



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 29, 2020 – 09:53 PM BST

PDB ID : 5X19
Title : CO bound cytochrome c oxidase at 100 micro sec after pump laser irradiation to release CO from O2 reduction center
Authors : Shimada, A.; Kubo, M.; Baba, S.; Yamashita, K.; Hirata, K.; Ueno, G.; Nomura, T.; Kimura, T.; Shinzawa-Itoh, K.; Baba, J.; Hatano, K.; Eto, Y.; Miyamoto, A.; Murakami, H.; Kumasaka, T.; Owada, S.; Tono, K.; Yabashi, M.; Yamaguchi, Y.; Yanagisawa, S.; Sakaguchi, M.; Ogura, T.; Komiya, R.; Yan, J.; Yamashita, E.; Yamamoto, M.; Ago, H.; Yoshikawa, S.; Tsukihara, T.
Deposited on : 2017-01-25
Resolution : 2.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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	:	2.13
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)	:	2.13

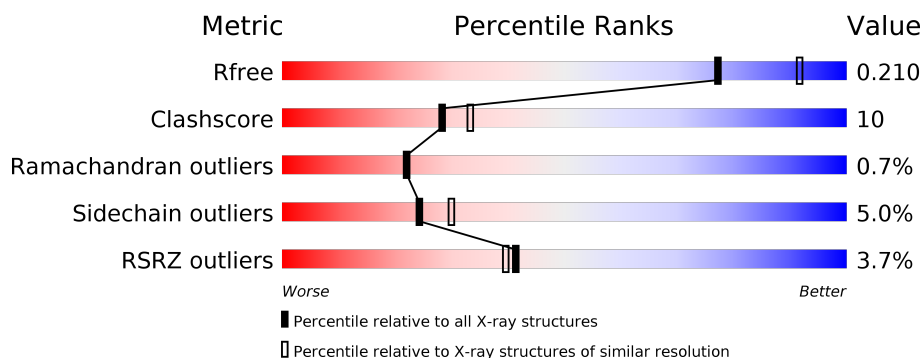
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



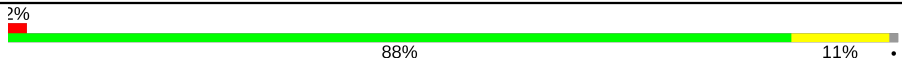

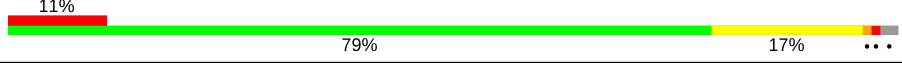
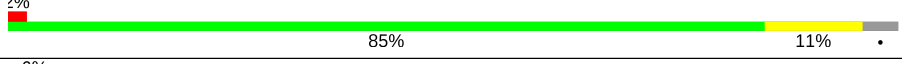

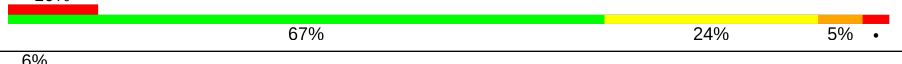
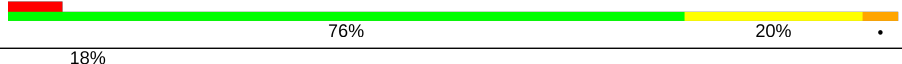

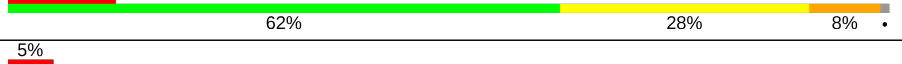


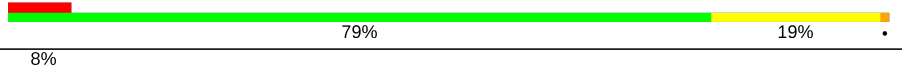



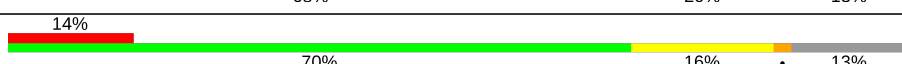
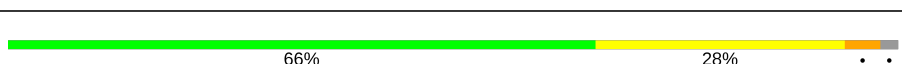
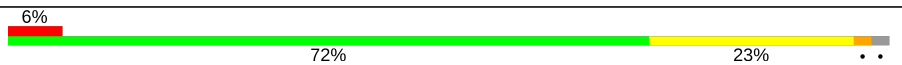
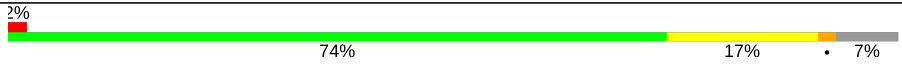


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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 $\leq 5\%$. 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	<div> <div>85%</div> <div>14%</div> <div>.</div> </div>
1	N	514	<div> <div>%</div> <div>81%</div> <div>18%</div> <div>.</div> </div>
2	B	227	<div> <div>%</div> <div>77%</div> <div>22%</div> <div>.</div> </div>
2	O	227	<div> <div>3%</div> <div>74%</div> <div>22%</div> <div>.</div> </div>
3	C	261	<div> <div>84%</div> <div>15%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
3	P	261	
4	D	147	
4	Q	147	
5	E	109	
5	R	109	
6	F	98	
6	S	98	
7	G	85	
7	T	85	
8	H	85	
8	U	85	
9	I	73	
9	V	73	
10	J	59	
10	W	59	
11	K	56	
11	X	56	
12	L	47	
12	Y	47	
13	M	46	
13	Z	46	

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

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CMO	N	606	-	-	X	-
21	EDO	A	612	-	-	X	-
21	EDO	A	613	-	-	X	-
21	EDO	C	310	-	-	-	X
21	EDO	N	610	-	-	-	X
21	EDO	T	105	-	-	X	-
25	UNX	P	302	-	-	-	X
26	CDL	T	104	-	-	X	-
27	PEK	G	103	-	-	-	X
27	PEK	T	102	-	-	-	X
9	SAC	V	1	-	-	-	X

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 32242 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
1	A	514	Total	C	N	O	S	0	7	0
			4068	2718	628	686	36			
1	N	514	Total	C	N	O	S	0	0	0
			4027	2691	623	678	35			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	73	Total	C	N	O	S	0	1	0
			609	398	107	100	4			
9	V	73	Total	C	N	O	S	0	2	0
			617	406	107	100	4			

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

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

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

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

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

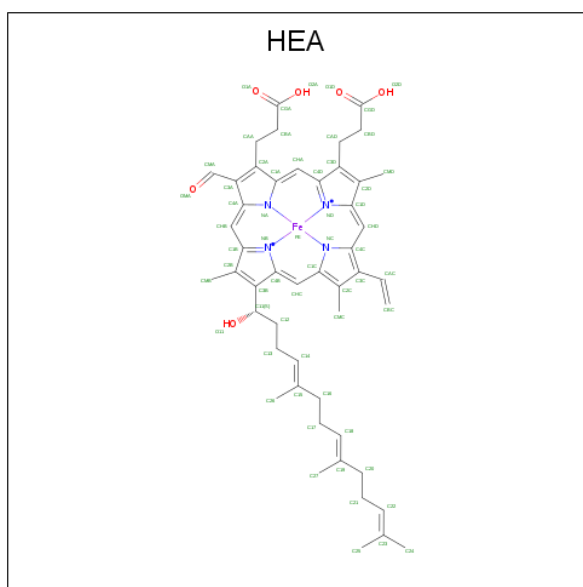
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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

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

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

- Molecule 14 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆).



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

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

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

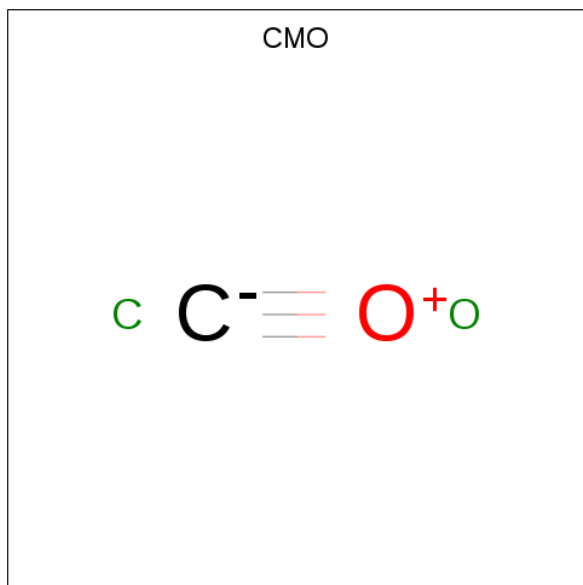
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

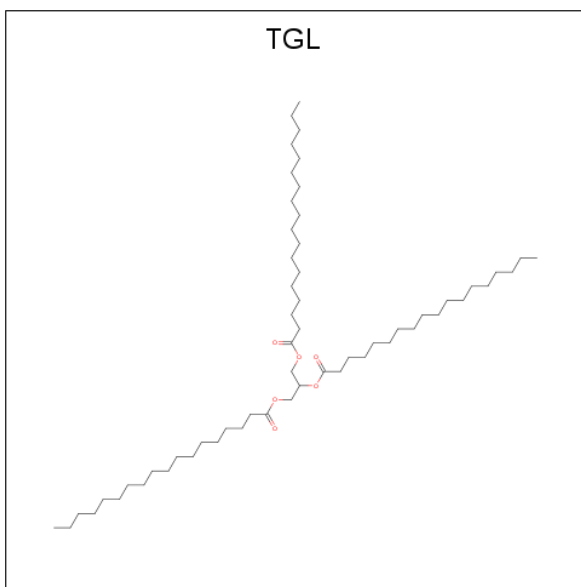
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Na	0	0
			1	1		
17	N	1	Total	Na	0	0
			1	1		

- Molecule 18 is CARBON MONOXIDE (three-letter code: CMO) (formula: CO).



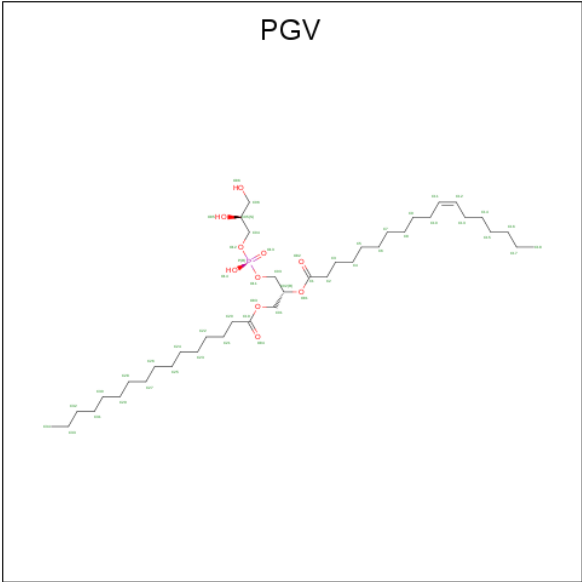
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	A	1	Total	C	O	0	0
			2	1	1		
18	N	1	Total	C	O	0	0
			2	1	1		

- Molecule 19 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C₅₇H₁₁₀O₆).



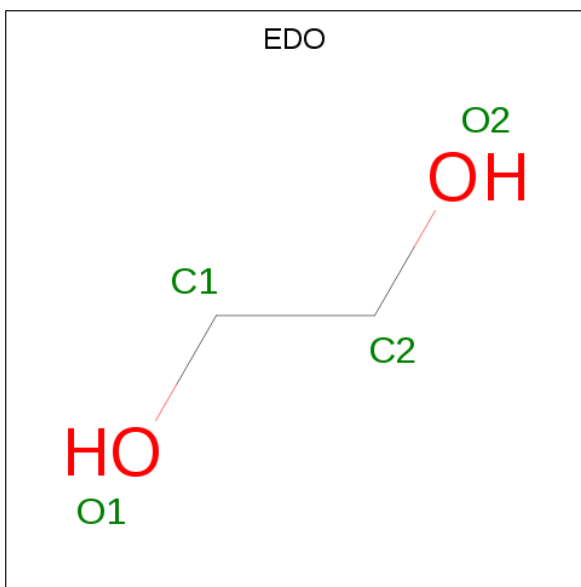
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	C	O	0	0
			63	57	6		
19	D	1	Total	C	O	0	0
			63	57	6		
19	L	1	Total	C	O	0	0
			63	57	6		
19	O	1	Total	C	O	0	0
			63	57	6		
19	Q	1	Total	C	O	0	0
			63	57	6		
19	Y	1	Total	C	O	0	0
			63	57	6		

- Molecule 20 is (1R)-2-{{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C₄₀H₇₇O₁₀P).



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

- Molecule 21 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



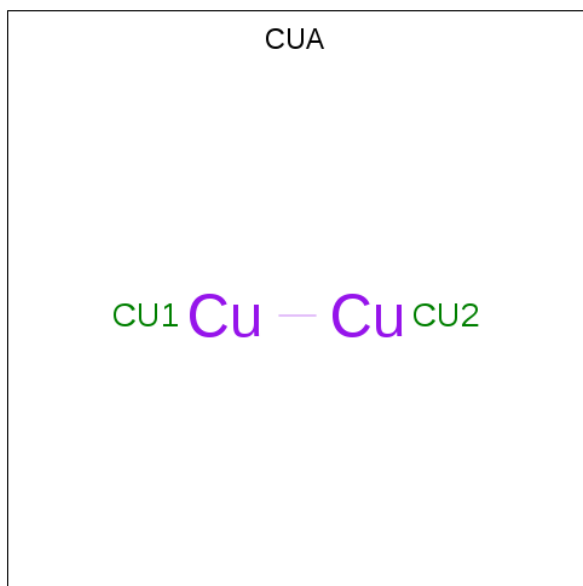
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	B	1	Total	C	O	0	0
			4	2	2		
21	B	1	Total	C	O	0	0
			4	2	2		
21	C	1	Total	C	O	0	0
			4	2	2		
21	C	1	Total	C	O	0	0
			4	2	2		
21	C	1	Total	C	O	0	0
			4	2	2		
21	C	1	Total	C	O	0	0
			4	2	2		
21	F	1	Total	C	O	0	0
			4	2	2		
21	F	1	Total	C	O	0	0
			4	2	2		
21	G	1	Total	C	O	0	0
			4	2	2		
21	H	1	Total	C	O	0	0
			4	2	2		

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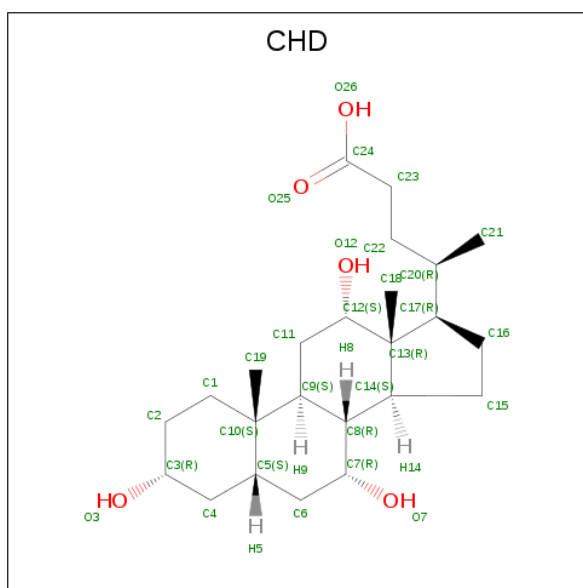
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	K	1	Total C O 4 2 2	0	0
21	K	1	Total C O 4 2 2	0	0
21	L	1	Total C O 4 2 2	0	0
21	N	1	Total C O 4 2 2	0	0
21	N	1	Total C O 4 2 2	0	0
21	O	1	Total C O 4 2 2	0	0
21	P	1	Total C O 4 2 2	0	0
21	P	1	Total C O 4 2 2	0	0
21	T	1	Total C O 4 2 2	0	0

- Molecule 22 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂).



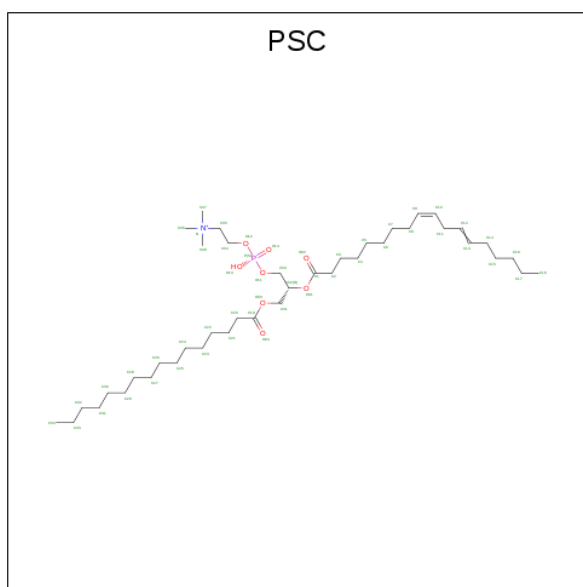
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	B	1	Total Cu 2 2	0	0
22	O	1	Total Cu 2 2	0	0

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



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

- Molecule 24 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: $C_{42}H_{81}NO_8P$).

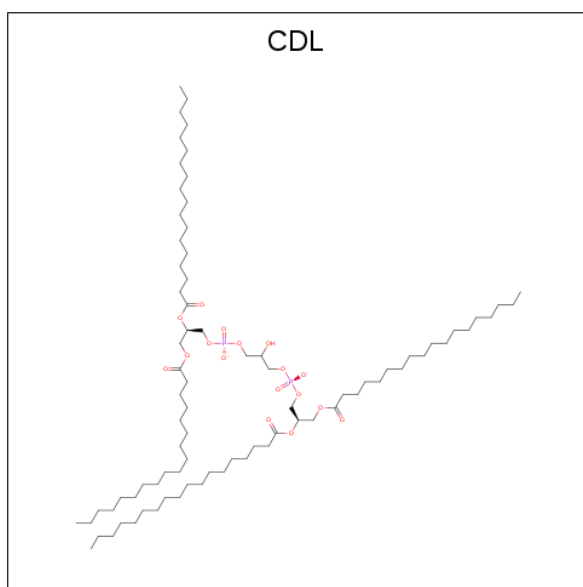


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
24	O	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 25 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

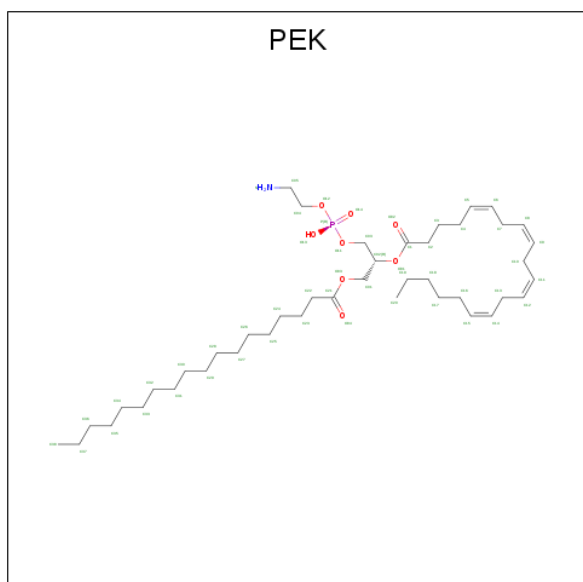
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	P	1	Total	X	0	0
			1	1		
25	C	1	Total	X	0	0
			1	1		

- Molecule 26 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



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

- Molecule 27 is (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: C₄₃H₇₈NO₈P).

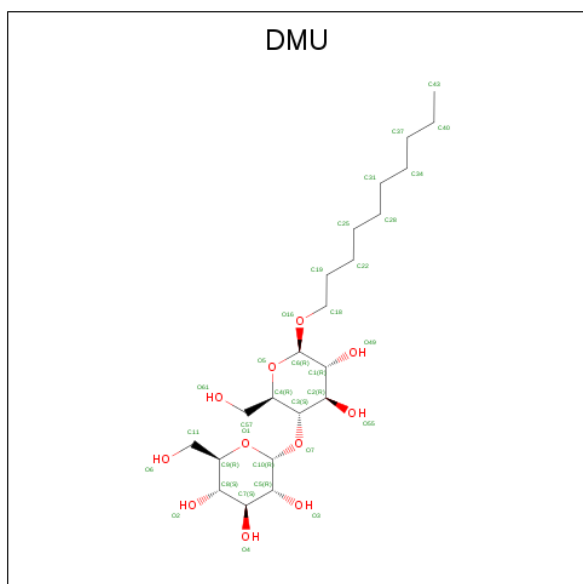


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
27	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

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

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

- Molecule 29 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: C₂₂H₄₂O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	M	1	Total	C	O	0	0
			33	22	11		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	Z	1	Total	C	O	0	0
			33	22	11		

- Molecule 30 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	191	Total	O		0	0
			191	191			
30	B	120	Total	O		0	1
			121	121			
30	C	83	Total	O		0	0
			83	83			
30	D	89	Total	O		0	0
			89	89			
30	E	45	Total	O		0	0
			45	45			
30	F	49	Total	O		0	0
			49	49			
30	G	40	Total	O		0	0
			40	40			
30	H	37	Total	O		0	0
			37	37			
30	I	19	Total	O		0	0
			19	19			
30	J	19	Total	O		0	0
			19	19			
30	K	27	Total	O		0	0
			27	27			
30	L	27	Total	O		0	0
			27	27			
30	M	18	Total	O		0	0
			18	18			
30	N	169	Total	O		0	0
			169	169			
30	O	100	Total	O		0	1
			101	101			
30	P	91	Total	O		0	0
			91	91			
30	Q	38	Total	O		0	0
			38	38			
30	R	40	Total	O		0	0
			40	40			

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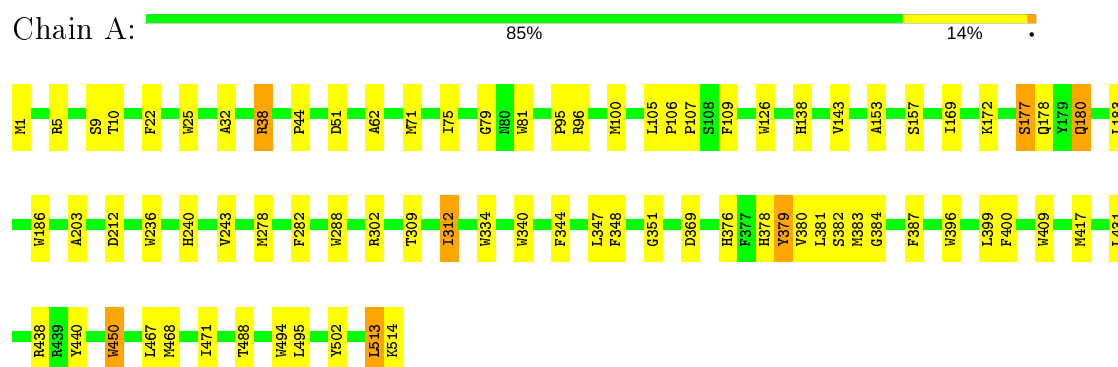
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	S	55	Total 55	O 55	0	0
30	T	45	Total 45	O 45	0	0
30	U	27	Total 27	O 27	0	0
30	V	23	Total 23	O 23	0	0
30	W	23	Total 23	O 23	0	0
30	X	16	Total 16	O 16	0	0
30	Y	18	Total 18	O 18	0	0
30	Z	4	Total 4	O 4	0	0

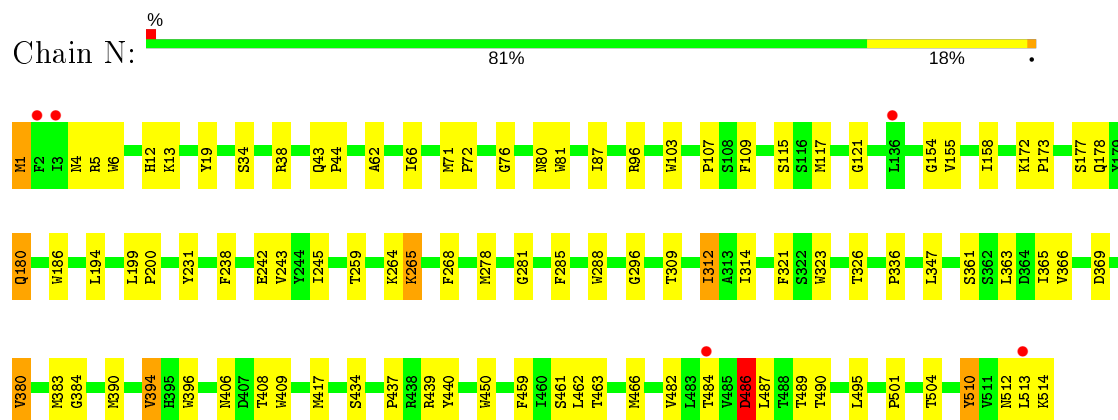
3 Residue-property plots

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.

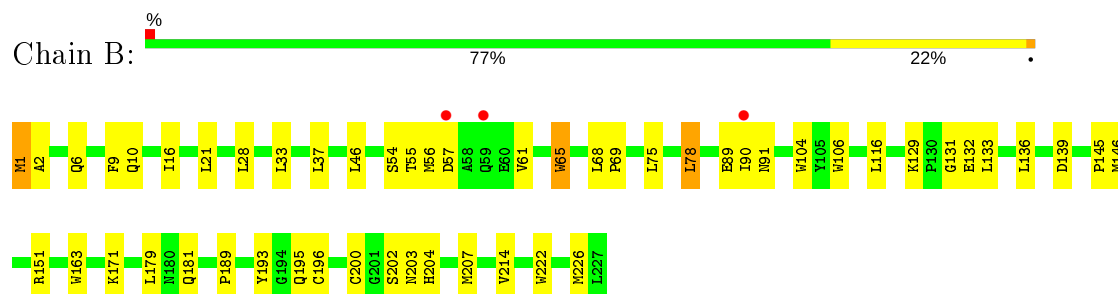
• Molecule 1: Cytochrome c oxidase subunit 1



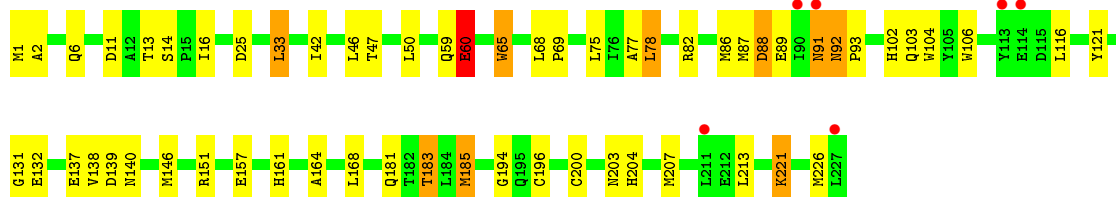
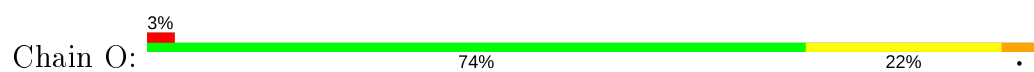
• Molecule 1: Cytochrome c oxidase subunit 1



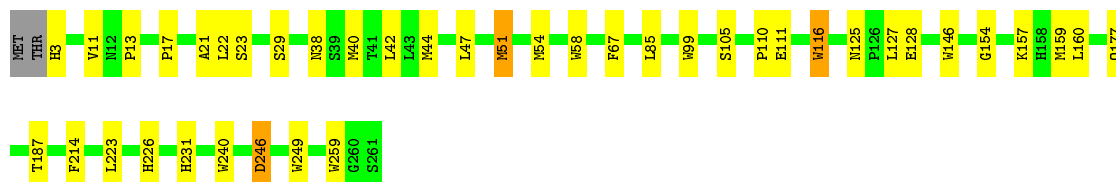
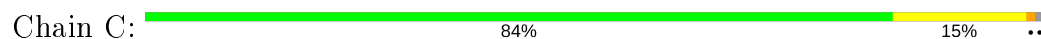
• Molecule 2: Cytochrome c oxidase subunit 2



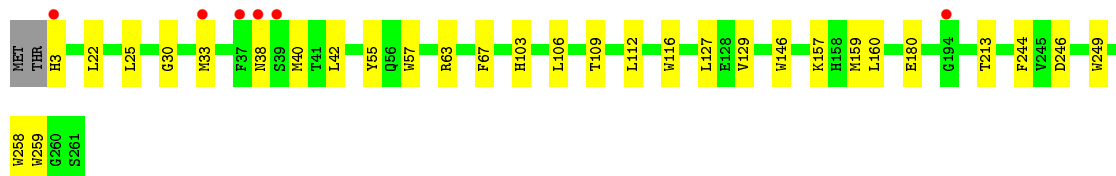
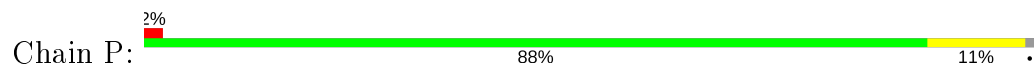
• Molecule 2: Cytochrome c oxidase subunit 2



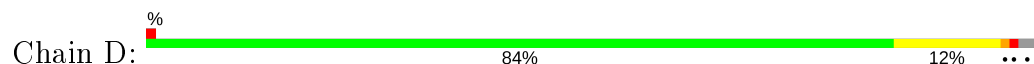
• Molecule 3: Cytochrome c oxidase subunit 3



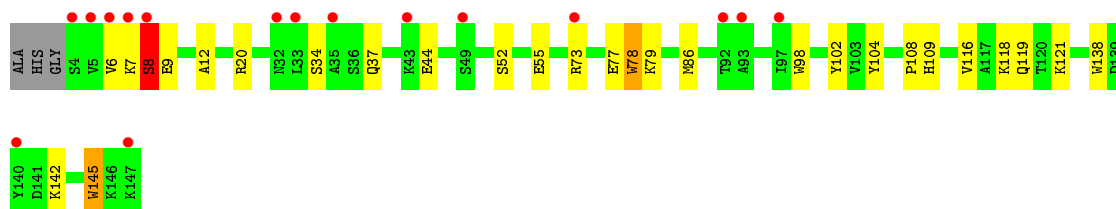
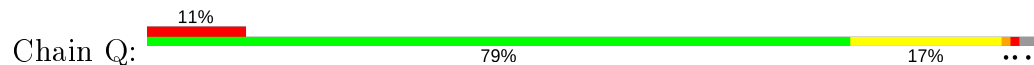
• Molecule 3: Cytochrome c oxidase subunit 3



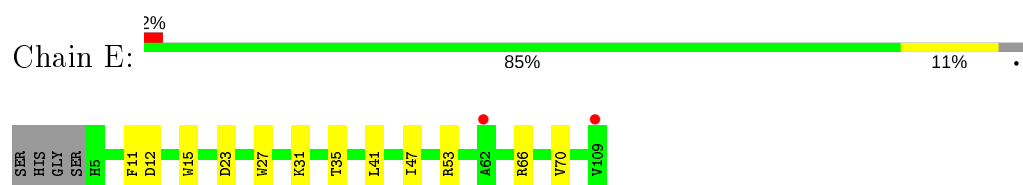
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



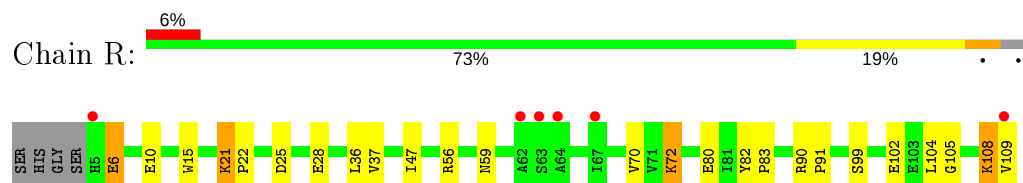
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



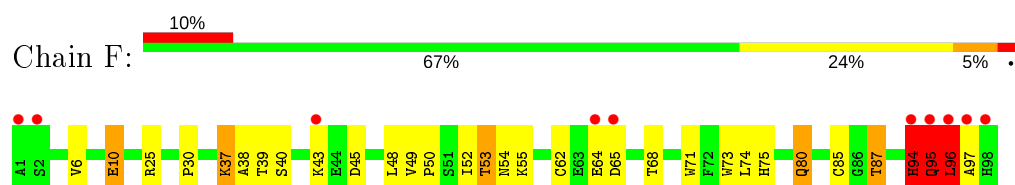
• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



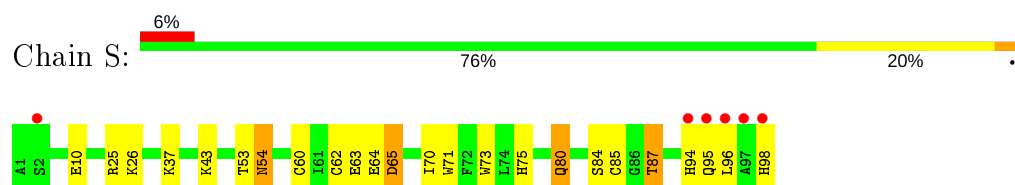
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



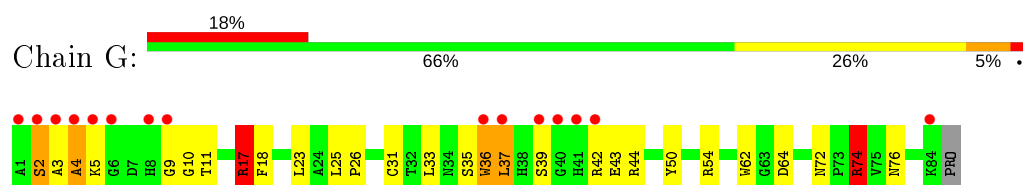
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



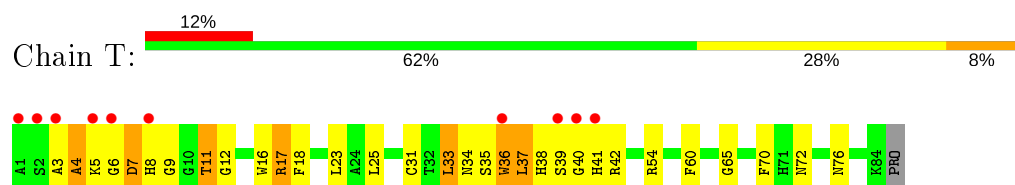
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



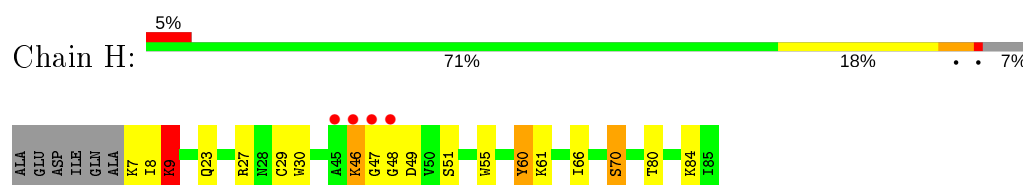
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



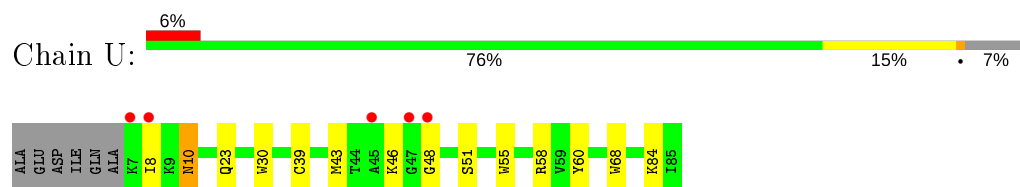
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



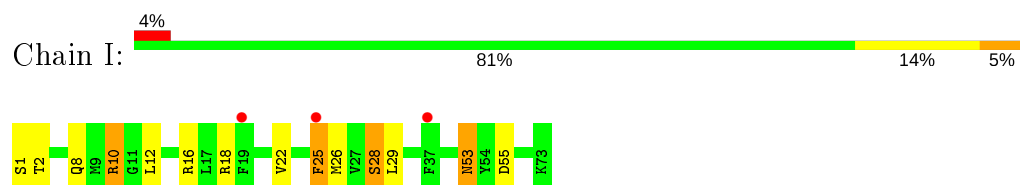
- Molecule 8: Cytochrome c oxidase subunit 6B1



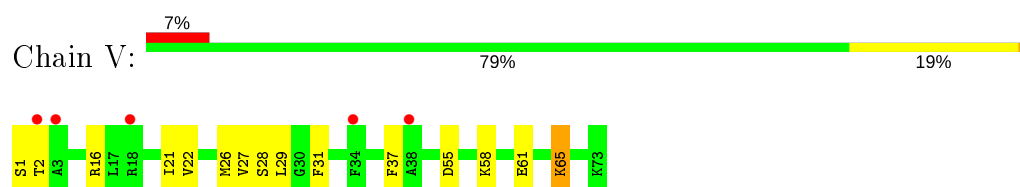
- Molecule 8: Cytochrome c oxidase subunit 6B1



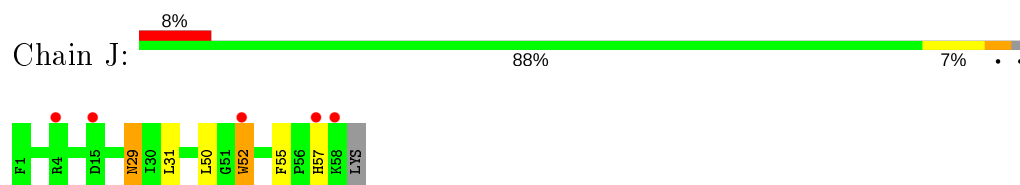
- Molecule 9: Cytochrome c oxidase subunit 6C



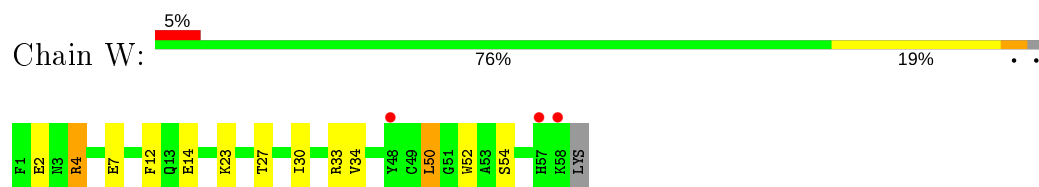
- Molecule 9: Cytochrome c oxidase subunit 6C



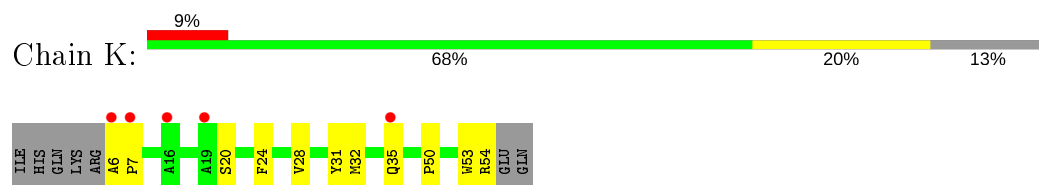
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



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



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



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





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

Chain L: 66% 28% ..



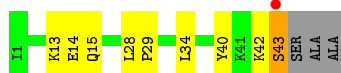
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain Y: 6% 72% 23% ..



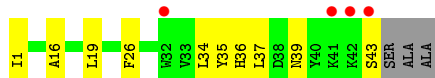
- Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

Chain M: 2% 74% 17% 7%



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

Chain Z: 9% 72% 22% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	185.03Å 208.85Å 178.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.20 24.99 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.8 (25.00-2.20) 96.9 (24.99-2.20)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.8.0048	Depositor
R, R_{free}	0.173 , 0.210 0.173 , 0.210	Depositor DCC
R_{free} test set	17156 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	51.4	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 63.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.028 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	32242	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CMO, ZN, CHD, HEA, SAC, CDL, PSC, PEK, MG, TGL, EDO, PGV, TPO, UNX, CUA, NA, FME, CU, DMU

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	1.05	12/4205 (0.3%)	0.95	5/5744 (0.1%)
1	N	1.02	9/4156 (0.2%)	0.92	4/5678 (0.1%)
2	B	0.94	3/1860 (0.2%)	0.96	4/2534 (0.2%)
2	O	0.83	2/1860 (0.1%)	0.91	2/2534 (0.1%)
3	C	1.06	5/2197 (0.2%)	0.92	1/3005 (0.0%)
3	P	1.01	4/2197 (0.2%)	0.87	1/3005 (0.0%)
4	D	0.94	5/1229 (0.4%)	0.88	2/1658 (0.1%)
4	Q	0.78	3/1229 (0.2%)	0.80	2/1658 (0.1%)
5	E	0.82	2/871 (0.2%)	0.94	2/1182 (0.2%)
5	R	0.72	1/871 (0.1%)	0.79	0/1182
6	F	0.86	2/765 (0.3%)	0.89	0/1038
6	S	0.80	0/765	0.89	1/1038 (0.1%)
7	G	0.97	2/690 (0.3%)	0.99	5/937 (0.5%)
7	T	0.90	1/690 (0.1%)	0.86	0/937
8	H	0.88	1/682 (0.1%)	0.88	0/921
8	U	0.84	3/682 (0.4%)	0.81	0/921
9	I	0.76	0/617	0.93	2/818 (0.2%)
9	V	0.70	0/629	0.83	1/834 (0.1%)
10	J	0.80	1/471 (0.2%)	0.84	0/636
10	W	0.71	1/471 (0.2%)	0.75	0/636
11	K	0.93	1/398 (0.3%)	0.75	0/546
11	X	0.85	2/398 (0.5%)	0.80	0/546
12	L	0.88	0/393	0.84	0/526
12	Y	0.77	0/393	0.76	0/526
13	M	0.85	0/345	0.82	0/470
13	Z	0.76	0/345	0.74	0/470
All	All	0.93	60/29409 (0.2%)	0.89	32/39980 (0.1%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
8	H	0	1

The worst 5 of 60 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	81	TRP	CD2-CE2	7.66	1.50	1.41
2	B	65	TRP	CD2-CE2	7.41	1.50	1.41
1	N	323	TRP	CD2-CE2	7.36	1.50	1.41
3	C	240	TRP	CD2-CE2	7.11	1.49	1.41
1	N	81	TRP	CD2-CE2	7.05	1.49	1.41

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	246	ASP	CB-CG-OD1	-8.98	110.22	118.30
9	I	10	ARG	NE-CZ-NH2	-8.12	116.24	120.30
1	A	71	MET	CG-SD-CE	-7.57	88.08	100.20
1	N	96	ARG	NE-CZ-NH2	-7.12	116.74	120.30
5	E	53	ARG	NE-CZ-NH1	6.43	123.52	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	H	9	LYS	Peptide

5.2 Too-close contacts

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	4068	0	4048	86	0
1	N	4027	0	4001	90	0
2	B	1824	0	1833	34	0
2	O	1824	0	1833	48	0
3	C	2110	0	2027	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	P	2110	0	2027	18	0
4	D	1195	0	1183	12	0
4	Q	1195	0	1183	28	0
5	E	852	0	845	4	0
5	R	852	0	845	13	0
6	F	748	0	728	24	0
6	S	748	0	728	17	0
7	G	675	0	643	23	0
7	T	675	0	643	29	0
8	H	662	0	623	9	0
8	U	662	0	623	7	0
9	I	609	0	622	11	0
9	V	617	0	631	7	0
10	J	460	0	459	3	0
10	W	460	0	459	13	0
11	K	384	0	366	5	0
11	X	384	0	366	7	0
12	L	380	0	380	20	0
12	Y	380	0	380	9	0
13	M	335	0	352	7	0
13	Z	335	0	352	8	0
14	A	120	0	108	13	0
14	N	120	0	108	11	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	2	0	0	1	0
18	N	2	0	0	2	0
19	A	63	0	110	3	0
19	D	63	0	110	5	0
19	L	63	0	110	9	0
19	O	63	0	110	7	0
19	Q	63	0	110	5	0
19	Y	63	0	110	3	0
20	A	102	0	152	5	0
20	C	102	0	152	4	0
20	N	102	0	152	6	0
20	P	102	0	152	3	0
21	A	16	0	24	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	B	8	0	12	1	0
21	C	16	0	24	2	0
21	F	8	0	12	2	0
21	G	4	0	6	0	0
21	H	4	0	6	2	0
21	K	8	0	12	0	0
21	L	4	0	6	0	0
21	N	8	0	12	3	0
21	O	4	0	6	0	0
21	P	8	0	12	0	0
21	T	4	0	6	4	0
22	B	2	0	0	0	0
22	O	2	0	0	0	0
23	B	29	0	39	1	0
23	C	58	0	78	5	0
23	G	29	0	39	1	0
23	J	29	0	38	0	0
23	P	58	0	78	6	0
23	W	29	0	38	9	0
24	B	52	0	80	4	0
24	O	52	0	80	5	0
25	C	1	0	0	0	0
25	P	1	0	0	0	0
26	C	100	0	156	6	0
26	G	100	0	156	6	0
26	P	100	0	156	7	0
26	T	100	0	156	21	0
27	C	53	0	77	3	0
27	G	106	0	154	6	0
27	T	159	0	231	13	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	M	33	0	42	0	0
29	Z	33	0	42	2	0
30	A	191	0	0	17	0
30	B	121	0	0	5	0
30	C	83	0	0	16	0
30	D	89	0	0	1	0
30	E	45	0	0	2	0
30	F	49	0	0	2	0
30	G	40	0	0	6	0
30	H	37	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	I	19	0	0	0	0
30	J	19	0	0	1	0
30	K	27	0	0	1	0
30	L	27	0	0	6	0
30	M	18	0	0	0	0
30	N	169	0	0	22	0
30	O	101	0	0	21	0
30	P	91	0	0	7	0
30	Q	38	0	0	8	0
30	R	40	0	0	0	0
30	S	55	0	0	5	0
30	T	45	0	0	3	0
30	U	27	0	0	0	0
30	V	23	0	0	1	0
30	W	23	0	0	4	0
30	X	16	0	0	1	0
30	Y	18	0	0	3	0
30	Z	4	0	0	0	0
All	All	32242	0	31442	611	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 10.

The worst 5 of 611 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:PHE:HE1	30:A:867:HOH:O	1.15	1.25
1:N:312:ILE:HB	30:N:844:HOH:O	1.31	1.23
7:G:50:TYR:HA	30:G:208:HOH:O	1.07	1.23
30:A:704:HOH:O	3:C:17:PRO:HB3	1.34	1.21
3:P:246:ASP:HB2	30:P:464:HOH:O	1.35	1.20

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	519/514 (101%)	503 (97%)	16 (3%)	0	100	100
1	N	512/514 (100%)	493 (96%)	19 (4%)	0	100	100
2	B	225/227 (99%)	215 (96%)	10 (4%)	0	100	100
2	O	225/227 (99%)	217 (96%)	6 (3%)	2 (1%)	17	16
3	C	257/261 (98%)	251 (98%)	5 (2%)	1 (0%)	34	37
3	P	257/261 (98%)	253 (98%)	4 (2%)	0	100	100
4	D	142/147 (97%)	139 (98%)	3 (2%)	0	100	100
4	Q	142/147 (97%)	137 (96%)	4 (3%)	1 (1%)	22	22
5	E	103/109 (94%)	101 (98%)	2 (2%)	0	100	100
5	R	103/109 (94%)	101 (98%)	2 (2%)	0	100	100
6	F	96/98 (98%)	89 (93%)	4 (4%)	3 (3%)	4	2
6	S	96/98 (98%)	88 (92%)	8 (8%)	0	100	100
7	G	81/85 (95%)	69 (85%)	9 (11%)	3 (4%)	3	1
7	T	81/85 (95%)	69 (85%)	5 (6%)	7 (9%)	1	0
8	H	77/85 (91%)	71 (92%)	4 (5%)	2 (3%)	5	3
8	U	77/85 (91%)	70 (91%)	4 (5%)	3 (4%)	3	1
9	I	72/73 (99%)	71 (99%)	1 (1%)	0	100	100
9	V	73/73 (100%)	71 (97%)	1 (1%)	1 (1%)	11	8
10	J	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
10	W	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
11	K	47/56 (84%)	47 (100%)	0	0	100	100
11	X	47/56 (84%)	42 (89%)	5 (11%)	0	100	100
12	L	44/47 (94%)	44 (100%)	0	0	100	100
12	Y	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
13	M	41/46 (89%)	41 (100%)	0	0	100	100
13	Z	41/46 (89%)	41 (100%)	0	0	100	100
All	All	3514/3614 (97%)	3374 (96%)	117 (3%)	23 (1%)	22	22

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	94	HIS
6	F	96	LEU
7	G	4	ALA
7	G	39	SER
7	T	4	ALA

5.3.2 Protein sidechains ⓘ

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	432/426 (101%)	423 (98%)	9 (2%)	53	67
1	N	426/426 (100%)	413 (97%)	13 (3%)	40	51
2	B	210/210 (100%)	204 (97%)	6 (3%)	42	54
2	O	210/210 (100%)	199 (95%)	11 (5%)	23	28
3	C	224/226 (99%)	218 (97%)	6 (3%)	44	57
3	P	224/226 (99%)	219 (98%)	5 (2%)	52	65
4	D	128/129 (99%)	122 (95%)	6 (5%)	26	33
4	Q	128/129 (99%)	124 (97%)	4 (3%)	40	51
5	E	92/95 (97%)	90 (98%)	2 (2%)	52	65
5	R	92/95 (97%)	87 (95%)	5 (5%)	22	26
6	F	81/81 (100%)	71 (88%)	10 (12%)	4	4
6	S	81/81 (100%)	72 (89%)	9 (11%)	6	5
7	G	67/68 (98%)	58 (87%)	9 (13%)	4	3
7	T	67/68 (98%)	60 (90%)	7 (10%)	7	6
8	H	71/75 (95%)	61 (86%)	10 (14%)	3	2
8	U	71/75 (95%)	67 (94%)	4 (6%)	21	25
9	I	58/57 (102%)	51 (88%)	7 (12%)	5	4
9	V	59/57 (104%)	53 (90%)	6 (10%)	7	6
10	J	49/50 (98%)	46 (94%)	3 (6%)	18	21
10	W	49/50 (98%)	46 (94%)	3 (6%)	18	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	39/46 (85%)	36 (92%)	3 (8%)	13	13
11	X	39/46 (85%)	36 (92%)	3 (8%)	13	13
12	L	39/40 (98%)	36 (92%)	3 (8%)	13	13
12	Y	39/40 (98%)	38 (97%)	1 (3%)	46	58
13	M	37/38 (97%)	33 (89%)	4 (11%)	6	6
13	Z	37/38 (97%)	33 (89%)	4 (11%)	6	6
All	All	3049/3082 (99%)	2896 (95%)	153 (5%)	24	30

5 of 153 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	K	32	MET
1	N	369	ASP
9	V	65	LYS
12	L	5	GLU
13	M	43	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
9	I	53	ASN
1	N	180	GLN
8	U	10	ASN
10	J	29	ASN
13	M	39	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	$\# Z > 2$
7	TPO	T	11	7	8,10,11	1.53	2 (25%)	10,14,16	1.10	1 (10%)
2	FME	B	1	2	8,9,10	1.12	0	7,9,11	5.86	2 (28%)
9	SAC	I	1	9	7,8,9	1.54	1 (14%)	8,9,11	1.05	0
7	TPO	G	11	7	8,10,11	1.72	2 (25%)	10,14,16	0.94	0
9	SAC	V	1	9	7,8,9	1.74	1 (14%)	8,9,11	1.68	2 (25%)
1	FME	N	1	1	8,9,10	0.47	0	7,9,11	3.11	3 (42%)
1	FME	A	1	1	8,9,10	0.97	0	7,9,11	5.70	4 (57%)
2	FME	O	1	2	8,9,10	1.07	1 (12%)	7,9,11	4.24	3 (42%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	TPO	T	11	7	-	3/9/11/13	-
2	FME	B	1	2	-	3/7/9/11	-
9	SAC	I	1	9	-	4/7/8/10	-
7	TPO	G	11	7	-	3/9/11/13	-
9	SAC	V	1	9	-	6/7/8/10	-
1	FME	N	1	1	-	4/7/9/11	-
1	FME	A	1	1	-	4/7/9/11	-
2	FME	O	1	2	-	2/7/9/11	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	V	1	SAC	CA-N	4.34	1.52	1.46
9	I	1	SAC	CA-N	3.81	1.51	1.46
7	G	11	TPO	P-O1P	2.85	1.59	1.50
7	T	11	TPO	P-O1P	2.78	1.59	1.50
7	G	11	TPO	P-OG1	2.52	1.64	1.59

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CA-N-CN	-14.94	99.85	122.82
1	A	1	FME	CA-N-CN	-13.87	101.50	122.82
2	O	1	FME	CA-N-CN	-10.10	107.28	122.82
1	N	1	FME	CA-N-CN	-7.45	111.36	122.82
2	O	1	FME	C-CA-N	3.84	116.67	109.73

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	T	11	TPO	N-CA-CB-CG2
7	T	11	TPO	N-CA-CB-OG1
7	T	11	TPO	C-CA-CB-CG2
2	B	1	FME	O1-CN-N-CA
9	I	1	SAC	C2A-C1A-N-CA

There are no ring outliers.

3 monomers are involved in 5 short contacts:

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 77 ligands modelled in this entry, 2 are unknown and 8 are monoatomic - leaving 67 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
23	CHD	B	302	-	29,32,32	0.70	0	48,51,51	1.42	10 (20%)
14	HEA	N	602	1	44,67,67	1.17	6 (13%)	37,103,103	2.07	10 (27%)
21	EDO	T	105	-	3,3,3	0.48	0	2,2,2	0.25	0
21	EDO	A	613	-	3,3,3	0.57	0	2,2,2	0.07	0
24	PSC	B	303	-	51,51,51	1.20	3 (5%)	57,59,59	1.13	4 (7%)
21	EDO	F	103	-	3,3,3	0.53	0	2,2,2	0.41	0
21	EDO	C	311	-	3,3,3	0.73	0	2,2,2	0.41	0
21	EDO	F	102	-	3,3,3	0.54	0	2,2,2	0.12	0
22	CUA	O	301	2,30	0,1,1	0.00	-	-		
14	HEA	A	601	1	44,67,67	0.90	1 (2%)	37,103,103	1.88	9 (24%)
20	PGV	C	302	-	50,50,50	0.88	2 (4%)	53,56,56	0.95	4 (7%)
23	CHD	C	304	-	29,32,32	0.49	0	48,51,51	2.00	17 (35%)
29	DMU	Z	101	-	34,34,34	0.49	0	45,45,45	0.85	2 (4%)
26	CDL	G	102	-	99,99,99	1.43	12 (12%)	105,111,111	1.21	9 (8%)
21	EDO	B	305	-	3,3,3	0.52	0	2,2,2	0.85	0
21	EDO	A	612	-	3,3,3	0.47	0	2,2,2	0.35	0
23	CHD	J	101	-	29,32,32	0.64	0	48,51,51	1.88	9 (18%)
21	EDO	A	610	-	3,3,3	0.49	0	2,2,2	0.29	0
21	EDO	K	102	-	3,3,3	0.47	0	2,2,2	0.30	0
21	EDO	P	307	-	3,3,3	0.54	0	2,2,2	0.17	0
14	HEA	A	602	1	44,67,67	1.23	3 (6%)	37,103,103	2.10	11 (29%)
21	EDO	L	102	-	3,3,3	0.41	0	2,2,2	0.31	0
20	PGV	N	607	-	50,50,50	1.04	2 (4%)	53,56,56	1.11	5 (9%)
24	PSC	O	303	-	51,51,51	1.19	3 (5%)	57,59,59	1.05	4 (7%)
21	EDO	N	609	-	3,3,3	0.41	0	2,2,2	0.65	0
27	PEK	T	103	-	52,52,52	1.13	2 (3%)	55,57,57	0.94	2 (3%)
20	PGV	N	608	-	50,50,50	0.87	2 (4%)	53,56,56	1.08	4 (7%)
27	PEK	G	103	-	52,52,52	1.17	2 (3%)	55,57,57	1.07	5 (9%)
21	EDO	P	308	-	3,3,3	0.59	0	2,2,2	0.16	0
21	EDO	G	105	-	3,3,3	0.42	0	2,2,2	0.56	0
27	PEK	T	102	-	52,52,52	1.12	2 (3%)	55,57,57	0.98	5 (9%)
19	TGL	O	302	-	62,62,62	1.12	3 (4%)	65,65,65	1.24	7 (10%)
19	TGL	Q	201	-	62,62,62	1.14	3 (4%)	65,65,65	1.05	5 (7%)
27	PEK	T	101	-	52,52,52	0.90	3 (5%)	55,57,57	1.01	3 (5%)
21	EDO	C	309	-	3,3,3	0.52	0	2,2,2	0.22	0
19	TGL	Y	101	-	62,62,62	1.14	3 (4%)	65,65,65	1.24	6 (9%)
23	CHD	C	305	-	29,32,32	0.84	1 (3%)	48,51,51	1.75	10 (20%)
18	CMO	N	606	-	0,1,1	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	PGV	C	307	-	50,50,50	1.04	2 (4%)	53,56,56	0.92	3 (5%)
27	PEK	G	101	-	52,52,52	0.87	3 (5%)	55,57,57	1.37	4 (7%)
23	CHD	P	305	-	29,32,32	0.51	0	48,51,51	1.80	14 (29%)
23	CHD	G	104	-	29,32,32	1.15	2 (6%)	48,51,51	1.48	9 (18%)
21	EDO	O	304	-	3,3,3	0.40	0	2,2,2	0.69	0
14	HEA	N	601	1	44,67,67	0.97	1 (2%)	37,103,103	1.44	7 (18%)
26	CDL	C	303	-	99,99,99	1.39	12 (12%)	105,111,111	1.23	9 (8%)
18	CMO	A	606	15	0,1,1	0.00	-	-		
22	CUA	B	301	2	0,1,1	0.00	-	-		
19	TGL	L	101	-	62,62,62	1.19	3 (4%)	65,65,65	1.43	8 (12%)
27	PEK	C	306	-	52,52,52	1.18	3 (5%)	55,57,57	1.17	5 (9%)
21	EDO	N	610	-	3,3,3	0.41	0	2,2,2	0.19	0
21	EDO	B	304	-	3,3,3	0.35	0	2,2,2	0.63	0
21	EDO	K	101	-	3,3,3	0.52	0	2,2,2	0.29	0
20	PGV	P	301	-	50,50,50	1.07	2 (4%)	53,56,56	1.11	4 (7%)
26	CDL	P	304	-	99,99,99	1.42	12 (12%)	105,111,111	1.27	7 (6%)
29	DMU	M	101	-	34,34,34	0.46	0	45,45,45	0.94	1 (2%)
20	PGV	P	303	-	50,50,50	0.86	3 (6%)	53,56,56	1.17	7 (13%)
23	CHD	P	306	-	29,32,32	0.78	0	48,51,51	1.66	11 (22%)
21	EDO	H	101	-	3,3,3	0.53	0	2,2,2	0.20	0
19	TGL	D	201	-	62,62,62	1.30	3 (4%)	65,65,65	1.07	6 (9%)
21	EDO	A	611	-	3,3,3	0.39	0	2,2,2	1.09	0
21	EDO	C	308	-	3,3,3	0.41	0	2,2,2	0.38	0
20	PGV	A	608	-	50,50,50	0.87	2 (4%)	53,56,56	1.45	4 (7%)
21	EDO	C	310	-	3,3,3	0.57	0	2,2,2	0.35	0
20	PGV	A	609	-	50,50,50	1.04	2 (4%)	53,56,56	1.17	7 (13%)
23	CHD	W	101	-	29,32,32	0.85	0	48,51,51	4.20	25 (52%)
26	CDL	T	104	-	99,99,99	1.37	12 (12%)	105,111,111	1.16	5 (4%)
19	TGL	A	607	-	62,62,62	1.19	4 (6%)	65,65,65	1.69	8 (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
23	CHD	B	302	-	-	1/7/74/74	0/4/4/4
14	HEA	N	602	1	-	4/24/76/76	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	EDO	T	105	-	-	1/1/1/1	-
21	EDO	A	613	-	-	1/1/1/1	-
24	PSC	B	303	-	-	38/55/55/55	-
21	EDO	F	103	-	-	0/1/1/1	-
21	EDO	C	311	-	-	0/1/1/1	-
21	EDO	F	102	-	-	0/1/1/1	-
20	PGV	C	302	-	-	10/55/55/55	-
23	CHD	C	304	-	-	0/7/74/74	0/4/4/4
29	DMU	Z	101	-	-	5/19/59/59	0/2/2/2
26	CDL	G	102	-	-	66/110/110/110	-
21	EDO	B	305	-	-	1/1/1/1	-
21	EDO	A	612	-	-	1/1/1/1	-
23	CHD	J	101	-	-	6/7/74/74	0/4/4/4
21	EDO	A	610	-	-	0/1/1/1	-
21	EDO	K	102	-	-	1/1/1/1	-
21	EDO	P	307	-	-	0/1/1/1	-
14	HEA	A	601	1	2/2/7/16	0/24/76/76	-
20	PGV	N	607	-	-	28/55/55/55	-
24	PSC	O	303	-	-	34/55/55/55	-
21	EDO	N	609	-	-	0/1/1/1	-
27	PEK	T	103	-	-	31/56/56/56	-
20	PGV	N	608	-	-	14/55/55/55	-
27	PEK	G	103	-	-	28/56/56/56	-
21	EDO	P	308	-	-	1/1/1/1	-
21	EDO	G	105	-	-	0/1/1/1	-
27	PEK	T	102	-	-	29/56/56/56	-
19	TGL	O	302	-	-	36/65/65/65	-
19	TGL	Q	201	-	-	35/65/65/65	-
27	PEK	T	101	-	-	23/56/56/56	-
21	EDO	C	309	-	-	0/1/1/1	-
19	TGL	Y	101	-	-	43/65/65/65	-
23	CHD	C	305	-	-	2/7/74/74	0/4/4/4
14	HEA	A	602	1	-	0/24/76/76	-
20	PGV	C	307	-	-	28/55/55/55	-
27	PEK	G	101	-	-	19/56/56/56	-
23	CHD	P	305	-	-	3/7/74/74	1/4/4/4
21	EDO	L	102	-	-	1/1/1/1	-
23	CHD	G	104	-	-	1/7/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	EDO	O	304	-	-	1/1/1/1	-
14	HEA	N	601	1	3/3/7/16	0/24/76/76	-
26	CDL	C	303	-	-	58/110/110/110	-
19	TGL	L	101	-	-	39/65/65/65	-
27	PEK	C	306	-	-	30/56/56/56	-
21	EDO	N	610	-	-	0/1/1/1	-
21	EDO	B	304	-	-	1/1/1/1	-
21	EDO	K	101	-	-	1/1/1/1	-
20	PGV	P	301	-	-	25/55/55/55	-
26	CDL	P	304	-	-	64/110/110/110	-
29	DMU	M	101	-	-	7/19/59/59	0/2/2/2
20	PGV	P	303	-	-	20/55/55/55	-
23	CHD	P	306	-	-	0/7/74/74	0/4/4/4
21	EDO	H	101	-	-	0/1/1/1	-
19	TGL	D	201	-	-	37/65/65/65	-
21	EDO	A	611	-	-	1/1/1/1	-
21	EDO	C	308	-	-	1/1/1/1	-
20	PGV	A	608	-	-	15/55/55/55	-
21	EDO	C	310	-	-	0/1/1/1	-
20	PGV	A	609	-	-	38/55/55/55	-
23	CHD	W	101	-	-	5/7/74/74	0/4/4/4
26	CDL	T	104	-	-	61/110/110/110	-
19	TGL	A	607	-	-	42/65/65/65	-

The worst 5 of 119 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	L	101	TGL	OG2-CB1	5.61	1.50	1.34
19	D	201	TGL	OG2-CB1	5.59	1.50	1.34
26	P	304	CDL	OA6-CA5	5.57	1.50	1.34
19	A	607	TGL	OG2-CB1	5.52	1.49	1.34
26	G	102	CDL	OB8-CB7	5.49	1.49	1.33

The worst 5 of 285 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	101	CHD	C14-C8-C9	-13.54	91.13	109.71
23	W	101	CHD	C18-C13-C12	-9.16	99.74	109.07
23	W	101	CHD	C14-C13-C12	9.14	115.91	107.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	101	CHD	C10-C9-C8	8.27	120.70	111.82
19	A	607	TGL	OG2-CB1-CB2	8.22	129.22	111.50

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	A	601	HEA	ND
14	A	601	HEA	NB
14	N	601	HEA	ND
14	N	601	HEA	NA
14	N	601	HEA	NB

5 of 937 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	T	102	PEK	C03-O11-P-O13
27	T	102	PEK	C12-C13-C14-C15
26	G	102	CDL	O1-C1-CA2-OA2
26	G	102	CDL	CA2-OA2-PA1-OA3
26	G	102	CDL	CA2-OA2-PA1-OA4

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	P	305	CHD	C1-C10-C2-C3-C4-C5

48 monomers are involved in 198 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	302	CHD	1	0
14	N	602	HEA	5	0
21	T	105	EDO	4	0
21	A	613	EDO	7	0
24	B	303	PSC	4	0
21	F	103	EDO	1	0
21	C	311	EDO	2	0
21	F	102	EDO	1	0
14	A	601	HEA	5	0
23	C	304	CHD	4	0
29	Z	101	DMU	2	0
26	G	102	CDL	6	0
21	A	612	EDO	12	0

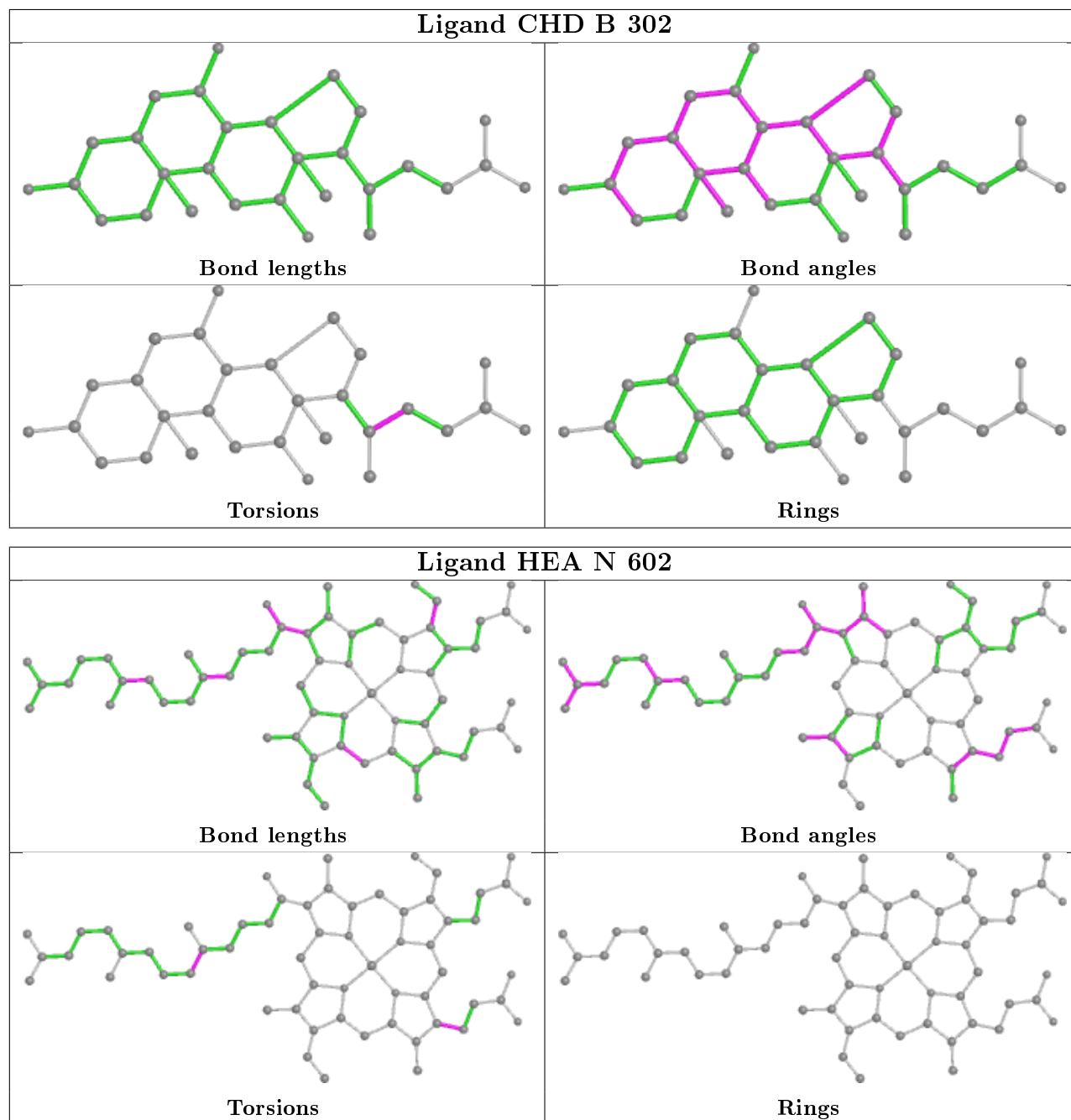
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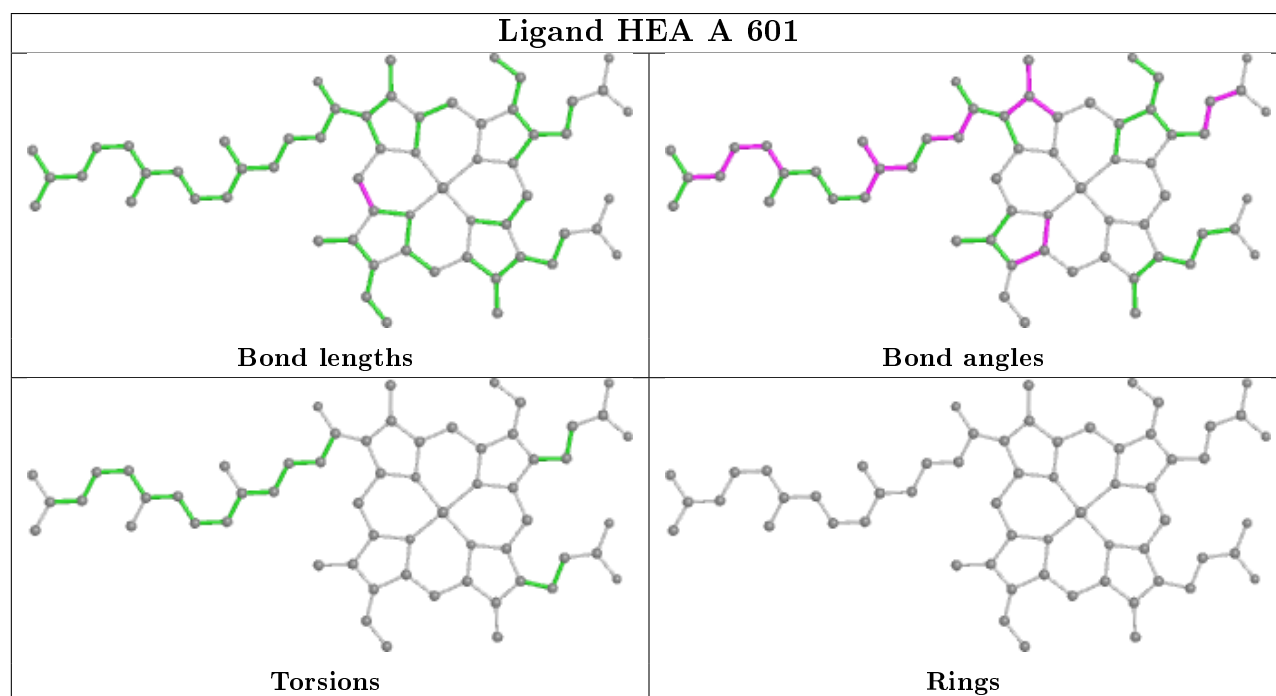
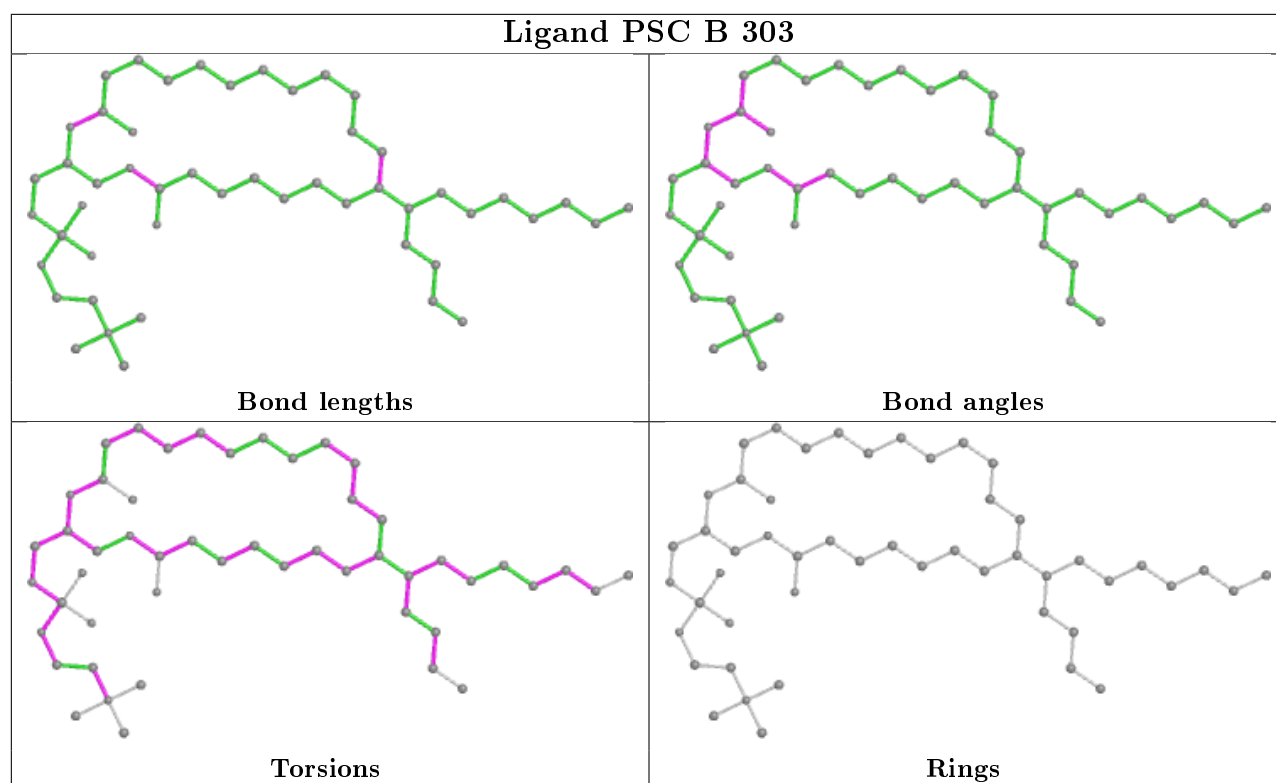
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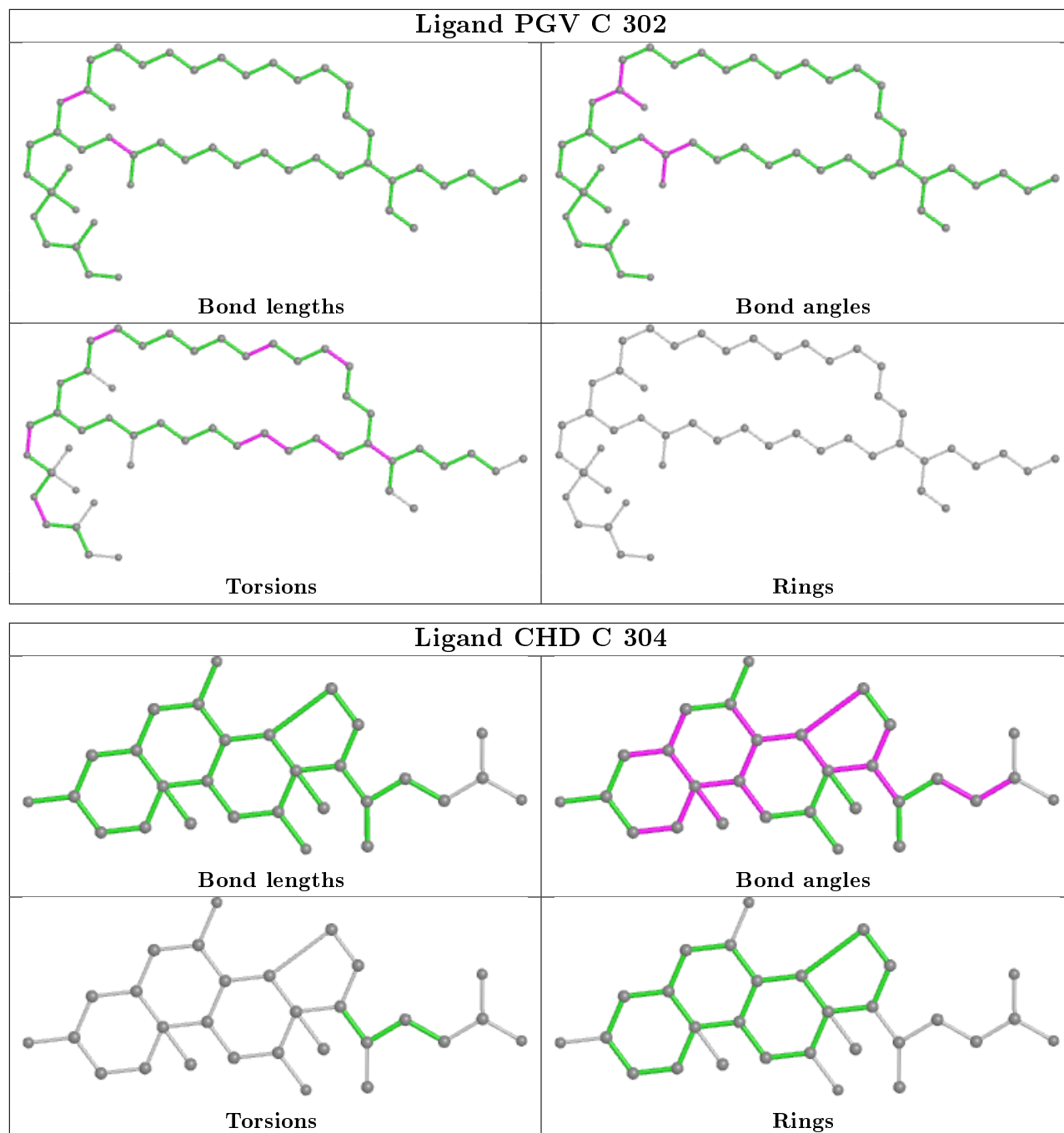
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	602	HEA	8	0
20	N	607	PGV	5	0
24	O	303	PSC	5	0
27	T	103	PEK	2	0
20	N	608	PGV	1	0
27	G	103	PEK	3	0
27	T	102	PEK	8	0
19	O	302	TGL	7	0
19	Q	201	TGL	5	0
27	T	101	PEK	3	0
19	Y	101	TGL	3	0
23	C	305	CHD	1	0
18	N	606	CMO	2	0
20	C	307	PGV	4	0
27	G	101	PEK	3	0
23	P	305	CHD	3	0
23	G	104	CHD	1	0
14	N	601	HEA	6	0
26	C	303	CDL	6	0
18	A	606	CMO	1	0
19	L	101	TGL	9	0
27	C	306	PEK	3	0
21	N	610	EDO	3	0
21	B	304	EDO	1	0
20	P	301	PGV	2	0
26	P	304	CDL	7	0
20	P	303	PGV	1	0
23	P	306	CHD	3	0
21	H	101	EDO	2	0
19	D	201	TGL	5	0
20	A	608	PGV	1	0
20	A	609	PGV	4	0
23	W	101	CHD	9	0
26	T	104	CDL	21	0
19	A	607	TGL	3	0

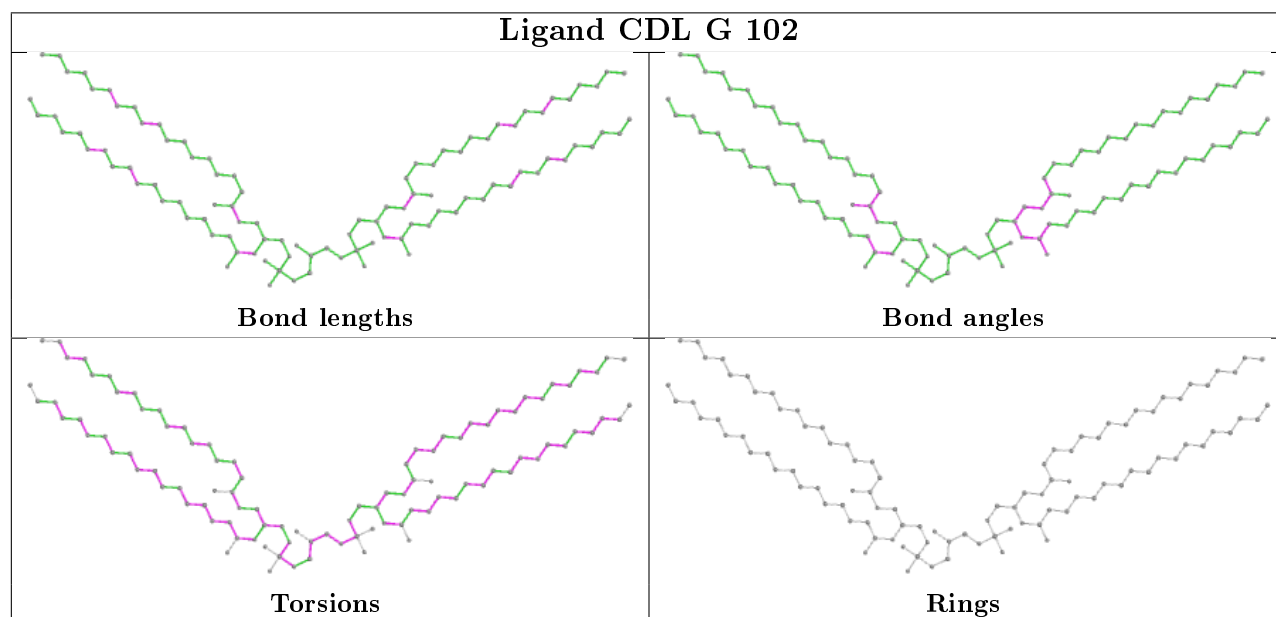
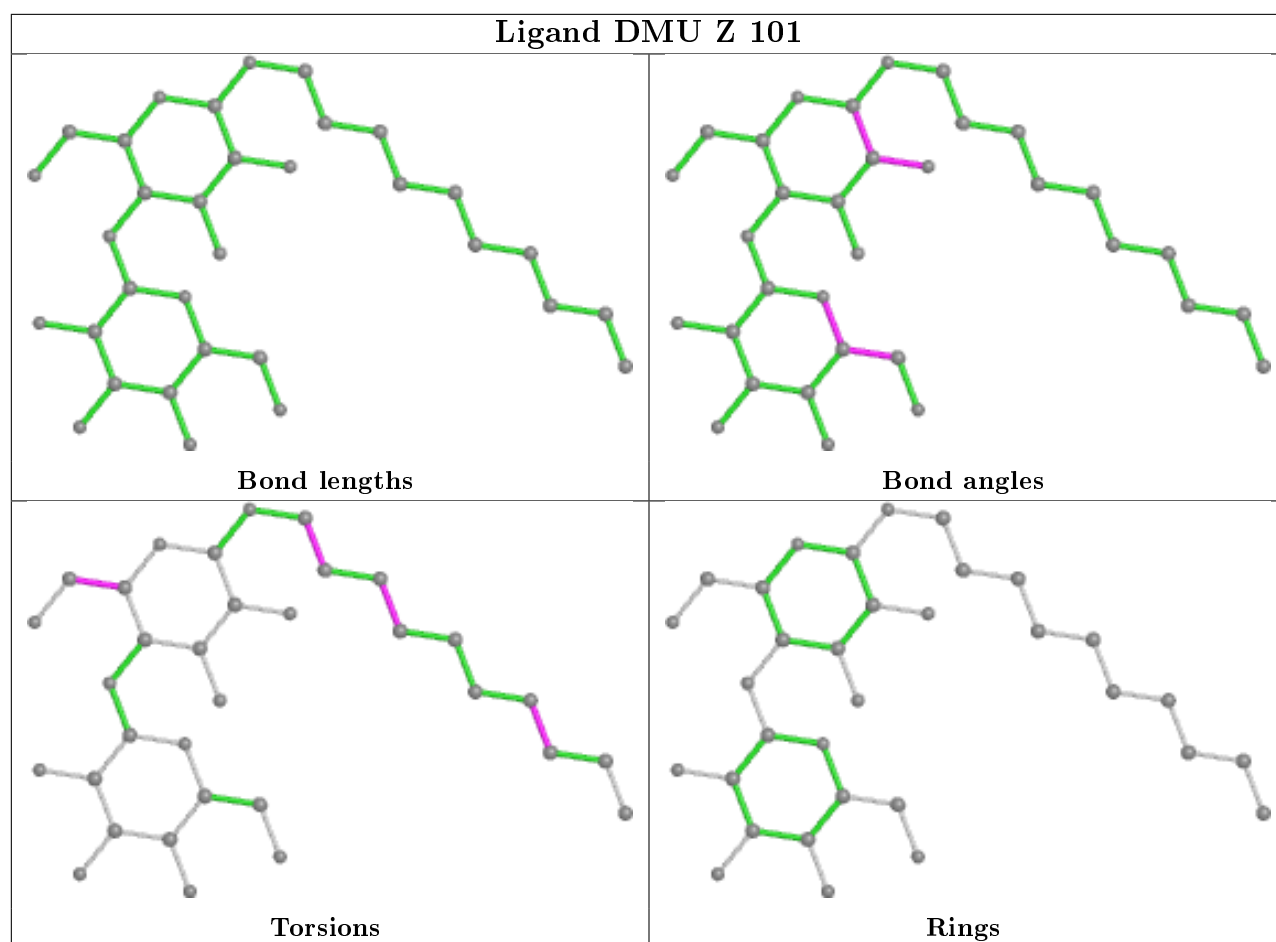
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.

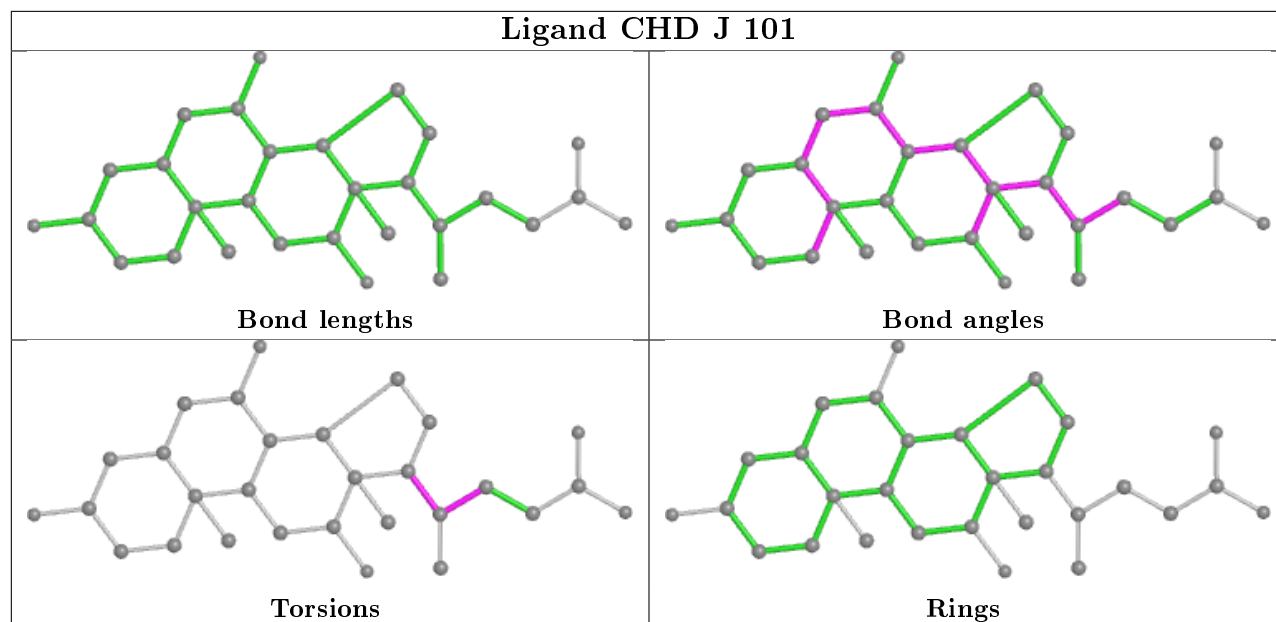




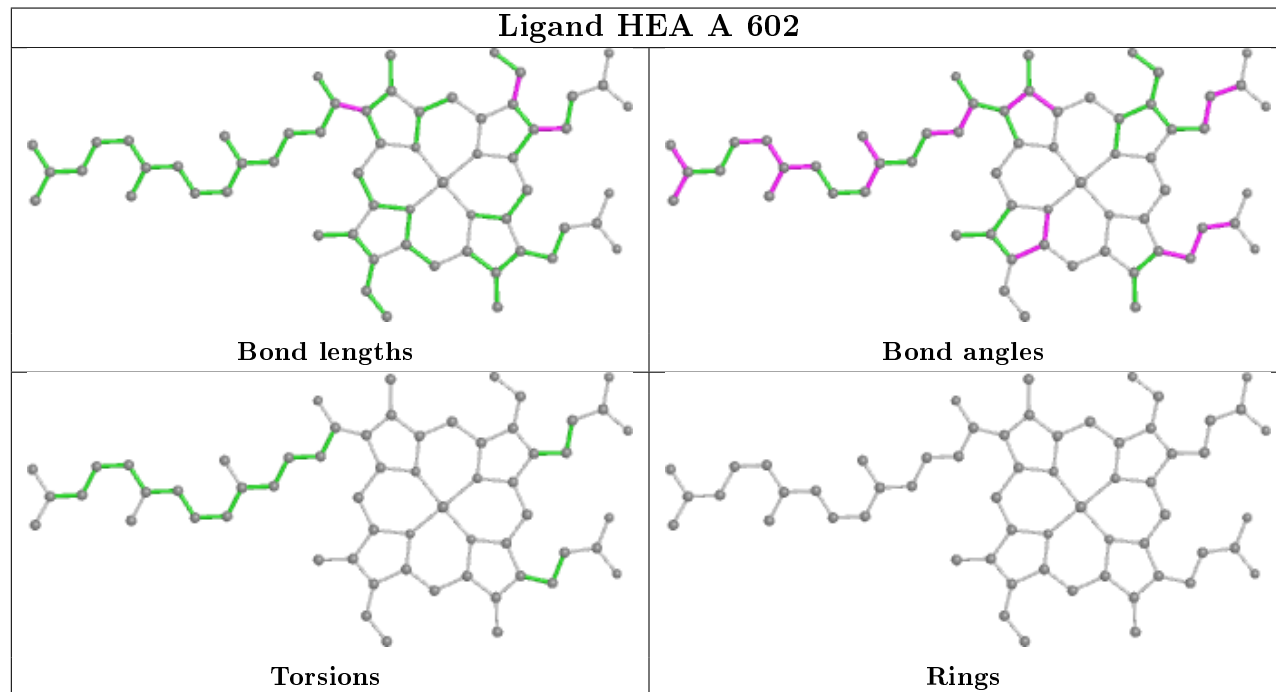


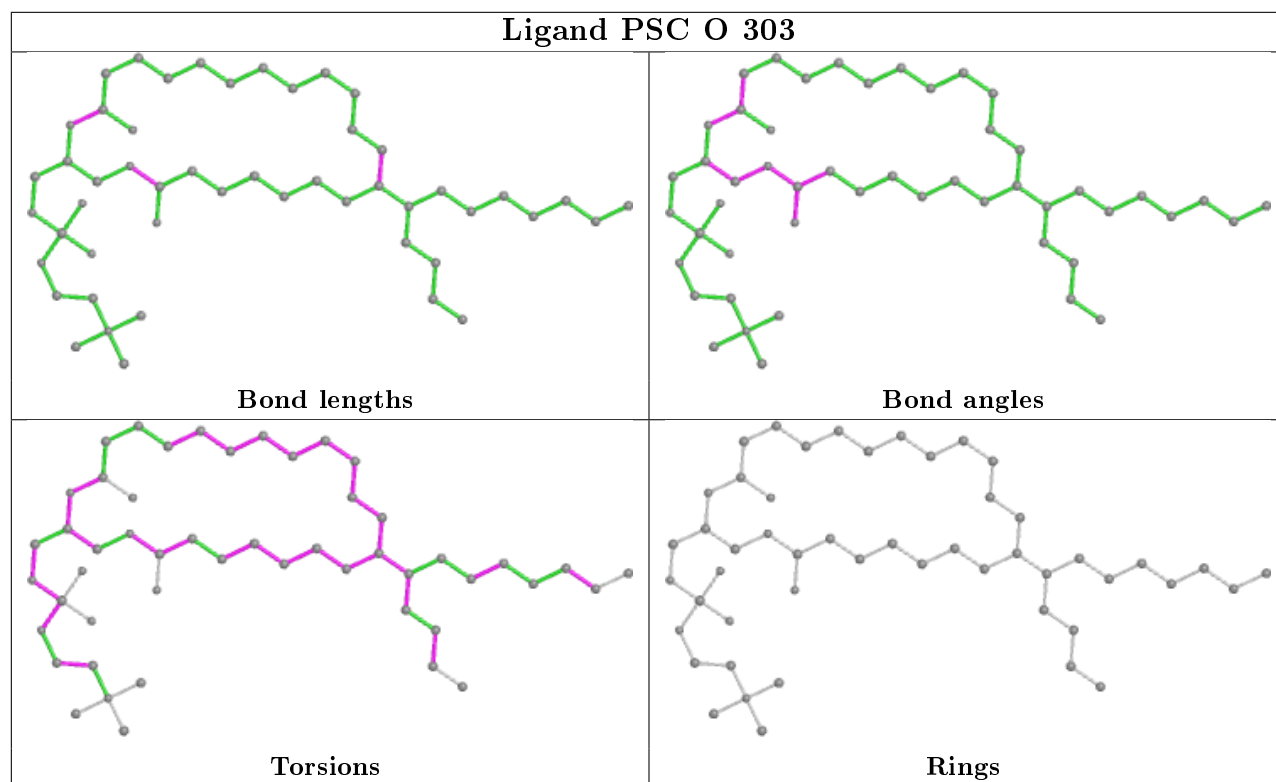
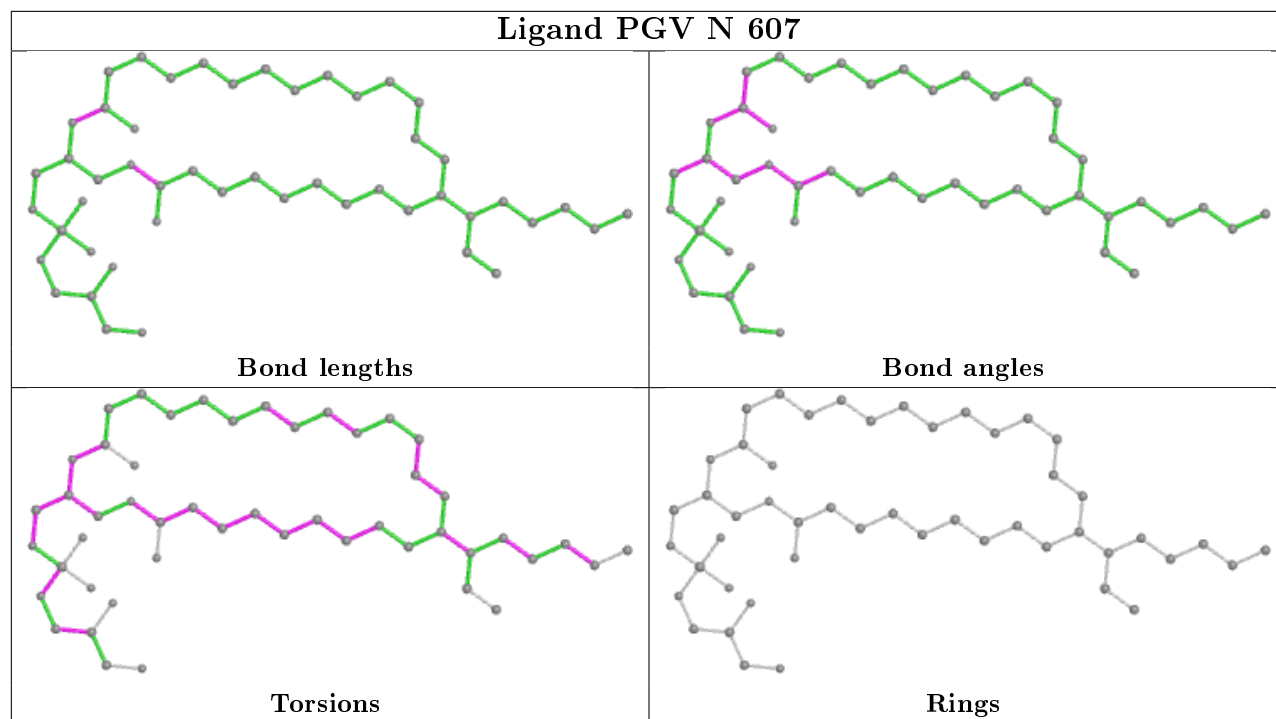


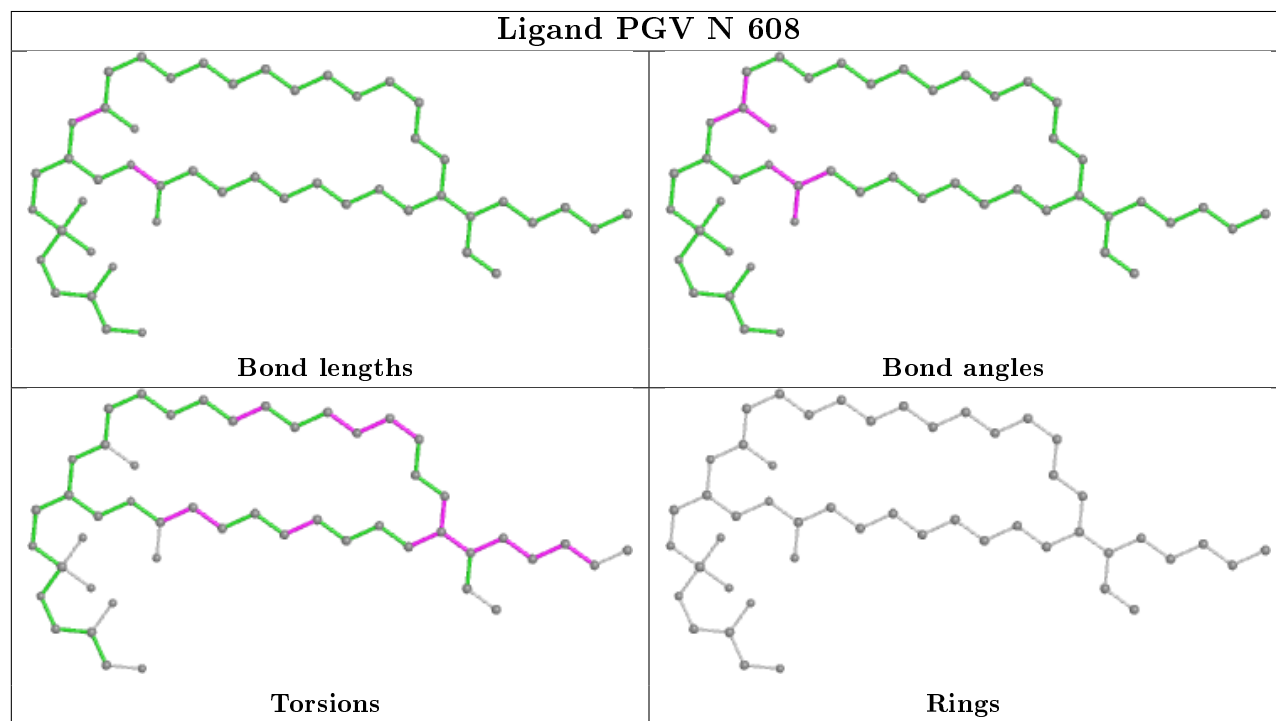
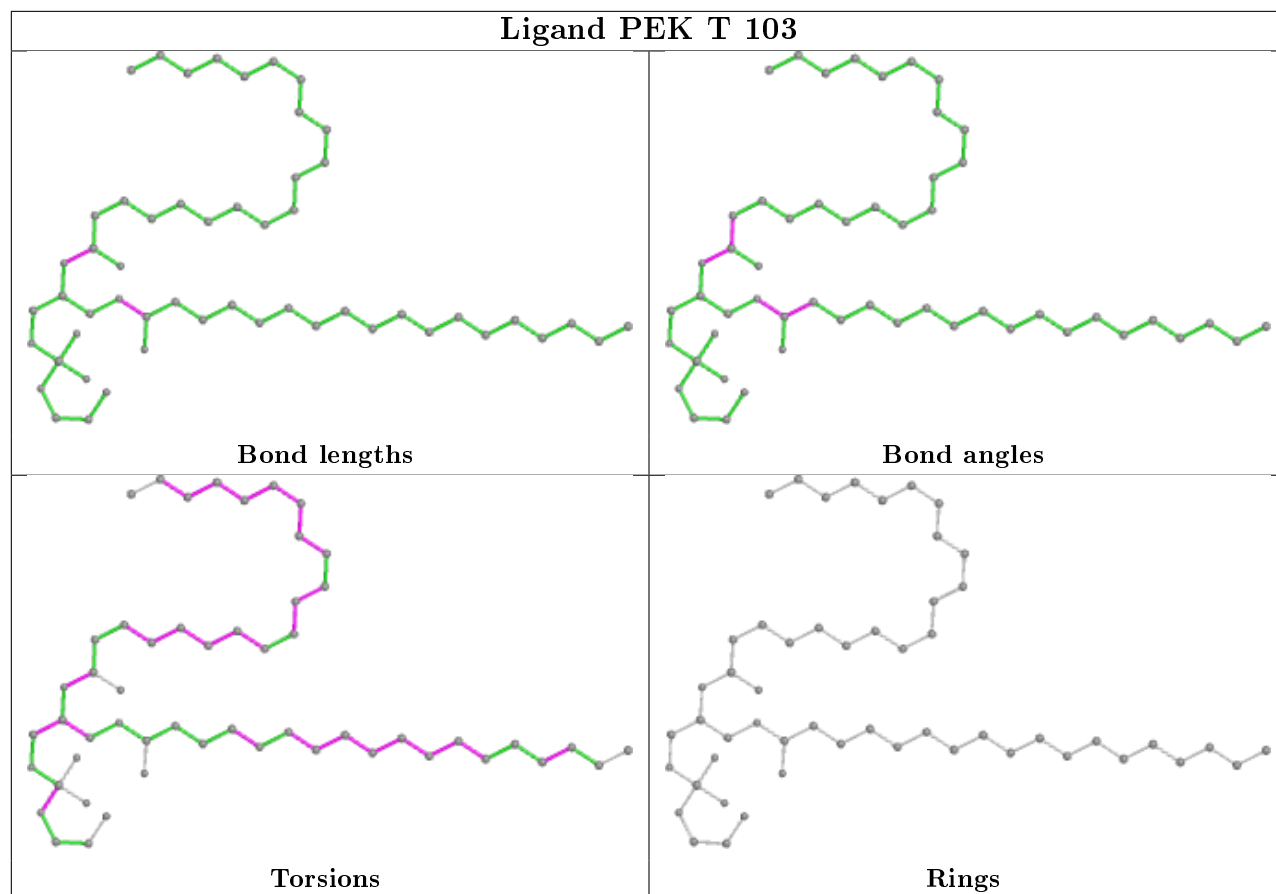
Ligand CHD J 101

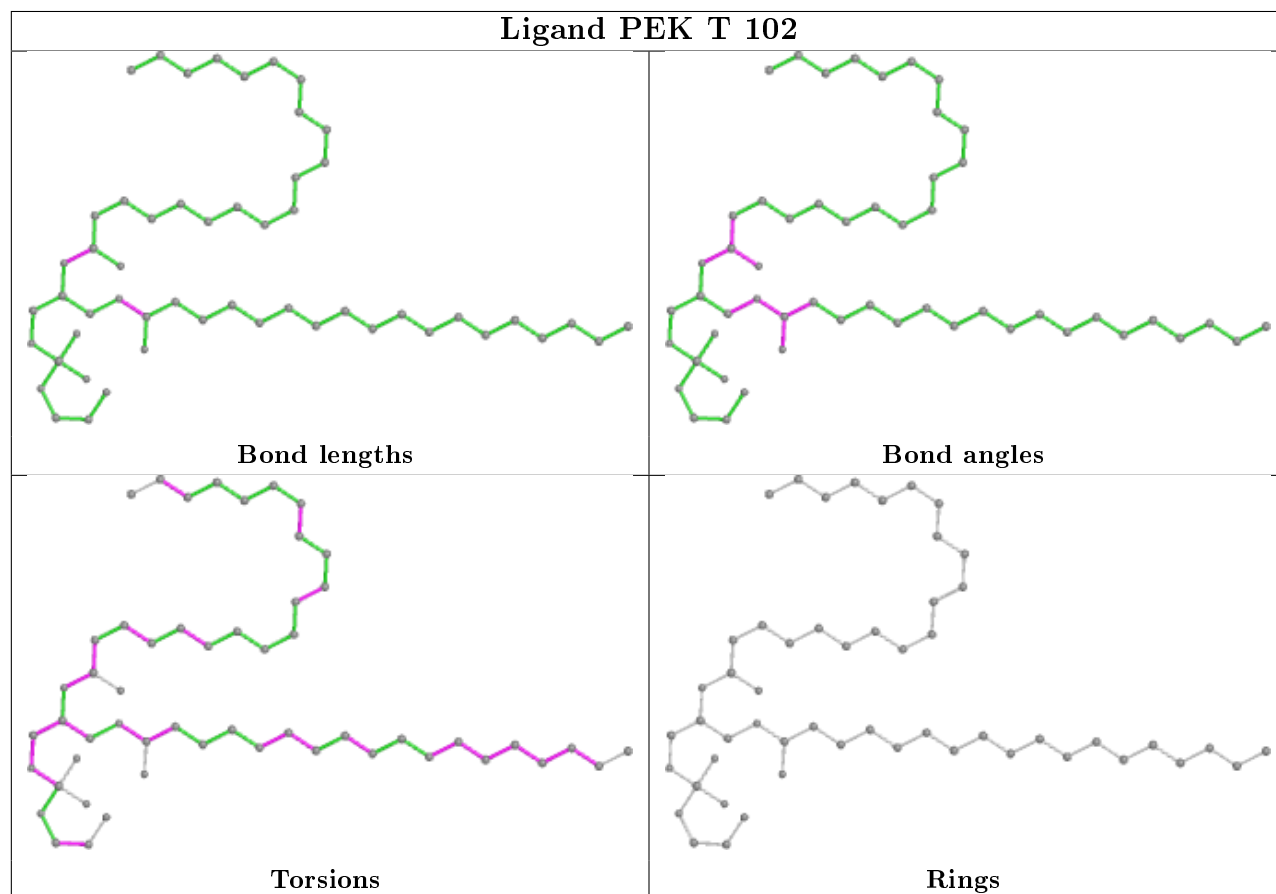
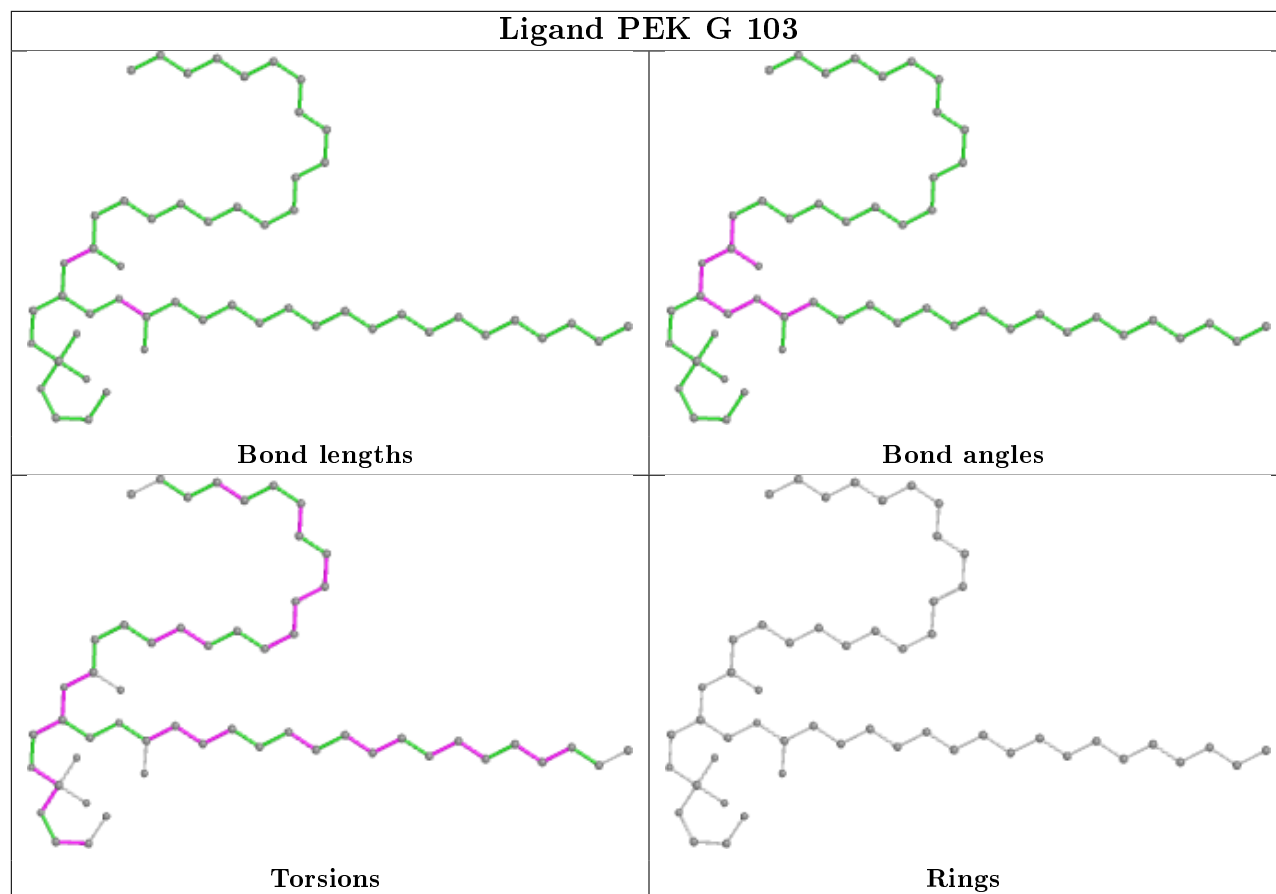


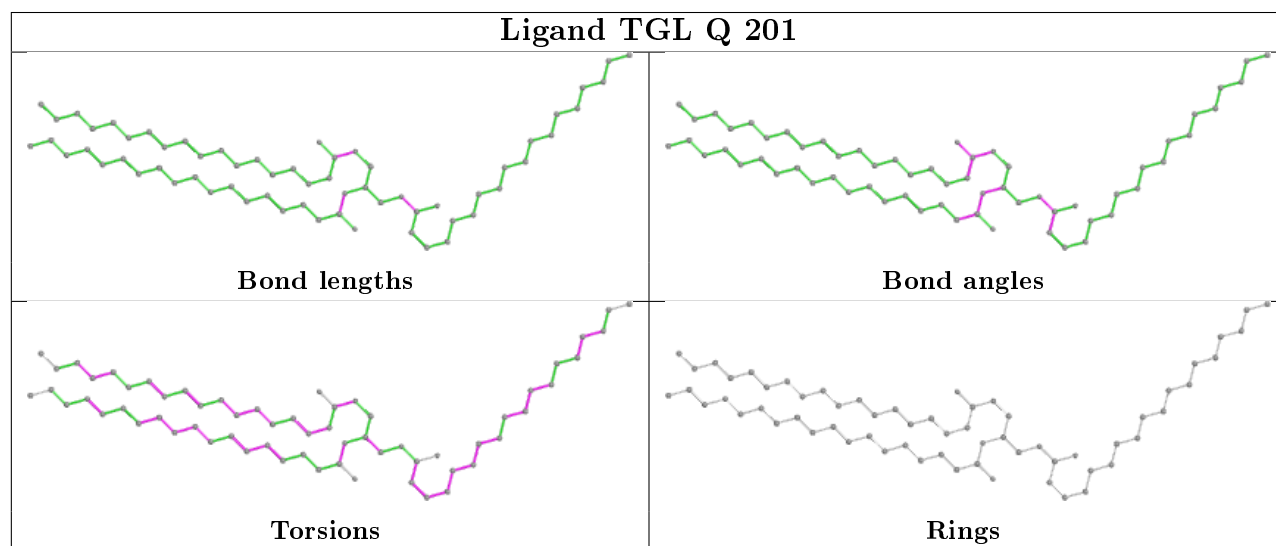
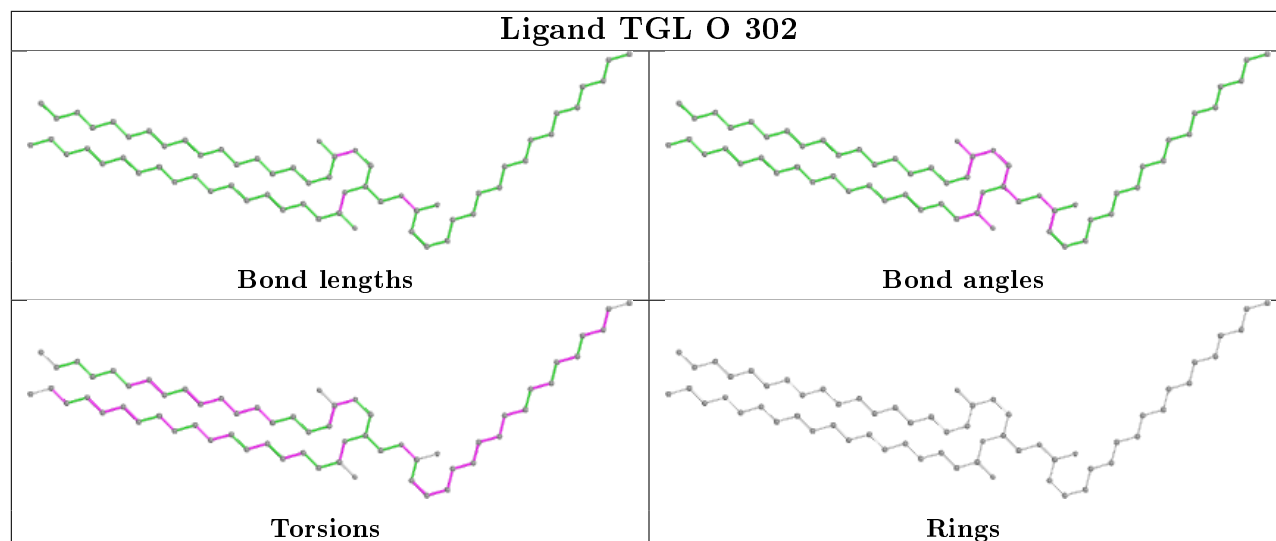
Ligand HEA A 602

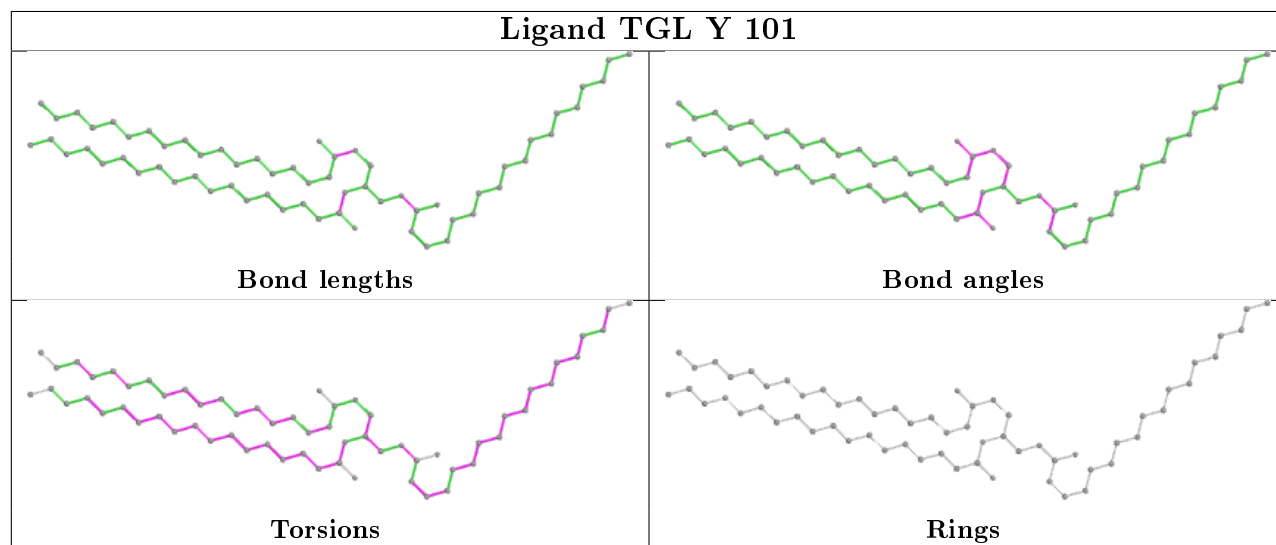
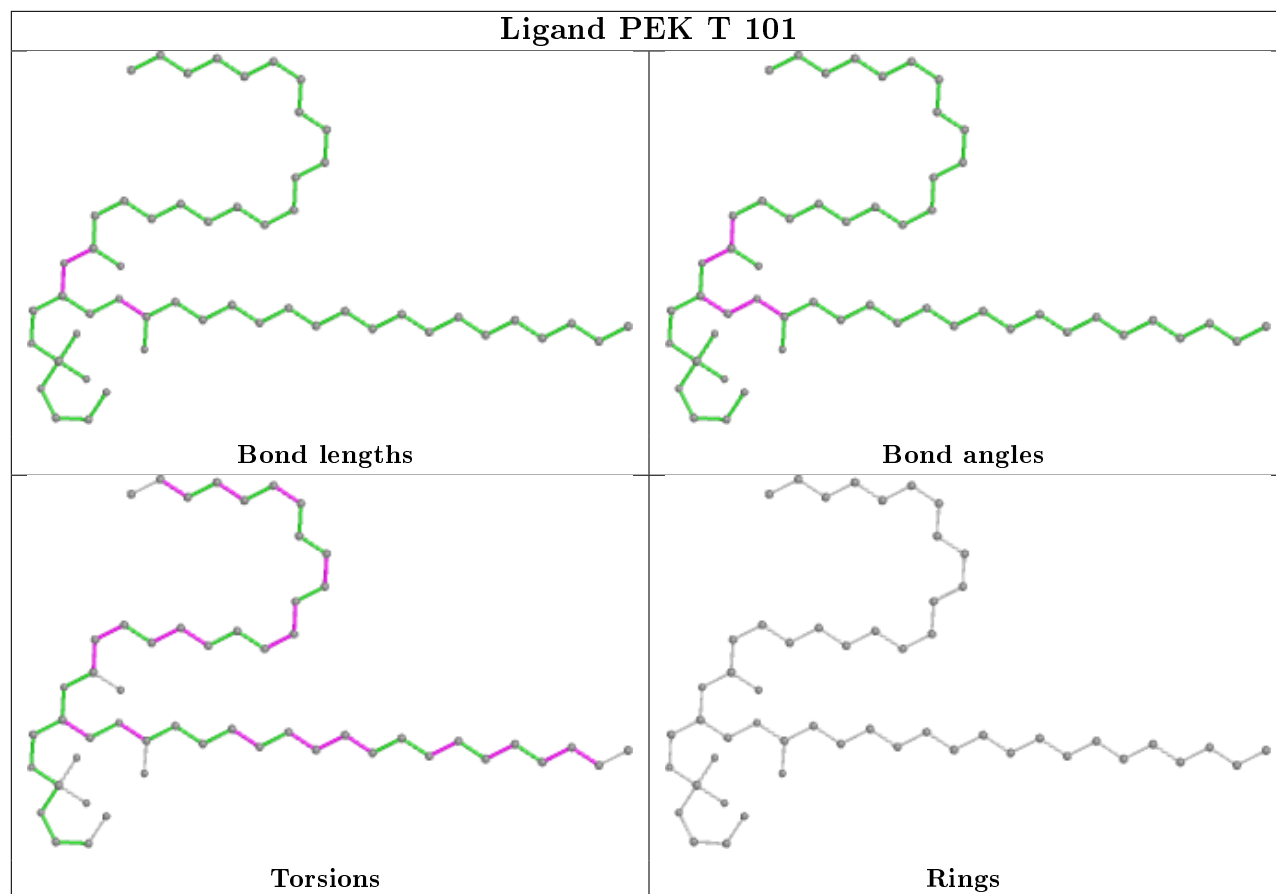


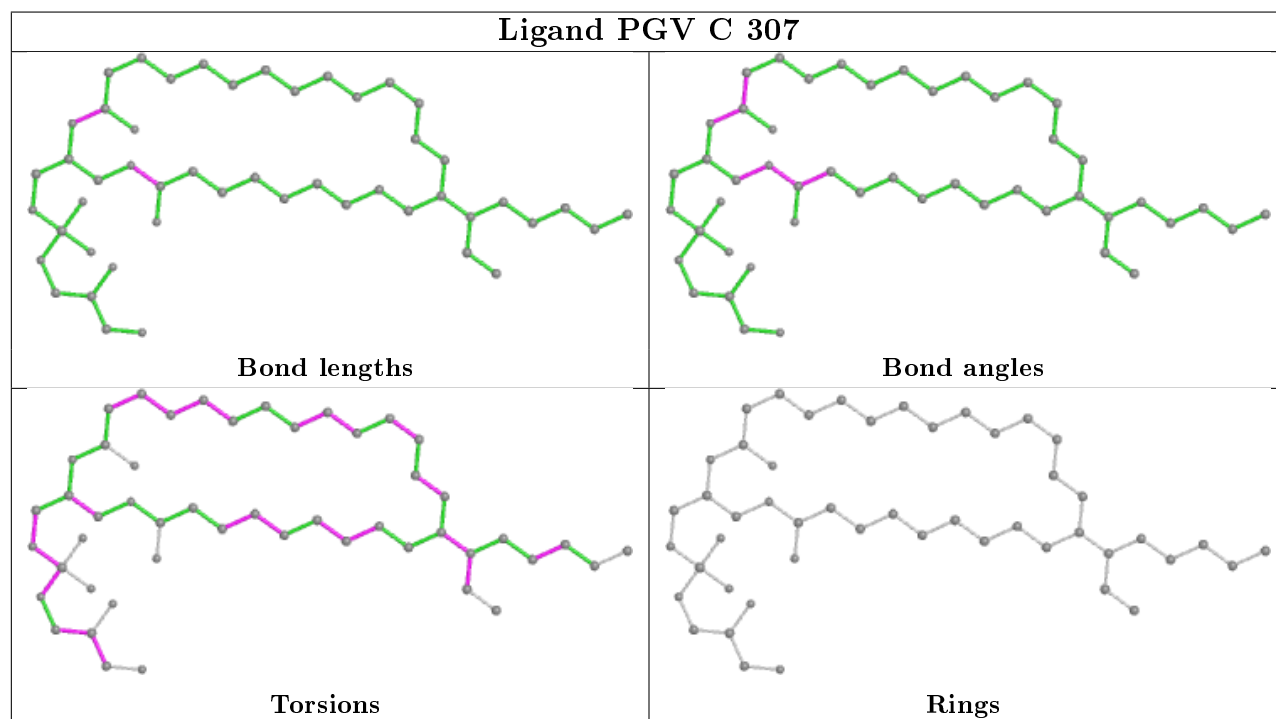
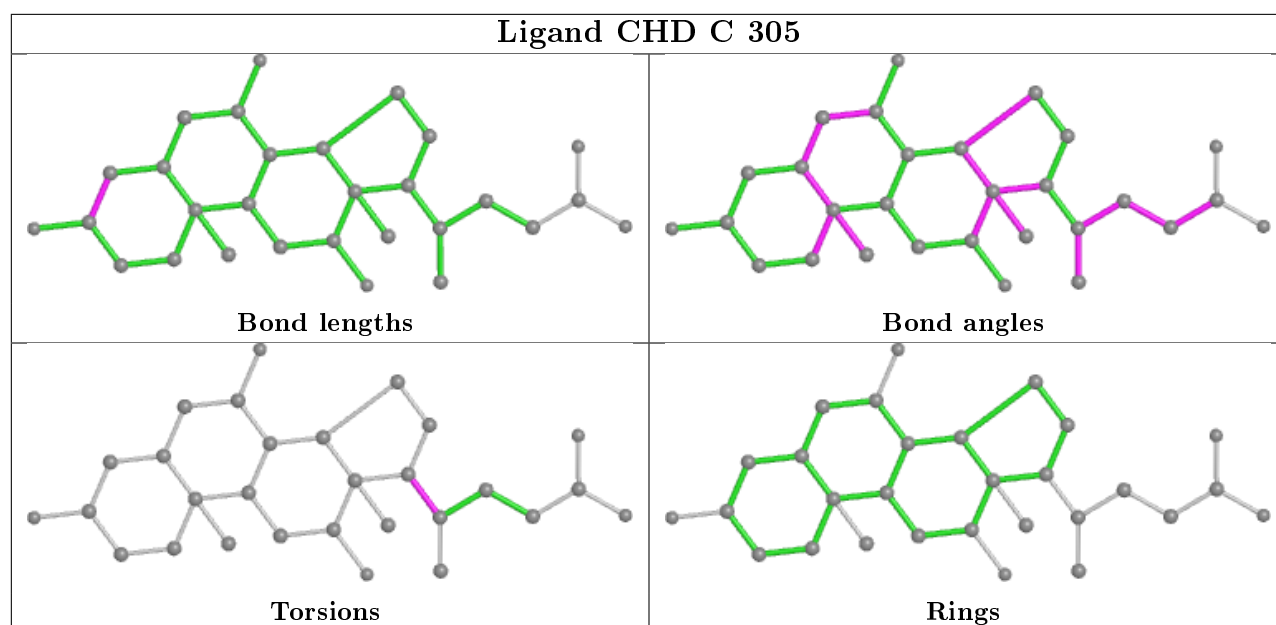


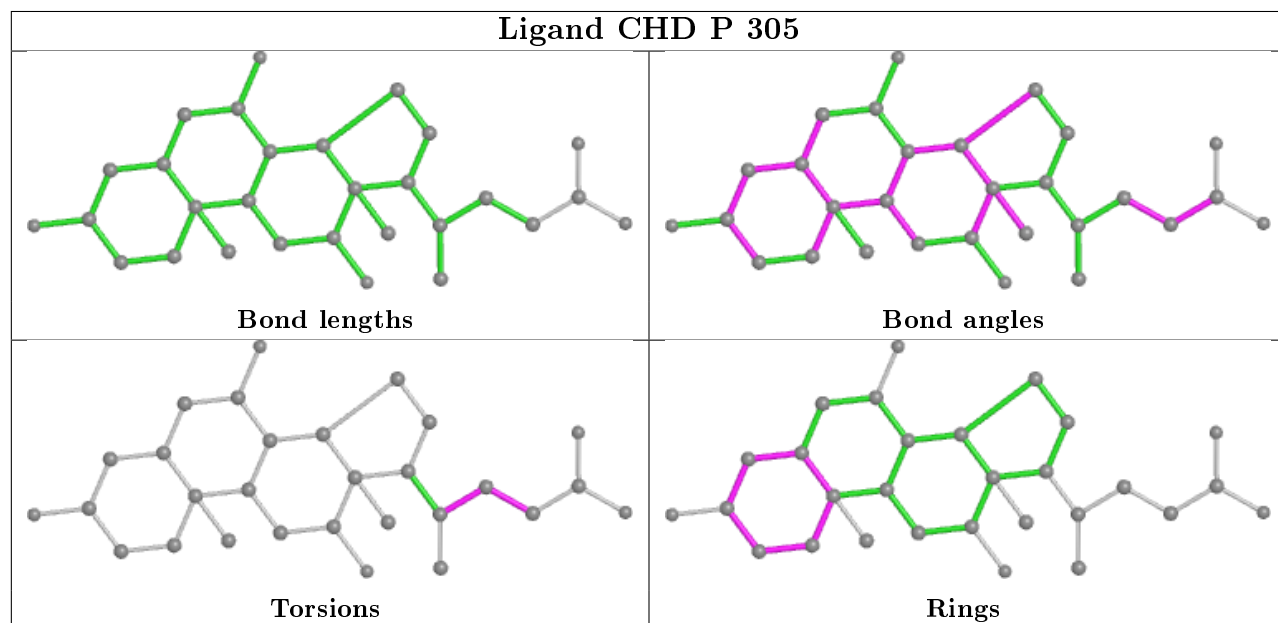
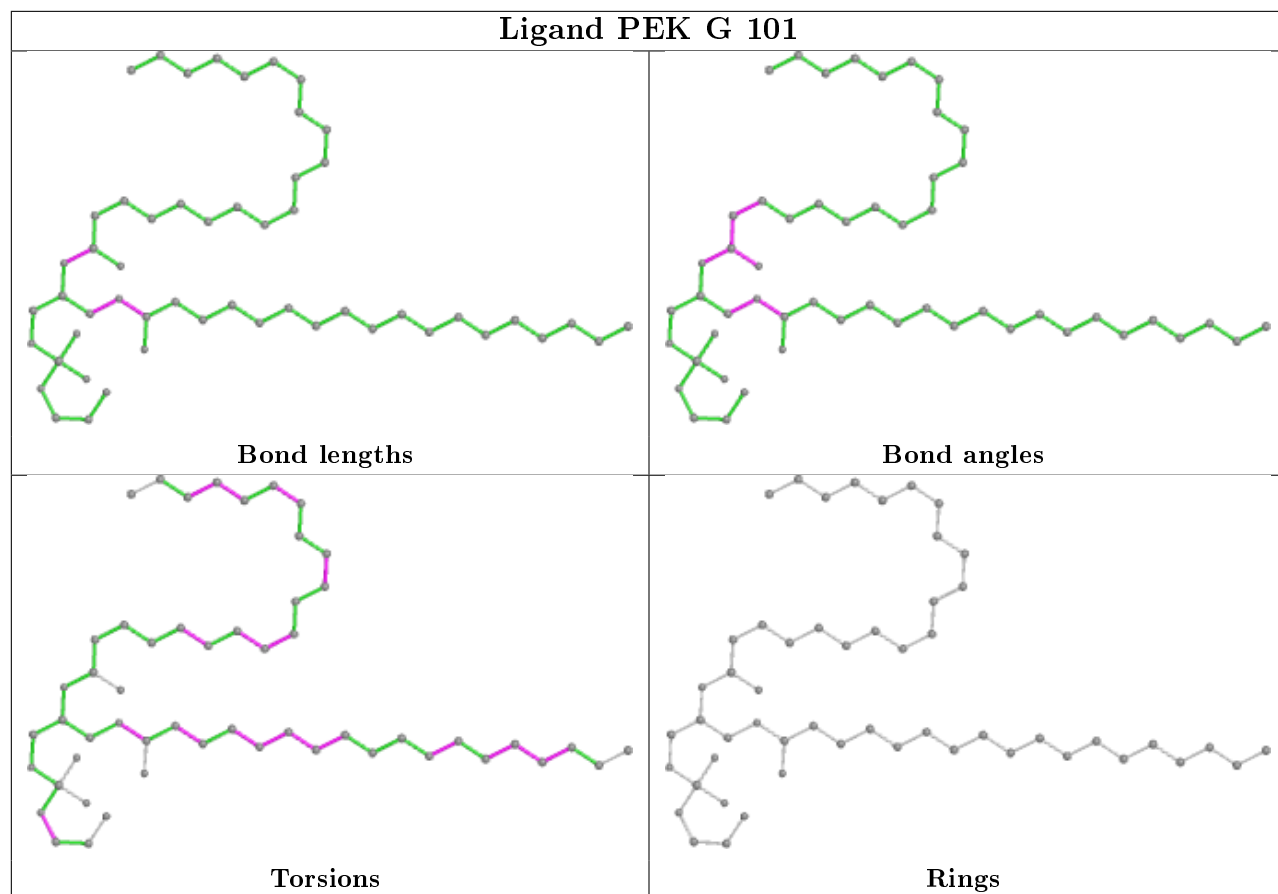


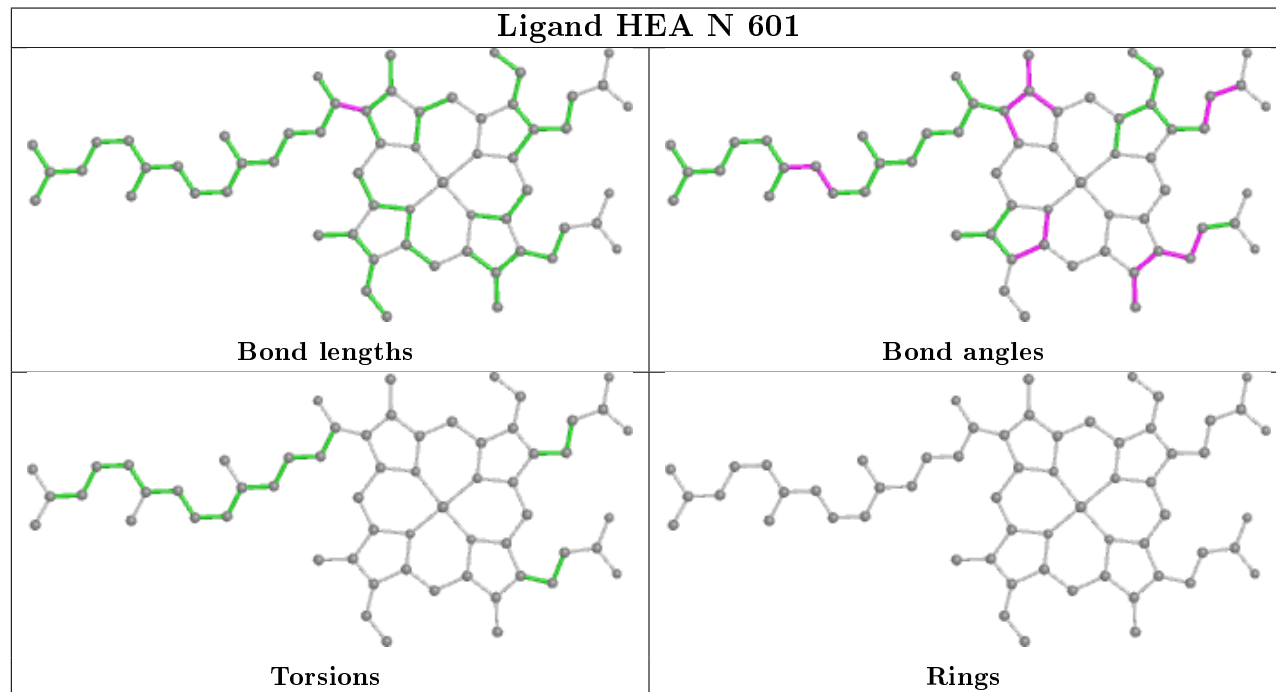
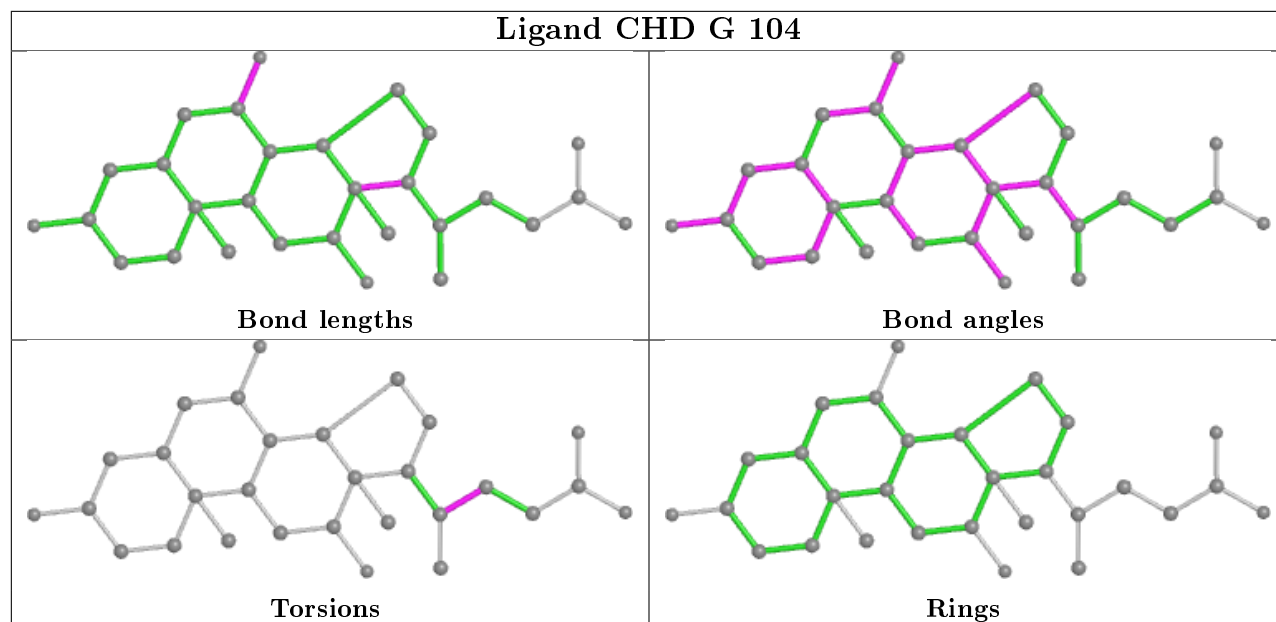


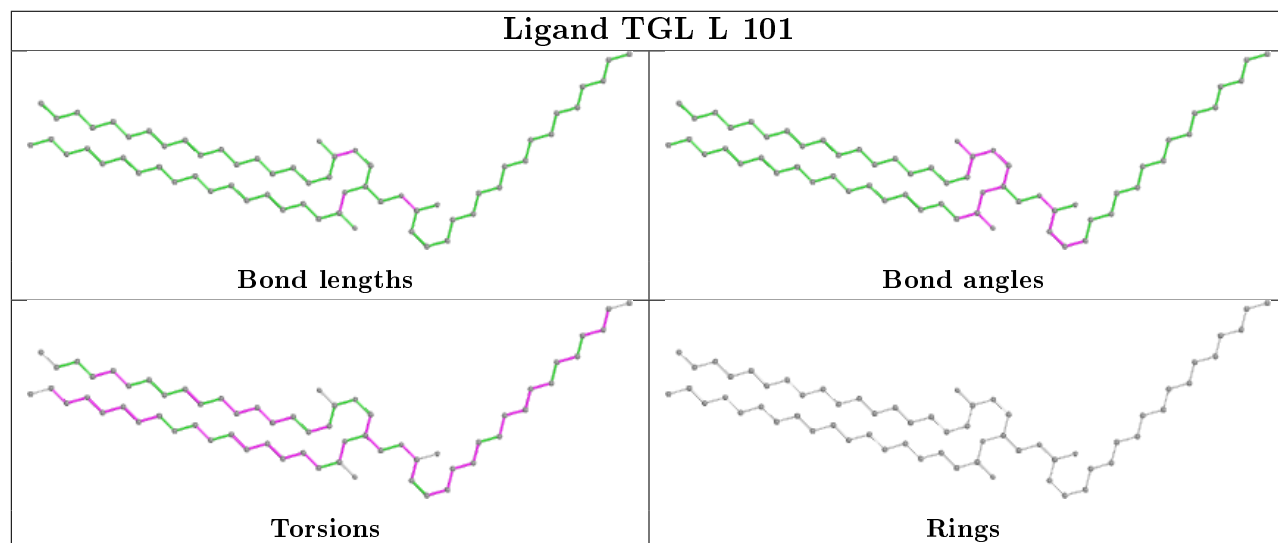
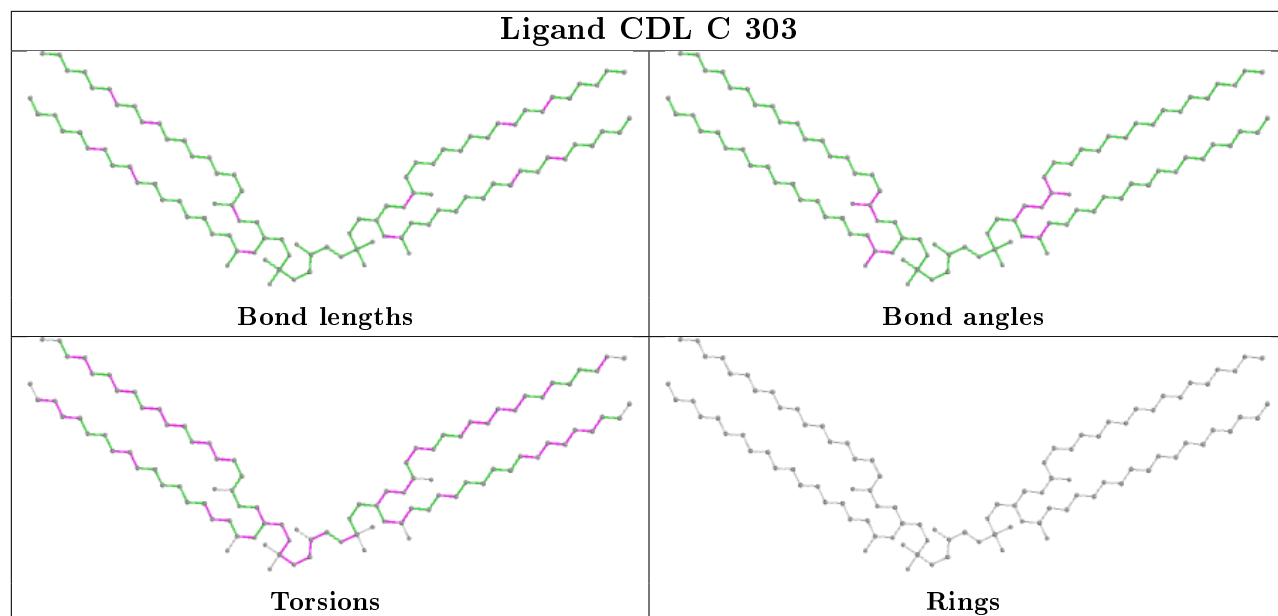




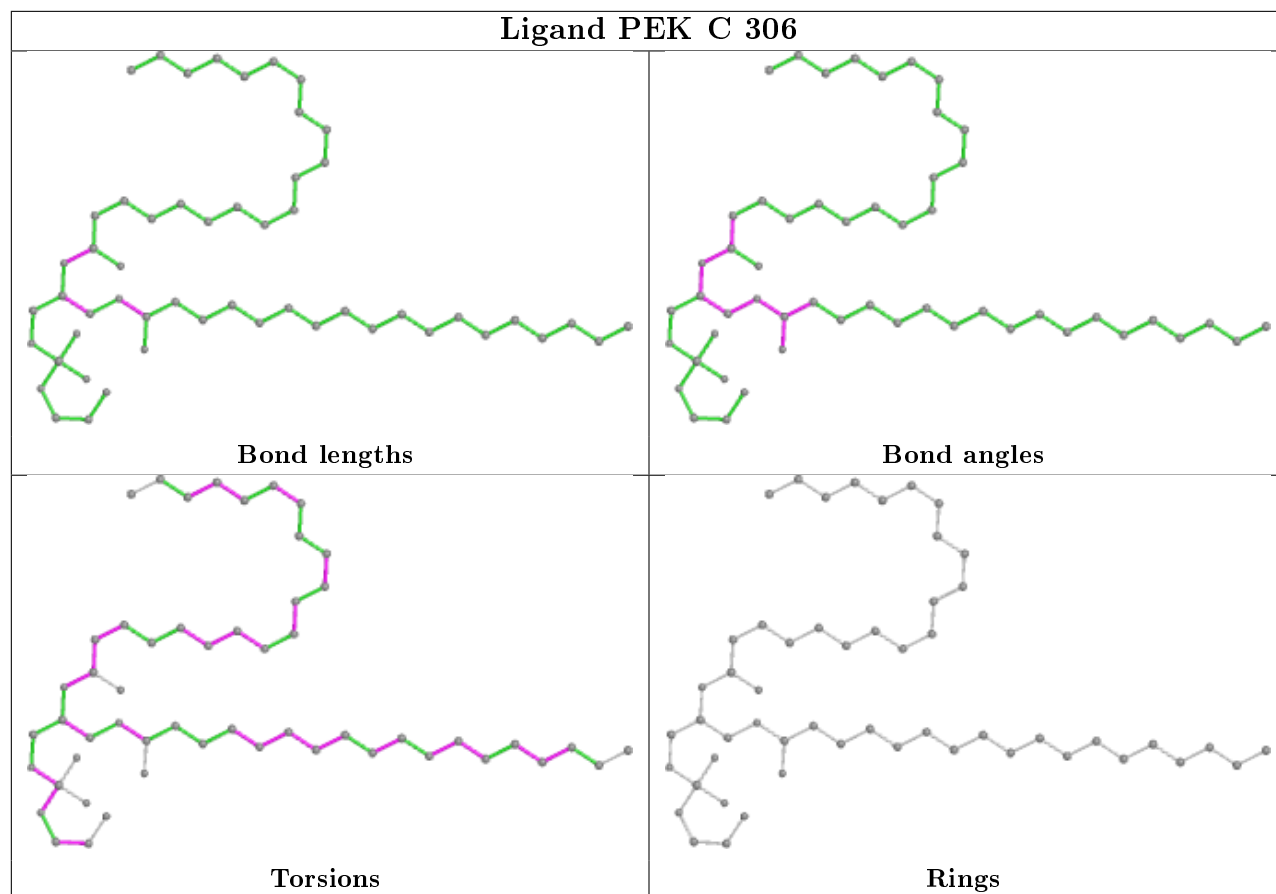




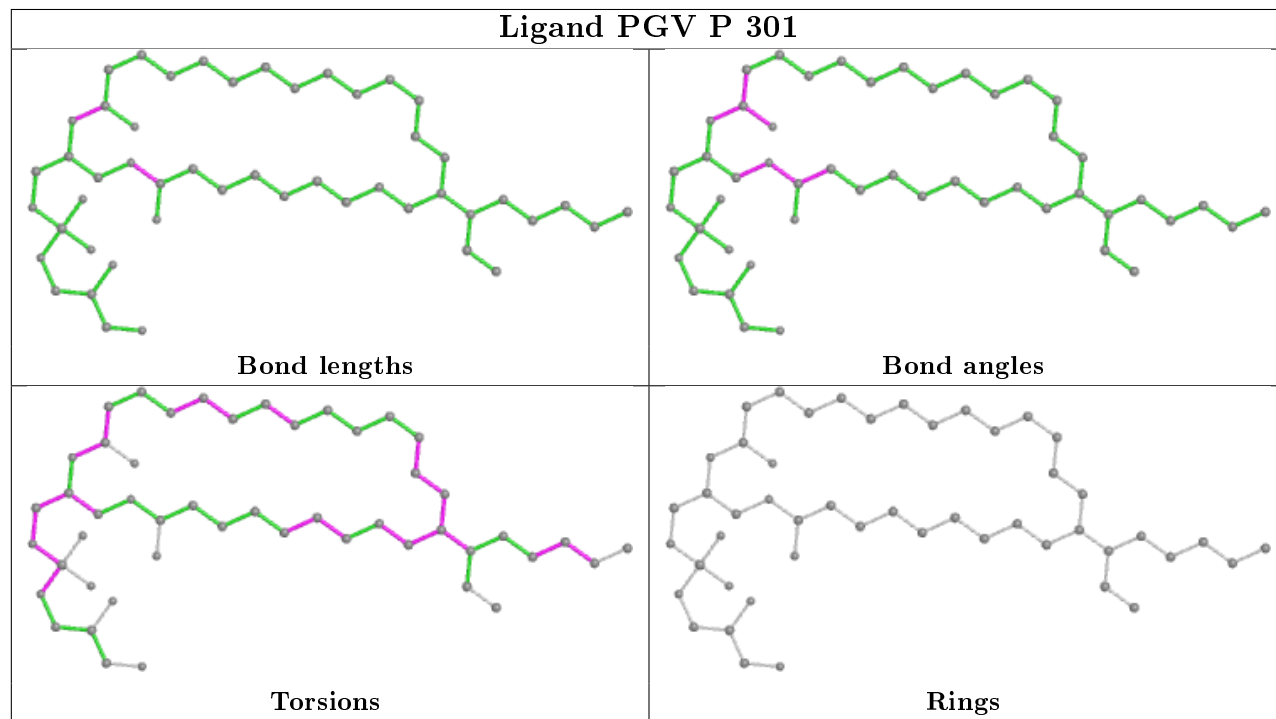


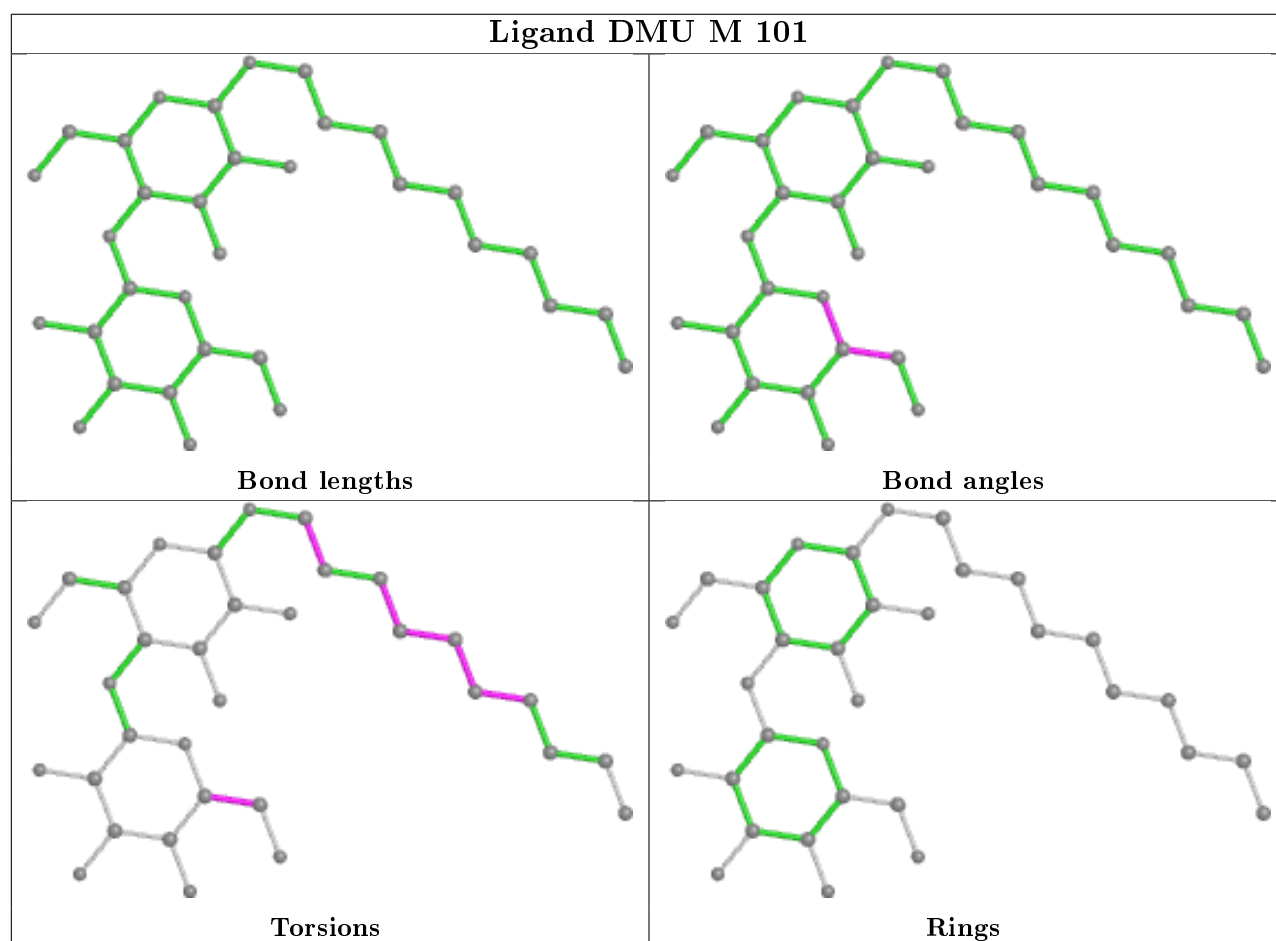
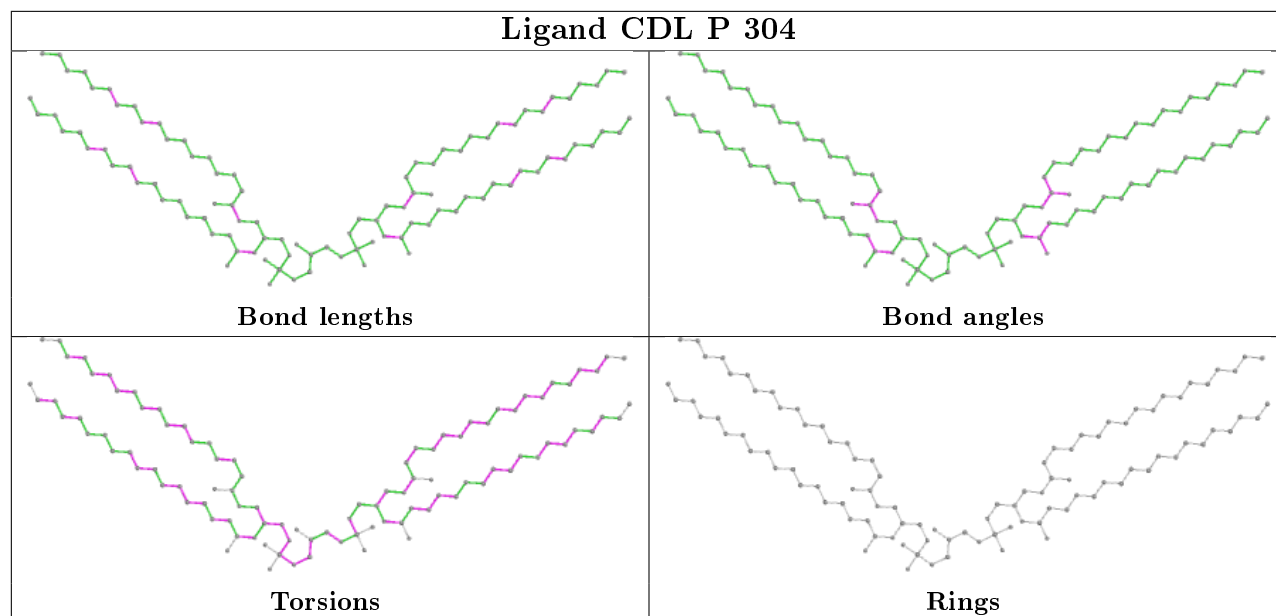


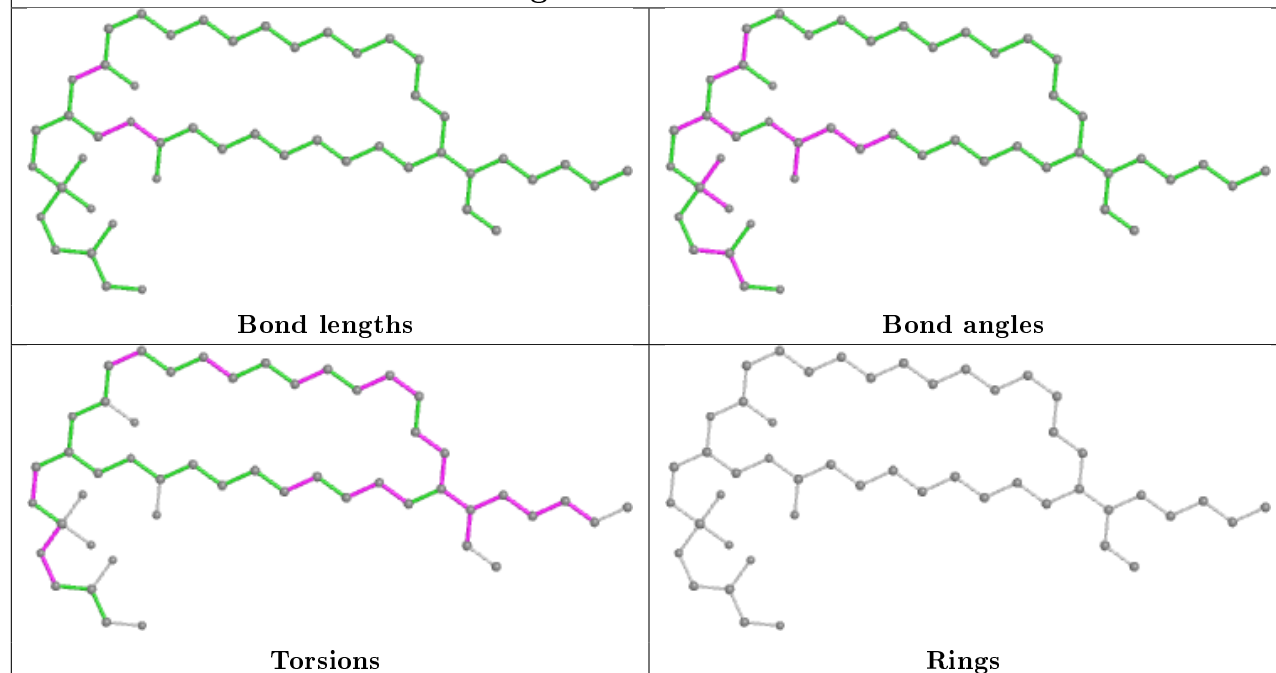
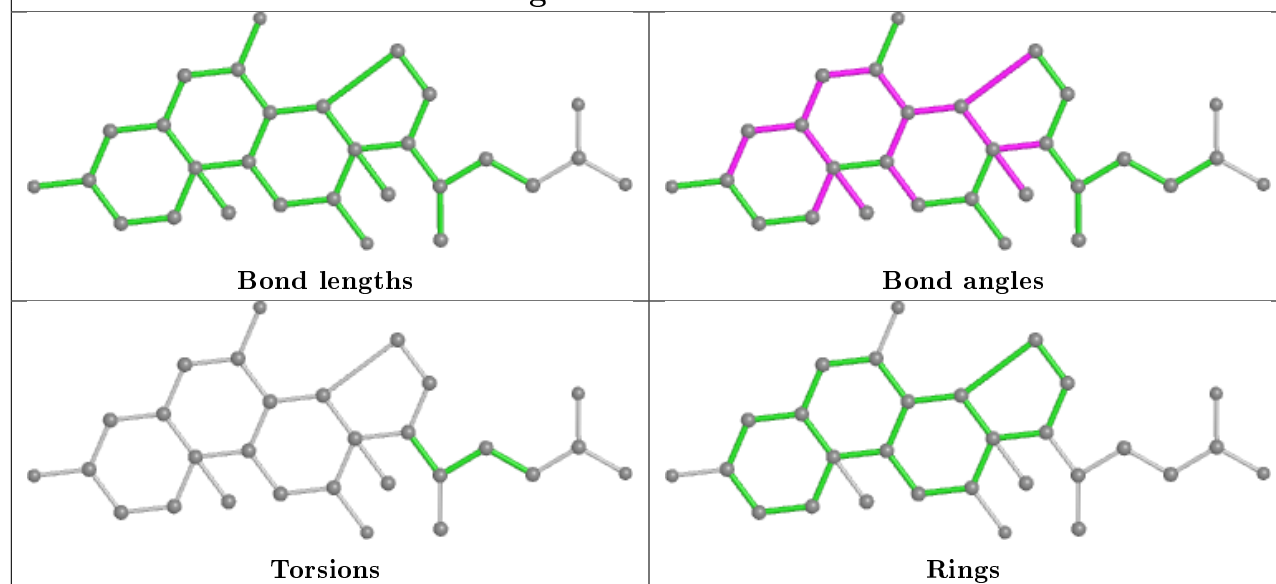
Ligand PEK C 306

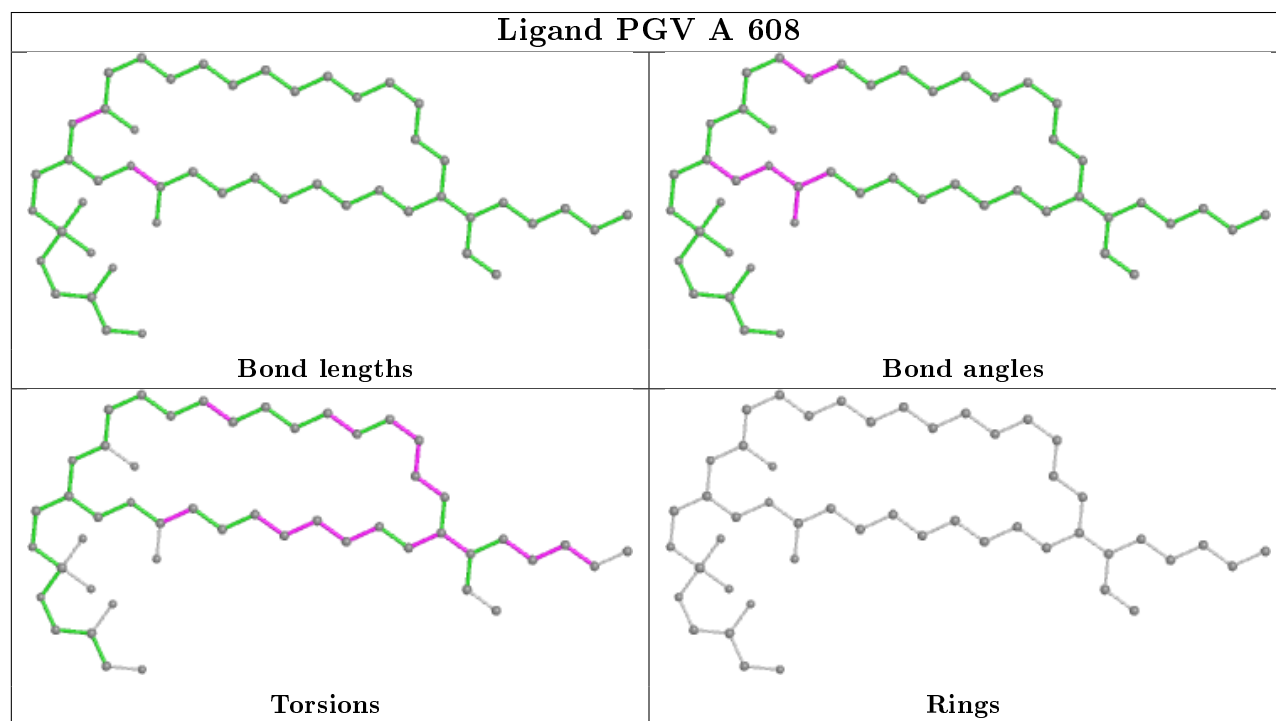
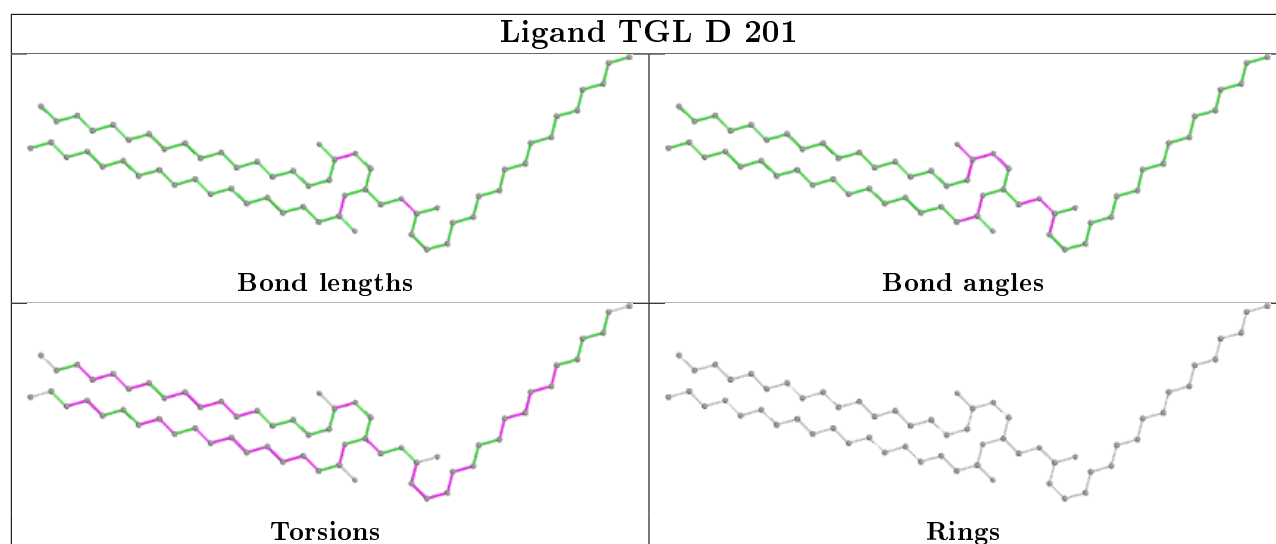


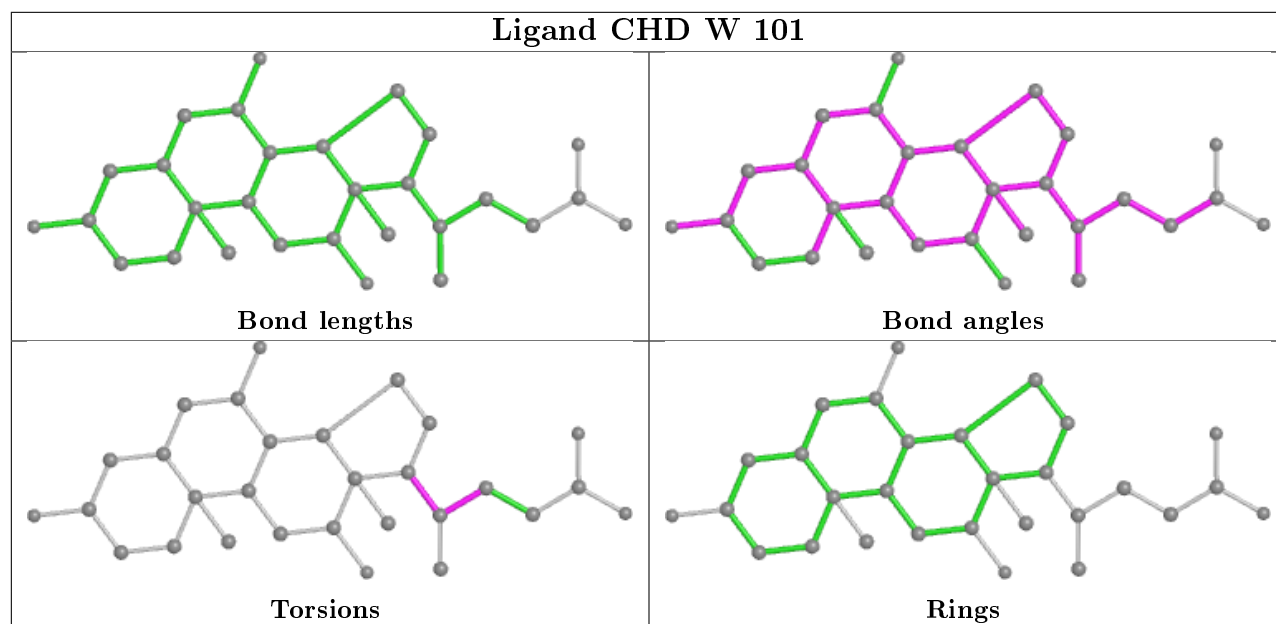
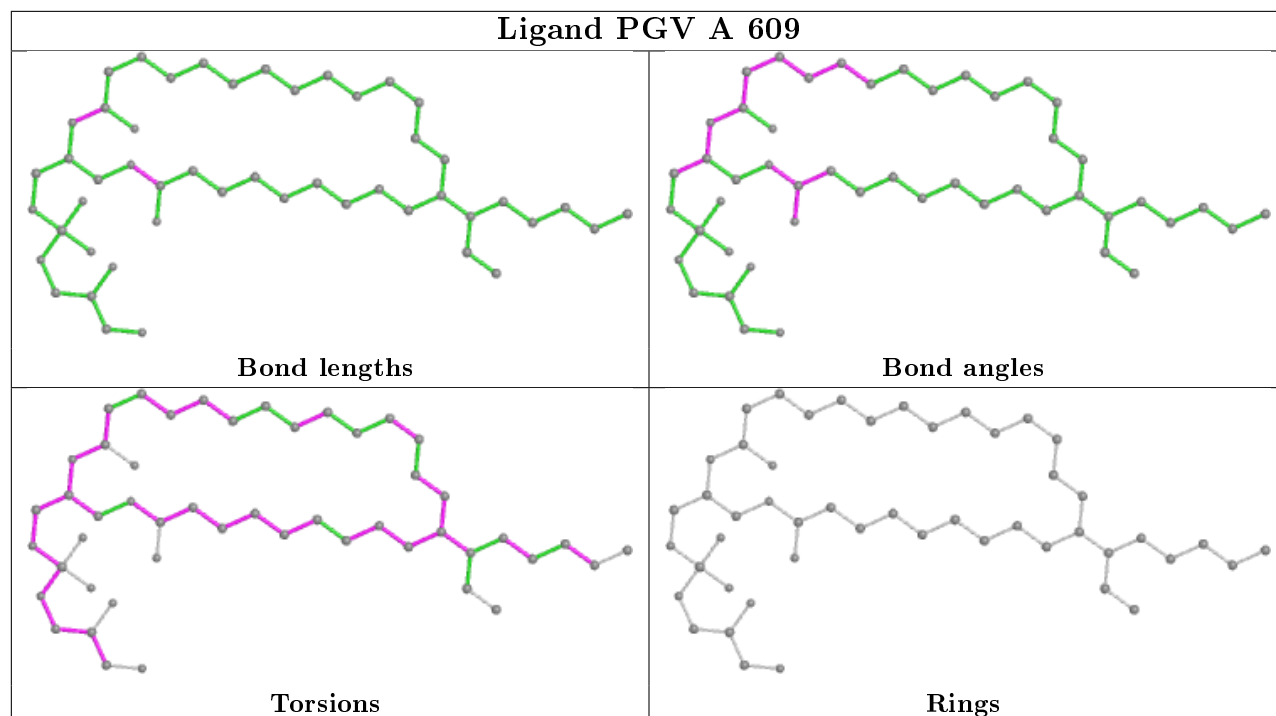
Ligand PGV P 301

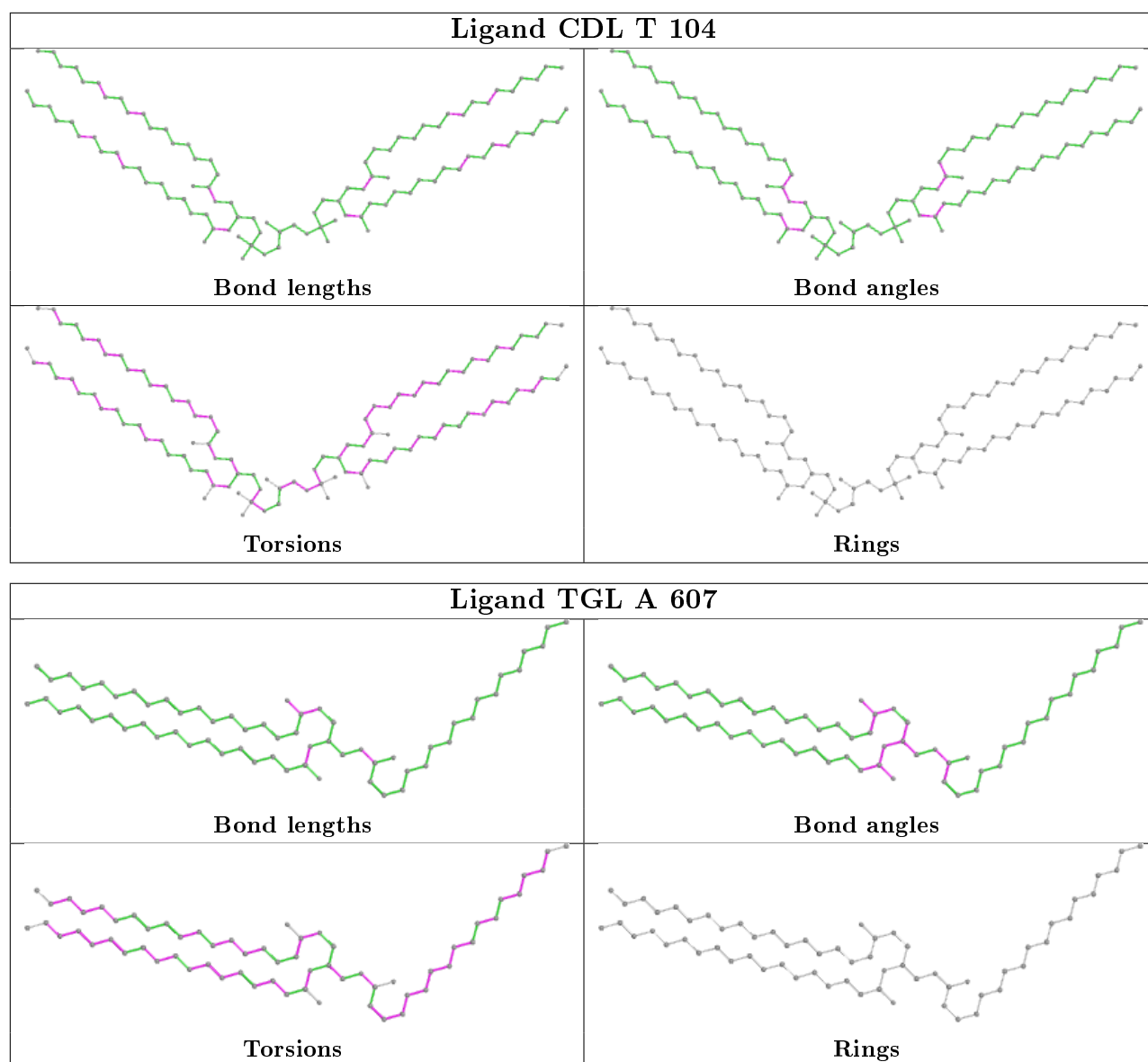




Ligand PGV P 303**Ligand CHD P 306**







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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	513/514 (99%)	-0.71	0 100 100	39, 47, 59, 90	0
1	N	513/514 (99%)	-0.71	5 (0%) 82 81	43, 55, 71, 103	0
2	B	226/227 (99%)	-0.74	3 (1%) 77 75	43, 54, 82, 118	0
2	O	226/227 (99%)	-0.48	6 (2%) 54 52	51, 64, 98, 140	0
3	C	259/261 (99%)	-0.55	0 100 100	44, 51, 69, 123	0
3	P	259/261 (99%)	-0.41	6 (2%) 60 58	46, 56, 75, 129	0
4	D	144/147 (97%)	-0.52	1 (0%) 87 86	49, 59, 87, 126	0
4	Q	144/147 (97%)	0.43	16 (11%) 5 4	60, 81, 126, 157	0
5	E	105/109 (96%)	-0.31	2 (1%) 66 65	49, 59, 88, 147	0
5	R	105/109 (96%)	-0.00	6 (5%) 23 22	56, 73, 104, 142	0
6	F	98/98 (100%)	-0.27	10 (10%) 6 6	47, 61, 138, 155	0
6	S	98/98 (100%)	-0.06	6 (6%) 21 20	51, 70, 140, 158	0
7	G	83/85 (97%)	0.62	15 (18%) 1 1	49, 62, 150, 157	0
7	T	83/85 (97%)	0.54	10 (12%) 4 3	49, 68, 143, 154	0
8	H	79/85 (92%)	-0.16	4 (5%) 28 26	49, 64, 129, 144	0
8	U	79/85 (92%)	-0.14	5 (6%) 20 19	56, 71, 143, 153	0
9	I	72/73 (98%)	-0.39	3 (4%) 36 34	53, 66, 96, 118	0
9	V	72/73 (98%)	-0.31	5 (6%) 16 15	50, 77, 105, 140	0
10	J	58/59 (98%)	0.06	5 (8%) 10 9	52, 64, 98, 150	0
10	W	58/59 (98%)	-0.17	3 (5%) 27 26	59, 76, 110, 157	0
11	K	49/56 (87%)	-0.08	5 (10%) 6 6	57, 67, 88, 105	0
11	X	49/56 (87%)	0.33	8 (16%) 1 1	69, 80, 109, 122	0
12	L	46/47 (97%)	-0.84	0 100 100	47, 55, 75, 109	0
12	Y	46/47 (97%)	-0.35	3 (6%) 18 17	57, 72, 98, 140	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	-0.41	1 (2%) 60 58	51, 57, 89, 130	0
13	Z	43/46 (93%)	-0.13	4 (9%) 8 7	66, 78, 113, 150	0
All	All	3550/3614 (98%)	-0.39	132 (3%) 41 39	39, 59, 103, 158	0

The worst 5 of 132 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	S	97	ALA	16.4
7	T	3	ALA	12.1
7	G	1	ALA	11.1
7	G	2	SER	10.3
4	Q	6	VAL	9.9

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

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	0.58	0.59	134,154,162,162	0
9	SAC	I	1	9/10	0.73	0.27	108,138,147,149	0
7	TPO	G	11	11/12	0.74	0.13	105,144,154,158	0
7	TPO	T	11	11/12	0.77	0.24	100,127,155,158	0
1	FME	A	1	10/11	0.96	0.28	58,69,114,141	0
1	FME	N	1	10/11	0.98	0.48	77,90,144,145	0
2	FME	B	1	10/11	0.98	0.08	51,56,62,76	0
2	FME	O	1	10/11	0.98	0.15	62,65,74,76	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
27	PEK	T	102	53/53	0.50	0.51	74,133,150,150	0
21	EDO	C	310	4/4	0.57	0.84	146,146,149,149	0
25	UNX	P	302	1/1	0.58	0.71	20,20,20,20	1
24	PSC	O	303	52/52	0.61	0.33	72,134,150,150	0
27	PEK	C	306	53/53	0.61	0.30	68,138,150,150	0
23	CHD	W	101	29/29	0.61	0.35	108,149,150,150	0
26	CDL	G	102	100/100	0.63	0.37	99,145,150,150	0
26	CDL	T	104	100/100	0.63	0.33	83,136,150,150	0
26	CDL	P	304	100/100	0.67	0.27	70,139,150,150	0
19	TGL	D	201	63/63	0.68	0.29	68,117,150,150	0
21	EDO	P	308	4/4	0.68	0.22	89,95,98,99	0
21	EDO	P	307	4/4	0.68	0.30	92,96,107,115	0
19	TGL	Y	101	63/63	0.68	0.35	78,127,150,150	0
21	EDO	K	101	4/4	0.69	0.16	87,91,96,105	0
24	PSC	B	303	52/52	0.70	0.27	73,142,150,150	0
27	PEK	G	103	53/53	0.70	0.47	84,136,150,150	0
20	PGV	A	609	51/51	0.72	0.30	62,112,152,160	0
19	TGL	Q	201	63/63	0.75	0.23	76,124,150,150	0
20	PGV	N	607	51/51	0.75	0.39	66,140,150,150	0
21	EDO	N	610	4/4	0.75	0.91	125,132,135,138	0
27	PEK	T	103	53/53	0.77	0.26	67,132,150,150	0
26	CDL	C	303	100/100	0.77	0.24	56,121,153,157	0
19	TGL	O	302	63/63	0.78	0.21	67,115,150,150	0
21	EDO	H	101	4/4	0.78	0.33	111,112,118,127	0
19	TGL	A	607	63/63	0.78	0.24	50,96,139,151	0
19	TGL	L	101	63/63	0.79	0.26	67,106,149,150	0
20	PGV	C	307	51/51	0.80	0.26	61,126,150,150	0
20	PGV	P	301	51/51	0.81	0.21	73,119,150,150	0
21	EDO	F	103	4/4	0.82	0.55	71,125,128,147	0
21	EDO	B	305	4/4	0.82	0.32	84,86,91,94	0
29	DMU	Z	101	33/33	0.83	0.30	95,106,138,147	0
23	CHD	J	101	29/29	0.84	0.33	90,142,150,150	0
21	EDO	A	611	4/4	0.84	0.16	81,82,106,109	0
25	UNX	C	301	1/1	0.85	0.75	17,17,17,17	1
21	EDO	G	105	4/4	0.87	0.17	74,78,88,97	0
21	EDO	A	613	4/4	0.88	0.47	96,116,120,122	0
23	CHD	C	304	29/29	0.89	0.27	89,104,112,113	0
29	DMU	M	101	33/33	0.89	0.23	61,78,111,115	0
21	EDO	C	309	4/4	0.89	0.25	80,86,89,95	0
18	CMO	N	606	2/2	0.89	0.12	47,47,47,50	2
23	CHD	P	305	29/29	0.89	0.21	82,131,147,148	0
21	EDO	C	308	4/4	0.91	0.22	89,93,96,106	0

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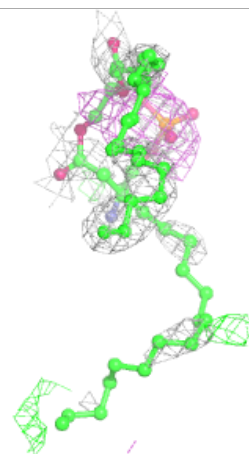
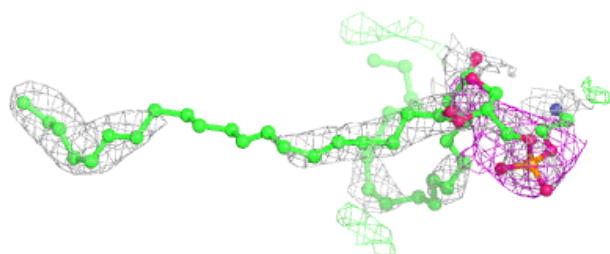
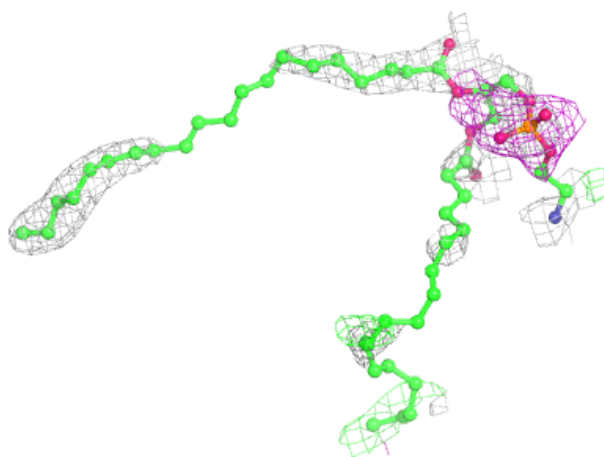
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
21	EDO	T	105	4/4	0.91	0.22	121,130,135,136	0
21	EDO	F	102	4/4	0.92	0.17	82,82,101,101	0
21	EDO	K	102	4/4	0.92	0.60	89,96,101,112	0
21	EDO	N	609	4/4	0.93	0.09	88,91,100,108	0
21	EDO	L	102	4/4	0.93	0.16	83,86,90,95	0
20	PGV	P	303	51/51	0.94	0.22	53,65,143,148	0
21	EDO	A	612	4/4	0.94	0.28	62,76,80,93	0
27	PEK	T	101	53/53	0.95	0.18	62,77,149,150	0
21	EDO	C	311	4/4	0.95	0.12	60,77,78,84	0
27	PEK	G	101	53/53	0.96	0.15	50,67,123,137	0
21	EDO	O	304	4/4	0.96	0.18	68,70,73,77	0
23	CHD	P	306	29/29	0.97	0.10	52,60,64,66	0
20	PGV	A	608	51/51	0.97	0.12	43,65,86,105	0
21	EDO	B	304	4/4	0.97	0.14	64,66,67,75	0
23	CHD	G	104	29/29	0.97	0.11	42,51,59,66	0
20	PGV	C	302	51/51	0.97	0.13	46,57,107,115	0
23	CHD	C	305	29/29	0.97	0.09	48,56,63,68	0
14	HEA	A	602	60/60	0.98	0.08	37,44,53,64	0
14	HEA	A	601	60/60	0.98	0.09	38,44,59,72	0
23	CHD	B	302	29/29	0.98	0.09	49,57,63,73	0
20	PGV	N	608	51/51	0.98	0.13	50,71,101,113	0
21	EDO	A	610	4/4	0.98	0.08	54,63,68,71	0
16	MG	N	604	1/1	0.98	0.03	52,52,52,52	0
14	HEA	N	601	60/60	0.98	0.11	48,57,76,84	0
17	NA	N	605	1/1	0.98	0.05	65,65,65,65	0
18	CMO	A	606	2/2	0.98	0.25	33,33,33,35	2
28	ZN	S	101	1/1	0.99	0.03	64,64,64,64	0
22	CUA	B	301	2/2	0.99	0.07	48,48,48,50	0
14	HEA	N	602	60/60	0.99	0.08	40,49,58,65	0
22	CUA	O	301	2/2	0.99	0.03	56,56,56,59	0
16	MG	A	604	1/1	1.00	0.02	41,41,41,41	0
15	CU	A	603	1/1	1.00	0.04	45,45,45,45	0
15	CU	N	603	1/1	1.00	0.05	51,51,51,51	0
17	NA	A	605	1/1	1.00	0.10	53,53,53,53	0
28	ZN	F	101	1/1	1.00	0.05	57,57,57,57	0

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

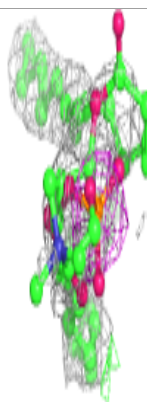
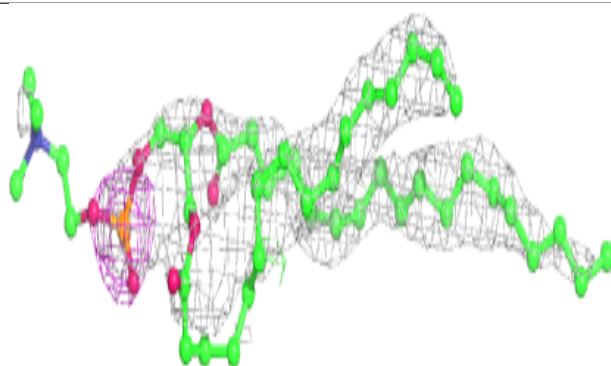
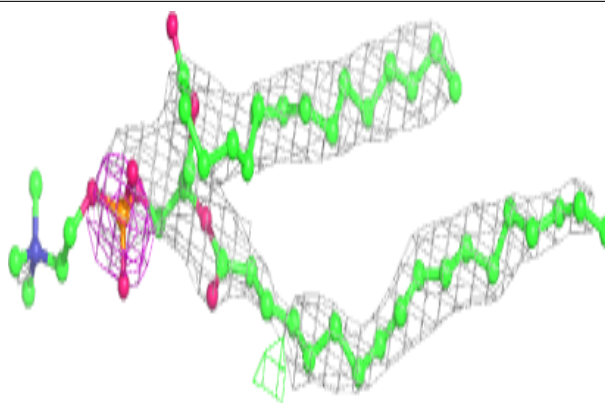
Electron density around PEK T 102:

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

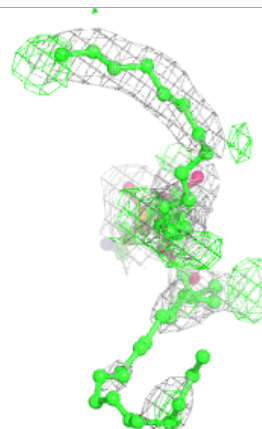
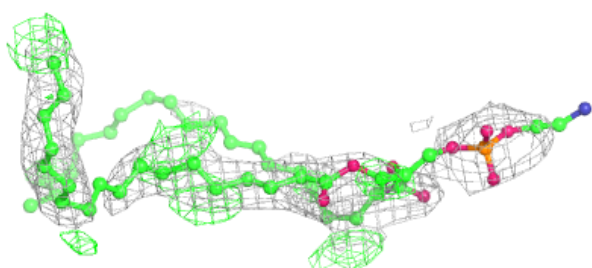
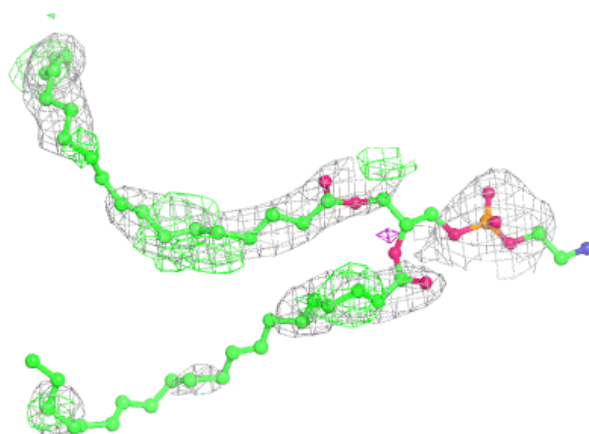


Electron density around PSC O 303:

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

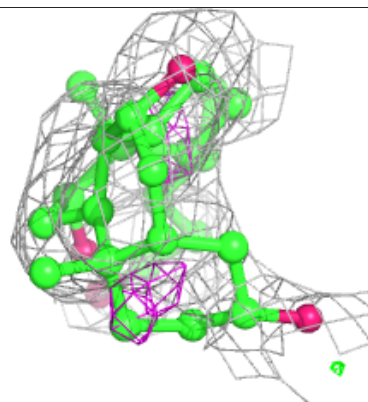
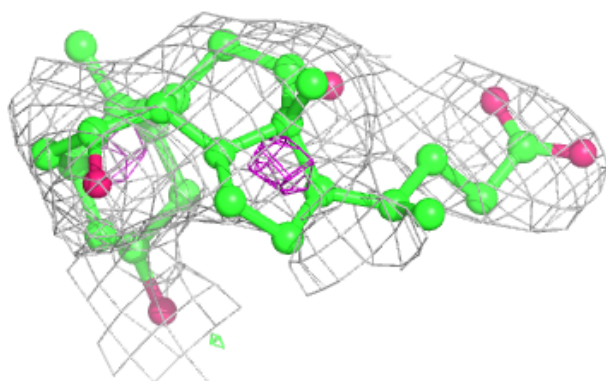
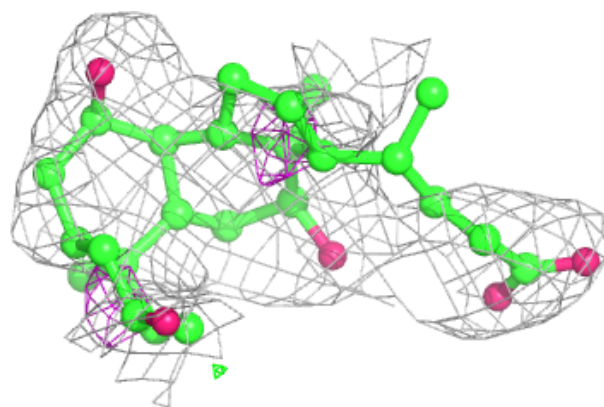
**Electron density around PEK C 306:**

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

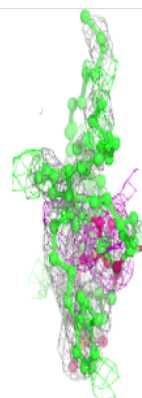
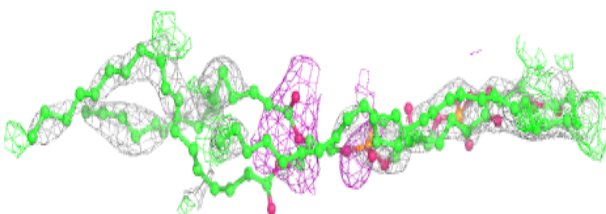
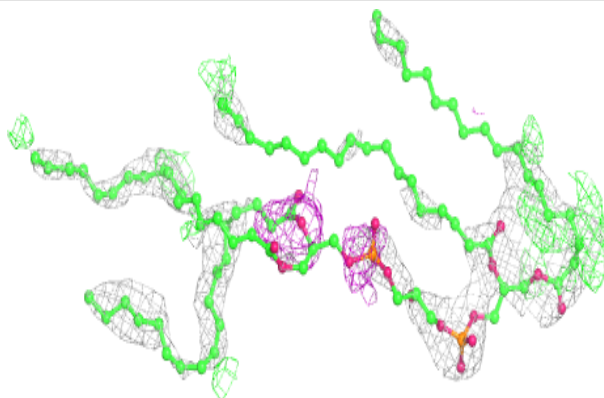


Electron density around CHD W 101:

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

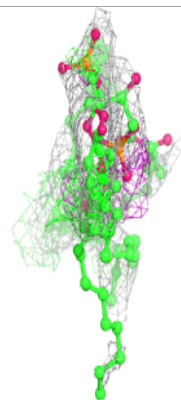
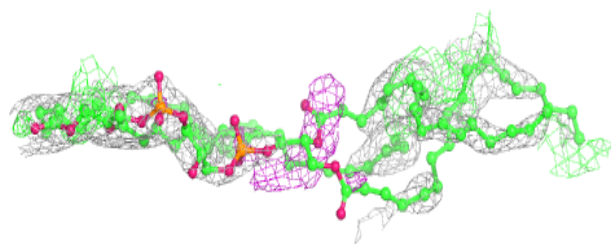
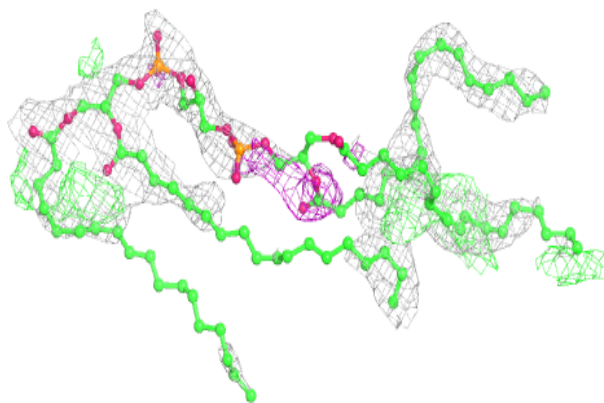
**Electron density around CDL G 102:**

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



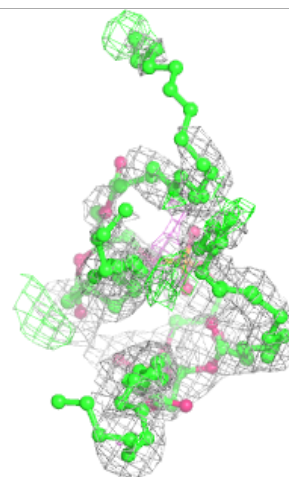
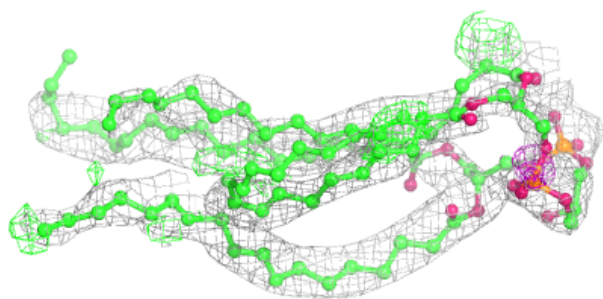
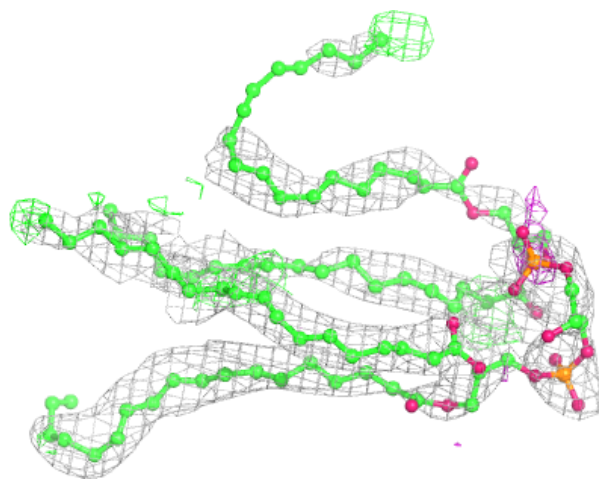
Electron density around CDL T 104:

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



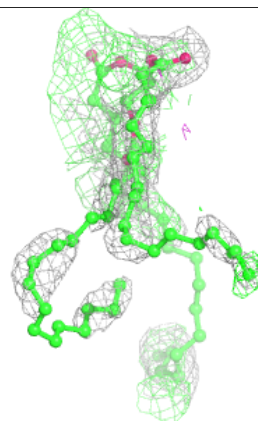
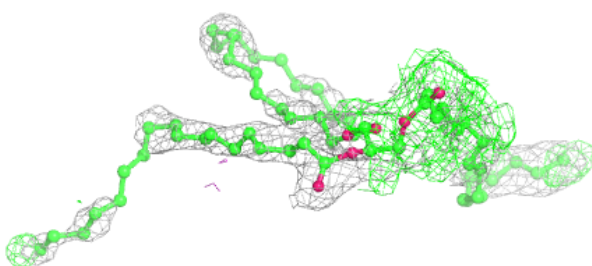
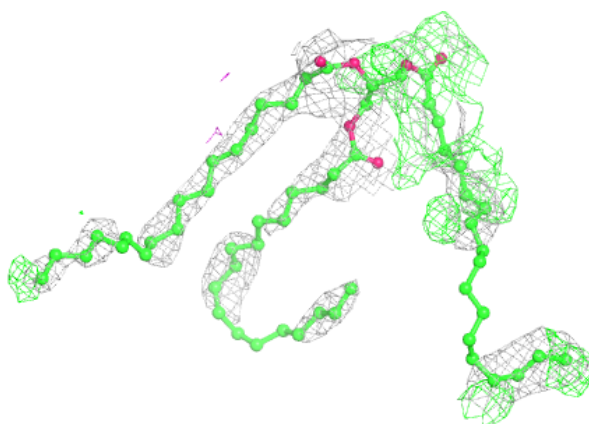
Electron density around CDL P 304:

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



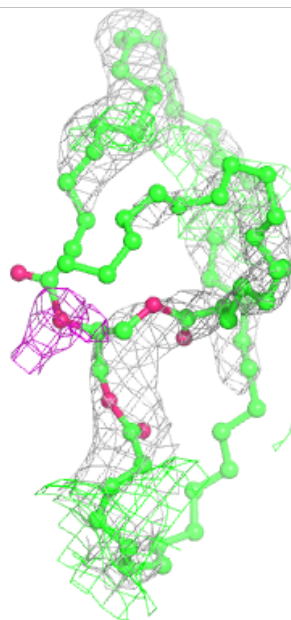
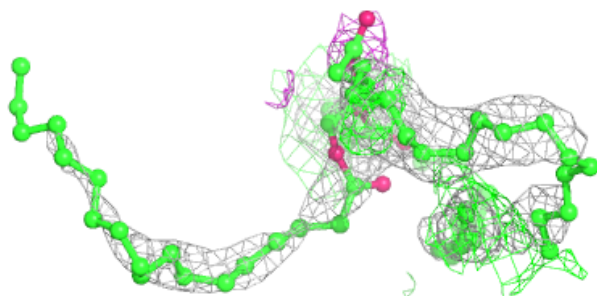
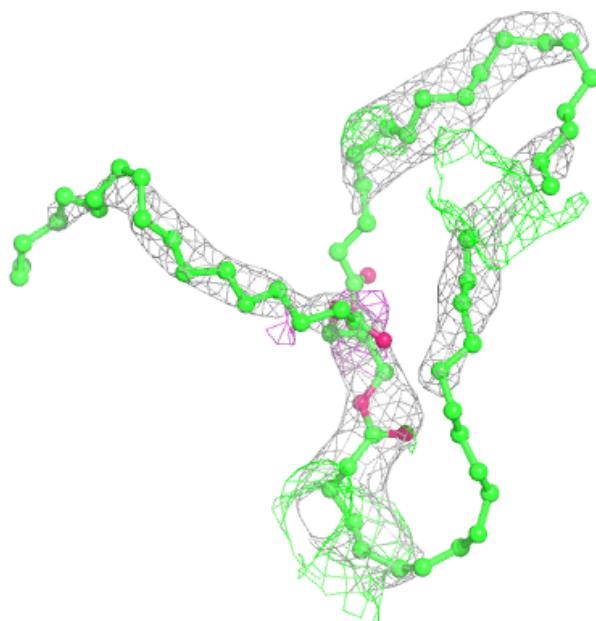
Electron density around TGL D 201:

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



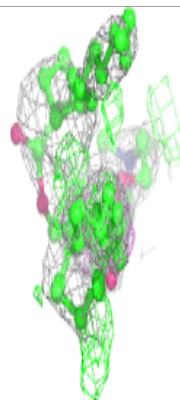
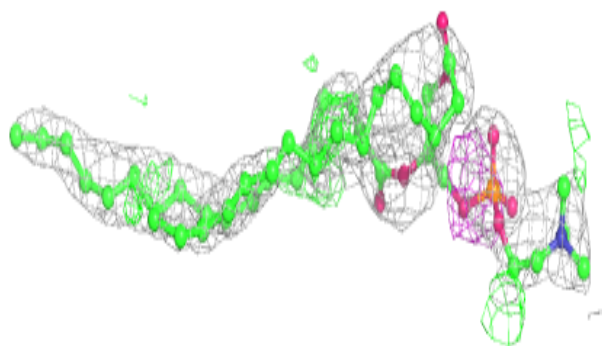
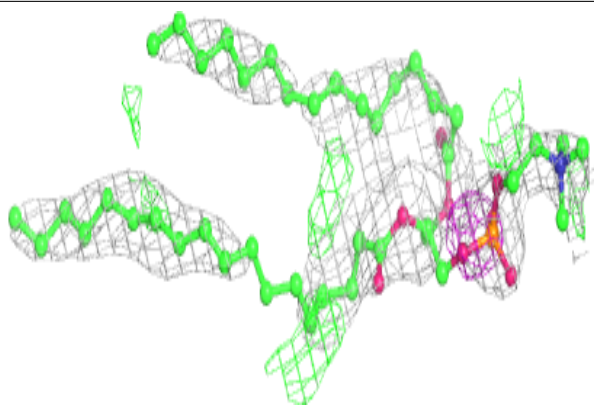
Electron density around TGL Y 101:

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



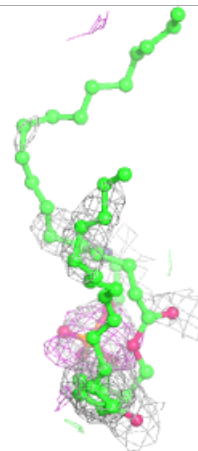
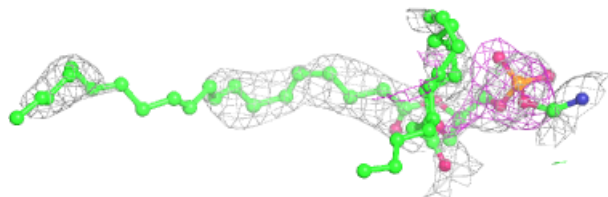
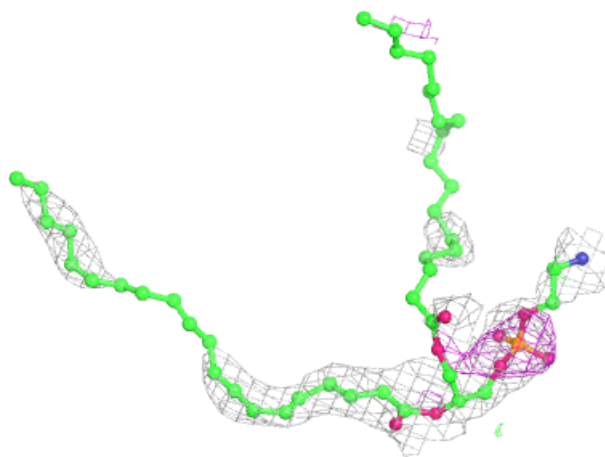
Electron density around PSC B 303:

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and green (positive)



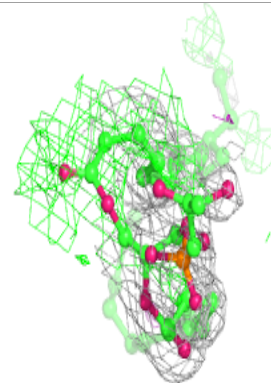
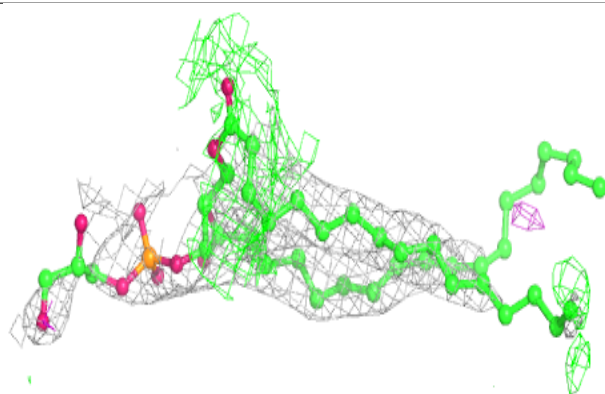
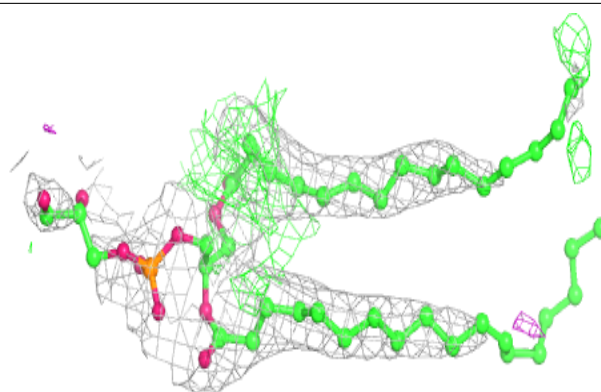
Electron density around PEK G 103:

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

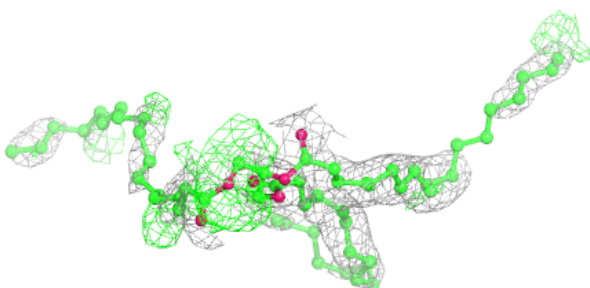
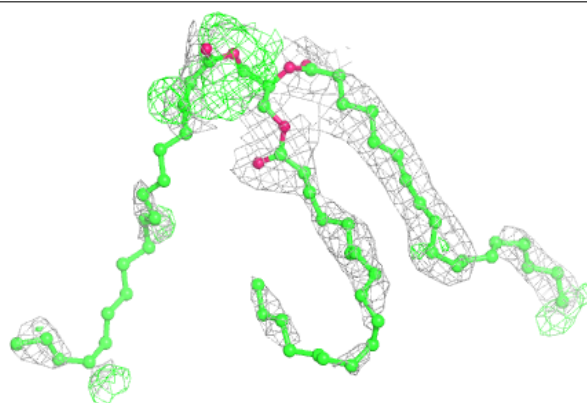


Electron density around PGV A 609:

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

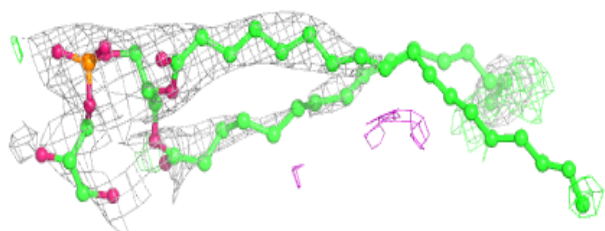
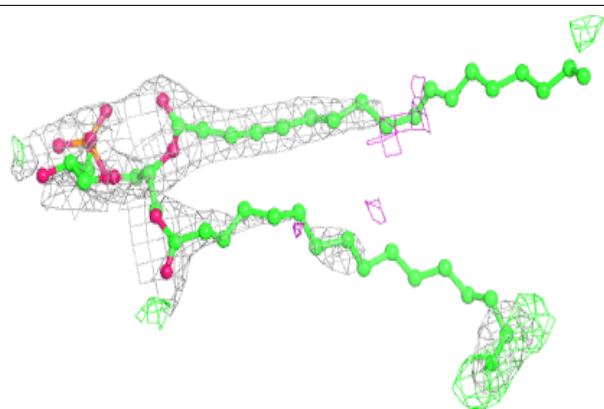
**Electron density around TGL Q 201:**

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

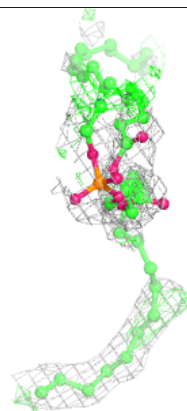
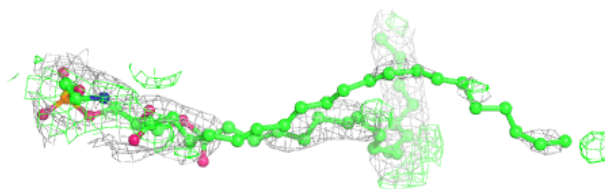
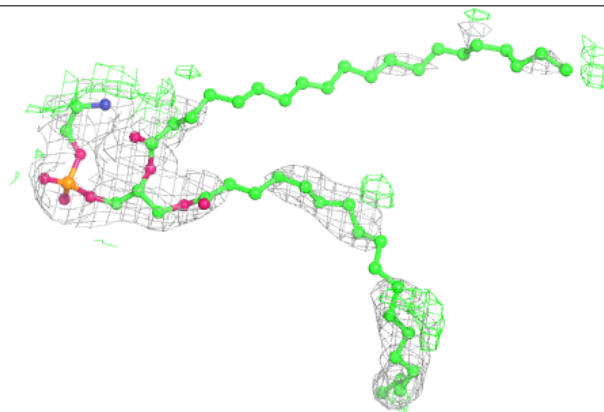


Electron density around PGV N 607:

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

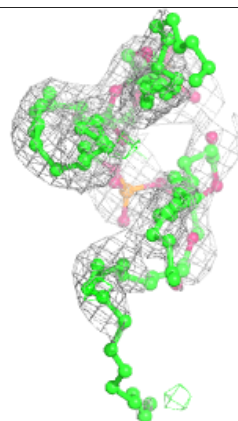
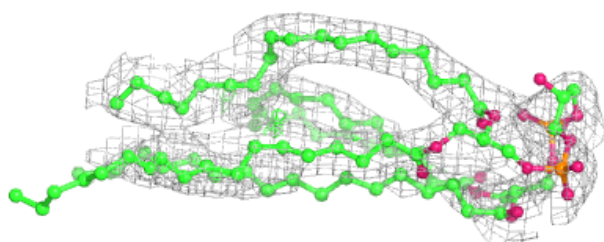
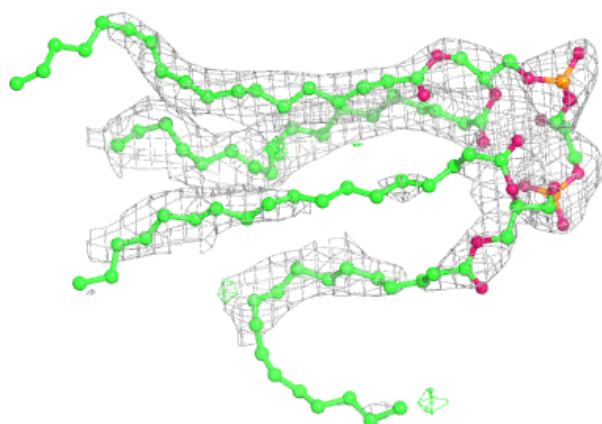
**Electron density around PEK T 103:**

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

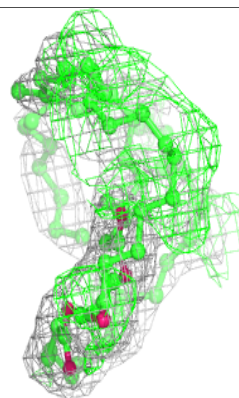
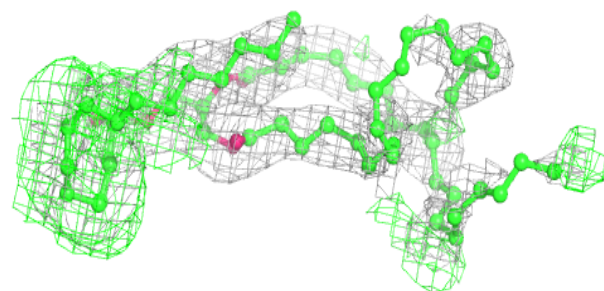
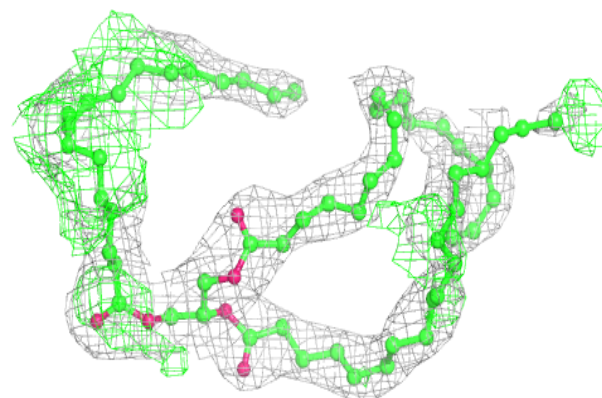


Electron density around CDL C 303:

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

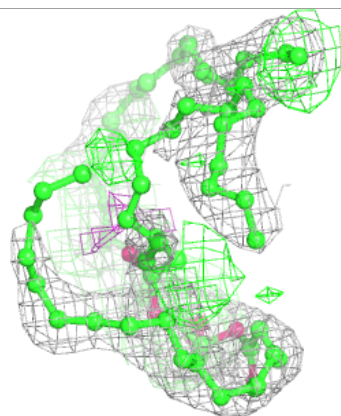
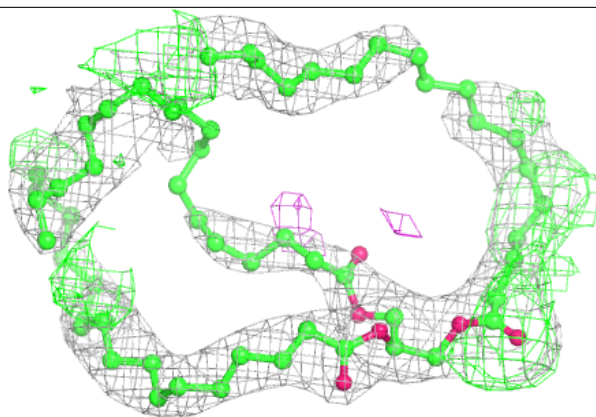
**Electron density around TGL O 302:**

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



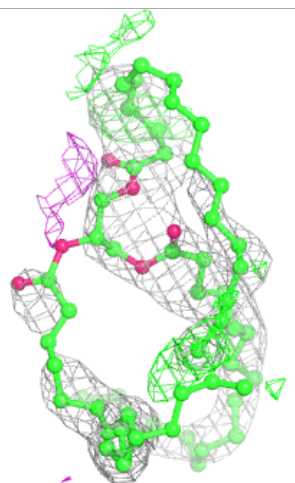
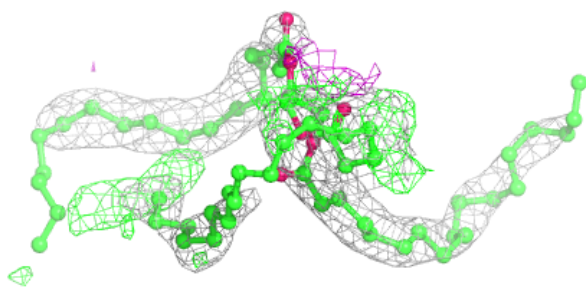
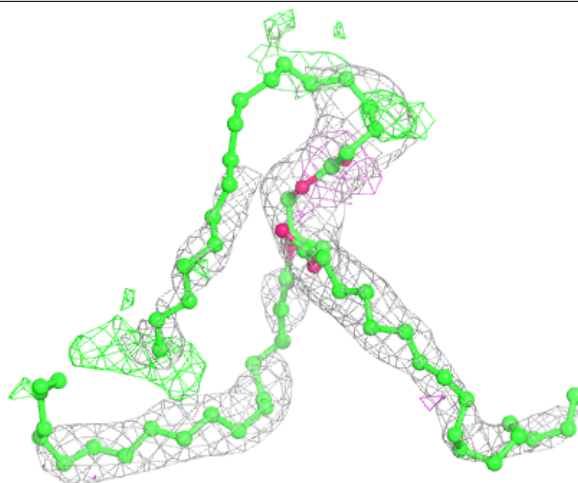
Electron density around TGL A 607:

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



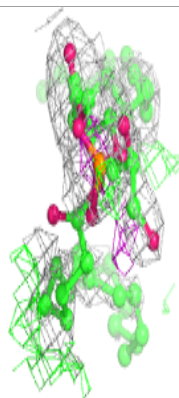
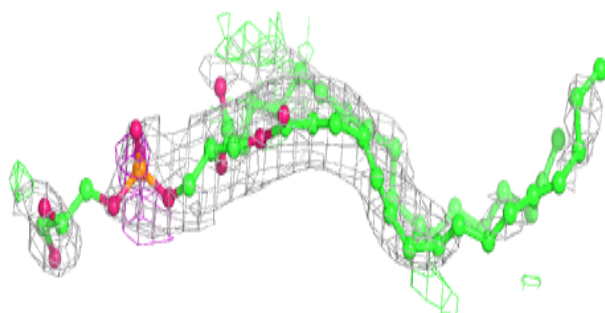
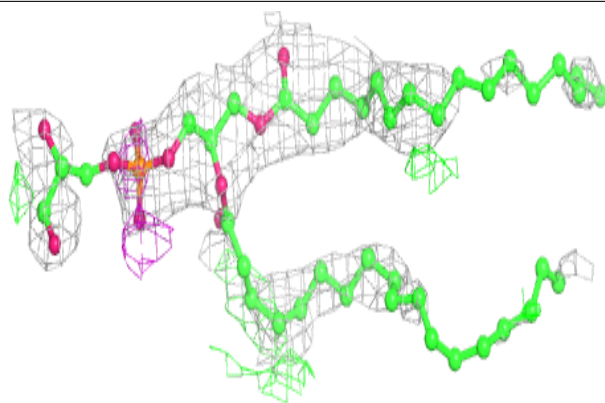
Electron density around TGL L 101:

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

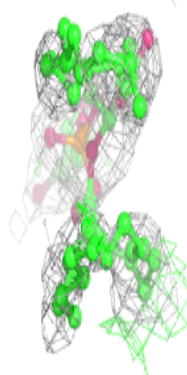
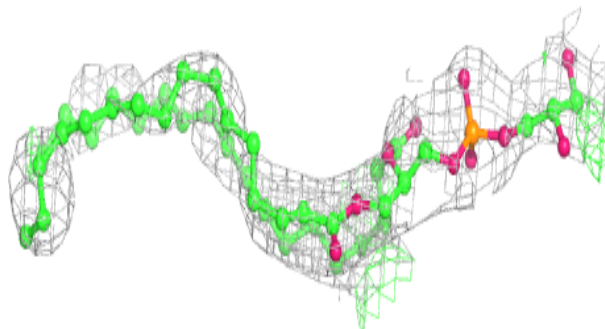
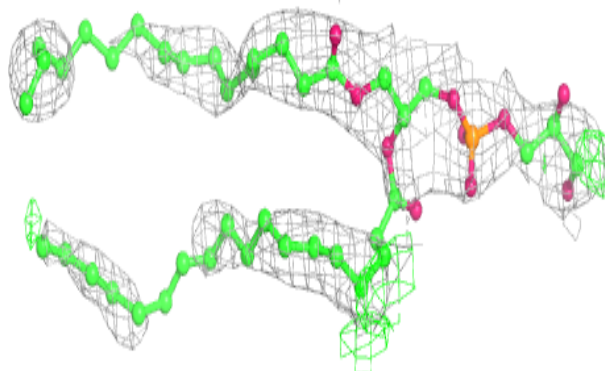


Electron density around PGV C 307:

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

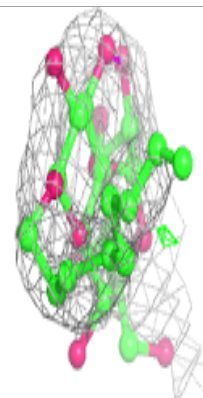
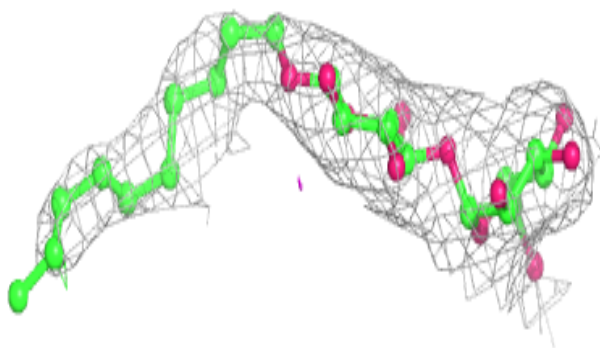
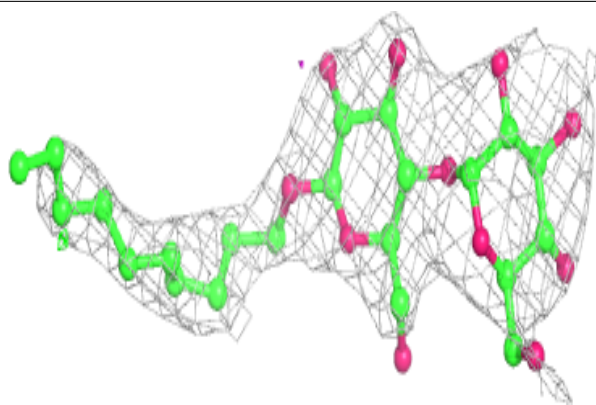
**Electron density around PGV P 301:**

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

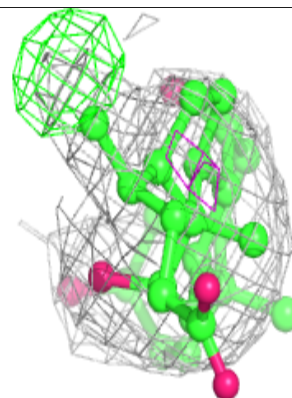
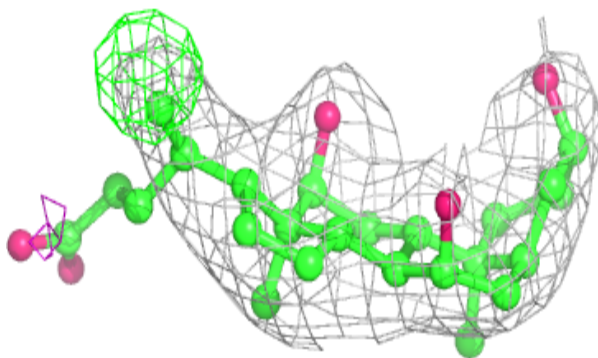
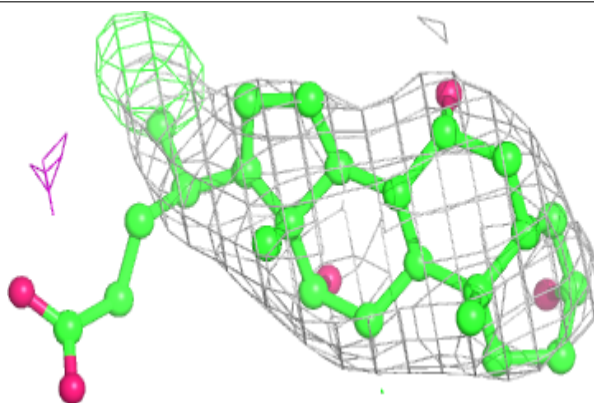


Electron density around DMU Z 101:

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

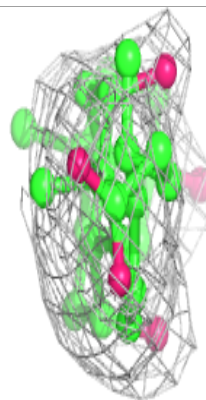
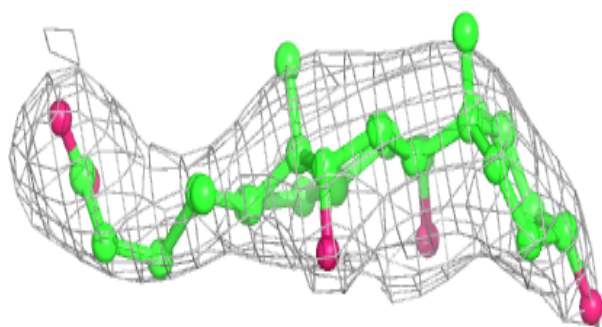
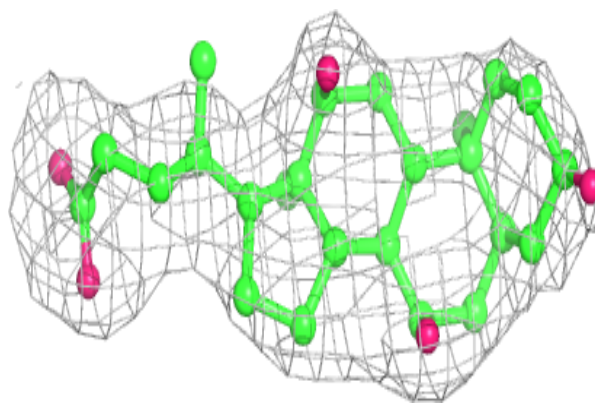
**Electron density around CHD J 101:**

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

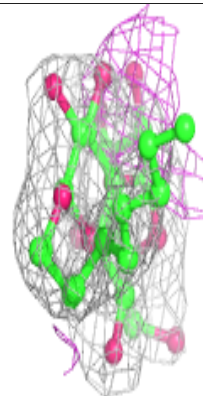
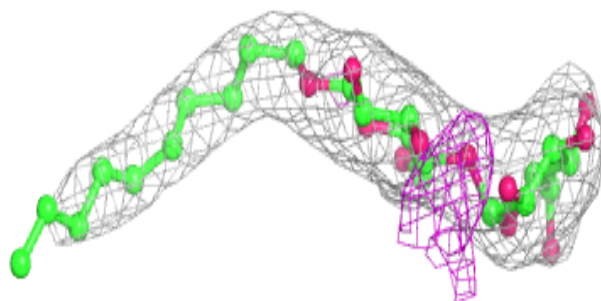
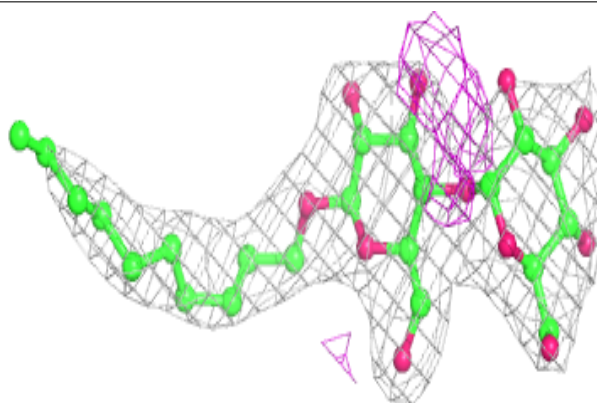


Electron density around CHD C 304:

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

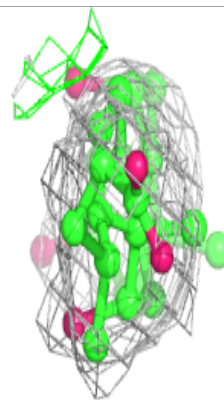
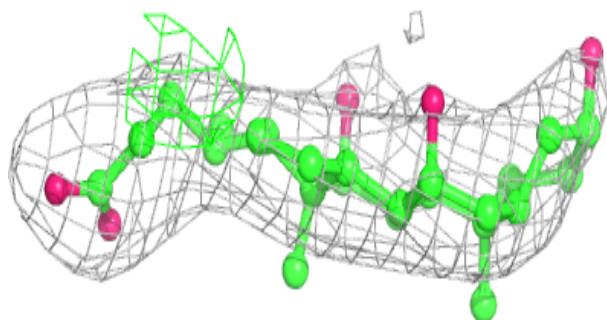
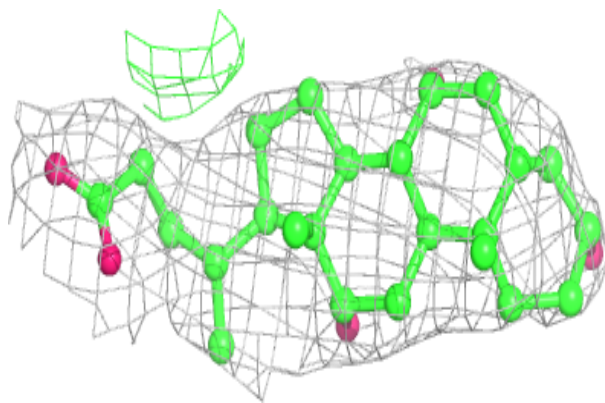
**Electron density around DMU M 101:**

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

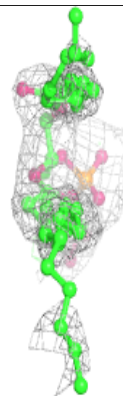
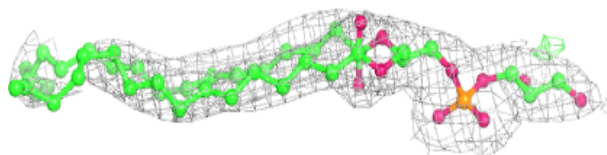
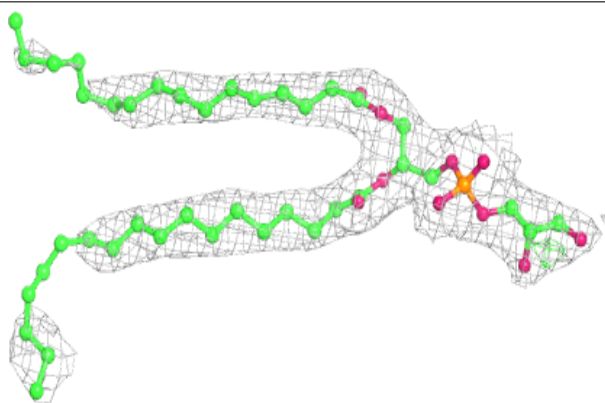


Electron density around CHD P 305:

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

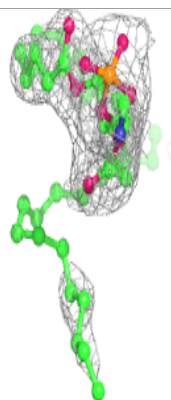
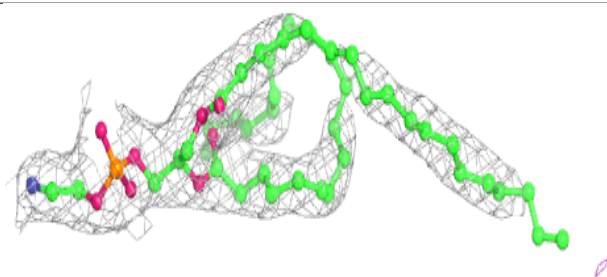
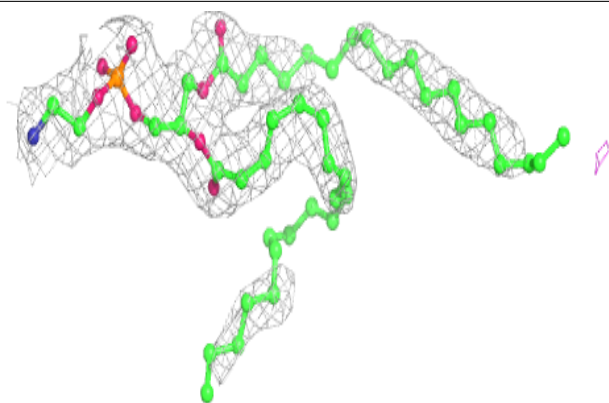
**Electron density around PGV P 303:**

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

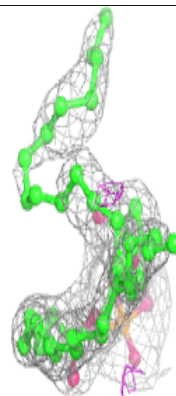
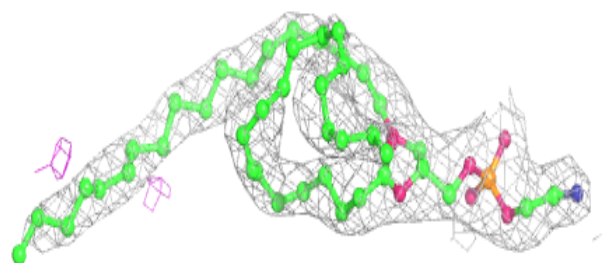
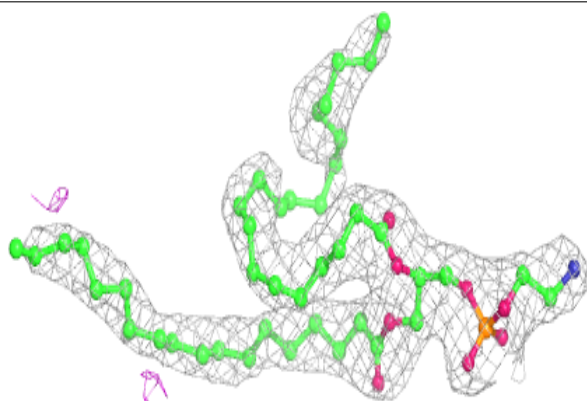


Electron density around PEK T 101:

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

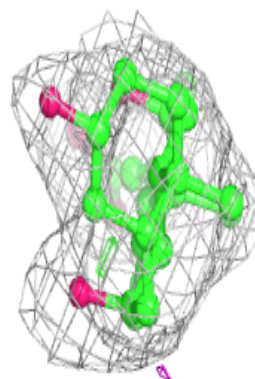
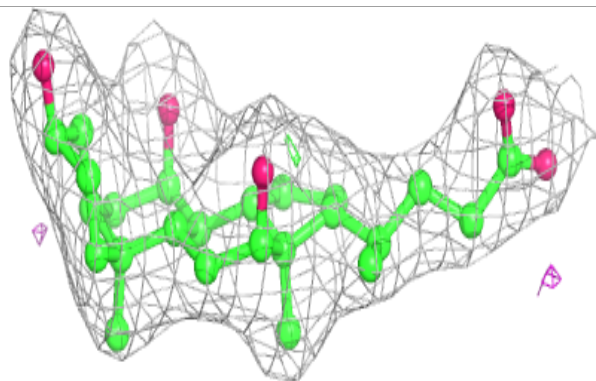
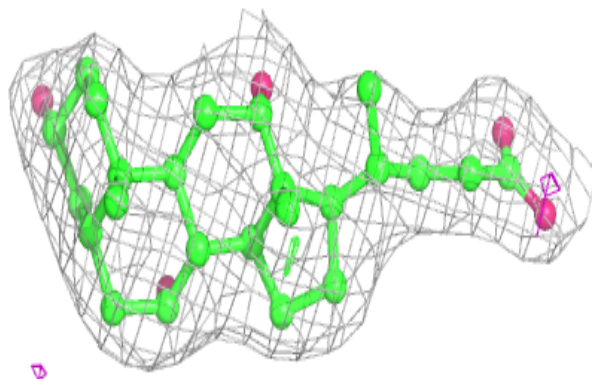
**Electron density around PEK G 101:**

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

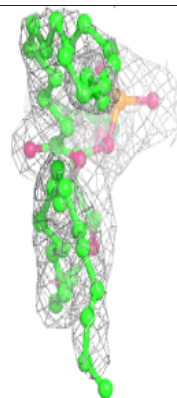
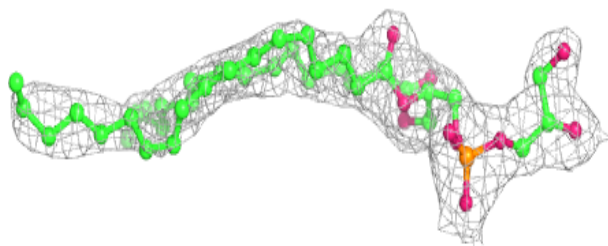
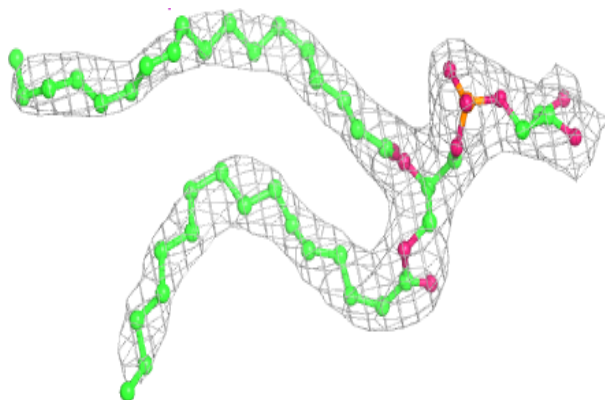


Electron density around CHD P 306:

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

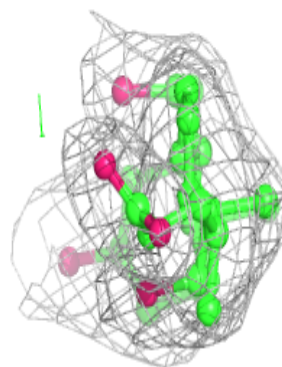
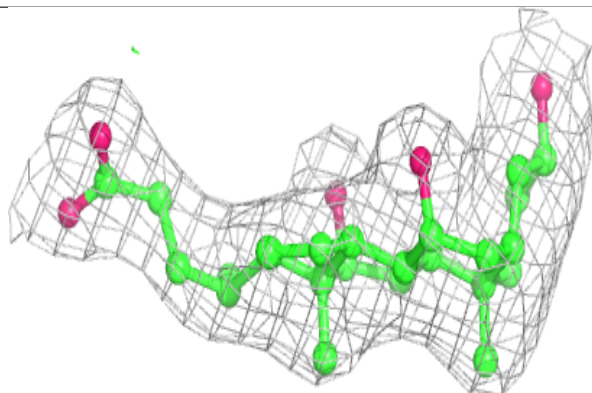
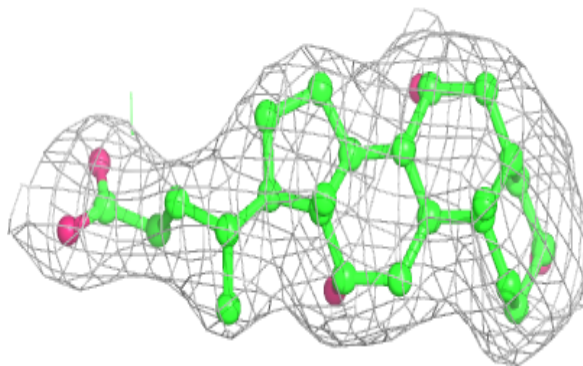
**Electron density around PGV A 608:**

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

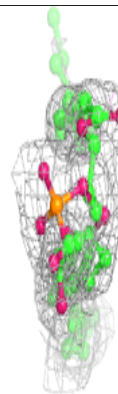
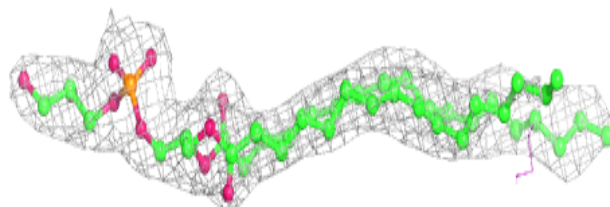
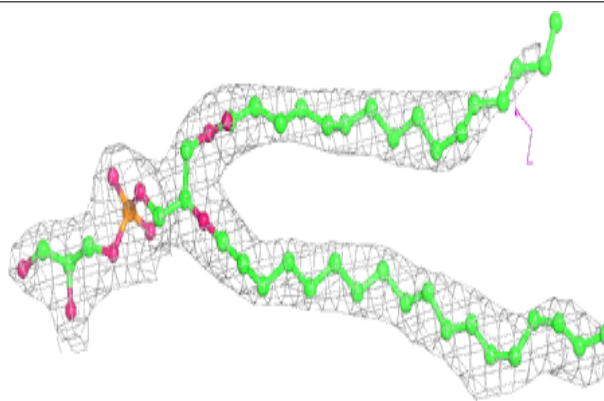


Electron density around CHD G 104:

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

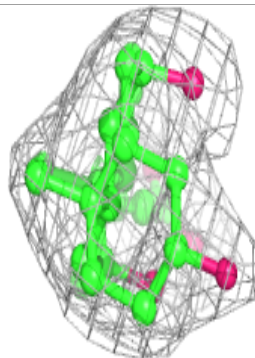
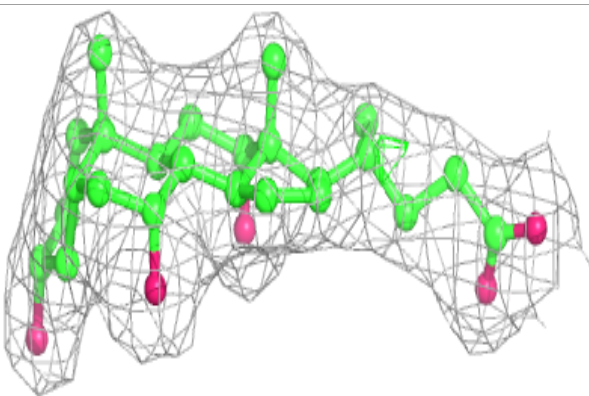
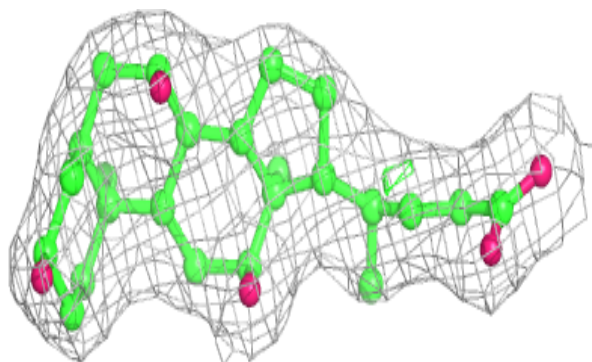
**Electron density around PGV C 302:**

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

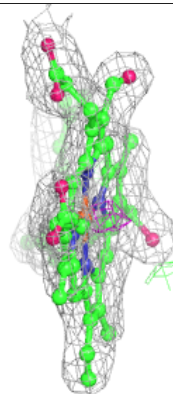
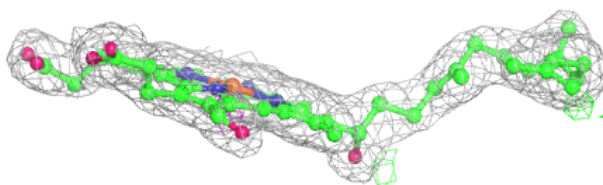
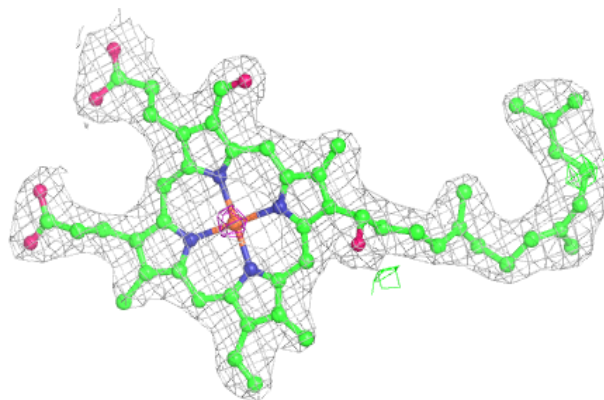


Electron density around CHD C 305:

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

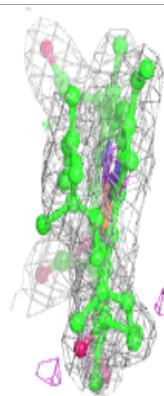
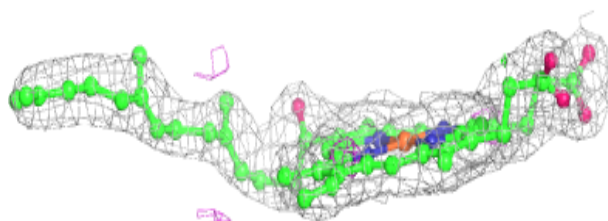
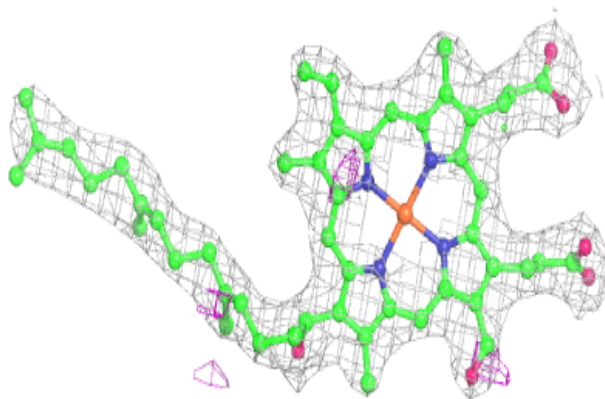
**Electron density around HEA A 602:**

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

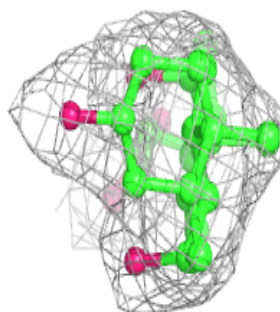
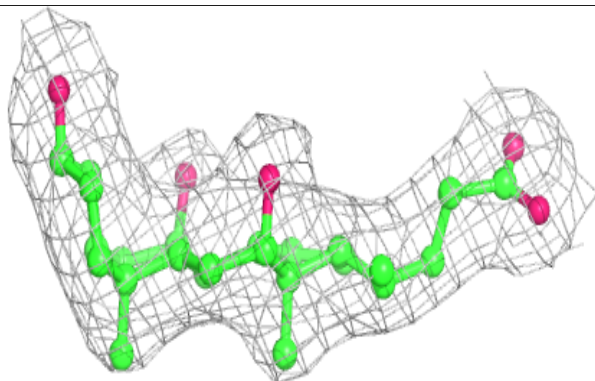
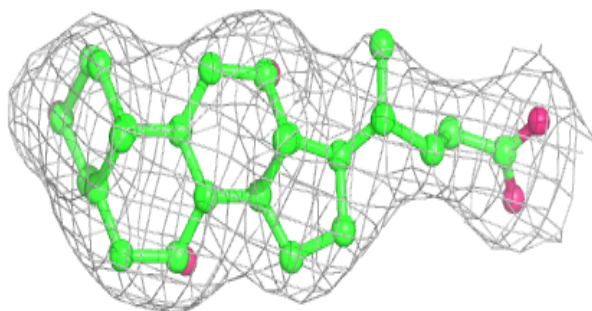


Electron density around HEA A 601:

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

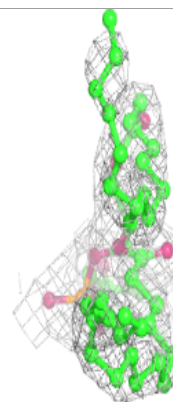
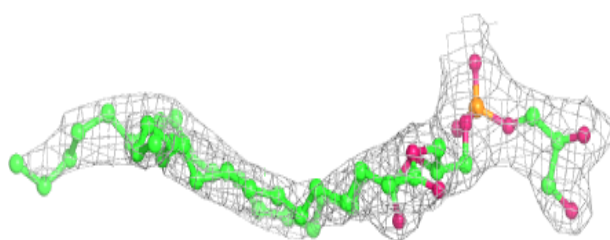
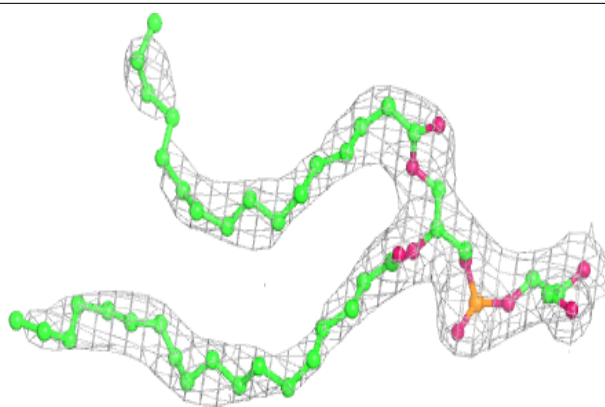
**Electron density around CHD B 302:**

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

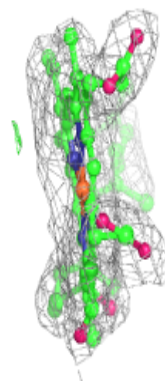
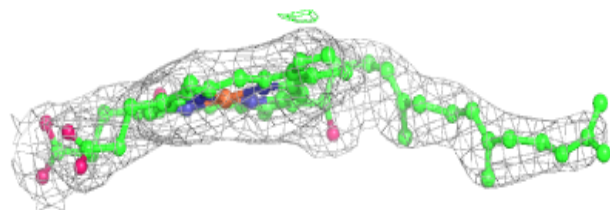
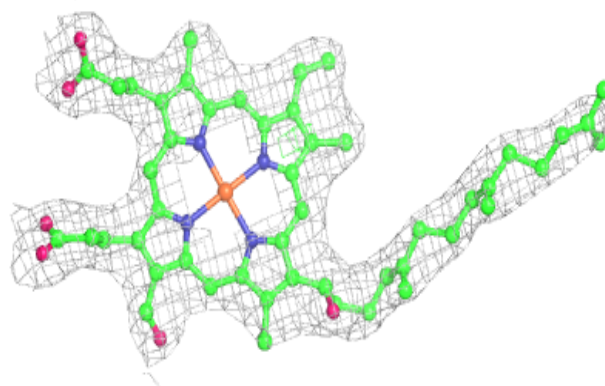


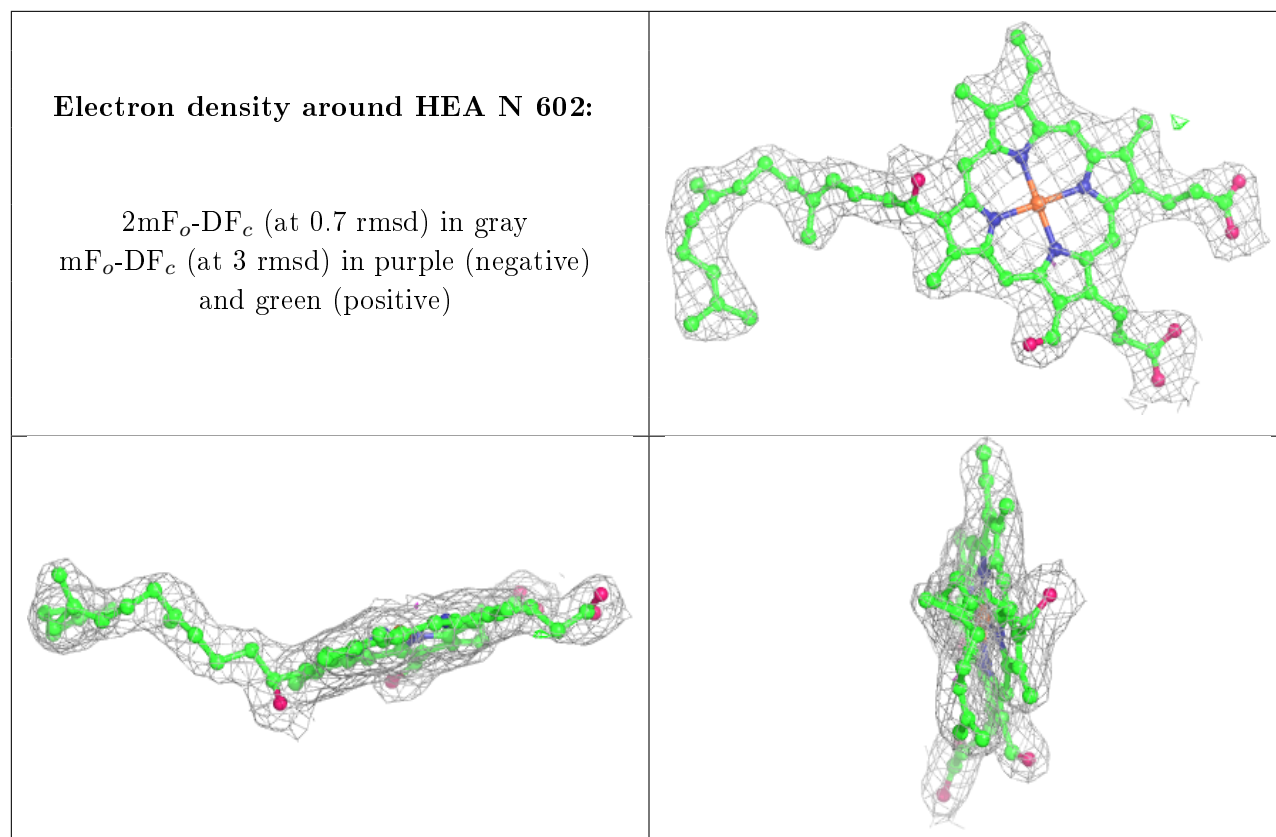
Electron density around PGV N 608:

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

**Electron density around HEA N 601:**

$2mF_o-DF_c$ (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.