	C	1	29	24	5	0	0
			Total	C	O		
22	N	1	29	24	5	0	0
			Total	C	O		
22	O	1	29	24	5	0	0
			Total	C	O		
22	P	1	29	24	5	0	0

- Molecule 23 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		
23	B	1	52	42	1	8	1	0	0
23	O	1	52	42	1	8	1	0	0

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



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

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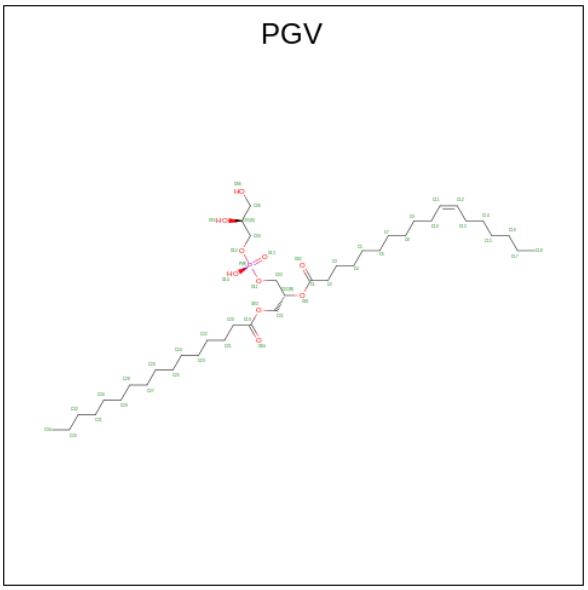
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
24	C	1	53	43	1	8	1	0	0
			Total	C	N	O	P		
24	C	1	53	43	1	8	1	0	0
			Total	C	N	O	P		
24	G	1	53	43	1	8	1	0	0
			Total	C	N	O	P		
24	P	1	53	43	1	8	1	0	0
			Total	C	N	O	P		
24	P	1	53	43	1	8	1	0	0

- Molecule 25 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		
25	C	1	51	40	10	1	0	0
			Total	C	O	P		
25	C	1	51	40	10	1	0	0
			Total	C	O	P		
25	C	1	51	40	10	1	0	0
			Total	C	O	P		
25	D	1	51	40	10	1	0	0
			Total	C	O	P		
25	N	1	51	40	10	1	0	0

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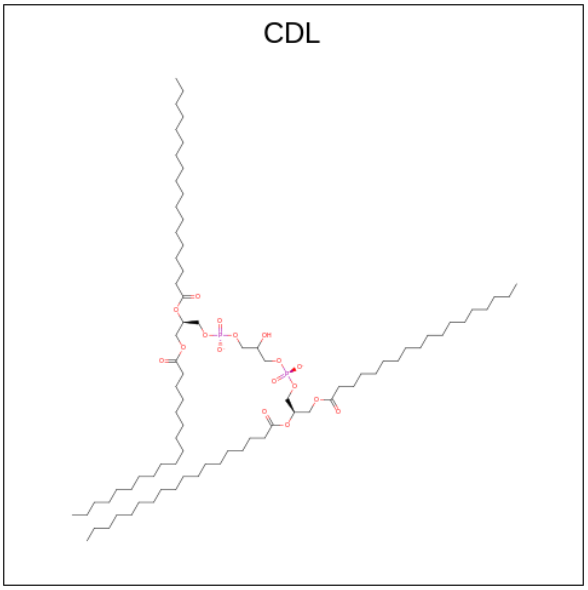
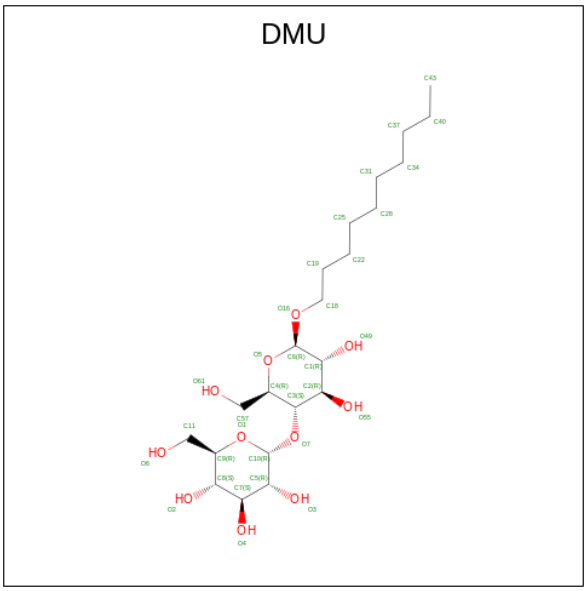
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
25	N	1	51	40	10	1	0	0
			Total	C	O	P		
25	P	1	51	40	10	1	0	0
			Total	C	O	P		
25	P	1	51	40	10	1	0	0

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



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

- Molecule 27 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).



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

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

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

- Molecule 29 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	A	274	Total	O	0	0
			274	274		
29	B	193	Total	O	0	1
			193	193		
29	C	152	Total	O	0	0
			152	152		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	D	179	Total O 179 179	0	0
29	E	126	Total O 126 126	0	0
29	F	119	Total O 119 119	0	0
29	G	60	Total O 60 60	0	0
29	H	74	Total O 74 74	0	0
29	I	48	Total O 48 48	0	0
29	J	38	Total O 38 38	0	0
29	K	38	Total O 38 38	0	0
29	L	39	Total O 39 39	0	0
29	M	35	Total O 35 35	0	0
29	N	288	Total O 288 288	0	0
29	O	148	Total O 148 148	0	1
29	P	143	Total O 143 143	0	0
29	Q	71	Total O 71 71	0	0
29	R	84	Total O 84 84	0	0
29	S	115	Total O 115 115	0	0
29	T	59	Total O 59 59	0	0
29	U	63	Total O 63 63	0	0
29	V	28	Total O 28 28	0	0
29	W	35	Total O 35 35	0	0
29	X	25	Total O 25 25	0	0

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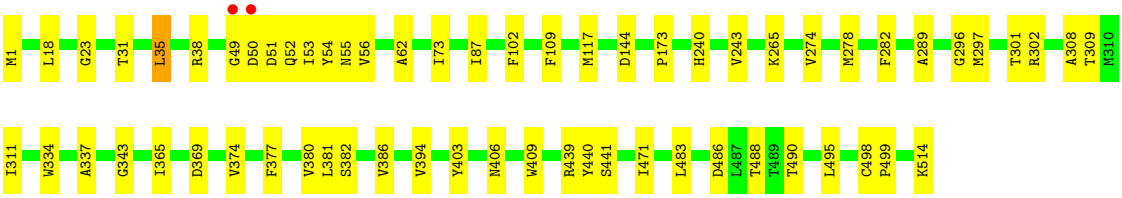
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	Y	39	Total O 39 39	0	0
29	Z	22	Total O 22 22	0	0

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.

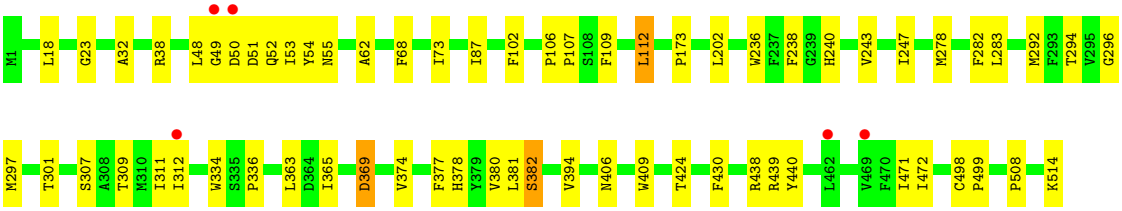
• Molecule 1: Cytochrome c oxidase subunit 1

Chain A:



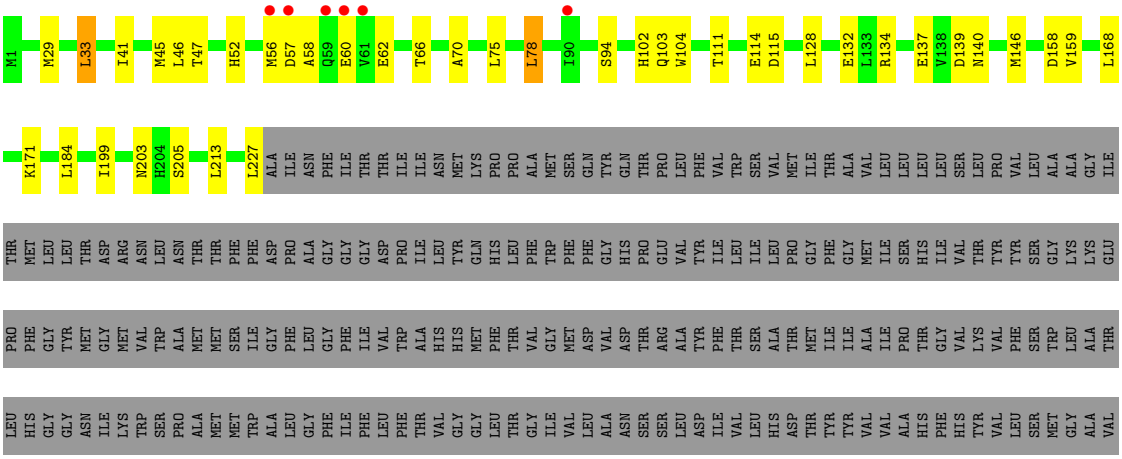
• Molecule 1: Cytochrome c oxidase subunit 1

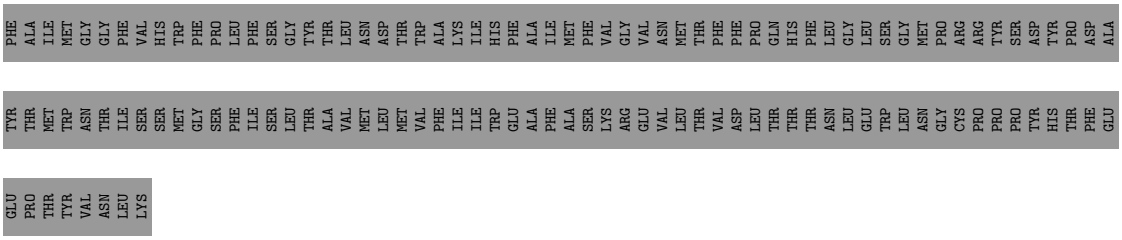
Chain N:



• Molecule 2: CYTOCHROME C OXIDASE

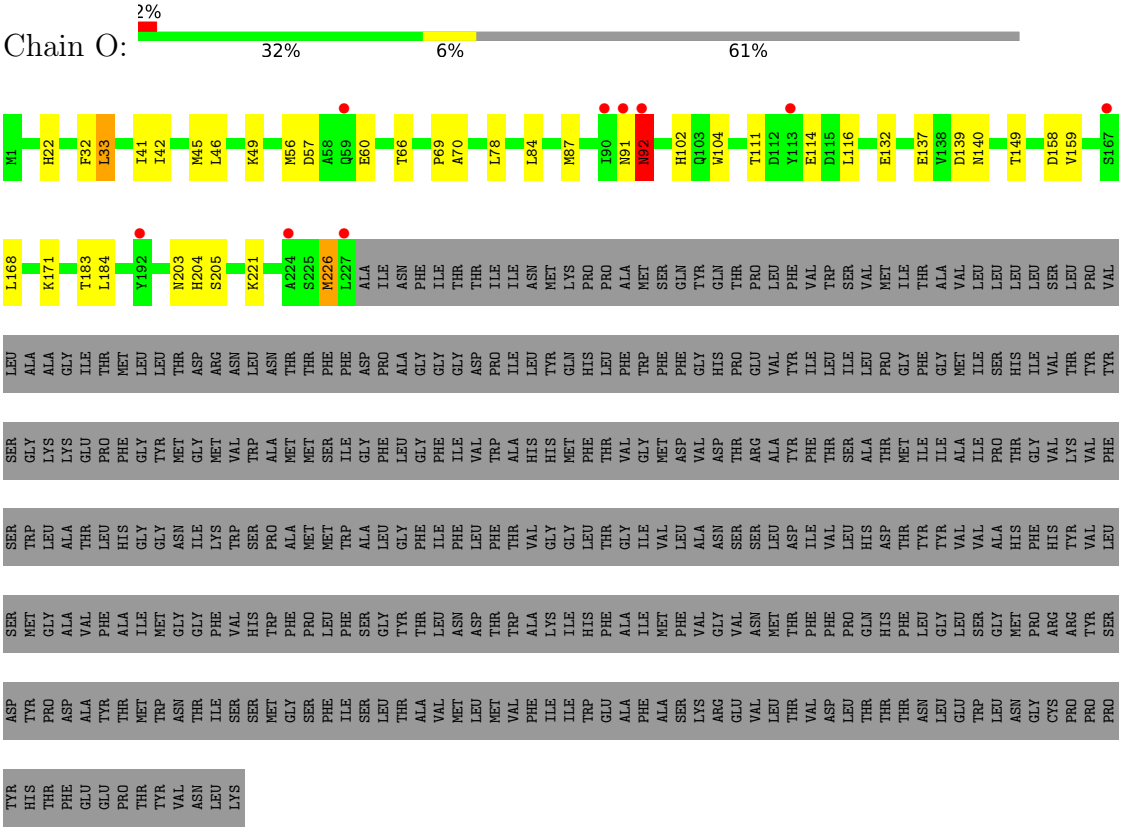
Chain B:





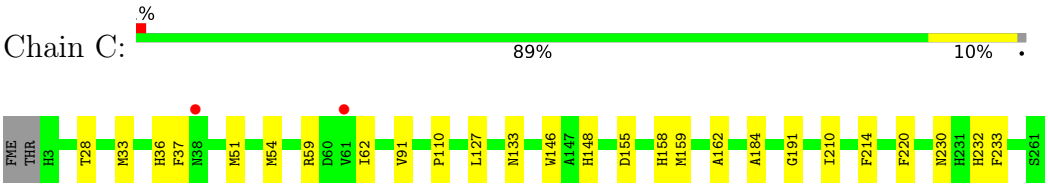
- Molecule 2: CYTOCHROME C OXIDASE

Chain O:



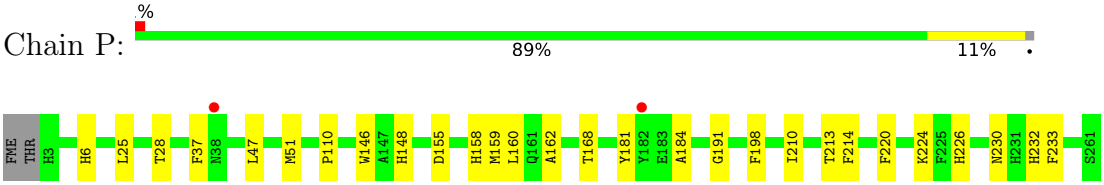
- Molecule 3: Cytochrome c oxidase subunit 3

Chain C:



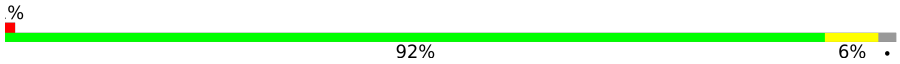
- Molecule 3: Cytochrome c oxidase subunit 3

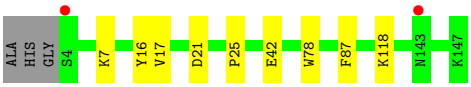
Chain P:



- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

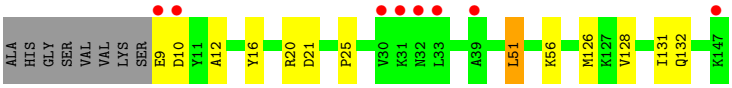
Chain D:





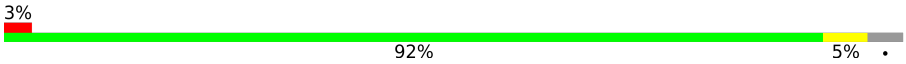
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

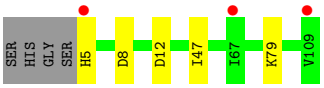
Chain Q:



• Molecule 5: Cytochrome c oxidase subunit 5A

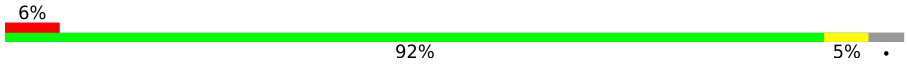
Chain E:

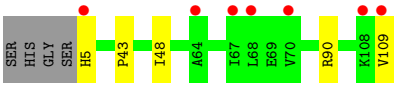




• Molecule 5: Cytochrome c oxidase subunit 5A

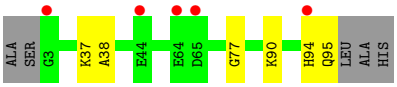
Chain R:





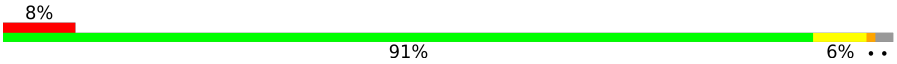
• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

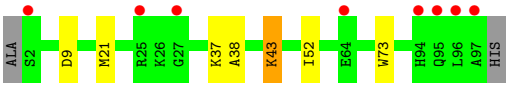
Chain F:



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

Chain S:



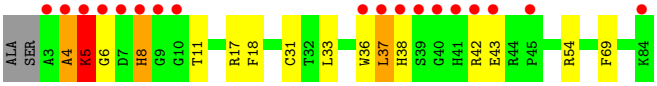


• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain G:

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

Chain T:

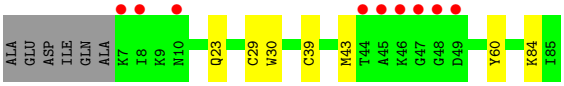


• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain H:

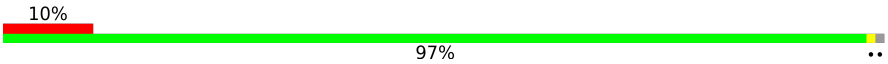
• Molecule 8: Cytochrome c oxidase subunit 6B1

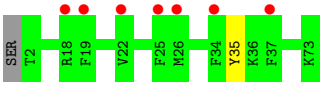
Chain U:



• Molecule 9: Cytochrome c oxidase subunit 6C

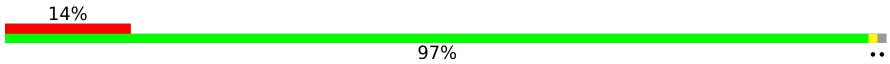
Chain I:

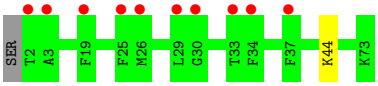




• Molecule 9: Cytochrome c oxidase subunit 6C

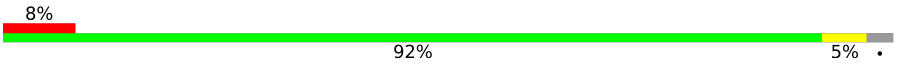
Chain V:

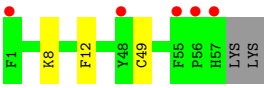




• Molecule 10: Cytochrome c oxidase subunit 7A1

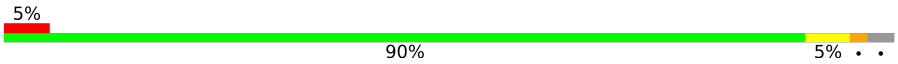
Chain J:

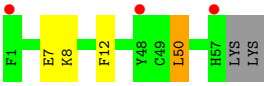




• Molecule 10: Cytochrome c oxidase subunit 7A1

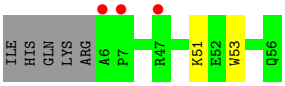
Chain W:





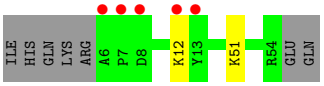
• Molecule 11: Cytochrome c oxidase subunit 7B

Chain K:



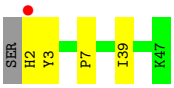
• Molecule 11: Cytochrome c oxidase subunit 7B

Chain X:



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

Chain L:

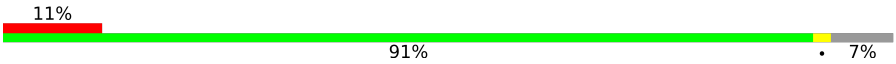


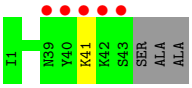
• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain Y:

• Molecule 13: Cytochrome c oxidase subunit 8B

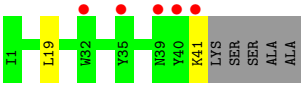
Chain M:





• Molecule 13: Cytochrome c oxidase subunit 8B

Chain Z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	182.10Å 204.34Å 177.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.98 – 2.20 29.98 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.98-2.20) 99.9 (29.98-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.50 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5, PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.178 , 0.204 0.181 , 0.207	Depositor DCC
R_{free} test set	16655 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	32.5	Xtriage
Anisotropy	0.787	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 68.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	33764	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% 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: MG, CDL, PER, DMU, CUA, PEK, CHD, TPO, HEA, FME, PGV, J6X, ZN, TGL, CU, NA, PSC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.26	0/4324	0.43	0/5905
1	N	0.26	0/4338	0.44	0/5923
2	B	0.25	0/1899	0.47	0/2587
2	O	0.25	0/1916	0.46	0/2609
3	C	0.25	0/2253	0.40	0/3077
3	P	0.25	0/2244	0.40	0/3065
4	D	0.24	0/1248	0.41	0/1684
4	Q	0.24	0/1213	0.42	0/1637
5	E	0.24	0/882	0.47	0/1196
5	R	0.26	0/882	0.48	0/1196
6	F	0.25	0/745	0.50	0/1011
6	S	0.24	0/756	0.50	0/1026
7	G	0.30	0/695	0.52	0/945
7	T	0.29	0/695	0.58	0/945
8	H	0.25	0/682	0.51	0/921
8	U	0.26	0/682	0.52	0/921
9	I	0.28	0/605	0.51	0/802
9	V	0.27	0/605	0.50	0/802
10	J	0.25	0/462	0.43	0/625
10	W	0.26	0/471	0.44	0/637
11	K	0.27	0/416	0.48	0/570
11	X	0.24	0/405	0.46	0/556
12	L	0.26	0/393	0.43	0/526
12	Y	0.27	0/391	0.43	0/525
13	M	0.24	0/345	0.40	0/470
13	Z	0.24	0/330	0.39	0/451
All	All	0.26	0/29877	0.45	0/40612

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4194	0	4168	52	0
1	N	4208	0	4180	59	0
2	B	1861	0	1860	27	0
2	O	1878	0	1873	31	0
3	C	2166	0	2075	27	0
3	P	2157	0	2068	25	0
4	D	1213	0	1199	15	0
4	Q	1178	0	1158	9	0
5	E	863	0	857	3	0
5	R	863	0	857	2	0
6	F	729	0	705	3	0
6	S	740	0	721	6	0
7	G	678	0	639	8	0
7	T	678	0	639	11	0
8	H	662	0	623	4	0
8	U	662	0	623	3	0
9	I	592	0	604	1	0
9	V	592	0	604	1	0
10	J	451	0	446	5	0
10	W	460	0	451	4	0
11	K	402	0	380	1	0
11	X	391	0	374	0	0
12	L	380	0	380	3	0
12	Y	378	0	375	6	0
13	M	335	0	352	1	0
13	Z	320	0	334	1	0
14	A	138	0	112	6	0
14	N	138	0	112	12	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	N	1	0	0	0	0
18	A	2	0	0	0	0
18	N	2	0	0	0	0
19	A	63	0	110	0	0
19	D	63	0	110	5	0
19	L	63	0	110	1	0
19	N	63	0	110	4	0
19	Q	63	0	110	2	0
19	Y	63	0	110	7	0
20	A	16	0	0	2	0
20	N	16	0	0	1	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	29	0	39	0	0
22	C	58	0	78	1	0
22	N	29	0	39	1	0
22	O	29	0	39	1	0
22	P	29	0	39	1	0
23	B	52	0	80	5	0
23	O	52	0	80	10	0
24	B	53	0	77	4	0
24	C	106	0	154	10	0
24	G	53	0	77	2	0
24	P	106	0	154	6	0
25	C	153	0	228	8	0
25	D	51	0	76	12	0
25	N	102	0	152	4	0
25	P	102	0	152	8	0
26	C	100	0	156	13	0
26	G	100	0	156	11	0
26	P	100	0	156	12	0
26	T	100	0	156	17	0
27	C	33	0	42	7	0
27	M	33	0	42	0	0
27	W	33	0	42	2	0
27	Z	33	0	42	0	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	A	274	0	0	8	0
29	B	193	0	0	3	0
29	C	152	0	0	4	0
29	D	179	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	E	126	0	0	1	0
29	F	119	0	0	1	0
29	G	60	0	0	1	0
29	H	74	0	0	0	0
29	I	48	0	0	0	0
29	J	38	0	0	0	0
29	K	38	0	0	0	0
29	L	39	0	0	0	0
29	M	35	0	0	0	0
29	N	288	0	0	12	0
29	O	148	0	0	3	0
29	P	143	0	0	2	0
29	Q	71	0	0	0	0
29	R	84	0	0	1	0
29	S	115	0	0	1	0
29	T	59	0	0	1	0
29	U	63	0	0	0	0
29	V	28	0	0	0	0
29	W	35	0	0	0	0
29	X	25	0	0	0	0
29	Y	39	0	0	1	0
29	Z	22	0	0	0	0
All	All	33764	0	31685	344	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 5.

The worst 5 of 344 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)
26:P:304:CDL:H1O1	10:W:12:PHE:HE2	1.13	0.94
4:D:87[A]:PHE:CD2	25:D:201:PGV:H141	2.04	0.93
19:D:202:TGL:HC32	19:D:202:TGL:HG12	1.60	0.81
1:A:50[D]:ASP:OD1	29:A:701:HOH:O	2.01	0.79
1:N:439:ARG:O	29:N:701:HOH:O	2.02	0.77

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	533/514 (104%)	518 (97%)	15 (3%)	0	100	100
1	N	535/514 (104%)	520 (97%)	15 (3%)	0	100	100
2	B	229/581 (39%)	225 (98%)	4 (2%)	0	100	100
2	O	231/581 (40%)	225 (97%)	5 (2%)	1 (0%)	34	37
3	C	264/261 (101%)	260 (98%)	4 (2%)	0	100	100
3	P	263/261 (101%)	259 (98%)	4 (2%)	0	100	100
4	D	144/147 (98%)	141 (98%)	3 (2%)	0	100	100
4	Q	139/147 (95%)	136 (98%)	3 (2%)	0	100	100
5	E	104/109 (95%)	104 (100%)	0	0	100	100
5	R	104/109 (95%)	104 (100%)	0	0	100	100
6	F	93/98 (95%)	92 (99%)	1 (1%)	0	100	100
6	S	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
7	G	80/84 (95%)	75 (94%)	4 (5%)	1 (1%)	12	9
7	T	80/84 (95%)	71 (89%)	5 (6%)	4 (5%)	2	0
8	H	77/85 (91%)	74 (96%)	3 (4%)	0	100	100
8	U	77/85 (91%)	75 (97%)	2 (3%)	0	100	100
9	I	70/73 (96%)	69 (99%)	1 (1%)	0	100	100
9	V	70/73 (96%)	69 (99%)	1 (1%)	0	100	100
10	J	55/59 (93%)	55 (100%)	0	0	100	100
10	W	56/59 (95%)	56 (100%)	0	0	100	100
11	K	49/56 (88%)	48 (98%)	1 (2%)	0	100	100
11	X	48/56 (86%)	47 (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%)	40 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	Z	39/46 (85%)	39 (100%)	0	0	100	100
All	All	3564/4320 (82%)	3481 (98%)	77 (2%)	6 (0%)	51	55

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	T	5	LYS
7	G	6	GLY
7	T	4	ALA
7	T	36[A]	TRP
7	T	36[B]	TRP

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	446/426 (105%)	440 (99%)	6 (1%)	69	81
1	N	448/426 (105%)	439 (98%)	9 (2%)	55	69
2	B	214/511 (42%)	205 (96%)	9 (4%)	30	38
2	O	216/511 (42%)	207 (96%)	9 (4%)	30	38
3	C	231/225 (103%)	227 (98%)	4 (2%)	60	74
3	P	230/225 (102%)	227 (99%)	3 (1%)	69	81
4	D	130/129 (101%)	129 (99%)	1 (1%)	81	90
4	Q	125/129 (97%)	124 (99%)	1 (1%)	81	90
5	E	93/95 (98%)	92 (99%)	1 (1%)	73	85
5	R	93/95 (98%)	91 (98%)	2 (2%)	52	65
6	F	80/81 (99%)	78 (98%)	2 (2%)	47	60
6	S	81/81 (100%)	80 (99%)	1 (1%)	71	83
7	G	67/67 (100%)	56 (84%)	11 (16%)	2	2
7	T	67/67 (100%)	58 (87%)	9 (13%)	4	3
8	H	71/75 (95%)	68 (96%)	3 (4%)	30	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	U	71/75 (95%)	68 (96%)	3 (4%)	30	38
9	I	57/58 (98%)	57 (100%)	0	100	100
9	V	57/58 (98%)	57 (100%)	0	100	100
10	J	48/50 (96%)	48 (100%)	0	100	100
10	W	49/50 (98%)	47 (96%)	2 (4%)	30	39
11	K	41/46 (89%)	40 (98%)	1 (2%)	49	62
11	X	40/46 (87%)	38 (95%)	2 (5%)	24	30
12	L	39/40 (98%)	39 (100%)	0	100	100
12	Y	39/40 (98%)	37 (95%)	2 (5%)	24	29
13	M	37/38 (97%)	37 (100%)	0	100	100
13	Z	35/38 (92%)	34 (97%)	1 (3%)	42	54
All	All	3105/3682 (84%)	3023 (97%)	82 (3%)	47	58

5 of 82 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	P	214	PHE
7	T	54	ARG
4	Q	51	LEU
7	T	18	PHE
10	W	7	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
2	O	92	ASN
5	R	78	HIS
8	U	37	HIS
7	G	38	HIS
7	G	34	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	FME	A	1	1	8,9,10	0.48	0	7,9,11	1.37	1 (14%)
7	TPO	G	11	7	8,10,11	1.28	1 (12%)	10,14,16	1.10	1 (10%)
2	FME	O	1	2	8,9,10	0.49	0	7,9,11	1.29	0
2	FME	B	1	2	8,9,10	0.49	0	7,9,11	1.32	0
7	TPO	T	11	7	8,10,11	1.31	1 (12%)	10,14,16	0.83	0
1	FME	N	1	1	8,9,10	0.45	0	7,9,11	1.17	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	A	1	1	-	6/7/9/11	-
7	TPO	G	11	7	-	4/9/11/13	-
2	FME	O	1	2	-	0/7/9/11	-
2	FME	B	1	2	-	0/7/9/11	-
7	TPO	T	11	7	-	6/9/11/13	-
1	FME	N	1	1	-	5/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	11	TPO	P-O1P	2.76	1.59	1.50
7	T	11	TPO	P-O1P	2.74	1.59	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	11	TPO	CG2-CB-CA	3.12	119.32	113.16
1	A	1	FME	O1-CN-N	-2.26	119.31	125.27

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	11	TPO	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 56 ligands modelled in this entry, 8 are monoatomic - leaving 48 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
21	CUA	B	601	2	0,1,1	-	-	-		
19	TGL	Q	201	-	62,62,62	0.98	3 (4%)	65,65,65	1.10	5 (7%)
20	J6X	N	611	-	11,18,18	3.54	5 (45%)	6,26,26	1.37	1 (16%)
25	PGV	C	301	-	50,50,50	0.35	0	53,56,56	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
25	PGV	N	610	-	50,50,50	0.92	2 (4%)	53,56,56	1.16	7 (13%)
22	CHD	O	602	-	32,32,32	0.81	1 (3%)	51,51,51	1.04	2 (3%)
25	PGV	C	302	-	50,50,50	0.97	2 (4%)	53,56,56	1.11	4 (7%)
19	TGL	L	101	-	62,62,62	1.00	3 (4%)	65,65,65	0.99	4 (6%)
26	CDL	P	304	-	99,99,99	1.31	12 (12%)	105,111,111	1.56	13 (12%)
18	PER	A	606	14,15	0,1,1	-	-	-		
21	CUA	O	601	2	0,1,1	-	-	-		
22	CHD	N	609	-	32,32,32	0.80	0	51,51,51	0.97	0
19	TGL	Y	101	-	62,62,62	1.01	3 (4%)	65,65,65	1.15	4 (6%)
14	HEA	N	601[C]	-	57,67,67	1.49	9 (15%)	61,103,103	1.56	12 (19%)
26	CDL	T	101	-	99,99,99	1.32	12 (12%)	105,111,111	1.34	9 (8%)
24	PEK	C	306	-	52,52,52	0.86	2 (3%)	55,57,57	1.34	9 (16%)
14	HEA	A	602	18,1	57,67,67	1.49	9 (15%)	61,103,103	1.67	18 (29%)
27	DMU	C	308	-	34,34,34	0.45	1 (2%)	45,45,45	0.99	2 (4%)
24	PEK	P	306	-	52,52,52	0.94	2 (3%)	55,57,57	1.28	6 (10%)
19	TGL	D	202	-	62,62,62	0.97	3 (4%)	65,65,65	0.99	4 (6%)
23	PSC	O	603	-	51,51,51	1.10	3 (5%)	57,59,59	1.55	5 (8%)
24	PEK	C	309	-	52,52,52	0.92	2 (3%)	55,57,57	1.14	5 (9%)
24	PEK	G	101	-	52,52,52	0.93	2 (3%)	55,57,57	1.18	5 (9%)
25	PGV	D	201	-	50,50,50	0.35	0	53,56,56	0.31	0
27	DMU	Z	101	-	34,34,34	0.38	0	45,45,45	0.87	1 (2%)
24	PEK	B	604	-	52,52,52	0.91	2 (3%)	55,57,57	1.45	8 (14%)
14	HEA	A	601[C]	-	57,67,67	1.50	9 (15%)	61,103,103	1.57	9 (14%)
26	CDL	G	102	-	99,99,99	1.32	12 (12%)	105,111,111	1.38	10 (9%)
14	HEA	N	602	18,1	57,67,67	1.50	9 (15%)	61,103,103	1.66	15 (24%)
25	PGV	P	302	-	50,50,50	0.96	2 (4%)	53,56,56	1.55	10 (18%)
19	TGL	A	607	-	62,62,62	0.98	3 (4%)	65,65,65	1.11	5 (7%)
25	PGV	N	607	-	50,50,50	0.36	0	53,56,56	0.40	0
24	PEK	P	301	-	52,52,52	0.27	0	55,57,57	0.42	0
22	CHD	C	304	-	32,32,32	0.84	1 (3%)	51,51,51	1.30	8 (15%)
27	DMU	M	101	-	34,34,34	0.35	0	45,45,45	0.83	1 (2%)
25	PGV	C	307	-	50,50,50	0.98	2 (4%)	53,56,56	1.38	6 (11%)
14	HEA	N	601[D]	-	57,67,67	1.49	9 (15%)	61,103,103	1.57	11 (18%)
23	PSC	B	603	-	51,51,51	1.09	3 (5%)	57,59,59	1.25	5 (8%)
22	CHD	B	602	-	32,32,32	0.81	1 (3%)	51,51,51	1.07	4 (7%)
27	DMU	W	101	-	34,34,34	0.35	0	45,45,45	0.83	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	CHD	P	305	-	32,32,32	0.82	1 (3%)	51,51,51	1.25	6 (11%)
19	TGL	N	608	-	62,62,62	0.99	3 (4%)	65,65,65	1.06	5 (7%)
18	PER	N	606	14,15	0,1,1	-	-	-		
22	CHD	C	305	-	32,32,32	0.81	1 (3%)	51,51,51	1.00	0
26	CDL	C	303	-	99,99,99	1.33	12 (12%)	105,111,111	1.51	14 (13%)
25	PGV	P	303	-	50,50,50	0.99	2 (4%)	53,56,56	1.23	5 (9%)
20	J6X	A	608	-	11,18,18	4.02	5 (45%)	6,26,26	1.44	1 (16%)
14	HEA	A	601[D]	-	57,67,67	1.50	9 (15%)	61,103,103	1.57	11 (18%)

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
19	TGL	Q	201	-	-	28/65/65/65	-
20	J6X	N	611	-	-	0/0/4/4	0/3/3/3
25	PGV	C	301	-	-	15/55/55/55	-
25	PGV	N	610	-	-	18/55/55/55	-
22	CHD	O	602	-	-	2/9/74/74	0/4/4/4
25	PGV	C	302	-	-	14/55/55/55	-
19	TGL	L	101	-	-	31/65/65/65	-
26	CDL	P	304	-	-	35/110/110/110	-
22	CHD	N	609	-	-	3/9/74/74	0/4/4/4
19	TGL	Y	101	-	-	38/65/65/65	-
14	HEA	N	601[C]	-	-	6/32/76/76	-
26	CDL	T	101	-	-	40/110/110/110	-
24	PEK	C	306	-	-	17/56/56/56	-
14	HEA	A	602	18,1	-	7/32/76/76	-
27	DMU	C	308	-	-	4/19/59/59	0/2/2/2
24	PEK	P	306	-	-	20/56/56/56	-
19	TGL	D	202	-	-	29/65/65/65	-
23	PSC	O	603	-	-	28/55/55/55	-
24	PEK	C	309	-	-	21/56/56/56	-
24	PEK	G	101	-	-	16/56/56/56	-
25	PGV	D	201	-	-	34/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	DMU	Z	101	-	-	4/19/59/59	0/2/2/2
24	PEK	B	604	-	-	24/56/56/56	-
14	HEA	A	601[C]	-	-	6/32/76/76	-
26	CDL	G	102	-	-	41/110/110/110	-
14	HEA	N	602	18,1	-	6/32/76/76	-
25	PGV	P	302	-	-	19/55/55/55	-
19	TGL	A	607	-	-	20/65/65/65	-
25	PGV	N	607	-	-	14/55/55/55	-
24	PEK	P	301	-	-	28/56/56/56	-
22	CHD	C	304	-	-	8/9/74/74	0/4/4/4
27	DMU	M	101	-	-	4/19/59/59	0/2/2/2
25	PGV	C	307	-	-	22/55/55/55	-
14	HEA	N	601[D]	-	-	6/32/76/76	-
23	PSC	B	603	-	-	28/55/55/55	-
22	CHD	B	602	-	-	2/9/74/74	0/4/4/4
27	DMU	W	101	-	-	4/19/59/59	0/2/2/2
22	CHD	P	305	-	-	4/9/74/74	0/4/4/4
19	TGL	N	608	-	-	26/65/65/65	-
22	CHD	C	305	-	-	1/9/74/74	0/4/4/4
26	CDL	C	303	-	-	52/110/110/110	-
25	PGV	P	303	-	-	17/55/55/55	-
20	J6X	A	608	-	-	0/0/4/4	0/3/3/3
14	HEA	A	601[D]	-	-	5/32/76/76	-

The worst 5 of 162 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	608	J6X	C9-S2	-11.16	1.58	1.73
20	N	611	J6X	C9-S2	-9.31	1.60	1.73
25	C	307	PGV	O03-C19	4.77	1.47	1.33
24	P	306	PEK	O03-C21	4.64	1.46	1.33
26	C	303	CDL	OA6-CA5	4.58	1.47	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	O	603	PSC	O01-C1-C2	7.81	128.34	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	P	304	CDL	CA6-CA4-CA3	-6.43	96.58	111.79
26	C	303	CDL	CB4-OB6-CB5	-6.13	102.70	117.79
26	T	101	CDL	OA6-CA5-C11	5.63	123.63	111.50
19	Y	101	TGL	OG2-CB1-CB2	5.42	123.19	111.50

There are no chirality outliers.

5 of 747 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	N	601[C]	HEA	C19-C20-C21-C22
14	N	602	HEA	C2D-C3D-CAD-CBD
14	N	602	HEA	C4D-C3D-CAD-CBD
19	L	101	TGL	CB2-CB1-OG2-CG2
19	Y	101	TGL	CB2-CB1-OG2-CG2

There are no ring outliers.

38 monomers are involved in 168 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	Q	201	TGL	2	0
20	N	611	J6X	1	0
25	C	301	PGV	3	0
25	N	610	PGV	3	0
22	O	602	CHD	1	0
25	C	302	PGV	5	0
19	L	101	TGL	1	0
26	P	304	CDL	12	0
22	N	609	CHD	1	0
19	Y	101	TGL	7	0
14	N	601[C]	HEA	3	0
26	T	101	CDL	17	0
24	C	306	PEK	4	0
14	A	602	HEA	2	0
27	C	308	DMU	7	0
24	P	306	PEK	5	0
19	D	202	TGL	5	0
23	O	603	PSC	10	0
24	C	309	PEK	6	0
24	G	101	PEK	2	0
25	D	201	PGV	12	0
24	B	604	PEK	4	0

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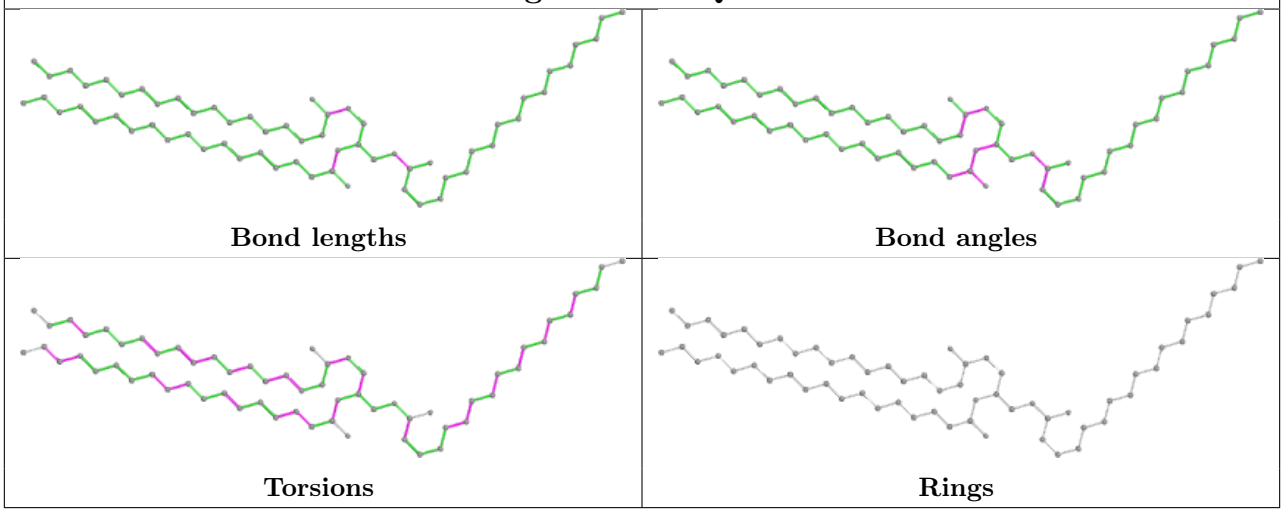
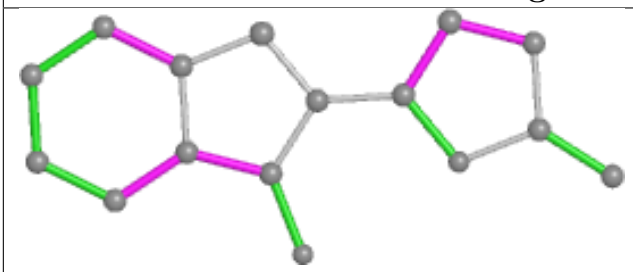
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	601[C]	HEA	3	0
26	G	102	CDL	11	0
14	N	602	HEA	8	0
25	P	302	PGV	2	0
25	N	607	PGV	1	0
24	P	301	PEK	1	0
22	C	304	CHD	1	0
14	N	601[D]	HEA	1	0
23	B	603	PSC	5	0
27	W	101	DMU	2	0
22	P	305	CHD	1	0
19	N	608	TGL	4	0
26	C	303	CDL	13	0
25	P	303	PGV	6	0
20	A	608	J6X	2	0
14	A	601[D]	HEA	1	0

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

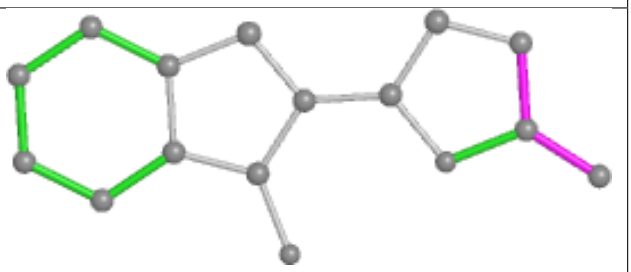
Ligand TGL Q 201



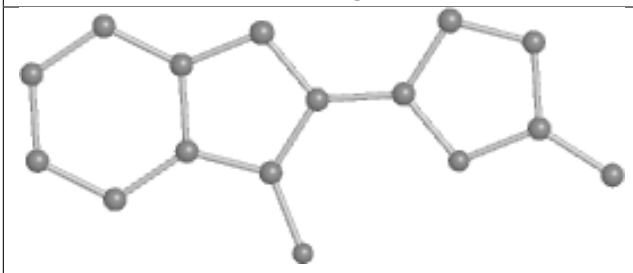
Ligand J6X N 611



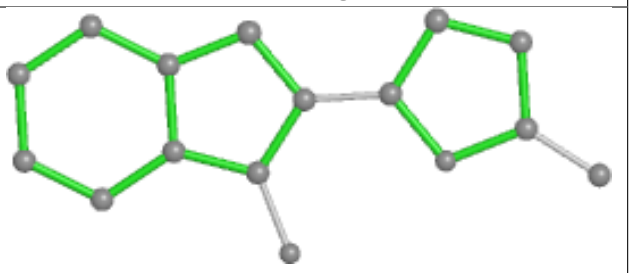
Bond lengths



Bond angles

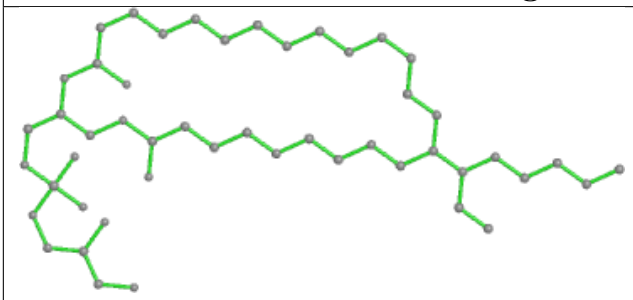


Torsions

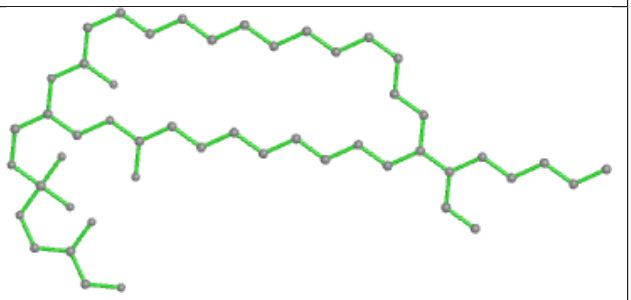


Rings

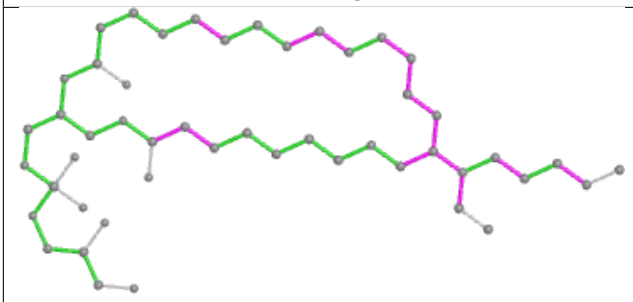
Ligand PGV C 301



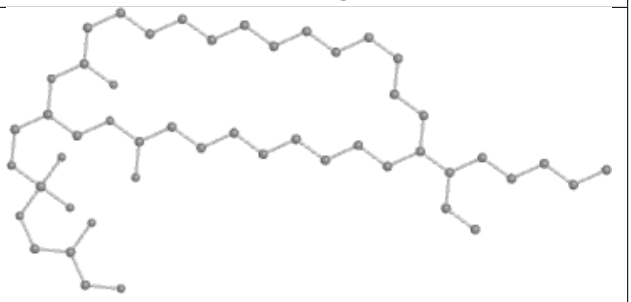
Bond lengths



Bond angles

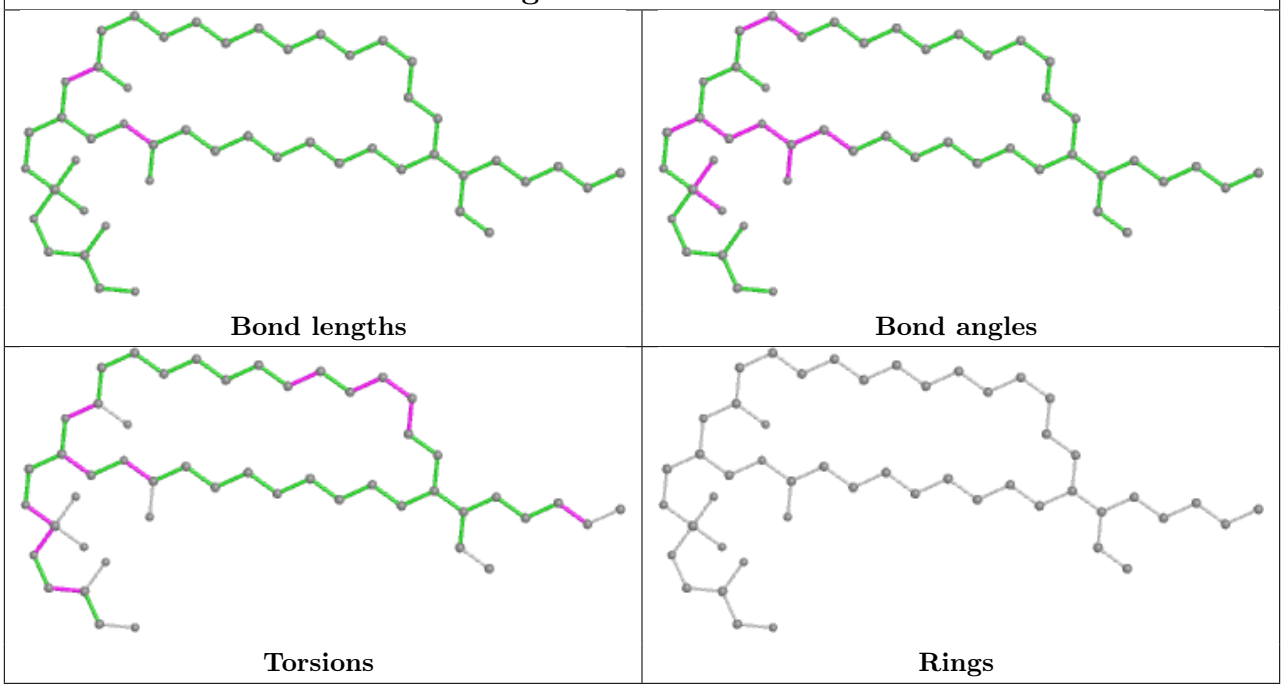


Torsions

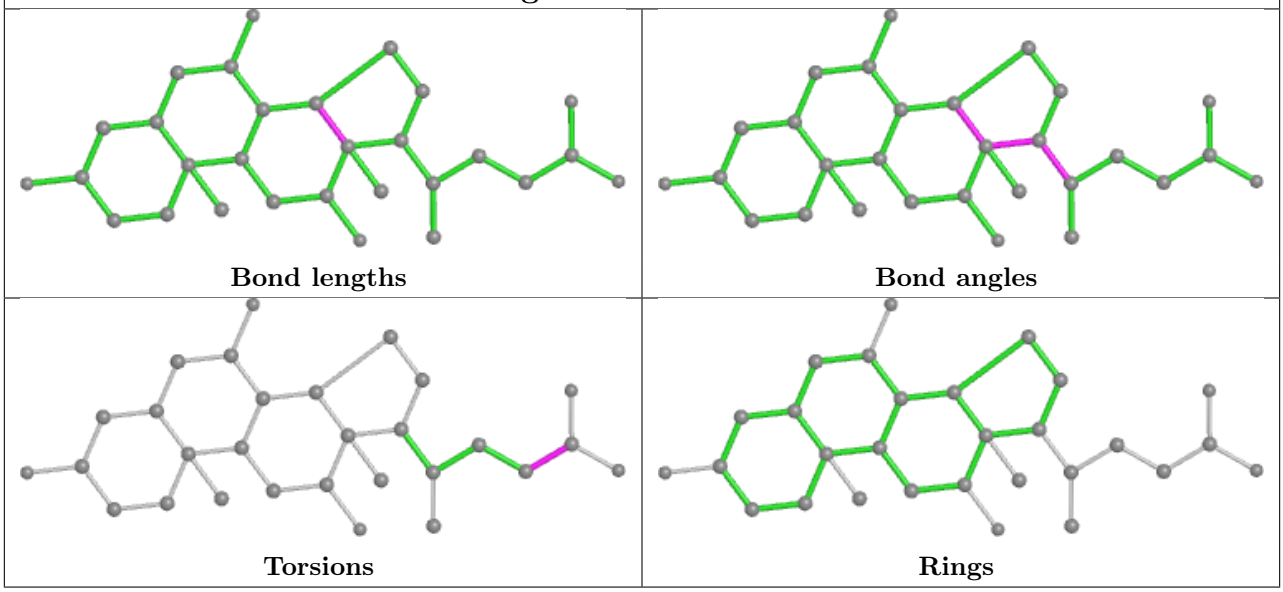


Rings

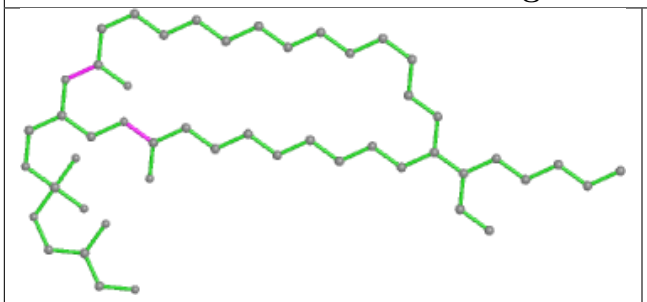
Ligand PGV N 610



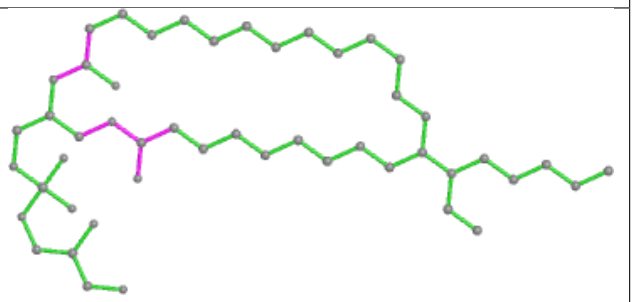
Ligand CHD O 602



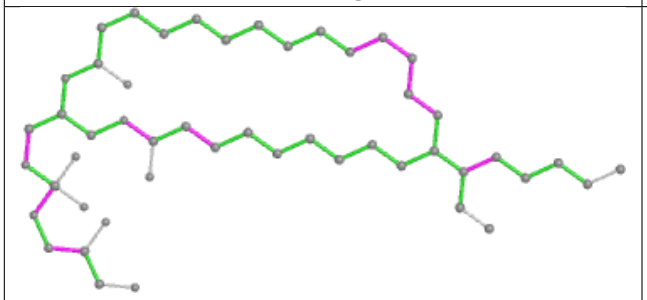
Ligand PGV C 302



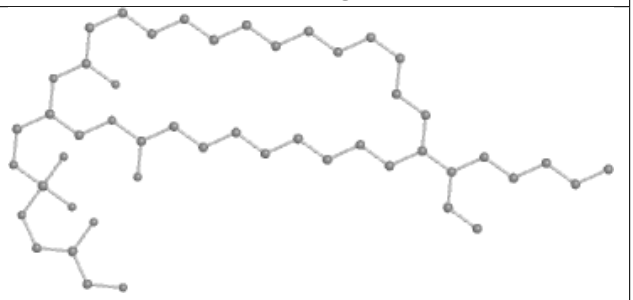
Bond lengths



Bond angles

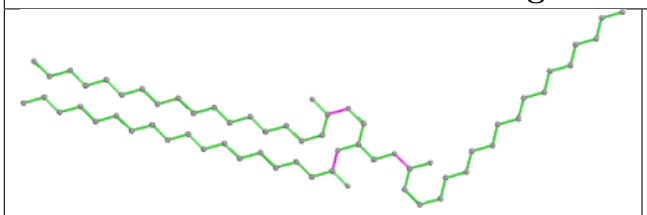


Torsions

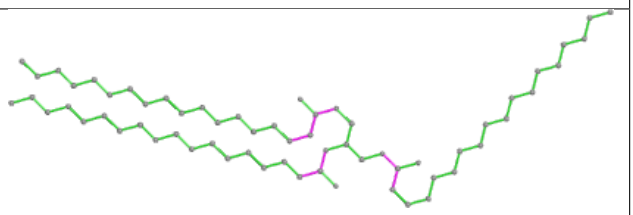


Rings

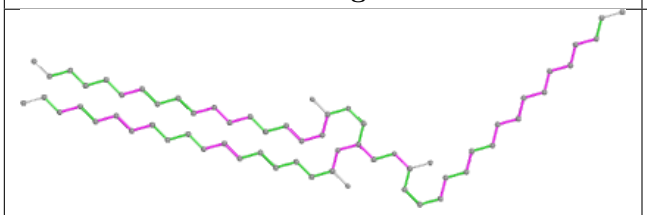
Ligand TGL L 101



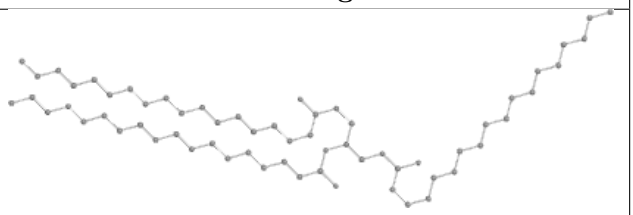
Bond lengths



Bond angles

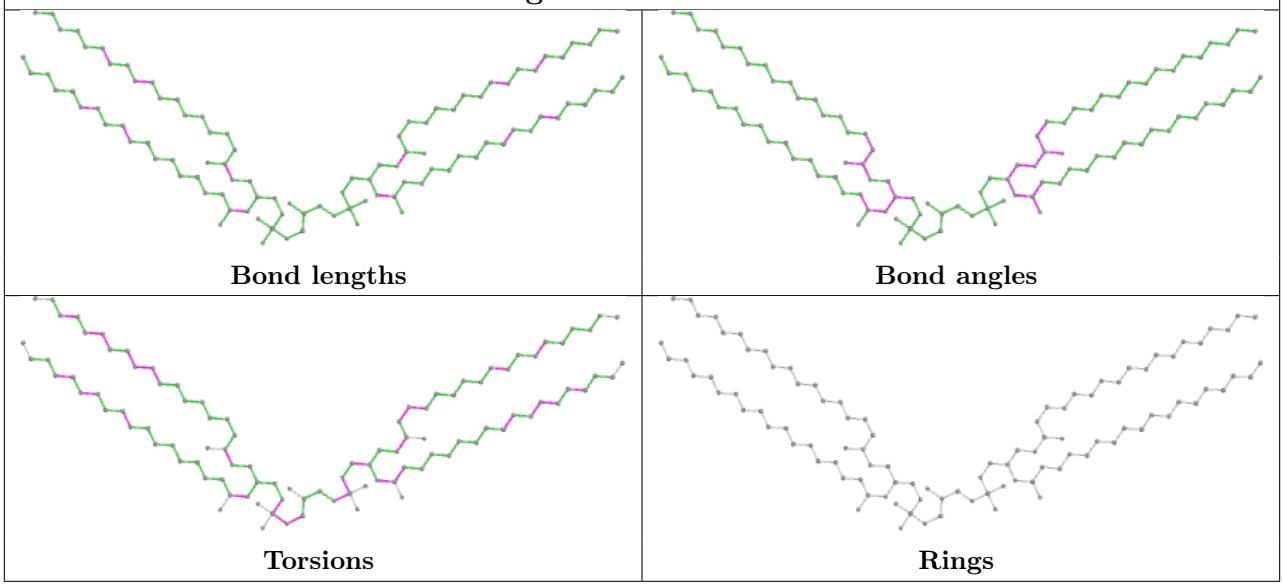


Torsions

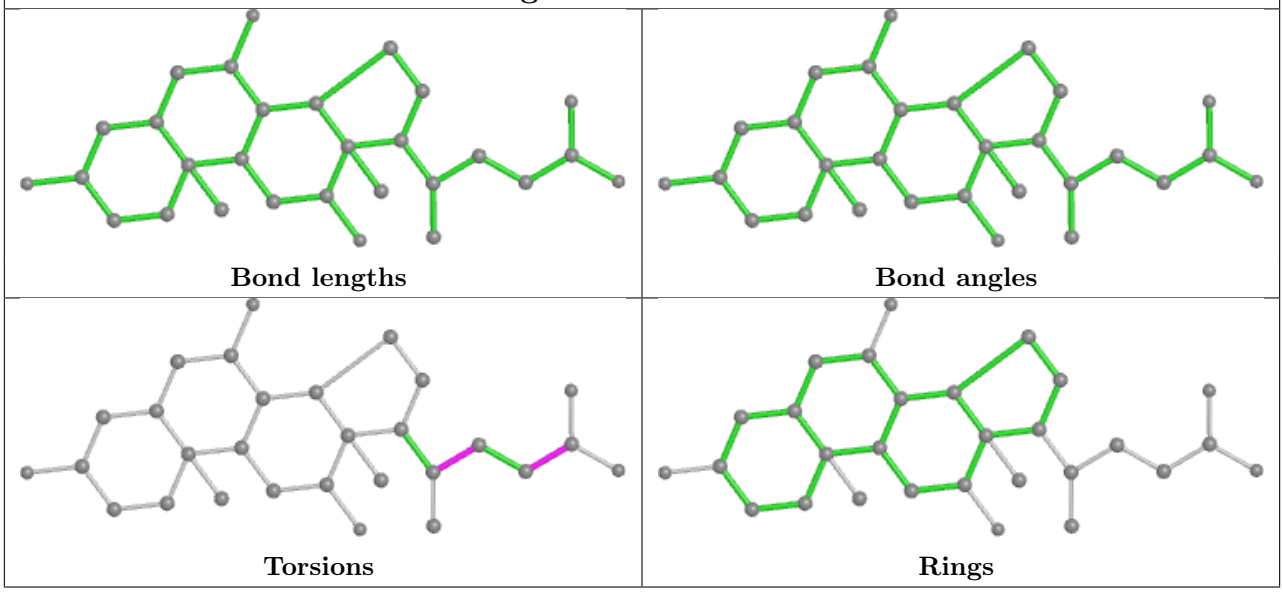


Rings

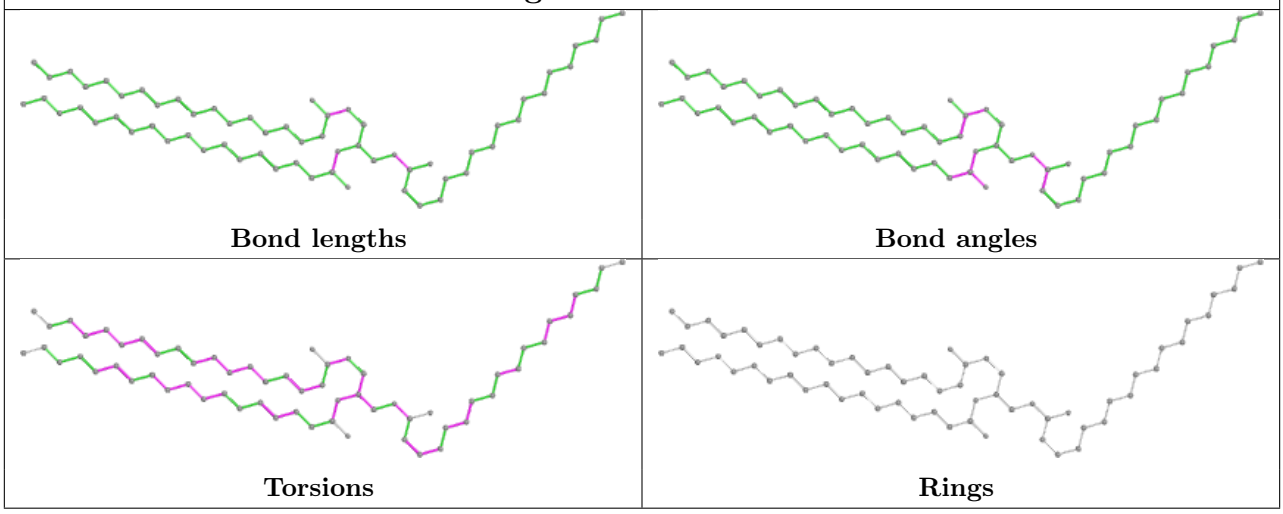
Ligand CDL P 304



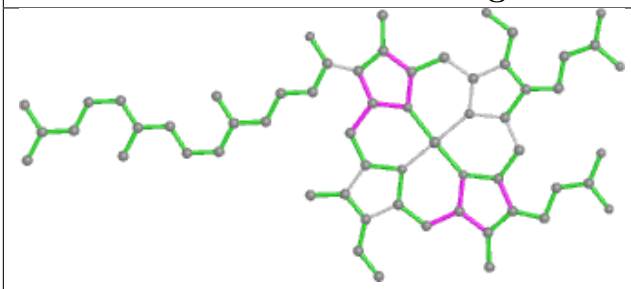
Ligand CHD N 609



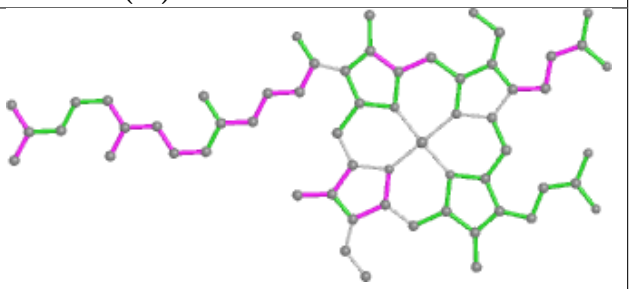
Ligand TGL Y 101



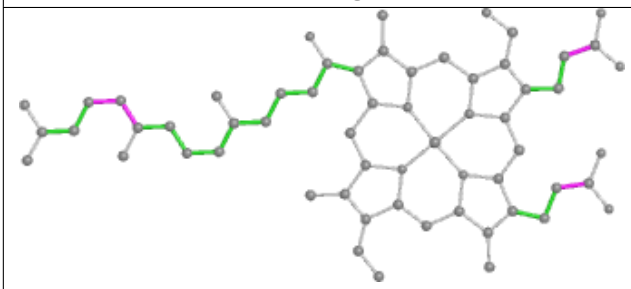
Ligand HEA N 601 (C)



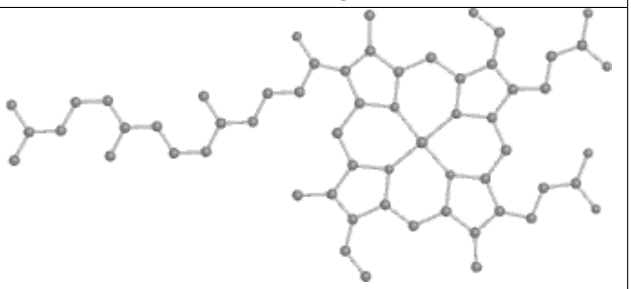
Bond lengths



Bond angles

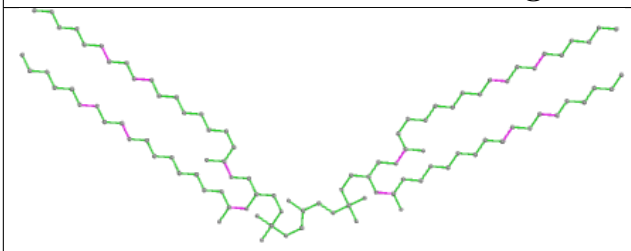


Torsions

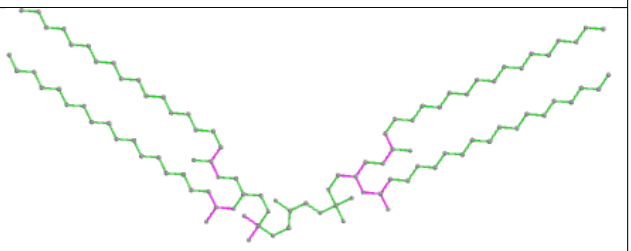


Rings

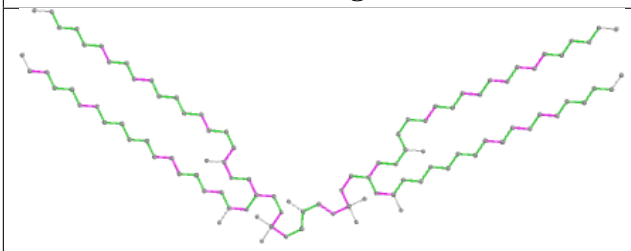
Ligand CDL T 101



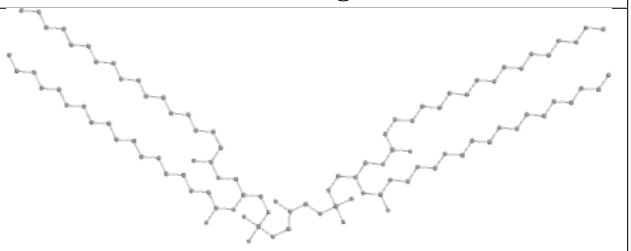
Bond lengths



Bond angles

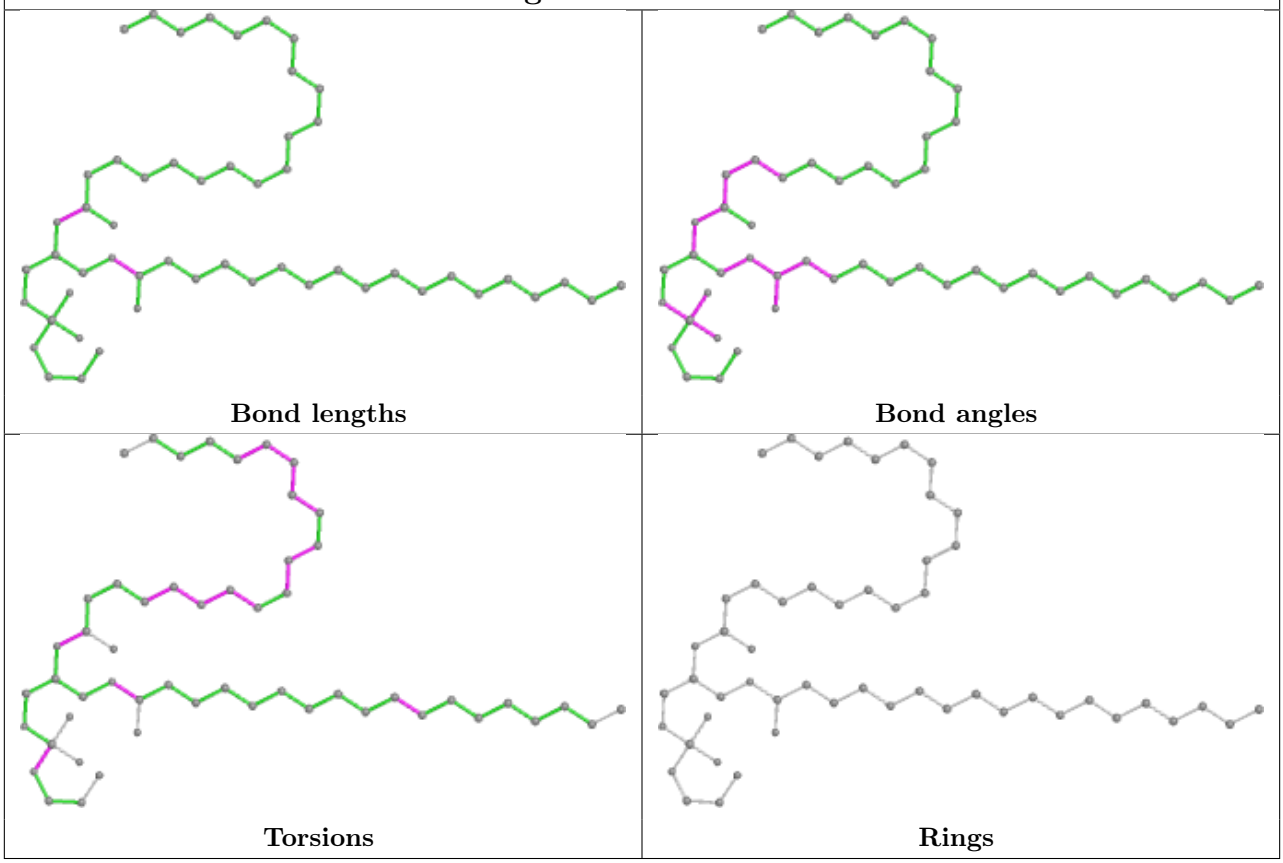


Torsions

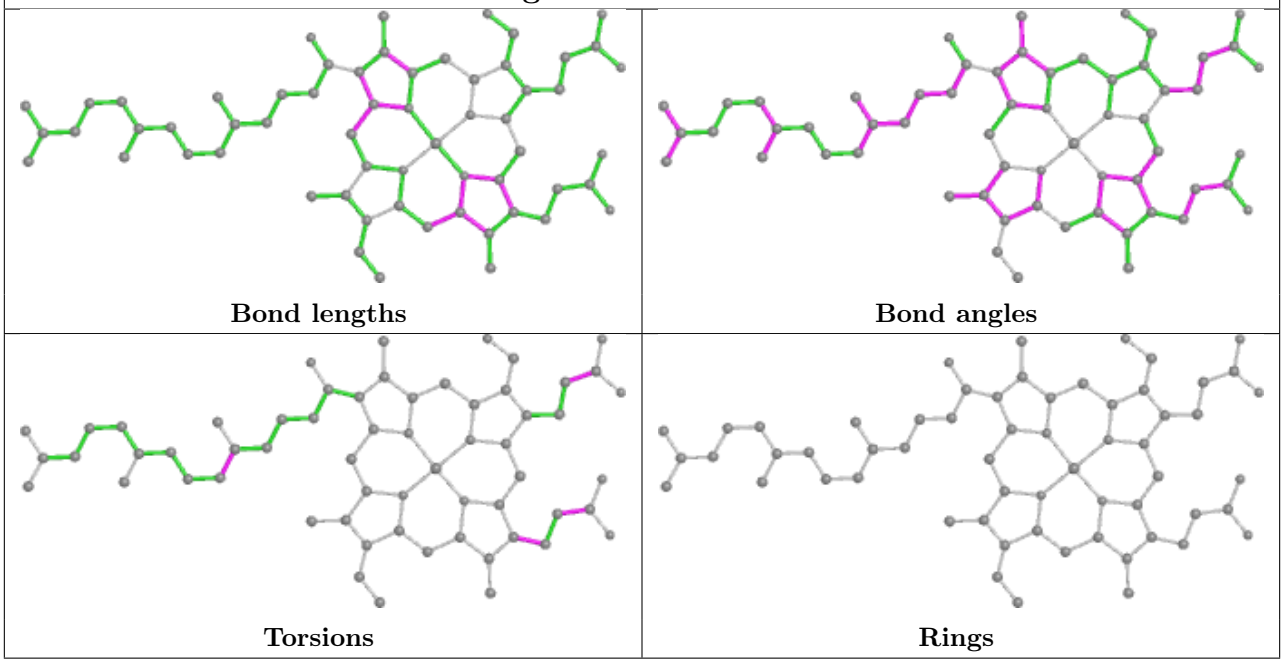


Rings

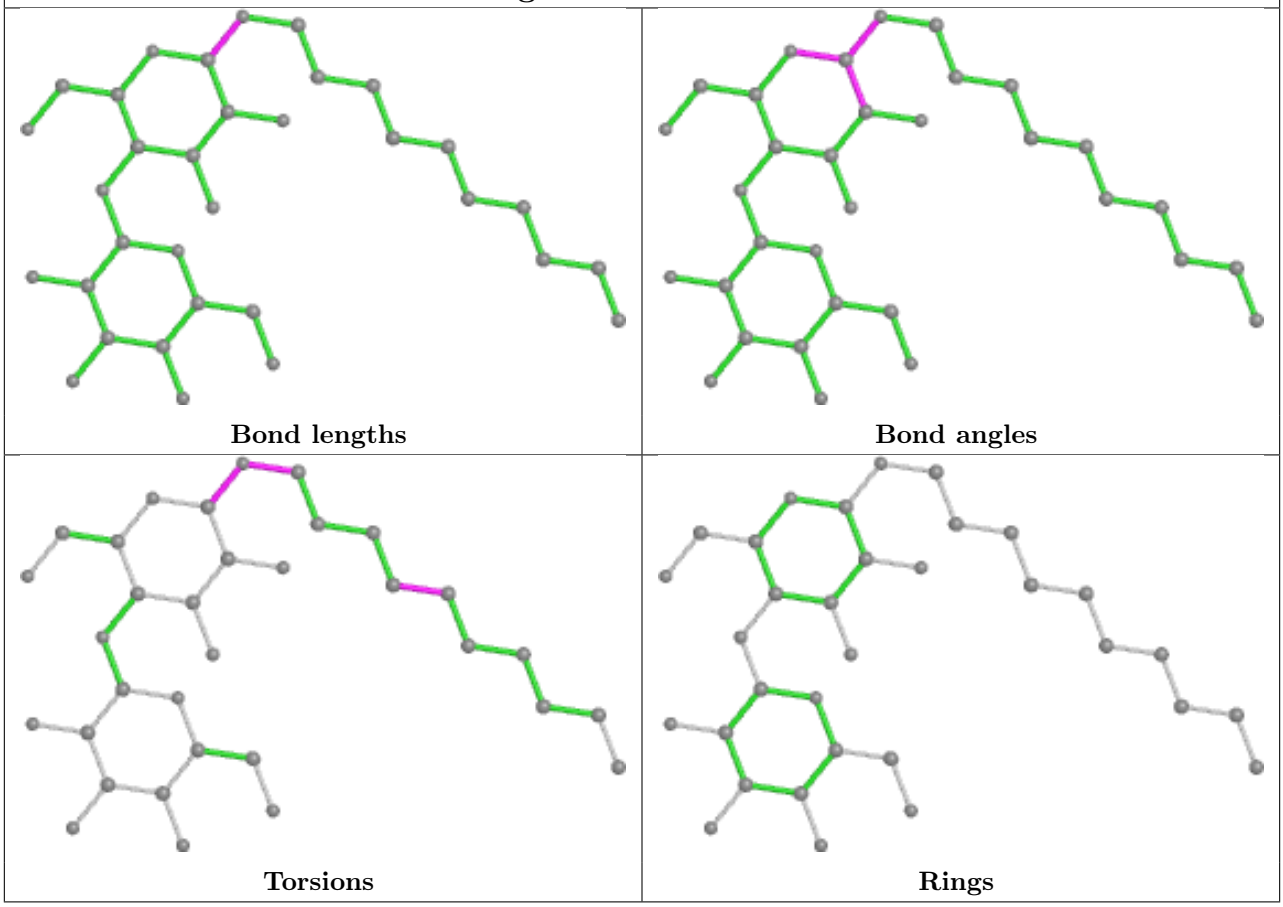
Ligand PEK C 306



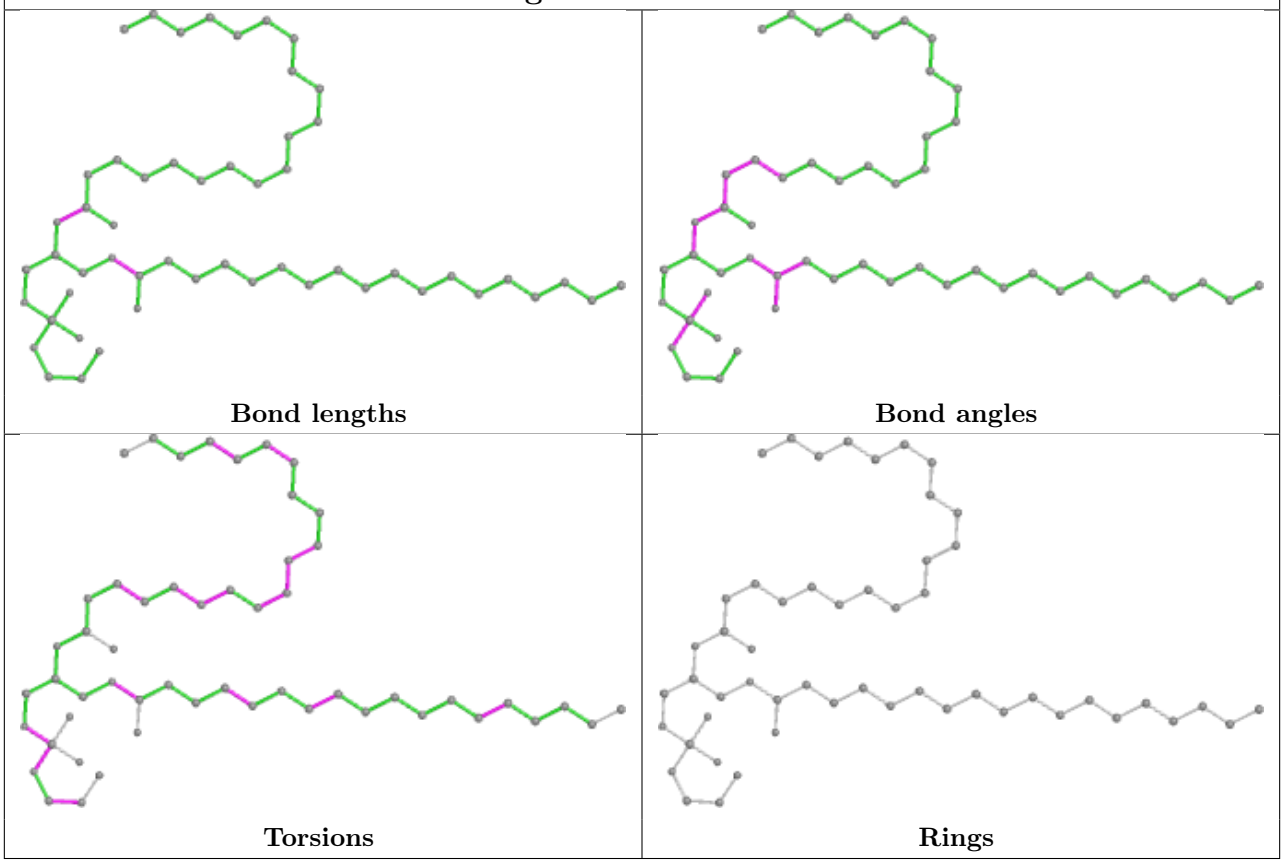
Ligand HEA A 602



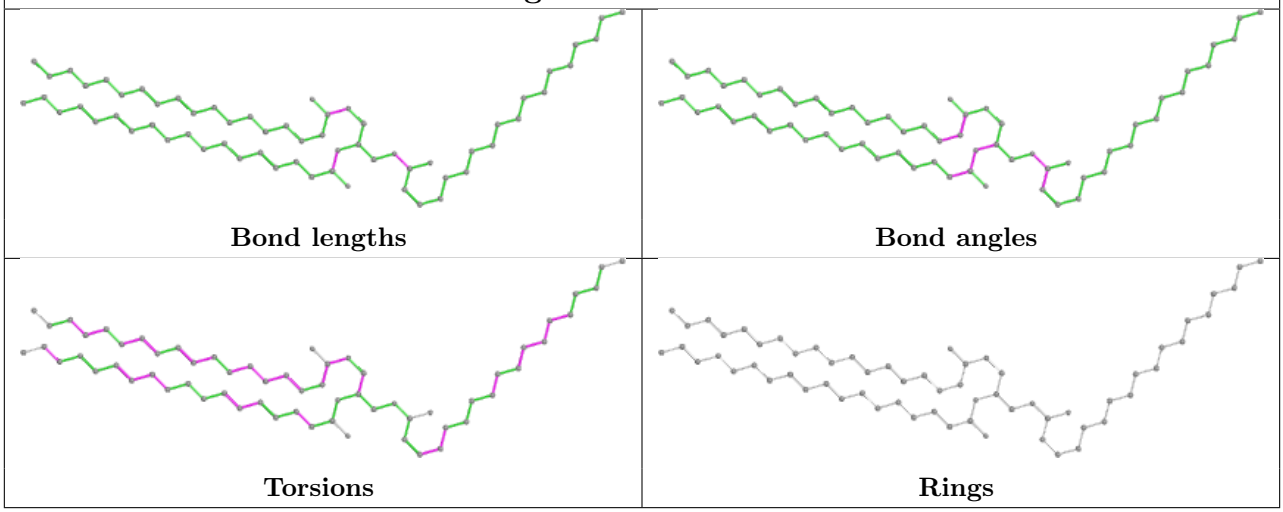
Ligand DMU C 308



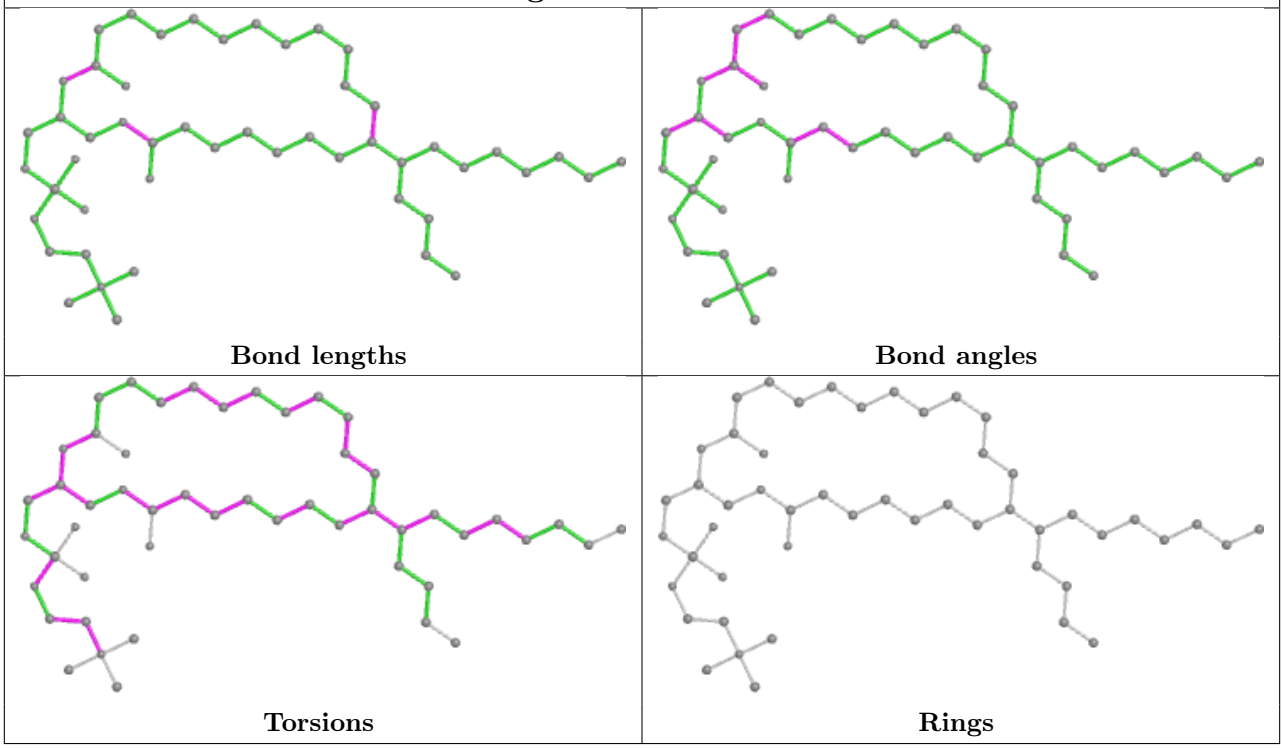
Ligand PEK P 306



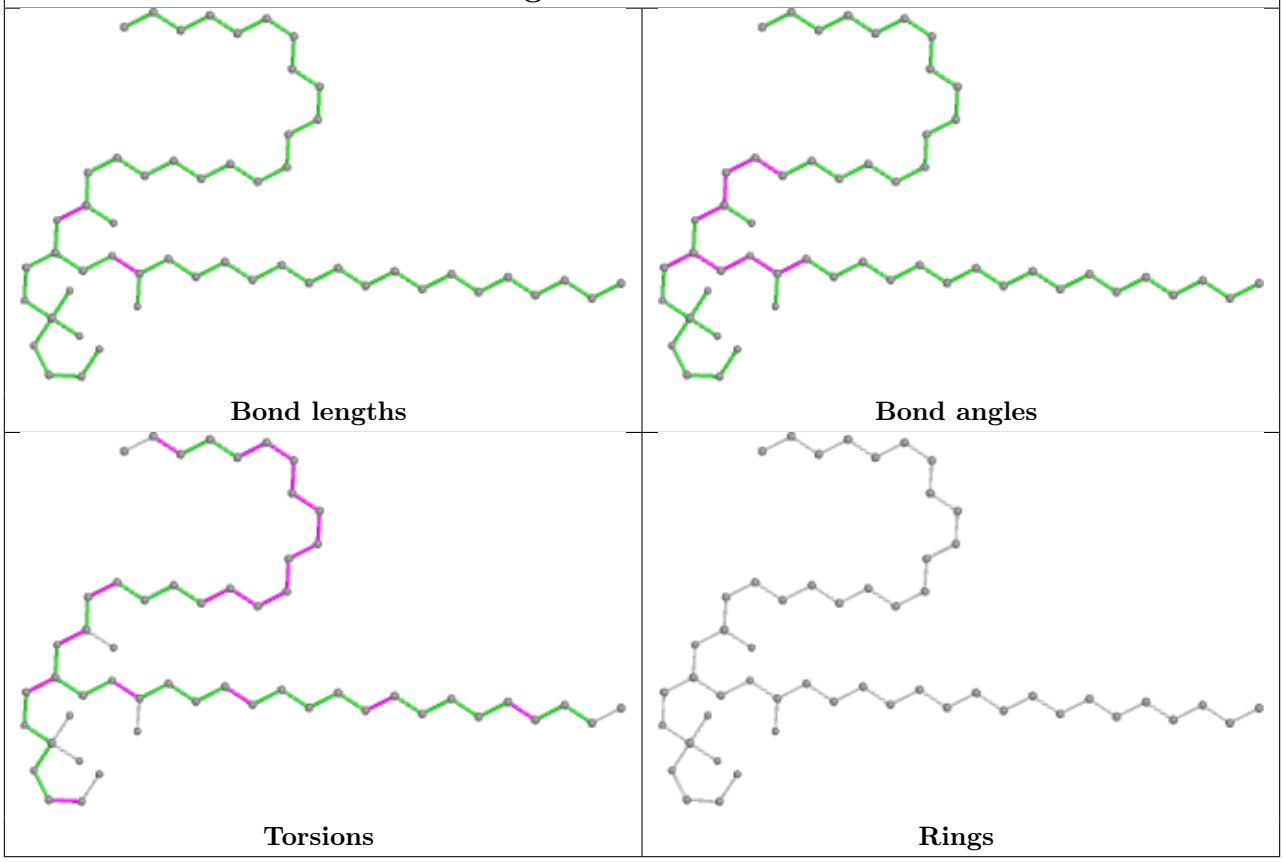
Ligand TGL D 202



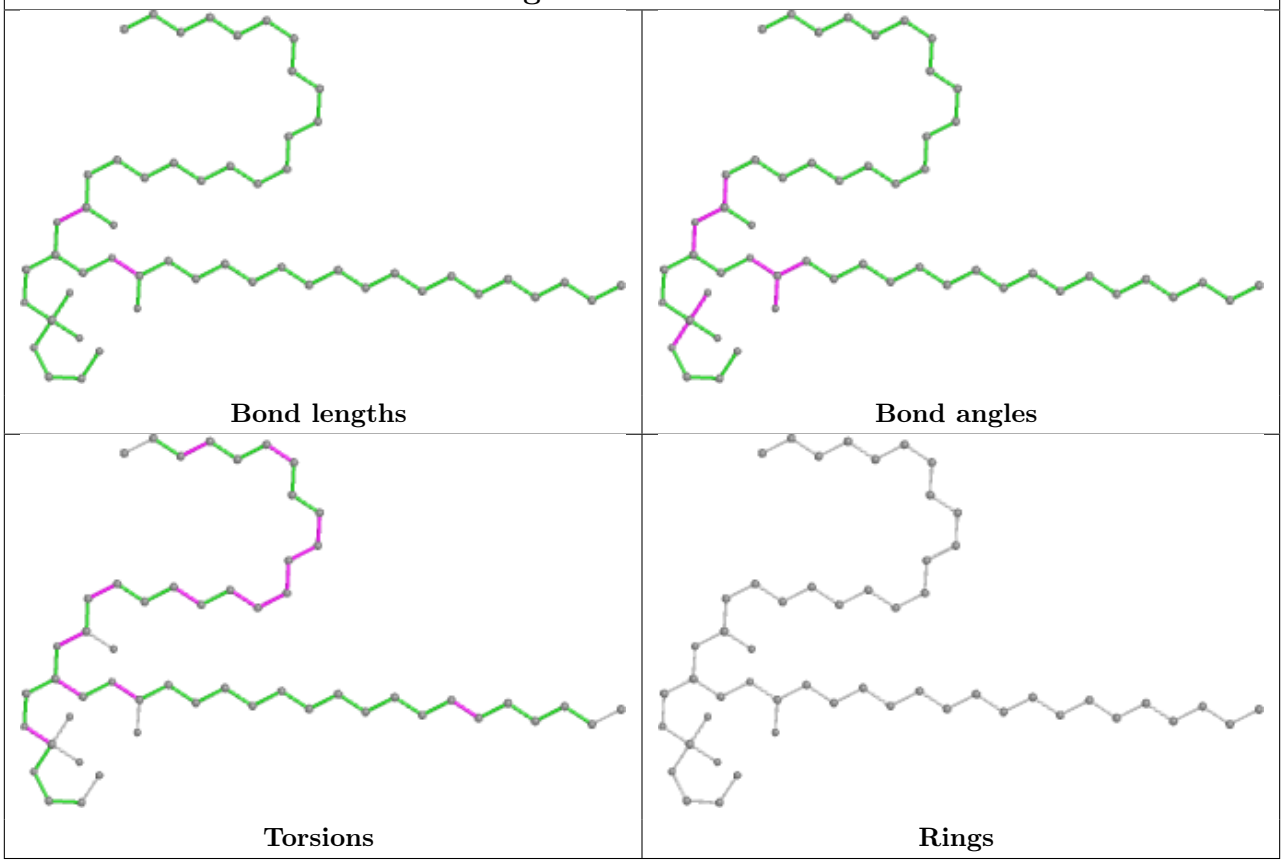
Ligand PSC O 603



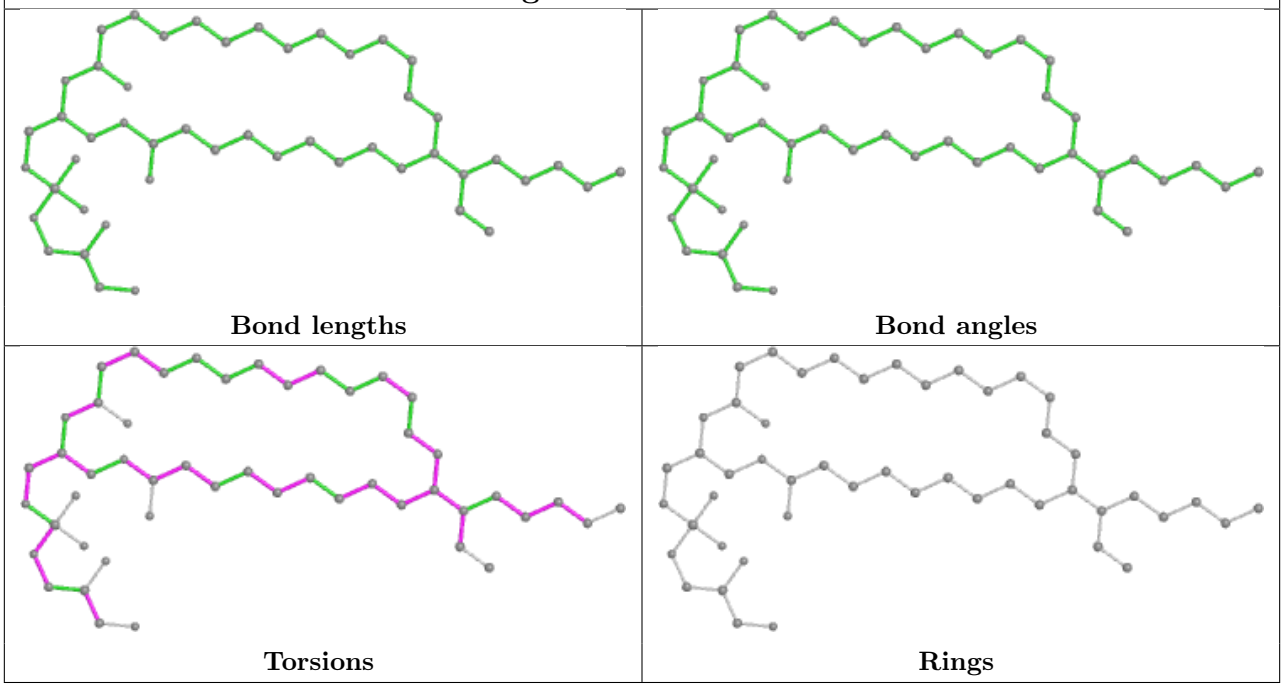
Ligand PEK C 309



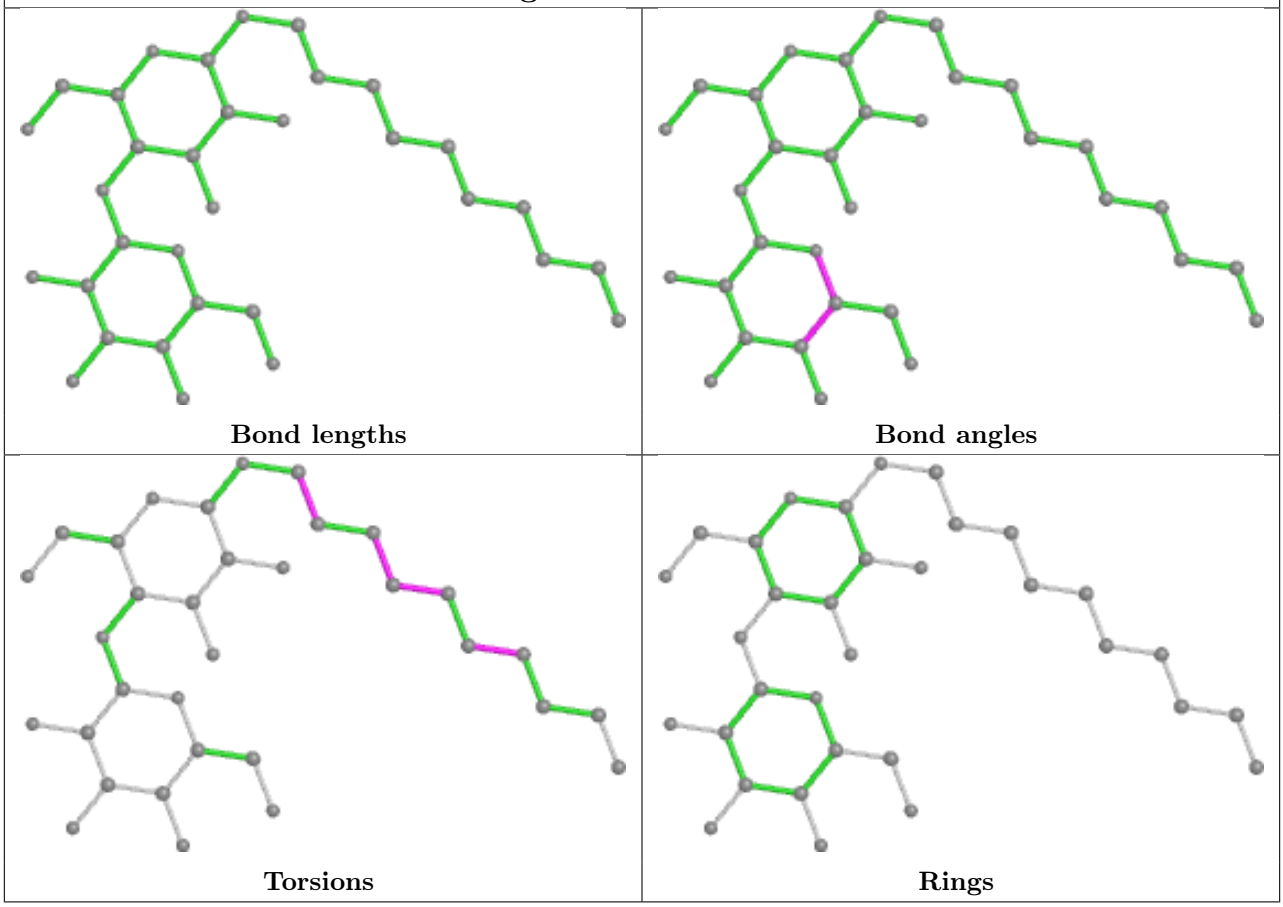
Ligand PEK G 101



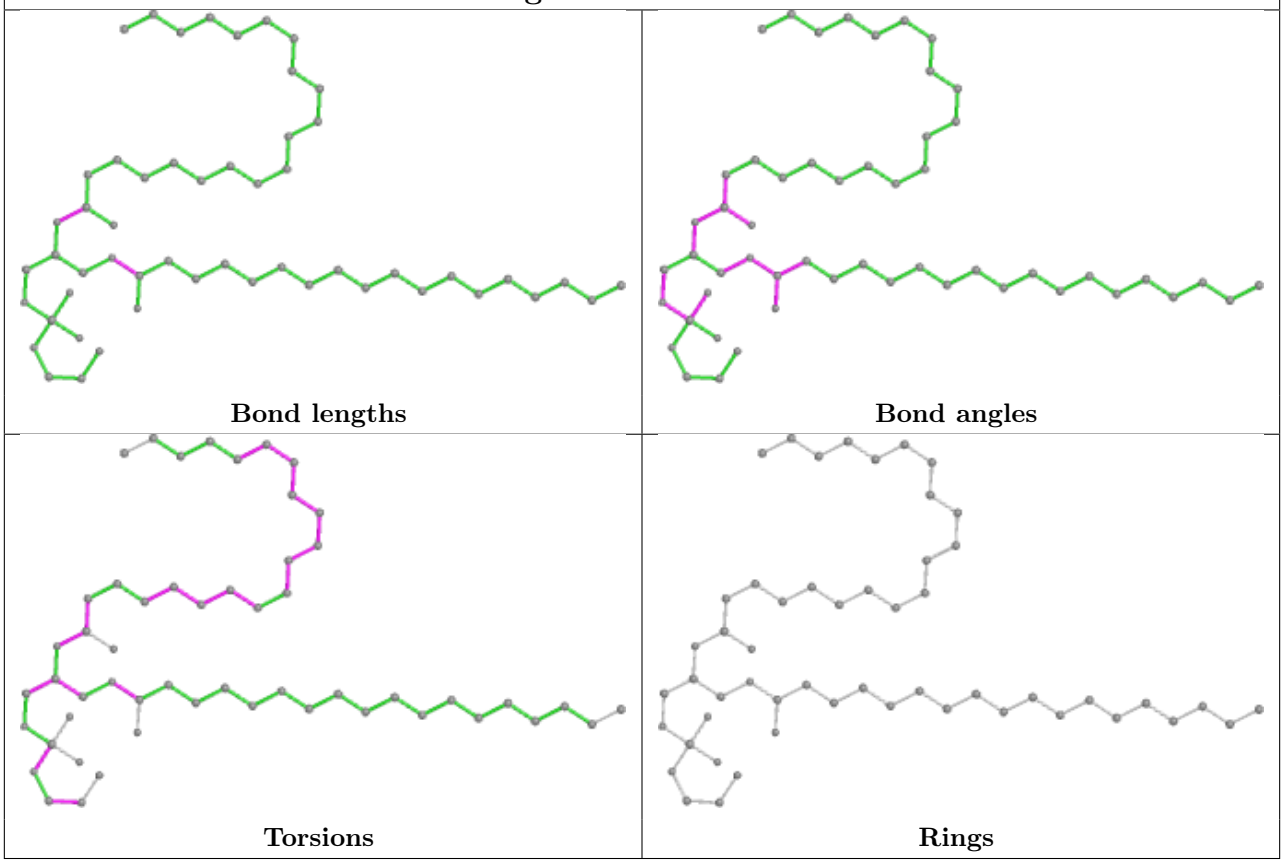
Ligand PGV D 201



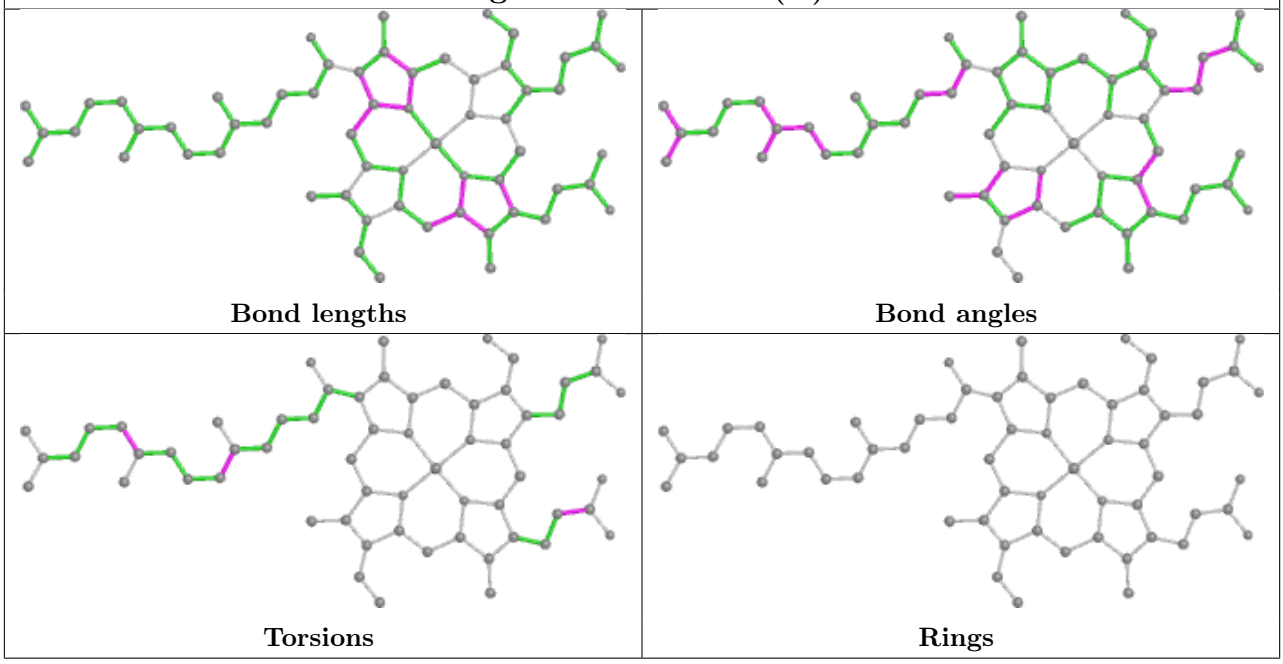
Ligand DMU Z 101



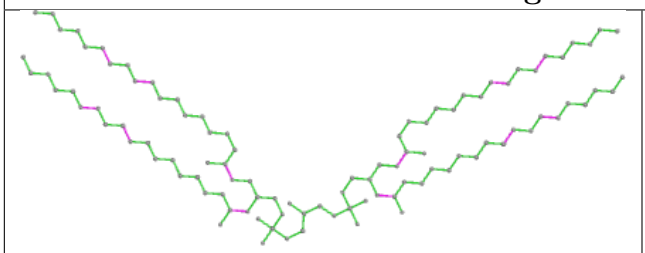
Ligand PEK B 604



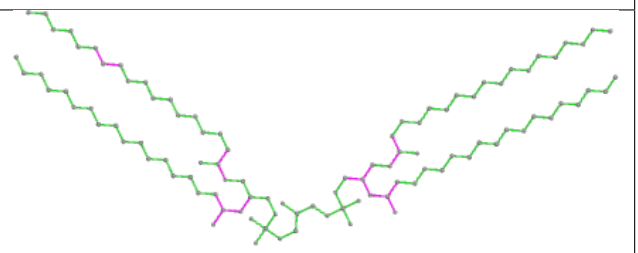
Ligand HEA A 601 (C)



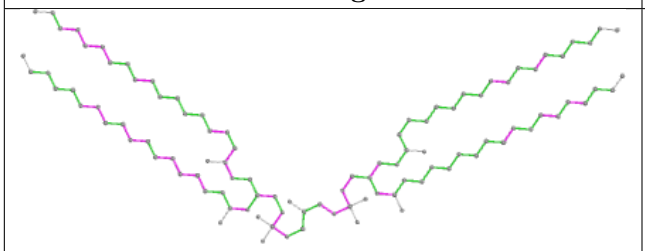
Ligand CDL G 102



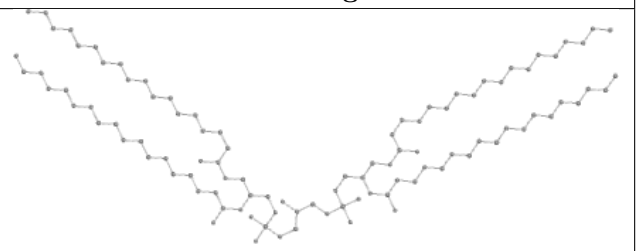
Bond lengths



Bond angles

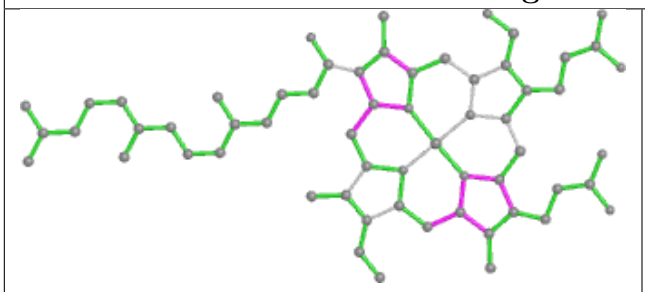


Torsions

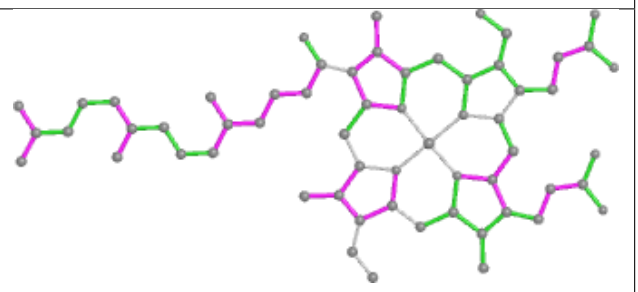


Rings

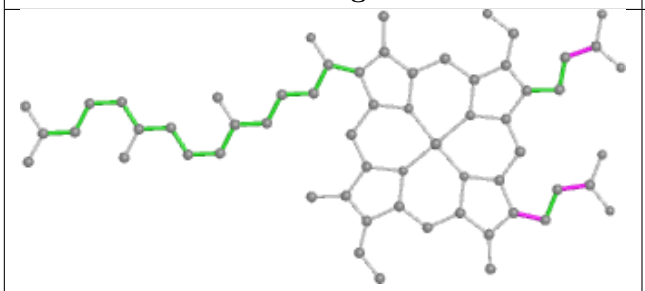
Ligand HEA N 602



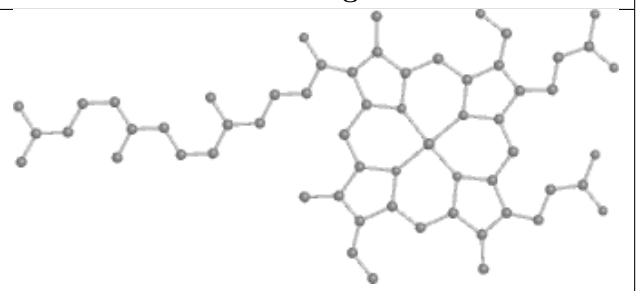
Bond lengths



Bond angles

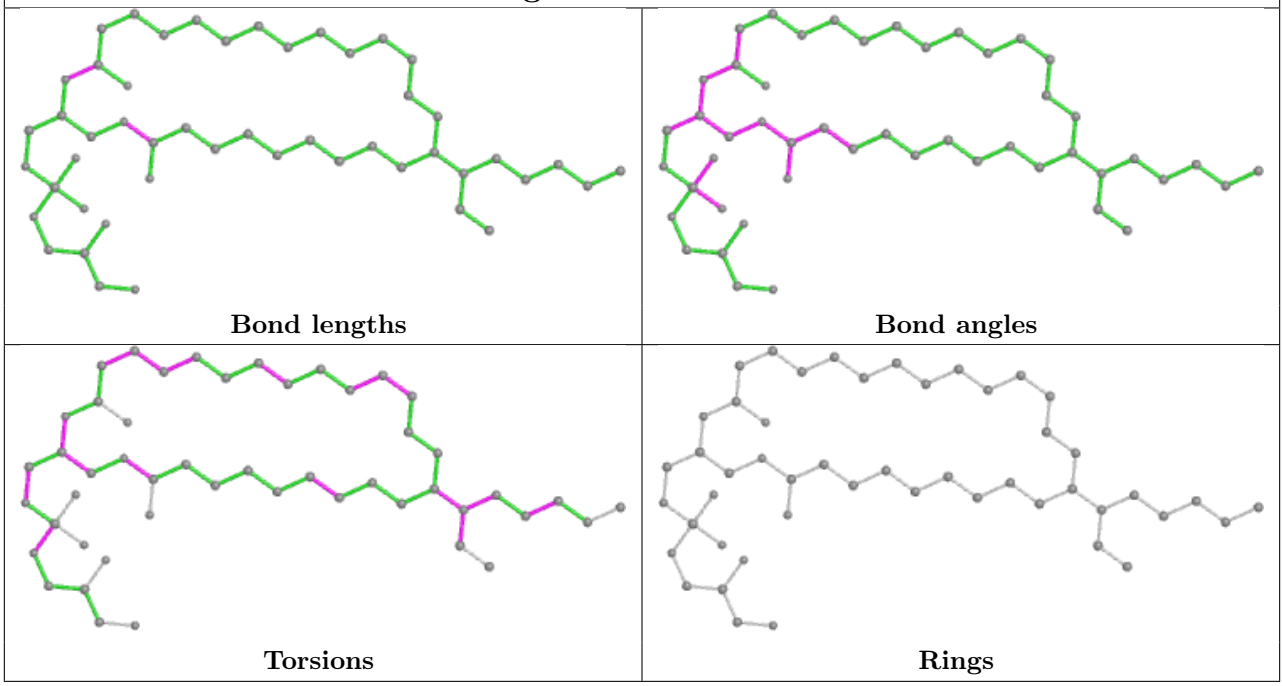


Torsions

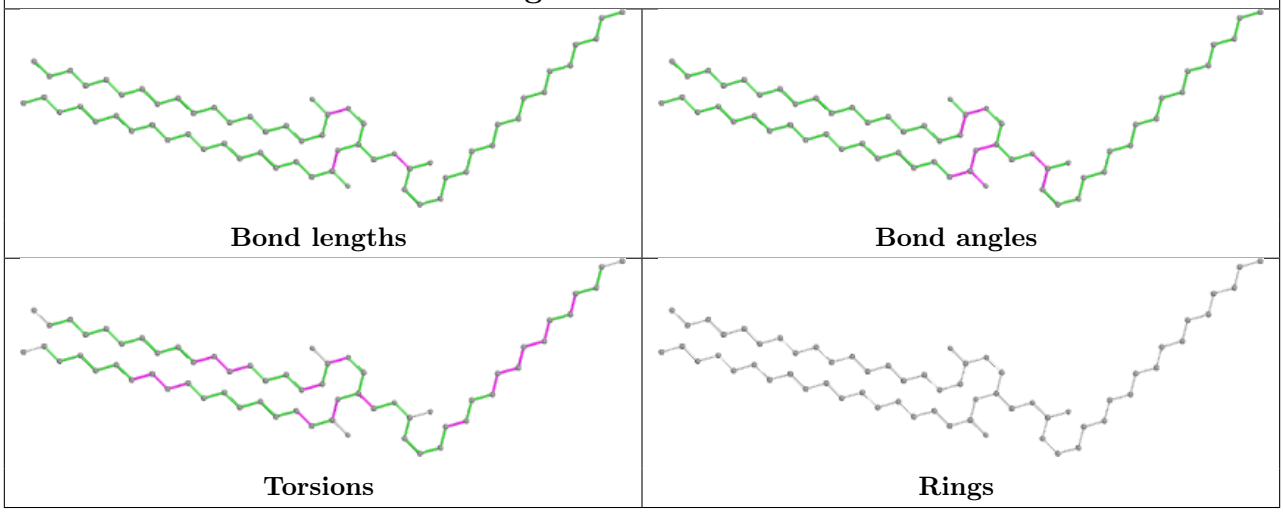


Rings

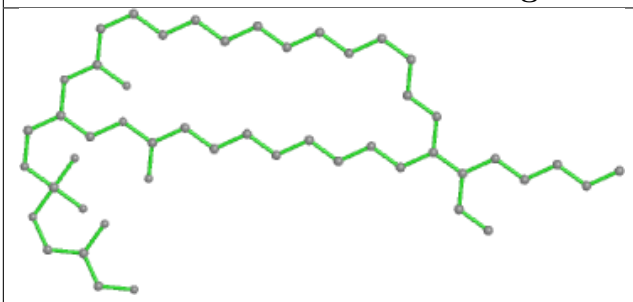
Ligand PGV P 302



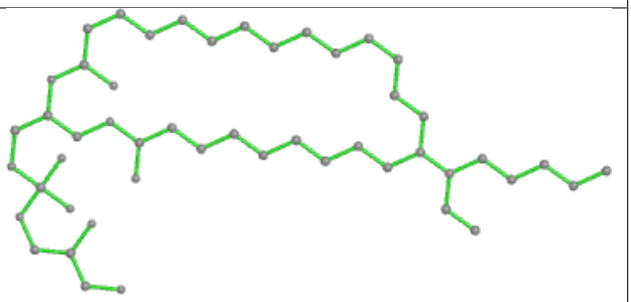
Ligand TGL A 607



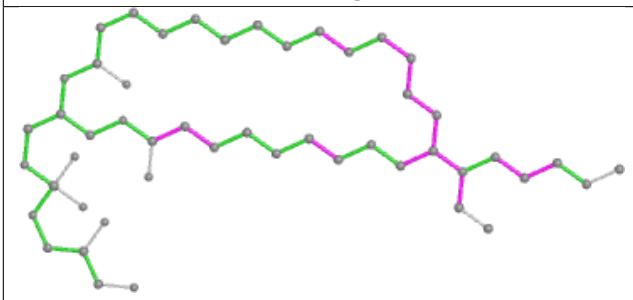
Ligand PGV N 607



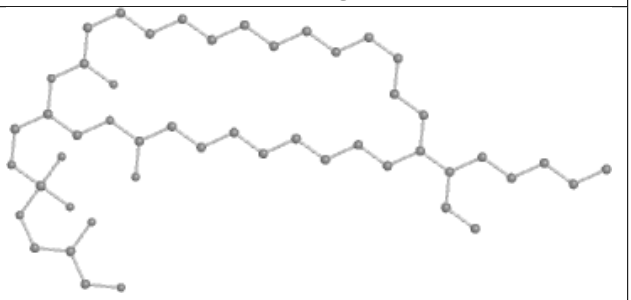
Bond lengths



Bond angles

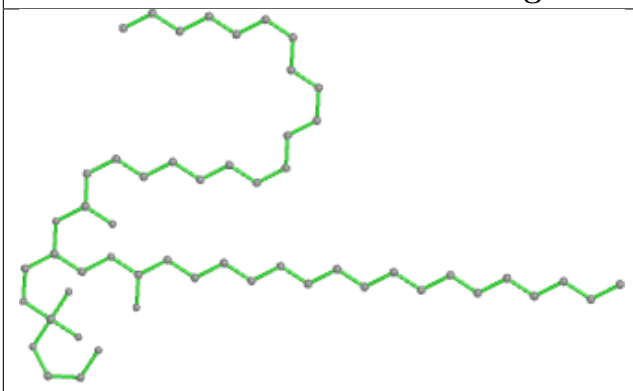


Torsions

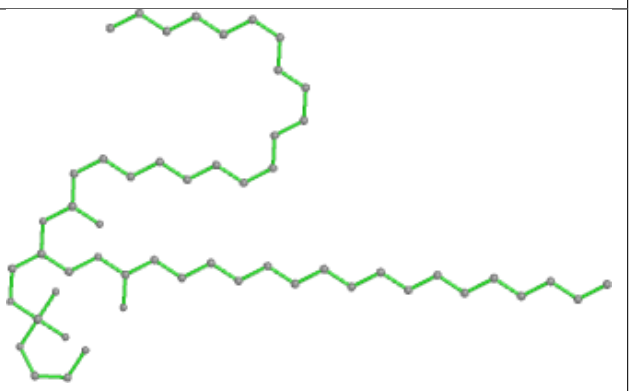


Rings

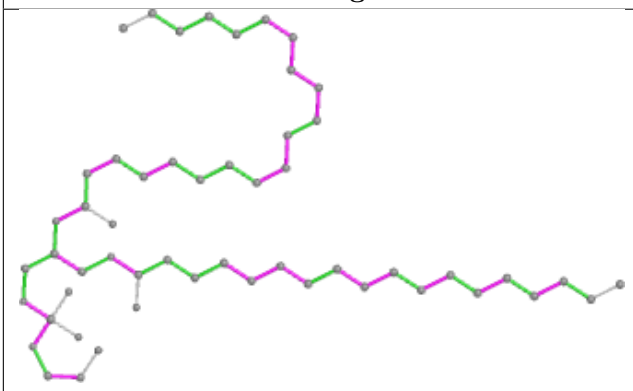
Ligand PEK P 301



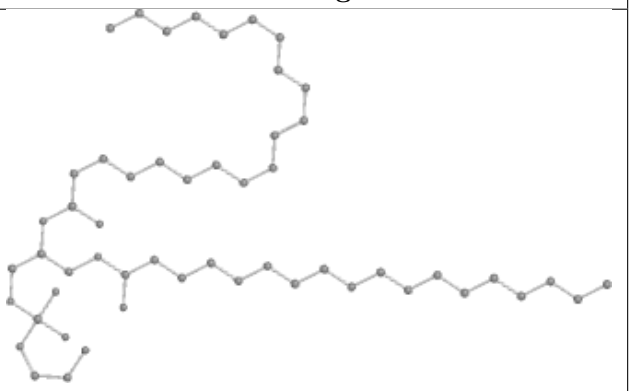
Bond lengths



Bond angles

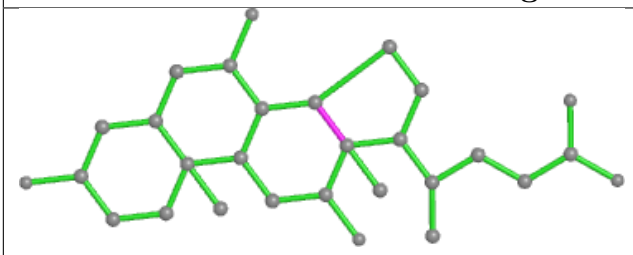


Torsions

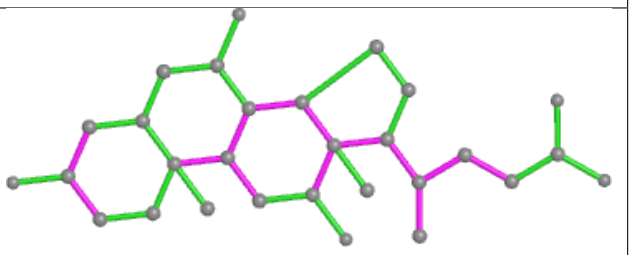


Rings

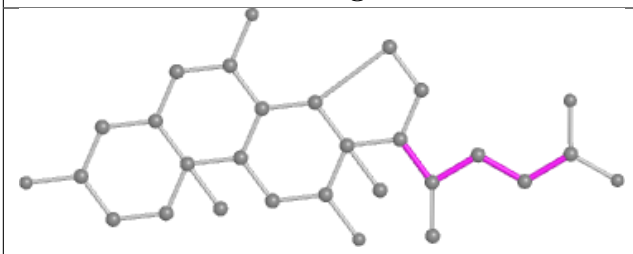
Ligand CHD C 304



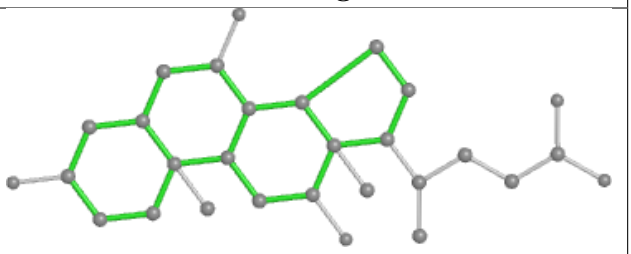
Bond lengths



Bond angles

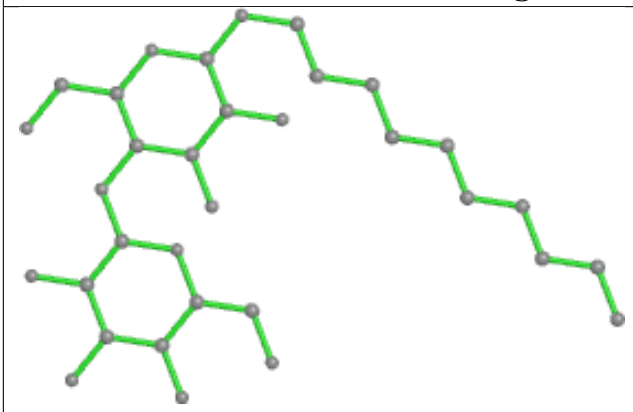


Torsions

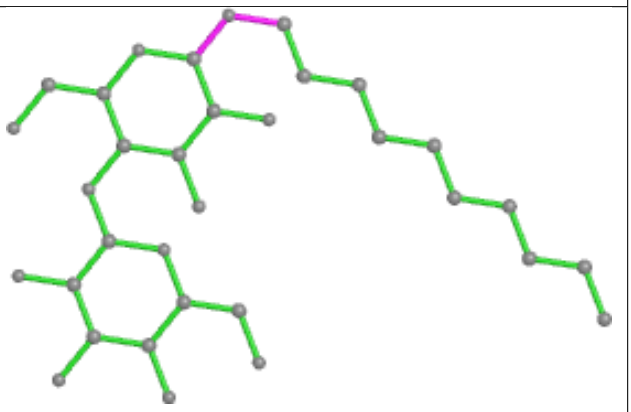


Rings

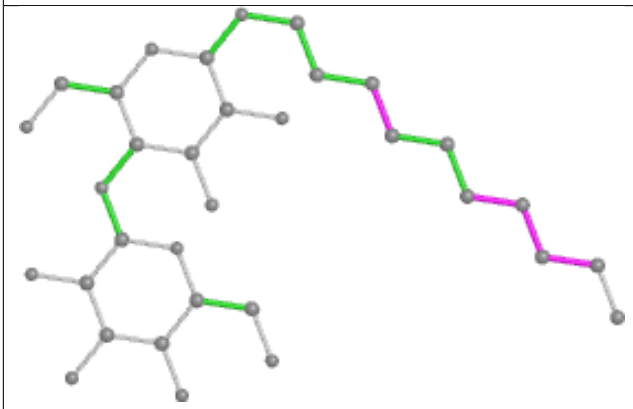
Ligand DMU M 101



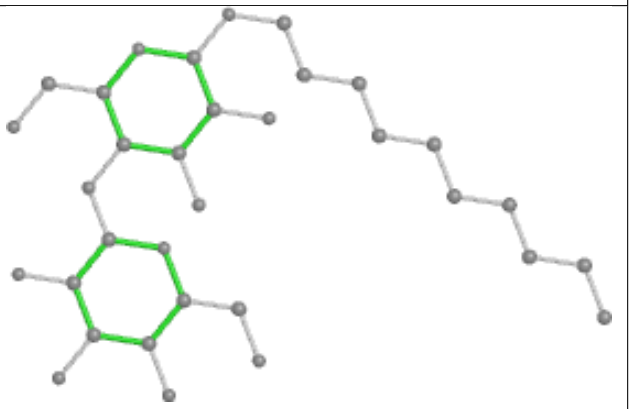
Bond lengths



Bond angles

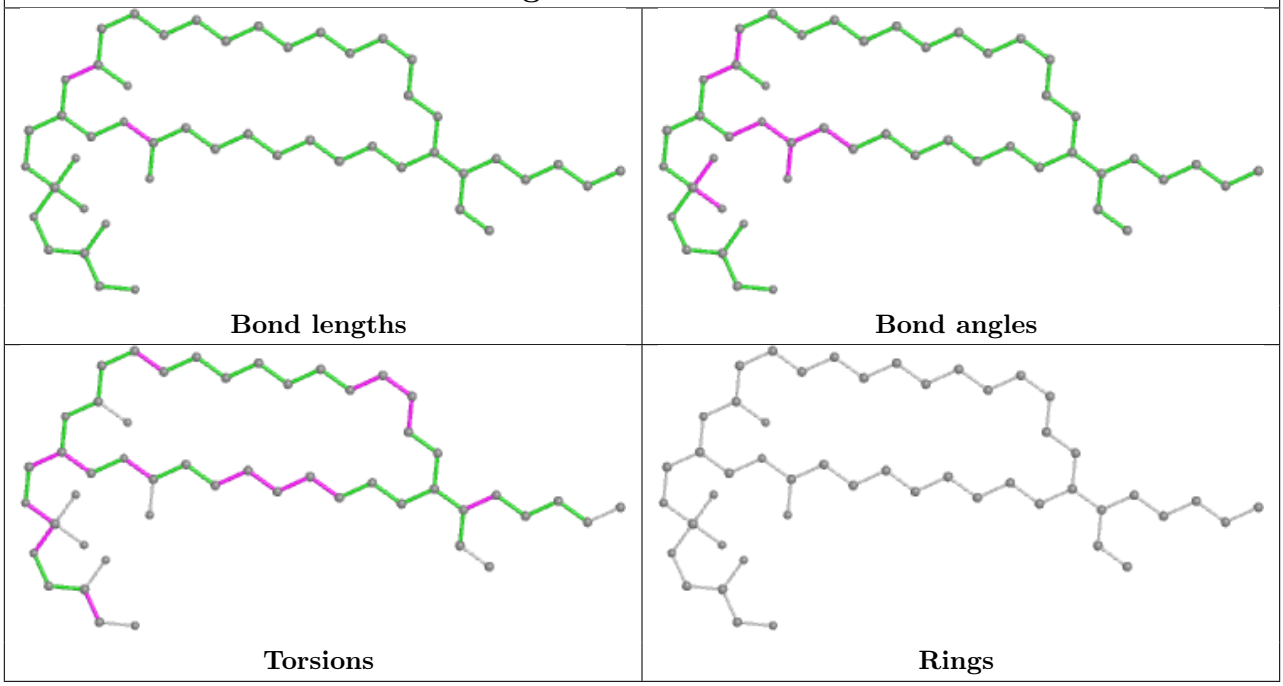


Torsions

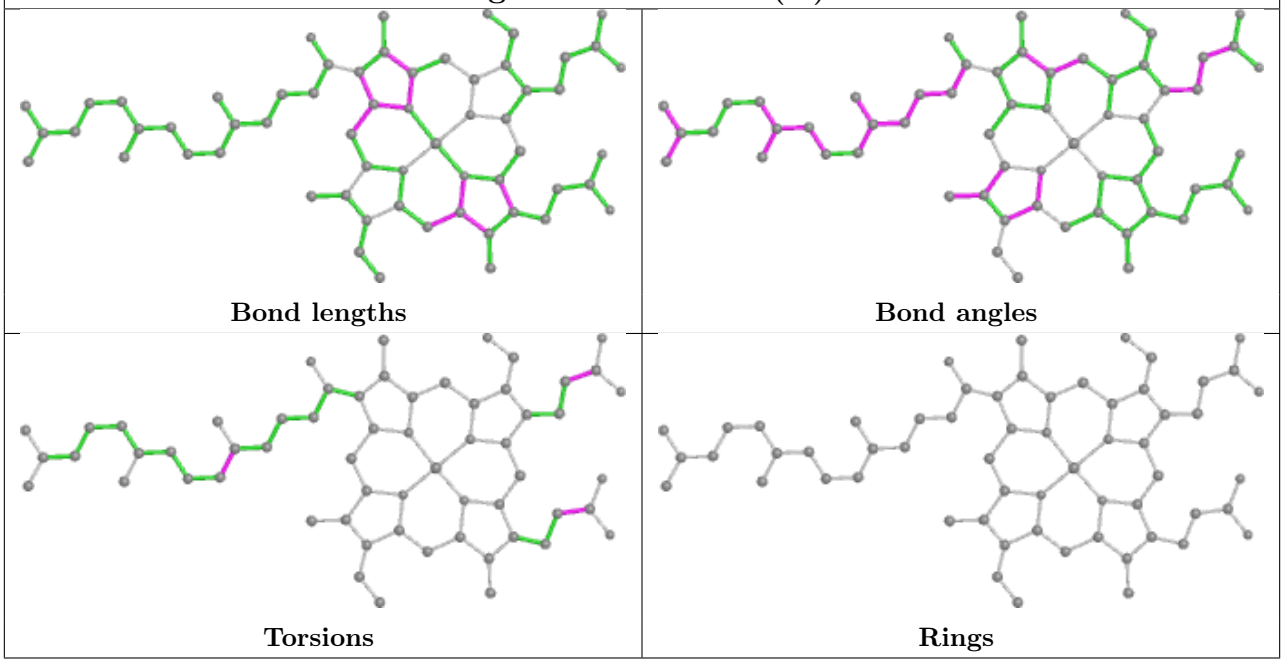


Rings

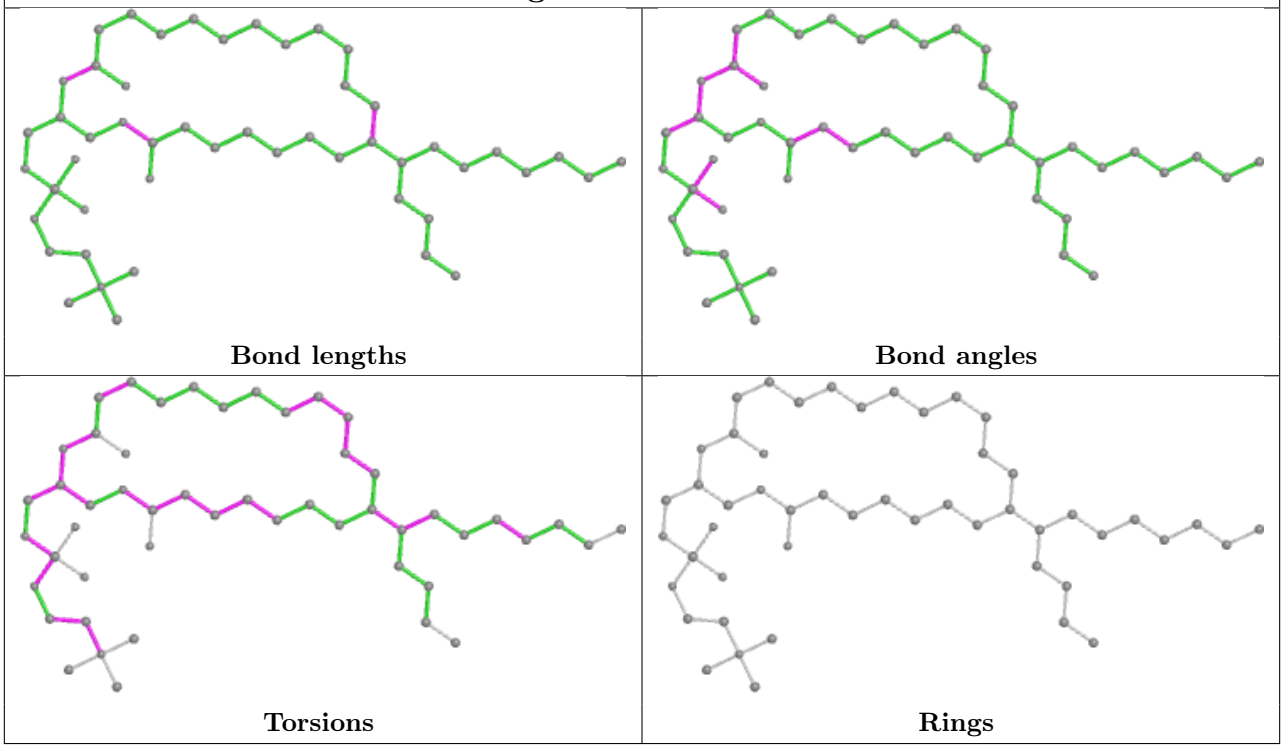
Ligand PGV C 307



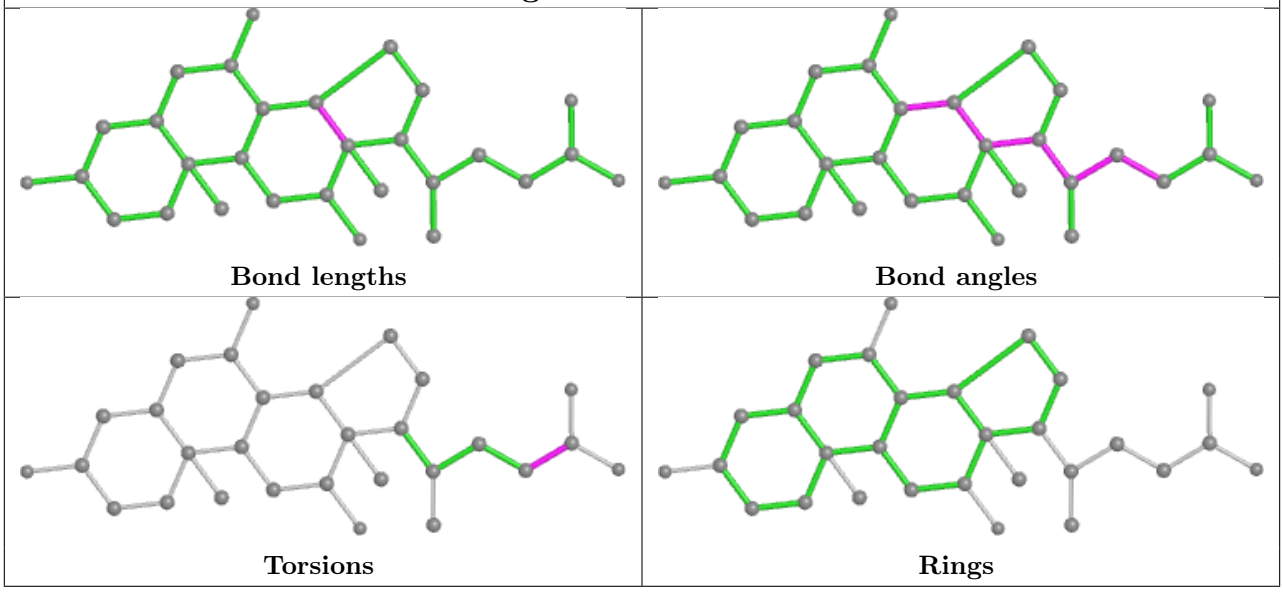
Ligand HEA N 601 (D)



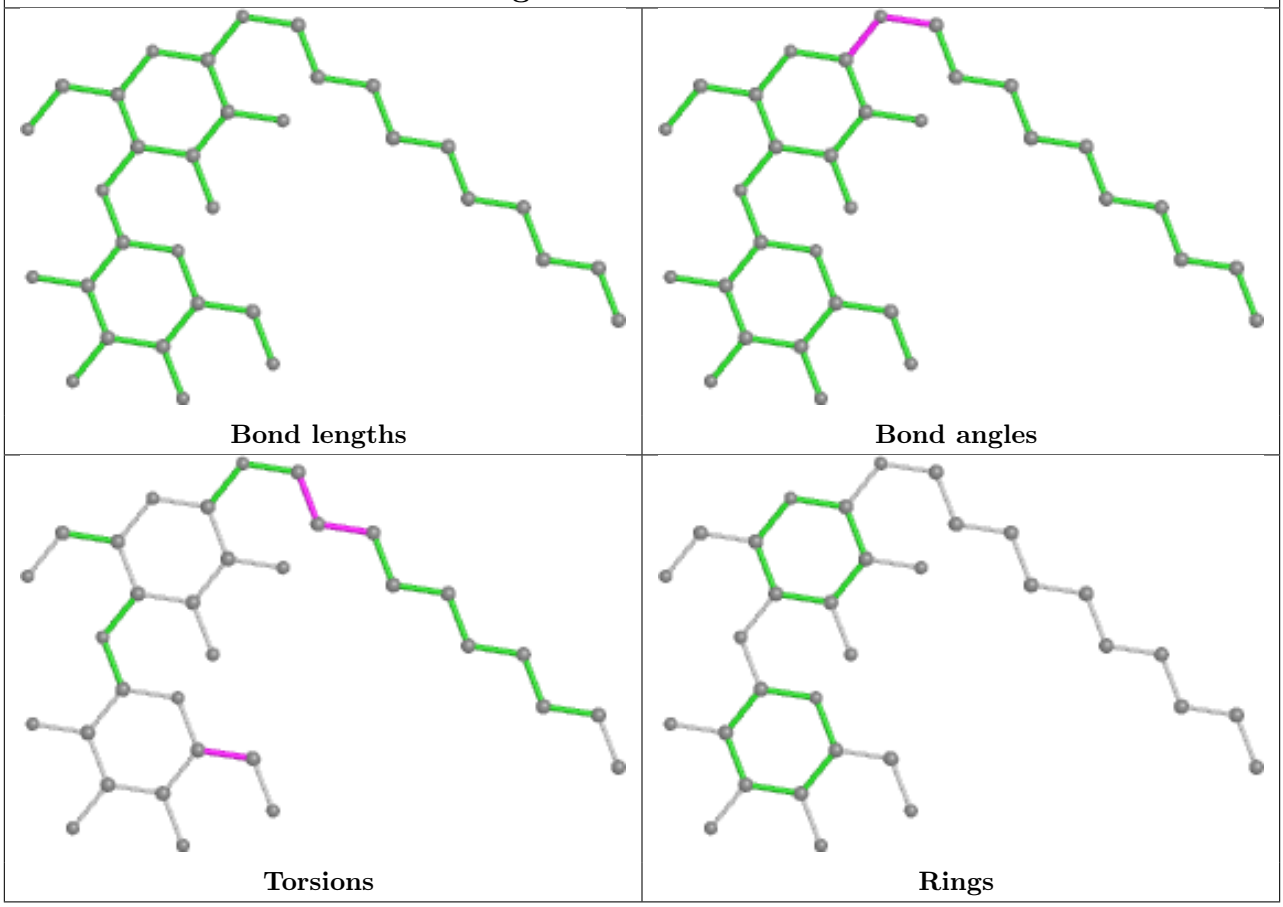
Ligand PSC B 603



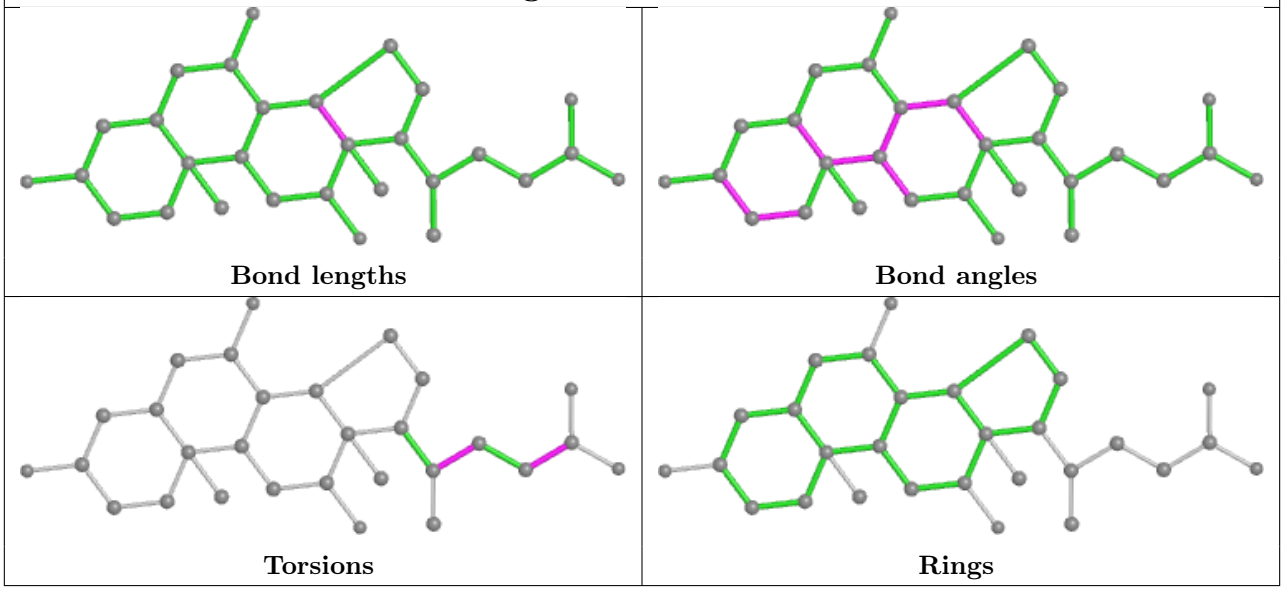
Ligand CHD B 602



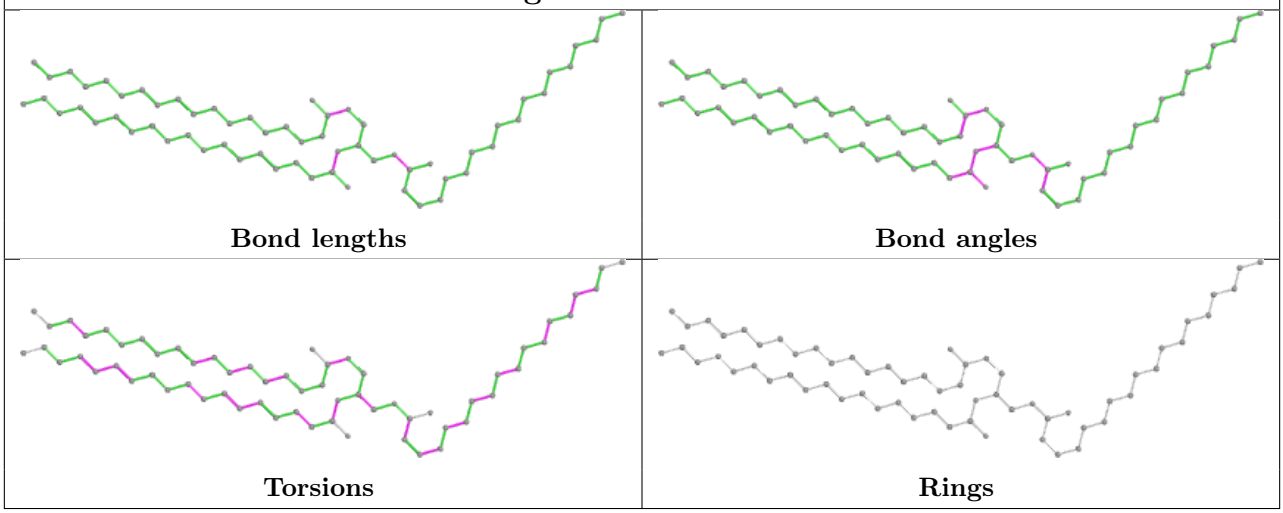
Ligand DMU W 101



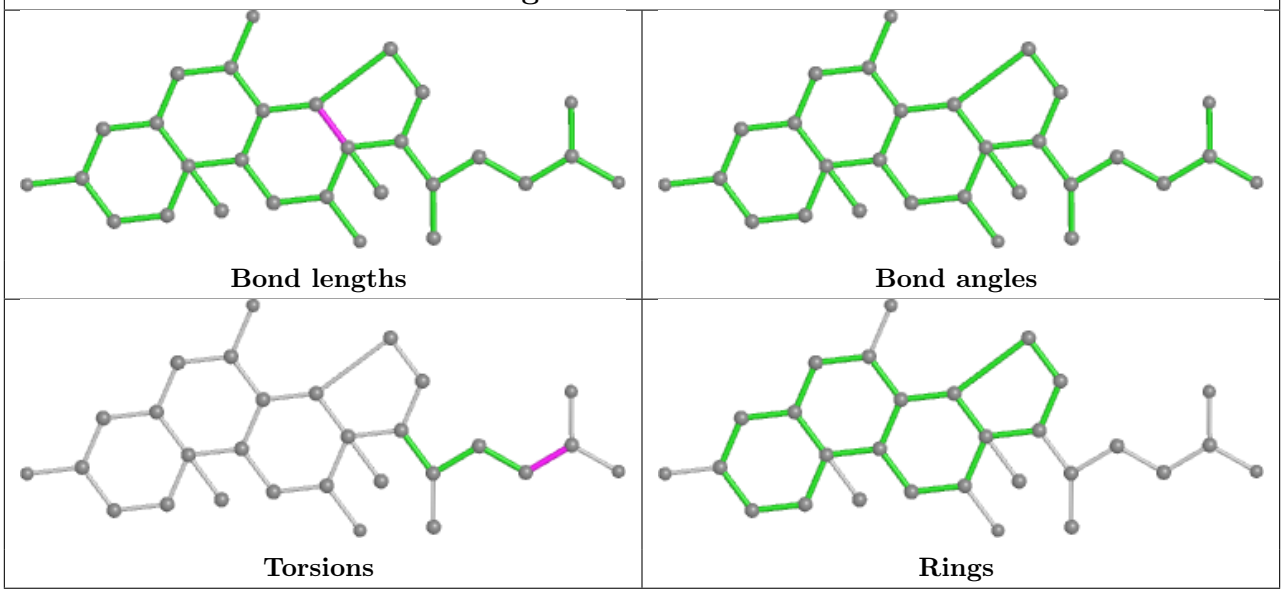
Ligand CHD P 305



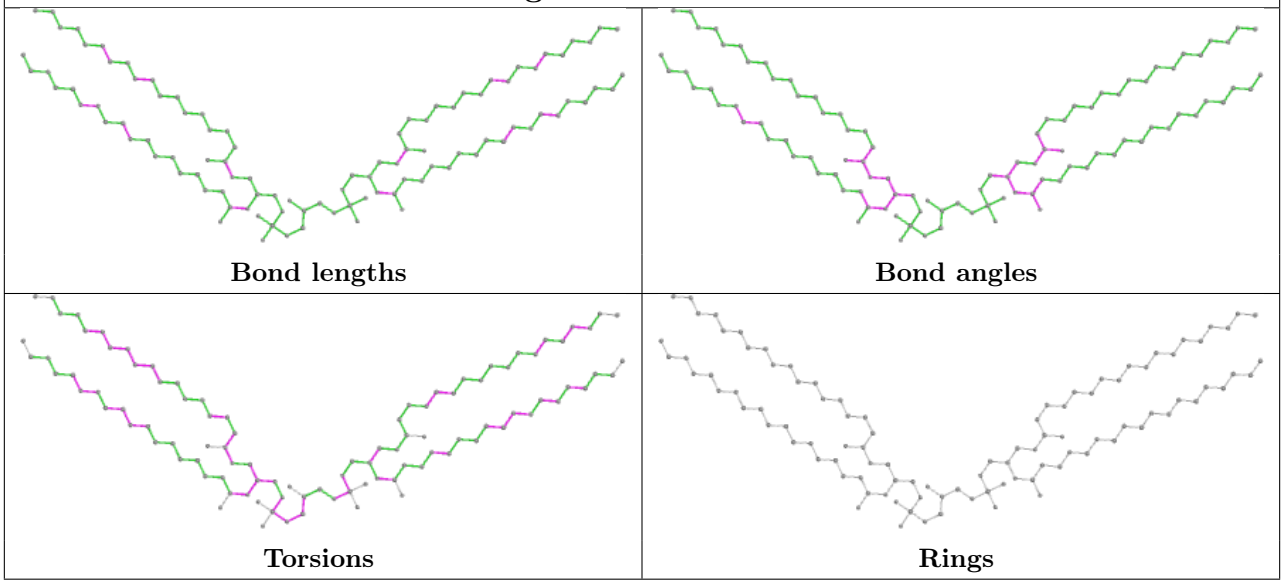
Ligand TGL N 608



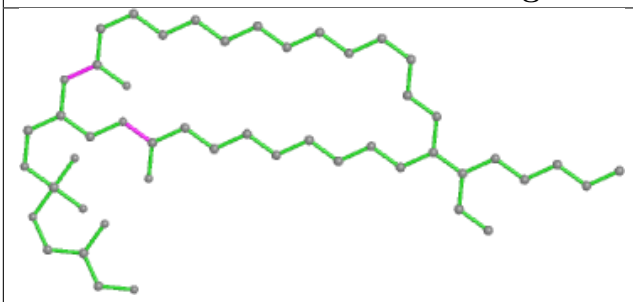
Ligand CHD C 305



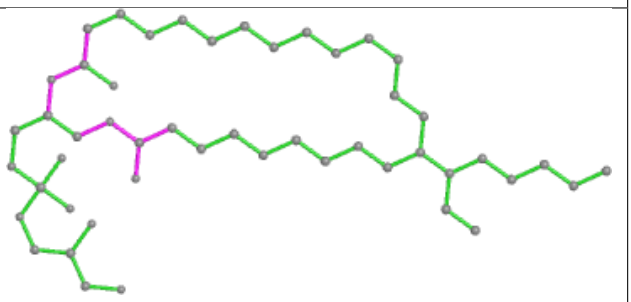
Ligand CDL C 303



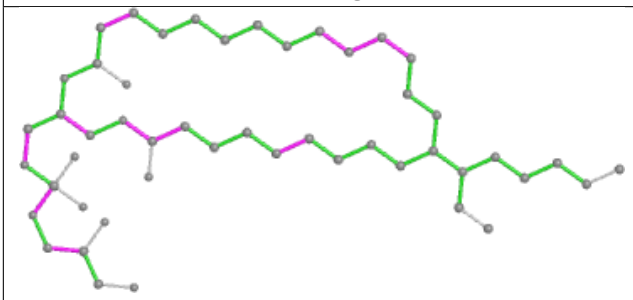
Ligand PGV P 303



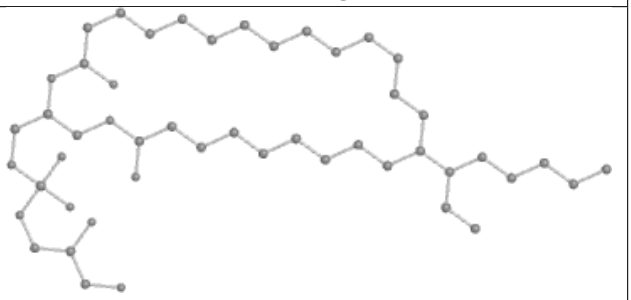
Bond lengths



Bond angles

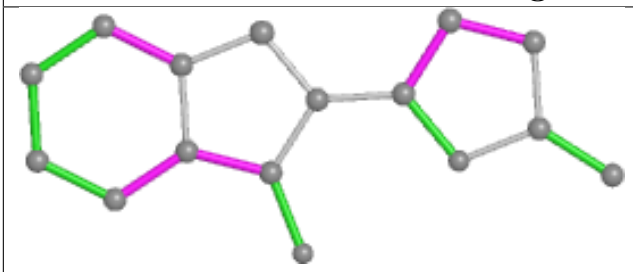


Torsions

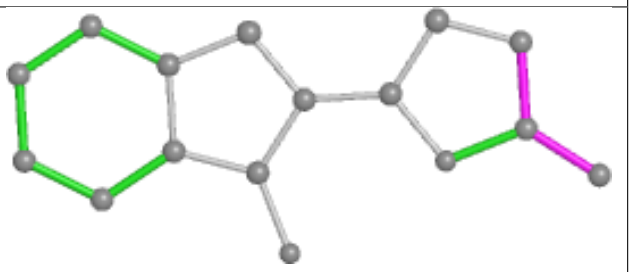


Rings

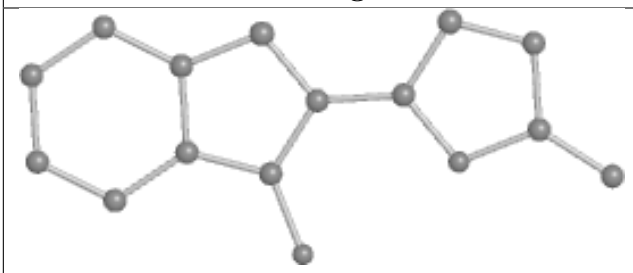
Ligand J6X A 608



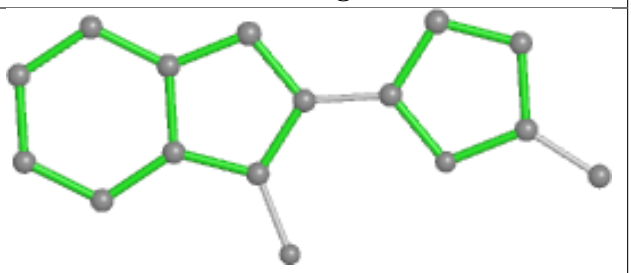
Bond lengths



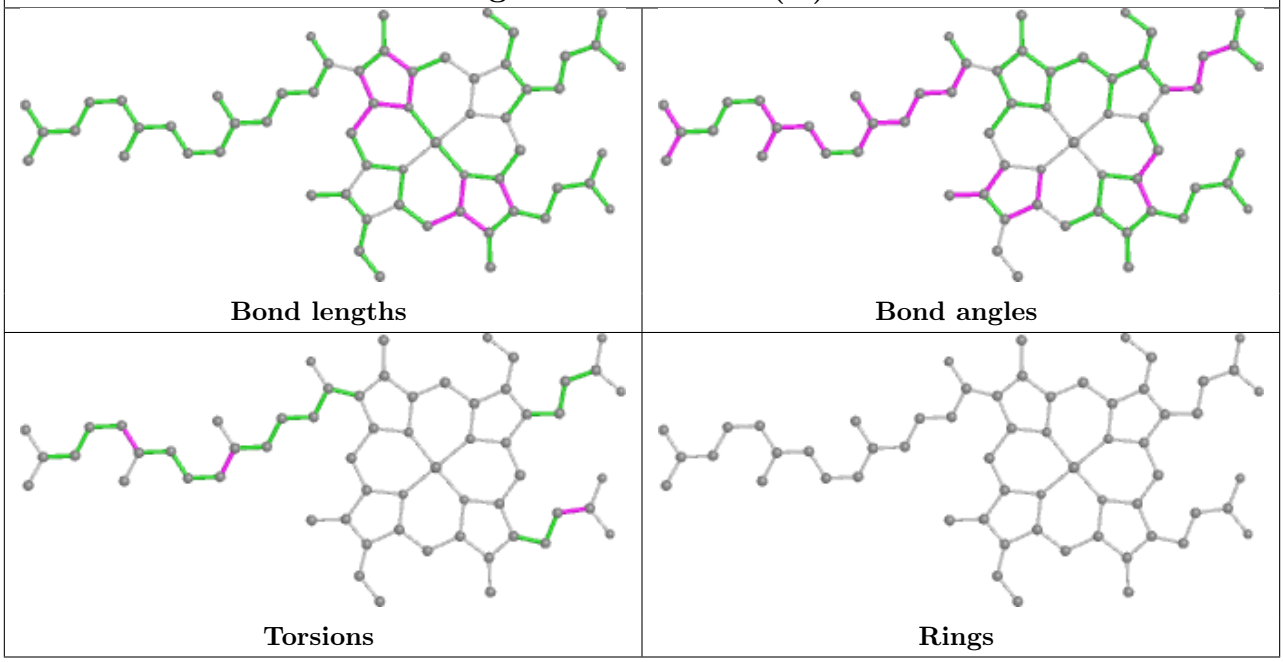
Bond angles



Torsions



Rings

Ligand HEA A 601 (D)	
 Bond lengths	Bond angles
Torsions	Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	513/514 (99%)	-0.50	2 (0%)	92	91	20, 27, 37, 94	0
1	N	513/514 (99%)	-0.44	5 (0%)	82	81	20, 29, 40, 81	0
2	B	226/581 (38%)	-0.22	6 (2%)	54	52	22, 35, 63, 118	0
2	O	226/581 (38%)	-0.12	9 (3%)	38	36	28, 40, 68, 122	0
3	C	259/261 (99%)	-0.52	2 (0%)	86	85	22, 30, 46, 95	0
3	P	259/261 (99%)	-0.45	2 (0%)	86	85	23, 31, 48, 91	0
4	D	144/147 (97%)	-0.42	2 (1%)	75	73	27, 37, 60, 96	0
4	Q	139/147 (94%)	0.12	8 (5%)	23	22	34, 49, 78, 126	0
5	E	105/109 (96%)	-0.23	3 (2%)	51	49	28, 37, 65, 125	0
5	R	105/109 (96%)	0.13	7 (6%)	17	16	32, 45, 75, 139	0
6	F	93/98 (94%)	-0.12	5 (5%)	25	24	25, 38, 65, 120	0
6	S	96/98 (97%)	-0.04	8 (8%)	11	10	24, 37, 74, 105	0
7	G	81/84 (96%)	0.59	17 (20%)	1	1	26, 39, 121, 185	0
7	T	81/84 (96%)	0.68	18 (22%)	0	0	26, 42, 118, 163	0
8	H	79/85 (92%)	0.05	9 (11%)	5	4	29, 39, 113, 130	0
8	U	79/85 (92%)	0.31	9 (11%)	5	4	33, 44, 123, 153	0
9	I	72/73 (98%)	0.38	7 (9%)	7	6	34, 48, 74, 94	0
9	V	72/73 (98%)	0.62	10 (13%)	2	2	33, 54, 84, 112	0
10	J	57/59 (96%)	0.05	5 (8%)	10	8	30, 42, 79, 90	0
10	W	57/59 (96%)	0.03	3 (5%)	26	25	30, 43, 78, 116	0
11	K	51/56 (91%)	0.32	3 (5%)	22	21	33, 41, 63, 87	0
11	X	49/56 (87%)	0.60	5 (10%)	6	6	41, 50, 75, 83	0
12	L	46/47 (97%)	-0.50	1 (2%)	62	59	26, 33, 54, 112	0
12	Y	45/47 (95%)	-0.41	0	100	100	30, 40, 66, 79	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
13	M	43/46 (93%)	-0.09	5 (11%)	4	4	28, 33, 81, 127	0
13	Z	41/46 (89%)	-0.02	5 (12%)	4	3	36, 42, 76, 89	0
All	All	3531/4320 (81%)	-0.19	156 (4%)	34	32	20, 35, 70, 185	0

The worst 5 of 156 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	T	8	HIS	9.8
8	H	45	ALA	8.2
5	R	5	HIS	8.0
11	X	6	ALA	7.1
5	R	109	VAL	6.9

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	TPO	G	11	11/12	0.63	0.44	81,125,214,234	0
7	TPO	T	11	11/12	0.71	0.42	106,148,176,206	0
1	FME	N	1	10/11	0.90	0.25	42,45,80,87	0
1	FME	A	1	10/11	0.95	0.30	40,50,64,117	0
2	FME	B	1	10/11	0.97	0.18	29,33,43,90	0
2	FME	O	1	10/11	0.97	0.14	32,40,48,69	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
24	PEK	C	309	53/53	0.49	0.49	38,93,179,194	0
24	PEK	C	306	53/53	0.51	0.34	42,80,164,192	0
24	PEK	B	604	53/53	0.51	0.38	45,88,160,182	0
22	CHD	P	305	29/29	0.53	0.39	67,107,138,141	0
22	CHD	C	304	29/29	0.59	0.45	77,111,137,141	0
23	PSC	B	603	52/52	0.60	0.37	42,121,226,245	0
24	PEK	P	301	53/53	0.61	0.30	46,91,158,171	0
26	CDL	T	101	100/100	0.63	0.33	47,91,167,201	0
19	TGL	Y	101	63/63	0.64	0.28	35,66,126,160	0
26	CDL	G	102	100/100	0.65	0.37	53,101,153,190	0
27	DMU	C	308	33/33	0.65	0.35	43,87,112,117	0
23	PSC	O	603	52/52	0.66	0.37	39,92,202,217	0
26	CDL	P	304	100/100	0.66	0.31	35,86,132,143	0
25	PGV	P	302	51/51	0.68	0.31	53,88,141,169	0
25	PGV	N	610	51/51	0.70	0.37	36,86,170,185	0
27	DMU	W	101	33/33	0.70	0.38	42,80,102,106	0
26	CDL	C	303	100/100	0.71	0.33	39,84,145,168	0
19	TGL	Q	201	63/63	0.71	0.23	40,80,119,139	0
19	TGL	L	101	63/63	0.75	0.22	39,58,106,124	0
27	DMU	Z	101	33/33	0.76	0.31	40,56,78,86	0
25	PGV	C	307	51/51	0.77	0.32	39,89,133,173	0
19	TGL	A	607	63/63	0.78	0.22	39,77,104,126	0
27	DMU	M	101	33/33	0.78	0.26	30,46,66,80	0
20	J6X	A	608	16/16	0.78	0.43	38,55,103,128	16
20	J6X	N	611	16/16	0.78	0.33	31,52,82,113	16
19	TGL	N	608	63/63	0.79	0.22	39,77,118,138	0
19	TGL	D	202	63/63	0.81	0.20	41,71,106,123	0
25	PGV	D	201	51/51	0.81	0.29	29,78,125,170	0
24	PEK	P	306	53/53	0.89	0.23	30,49,100,115	0
25	PGV	P	303	51/51	0.90	0.26	23,40,95,105	0
22	CHD	C	305	29/29	0.90	0.11	20,32,40,51	0
25	PGV	C	302	51/51	0.90	0.29	21,41,85,88	0
22	CHD	N	609	29/29	0.91	0.11	22,35,45,47	0
24	PEK	G	101	53/53	0.91	0.23	28,52,111,133	0
22	CHD	O	602	29/29	0.94	0.09	17,26,37,46	0
14	HEA	A	601[C]	60/60	0.95	0.14	10,28,49,53	18
14	HEA	A	601[D]	60/60	0.95	0.14	6,28,44,55	18
14	HEA	N	601[C]	60/60	0.95	0.17	17,33,60,66	18
25	PGV	C	301	51/51	0.95	0.23	18,41,60,72	0
14	HEA	N	601[D]	60/60	0.95	0.17	7,28,41,43	18
22	CHD	B	602	29/29	0.95	0.08	16,27,39,50	0
28	ZN	S	101	1/1	0.95	0.14	25,25,25,25	0
14	HEA	A	602	60/60	0.96	0.12	15,24,39,44	0

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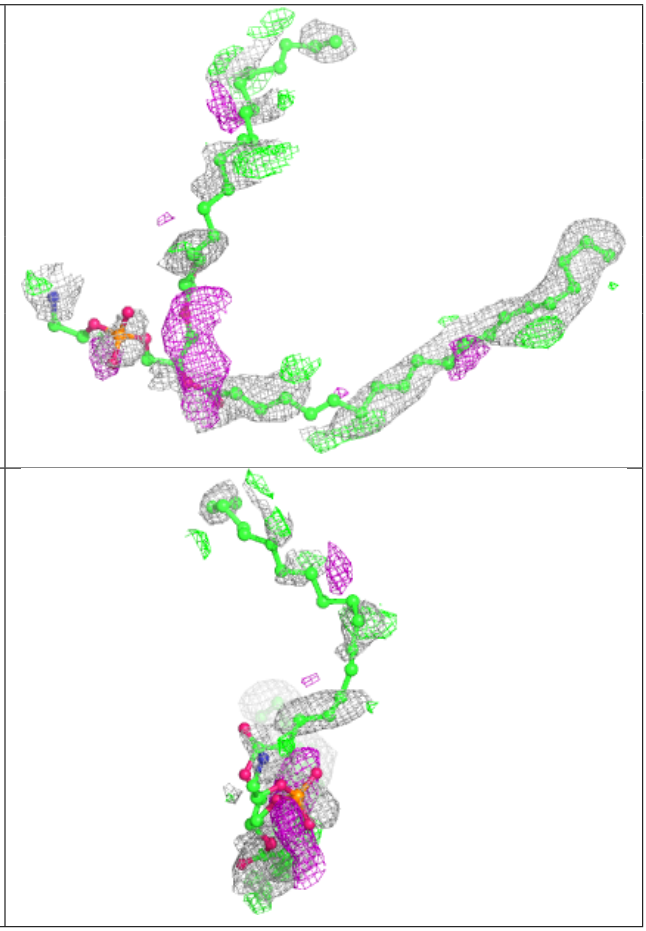
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	HEA	N	602	60/60	0.96	0.12	17,26,38,41	0
25	PGV	N	607	51/51	0.96	0.18	18,43,66,75	0
28	ZN	F	101	1/1	0.97	0.17	25,25,25,25	0
18	PER	N	606	2/2	0.97	0.25	50,50,50,61	0
16	MG	A	604	1/1	0.98	0.10	14,14,14,14	0
17	NA	N	605	1/1	0.98	0.08	19,19,19,19	0
18	PER	A	606	2/2	0.98	0.13	45,45,45,54	0
15	CU	N	603	1/1	0.98	0.03	20,20,20,20	0
16	MG	N	604	1/1	0.99	0.10	16,16,16,16	0
21	CUA	B	601	2/2	0.99	0.02	19,19,19,21	0
21	CUA	O	601	2/2	0.99	0.03	22,22,22,23	0
17	NA	A	605	1/1	0.99	0.07	16,16,16,16	0
15	CU	A	603	1/1	0.99	0.03	19,19,19,19	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.

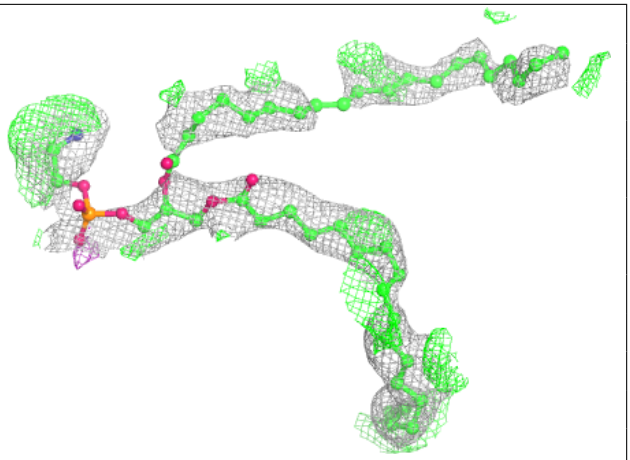
Electron density around PEK C 309:

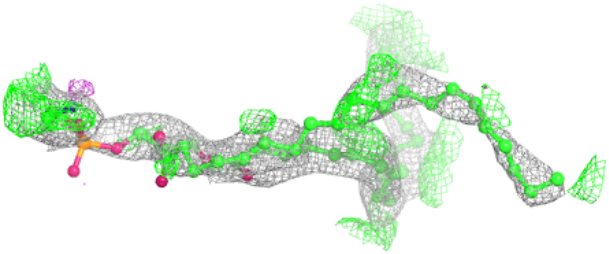
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around PEK C 306:

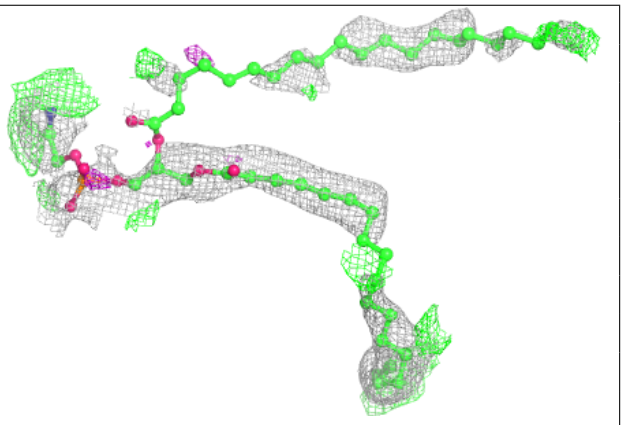
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

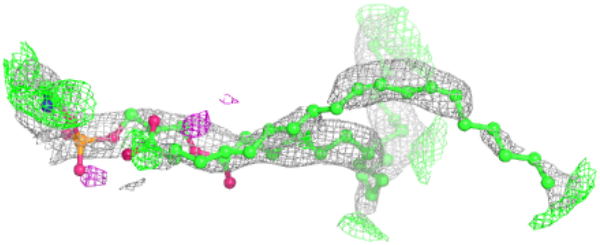


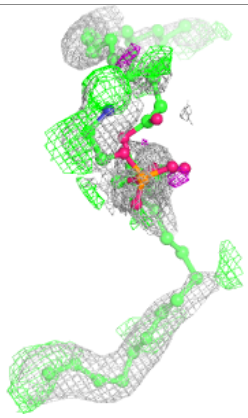


Electron density around PEK B 604:

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

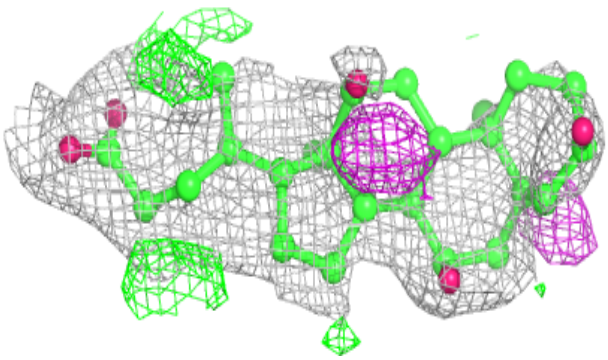


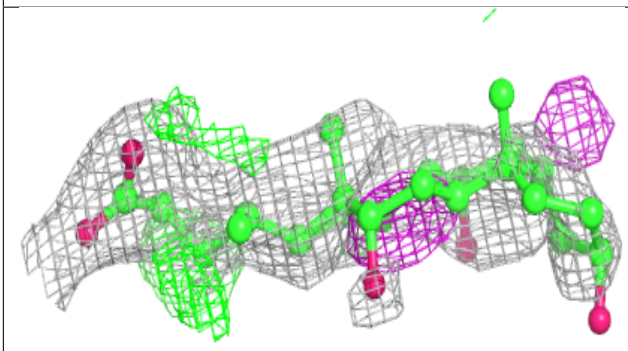


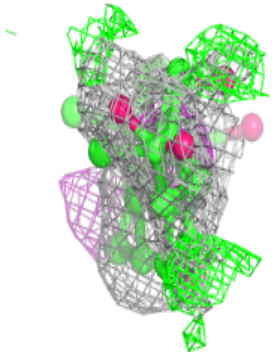


Electron density around CHD P 305:

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

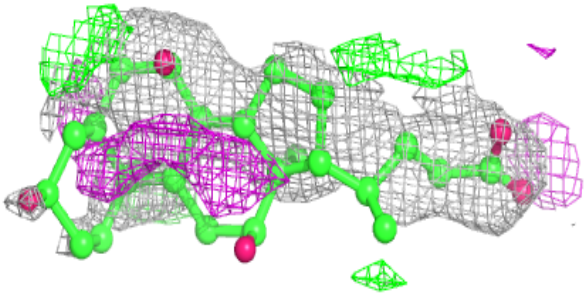


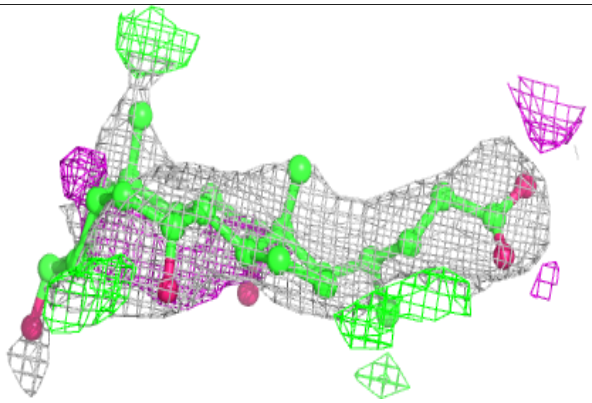


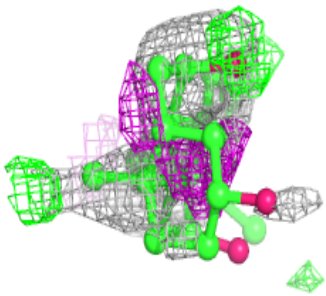


Electron density around CHD C 304:

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

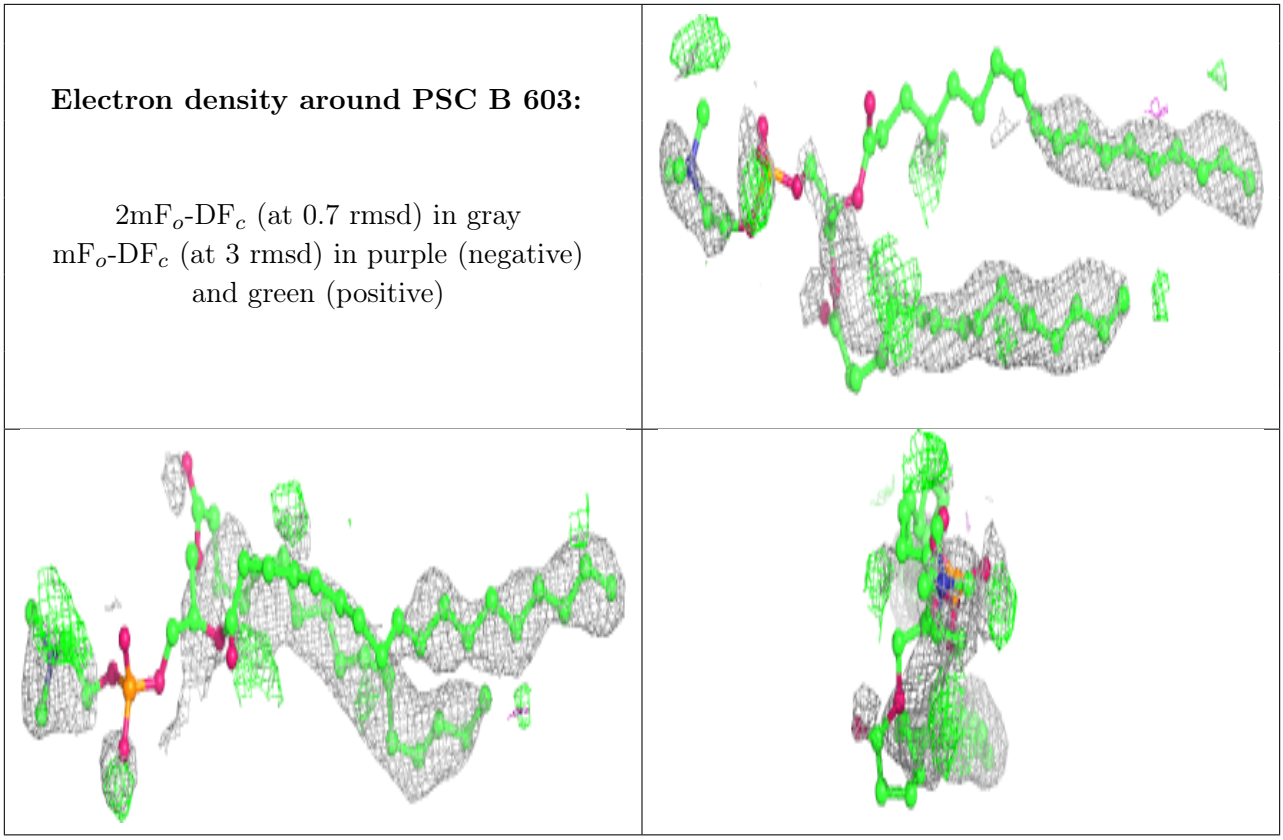






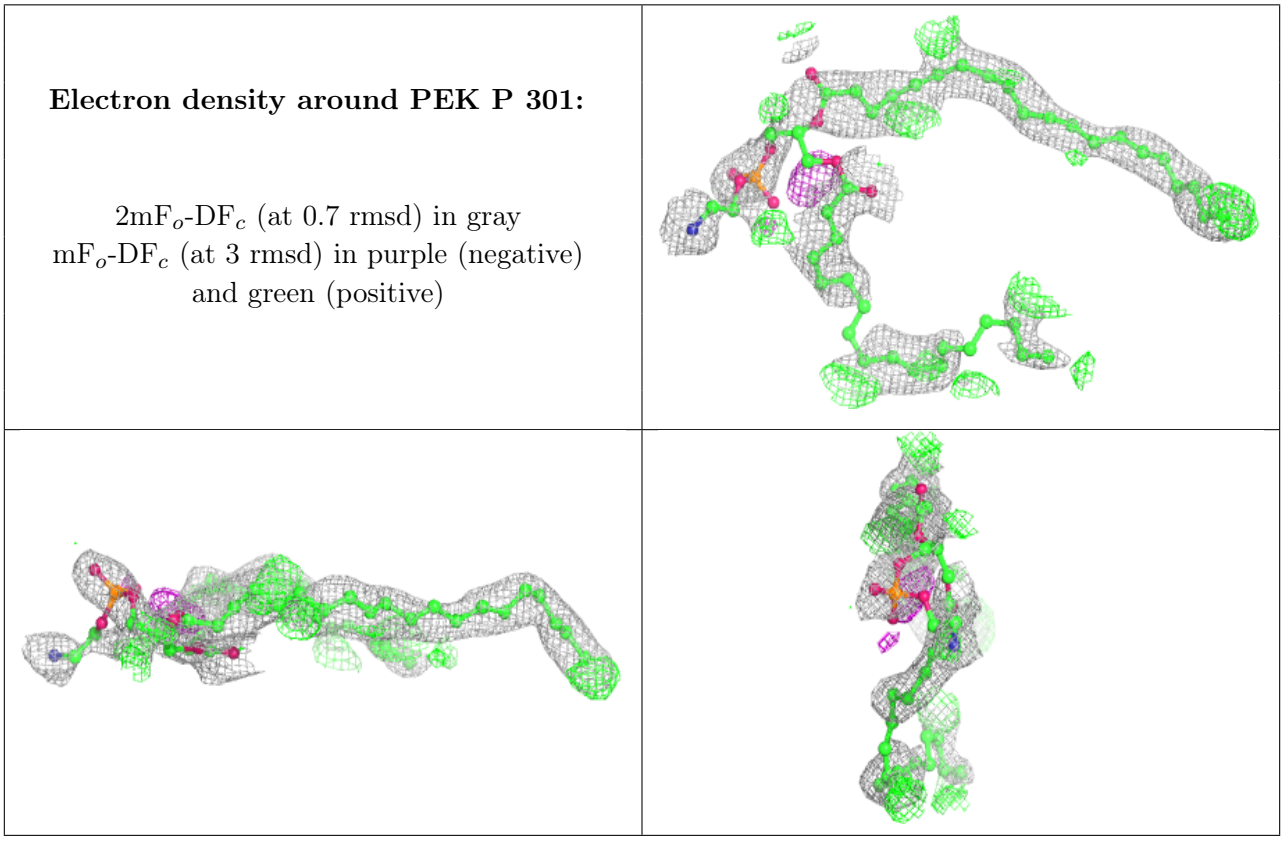
Electron density around PSC B 603:

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



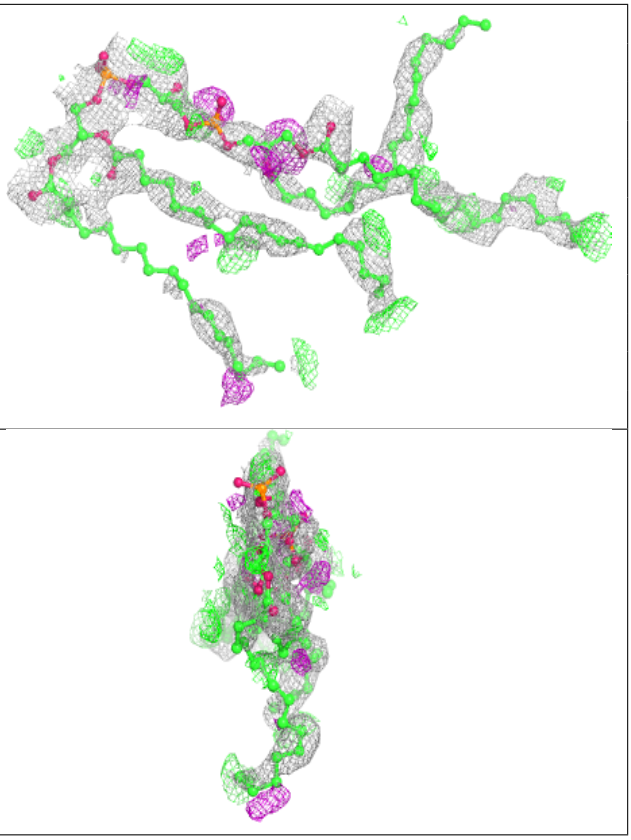
Electron density around PEK P 301:

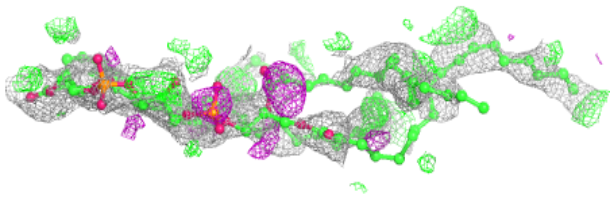
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CDL T 101:

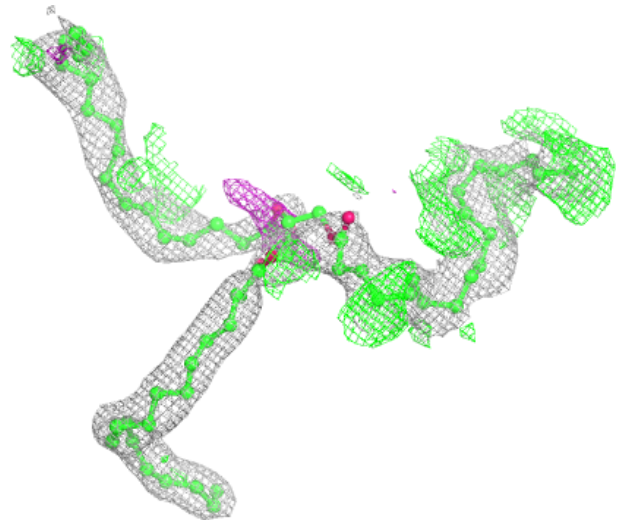
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

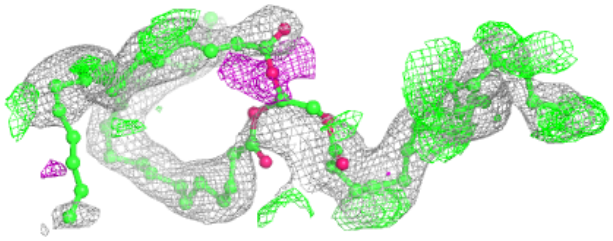


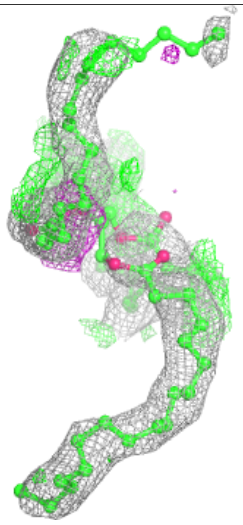


Electron density around TGL Y 101:

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

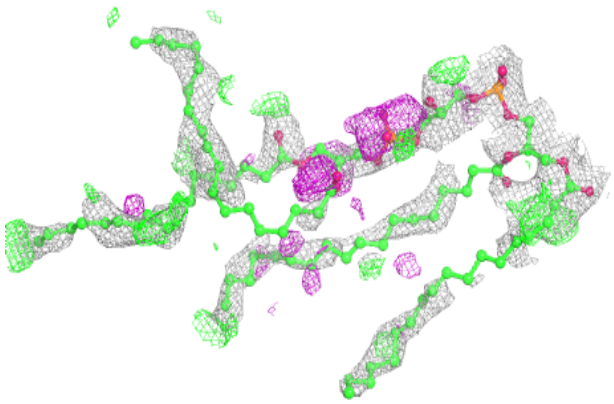


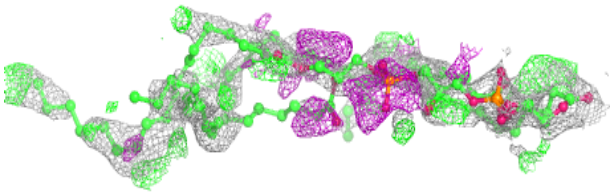


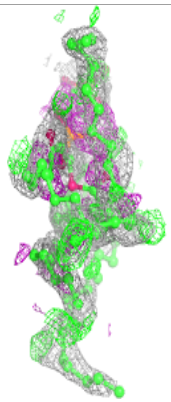


Electron density around CDL G 102:

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

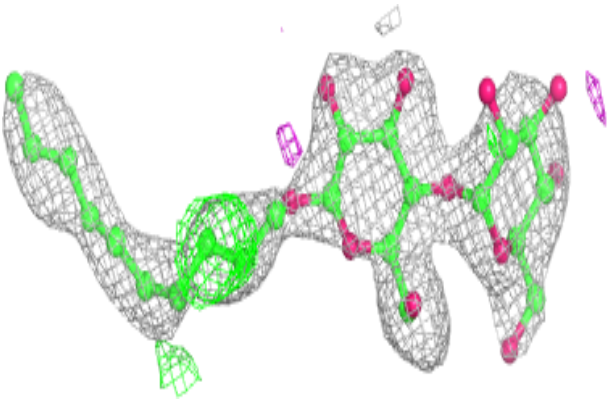


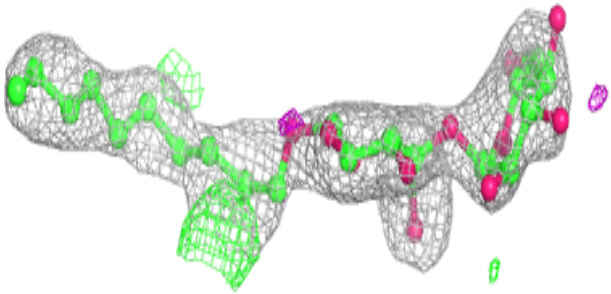


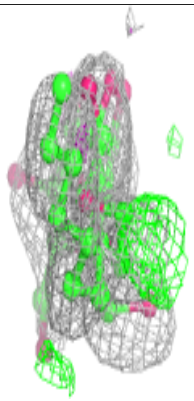


Electron density around DMU C 308:

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

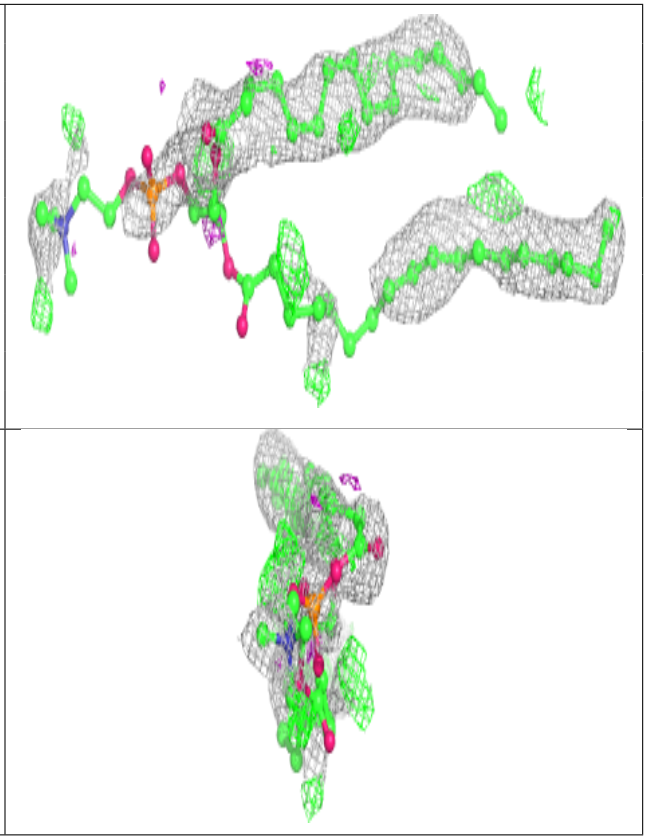


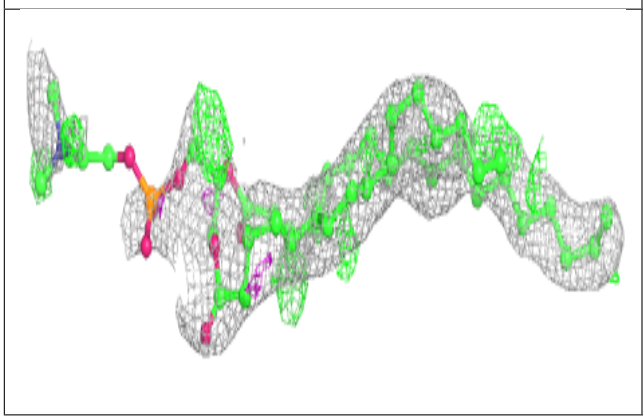




Electron density around PSC O 603:

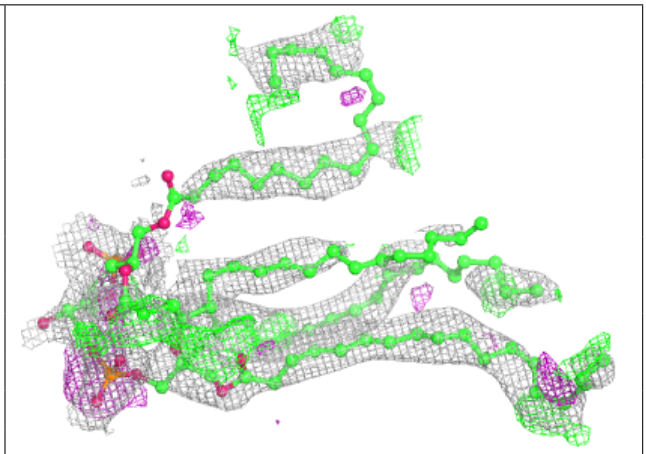
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

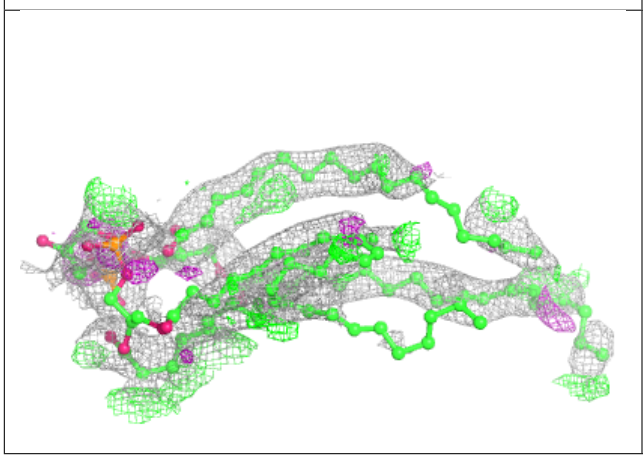


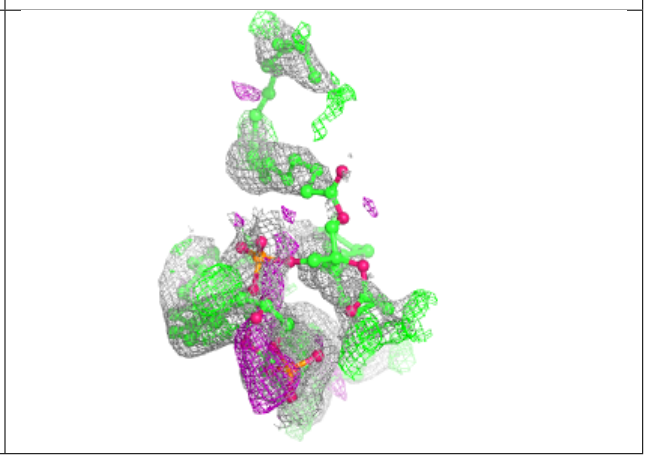


Electron density around CDL P 304:

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

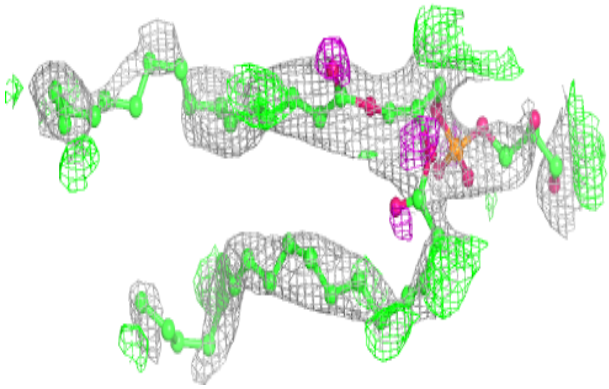


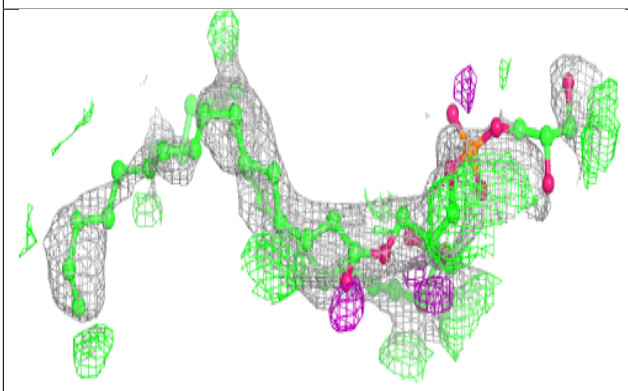


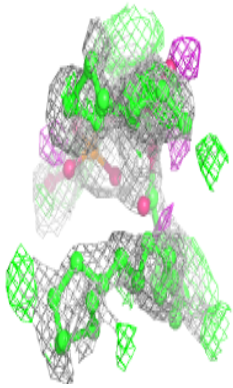


Electron density around PGV P 302:

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

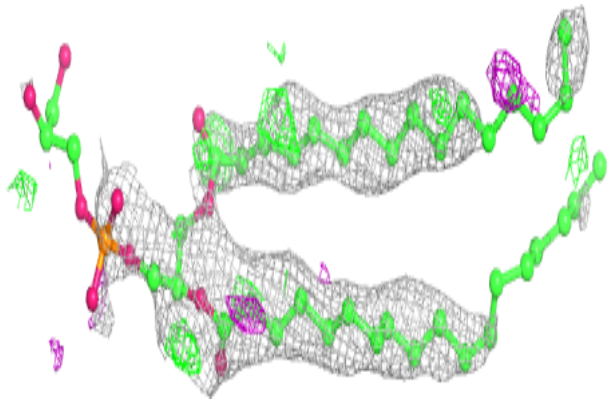


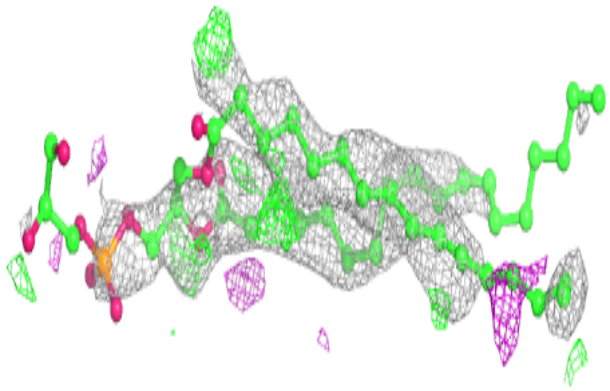


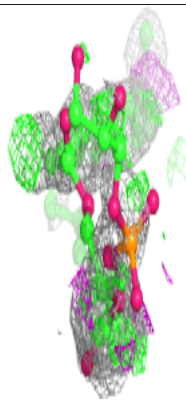


Electron density around PGV N 610:

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

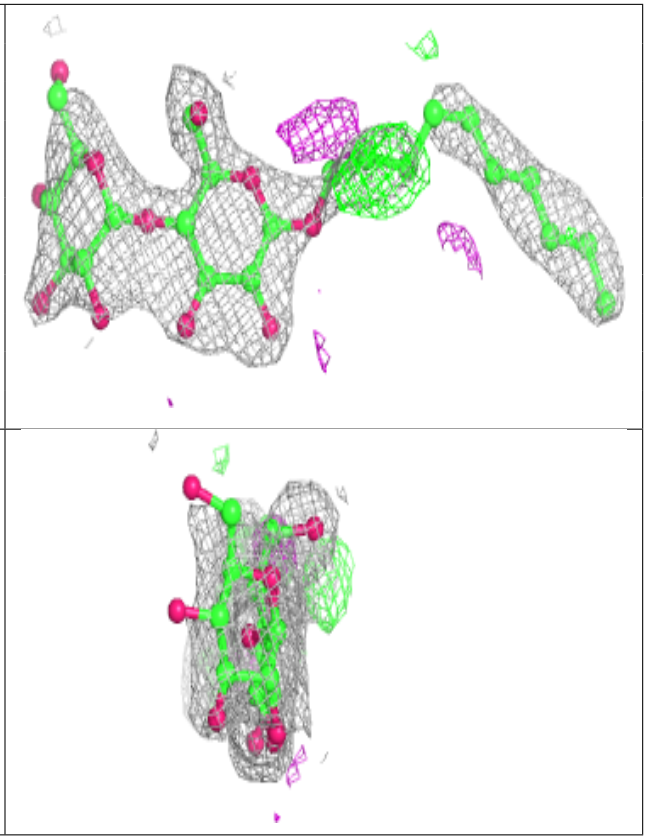






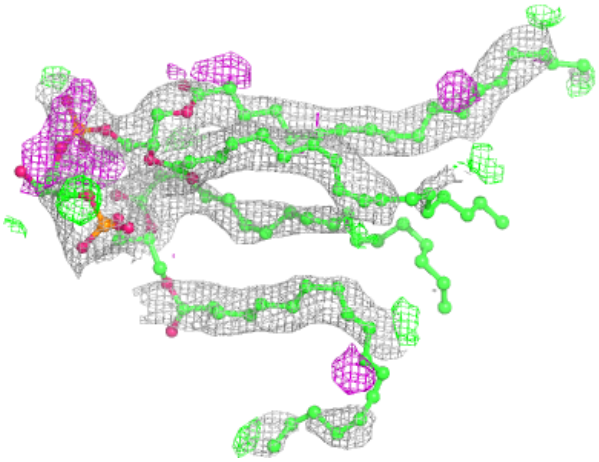
Electron density around DMU W 101:

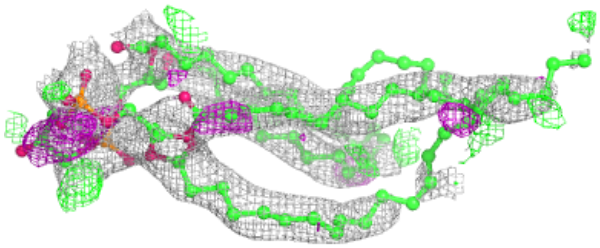
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

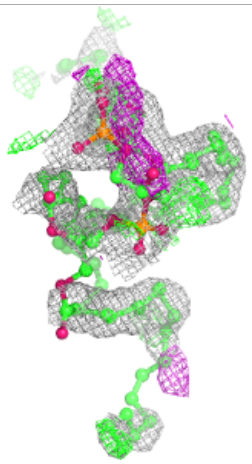


Electron density around CDL C 303:

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

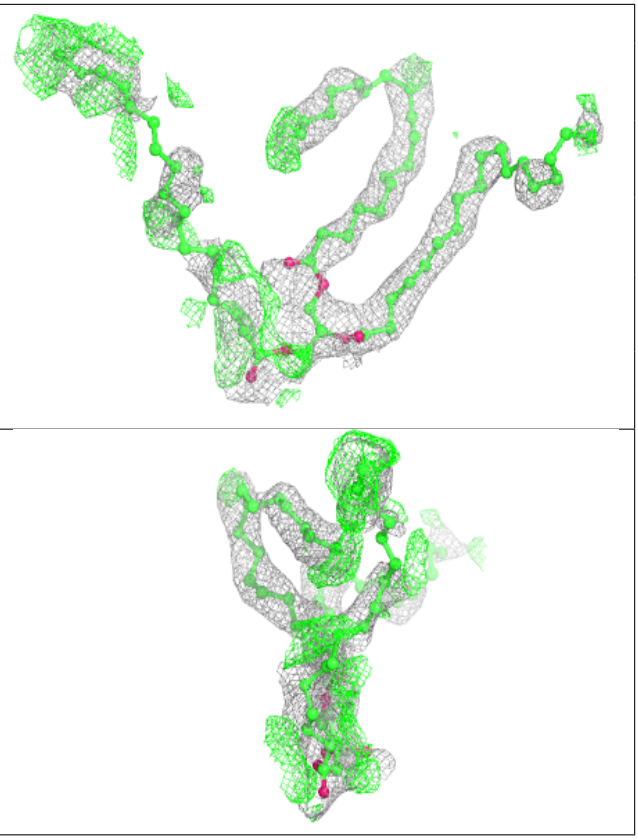


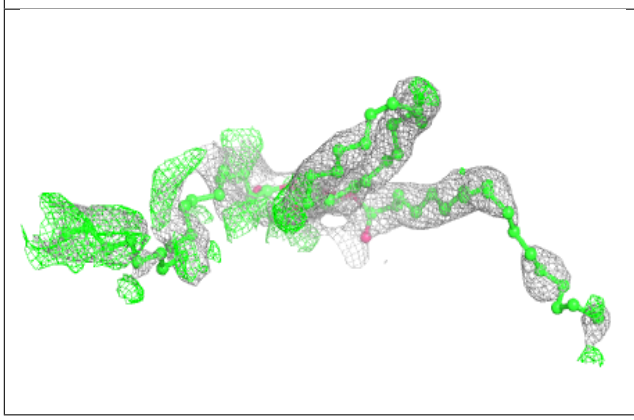




Electron density around TGL Q 201:

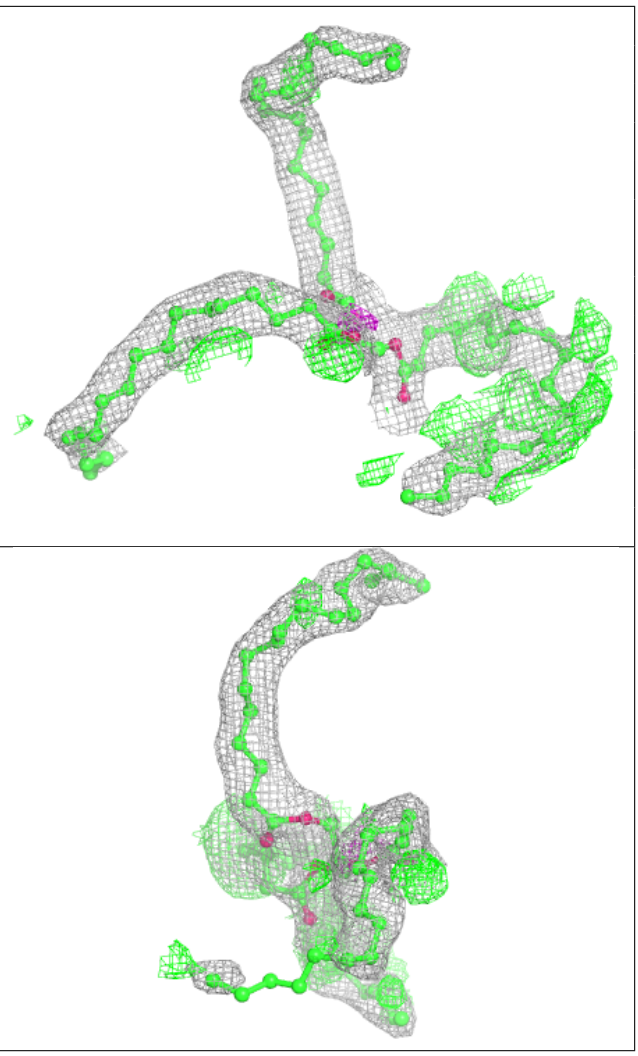
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





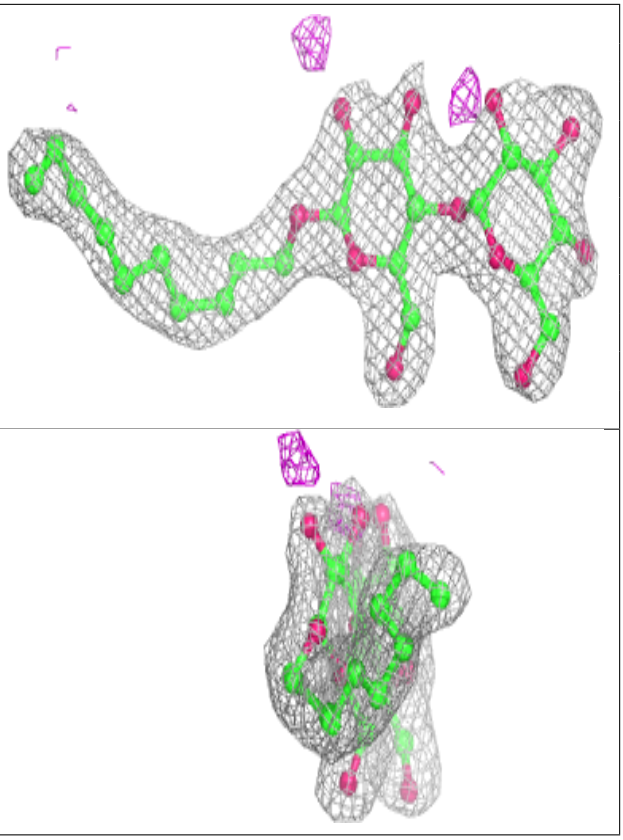
Electron density around TGL L 101:

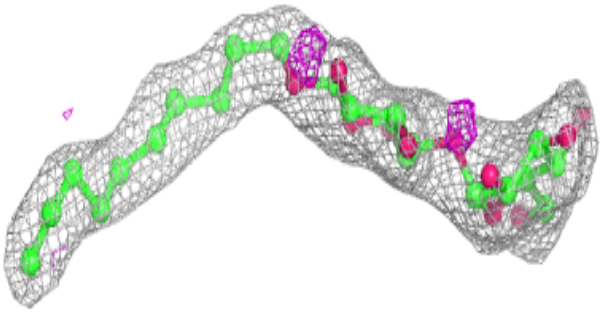
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around DMU Z 101:

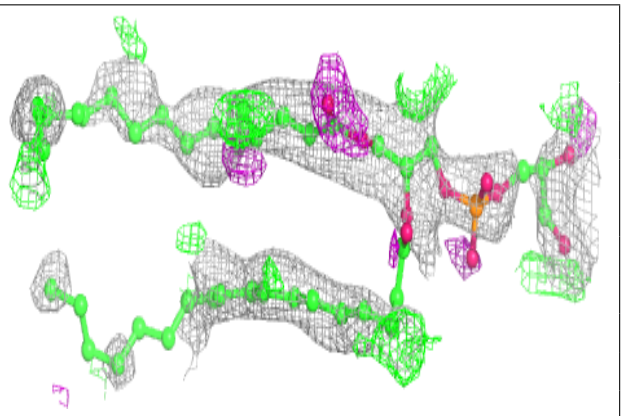
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

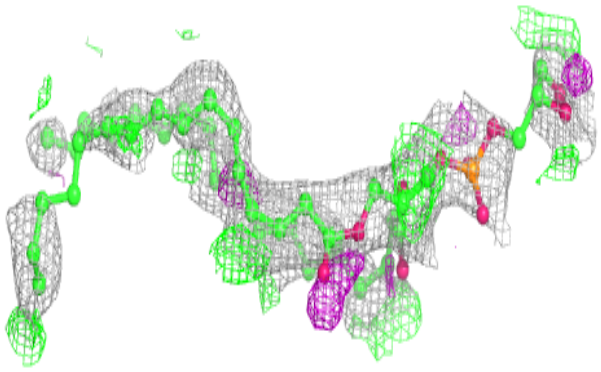


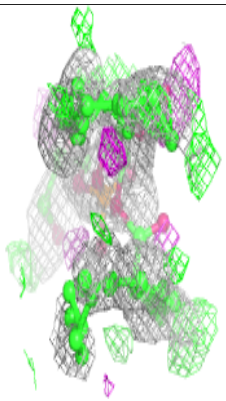


Electron density around PGV C 307:

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

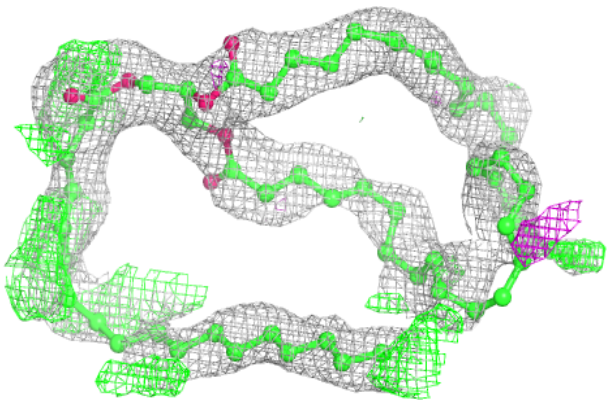


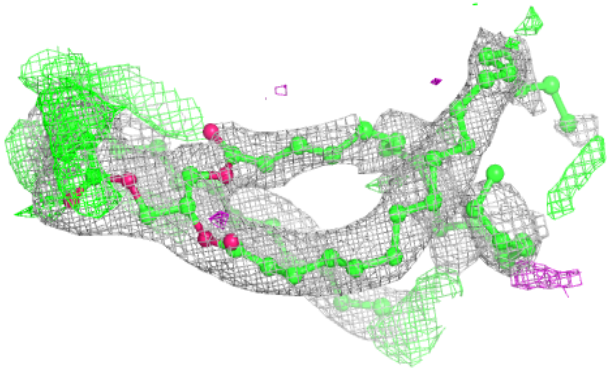


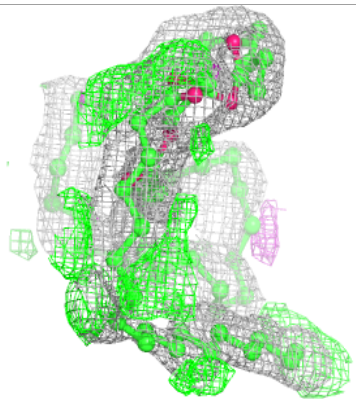


Electron density around TGL A 607:

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

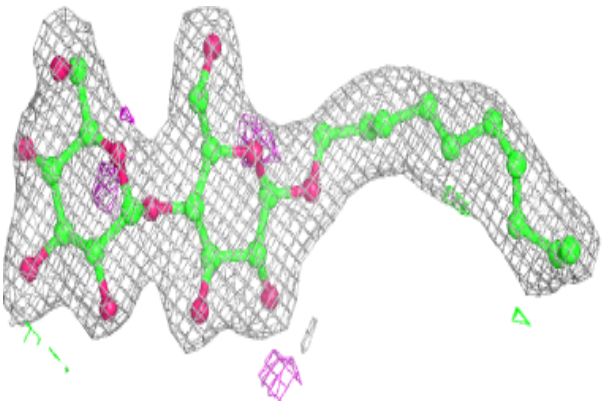


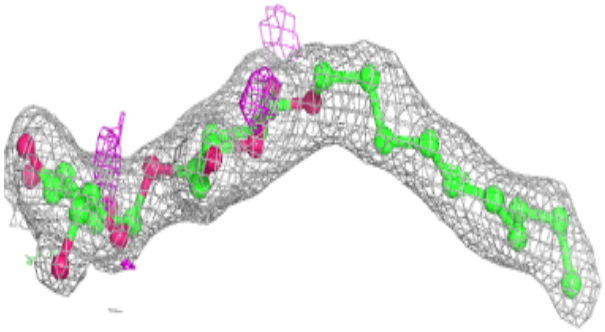


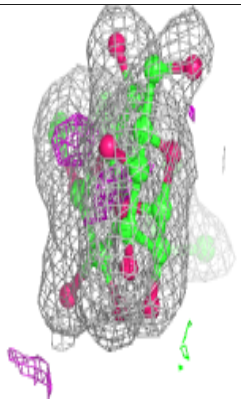


Electron density around DMU M 101:

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

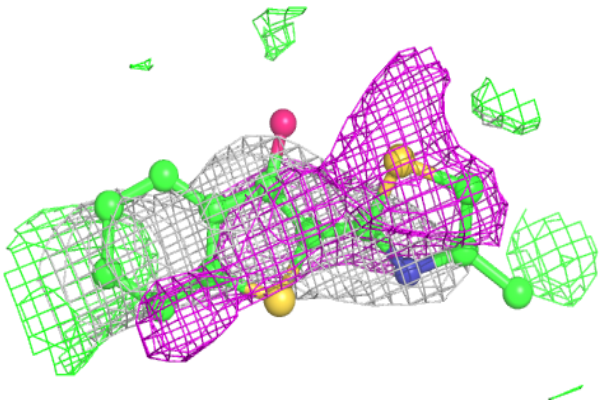


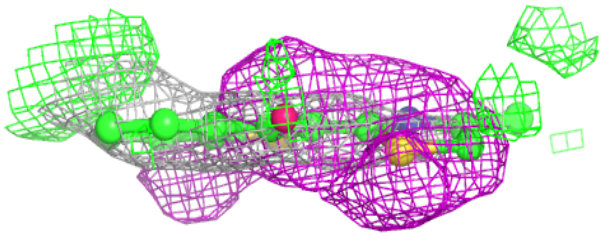


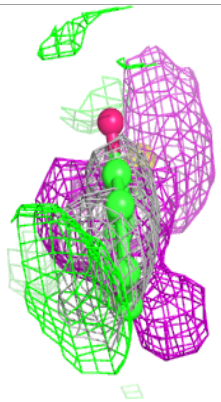


Electron density around J6X A 608:

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

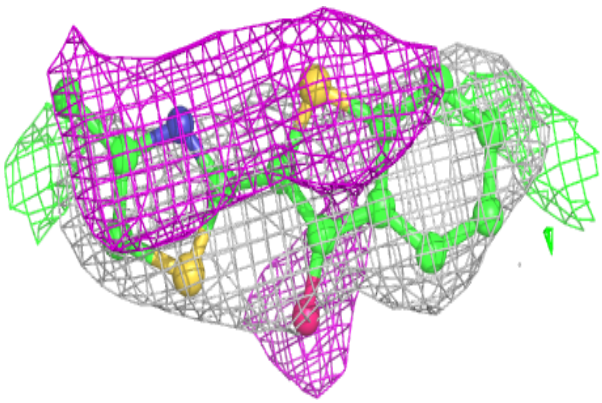


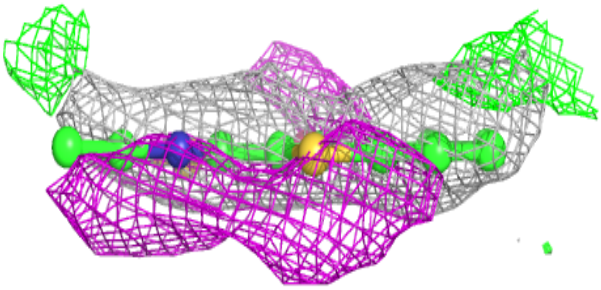


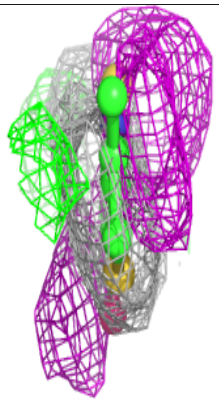


Electron density around J6X N 611:

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

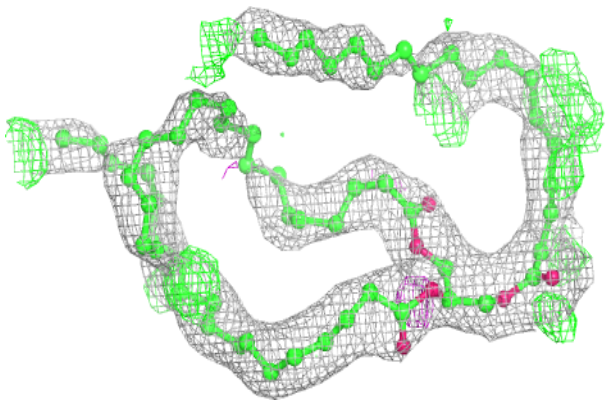


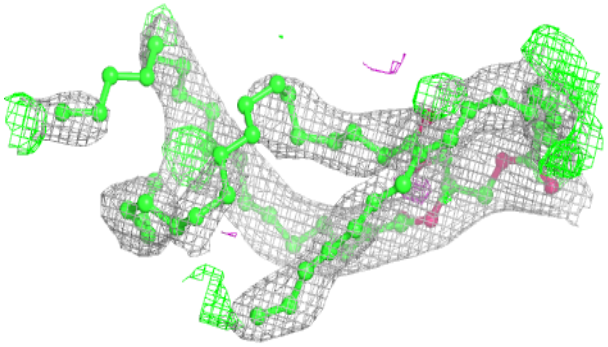


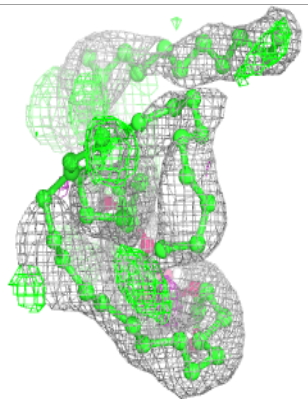


Electron density around TGL N 608:

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

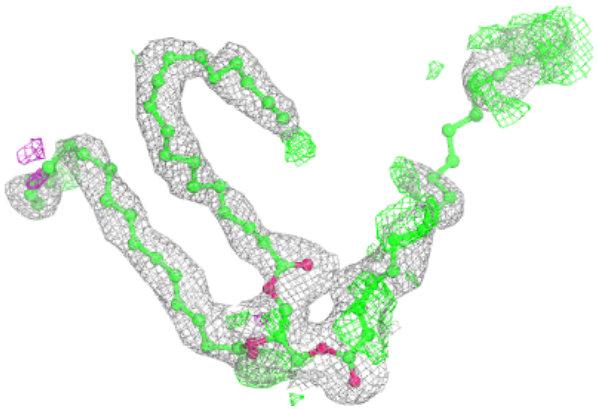


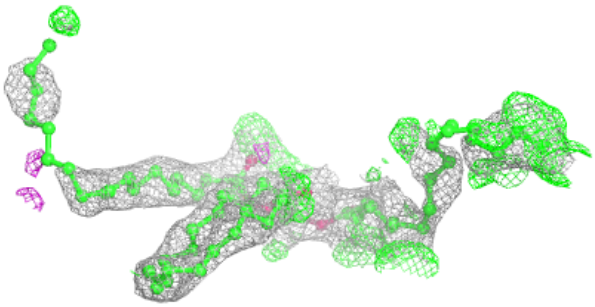


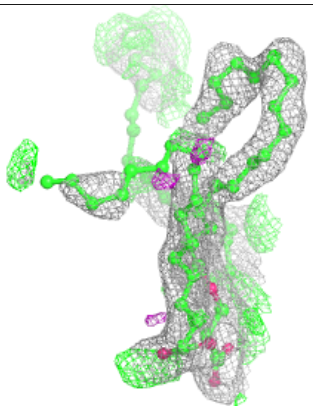


Electron density around TGL D 202:

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

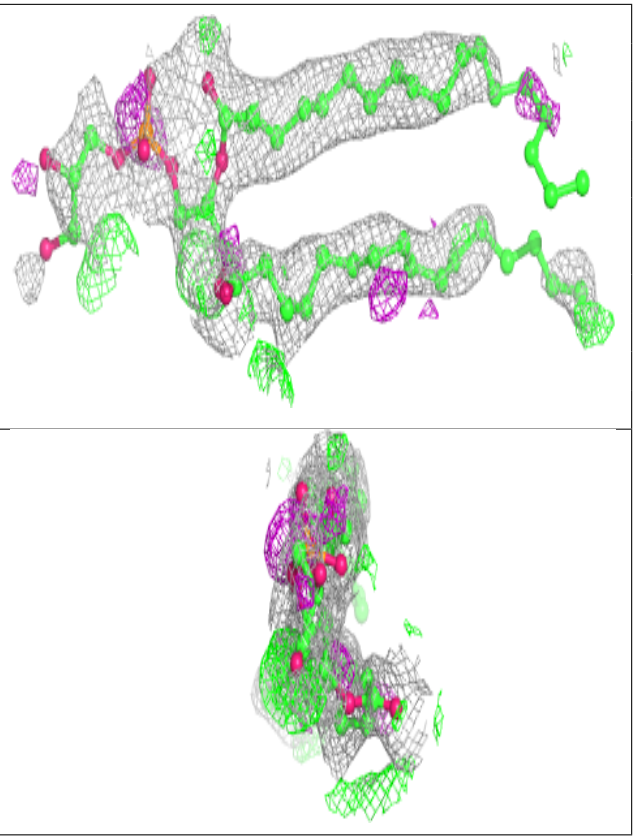


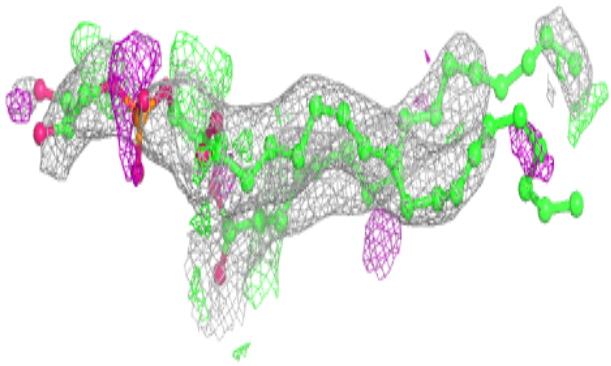




Electron density around PGV D 201:

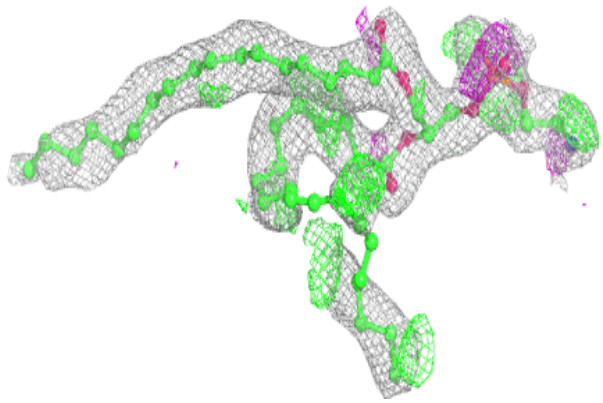
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

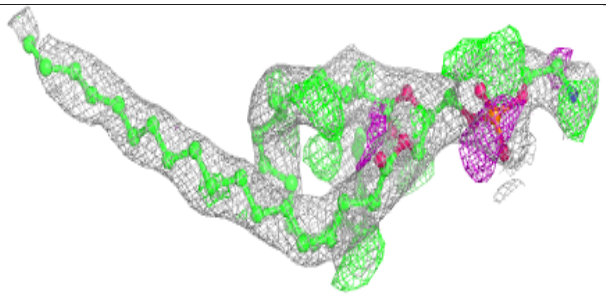


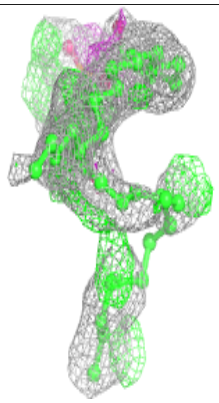


Electron density around PEK P 306:

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

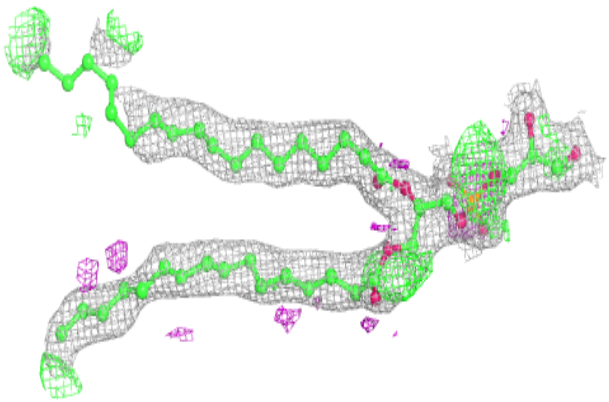


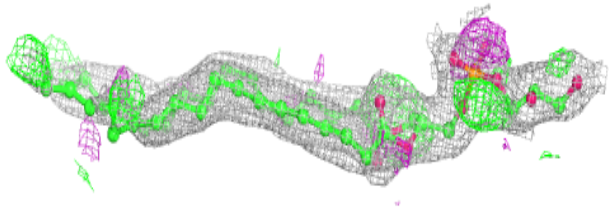


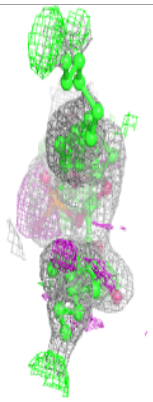


Electron density around PGV P 303:

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

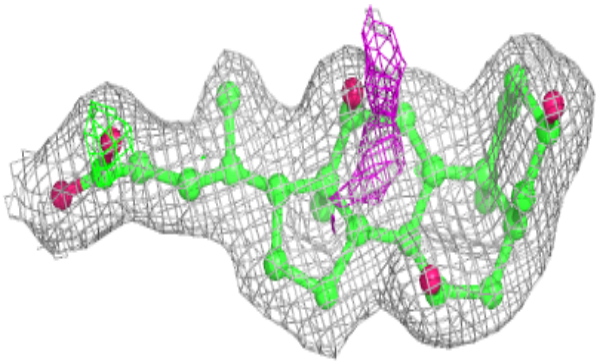


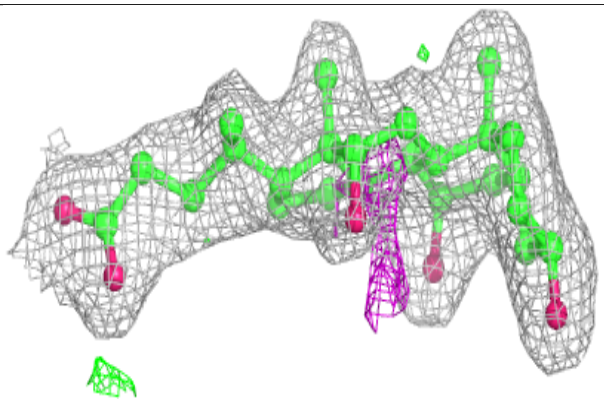


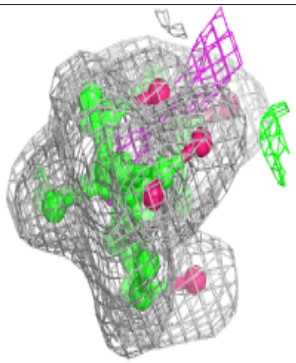


Electron density around CHD C 305:

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

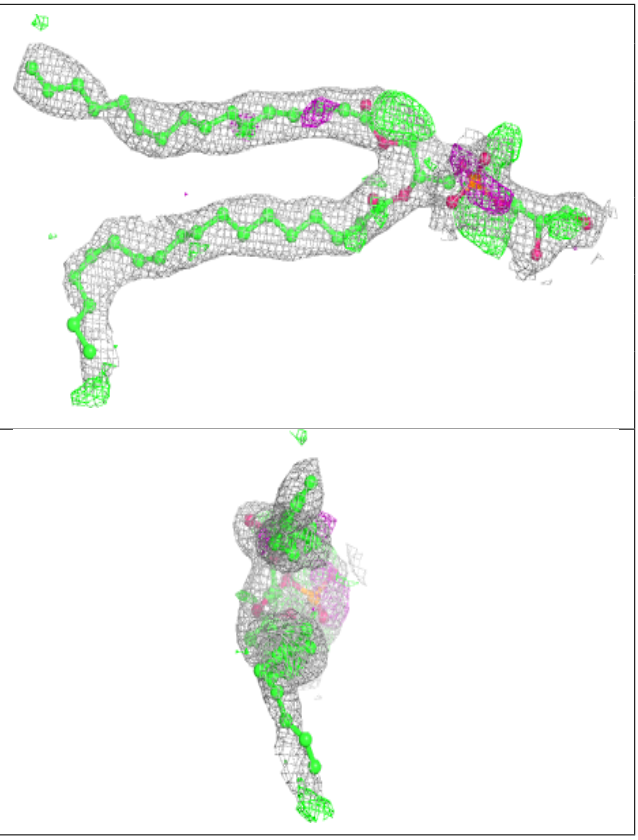






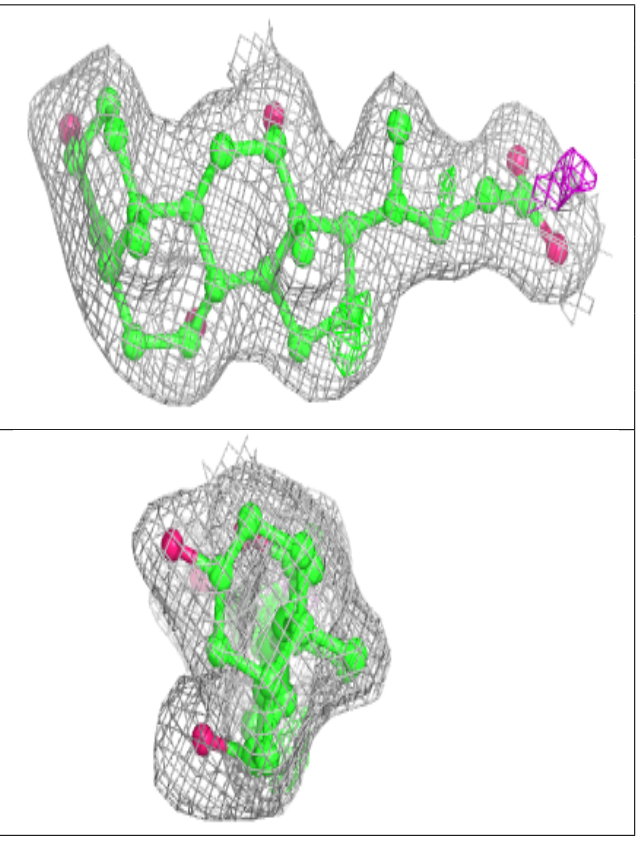
Electron density around PGV C 302:

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



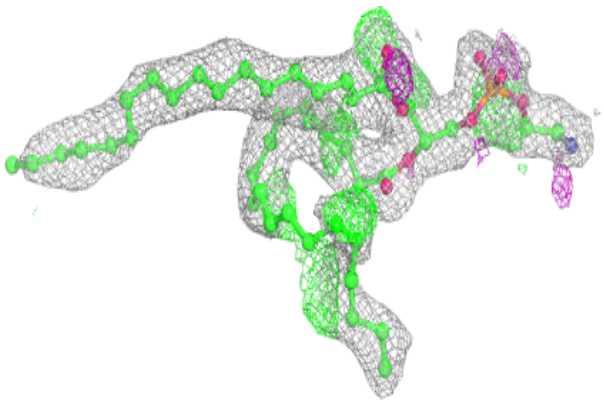
Electron density around CHD N 609:

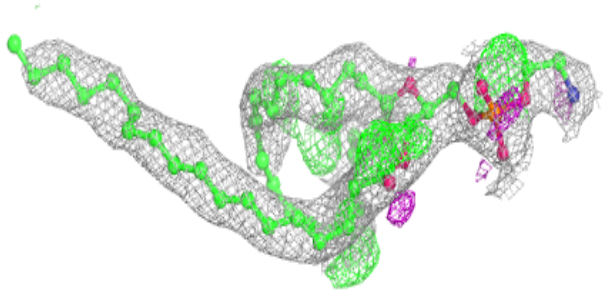
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

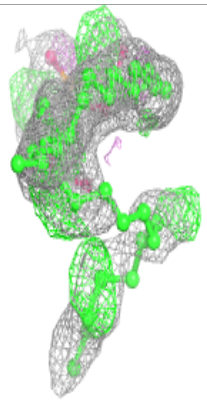


Electron density around PEK G 101:

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

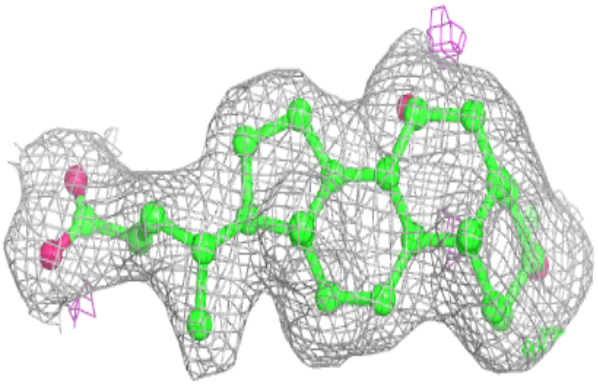


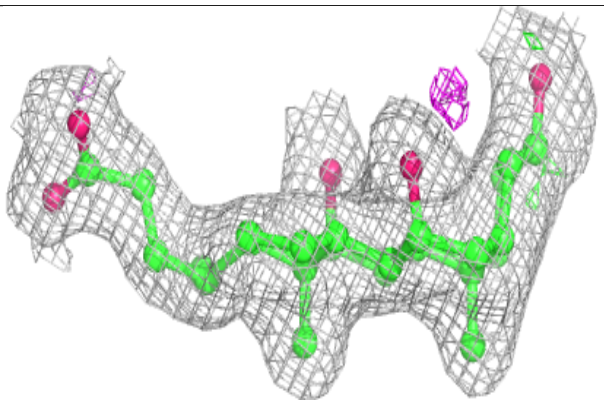


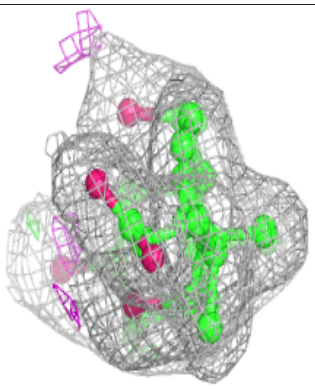


Electron density around CHD O 602:

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

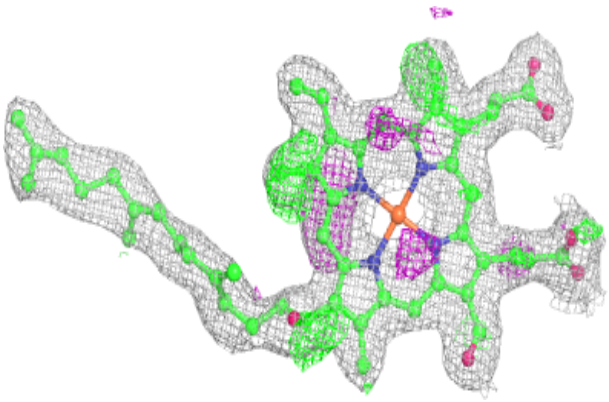


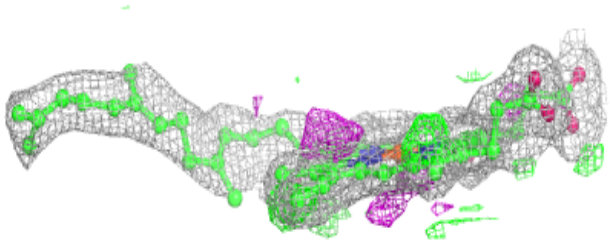


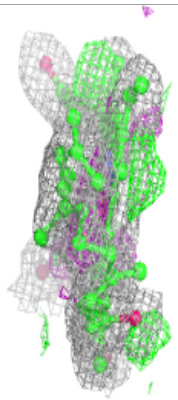


Electron density around HEA A 601 (C):

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

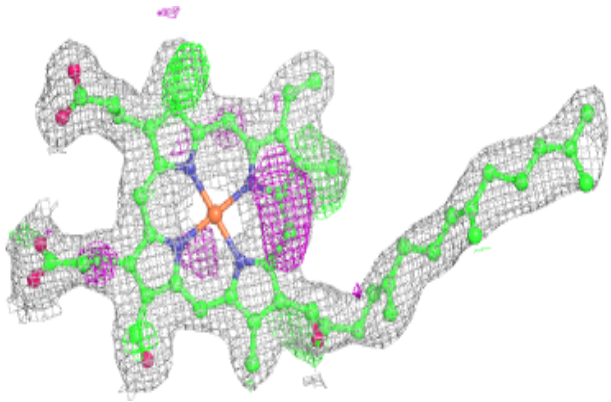


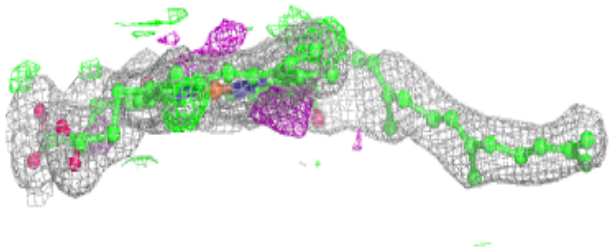


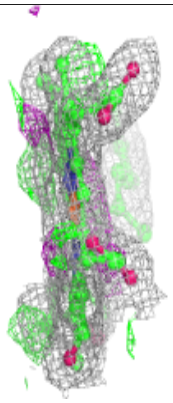


Electron density around HEA A 601 (D):

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

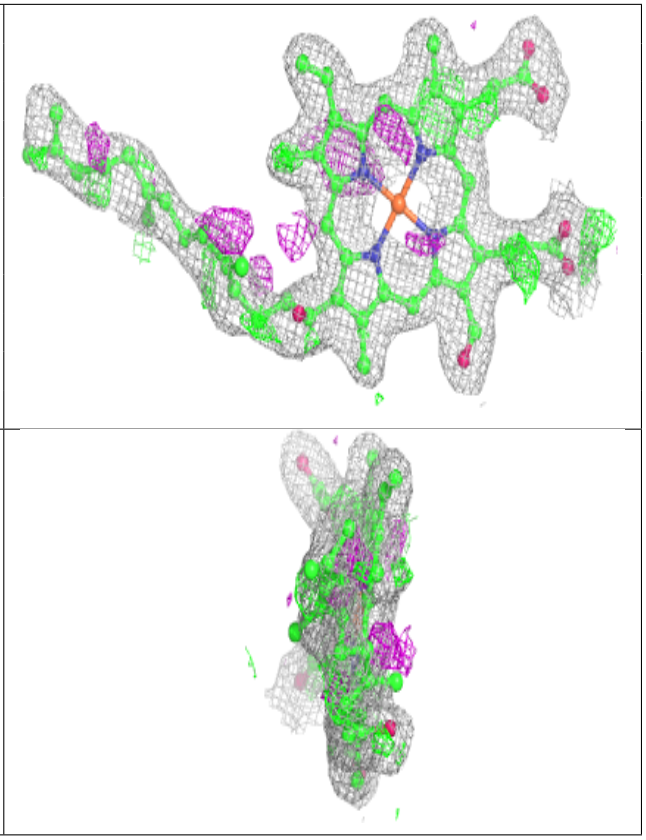






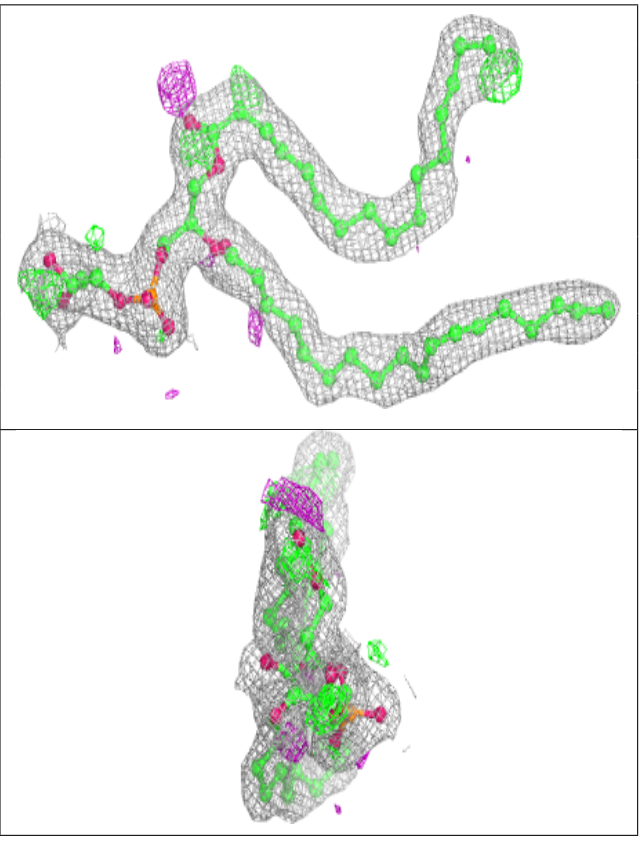
Electron density around HEA N 601 (C):

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



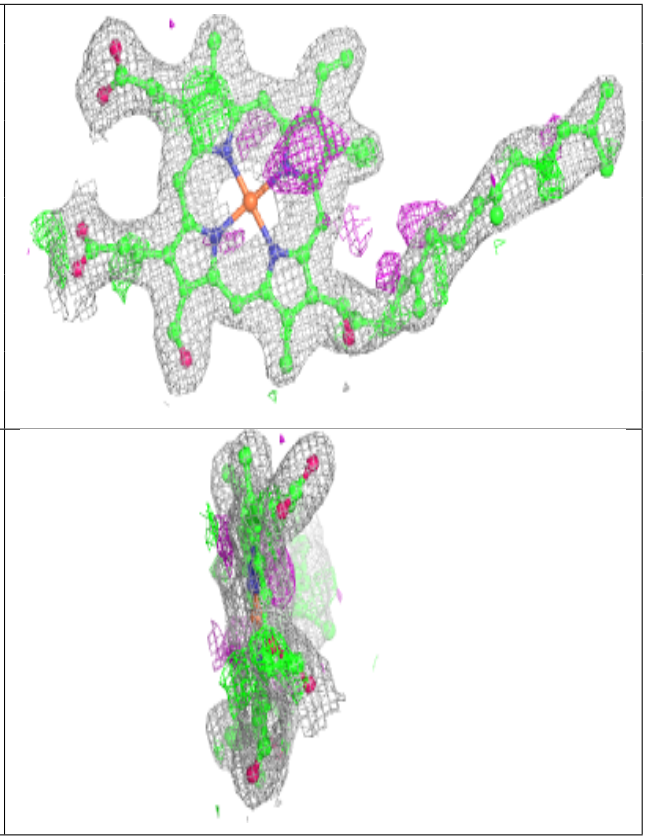
Electron density around PGV C 301:

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



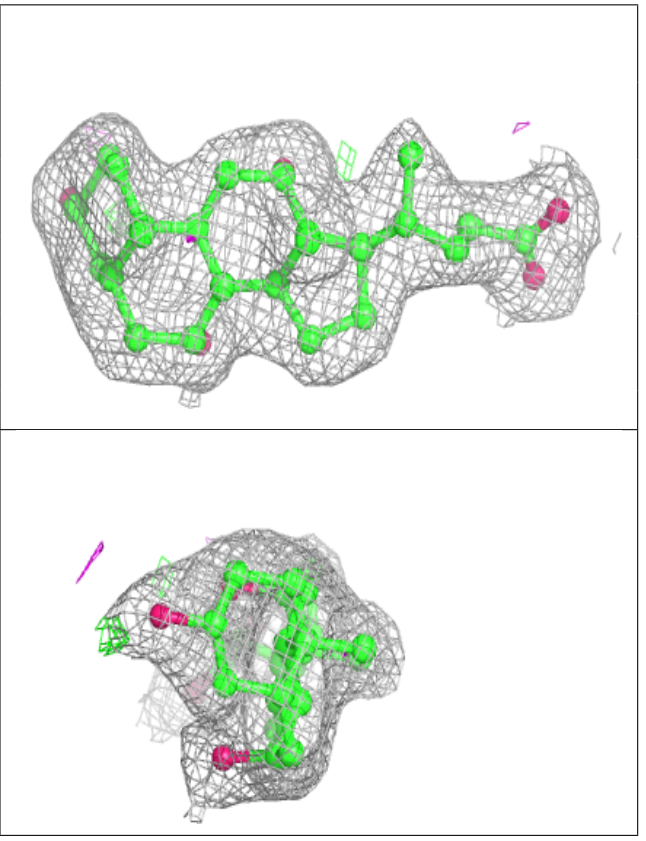
Electron density around HEA N 601 (D):

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



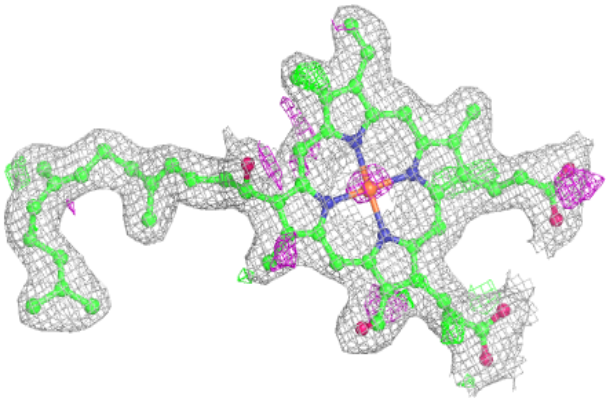
Electron density around CHD B 602:

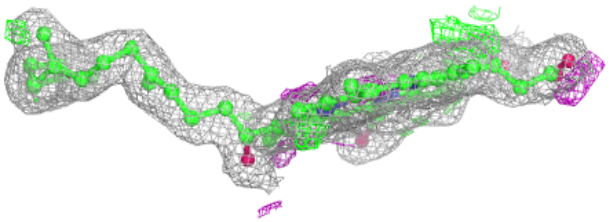
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

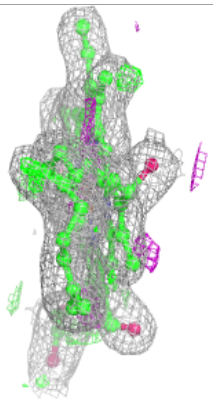


Electron density around HEA A 602:

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

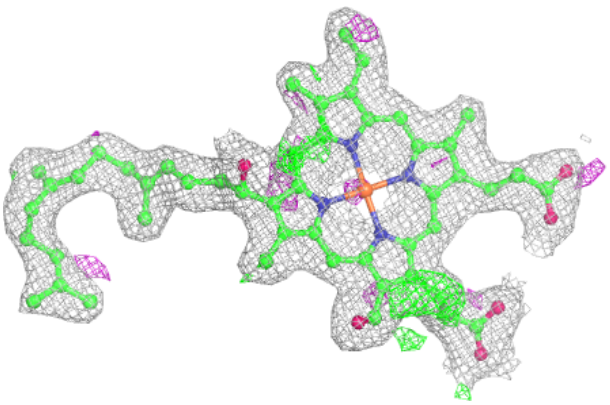


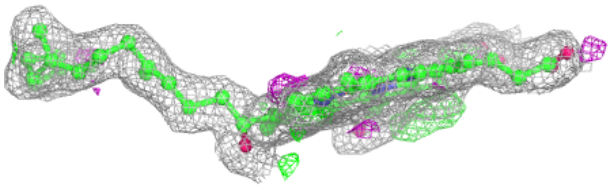


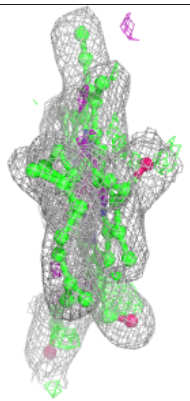


Electron density around HEA N 602:

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

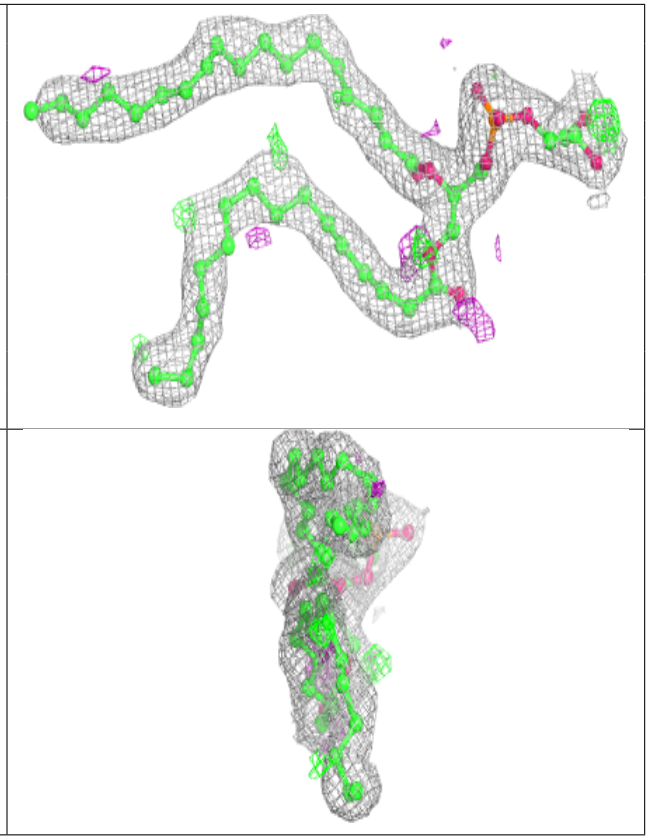






Electron density around PGV N 607:

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



6.5 Other polymers (i)

There are no such residues in this entry.