



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 29, 2020 – 09:20 PM BST

PDB ID : 5X1B  
Title : CO bound cytochrome c oxidase at 20 nsec 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 : 2.40 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](mailto: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.

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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

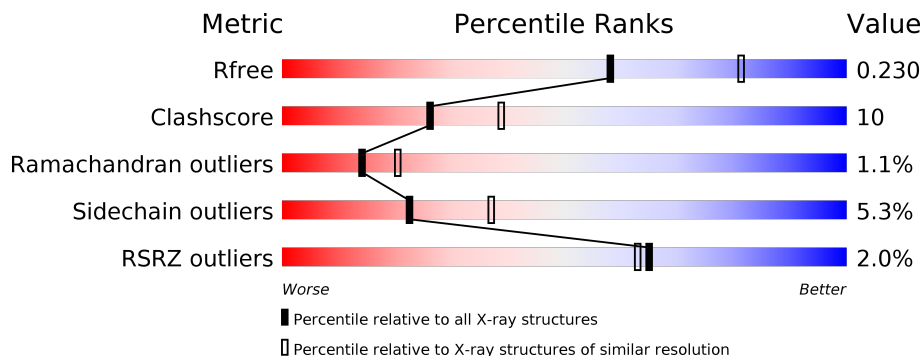
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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  $\geq 3$ , 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	
1	N	514	
2	B	227	
2	O	227	
3	C	261	

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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	A	602	X	-	-	-

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<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
14	HEA	N	601	X	-	-	-
21	EDO	A	612	-	-	-	X
21	EDO	A	614	-	-	X	-
9	SAC	V	1	-	-	-	X



## 2 Entry composition [i](#)

There are 30 unique types of molecules in this entry. The entry contains 31717 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	514	Total	C	N	O	S	0	1	0
			4030	2694	623	678	35			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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	0
			675	431	129	113	1	1			
7	T	84	Total	C	N	O	P	S	0	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	0	0
			601	390	107	100	4			
9	V	73	Total	C	N	O	S	0	0	0
			601	390	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			

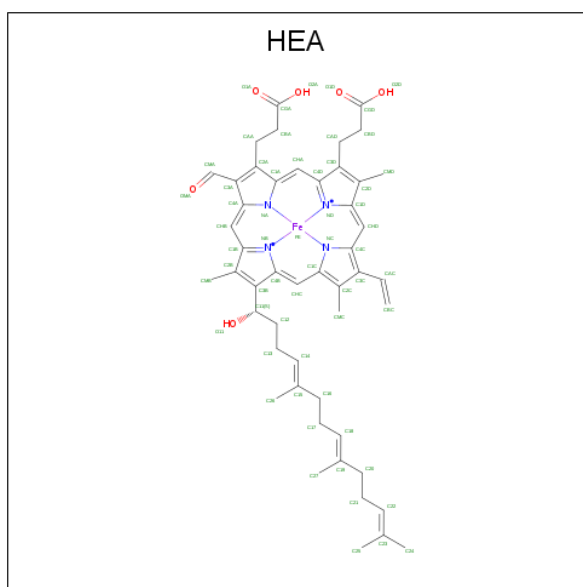
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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: C<sub>49</sub>H<sub>56</sub>FeN<sub>4</sub>O<sub>6</sub>).



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

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

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

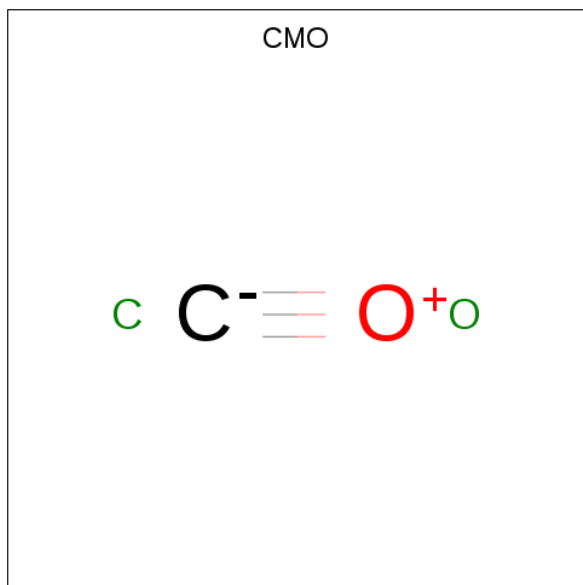
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

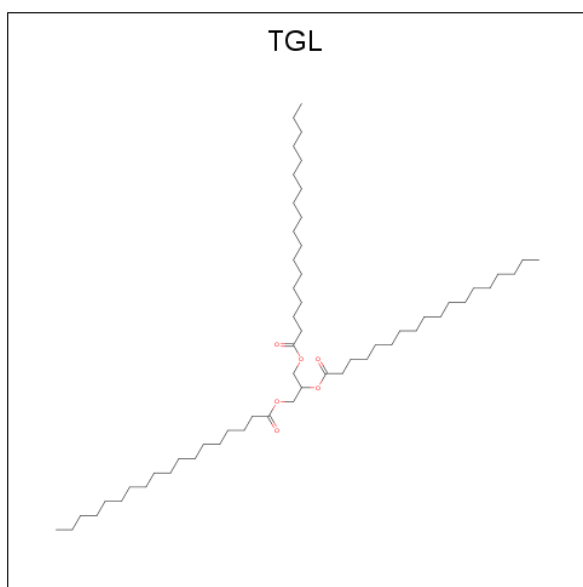
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Na 1 1	0	0
17	N	1	Total Na 1 1	0	0

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



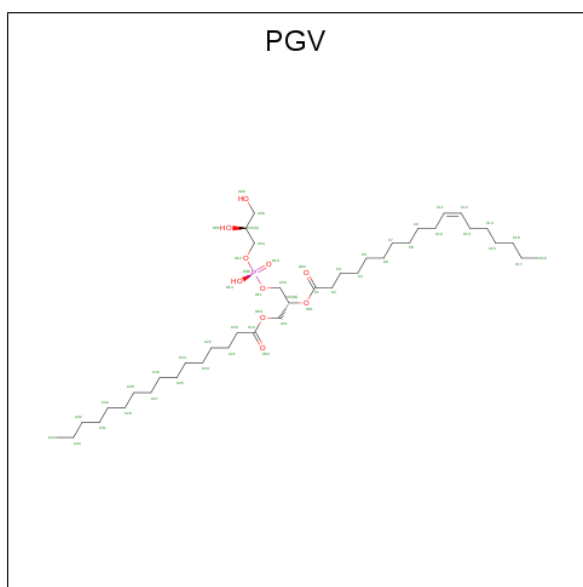
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total C O 2 1 1	0	0
18	N	1	Total C O 2 1 1	0	0

- Molecule 19 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C<sub>57</sub>H<sub>110</sub>O<sub>6</sub>).



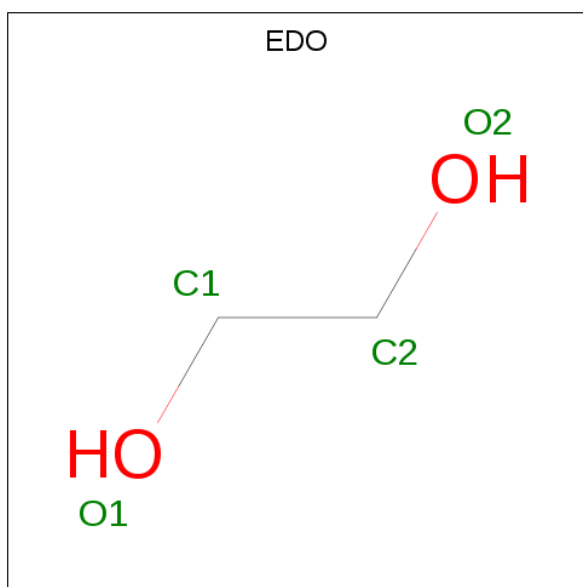
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	C	O	0	0
			63	57	6		
19	D	1	Total	C	O	0	0
			63	57	6		
19	L	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		

- 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: C<sub>40</sub>H<sub>77</sub>O<sub>10</sub>P).



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

- Molecule 21 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).

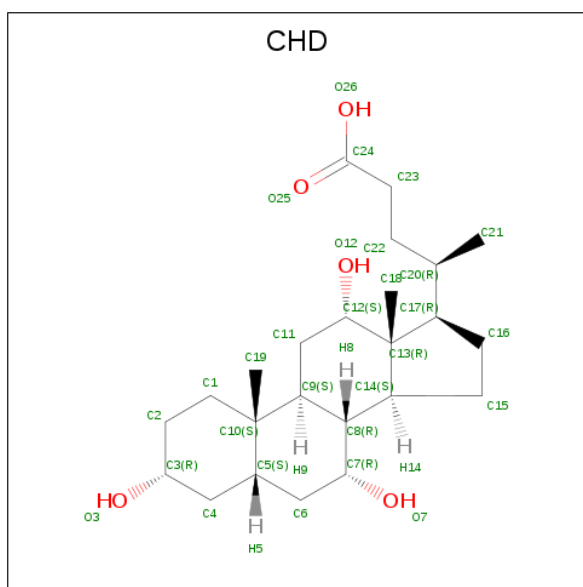


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	A	1	Total C O 4 2 2	0	0
21	A	1	Total C O 4 2 2	0	0
21	A	1	Total C O 4 2 2	0	0
21	A	1	Total C O 4 2 2	0	0
21	A	1	Total C O 4 2 2	0	0
21	B	1	Total C O 4 2 2	0	0
21	B	1	Total C O 4 2 2	0	0
21	C	1	Total C O 4 2 2	0	0
21	C	1	Total C O 4 2 2	0	0
21	C	1	Total C O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

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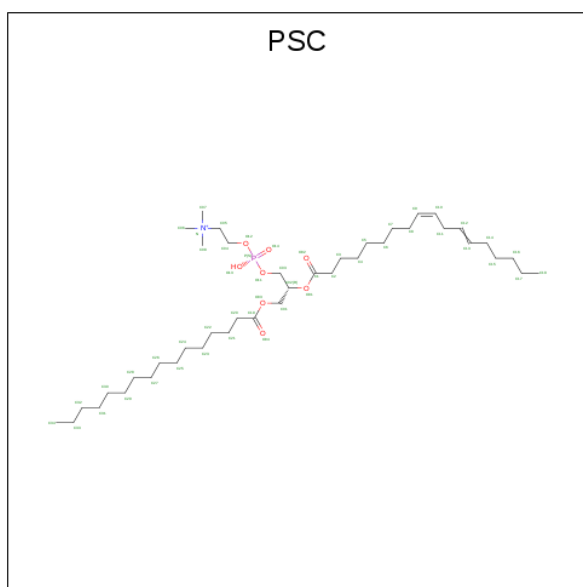






Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	B	1	Total C O 29 24 5	0	0
23	C	1	Total C O 29 24 5	0	0
23	C	1	Total C O 29 24 5	0	0
23	J	1	Total C O 29 24 5	0	0
23	O	1	Total C O 29 24 5	0	0
23	P	1	Total C O 29 24 5	0	0
23	P	1	Total C O 29 24 5	0	0
23	W	1	Total C O 29 24 5	0	0

- 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<sub>42</sub>H<sub>81</sub>NO<sub>8</sub>P).

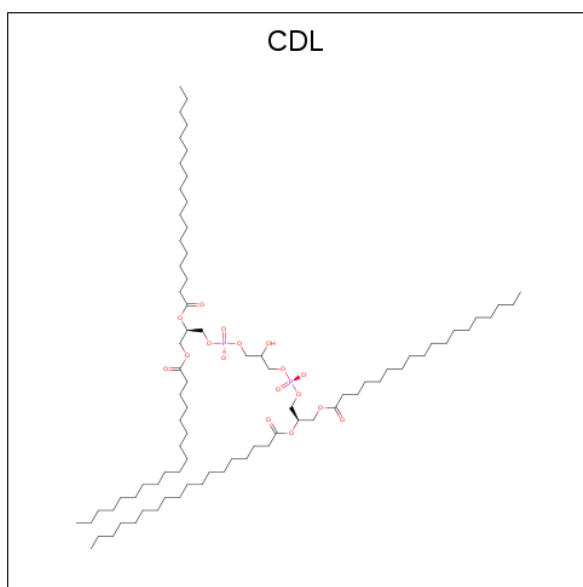


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
24	B	1	52	42	1	8	1	0	0
24	R	1	52	42	1	8	1	0	0

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

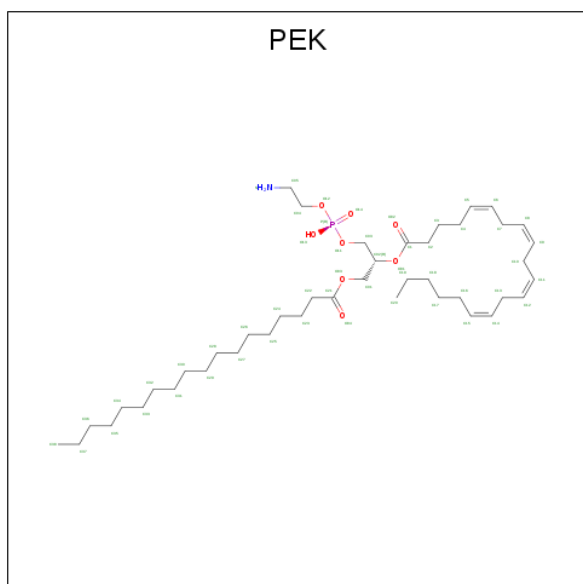
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	X		
25	P	1	1	1	0	0
25	C	1	1	1	0	0

- Molecule 26 is CARDIOLIPIN (three-letter code: CDL) (formula: C<sub>81</sub>H<sub>156</sub>O<sub>17</sub>P<sub>2</sub>).



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

- 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: C<sub>43</sub>H<sub>78</sub>NO<sub>8</sub>P).

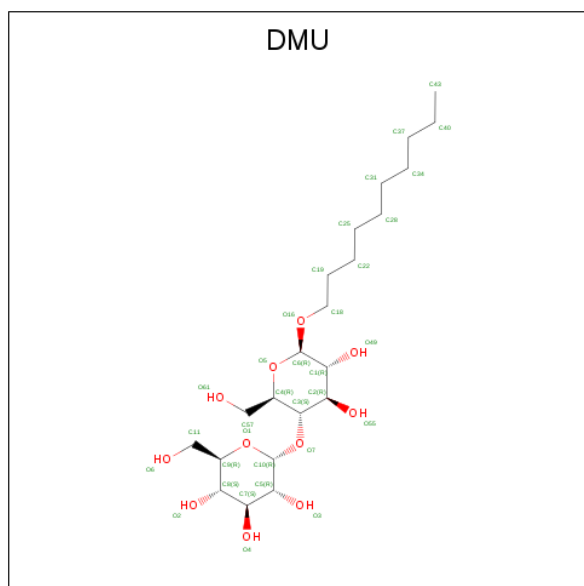


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
27	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- 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: C<sub>22</sub>H<sub>42</sub>O<sub>11</sub>).



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	125	Total	O	0	0
			125	125		
30	B	77	Total	O	0	1
			78	78		
30	C	70	Total	O	0	0
			70	70		
30	D	41	Total	O	0	0
			41	41		
30	E	24	Total	O	0	0
			24	24		
30	F	36	Total	O	0	0
			36	36		
30	G	31	Total	O	0	0
			31	31		
30	H	33	Total	O	0	0
			33	33		
30	I	12	Total	O	0	0
			12	12		
30	J	19	Total	O	0	0
			19	19		
30	K	19	Total	O	0	0
			19	19		
30	L	14	Total	O	0	0
			14	14		
30	M	15	Total	O	0	0
			15	15		
30	N	117	Total	O	0	0
			117	117		
30	O	76	Total	O	0	1
			77	77		
30	P	54	Total	O	0	0
			54	54		
30	Q	29	Total	O	0	0
			29	29		
30	R	29	Total	O	0	0
			29	29		

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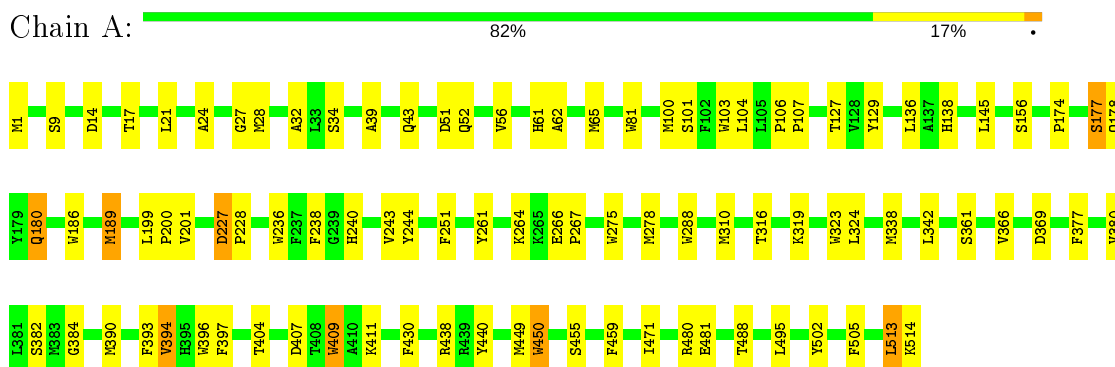
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
30	S	43	Total O 43 43	0	0
30	T	20	Total O 20 20	0	0
30	U	31	Total O 31 31	0	0
30	V	19	Total O 19 19	0	0
30	W	17	Total O 17 17	0	0
30	X	9	Total O 9 9	0	0
30	Y	6	Total O 6 6	0	0
30	Z	4	Total O 4 4	0	0

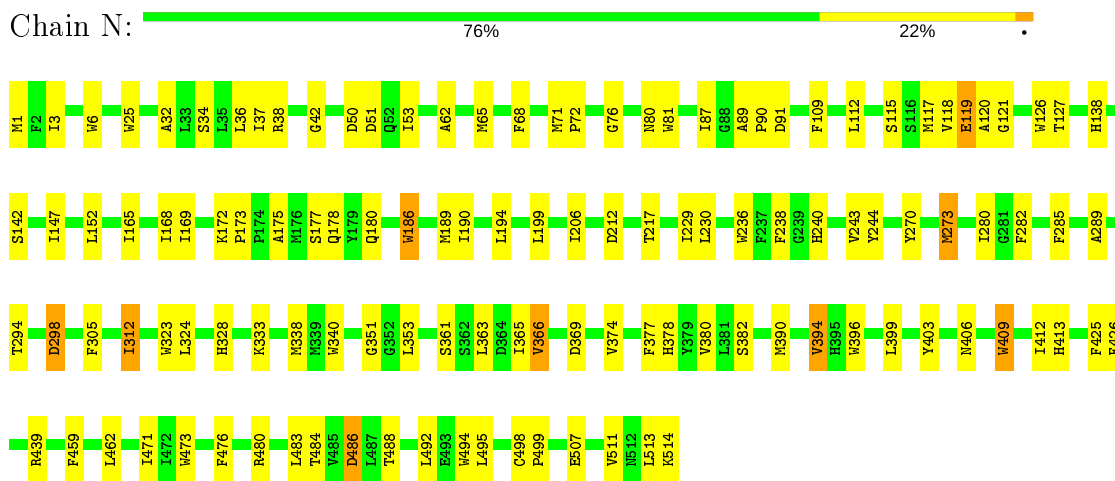
### 3 Residue-property plots [i](#)

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

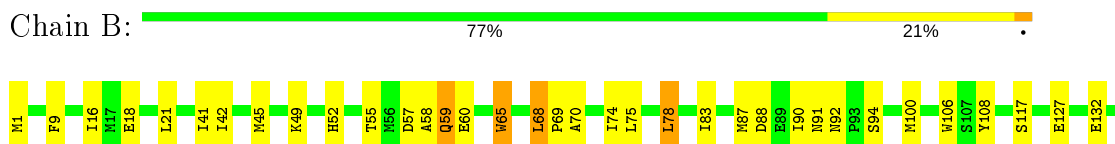
- Molecule 1: Cytochrome c oxidase subunit 1



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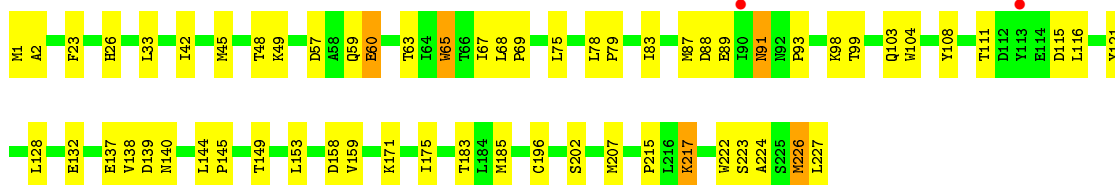
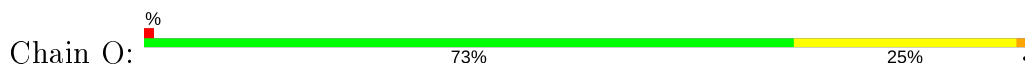
- Molecule 2: Cytochrome c oxidase subunit 2



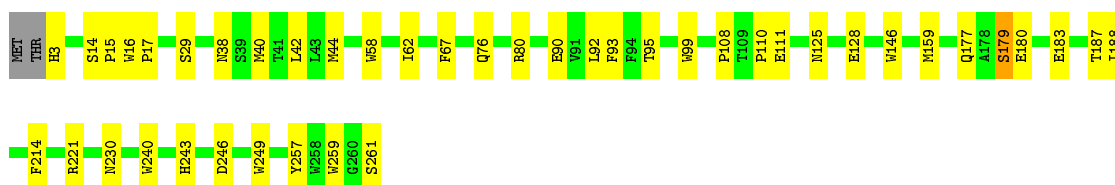
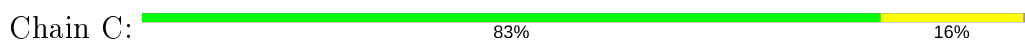




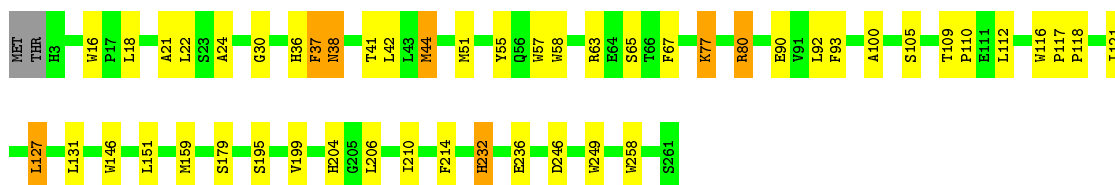
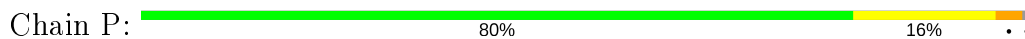
- Molecule 2: Cytochrome c oxidase subunit 2



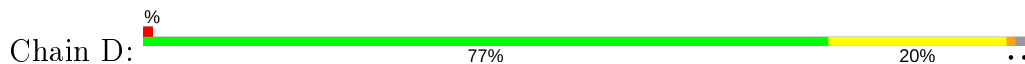
- Molecule 3: Cytochrome c oxidase subunit 3



- Molecule 3: Cytochrome c oxidase subunit 3



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

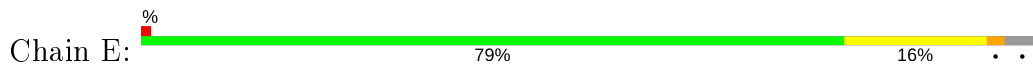


- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial





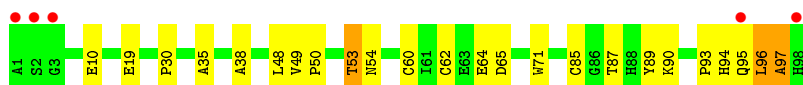
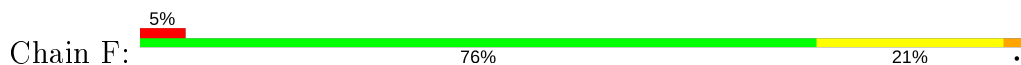
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



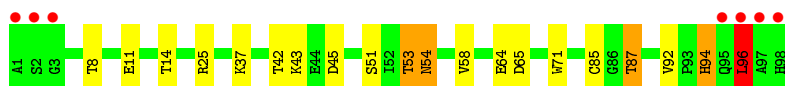
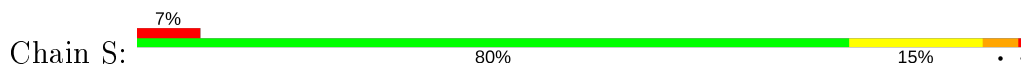
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



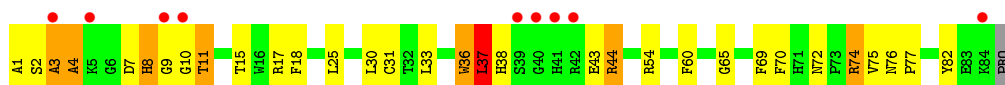
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



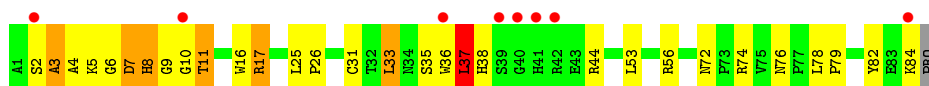
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



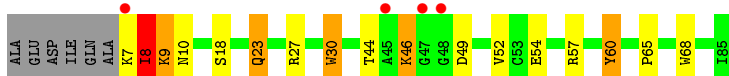
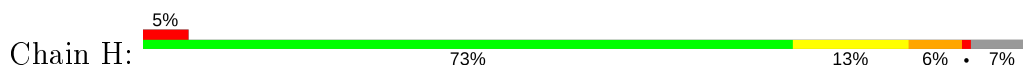
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



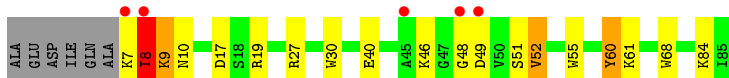
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



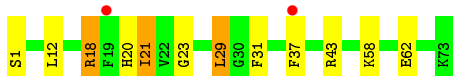
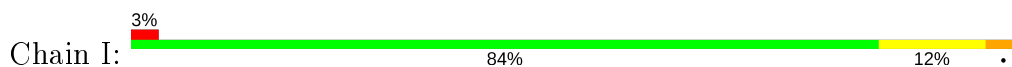
- Molecule 8: Cytochrome c oxidase subunit 6B1



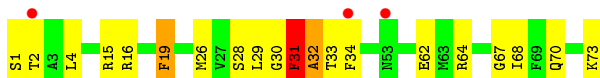
- Molecule 8: Cytochrome c oxidase subunit 6B1



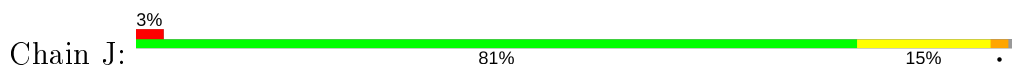
- Molecule 9: Cytochrome c oxidase subunit 6C



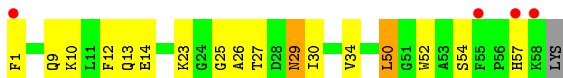
- Molecule 9: Cytochrome c oxidase subunit 6C



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



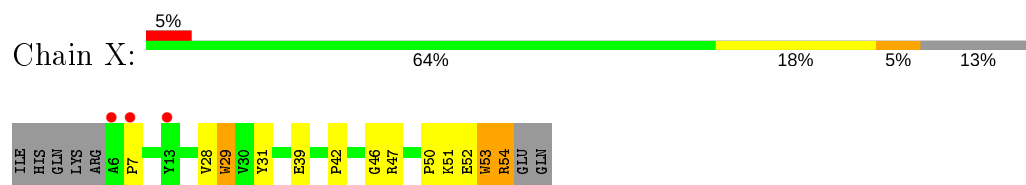
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



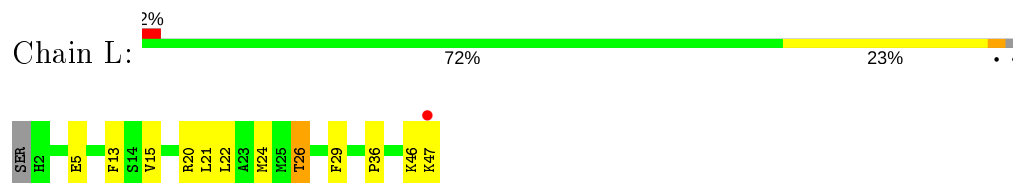
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



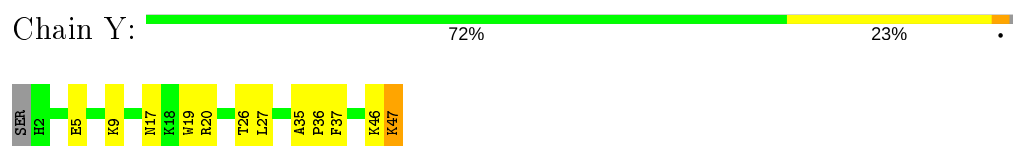
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



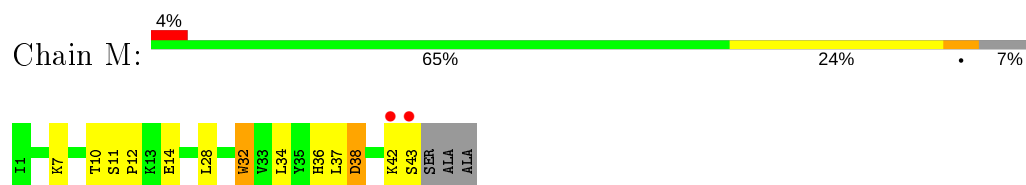
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



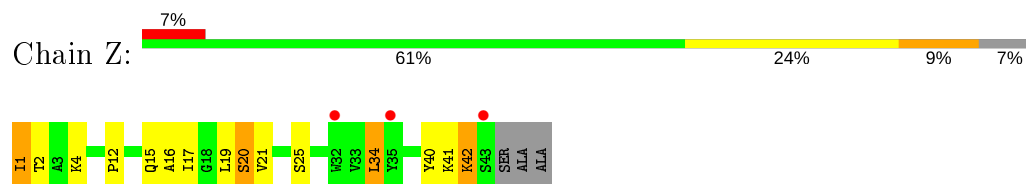
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	185.85Å 209.49Å 179.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.40 14.99 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.7 (15.00-2.40) 98.2 (14.99-2.40)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.32 (at 2.39Å)	Xtrriage
Refinement program	REFMAC 5.8.0048	Depositor
R, $R_{free}$	0.182 , 0.230 0.182 , 0.230	Depositor DCC
$R_{free}$ test set	13569 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.1	Xtrriage
Anisotropy	0.221	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 72.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.21$	Xtrriage
Estimated twinning fraction	0.045 for l,-k,h	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	31717	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.91	10/4164 (0.2%)	0.89	4/5689 (0.1%)
1	N	0.86	11/4156 (0.3%)	0.82	0/5678
2	B	0.81	2/1860 (0.1%)	0.90	1/2534 (0.0%)
2	O	0.73	2/1860 (0.1%)	0.83	0/2534
3	C	0.92	7/2197 (0.3%)	0.81	0/3005
3	P	0.89	4/2197 (0.2%)	0.80	0/3005
4	D	0.82	4/1229 (0.3%)	0.79	0/1658
4	Q	0.76	4/1229 (0.3%)	0.74	0/1658
5	E	0.67	1/871 (0.1%)	0.80	0/1182
5	R	0.65	0/871	0.74	0/1182
6	F	0.74	1/765 (0.1%)	0.86	2/1038 (0.2%)
6	S	0.72	0/765	0.82	1/1038 (0.1%)
7	G	0.86	1/690 (0.1%)	0.87	1/937 (0.1%)
7	T	0.80	1/690 (0.1%)	0.83	1/937 (0.1%)
8	H	0.85	2/682 (0.3%)	0.86	0/921
8	U	0.79	3/682 (0.4%)	0.79	0/921
9	I	0.69	0/605	0.83	0/802
9	V	0.60	0/605	0.80	1/802 (0.1%)
10	J	0.72	0/471	0.75	0/636
10	W	0.66	1/471 (0.2%)	0.77	0/636
11	K	0.81	1/398 (0.3%)	0.76	0/546
11	X	0.80	2/398 (0.5%)	0.75	0/546
12	L	0.80	0/393	0.76	0/526
12	Y	0.75	1/393 (0.3%)	0.75	0/526
13	M	0.81	1/345 (0.3%)	0.78	0/470
13	Z	0.68	0/345	0.75	0/470
All	All	0.82	59/29332 (0.2%)	0.82	11/39877 (0.0%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	G	0	1
7	T	0	2
All	All	0	3

The worst 5 of 59 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	58	TRP	CD2-CE2	7.46	1.50	1.41
1	N	126	TRP	CD2-CE2	7.33	1.50	1.41
1	A	396	TRP	CD2-CE2	6.55	1.49	1.41
2	B	106	TRP	CD2-CE2	6.42	1.49	1.41
1	N	340	TRP	CD2-CE2	6.38	1.49	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	227	ASP	CB-CG-OD1	7.54	125.08	118.30
1	A	438	ARG	NE-CZ-NH1	-6.50	117.05	120.30
6	S	96	LEU	CA-CB-CG	6.36	129.92	115.30
7	G	37	LEU	CA-CB-CG	6.03	129.17	115.30
6	F	48	LEU	CB-CG-CD2	-6.00	100.81	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	G	11	TPO	Peptide
7	T	10	GLY	Peptide
7	T	11	TPO	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	4030	0	4009	73	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	4027	0	4002	99	0
2	B	1824	0	1833	34	0
2	O	1824	0	1833	38	0
3	C	2110	0	2027	31	0
3	P	2110	0	2027	40	0
4	D	1195	0	1183	21	0
4	Q	1195	0	1183	31	0
5	E	852	0	845	8	0
5	R	852	0	845	21	0
6	F	748	0	728	13	0
6	S	748	0	728	18	0
7	G	675	0	643	29	0
7	T	675	0	643	23	0
8	H	662	0	623	13	0
8	U	662	0	623	9	0
9	I	601	0	613	8	0
9	V	601	0	613	23	0
10	J	460	0	459	8	0
10	W	460	0	459	11	0
11	K	384	0	366	6	0
11	X	384	0	366	12	0
12	L	380	0	380	12	0
12	Y	380	0	380	13	0
13	M	335	0	352	9	0
13	Z	335	0	352	15	0
14	A	120	0	108	12	0
14	N	120	0	108	13	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	0	0
19	A	63	0	110	3	0
19	D	63	0	110	1	0
19	L	63	0	110	4	0
19	N	189	0	330	11	0
20	A	102	0	152	3	0
20	C	102	0	152	0	0
20	G	51	0	76	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	N	102	0	152	8	0
20	P	51	0	76	3	0
21	A	20	0	30	9	0
21	B	8	0	12	1	0
21	C	12	0	18	0	0
21	F	4	0	6	0	0
21	G	4	0	6	0	0
21	K	12	0	18	0	0
21	L	4	0	6	0	0
21	N	4	0	6	1	0
21	T	4	0	6	1	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	3	0
23	J	29	0	39	1	0
23	O	29	0	39	1	0
23	P	58	0	78	2	0
23	W	29	0	38	1	0
24	B	52	0	80	12	0
24	R	52	0	80	6	0
25	C	1	0	0	0	0
25	P	1	0	0	0	0
26	C	200	0	312	15	0
26	P	100	0	156	7	0
26	T	100	0	156	13	0
27	C	53	0	77	3	0
27	G	106	0	154	10	0
27	P	53	0	77	4	0
27	T	106	0	154	4	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	M	33	0	42	1	0
29	Z	33	0	42	1	0
30	A	125	0	0	22	0
30	B	78	0	0	6	0
30	C	70	0	0	18	0
30	D	41	0	0	2	0
30	E	24	0	0	2	0
30	F	36	0	0	2	0
30	G	31	0	0	2	0
30	H	33	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	I	12	0	0	0	0
30	J	19	0	0	2	0
30	K	19	0	0	3	0
30	L	14	0	0	2	0
30	M	15	0	0	1	0
30	N	117	0	0	16	0
30	O	77	0	0	8	0
30	P	54	0	0	5	0
30	Q	29	0	0	7	0
30	R	29	0	0	3	0
30	S	43	0	0	4	0
30	T	20	0	0	6	0
30	U	31	0	0	3	0
30	V	19	0	0	4	0
30	W	17	0	0	1	0
30	X	9	0	0	4	0
30	Y	6	0	0	1	0
30	Z	4	0	0	0	0
All	All	31717	0	31348	645	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 645 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:N:240:HIS:NE2	1:N:244:TYR:CE2	1.73	1.45
1:A:240:HIS:NE2	1:A:244:TYR:HE2	1.01	1.42
1:A:240:HIS:NE2	1:A:244:TYR:CE2	1.78	1.30
1:A:240:HIS:CD2	1:A:244:TYR:HE2	1.49	1.29
1:N:240:HIS:NE2	1:N:244:TYR:HE2	0.80	1.28

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	513/514 (100%)	494 (96%)	19 (4%)	0	100	100
1	N	512/514 (100%)	488 (95%)	23 (4%)	1 (0%)	47	62
2	B	225/227 (99%)	213 (95%)	11 (5%)	1 (0%)	34	48
2	O	225/227 (99%)	211 (94%)	12 (5%)	2 (1%)	17	25
3	C	257/261 (98%)	250 (97%)	7 (3%)	0	100	100
3	P	257/261 (98%)	248 (96%)	6 (2%)	3 (1%)	13	19
4	D	142/147 (97%)	133 (94%)	9 (6%)	0	100	100
4	Q	142/147 (97%)	130 (92%)	9 (6%)	3 (2%)	7	8
5	E	103/109 (94%)	98 (95%)	4 (4%)	1 (1%)	15	23
5	R	103/109 (94%)	99 (96%)	3 (3%)	1 (1%)	15	23
6	F	96/98 (98%)	87 (91%)	7 (7%)	2 (2%)	7	8
6	S	96/98 (98%)	90 (94%)	5 (5%)	1 (1%)	15	23
7	G	81/85 (95%)	69 (85%)	8 (10%)	4 (5%)	2	1
7	T	81/85 (95%)	68 (84%)	5 (6%)	8 (10%)	0	0
8	H	77/85 (91%)	67 (87%)	9 (12%)	1 (1%)	12	17
8	U	77/85 (91%)	69 (90%)	4 (5%)	4 (5%)	2	1
9	I	71/73 (97%)	66 (93%)	5 (7%)	0	100	100
9	V	71/73 (97%)	64 (90%)	6 (8%)	1 (1%)	11	15
10	J	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
10	W	56/59 (95%)	53 (95%)	2 (4%)	1 (2%)	8	10
11	K	47/56 (84%)	47 (100%)	0	0	100	100
11	X	47/56 (84%)	41 (87%)	5 (11%)	1 (2%)	7	8
12	L	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
12	Y	44/47 (94%)	40 (91%)	4 (9%)	0	100	100
13	M	41/46 (89%)	40 (98%)	0	1 (2%)	6	6
13	Z	41/46 (89%)	38 (93%)	2 (5%)	1 (2%)	6	6
All	All	3505/3614 (97%)	3301 (94%)	167 (5%)	37 (1%)	14	20

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	97	ALA
7	G	3	ALA
7	G	4	ALA
7	G	8	HIS
8	H	8	ILE

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	427/426 (100%)	411 (96%)	16 (4%)	34	53
1	N	426/426 (100%)	408 (96%)	18 (4%)	30	47
2	B	210/210 (100%)	198 (94%)	12 (6%)	20	33
2	O	210/210 (100%)	198 (94%)	12 (6%)	20	33
3	C	224/226 (99%)	220 (98%)	4 (2%)	59	76
3	P	224/226 (99%)	216 (96%)	8 (4%)	35	54
4	D	128/129 (99%)	125 (98%)	3 (2%)	50	70
4	Q	128/129 (99%)	121 (94%)	7 (6%)	21	35
5	E	92/95 (97%)	86 (94%)	6 (6%)	17	27
5	R	92/95 (97%)	87 (95%)	5 (5%)	22	36
6	F	81/81 (100%)	77 (95%)	4 (5%)	25	40
6	S	81/81 (100%)	74 (91%)	7 (9%)	10	16
7	G	67/68 (98%)	61 (91%)	6 (9%)	9	14
7	T	67/68 (98%)	63 (94%)	4 (6%)	19	31
8	H	71/75 (95%)	63 (89%)	8 (11%)	6	8
8	U	71/75 (95%)	65 (92%)	6 (8%)	10	16
9	I	57/57 (100%)	52 (91%)	5 (9%)	10	15
9	V	57/57 (100%)	51 (90%)	6 (10%)	7	9
10	J	49/50 (98%)	46 (94%)	3 (6%)	18	30
10	W	49/50 (98%)	43 (88%)	6 (12%)	5	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	39/46 (85%)	37 (95%)	2 (5%)	24	39
11	X	39/46 (85%)	37 (95%)	2 (5%)	24	39
12	L	39/40 (98%)	37 (95%)	2 (5%)	24	39
12	Y	39/40 (98%)	37 (95%)	2 (5%)	24	39
13	M	37/38 (97%)	35 (95%)	2 (5%)	22	36
13	Z	37/38 (97%)	32 (86%)	5 (14%)	4	4
All	All	3041/3082 (99%)	2880 (95%)	161 (5%)	22	37

5 of 161 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	M	38	ASP
1	N	486	ASP
10	W	14	GLU
1	N	91	ASP
1	N	273	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
10	J	57	HIS
1	N	413	HIS
8	U	23	GLN
11	K	35	GLN
1	N	180	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	FME	N	1	1	8,9,10	0.45	0	7,9,11	1.59	2 (28%)
7	TPO	T	11	7	8,10,11	1.73	2 (25%)	10,14,16	1.02	1 (10%)
9	SAC	I	1	9	7,8,9	1.30	1 (14%)	8,9,11	0.99	0
1	FME	A	1	1	8,9,10	0.44	0	7,9,11	1.97	4 (57%)
2	FME	O	1	2	8,9,10	0.85	0	7,9,11	1.63	1 (14%)
7	TPO	G	11	7	8,10,11	1.45	1 (12%)	10,14,16	0.92	1 (10%)
2	FME	B	1	2	8,9,10	0.97	0	7,9,11	1.45	3 (42%)
9	SAC	V	1	9	7,8,9	1.70	1 (14%)	8,9,11	1.82	2 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	N	1	1	-	2/7/9/11	-
7	TPO	T	11	7	-	2/9/11/13	-
9	SAC	I	1	9	-	4/7/8/10	-
1	FME	A	1	1	-	3/7/9/11	-
2	FME	O	1	2	-	0/7/9/11	-
7	TPO	G	11	7	-	2/9/11/13	-
2	FME	B	1	2	-	1/7/9/11	-
9	SAC	V	1	9	-	4/7/8/10	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	V	1	SAC	CA-N	4.27	1.52	1.46
9	I	1	SAC	CA-N	3.22	1.50	1.46
7	T	11	TPO	P-O1P	2.85	1.59	1.50
7	G	11	TPO	P-O1P	2.83	1.59	1.50
7	T	11	TPO	P-OG1	2.33	1.63	1.59

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	V	1	SAC	C-CA-N	3.75	116.49	109.73
2	O	1	FME	CA-N-CN	3.70	128.51	122.82
1	N	1	FME	C-CA-N	2.76	114.71	109.73
1	A	1	FME	C-CA-N	2.75	114.69	109.73
1	A	1	FME	CE-SD-CG	2.60	109.33	100.40

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	N	1	FME	CA-CB-CG-SD
7	T	11	TPO	N-CA-CB-OG1
9	I	1	SAC	C2A-C1A-N-CA
9	I	1	SAC	OAC-C1A-N-CA
9	I	1	SAC	C-CA-N-C1A

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 72 ligands modelled in this entry, 2 are unknown and 8 are monoatomic - leaving 62 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
20	PGV	N	608	-	50,50,50	0.90	3 (6%)	53,56,56	1.17	4 (7%)
22	CUA	O	301	2	0,1,1	0.00	-	-		
19	TGL	N	609	-	62,62,62	1.12	3 (4%)	65,65,65	1.29	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	PGV	A	609	-	50,50,50	1.10	2 (4%)	53,56,56	1.08	5 (9%)
27	PEK	G	102	-	52,52,52	1.21	2 (3%)	55,57,57	1.06	5 (9%)
20	PGV	C	308	-	50,50,50	1.21	2 (4%)	53,56,56	1.01	3 (5%)
23	CHD	W	101	-	29,32,32	0.83	1 (3%)	48,51,51	2.13	16 (33%)
27	PEK	P	302	-	52,52,52	0.87	2 (3%)	55,57,57	1.35	5 (9%)
23	CHD	P	305	-	29,32,32	0.50	0	48,51,51	1.87	13 (27%)
23	CHD	J	101	-	29,32,32	0.60	0	48,51,51	1.60	10 (20%)
19	TGL	D	201	-	62,62,62	1.13	3 (4%)	65,65,65	0.99	5 (7%)
21	EDO	K	101	-	3,3,3	0.47	0	2,2,2	0.33	0
21	EDO	A	610	-	3,3,3	0.52	0	2,2,2	0.57	0
14	HEA	A	602	1	44,67,67	0.91	2 (4%)	37,103,103	1.75	7 (18%)
29	DMU	Z	101	-	34,34,34	0.53	0	45,45,45	1.13	4 (8%)
23	CHD	B	302	-	29,32,32	0.79	0	48,51,51	1.25	4 (8%)
14	HEA	A	601	1	44,67,67	1.04	3 (6%)	37,103,103	1.89	9 (24%)
26	CDL	P	304	-	99,99,99	1.39	12 (12%)	105,111,111	1.16	7 (6%)
14	HEA	N	602	1	44,67,67	1.07	1 (2%)	37,103,103	1.97	11 (29%)
24	PSC	R	201	-	51,51,51	1.22	3 (5%)	57,59,59	0.99	4 (7%)
21	EDO	K	103	-	3,3,3	0.56	0	2,2,2	0.11	0
27	PEK	T	102	-	52,52,52	1.19	2 (3%)	55,57,57	1.13	4 (7%)
21	EDO	L	102	-	3,3,3	0.46	0	2,2,2	0.40	0
21	EDO	B	305	-	3,3,3	0.39	0	2,2,2	0.49	0
14	HEA	N	601	1	44,67,67	1.04	3 (6%)	37,103,103	1.72	8 (21%)
21	EDO	K	102	-	3,3,3	0.50	0	2,2,2	0.26	0
18	CMO	N	606	-	0,1,1	0.00	-	-	-	-
18	CMO	A	606	15	0,1,1	0.00	-	-	-	-
27	PEK	C	306	-	52,52,52	1.03	2 (3%)	55,57,57	0.90	3 (5%)
21	EDO	C	309	-	3,3,3	0.38	0	2,2,2	0.68	0
20	PGV	C	302	-	50,50,50	0.92	2 (4%)	53,56,56	0.93	4 (7%)
20	PGV	P	303	-	50,50,50	0.93	2 (4%)	53,56,56	1.08	5 (9%)
24	PSC	B	303	-	51,51,51	1.28	3 (5%)	57,59,59	1.07	5 (8%)
26	CDL	T	103	-	99,99,99	1.37	12 (12%)	105,111,111	1.31	11 (10%)
21	EDO	B	304	-	3,3,3	0.40	0	2,2,2	0.60	0
27	PEK	T	101	-	52,52,52	1.16	2 (3%)	55,57,57	1.06	4 (7%)
19	TGL	A	607	-	62,62,62	1.23	4 (6%)	65,65,65	1.38	10 (15%)
19	TGL	N	611	-	62,62,62	1.18	3 (4%)	65,65,65	1.24	7 (10%)
20	PGV	N	607	-	50,50,50	1.09	2 (4%)	53,56,56	1.07	4 (7%)
21	EDO	C	310	-	3,3,3	0.53	0	2,2,2	0.33	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	PGV	A	608	-	50,50,50	0.79	2 (4%)	53,56,56	1.44	5 (9%)
23	CHD	P	306	-	29,32,32	0.72	1 (3%)	48,51,51	1.52	11 (22%)
26	CDL	C	303	-	99,99,99	1.39	12 (12%)	105,111,111	1.22	7 (6%)
21	EDO	N	612	-	3,3,3	0.56	0	2,2,2	0.16	0
27	PEK	G	101	-	52,52,52	0.94	2 (3%)	55,57,57	1.23	4 (7%)
19	TGL	L	101	-	62,62,62	1.19	3 (4%)	65,65,65	1.25	5 (7%)
23	CHD	C	305	-	29,32,32	0.93	1 (3%)	48,51,51	1.22	7 (14%)
21	EDO	C	311	-	3,3,3	0.53	0	2,2,2	0.30	0
21	EDO	G	104	-	3,3,3	0.40	0	2,2,2	0.56	0
20	PGV	G	103	-	50,50,50	1.07	2 (4%)	53,56,56	0.95	2 (3%)
29	DMU	M	101	-	34,34,34	0.53	0	45,45,45	1.14	4 (8%)
22	CUA	B	301	2	0,1,1	0.00	-	-	-	-
21	EDO	A	613	-	3,3,3	0.54	0	2,2,2	0.24	0
23	CHD	O	302	-	29,32,32	1.00	1 (3%)	48,51,51	1.48	8 (16%)
21	EDO	F	102	-	3,3,3	0.57	0	2,2,2	0.06	0
19	TGL	N	610	-	62,62,62	1.13	3 (4%)	65,65,65	1.13	6 (9%)
23	CHD	C	304	-	29,32,32	0.58	0	48,51,51	2.06	16 (33%)
21	EDO	A	614	-	3,3,3	0.59	0	2,2,2	0.11	0
21	EDO	T	104	-	3,3,3	0.45	0	2,2,2	0.26	0
26	CDL	C	307	-	99,99,99	1.43	13 (13%)	105,111,111	1.23	8 (7%)
21	EDO	A	611	-	3,3,3	0.37	0	2,2,2	0.61	0
21	EDO	A	612	-	3,3,3	0.52	0	2,2,2	0.10	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	PGV	N	608	-	-	22/55/55/55	-
19	TGL	N	609	-	-	37/65/65/65	-
20	PGV	A	609	-	-	31/55/55/55	-
27	PEK	G	102	-	-	35/56/56/56	-
20	PGV	C	308	-	-	32/55/55/55	-
23	CHD	W	101	-	-	4/7/74/74	0/4/4/4
27	PEK	P	302	-	-	17/56/56/56	-
23	CHD	P	305	-	-	7/7/74/74	0/4/4/4
23	CHD	J	101	-	-	7/7/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	TGL	D	201	-	-	38/65/65/65	-
21	EDO	K	101	-	-	1/1/1/1	-
21	EDO	A	610	-	-	1/1/1/1	-
14	HEA	A	602	1	1/1/7/16	1/24/76/76	-
29	DMU	Z	101	-	-	9/19/59/59	0/2/2/2
23	CHD	B	302	-	-	0/7/74/74	0/4/4/4
14	HEA	A	601	1	3/3/7/16	6/24/76/76	-
26	CDL	P	304	-	-	66/110/110/110	-
14	HEA	N	602	1	-	3/24/76/76	-
24	PSC	R	201	-	-	29/55/55/55	-
21	EDO	K	103	-	-	0/1/1/1	-
27	PEK	T	102	-	-	29/56/56/56	-
21	EDO	L	102	-	-	1/1/1/1	-
21	EDO	B	305	-	-	0/1/1/1	-
14	HEA	N	601	1	3/3/7/16	1/24/76/76	-
21	EDO	K	102	-	-	1/1/1/1	-
27	PEK	C	306	-	-	30/56/56/56	-
21	EDO	C	309	-	-	1/1/1/1	-
20	PGV	C	302	-	-	15/55/55/55	-
20	PGV	P	303	-	-	21/55/55/55	-
24	PSC	B	303	-	-	30/55/55/55	-
26	CDL	T	103	-	-	63/110/110/110	-
21	EDO	B	304	-	-	1/1/1/1	-
27	PEK	T	101	-	-	22/56/56/56	-
19	TGL	A	607	-	-	36/65/65/65	-
19	TGL	N	611	-	-	34/65/65/65	-
20	PGV	N	607	-	-	33/55/55/55	-
21	EDO	C	310	-	-	1/1/1/1	-
20	PGV	A	608	-	-	11/55/55/55	-
23	CHD	P	306	-	-	1/7/74/74	0/4/4/4
26	CDL	C	303	-	-	65/110/110/110	-
21	EDO	N	612	-	-	0/1/1/1	-
27	PEK	G	101	-	-	21/56/56/56	-
19	TGL	L	101	-	-	35/65/65/65	-
23	CHD	C	305	-	-	0/7/74/74	0/4/4/4
21	EDO	C	311	-	-	0/1/1/1	-
21	EDO	G	104	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	PGV	G	103	-	-	33/55/55/55	-
29	DMU	M	101	-	-	5/19/59/59	0/2/2/2
21	EDO	A	613	-	-	1/1/1/1	-
23	CHD	O	302	-	-	2/7/74/74	0/4/4/4
21	EDO	F	102	-	-	0/1/1/1	-
19	TGL	N	610	-	-	42/65/65/65	-
23	CHD	C	304	-	-	3/7/74/74	0/4/4/4
21	EDO	A	614	-	-	0/1/1/1	-
21	EDO	T	104	-	-	1/1/1/1	-
26	CDL	C	307	-	-	64/110/110/110	-
21	EDO	A	611	-	-	1/1/1/1	-
21	EDO	A	612	-	-	1/1/1/1	-

The worst 5 of 116 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	L	101	TGL	OG2-CB1	5.59	1.50	1.34
19	A	607	TGL	OG1-CA1	5.58	1.49	1.33
27	T	102	PEK	O01-C1	5.50	1.49	1.34
19	A	607	TGL	OG2-CB1	5.44	1.49	1.34
20	C	308	PGV	O01-C1	5.43	1.49	1.34

The worst 5 of 268 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	101	CHD	C13-C17-C20	5.97	126.63	119.50
19	N	611	TGL	OG2-CB1-CB2	5.80	124.01	111.50
19	N	609	TGL	OG2-CB1-CB2	5.64	123.66	111.50
26	T	103	CDL	OB6-CB5-C51	5.53	123.42	111.50
26	C	303	CDL	OA6-CA5-C11	5.44	123.22	111.50

5 of 7 chirality outliers are listed below:

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

5 of 951 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	N	608	PGV	C10-C11-C12-C13
20	A	609	PGV	C03-O11-P-O12
20	A	609	PGV	C03-O11-P-O13
20	A	609	PGV	C03-O11-P-O14
20	A	609	PGV	C04-C05-C06-O06

There are no ring outliers.

46 monomers are involved in 154 short contacts:

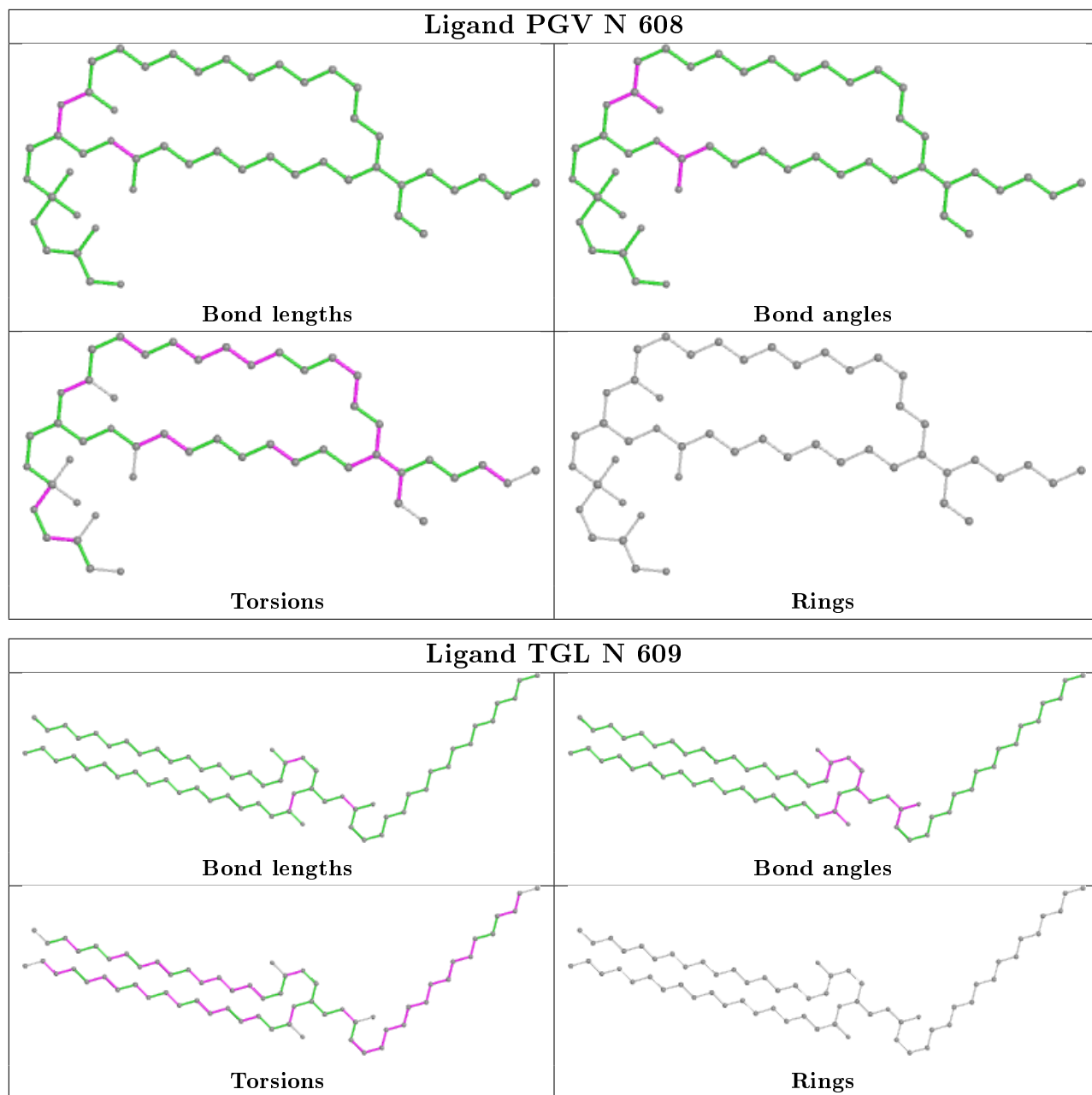
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	N	608	PGV	2	0
19	N	609	TGL	5	0
20	A	609	PGV	2	0
27	G	102	PEK	6	0
23	W	101	CHD	1	0
27	P	302	PEK	4	0
23	P	305	CHD	1	0
23	J	101	CHD	1	0
19	D	201	TGL	1	0
21	A	610	EDO	1	0
14	A	602	HEA	6	0
29	Z	101	DMU	1	0
23	B	302	CHD	1	0
14	A	601	HEA	6	0
26	P	304	CDL	7	0
14	N	602	HEA	3	0
24	R	201	PSC	6	0
27	T	102	PEK	1	0
21	B	305	EDO	1	0
14	N	601	HEA	10	0
18	A	606	CMO	1	0
27	C	306	PEK	3	0
20	P	303	PGV	3	0
24	B	303	PSC	12	0
26	T	103	CDL	13	0
27	T	101	PEK	3	0
19	A	607	TGL	3	0
19	N	611	TGL	4	0
20	N	607	PGV	6	0
20	A	608	PGV	1	0
23	P	306	CHD	1	0
26	C	303	CDL	2	0
21	N	612	EDO	1	0

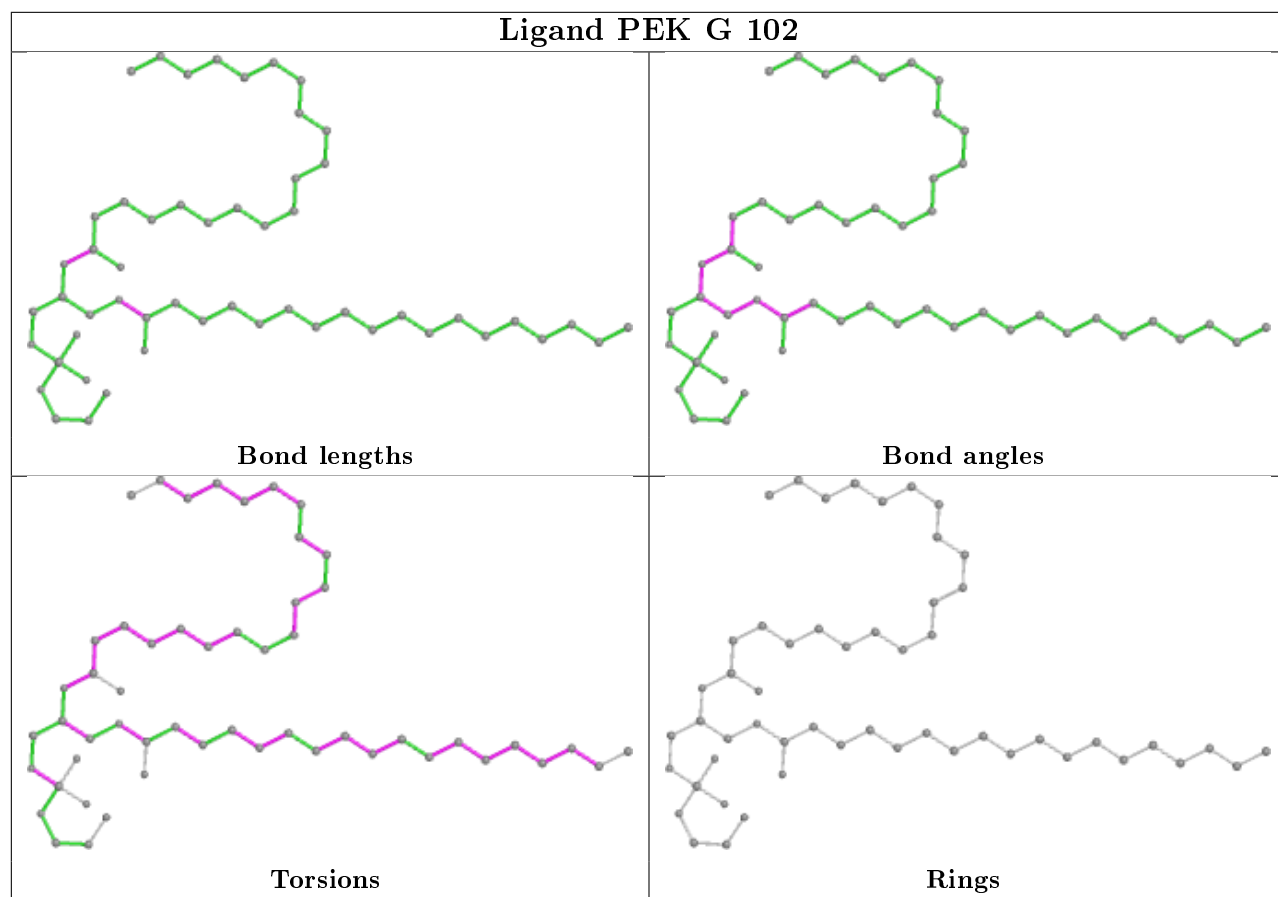
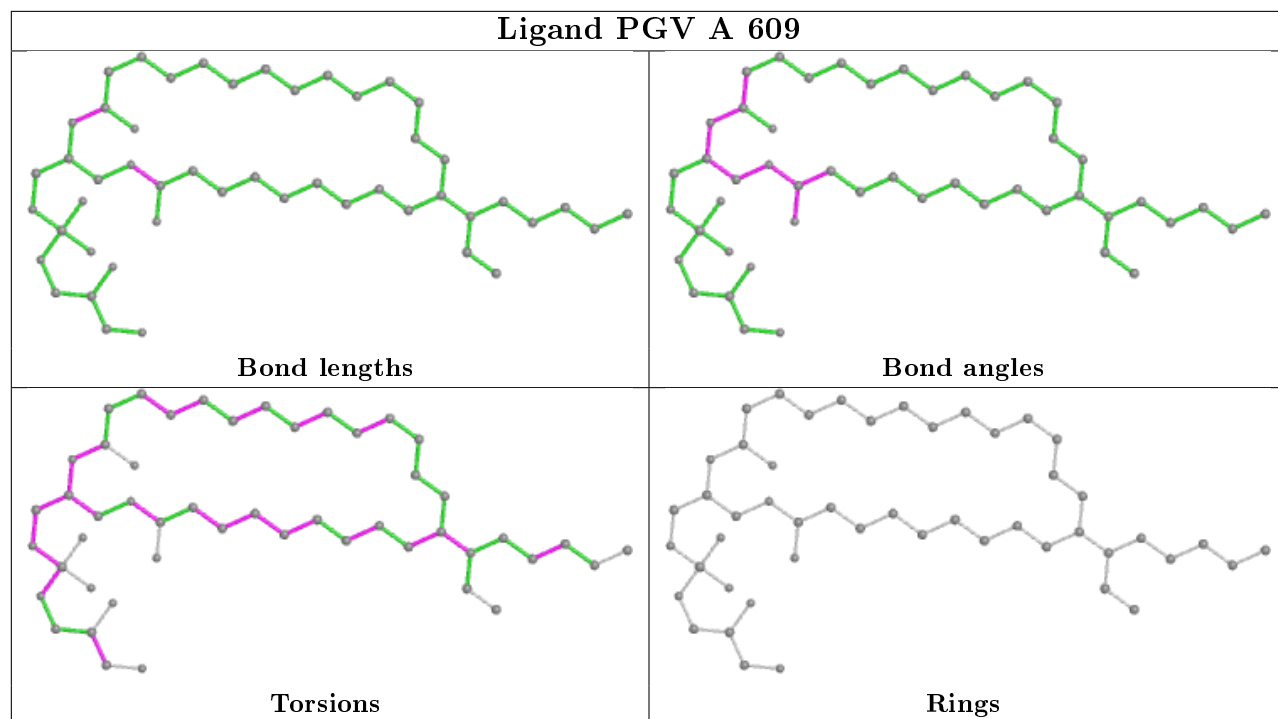
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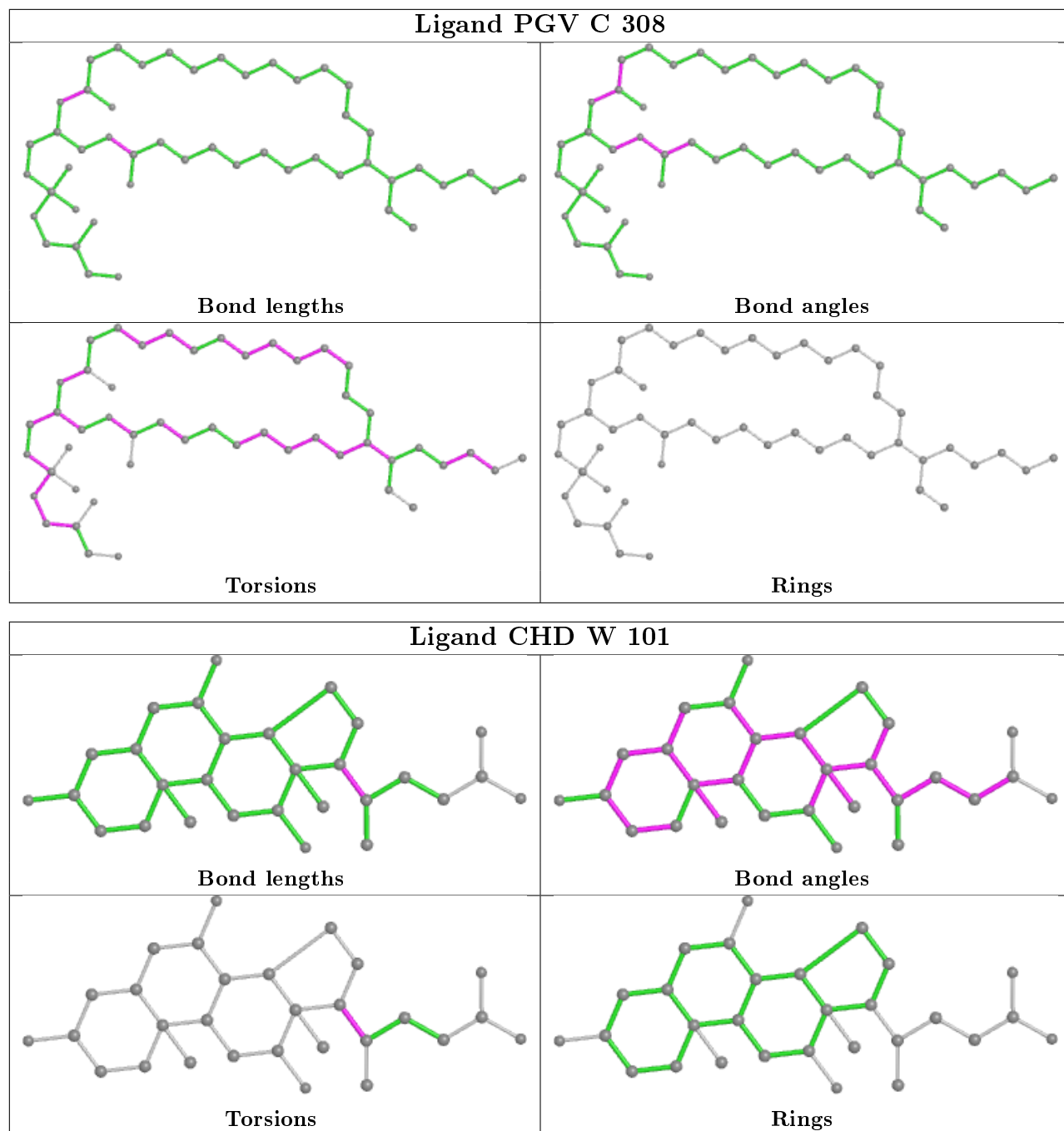
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	G	101	PEK	4	0
19	L	101	TGL	4	0
23	C	305	CHD	1	0
20	G	103	PGV	2	0
29	M	101	DMU	1	0
21	A	613	EDO	2	0
23	O	302	CHD	1	0
19	N	610	TGL	2	0
23	C	304	CHD	2	0
21	A	614	EDO	4	0
21	T	104	EDO	1	0
26	C	307	CDL	13	0
21	A	612	EDO	2	0

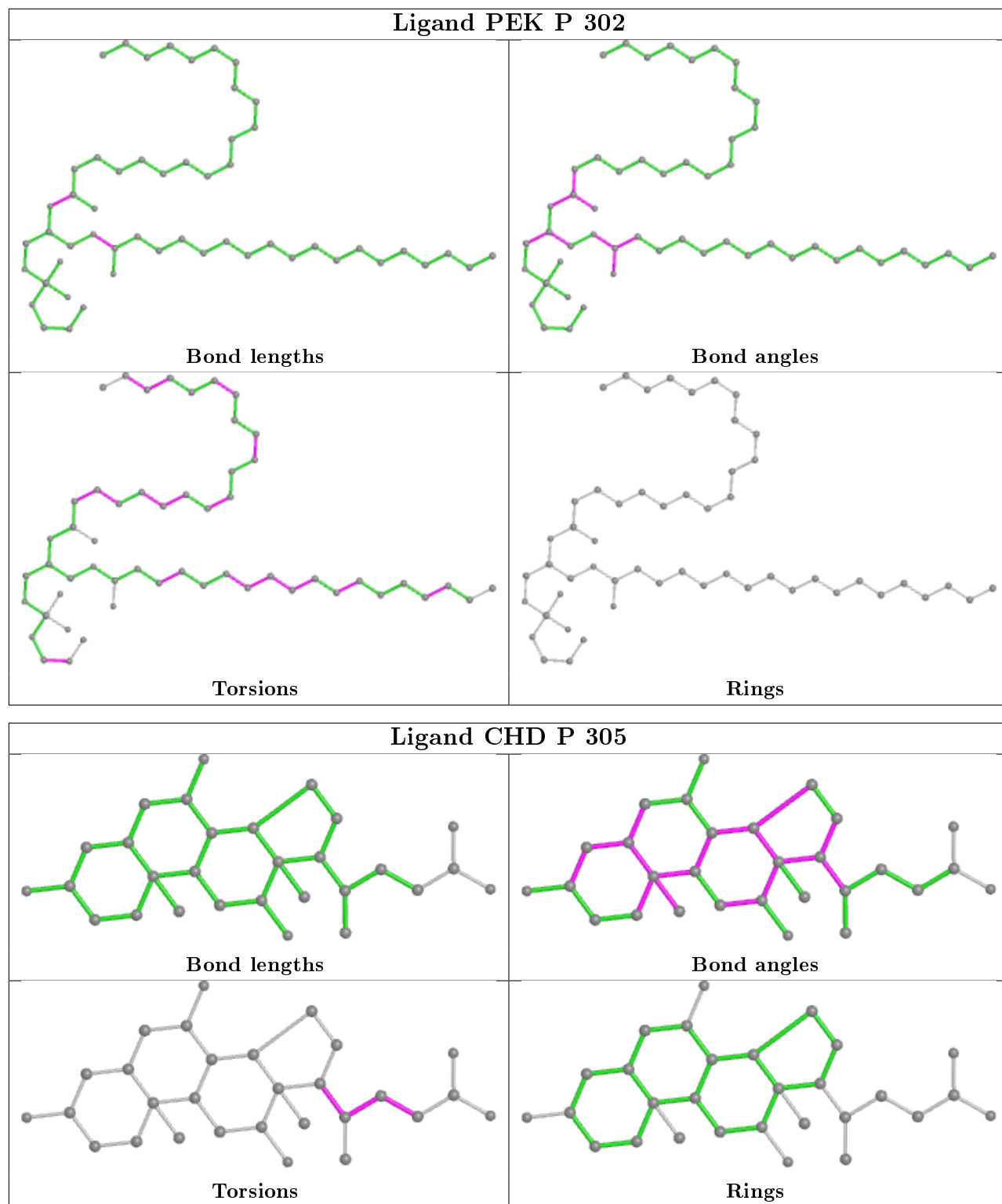
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

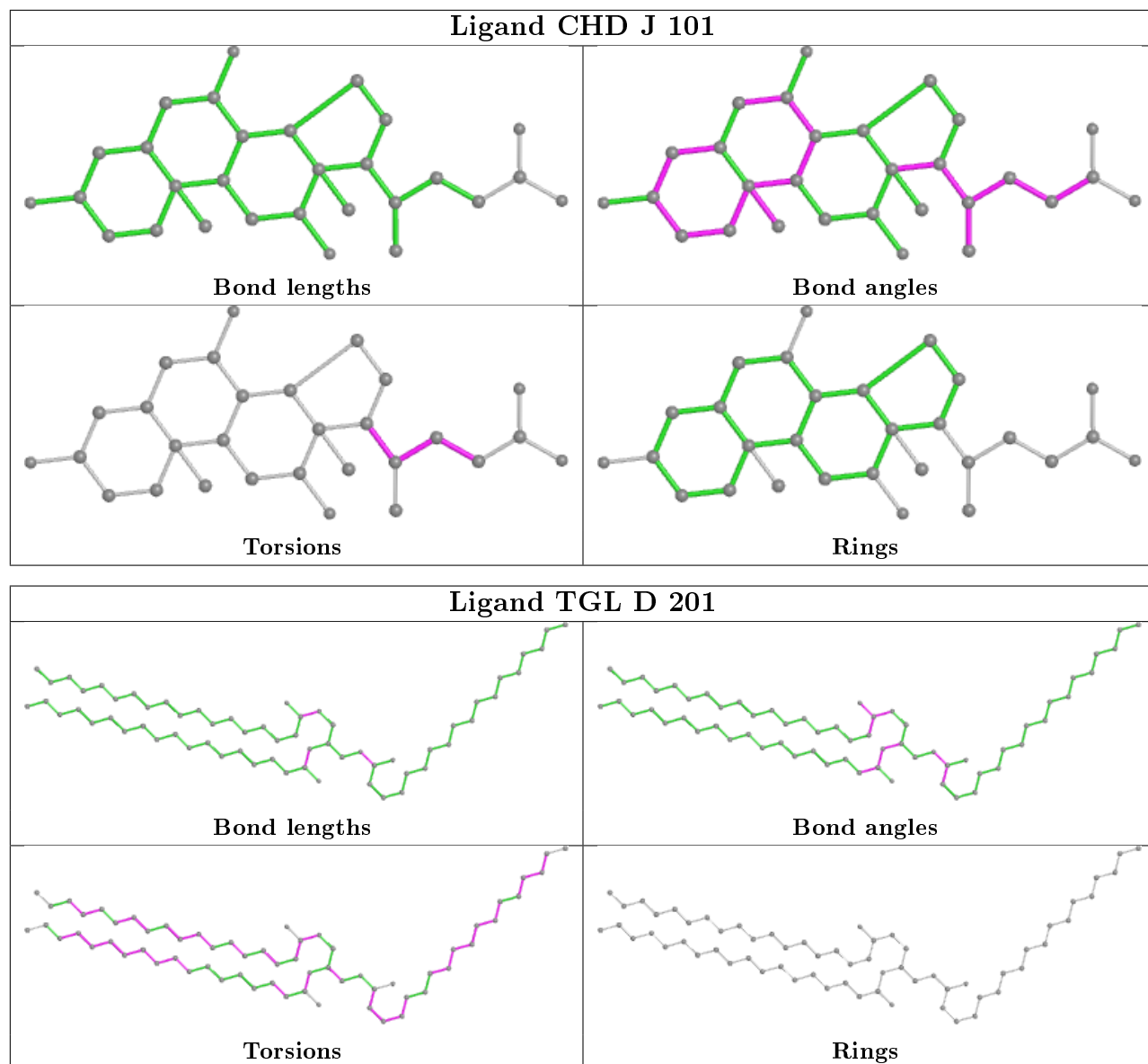


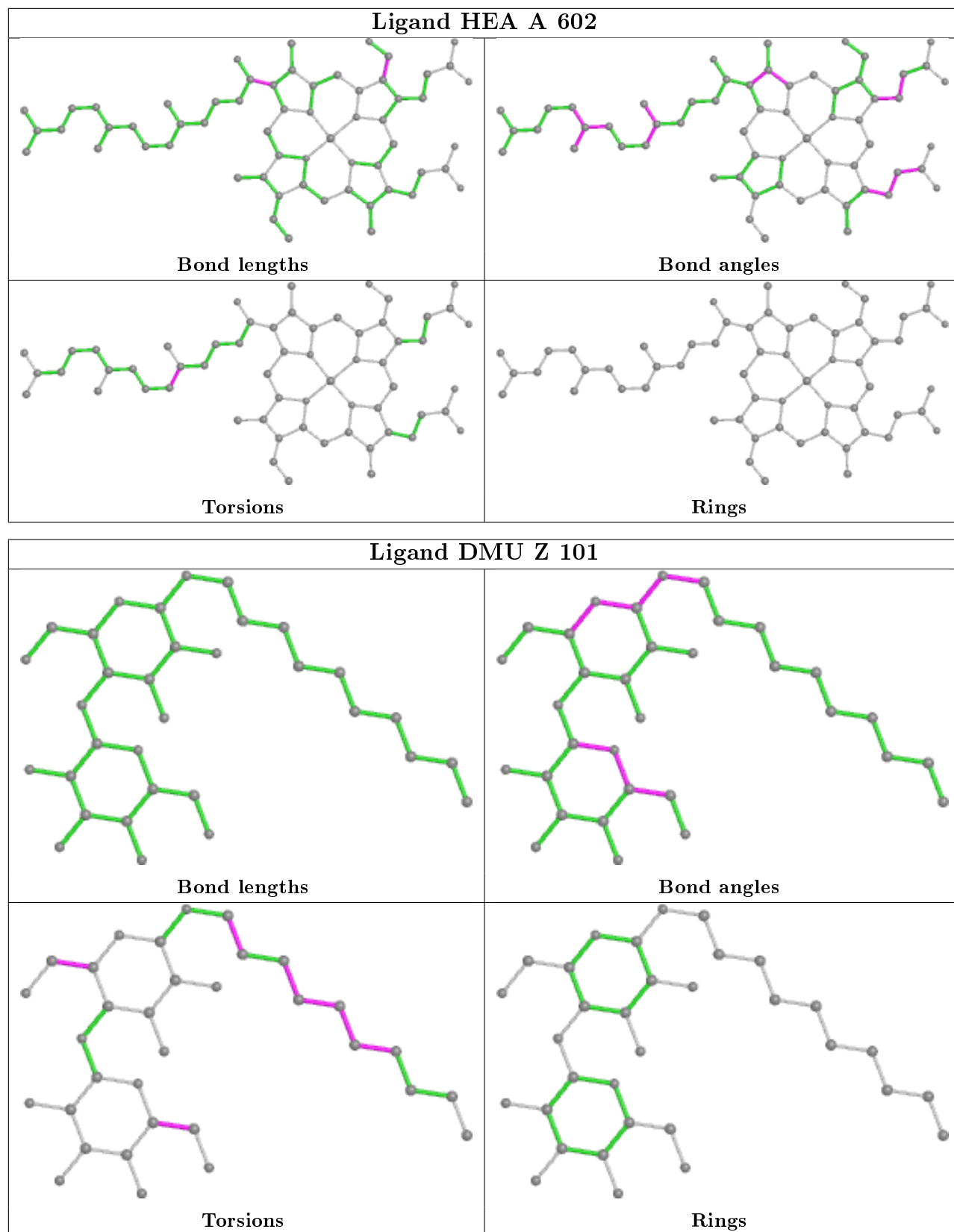


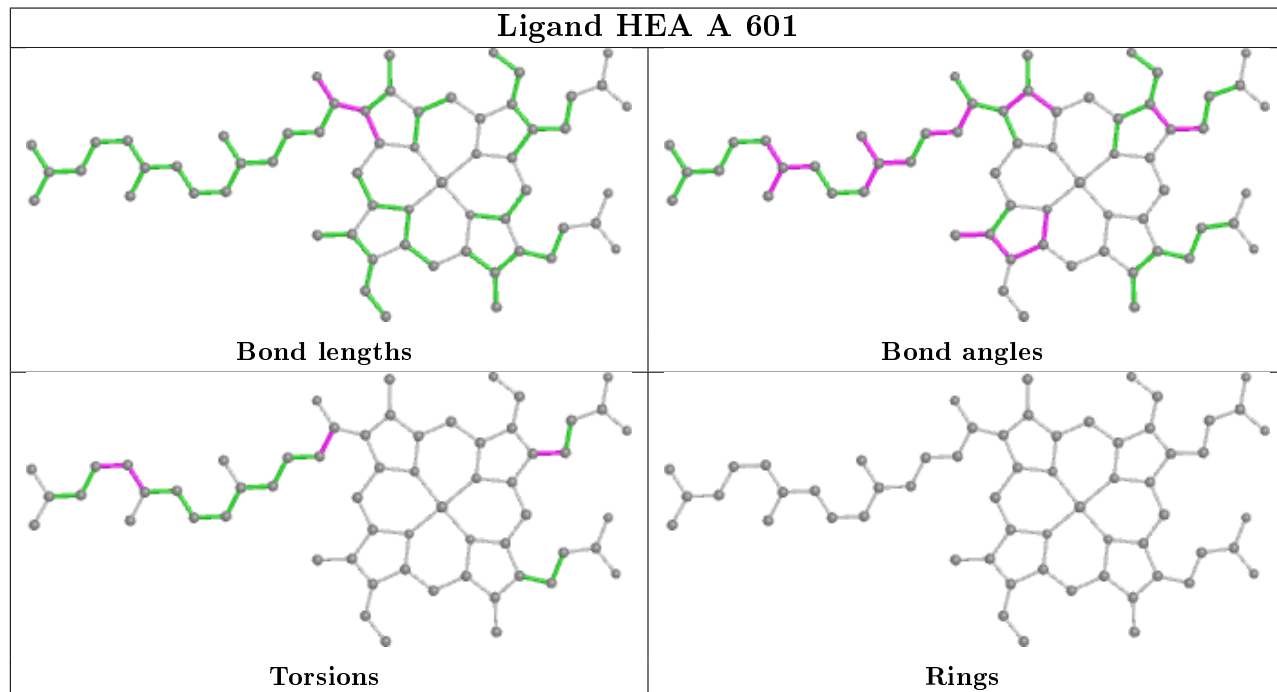
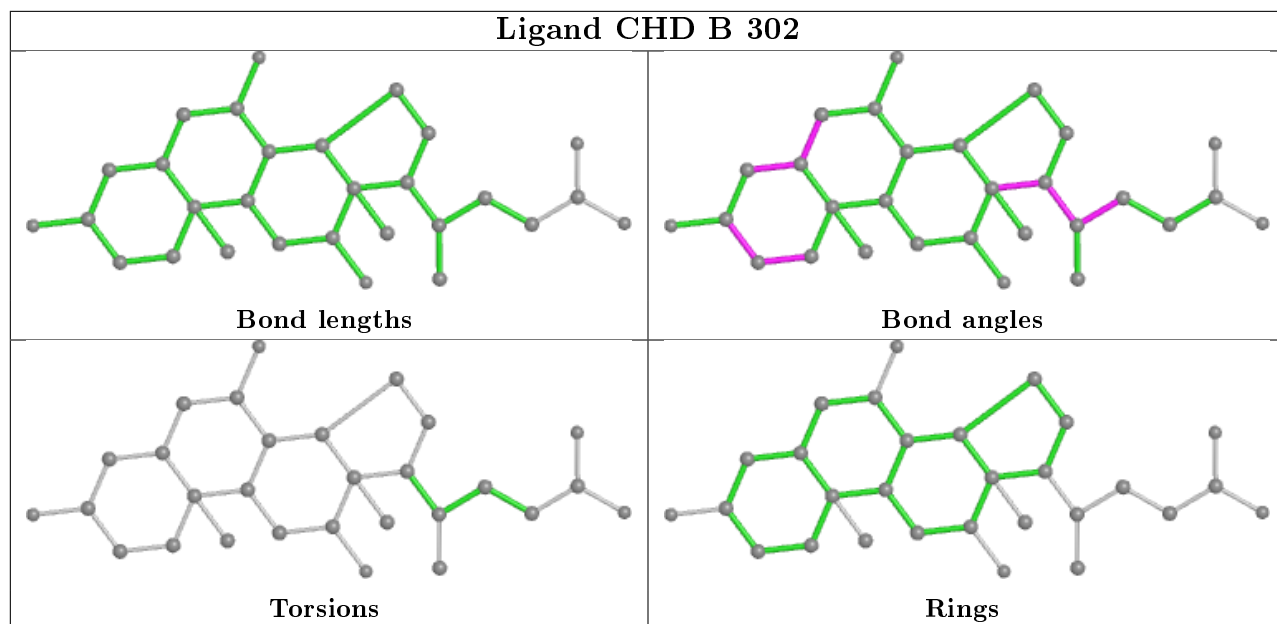


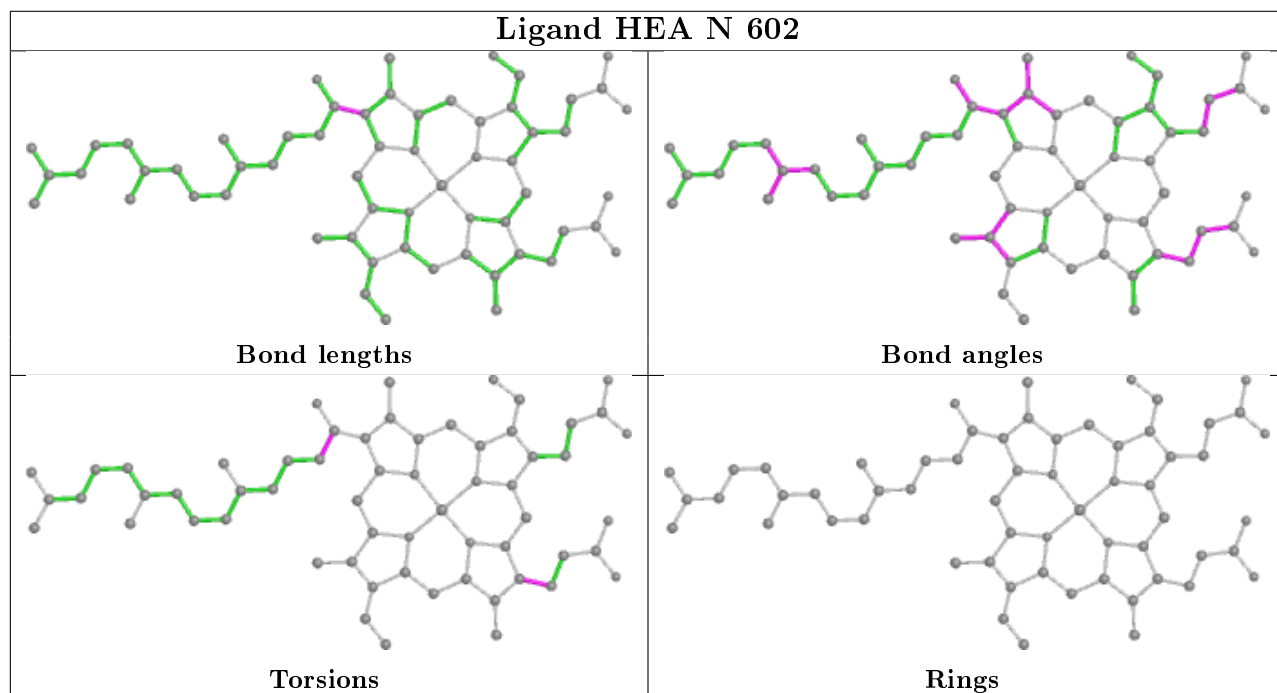
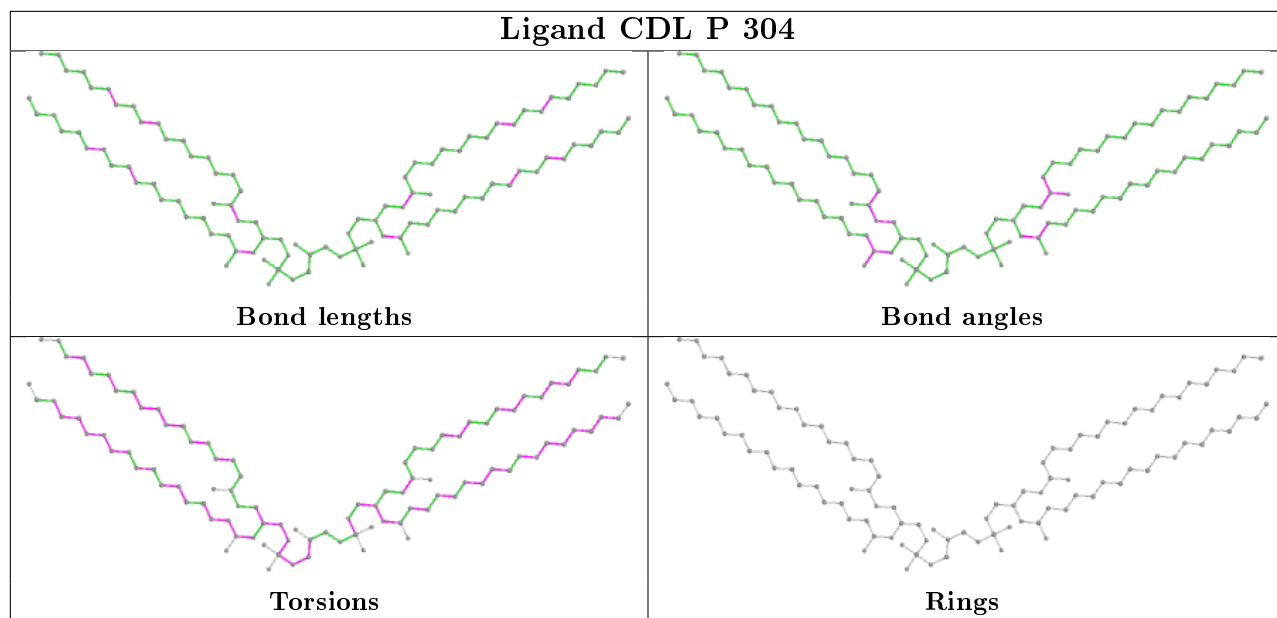


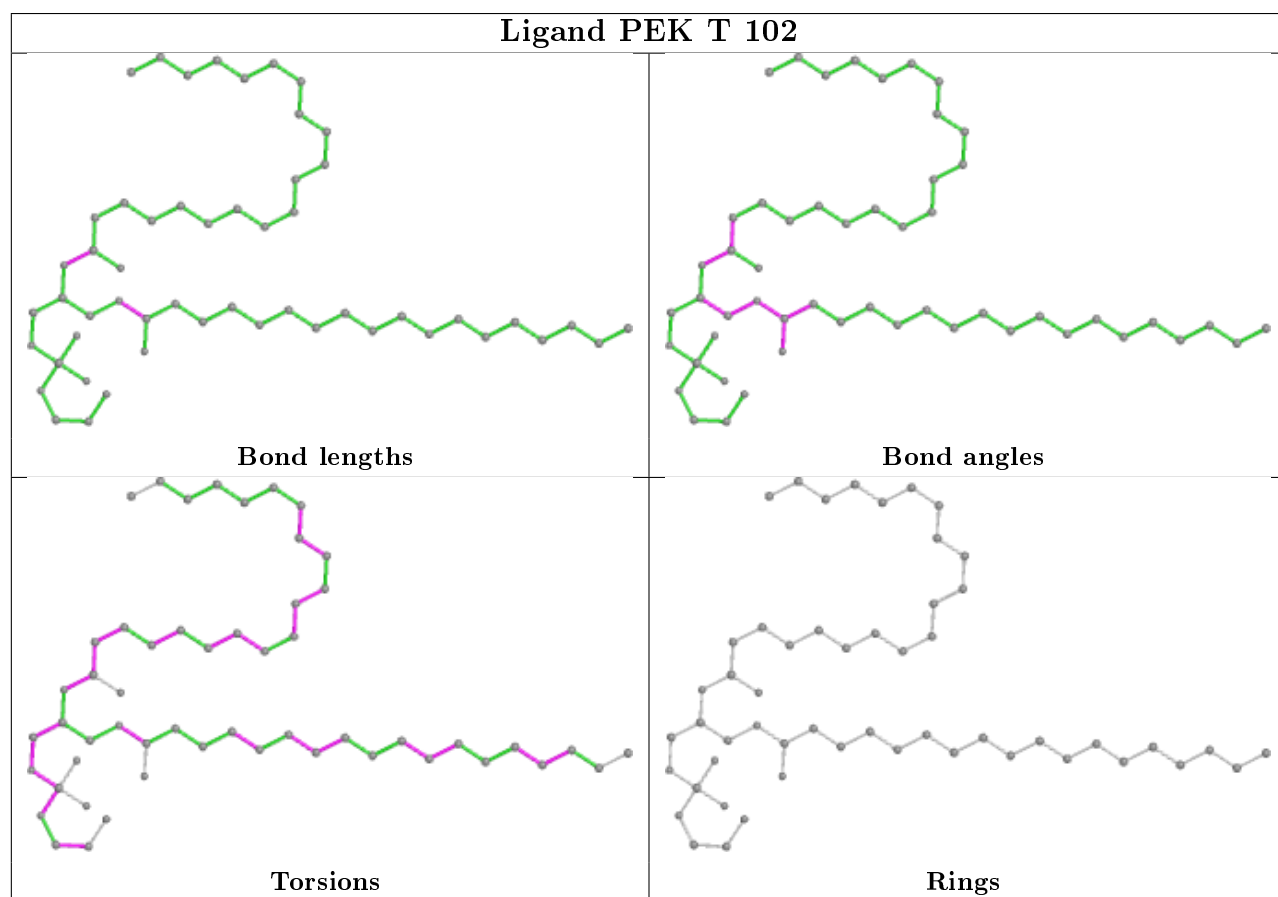
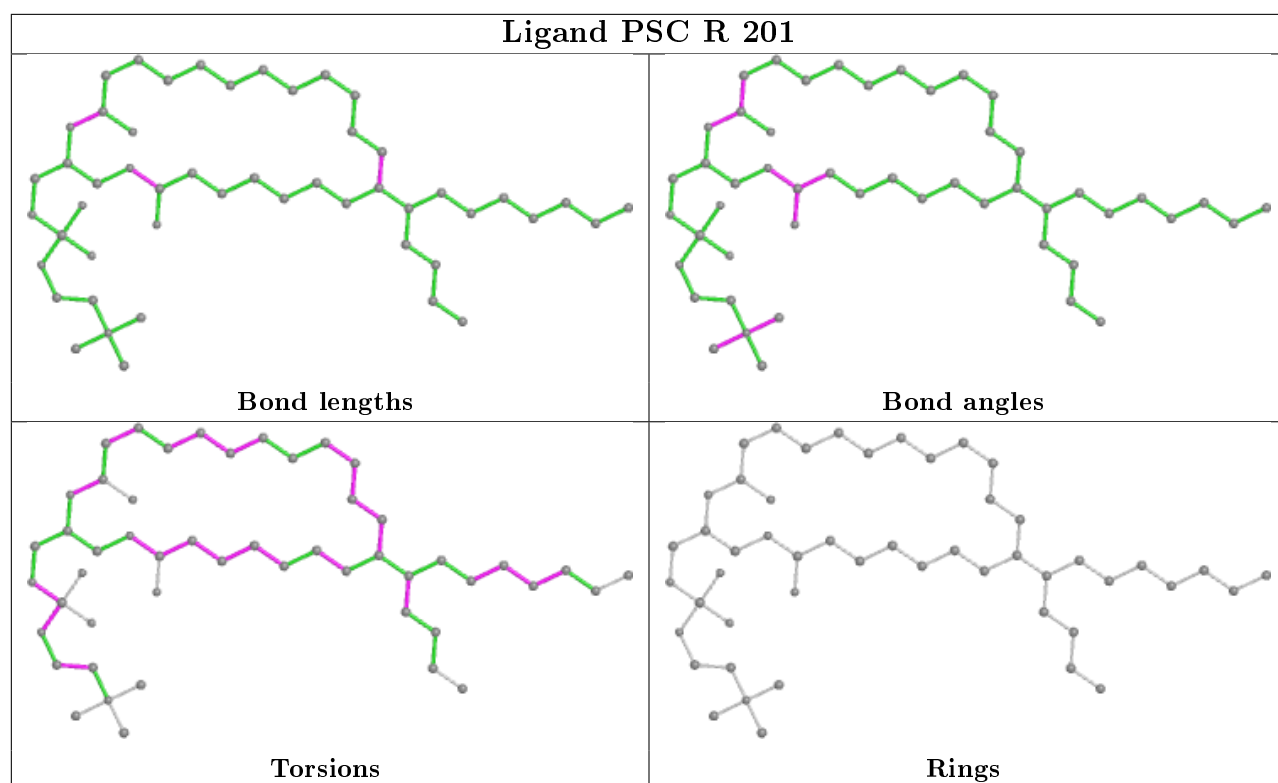


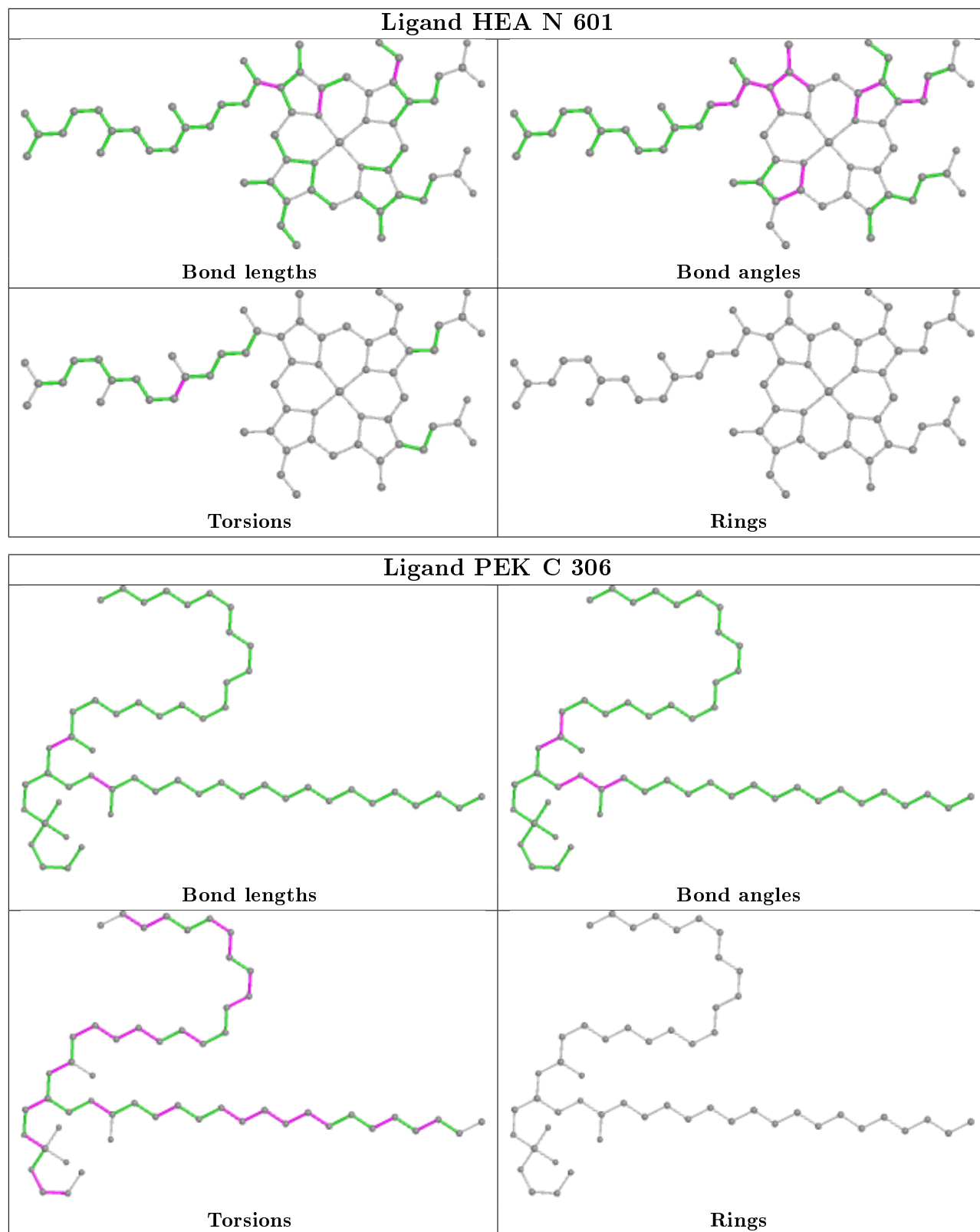


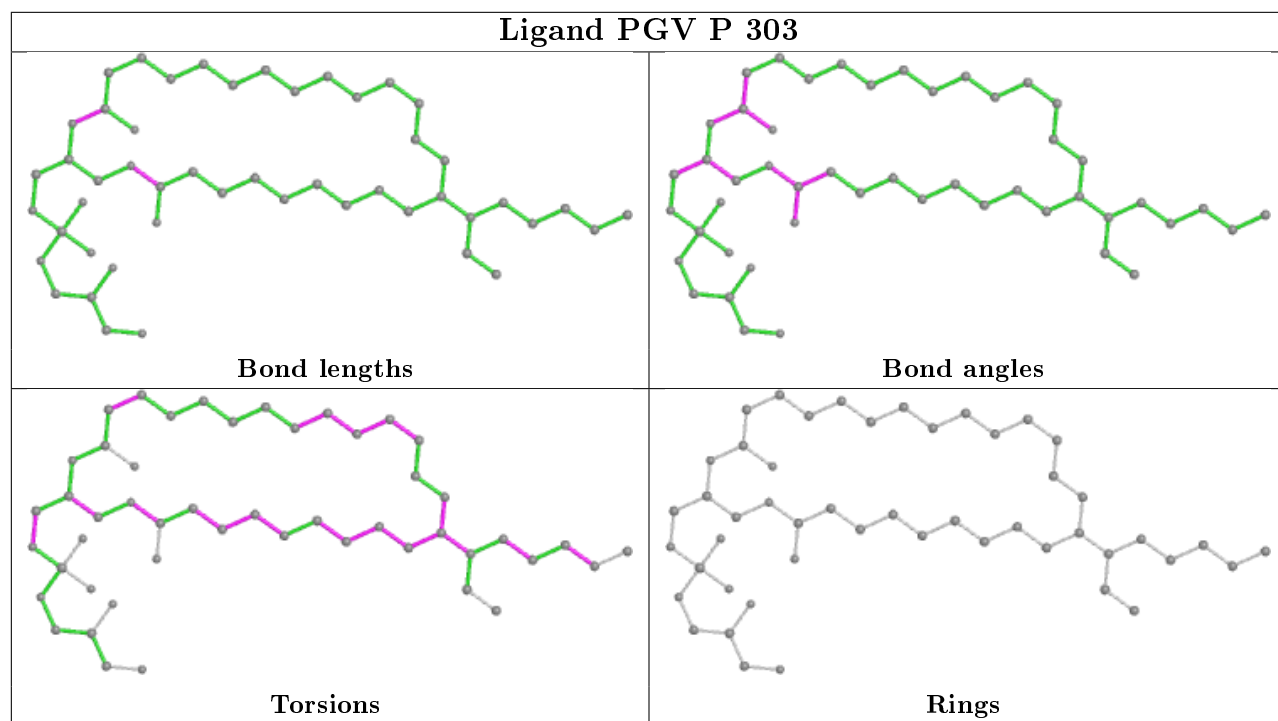
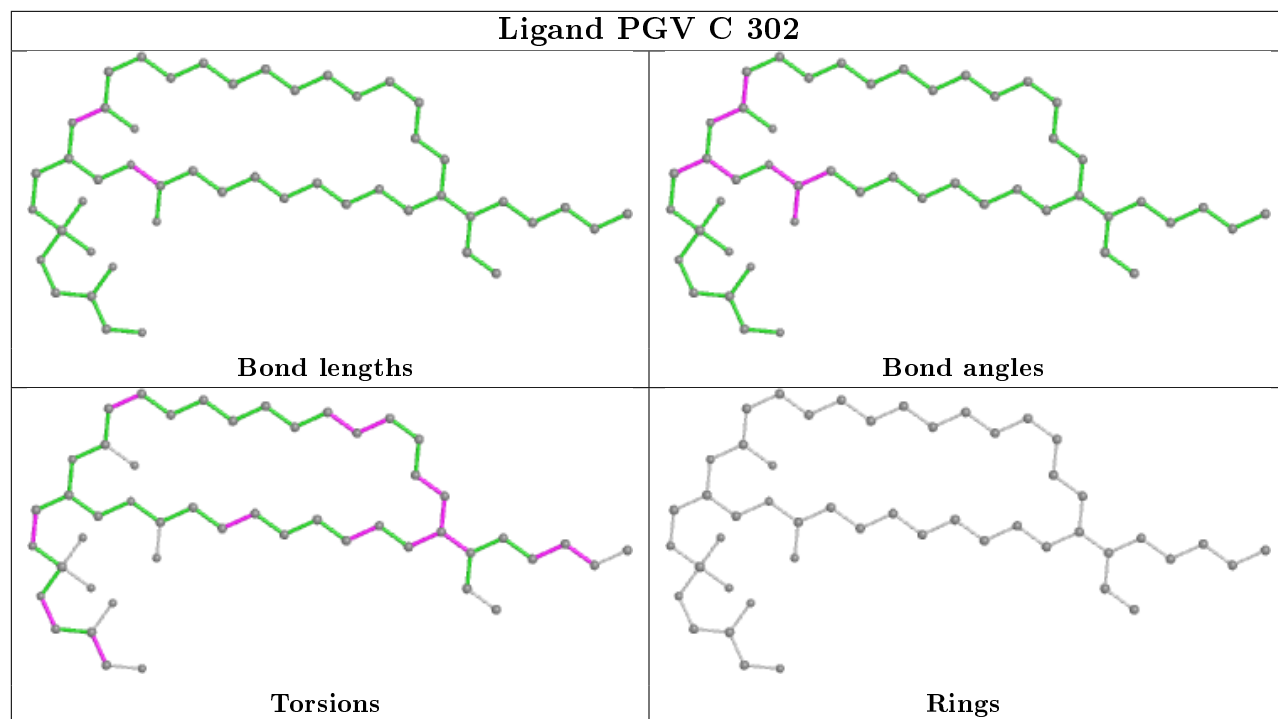




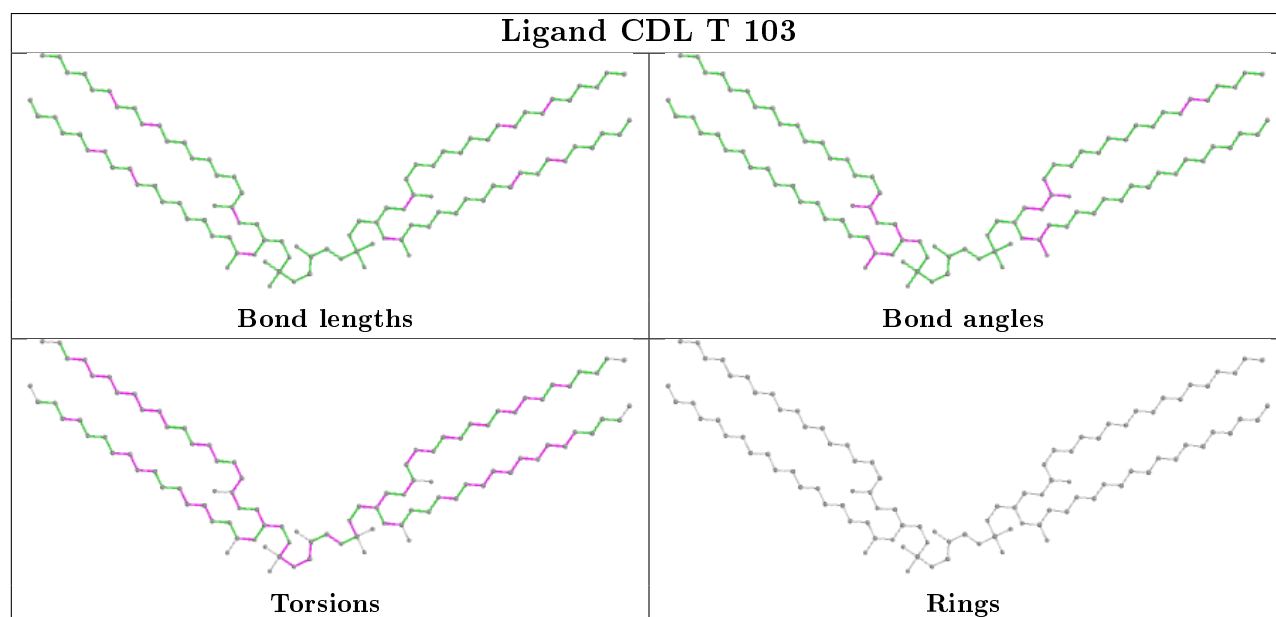
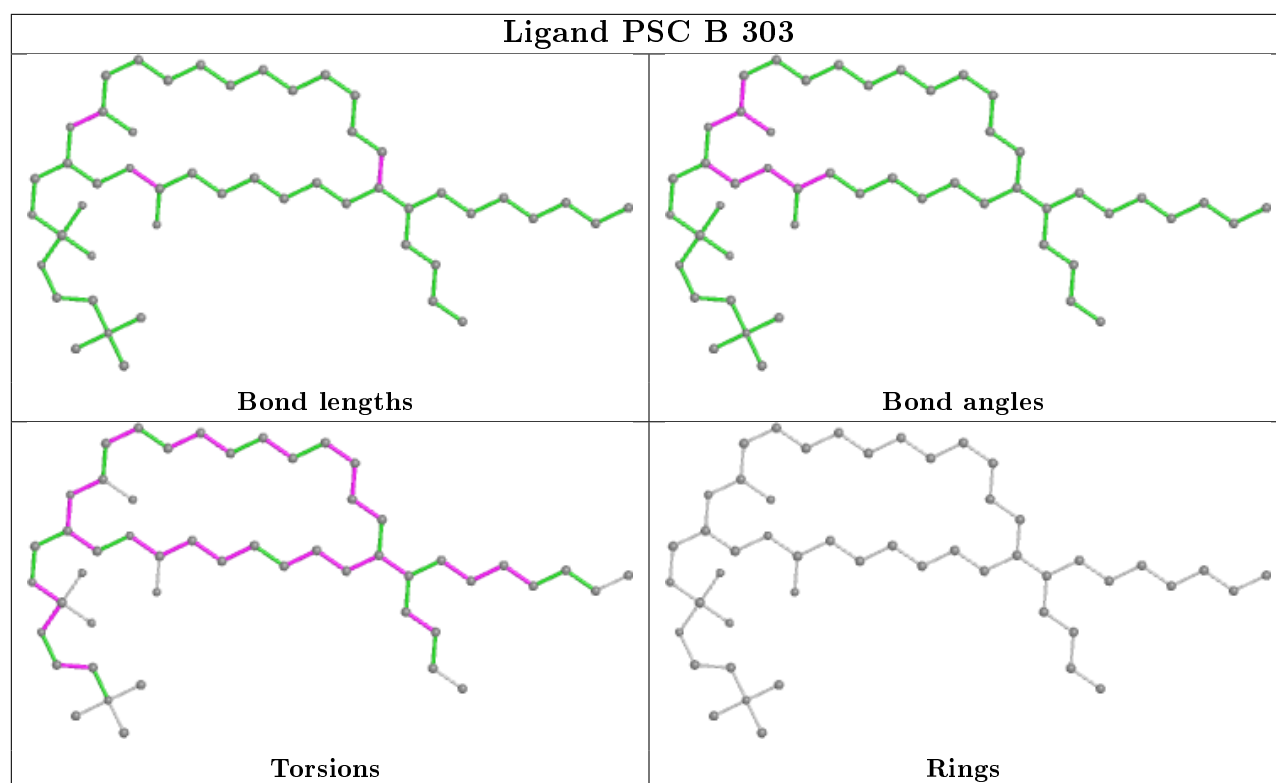


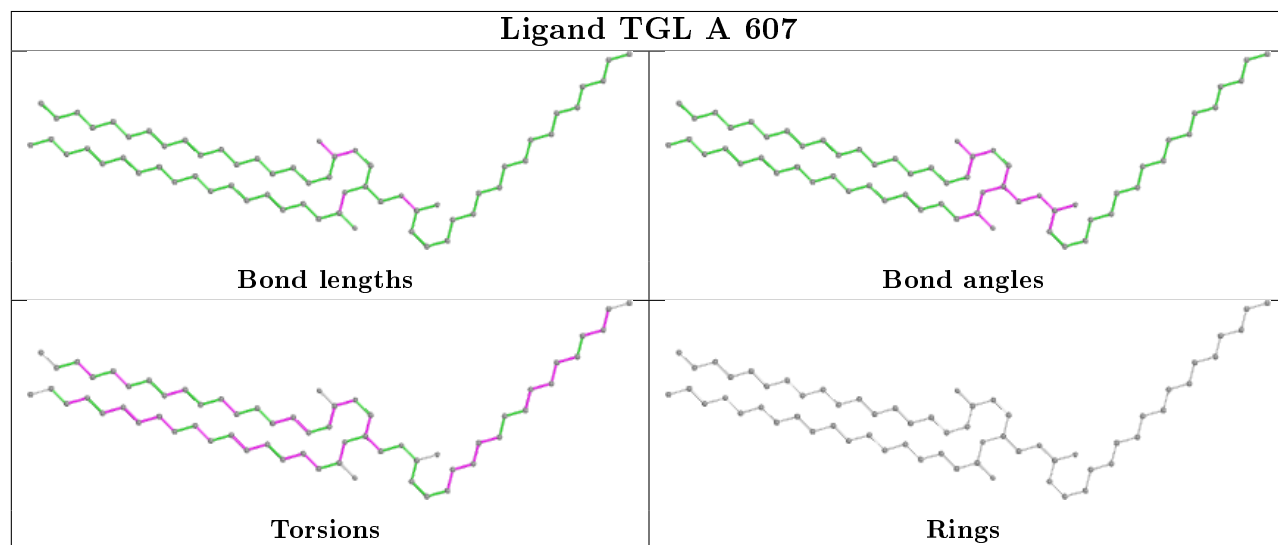
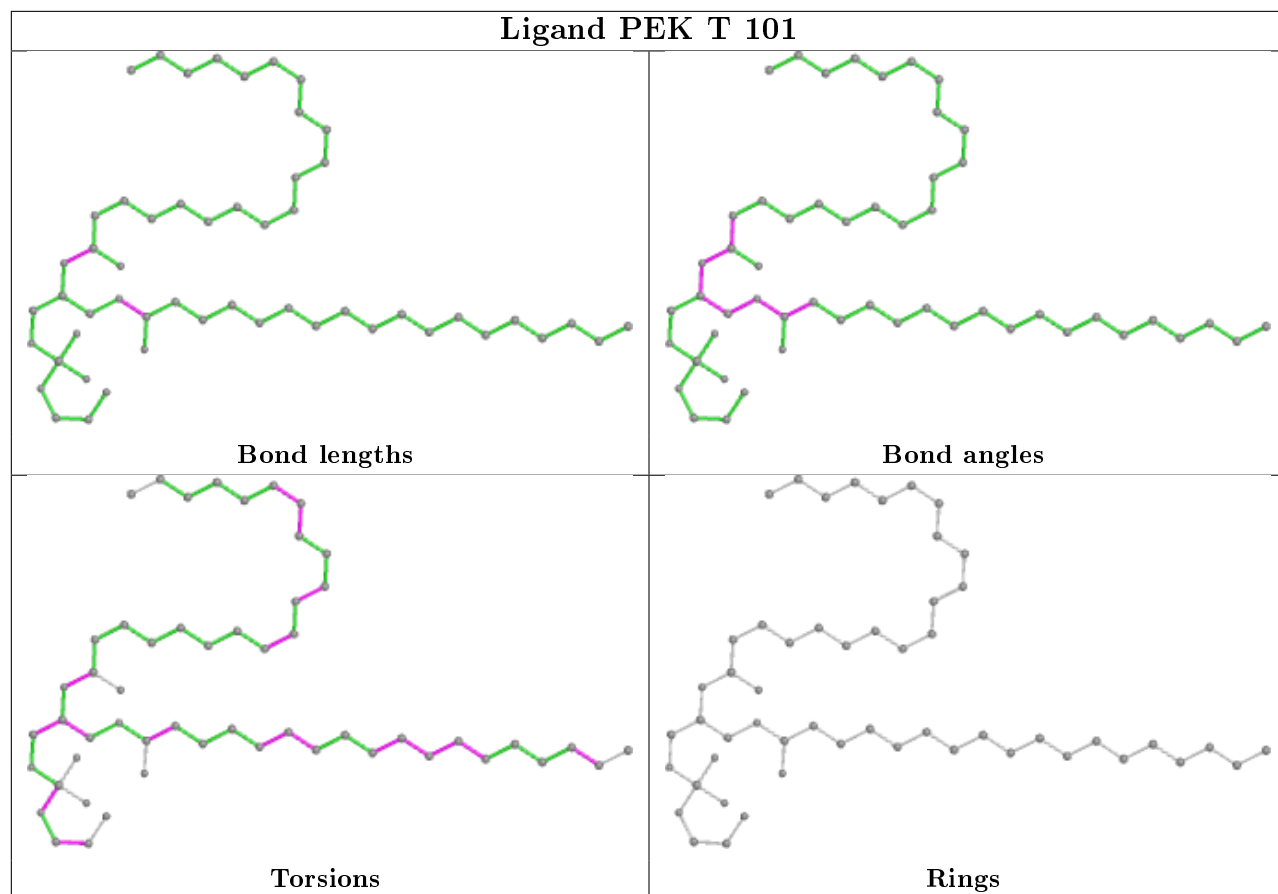


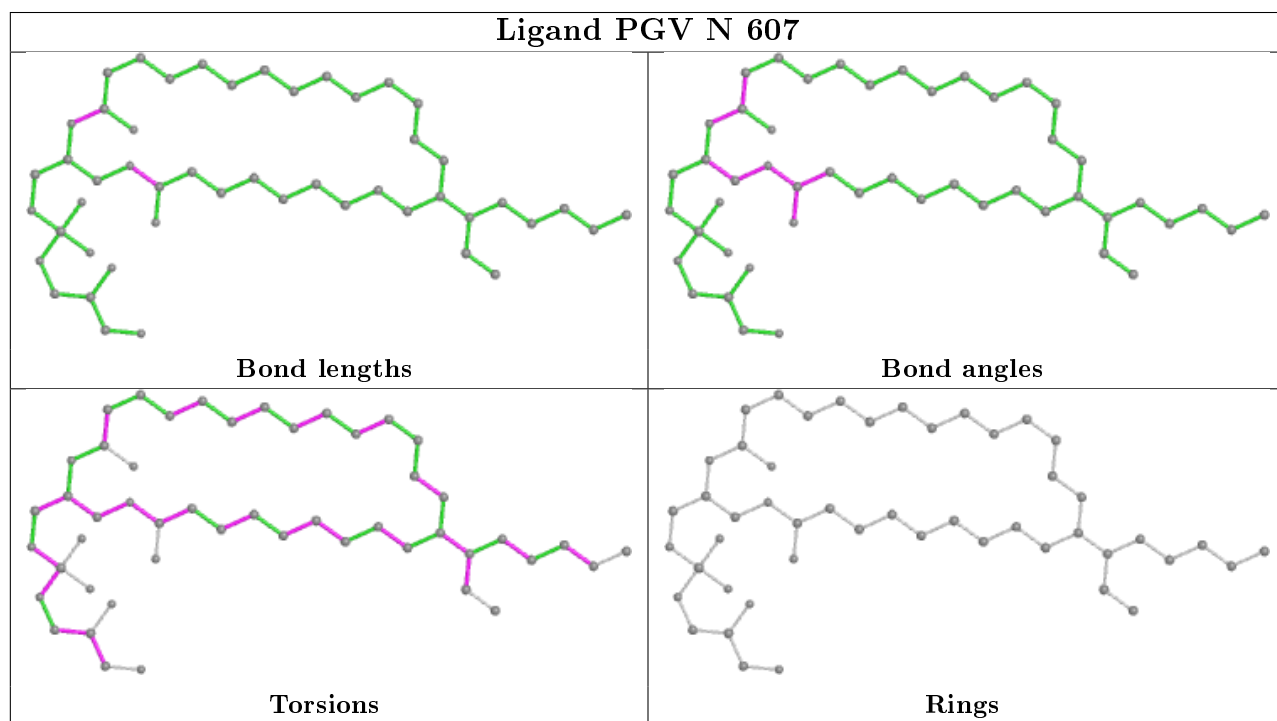
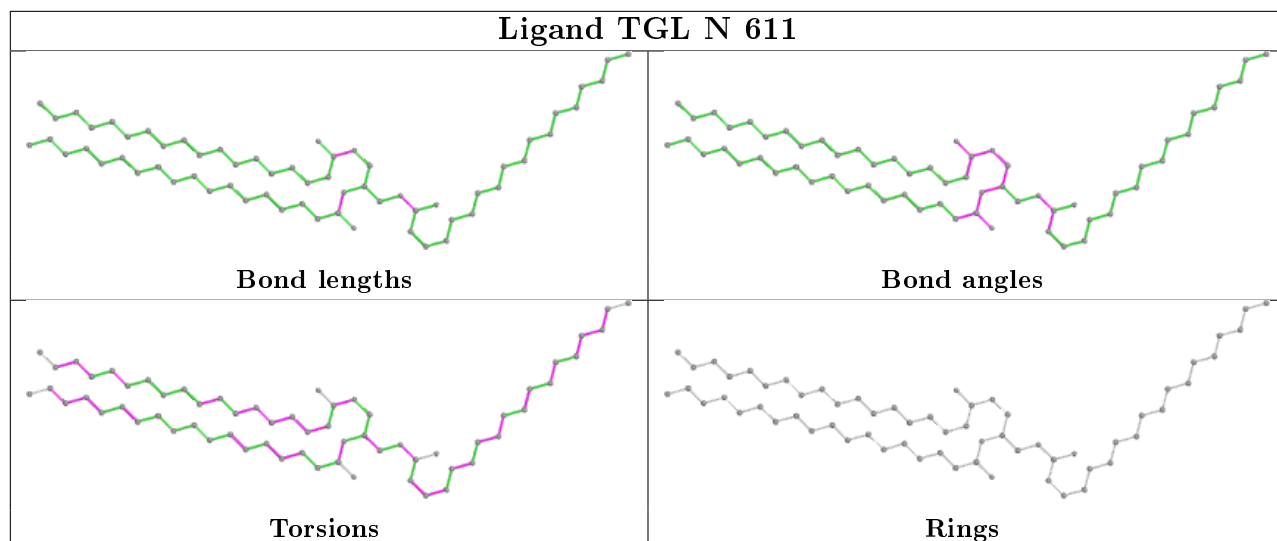


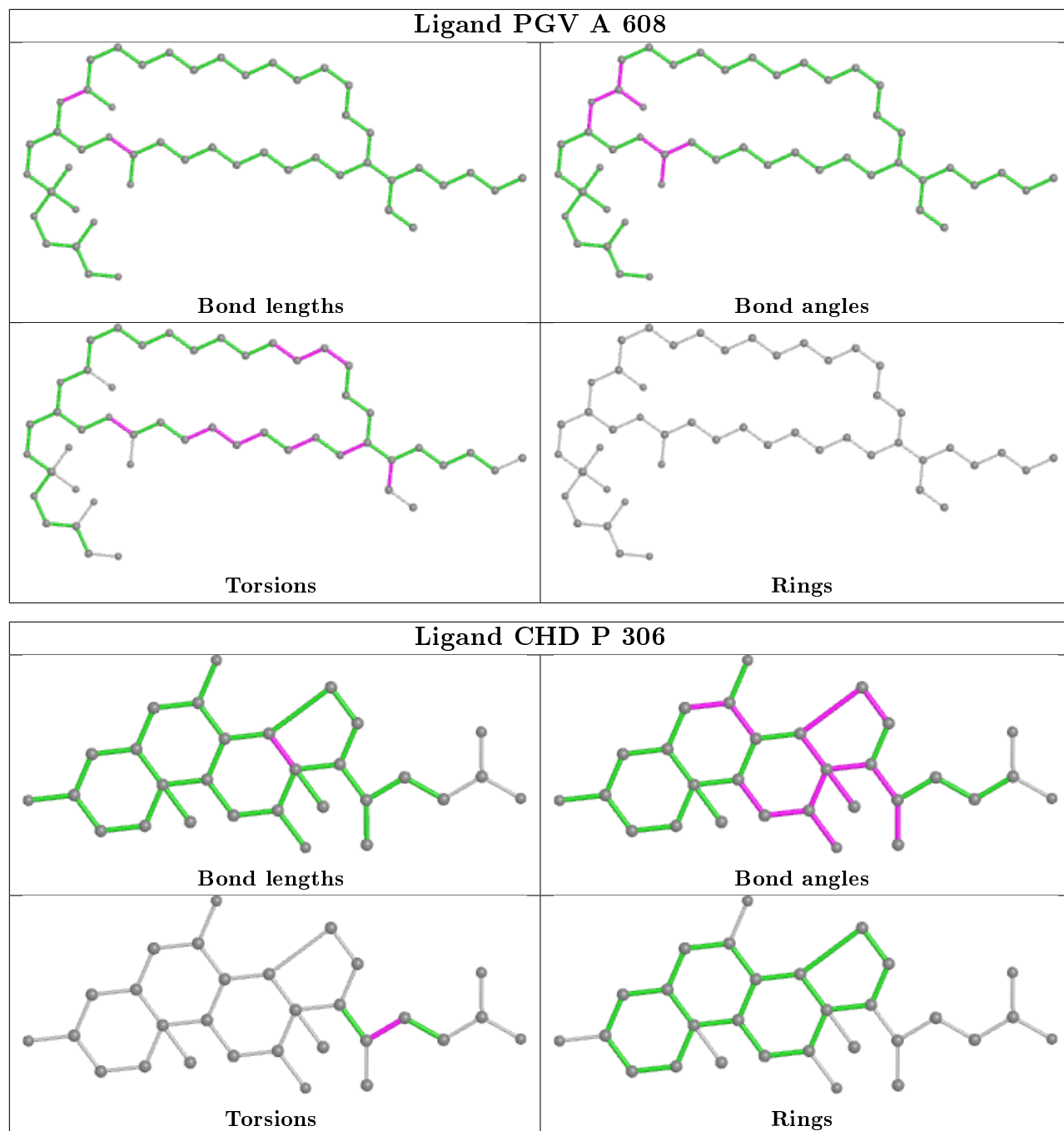


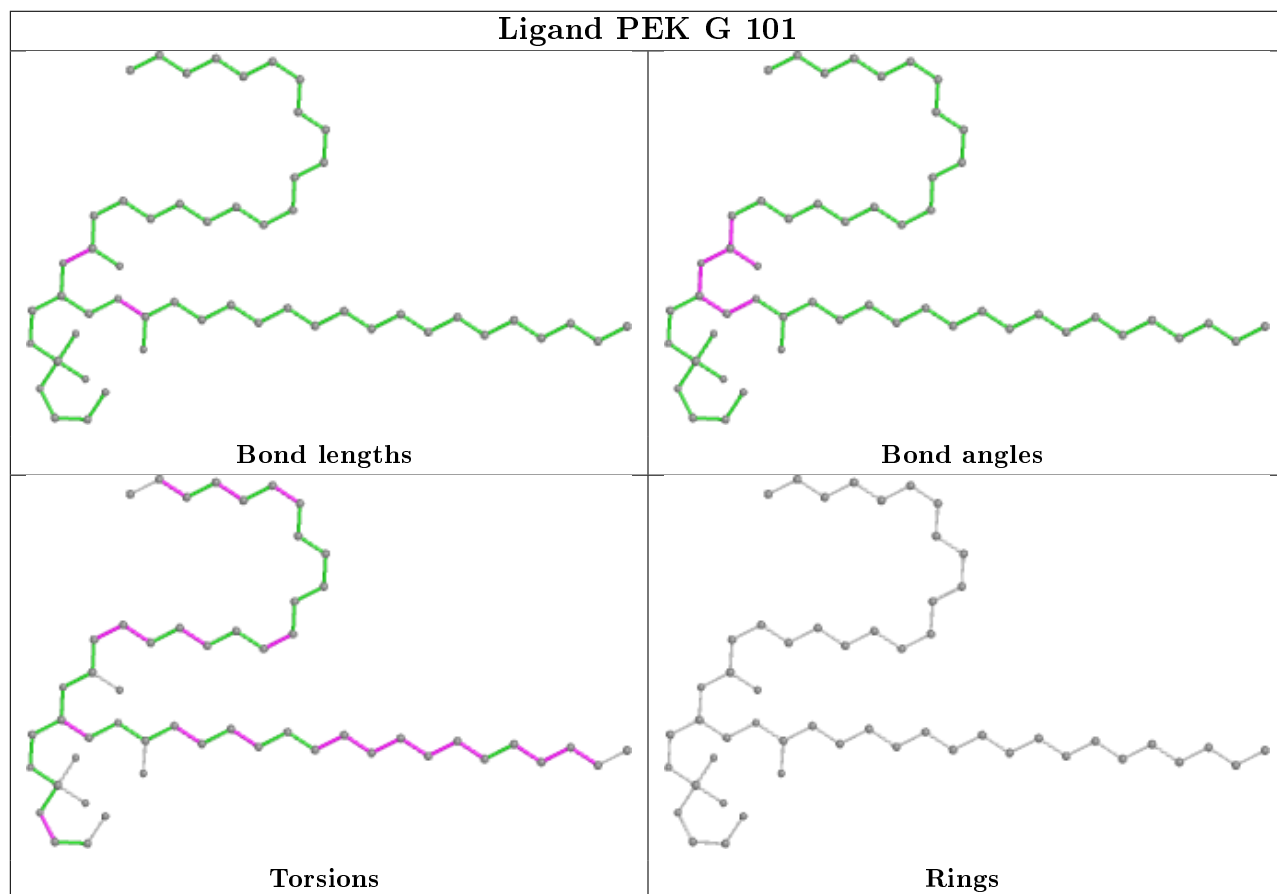
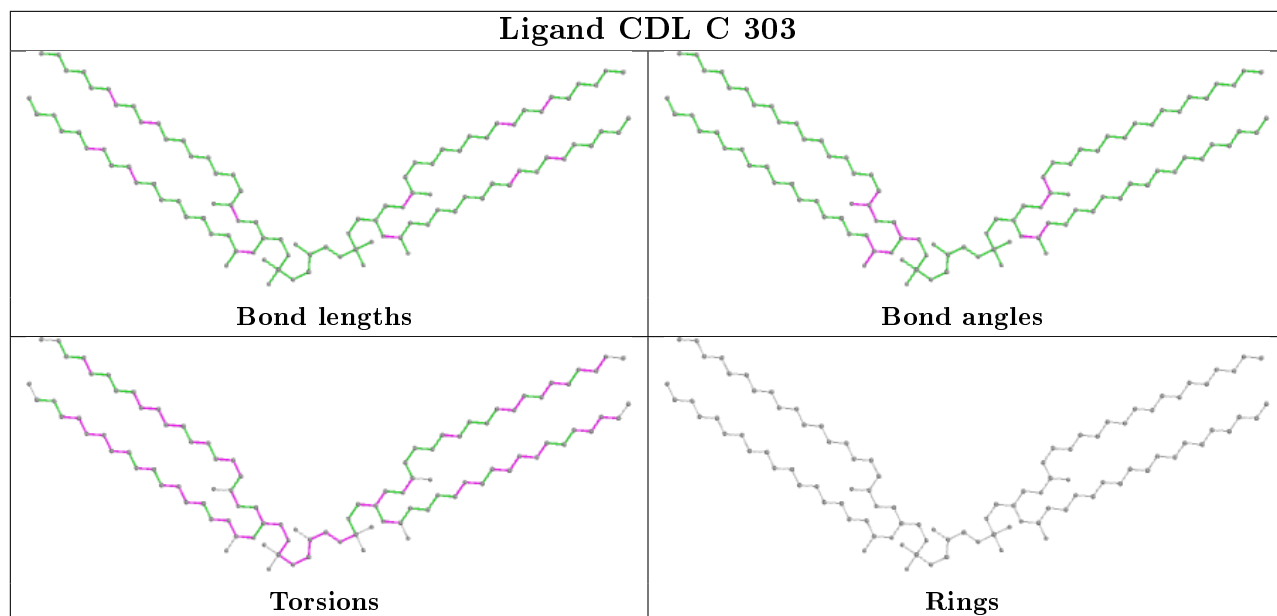


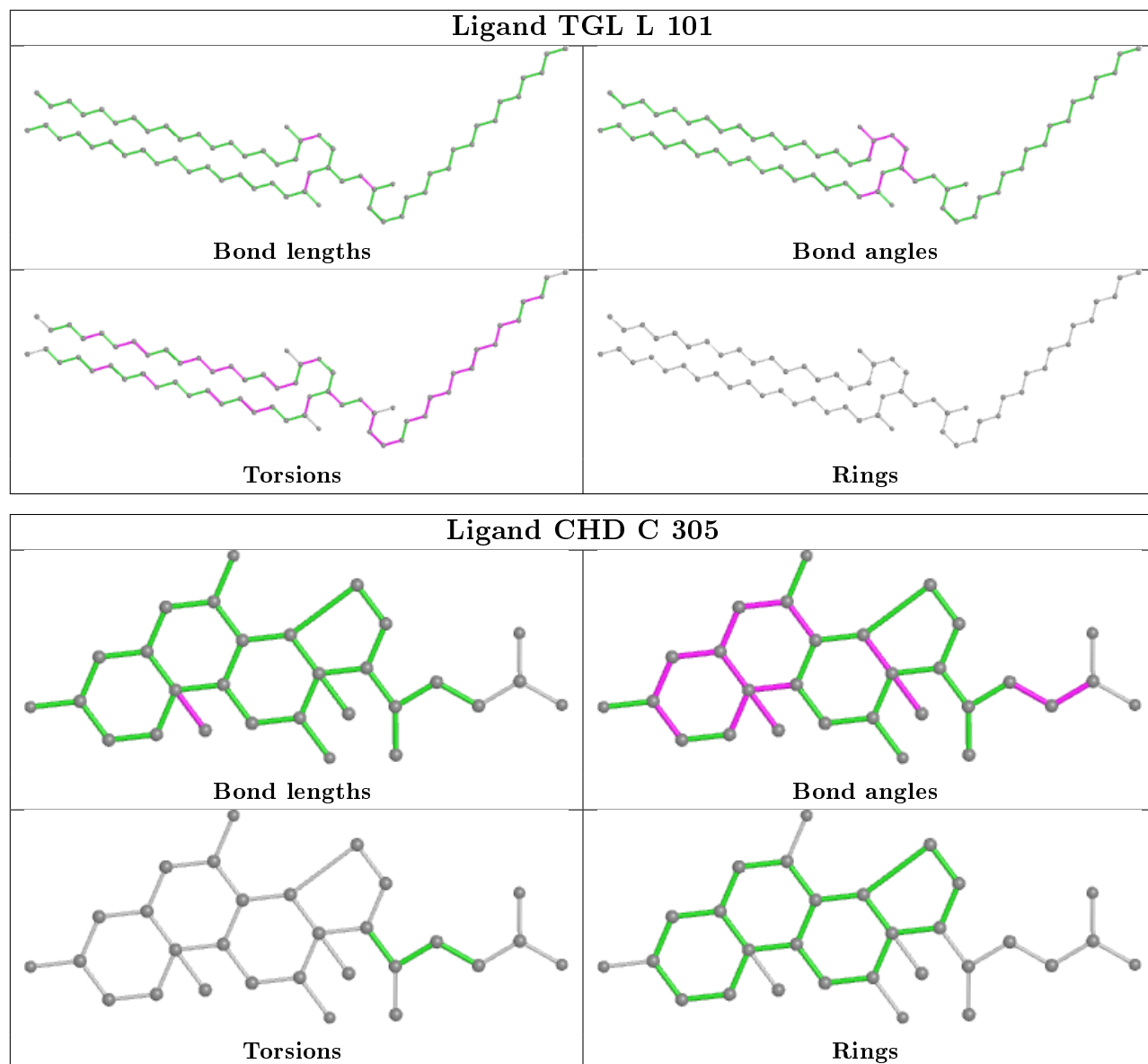


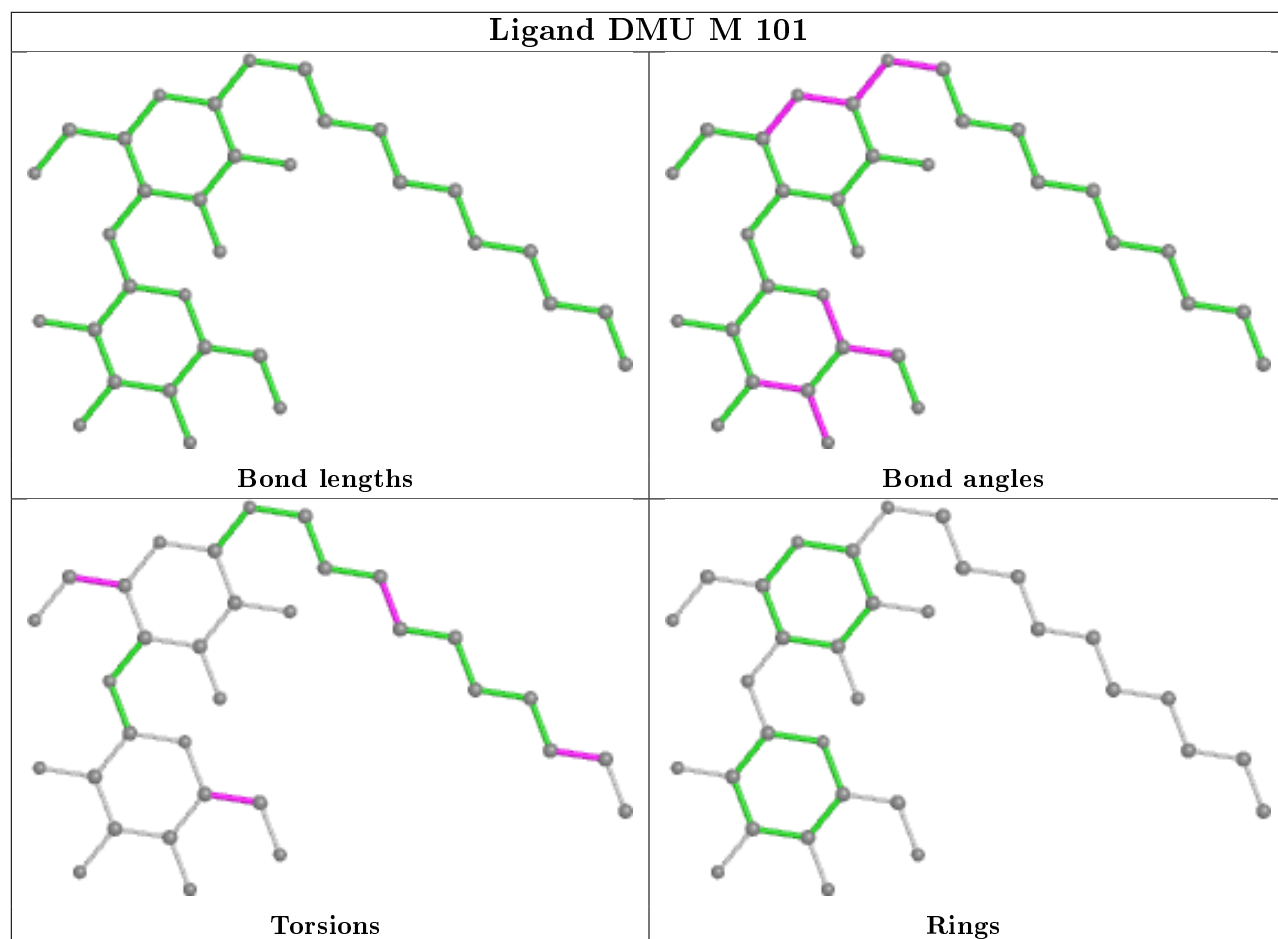
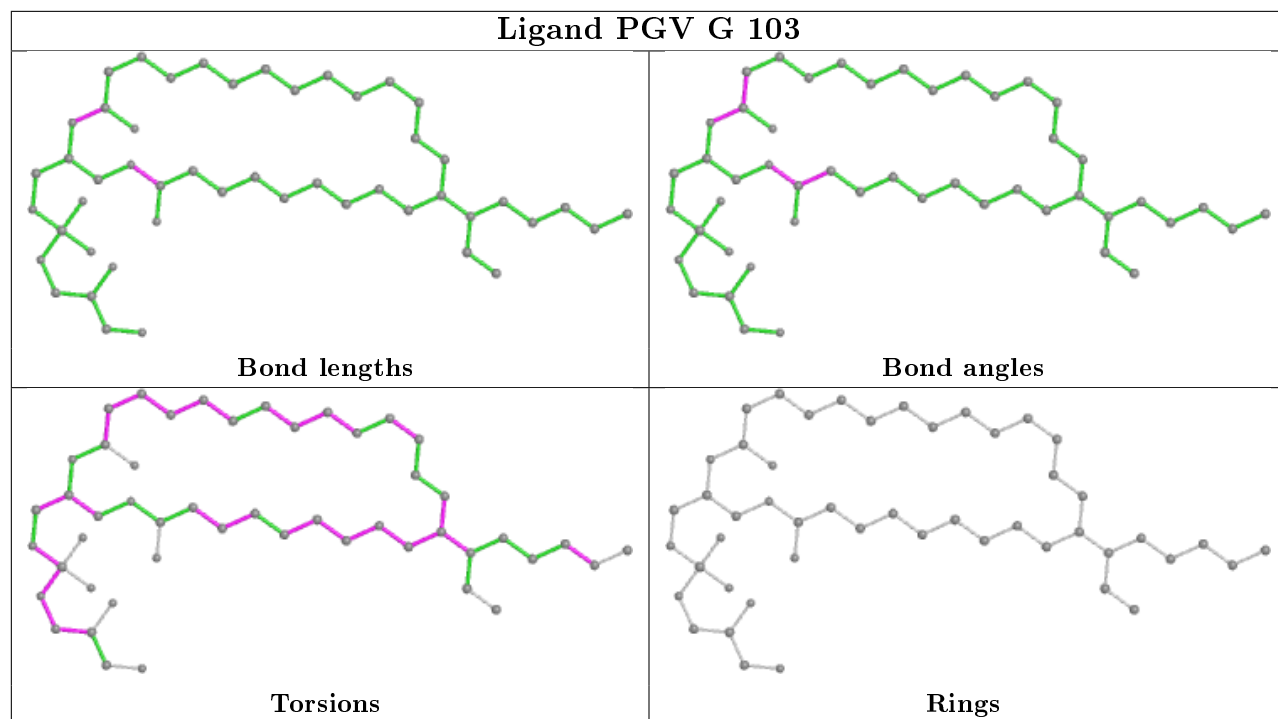


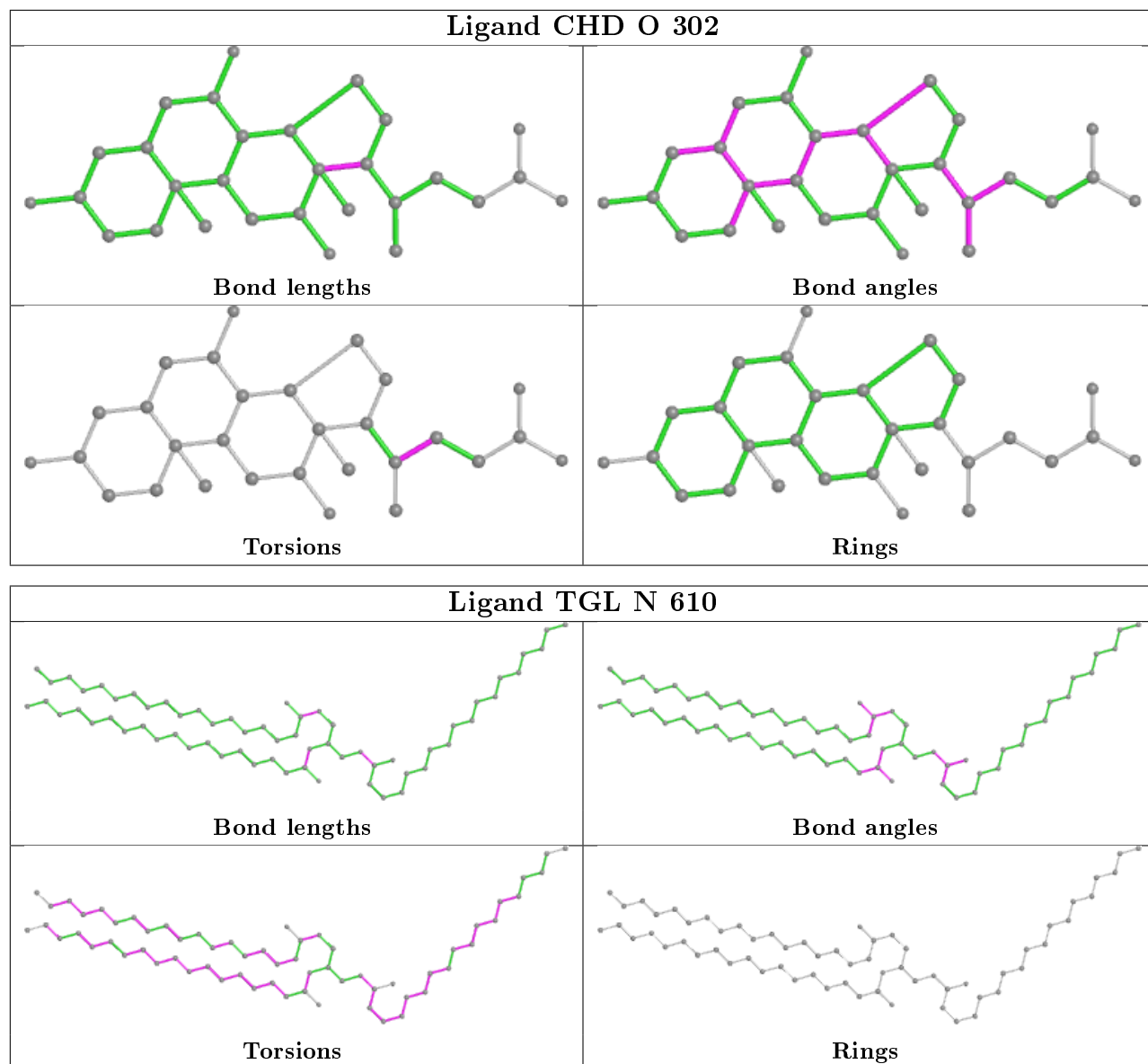




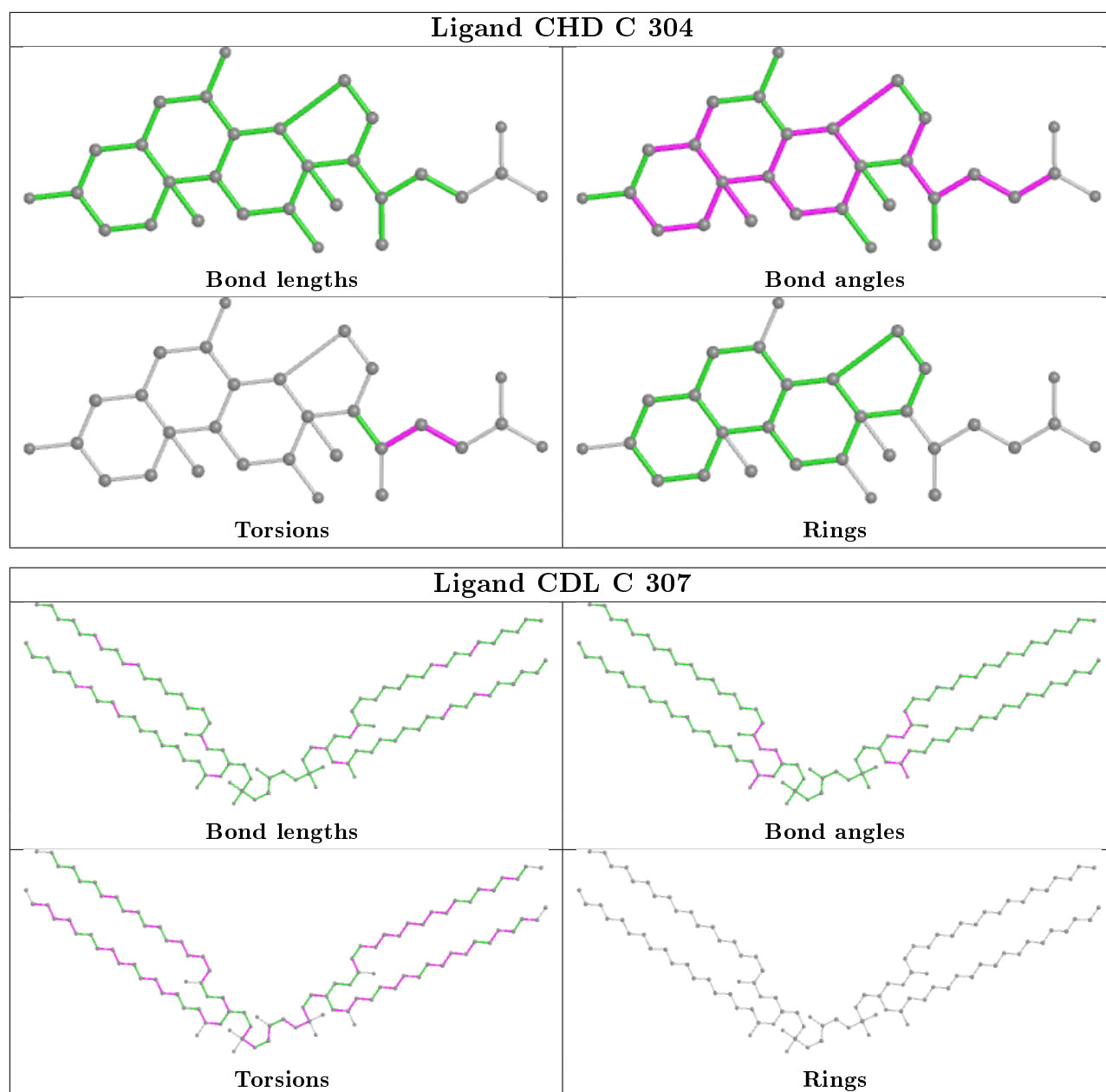












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

## 6 Fit of model and data i

### 6.1 Protein, DNA and RNA chains i

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	513/514 (99%)	-1.13	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	41, 53, 66, 101	0
1	N	513/514 (99%)	-1.08	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	43, 60, 76, 104	0
2	B	226/227 (99%)	-0.99	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	46, 59, 91, 128	0
2	O	226/227 (99%)	-0.81	2 (0%) <span style="border: 1px solid blue; padding: 2px;">84</span> <span style="border: 1px solid blue; padding: 2px;">82</span>	54, 69, 104, 151	0
3	C	259/261 (99%)	-0.90	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	46, 57, 75, 115	0
3	P	259/261 (99%)	-0.90	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	46, 62, 81, 121	0
4	D	144/147 (97%)	-0.68	1 (0%) <span style="border: 1px solid blue; padding: 2px;">87</span> <span style="border: 1px solid blue; padding: 2px;">86</span>	52, 66, 89, 117	0
4	Q	144/147 (97%)	-0.23	8 (5%) <span style="border: 1px solid red; padding: 2px;">24</span> <span style="border: 1px solid red; padding: 2px;">23</span>	64, 83, 125, 160	0
5	E	105/109 (96%)	-0.86	1 (0%) <span style="border: 1px solid blue; padding: 2px;">82</span> <span style="border: 1px solid blue; padding: 2px;">80</span>	50, 65, 92, 147	0
5	R	105/109 (96%)	-0.76	1 (0%) <span style="border: 1px solid blue; padding: 2px;">82</span> <span style="border: 1px solid blue; padding: 2px;">80</span>	62, 79, 105, 154	0
6	F	98/98 (100%)	-0.36	5 (5%) <span style="border: 1px solid red; padding: 2px;">28</span> <span style="border: 1px solid red; padding: 2px;">26</span>	52, 66, 134, 154	0
6	S	98/98 (100%)	-0.20	7 (7%) <span style="border: 1px solid red; padding: 2px;">16</span> <span style="border: 1px solid red; padding: 2px;">14</span>	58, 74, 145, 162	0
7	G	83/85 (97%)	-0.28	9 (10%) <span style="border: 1px solid red; padding: 2px;">5</span> <span style="border: 1px solid red; padding: 2px;">5</span>	55, 66, 143, 159	0
7	T	83/85 (97%)	-0.21	8 (9%) <span style="border: 1px solid red; padding: 2px;">8</span> <span style="border: 1px solid red; padding: 2px;">7</span>	53, 73, 147, 158	0
8	H	79/85 (92%)	-0.49	4 (5%) <span style="border: 1px solid red; padding: 2px;">28</span> <span style="border: 1px solid red; padding: 2px;">26</span>	54, 69, 141, 156	0
8	U	79/85 (92%)	-0.30	5 (6%) <span style="border: 1px solid red; padding: 2px;">20</span> <span style="border: 1px solid red; padding: 2px;">18</span>	61, 80, 139, 153	0
9	I	72/73 (98%)	-0.55	2 (2%) <span style="border: 1px solid gray; padding: 2px;">53</span> <span style="border: 1px solid gray; padding: 2px;">51</span>	58, 73, 101, 114	0
9	V	72/73 (98%)	-0.29	3 (4%) <span style="border: 1px solid red; padding: 2px;">36</span> <span style="border: 1px solid red; padding: 2px;">35</span>	59, 84, 114, 142	0
10	J	58/59 (98%)	-0.51	2 (3%) <span style="border: 1px solid gray; padding: 2px;">45</span> <span style="border: 1px solid gray; padding: 2px;">44</span>	57, 70, 111, 144	0
10	W	58/59 (98%)	-0.27	4 (6%) <span style="border: 1px solid red; padding: 2px;">16</span> <span style="border: 1px solid red; padding: 2px;">15</span>	66, 82, 123, 158	0
11	K	49/56 (87%)	-0.35	1 (2%) <span style="border: 1px solid blue; padding: 2px;">65</span> <span style="border: 1px solid blue; padding: 2px;">63</span>	59, 72, 93, 119	0
11	X	49/56 (87%)	-0.12	3 (6%) <span style="border: 1px solid red; padding: 2px;">21</span> <span style="border: 1px solid red; padding: 2px;">20</span>	70, 84, 119, 127	0
12	L	46/47 (97%)	-0.77	1 (2%) <span style="border: 1px solid blue; padding: 2px;">62</span> <span style="border: 1px solid blue; padding: 2px;">60</span>	49, 60, 80, 122	0
12	Y	46/47 (97%)	-0.64	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	60, 75, 102, 119	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	43/46 (93%)	-0.43	2 (4%) 31 30	50, 63, 99, 147	0
13	Z	43/46 (93%)	-0.01	3 (6%) 16 15	70, 79, 121, 164	0
All	All	3550/3614 (98%)	-0.76	72 (2%) 65 63	41, 64, 107, 164	0

The worst 5 of 72 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	Z	43	SER	10.6
2	O	90	ILE	9.5
6	F	1	ALA	9.2
7	G	40	GLY	6.7
6	S	2	SER	6.2

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
9	SAC	V	1	9/10	0.43	0.49	138,151,167,167	0
7	TPO	T	11	11/12	0.64	0.31	101,147,160,160	0
9	SAC	I	1	9/10	0.72	0.37	116,134,157,165	0
7	TPO	G	11	11/12	0.76	0.27	102,140,157,157	0
1	FME	N	1	10/11	0.92	0.31	80,86,125,151	0
1	FME	A	1	10/11	0.95	0.29	74,86,128,147	0
2	FME	B	1	10/11	0.98	0.07	58,65,72,72	0
2	FME	O	1	10/11	0.99	0.08	64,71,76,79	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
24	PSC	B	303	52/52	0.53	0.35	75,147,150,150	0
27	PEK	G	102	53/53	0.59	0.32	100,135,150,150	0
20	PGV	N	607	51/51	0.64	0.32	99,137,150,150	0
20	PGV	A	609	51/51	0.65	0.26	69,115,159,161	0
19	TGL	N	610	63/63	0.65	0.29	90,134,149,150	0
27	PEK	T	101	53/53	0.66	0.36	79,136,150,150	0
24	PSC	R	201	52/52	0.67	0.29	76,137,150,150	0
27	PEK	T	102	53/53	0.67	0.31	78,133,150,150	0
29	DMU	Z	101	33/33	0.68	0.30	80,128,149,150	0
23	CHD	W	101	29/29	0.69	0.40	107,145,150,150	0
26	CDL	C	307	100/100	0.71	0.30	89,138,150,150	0
26	CDL	P	304	100/100	0.72	0.25	71,140,150,150	0
21	EDO	C	310	4/4	0.72	0.24	94,105,106,112	0
19	TGL	N	611	63/63	0.73	0.25	90,126,148,150	0
19	TGL	D	201	63/63	0.75	0.24	87,126,147,150	0
21	EDO	A	612	4/4	0.75	0.51	88,115,122,127	0
21	EDO	K	101	4/4	0.76	0.18	86,107,118,131	0
20	PGV	C	308	51/51	0.76	0.22	75,125,150,150	0
26	CDL	T	103	100/100	0.77	0.26	76,140,150,150	0
19	TGL	L	101	63/63	0.79	0.23	67,113,143,150	0
27	PEK	C	306	53/53	0.79	0.26	71,132,149,150	0
20	PGV	G	103	51/51	0.80	0.20	96,127,150,150	0
23	CHD	J	101	29/29	0.81	0.36	123,142,150,150	0
26	CDL	C	303	100/100	0.82	0.22	66,123,153,155	0
21	EDO	C	311	4/4	0.83	0.26	80,95,109,118	0
19	TGL	A	607	63/63	0.84	0.18	54,97,122,132	0
25	UNX	P	301	1/1	0.84	0.41	15,15,15,15	1
21	EDO	A	614	4/4	0.84	0.58	133,137,141,148	0
19	TGL	N	609	63/63	0.85	0.18	60,120,149,150	0
21	EDO	K	103	4/4	0.85	0.23	90,92,99,101	0
21	EDO	G	104	4/4	0.86	0.21	97,101,102,105	0
23	CHD	C	304	29/29	0.87	0.26	93,117,125,127	0
21	EDO	F	102	4/4	0.88	0.28	80,88,96,96	0
21	EDO	K	102	4/4	0.89	0.21	101,108,112,116	0
29	DMU	M	101	33/33	0.90	0.16	70,102,129,136	0
23	CHD	P	305	29/29	0.90	0.20	120,135,145,147	0
25	UNX	C	301	1/1	0.93	0.36	26,26,26,26	1
21	EDO	A	611	4/4	0.93	0.13	86,94,107,113	0
21	EDO	A	613	4/4	0.93	0.19	112,112,121,122	0
27	PEK	P	302	53/53	0.94	0.13	59,91,150,150	0
27	PEK	G	101	53/53	0.94	0.12	57,72,126,136	0
21	EDO	B	305	4/4	0.94	0.20	105,110,115,123	0

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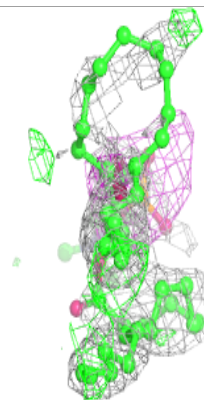
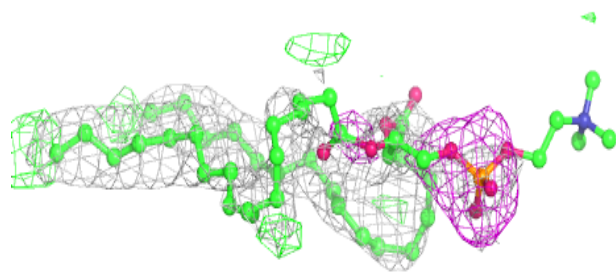
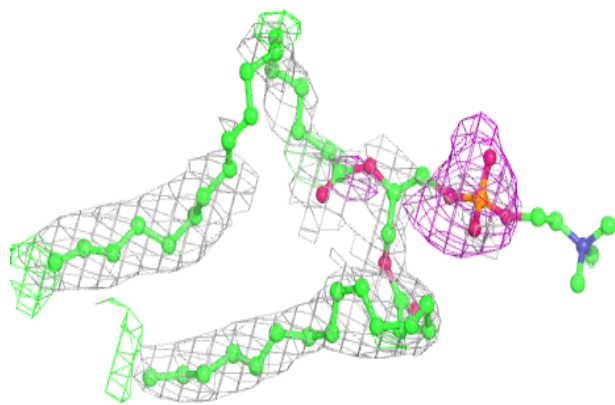
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
21	EDO	T	104	4/4	0.94	0.32	124,129,131,132	0
23	CHD	C	305	29/29	0.96	0.09	47,61,71,81	0
23	CHD	B	302	29/29	0.96	0.10	48,64,74,77	0
21	EDO	N	612	4/4	0.96	0.09	79,80,82,84	0
21	EDO	L	102	4/4	0.97	0.06	83,84,84,90	0
21	EDO	A	610	4/4	0.97	0.10	75,75,78,81	0
23	CHD	O	302	29/29	0.97	0.09	50,57,67,72	0
21	EDO	C	309	4/4	0.97	0.16	76,86,100,122	0
20	PGV	N	608	51/51	0.98	0.11	47,76,117,142	0
20	PGV	A	608	51/51	0.98	0.10	51,66,79,86	0
23	CHD	P	306	29/29	0.98	0.09	57,65,72,73	0
20	PGV	P	303	51/51	0.98	0.10	51,72,132,148	0
17	NA	N	605	1/1	0.98	0.11	70,70,70,70	0
16	MG	N	604	1/1	0.98	0.07	57,57,57,57	0
21	EDO	B	304	4/4	0.98	0.09	71,75,75,75	0
20	PGV	C	302	51/51	0.98	0.08	49,58,90,99	0
18	CMO	N	606	2/2	0.99	0.15	77,77,77,80	0
14	HEA	A	602	60/60	0.99	0.06	45,51,60,62	0
14	HEA	N	602	60/60	0.99	0.08	47,57,69,75	0
16	MG	A	604	1/1	0.99	0.06	51,51,51,51	0
22	CUA	O	301	2/2	0.99	0.06	66,66,66,67	0
14	HEA	N	601	60/60	0.99	0.09	47,56,78,84	0
17	NA	A	605	1/1	0.99	0.16	59,59,59,59	0
22	CUA	B	301	2/2	0.99	0.07	54,54,54,58	0
14	HEA	A	601	60/60	0.99	0.07	34,46,65,70	0
28	ZN	F	101	1/1	1.00	0.04	64,64,64,64	0
18	CMO	A	606	2/2	1.00	0.06	55,55,55,55	0
15	CU	N	603	1/1	1.00	0.03	55,55,55,55	0
15	CU	A	603	1/1	1.00	0.01	55,55,55,55	0
28	ZN	S	101	1/1	1.00	0.07	70,70,70,70	0

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

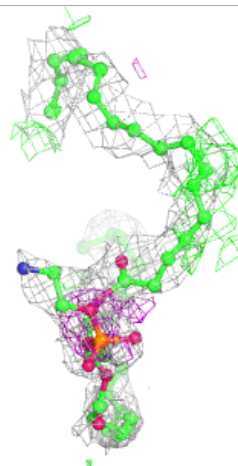
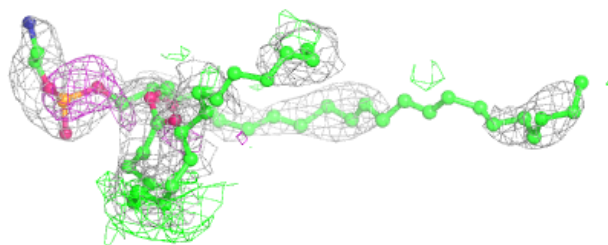
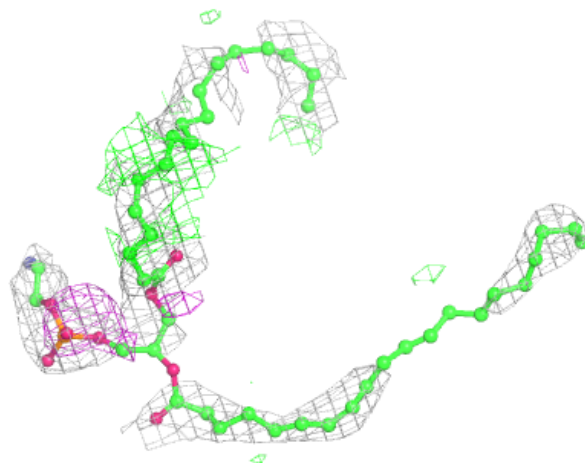
**Electron density around PSC B 303:**

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



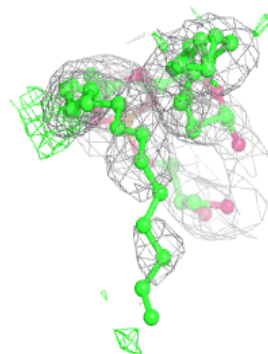
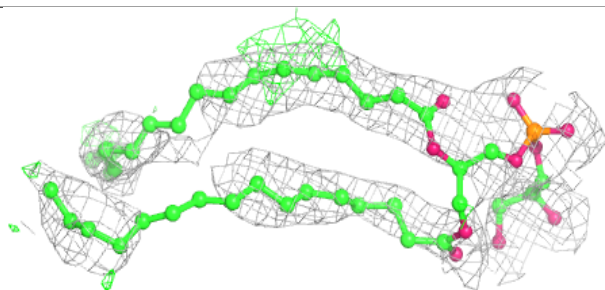
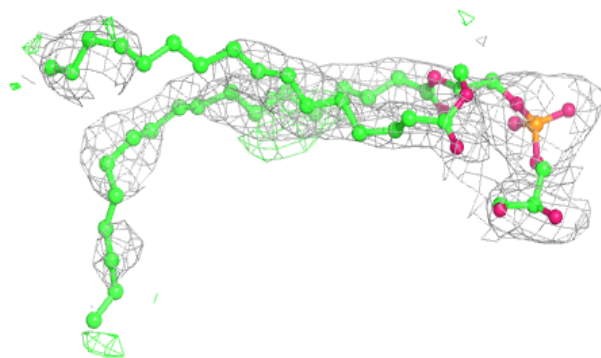
**Electron density around PEK G 102:**

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

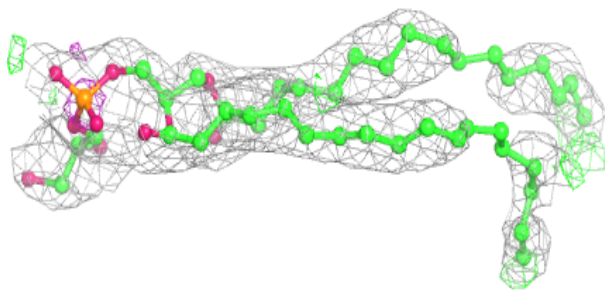
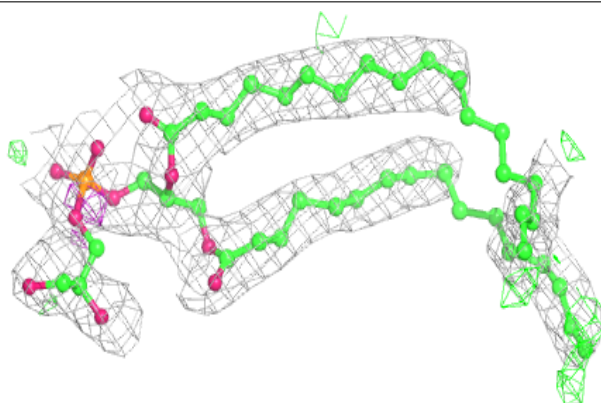


**Electron density around PGV N 607:**

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

**Electron density around PGV A 609:**

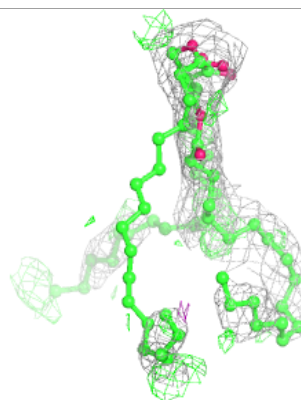
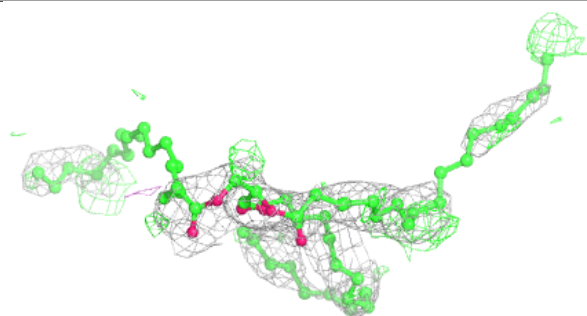
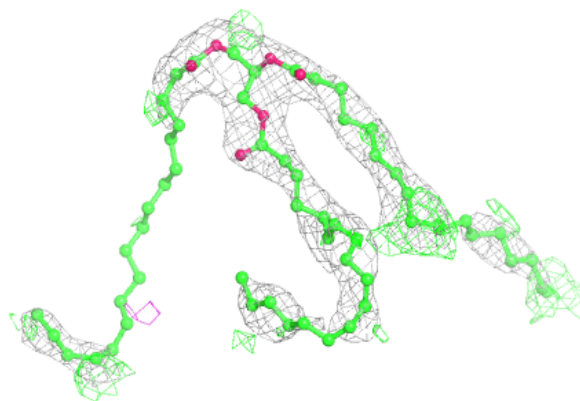
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



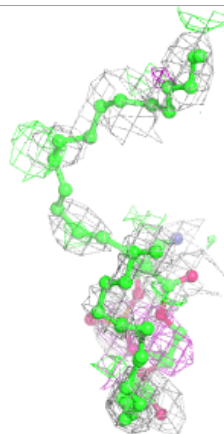
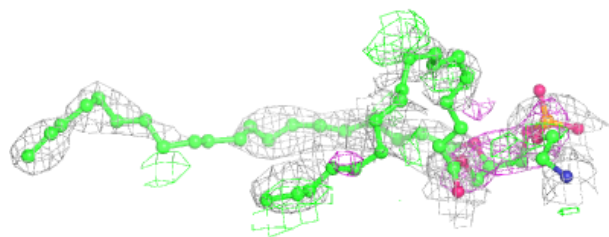
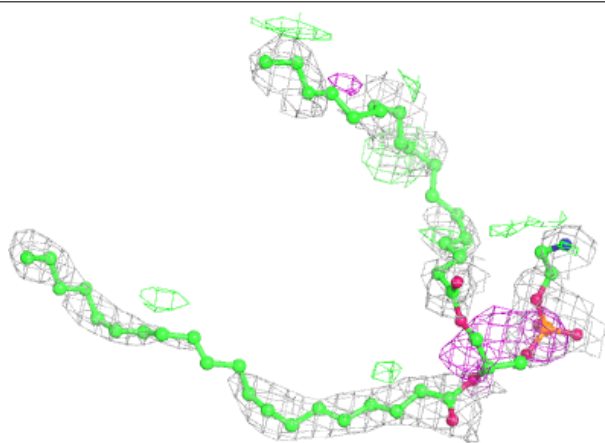


**Electron density around TGL N 610:**

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

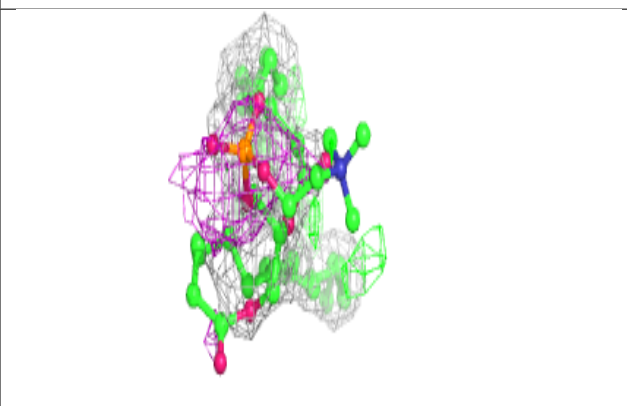
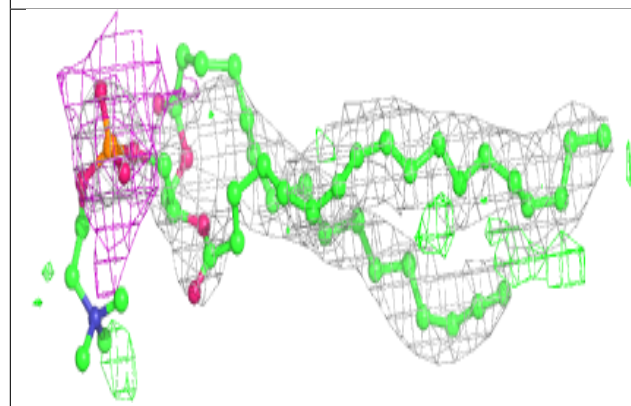
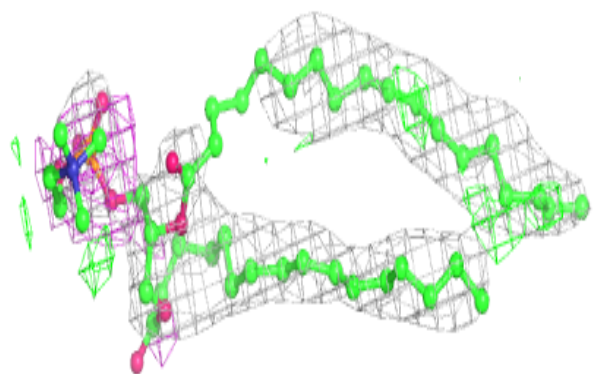
**Electron density around PEK T 101:**

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

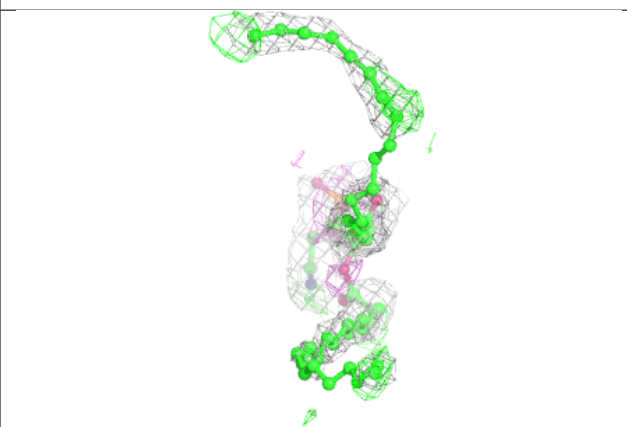
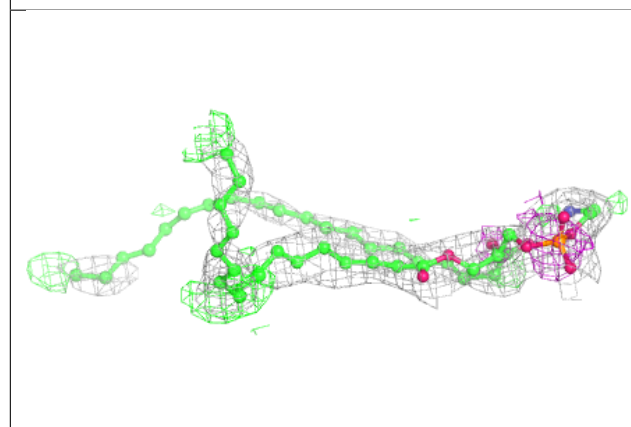
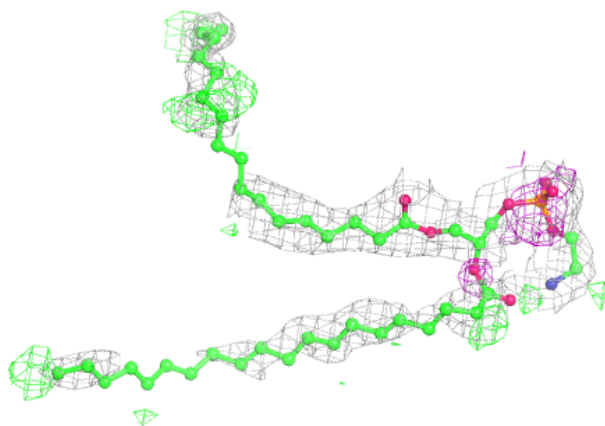


**Electron density around PSC R 201:**

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

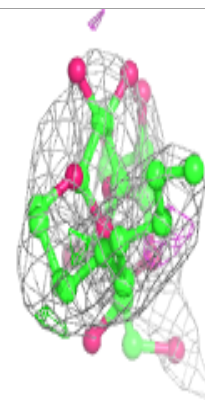
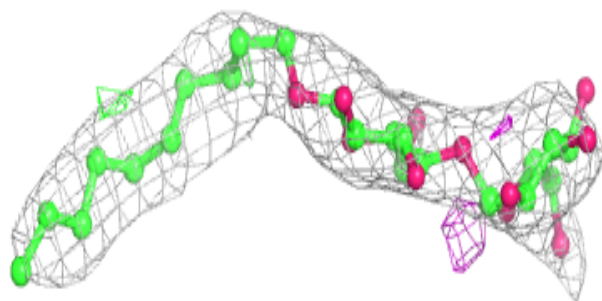
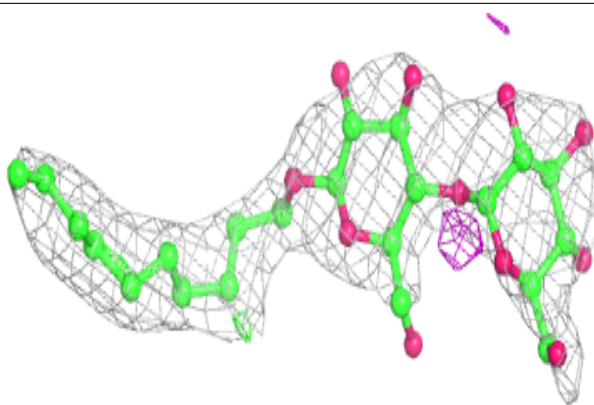
**Electron density around PEK T 102:**

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

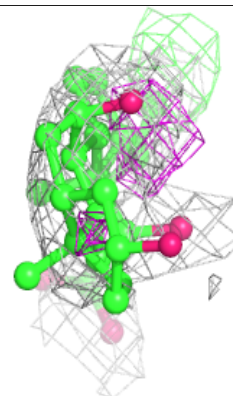
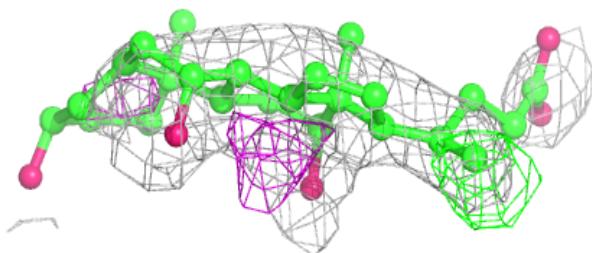
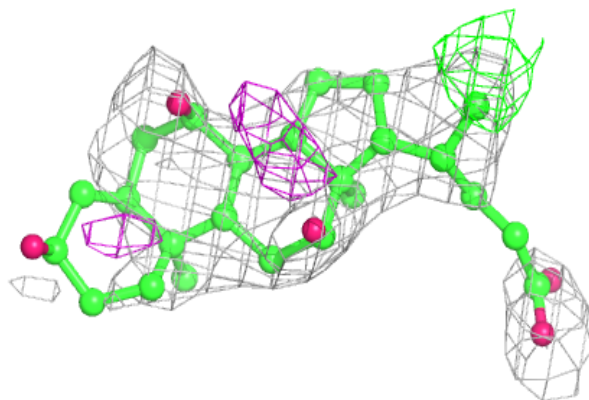


**Electron density around DMU Z 101:**

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

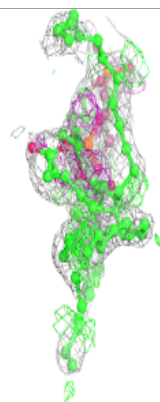
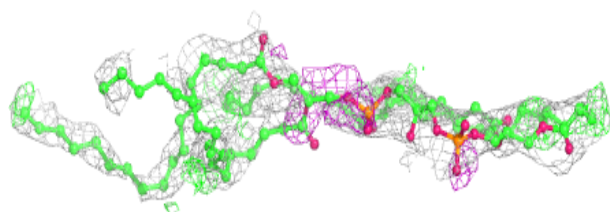
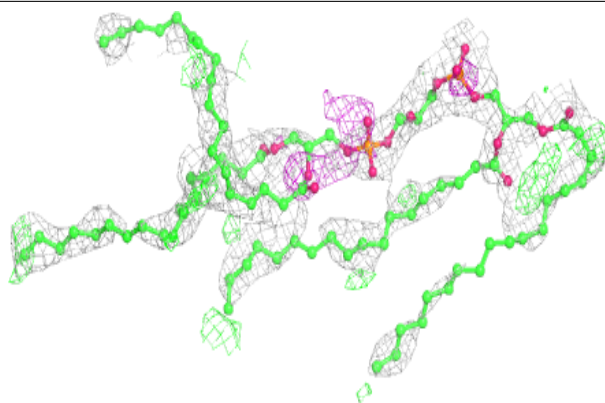
**Electron density around CHD W 101:**

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

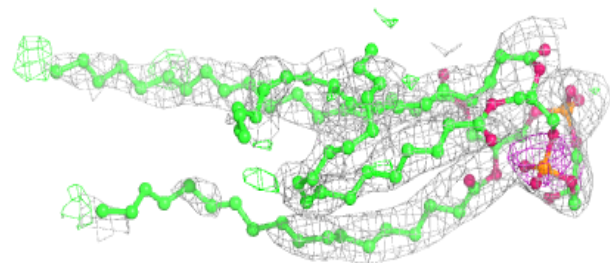
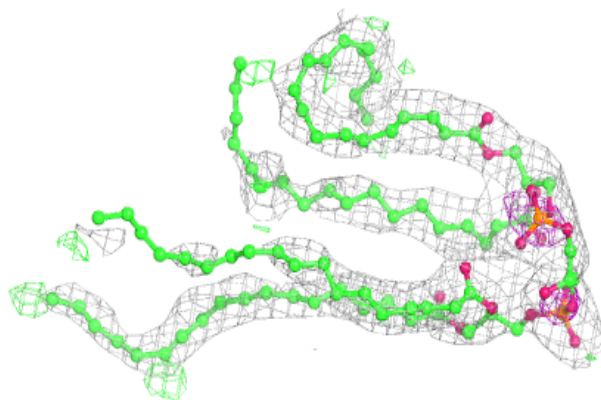


**Electron density around CDL C 307:**

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

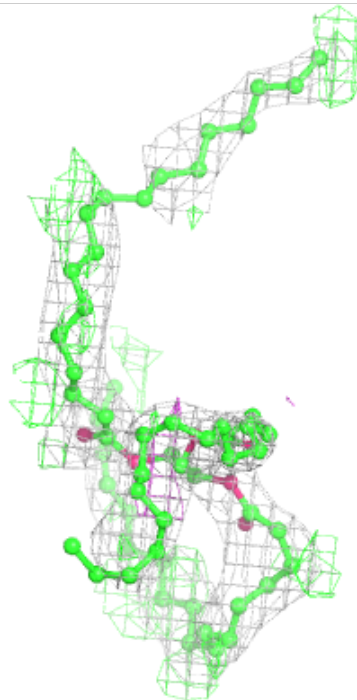
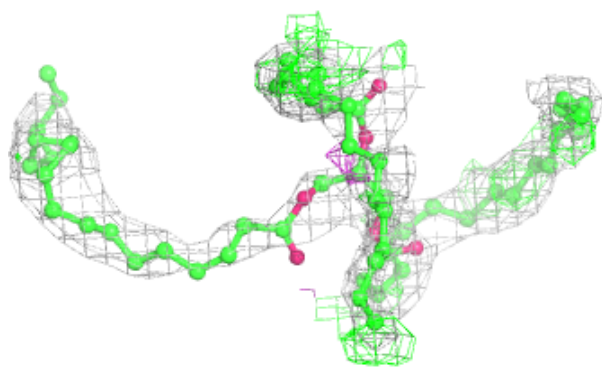
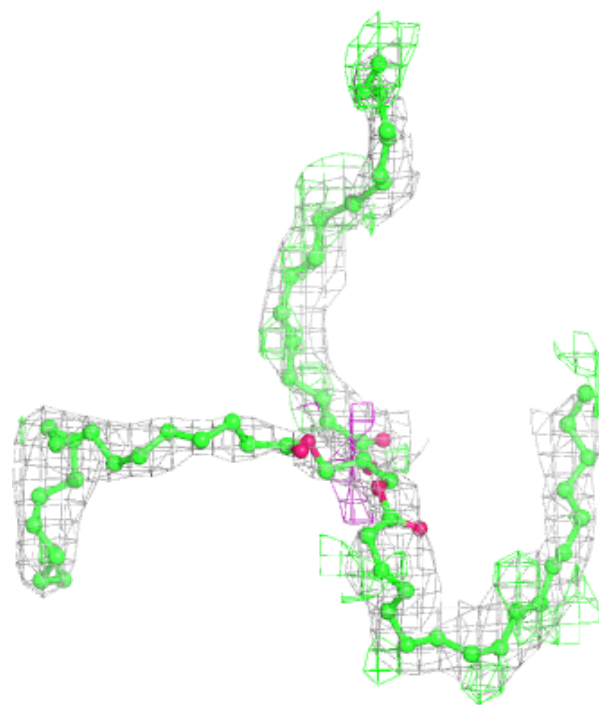
**Electron density around CDL P 304:**

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



**Electron density around TGL N 611:**

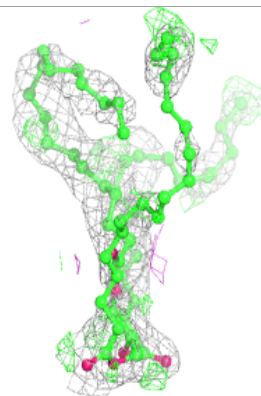
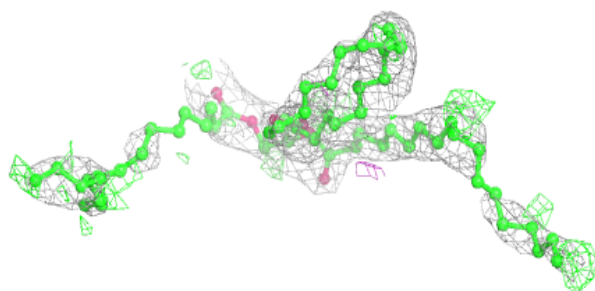
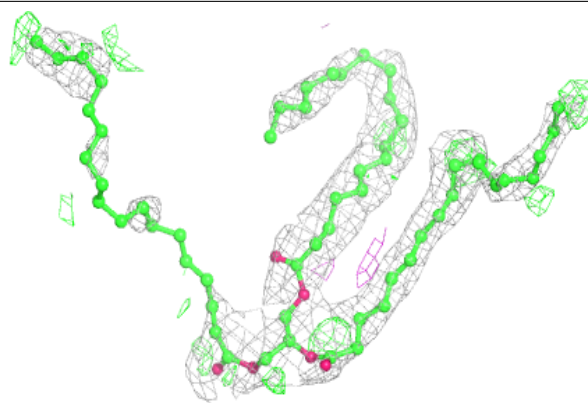
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



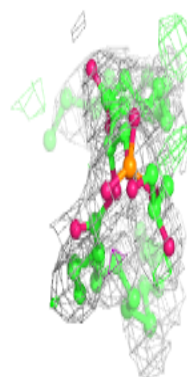
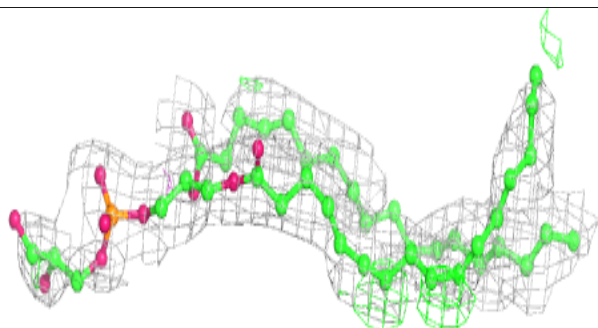
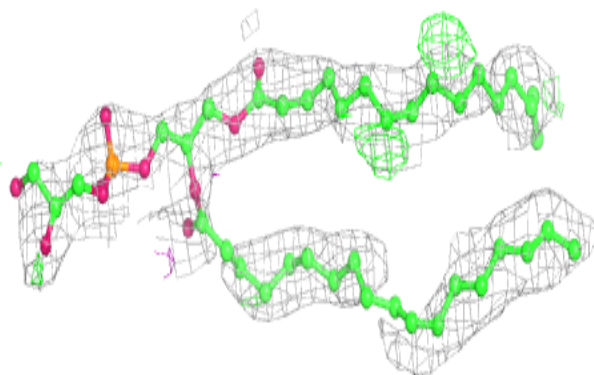


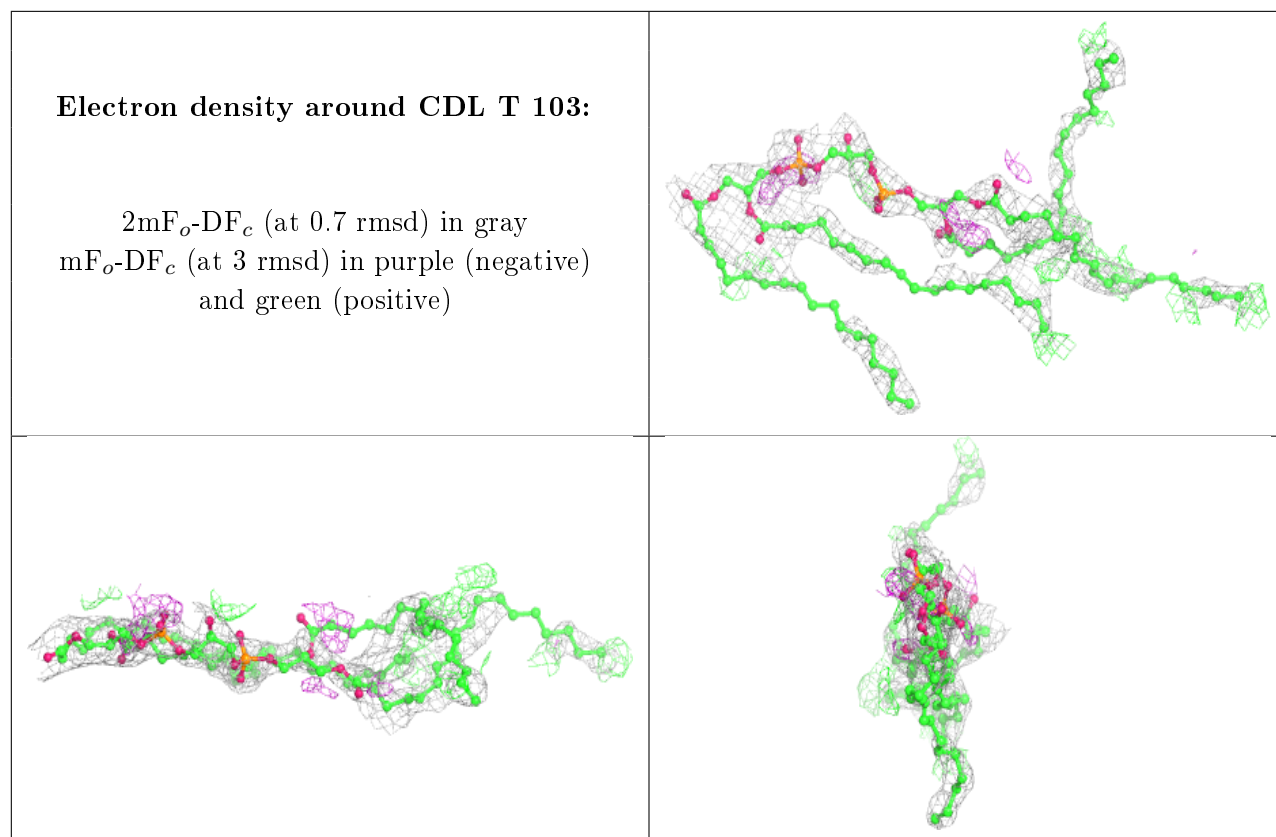
**Electron density around TGL D 201:**

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

**Electron density around PGV C 308:**

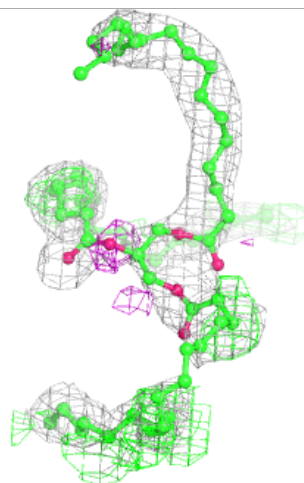
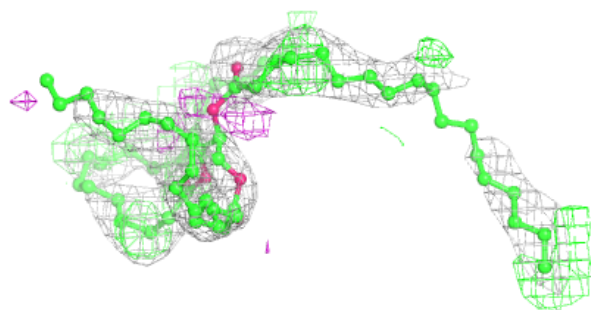
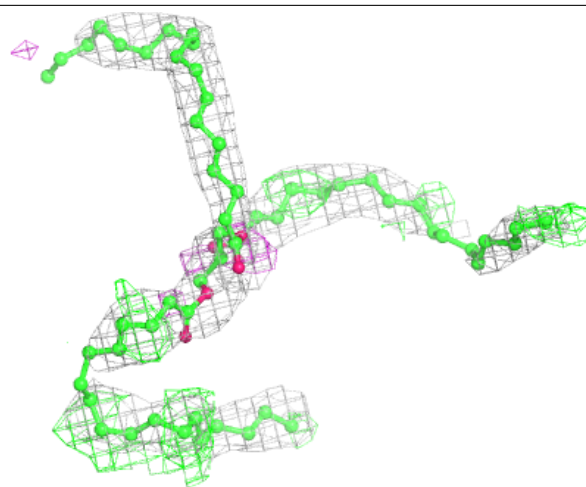
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



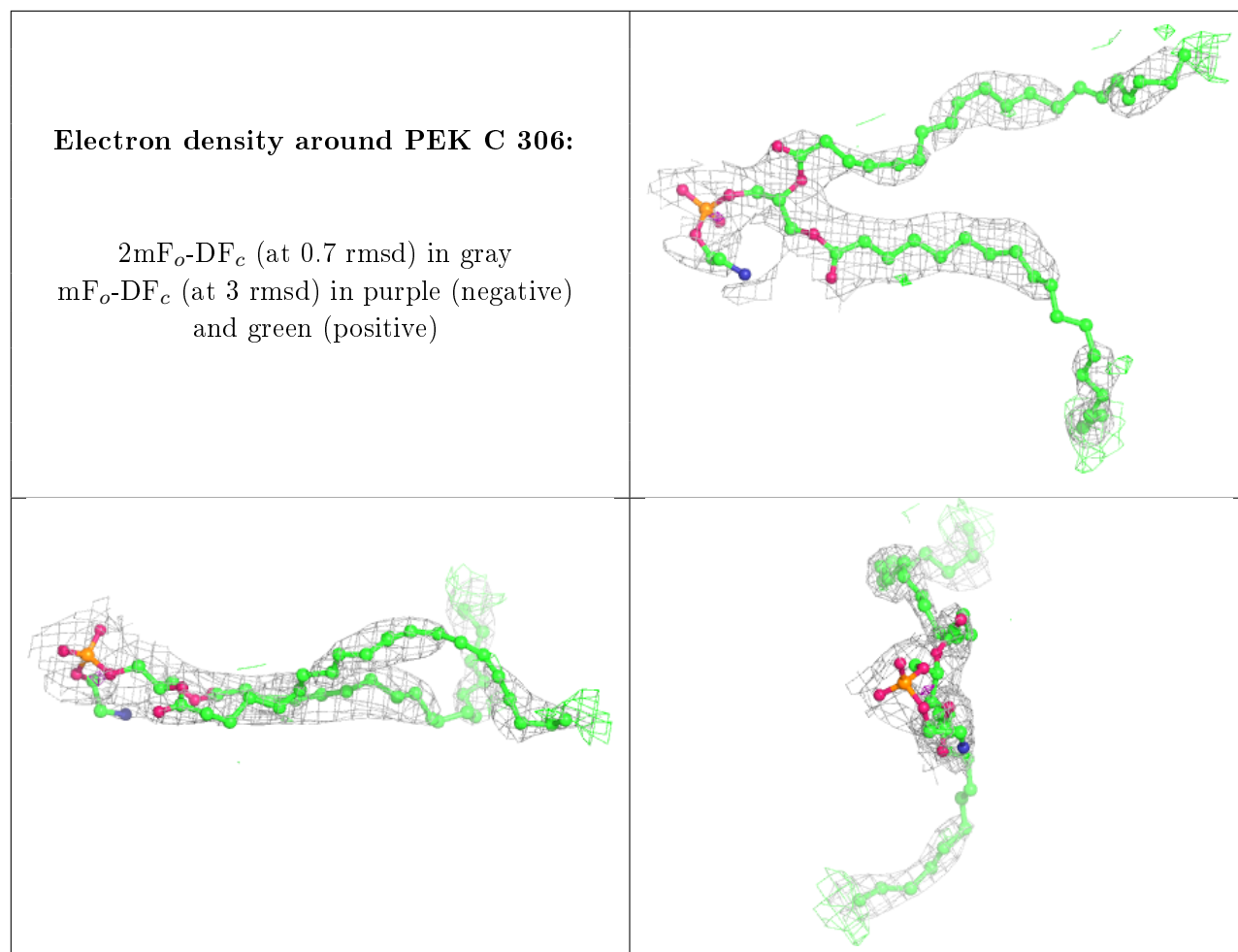


**Electron density around TGL L 101:**

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

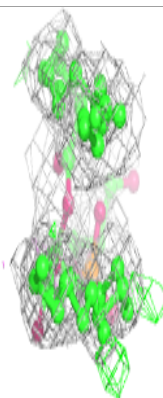
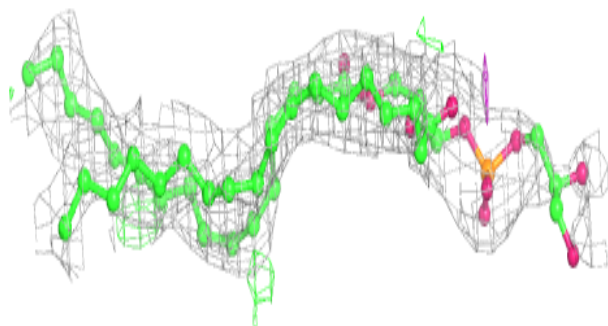
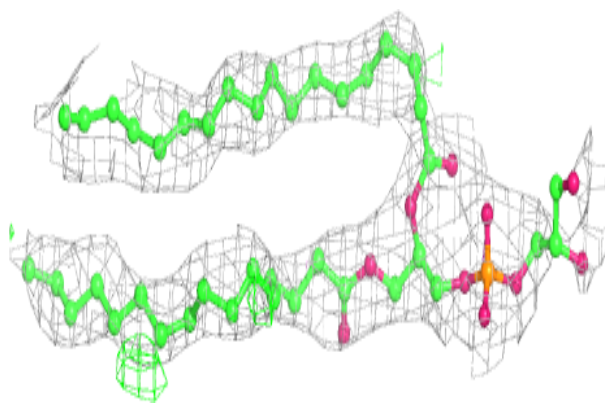




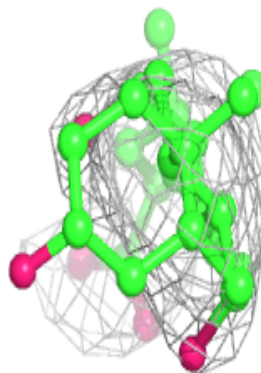
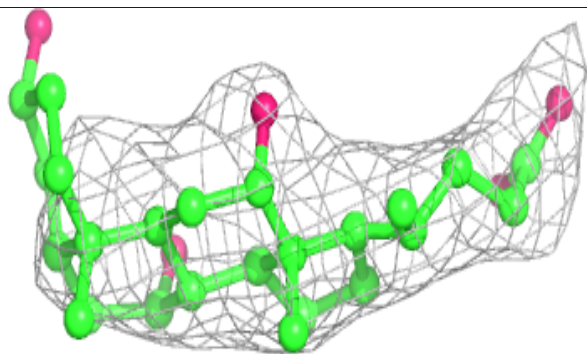
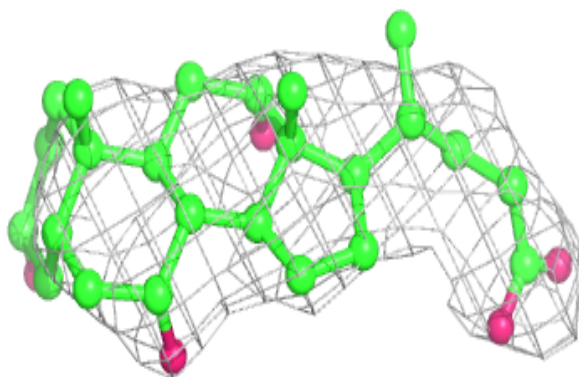


**Electron density around PGV G 103:**

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

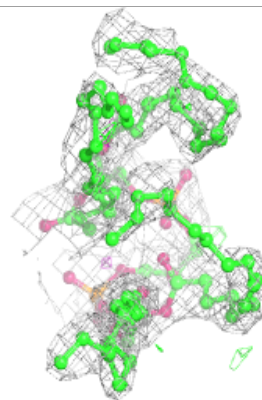
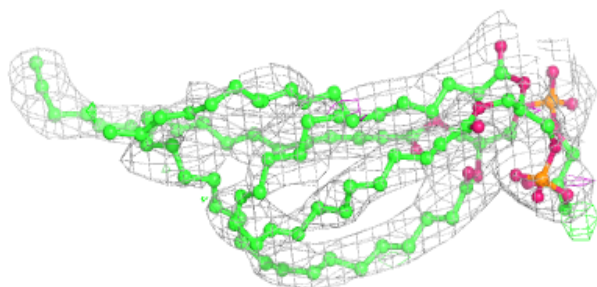
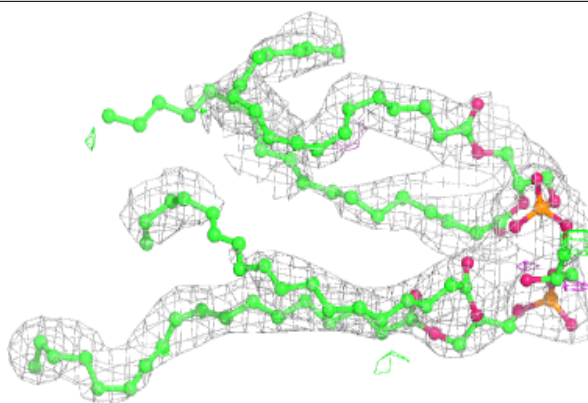
**Electron density around CHD J 101:**

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

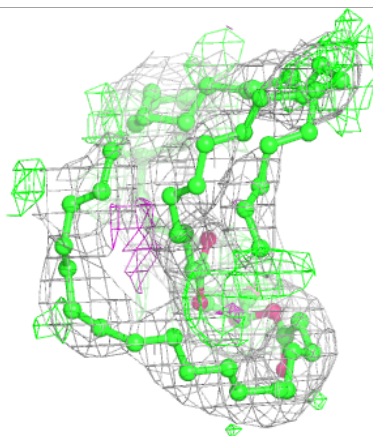
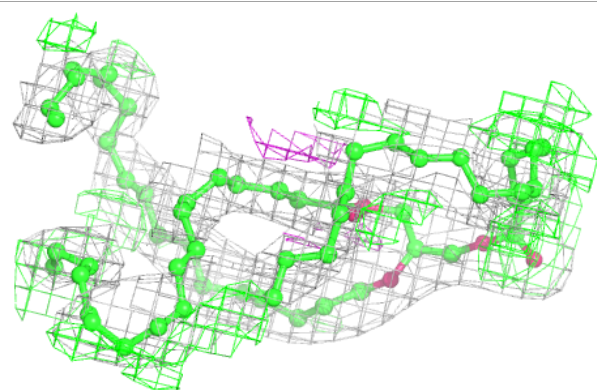
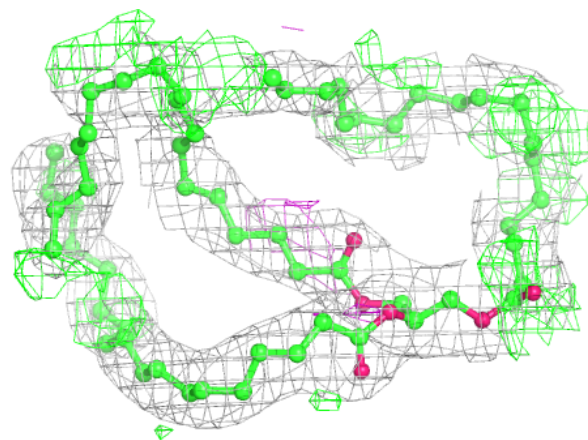


**Electron density around CDL C 303:**

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

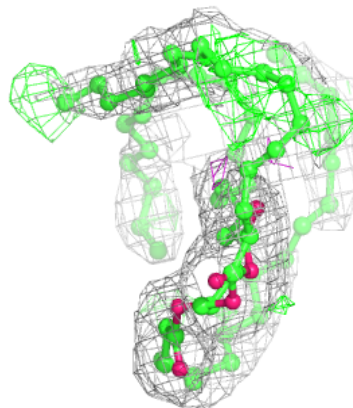
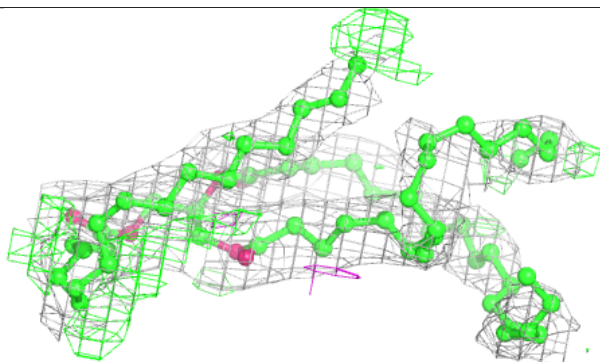
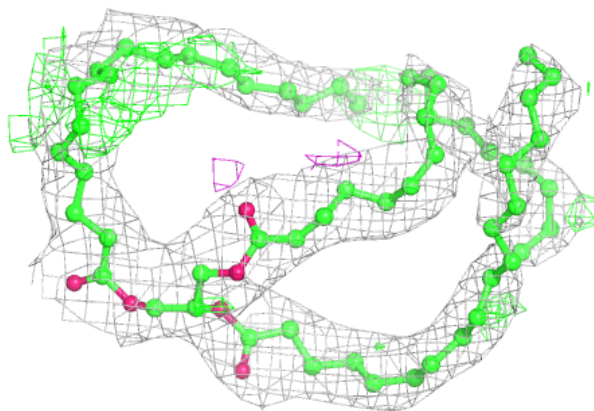
**Electron density around TGL A 607:**

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

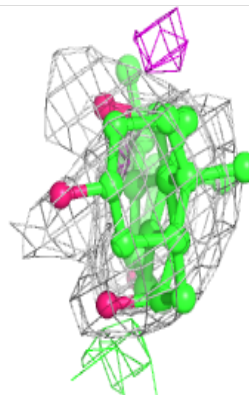
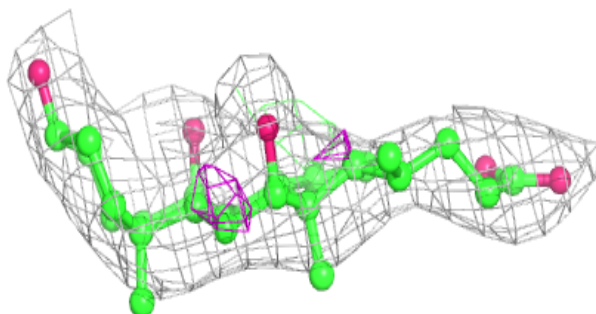
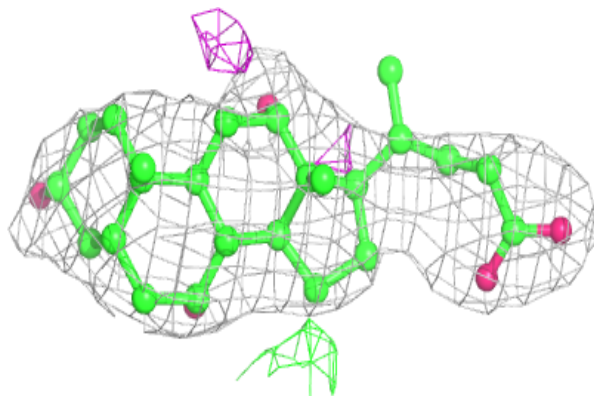


**Electron density around TGL N 609:**

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

**Electron density around CHD C 304:**

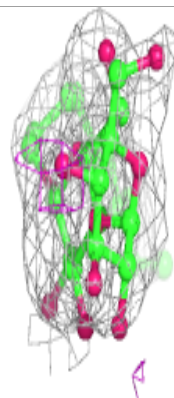
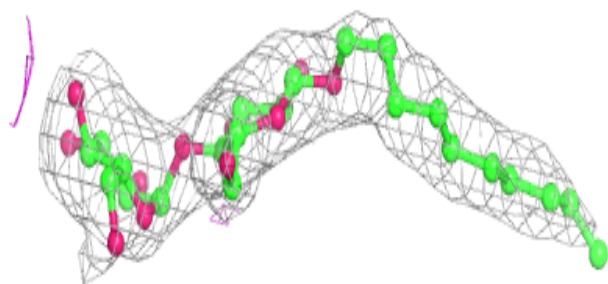
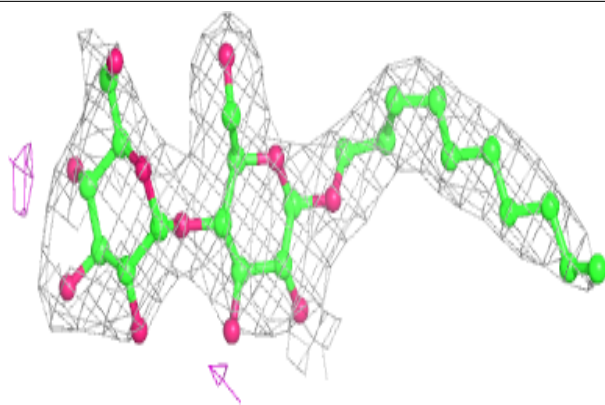
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



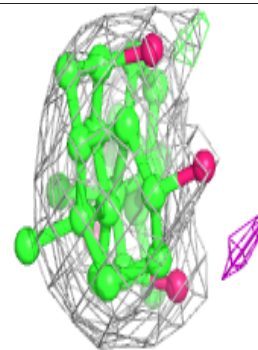
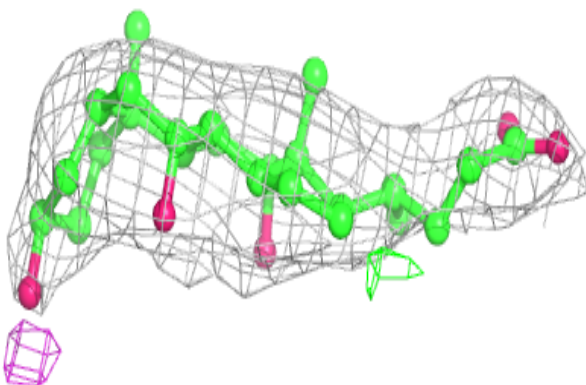
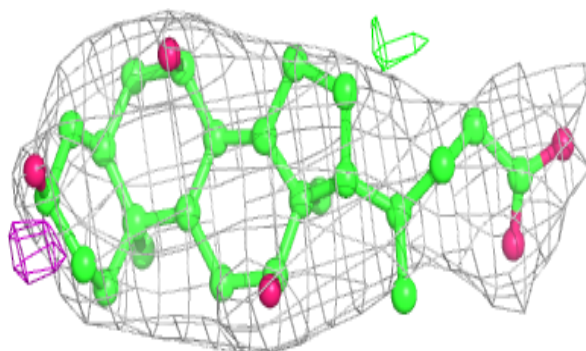


**Electron density around DMU M 101:**

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

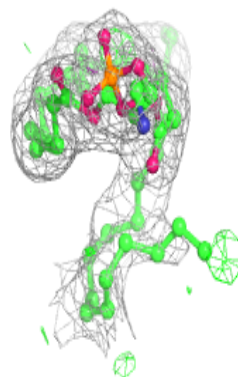
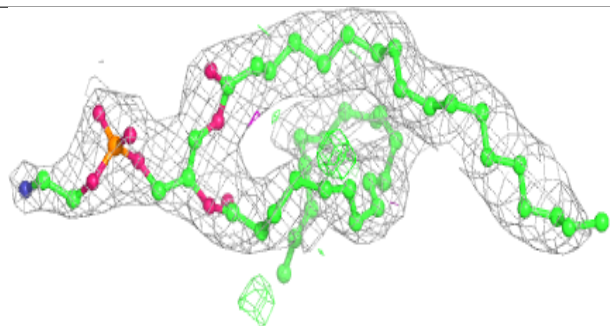
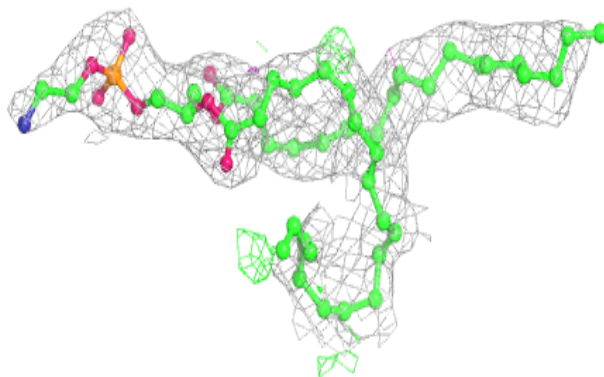
**Electron density around CHD P 305:**

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

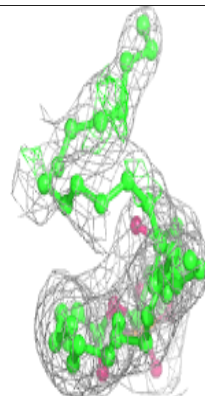
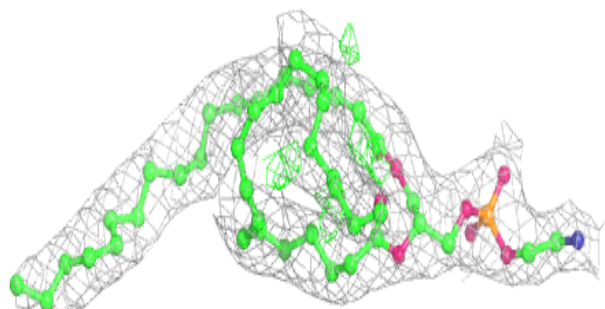
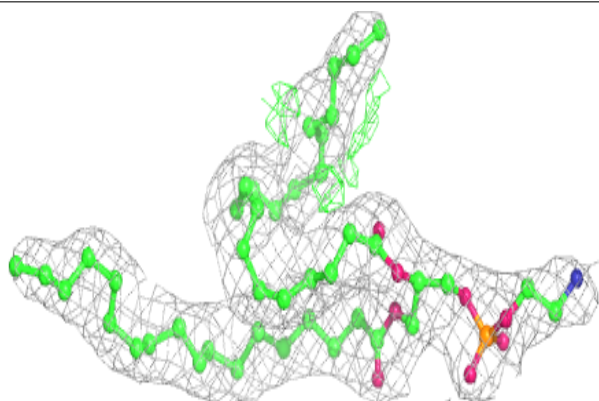


**Electron density around PEK P 302:**

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

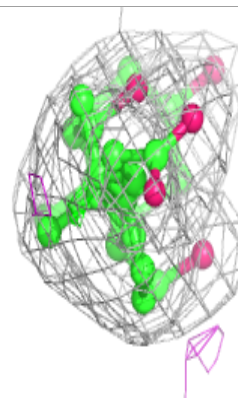
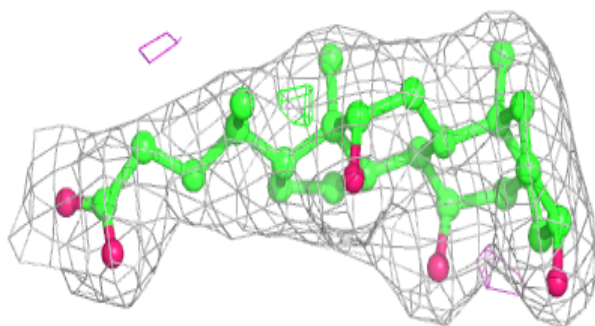
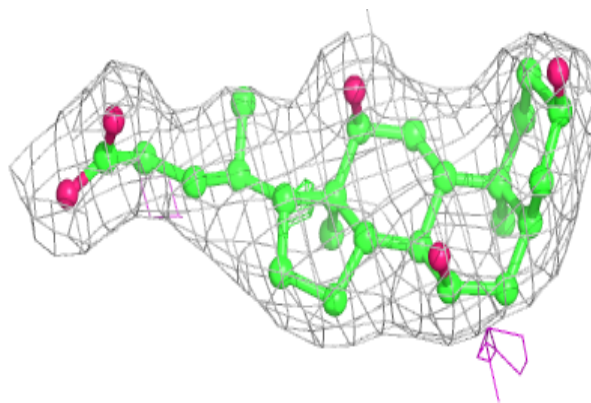
**Electron density around PEK G 101:**

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

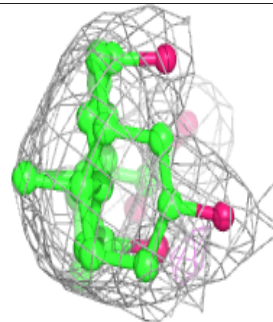
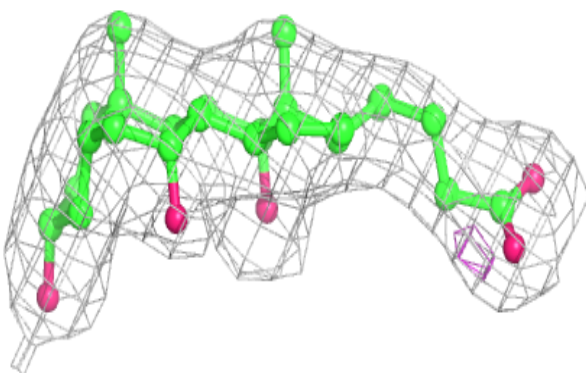
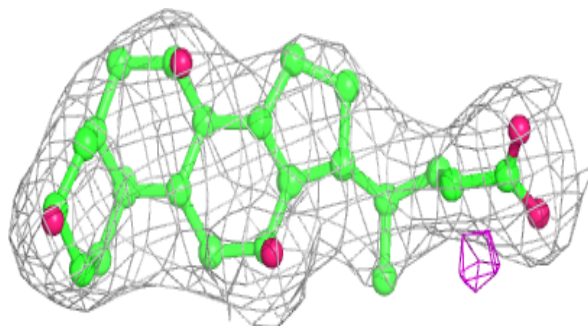


**Electron density around CHD C 305:**

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

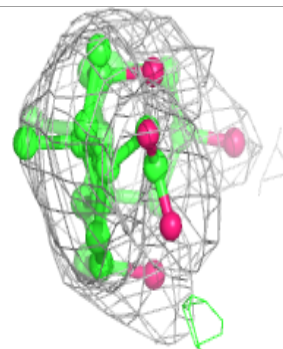
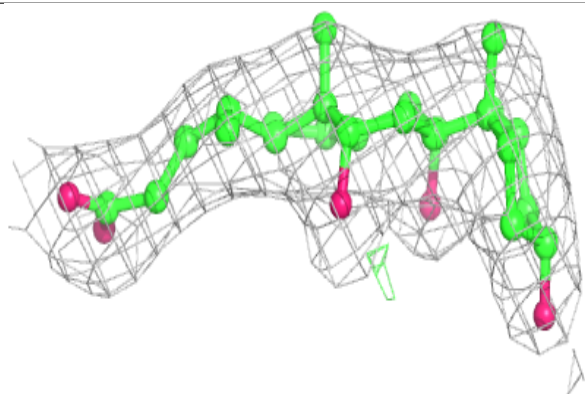
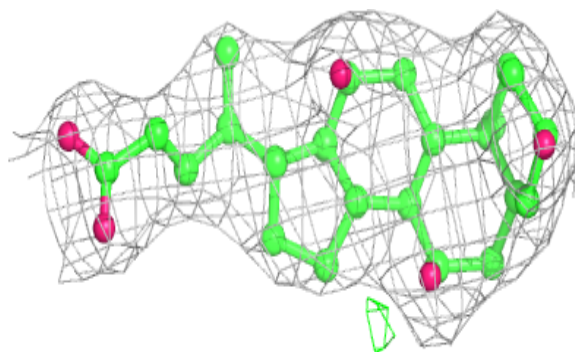
**Electron density around CHD B 302:**

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

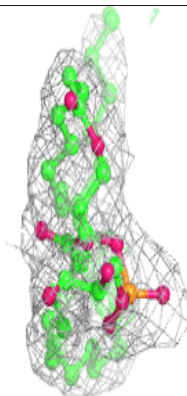
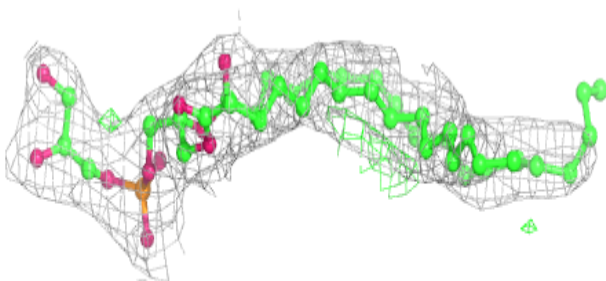
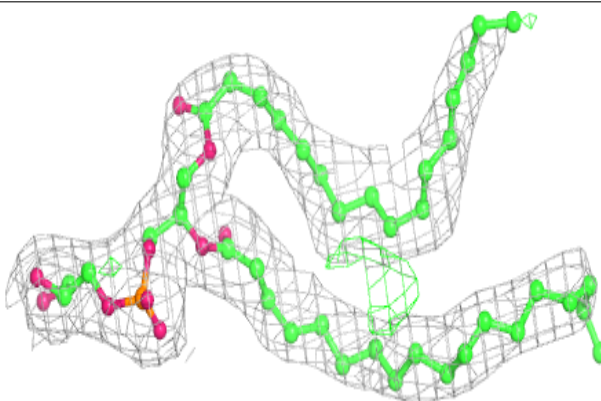


**Electron density around CHD O 302:**

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

**Electron density around PGV N 608:**

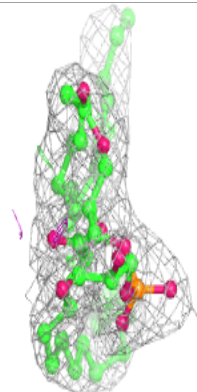
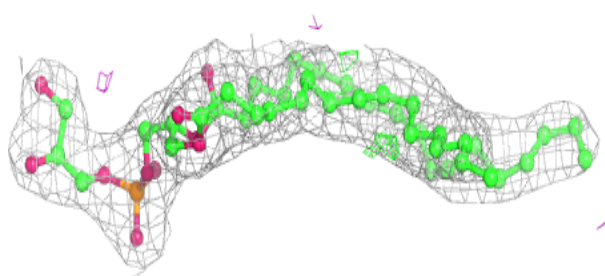
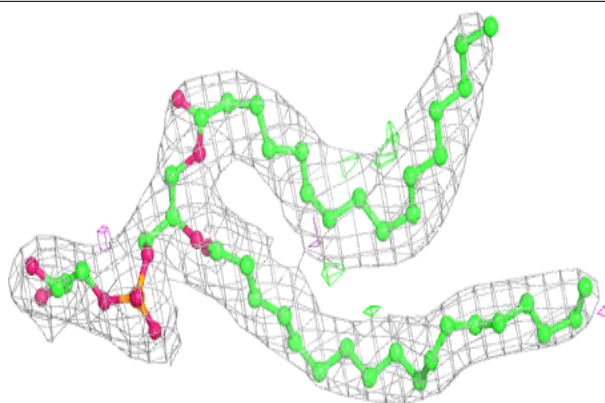
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



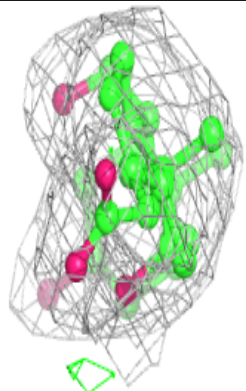
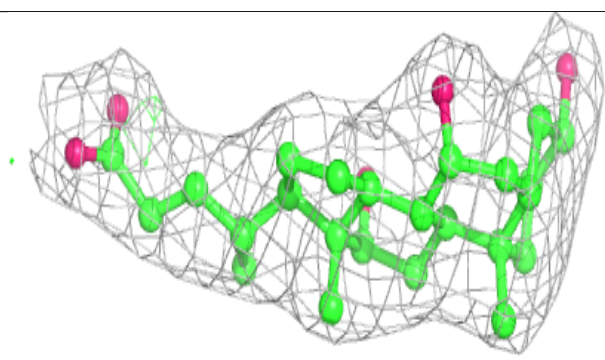
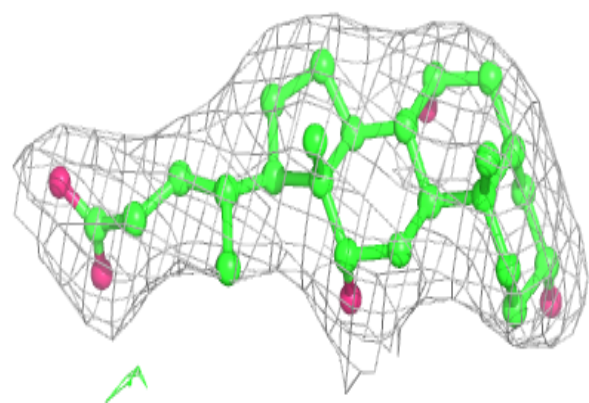


**Electron density around PGV A 608:**

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

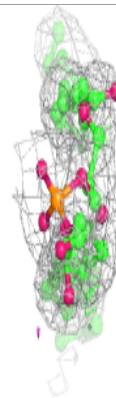
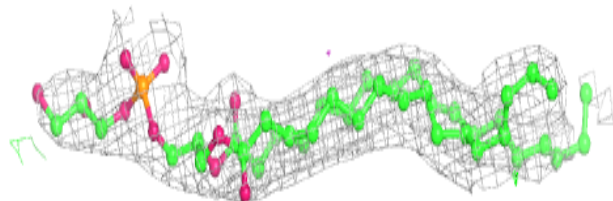
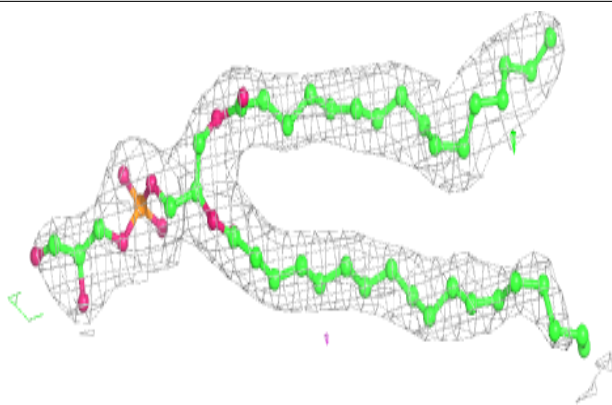
**Electron density around CHD P 306:**

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

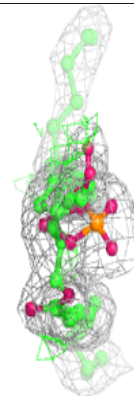
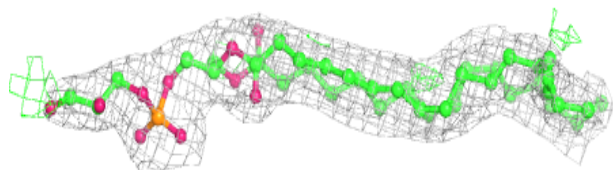
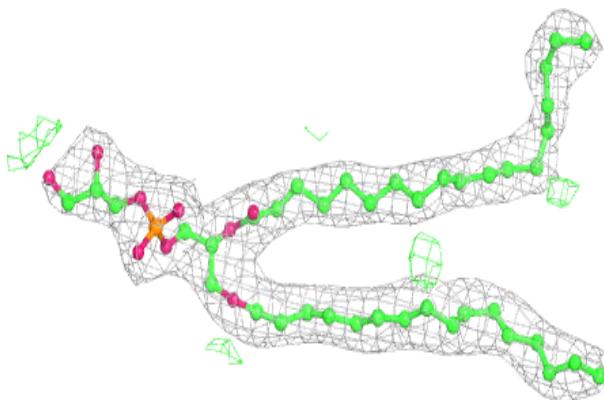


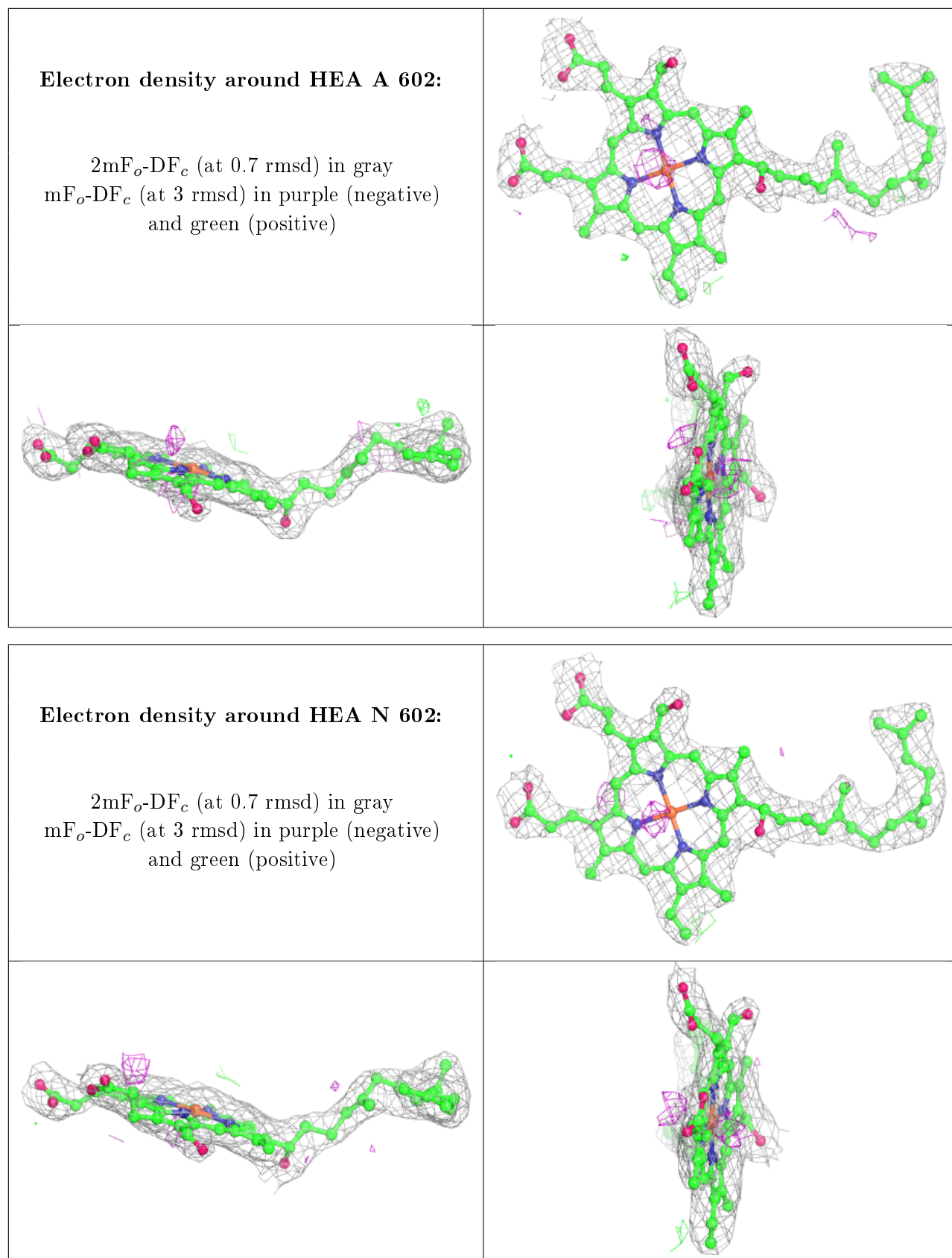
**Electron density around PGV P 303:**

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

**Electron density around PGV C 302:**

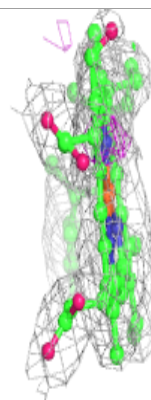
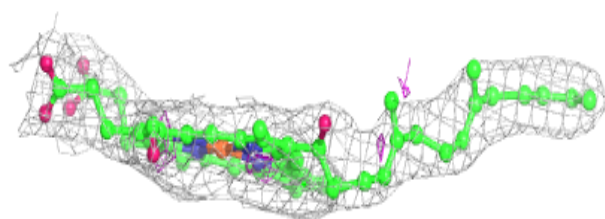
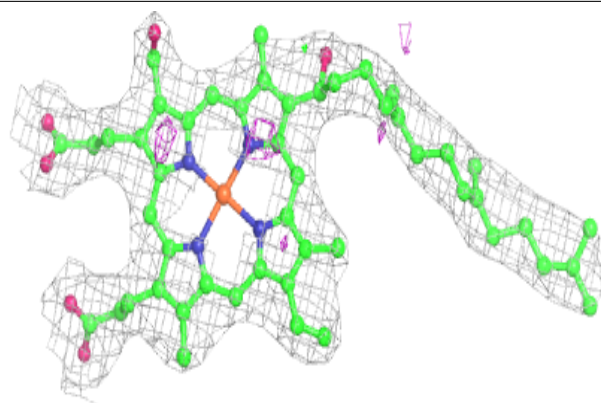
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



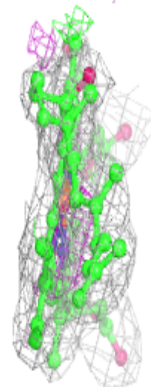
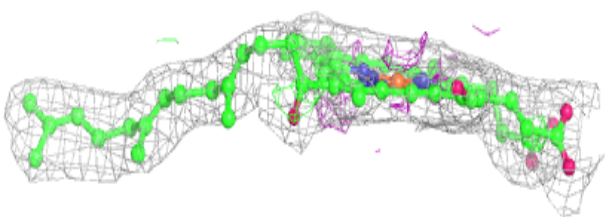
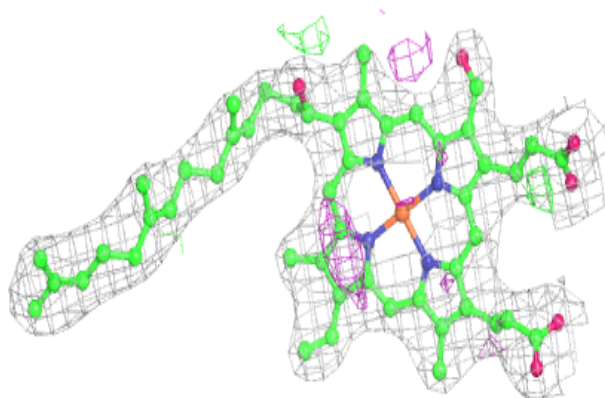


**Electron density around HEA N 601:**

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

**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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.