wwPDB X-ray Structure Validation Summary Report (i)

Oct 4, 2023 – 04:47 AM EDT

PDB ID	:	6NKN
Title	:	Time-resolved SFX structure of the PR intermediate of cytochrome c oxidase at room temperature
Authors	:	Rousseau, D.L.; Yeh, S.-R.; Ishigami, I.
Deposited on	:	2019-01-07
Resolution	:	2.50 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:

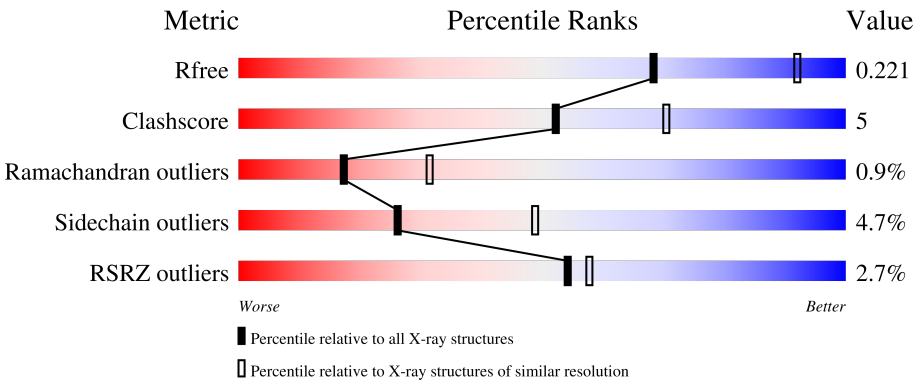
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	514	89% 10%
1	N	514	84% 15% •
2	B	227	% 80% 19% •
2	O	227	3% 77% 21% •
3	C	261	93% 6% •

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Mol	Chain	Length	Quality of chain
3	P	261	91% 8%
4	D	147	87% 10%
4	Q	147	5% 85% 10% 5%
5	E	109	2% 90% 6%
5	R	109	2% 89% 6%
6	F	98	5% 84% 9% 5%
6	S	98	5% 85% 10%
7	G	85	13% 75% 19% 5%
7	T	85	13% 73% 24%
8	H	85	5% 84% 8% 8%
8	U	85	7% 80% 12% 7%
9	I	73	5% 84% 15%
9	V	73	11% 85% 10% 5%
10	J	59	3% 92% 5%
10	W	59	8% 90% 7%
11	K	56	2% 82% 5% 12%
11	X	56	4% 59% 25% 12%
12	L	47	4% 87% 11%
12	Y	47	4% 79% 19%
13	M	46	4% 89% 7%
13	Z	46	11% 74% 20% 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
17	HEA	A	604	X	-	-	-
17	HEA	A	605	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	HEA	N	605	X	-	-	-
17	HEA	N	606	X	-	-	-
26	CDL	N	601	-	-	X	-
7	TPO	G	11	-	-	-	X
9	SAC	I	1	-	-	-	X
9	SAC	V	1	-	-	-	X

2 Entry composition (i)

There are 29 unique types of molecules in this entry. The entry contains 31419 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	144	1195	777	196	218	4	0	0	0
4	Q	139	1160	755	190	211	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	R	105	852	544	144	162	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	96	732	455	130	142	5	0	0	0
6	S	94	721	449	128	139	5	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	78	653	411	119	118	5	0	0	0
8	U	79	662	417	121	119	5	0	0	0

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

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

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

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

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

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

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

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

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

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

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

- Molecule 14 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

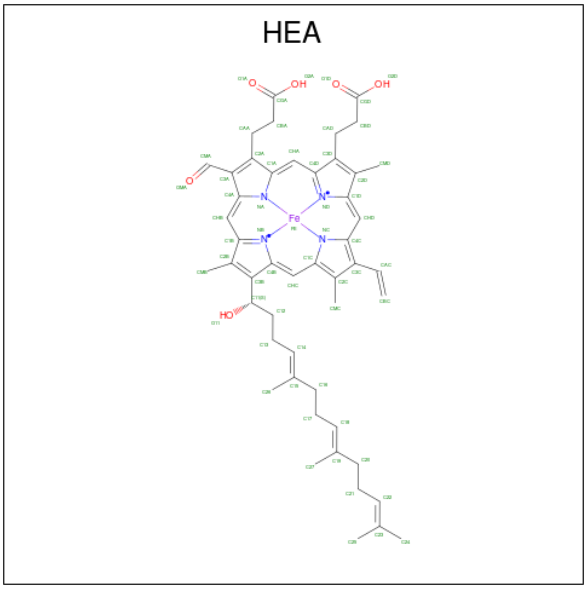
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

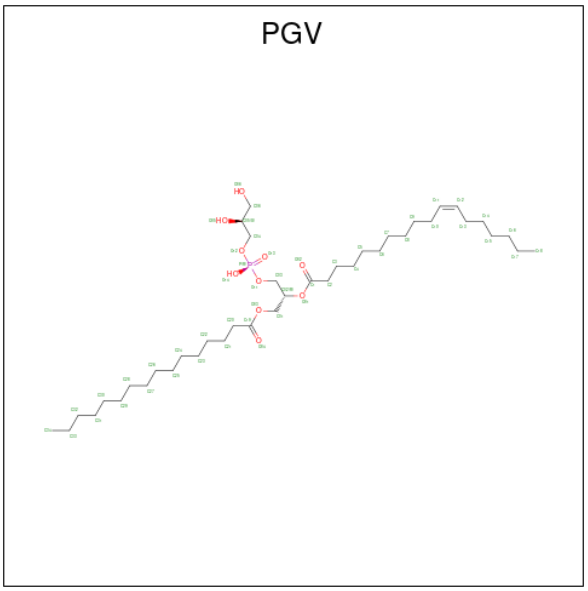
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
16	A	1	1	1	0	0
			Total	Na		
16	N	1	1	1	0	0

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



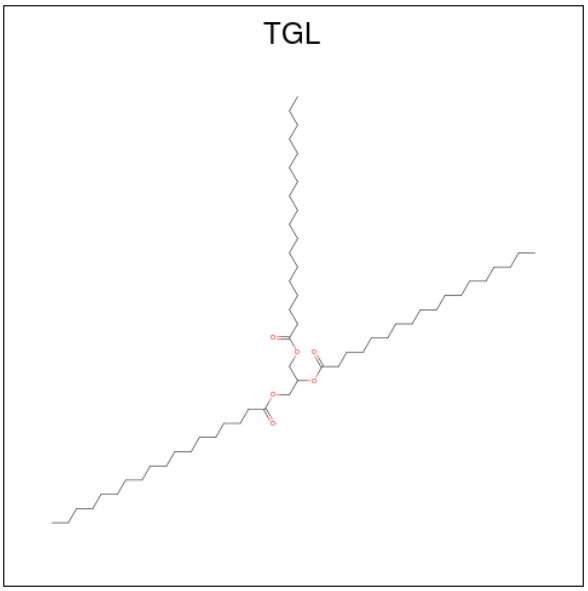
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
17	A	1	60	49	1	4	6	0	0
			Total	C	Fe	N	O		
17	A	1	60	49	1	4	6	0	0
			Total	C	Fe	N	O		
17	N	1	60	49	1	4	6	0	0
			Total	C	Fe	N	O		
17	N	1	60	49	1	4	6	0	0

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



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

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

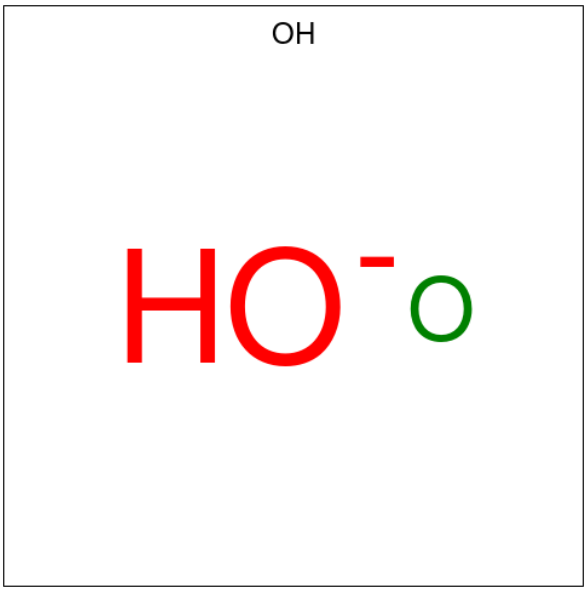


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
19	A	1	63	57	6	0	0
19	B	1	63	57	6	0	0
19	L	1	63	57	6	0	0
19	N	1	63	57	6	0	0
19	N	1	63	57	6	0	0
19	Y	1	63	57	6	0	0

- Molecule 20 is OXYGEN ATOM (three-letter code: O) (formula: O).

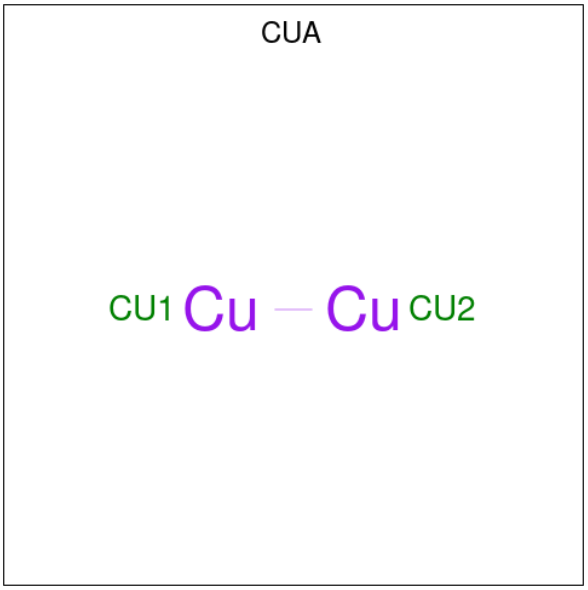
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
20	A	1	1	1	0	0
20	N	1	1	1	0	0

- Molecule 21 is HYDROXIDE ION (three-letter code: OH) (formula: HO).



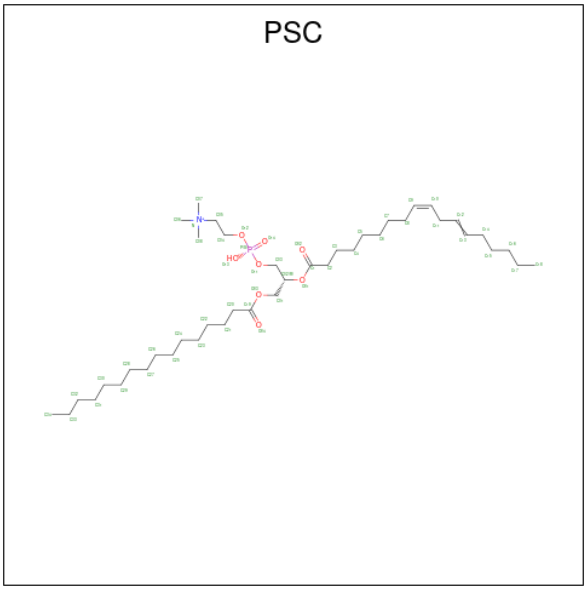
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	A	1	Total O 1 1	0	0
21	N	1	Total O 1 1	0	0

- Molecule 22 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).



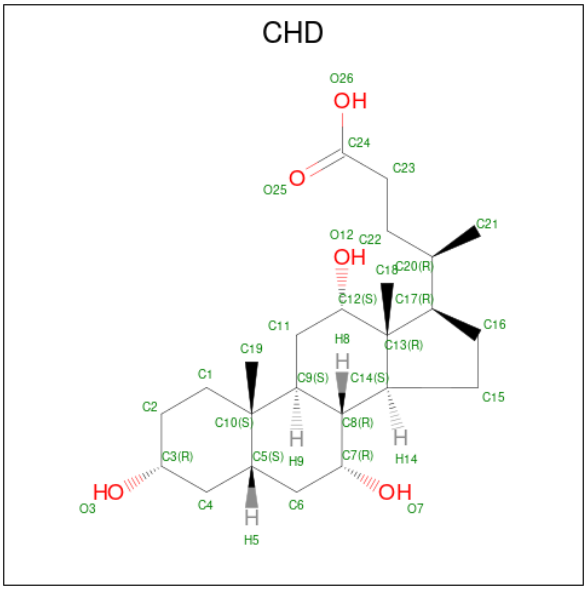
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	B	1	Total Cu 2 2	0	0
22	O	1	Total Cu 2 2	0	0

- Molecule 23 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: $C_{42}H_{81}NO_8P$).



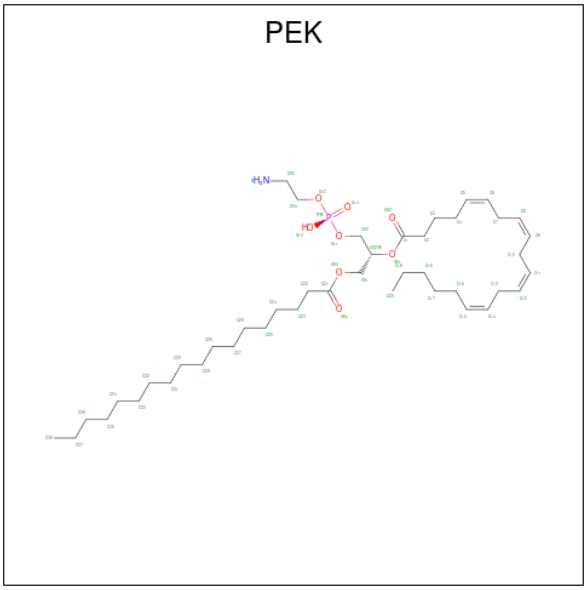
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
23	B	1	52	42	1	8	1	0	0
			Total	C	N	O	P		
23	O	1	52	42	1	8	1	0	0

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



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

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



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

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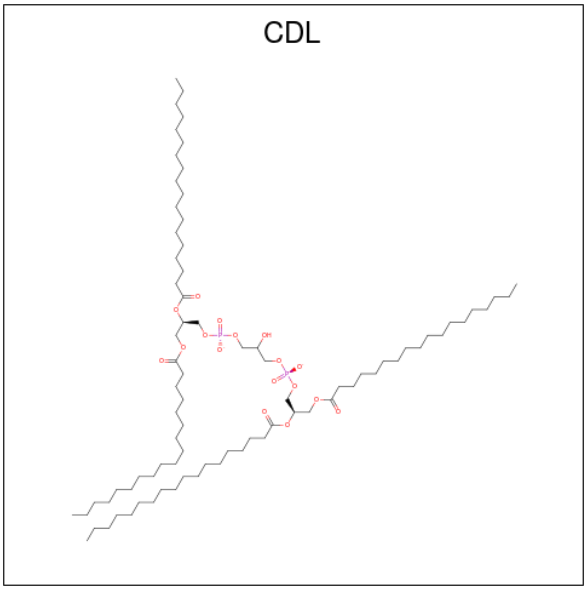
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
25	P	1	53	43	1	8	1	0	0
			Total	C	N	O	P		
25	P	1	53	43	1	8	1	0	0
			Total	C	N	O	P		
25	T	1	53	43	1	8	1	0	0

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

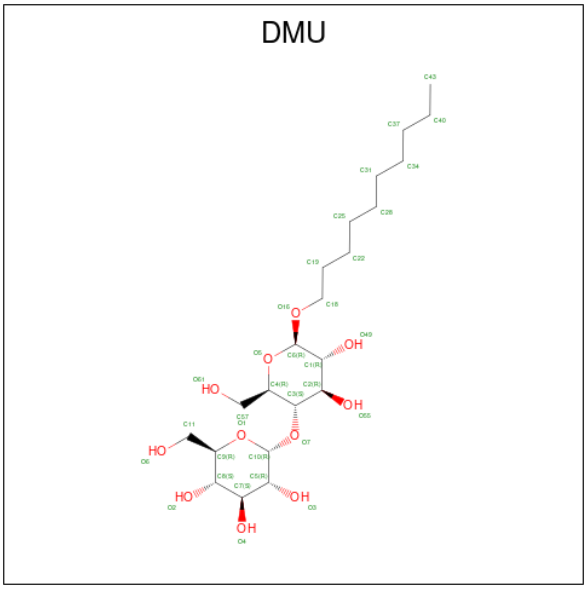


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
26	C	1	100	81	17	2	0	0
			Total	C	O	P		
26	N	1	100	81	17	2	0	0
			Total	C	O	P		
26	P	1	100	81	17	2	0	0
			Total	C	O	P		
26	T	1	100	81	17	2	0	0

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

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

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



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

- Molecule 29 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
29	A	152	152	152	0	0
29	B	102	102	102	0	0
29	C	58	58	58	0	0
29	D	45	45	45	0	0
29	E	26	26	26	0	0
29	F	36	36	36	0	0

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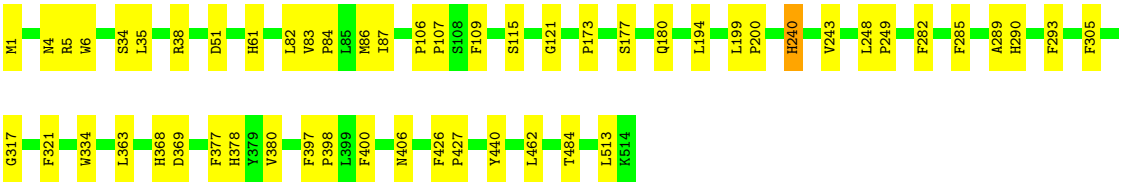
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	G	21	Total O 21 21	0	0
29	H	21	Total O 21 21	0	0
29	I	14	Total O 14 14	0	0
29	J	10	Total O 10 10	0	0
29	K	4	Total O 4 4	0	0
29	L	9	Total O 9 9	0	0
29	M	11	Total O 11 11	0	0
29	N	84	Total O 84 84	0	0
29	O	42	Total O 42 42	0	0
29	P	36	Total O 36 36	0	0
29	Q	18	Total O 18 18	0	0
29	R	11	Total O 11 11	0	0
29	S	22	Total O 22 22	0	0
29	T	15	Total O 15 15	0	0
29	U	7	Total O 7 7	0	0
29	V	8	Total O 8 8	0	0
29	W	7	Total O 7 7	0	0
29	X	6	Total O 6 6	0	0
29	Y	6	Total O 6 6	0	0
29	Z	1	Total O 1 1	0	0

3 Residue-property plots (i)

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

• Molecule 1: Cytochrome c oxidase subunit 1

Chain A:

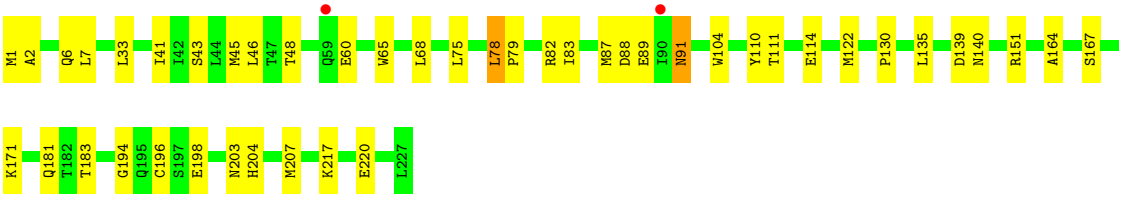


• Molecule 1: Cytochrome c oxidase subunit 1

Chain N:

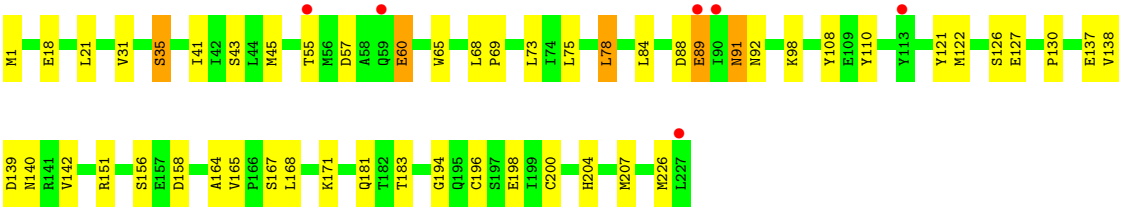
• Molecule 2: Cytochrome c oxidase subunit 2

Chain B:



• Molecule 2: Cytochrome c oxidase subunit 2

Chain O:

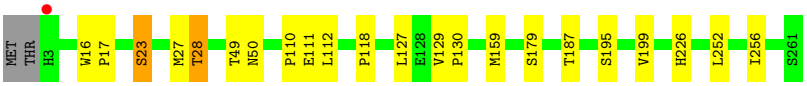


• Molecule 3: Cytochrome c oxidase subunit 3

Chain C: 93% 6%

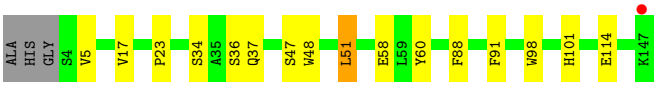
• Molecule 3: Cytochrome c oxidase subunit 3

Chain P: 91% 8%



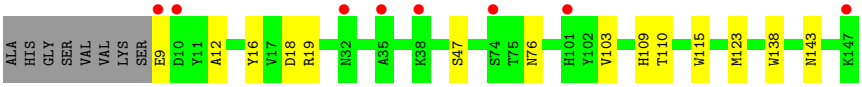
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain D: % 87% 10%



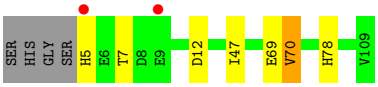
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain Q: 5% 85% 10% 5%



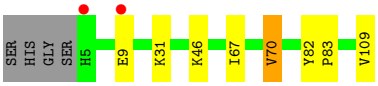
• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

Chain E: 2% 90% 6%



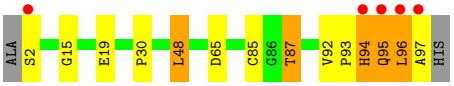
• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

Chain R: 2% 89% 6%



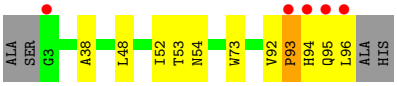
• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

Chain F:



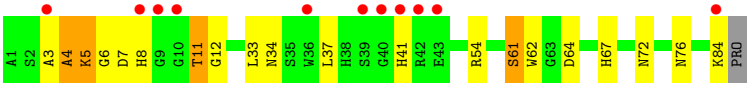
• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

Chain S:



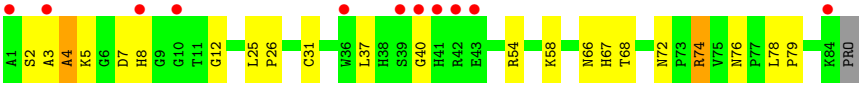
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain G:



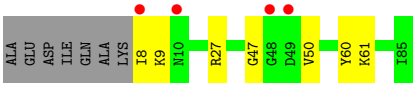
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain T:



• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain H:

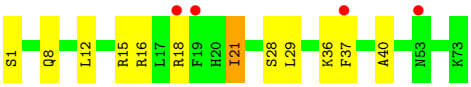


• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain U:

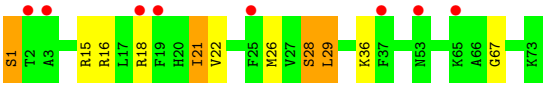
• Molecule 9: Cytochrome c oxidase subunit 6C

Chain I:

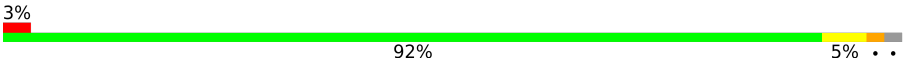


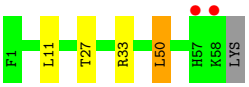
• Molecule 9: Cytochrome c oxidase subunit 6C

Chain V:



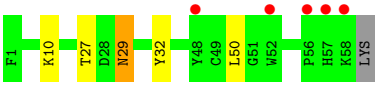
• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial

Chain J: 



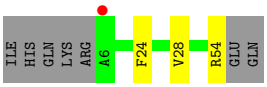
• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial

Chain W:



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

Chain K:

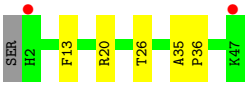


• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

Chain X:

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

Chain L:

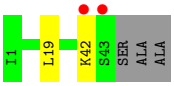


• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain Y:

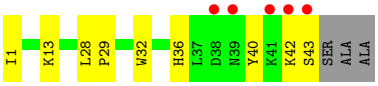
• Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

Chain M:



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

Chain Z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	178.70Å 189.80Å 211.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.50 – 2.50 10.50 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.5 (10.50-2.50) 100.0 (10.50-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.20 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.176 , 0.217 0.185 , 0.221	Depositor DCC
R_{free} test set	12143 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	53.8	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 60.0	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	0.97	EDS
Total number of atoms	31419	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% 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: FME, ZN, TPO, OH, CUA, PGV, CHD, DMU, CDL, SAC, MG, NA, CU, HEA, TGL, O, PSC, PEK

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	0.66	0/4156	0.78	0/5678
1	N	0.74	0/4156	0.79	0/5678
2	B	0.69	1/1860 (0.1%)	0.85	0/2534
2	O	0.69	1/1860 (0.1%)	0.83	0/2534
3	C	0.64	0/2197	0.76	0/3005
3	P	0.70	0/2197	0.77	0/3005
4	D	0.68	0/1229	0.80	0/1658
4	Q	0.69	0/1194	0.76	0/1611
5	E	0.67	0/871	0.78	0/1182
5	R	0.68	0/871	0.76	0/1182
6	F	0.66	0/748	0.91	0/1016
6	S	0.68	0/737	0.85	0/1001
7	G	0.68	0/690	0.88	0/937
7	T	0.67	0/690	0.86	0/937
8	H	0.67	0/673	0.87	0/910
8	U	0.65	0/682	0.81	0/921
9	I	0.66	0/605	0.85	0/802
9	V	0.70	0/605	0.86	0/802
10	J	0.70	0/471	0.76	0/636
10	W	0.73	0/471	0.80	0/636
11	K	0.71	0/398	0.81	0/546
11	X	0.73	0/398	0.77	0/546
12	L	0.65	0/393	0.84	0/526
12	Y	0.71	0/393	0.80	0/526
13	M	0.62	0/345	0.76	0/470
13	Z	0.70	0/345	0.77	0/470
All	All	0.69	2/29235 (0.0%)	0.80	0/39749

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	N	0	1
6	F	0	1
6	S	0	1
9	V	0	1
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	198	GLU	C-O	7.49	1.37	1.23
2	O	198	GLU	C-O	5.13	1.33	1.23

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	A	368	HIS	Sidechain
6	F	93	PRO	Peptide
1	N	291	HIS	Sidechain
6	S	93	PRO	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4027	0	4001	29	0
1	N	4027	0	4001	49	0
2	B	1824	0	1833	22	0
2	O	1824	0	1833	26	0
3	C	2110	0	2027	9	0
3	P	2110	0	2027	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1195	0	1183	7	0
4	Q	1160	0	1142	13	0
5	E	852	0	845	4	0
5	R	852	0	845	2	0
6	F	732	0	713	8	0
6	S	721	0	703	4	0
7	G	675	0	643	10	0
7	T	675	0	643	17	0
8	H	653	0	610	1	0
8	U	662	0	623	4	0
9	I	601	0	612	5	0
9	V	601	0	613	9	0
10	J	460	0	459	4	0
10	W	460	0	459	3	0
11	K	384	0	366	1	0
11	X	384	0	366	9	0
12	L	380	0	380	7	0
12	Y	380	0	380	6	0
13	M	335	0	352	0	0
13	Z	335	0	352	4	0
14	A	1	0	0	0	0
14	N	1	0	0	0	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	120	0	108	2	0
17	N	120	0	108	9	0
18	A	153	0	228	5	0
18	C	51	0	76	0	0
18	N	102	0	152	1	0
18	P	51	0	76	0	0
18	U	51	0	76	0	0
19	A	63	0	109	1	0
19	B	63	0	110	10	0
19	L	63	0	110	12	0
19	N	126	0	220	20	0
19	Y	63	0	110	2	0
20	A	1	0	0	1	0
20	N	1	0	0	0	0
21	A	1	0	0	1	0
21	N	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	B	2	0	0	0	0
22	O	2	0	0	0	0
23	B	52	0	80	6	0
23	O	52	0	80	3	0
24	B	29	0	39	0	0
24	C	29	0	39	1	0
24	G	29	0	39	0	0
24	J	58	0	78	4	0
24	P	29	0	39	1	0
24	W	58	0	78	2	0
25	C	53	0	77	3	0
25	G	106	0	154	2	0
25	P	106	0	154	2	0
25	T	53	0	77	2	0
26	C	100	0	156	14	0
26	N	100	0	156	23	0
26	P	100	0	156	9	0
26	T	100	0	156	1	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	G	33	0	42	3	0
28	M	33	0	42	2	0
28	Q	33	0	42	0	0
28	T	33	0	42	0	0
29	A	152	0	0	3	0
29	B	102	0	0	4	0
29	C	58	0	0	2	0
29	D	45	0	0	1	0
29	E	26	0	0	0	0
29	F	36	0	0	2	0
29	G	21	0	0	4	0
29	H	21	0	0	1	0
29	I	14	0	0	0	0
29	J	10	0	0	3	0
29	K	4	0	0	0	0
29	L	9	0	0	0	0
29	M	11	0	0	1	0
29	N	84	0	0	3	0
29	O	42	0	0	1	0
29	P	36	0	0	0	0
29	Q	18	0	0	8	0
29	R	11	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	S	22	0	0	2	0
29	T	15	0	0	4	0
29	U	7	0	0	2	0
29	V	8	0	0	6	0
29	W	7	0	0	1	0
29	X	6	0	0	2	0
29	Y	6	0	0	1	0
29	Z	1	0	0	0	0
All	All	31419	0	31220	338	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 338 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:N:607:TGL:OG1	29:N:701:HOH:O	1.67	1.11
12:L:20:ARG:HH22	19:L:101:TGL:HC52	1.12	1.06
4:Q:19:ARG:CD	29:Q:301:HOH:O	2.03	1.04
6:F:19:GLU:HG2	29:F:235:HOH:O	1.62	0.98
4:Q:19:ARG:HD3	29:Q:301:HOH:O	1.63	0.91

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	512/514 (100%)	492 (96%)	19 (4%)	1 (0%)	47 68
1	N	512/514 (100%)	488 (95%)	23 (4%)	1 (0%)	47 68
2	B	225/227 (99%)	213 (95%)	12 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	O	225/227 (99%)	210 (93%)	13 (6%)	2 (1%)	17	31
3	C	257/261 (98%)	251 (98%)	5 (2%)	1 (0%)	34	54
3	P	257/261 (98%)	248 (96%)	9 (4%)	0	100	100
4	D	142/147 (97%)	135 (95%)	6 (4%)	1 (1%)	22	39
4	Q	137/147 (93%)	123 (90%)	13 (10%)	1 (1%)	22	39
5	E	103/109 (94%)	100 (97%)	3 (3%)	0	100	100
5	R	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
6	F	94/98 (96%)	87 (93%)	3 (3%)	4 (4%)	2	3
6	S	92/98 (94%)	87 (95%)	3 (3%)	2 (2%)	6	10
7	G	81/85 (95%)	66 (82%)	9 (11%)	6 (7%)	1	1
7	T	81/85 (95%)	64 (79%)	12 (15%)	5 (6%)	1	1
8	H	76/85 (89%)	73 (96%)	1 (1%)	2 (3%)	5	8
8	U	77/85 (91%)	72 (94%)	3 (4%)	2 (3%)	5	8
9	I	71/73 (97%)	66 (93%)	4 (6%)	1 (1%)	11	20
9	V	71/73 (97%)	64 (90%)	6 (8%)	1 (1%)	11	20
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	W	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
11	K	47/56 (84%)	44 (94%)	3 (6%)	0	100	100
11	X	47/56 (84%)	39 (83%)	7 (15%)	1 (2%)	7	11
12	L	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
12	Y	44/47 (94%)	40 (91%)	3 (7%)	1 (2%)	6	10
13	M	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
13	Z	41/46 (89%)	36 (88%)	5 (12%)	0	100	100
All	All	3492/3614 (97%)	3293 (94%)	167 (5%)	32 (1%)	17	31

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	4	ALA
7	G	5	LYS
7	G	7	ASP
7	G	37	LEU
2	O	89	GLU

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%)	421 (99%)	5 (1%)	71	88
1	N	426/426 (100%)	412 (97%)	14 (3%)	38	64
2	B	210/210 (100%)	197 (94%)	13 (6%)	18	35
2	O	210/210 (100%)	191 (91%)	19 (9%)	9	19
3	C	224/226 (99%)	217 (97%)	7 (3%)	40	67
3	P	224/226 (99%)	217 (97%)	7 (3%)	40	67
4	D	128/129 (99%)	121 (94%)	7 (6%)	21	41
4	Q	123/129 (95%)	119 (97%)	4 (3%)	38	64
5	E	92/95 (97%)	89 (97%)	3 (3%)	38	64
5	R	92/95 (97%)	87 (95%)	5 (5%)	22	42
6	F	80/81 (99%)	77 (96%)	3 (4%)	33	58
6	S	79/81 (98%)	74 (94%)	5 (6%)	18	34
7	G	67/68 (98%)	61 (91%)	6 (9%)	9	19
7	T	67/68 (98%)	63 (94%)	4 (6%)	19	37
8	H	70/75 (93%)	66 (94%)	4 (6%)	20	39
8	U	71/75 (95%)	66 (93%)	5 (7%)	15	29
9	I	57/57 (100%)	52 (91%)	5 (9%)	10	19
9	V	57/57 (100%)	51 (90%)	6 (10%)	7	13
10	J	49/50 (98%)	47 (96%)	2 (4%)	30	55
10	W	49/50 (98%)	45 (92%)	4 (8%)	11	22
11	K	39/46 (85%)	38 (97%)	1 (3%)	46	72
11	X	39/46 (85%)	35 (90%)	4 (10%)	7	14
12	L	39/40 (98%)	38 (97%)	1 (3%)	46	72
12	Y	39/40 (98%)	37 (95%)	2 (5%)	24	45
13	M	37/38 (97%)	35 (95%)	2 (5%)	22	42
13	Z	37/38 (97%)	34 (92%)	3 (8%)	11	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3031/3082 (98%)	2890 (95%)	141 (5%)	26 49

5 of 141 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	T	54	ARG
8	U	27	ARG
10	W	29	ASN
9	I	8	GLN
8	H	61	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
5	R	94	ASN
8	U	37	HIS
6	S	54	ASN
7	T	76	ASN
13	Z	36	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	SAC	I	1	9	7,8,9	0.69	0	8,9,11	1.05	1 (12%)
7	TPO	T	11	7	8,10,11	0.91	0	10,14,16	0.81	0
1	FME	N	1	1	8,9,10	0.50	0	7,9,11	0.98	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	FME	A	1	1	8,9,10	0.48	0	7,9,11	0.96	0
7	TPO	G	11	7	8,10,11	1.30	1 (12%)	10,14,16	0.81	0
2	FME	O	1	2	8,9,10	0.44	0	7,9,11	1.63	2 (28%)
2	FME	B	1	2	8,9,10	0.56	0	7,9,11	2.08	2 (28%)
9	SAC	V	1	9	7,8,9	0.65	0	8,9,11	1.47	1 (12%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	11	TPO	P-OG1	3.30	1.65	1.59

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	FME	CA-N-CN	-4.15	116.43	122.82
9	V	1	SAC	O-C-CA	-4.01	114.27	124.78
2	B	1	FME	C-CA-N	3.12	115.37	109.73
2	O	1	FME	CA-N-CN	-2.95	118.28	122.82
2	O	1	FME	C-CA-N	2.88	114.92	109.73

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 56 ligands modelled in this entry, 10 are monoatomic and 2 are modelled with single atom - leaving 44 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
19	TGL	N	609	-	62,62,62	1.13	3 (4%)	65,65,65	1.03	5 (7%)
17	HEA	A	605	20,1	57,67,67	1.93	14 (24%)	61,103,103	2.31	22 (36%)
25	PEK	T	102	-	52,52,52	0.33	0	55,57,57	0.49	0
24	CHD	G	104	-	32,32,32	0.57	0	51,51,51	0.85	0
17	HEA	N	606	1	57,67,67	1.96	15 (26%)	61,103,103	2.37	22 (36%)
24	CHD	J	101	-	32,32,32	0.63	0	51,51,51	1.14	5 (9%)
24	CHD	W	101	-	32,32,32	0.56	0	51,51,51	0.71	0
24	CHD	P	301	-	32,32,32	0.62	0	51,51,51	0.75	0
18	PGV	A	608	-	50,50,50	1.18	2 (4%)	53,56,56	1.34	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
23	PSC	O	302	-	51,51,51	0.31	0	57,59,59	0.39	0
24	CHD	J	102	-	32,32,32	0.77	0	51,51,51	1.27	4 (7%)
25	PEK	P	302	-	52,52,52	0.30	0	55,57,57	0.55	0
28	DMU	Q	201	-	34,34,34	1.06	2 (5%)	45,45,45	1.29	5 (11%)
18	PGV	C	303	-	50,50,50	0.85	2 (4%)	53,56,56	1.14	6 (11%)
26	CDL	T	103	-	99,99,99	1.01	4 (4%)	105,111,111	0.69	4 (3%)
19	TGL	N	607	-	62,62,62	1.06	4 (6%)	65,65,65	1.09	5 (7%)
19	TGL	B	303	-	62,62,62	1.01	4 (6%)	65,65,65	1.07	7 (10%)
19	TGL	L	101	-	62,62,62	1.11	5 (8%)	65,65,65	1.09	4 (6%)
18	PGV	U	101	-	50,50,50	1.12	2 (4%)	53,56,56	1.21	5 (9%)
18	PGV	N	610	-	50,50,50	1.06	2 (4%)	53,56,56	0.95	3 (5%)
18	PGV	A	606	-	50,50,50	1.10	2 (4%)	53,56,56	1.14	4 (7%)
19	TGL	A	609	-	62,62,62	1.13	4 (6%)	65,65,65	1.05	5 (7%)
25	PEK	P	303	-	52,52,52	0.38	0	55,57,57	0.56	0
18	PGV	P	304	-	50,50,50	0.94	2 (4%)	53,56,56	1.02	4 (7%)
22	CUA	O	301	2	0,1,1	-	-	-		
26	CDL	P	305	-	99,99,99	0.98	4 (4%)	105,111,111	0.87	5 (4%)
17	HEA	A	604	1	57,67,67	2.00	17 (29%)	61,103,103	2.28	26 (42%)
28	DMU	M	101	-	34,34,34	1.08	3 (8%)	45,45,45	1.50	8 (17%)
24	CHD	B	304	-	32,32,32	0.47	0	51,51,51	0.70	0
25	PEK	C	302	-	52,52,52	0.34	0	55,57,57	0.46	0
26	CDL	N	601	-	99,99,99	0.96	4 (4%)	105,111,111	0.71	2 (1%)
28	DMU	T	101	-	34,34,34	1.84	6 (17%)	45,45,45	1.58	6 (13%)
26	CDL	C	304	-	99,99,99	0.98	4 (4%)	105,111,111	0.81	4 (3%)
18	PGV	N	608	-	50,50,50	0.87	2 (4%)	53,56,56	1.08	4 (7%)
22	CUA	B	301	2	0,1,1	-	-	-		
25	PEK	G	102	-	52,52,52	0.33	0	55,57,57	0.57	0
18	PGV	A	607	-	50,50,50	0.85	2 (4%)	53,56,56	1.34	5 (9%)
25	PEK	G	103	-	52,52,52	0.37	0	55,57,57	0.53	1 (1%)
24	CHD	C	301	-	32,32,32	0.64	1 (3%)	51,51,51	0.73	0
23	PSC	B	302	-	51,51,51	0.34	0	57,59,59	0.47	0
19	TGL	Y	101	-	62,62,62	1.09	4 (6%)	65,65,65	0.97	5 (7%)
17	HEA	N	605	1	57,67,67	1.96	14 (24%)	61,103,103	2.42	28 (45%)
24	CHD	W	102	-	32,32,32	0.69	0	51,51,51	1.04	4 (7%)
28	DMU	G	101	-	34,34,34	1.38	5 (14%)	45,45,45	1.71	9 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	TGL	N	609	-	-	42/65/65/65	-
17	HEA	A	605	20,1	3/3/7/16	5/32/76/76	-
25	PEK	T	102	-	-	30/56/56/56	-
24	CHD	G	104	-	-	4/9/74/74	0/4/4/4
17	HEA	N	606	1	3/3/7/16	5/32/76/76	-
24	CHD	J	101	-	-	4/9/74/74	1/4/4/4
24	CHD	W	101	-	-	2/9/74/74	1/4/4/4
24	CHD	P	301	-	-	3/9/74/74	0/4/4/4
18	PGV	A	608	-	-	26/55/55/55	-
23	PSC	O	302	-	-	31/55/55/55	-
24	CHD	J	102	-	-	6/9/74/74	0/4/4/4
25	PEK	P	302	-	-	21/56/56/56	-
28	DMU	Q	201	-	-	10/19/59/59	0/2/2/2
18	PGV	C	303	-	-	13/55/55/55	-
26	CDL	T	103	-	-	65/110/110/110	-
19	TGL	N	607	-	-	39/65/65/65	-
19	TGL	B	303	-	-	40/65/65/65	-
19	TGL	L	101	-	-	37/65/65/65	-
18	PGV	U	101	-	-	29/55/55/55	-
18	PGV	N	610	-	-	33/55/55/55	-
18	PGV	A	606	-	-	32/55/55/55	-
19	TGL	A	609	-	-	39/65/65/65	-
25	PEK	P	303	-	-	21/56/56/56	-
18	PGV	P	304	-	-	14/55/55/55	-
26	CDL	P	305	-	-	71/110/110/110	-
17	HEA	A	604	1	3/3/7/16	5/32/76/76	-
28	DMU	M	101	-	-	10/19/59/59	0/2/2/2
24	CHD	B	304	-	-	4/9/74/74	0/4/4/4
25	PEK	C	302	-	-	25/56/56/56	-
26	CDL	N	601	-	-	58/110/110/110	-
28	DMU	T	101	-	-	10/19/59/59	0/2/2/2
26	CDL	C	304	-	-	59/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	PGV	N	608	-	-	15/55/55/55	-
25	PEK	G	102	-	-	21/56/56/56	-
18	PGV	A	607	-	-	17/55/55/55	-
25	PEK	G	103	-	-	25/56/56/56	-
24	CHD	C	301	-	-	0/9/74/74	0/4/4/4
23	PSC	B	302	-	-	29/55/55/55	-
19	TGL	Y	101	-	-	32/65/65/65	-
17	HEA	N	605	1	3/3/7/16	5/32/76/76	-
24	CHD	W	102	-	-	6/9/74/74	0/4/4/4
28	DMU	G	101	-	-	12/19/59/59	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	T	101	DMU	O16-C6	6.46	1.51	1.40
17	N	606	HEA	C3B-C2B	6.00	1.48	1.34
17	N	605	HEA	C3B-C2B	5.68	1.47	1.34
18	A	608	PGV	O01-C1	5.49	1.49	1.34
18	A	606	PGV	O03-C19	5.15	1.48	1.33

The worst 5 of 221 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	608	PGV	O01-C1-C2	6.28	125.04	111.50
17	N	606	HEA	C2D-C1D-ND	6.27	117.27	109.84
17	A	605	HEA	CAD-CBD-CGD	-6.09	100.50	113.60
17	N	606	HEA	C3D-C4D-ND	6.02	116.19	110.36
17	N	605	HEA	C3D-C4D-ND	6.00	116.17	110.36

5 of 12 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	A	604	HEA	ND
17	A	604	HEA	NA
17	A	604	HEA	NB
17	A	605	HEA	ND
17	A	605	HEA	NA

5 of 955 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	606	PGV	C04-O12-P-O13
18	A	606	PGV	C04-O12-P-O14
18	A	606	PGV	C02-C03-O11-P
18	A	606	PGV	C04-C05-C06-O06
18	A	606	PGV	O05-C05-C06-O06

All (2) ring outliers are listed below:

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

31 monomers are involved in 138 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	N	609	TGL	7	0
17	A	605	HEA	1	0
25	T	102	PEK	2	0
17	N	606	HEA	4	0
24	J	101	CHD	2	0
24	P	301	CHD	1	0
18	A	608	PGV	2	0
23	O	302	PSC	3	0
24	J	102	CHD	2	0
25	P	302	PEK	2	0
26	T	103	CDL	1	0
19	N	607	TGL	13	0
19	B	303	TGL	10	0
19	L	101	TGL	12	0
18	N	610	PGV	1	0
18	A	606	PGV	3	0
19	A	609	TGL	1	0
26	P	305	CDL	9	0
17	A	604	HEA	1	0
28	M	101	DMU	2	0
25	C	302	PEK	3	0
26	N	601	CDL	23	0
26	C	304	CDL	14	0
25	G	102	PEK	1	0
25	G	103	PEK	1	0
24	C	301	CHD	1	0
23	B	302	PSC	6	0
19	Y	101	TGL	2	0

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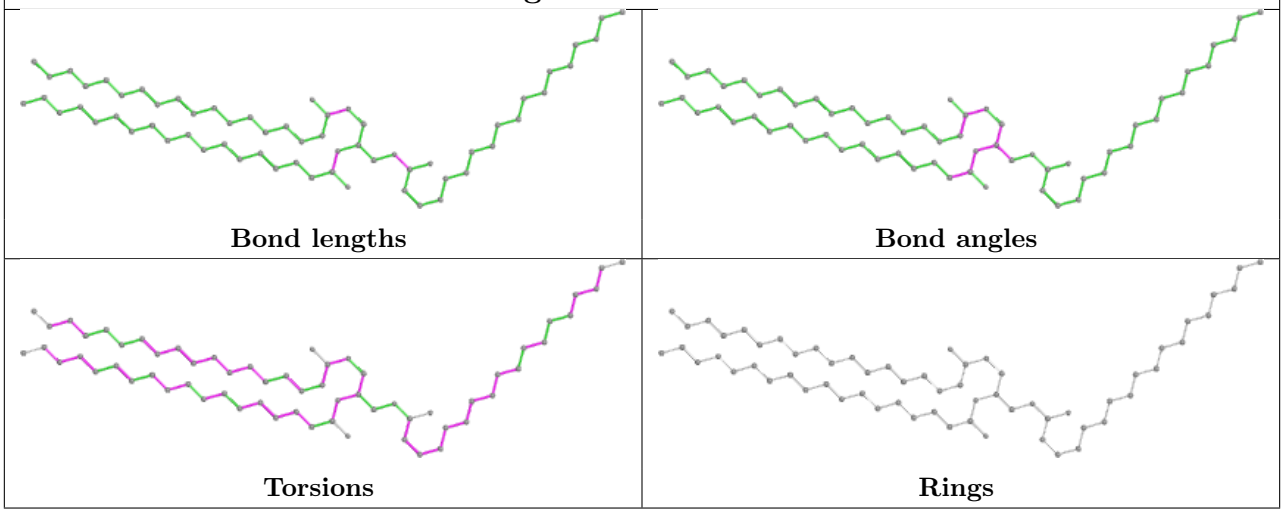
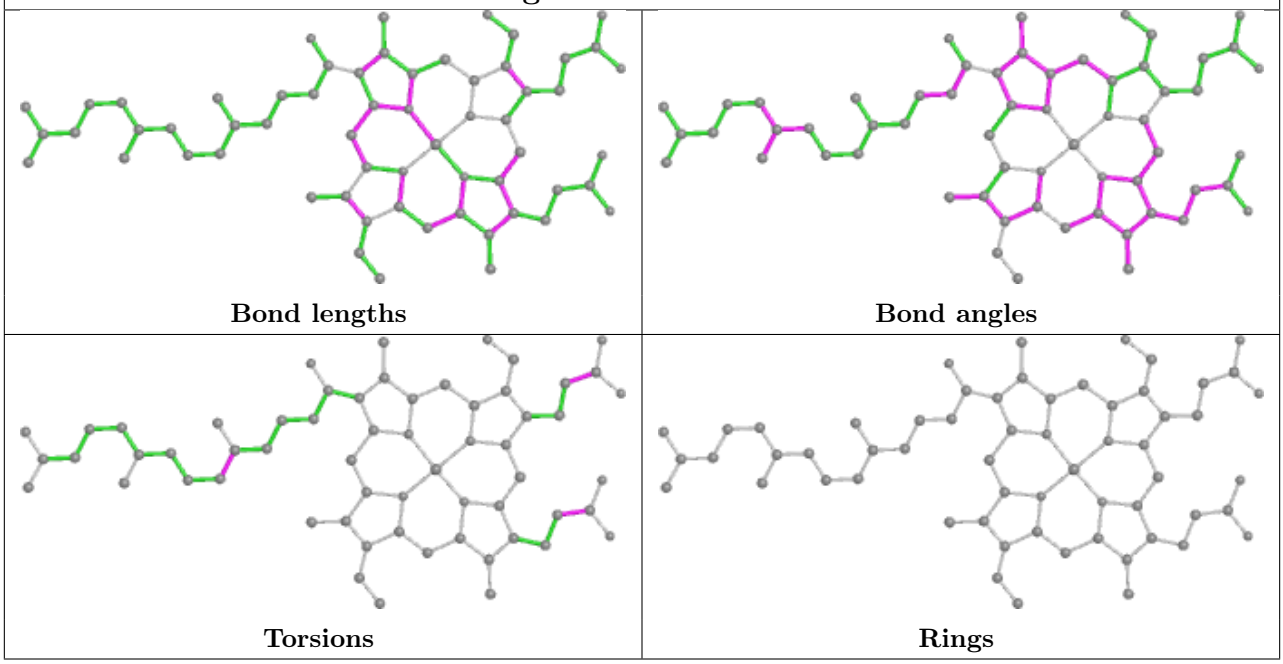
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	N	605	HEA	5	0
24	W	102	CHD	2	0
28	G	101	DMU	3	0

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

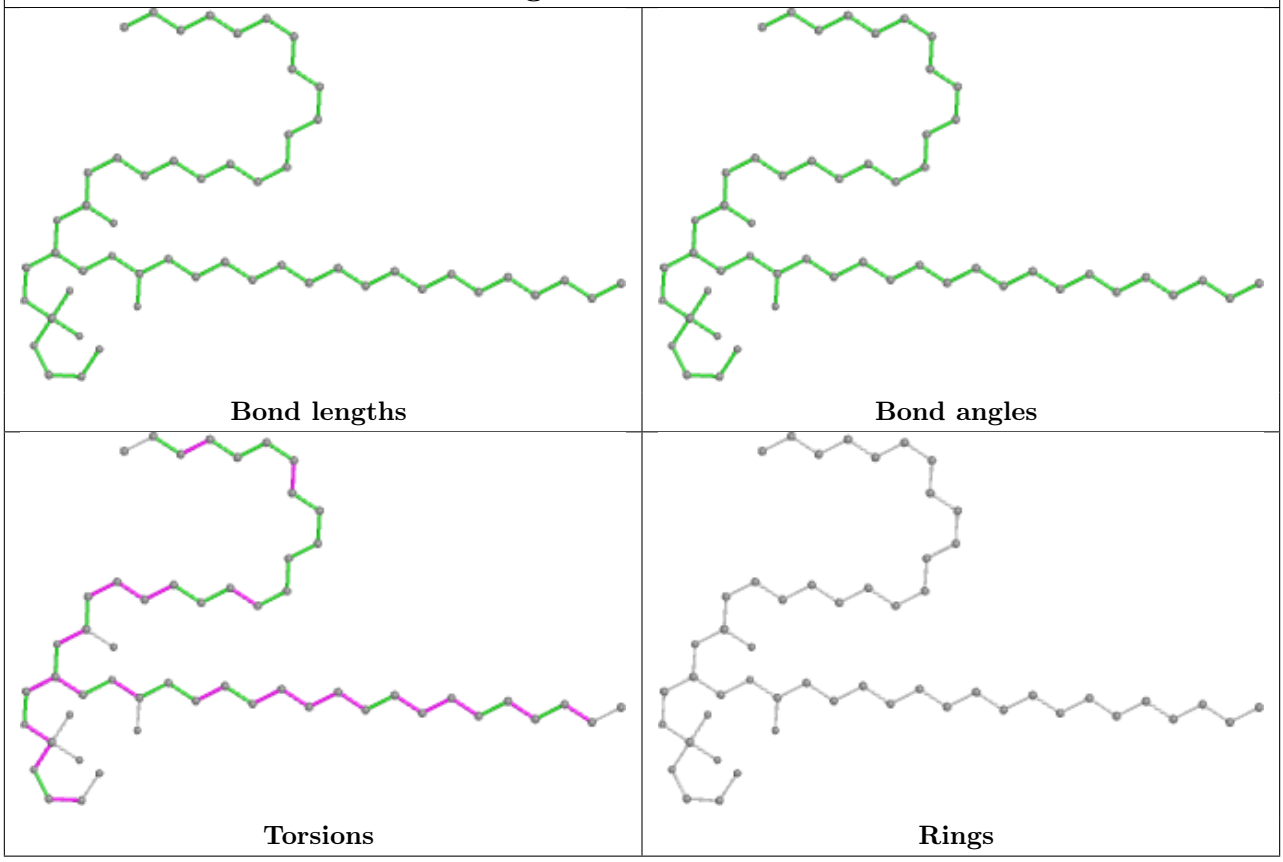
Ligand TGL N 609



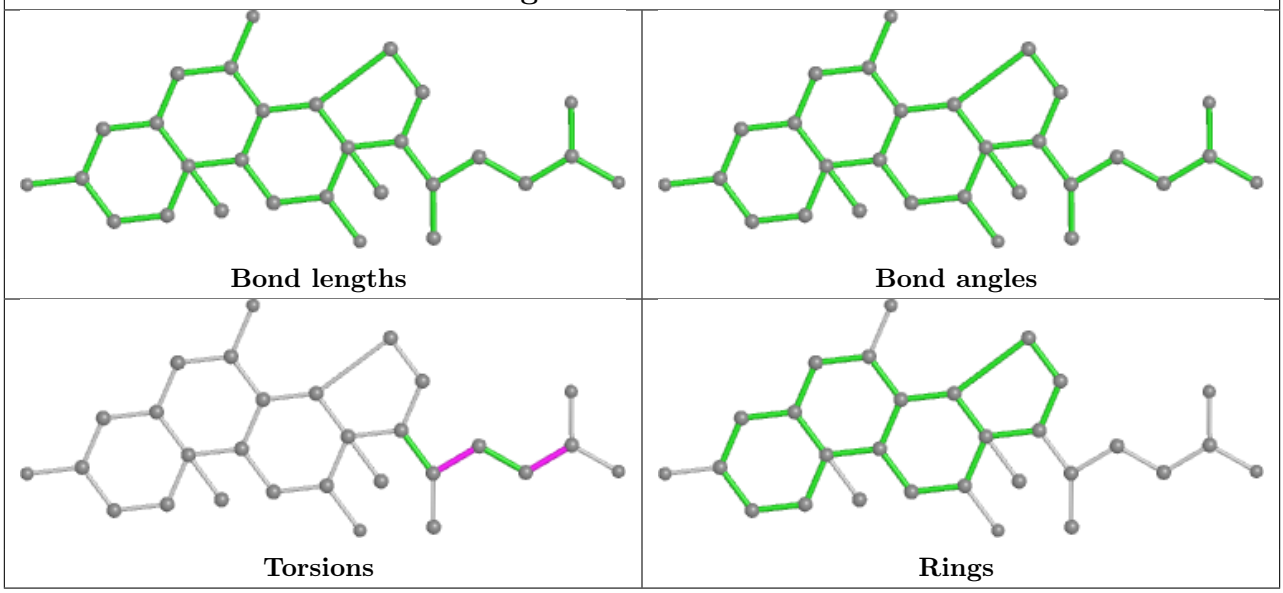
Ligand HEA A 605



Ligand PEK T 102



Ligand CHD G 104



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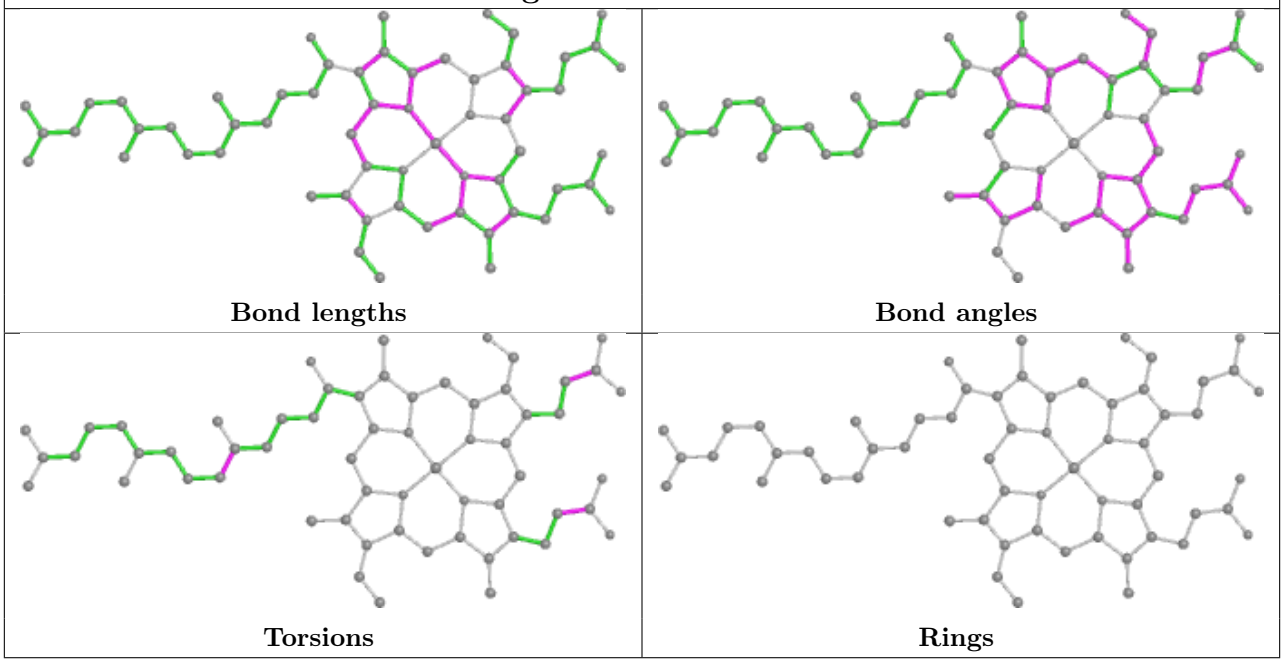
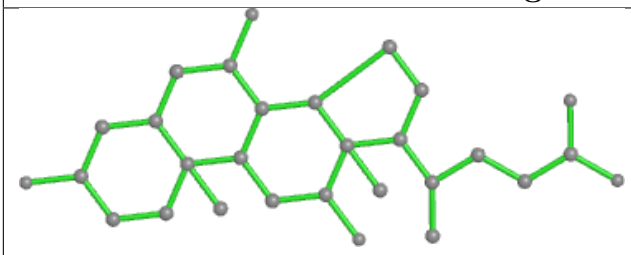
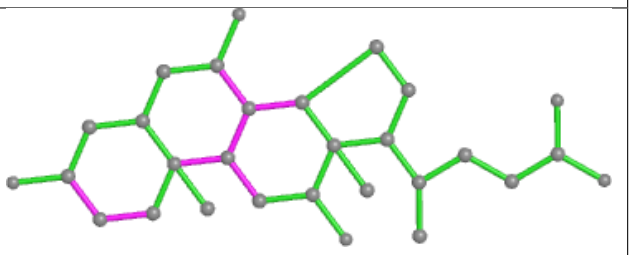
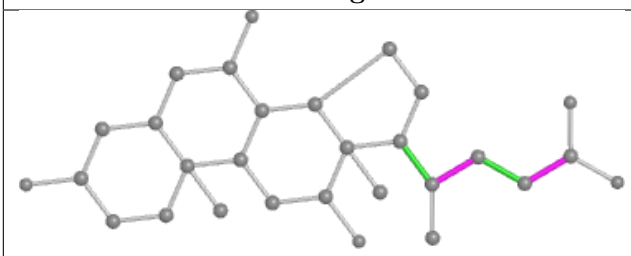
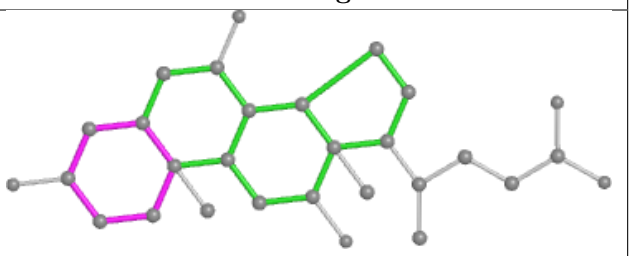
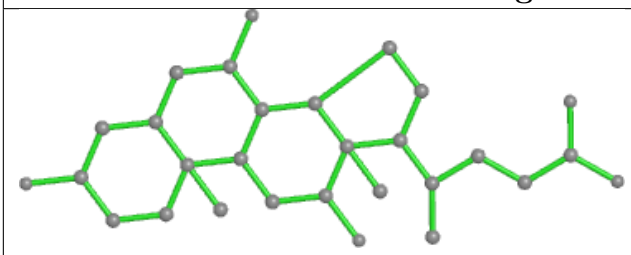
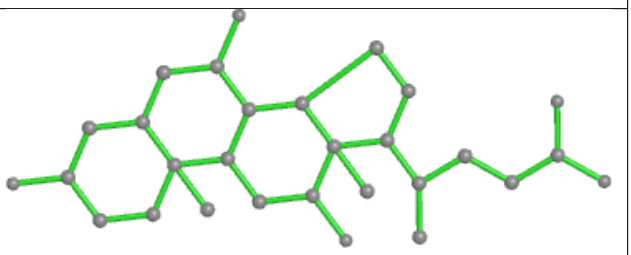
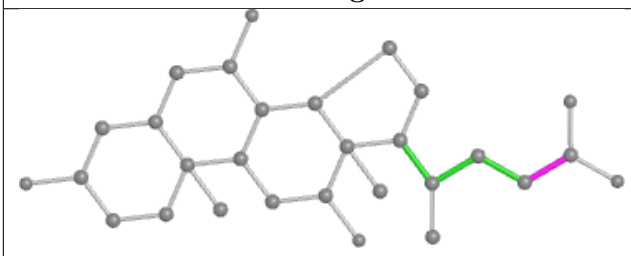
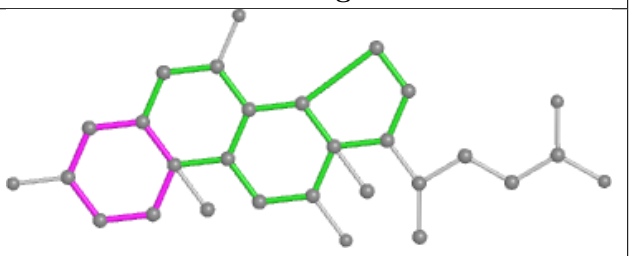
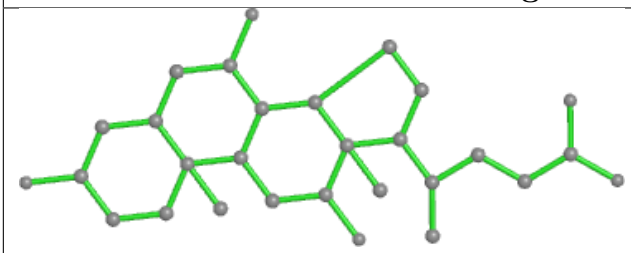


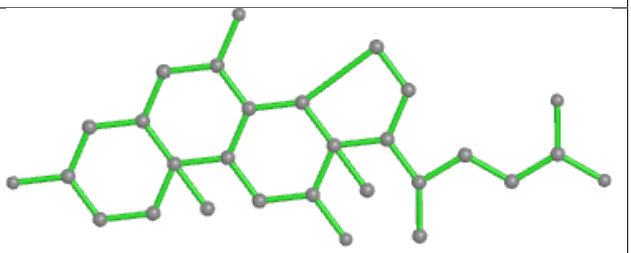
Ligand CHD J 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHD W 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

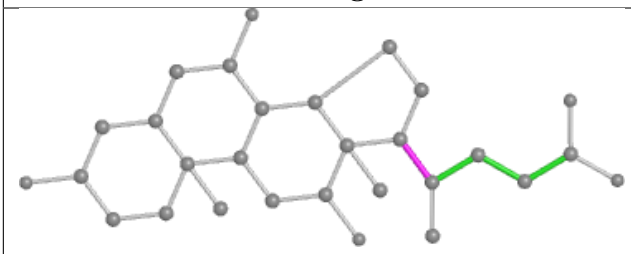
Ligand CHD P 301



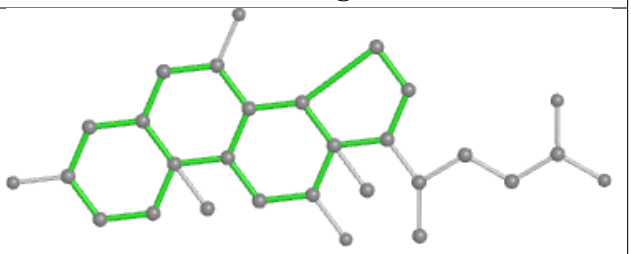
Bond lengths



Bond angles

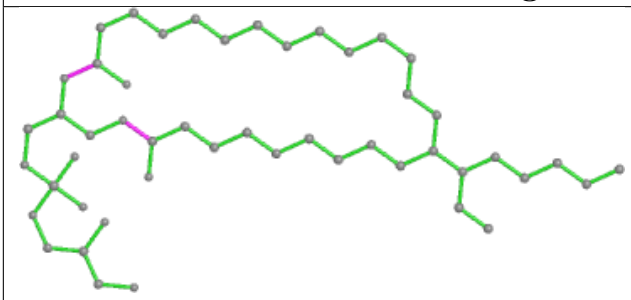


Torsions



Rings

Ligand PGV A 608



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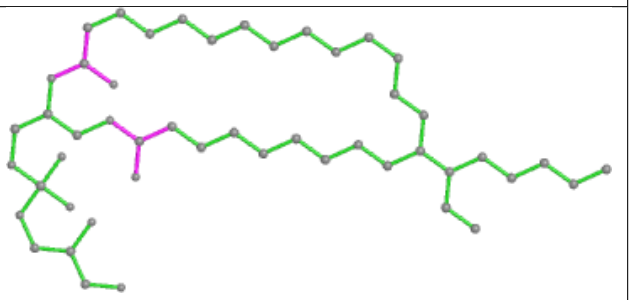
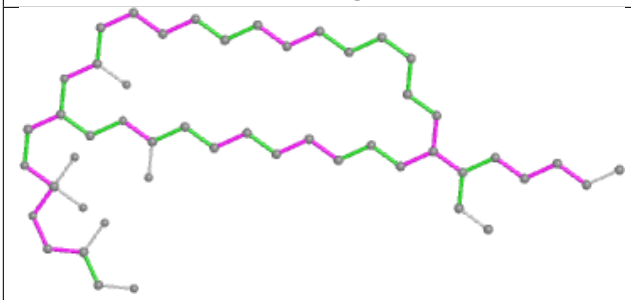
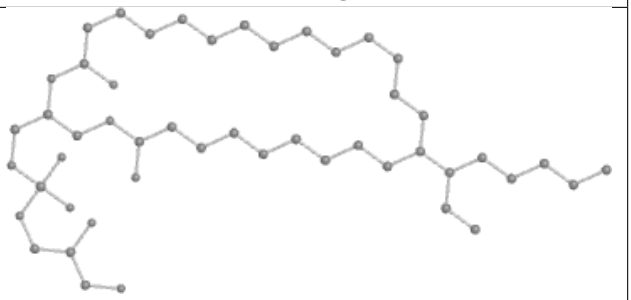


Bond angles

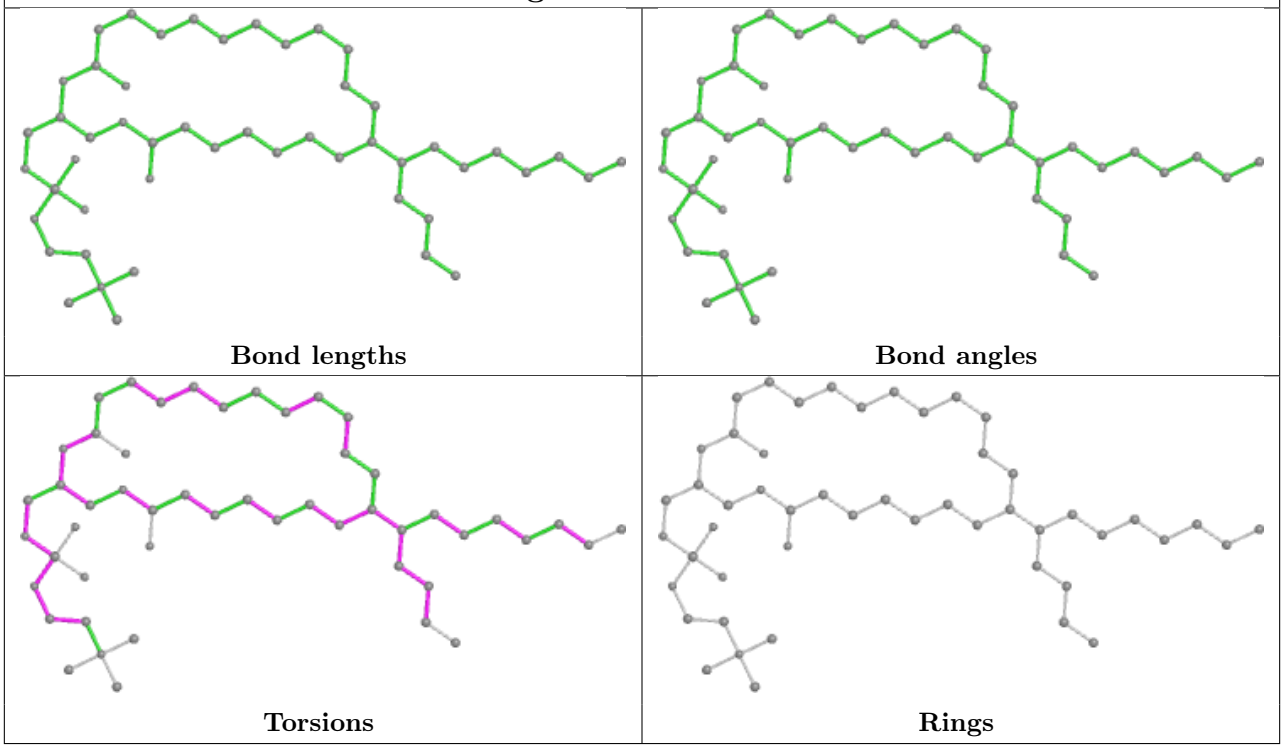


Torsions

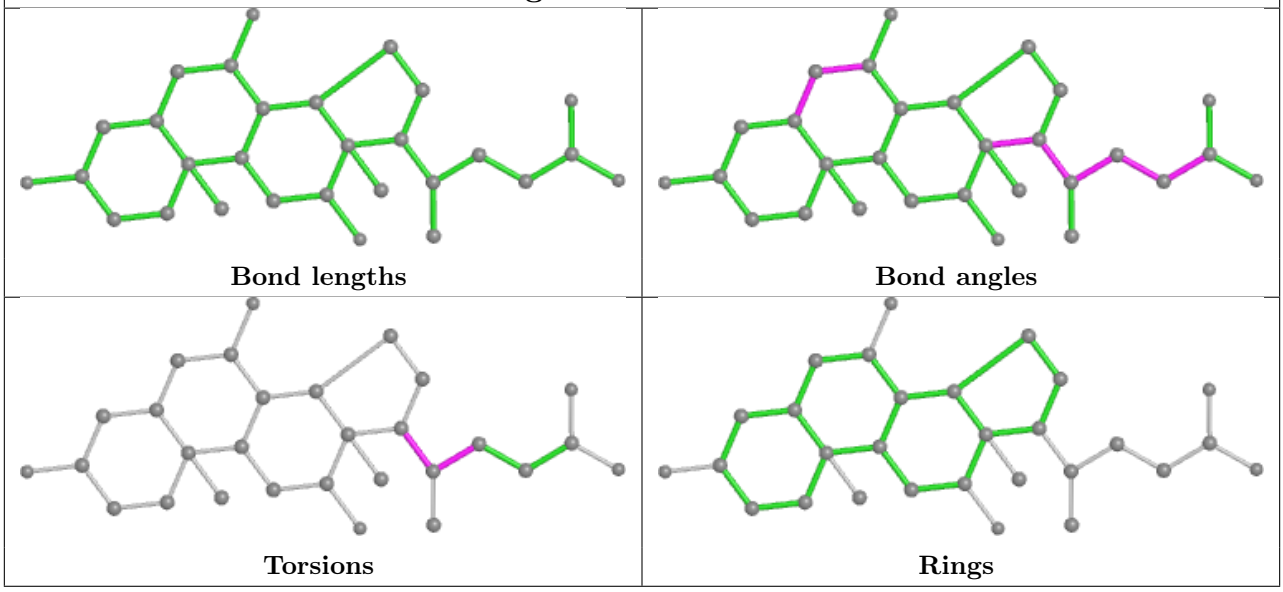


Rings

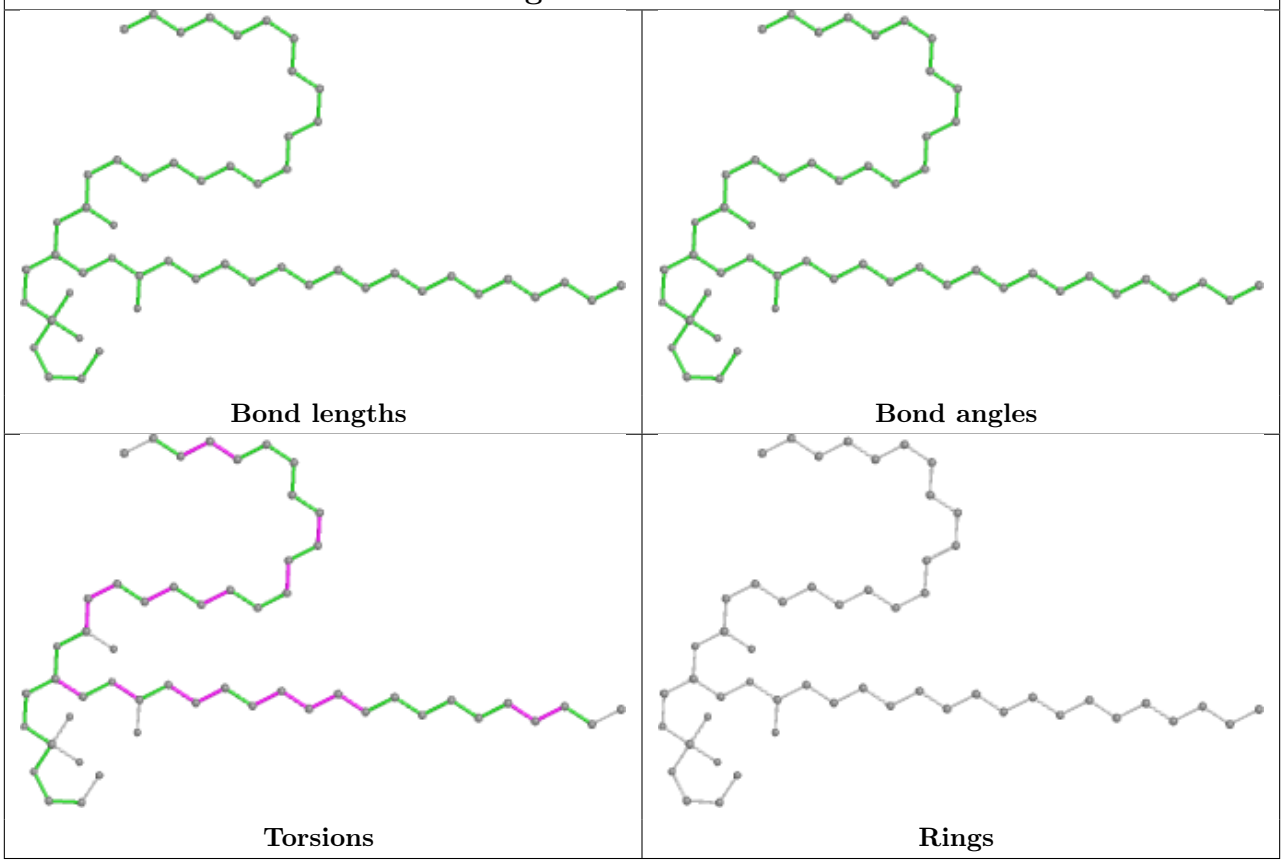
Ligand PSC O 302



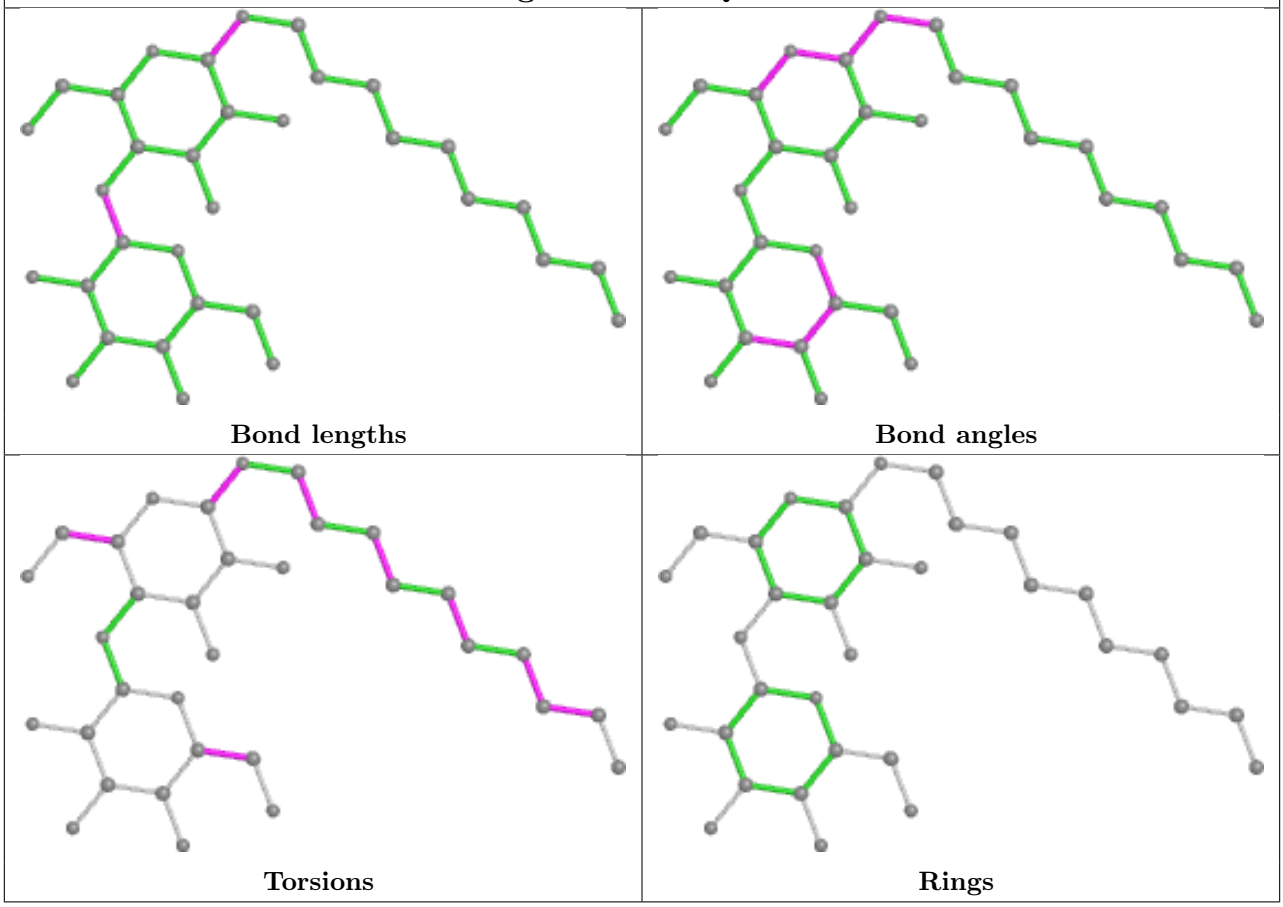
Ligand CHD J 102



Ligand PEK P 302



Ligand DMU Q 201



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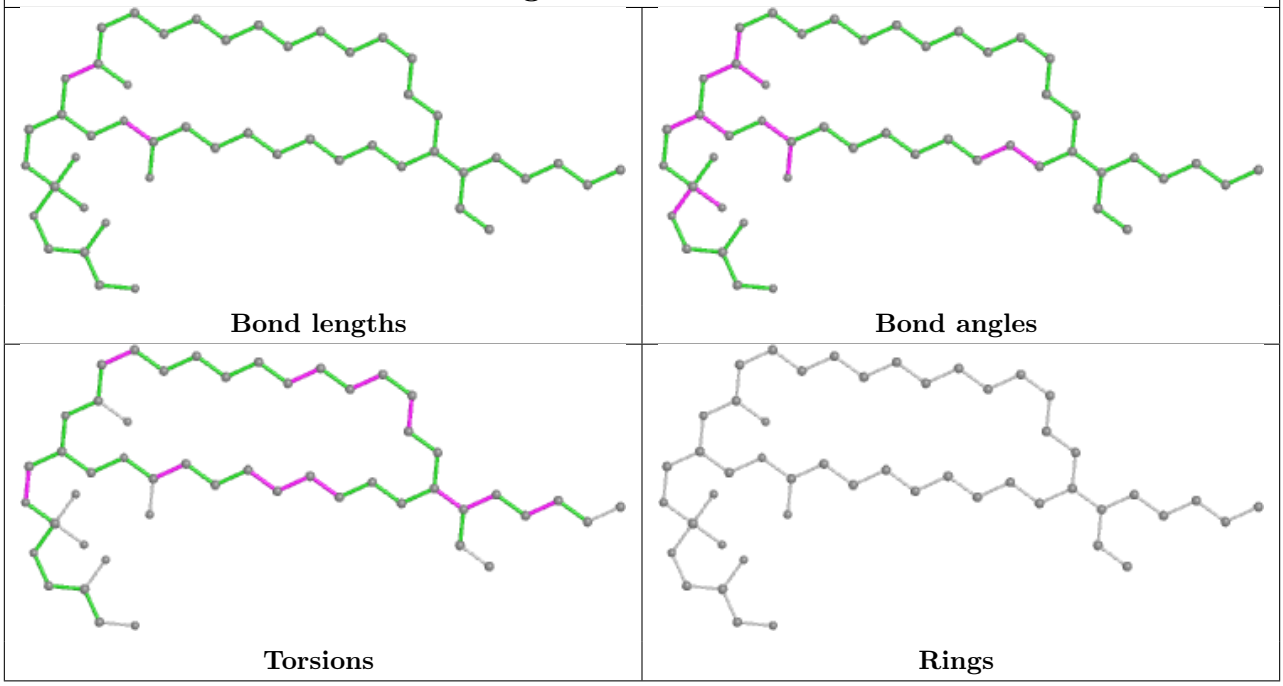

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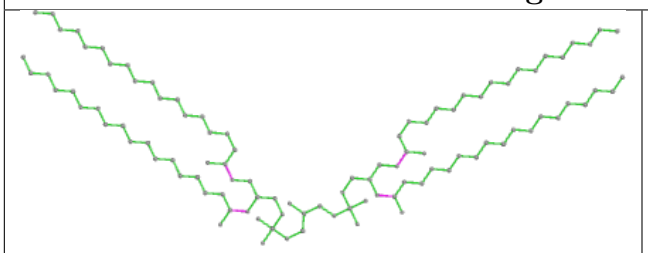
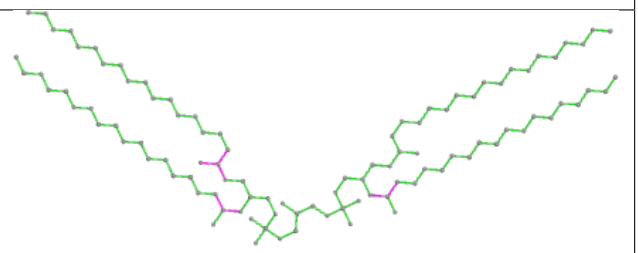
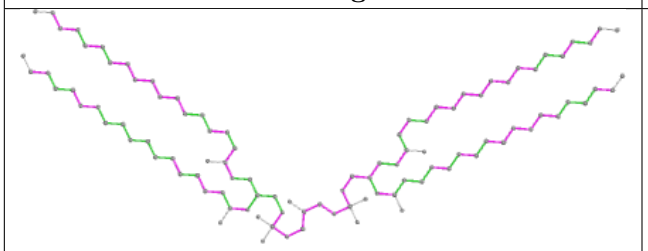


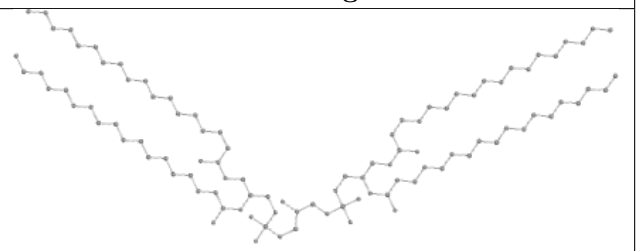
Bond lengths



Bond angles

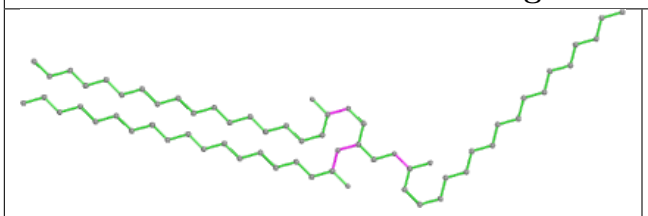


Torsions



Rings

Ligand TGL N 607



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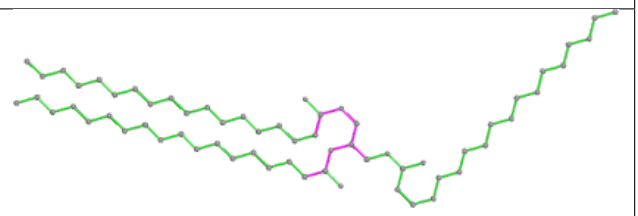
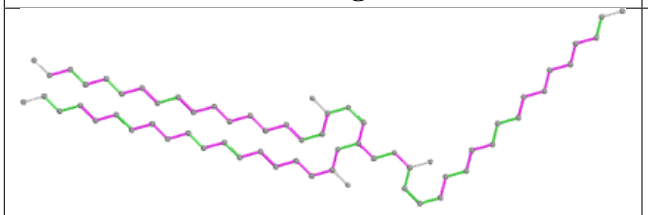


Bond angles



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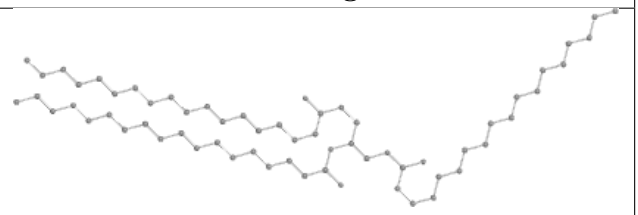
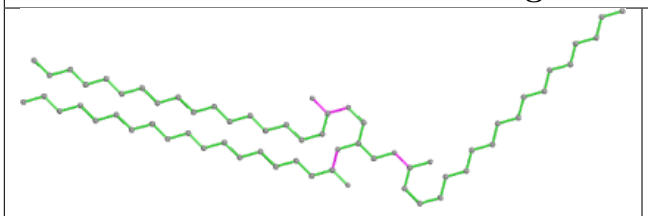


Rings

Ligand TGL B 303



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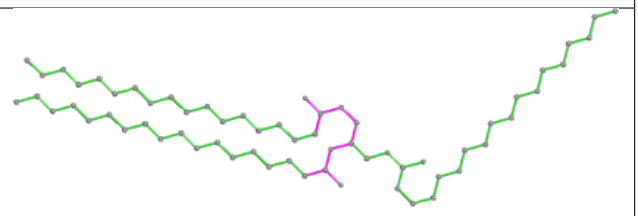
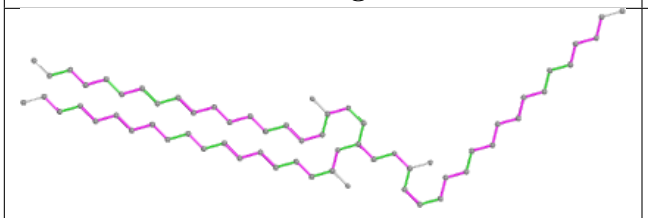


Bond angles



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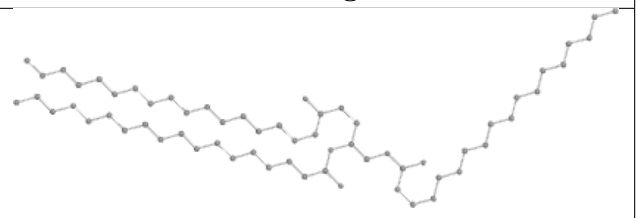
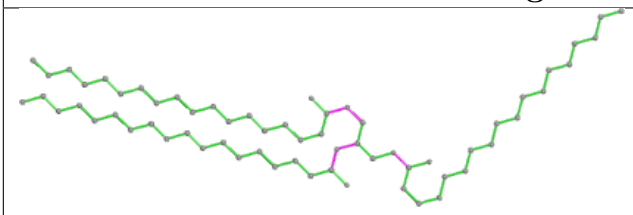


Rings

Ligand TGL L 101



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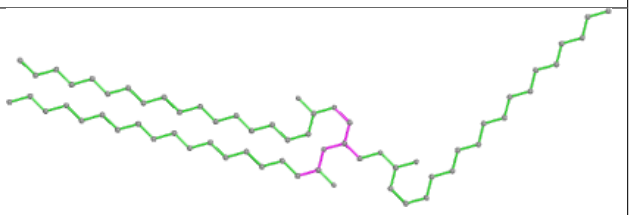

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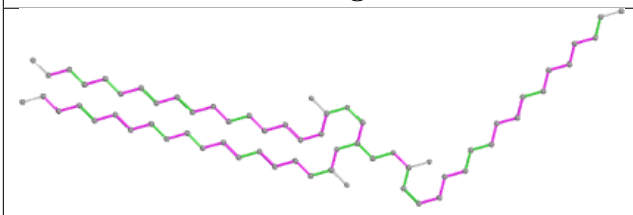

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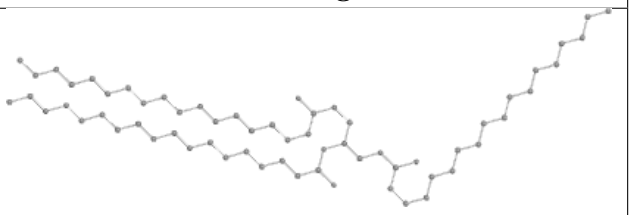
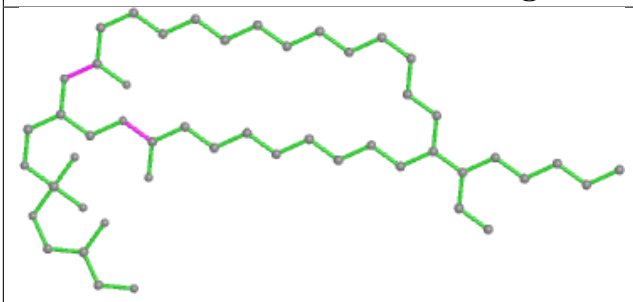


Rings

Ligand PGV U 101



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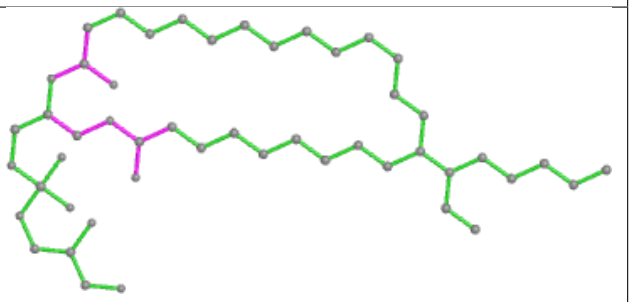
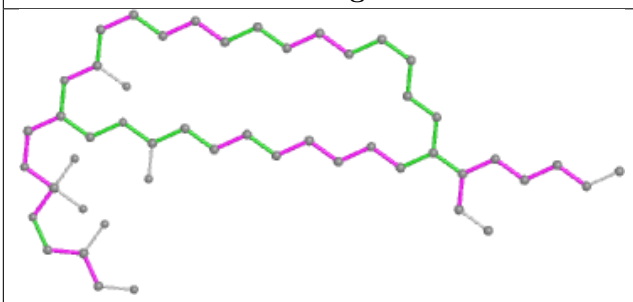
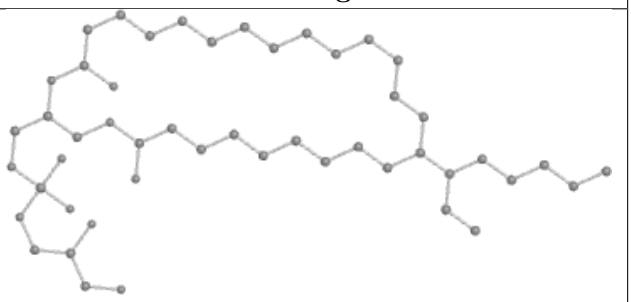


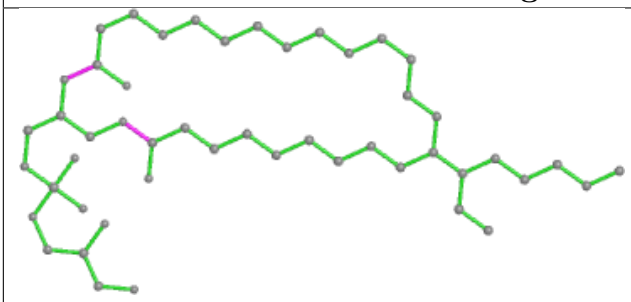
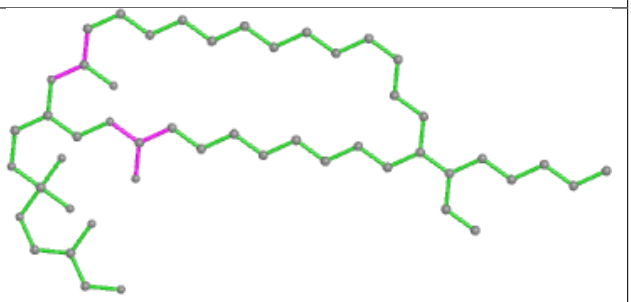
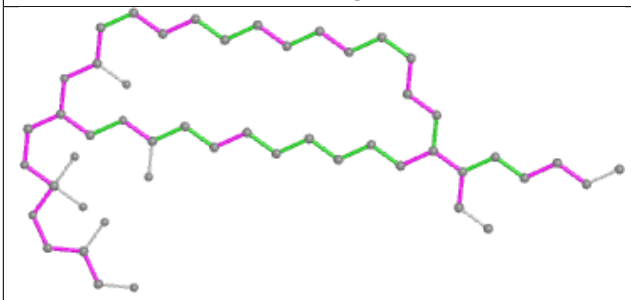
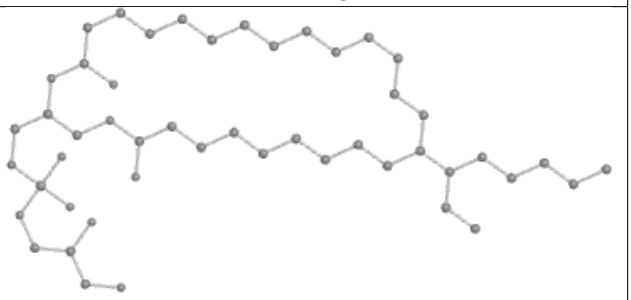
Bond angles

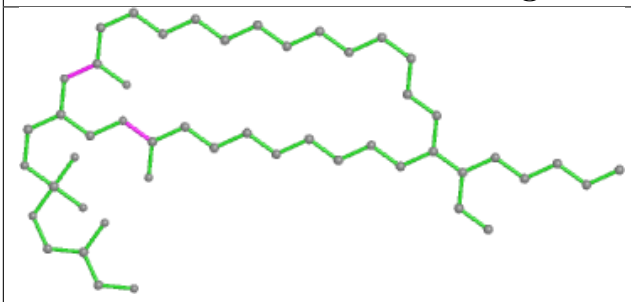
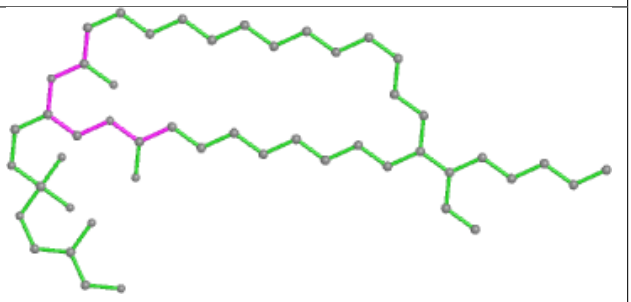
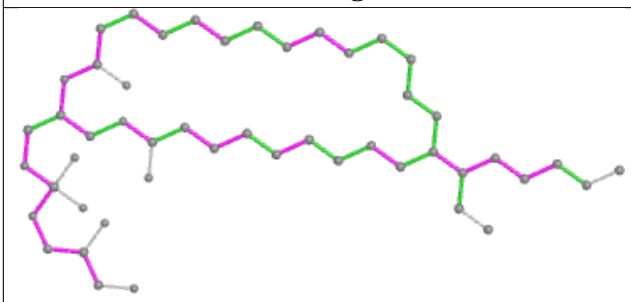
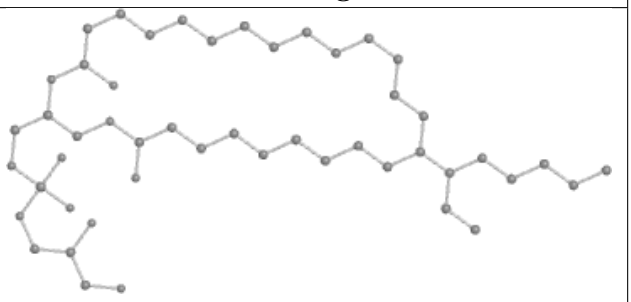


Torsions

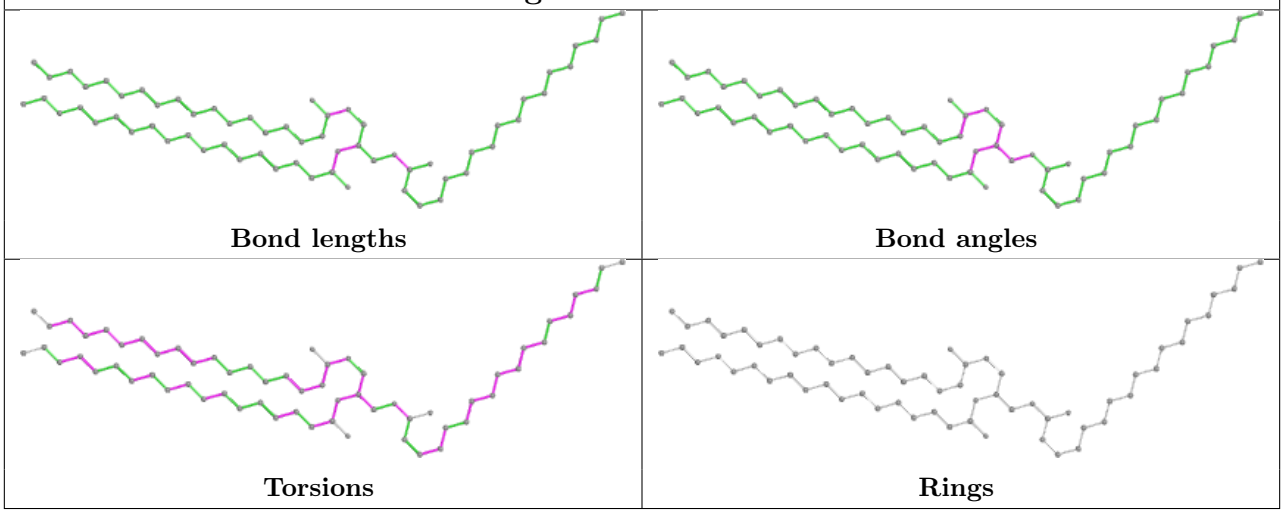


Rings

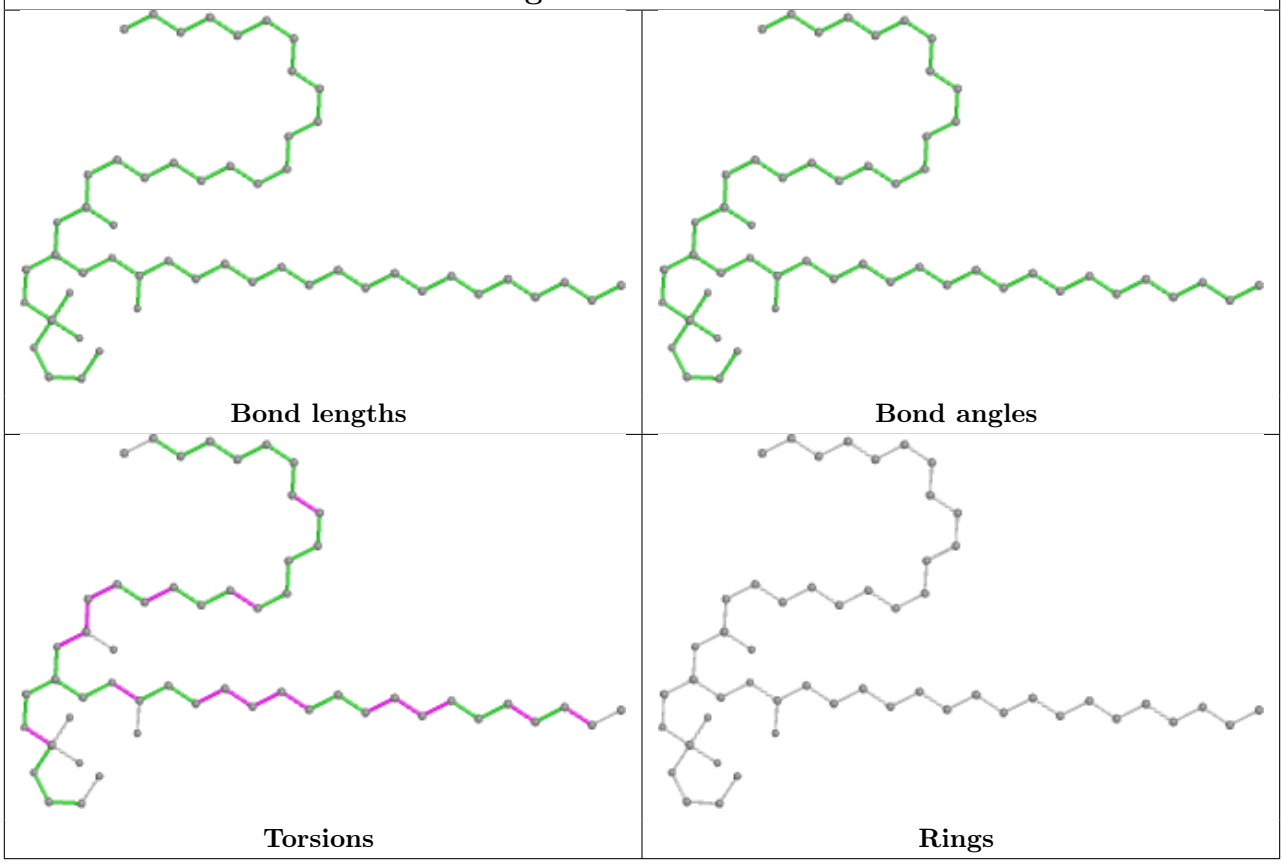
Ligand PGV N 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PGV A 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

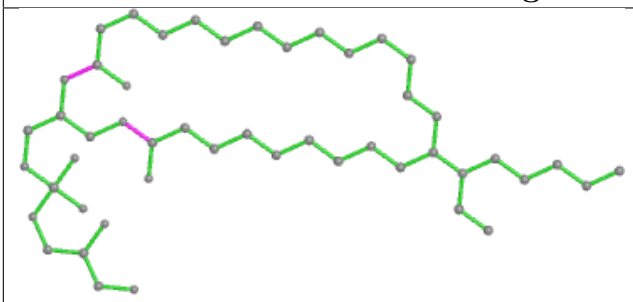
Ligand TGL A 609



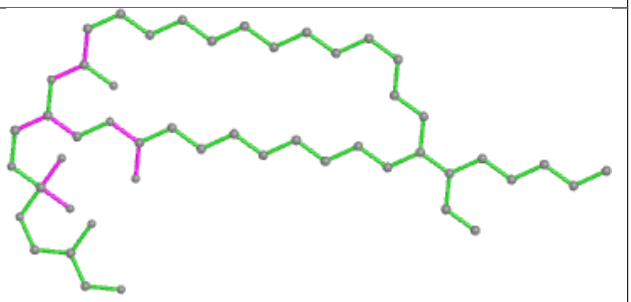
Ligand PEK P 303



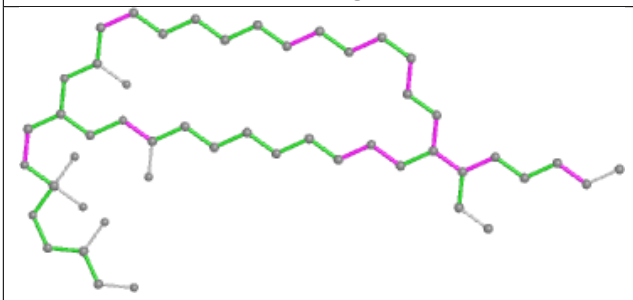
Ligand PGV P 304



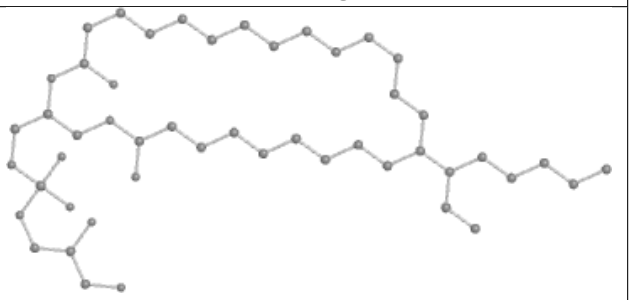
Bond lengths



Bond angles

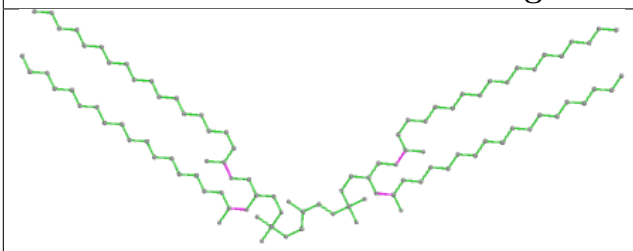


Torsions

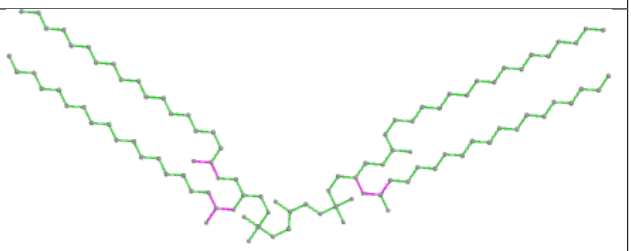


Rings

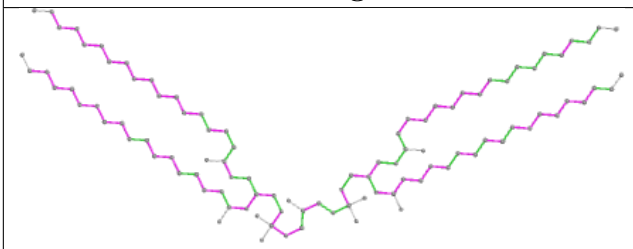
Ligand CDL P 305



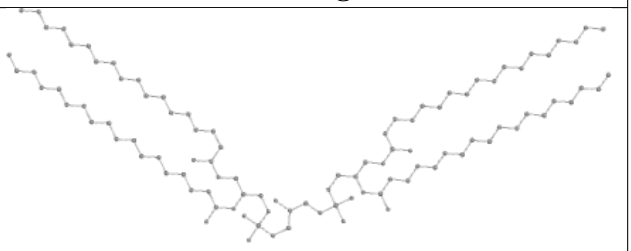
Bond lengths



Bond angles

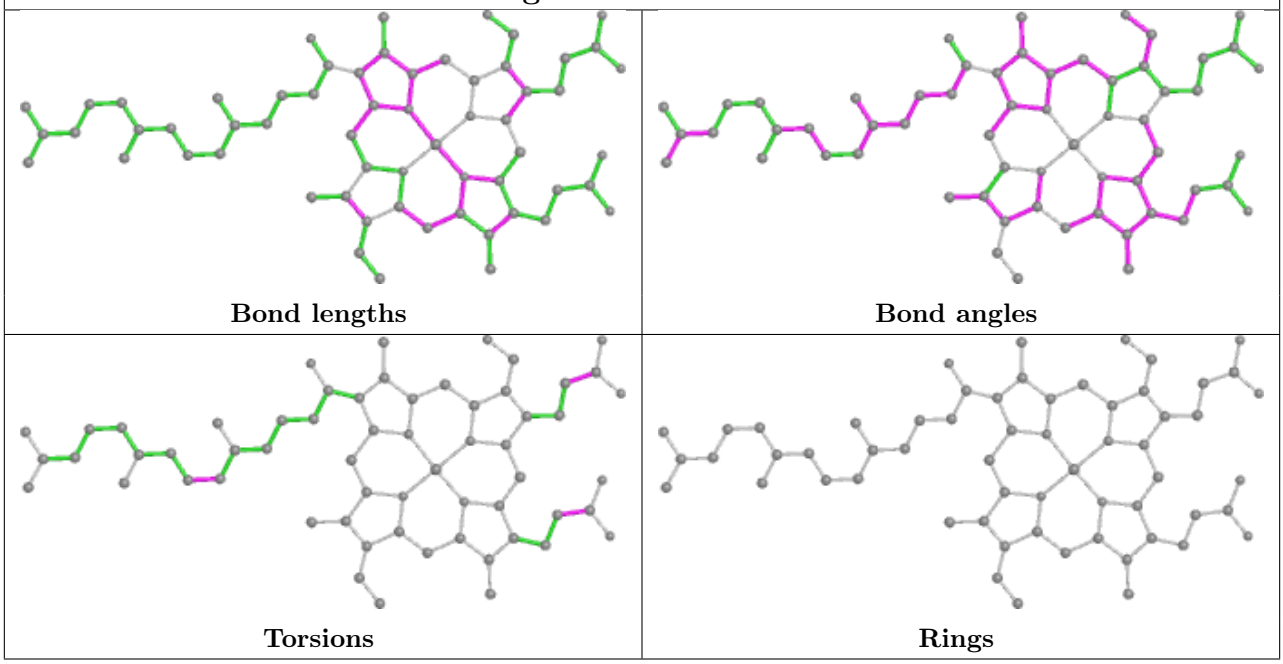


Torsions

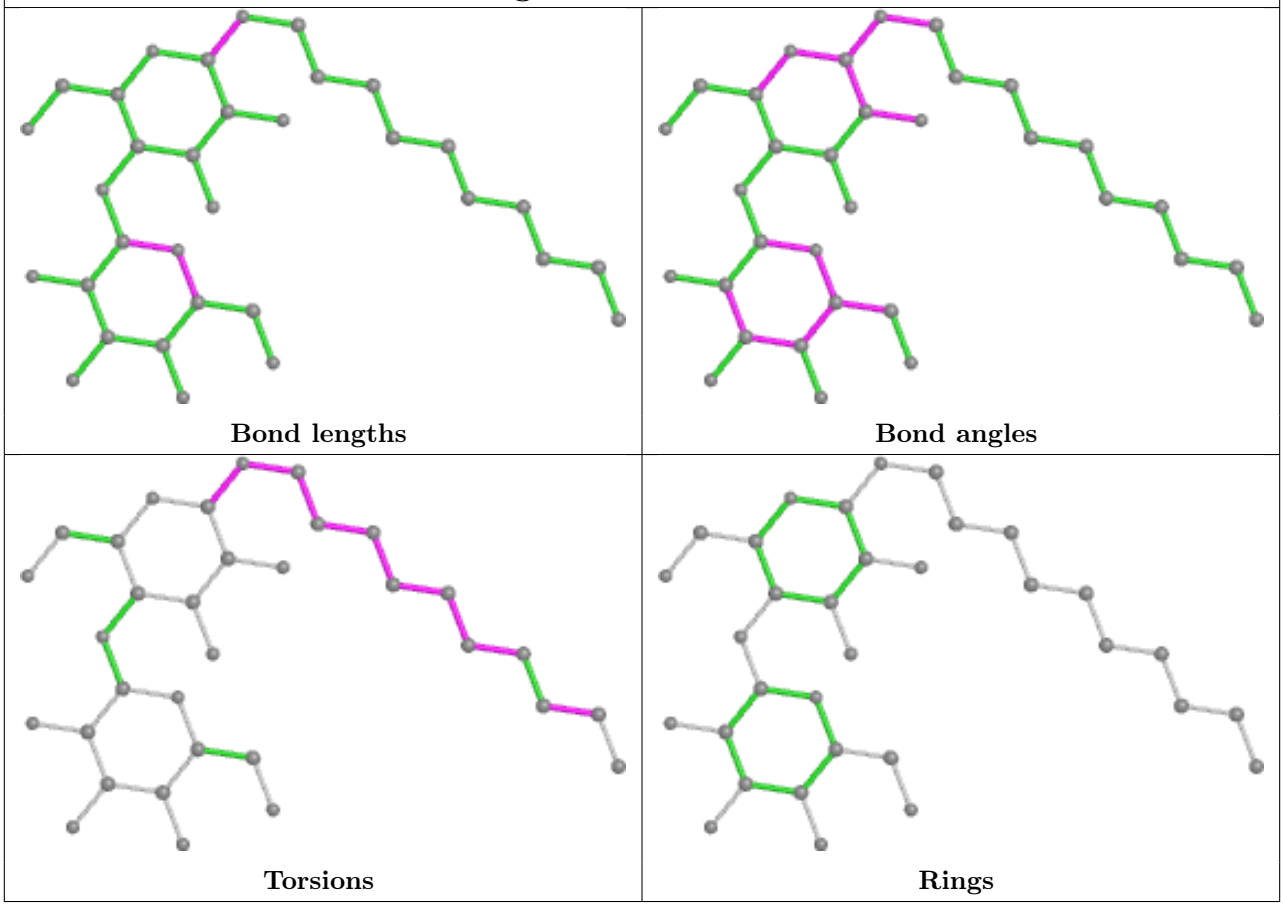


Rings

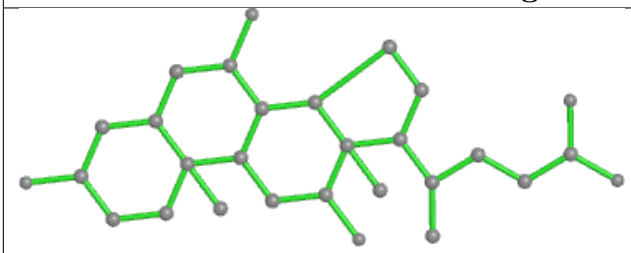
Ligand HEA A 604



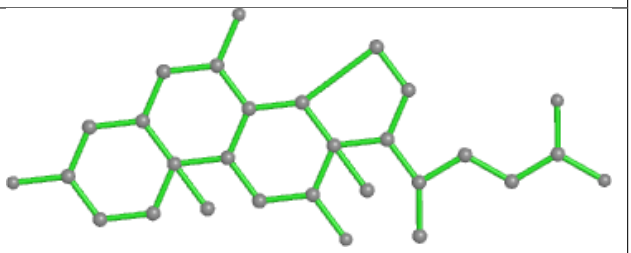
Ligand DMU M 101



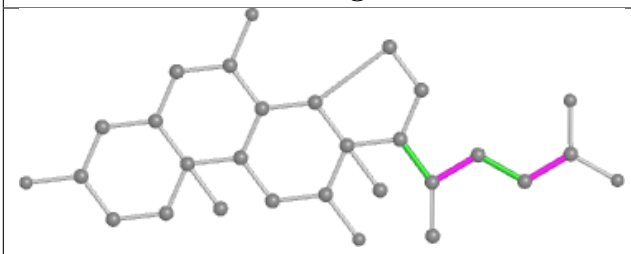
Ligand CHD B 304



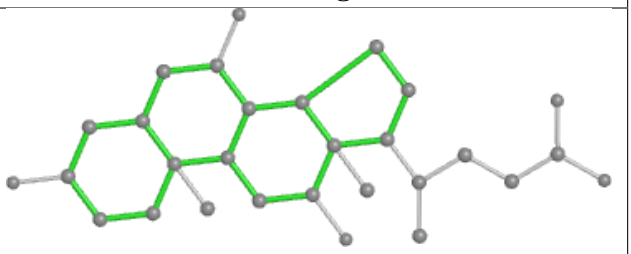
Bond lengths



Bond angles

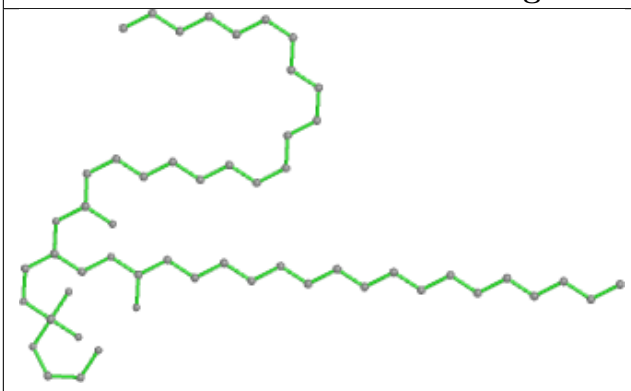


Torsions

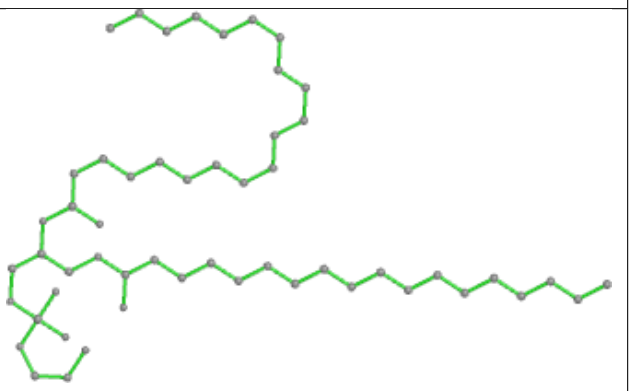


Rings

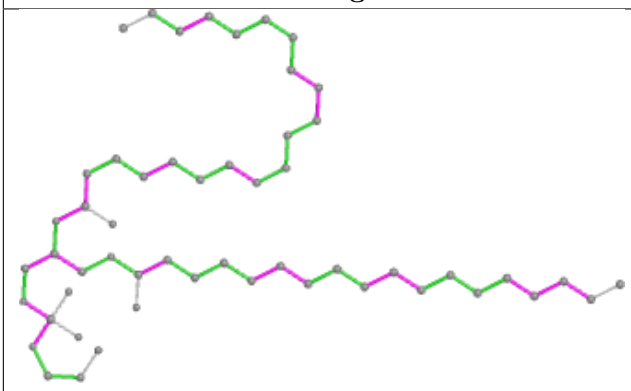
Ligand PEK C 302



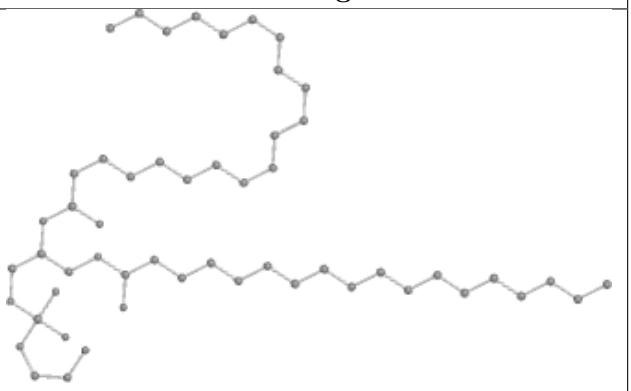
Bond lengths



Bond angles

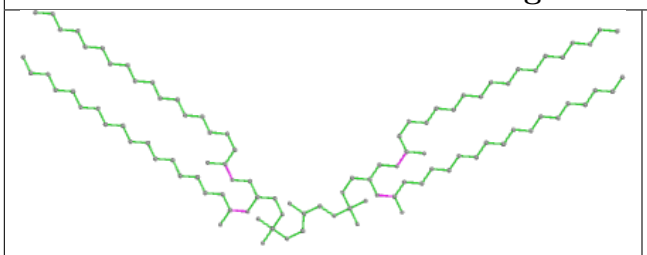


Torsions

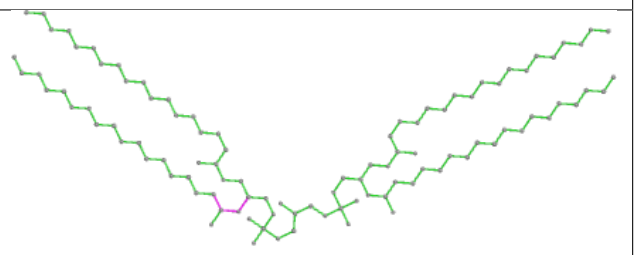


Rings

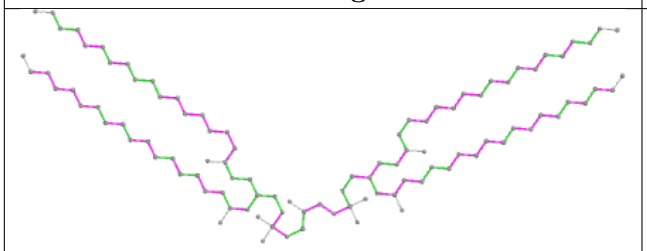
Ligand CDL N 601



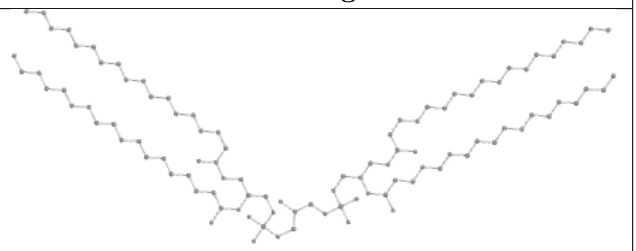
Bond lengths



Bond angles

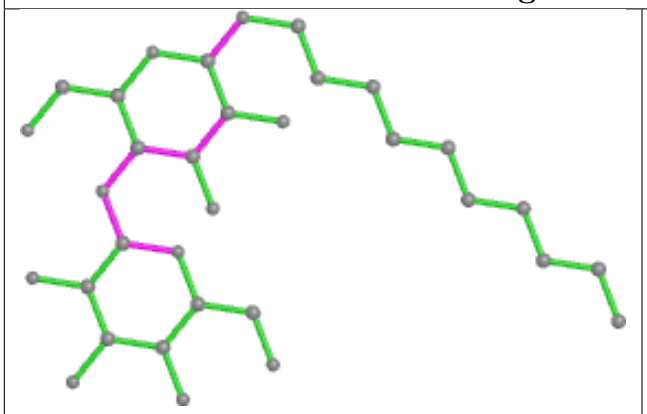


Torsions



Rings

Ligand DMU T 101



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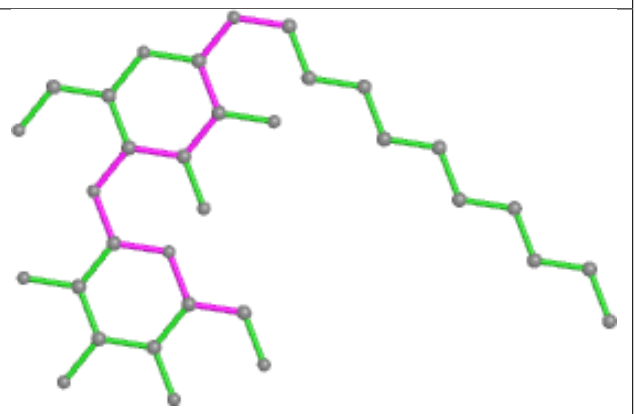
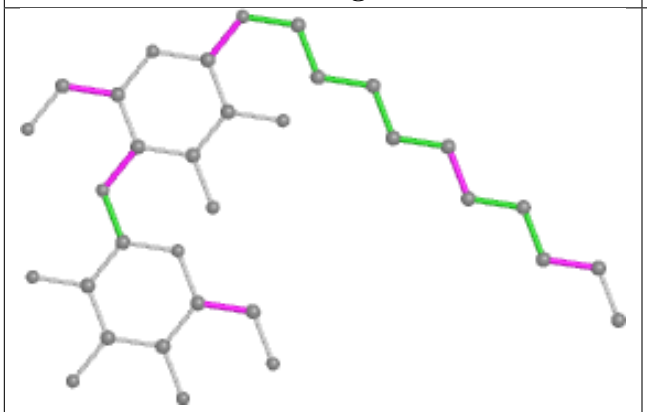
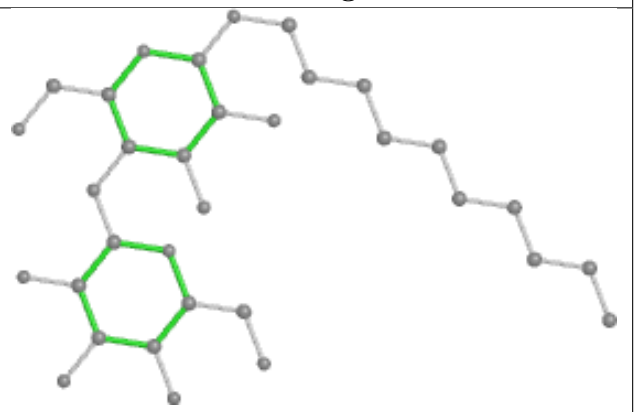


Bond angles

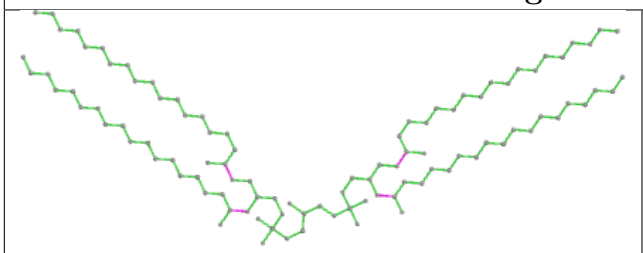


Torsions



Rings

Ligand CDL C 304



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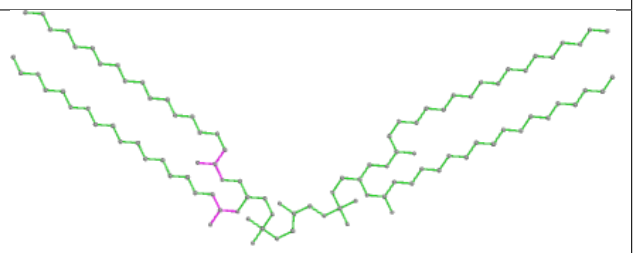
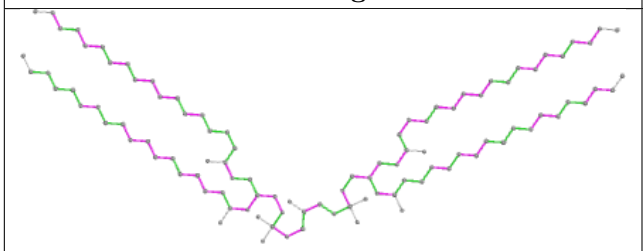
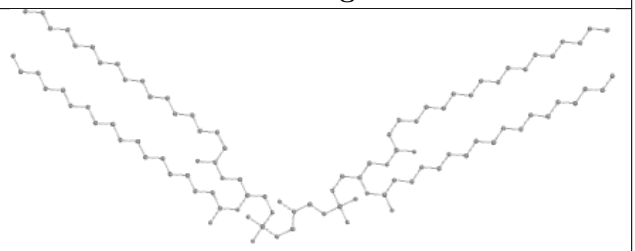


Bond angles

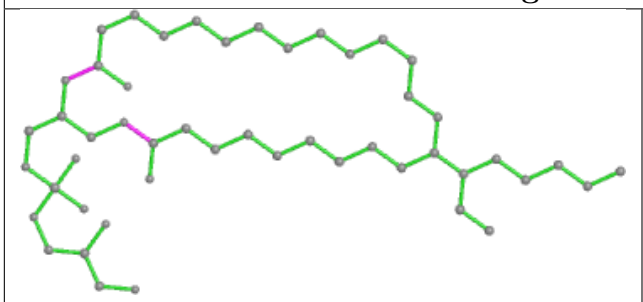


Torsions

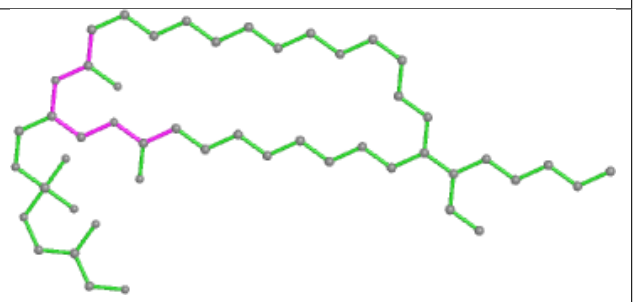


Rings

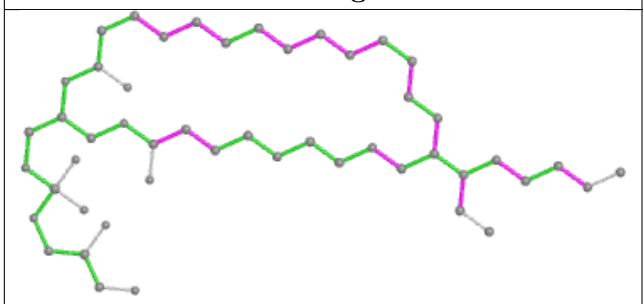
Ligand PGV N 608



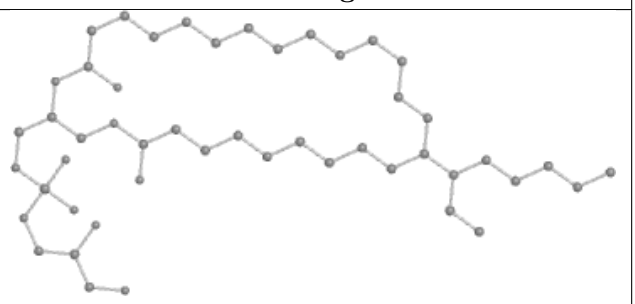
Bond lengths



Bond angles

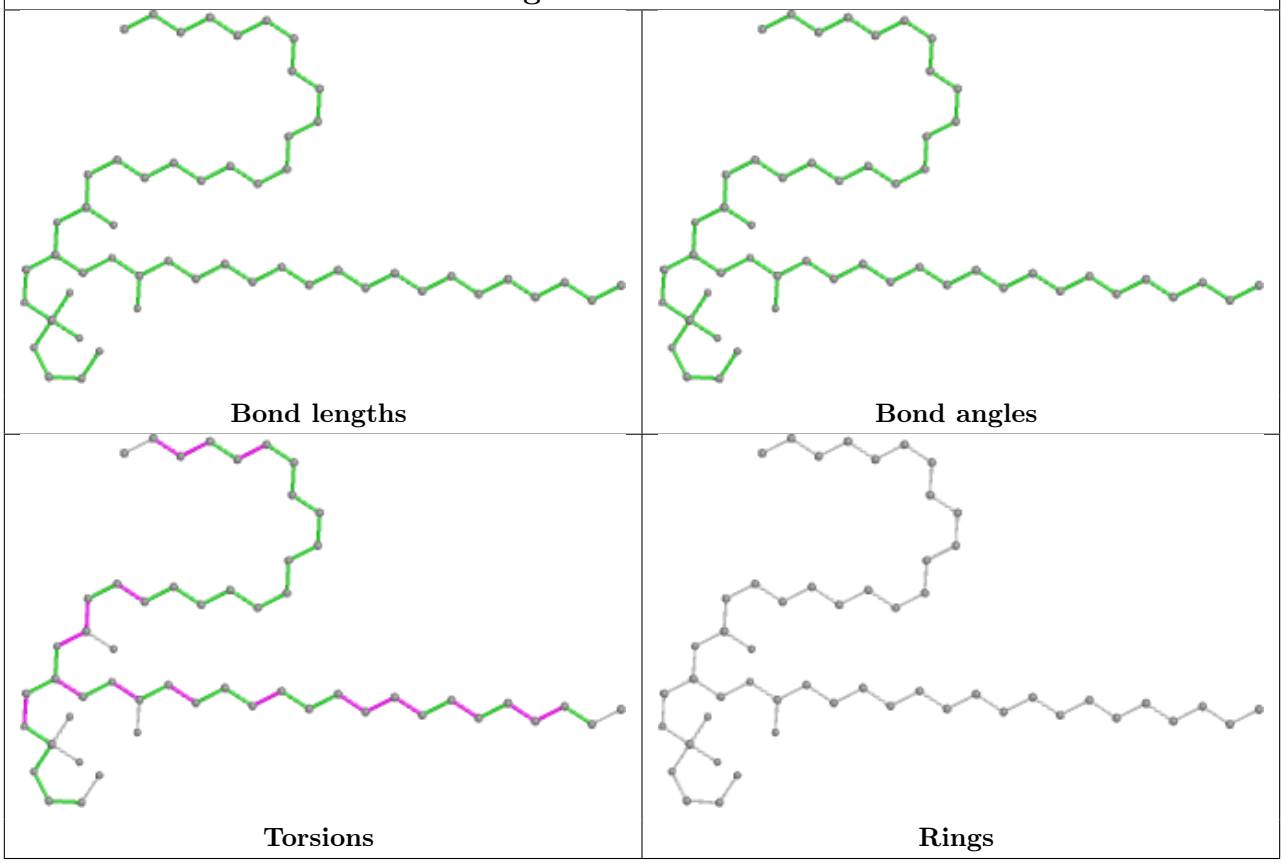


Torsions

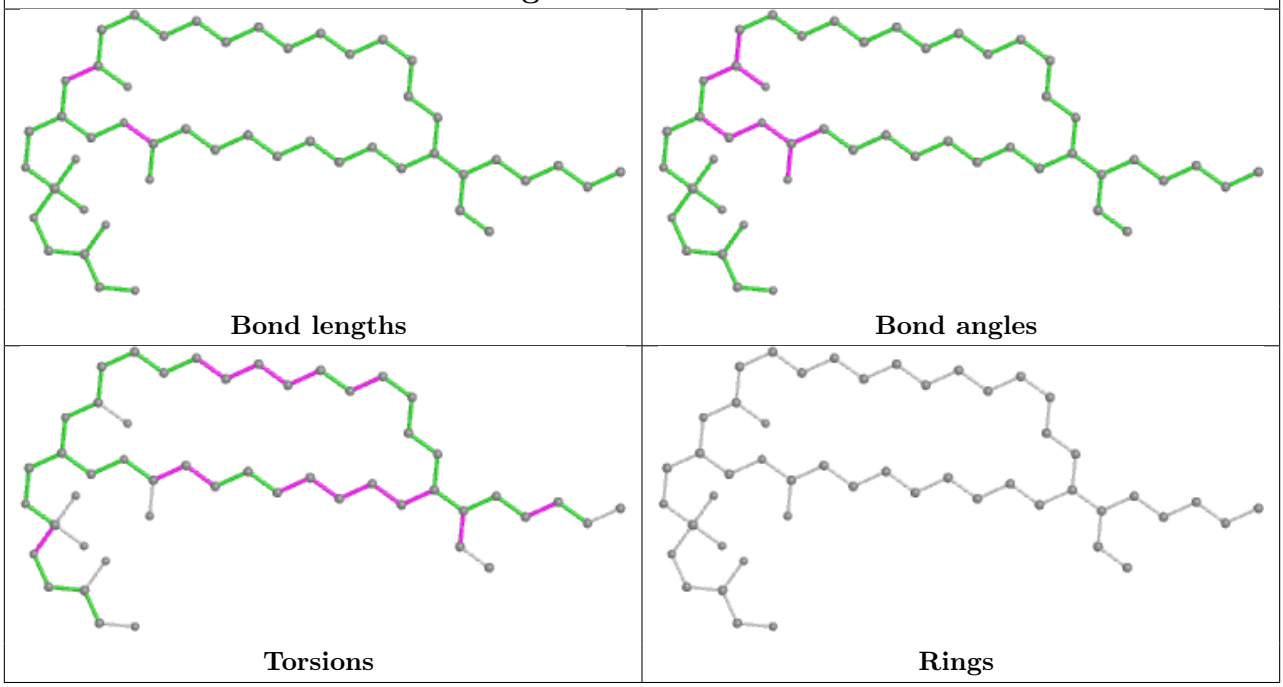


Rings

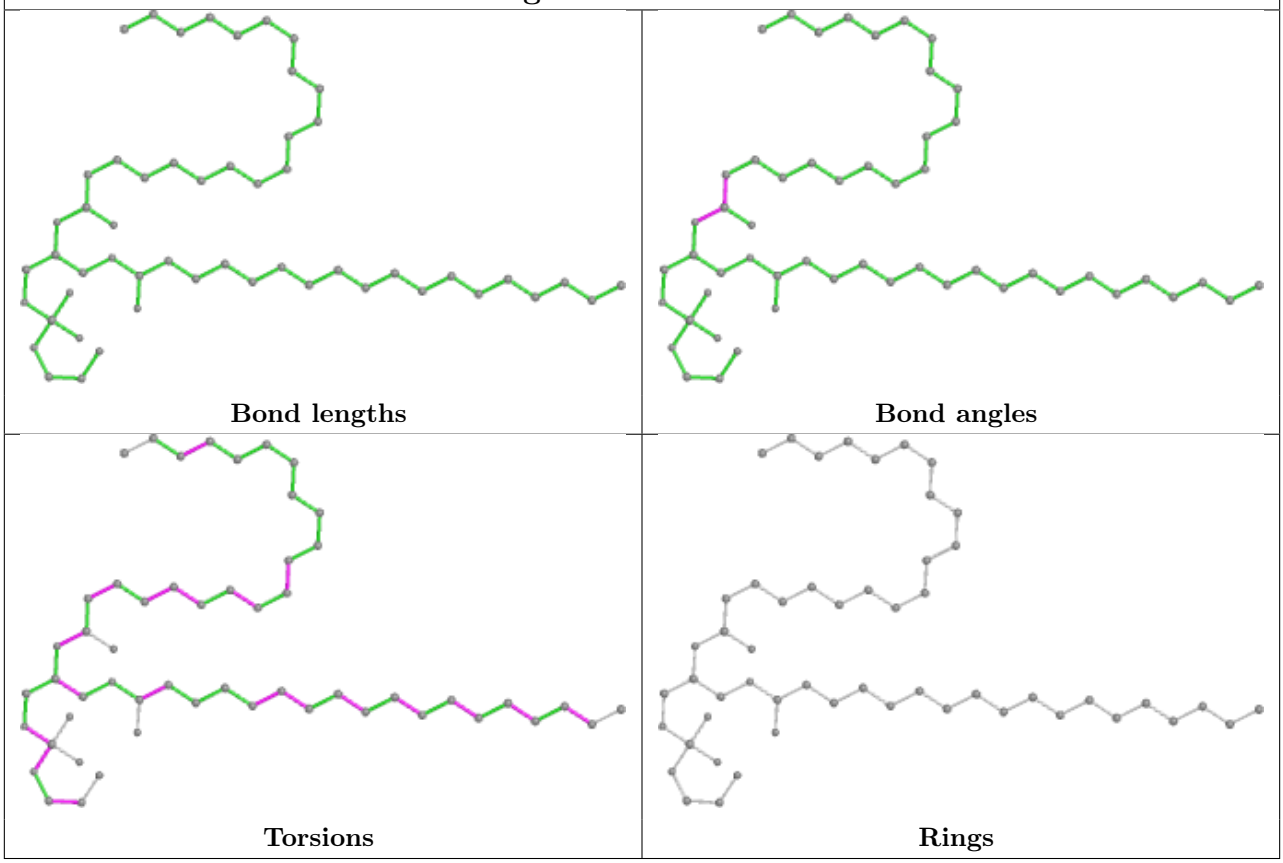
Ligand PEK G 102



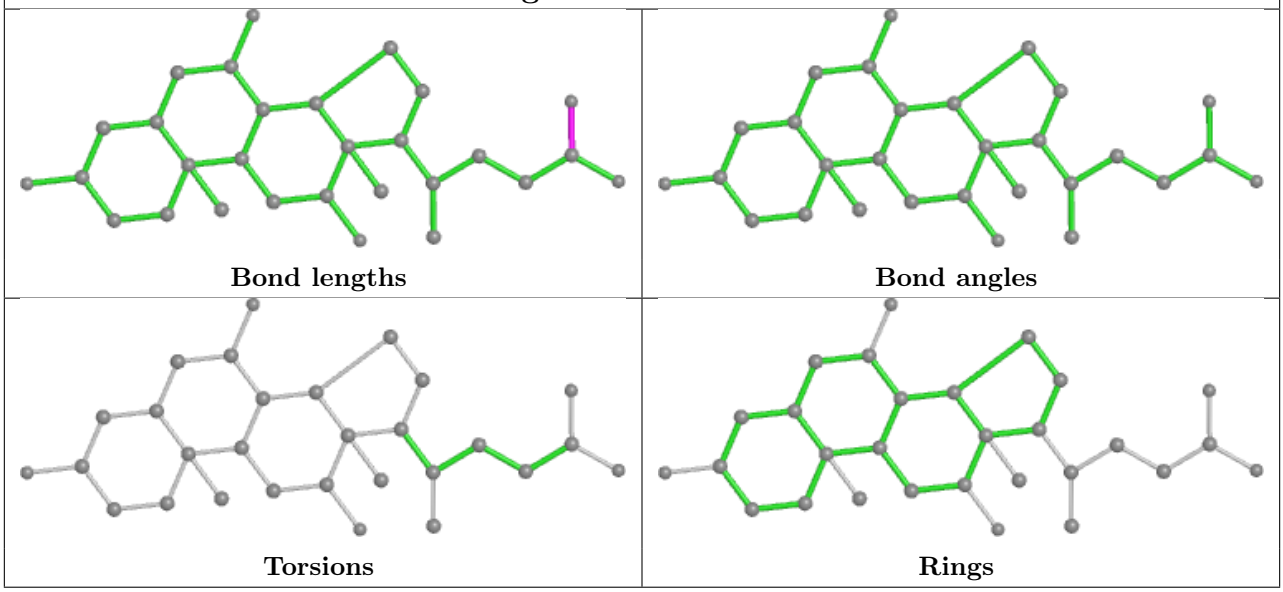
Ligand PGV A 607



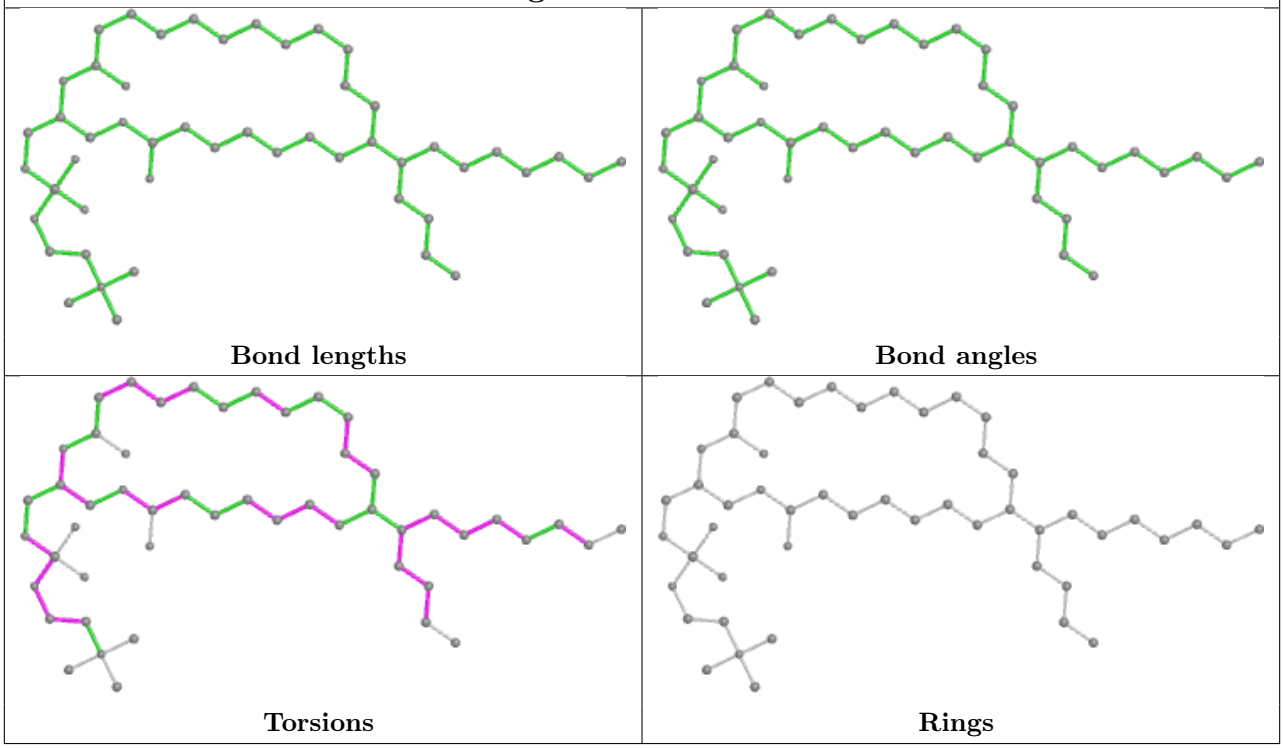
Ligand PEK G 103



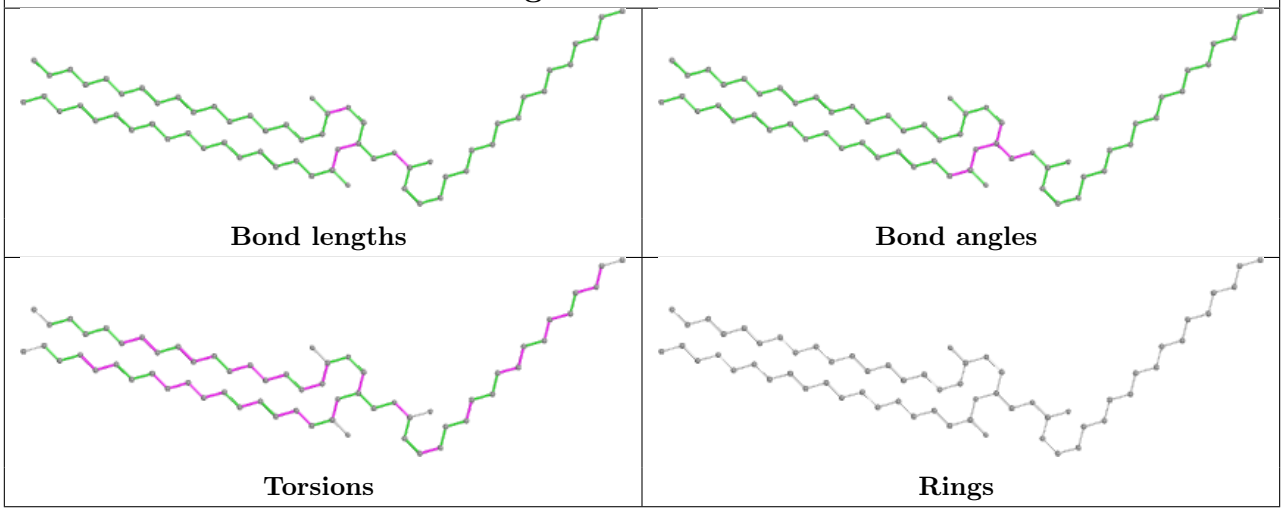
Ligand CHD C 301

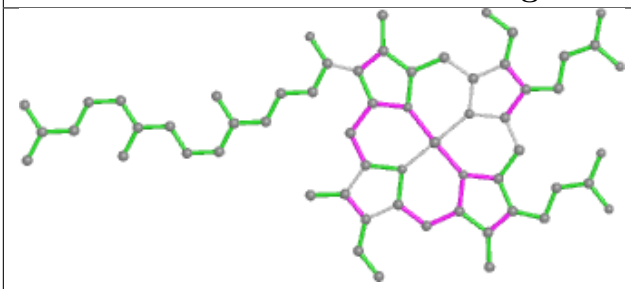
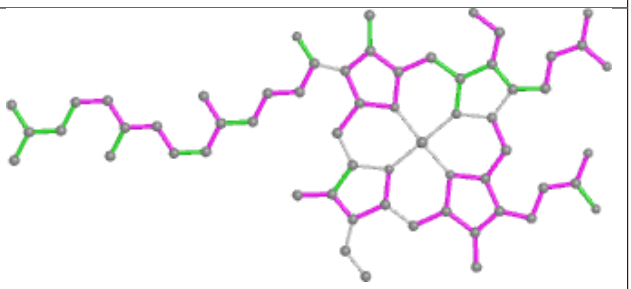
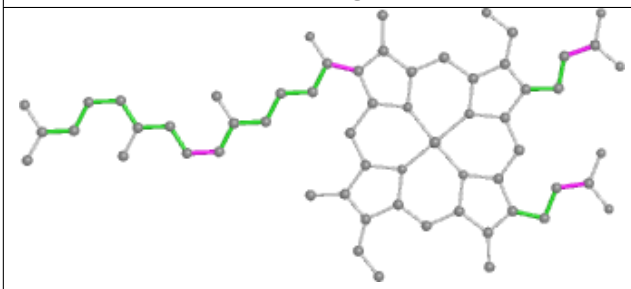
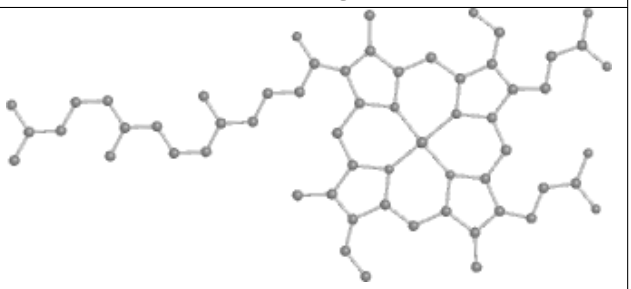


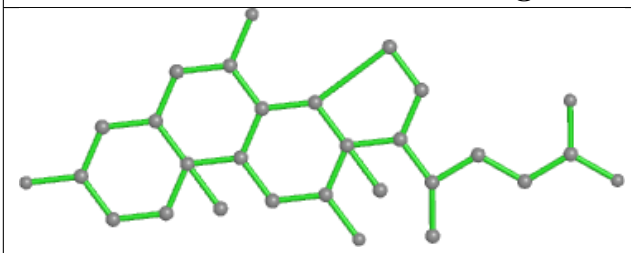
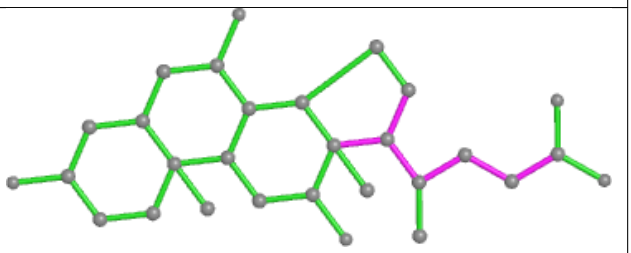
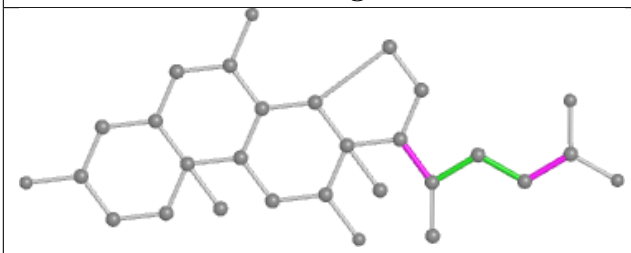
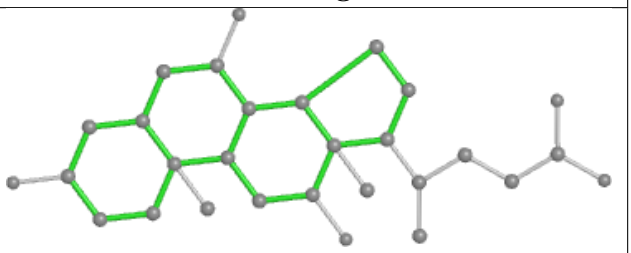
Ligand PSC B 302

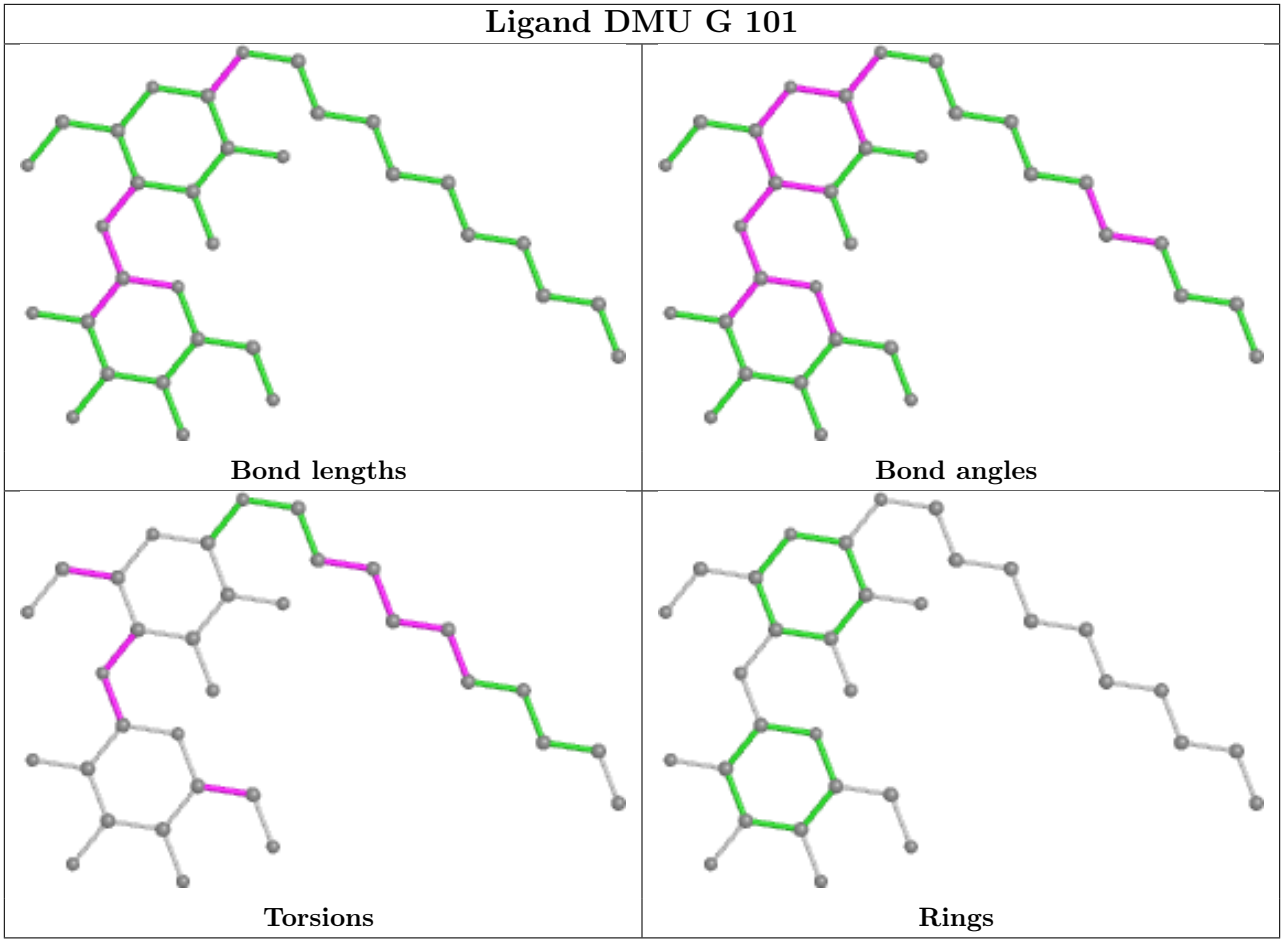


Ligand TGL Y 101



Ligand HEA N 605	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHD W 102	
 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%)	-1.12	0	100	100	35, 43, 55, 103	0
1	N	513/514 (99%)	-0.95	0	100	100	41, 57, 75, 129	0
2	B	226/227 (99%)	-0.83	2 (0%)	84	86	36, 50, 84, 158	0
2	O	226/227 (99%)	-0.46	6 (2%)	54	58	48, 70, 109, 160	0
3	C	259/261 (99%)	-0.97	0	100	100	39, 48, 66, 114	0
3	P	259/261 (99%)	-0.83	1 (0%)	92	93	45, 59, 86, 127	0
4	D	144/147 (97%)	-0.68	1 (0%)	87	89	43, 54, 81, 124	0
4	Q	139/147 (94%)	-0.01	8 (5%)	23	24	62, 86, 118, 135	0
5	E	105/109 (96%)	-0.68	2 (1%)	66	69	41, 54, 92, 147	0
5	R	105/109 (96%)	-0.36	2 (1%)	66	69	53, 73, 97, 152	0
6	F	96/98 (97%)	-0.37	5 (5%)	27	29	42, 55, 103, 145	0
6	S	94/98 (95%)	-0.24	5 (5%)	26	28	50, 70, 112, 153	0
7	G	83/85 (97%)	0.15	11 (13%)	3	2	44, 59, 156, 192	0
7	T	83/85 (97%)	0.25	11 (13%)	3	2	49, 74, 152, 192	0
8	H	78/85 (91%)	-0.29	4 (5%)	28	29	44, 59, 126, 160	0
8	U	79/85 (92%)	0.16	6 (7%)	13	14	51, 78, 144, 179	0
9	I	72/73 (98%)	-0.29	4 (5%)	24	25	50, 62, 95, 118	0
9	V	72/73 (98%)	0.17	8 (11%)	5	5	50, 82, 115, 137	0
10	J	58/59 (98%)	-0.19	2 (3%)	45	48	50, 62, 112, 160	0
10	W	58/59 (98%)	0.20	5 (8%)	10	10	64, 81, 124, 158	0
11	K	49/56 (87%)	-0.40	1 (2%)	65	68	41, 58, 78, 110	0
11	X	49/56 (87%)	0.27	2 (4%)	37	40	73, 86, 109, 144	0
12	L	46/47 (97%)	-0.78	2 (4%)	35	38	41, 49, 78, 137	0
12	Y	46/47 (97%)	-0.29	2 (4%)	35	38	56, 80, 108, 144	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	43/46 (93%)	-0.53	2 (4%) 31 33	44, 51, 89, 143	0
13	Z	43/46 (93%)	0.34	5 (11%) 4 4	67, 81, 126, 158	0
All	All	3538/3614 (97%)	-0.60	97 (2%) 54 58	35, 58, 105, 192	0

The worst 5 of 97 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	G	40	GLY	13.8
13	Z	43	SER	8.6
7	T	10	GLY	8.3
7	T	40	GLY	8.1
7	T	8	HIS	7.8

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	SAC	V	1	9/10	0.40	0.78	140,158,175,179	0
7	TPO	G	11	11/12	0.67	0.40	116,142,176,188	0
9	SAC	I	1	9/10	0.69	0.60	128,141,151,154	0
7	TPO	T	11	11/12	0.79	0.35	139,157,180,188	0
1	FME	N	1	10/11	0.87	0.29	89,103,132,152	0
1	FME	A	1	10/11	0.94	0.17	69,80,105,120	0
2	FME	O	1	10/11	0.95	0.12	59,73,86,88	0
2	FME	B	1	10/11	0.97	0.11	48,54,56,64	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	PEK	G	103	53/53	0.62	0.28	78,133,201,215	0
28	DMU	T	101	33/33	0.66	0.29	117,166,199,205	0
25	PEK	P	303	53/53	0.69	0.25	78,129,162,178	0
18	PGV	N	610	51/51	0.70	0.29	67,113,153,166	0
26	CDL	T	103	100/100	0.72	0.22	86,134,181,206	0
25	PEK	C	302	53/53	0.72	0.23	80,123,194,208	0
23	PSC	B	302	52/52	0.74	0.27	78,132,259,284	0
18	PGV	A	608	51/51	0.74	0.28	76,120,154,156	0
18	PGV	U	101	51/51	0.75	0.28	75,119,151,156	0
19	TGL	N	609	63/63	0.76	0.21	91,125,149,159	0
25	PEK	T	102	53/53	0.76	0.24	72,147,234,241	0
28	DMU	G	101	33/33	0.77	0.27	101,139,187,198	0
19	TGL	A	609	63/63	0.77	0.20	75,106,129,133	0
23	PSC	O	302	52/52	0.78	0.25	73,139,232,252	0
24	CHD	W	102	29/29	0.78	0.26	98,143,157,162	0
18	PGV	A	606	51/51	0.78	0.22	53,107,152,185	0
26	CDL	N	601	100/100	0.81	0.18	90,125,171,189	0
19	TGL	Y	101	63/63	0.81	0.21	74,117,173,182	0
26	CDL	P	305	100/100	0.82	0.22	54,129,159,162	0
24	CHD	J	102	29/29	0.82	0.19	97,115,137,144	0
26	CDL	C	304	100/100	0.83	0.22	59,124,167,174	0
28	DMU	Q	201	33/33	0.84	0.18	96,111,126,131	0
19	TGL	N	607	63/63	0.86	0.18	53,109,152,162	0
19	TGL	L	101	63/63	0.87	0.17	58,95,149,160	0
19	TGL	B	303	63/63	0.88	0.18	47,99,151,158	0
24	CHD	J	101	29/29	0.89	0.17	89,107,119,123	0
24	CHD	W	101	29/29	0.89	0.18	102,115,125,128	0
28	DMU	M	101	33/33	0.91	0.12	56,65,83,87	0
16	NA	N	604	1/1	0.92	0.17	62,62,62,62	0
24	CHD	P	301	29/29	0.94	0.10	51,58,61,64	0
25	PEK	G	102	53/53	0.95	0.13	40,83,126,143	0
25	PEK	P	302	53/53	0.95	0.14	54,94,153,177	0
24	CHD	C	301	29/29	0.96	0.09	41,48,54,61	0
24	CHD	G	104	29/29	0.96	0.09	45,52,60,66	0
15	MG	N	603	1/1	0.96	0.04	55,55,55,55	0
18	PGV	C	303	51/51	0.97	0.10	38,54,123,140	0
18	PGV	P	304	51/51	0.97	0.11	45,59,172,183	0
24	CHD	B	304	29/29	0.97	0.08	46,50,60,66	0
18	PGV	N	608	51/51	0.97	0.09	43,73,91,94	0
17	HEA	N	606	60/60	0.98	0.08	42,46,56,60	0
16	NA	A	603	1/1	0.98	0.04	45,45,45,45	0
18	PGV	A	607	51/51	0.98	0.09	32,68,86,90	0

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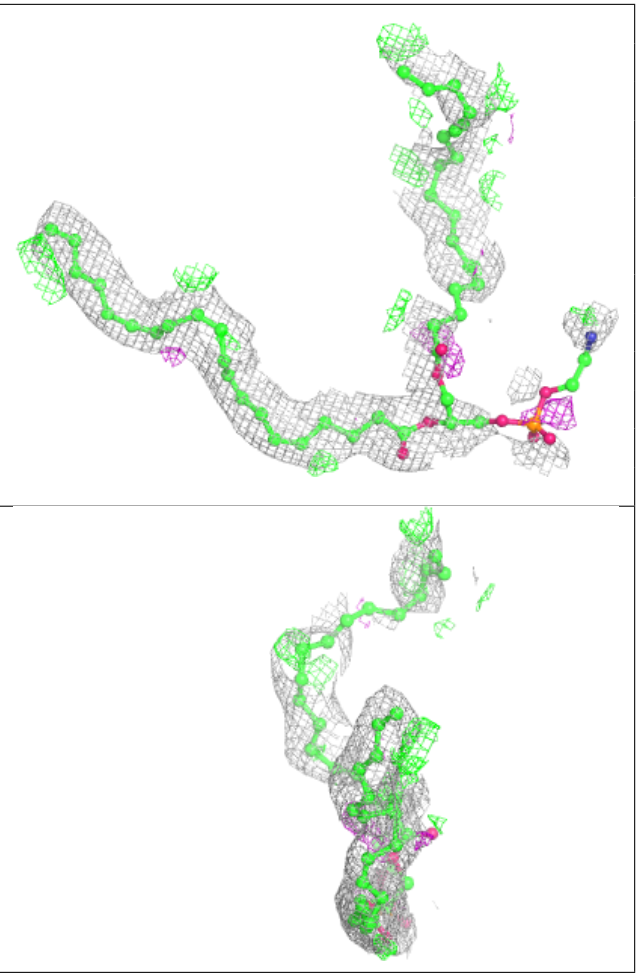
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	CUA	O	301	2/2	0.98	0.04	59,59,59,61	0
17	HEA	A	604	60/60	0.98	0.07	32,39,75,81	0
17	HEA	A	605	60/60	0.98	0.07	32,39,51,55	0
17	HEA	N	605	60/60	0.98	0.08	45,56,74,86	0
15	MG	A	602	1/1	0.99	0.05	38,38,38,38	0
14	CU	A	601	1/1	0.99	0.02	46,46,46,46	0
22	CUA	B	301	2/2	0.99	0.03	42,42,42,45	0
27	ZN	F	101	1/1	0.99	0.02	58,58,58,58	0
20	O	N	611	1/1	1.00	0.05	50,50,50,50	0
27	ZN	S	101	1/1	1.00	0.01	64,64,64,64	0
21	OH	A	611	1/1	1.00	0.06	44,44,44,44	0
21	OH	N	612	1/1	1.00	0.05	64,64,64,64	0
14	CU	N	602	1/1	1.00	0.02	58,58,58,58	0
20	O	A	610	1/1	1.00	0.03	35,35,35,35	0

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

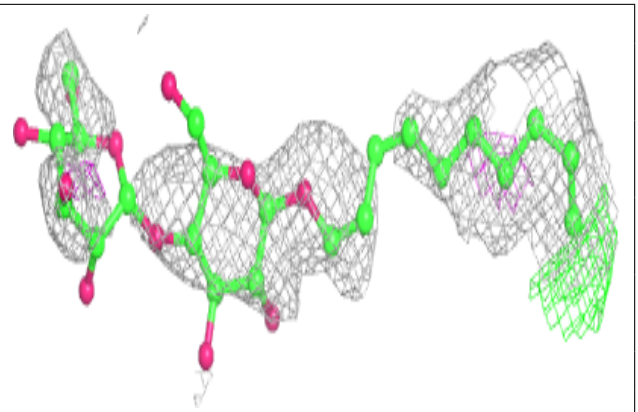
Electron density around PEK G 103:

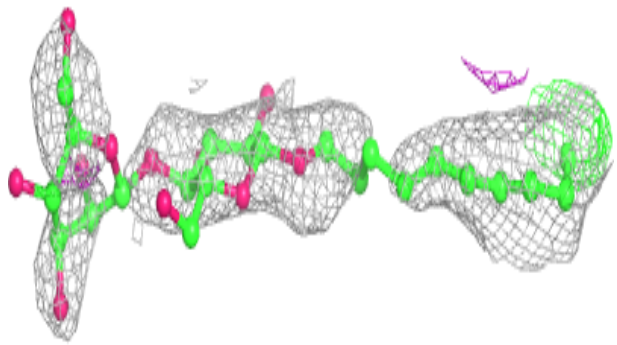
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

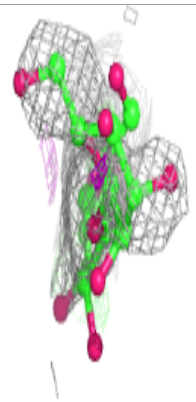


Electron density around DMU T 101:

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

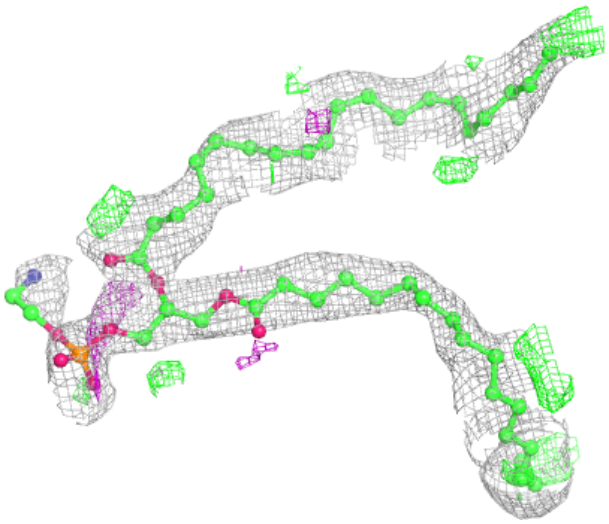


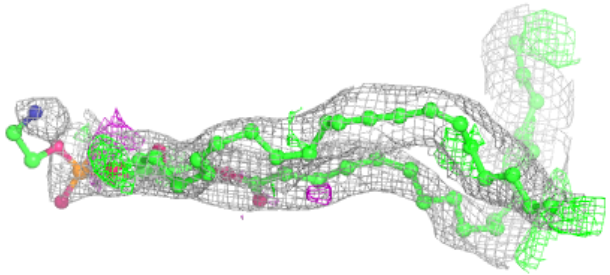


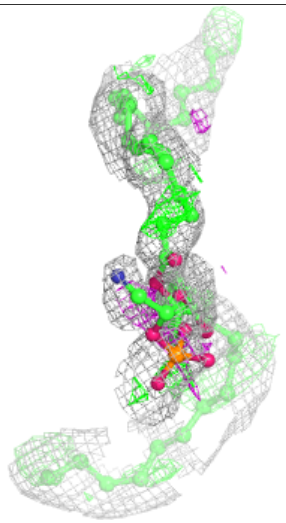


Electron density around PEK P 303:

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

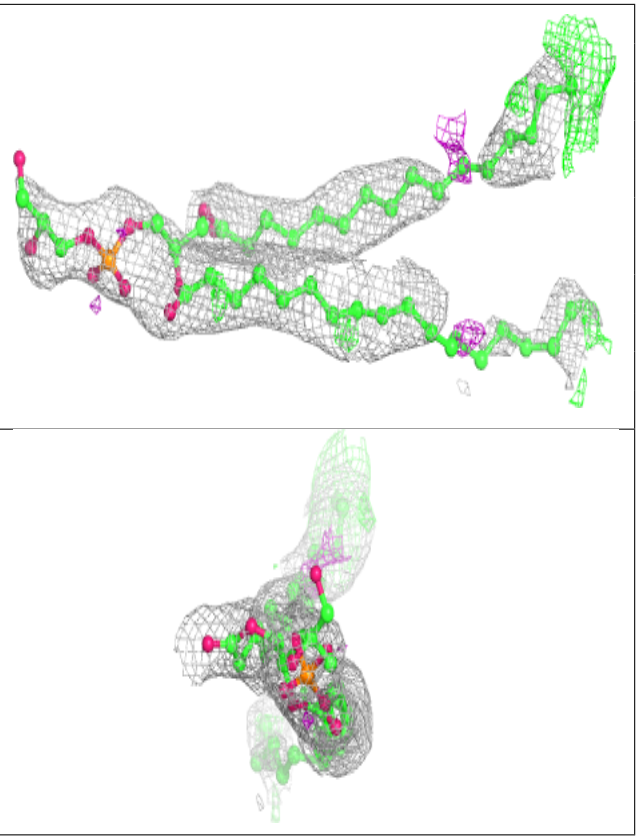






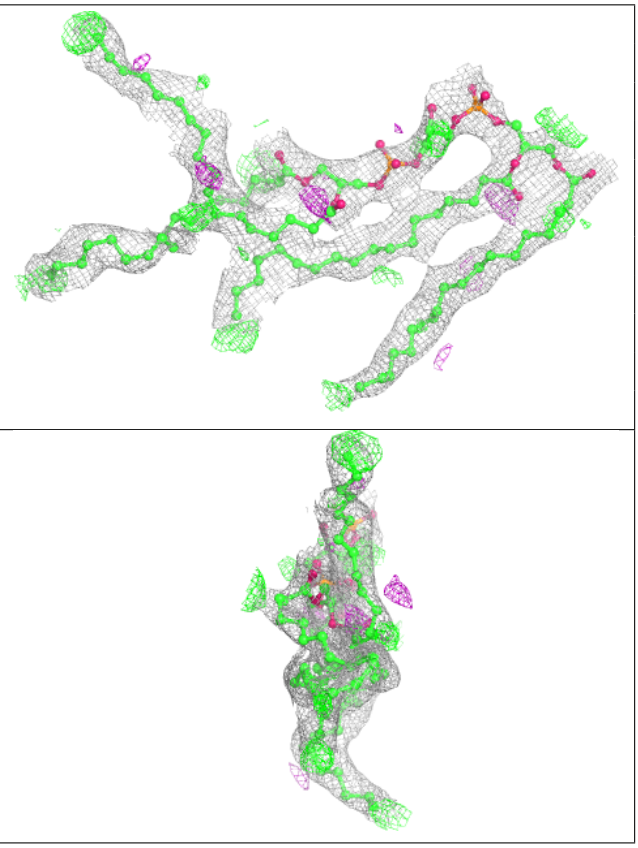
Electron density around PGV N 610:

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



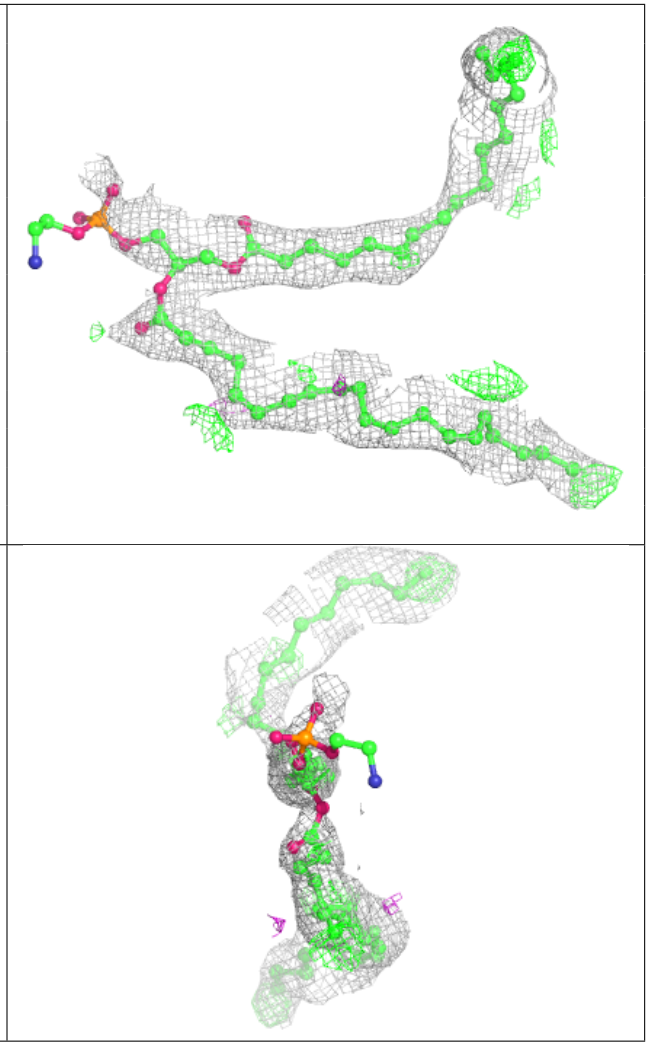
Electron density around CDL T 103:

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



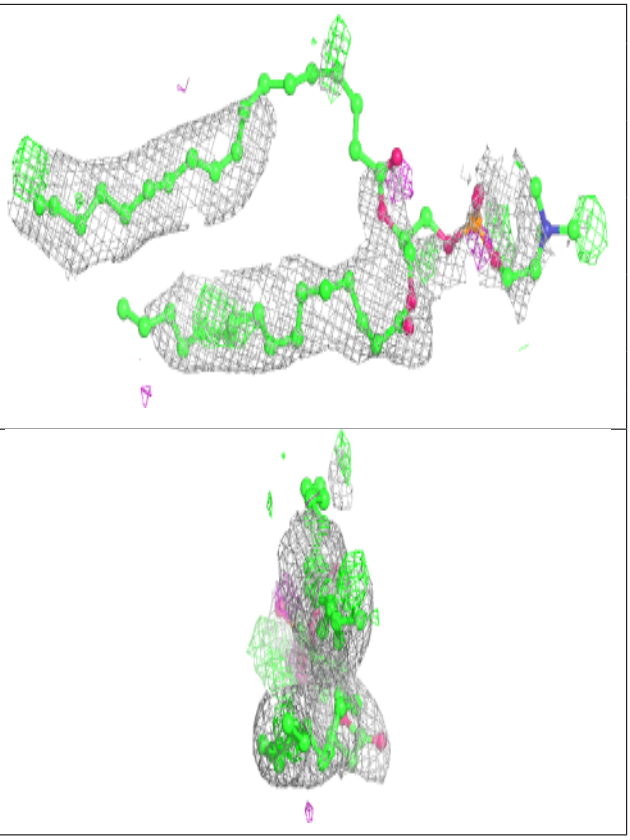
Electron density around PEK C 302:

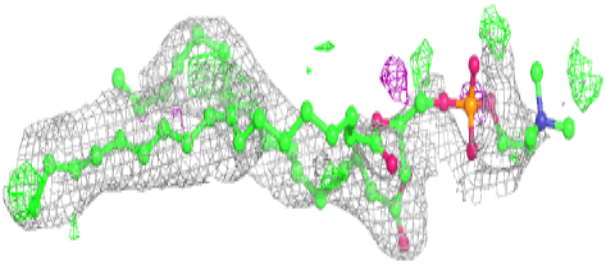
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PSC B 302:

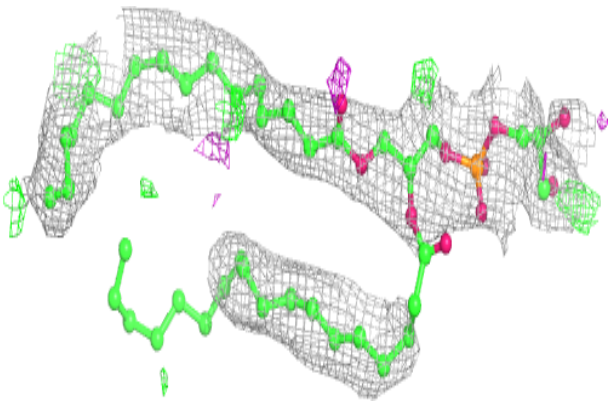
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

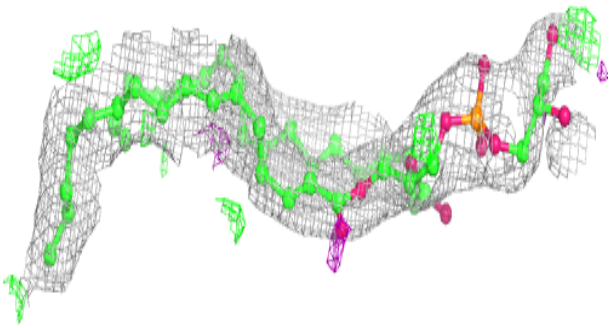


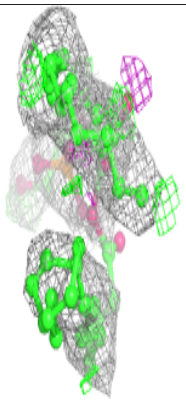


Electron density around PGV A 608:

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

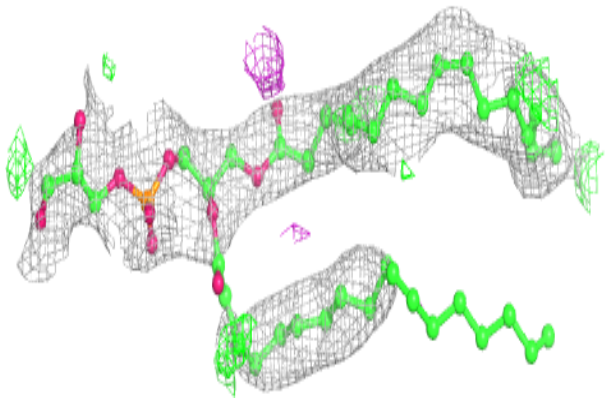


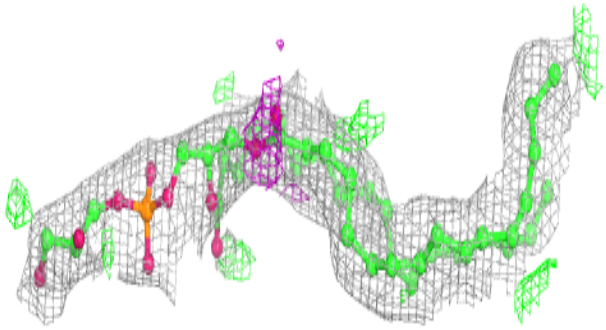


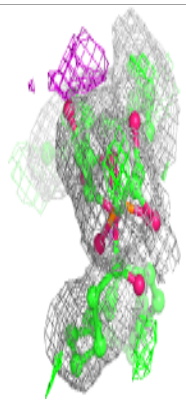


Electron density around PGV U 101:

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

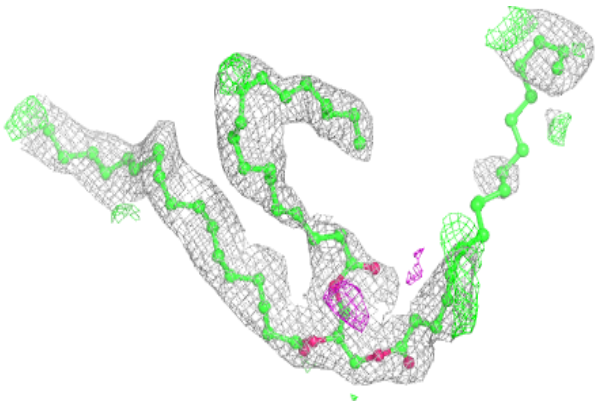


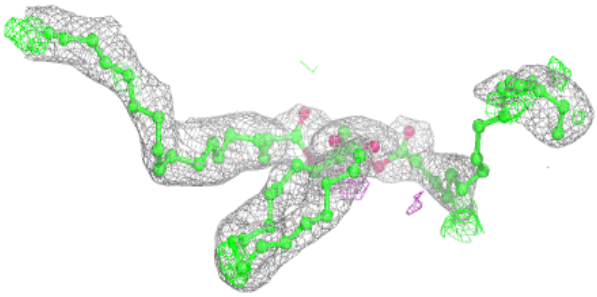


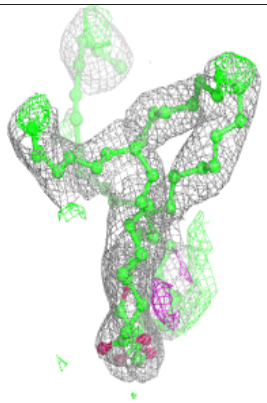


Electron density around TGL N 609:

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

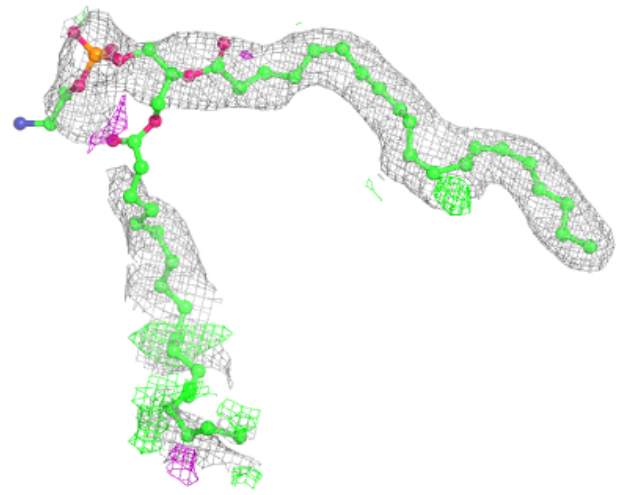


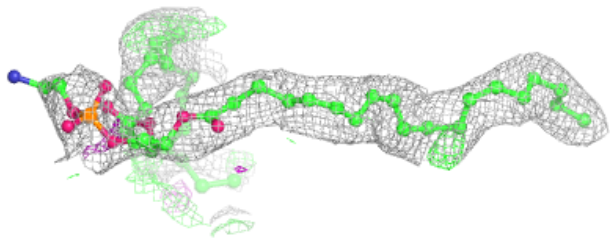


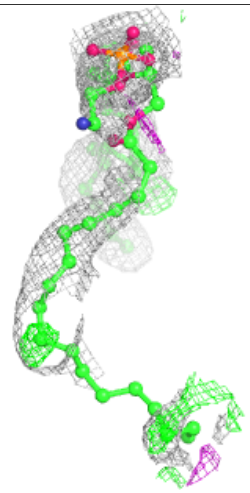


Electron density around PEK T 102:

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

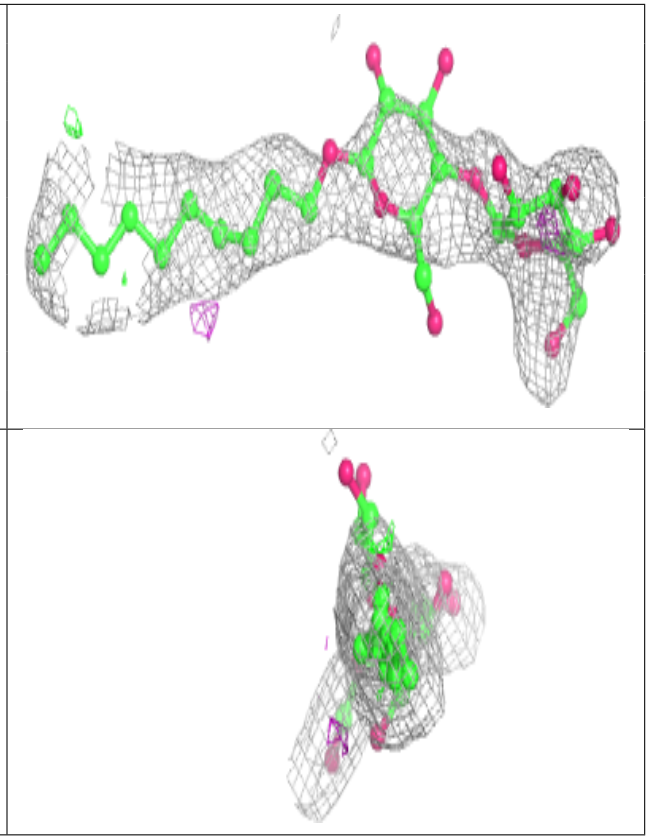






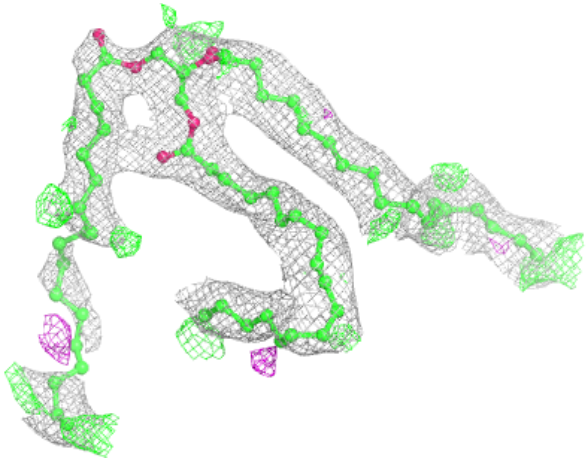
Electron density around DMU G 101:

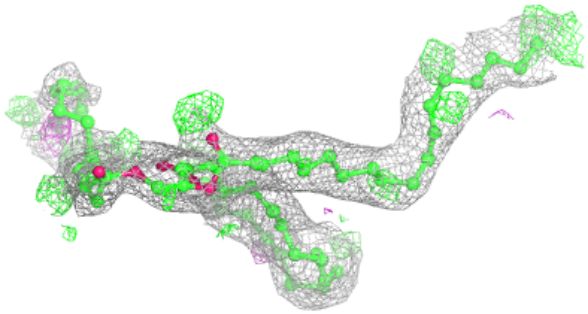
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

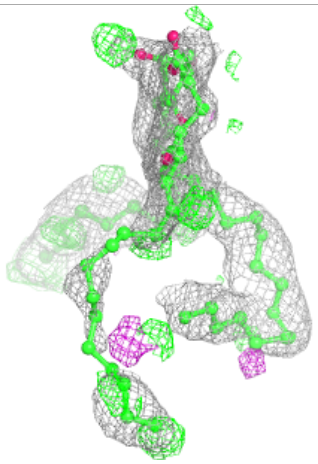


Electron density around TGL A 609:

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







Electron density around PSC O 302:

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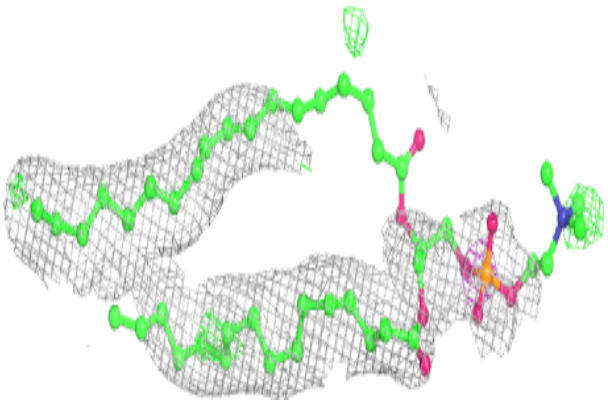
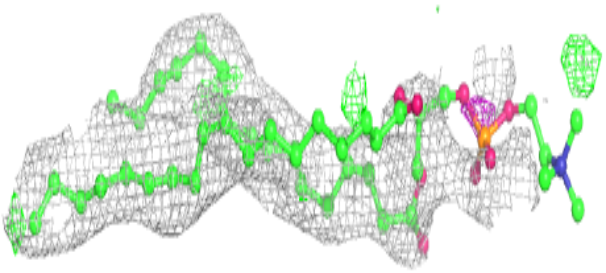
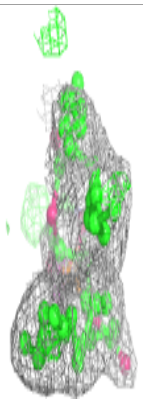
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

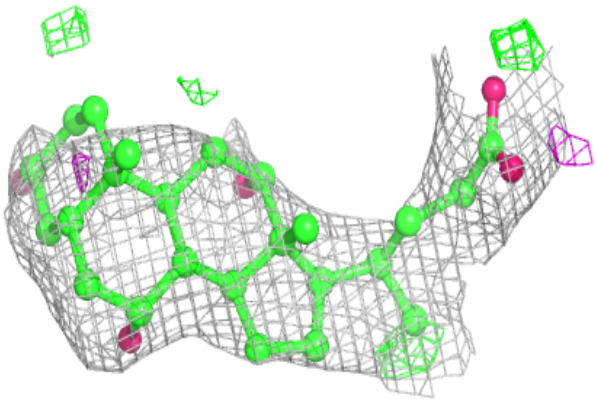


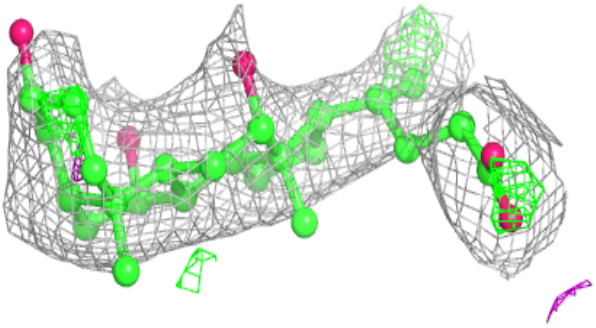


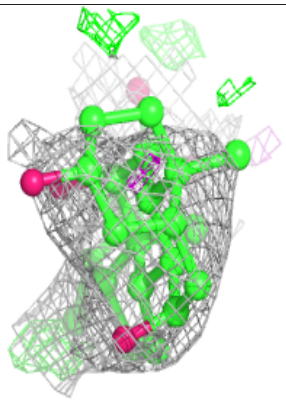


Electron density around CHD W 102:

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

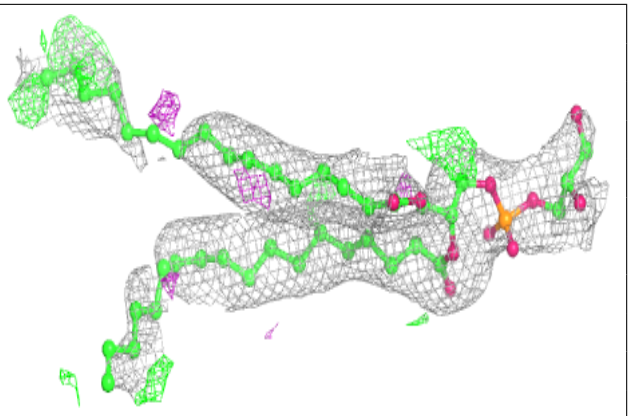


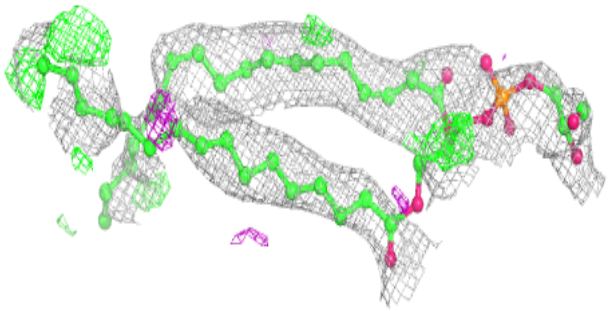


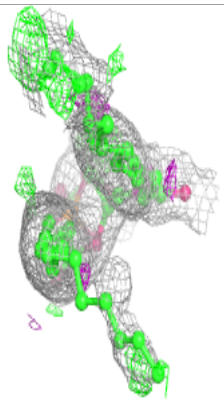


Electron density around PGV A 606:

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

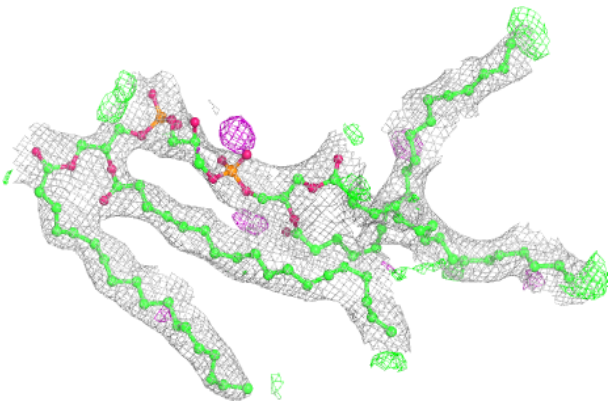


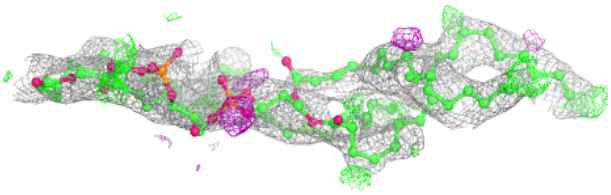


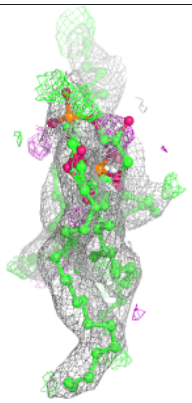


Electron density around CDL N 601:

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

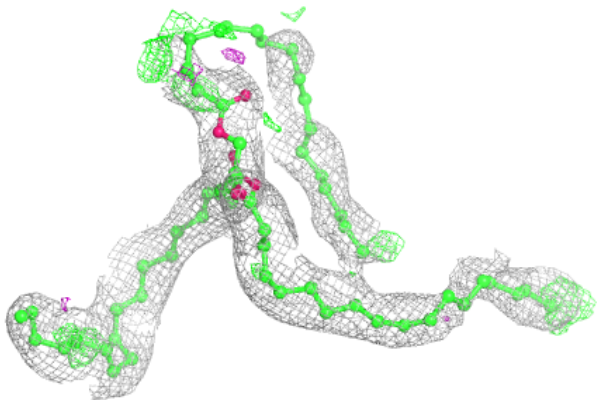


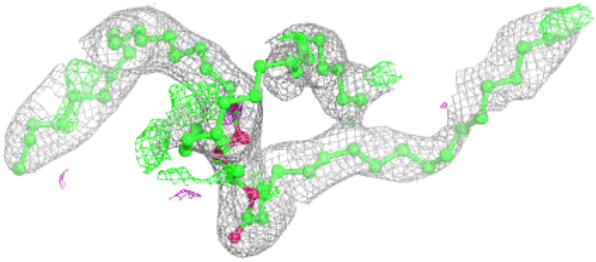


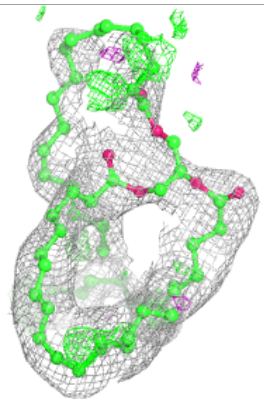


Electron density around TGL Y 101:

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

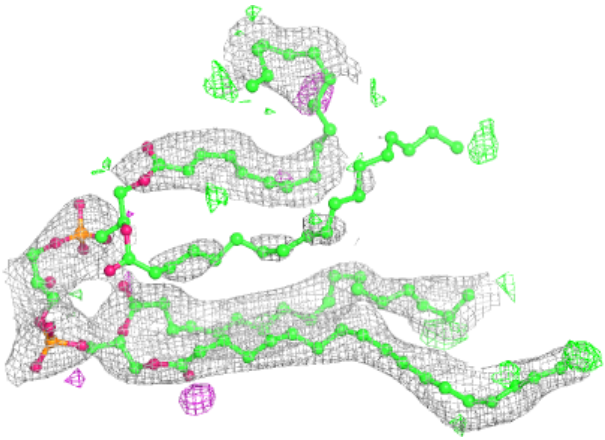


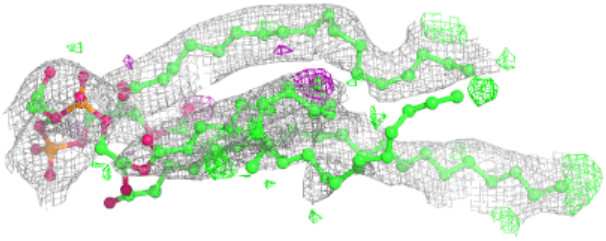


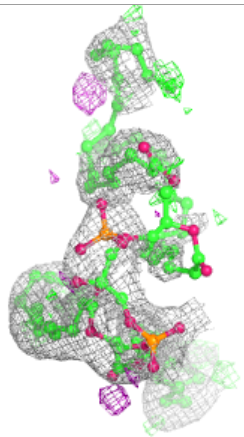


Electron density around CDL P 305:

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

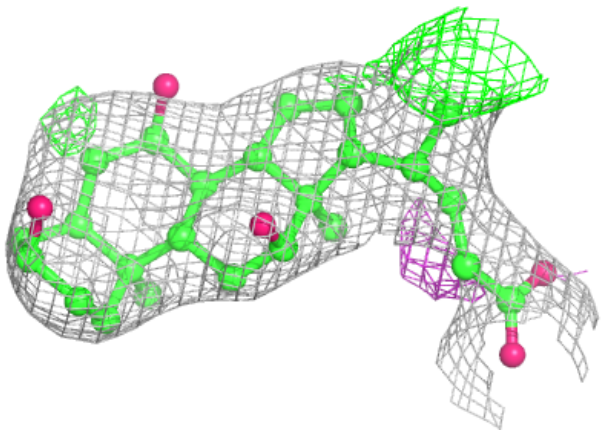


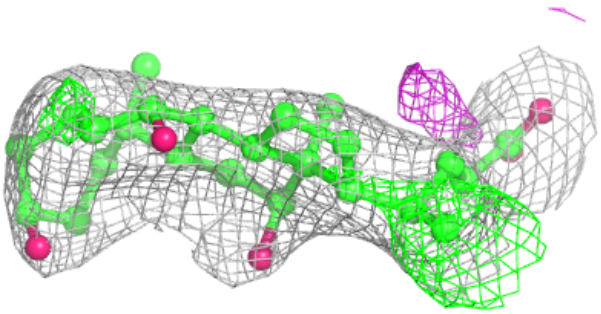


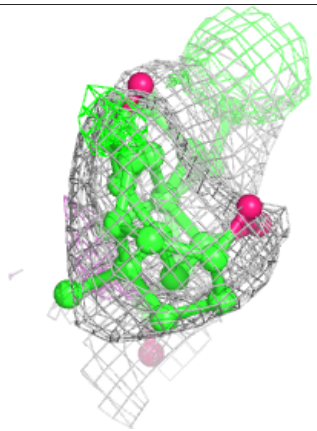


Electron density around CHD J 102:

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

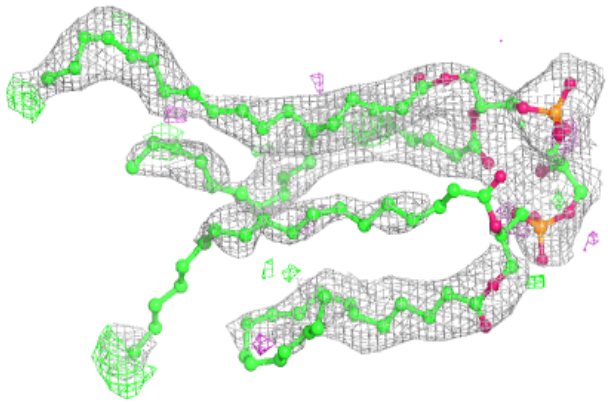


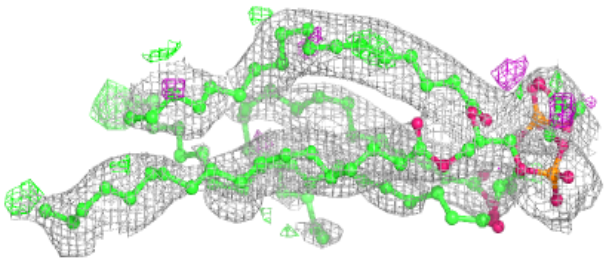


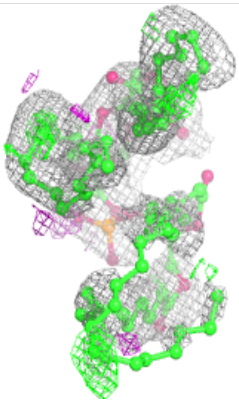


Electron density around CDL C 304:

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

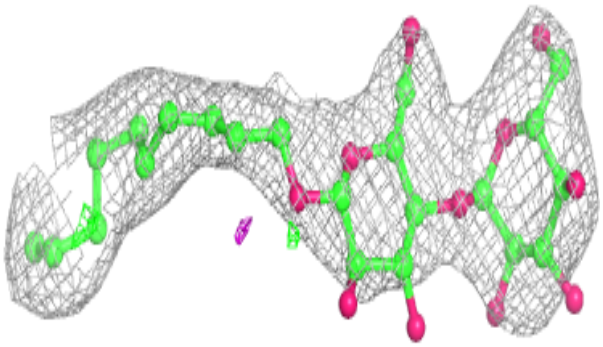


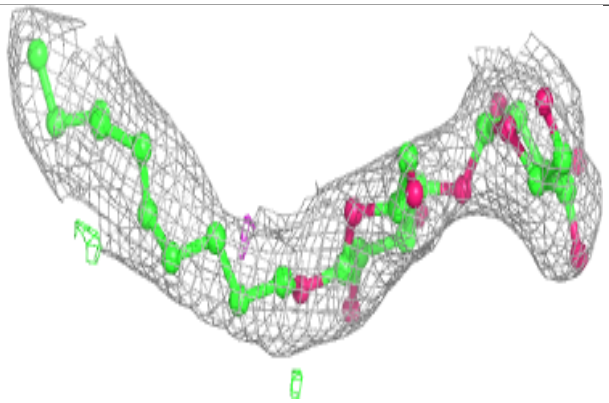


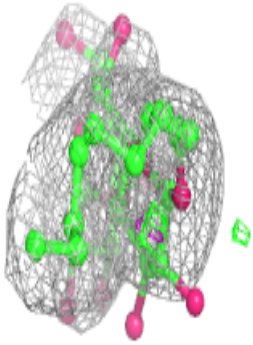


Electron density around DMU Q 201:

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

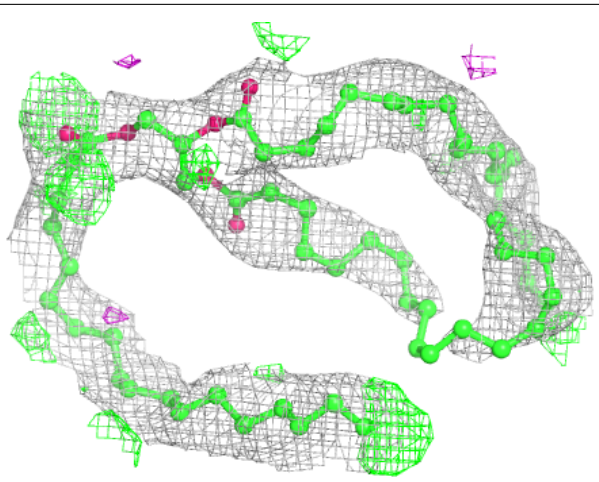


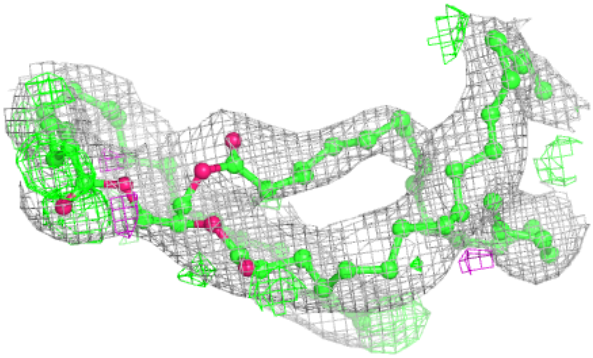


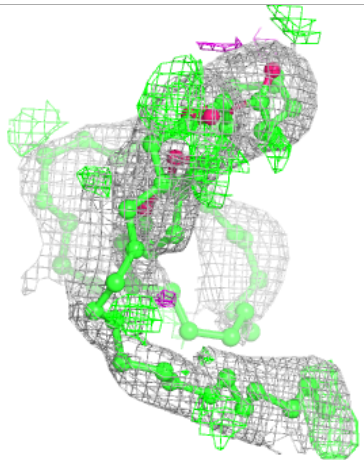


Electron density around TGL N 607:

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

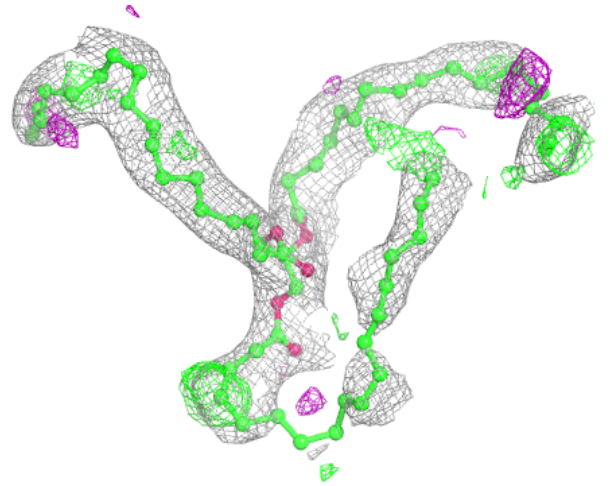


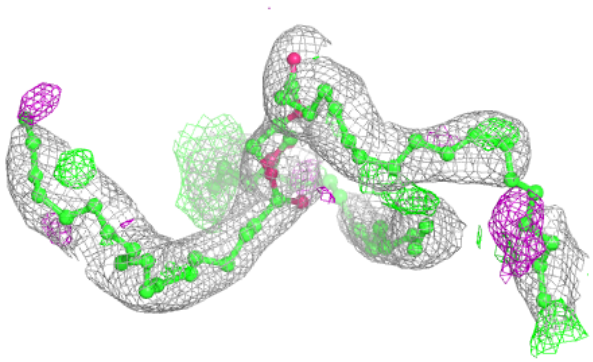


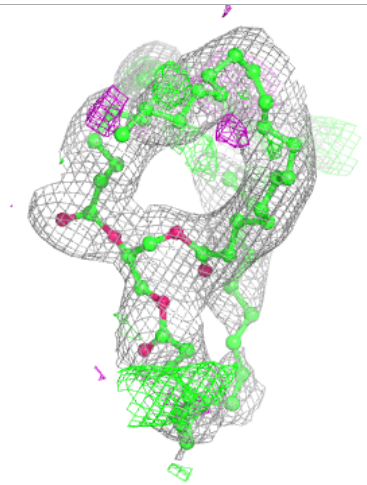


Electron density around TGL L 101:

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

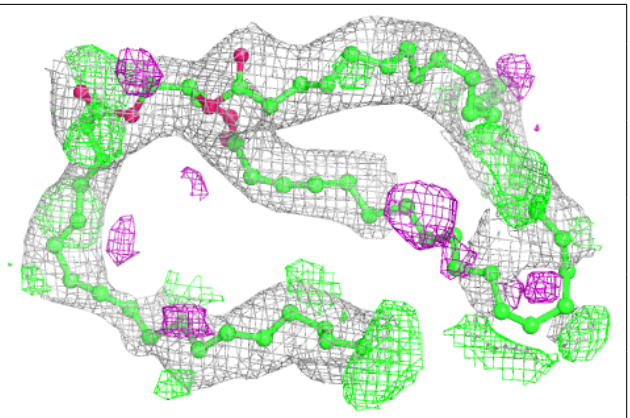


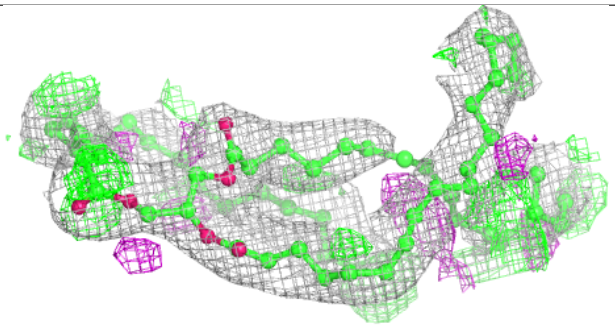


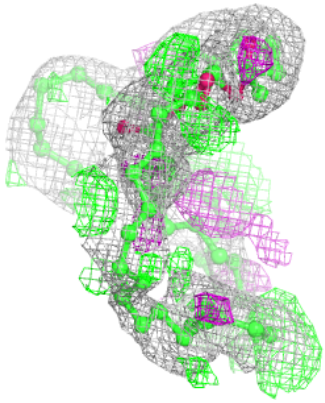


Electron density around TGL B 303:

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

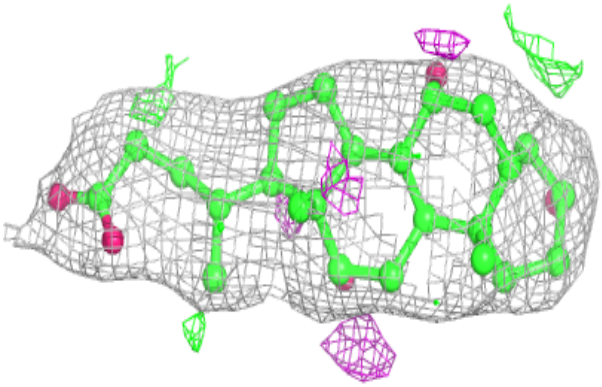


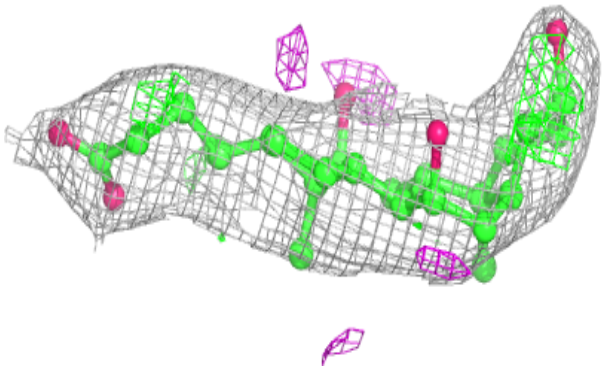


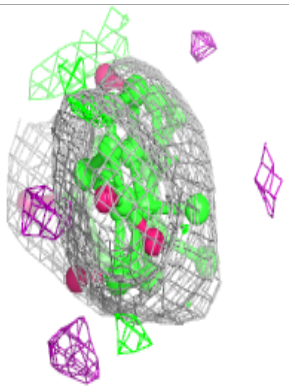


Electron density around CHD J 101:

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

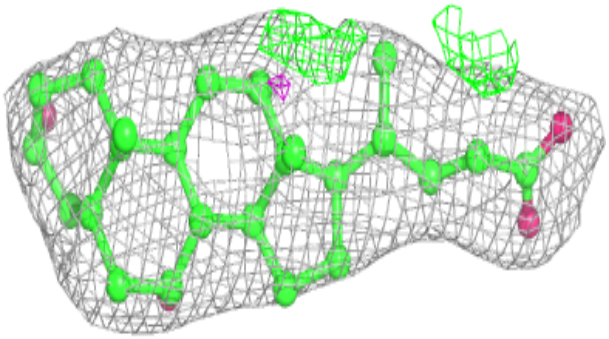


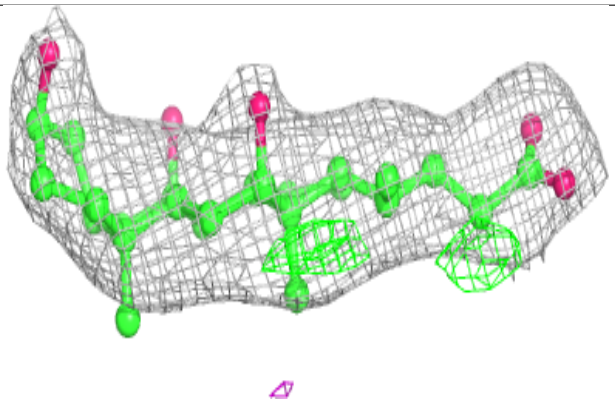


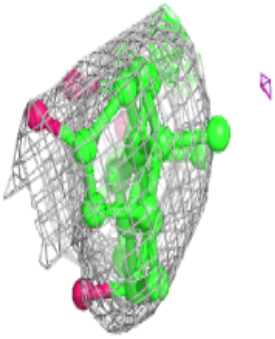


Electron density around CHD W 101:

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

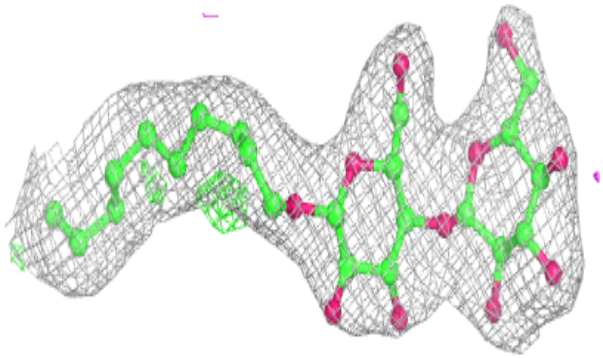


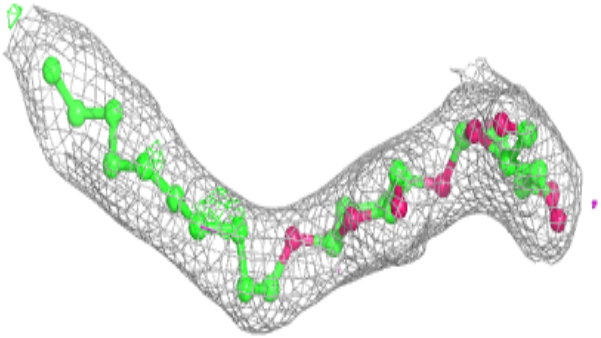


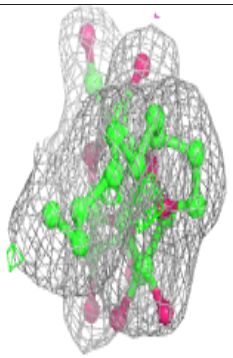


Electron density around DMU M 101:

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

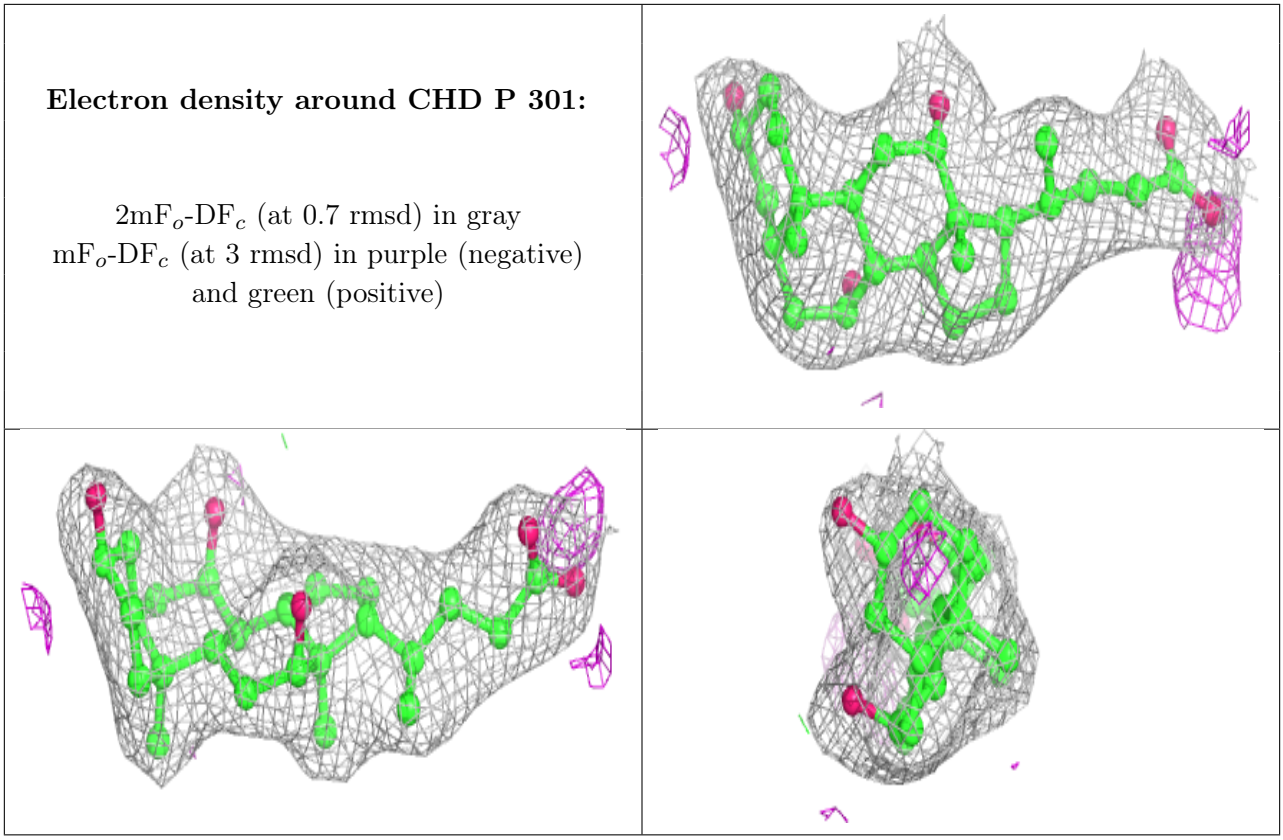






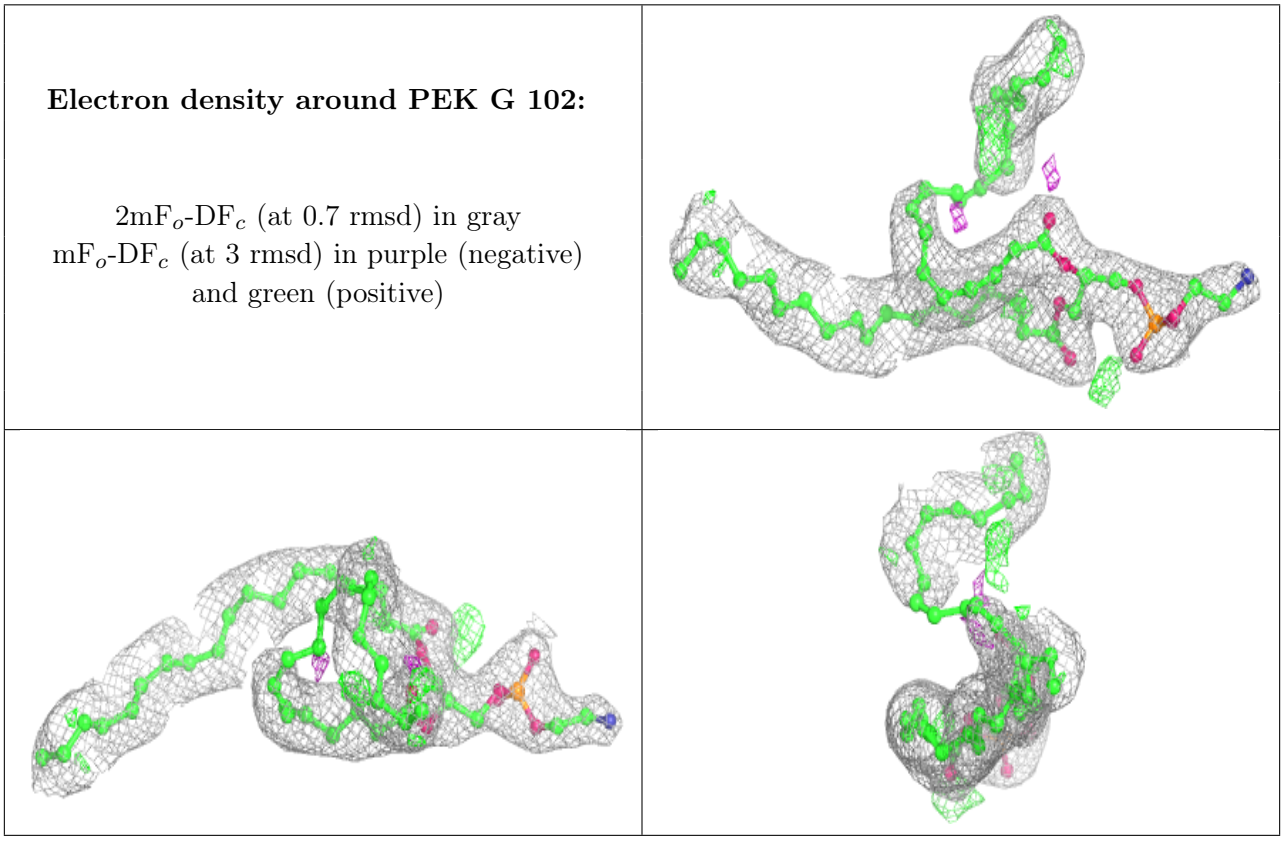
Electron density around CHD P 301:

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



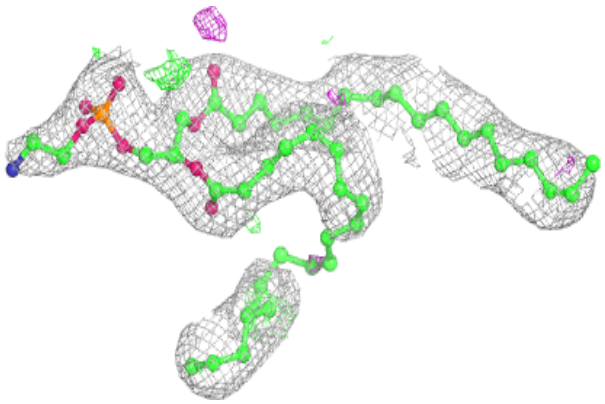
Electron density around PEK G 102:

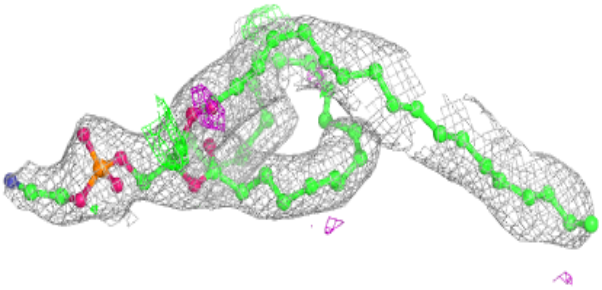
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

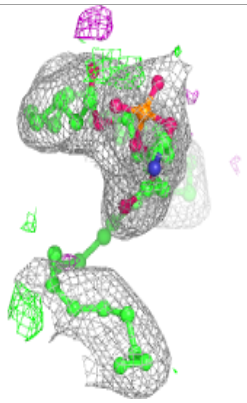


Electron density around PEK P 302:

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

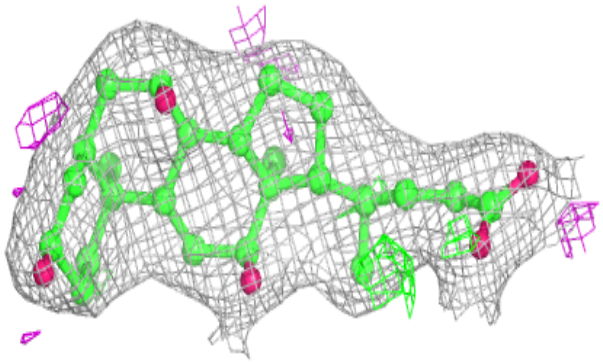


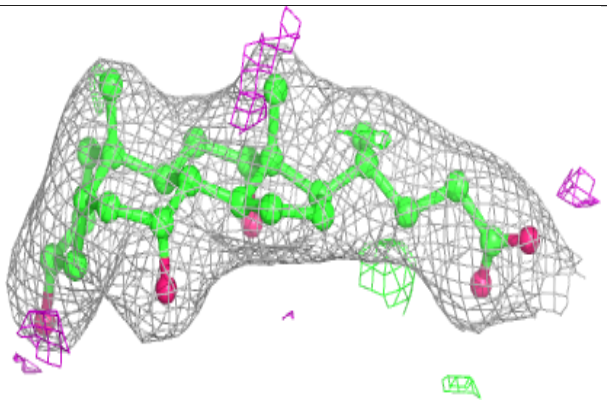


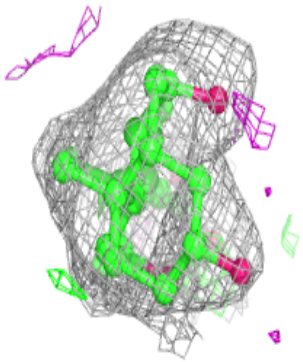


Electron density around CHD C 301:

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

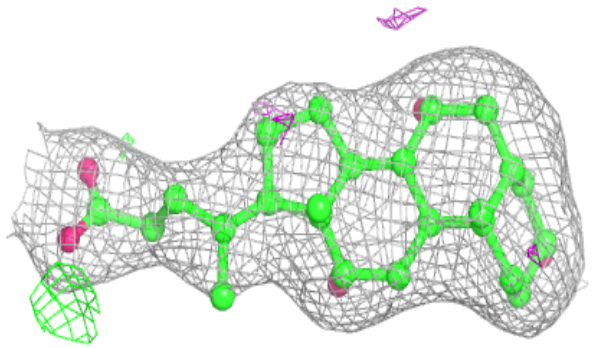


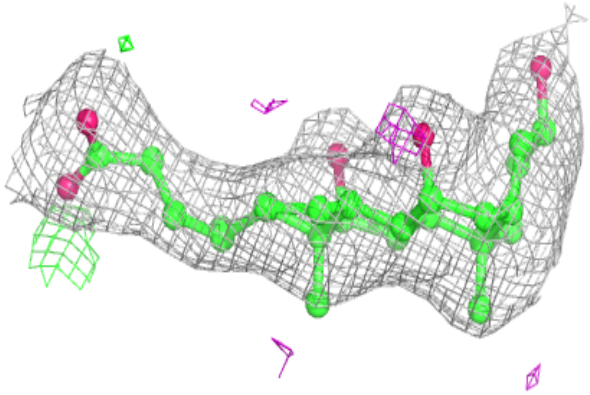


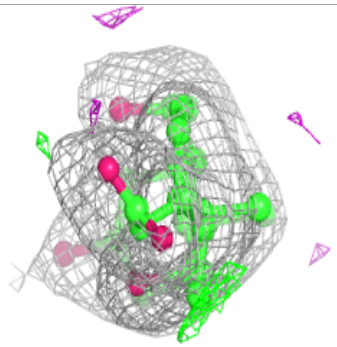


Electron density around CHD G 104:

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

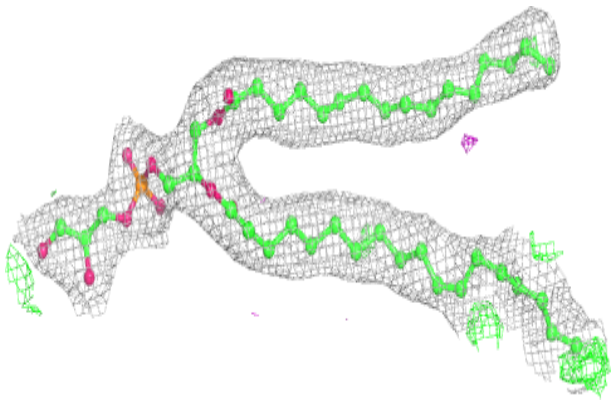


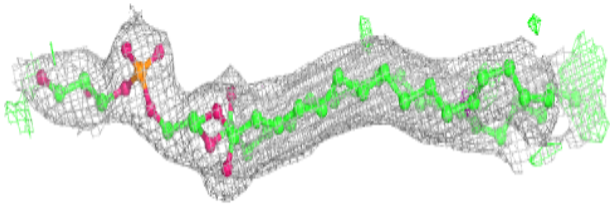


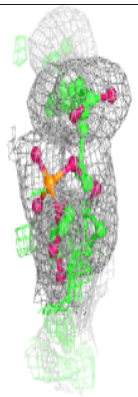


Electron density around PGV C 303:

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

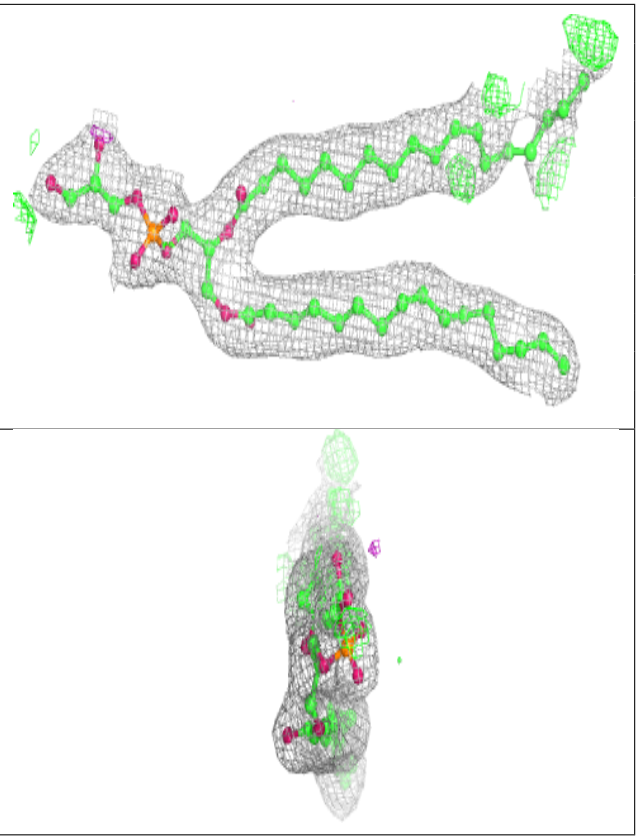






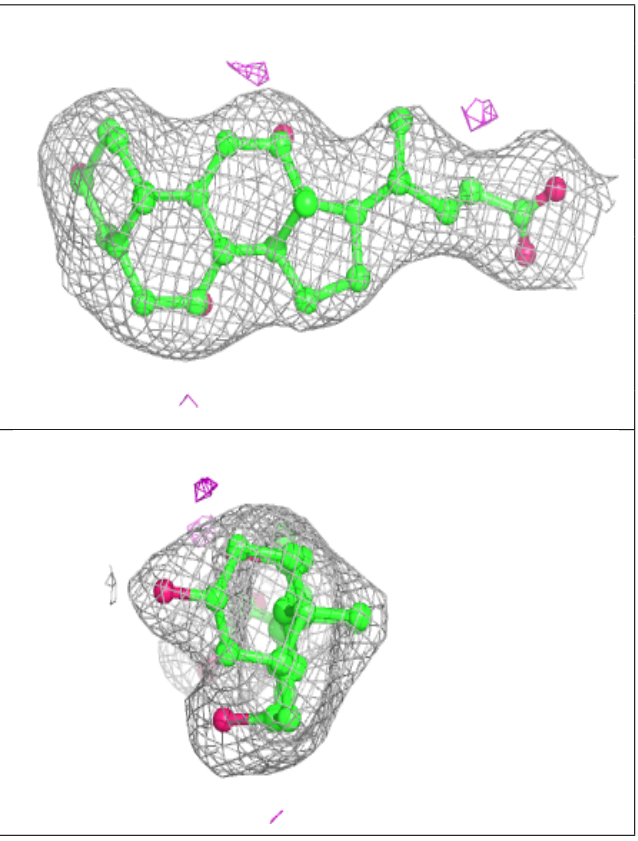
Electron density around PGV P 304:

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



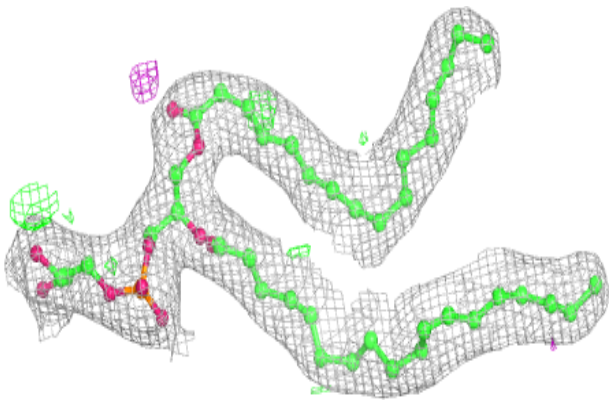
Electron density around CHD B 304:

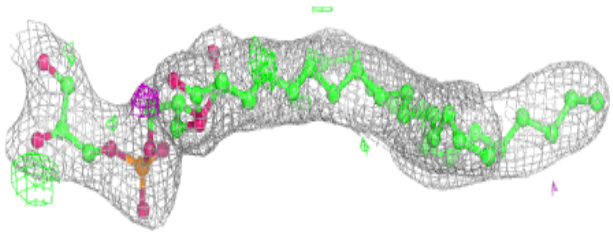
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

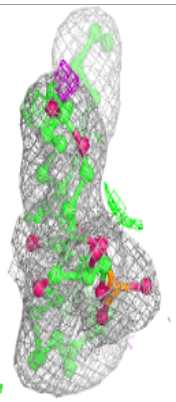


Electron density around PGV N 608:

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

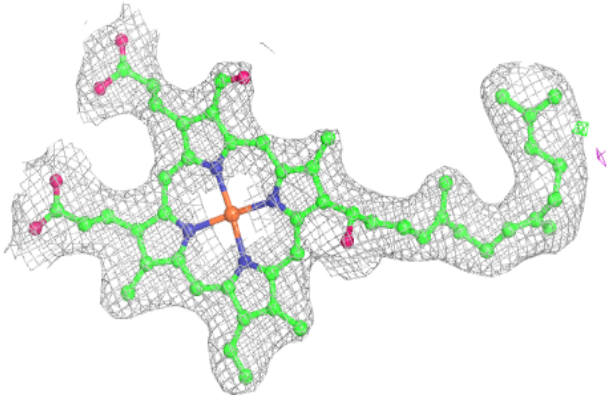


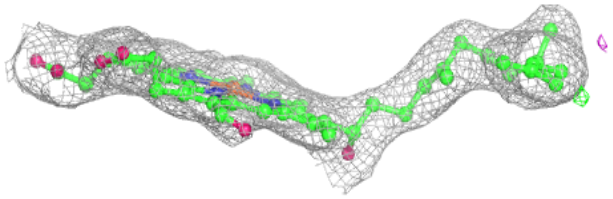


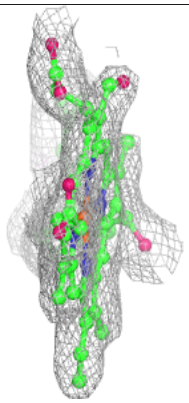


Electron density around HEA N 606:

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

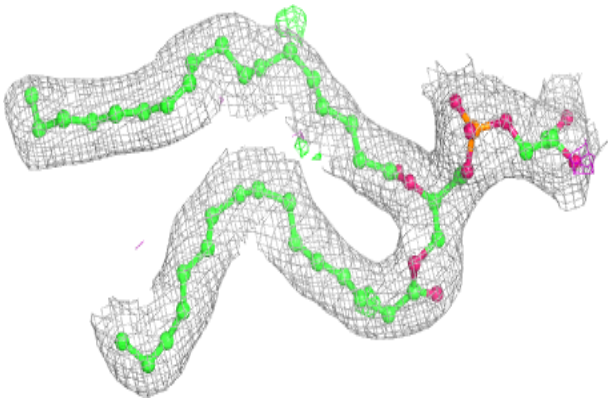


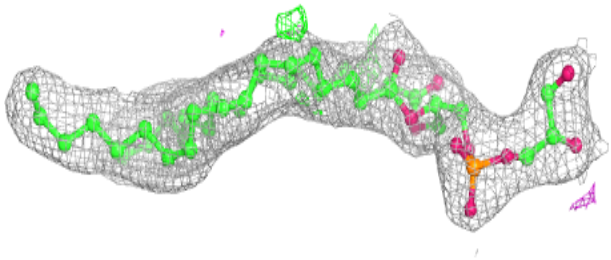


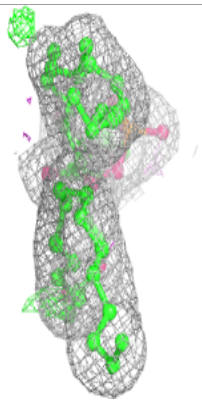


Electron density around PGV A 607:

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

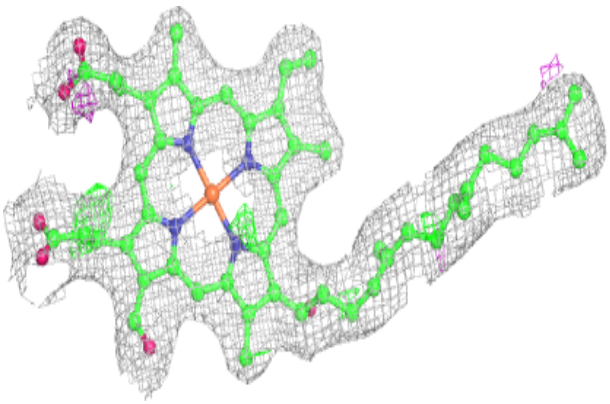


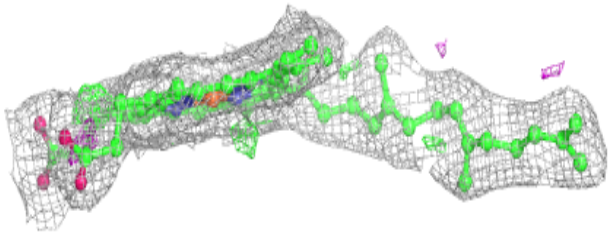


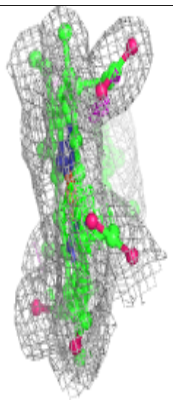


Electron density around HEA A 604:

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

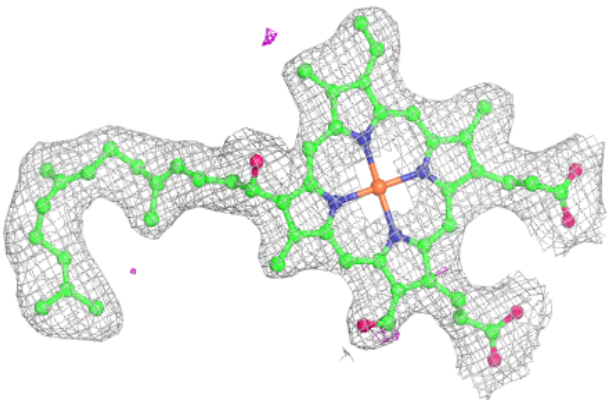


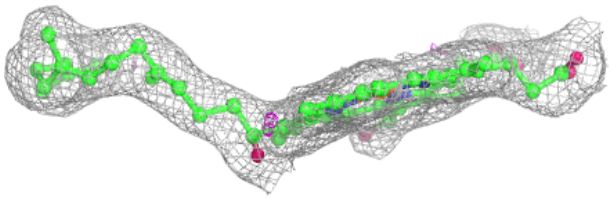


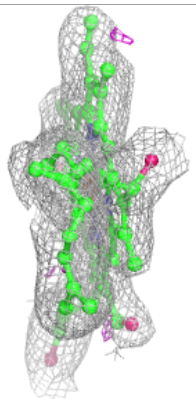


Electron density around HEA A 605:

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

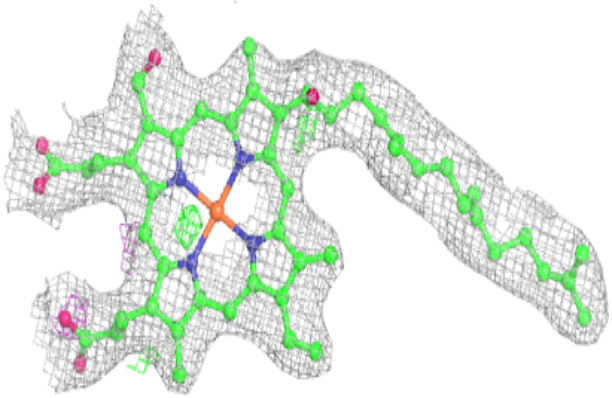


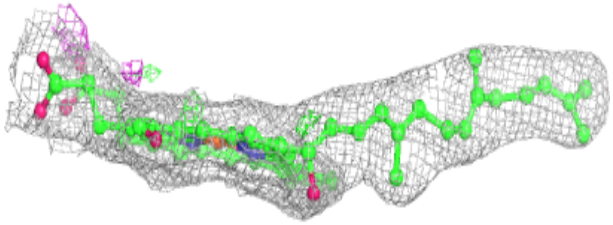


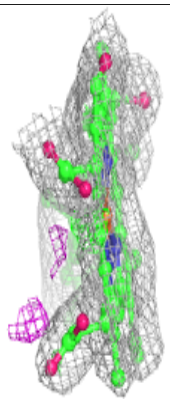


Electron density around HEA N 605:

$2mF_o$-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.