



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 06:43 pm BST

PDB ID : 6J8M  
Title : Low-dose structure of bovine heart cytochrome c oxidase in the fully oxidized state determined using 30 keV X-ray  
Authors : Ueno, G.; Shimada, A.; Yamashita, E.; Hasegawa, K.; Kumasaka, T.; Shinzawa-Itoh, K.; Yoshikawa, S.; Tsukihara, T.; Yamamoto, M.  
Deposited on : 2019-01-20  
Resolution : 1.90 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 : 2.11  
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) : 2.11

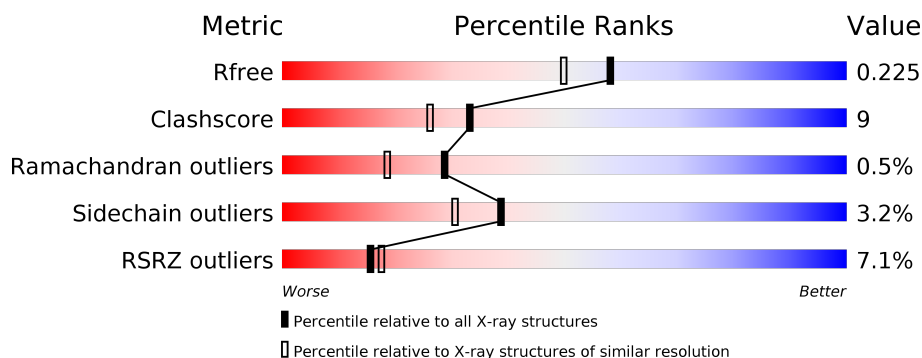
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	<div> <div>89%</div> <div>10%</div> <div>.</div> </div>
1	N	514	<div> <div>%</div> <div>87%</div> <div>12%</div> </div>
2	B	227	<div> <div>4%</div> <div>84%</div> <div>14%</div> <div>.</div> </div>
2	O	227	<div> <div>7%</div> <div>77%</div> <div>21%</div> <div>.</div> </div>
3	C	261	<div> <div>%</div> <div>89%</div> <div>10%</div> <div>.</div> </div>
3	P	261	<div> <div>2%</div> <div>89%</div> <div>11%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
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	-	-	-
14	HEA	N	601	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	N	602	X	-	-	-
19	PER	A	607[B]	-	-	X	-
22	CHD	W	101	-	-	-	X
25	DMU	C	309	-	-	-	X
25	DMU	P	307	-	-	-	X
7	TPO	G	11	-	-	-	X
7	TPO	T	11	-	-	-	X
9	SAC	I	1	-	-	-	X
9	SAC	V	1	-	-	-	X



## 2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 33893 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	12	0
			4124	2753	638	693	40			
1	N	514	Total	C	N	O	S	0	13	0
			4123	2752	638	693	40			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	6	0
			1868	1213	288	348	19			
2	O	227	Total	C	N	O	S	0	5	0
			1870	1215	289	348	18			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	259	Total	C	N	O	S	0	8	0
			2174	1451	345	364	14			
3	P	259	Total	C	N	O	S	0	8	0
			2173	1451	344	363	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	144	Total	C	N	O	S	0	6	0
			1249	814	206	224	5			
4	Q	144	Total	C	N	O	S	0	1	0
			1203	782	197	219	5			

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	98	Total	C	N	O	S	0	5	0
			789	489	142	152	6			
6	S	98	Total	C	N	O	S	0	1	0
			755	468	135	147	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
7	G	84	Total 686	C 440	N 130	O 114	P 1	S 1	0	1	0
7	T	84	Total 706	C 454	N 133	O 117	P 1	S 1	0	3	0

- 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	1	0
			609	395	108	101	5			

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

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.

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

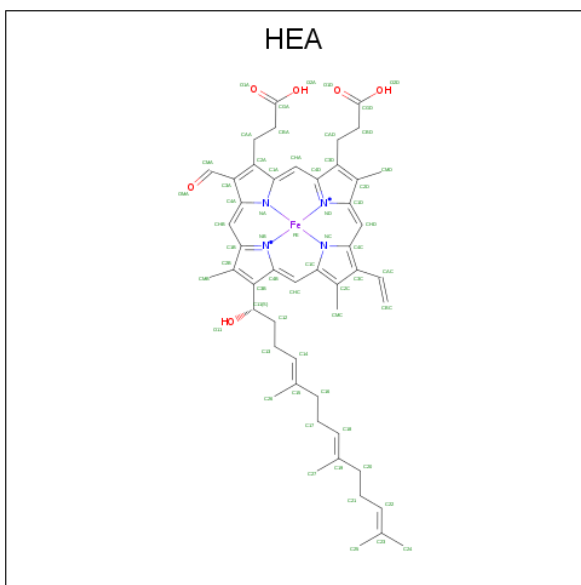
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C.

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.

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	
			60	49	1	4	6	0
14	A	1	Total	C	Fe	N	O	
			60	49	1	4	6	0
14	N	1	Total	C	Fe	N	O	
			60	49	1	4	6	0
14	N	1	Total	C	Fe	N	O	
			60	49	1	4	6	0

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

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

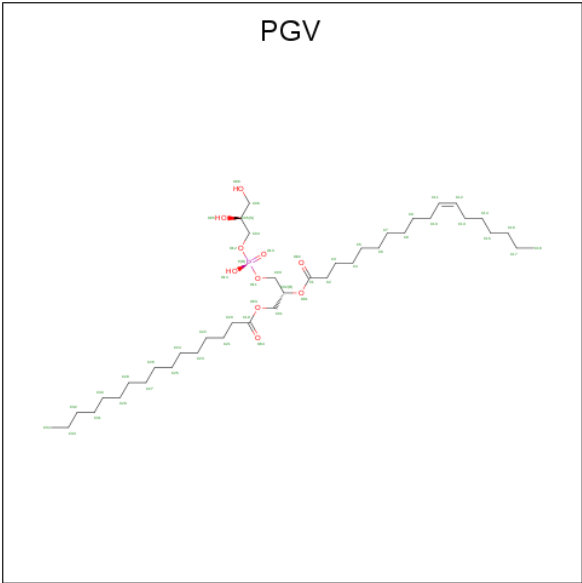
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

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

- Molecule 18 is (1R)-2-{{[[(2S)-2,3-DIHYDROXYPROPYL|OXY}(HYDROXY)PHOSPHORYL|OXY]}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C<sub>40</sub>H<sub>77</sub>O<sub>10</sub>P).



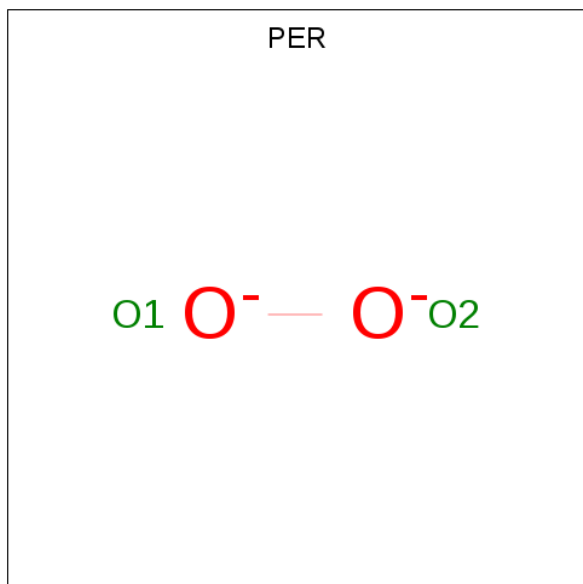
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total C O P 51 40 10 1	0	0
18	A	1	Total C O P 51 40 10 1	0	0
18	C	1	Total C O P 51 40 10 1	0	0
18	C	1	Total C O P 51 40 10 1	0	0
18	N	1	Total C O P 51 40 10 1	0	0
18	N	1	Total C O P 51 40 10 1	0	0
18	P	1	Total C O P 51 40 10 1	0	0

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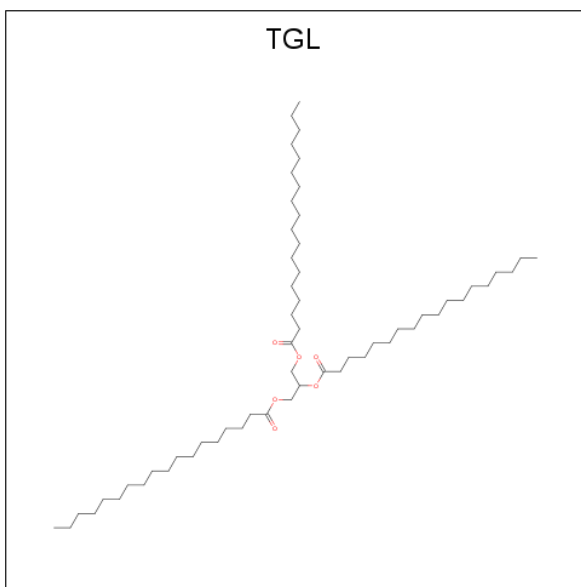
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	P	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 19 is PEROXIDE ION (three-letter code: PER) (formula: O<sub>2</sub>).



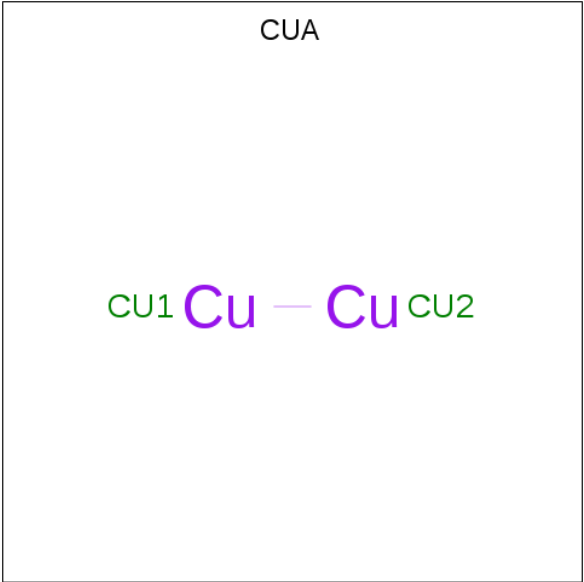
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	1	Total	O	0	1
			4	4		
19	N	1	Total	O	0	1
			4	4		

- Molecule 20 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C<sub>57</sub>H<sub>110</sub>O<sub>6</sub>).



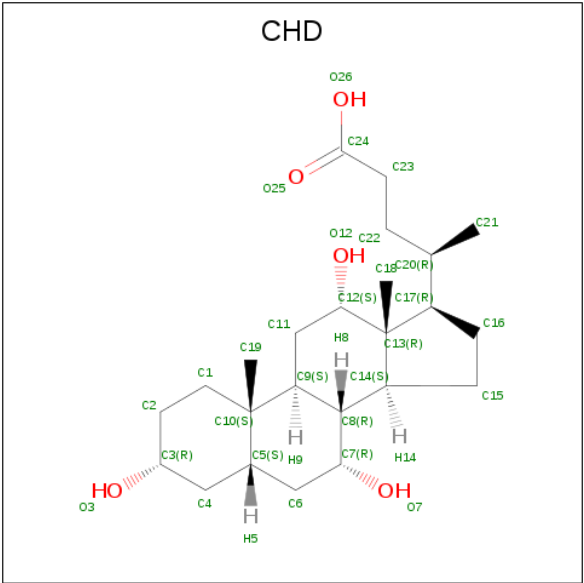
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	B	1	Total	C	O	0	0
			63	57	6		
20	D	1	Total	C	O	0	0
			63	57	6		
20	L	1	Total	C	O	0	0
			63	57	6		
20	N	1	Total	C	O	0	0
			63	57	6		
20	N	1	Total	C	O	0	0
			63	57	6		
20	Q	1	Total	C	O	0	0
			63	57	6		

- Molecule 21 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu<sub>2</sub>).



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

- Molecule 22 is CHOLIC ACID (three-letter code: CHD) (formula: C<sub>24</sub>H<sub>40</sub>O<sub>5</sub>).



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

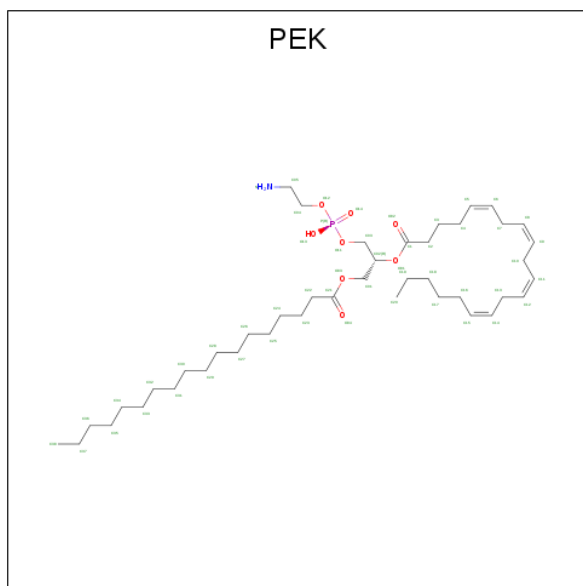
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	C	1	Total	C	O	0	0
			29	24	5		
22	J	1	Total	C	O	0	0
			29	24	5		
22	N	1	Total	C	O	0	0
			29	24	5		
22	O	1	Total	C	O	0	0
			29	24	5		
22	P	1	Total	C	O	0	0
			29	24	5		
22	W	1	Total	C	O	0	0
			29	24	5		

- Molecule 23 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).



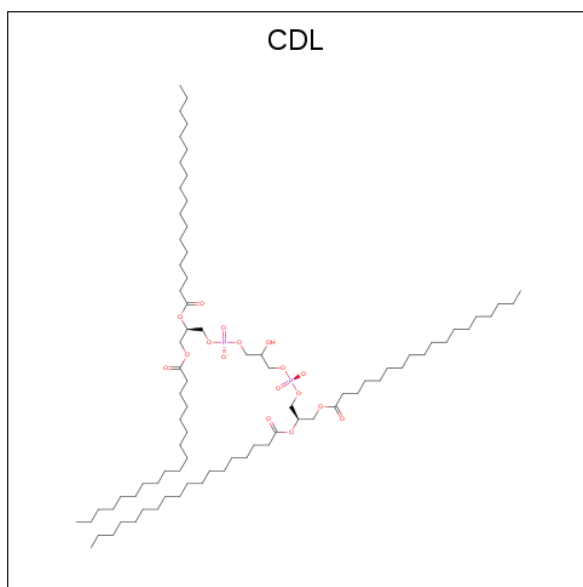
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

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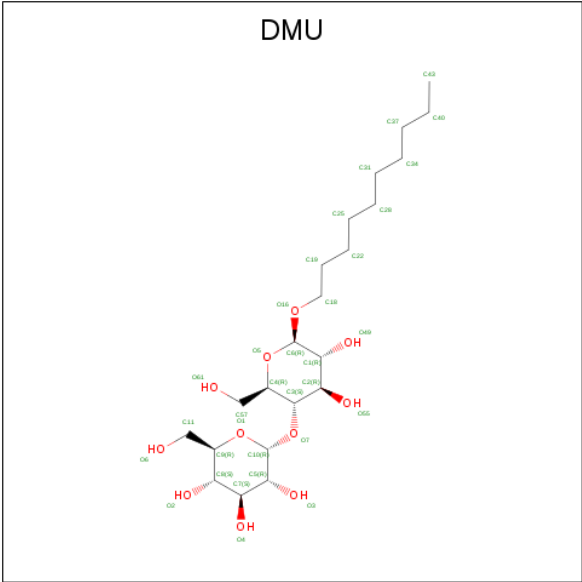
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 24 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



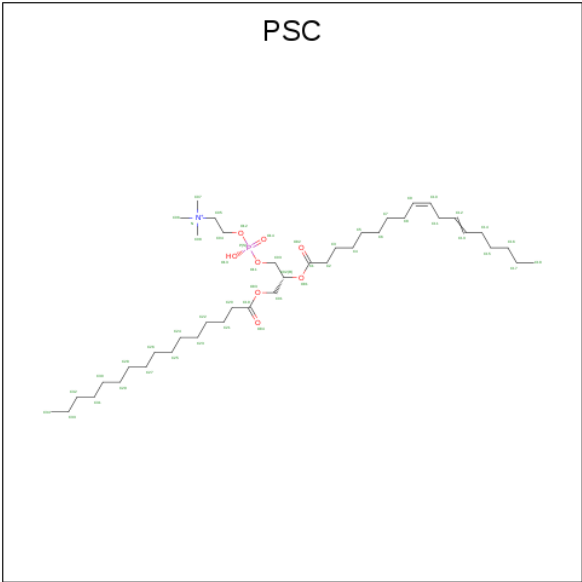
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	C	1	Total	C	O	P		0	0
			100	81	17	2			
24	G	1	Total	C	O	P		0	0
			100	81	17	2			
24	P	1	Total	C	O	P		0	0
			100	81	17	2			
24	T	1	Total	C	O	P		0	0
			100	81	17	2			

- Molecule 25 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula:  $C_{22}H_{42}O_{11}$ ).



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

- Molecule 26 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
26	E	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
26	R	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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

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

- Molecule 28 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	270	Total	O	0	0
			270	270		
28	B	206	Total	O	0	0
			206	206		
28	C	145	Total	O	0	0
			145	145		
28	D	167	Total	O	0	0
			167	167		
28	E	113	Total	O	0	0
			113	113		
28	F	137	Total	O	0	0
			137	137		
28	G	77	Total	O	0	0
			77	77		
28	H	83	Total	O	0	0
			83	83		
28	I	50	Total	O	0	0
			50	50		
28	J	42	Total	O	0	0
			42	42		
28	K	44	Total	O	0	0
			44	44		
28	L	36	Total	O	0	0
			36	36		
28	M	28	Total	O	0	0
			28	28		
28	N	266	Total	O	0	0
			266	266		

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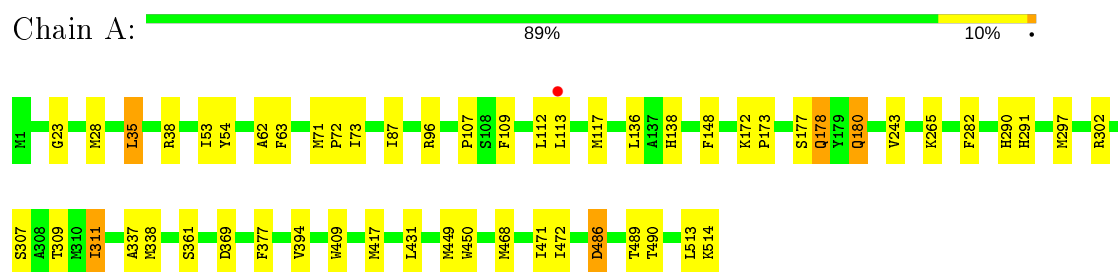
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	O	168	Total 168	O 168	0	0
28	P	138	Total 138	O 138	0	0
28	Q	84	Total 84	O 84	0	0
28	R	91	Total 91	O 91	0	0
28	S	126	Total 126	O 126	0	0
28	T	62	Total 62	O 62	0	0
28	U	68	Total 68	O 68	0	0
28	V	41	Total 41	O 41	0	0
28	W	44	Total 44	O 44	0	0
28	X	28	Total 28	O 28	0	0
28	Y	24	Total 24	O 24	0	0
28	Z	20	Total 20	O 20	0	0

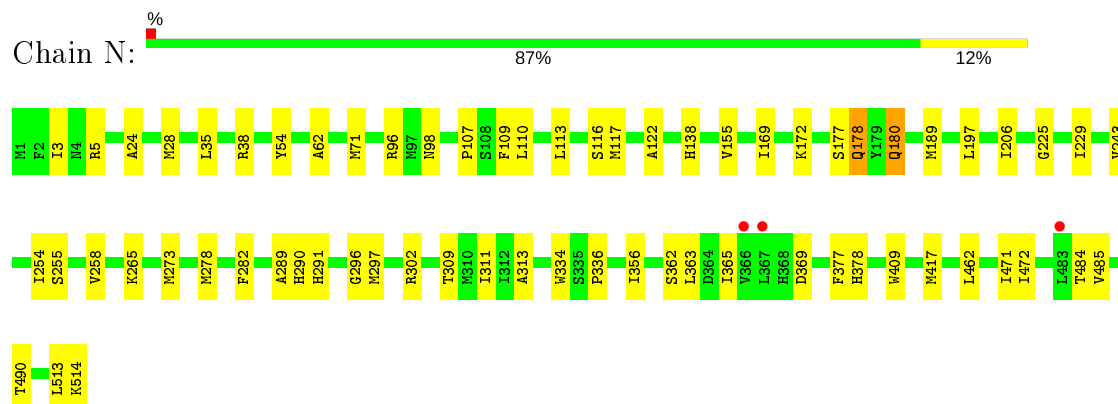
### 3 Residue-property plots [i](#)

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

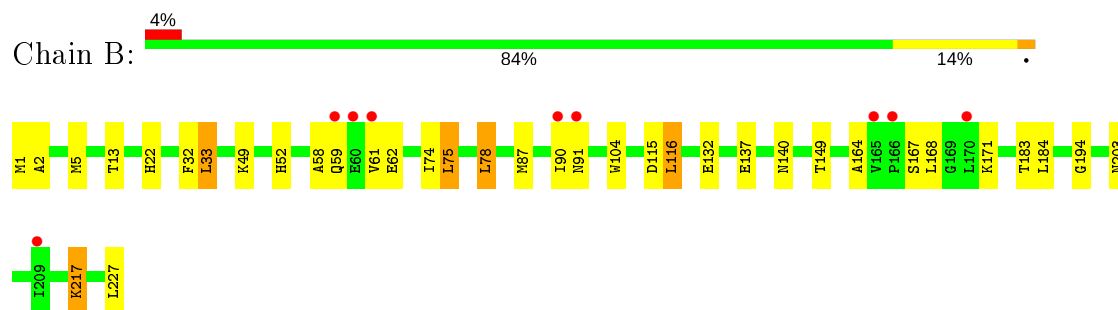
- Molecule 1: Cytochrome c oxidase subunit 1



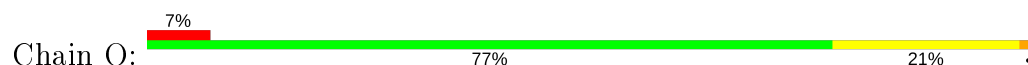
- Molecule 1: Cytochrome c oxidase subunit 1



- Molecule 2: Cytochrome c oxidase subunit 2



- Molecule 2: Cytochrome c oxidase subunit 2



- Molecule 3: Cytochrome c oxidase subunit 3

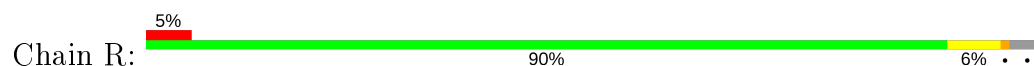
- Molecule 3: Cytochrome c oxidase subunit 3

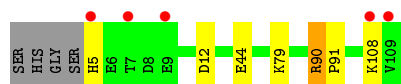
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

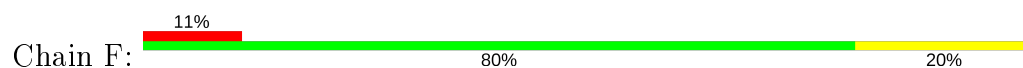
- Molecule 5: Cytochrome c oxidase subunit 5A

- Molecule 5: Cytochrome c oxidase subunit 5A

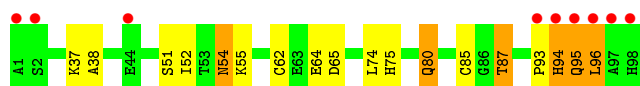
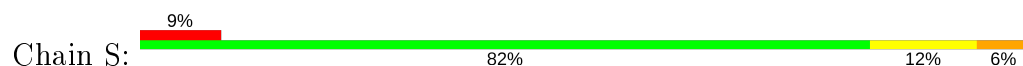




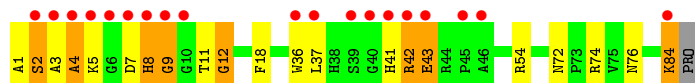
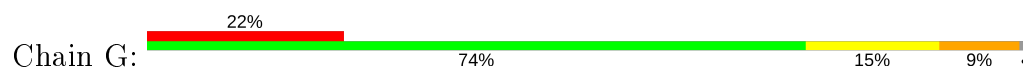
- Molecule 6: Cytochrome c oxidase subunit 5B



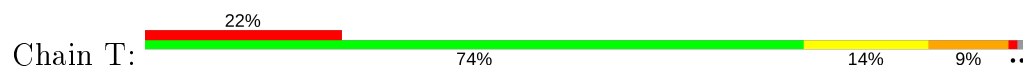
- Molecule 6: Cytochrome c oxidase subunit 5B



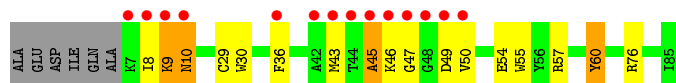
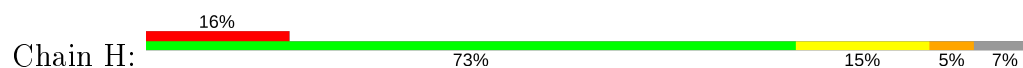
- Molecule 7: Cytochrome c oxidase subunit 6A2



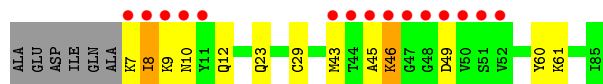
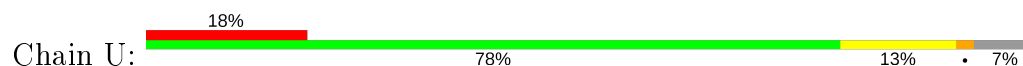
- Molecule 7: Cytochrome c oxidase subunit 6A2



- Molecule 8: Cytochrome c oxidase subunit 6B1

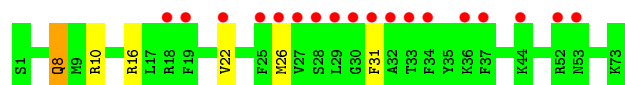
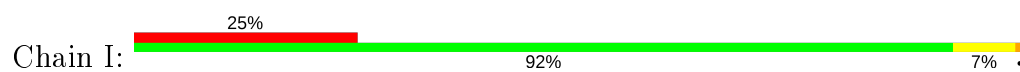


- Molecule 8: Cytochrome c oxidase subunit 6B1

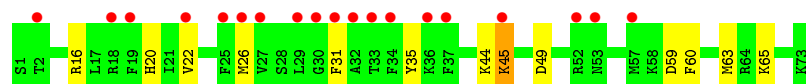
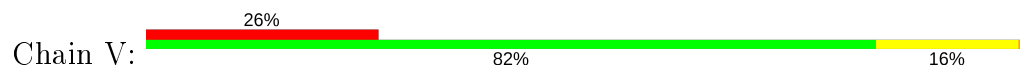


- Molecule 9: Cytochrome c oxidase subunit 6C

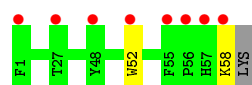
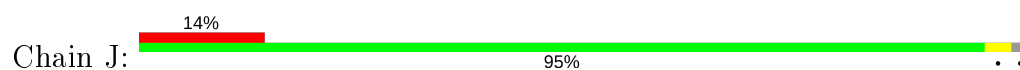




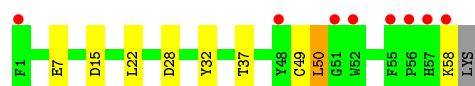
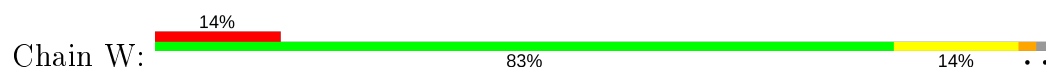
- Molecule 9: Cytochrome c oxidase subunit 6C



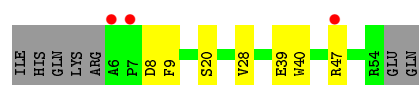
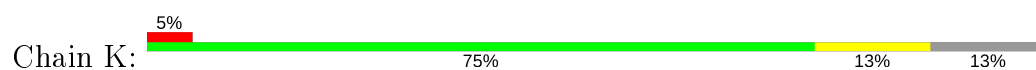
- Molecule 10: Cytochrome c oxidase subunit 7A1



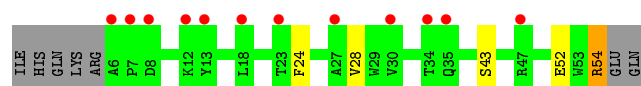
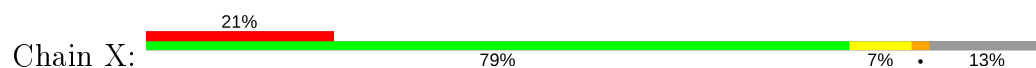
- Molecule 10: Cytochrome c oxidase subunit 7A1



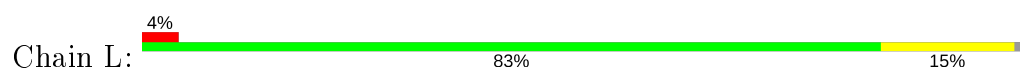
- Molecule 11: Cytochrome c oxidase subunit 7B




- Molecule 11: Cytochrome c oxidase subunit 7B

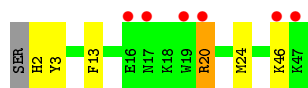


- Molecule 12: Cytochrome c oxidase subunit 7C




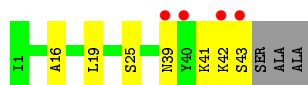
## • Molecule 12: Cytochrome c oxidase subunit 7C

Chain Y:  13% 85% 11% ..




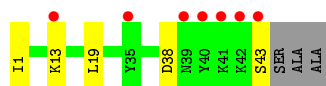
## • Molecule 13: Cytochrome c oxidase subunit 8B

Chain M:  9% 78% 15% 7%



## • Molecule 13: Cytochrome c oxidase subunit 8B

Chain Z:  15% 83% 11% 7%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	182.02Å 203.54Å 177.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.90 36.37 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.0 (40.00-1.90) 98.1 (36.37-1.90)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.78 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.8.0048	Depositor
R, $R_{free}$	0.172 , 0.199 0.174 , 0.225	Depositor DCC
$R_{free}$ test set	33115 reflections (6.58%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.9	Xtriage
Anisotropy	0.649	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 69.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.008 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	33893	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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: ZN, TPO, CHD, TGL, CDL, PSC, PEK, MG, PER, PGV, SAC, DMU, CUA, NA, FME, CU, HEA

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	0.83	0/4253	0.78	3/5805 (0.1%)
1	N	0.77	0/4252	0.76	3/5804 (0.1%)
2	B	0.74	0/1906	0.82	1/2595 (0.0%)
2	O	0.63	0/1908	0.78	1/2599 (0.0%)
3	C	0.75	0/2261	0.68	0/3090
3	P	0.72	0/2260	0.67	0/3088
4	D	0.66	0/1284	0.80	3/1730 (0.2%)
4	Q	0.52	0/1237	0.66	0/1668
5	E	0.65	0/882	0.66	0/1196
5	R	0.55	0/871	0.68	1/1182 (0.1%)
6	F	0.67	0/806	0.80	0/1093
6	S	0.69	0/772	0.79	1/1048 (0.1%)
7	G	0.72	0/702	0.77	1/953 (0.1%)
7	T	0.67	0/724	0.85	3/984 (0.3%)
8	H	0.66	0/682	0.70	0/921
8	U	0.63	0/682	0.67	0/921
9	I	0.62	0/605	0.69	0/802
9	V	0.53	0/613	0.66	0/812
10	J	0.54	0/471	0.61	0/636
10	W	0.55	0/471	0.66	0/636
11	K	0.65	0/405	0.66	0/556
11	X	0.53	0/405	0.55	0/556
12	L	0.73	0/393	0.69	0/526
12	Y	0.65	0/393	0.60	0/526
13	M	0.64	0/345	0.67	0/470
13	Z	0.60	0/345	0.61	0/470
All	All	0.70	0/29928	0.73	17/40667 (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
6	F	0	1
6	S	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	20	ARG	NE-CZ-NH2	-12.07	114.27	120.30
4	D	20	ARG	NE-CZ-NH1	10.37	125.49	120.30
7	T	17	ARG	NE-CZ-NH2	-10.02	115.29	120.30
1	A	35	LEU	CA-CB-CG	-9.63	93.15	115.30
1	A	96	ARG	NE-CZ-NH2	-7.36	116.62	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	F	93	PRO	Peptide
6	S	93	PRO	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	4124	0	4102	57	0
1	N	4123	0	4098	74	0
2	B	1868	0	1864	27	0
2	O	1870	0	1867	37	0
3	C	2174	0	2082	32	0
3	P	2173	0	2083	30	0
4	D	1249	0	1242	27	1
4	Q	1203	0	1191	10	0
5	E	863	0	857	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	R	852	0	845	3	0
6	F	789	0	769	22	0
6	S	755	0	734	17	0
7	G	686	0	651	32	0
7	T	706	0	664	27	0
8	H	662	0	623	15	0
8	U	662	0	623	13	0
9	I	601	0	613	7	0
9	V	609	0	621	12	0
10	J	460	0	459	2	0
10	W	460	0	459	8	0
11	K	391	0	374	7	0
11	X	391	0	374	6	0
12	L	380	0	380	8	0
12	Y	380	0	380	9	0
13	M	335	0	352	9	0
13	Z	335	0	352	2	0
14	A	120	0	108	14	0
14	N	120	0	108	14	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	C	1	0	0	0	0
17	N	1	0	0	0	0
17	P	1	0	0	0	0
18	A	102	0	152	16	0
18	C	102	0	152	3	0
18	N	102	0	152	8	0
18	P	102	0	152	8	0
19	A	4	0	0	3	0
19	N	4	0	0	2	0
20	B	63	0	110	1	0
20	D	63	0	110	11	0
20	L	63	0	110	11	0
20	N	126	0	220	10	0
20	Q	63	0	110	6	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	29	0	39	1	0
22	C	58	0	78	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	J	29	0	38	0	0
22	N	29	0	39	1	0
22	O	29	0	39	1	0
22	P	29	0	39	1	0
22	W	29	0	39	5	0
23	C	106	0	154	21	0
23	G	53	0	77	7	0
23	P	53	0	77	11	0
23	T	106	0	154	8	0
24	C	100	0	156	13	0
24	G	100	0	156	17	0
24	P	100	0	156	10	0
24	T	100	0	156	20	0
25	C	33	0	42	6	0
25	M	33	0	42	0	0
25	P	33	0	42	4	0
25	Z	33	0	42	1	0
26	E	52	0	80	7	0
26	R	52	0	80	6	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	A	270	0	0	9	0
28	B	206	0	0	13	2
28	C	145	0	0	4	0
28	D	167	0	0	10	1
28	E	113	0	0	1	0
28	F	137	0	0	6	0
28	G	77	0	0	3	0
28	H	83	0	0	2	0
28	I	50	0	0	0	0
28	J	42	0	0	0	0
28	K	44	0	0	2	0
28	L	36	0	0	0	0
28	M	28	0	0	0	0
28	N	266	0	0	16	0
28	O	168	0	0	4	0
28	P	138	0	0	8	0
28	Q	84	0	0	0	0
28	R	91	0	0	2	0
28	S	126	0	0	1	0
28	T	62	0	0	2	0
28	U	68	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	V	41	0	0	1	0
28	W	44	0	0	2	0
28	X	28	0	0	0	0
28	Y	24	0	0	1	0
28	Z	20	0	0	0	0
All	All	33893	0	31868	544	2

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 9.

The worst 5 of 544 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)
4:D:4:SER:HB3	28:D:389:HOH:O	1.32	1.26
23:P:302:PEK:H383	24:T:103:CDL:C27	1.65	1.25
6:F:53:THR:HB	28:F:201:HOH:O	1.14	1.24
19:N:607[B]:PER:O2	19:N:607[B]:PER:O1	1.55	1.23
19:N:607[A]:PER:O2	19:N:607[A]:PER:O1	1.55	1.22

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:31:LYS:CE	28:B:402:HOH:O[2_585]	2.12	0.08
28:B:482:HOH:O	28:D:361:HOH:O[2_584]	2.19	0.01

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	524/514 (102%)	510 (97%)	14 (3%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	524/514 (102%)	511 (98%)	13 (2%)	0	100	100
2	B	230/227 (101%)	223 (97%)	7 (3%)	0	100	100
2	O	230/227 (101%)	221 (96%)	9 (4%)	0	100	100
3	C	265/261 (102%)	261 (98%)	4 (2%)	0	100	100
3	P	265/261 (102%)	260 (98%)	5 (2%)	0	100	100
4	D	148/147 (101%)	144 (97%)	4 (3%)	0	100	100
4	Q	143/147 (97%)	138 (96%)	5 (4%)	0	100	100
5	E	104/109 (95%)	104 (100%)	0	0	100	100
5	R	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
6	F	101/98 (103%)	94 (93%)	3 (3%)	4 (4%)	3	0
6	S	97/98 (99%)	91 (94%)	6 (6%)	0	100	100
7	G	82/85 (96%)	71 (87%)	8 (10%)	3 (4%)	3	0
7	T	84/85 (99%)	73 (87%)	8 (10%)	3 (4%)	3	0
8	H	77/85 (91%)	73 (95%)	1 (1%)	3 (4%)	3	0
8	U	77/85 (91%)	69 (90%)	5 (6%)	3 (4%)	3	0
9	I	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
9	V	72/73 (99%)	70 (97%)	2 (3%)	0	100	100
10	J	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
10	W	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
11	K	48/56 (86%)	47 (98%)	1 (2%)	0	100	100
11	X	48/56 (86%)	46 (96%)	2 (4%)	0	100	100
12	L	44/47 (94%)	41 (93%)	3 (7%)	0	100	100
12	Y	44/47 (94%)	41 (93%)	2 (4%)	1 (2%)	6	1
13	M	41/46 (89%)	39 (95%)	1 (2%)	1 (2%)	6	1
13	Z	41/46 (89%)	39 (95%)	2 (5%)	0	100	100
All	All	3575/3614 (99%)	3448 (96%)	109 (3%)	18 (0%)	29	18

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	94	HIS
7	G	4	ALA
7	T	4	ALA

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Mol	Chain	Res	Type
8	U	8	ILE
8	U	45	ALA

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	438/426 (103%)	428 (98%)	10 (2%)	50	45
1	N	438/426 (103%)	427 (98%)	11 (2%)	47	41
2	B	215/210 (102%)	208 (97%)	7 (3%)	38	29
2	O	215/210 (102%)	203 (94%)	12 (6%)	21	11
3	C	232/226 (103%)	229 (99%)	3 (1%)	69	68
3	P	232/226 (103%)	229 (99%)	3 (1%)	69	68
4	D	134/129 (104%)	133 (99%)	1 (1%)	84	84
4	Q	129/129 (100%)	123 (95%)	6 (5%)	26	16
5	E	93/95 (98%)	91 (98%)	2 (2%)	52	47
5	R	92/95 (97%)	90 (98%)	2 (2%)	52	47
6	F	86/81 (106%)	85 (99%)	1 (1%)	71	70
6	S	82/81 (101%)	75 (92%)	7 (8%)	10	4
7	G	68/68 (100%)	59 (87%)	9 (13%)	4	1
7	T	70/68 (103%)	60 (86%)	10 (14%)	3	1
8	H	71/75 (95%)	67 (94%)	4 (6%)	21	11
8	U	71/75 (95%)	69 (97%)	2 (3%)	43	36
9	I	57/57 (100%)	56 (98%)	1 (2%)	59	55
9	V	58/57 (102%)	57 (98%)	1 (2%)	60	57
10	J	49/50 (98%)	48 (98%)	1 (2%)	55	51
10	W	49/50 (98%)	47 (96%)	2 (4%)	30	21
11	K	40/46 (87%)	40 (100%)	0	100	100
11	X	40/46 (87%)	38 (95%)	2 (5%)	24	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	39/40 (98%)	38 (97%)	1 (3%)	46	39
12	Y	39/40 (98%)	38 (97%)	1 (3%)	46	39
13	M	37/38 (97%)	36 (97%)	1 (3%)	44	38
13	Z	37/38 (97%)	34 (92%)	3 (8%)	11	4
All	All	3111/3082 (101%)	3008 (97%)	103 (3%)	39	29

5 of 103 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	180	GLN
2	O	94	SER
10	W	50	LEU
1	N	336	PRO
2	O	33	LEU

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

Mol	Chain	Res	Type
1	N	180	GLN
3	P	50	ASN
9	V	20	HIS
1	N	512	ASN
2	O	181	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FME	O	1	2	8,9,10	0.77	0	7,9,11	1.50	1 (14%)
7	TPO	G	11	7	8,10,11	1.52	1 (12%)	10,14,16	1.12	1 (10%)
9	SAC	V	1	9	7,8,9	1.25	1 (14%)	8,9,11	1.76	1 (12%)
9	SAC	I	1	9	7,8,9	1.52	1 (14%)	8,9,11	1.71	2 (25%)
1	FME	A	1	1	8,9,10	0.64	0	7,9,11	1.54	2 (28%)
7	TPO	T	11	7	8,10,11	1.50	1 (12%)	10,14,16	0.81	0
2	FME	B	1	2	8,9,10	1.75	1 (12%)	7,9,11	6.65	3 (42%)
1	FME	N	1	1	8,9,10	0.65	0	7,9,11	1.40	2 (28%)

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
2	FME	O	1	2	-	0/7/9/11	-
7	TPO	G	11	7	-	5/9/11/13	-
9	SAC	V	1	9	-	2/7/8/10	-
9	SAC	I	1	9	-	4/7/8/10	-
1	FME	A	1	1	-	3/7/9/11	-
7	TPO	T	11	7	-	6/9/11/13	-
2	FME	B	1	2	-	1/7/9/11	-
1	FME	N	1	1	-	1/7/9/11	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	O1-CN	-4.41	1.09	1.22
9	I	1	SAC	CA-N	3.95	1.51	1.46
9	V	1	SAC	CA-N	3.08	1.50	1.46
7	T	11	TPO	P-O1P	2.88	1.59	1.50
7	G	11	TPO	P-O1P	2.86	1.59	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CA-N-CN	-17.25	96.30	122.82
9	V	1	SAC	C-CA-N	4.13	117.19	109.73
9	I	1	SAC	C-CA-N	3.35	115.78	109.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	1	FME	CG-CB-CA	-2.58	105.79	112.95
1	A	1	FME	C-CA-N	2.50	114.25	109.73

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	G	11	TPO	N-CA-CB-CG2
7	G	11	TPO	N-CA-CB-OG1
7	G	11	TPO	C-CA-CB-CG2
7	G	11	TPO	O-C-CA-CB
7	G	11	TPO	CA-CB-OG1-P

There are no ring outliers.

4 monomers are involved in 4 short contacts:

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 58 ligands modelled in this entry, 10 are monoatomic - leaving 48 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
19	PER	A	607[A]	15,14	0,1,1	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CHD	P	306	-	29,32,32	0.53	0	48,51,51	1.56	10 (20%)
20	TGL	B	301	-	62,62,62	1.12	3 (4%)	65,65,65	1.48	7 (10%)
18	PGV	P	304	-	50,50,50	1.15	2 (4%)	53,56,56	1.03	3 (5%)
19	PER	A	607[B]	15	0,1,1	0.00	-	-		
18	PGV	N	606	-	50,50,50	1.00	2 (4%)	53,56,56	1.36	7 (13%)
18	PGV	C	305	-	50,50,50	1.08	2 (4%)	53,56,56	0.95	3 (5%)
22	CHD	C	307	-	29,32,32	0.55	0	48,51,51	2.27	18 (37%)
26	PSC	R	201	-	51,51,51	1.19	3 (5%)	57,59,59	1.02	2 (3%)
14	HEA	A	601	1	44,67,67	0.95	3 (6%)	37,103,103	2.42	16 (43%)
25	DMU	Z	101	-	34,34,34	0.50	0	45,45,45	0.85	1 (2%)
24	CDL	G	101	-	99,99,99	1.39	12 (12%)	105,111,111	1.20	6 (5%)
19	PER	N	607[A]	15,14	0,1,1	0.00	-	-		
18	PGV	A	606	-	50,50,50	0.95	2 (4%)	53,56,56	1.37	7 (13%)
23	PEK	T	102	-	52,52,52	0.91	3 (5%)	55,57,57	1.30	6 (10%)
22	CHD	N	610	-	29,32,32	0.84	0	48,51,51	1.14	3 (6%)
23	PEK	C	303	-	52,52,52	1.06	2 (3%)	55,57,57	1.00	5 (9%)
20	TGL	Q	201	-	62,62,62	1.16	3 (4%)	65,65,65	0.88	4 (6%)
23	PEK	T	101	-	52,52,52	1.07	2 (3%)	55,57,57	0.95	3 (5%)
19	PER	N	607[B]	15	0,1,1	0.00	-	-		
24	CDL	C	306	-	99,99,99	1.32	12 (12%)	105,111,111	1.25	10 (9%)
14	HEA	N	601	1	44,67,67	1.09	5 (11%)	37,103,103	1.88	15 (40%)
21	CUA	B	302	2	0,1,1	0.00	-	-		
14	HEA	N	602	1,19	44,67,67	0.90	0	37,103,103	1.71	11 (29%)
24	CDL	T	103	-	99,99,99	1.33	12 (12%)	105,111,111	1.20	7 (6%)
20	TGL	N	611	-	62,62,62	1.16	3 (4%)	65,65,65	1.24	4 (6%)
14	HEA	A	602	1,19	44,67,67	1.05	2 (4%)	37,103,103	2.06	12 (32%)
23	PEK	C	302	-	52,52,52	0.85	2 (3%)	55,57,57	0.90	3 (5%)
22	CHD	C	308	-	29,32,32	0.94	1 (3%)	48,51,51	1.29	6 (12%)
22	CHD	W	101	-	29,32,32	0.55	0	48,51,51	2.38	20 (41%)
21	CUA	O	302	2	0,1,1	0.00	-	-		
18	PGV	C	304	-	50,50,50	0.83	2 (4%)	53,56,56	0.97	2 (3%)
20	TGL	N	608	-	62,62,62	1.10	3 (4%)	65,65,65	1.13	4 (6%)
25	DMU	P	307	-	34,34,34	0.74	1 (2%)	45,45,45	0.97	2 (4%)
26	PSC	E	201	-	51,51,51	1.17	3 (5%)	57,59,59	0.94	2 (3%)
22	CHD	B	303	-	29,32,32	1.00	2 (6%)	48,51,51	1.24	4 (8%)
18	PGV	P	303	-	50,50,50	0.90	3 (6%)	53,56,56	0.82	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CHD	J	101	-	29,32,32	0.49	0	48,51,51	2.01	14 (29%)
20	TGL	D	201	-	62,62,62	1.12	4 (6%)	65,65,65	0.84	4 (6%)
25	DMU	C	309	-	34,34,34	0.61	0	45,45,45	1.21	4 (8%)
23	PEK	G	102	-	52,52,52	1.04	2 (3%)	55,57,57	1.09	3 (5%)
18	PGV	A	608	-	50,50,50	0.93	2 (4%)	53,56,56	1.22	4 (7%)
20	TGL	L	101	-	62,62,62	1.17	3 (4%)	65,65,65	1.47	9 (13%)
25	DMU	M	101	-	34,34,34	0.50	0	45,45,45	1.13	3 (6%)
22	CHD	O	301	-	29,32,32	0.88	0	48,51,51	1.53	9 (18%)
24	CDL	P	305	-	99,99,99	1.36	12 (12%)	105,111,111	1.28	8 (7%)
18	PGV	N	609	-	50,50,50	0.93	2 (4%)	53,56,56	1.26	5 (9%)
23	PEK	P	302	-	52,52,52	1.07	2 (3%)	55,57,57	1.05	3 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CHD	P	306	-	-	2/7/74/74	0/4/4/4
20	TGL	B	301	-	-	36/65/65/65	-
18	PGV	P	304	-	-	28/55/55/55	-
14	HEA	N	601	1	3/3/7/16	2/24/76/76	-
18	PGV	N	606	-	-	36/55/55/55	-
18	PGV	C	305	-	-	30/55/55/55	-
22	CHD	C	307	-	-	5/7/74/74	0/4/4/4
26	PSC	R	201	-	-	22/55/55/55	-
14	HEA	A	601	1	2/2/7/16	3/24/76/76	-
25	DMU	Z	101	-	-	5/19/59/59	0/2/2/2
24	CDL	G	101	-	-	68/110/110/110	-
18	PGV	A	606	-	-	32/55/55/55	-
23	PEK	T	102	-	-	20/56/56/56	-
22	CHD	N	610	-	-	0/7/74/74	0/4/4/4
23	PEK	C	303	-	-	32/56/56/56	-
20	TGL	Q	201	-	-	34/65/65/65	-
23	PEK	T	101	-	-	21/56/56/56	-
24	CDL	C	306	-	-	63/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CHD	O	301	-	-	0/7/74/74	0/4/4/4
14	HEA	N	602	1,19	2/2/7/16	1/24/76/76	-
24	CDL	T	103	-	-	60/110/110/110	-
20	TGL	N	611	-	-	30/65/65/65	-
14	HEA	A	602	1,19	2/2/7/16	1/24/76/76	-
23	PEK	C	302	-	-	15/56/56/56	-
22	CHD	C	308	-	-	0/7/74/74	0/4/4/4
22	CHD	W	101	-	-	6/7/74/74	1/4/4/4
18	PGV	C	304	-	-	15/55/55/55	-
20	TGL	N	608	-	-	38/65/65/65	-
25	DMU	P	307	-	-	8/19/59/59	0/2/2/2
26	PSC	E	201	-	-	24/55/55/55	-
22	CHD	B	303	-	-	0/7/74/74	0/4/4/4
18	PGV	P	303	-	-	13/55/55/55	-
22	CHD	J	101	-	-	3/7/74/74	0/4/4/4
20	TGL	D	201	-	-	41/65/65/65	-
25	DMU	C	309	-	-	9/19/59/59	0/2/2/2
23	PEK	G	102	-	-	31/56/56/56	-
18	PGV	A	608	-	-	6/55/55/55	-
20	TGL	L	101	-	-	37/65/65/65	-
25	DMU	M	101	-	-	5/19/59/59	0/2/2/2
18	PGV	N	609	-	-	11/55/55/55	-
24	CDL	P	305	-	-	72/110/110/110	-
23	PEK	P	302	-	-	27/56/56/56	-

The worst 5 of 117 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	L	101	TGL	OG2-CB1	5.66	1.50	1.34
20	N	611	TGL	OG2-CB1	5.58	1.50	1.34
18	P	304	PGV	O03-C19	5.22	1.48	1.33
20	B	301	TGL	OG1-CA1	5.17	1.48	1.33
24	G	101	CDL	OB6-CB5	5.11	1.48	1.34

The worst 5 of 272 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	301	TGL	OG2-CB1-CB2	7.35	127.34	111.50
14	A	602	HEA	CAD-CBD-CGD	-6.46	101.83	112.67
22	C	307	CHD	C16-C17-C20	6.33	121.95	112.15
22	C	307	CHD	C14-C13-C12	6.16	113.13	107.40
22	J	101	CHD	C17-C13-C14	-5.92	94.13	100.09

5 of 9 chirality outliers are listed below:

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

5 of 892 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	P	304	PGV	C10-C11-C12-C13
18	N	606	PGV	C03-O11-P-O13
18	N	606	PGV	C03-O11-P-O14
18	N	606	PGV	C02-C03-O11-P
18	N	606	PGV	C04-C05-C06-O06

All (1) ring outliers are listed below:

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

43 monomers are involved in 223 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	607[A]	PER	1	0
22	P	306	CHD	1	0
20	B	301	TGL	1	0
18	P	304	PGV	4	0
19	A	607[B]	PER	2	0
18	N	606	PGV	6	0
18	C	305	PGV	1	0
22	C	307	CHD	1	0
26	R	201	PSC	6	0
14	A	601	HEA	9	0
25	Z	101	DMU	1	0

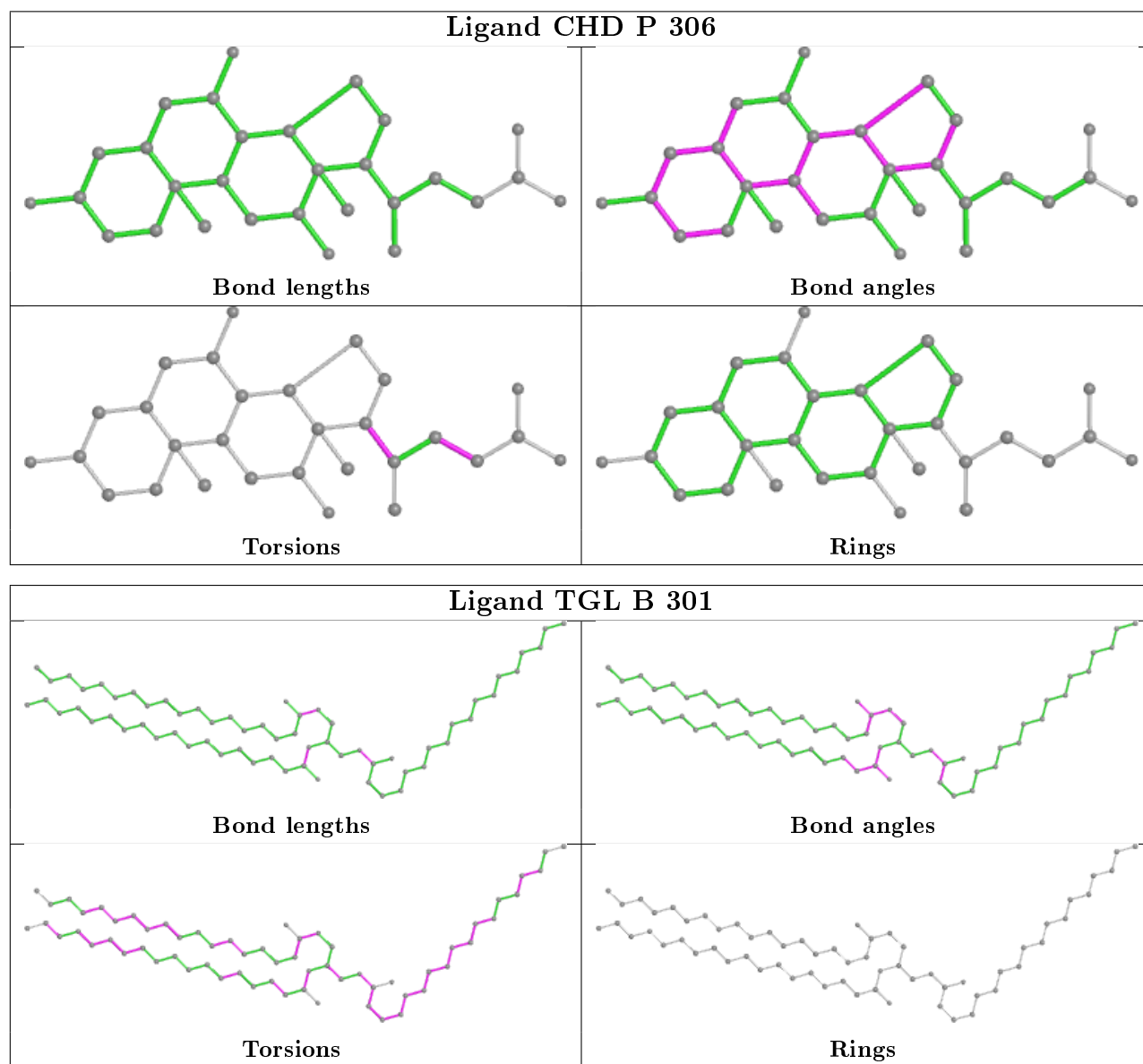
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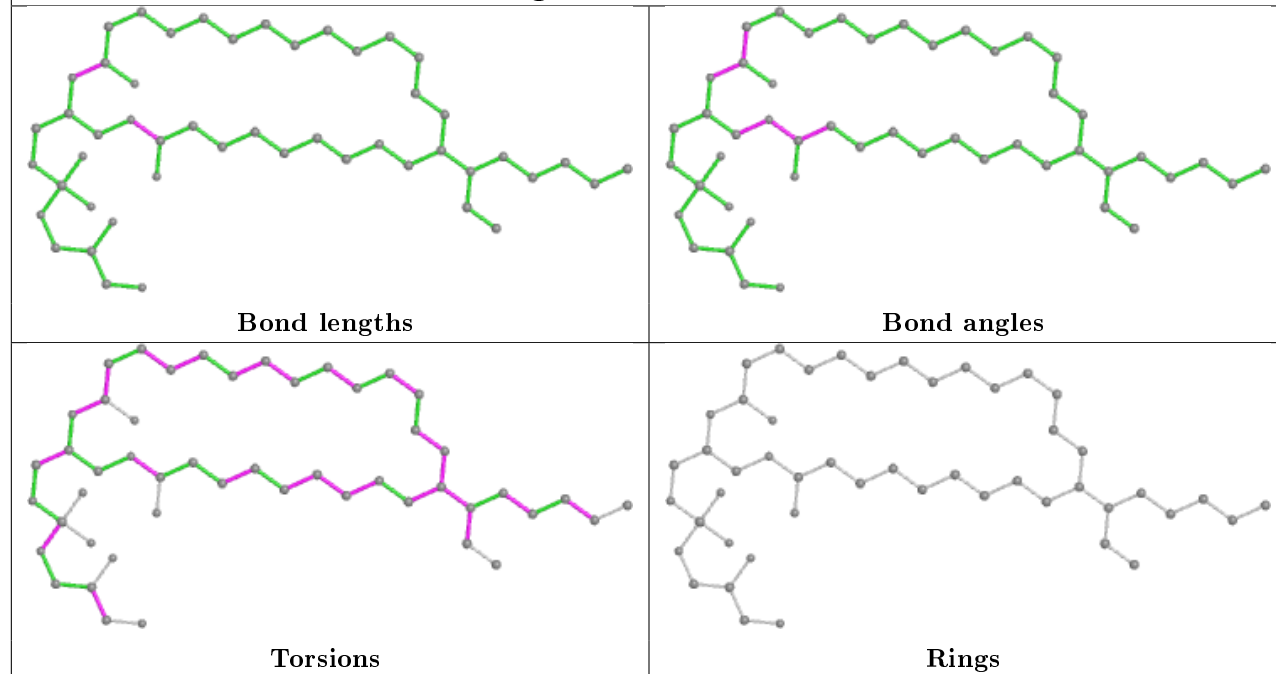
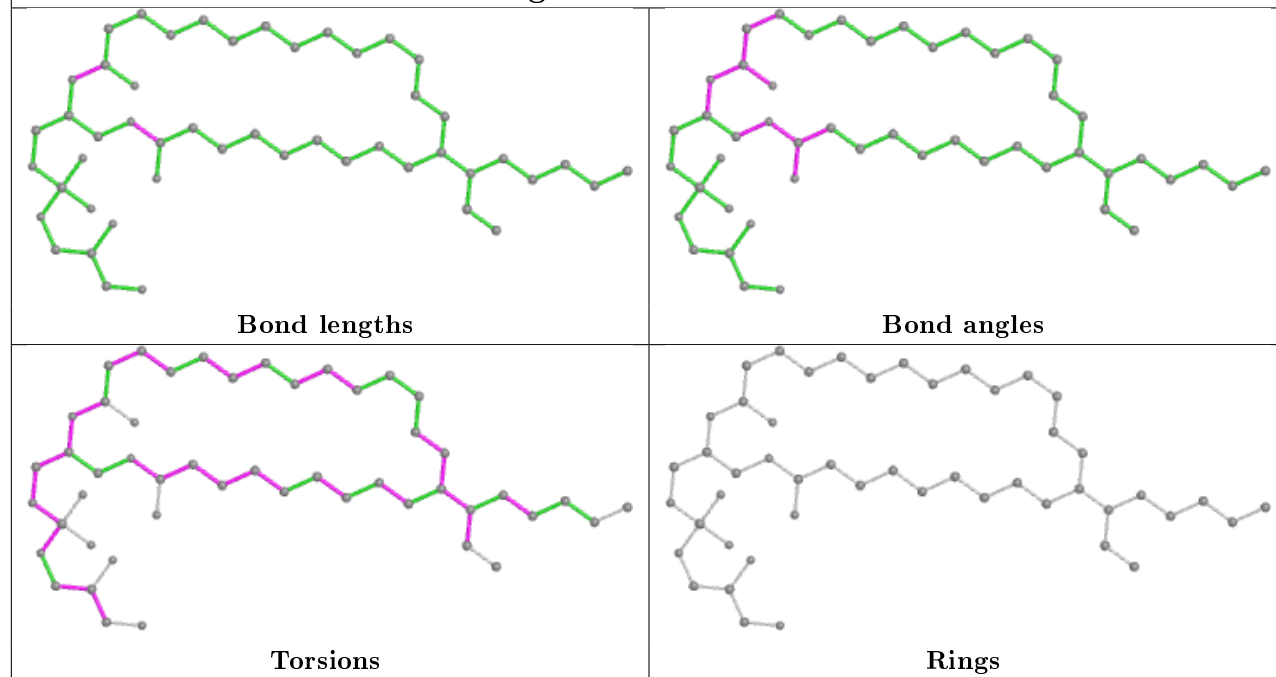
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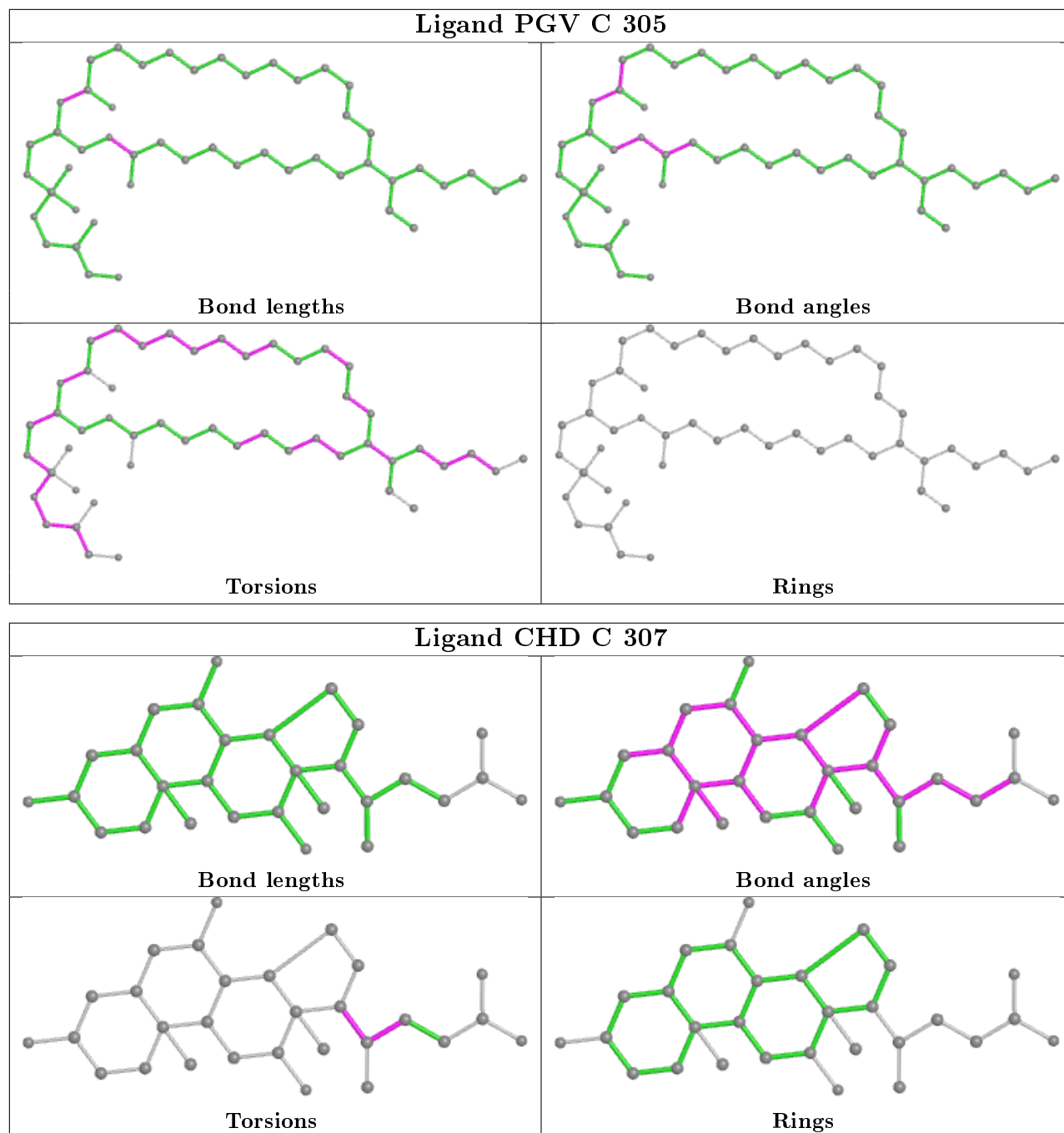
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	G	101	CDL	17	0
19	N	607[A]	PER	1	0
18	A	606	PGV	11	0
23	T	102	PEK	1	0
22	N	610	CHD	1	0
23	C	303	PEK	15	0
20	Q	201	TGL	6	0
23	T	101	PEK	7	0
19	N	607[B]	PER	1	0
24	C	306	CDL	13	0
14	N	601	HEA	9	0
14	N	602	HEA	5	0
24	T	103	CDL	20	0
20	N	611	TGL	7	0
14	A	602	HEA	5	0
23	C	302	PEK	6	0
22	W	101	CHD	5	0
18	C	304	PGV	2	0
20	N	608	TGL	3	0
25	P	307	DMU	4	0
26	E	201	PSC	7	0
22	B	303	CHD	1	0
18	P	303	PGV	4	0
20	D	201	TGL	11	0
25	C	309	DMU	6	0
23	G	102	PEK	7	0
18	A	608	PGV	5	0
20	L	101	TGL	11	0
22	O	301	CHD	1	0
24	P	305	CDL	10	0
18	N	609	PGV	2	0
23	P	302	PEK	11	0

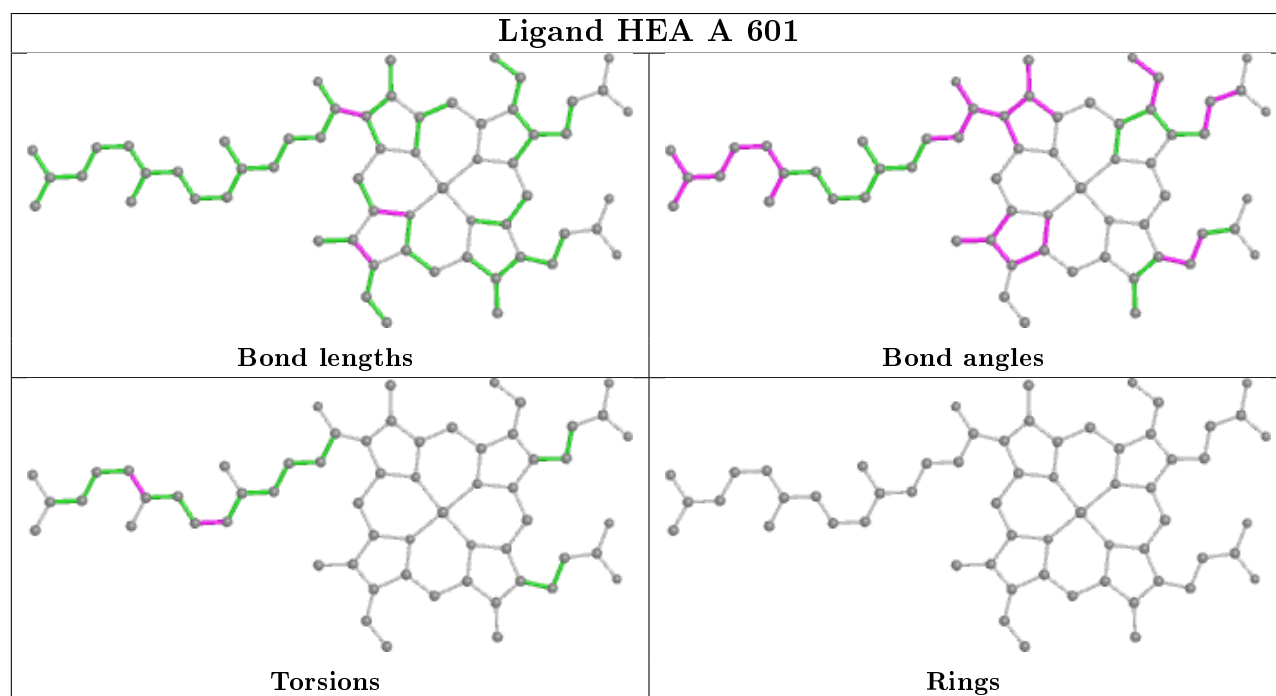
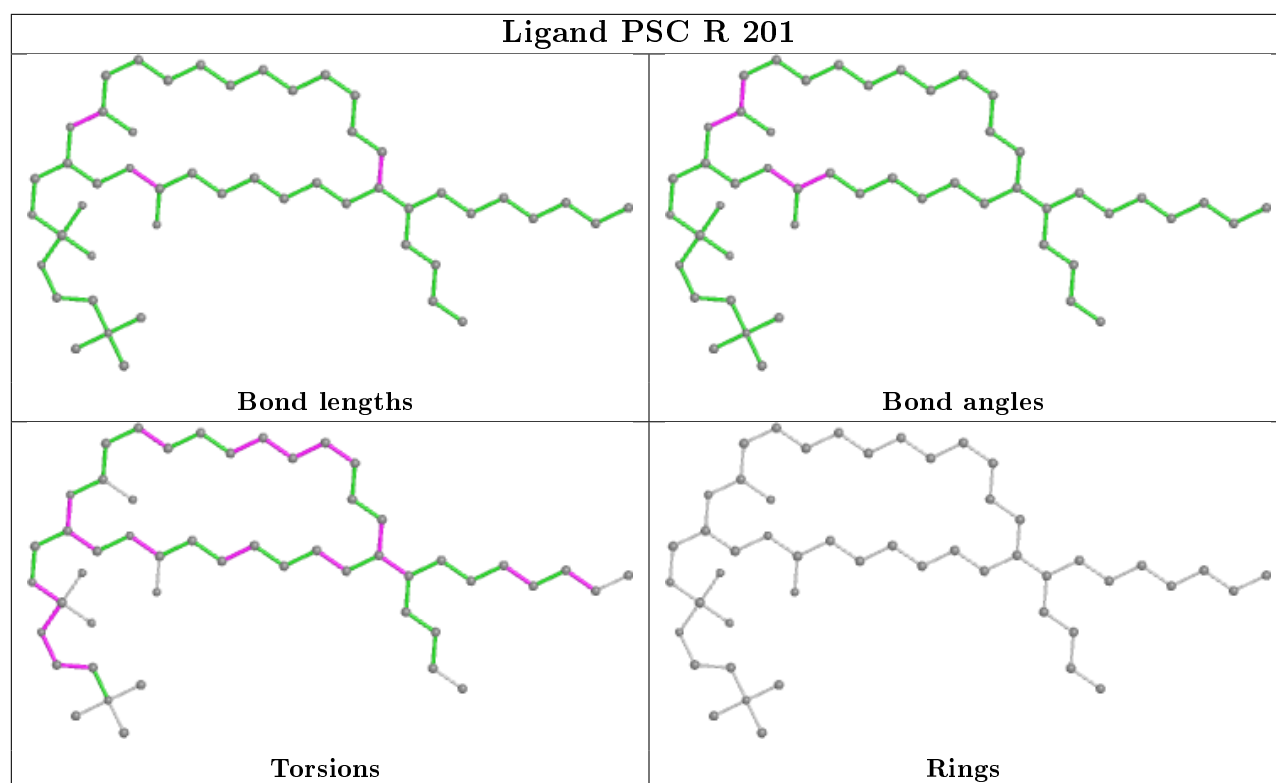
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

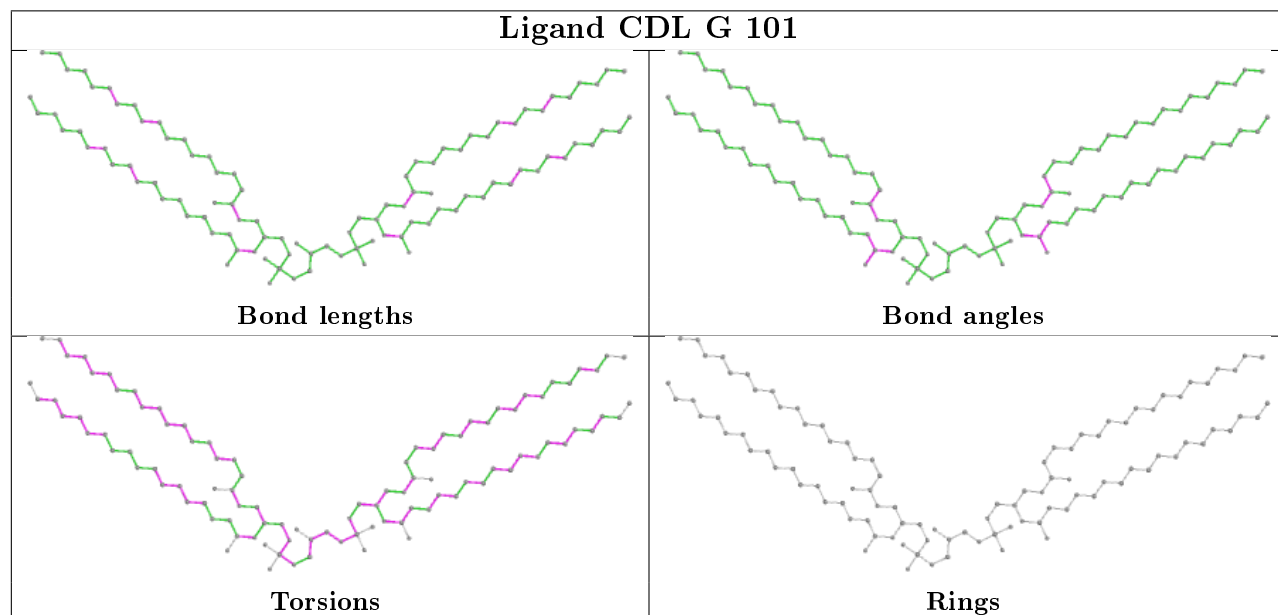
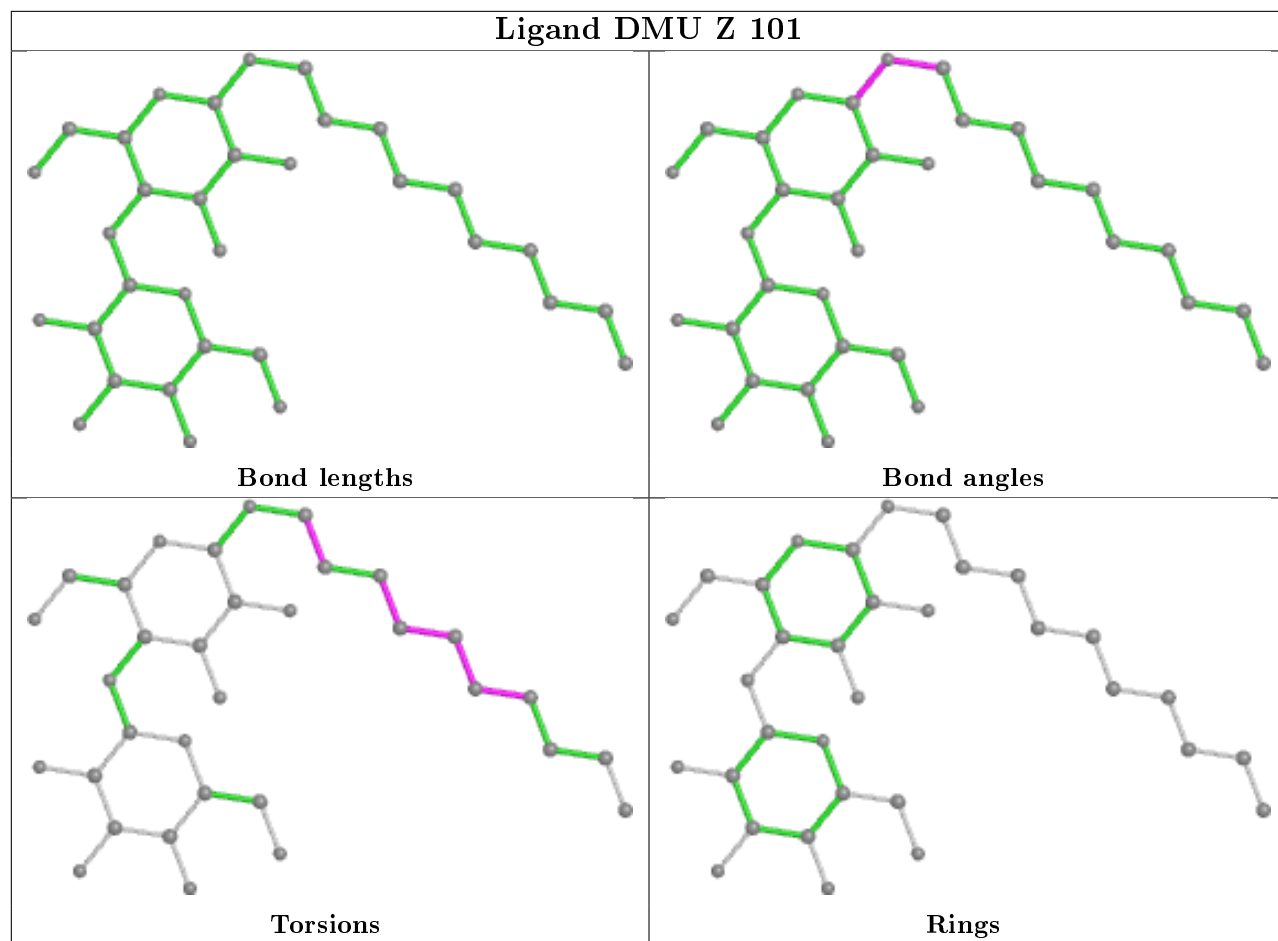
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

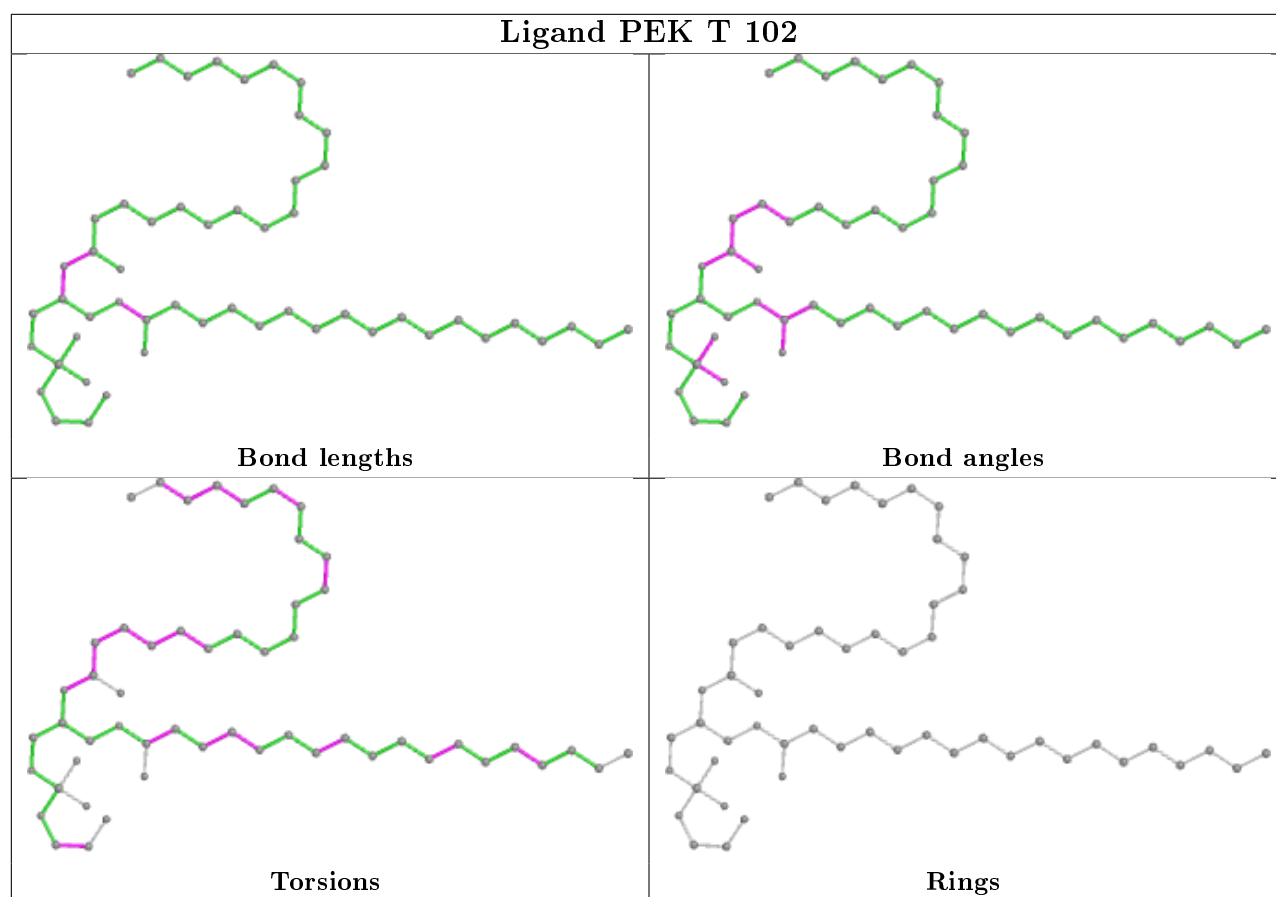
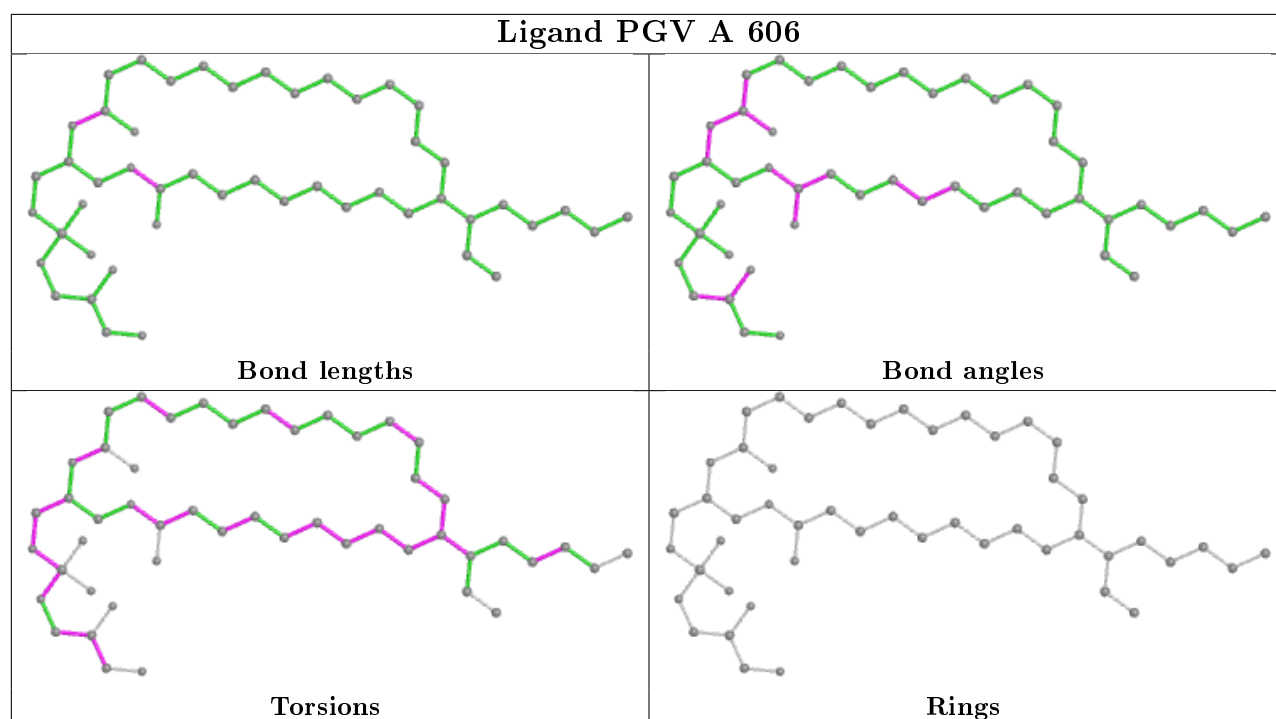


**Ligand PGV P 304****Ligand PGV N 606**

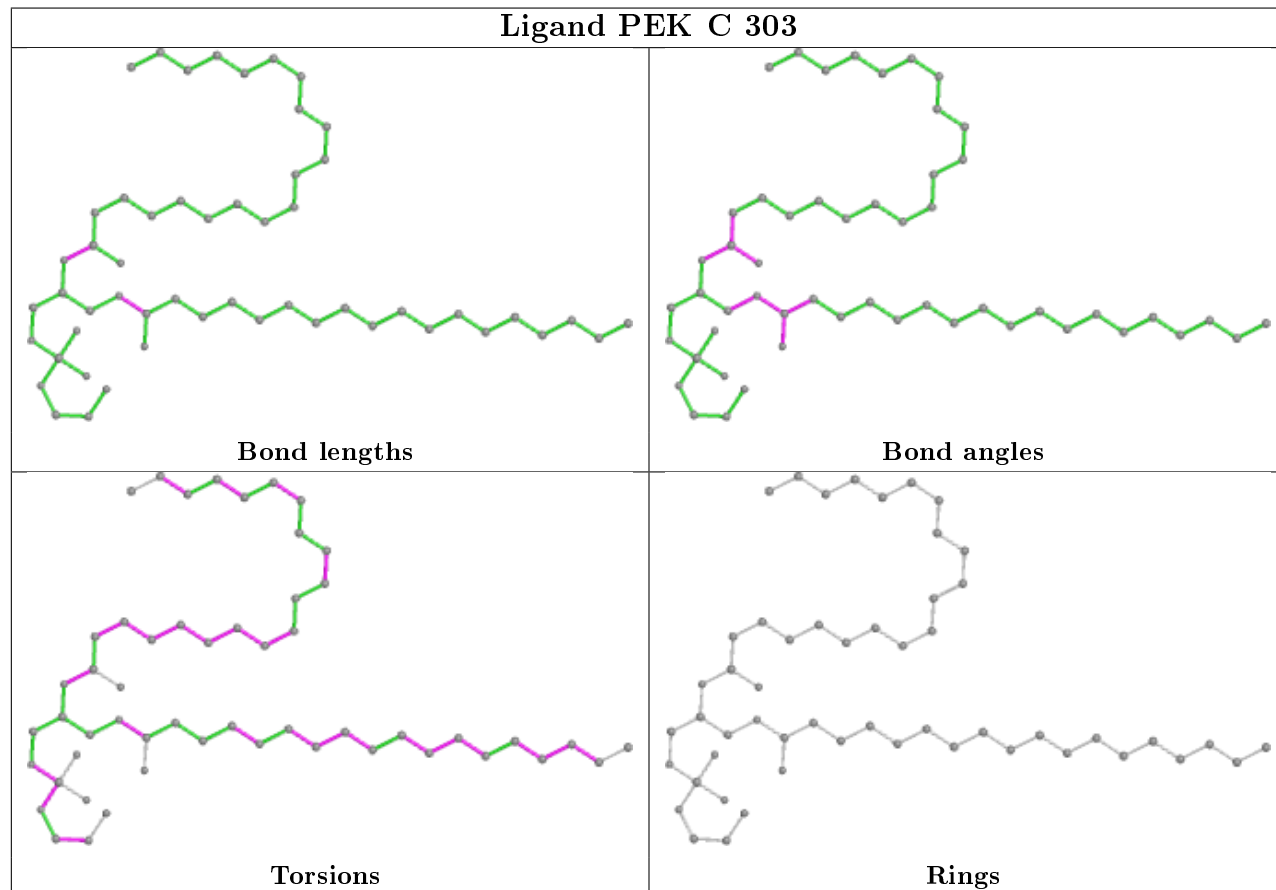
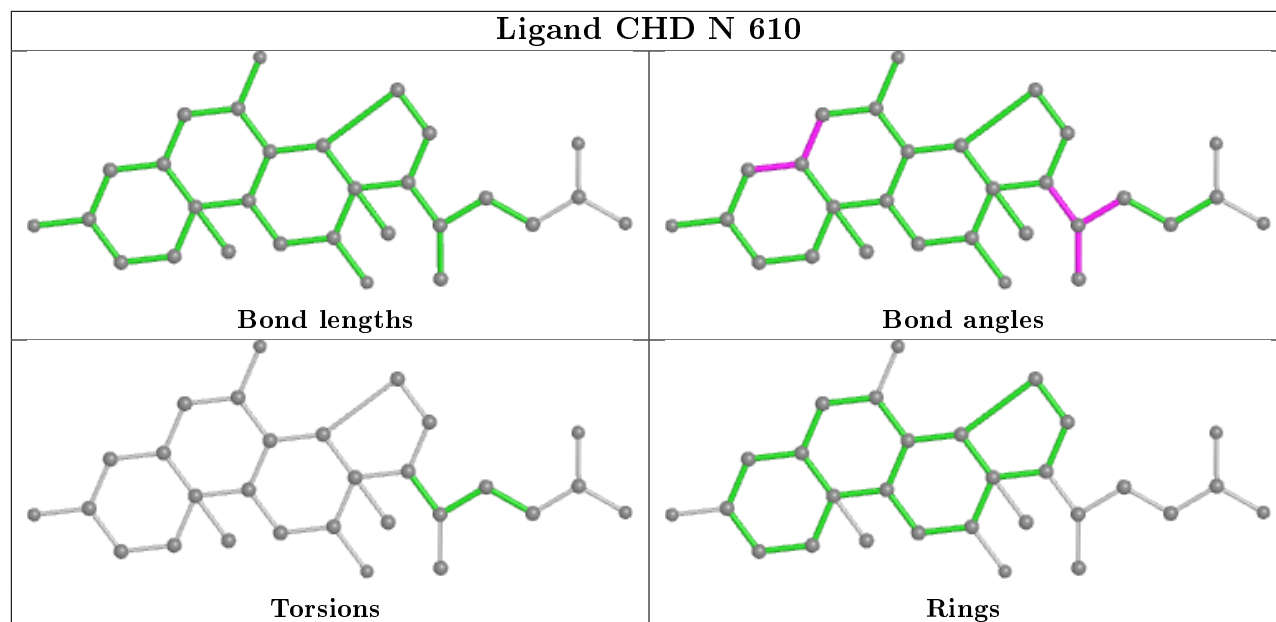


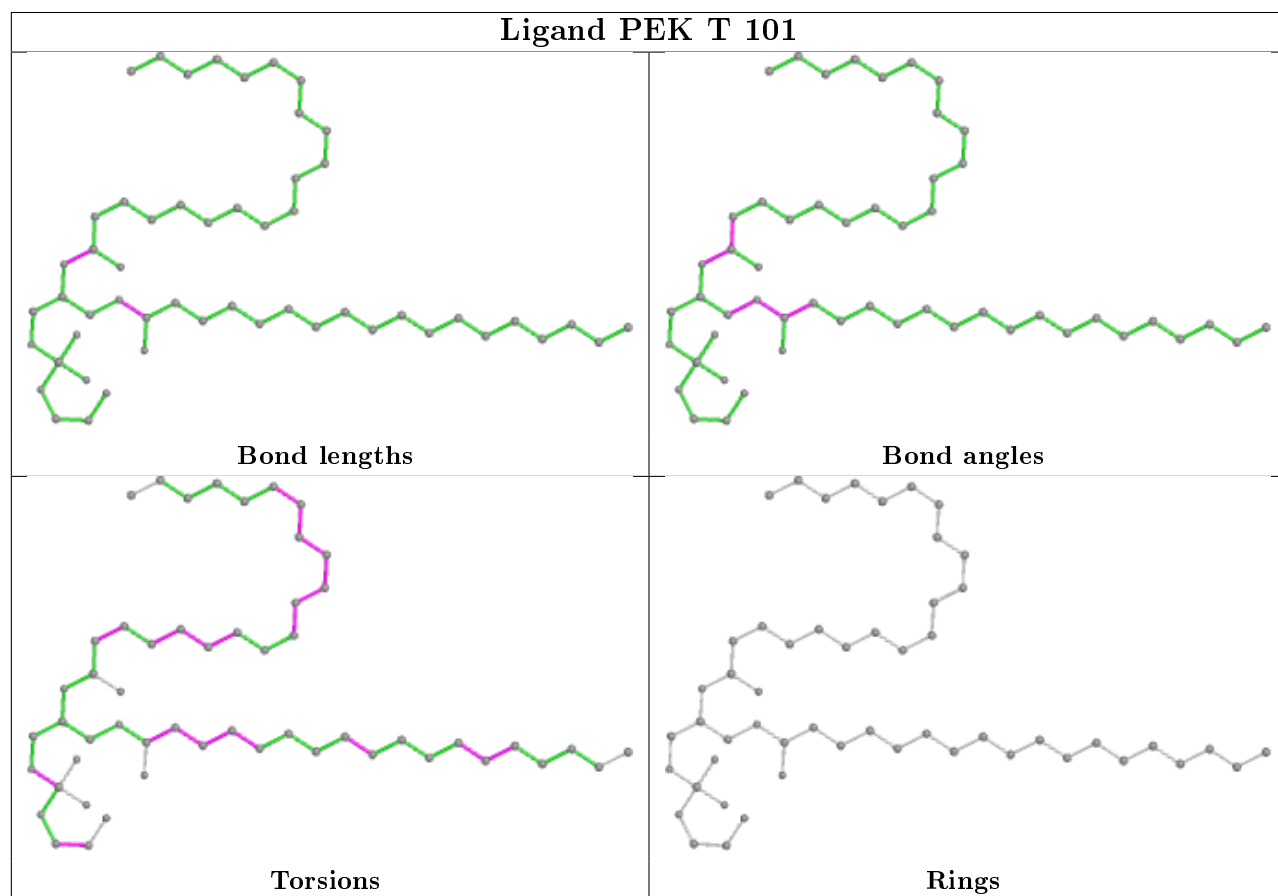
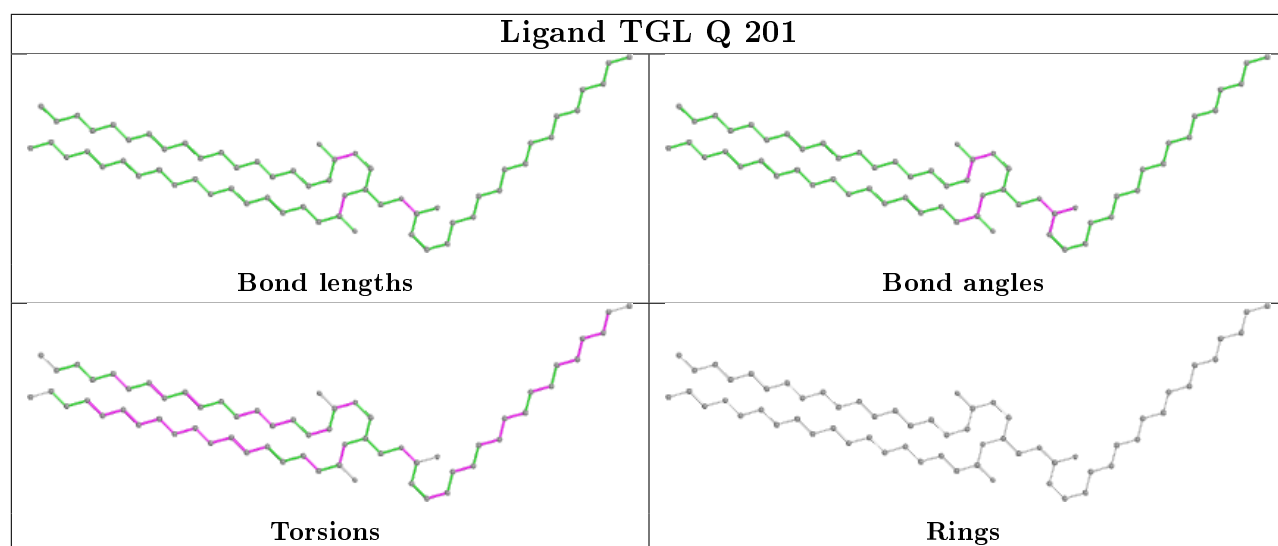


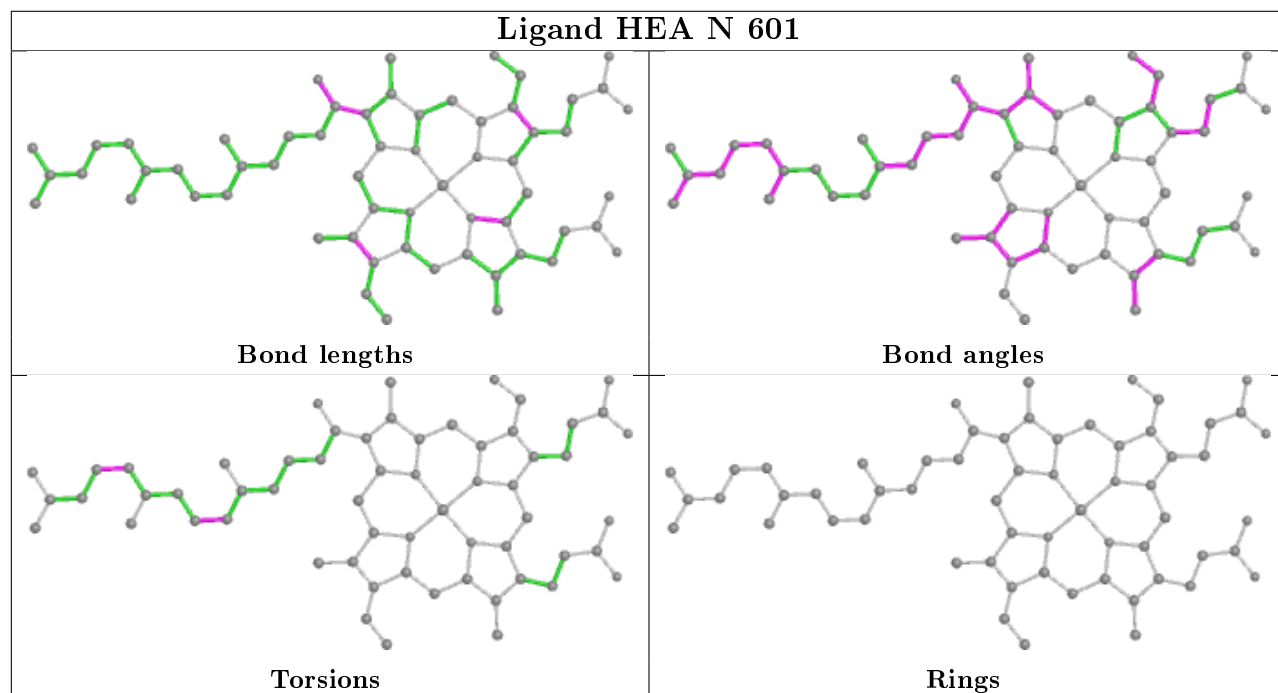
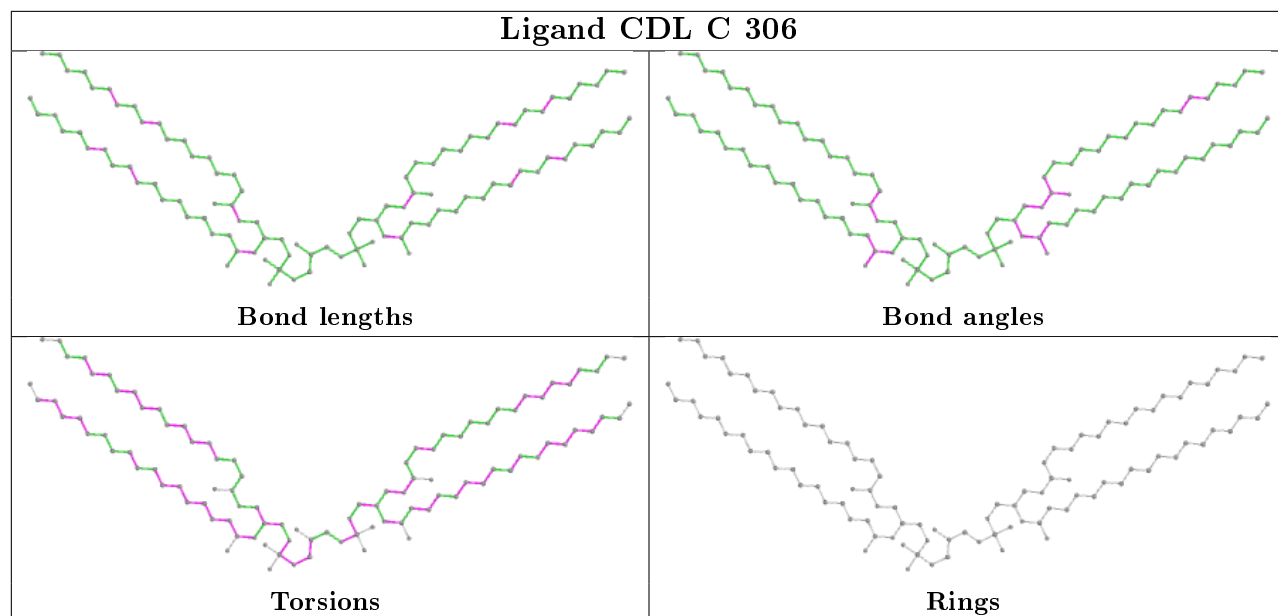


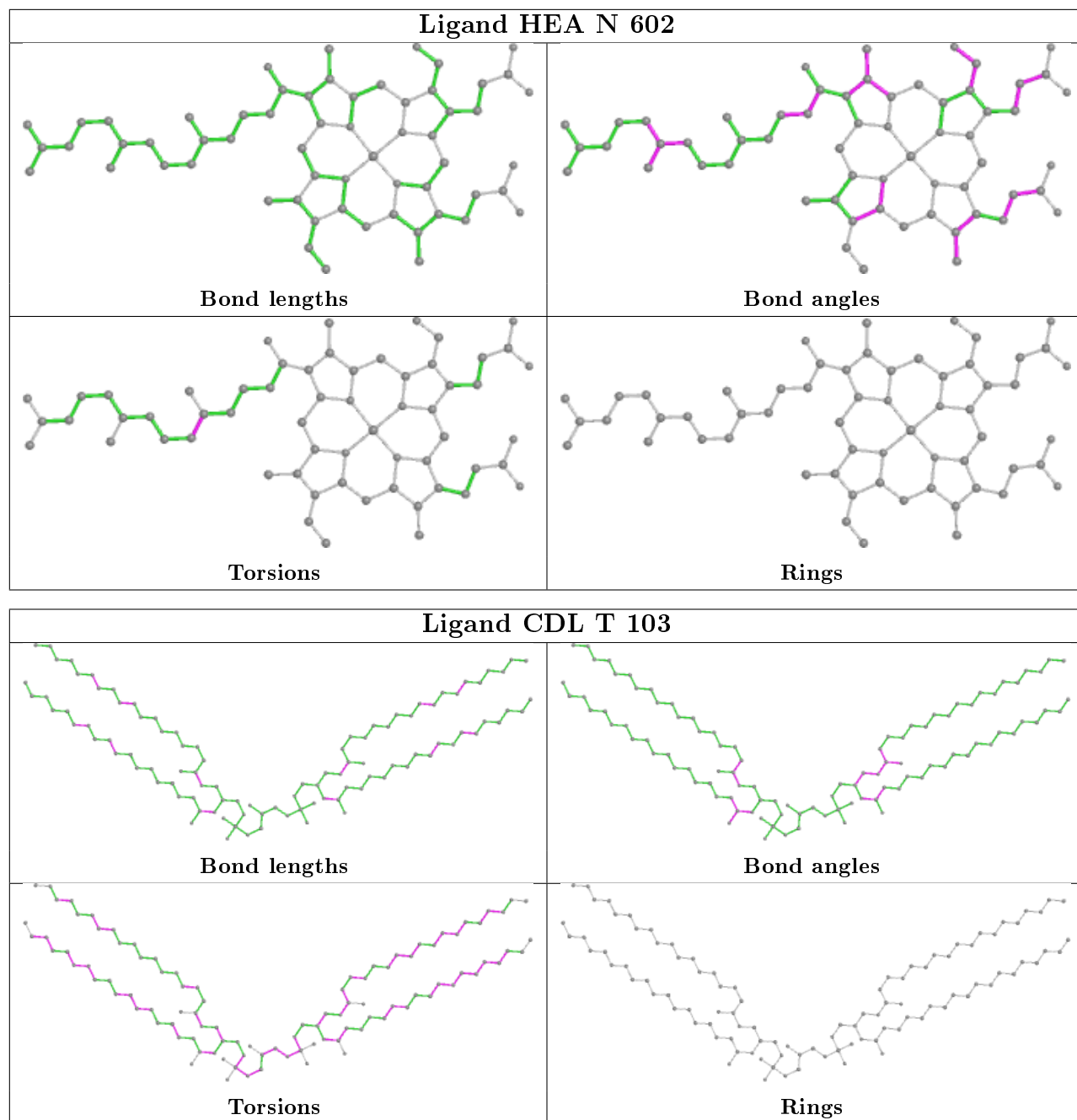


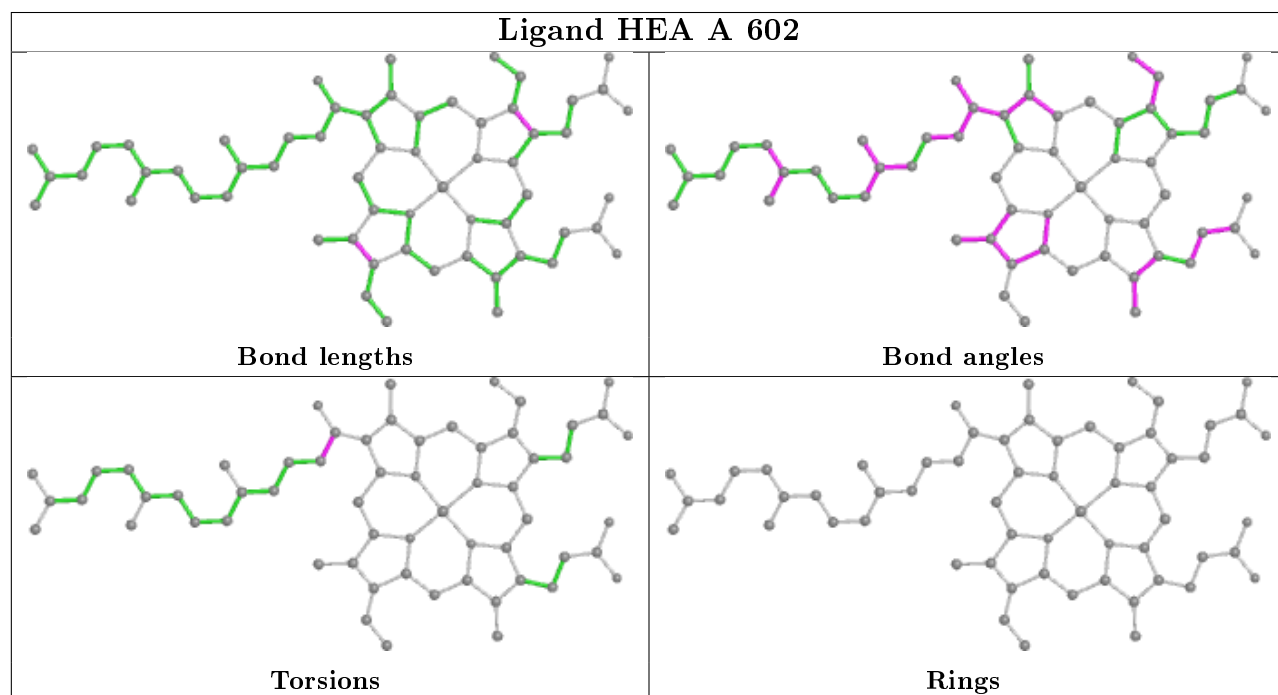
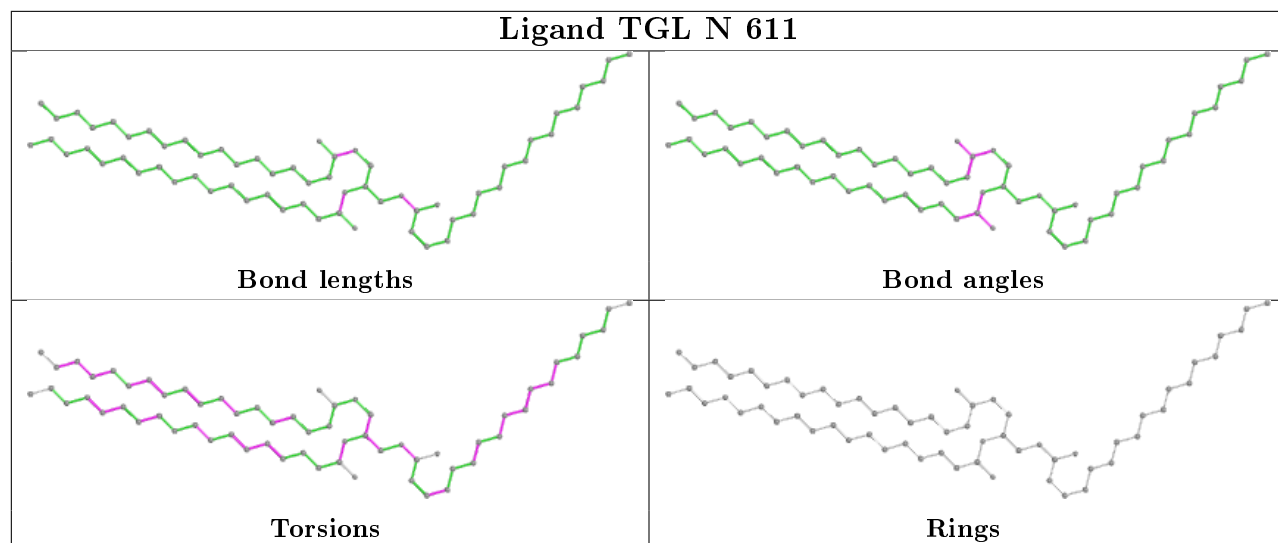




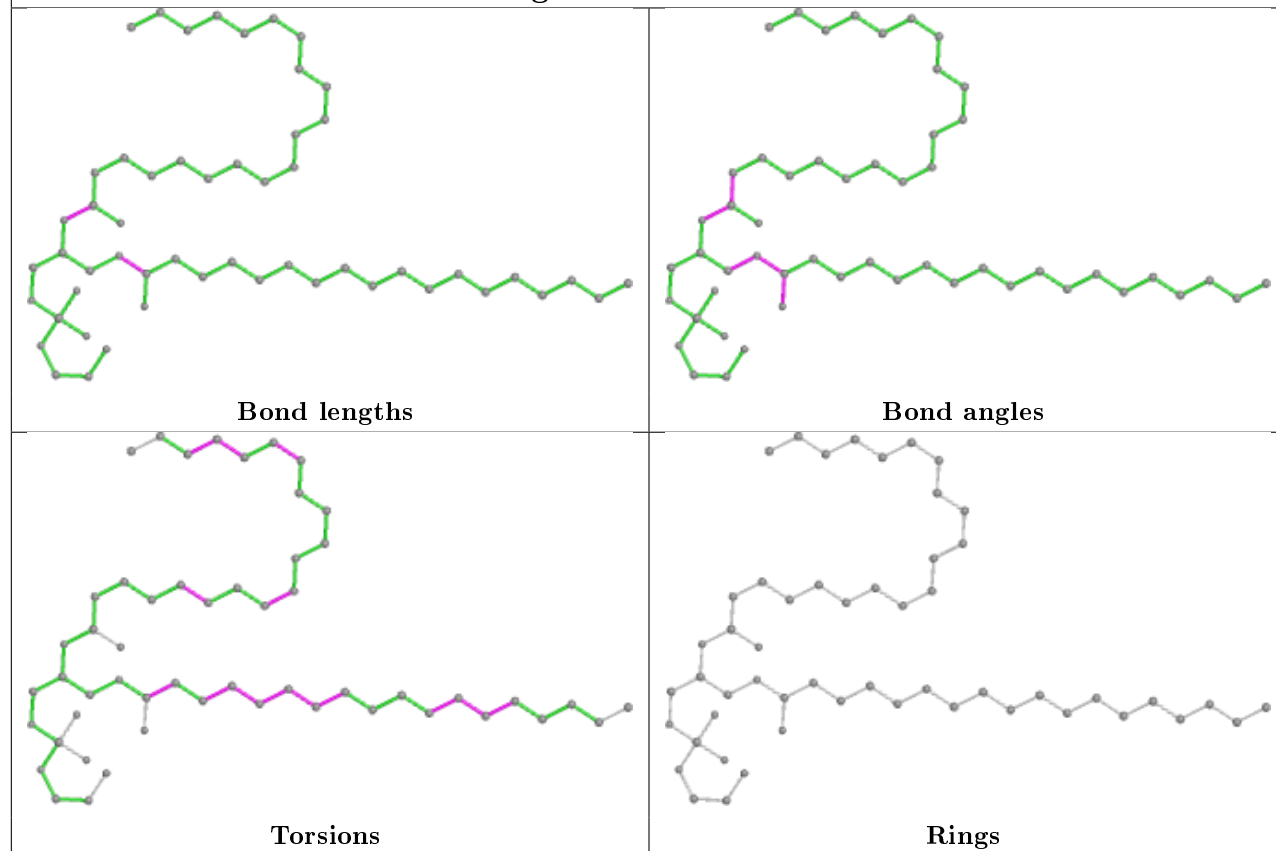




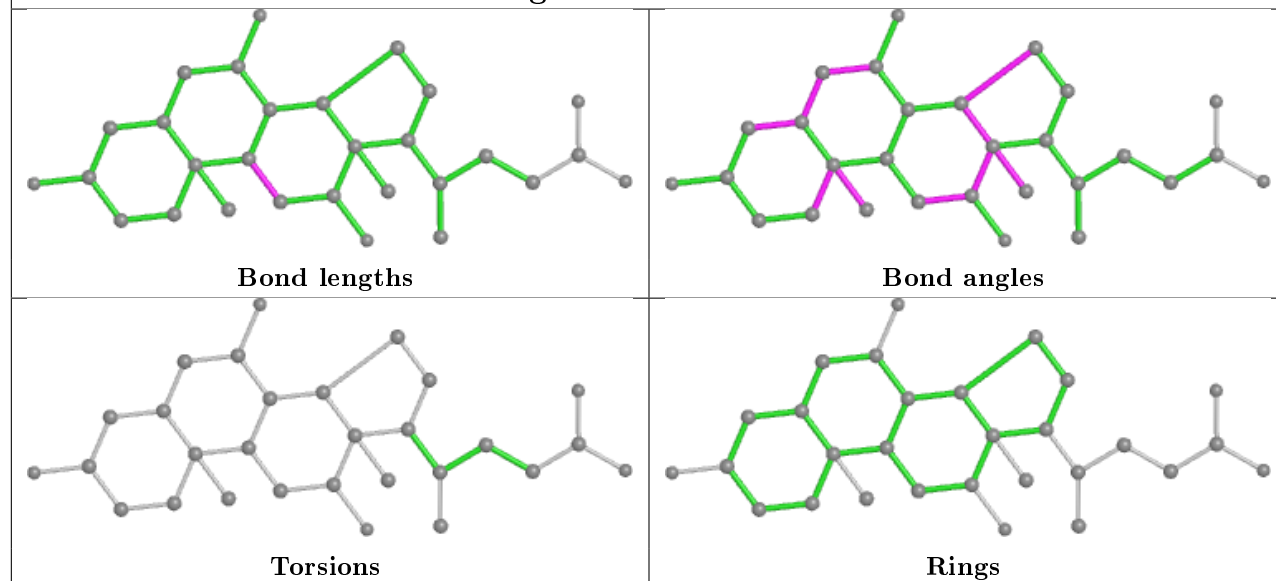


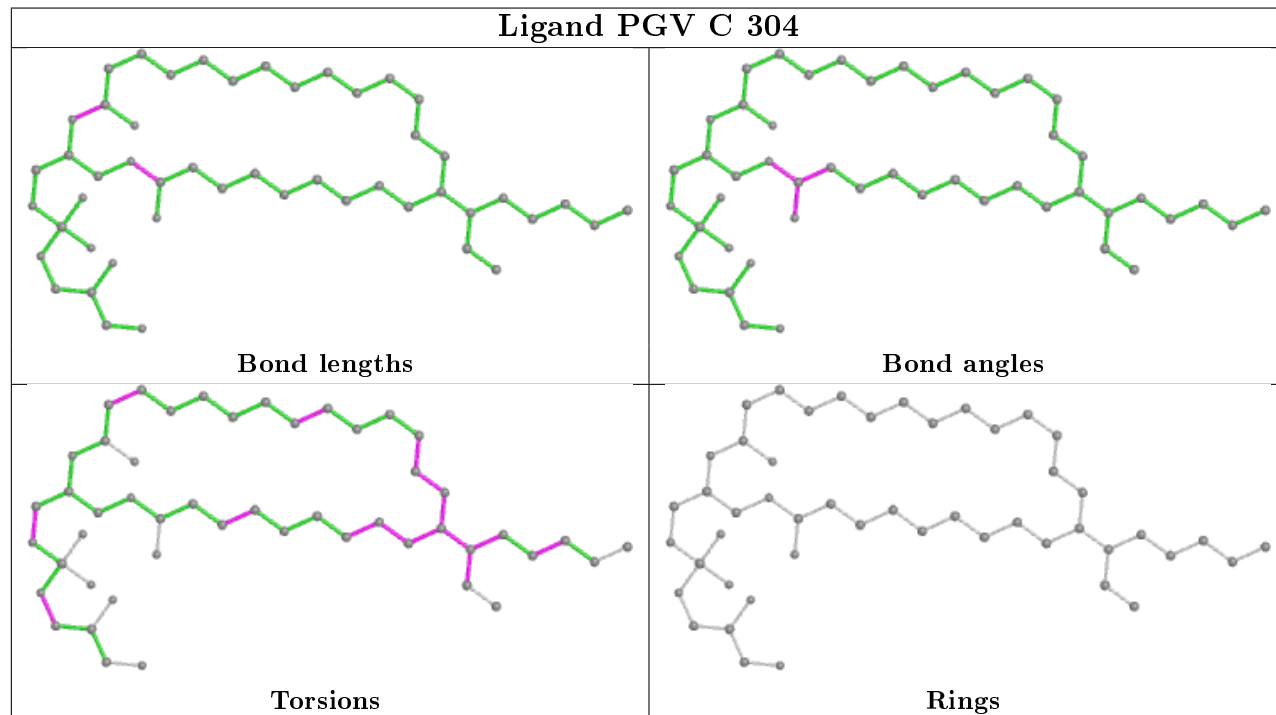
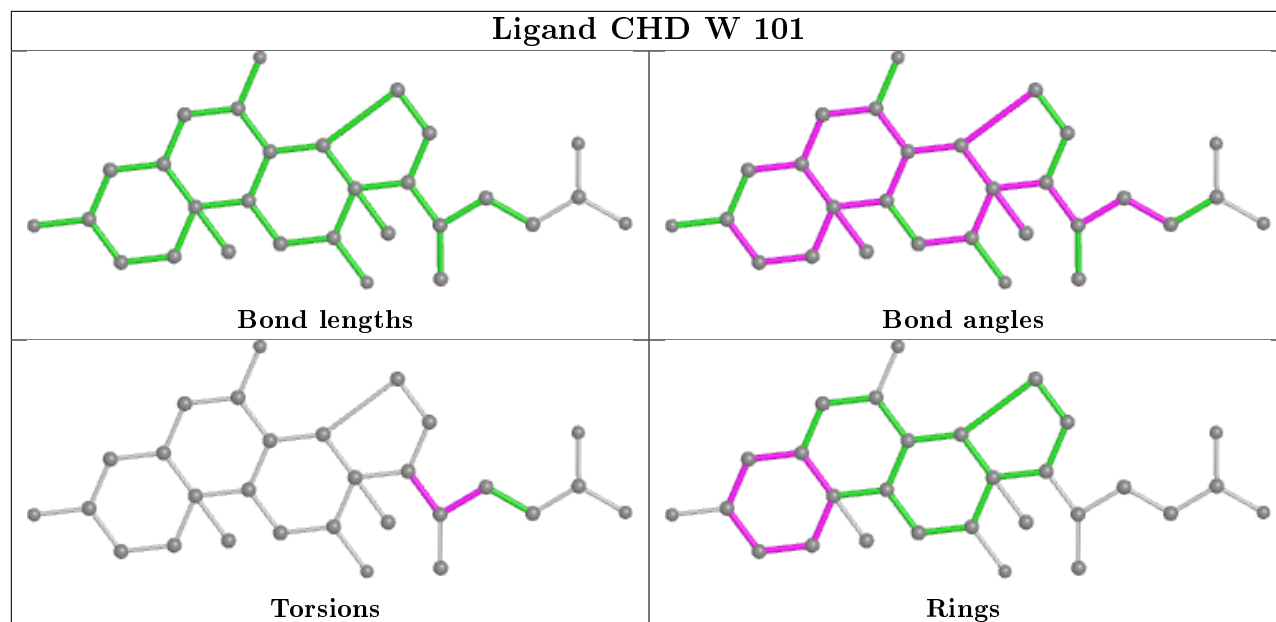


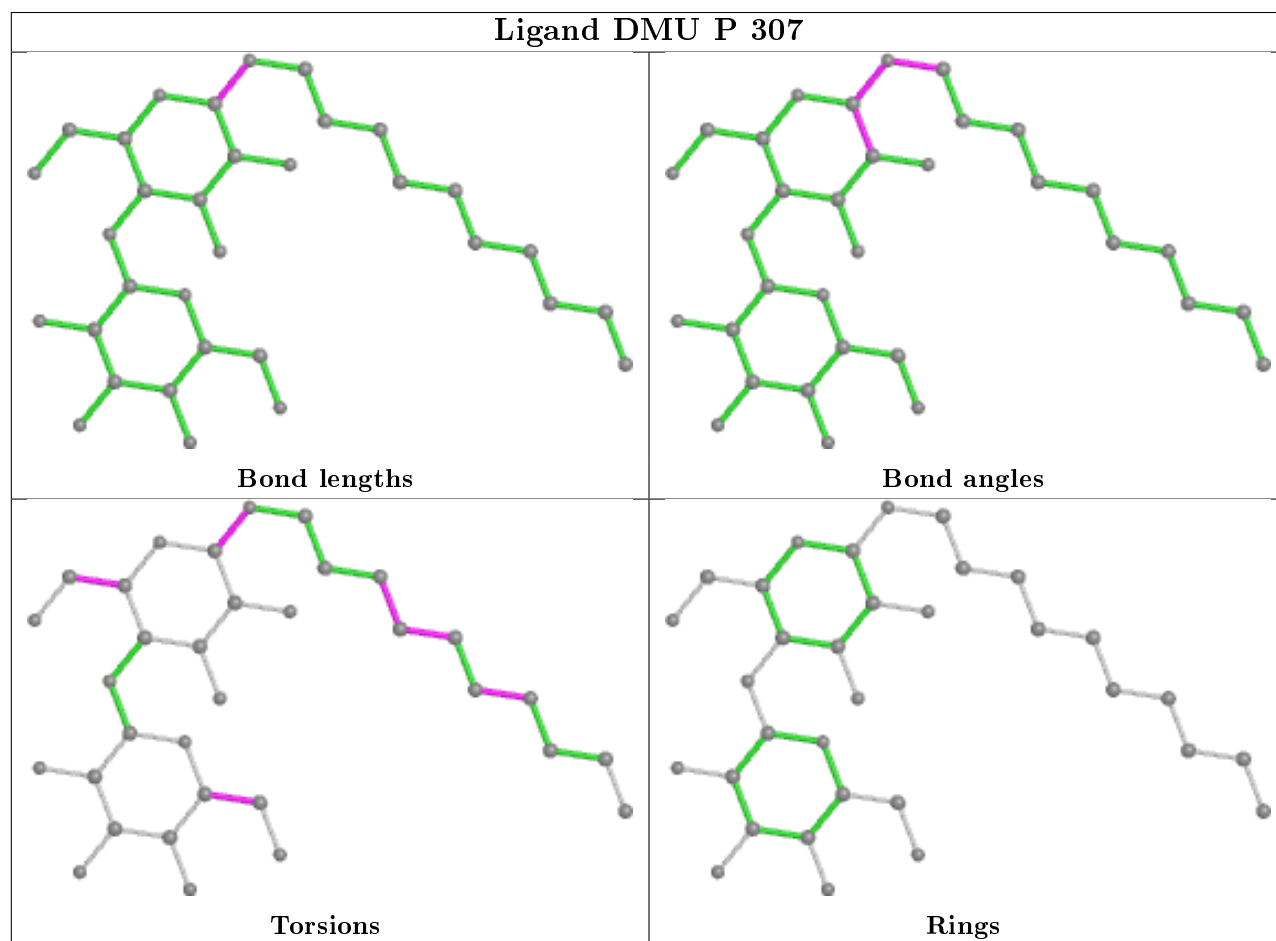
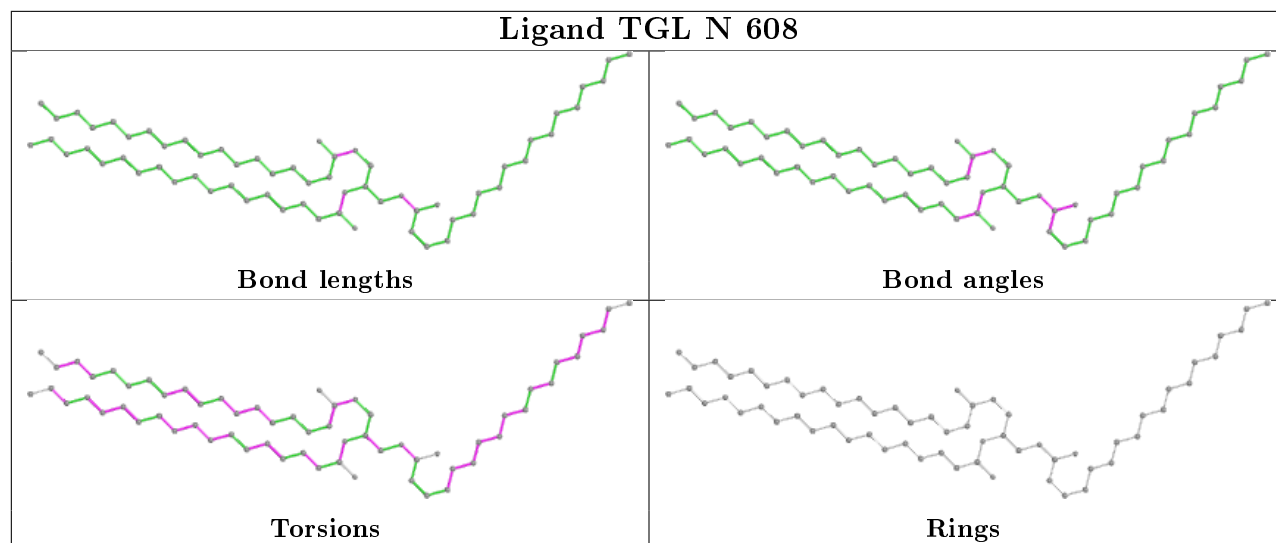
## Ligand PEK C 302



## Ligand CHD C 308

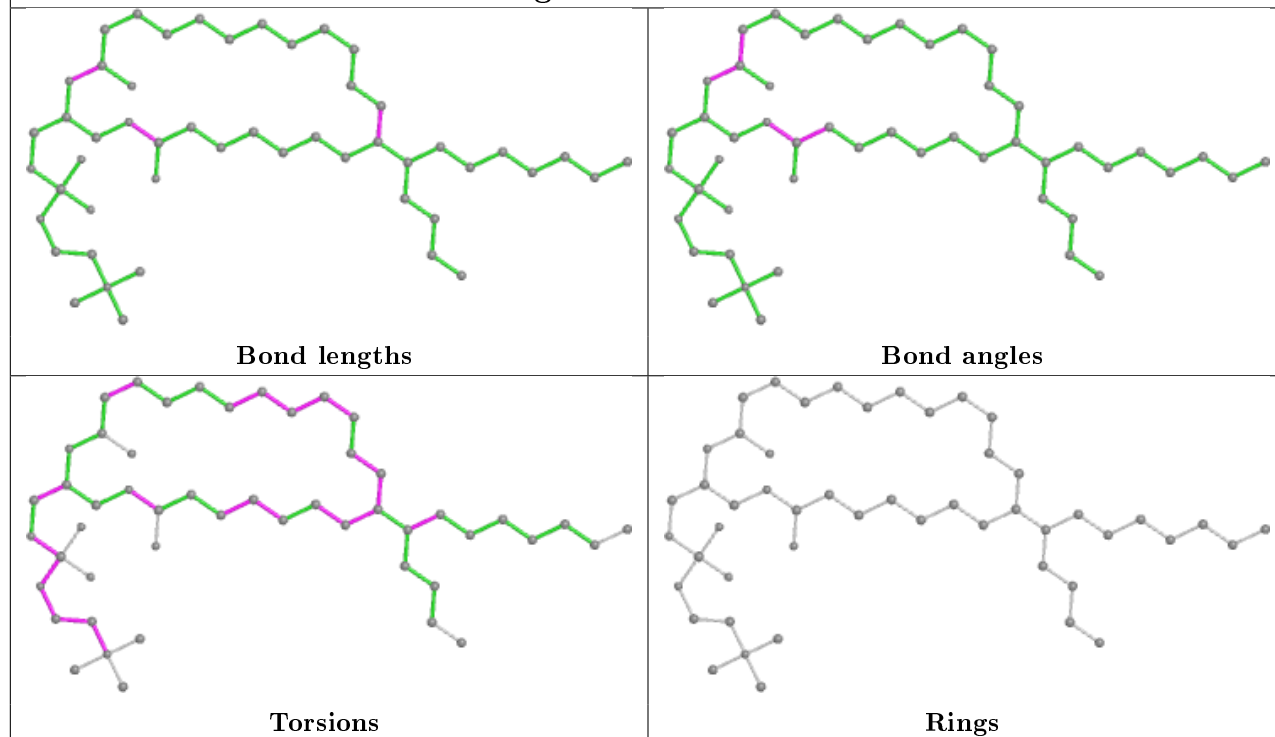




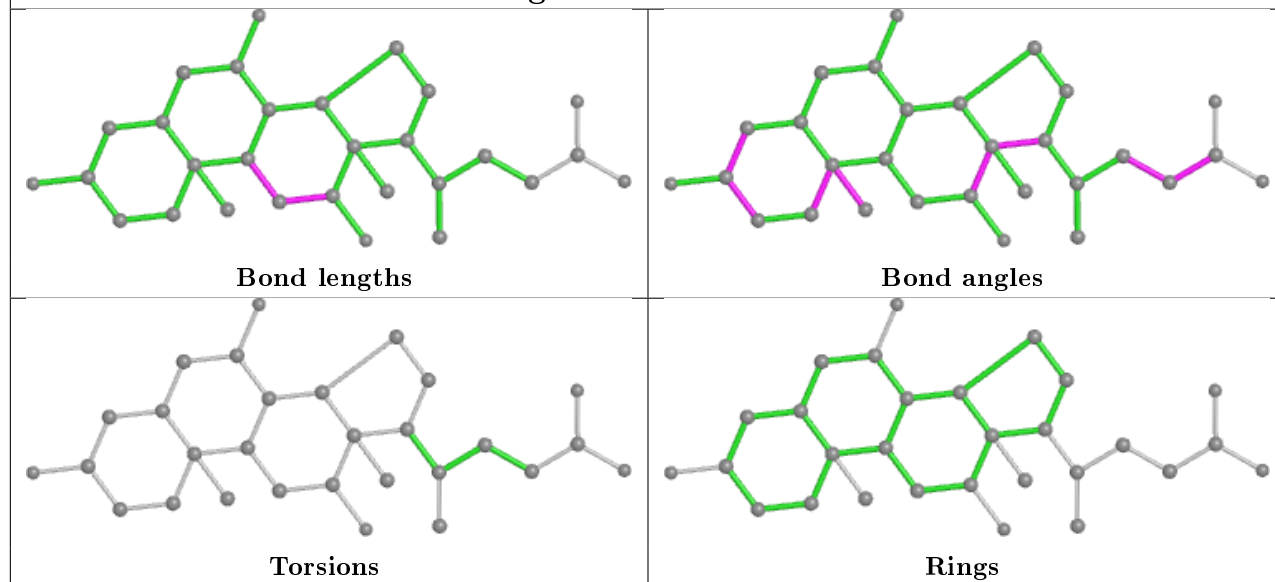




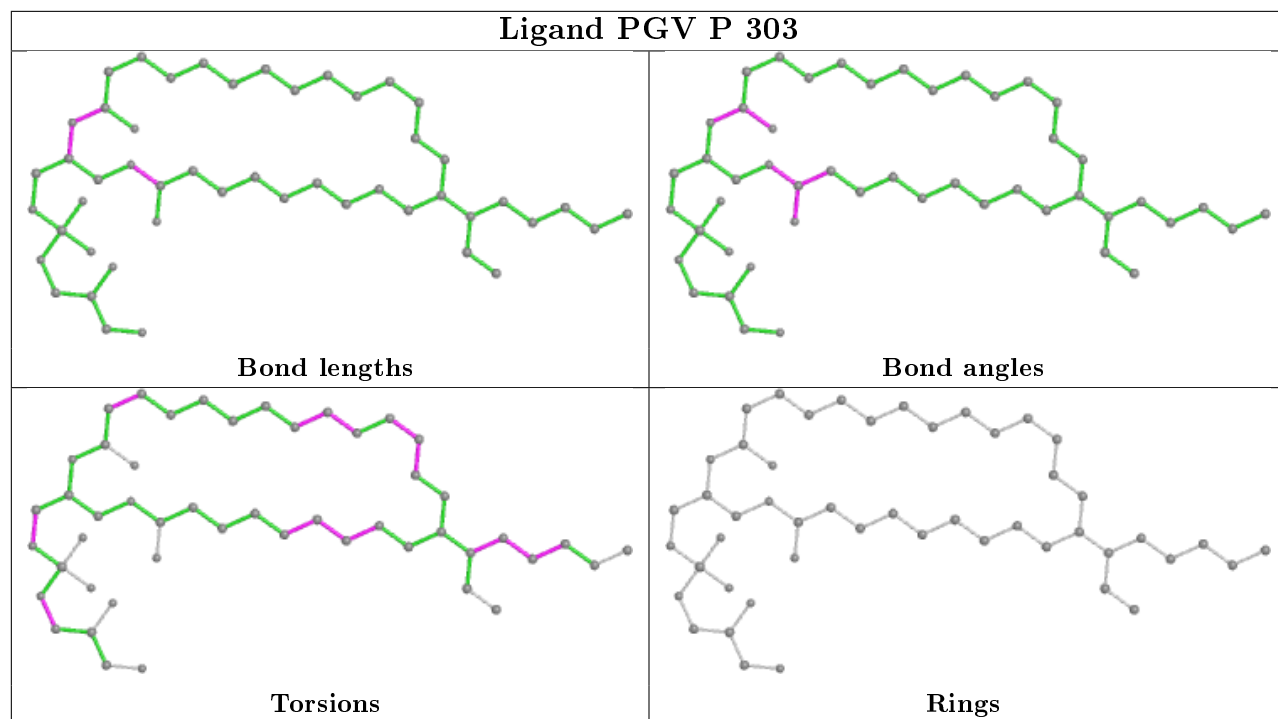
## Ligand PSC E 201



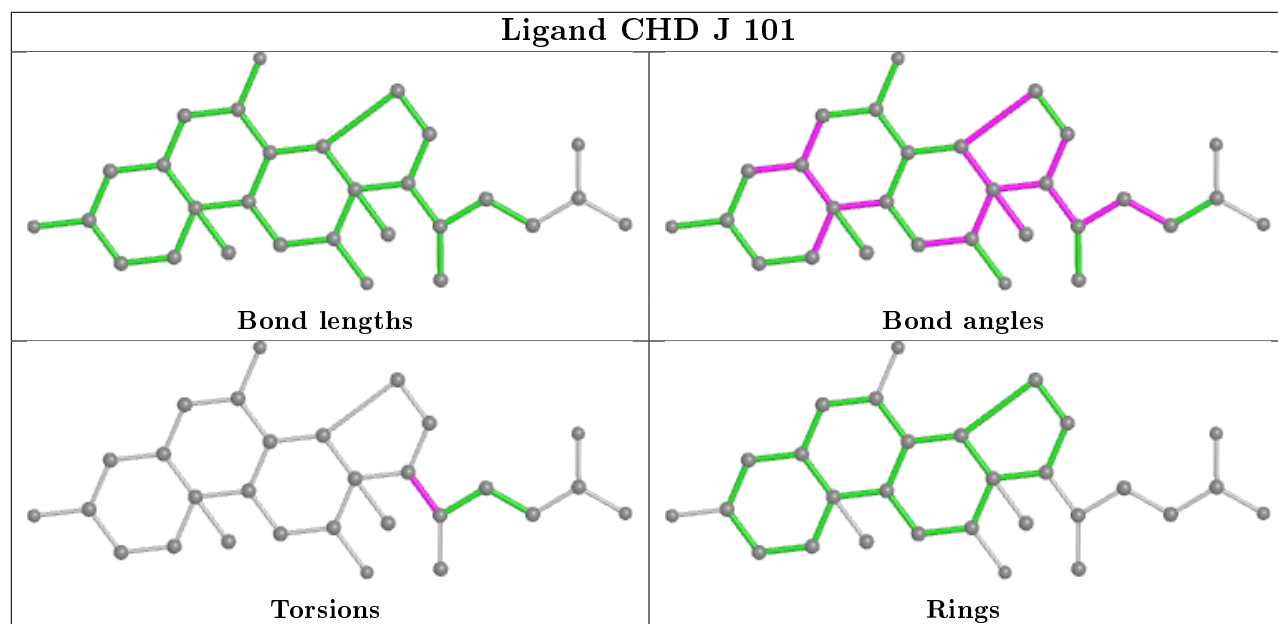
## Ligand CHD B 303

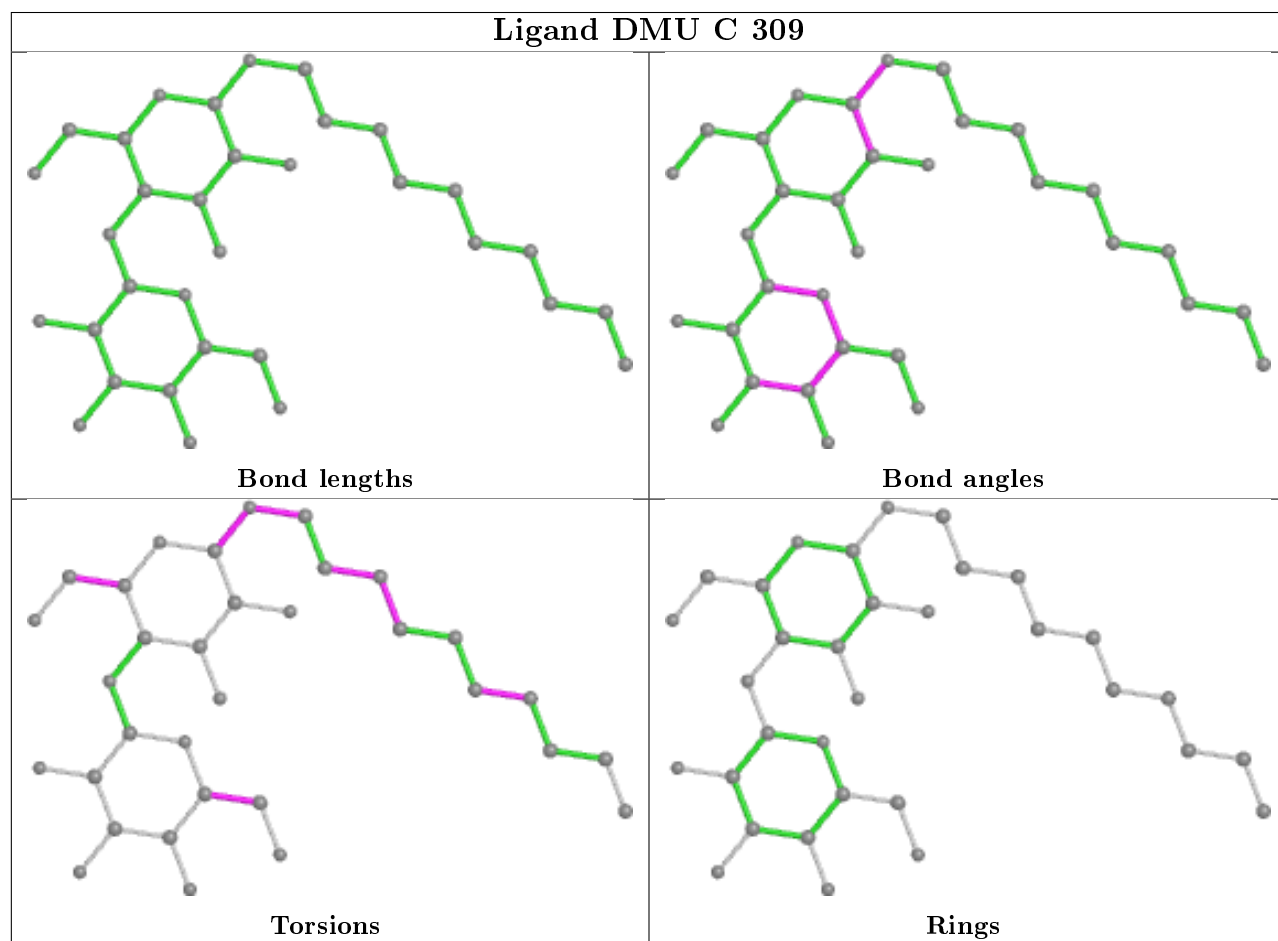
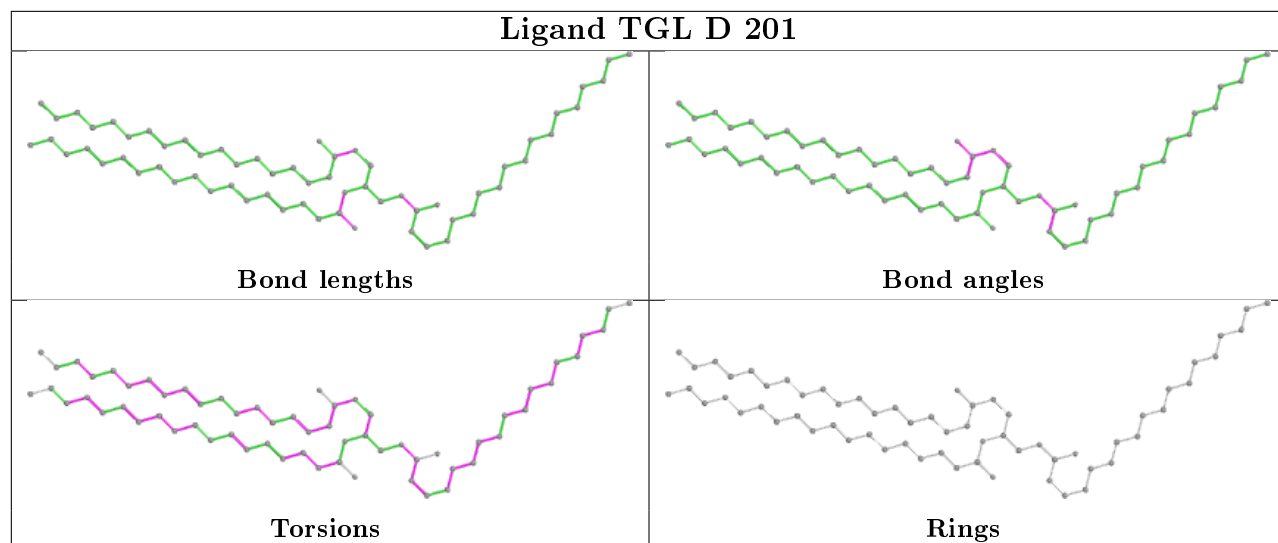


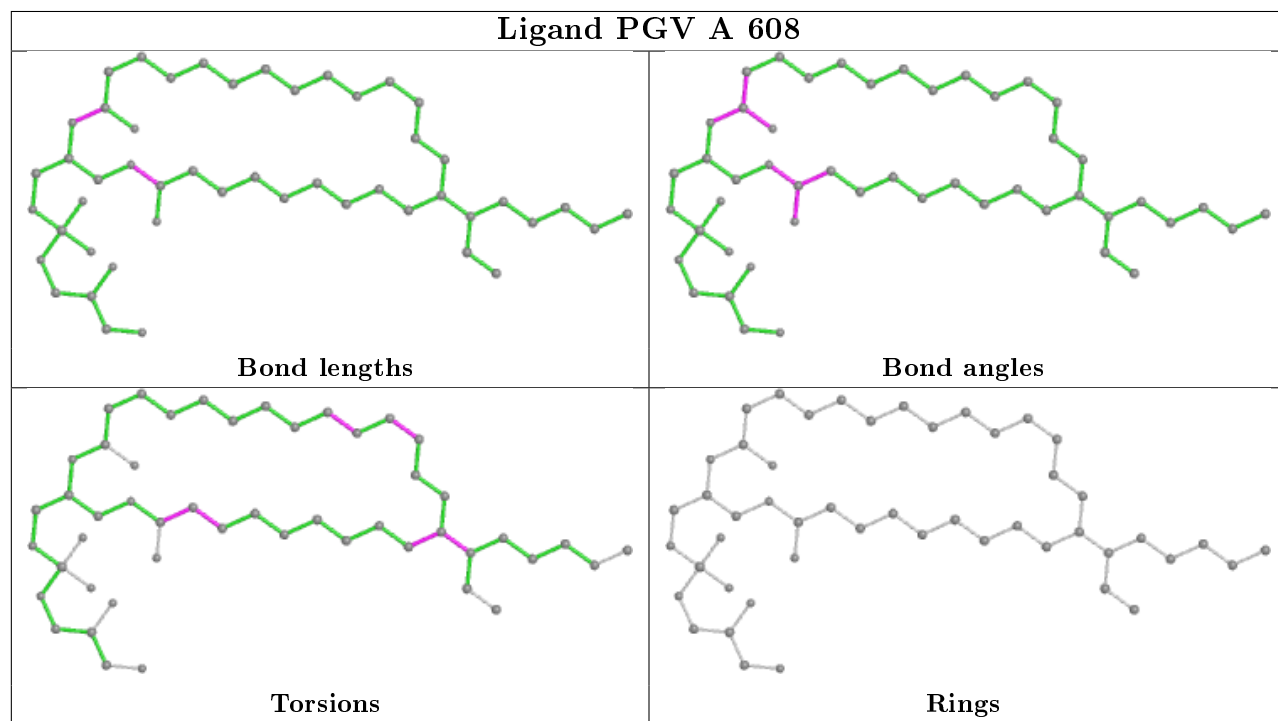
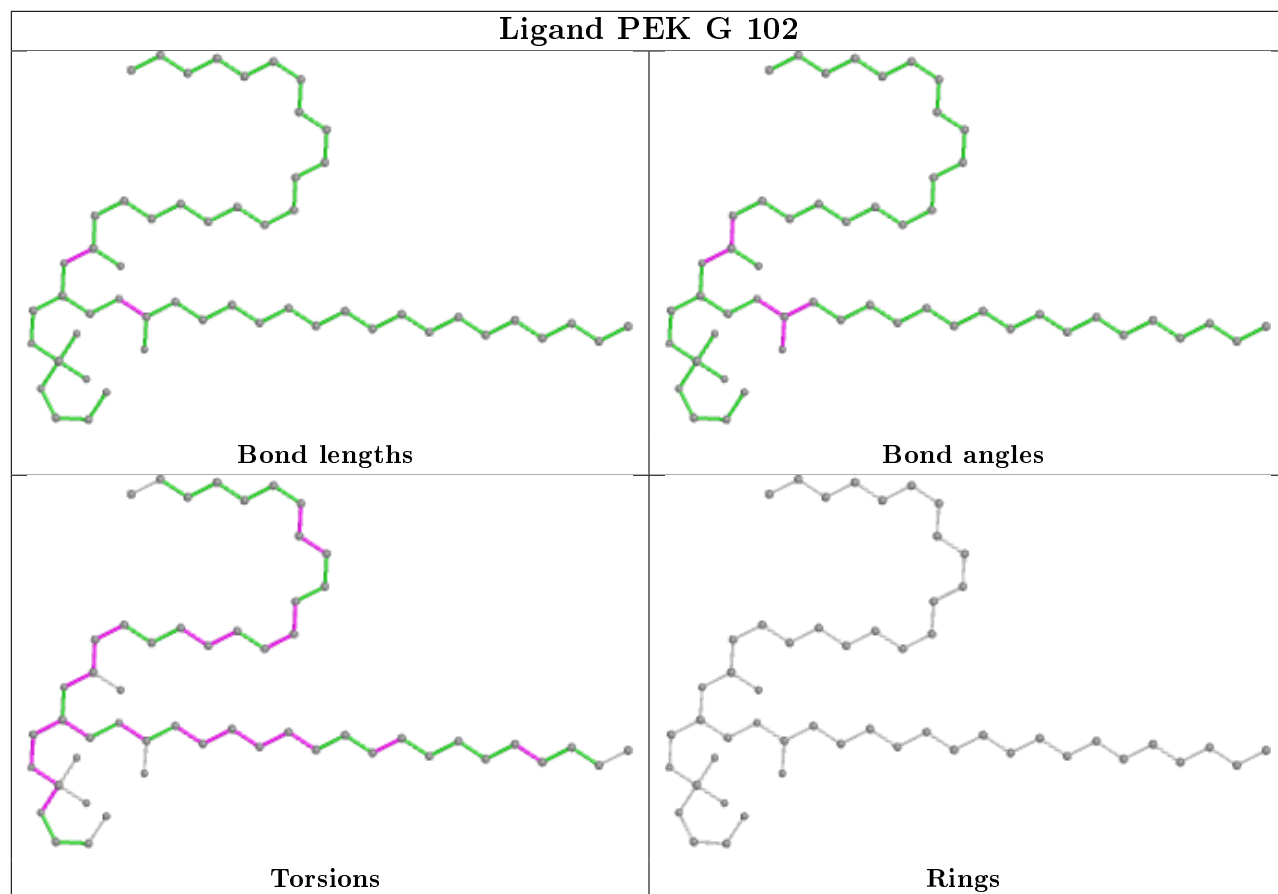
## Ligand PGV P 303

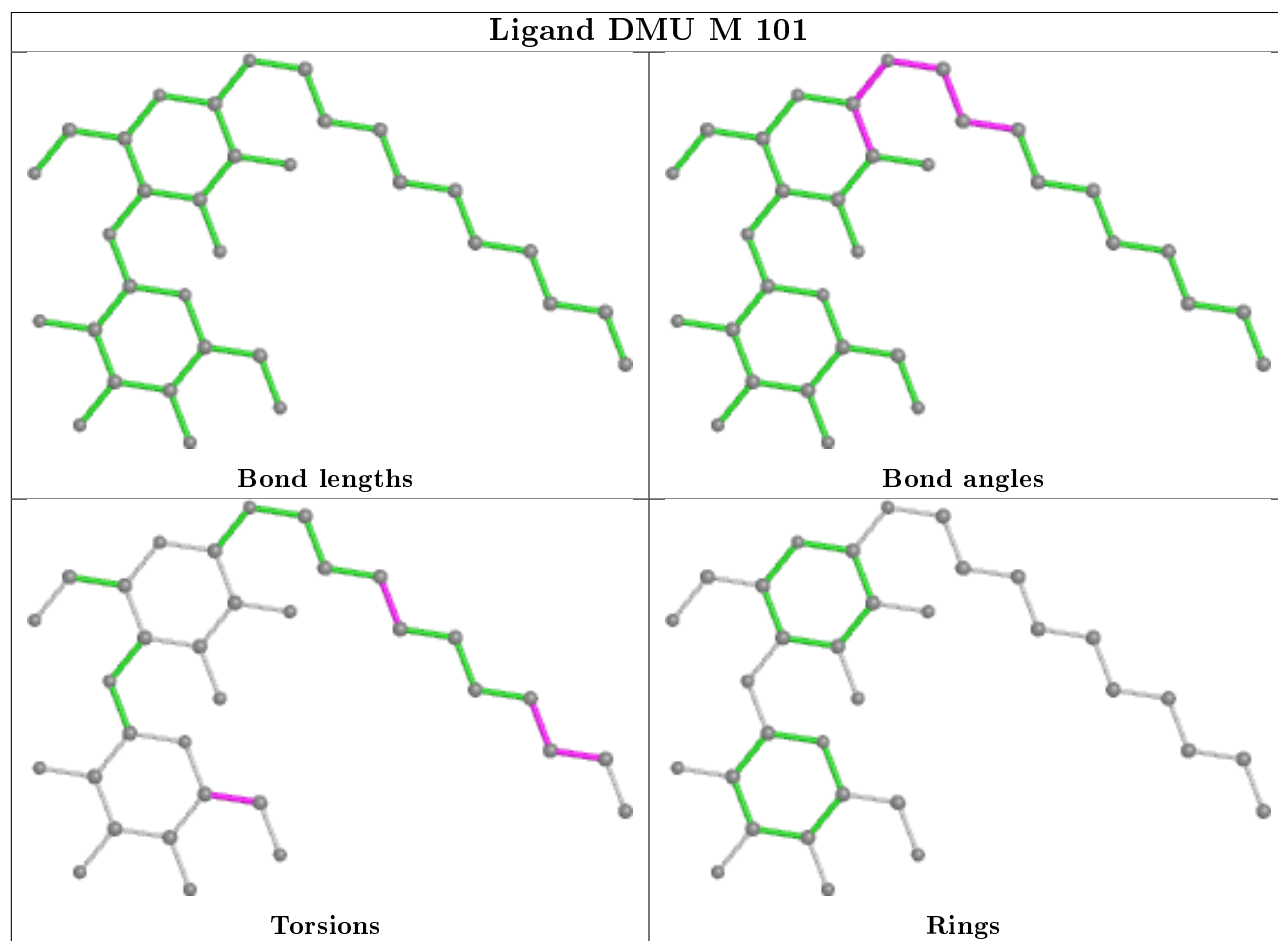
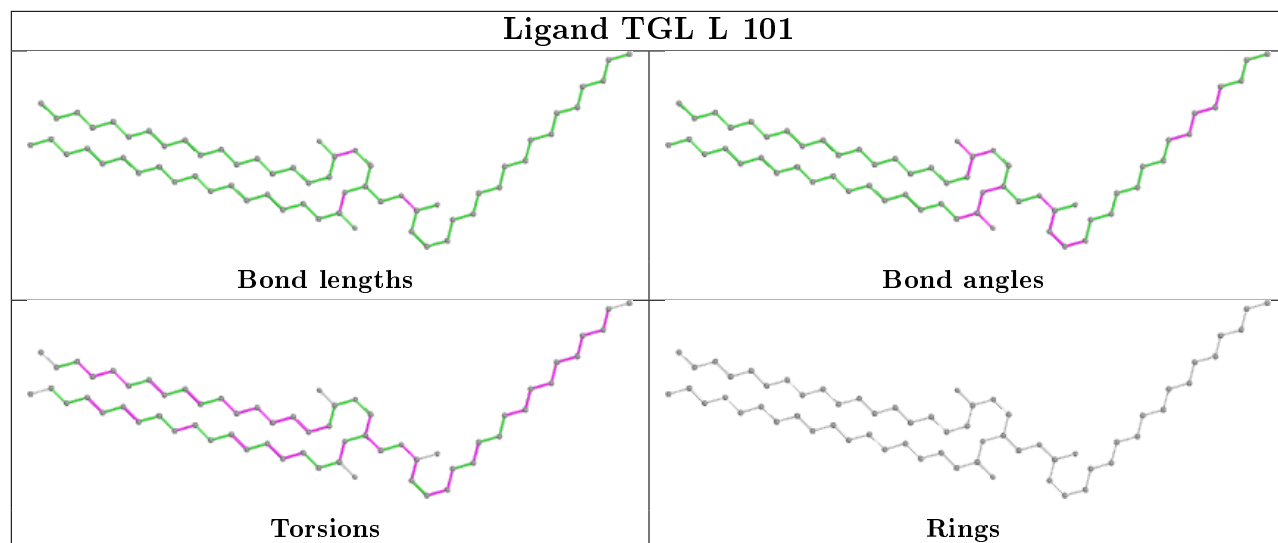


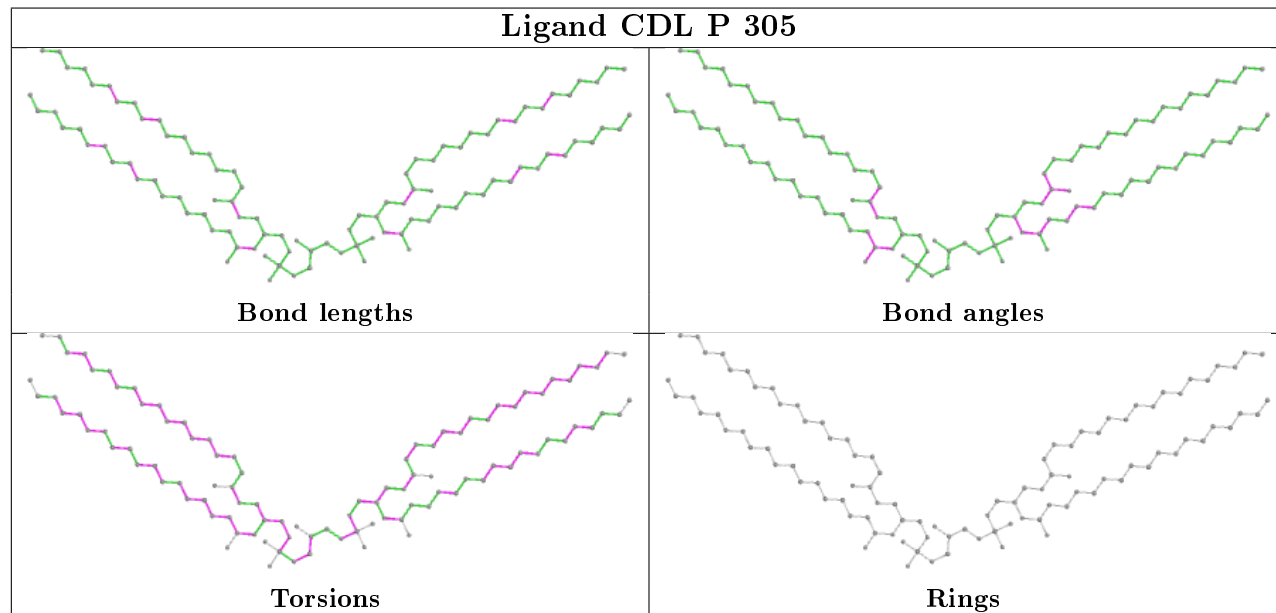
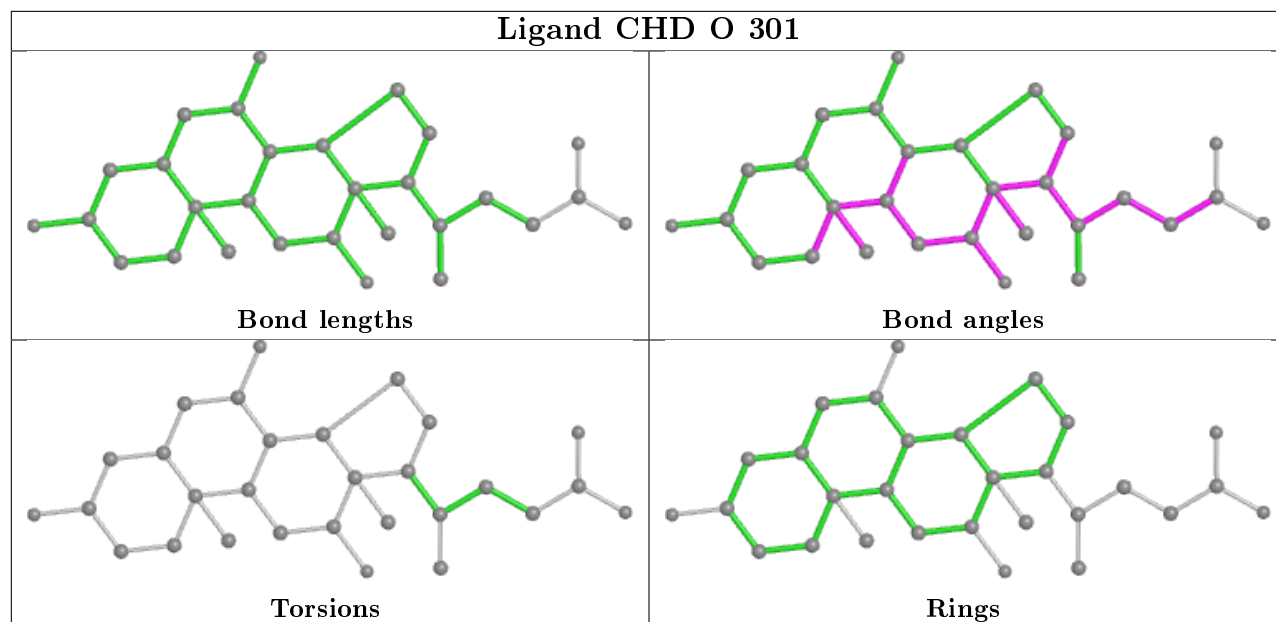
## Ligand CHD J 101

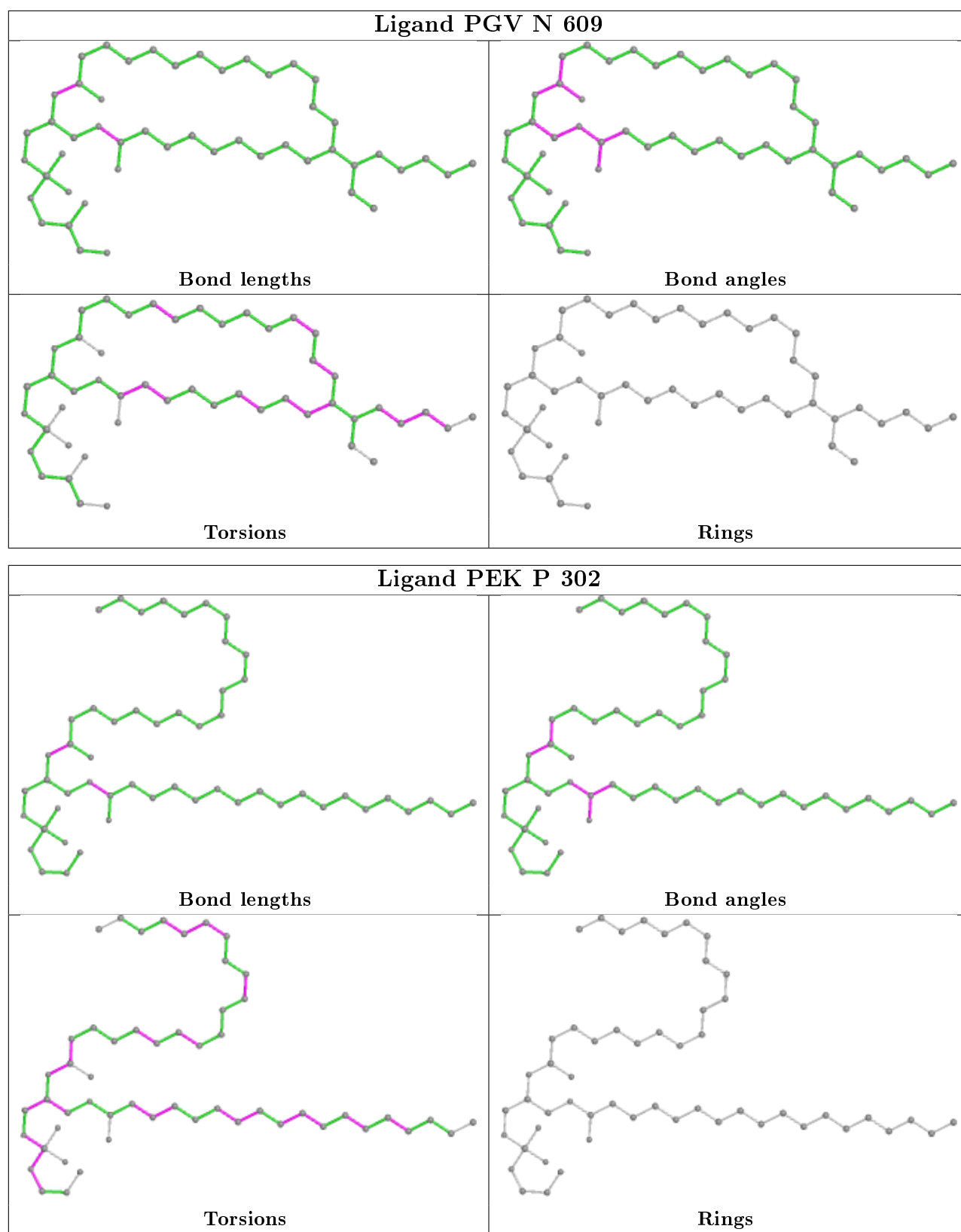












## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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%)	-0.07	1 (0%) 95 95	24, 28, 36, 71	0
1	N	513/514 (99%)	-0.07	3 (0%) 89 90	24, 31, 40, 70	0
2	B	226/227 (99%)	0.01	9 (3%) 38 41	26, 35, 56, 91	1 (0%)
2	O	226/227 (99%)	0.02	16 (7%) 16 17	31, 40, 63, 84	0
3	C	259/261 (99%)	-0.35	3 (1%) 79 81	26, 32, 43, 78	0
3	P	259/261 (99%)	-0.32	4 (1%) 73 76	25, 32, 45, 76	0
4	D	144/147 (97%)	-0.06	6 (4%) 36 39	30, 37, 57, 76	0
4	Q	144/147 (97%)	1.01	25 (17%) 1 1	37, 49, 78, 148	0
5	E	105/109 (96%)	-0.02	5 (4%) 30 33	31, 37, 58, 103	0
5	R	105/109 (96%)	0.14	5 (4%) 30 33	34, 45, 63, 113	0
6	F	98/98 (100%)	0.63	11 (11%) 5 6	28, 38, 93, 145	0
6	S	98/98 (100%)	0.84	9 (9%) 9 10	27, 37, 97, 149	0
7	G	83/85 (97%)	1.03	19 (22%) 0 0	30, 41, 104, 128	0
7	T	83/85 (97%)	1.06	19 (22%) 0 0	31, 42, 105, 134	0
8	H	79/85 (92%)	0.89	14 (17%) 1 1	32, 41, 95, 109	0
8	U	79/85 (92%)	0.92	15 (18%) 1 1	36, 46, 96, 121	0
9	I	72/73 (98%)	1.16	18 (25%) 0 0	35, 47, 74, 86	0
9	V	72/73 (98%)	1.35	19 (26%) 0 0	34, 55, 73, 91	0
10	J	58/59 (98%)	0.52	8 (13%) 2 3	32, 43, 65, 107	0
10	W	58/59 (98%)	0.54	8 (13%) 2 3	34, 44, 70, 109	0
11	K	49/56 (87%)	0.53	3 (6%) 21 24	33, 41, 54, 60	0
11	X	49/56 (87%)	1.37	12 (24%) 0 0	42, 51, 69, 79	0
12	L	46/47 (97%)	-0.20	2 (4%) 35 38	30, 34, 54, 88	0
12	Y	46/47 (97%)	0.22	6 (13%) 3 3	33, 41, 61, 107	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	43/46 (93%)	0.20	4 (9%) 8 10	29, 34, 65, 99	0
13	Z	43/46 (93%)	0.63	7 (16%) 1 1	36, 42, 75, 108	0
All	All	3550/3614 (98%)	0.21	251 (7%) 16 17	24, 36, 67, 149	1 (0%)

The worst 5 of 251 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	S	97	ALA	29.1
4	Q	6	VAL	18.0
4	Q	5	VAL	16.2
6	S	1	ALA	15.6
6	S	98	HIS	12.7

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
7	TPO	G	11	11/12	0.11	0.53	106,116,133,137	0
7	TPO	T	11	11/12	0.14	0.62	110,123,134,135	0
9	SAC	V	1	9/10	0.43	0.64	117,122,125,126	0
9	SAC	I	1	9/10	0.65	0.43	85,97,109,115	0
1	FME	A	1	10/11	0.94	0.21	41,46,68,84	0
1	FME	N	1	10/11	0.94	0.17	43,49,71,73	0
2	FME	B	1	10/11	0.96	0.14	32,34,43,57	0
2	FME	O	1	10/11	0.98	0.14	40,41,51,57	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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( $\text{\AA}^2$ )	Q<0.9
23	PEK	C	303	53/53	0.49	0.32	50,79,121,126	0
26	PSC	E	201	52/52	0.49	0.33	49,98,155,160	0
25	DMU	C	309	33/33	0.53	0.47	45,99,129,131	0
24	CDL	G	101	100/100	0.55	0.27	63,90,131,148	0
23	PEK	P	302	53/53	0.55	0.30	51,74,133,139	0
23	PEK	G	102	53/53	0.57	0.37	49,105,138,154	0
23	PEK	T	101	53/53	0.58	0.34	52,96,152,157	0
20	TGL	Q	201	63/63	0.59	0.27	58,81,112,118	0
24	CDL	T	103	100/100	0.59	0.28	61,90,141,150	0
22	CHD	W	101	29/29	0.59	0.42	96,123,135,140	0
25	DMU	P	307	33/33	0.59	0.43	48,98,126,136	0
24	CDL	P	305	100/100	0.60	0.32	46,83,127,140	0
24	CDL	C	306	100/100	0.63	0.28	50,82,111,115	0
20	TGL	N	611	63/63	0.65	0.29	51,77,104,121	0
18	PGV	N	606	51/51	0.66	0.31	55,79,121,126	0
18	PGV	P	304	51/51	0.68	0.24	60,80,108,116	0
22	CHD	J	101	29/29	0.69	0.29	62,80,116,123	0
26	PSC	R	201	52/52	0.70	0.27	43,73,150,161	0
18	PGV	C	305	51/51	0.72	0.23	53,79,113,119	0
18	PGV	A	606	51/51	0.74	0.29	41,78,96,100	0
20	TGL	L	101	63/63	0.74	0.26	39,68,100,105	0
20	TGL	D	201	63/63	0.76	0.19	47,70,96,99	0
20	TGL	N	608	63/63	0.77	0.24	53,78,123,143	0
25	DMU	Z	101	33/33	0.80	0.23	51,56,65,65	0
20	TGL	B	301	63/63	0.82	0.20	46,70,96,102	0
25	DMU	M	101	33/33	0.82	0.17	41,46,55,61	0
22	CHD	C	307	29/29	0.86	0.22	55,60,71,81	0
22	CHD	P	306	29/29	0.89	0.23	48,59,64,70	0
23	PEK	T	102	53/53	0.93	0.21	35,47,81,85	0
17	NA	P	301	1/1	0.93	0.08	47,47,47,47	0
17	NA	C	301	1/1	0.94	0.13	49,49,49,49	0
22	CHD	C	308	29/29	0.95	0.08	30,33,38,41	0
23	PEK	C	302	53/53	0.95	0.20	31,48,80,85	0
22	CHD	N	610	29/29	0.96	0.08	30,33,38,44	0
18	PGV	N	609	51/51	0.96	0.19	29,41,63,69	0
18	PGV	C	304	51/51	0.96	0.22	29,36,75,80	0
18	PGV	P	303	51/51	0.96	0.20	28,38,72,76	0
16	MG	N	604	1/1	0.97	0.11	36,36,36,36	0
18	PGV	A	608	51/51	0.97	0.21	28,39,64,70	0
22	CHD	O	301	29/29	0.97	0.07	26,30,34,41	0
22	CHD	B	303	29/29	0.97	0.08	28,30,34,43	0
14	HEA	N	602	60/60	0.98	0.12	25,28,33,36	0

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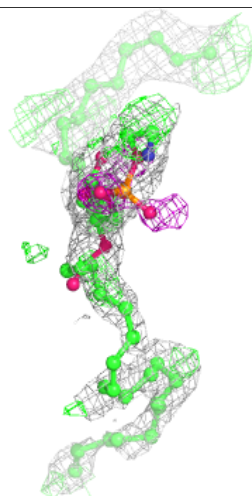
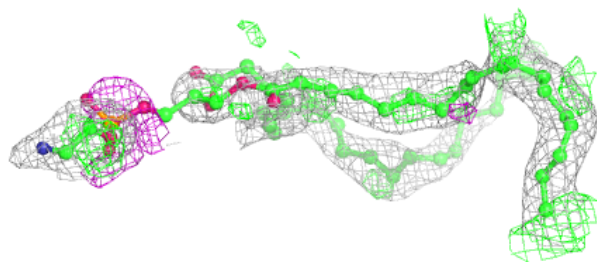
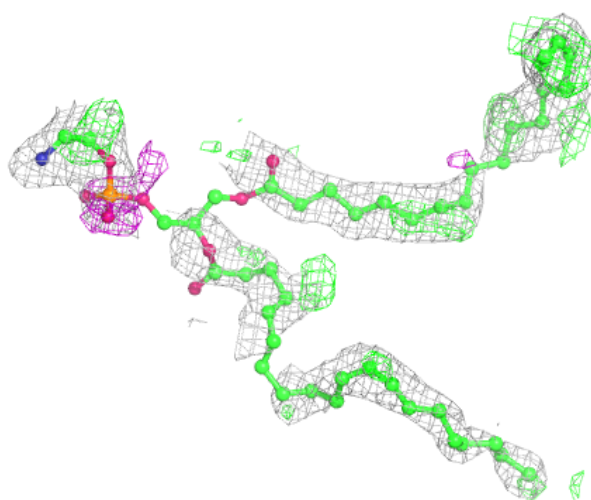
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
14	HEA	N	601	60/60	0.98	0.14	26,31,52,58	0
14	HEA	A	602	60/60	0.98	0.11	23,26,33,34	0
14	HEA	A	601	60/60	0.98	0.12	22,26,51,55	0
19	PER	N	607[A]	2/2	0.99	0.17	21,21,21,25	0
16	MG	A	604	1/1	0.99	0.08	29,29,29,29	0
19	PER	N	607[B]	2/2	0.99	0.17	19,19,19,19	2
17	NA	A	605	1/1	0.99	0.05	30,30,30,30	0
15	CU	N	603	1/1	1.00	0.12	29,29,29,29	0
19	PER	A	607[A]	2/2	1.00	0.13	19,19,19,25	0
17	NA	N	605	1/1	1.00	0.07	35,35,35,35	0
21	CUA	O	302	2/2	1.00	0.07	34,34,34,35	0
27	ZN	S	101	1/1	1.00	0.06	34,34,34,34	0
19	PER	A	607[B]	2/2	1.00	0.13	15,15,15,15	2
21	CUA	B	302	2/2	1.00	0.09	29,29,29,30	0
15	CU	A	603	1/1	1.00	0.09	27,27,27,27	0
27	ZN	F	101	1/1	1.00	0.05	33,33,33,33	0

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

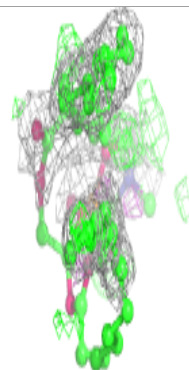
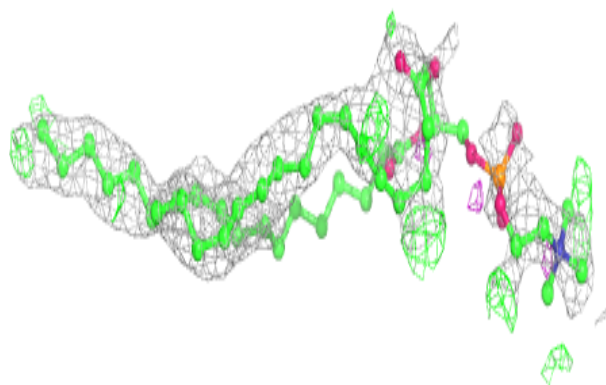
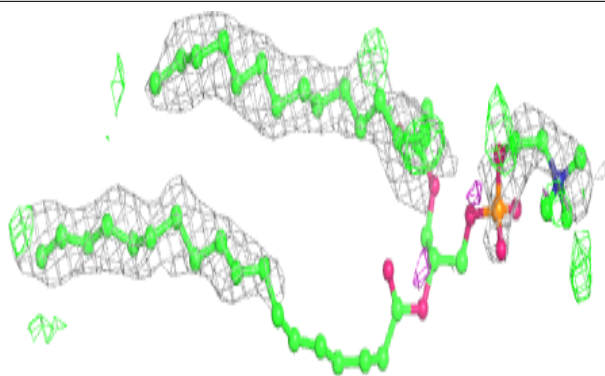
**Electron density around PEK C 303:**

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

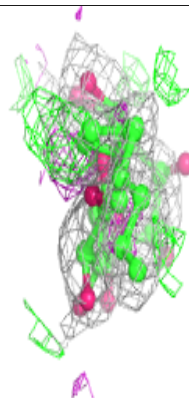
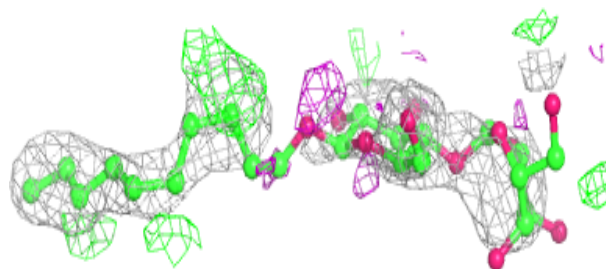
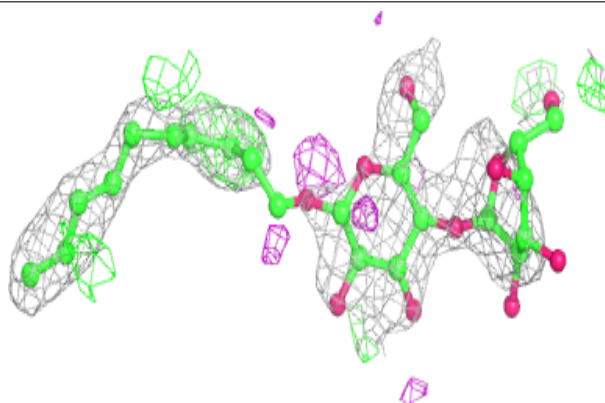


**Electron density around PSC E 201:**

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

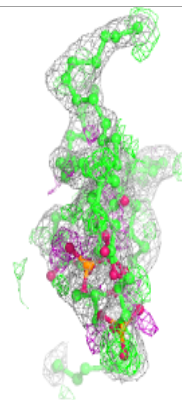
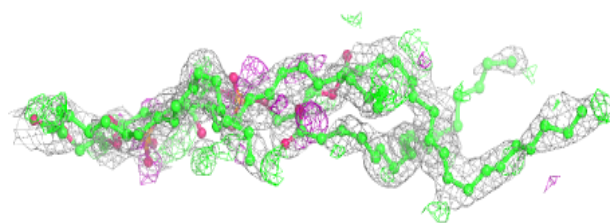
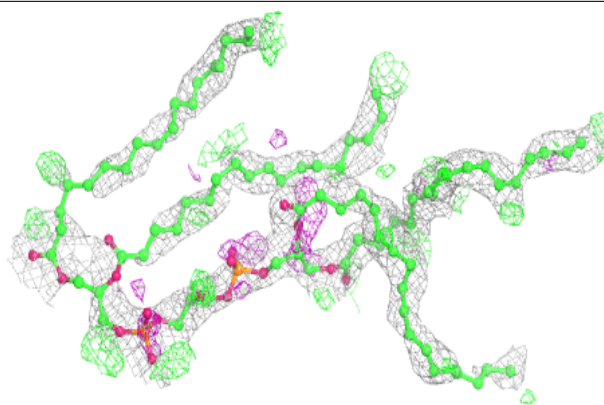
**Electron density around DMU C 309:**

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

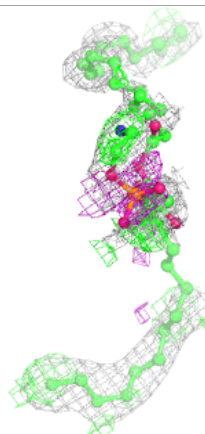
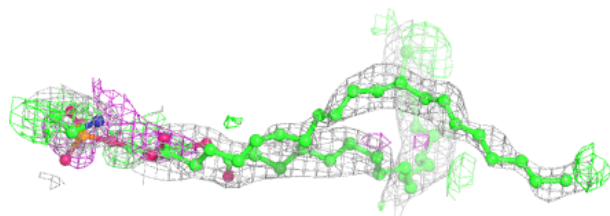
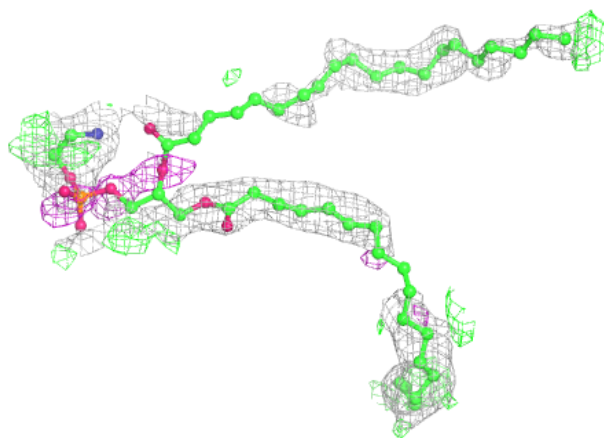


**Electron density around CDL G 101:**

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and green (positive)

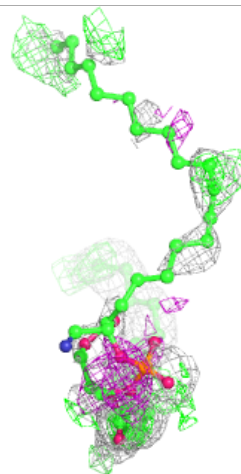
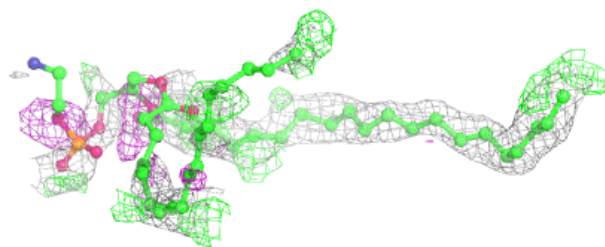
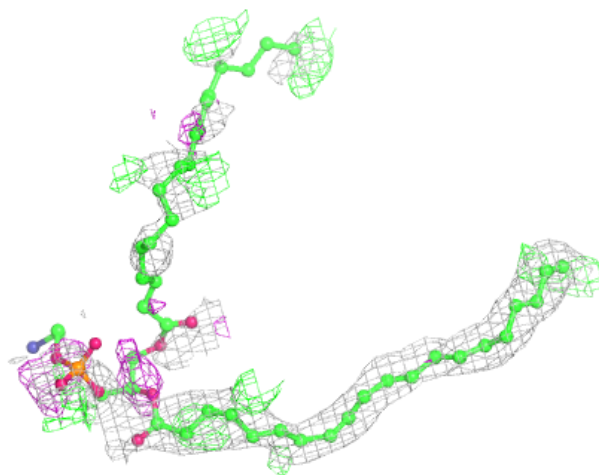
**Electron density around PEK P 302:**

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



**Electron density around PEK G 102:**

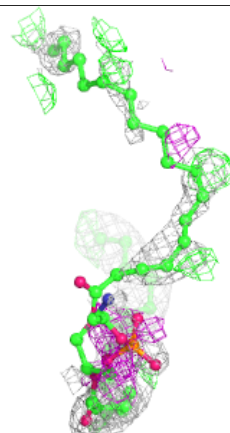
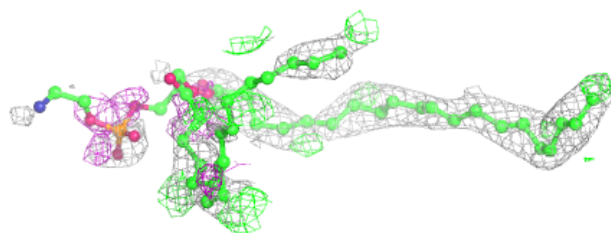
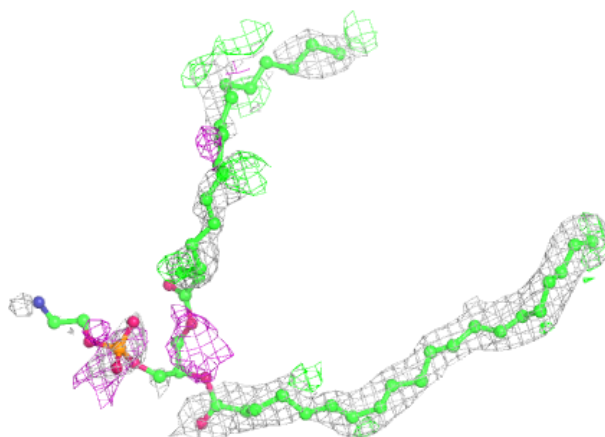
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



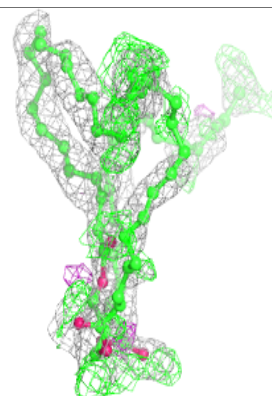
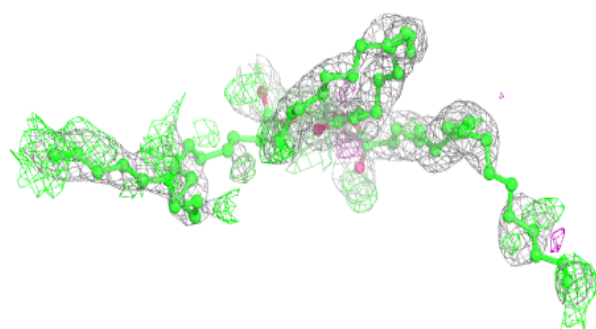
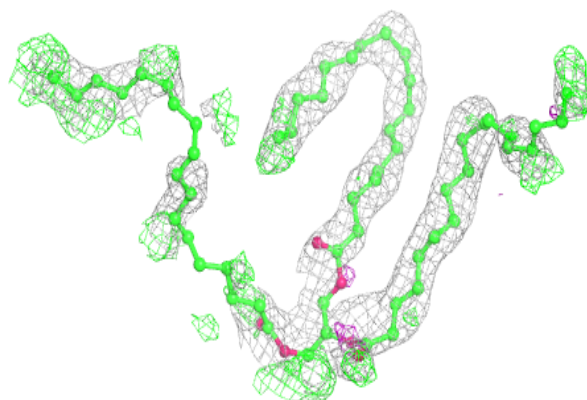


**Electron density around PEK T 101:**

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

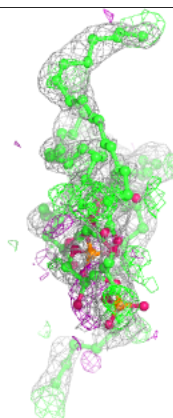
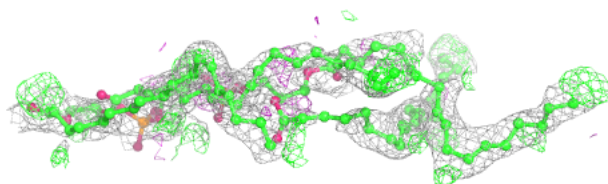
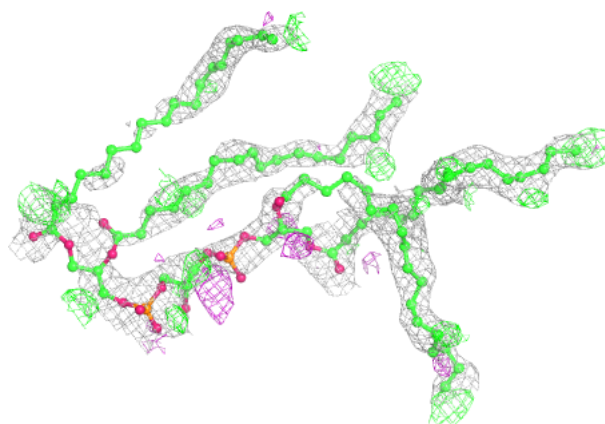
**Electron density around TGL Q 201:**

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

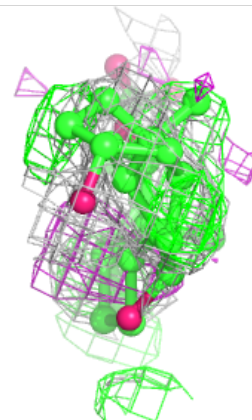
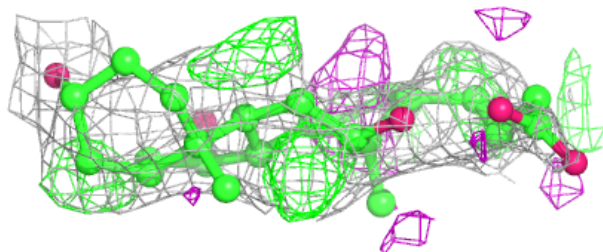
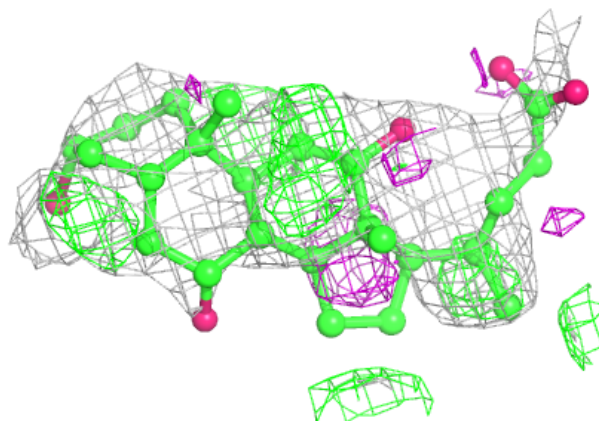


**Electron density around CDL T 103:**

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

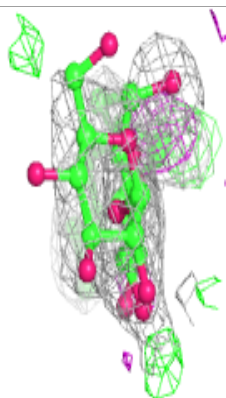
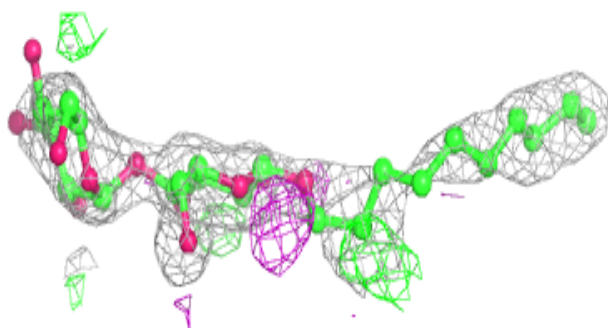
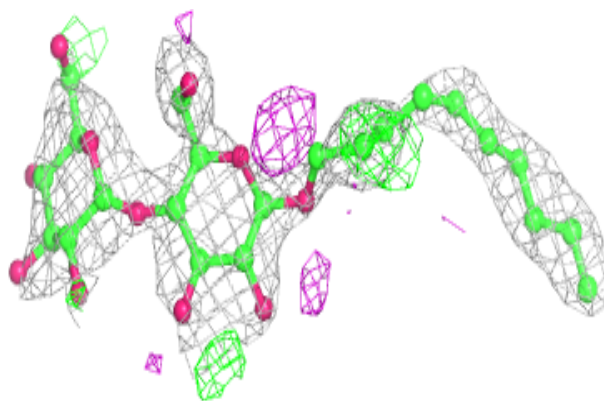
**Electron density around CHD W 101:**

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

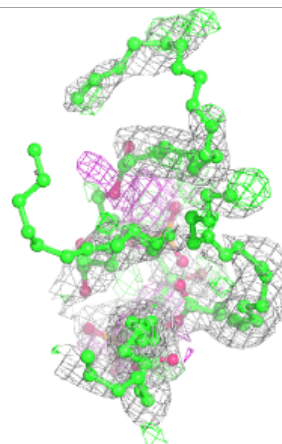
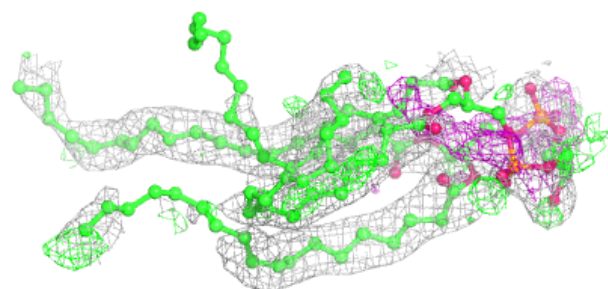
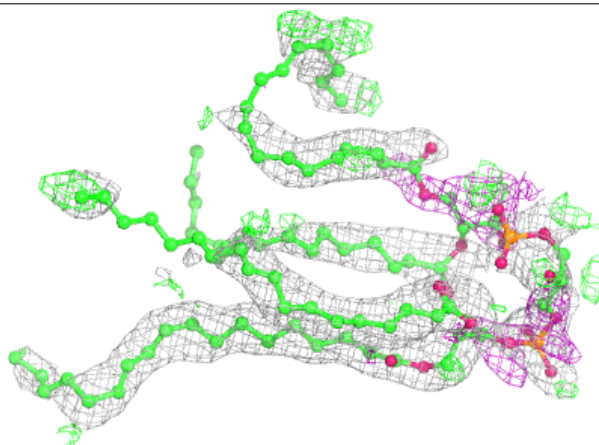


**Electron density around DMU P 307:**

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

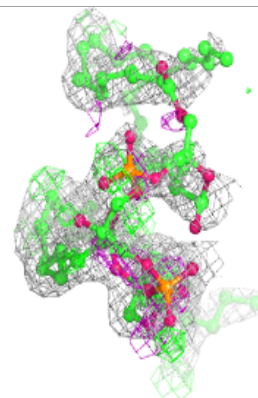
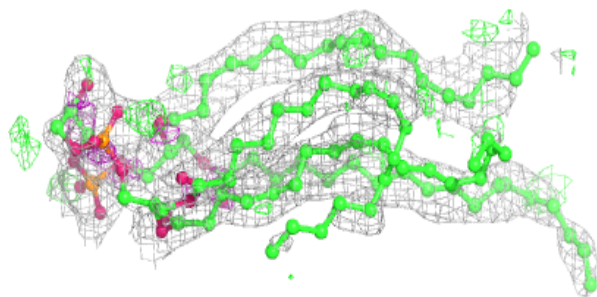
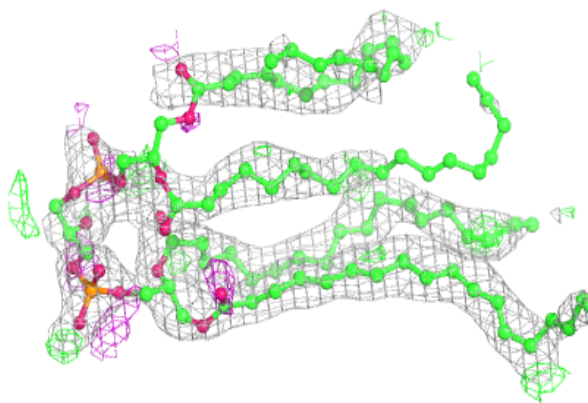
**Electron density around CDL P 305:**

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



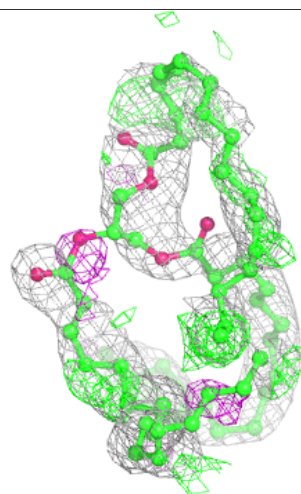
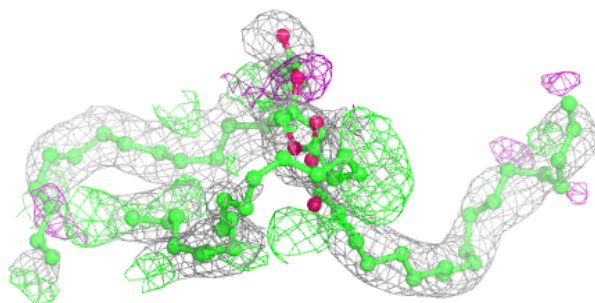
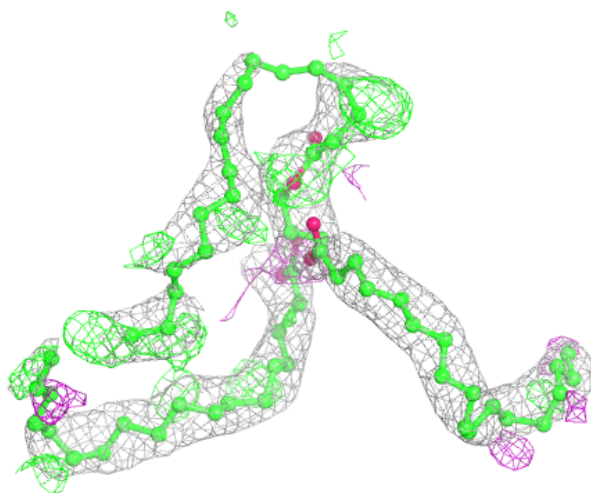
**Electron density around CDL C 306:**

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



**Electron density around TGL N 611:**

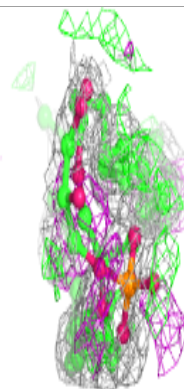
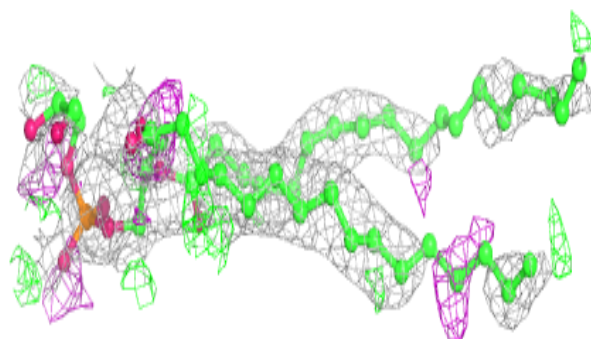
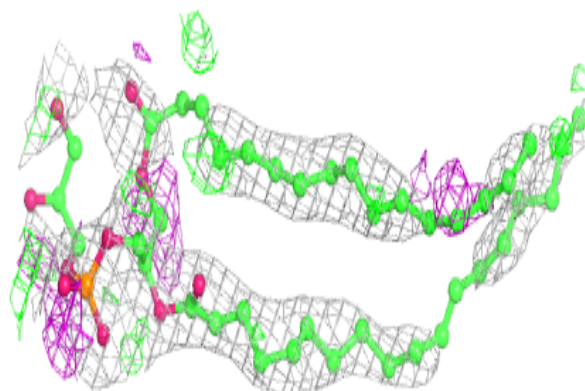
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



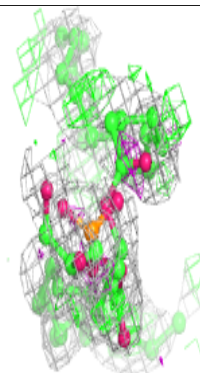
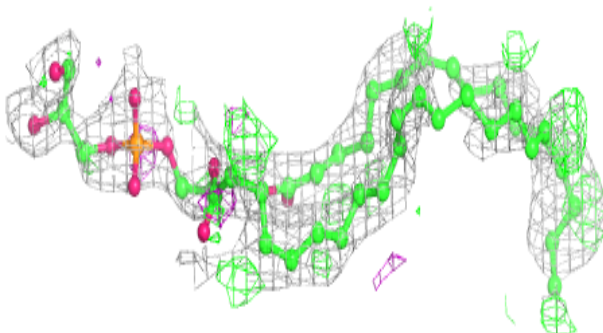
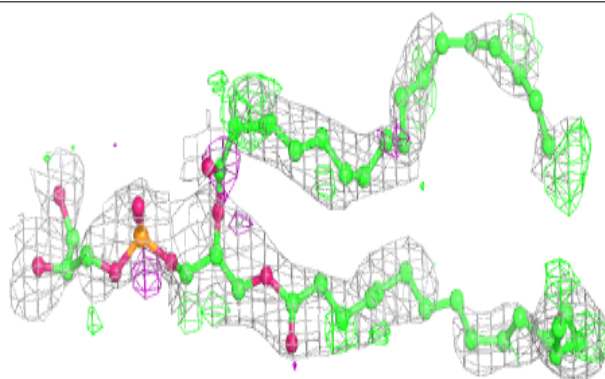


**Electron density around PGV N 606:**

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

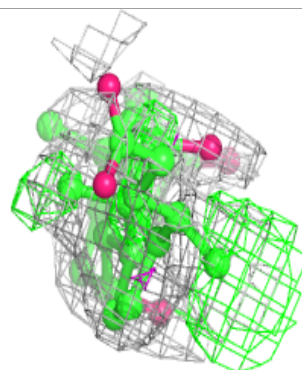
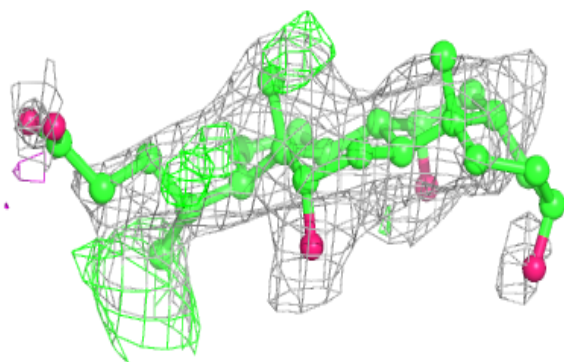
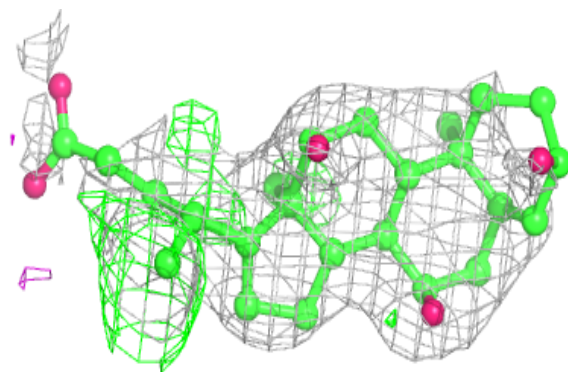
**Electron density around PGV P 304:**

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

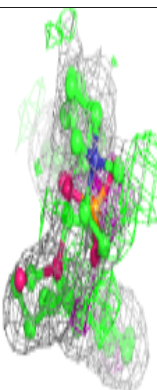
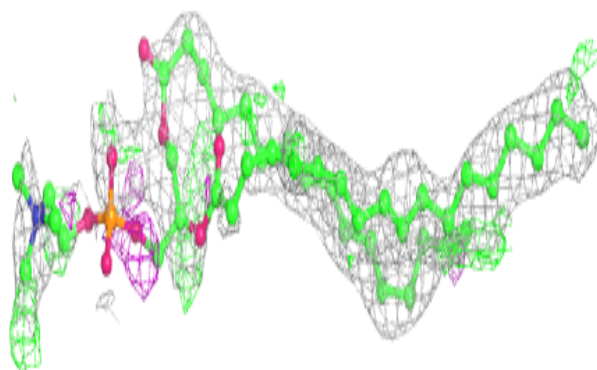
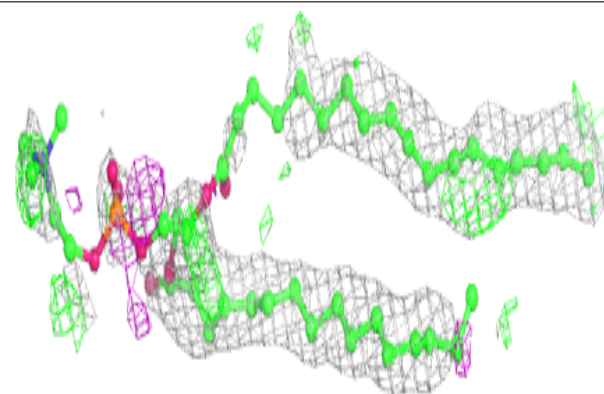


**Electron density around CHD J 101:**

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

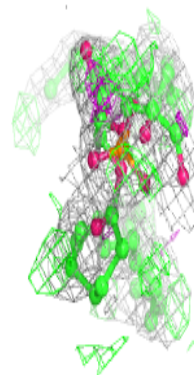
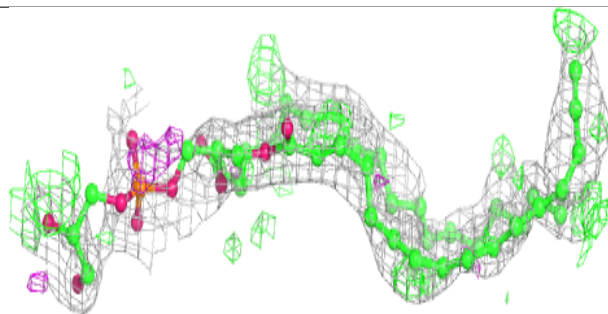
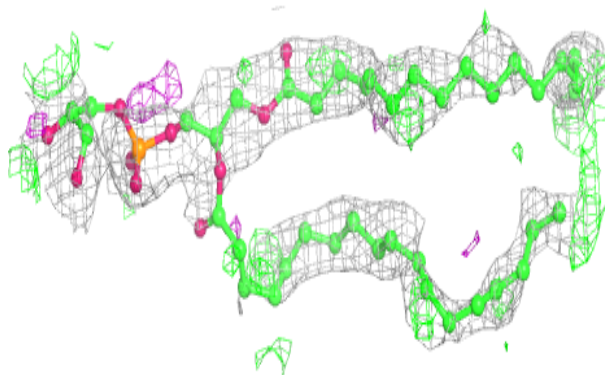
**Electron density around PSC R 201:**

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

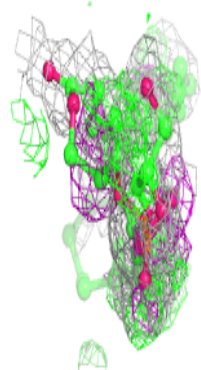
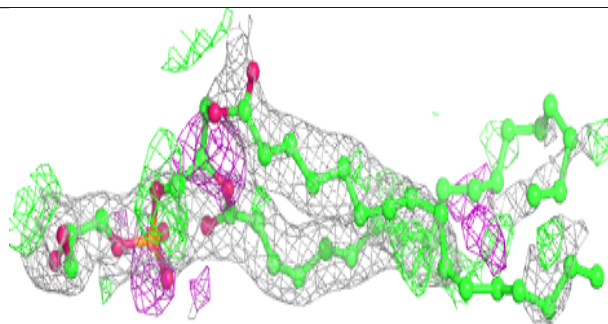
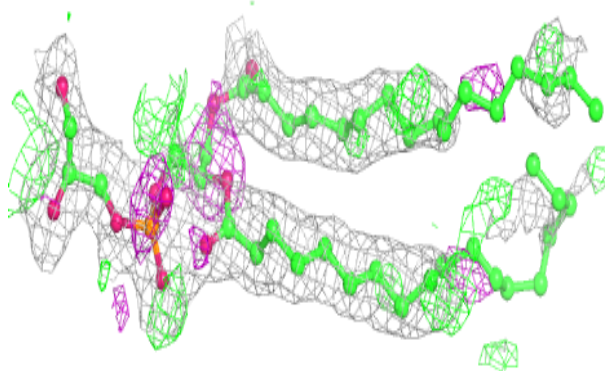


**Electron density around PGV C 305:**

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

**Electron density around PGV A 606:**

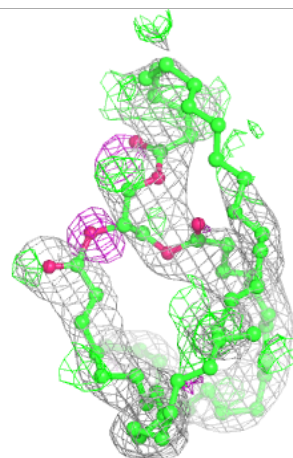
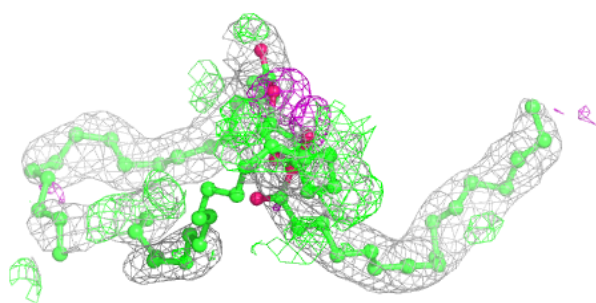
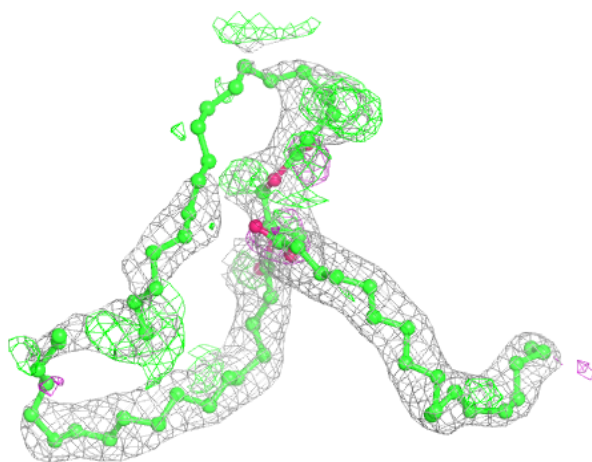
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





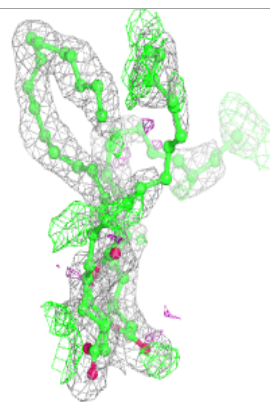
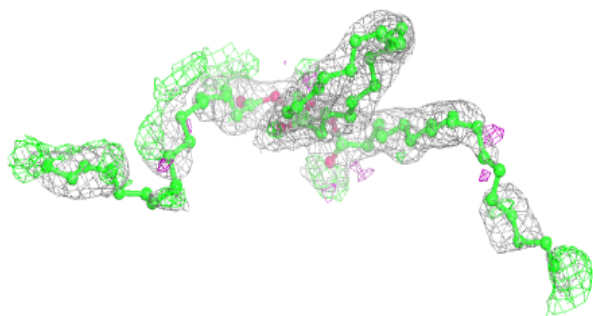
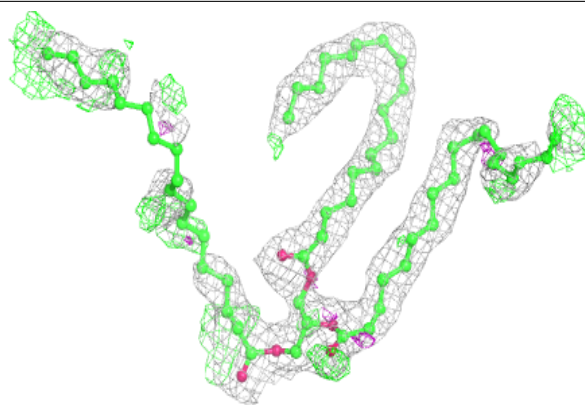
**Electron density around TGL L 101:**

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

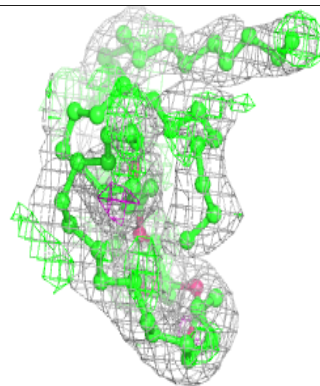
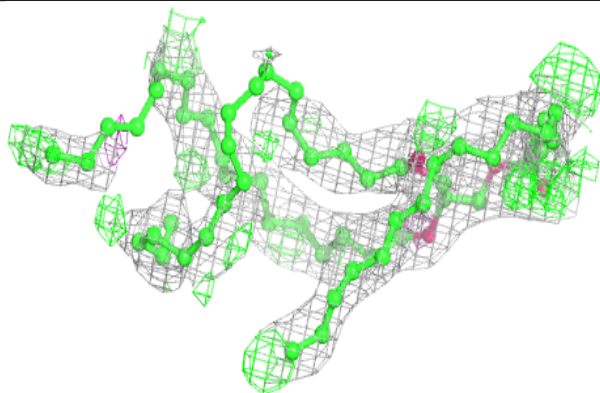
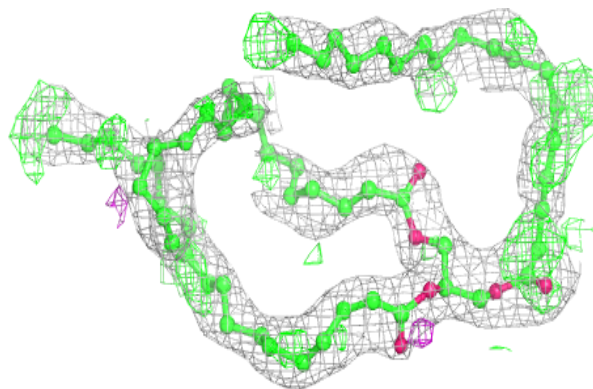


**Electron density around TGL D 201:**

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

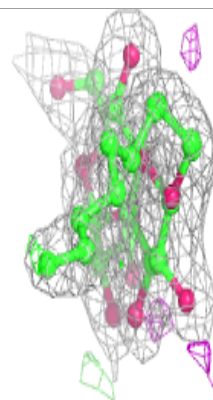
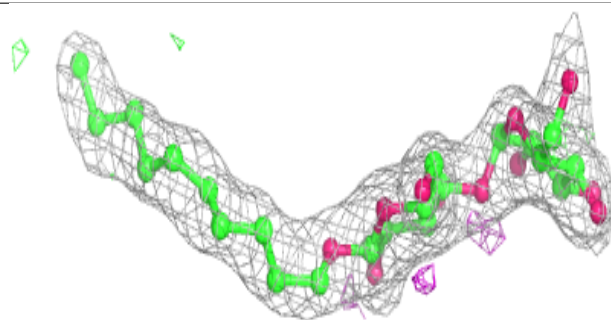
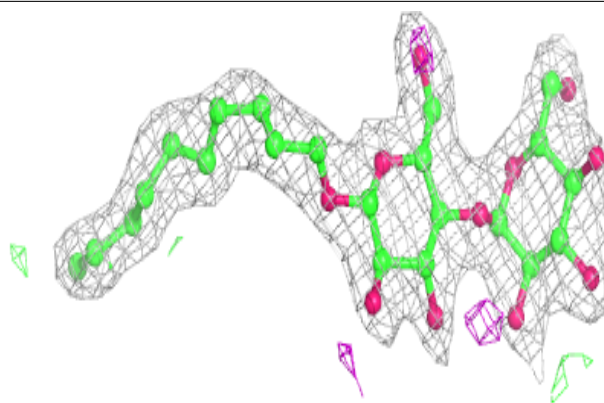
**Electron density around TGL N 608:**

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

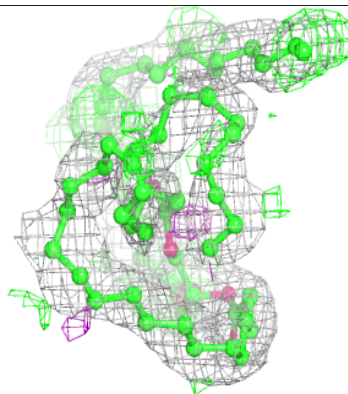
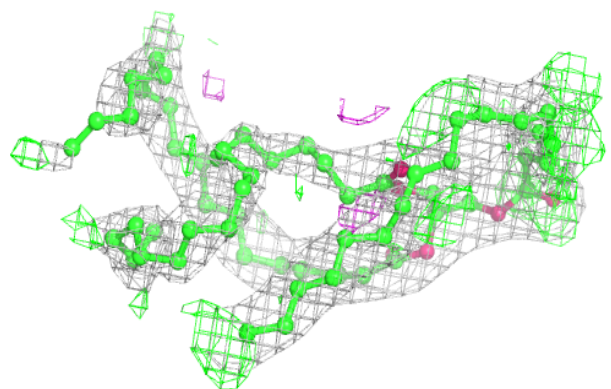
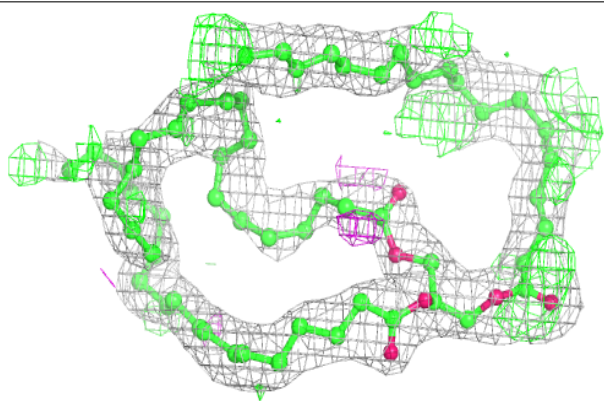


**Electron density around DMU Z 101:**

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

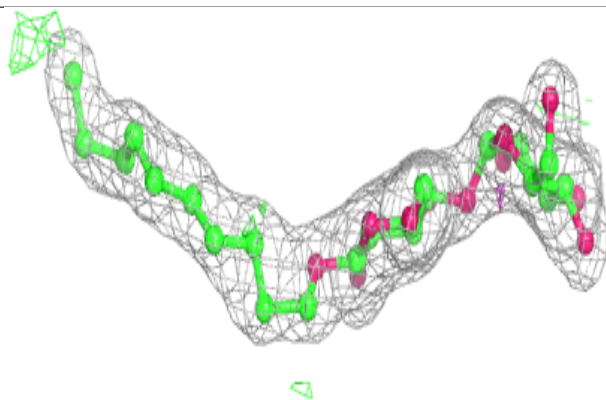
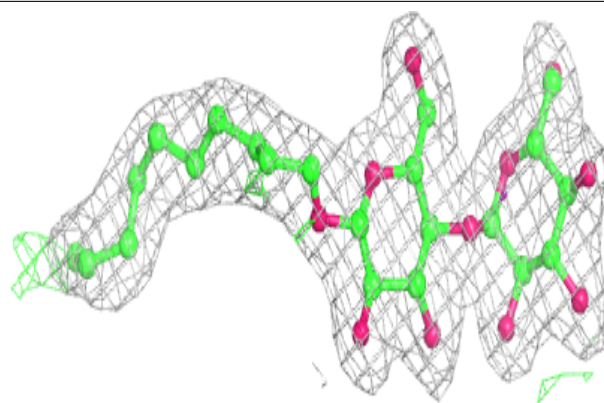
**Electron density around TGL B 301:**

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

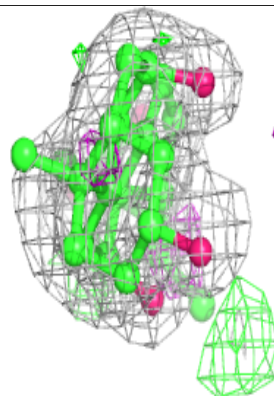
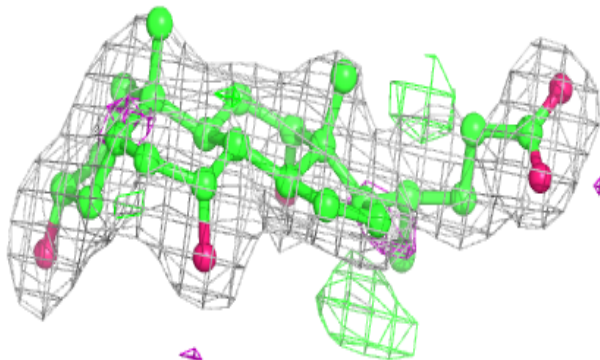
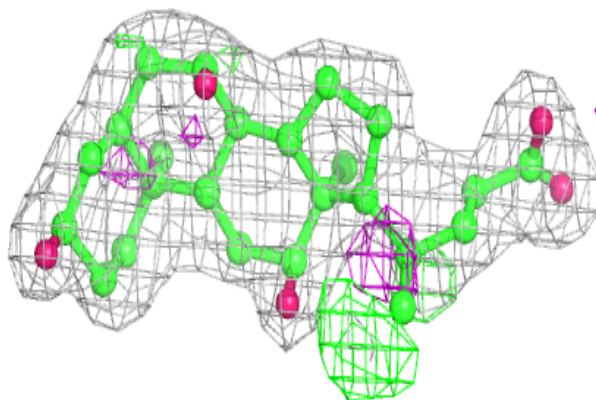


**Electron density around DMU M 101:**

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

**Electron density around CHD C 307:**

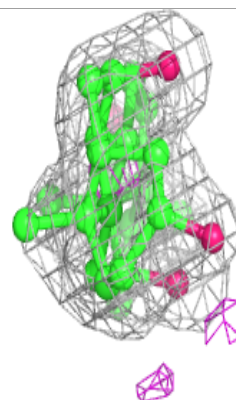
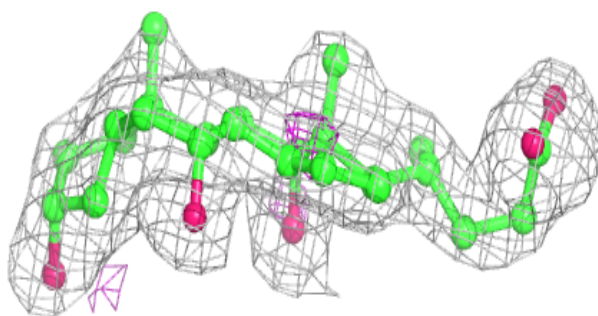
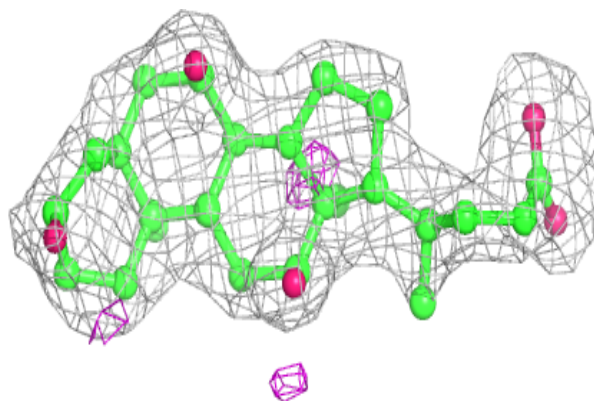
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



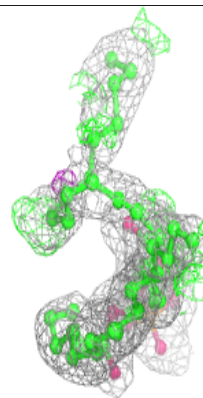
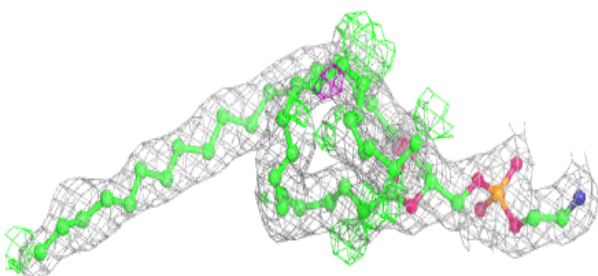
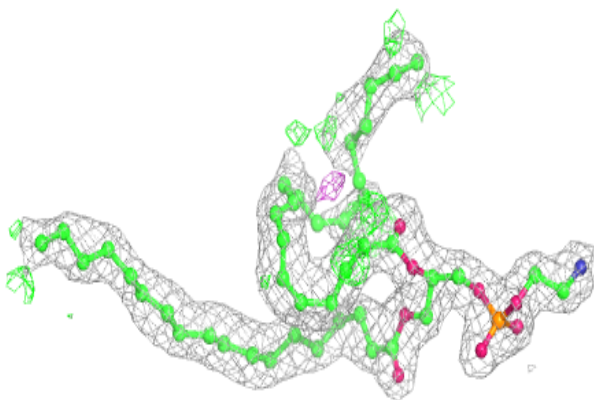


**Electron density around CHD P 306:**

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

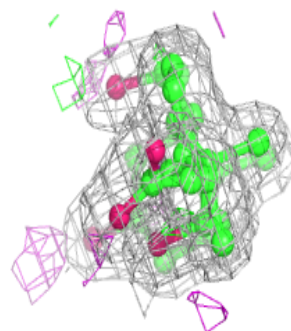
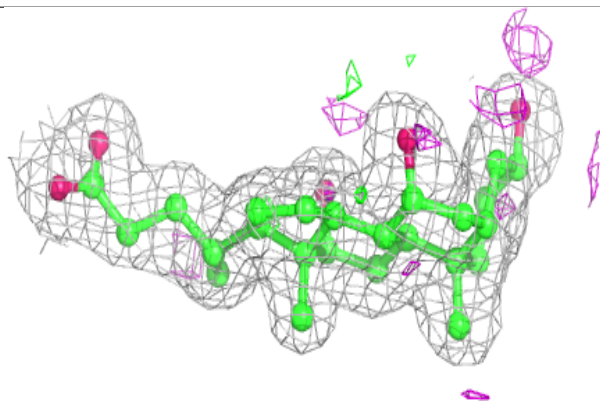
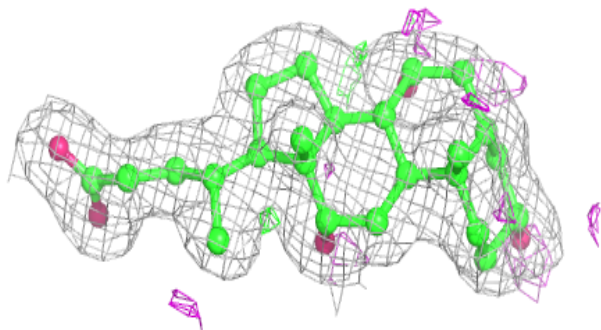
**Electron density around PEK T 102:**

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

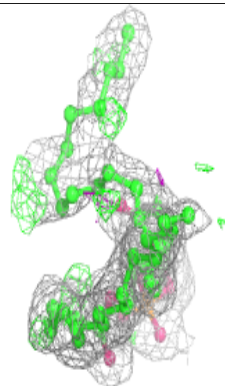
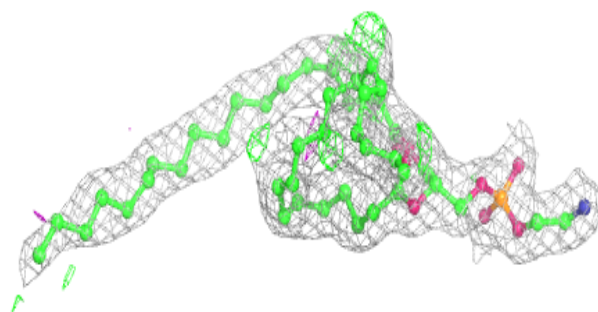
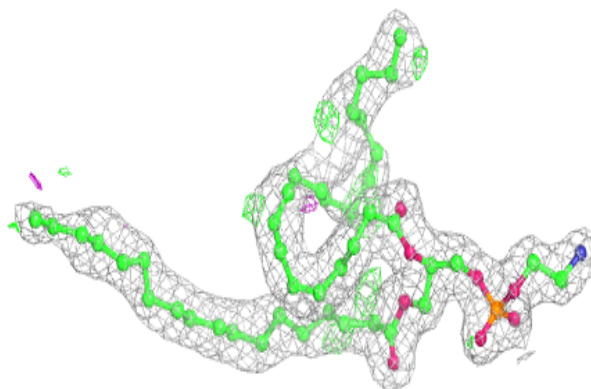


**Electron density around CHD C 308:**

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

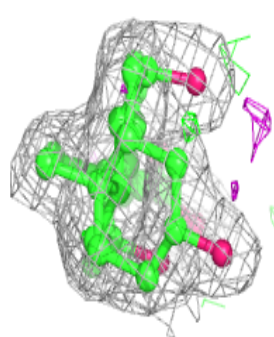
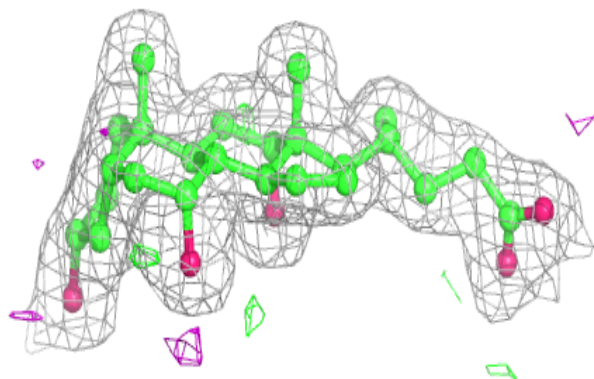
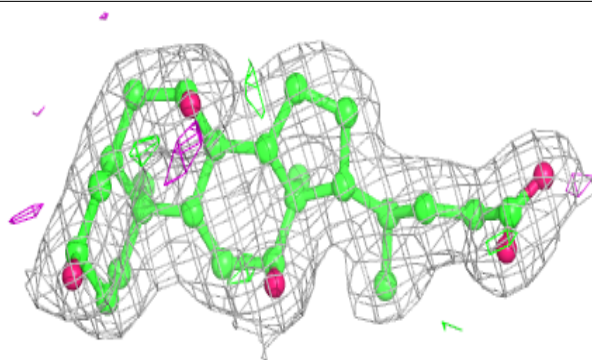
**Electron density around PEK C 302:**

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

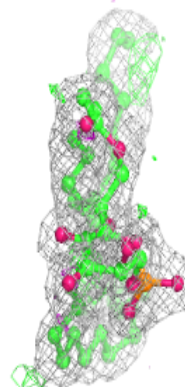
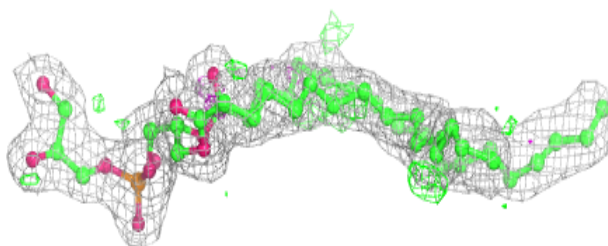
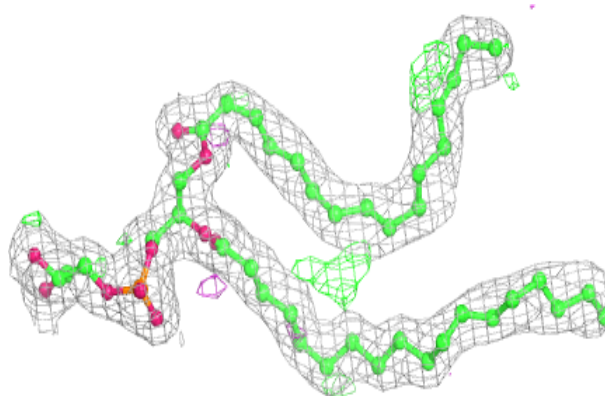


**Electron density around CHD N 610:**

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

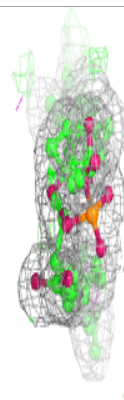
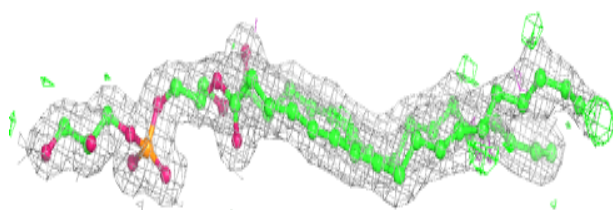
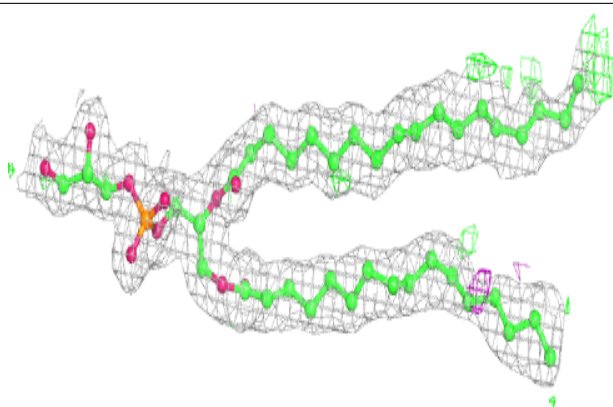
**Electron density around PGV N 609:**

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

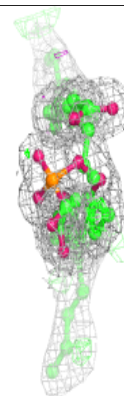
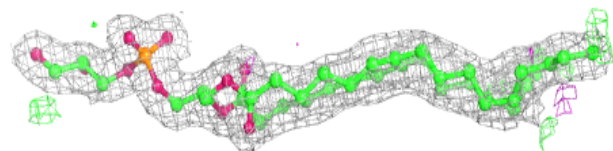
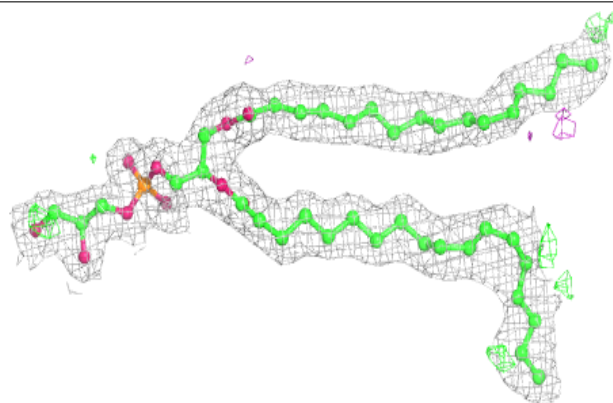


**Electron density around PGV C 304:**

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

**Electron density around PGV P 303:**

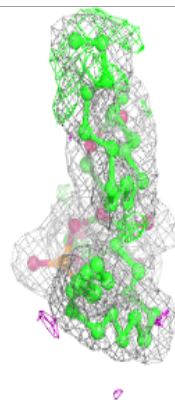
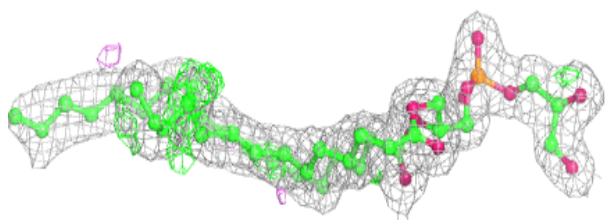
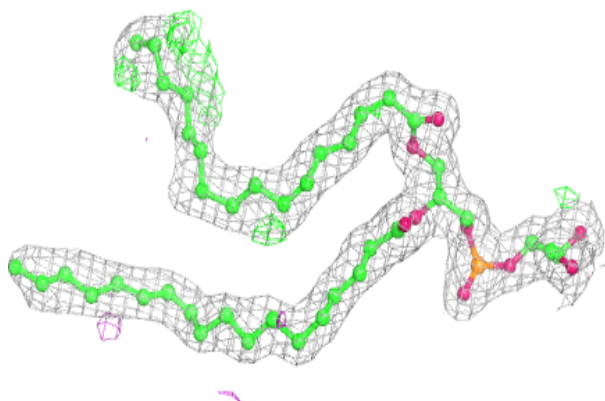
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



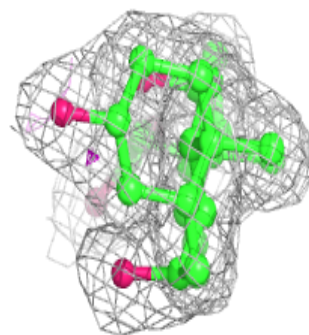
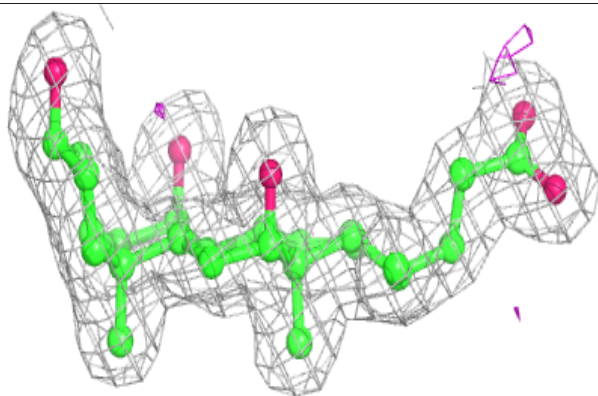
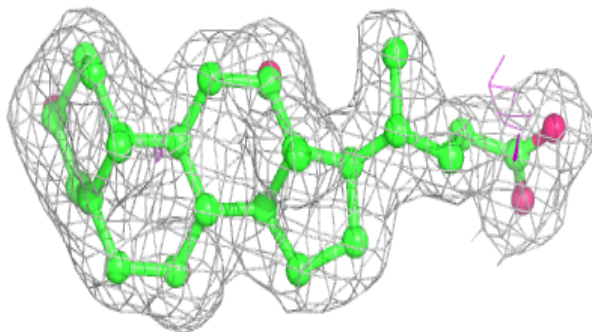


**Electron density around PGV A 608:**

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

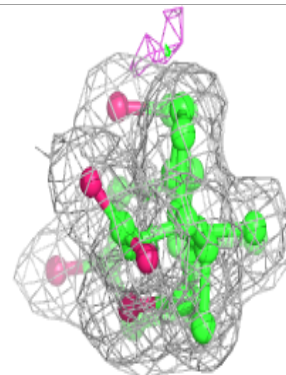
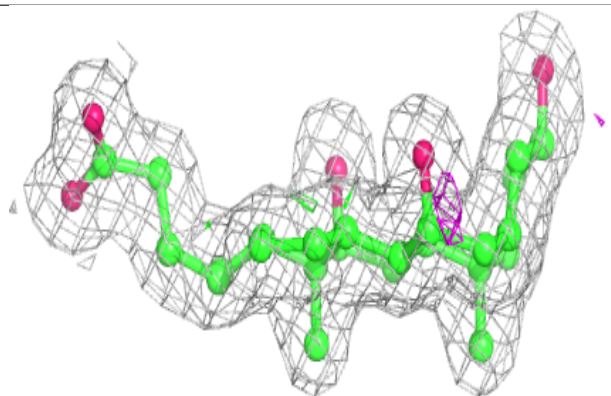
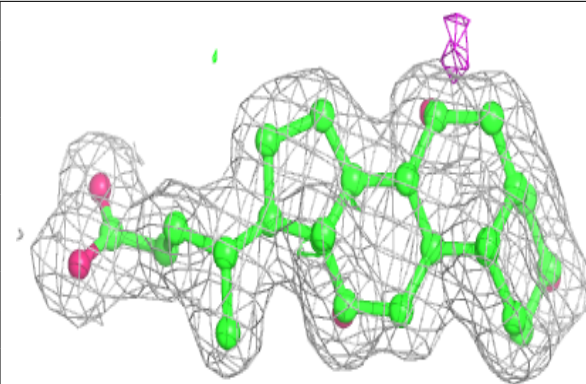
**Electron density around CHD O 301:**

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

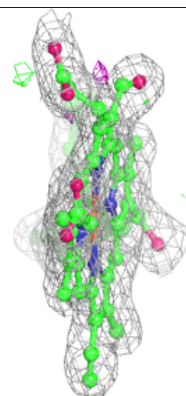
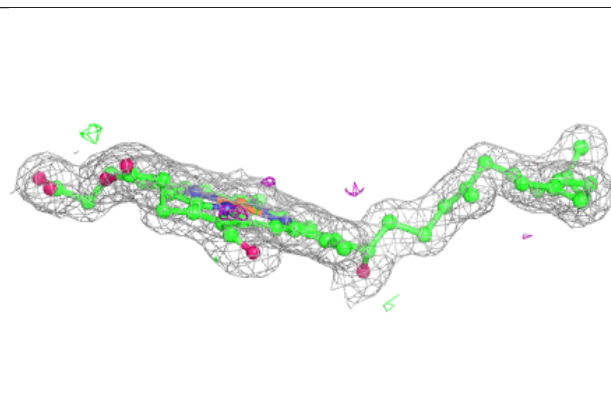
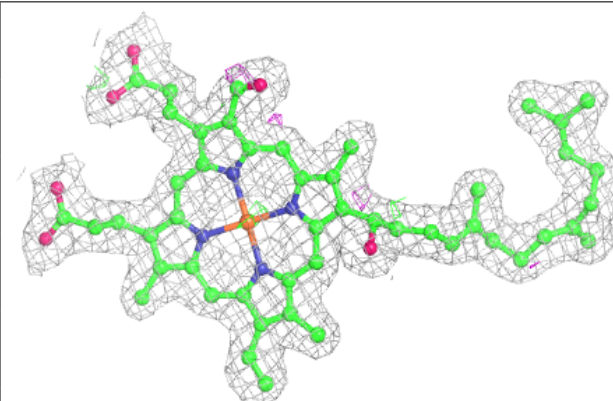


**Electron density around CHD B 303:**

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

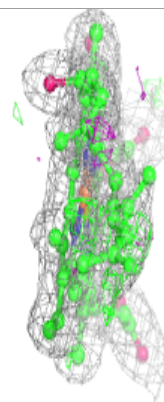
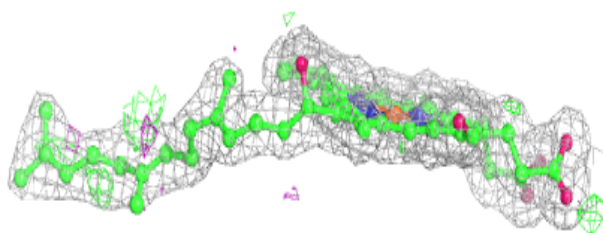
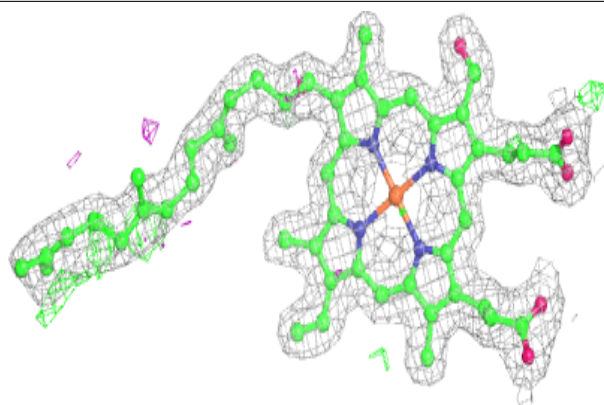
**Electron density around HEA N 602:**

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

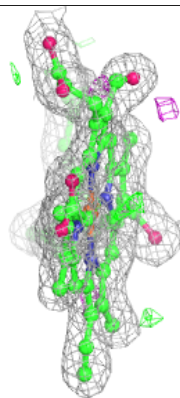
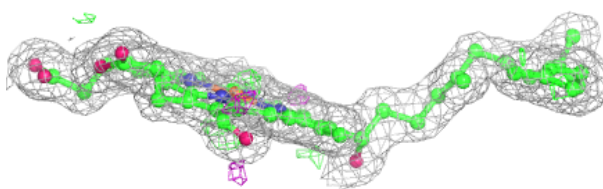
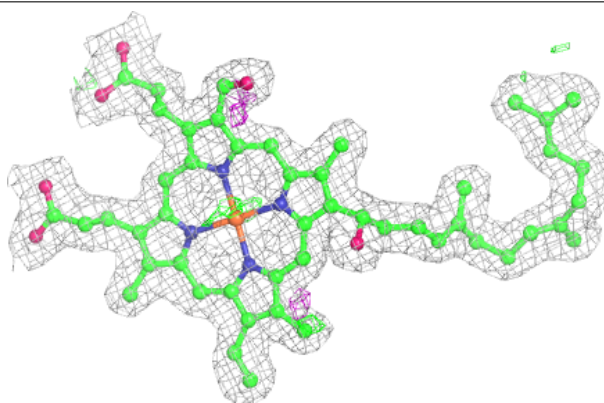


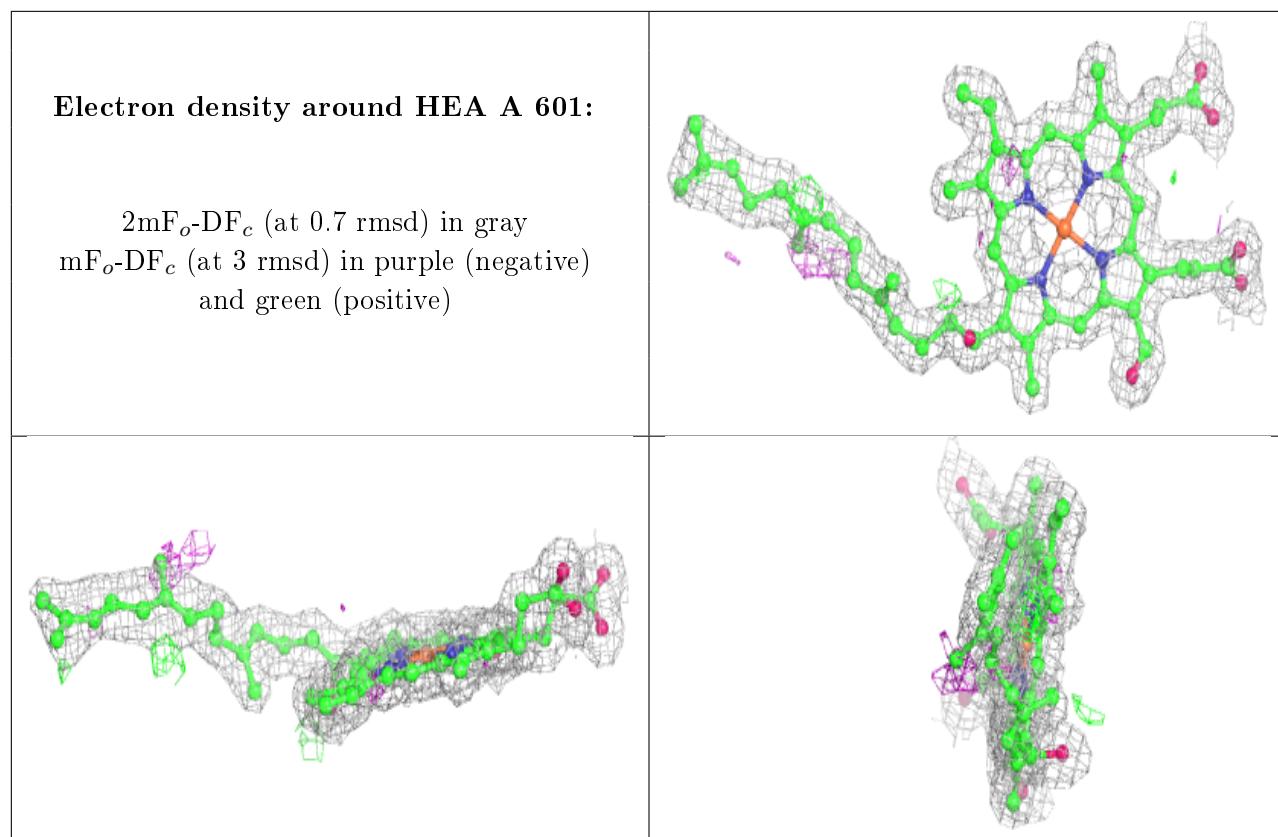
**Electron density around HEA N 601:**

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

**Electron density around HEA A 602:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.