wwPDB X-ray Structure Validation Summary Report (i)

Sep 25, 2023 – 07:47 AM EDT

PDB ID	:	5W97
Title	:	Crystal Structure of CO-bound Cytochrome c Oxidase determined by Serial Femtosecond X-Ray Crystallography at Room Temperature
Authors	:	Rousseau, D.L.; Yeh, S.-R.; Ishigami, I.; Zatsepin, N.A.; Grant, T.D.; Fromme, P.; Fromme, R.
Deposited on	:	2017-06-22
Resolution	:	2.30 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:

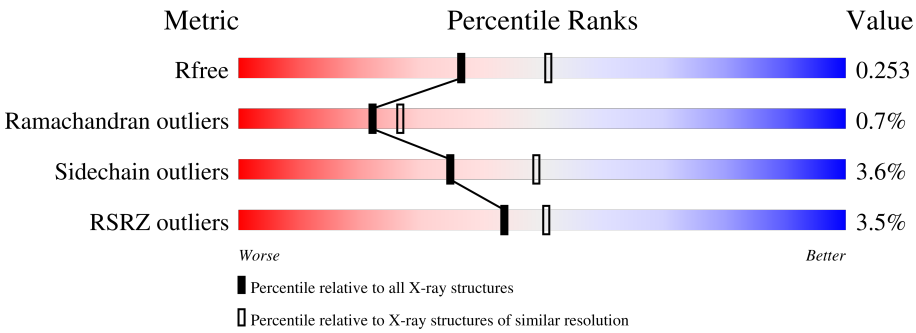
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.30 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	5042 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	98% ·
1	a	514	96% ·
2	B	227	94% 6%
2	b	227	5% 94% 6%
3	C	261	97% · ·
3	c	261	97% · ·

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	147	%, 93%, 5%
4	d	147	8%, 93%, 5%
5	E	109	2%, 93%
5	e	109	2%, 93%
6	F	98	6%, 93%, 6%
6	f	98	7%, 98%
7	G	85	16%, 88%, 11%
7	g	85	13%, 87%, 11%
8	H	85	8%, 82%, 8%, 7%
8	h	85	7%, 91%, 7%
9	I	73	4%, 93%, 7%
9	i	73	11%, 93%, 7%
10	J	59	5%, 97%
10	j	59	8%, 81%, 15%
11	K	56	5%, 77%, 9%, 12%
11	k	56	14%, 86%, 12%
12	L	47	2%, 96%
12	l	47	2%, 85%, 11%
13	M	46	4%, 93%, 7%
13	m	46	15%, 87%, 7%, 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	A	601	X	-	-	-
14	HEA	A	602	X	-	-	-
14	HEA	a	601	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	a	602	X	-	-	-
22	PSC	e	201	-	-	-	X
9	SAC	i	1	-	-	-	X

2 Entry composition (i)

There are 28 unique types of molecules in this entry. The entry contains 32025 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	514	4027	2691	623	678	35	0	0	0
1	a	514	4027	2691	623	678	35	0	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	144	1195	777	196	218	4	0	0	0
4	d	144	1195	777	196	218	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	105	852	544	144	162	2	0	0	0
5	e	105	852	544	144	162	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	98	748	464	134	145	5	0	0	0
6	f	98	748	464	134	145	5	0	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	I	73	601	390	107	100	4	0	0	0
9	i	73	601	390	107	100	4	0	0	0

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

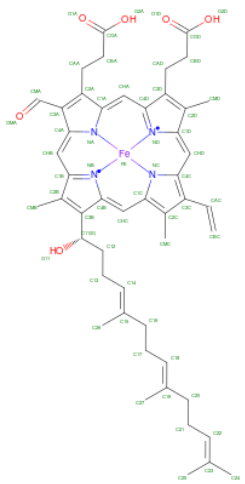
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	L	46	380	254	64	60	2	0	0	0
			Total	C	N	O	S			
12	l	46	380	254	64	60	2	0	0	0

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

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

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

HEA



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

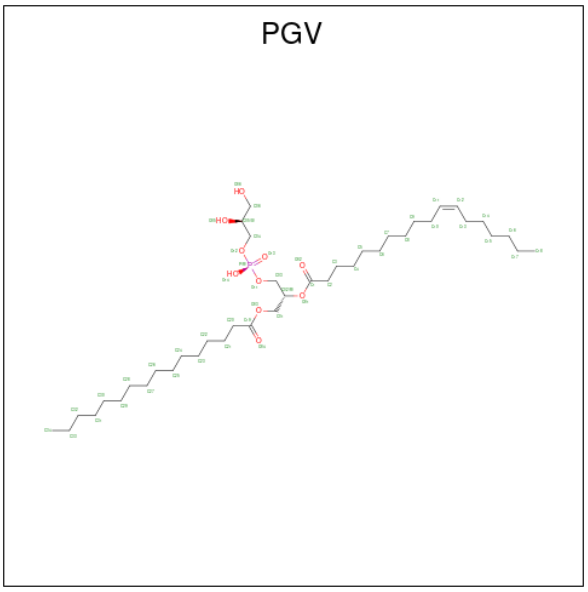
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

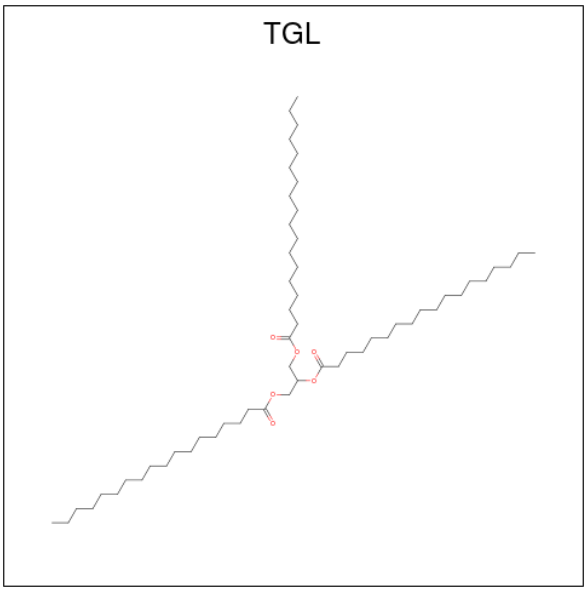
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
17	A	1	1	1	0	0
			Total	Na		
17	a	1	1	1	0	0

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



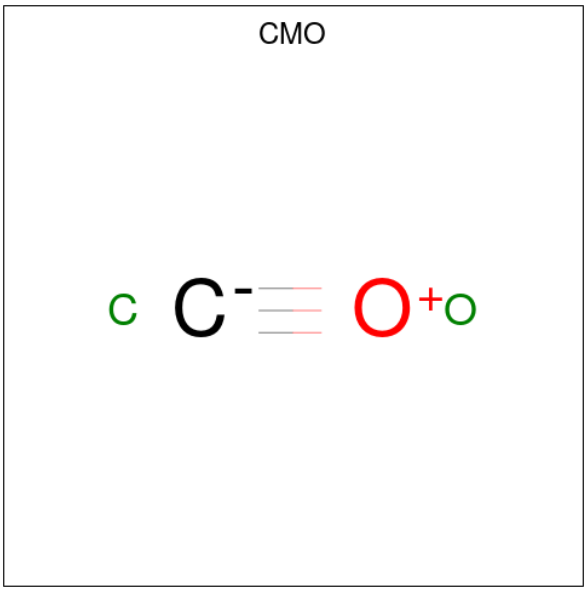
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
18	A	1	51	40	10	1	0	0
			Total	C	O	P		
18	A	1	51	40	10	1	0	0
			Total	C	O	P		
18	C	1	51	40	10	1	0	0
			Total	C	O	P		
18	C	1	51	40	10	1	0	0
			Total	C	O	P		
18	G	1	51	40	10	1	0	0
			Total	C	O	P		
18	a	1	51	40	10	1	0	0
			Total	C	O	P		
18	c	1	51	40	10	1	0	0
			Total	C	O	P		
18	c	1	51	40	10	1	0	0

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



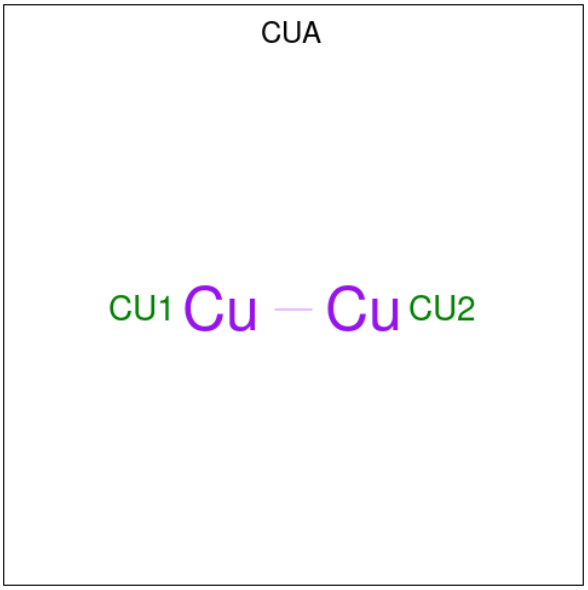
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
19	A	1	63	57	6	0	0
19	D	1	63	57	6	0	0
19	L	1	63	57	6	0	0
19	a	1	63	57	6	0	0
19	i	1	63	57	6	0	0
19	l	1	63	57	6	0	0

- Molecule 20 is CARBON MONOXIDE (three-letter code: CMO) (formula: CO).



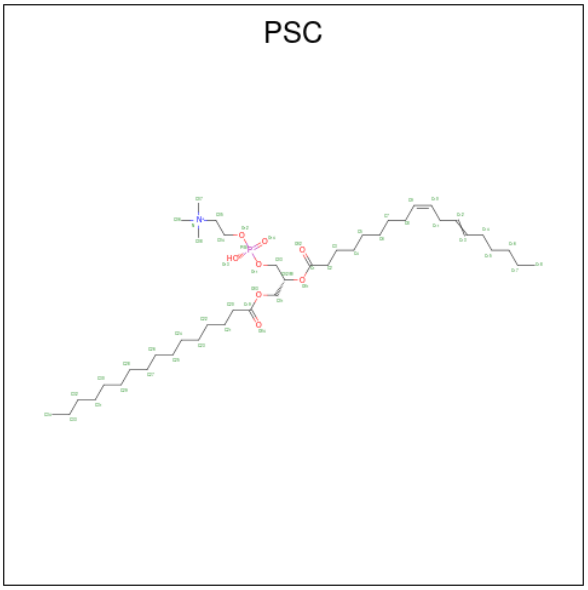
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	A	1	Total C O 2 1 1	0	0
20	a	1	Total C O 2 1 1	0	0

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



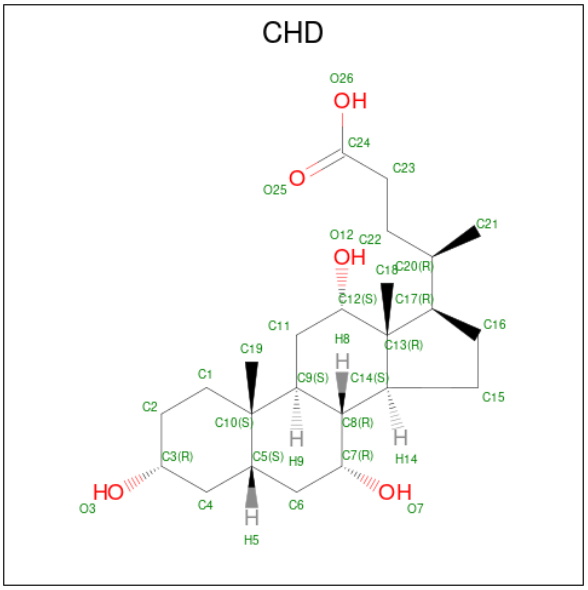
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	B	1	Total Cu 2 2	0	0
21	b	1	Total Cu 2 2	0	0

- Molecule 22 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: $C_{42}H_{81}NO_8P$).



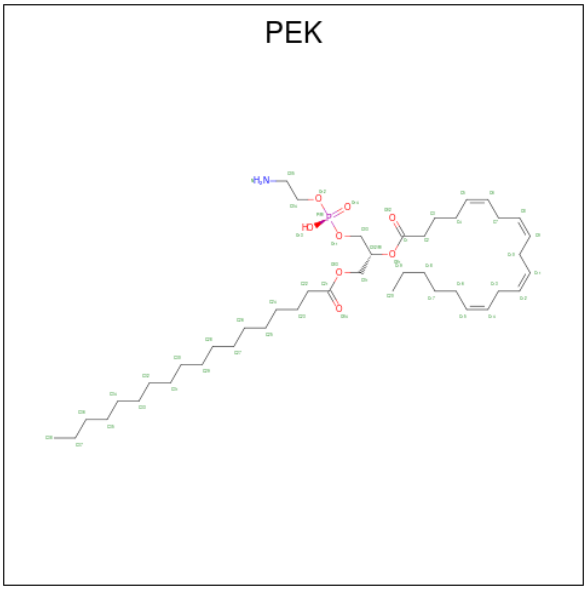
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
22	B	1	52	42	1	8	1	0	0
			Total	C	N	O	P		
22	e	1	52	42	1	8	1	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
23	B	1	29	24	5		0	0
			Total	C	O			
23	C	1	29	24	5		0	0
			Total	C	O			
23	C	1	29	24	5		0	0
			Total	C	O			
23	J	1	29	24	5		0	0
			Total	C	O			
23	b	1	29	24	5		0	0
			Total	C	O			
23	c	1	29	24	5		0	0
			Total	C	O			
23	c	1	29	24	5		0	0
			Total	C	O			
23	j	1	29	24	5		0	0

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



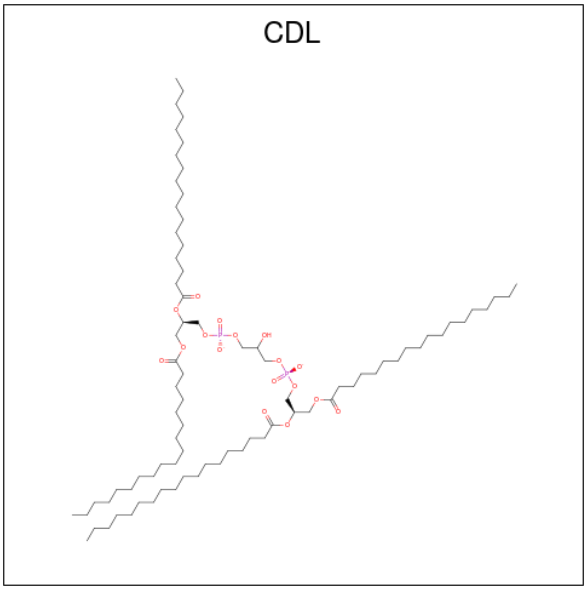
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
24	C	1	53	43	1	8	1	0	0
			Total	C	N	O	P		
24	C	1	53	43	1	8	1	0	0
			Total	C	N	O	P		
24	C	1	53	43	1	8	1	0	0

Continued on next page...

Continued from previous page...

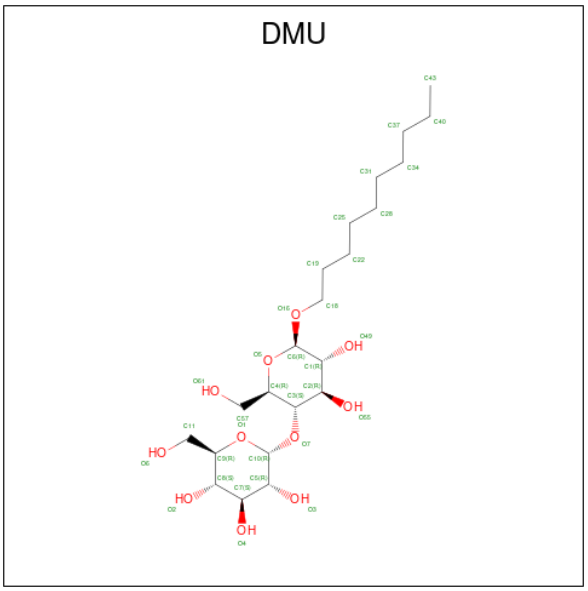
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
24	G	1	53	43	1	8	1	0	0
			Total	C	N	O	P		
24	c	1	53	43	1	8	1	0	0
			Total	C	N	O	P		
24	g	1	53	43	1	8	1	0	0

- Molecule 25 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		
25	C	1	100	81	17	2	0	0
			Total	C	O	P		
25	G	1	100	81	17	2	0	0
			Total	C	O	P		
25	c	1	100	81	17	2	0	0
			Total	C	O	P		
25	g	1	100	81	17	2	0	0

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
26	C	1	33	22	11	0	0
26	M	1	33	22	11	0	0
26	c	1	33	22	11	0	0
26	m	1	33	22	11	0	0

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

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

- Molecule 28 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
28	A	197	197	197	0	0
28	B	120	120	120	0	0
28	C	81	81	81	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	D	85	Total O 85 85	0	0
28	E	51	Total O 51 51	0	0
28	F	66	Total O 66 66	0	0
28	G	51	Total O 51 51	0	0
28	H	33	Total O 33 33	0	0
28	I	33	Total O 33 33	0	0
28	J	26	Total O 26 26	0	0
28	K	30	Total O 30 30	0	0
28	L	35	Total O 35 35	0	0
28	M	22	Total O 22 22	0	0
28	a	140	Total O 140 140	0	0
28	b	63	Total O 63 63	0	0
28	c	59	Total O 59 59	0	0
28	d	25	Total O 25 25	0	0
28	e	36	Total O 36 36	0	0
28	f	29	Total O 29 29	0	0
28	g	29	Total O 29 29	0	0
28	h	24	Total O 24 24	0	0
28	i	14	Total O 14 14	0	0
28	j	8	Total O 8 8	0	0
28	k	8	Total O 8 8	0	0

Continued on next page...

Continued from previous page...

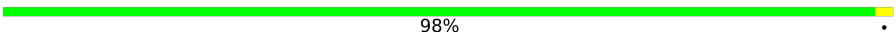
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	l	19	Total O 19 19	0	0
28	m	7	Total O 7 7	0	0

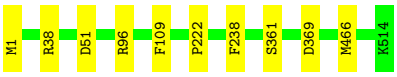
3 Residue-property plots (i)

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

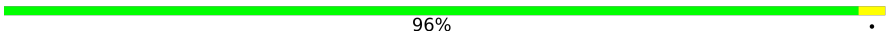
Chain A:





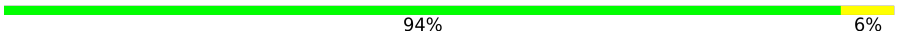
• Molecule 1: Cytochrome c oxidase subunit 1

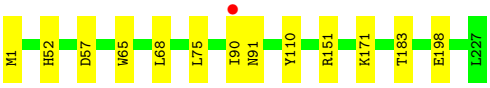
Chain a:



• Molecule 2: Cytochrome c oxidase subunit 2

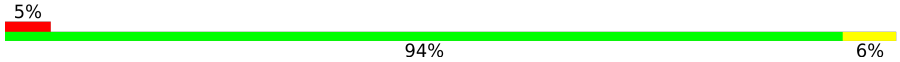
Chain B:





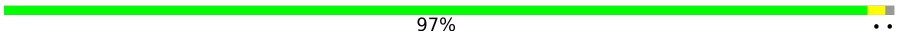
• Molecule 2: Cytochrome c oxidase subunit 2

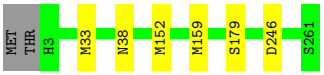
Chain b:



• Molecule 3: Cytochrome c oxidase subunit 3

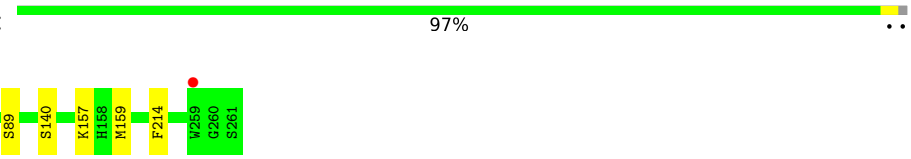
Chain C:





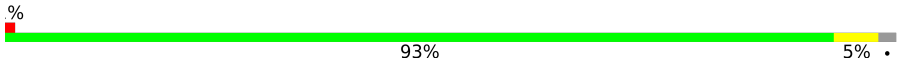
• Molecule 3: Cytochrome c oxidase subunit 3

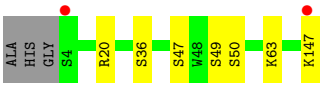
Chain c:



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

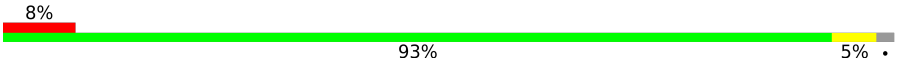
Chain D:

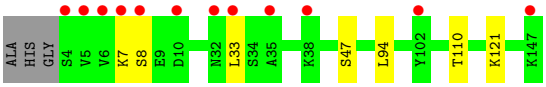




• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

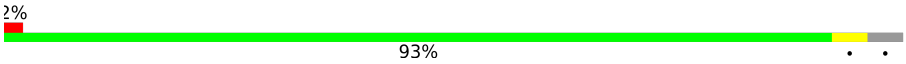
Chain d:





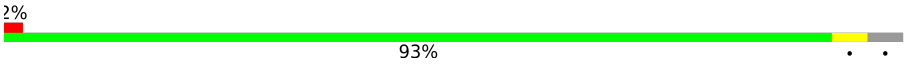
• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

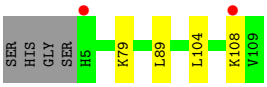
Chain E:



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

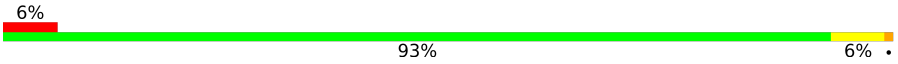
Chain e:

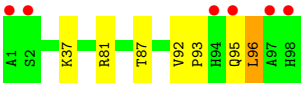




• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

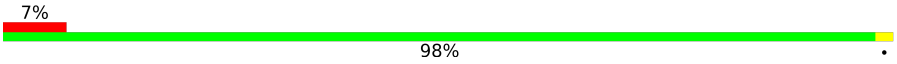
Chain F:

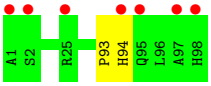




• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

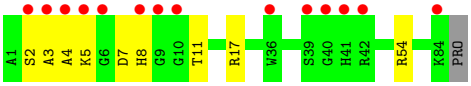
Chain f:





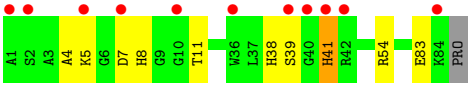
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain G:



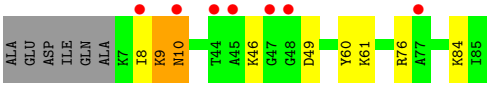
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain g:



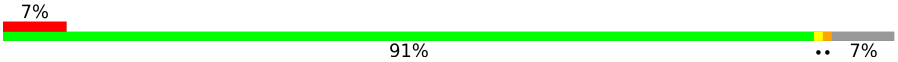
• Molecule 8: Cytochrome c oxidase subunit 6B1

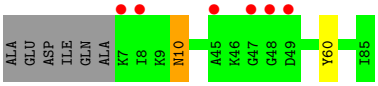
Chain H:



• Molecule 8: Cytochrome c oxidase subunit 6B1

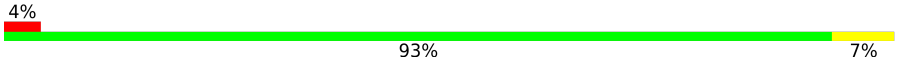
Chain h:

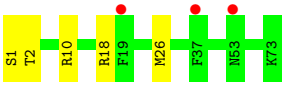




• Molecule 9: Cytochrome c oxidase subunit 6C

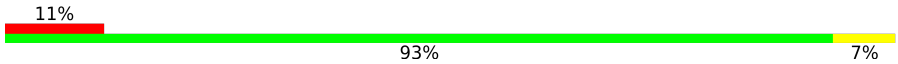
Chain I:

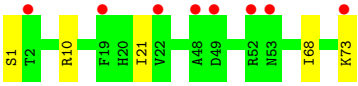




• Molecule 9: Cytochrome c oxidase subunit 6C

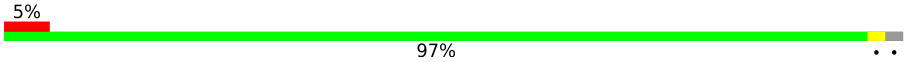
Chain i:

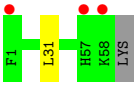




• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial

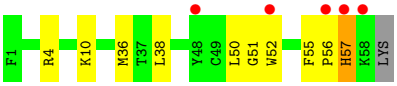
Chain J:





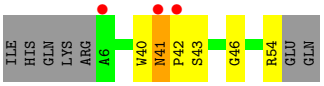
• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial

Chain j:



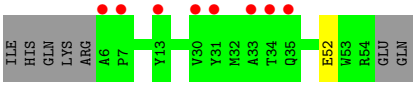
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

Chain K:



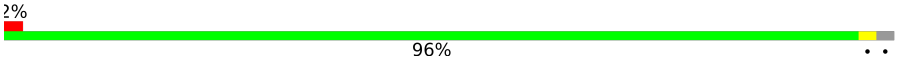
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

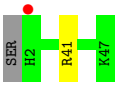
Chain k:



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

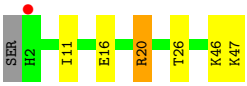
Chain L:





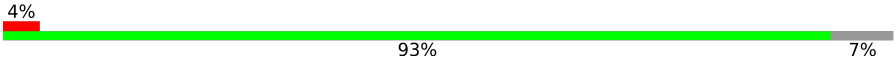
• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

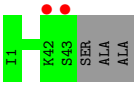
Chain l:



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

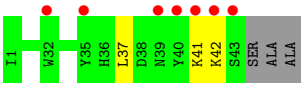
Chain M:





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

Chain m:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	178.30Å 189.00Å 209.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.86 – 2.30 29.86 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.86-2.30) 100.0 (29.86-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.19 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.208 , 0.252 0.215 , 0.253	Depositor DCC
R_{free} test set	2994 reflections (0.96%)	wwPDB-VP
Wilson B-factor (Å^2)	34.1	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 59.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	32025	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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: DMU, CMO, HEA, PGV, CDL, CU, CUA, CHD, SAC, NA, TPO, FME, MG, PEK, PSC, TGL, ZN

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	0.70	0/4156	0.78	4/5678 (0.1%)
1	a	0.65	0/4156	0.76	2/5678 (0.0%)
2	B	0.70	1/1860 (0.1%)	0.88	1/2534 (0.0%)
2	b	0.61	1/1860 (0.1%)	0.81	0/2534
3	C	0.67	0/2197	0.75	2/3005 (0.1%)
3	c	0.64	0/2197	0.72	0/3005
4	D	0.66	0/1229	0.75	1/1658 (0.1%)
4	d	0.56	0/1229	0.75	0/1658
5	E	0.59	0/871	0.72	0/1182
5	e	0.53	0/871	0.79	0/1182
6	F	0.73	0/765	0.88	1/1038 (0.1%)
6	f	0.57	0/765	0.78	0/1038
7	G	0.68	0/690	0.80	2/937 (0.2%)
7	g	0.64	0/690	0.74	0/937
8	H	0.66	0/682	0.86	0/921
8	h	0.61	0/682	0.81	0/921
9	I	0.66	0/605	0.84	1/802 (0.1%)
9	i	0.63	0/605	0.81	1/802 (0.1%)
10	J	0.62	0/471	0.77	0/636
10	j	0.72	1/471 (0.2%)	0.75	0/636
11	K	0.75	0/398	0.99	4/546 (0.7%)
11	k	0.63	0/398	0.72	0/546
12	L	0.71	0/393	0.76	1/526 (0.2%)
12	l	0.61	0/393	0.74	1/526 (0.2%)
13	M	0.59	0/345	0.68	0/470
13	m	0.56	0/345	0.66	0/470
All	All	0.65	3/29324 (0.0%)	0.78	21/39866 (0.1%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	d	0	1
6	F	0	1
7	g	0	1
8	H	0	2
8	h	0	1
10	j	0	1
11	K	0	4
All	All	0	11

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	198	GLU	C-O	7.01	1.36	1.23
2	b	198	GLU	C-O	6.79	1.36	1.23
10	j	52	TRP	CB-CG	5.73	1.60	1.50

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	152	MET	CG-SD-CE	11.06	117.90	100.20
9	i	10	ARG	NE-CZ-NH2	-7.00	116.80	120.30
11	K	41	ASN	C-N-CA	-6.90	93.00	122.00
11	K	41	ASN	C-N-CD	6.46	141.96	128.40
11	K	43	SER	N-CA-CB	6.42	120.13	110.50

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	F	92	VAL	Peptide
8	H	10	ASN	Peptide
8	H	9	LYS	Peptide
11	K	40	TRP	Peptide
11	K	41	ASN	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	512/514 (100%)	497 (97%)	15 (3%)	0	100	100
1	a	512/514 (100%)	495 (97%)	16 (3%)	1 (0%)	47	58
2	B	225/227 (99%)	214 (95%)	10 (4%)	1 (0%)	34	42
2	b	225/227 (99%)	218 (97%)	7 (3%)	0	100	100
3	C	257/261 (98%)	251 (98%)	5 (2%)	1 (0%)	34	42
3	c	257/261 (98%)	248 (96%)	8 (3%)	1 (0%)	34	42
4	D	142/147 (97%)	139 (98%)	3 (2%)	0	100	100
4	d	142/147 (97%)	133 (94%)	8 (6%)	1 (1%)	22	26
5	E	103/109 (94%)	100 (97%)	3 (3%)	0	100	100
5	e	103/109 (94%)	101 (98%)	2 (2%)	0	100	100
6	F	96/98 (98%)	90 (94%)	4 (4%)	2 (2%)	7	5
6	f	96/98 (98%)	91 (95%)	3 (3%)	2 (2%)	7	5
7	G	81/85 (95%)	71 (88%)	7 (9%)	3 (4%)	3	2
7	g	81/85 (95%)	66 (82%)	9 (11%)	6 (7%)	1	0
8	H	77/85 (91%)	72 (94%)	3 (4%)	2 (3%)	5	4
8	h	77/85 (91%)	73 (95%)	4 (5%)	0	100	100
9	I	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
9	i	71/73 (97%)	66 (93%)	4 (6%)	1 (1%)	11	11
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	j	56/59 (95%)	53 (95%)	0	3 (5%)	2	1
11	K	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
11	k	47/56 (84%)	44 (94%)	3 (6%)	0	100	100
12	L	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
12	l	44/47 (94%)	41 (93%)	2 (4%)	1 (2%)	6	5
13	M	41/46 (89%)	40 (98%)	1 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
13	m	41/46 (89%)	38 (93%)	2 (5%)	1 (2%)	6 4
All	All	3504/3614 (97%)	3355 (96%)	123 (4%)	26 (1%)	22 26

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	96	LEU
8	H	10	ASN
7	g	4	ALA
12	l	46	LYS
2	B	90	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	426/426 (100%)	420 (99%)	6 (1%)	67 81
1	a	426/426 (100%)	411 (96%)	15 (4%)	36 50
2	B	210/210 (100%)	201 (96%)	9 (4%)	29 40
2	b	210/210 (100%)	198 (94%)	12 (6%)	20 28
3	C	224/226 (99%)	221 (99%)	3 (1%)	69 82
3	c	224/226 (99%)	218 (97%)	6 (3%)	44 61
4	D	128/129 (99%)	122 (95%)	6 (5%)	26 37
4	d	128/129 (99%)	123 (96%)	5 (4%)	32 46
5	E	92/95 (97%)	88 (96%)	4 (4%)	29 40
5	e	92/95 (97%)	88 (96%)	4 (4%)	29 40
6	F	81/81 (100%)	77 (95%)	4 (5%)	25 35
6	f	81/81 (100%)	81 (100%)	0	100 100
7	G	67/68 (98%)	63 (94%)	4 (6%)	19 26
7	g	67/68 (98%)	64 (96%)	3 (4%)	27 39
8	H	71/75 (95%)	64 (90%)	7 (10%)	8 9

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	h	71/75 (95%)	69 (97%)	2 (3%)	43	60
9	I	57/57 (100%)	54 (95%)	3 (5%)	22	31
9	i	57/57 (100%)	55 (96%)	2 (4%)	36	50
10	J	49/50 (98%)	48 (98%)	1 (2%)	55	72
10	j	49/50 (98%)	43 (88%)	6 (12%)	5	5
11	K	39/46 (85%)	39 (100%)	0	100	100
11	k	39/46 (85%)	38 (97%)	1 (3%)	46	63
12	L	39/40 (98%)	39 (100%)	0	100	100
12	l	39/40 (98%)	34 (87%)	5 (13%)	4	4
13	M	37/38 (97%)	37 (100%)	0	100	100
13	m	37/38 (97%)	35 (95%)	2 (5%)	22	30
All	All	3040/3082 (99%)	2930 (96%)	110 (4%)	35	49

5 of 110 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	417	MET
2	b	183	THR
13	m	41	LYS
10	j	38	LEU
1	a	483	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
2	b	6	GLN
13	m	15	GLN
3	c	50	ASN
6	f	95	GLN
5	E	59	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	SAC	i	1	9	7,8,9	1.88	1 (14%)	8,9,11	1.85	2 (25%)
2	FME	b	1	2	8,9,10	0.60	0	7,9,11	2.48	2 (28%)
1	FME	a	1	1	8,9,10	0.55	0	7,9,11	1.94	2 (28%)
1	FME	A	1	1	8,9,10	0.55	0	7,9,11	2.78	3 (42%)
7	TPO	G	11	7	8,10,11	1.52	2 (25%)	10,14,16	0.88	0
7	TPO	g	11	7	8,10,11	1.35	1 (12%)	10,14,16	0.74	0
9	SAC	I	1	9	7,8,9	1.58	1 (14%)	8,9,11	1.09	0
2	FME	B	1	2	8,9,10	1.08	0	7,9,11	3.79	3 (42%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	SAC	i	1	9	-	2/7/8/10	-
2	FME	b	1	2	-	1/7/9/11	-
1	FME	a	1	1	-	5/7/9/11	-
1	FME	A	1	1	-	5/7/9/11	-
7	TPO	G	11	7	-	5/9/11/13	-
7	TPO	g	11	7	-	5/9/11/13	-
9	SAC	I	1	9	-	1/7/8/10	-
2	FME	B	1	2	-	1/7/9/11	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	i	1	SAC	CA-N	4.51	1.52	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	1	SAC	CA-N	3.68	1.51	1.46
7	G	11	TPO	P-OG1	2.81	1.64	1.59
7	G	11	TPO	CB-CA	2.52	1.59	1.53
7	g	11	TPO	P-OG1	2.45	1.63	1.59

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	FME	CA-N-CN	-8.96	109.04	122.82
1	A	1	FME	CA-N-CN	-6.41	112.97	122.82
2	b	1	FME	CA-N-CN	-5.22	114.80	122.82
1	a	1	FME	CA-N-CN	-4.24	116.30	122.82
9	i	1	SAC	C-CA-N	3.40	115.86	109.73

There are no chirality outliers.

5 of 25 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
2	B	1	FME	O1-CN-N-CA
7	G	11	TPO	N-CA-CB-CG2
7	G	11	TPO	N-CA-CB-OG1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 54 ligands modelled in this entry, 8 are monoatomic - leaving 46 for Mogul analysis.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
18	PGV	C	304	-	50,50,50	1.14	2 (4%)	53,56,56	1.14	3 (5%)
25	CDL	c	305	-	99,99,99	1.09	4 (4%)	105,111,111	1.08	8 (7%)
19	TGL	L	101	-	62,62,62	1.10	3 (4%)	65,65,65	1.04	4 (6%)
25	CDL	C	305	-	99,99,99	1.02	4 (4%)	105,111,111	1.12	10 (9%)
18	PGV	A	607	-	50,50,50	0.73	2 (4%)	53,56,56	0.94	3 (5%)
14	HEA	A	602	20,1	57,67,67	1.83	15 (26%)	61,103,103	2.52	21 (34%)
21	CUA	b	302	2	0,1,1	-	-	-		
23	CHD	c	302	-	32,32,32	0.78	0	51,51,51	1.61	12 (23%)
23	CHD	C	306	-	32,32,32	0.55	0	51,51,51	1.23	5 (9%)
18	PGV	c	301	-	50,50,50	0.79	2 (4%)	53,56,56	0.85	2 (3%)
24	PEK	C	308	-	52,52,52	1.00	2 (3%)	55,57,57	1.19	4 (7%)
22	PSC	B	302	-	51,51,51	1.08	2 (3%)	57,59,59	1.91	9 (15%)
24	PEK	c	303	-	52,52,52	1.09	2 (3%)	55,57,57	1.03	3 (5%)
22	PSC	e	201	-	51,51,51	1.06	2 (3%)	57,59,59	1.83	10 (17%)
19	TGL	i	101	-	62,62,62	1.05	3 (4%)	65,65,65	1.23	5 (7%)
18	PGV	A	606	-	50,50,50	1.25	3 (6%)	53,56,56	1.28	8 (15%)
18	PGV	a	607	-	50,50,50	1.08	2 (4%)	53,56,56	0.96	3 (5%)
24	PEK	C	302	-	52,52,52	0.95	4 (7%)	55,57,57	0.97	2 (3%)
23	CHD	C	301	-	32,32,32	0.84	0	51,51,51	1.23	6 (11%)
19	TGL	A	608	-	62,62,62	1.28	3 (4%)	65,65,65	1.31	6 (9%)
19	TGL	a	606	-	62,62,62	1.16	3 (4%)	65,65,65	0.95	3 (4%)
26	DMU	M	101	-	34,34,34	0.47	0	45,45,45	1.05	4 (8%)
26	DMU	c	307	-	34,34,34	0.82	1 (2%)	45,45,45	1.13	2 (4%)
24	PEK	C	309	-	52,52,52	1.14	2 (3%)	55,57,57	0.96	4 (7%)
23	CHD	J	101	-	32,32,32	0.82	0	51,51,51	2.04	12 (23%)
19	TGL	l	101	-	62,62,62	1.16	3 (4%)	65,65,65	1.17	5 (7%)
14	HEA	a	602	20,1	57,67,67	1.85	15 (26%)	61,103,103	2.58	25 (40%)
14	HEA	a	601	1	57,67,67	2.05	15 (26%)	61,103,103	2.48	21 (34%)
20	CMO	a	608	14	0,1,1	-	-	-		
14	HEA	A	601	1	57,67,67	2.04	15 (26%)	61,103,103	2.43	25 (40%)
21	CUA	B	301	2	0,1,1	-	-	-		
18	PGV	C	303	-	50,50,50	0.87	2 (4%)	53,56,56	0.91	3 (5%)
18	PGV	c	304	-	50,50,50	0.90	2 (4%)	53,56,56	1.05	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
23	CHD	c	306	-	32,32,32	0.59	0	51,51,51	1.49	12 (23%)
26	DMU	m	401	-	34,34,34	0.52	0	45,45,45	1.13	3 (6%)
23	CHD	B	303	-	32,32,32	1.00	1 (3%)	51,51,51	1.22	7 (13%)
24	PEK	g	102	-	52,52,52	0.89	3 (5%)	55,57,57	0.85	2 (3%)
23	CHD	j	101	-	32,32,32	0.80	0	51,51,51	2.04	12 (23%)
23	CHD	b	301	-	32,32,32	0.80	0	51,51,51	1.54	13 (25%)
25	CDL	g	103	-	99,99,99	1.07	4 (4%)	105,111,111	0.95	6 (5%)
19	TGL	D	201	-	62,62,62	1.28	3 (4%)	65,65,65	1.24	6 (9%)
24	PEK	G	102	-	52,52,52	1.11	2 (3%)	55,57,57	0.92	4 (7%)
20	CMO	A	609	14	0,1,1	-	-	-		
26	DMU	C	307	-	34,34,34	0.98	1 (2%)	45,45,45	1.46	8 (17%)
18	PGV	G	103	-	50,50,50	1.08	2 (4%)	53,56,56	0.98	4 (7%)
25	CDL	G	101	-	99,99,99	1.08	4 (4%)	105,111,111	0.95	6 (5%)

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
18	PGV	C	304	-	-	24/55/55/55	-
25	CDL	c	305	-	-	57/110/110/110	-
19	TGL	L	101	-	-	38/65/65/65	-
25	CDL	C	305	-	-	46/110/110/110	-
18	PGV	A	607	-	-	16/55/55/55	-
14	HEA	A	602	20,1	2/2/7/16	4/32/76/76	-
23	CHD	c	302	-	-	3/9/74/74	0/4/4/4
23	CHD	C	306	-	-	2/9/74/74	0/4/4/4
18	PGV	c	301	-	-	18/55/55/55	-
24	PEK	C	308	-	-	20/56/56/56	-
22	PSC	B	302	-	-	30/55/55/55	-
24	PEK	c	303	-	-	25/56/56/56	-
22	PSC	e	201	-	-	25/55/55/55	-
19	TGL	i	101	-	-	23/65/65/65	-
18	PGV	A	606	-	-	32/55/55/55	-
18	PGV	a	607	-	-	21/55/55/55	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PEK	C	302	-	-	13/56/56/56	-
23	CHD	C	301	-	-	3/9/74/74	0/4/4/4
19	TGL	A	608	-	-	33/65/65/65	-
19	TGL	a	606	-	-	28/65/65/65	-
26	DMU	M	101	-	-	3/19/59/59	0/2/2/2
26	DMU	c	307	-	-	11/19/59/59	0/2/2/2
24	PEK	C	309	-	-	25/56/56/56	-
23	CHD	J	101	-	-	6/9/74/74	1/4/4/4
19	TGL	l	101	-	-	34/65/65/65	-
14	HEA	a	602	20,1	2/2/7/16	5/32/76/76	-
14	HEA	a	601	1	2/2/7/16	2/32/76/76	-
14	HEA	A	601	1	2/2/7/16	3/32/76/76	-
18	PGV	C	303	-	-	12/55/55/55	-
18	PGV	c	304	-	-	15/55/55/55	-
23	CHD	c	306	-	-	3/9/74/74	0/4/4/4
26	DMU	m	401	-	-	6/19/59/59	0/2/2/2
23	CHD	B	303	-	-	2/9/74/74	0/4/4/4
24	PEK	g	102	-	-	17/56/56/56	-
23	CHD	j	101	-	-	7/9/74/74	0/4/4/4
23	CHD	b	301	-	-	3/9/74/74	0/4/4/4
25	CDL	g	103	-	-	58/110/110/110	-
19	TGL	D	201	-	-	30/65/65/65	-
24	PEK	G	102	-	-	24/56/56/56	-
26	DMU	C	307	-	-	8/19/59/59	0/2/2/2
18	PGV	G	103	-	-	26/55/55/55	-
25	CDL	G	101	-	-	58/110/110/110	-

The worst 5 of 133 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	608	TGL	OG1-CA1	6.07	1.51	1.33
14	a	601	HEA	C3B-C2B	5.81	1.47	1.34
14	A	601	HEA	C3D-C2D	5.67	1.48	1.36
19	D	201	TGL	OG2-CB1	5.55	1.50	1.34
14	a	601	HEA	C3C-C2C	5.35	1.47	1.40

The worst 5 of 314 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	302	PSC	C08-N-C07	-7.43	89.88	108.97
14	a	602	HEA	C3D-C4D-ND	7.21	117.33	110.36
14	a	601	HEA	C3D-C4D-ND	6.91	117.05	110.36
22	B	302	PSC	C08-N-C06	-6.65	91.89	108.97
14	a	602	HEA	C2D-C1D-ND	6.46	117.50	109.84

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	A	601	HEA	ND
14	A	601	HEA	NB
14	A	602	HEA	ND
14	A	602	HEA	NB
14	a	601	HEA	ND

5 of 819 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	606	PGV	C03-O11-P-O12
18	A	606	PGV	C03-O11-P-O13
18	A	606	PGV	C03-O11-P-O14
18	A	606	PGV	O12-C04-C05-O05
18	C	304	PGV	C03-O11-P-O12

All (1) ring outliers are listed below:

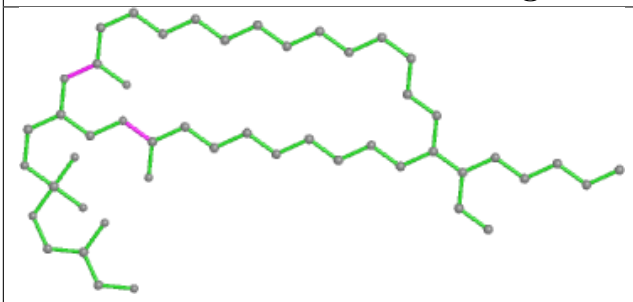
Mol	Chain	Res	Type	Atoms
23	J	101	CHD	C1-C10-C2-C3-C4-C5

No monomer is involved in short contacts.

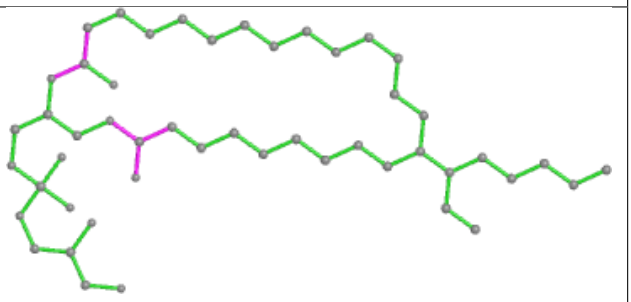
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

equivalents in the CSD to analyse the geometry.

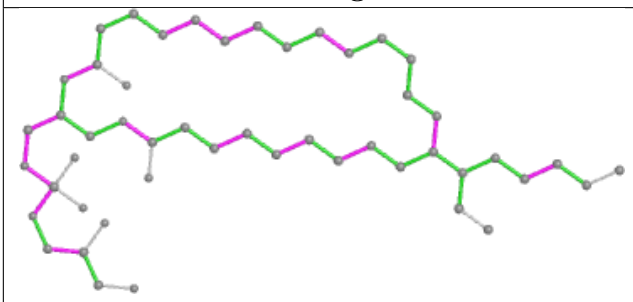
Ligand PGV C 304



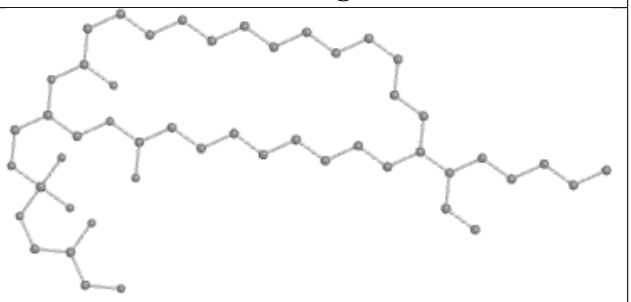
Bond lengths



Bond angles

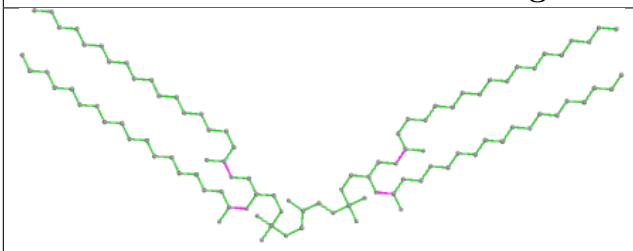


Torsions

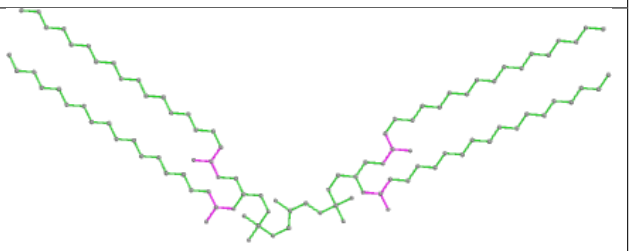


Rings

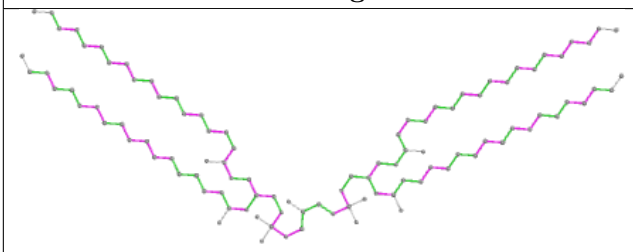
Ligand CDL c 305



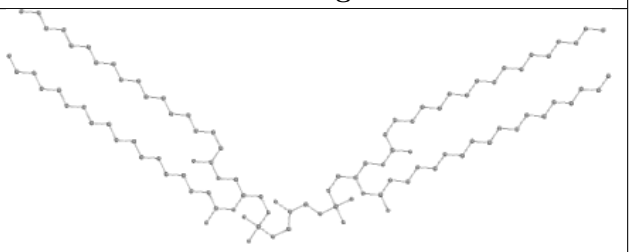
Bond lengths



Bond angles

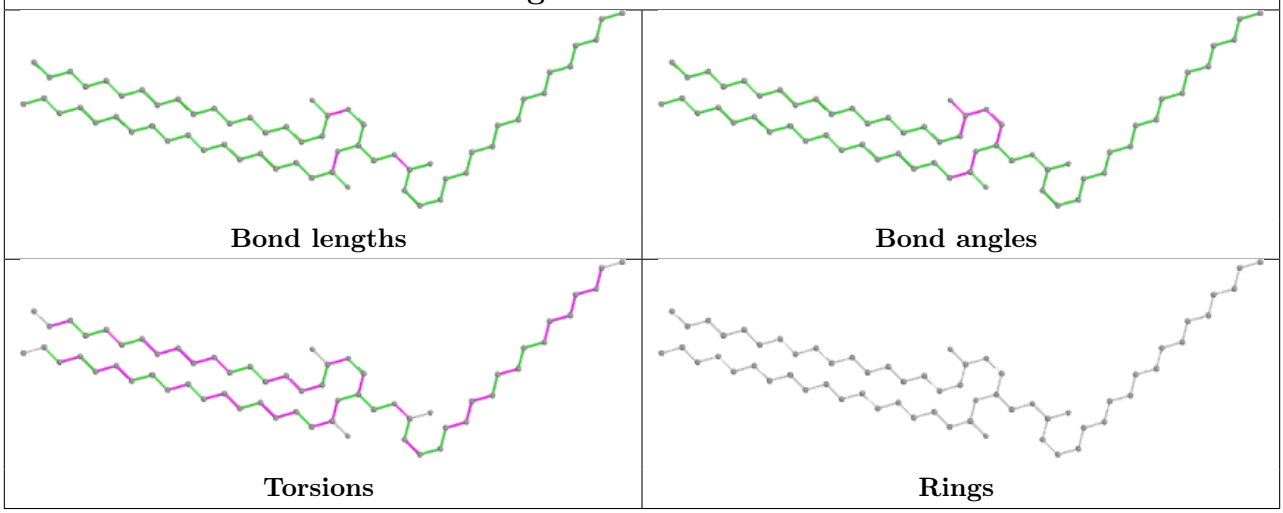


Torsions

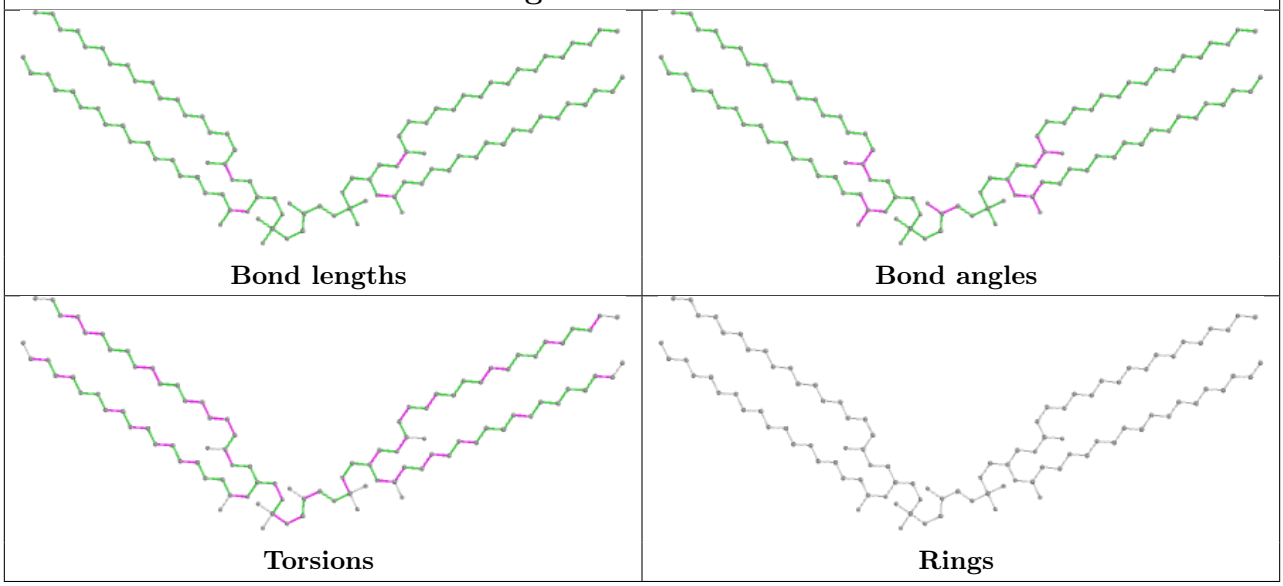


Rings

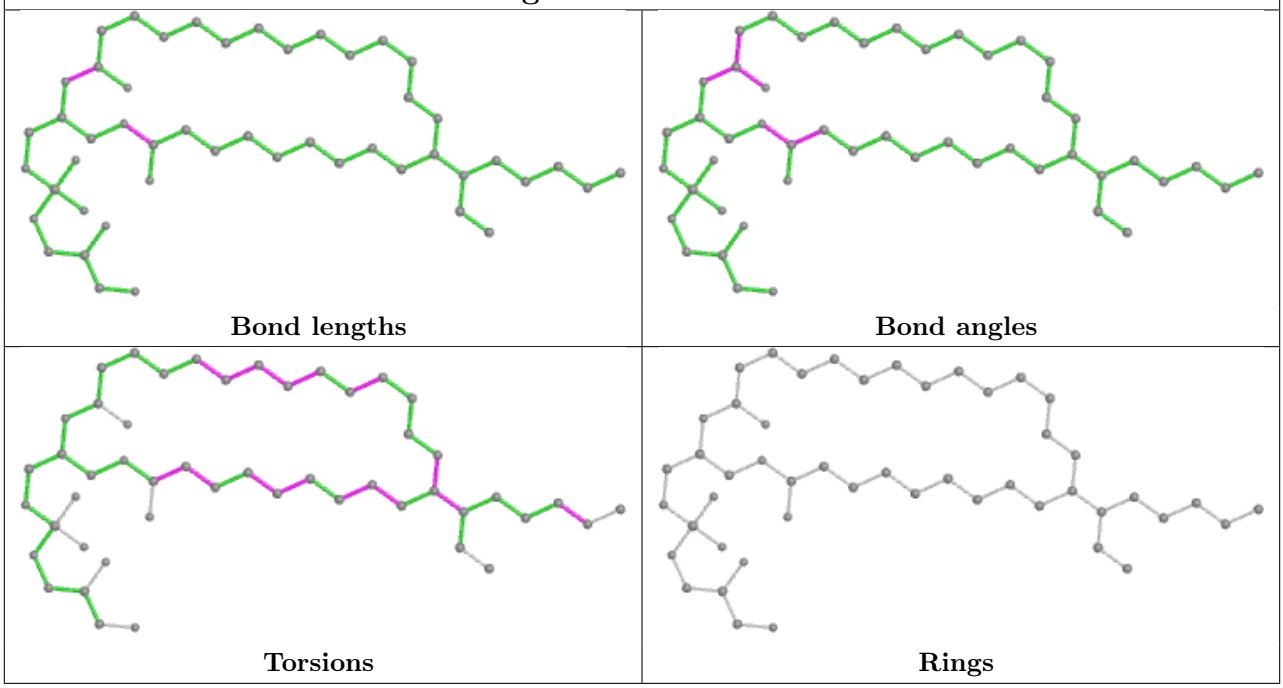
Ligand TGL L 101



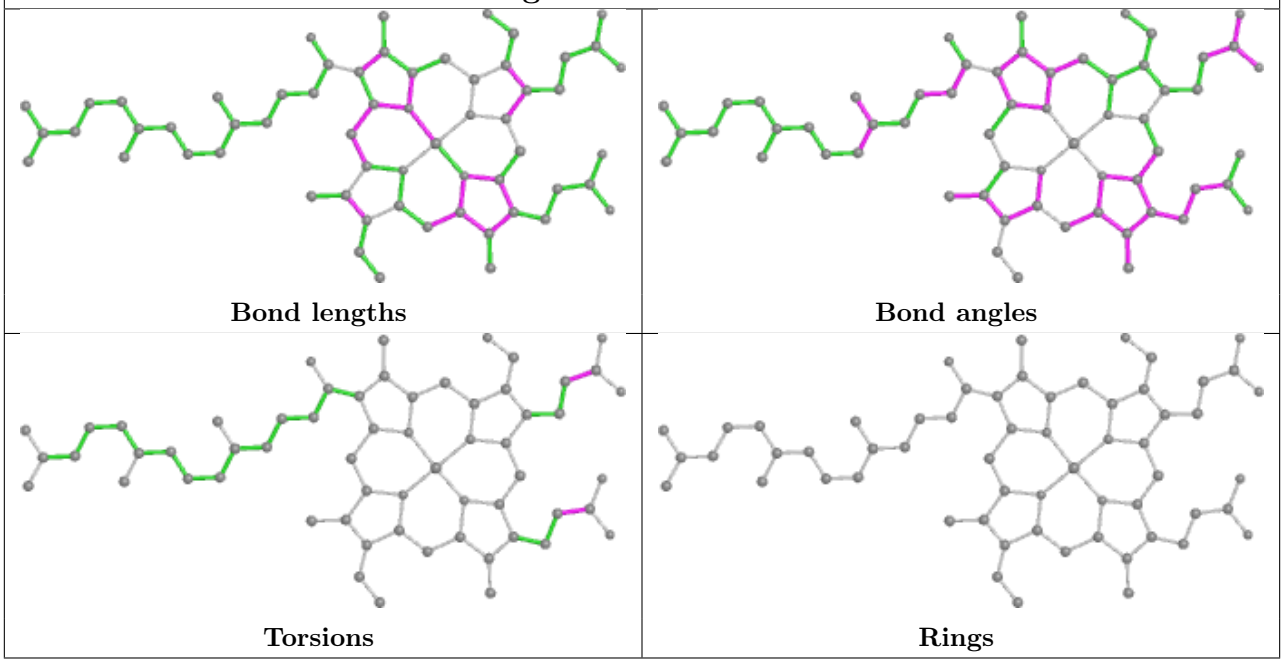
Ligand CDL C 305



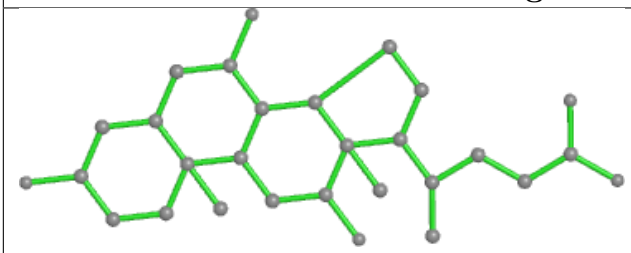
Ligand PGV A 607



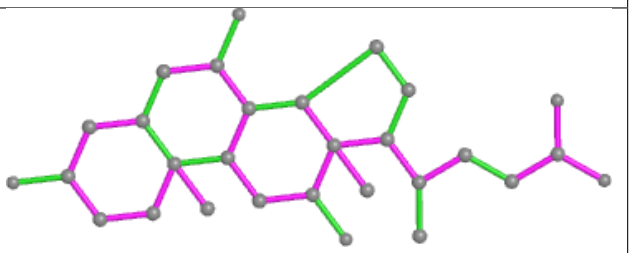
Ligand HEA A 602



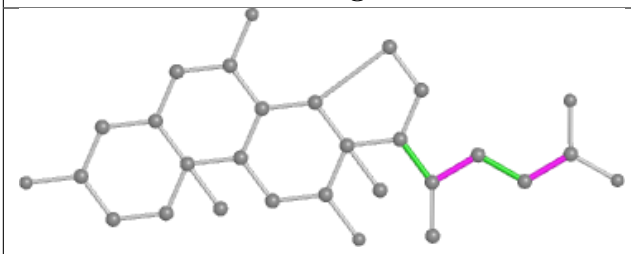
Ligand CHD c 302



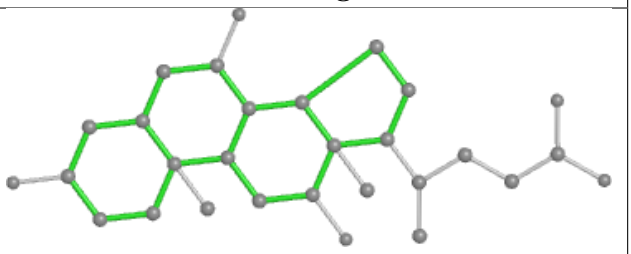
Bond lengths



Bond angles

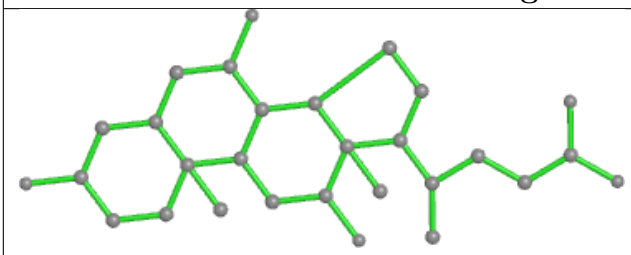


Torsions

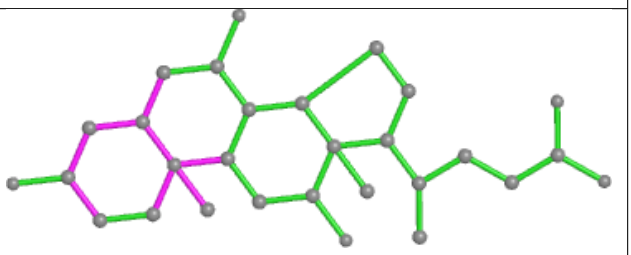


Rings

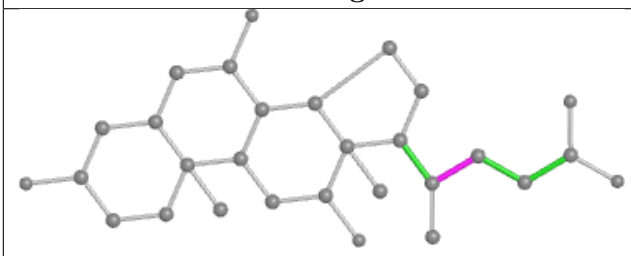
Ligand CHD C 306



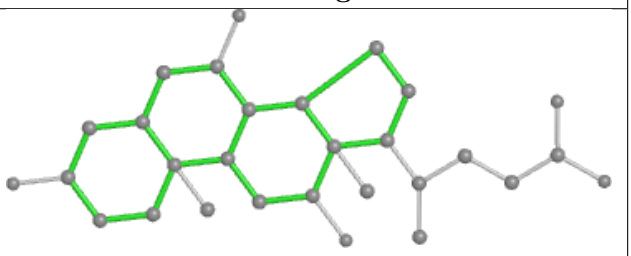
Bond lengths



Bond angles

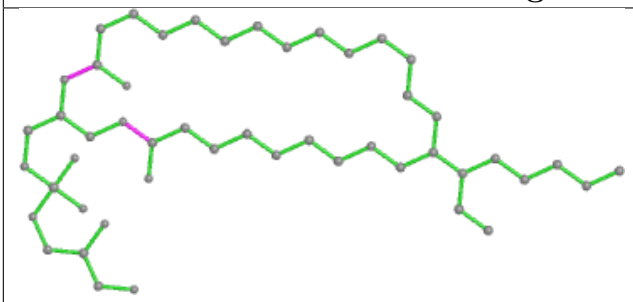


Torsions

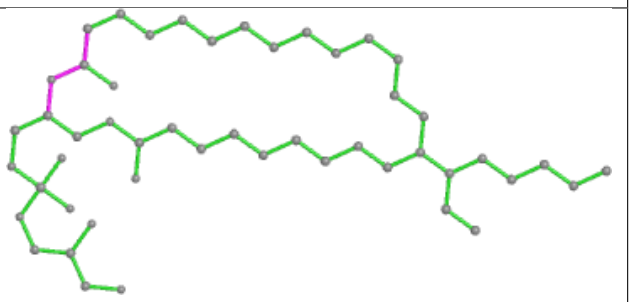


Rings

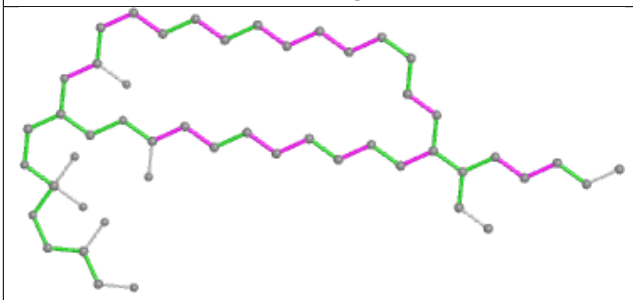
Ligand PGV c 301



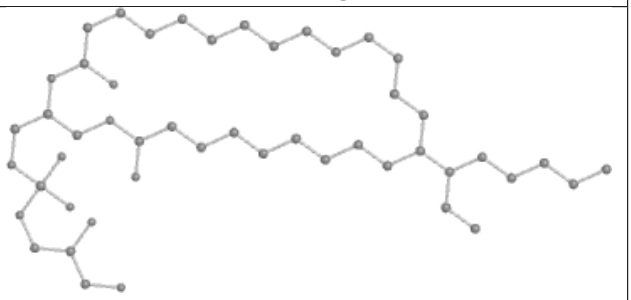
Bond lengths



Bond angles

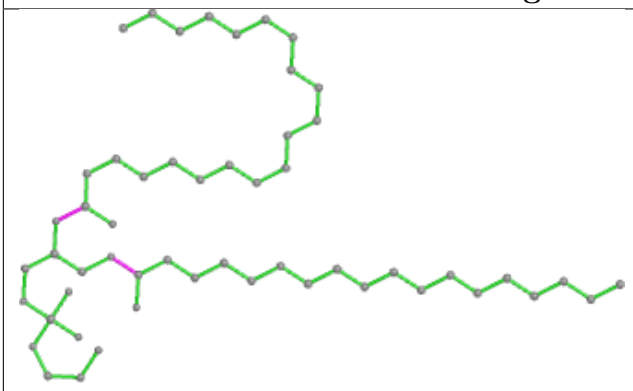


Torsions

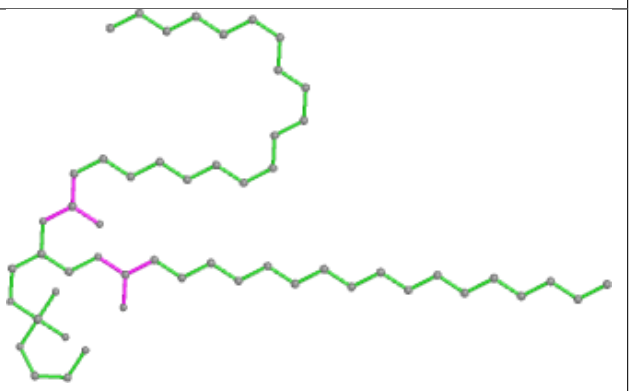


Rings

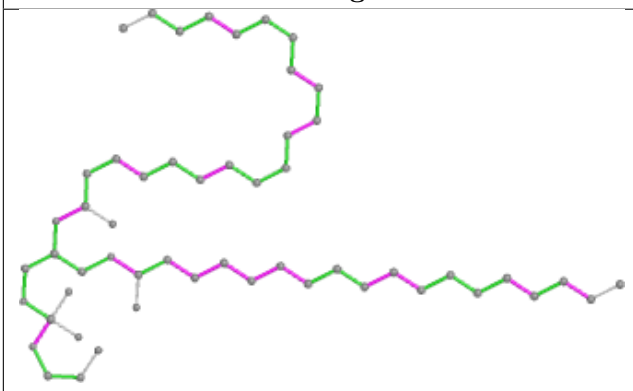
Ligand PEK C 308



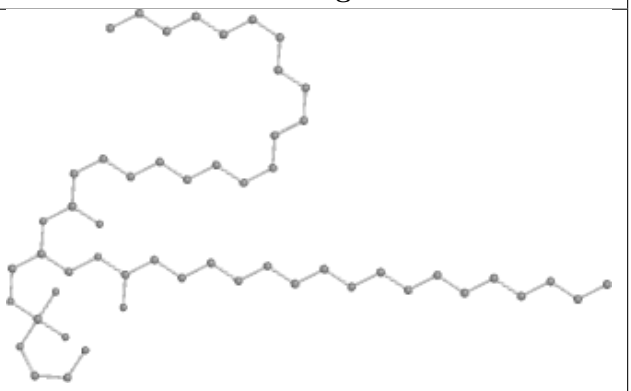
Bond lengths



Bond angles

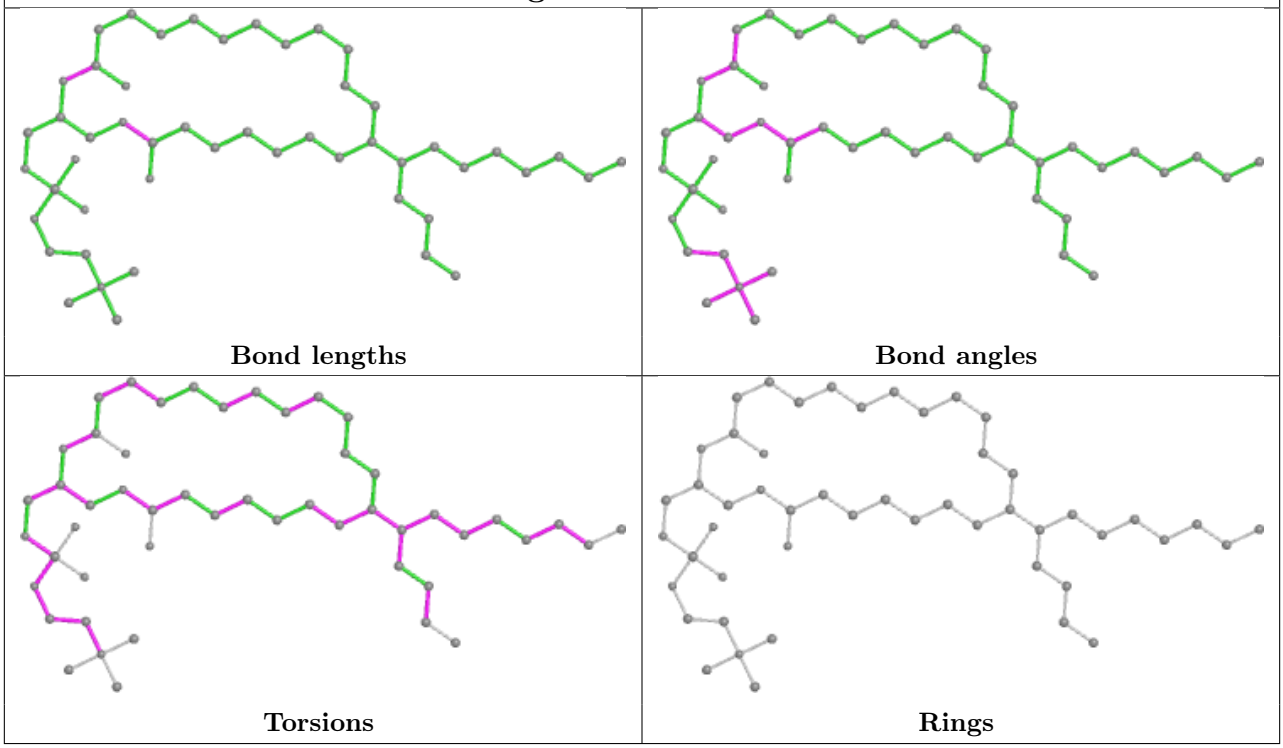


Torsions

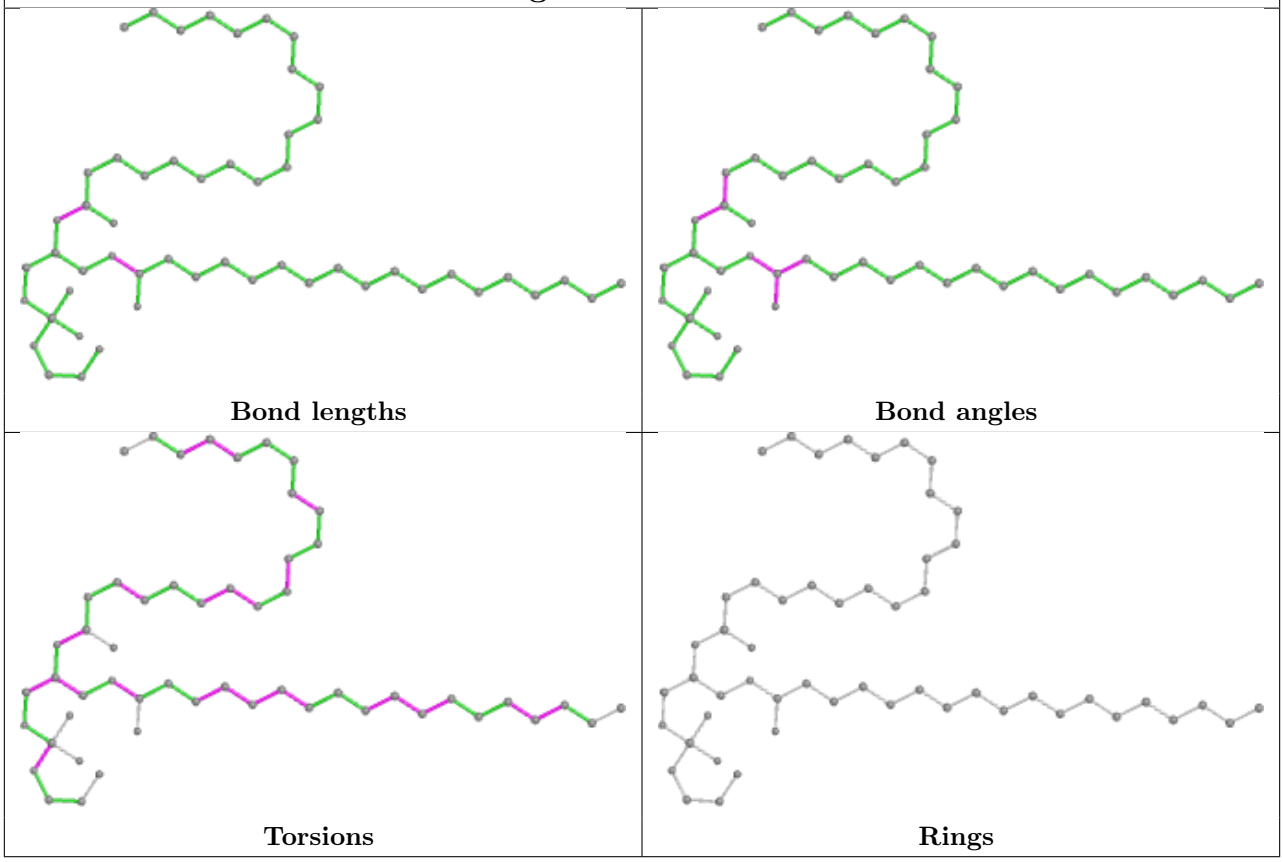


Rings

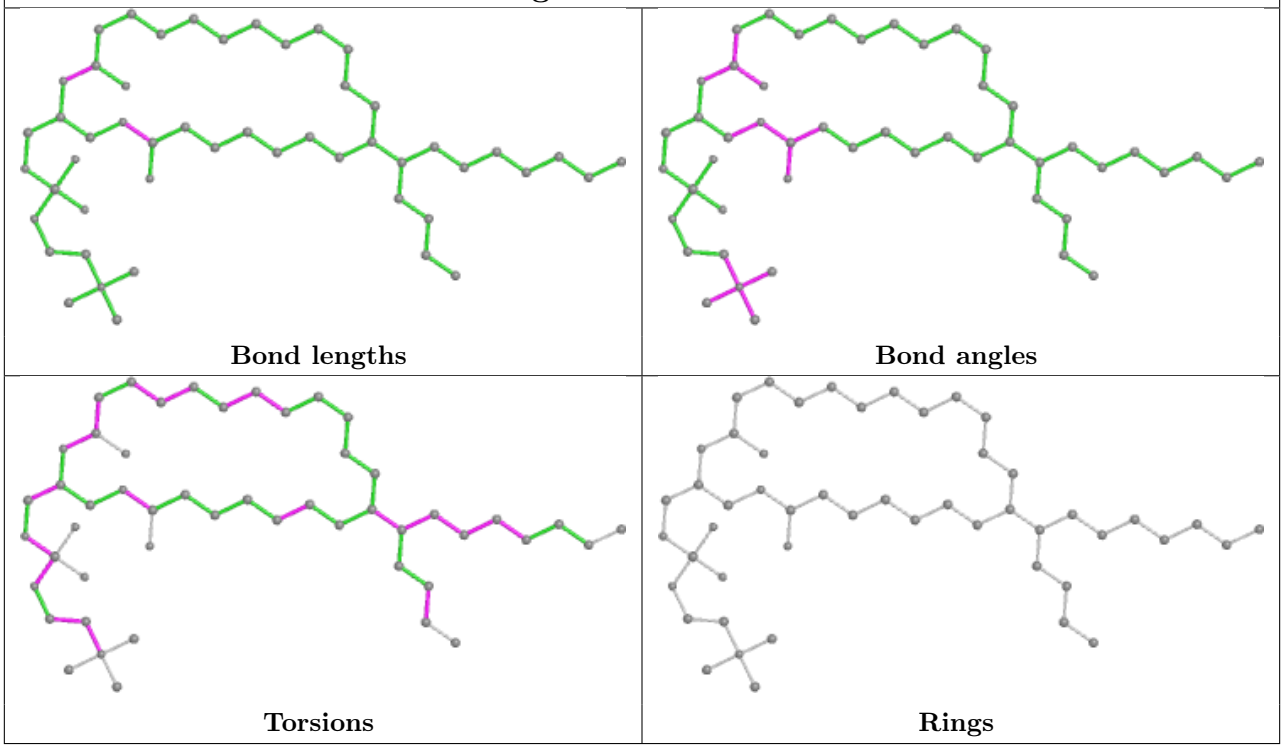
Ligand PSC B 302



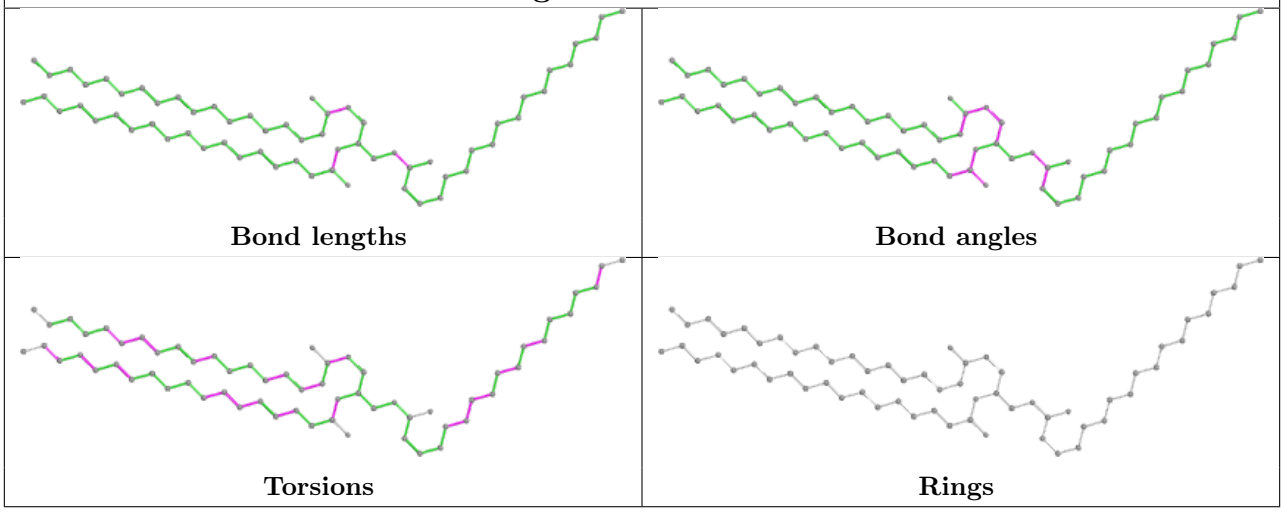
Ligand PEK c 303



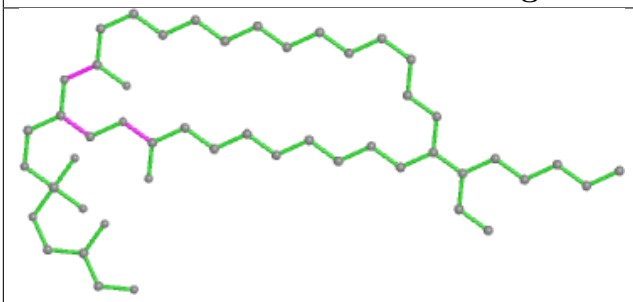
Ligand PSC e 201



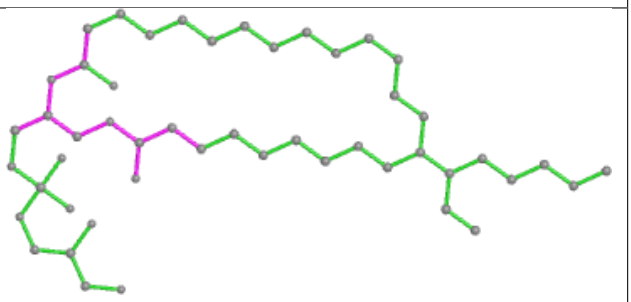
Ligand TGL i 101



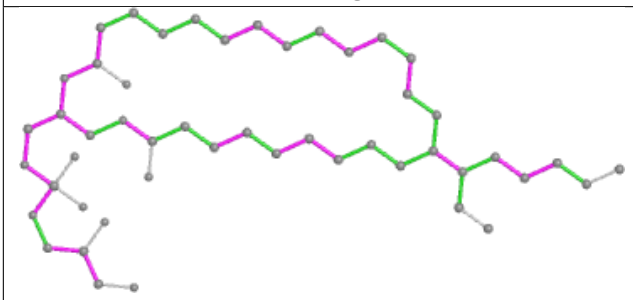
Ligand PGV A 606



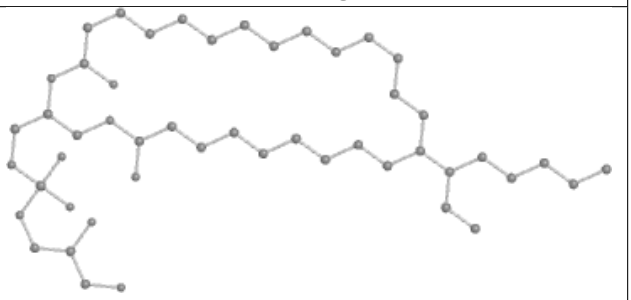
Bond lengths



Bond angles

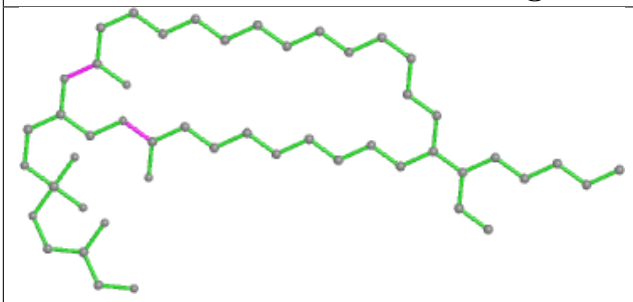


Torsions

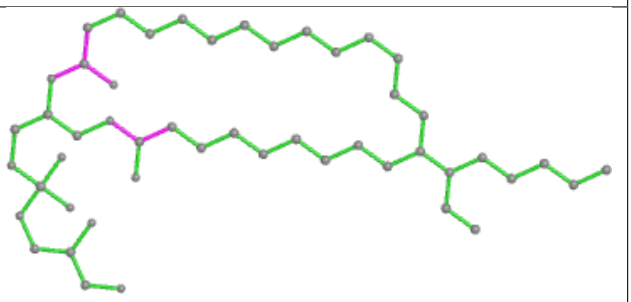


Rings

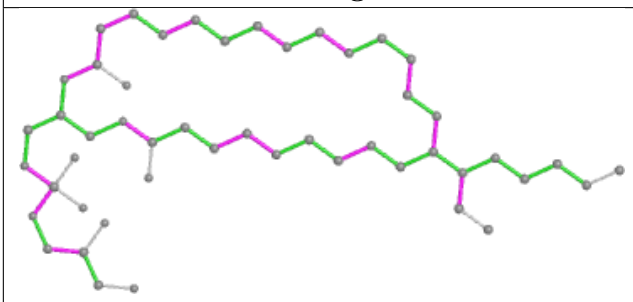
Ligand PGV a 607



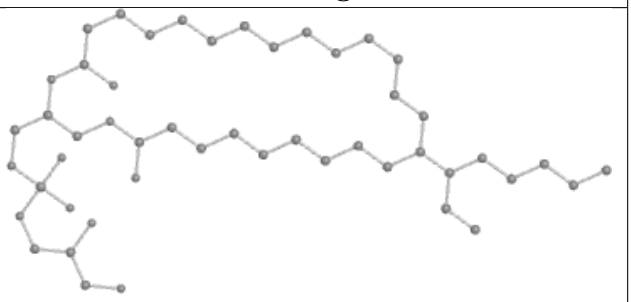
Bond lengths



Bond angles

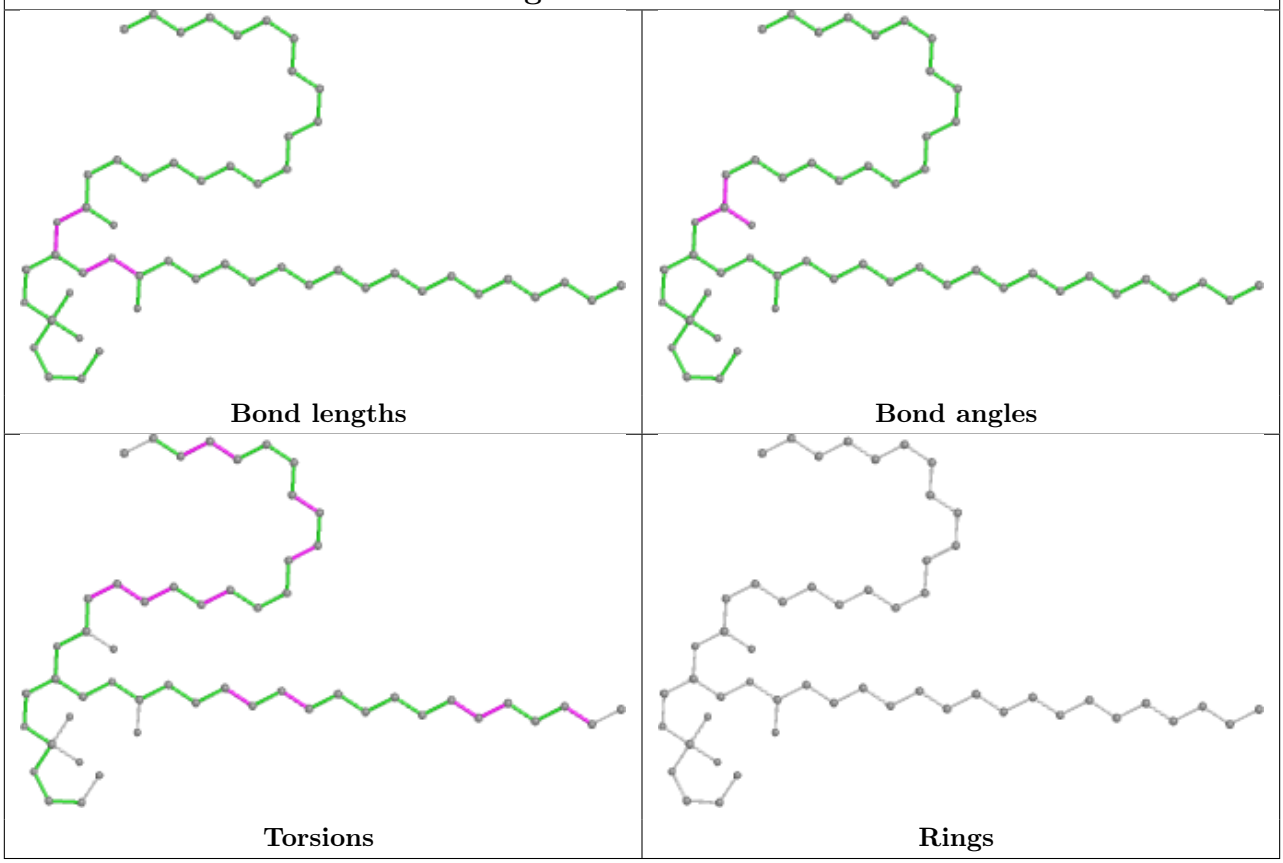


Torsions

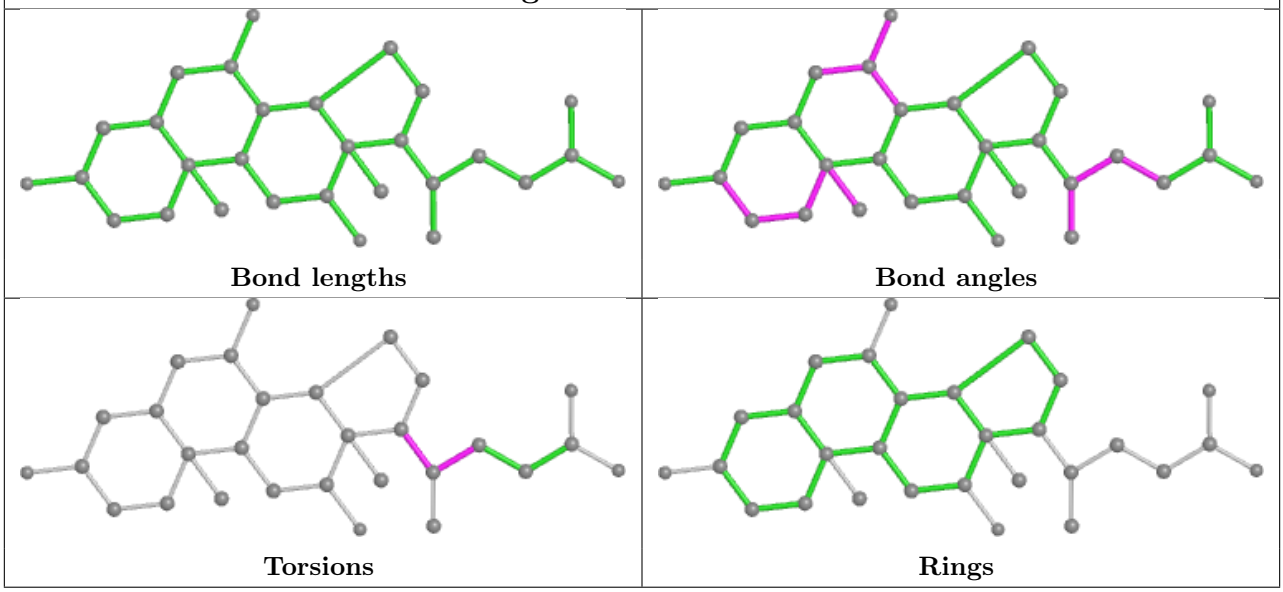


Rings

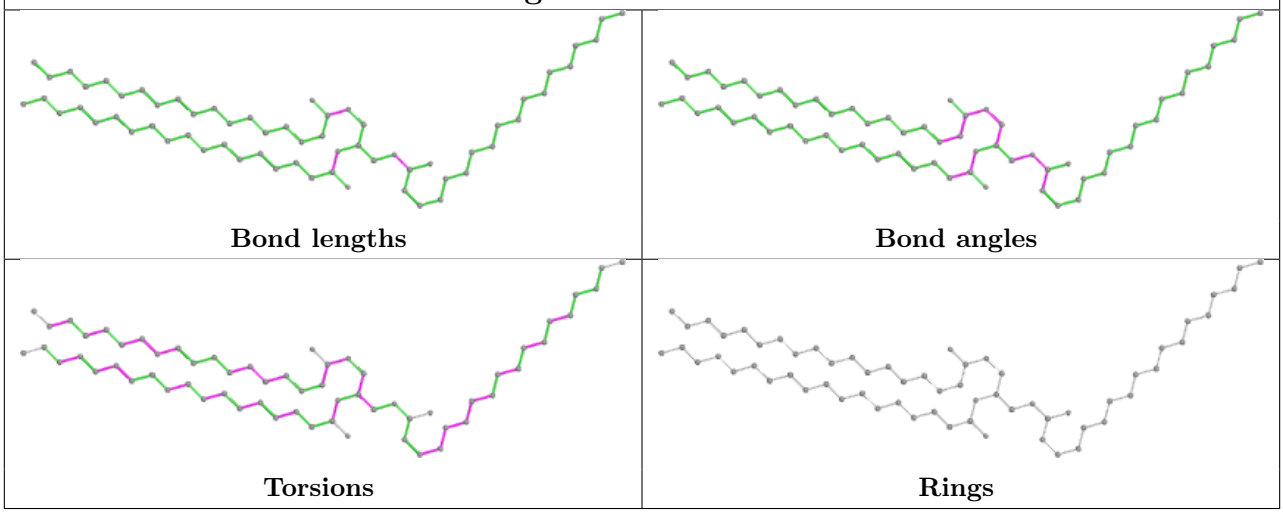
Ligand PEK C 302



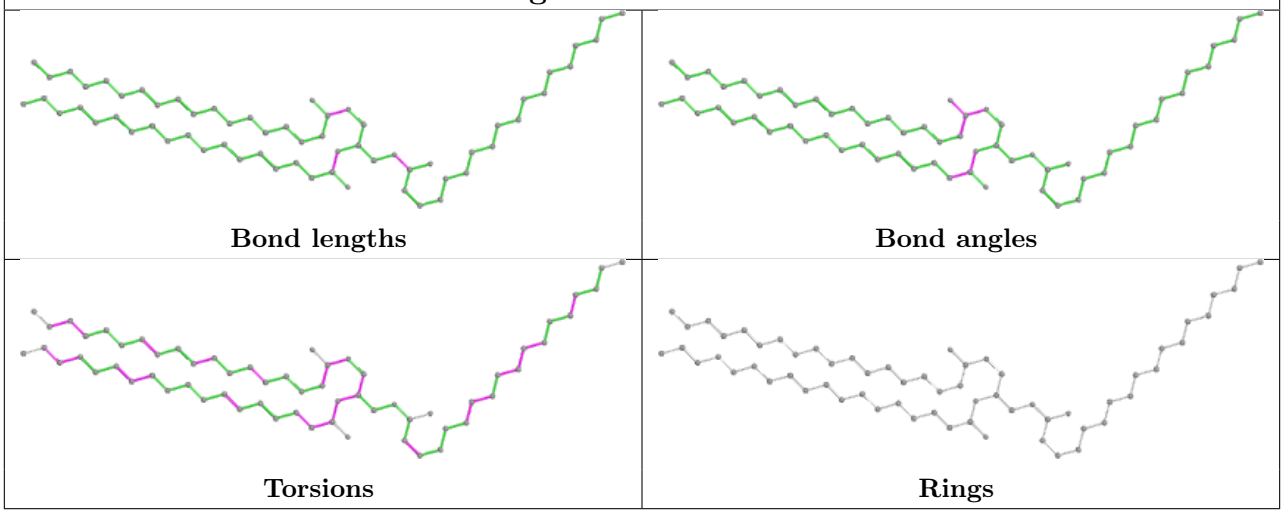
Ligand CHD C 301

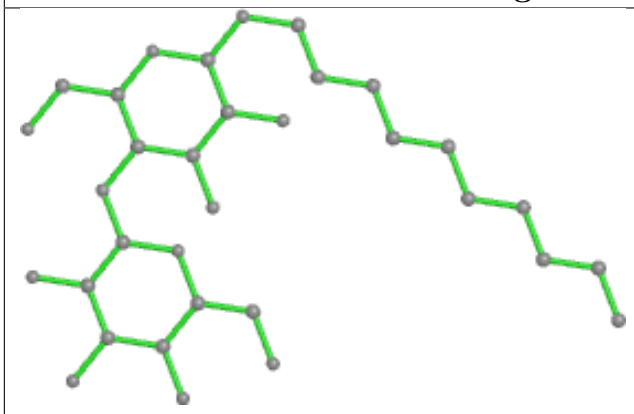
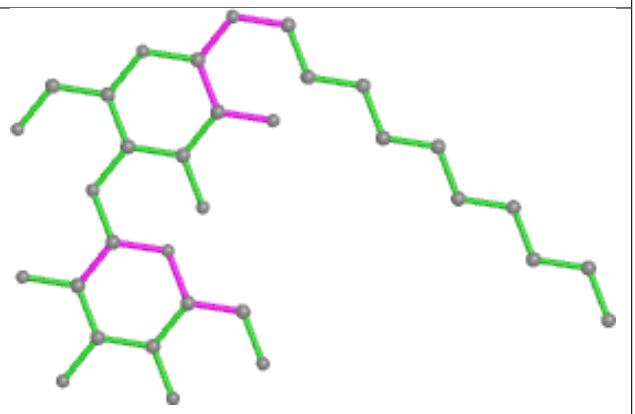
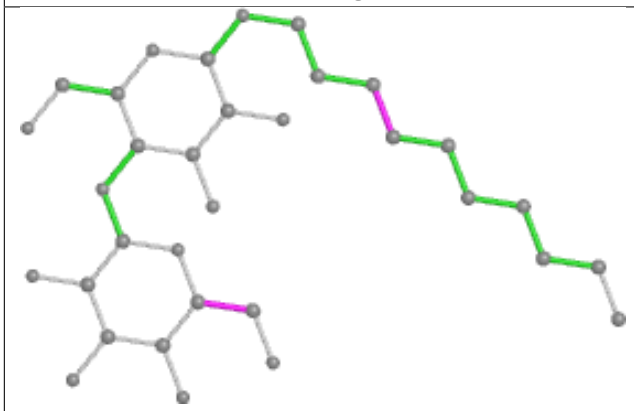
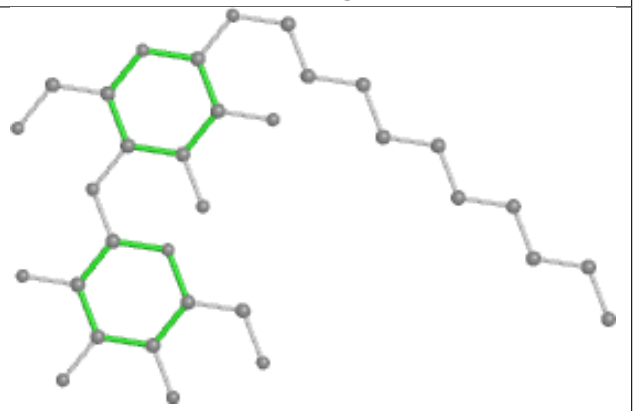


Ligand TGL A 608

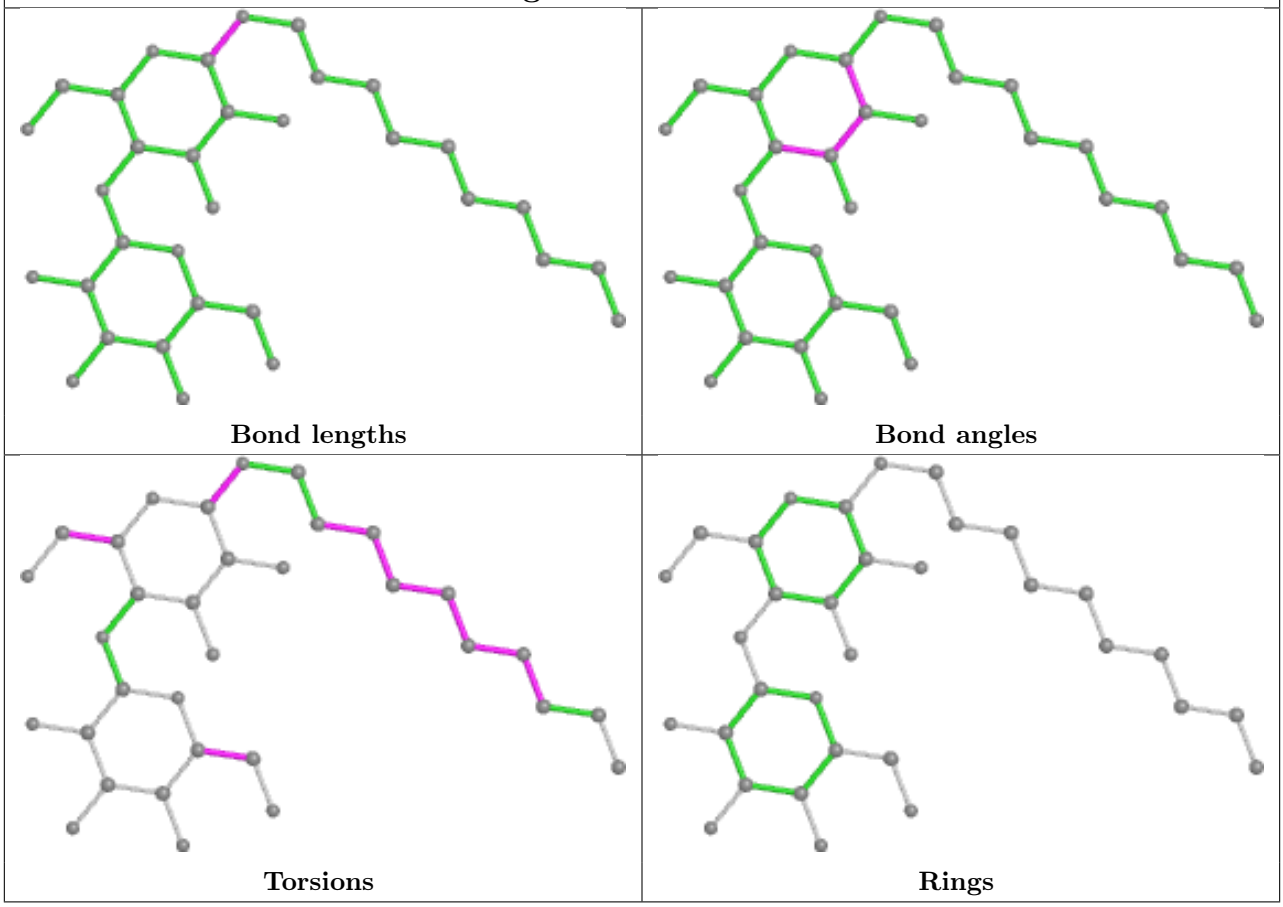


Ligand TGL a 606

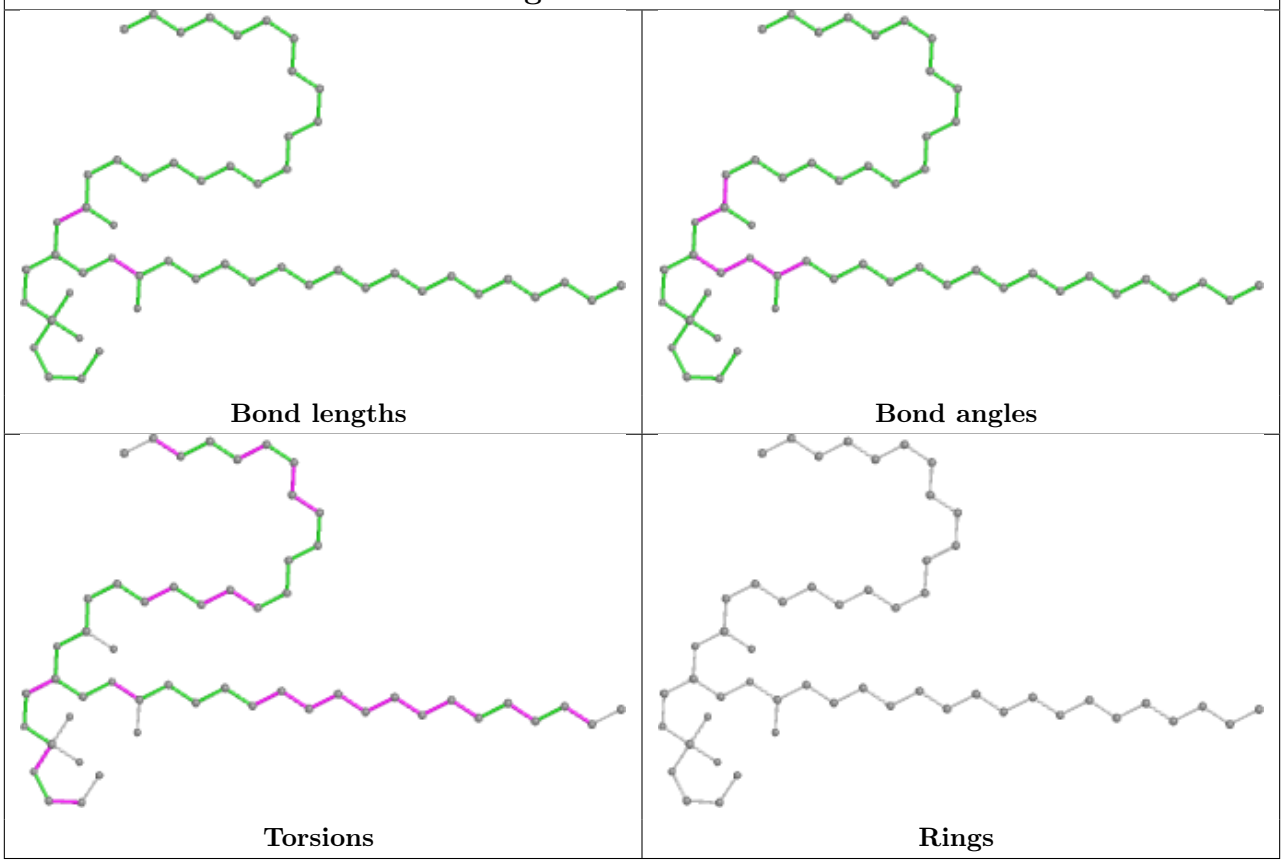


Ligand DMU M 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

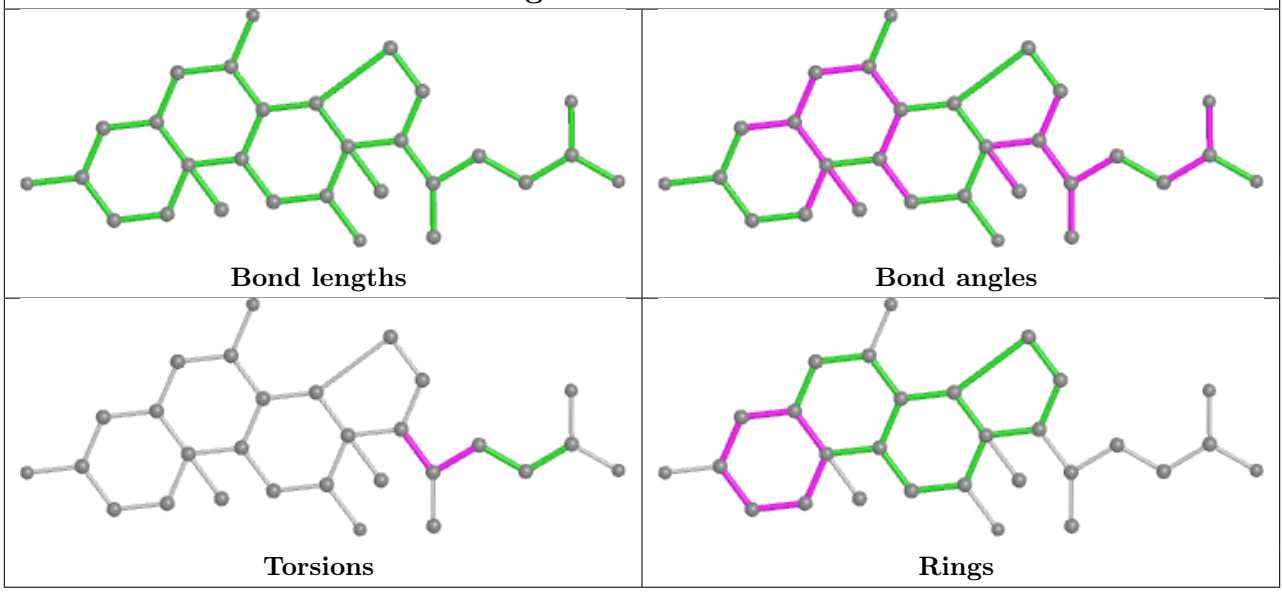
Ligand DMU c 307



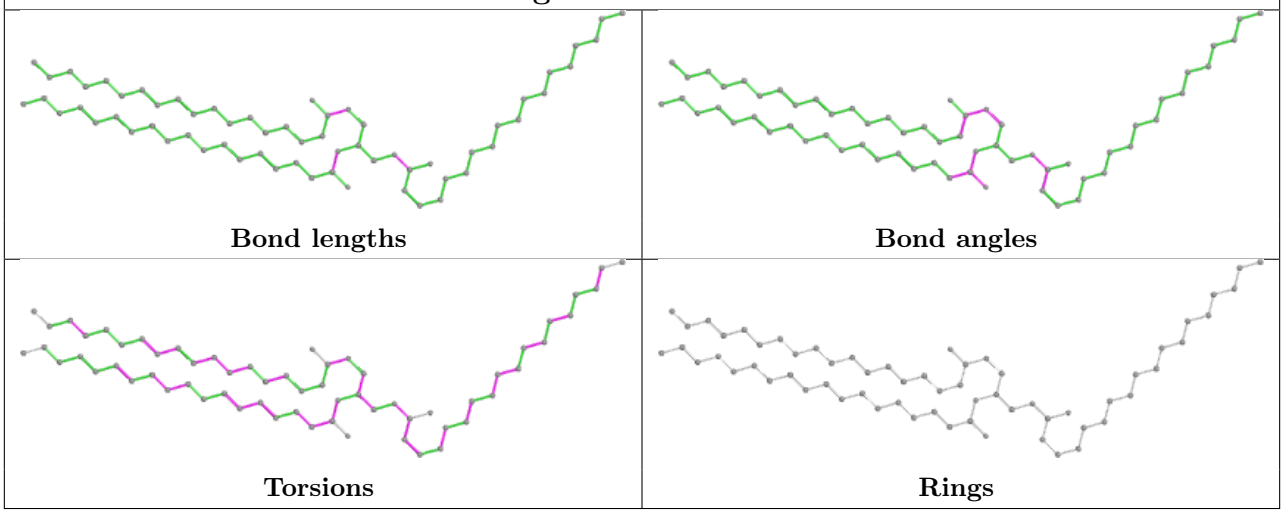
Ligand PEK C 309



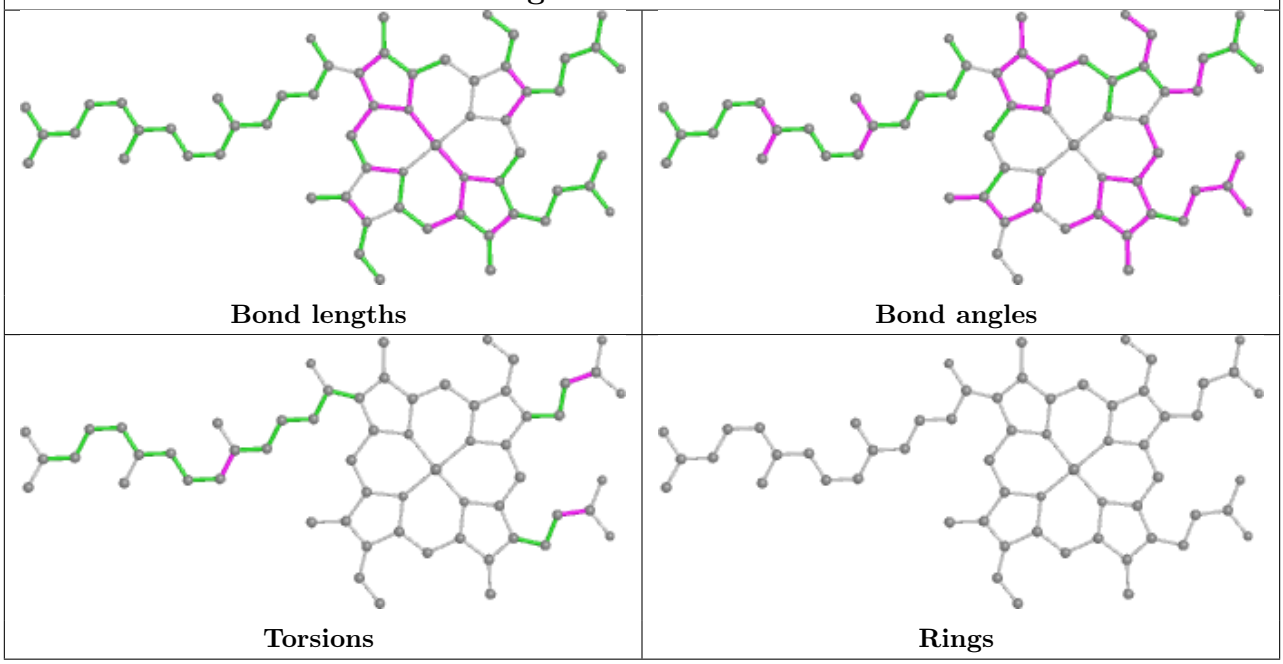
Ligand CHD J 101

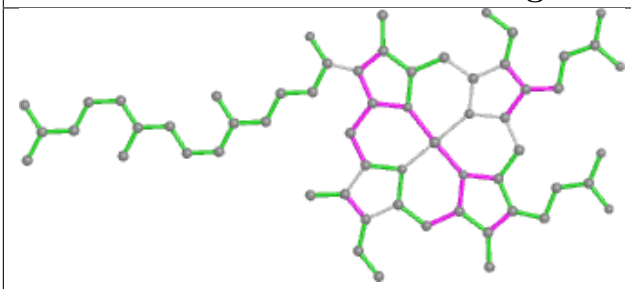
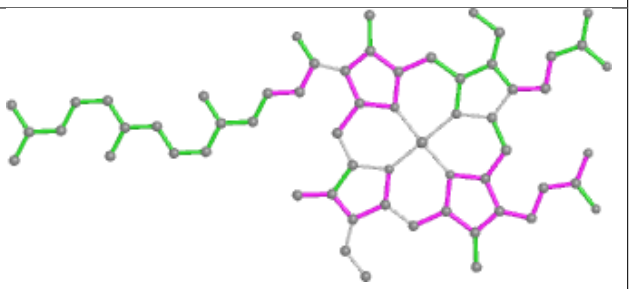
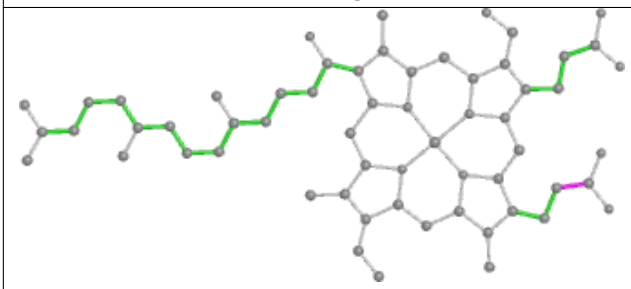
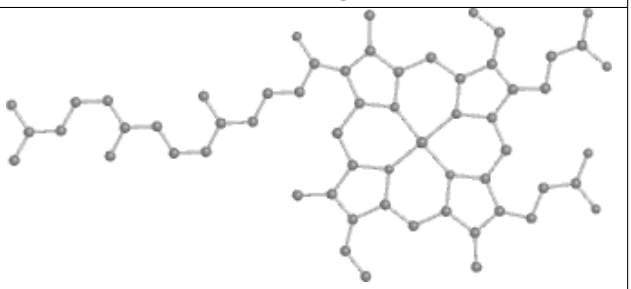


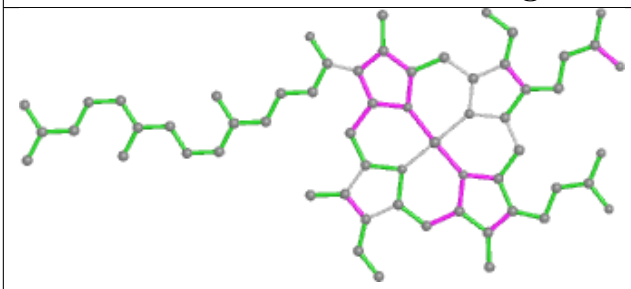
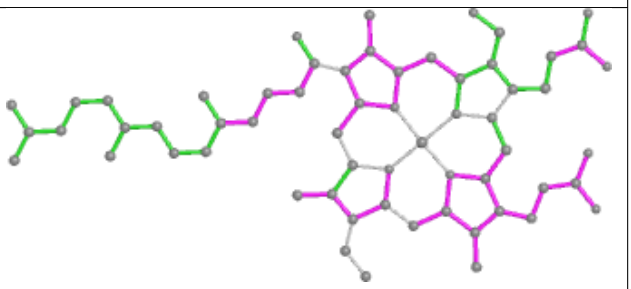
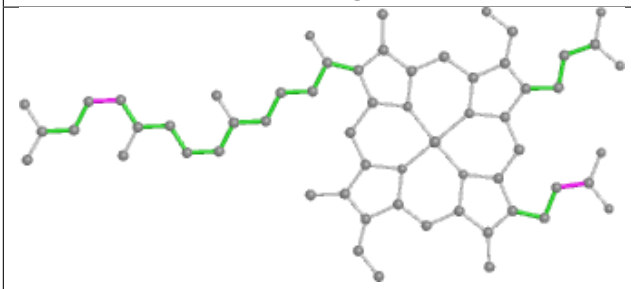
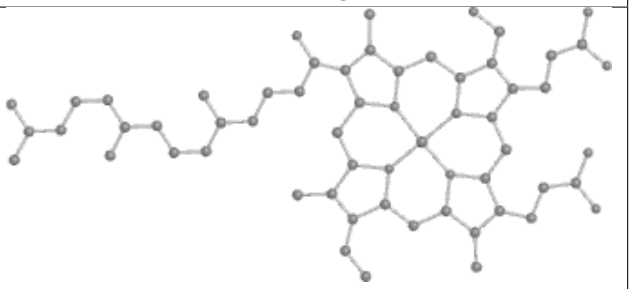
Ligand TGL l 101

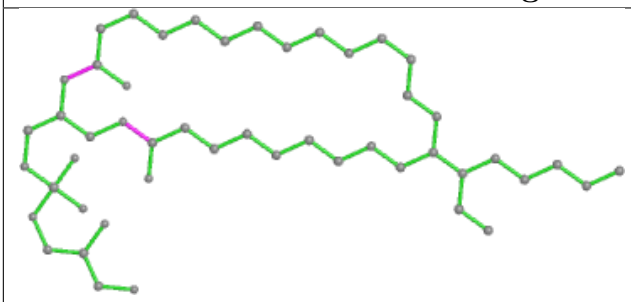
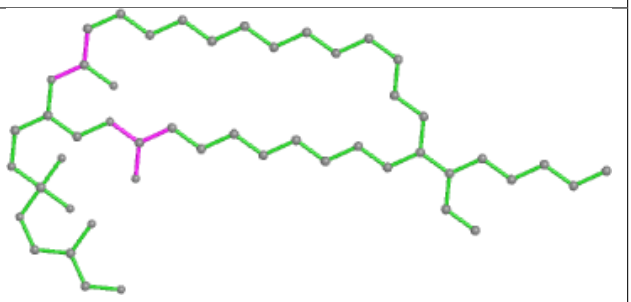
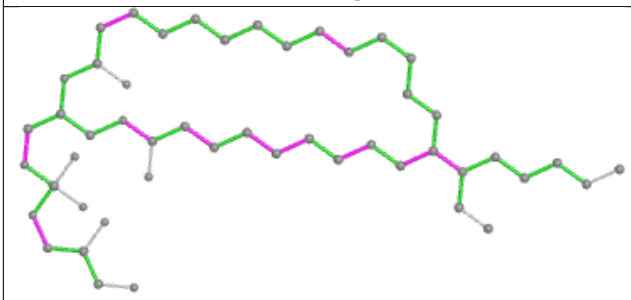
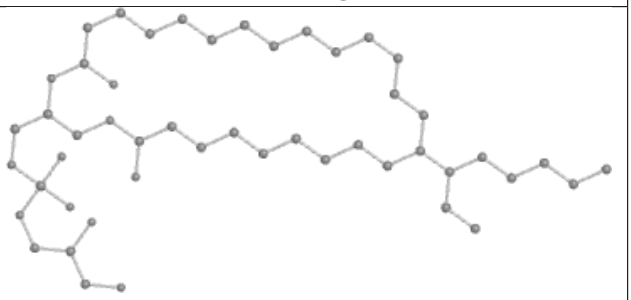


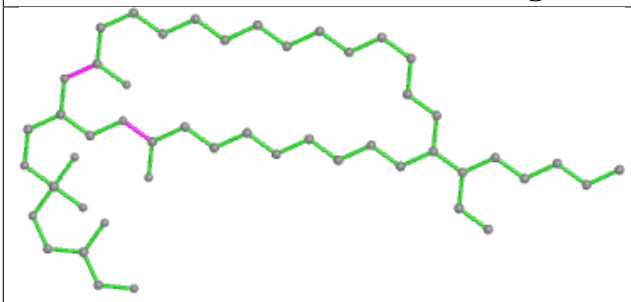
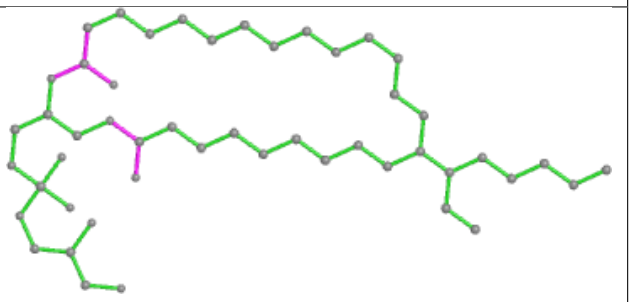
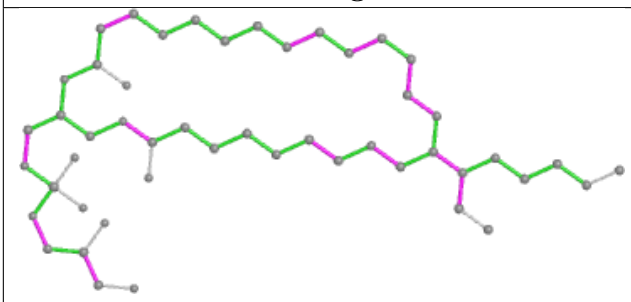
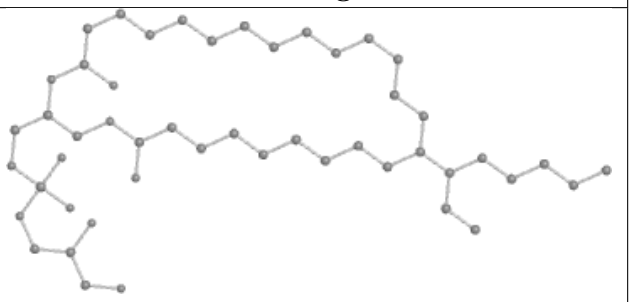
Ligand HEA a 602



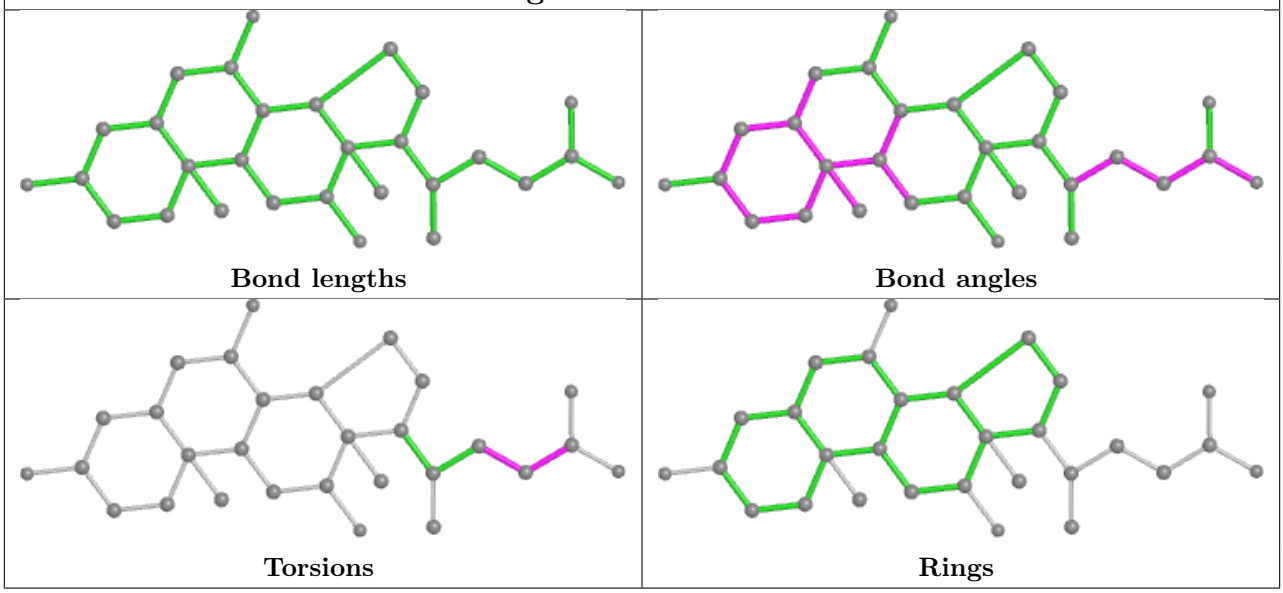
Ligand HEA a 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HEA A 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

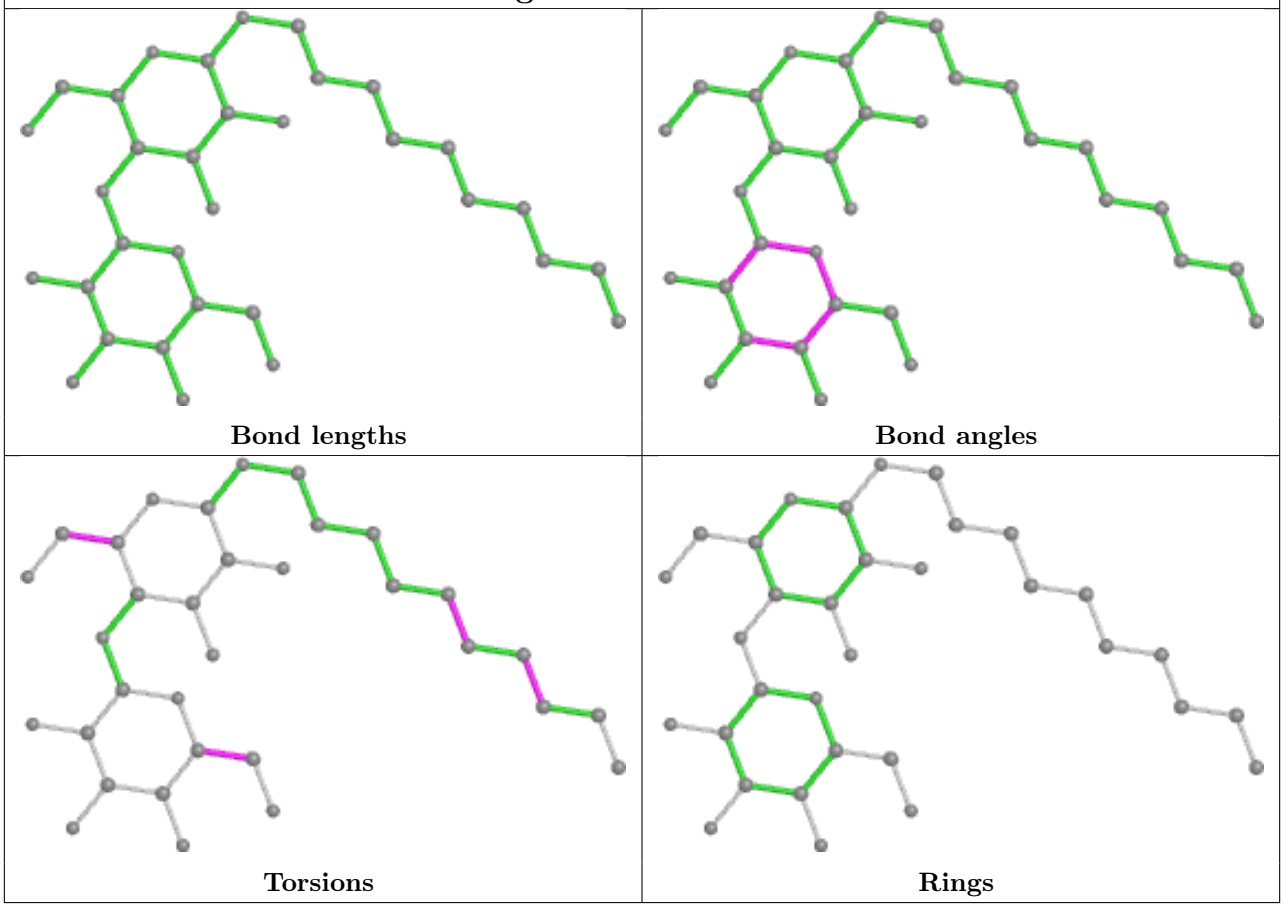
Ligand PGV C 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PGV c 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

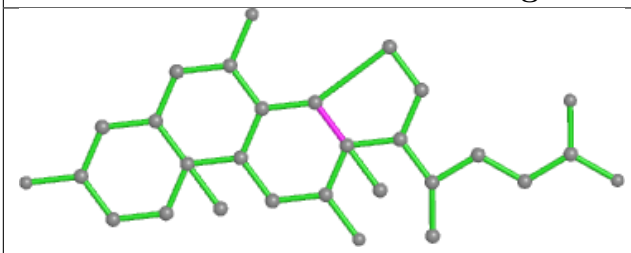
Ligand CHD c 306



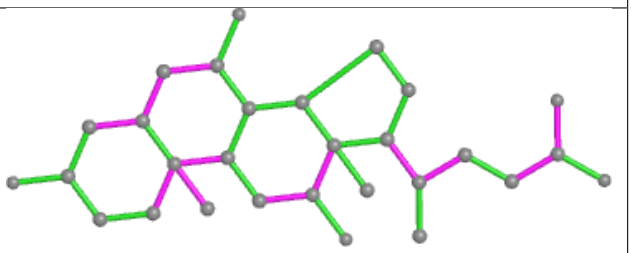
Ligand DMU m 401



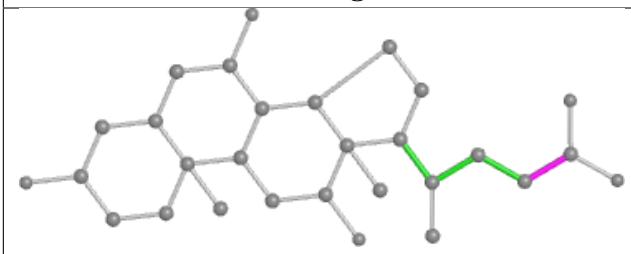
Ligand CHD B 303



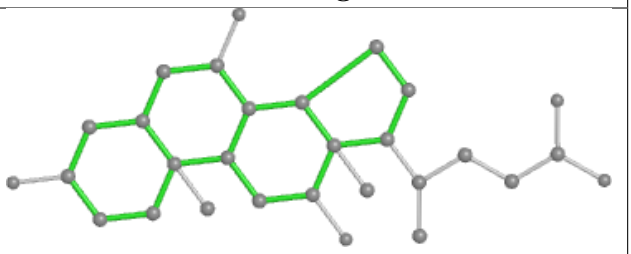
Bond lengths



Bond angles

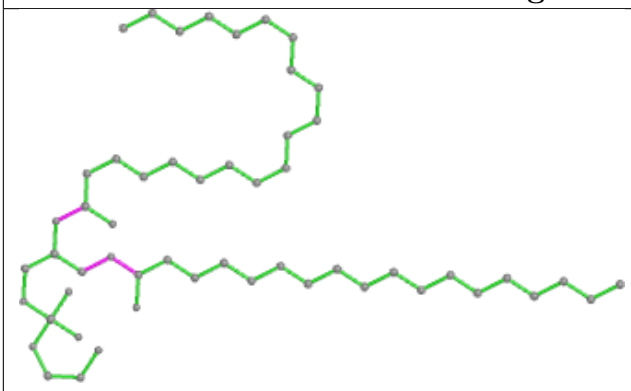


Torsions

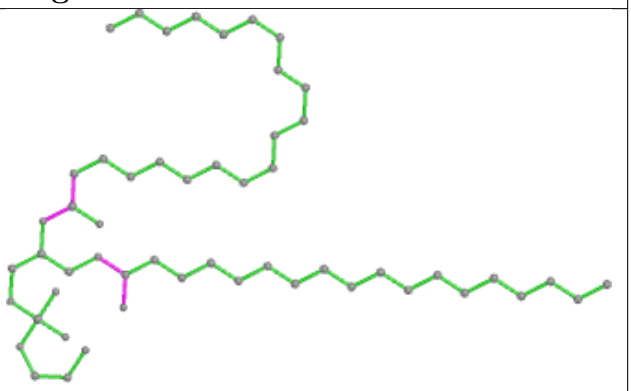


Rings

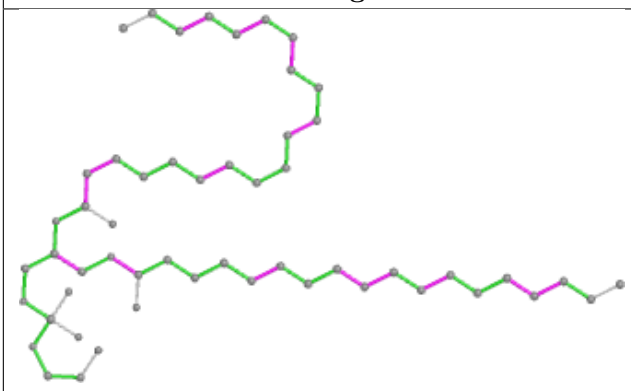
Ligand PEK g 102



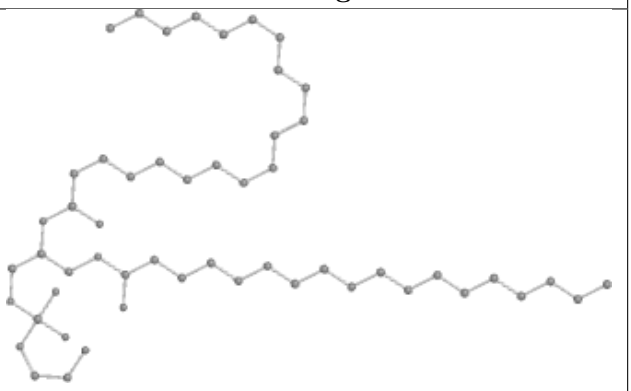
Bond lengths



Bond angles

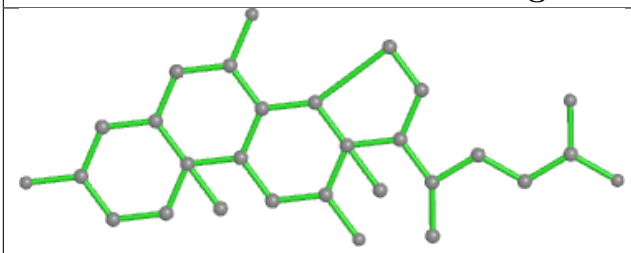


Torsions

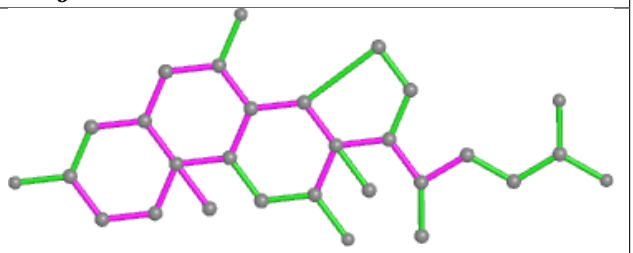


Rings

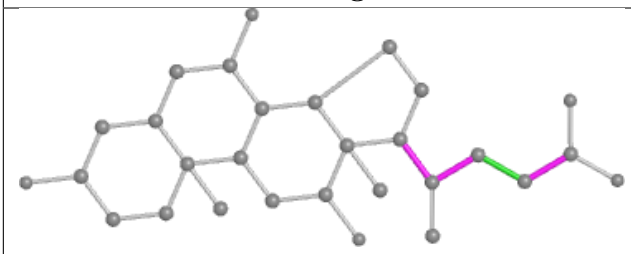
Ligand CHD j 101



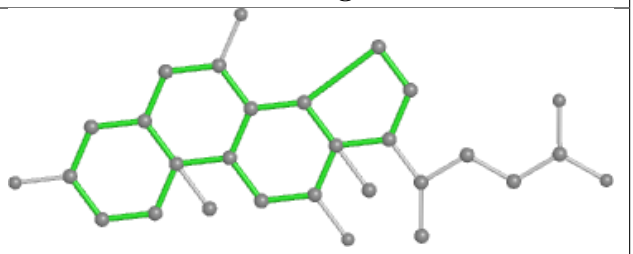
Bond lengths



Bond angles

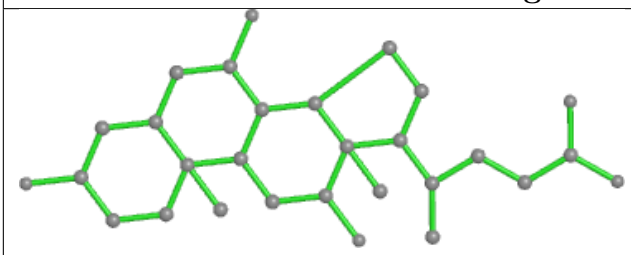


Torsions

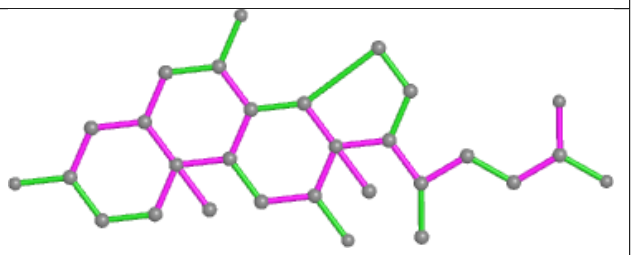


Rings

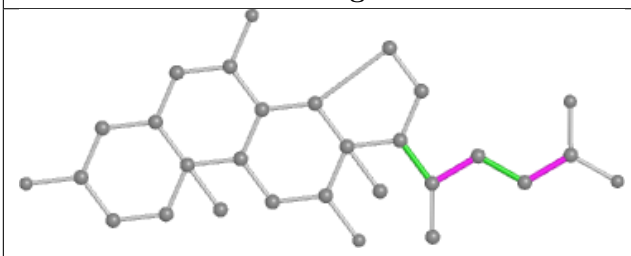
Ligand CHD b 301



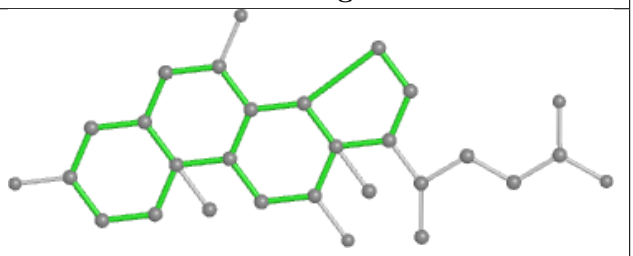
Bond lengths



Bond angles

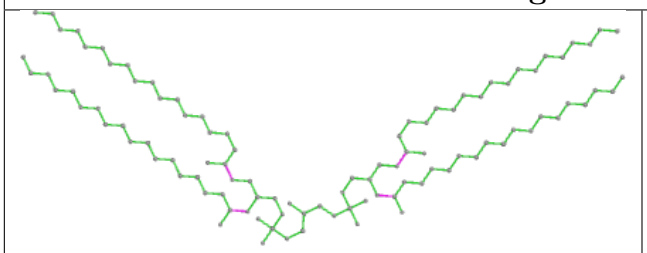


Torsions

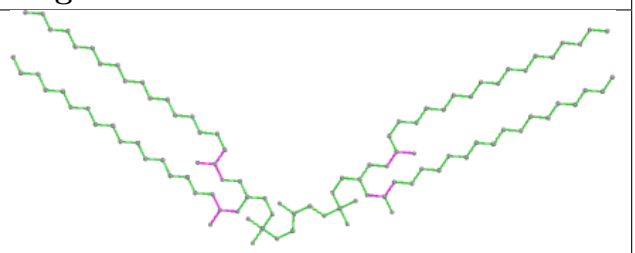


Rings

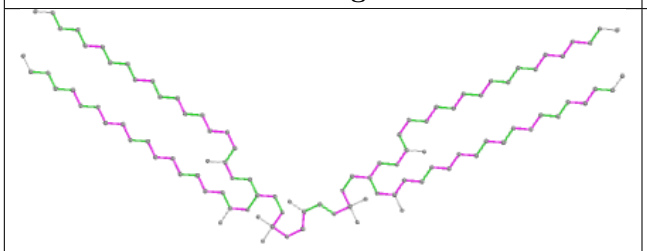
Ligand CDL g 103



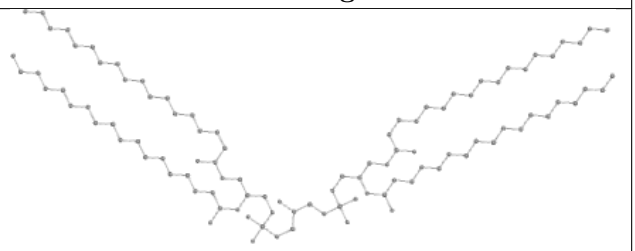
Bond lengths



Bond angles

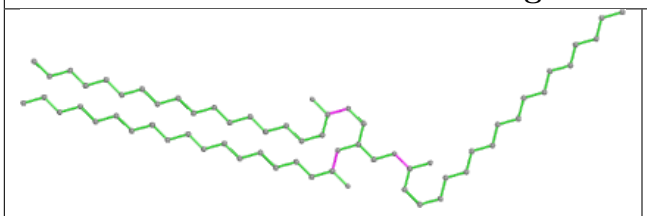


Torsions

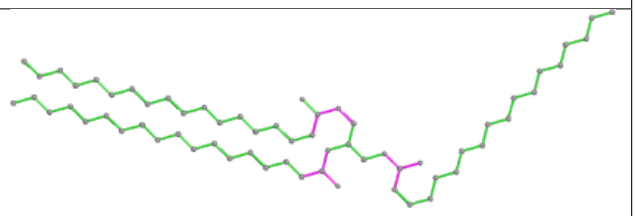


Rings

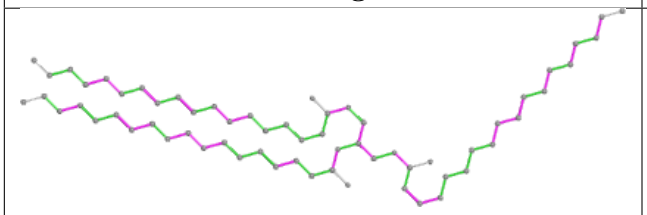
Ligand TGL D 201



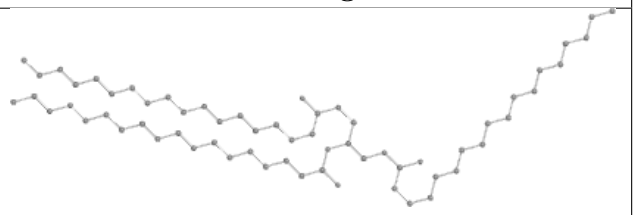
Bond lengths



Bond angles

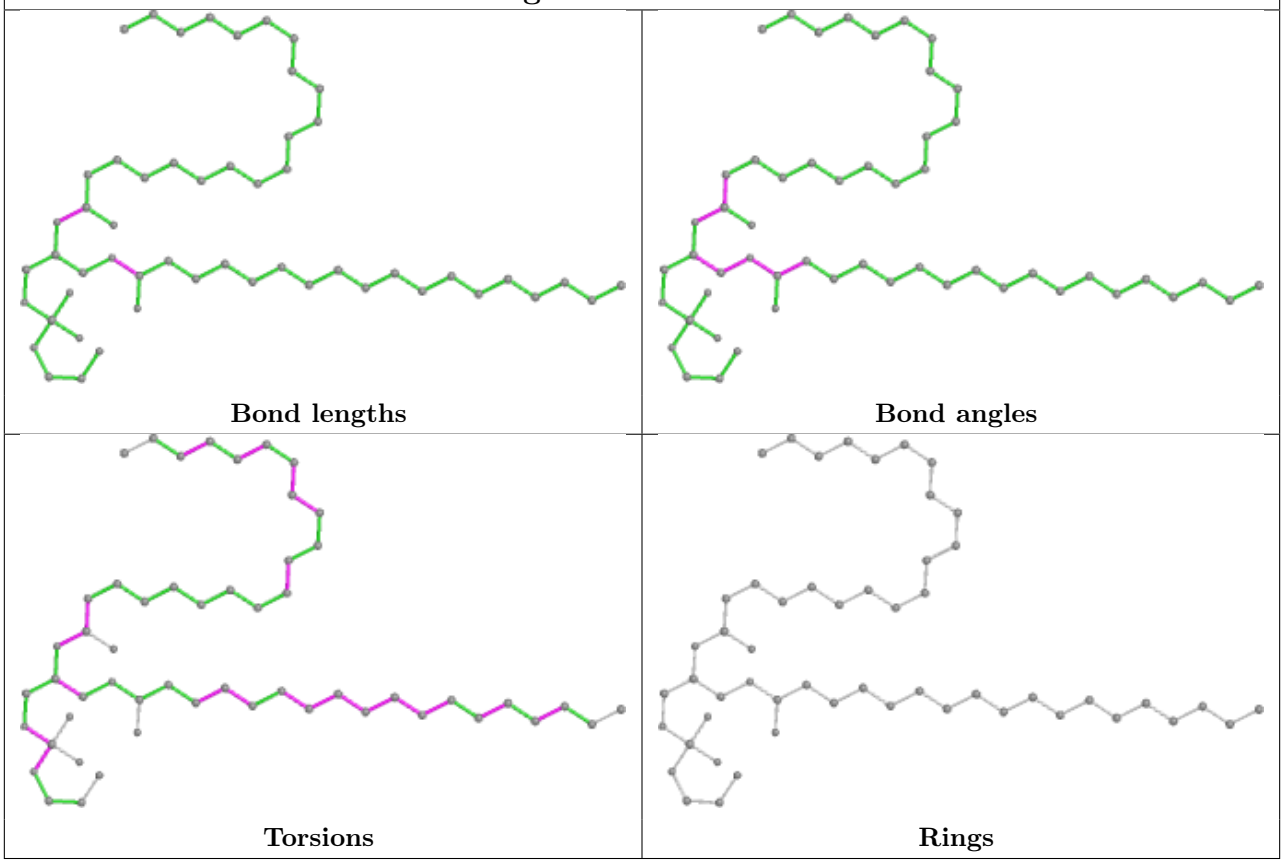


Torsions

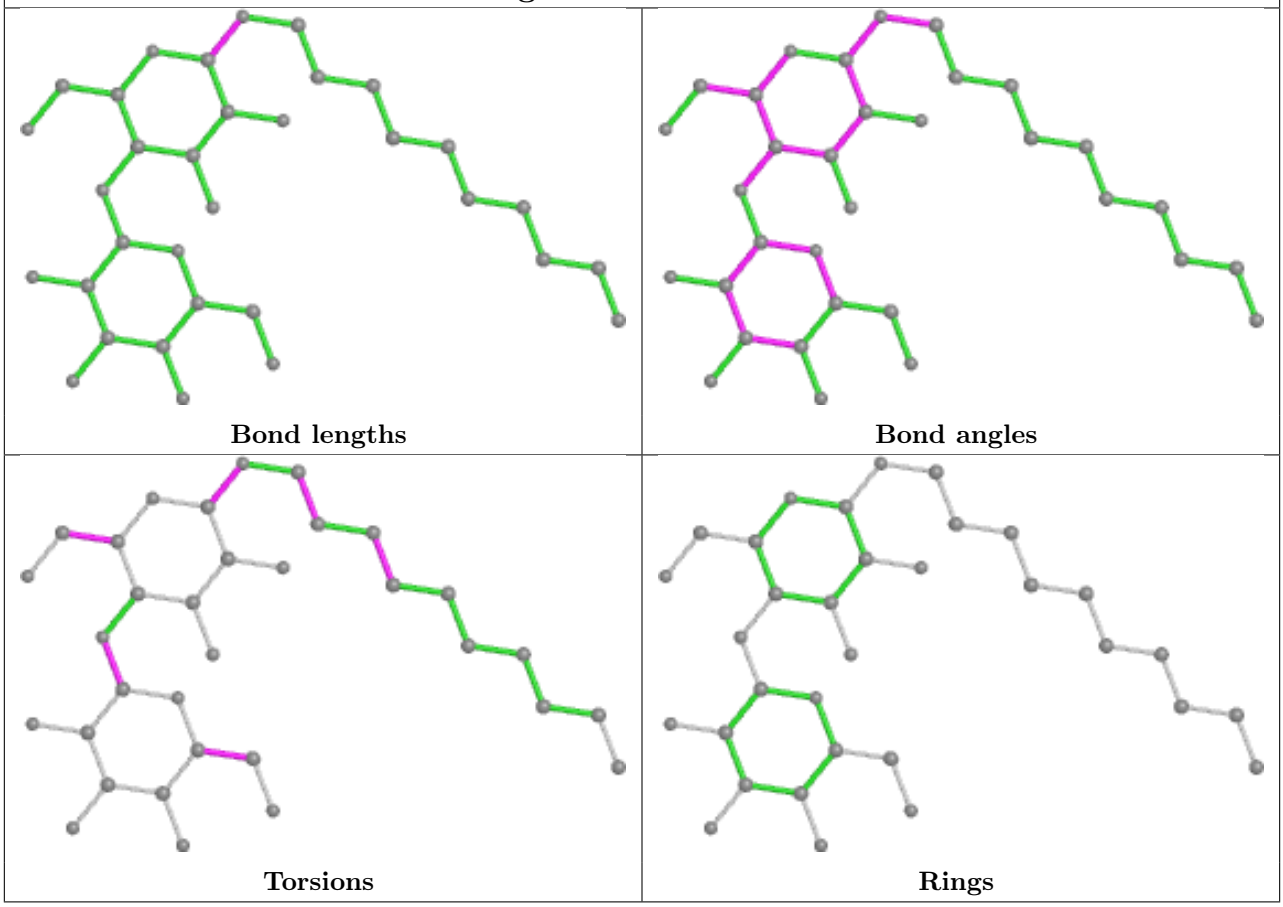


Rings

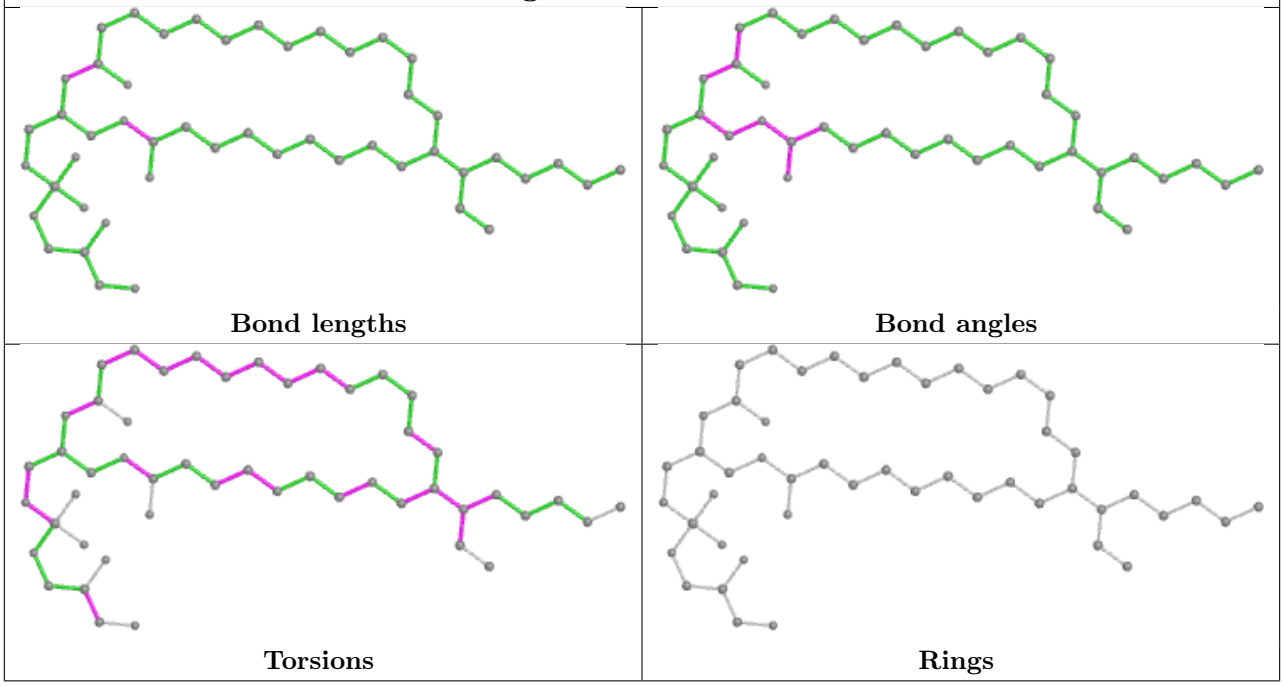
Ligand PEK G 102

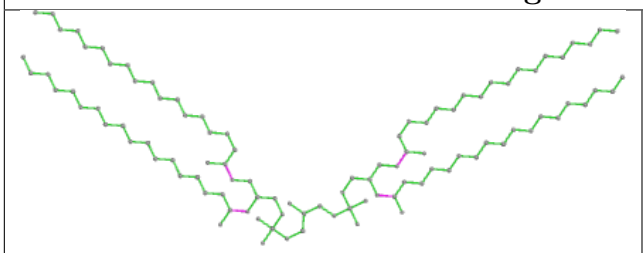
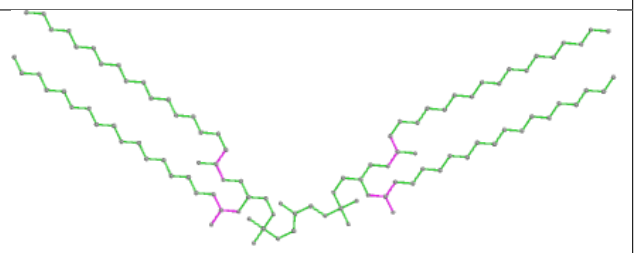
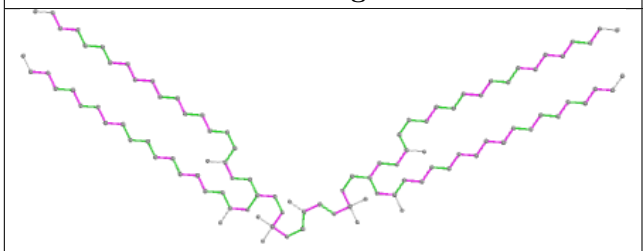
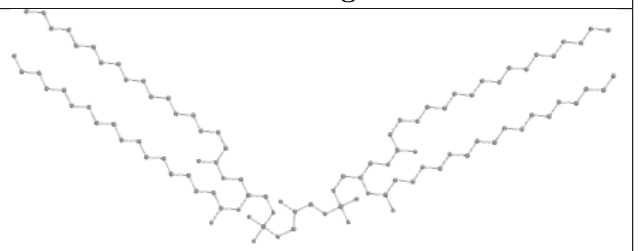


Ligand DMU C 307



Ligand PGV G 103



Ligand CDL G 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	513/514 (99%)	-0.64	0 100 100	22, 28, 39, 85	0
1	a	513/514 (99%)	-0.50	0 100 100	27, 41, 58, 93	0
2	B	226/227 (99%)	-0.53	1 (0%) 92 95	23, 35, 62, 123	0
2	b	226/227 (99%)	-0.08	11 (4%) 29 36	36, 52, 90, 134	0
3	C	259/261 (99%)	-0.62	0 100 100	25, 33, 52, 87	0
3	c	259/261 (99%)	-0.50	1 (0%) 92 95	31, 41, 64, 92	0
4	D	144/147 (97%)	-0.52	2 (1%) 75 80	29, 39, 65, 108	0
4	d	144/147 (97%)	0.35	12 (8%) 11 15	49, 67, 109, 200	0
5	E	105/109 (96%)	-0.40	2 (1%) 66 73	29, 40, 77, 124	0
5	e	105/109 (96%)	-0.12	2 (1%) 66 73	37, 56, 79, 118	0
6	F	98/98 (100%)	-0.10	6 (6%) 21 27	28, 43, 118, 148	0
6	f	98/98 (100%)	0.23	7 (7%) 16 21	37, 53, 130, 160	0
7	G	83/85 (97%)	0.17	14 (16%) 1 2	31, 43, 128, 140	0
7	g	83/85 (97%)	0.31	11 (13%) 3 4	33, 55, 133, 156	0
8	H	79/85 (92%)	-0.15	7 (8%) 9 13	30, 46, 113, 133	0
8	h	79/85 (92%)	0.19	6 (7%) 13 18	40, 62, 133, 154	0
9	I	72/73 (98%)	-0.20	3 (4%) 36 43	33, 47, 73, 76	0
9	i	72/73 (98%)	0.30	8 (11%) 5 7	38, 65, 90, 129	0
10	J	58/59 (98%)	-0.16	3 (5%) 27 34	36, 48, 82, 130	0
10	j	58/59 (98%)	0.09	5 (8%) 10 14	49, 62, 106, 176	0
11	K	49/56 (87%)	-0.03	3 (6%) 21 27	30, 46, 76, 107	0
11	k	49/56 (87%)	0.58	8 (16%) 1 2	53, 68, 91, 111	0
12	L	46/47 (97%)	-0.69	1 (2%) 62 69	28, 36, 58, 118	0
12	l	46/47 (97%)	-0.31	1 (2%) 62 69	42, 59, 89, 140	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	43/46 (93%)	-0.36	2 (4%) 31 38	33, 38, 69, 116	0
13	m	43/46 (93%)	0.50	7 (16%) 1 2	51, 60, 97, 163	0
All	All	3550/3614 (98%)	-0.29	123 (3%) 44 51	22, 42, 87, 200	0

The worst 5 of 123 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	f	1	ALA	18.4
4	d	6	VAL	14.3
4	d	5	VAL	9.7
13	m	43	SER	9.7
10	j	57	HIS	9.3

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	0.66	0.30	92,134,145,151	0
9	SAC	i	1	9/10	0.66	0.60	117,152,162,171	0
7	TPO	g	11	11/12	0.77	0.26	93,121,137,145	0
9	SAC	I	1	9/10	0.82	0.32	86,107,126,130	0
1	FME	a	1	10/11	0.89	0.32	80,89,130,142	0
1	FME	A	1	10/11	0.95	0.23	53,62,98,100	0
2	FME	b	1	10/11	0.95	0.23	48,55,57,58	0
2	FME	B	1	10/11	0.97	0.22	29,35,42,44	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
22	PSC	e	201	52/52	0.48	0.42	56,121,231,239	0
24	PEK	G	102	53/53	0.54	0.35	64,117,204,226	0
26	DMU	C	307	33/33	0.54	0.32	66,126,146,150	0
24	PEK	C	309	53/53	0.55	0.36	66,98,168,173	0
19	TGL	l	101	63/63	0.59	0.27	55,100,146,161	0
22	PSC	B	302	52/52	0.59	0.35	57,118,223,244	0
24	PEK	C	308	53/53	0.62	0.29	67,103,158,173	0
26	DMU	c	307	33/33	0.62	0.38	90,138,163,171	0
24	PEK	c	303	53/53	0.63	0.26	59,104,133,143	0
25	CDL	c	305	100/100	0.65	0.29	49,107,143,157	0
19	TGL	a	606	63/63	0.65	0.23	74,95,131,133	0
25	CDL	C	305	100/100	0.65	0.29	46,102,140,147	0
25	CDL	g	103	100/100	0.67	0.30	63,112,158,182	0
25	CDL	G	101	100/100	0.70	0.28	71,112,154,164	0
17	NA	a	605	1/1	0.71	0.12	50,50,50,50	0
19	TGL	L	101	63/63	0.71	0.27	43,88,128,130	0
19	TGL	D	201	63/63	0.72	0.21	66,92,121,126	0
18	PGV	A	606	51/51	0.73	0.26	53,89,136,151	0
18	PGV	a	607	51/51	0.74	0.29	58,96,149,171	0
26	DMU	m	401	33/33	0.75	0.31	67,94,108,112	0
18	PGV	G	103	51/51	0.78	0.21	54,108,130,139	0
23	CHD	j	101	29/29	0.82	0.24	104,119,130,134	0
18	PGV	C	304	51/51	0.83	0.20	61,95,132,142	0
26	DMU	M	101	33/33	0.83	0.19	42,54,66,67	0
19	TGL	A	608	63/63	0.85	0.21	37,87,127,146	0
19	TGL	i	101	63/63	0.85	0.21	46,99,142,151	0
23	CHD	J	101	29/29	0.88	0.23	76,89,111,117	0
23	CHD	C	306	29/29	0.89	0.21	72,84,88,90	0
23	CHD	c	306	29/29	0.92	0.19	78,83,100,101	0
24	PEK	g	102	53/53	0.94	0.20	41,65,100,105	0
18	PGV	C	303	51/51	0.95	0.23	27,39,95,97	0
23	CHD	b	301	29/29	0.96	0.10	32,39,46,51	0
23	CHD	c	302	29/29	0.96	0.08	34,38,40,44	0
16	MG	a	604	1/1	0.96	0.15	42,42,42,42	0
18	PGV	c	304	51/51	0.96	0.24	31,44,93,100	0
24	PEK	C	302	53/53	0.96	0.21	28,56,114,116	0
14	HEA	a	601	60/60	0.96	0.13	34,41,52,53	0
18	PGV	c	301	51/51	0.97	0.21	29,56,75,82	0
20	CMO	a	608	2/2	0.97	0.11	33,33,33,36	0
23	CHD	B	303	29/29	0.97	0.10	32,36,45,49	0
23	CHD	C	301	29/29	0.97	0.07	29,32,37,41	0
21	CUA	B	301	2/2	0.97	0.04	29,29,29,31	0

Continued on next page...

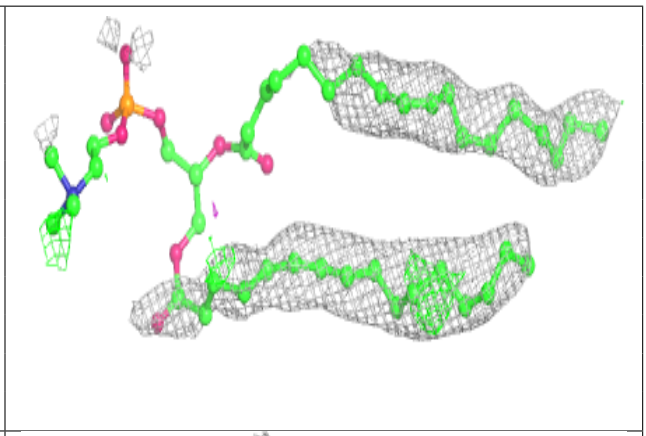
Continued from previous page...

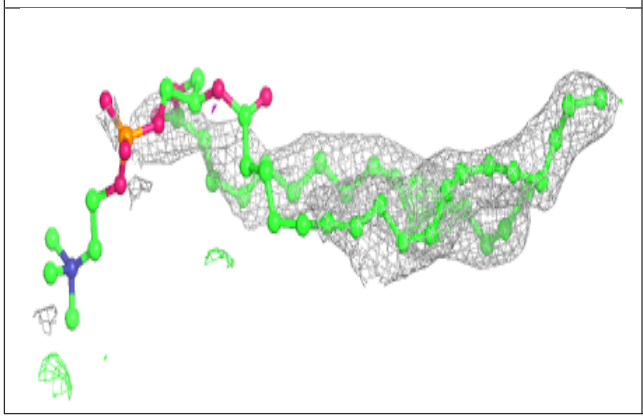
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
21	CUA	b	302	2/2	0.97	0.03	46,46,46,47	0
14	HEA	A	601	60/60	0.98	0.10	20,25,42,54	0
14	HEA	a	602	60/60	0.98	0.13	27,31,41,45	0
18	PGV	A	607	51/51	0.98	0.21	24,46,64,72	0
16	MG	A	604	1/1	0.98	0.07	26,26,26,26	0
14	HEA	A	602	60/60	0.98	0.12	20,23,36,43	0
17	NA	A	605	1/1	0.98	0.04	31,31,31,31	0
20	CMO	A	609	2/2	0.99	0.09	23,23,23,24	0
15	CU	a	603	1/1	0.99	0.06	39,39,39,39	0
27	ZN	F	101	1/1	0.99	0.02	45,45,45,45	0
15	CU	A	603	1/1	1.00	0.05	28,28,28,28	0
27	ZN	f	101	1/1	1.00	0.03	52,52,52,52	0

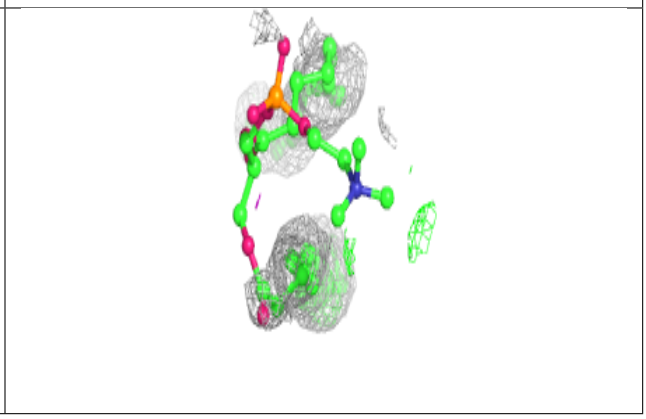
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PSC e 201:

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

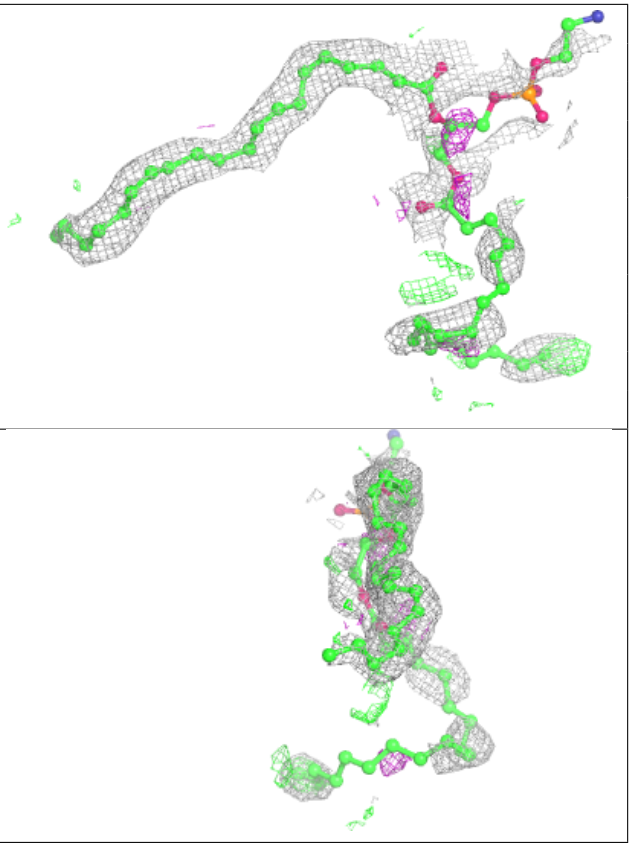






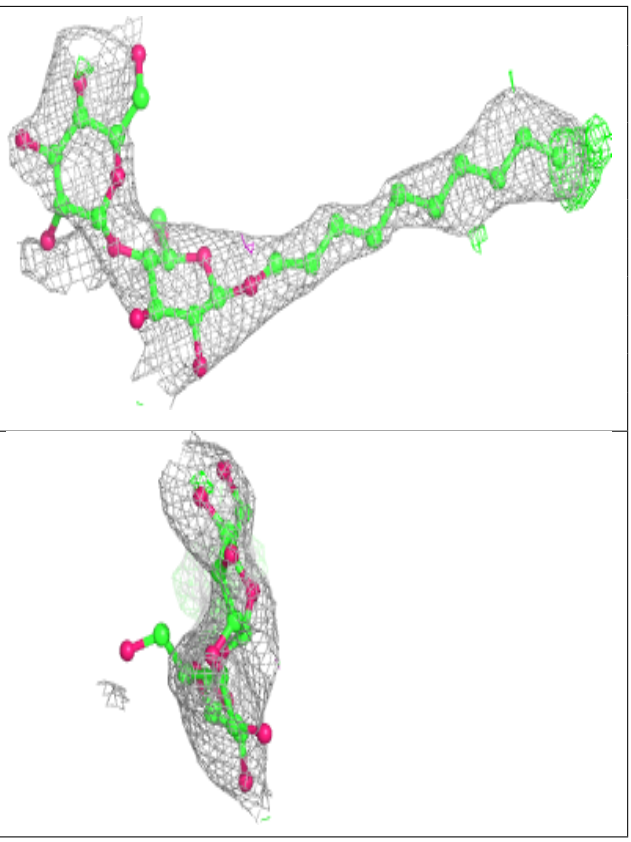
Electron density around PEK G 102:

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



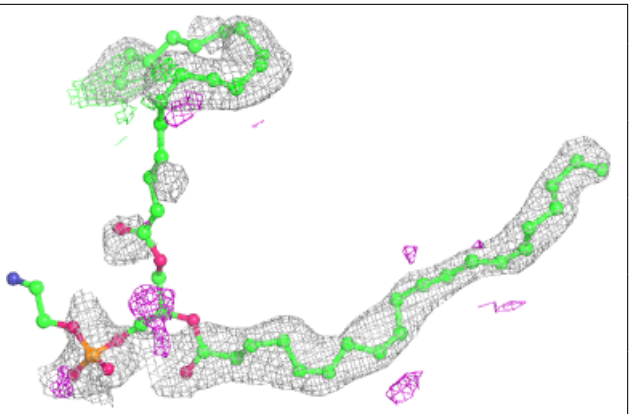
Electron density around DMU C 307:

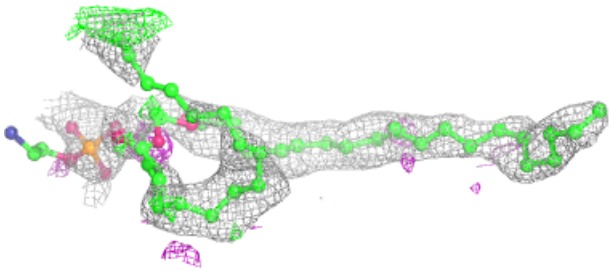
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

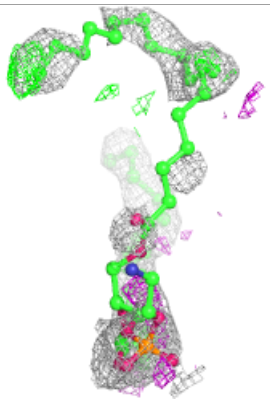


Electron density around PEK C 309:

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

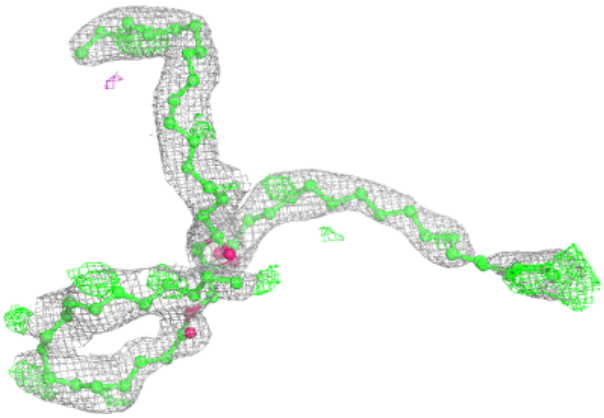


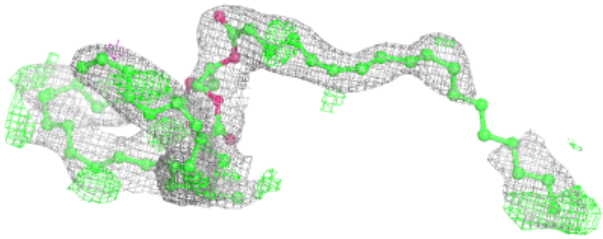


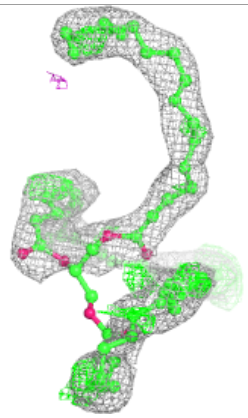


Electron density around TGL l 101:

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

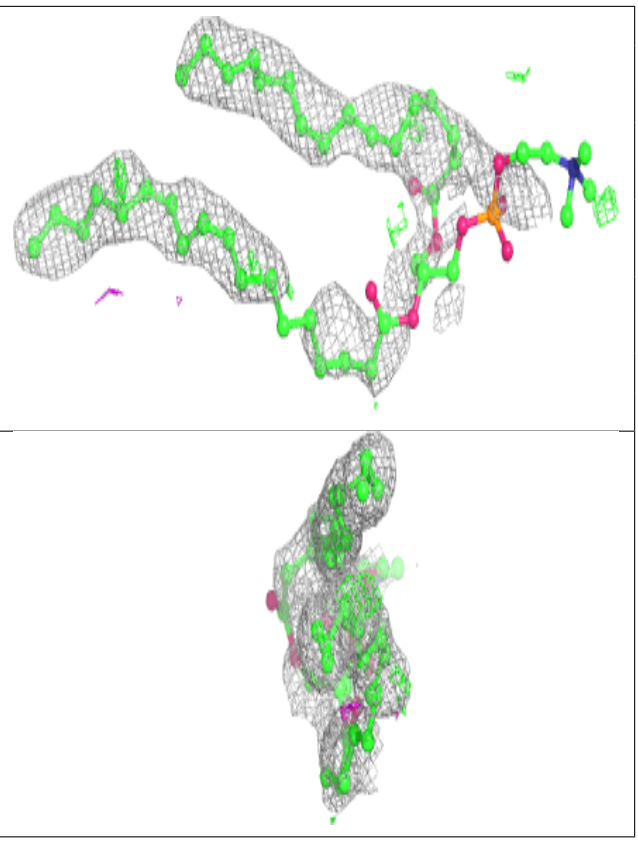






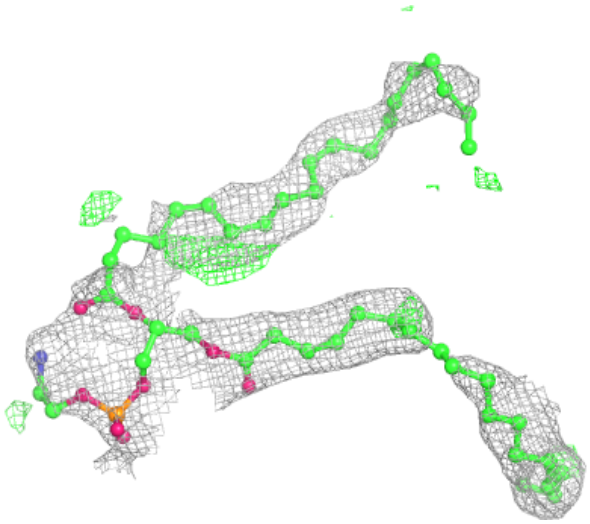
Electron density around PSC B 302:

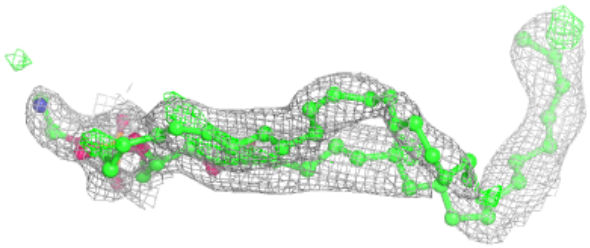
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

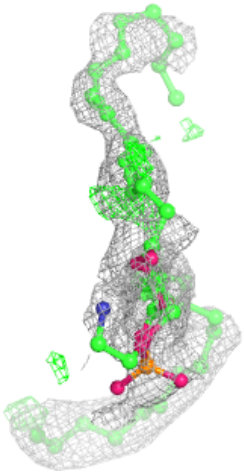


Electron density around PEK C 308:

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

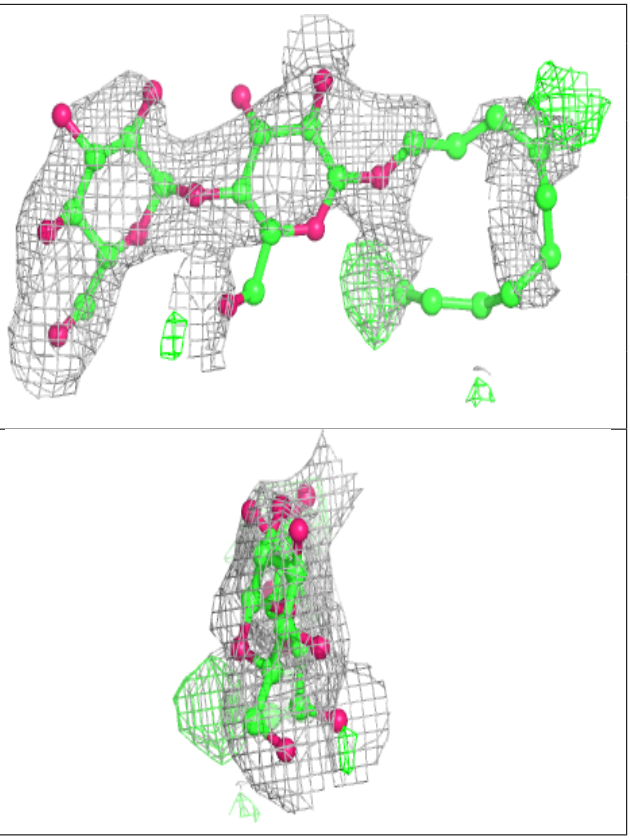


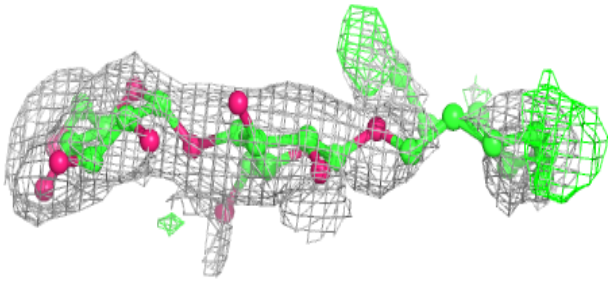




Electron density around DMU c 307:

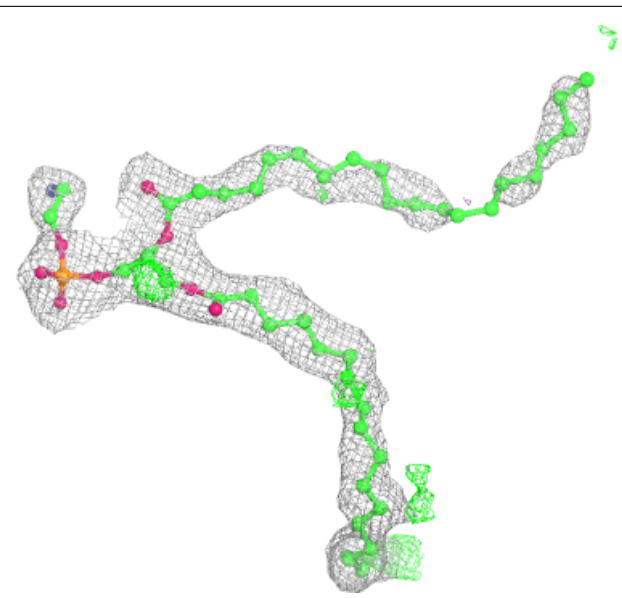
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

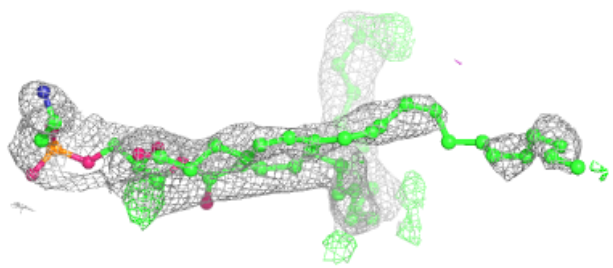


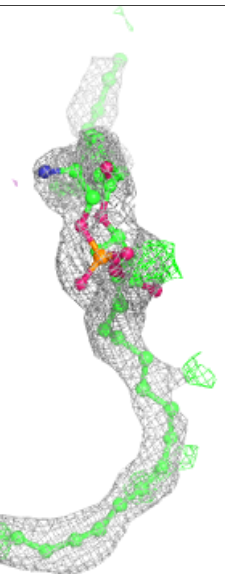


Electron density around PEK c 303:

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

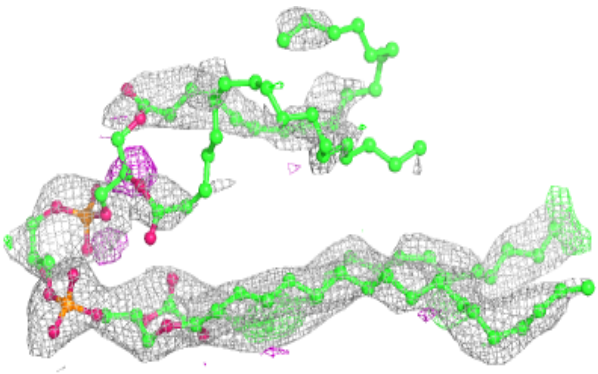


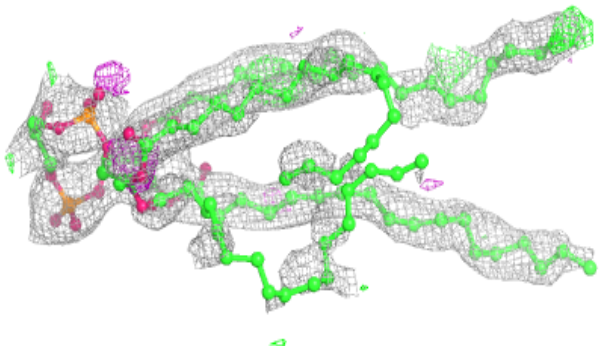


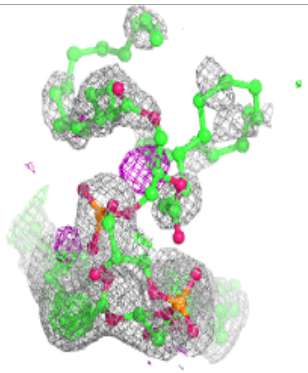


Electron density around CDL c 305:

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

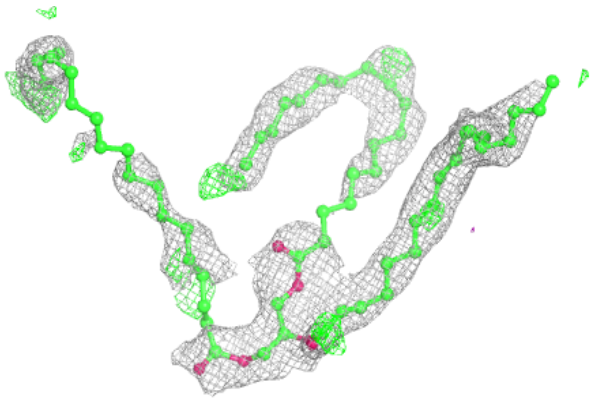


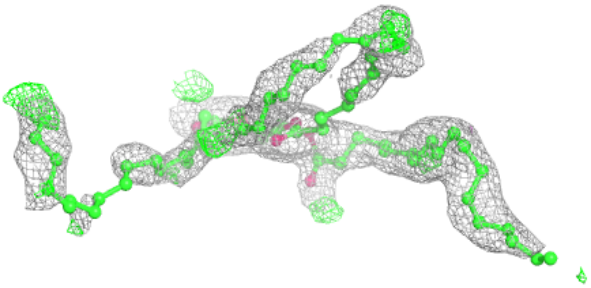


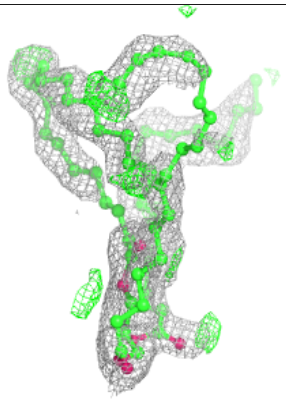


Electron density around TGL a 606:

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

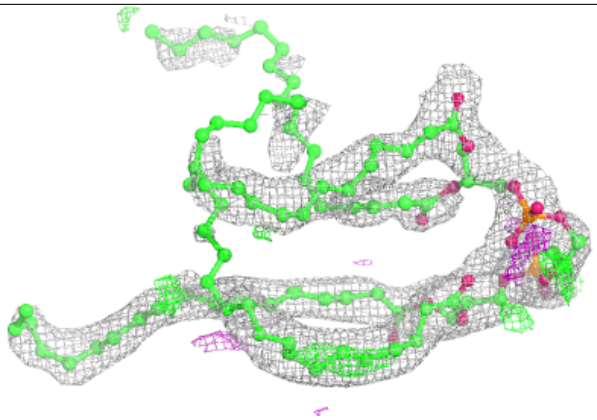


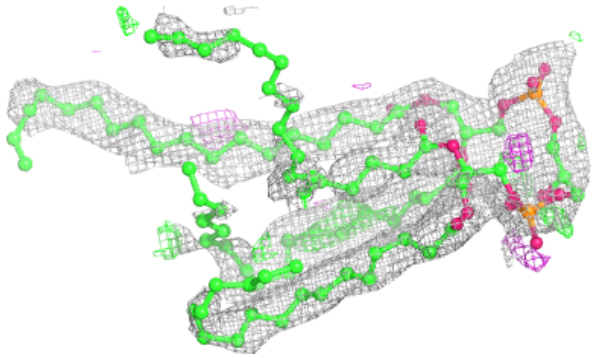


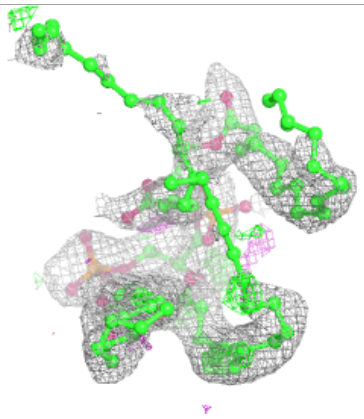


Electron density around CDL C 305:

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

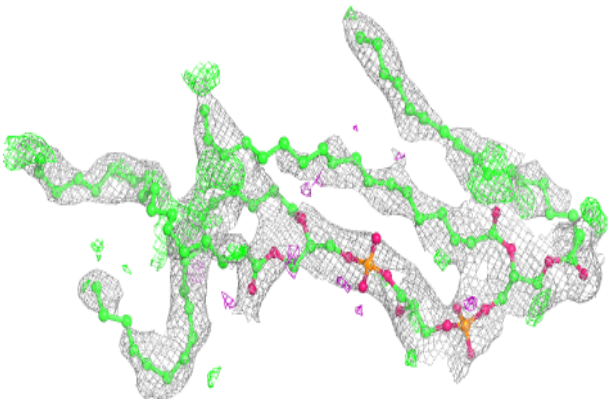


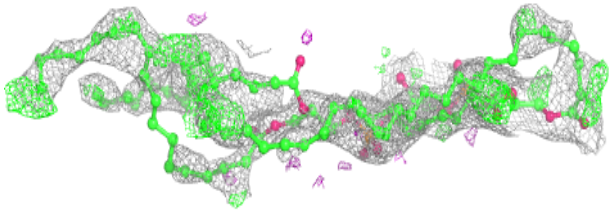


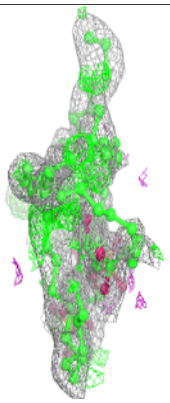


Electron density around CDL g 103:

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

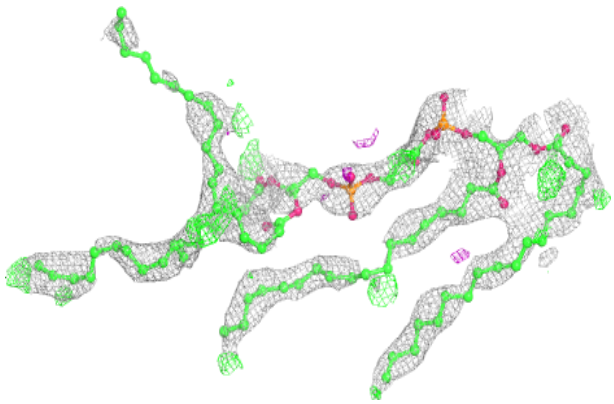


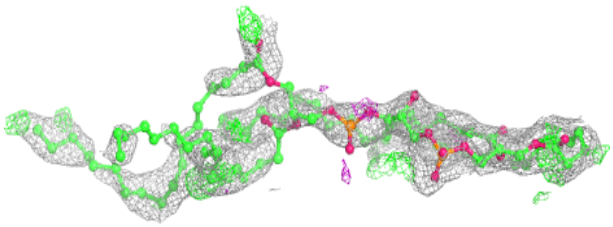


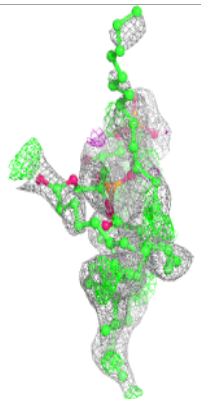


Electron density around CDL G 101:

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

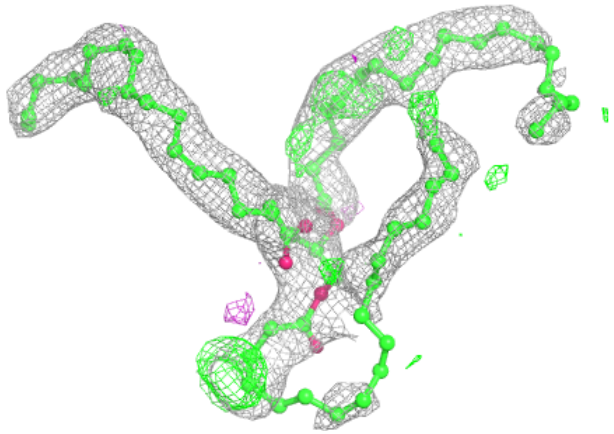


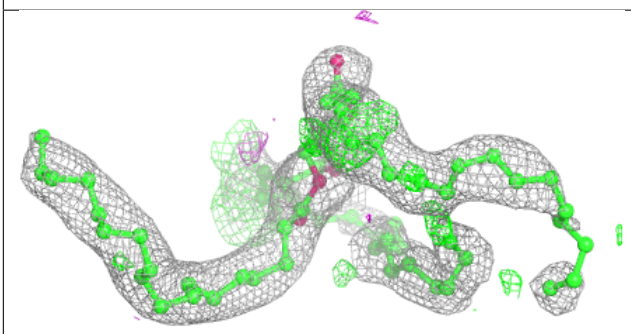


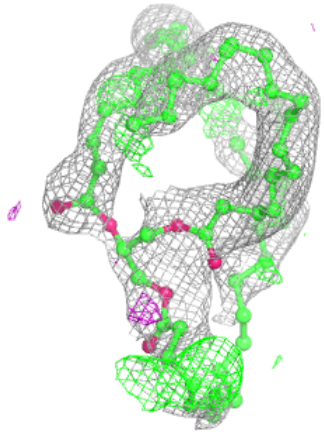


Electron density around TGL L 101:

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

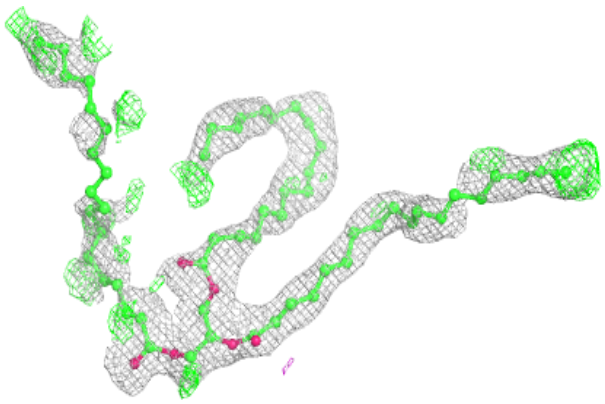


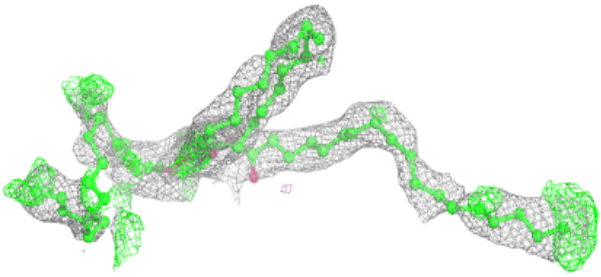


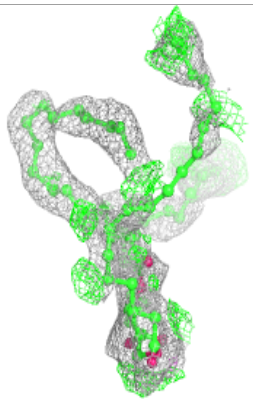


Electron density around TGL D 201:

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

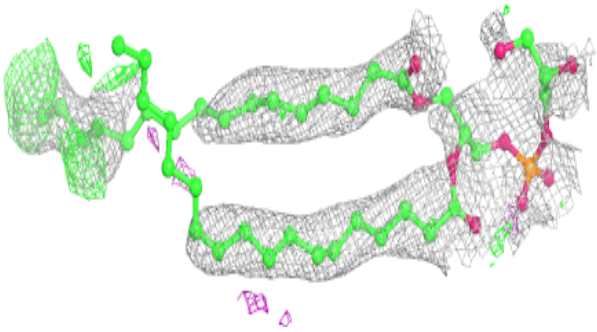


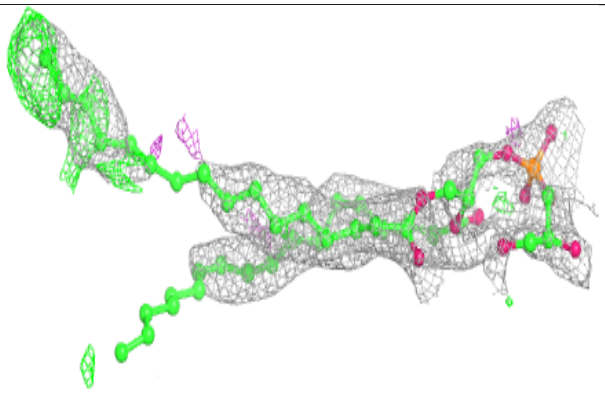


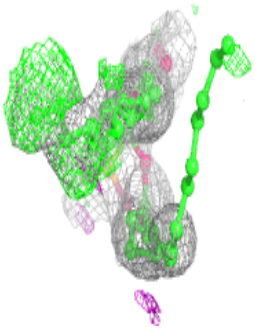


Electron density around PGV A 606:

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

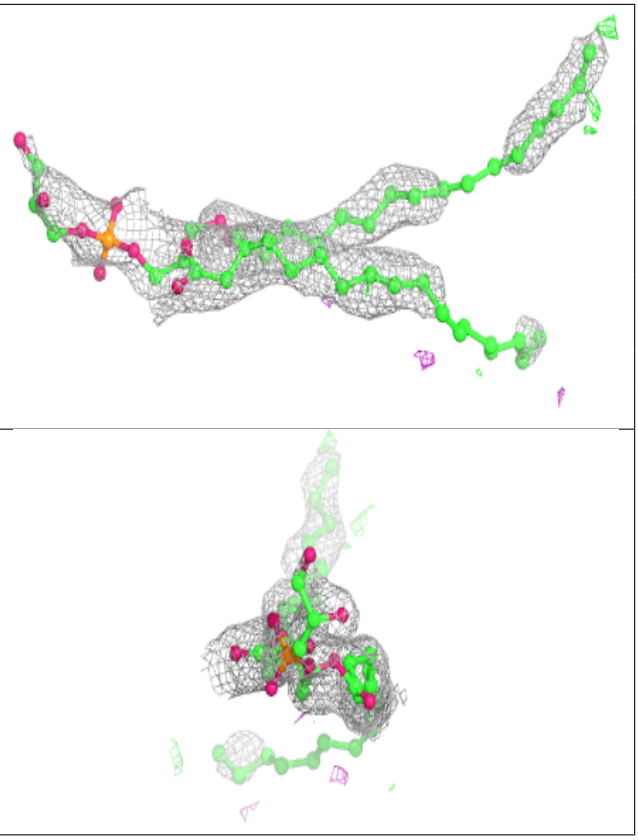


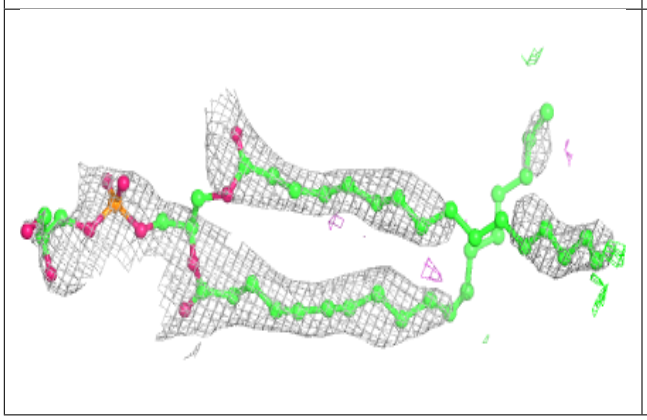




Electron density around PGV a 607:

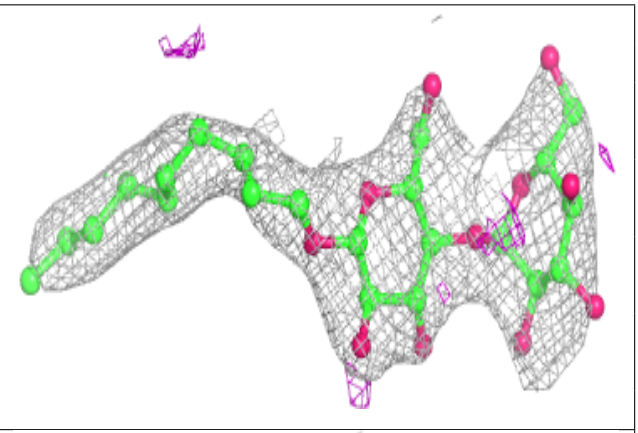
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

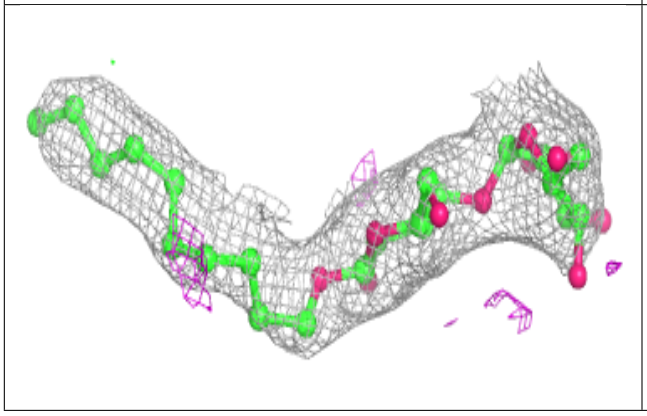


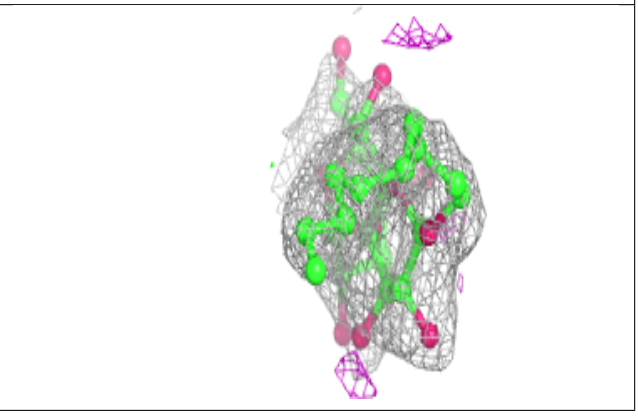


Electron density around DMU m 401:

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

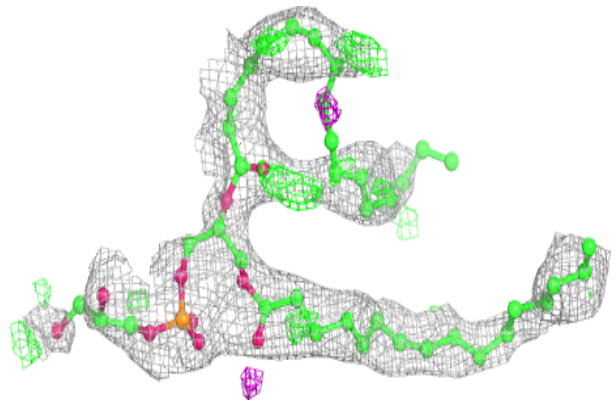


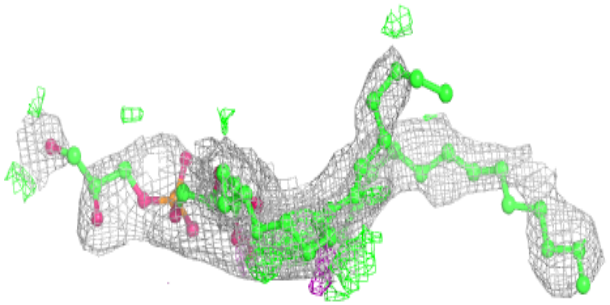


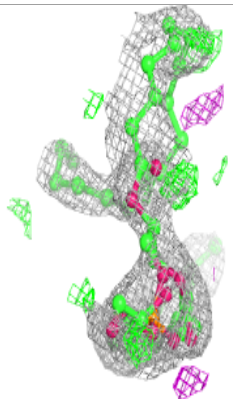


Electron density around PGV G 103:

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

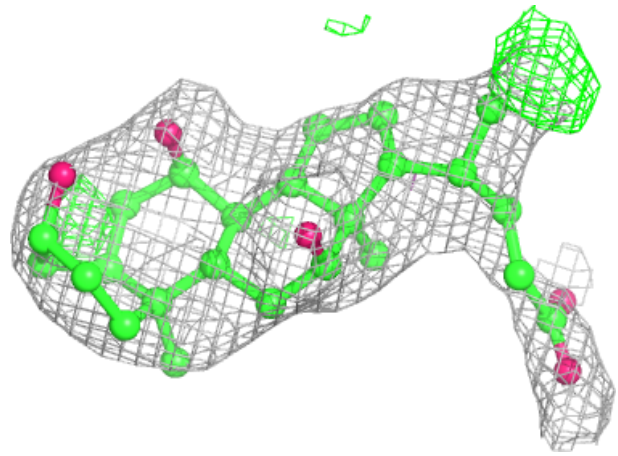


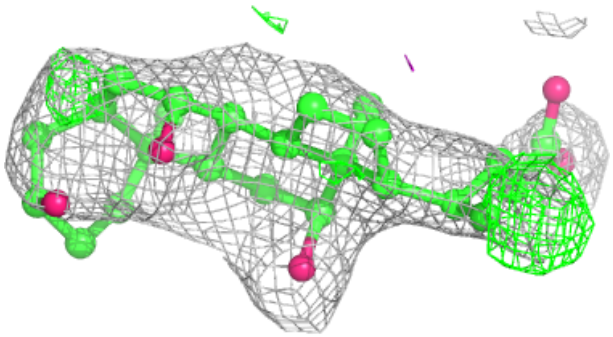


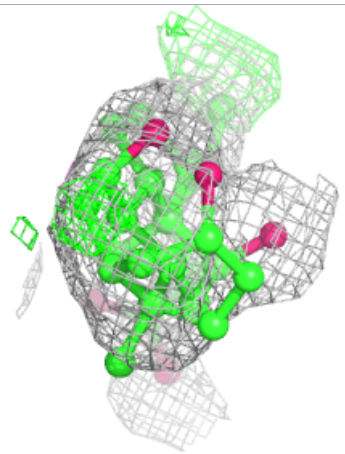


Electron density around CHD j 101:

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

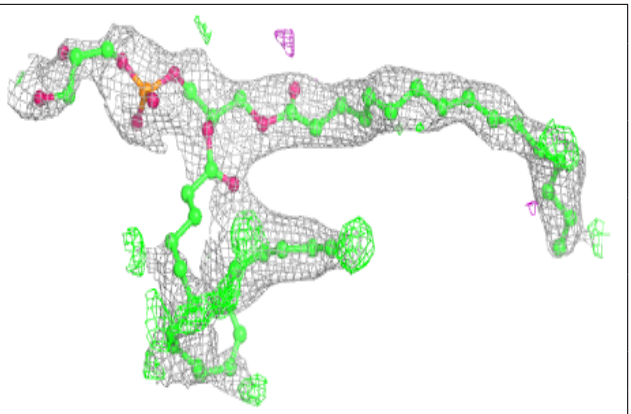


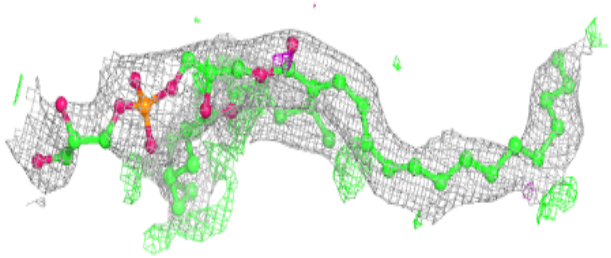


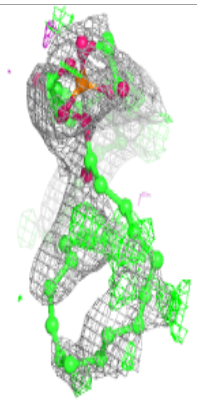


Electron density around PGV C 304:

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

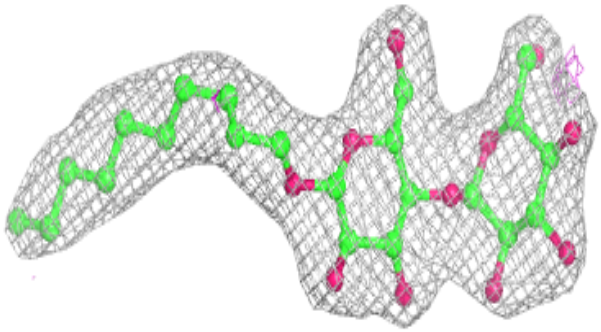


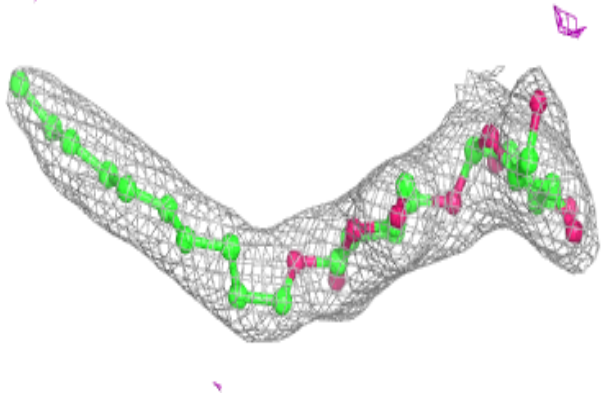


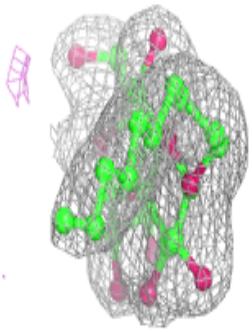


Electron density around DMU M 101:

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

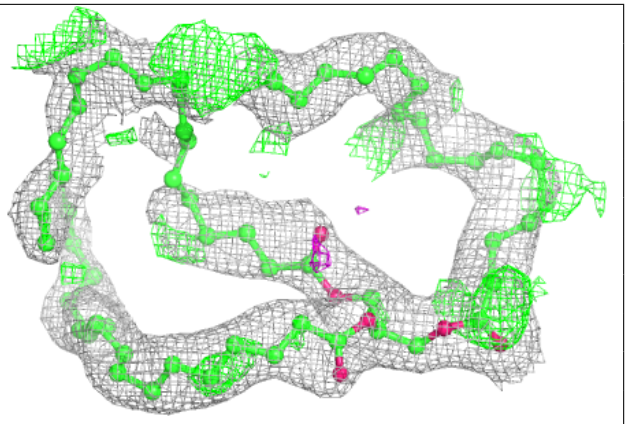


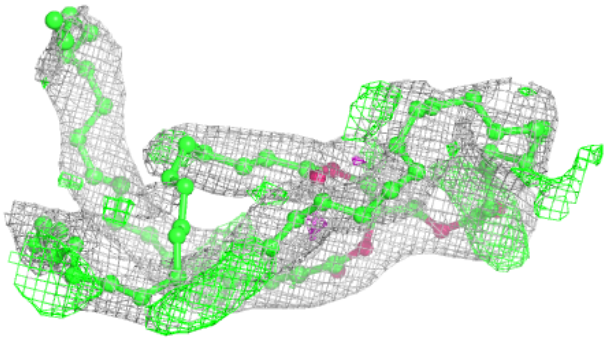


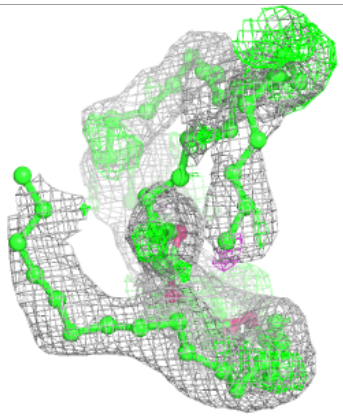


Electron density around TGL A 608:

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

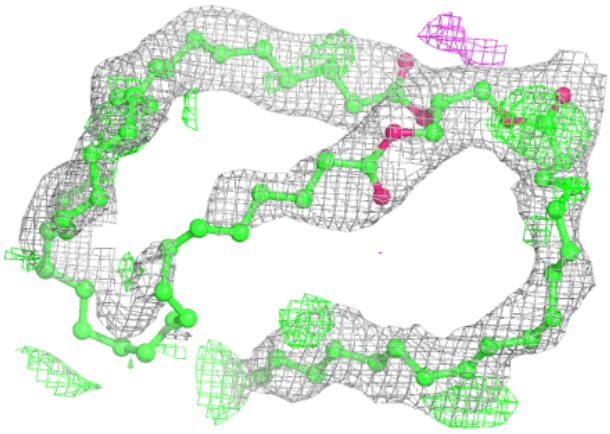


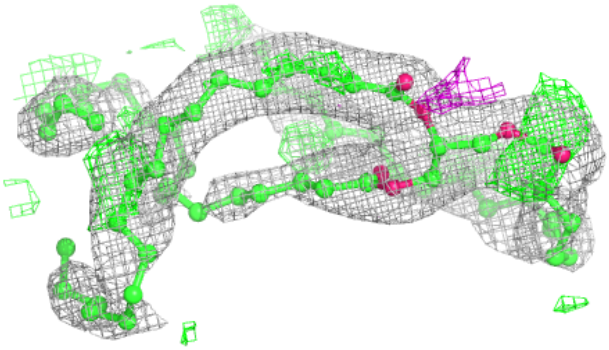


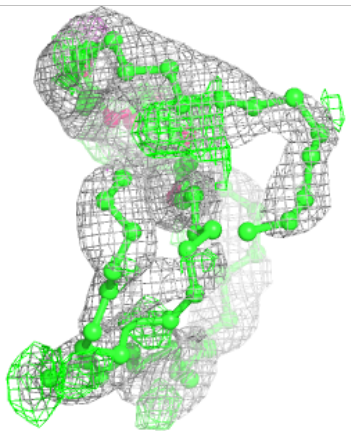


Electron density around TGL i 101:

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

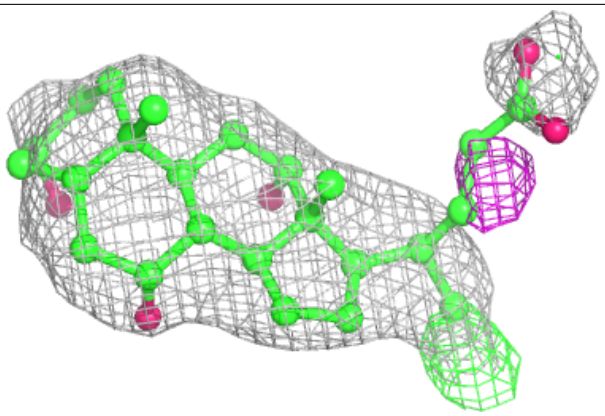


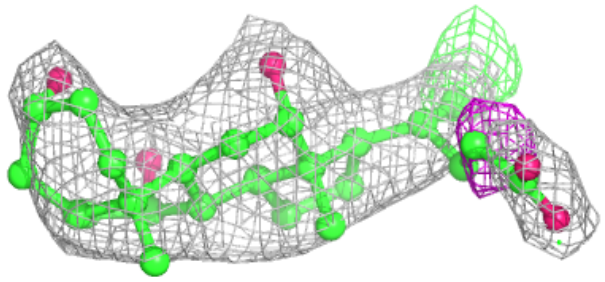


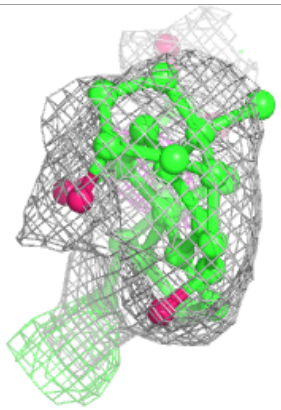


Electron density around CHD J 101:

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

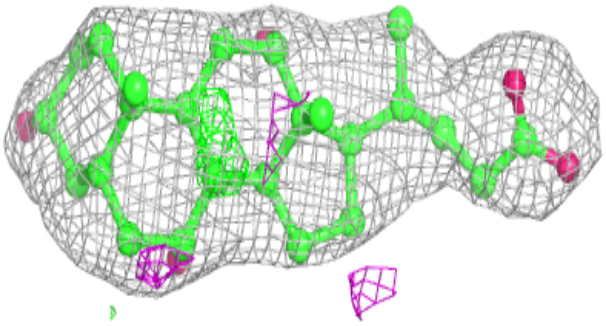


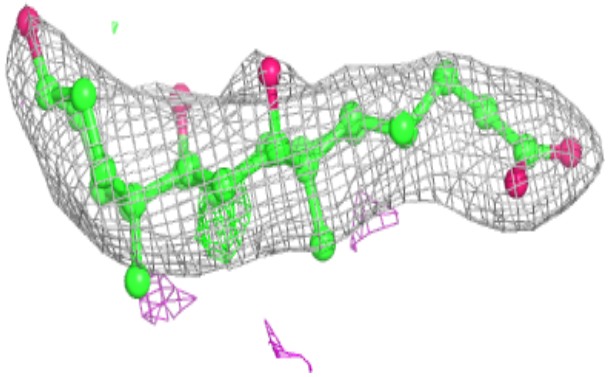


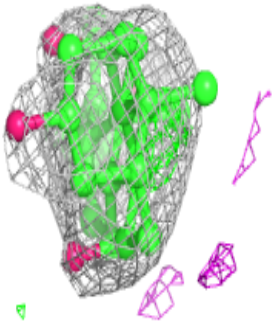


Electron density around CHD C 306:

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

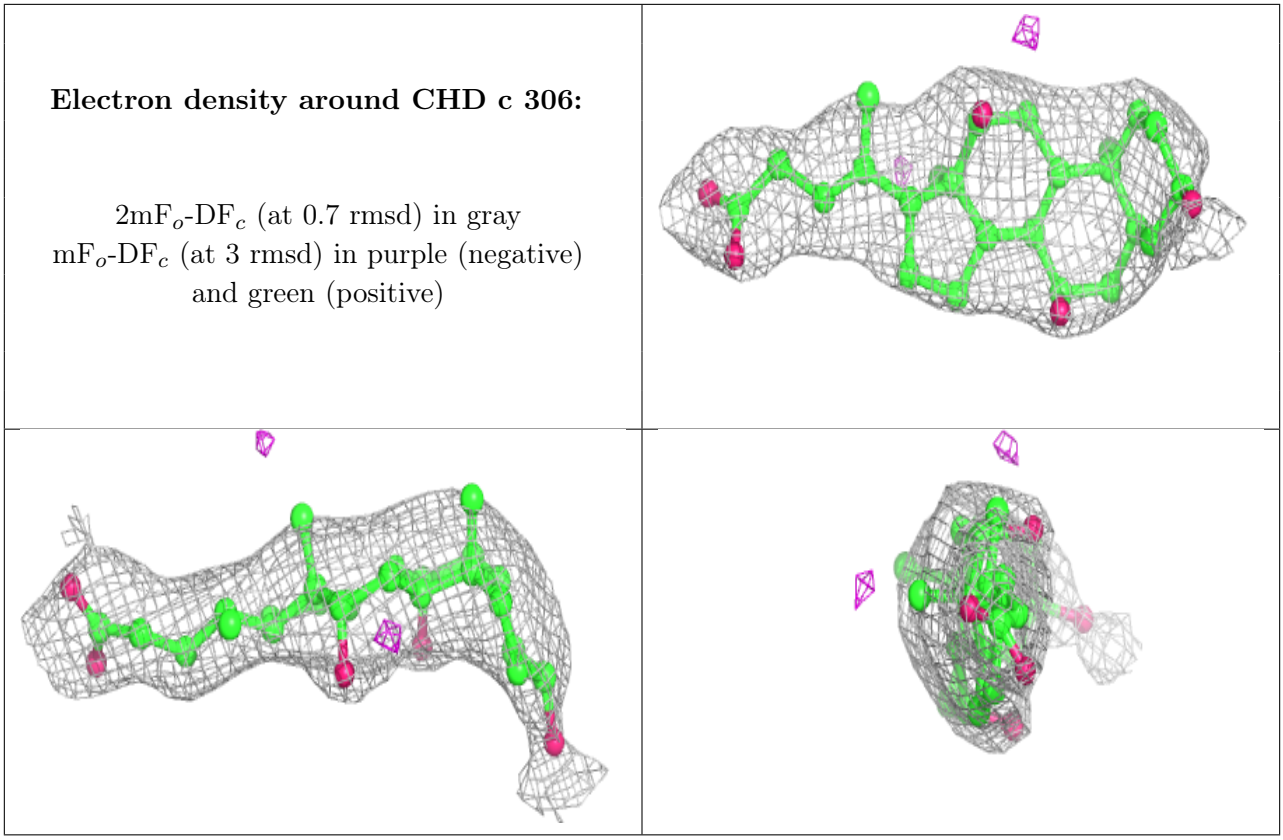






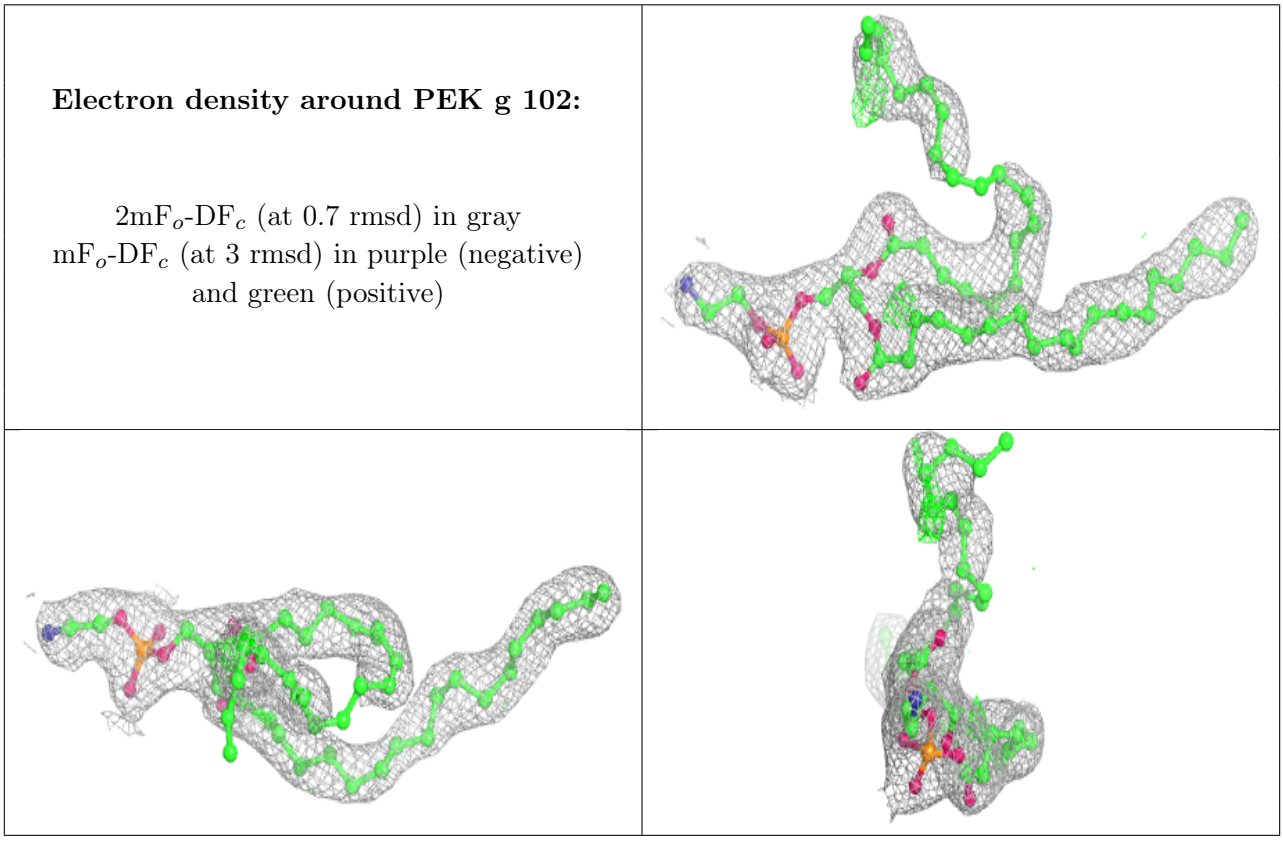
Electron density around CHD c 306:

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



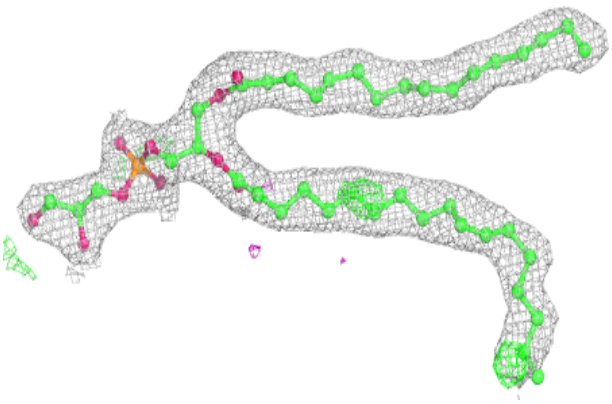
Electron density around PEK g 102:

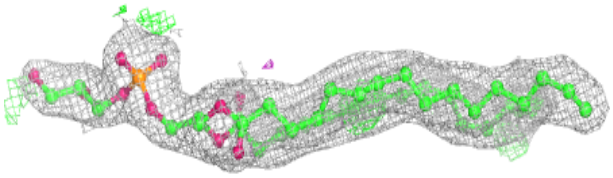
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

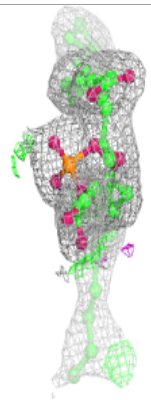


Electron density around PGV C 303:

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

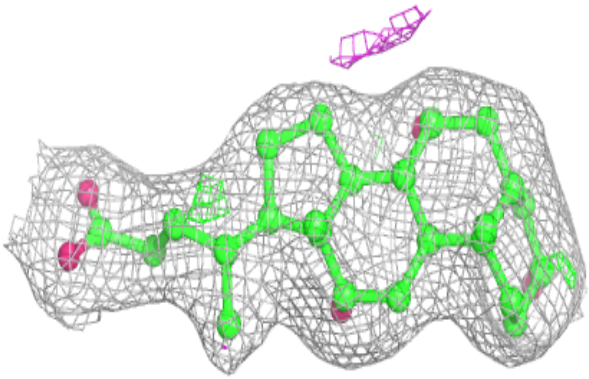


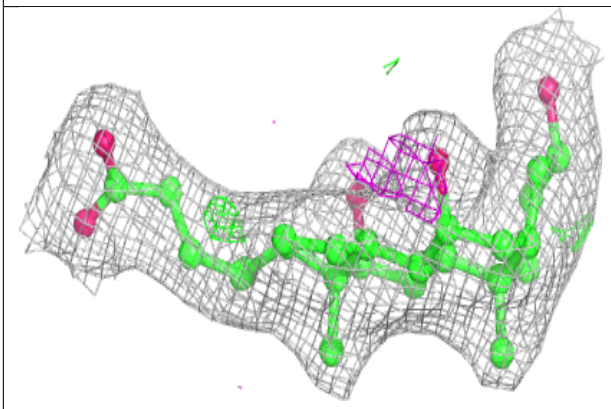


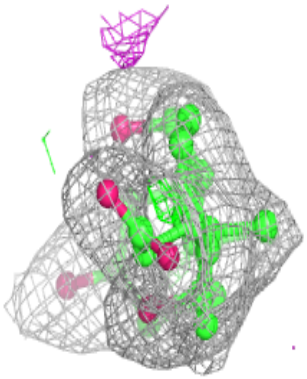


Electron density around CHD b 301:

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

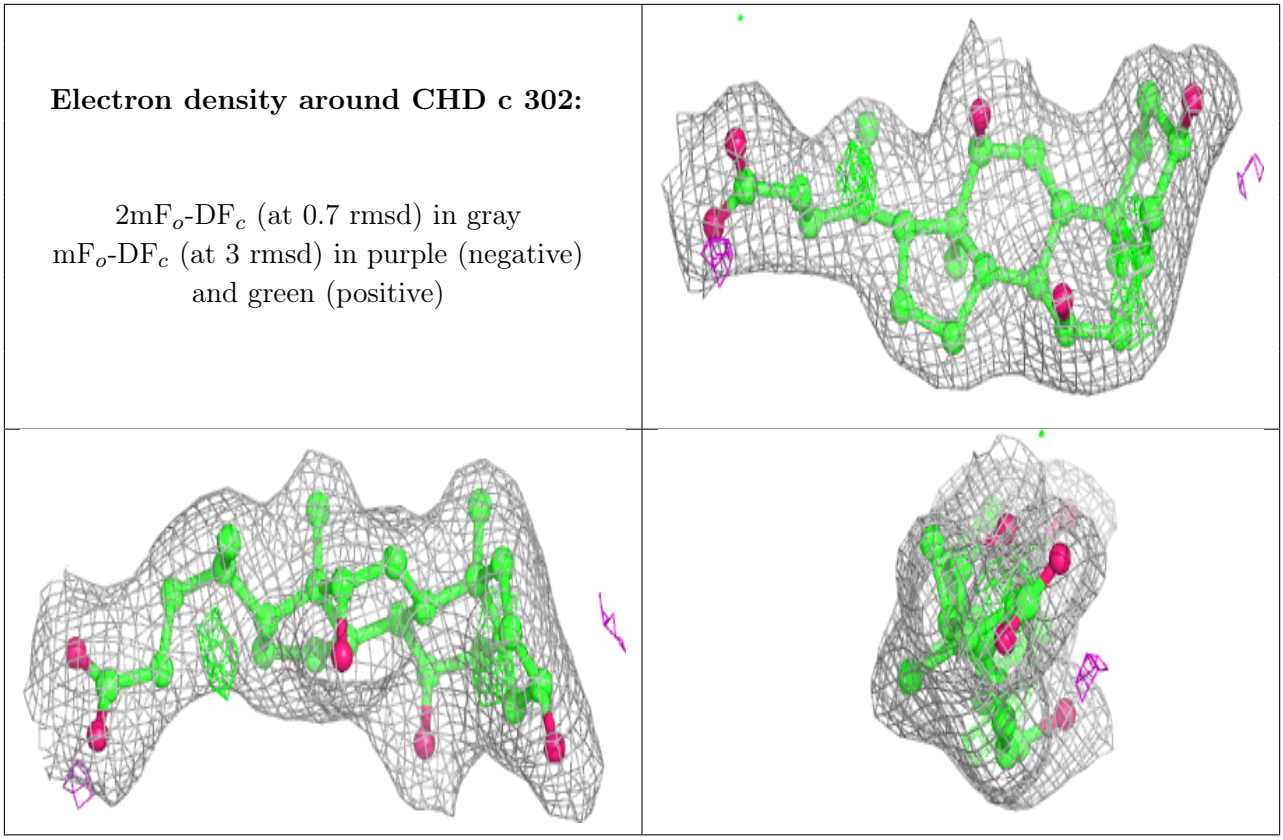






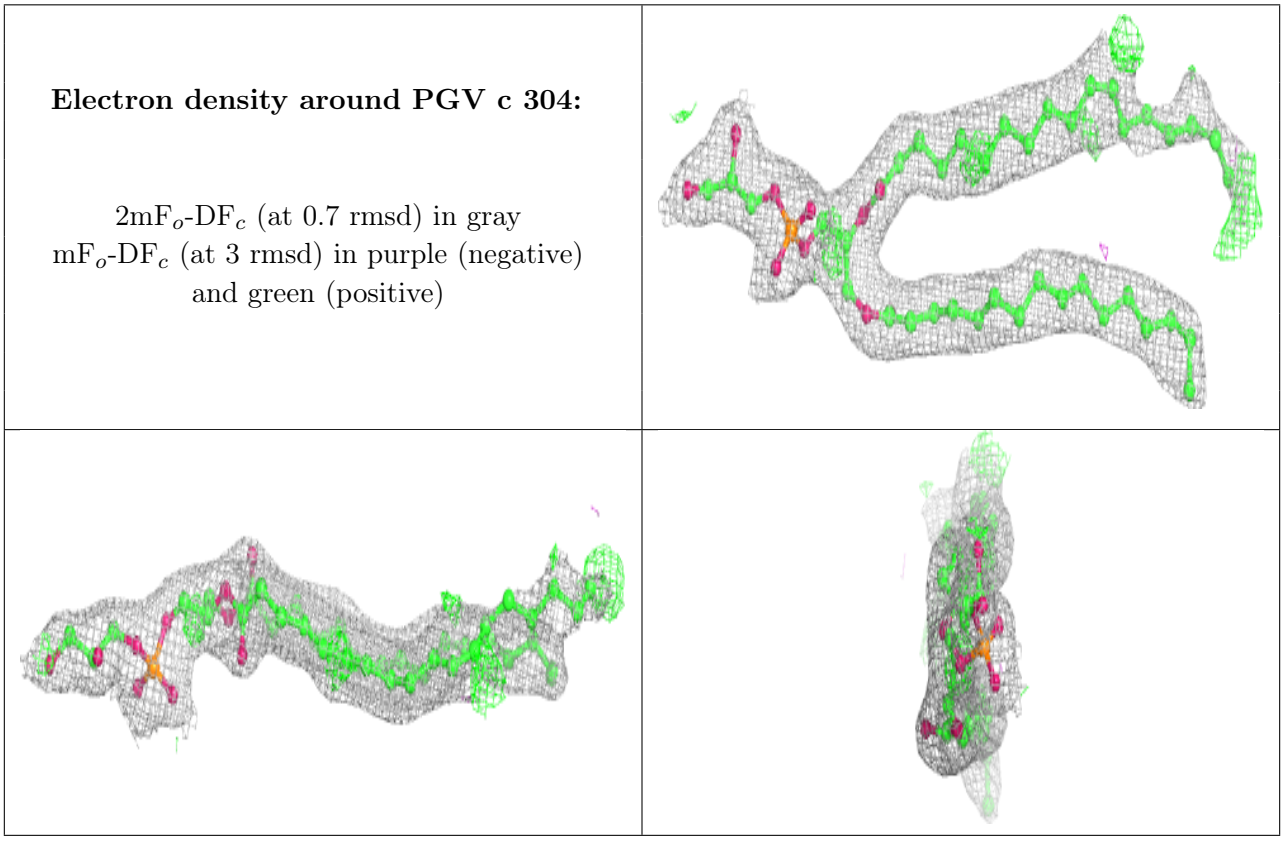
Electron density around CHD c 302:

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



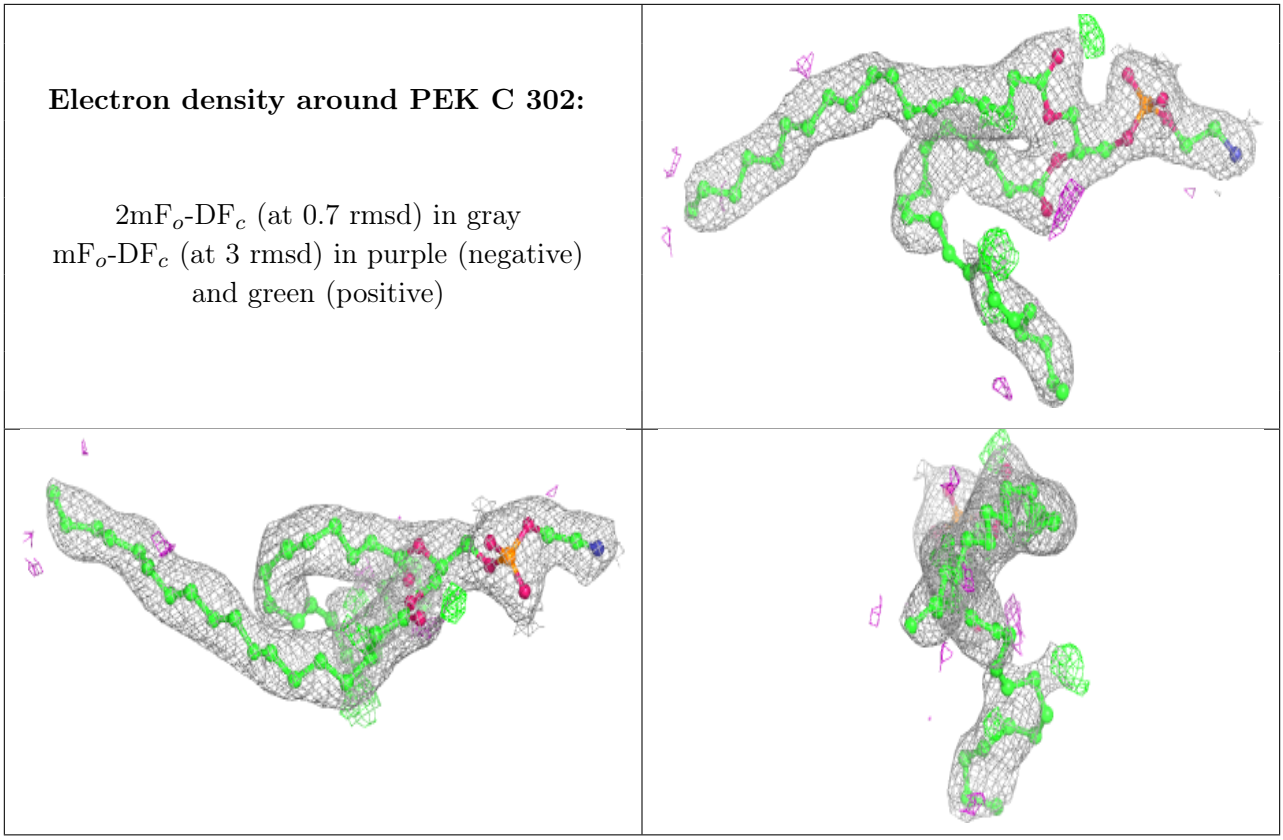
Electron density around PGV c 304:

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



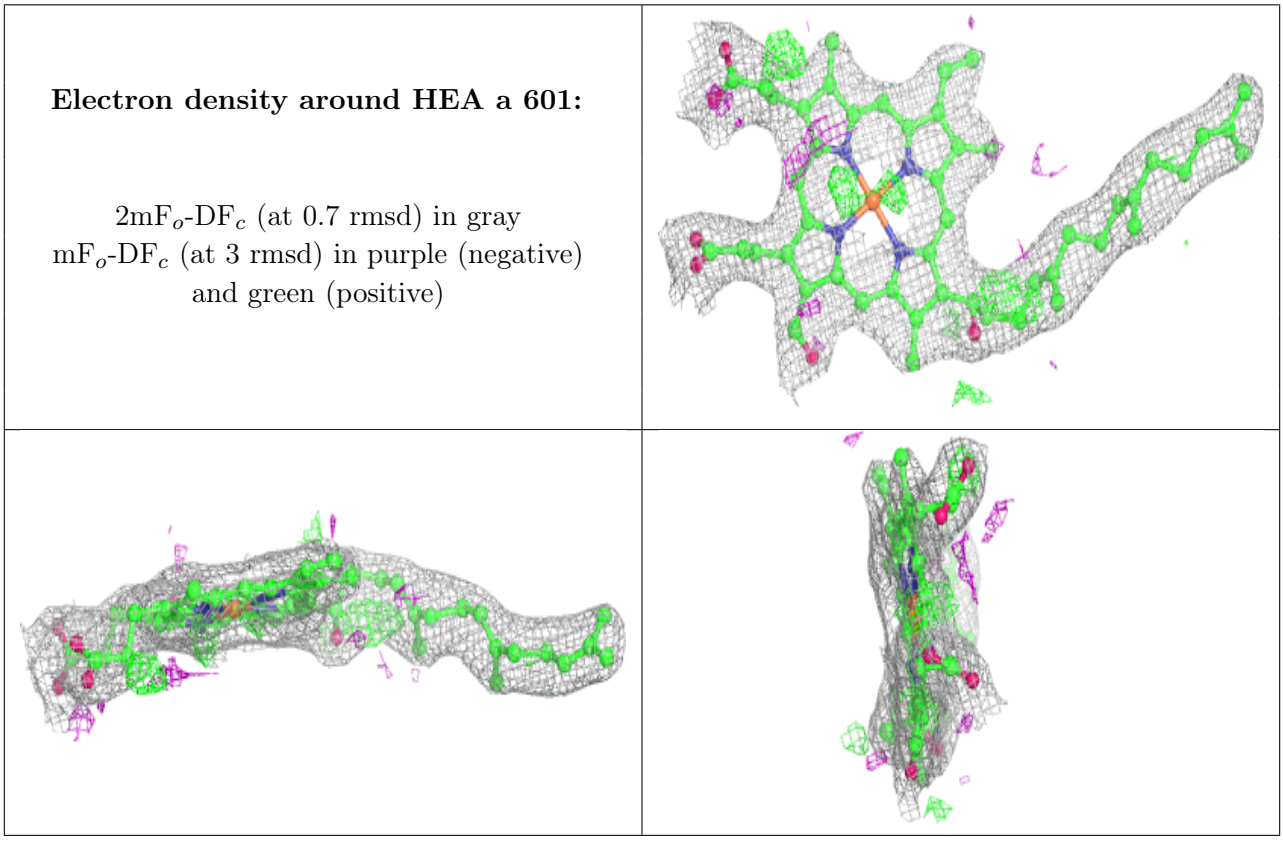
Electron density around PEK C 302:

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



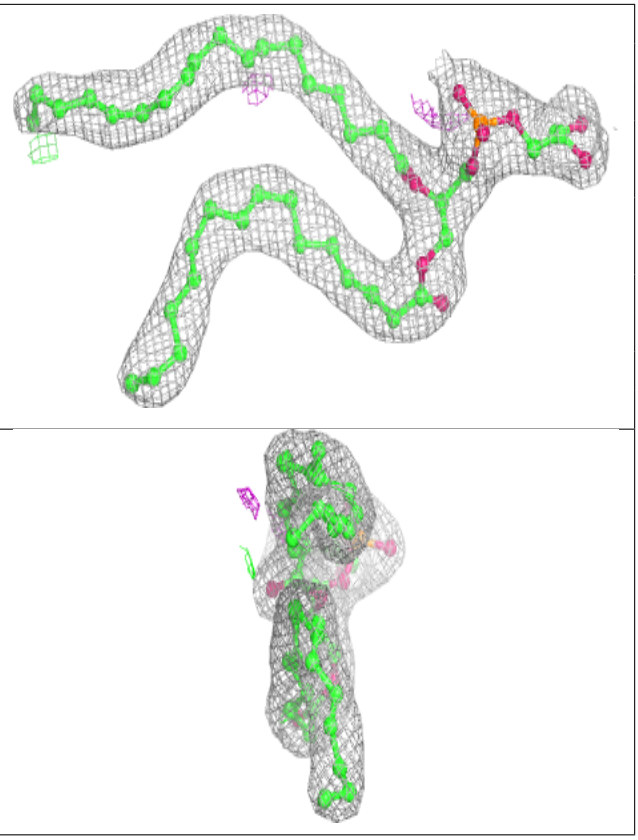
Electron density around HEA a 601:

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



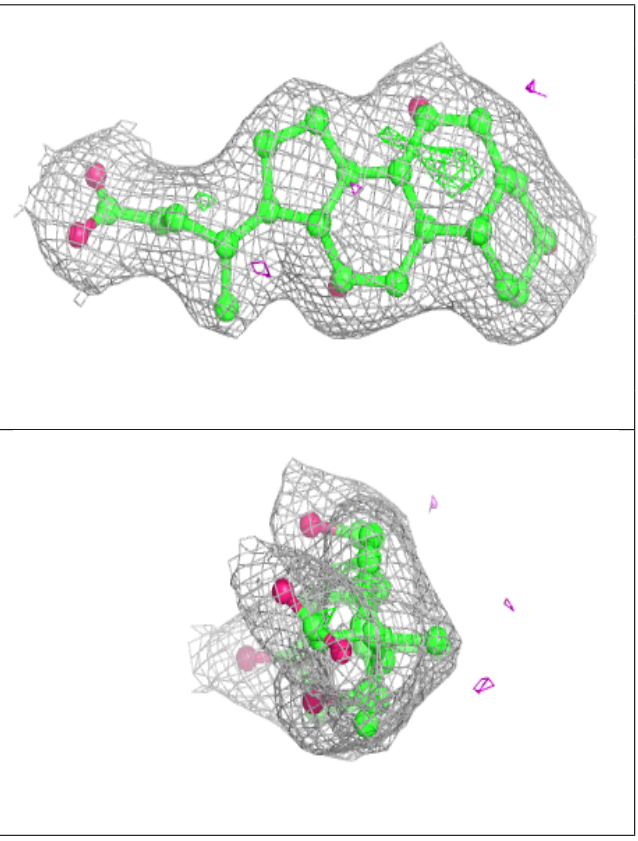
Electron density around PGV c 301:

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



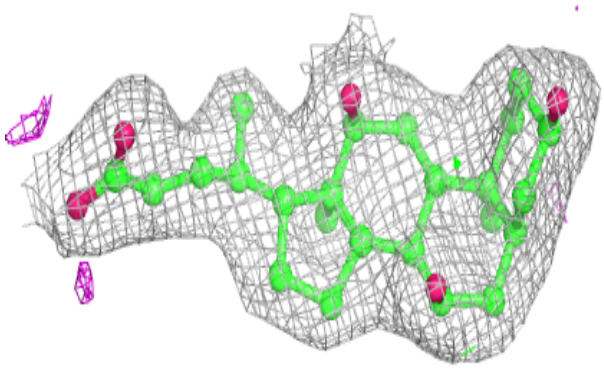
Electron density around CHD B 303:

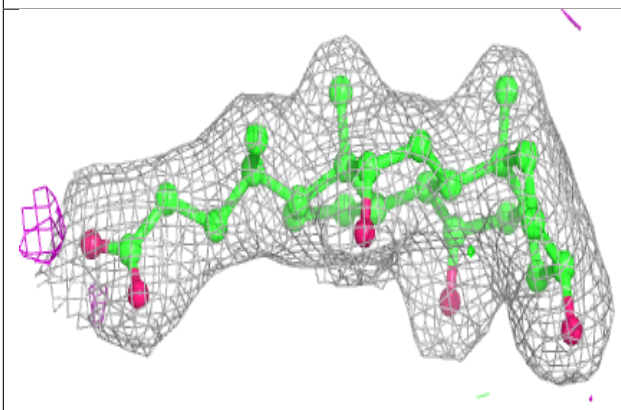
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

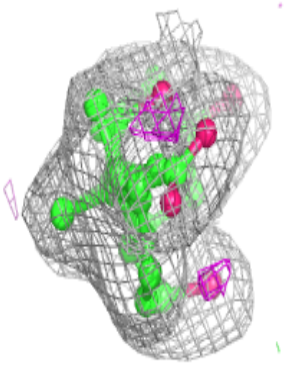


Electron density around CHD C 301:

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

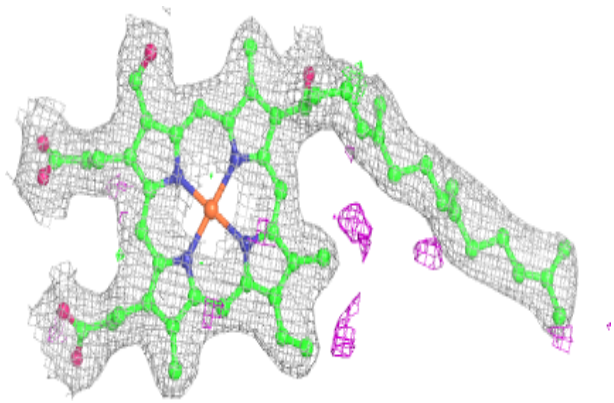


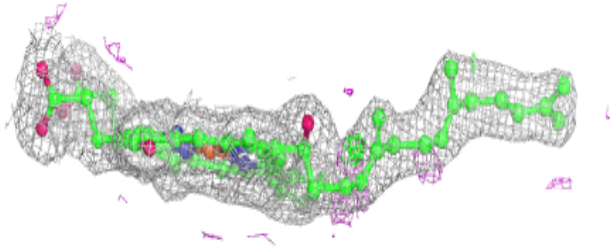


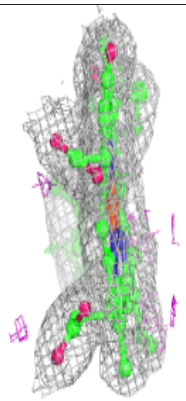


Electron density around HEA A 601:

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

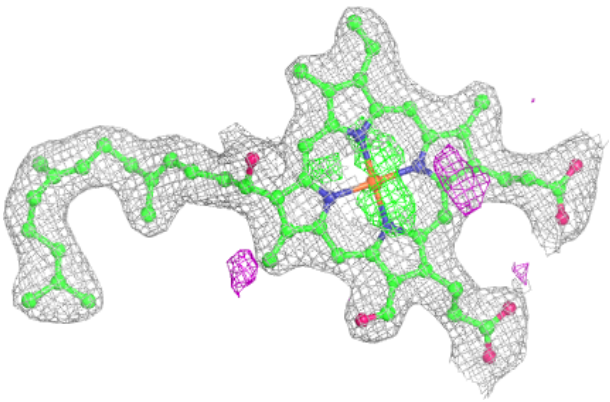


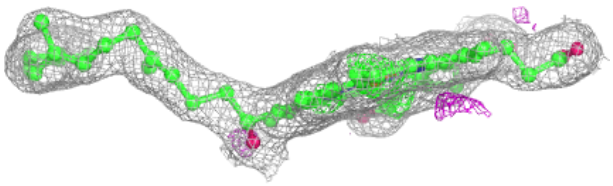


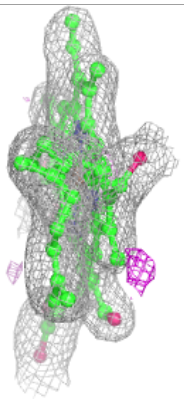


Electron density around HEA a 602:

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

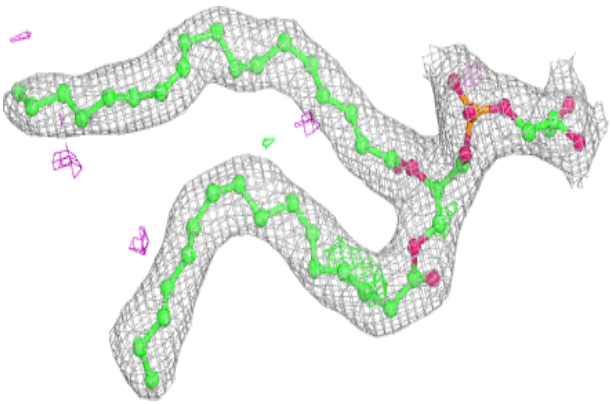


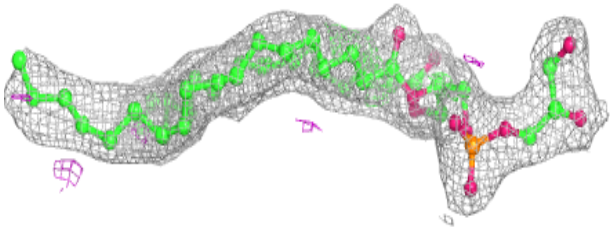


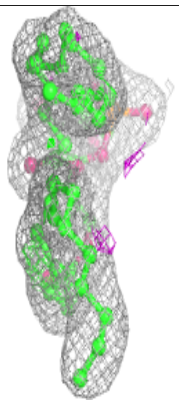


Electron density around PGV A 607:

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

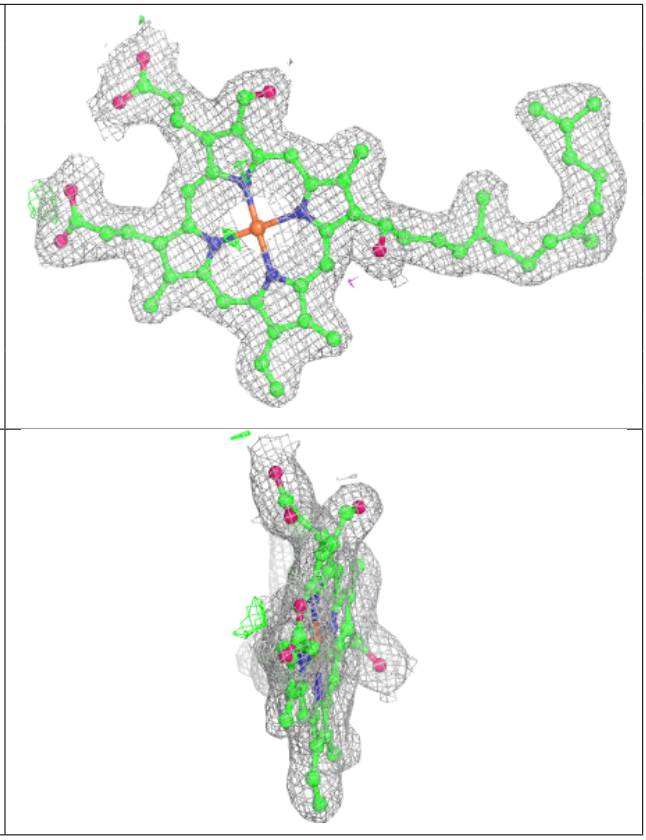






Electron density around HEA A 602:

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



6.5 Other polymers (i)

There are no such residues in this entry.