



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2026 – 03:40 PM JST

PDB ID : 7XMA / pdb_00007xma
Title : Crystal structure of Bovine heart cytochrome c oxidase, apo structure with DMSO
Authors : Nishida, Y.; Shinzawa-Itoh, K.; Mizuno, N.; Kumasaka, T.; Yoshikawa, S.; Tsukihara, T.; Takashima, S.; Shintani, Y.
Deposited on : 2022-04-25
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

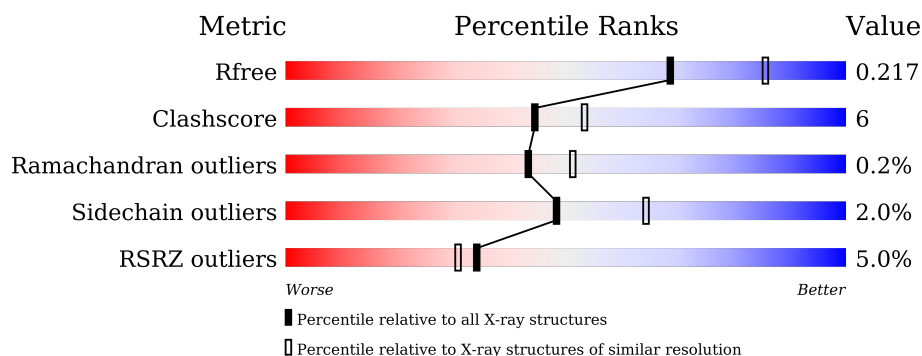
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	514	
1	N	514	
2	B	581	
2	O	581	
3	C	261	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	P	261	 % 90% 10% .
4	D	147	 3% 87% 11% .
4	Q	147	 6% 85% 10% 5%
5	E	109	 2% 93% . .
5	R	109	 6% 94% . .
6	F	98	 4% 88% 6% 5%
6	S	98	 9% 92% 6% .
7	G	84	 21% 77% 15% 5% .
7	T	84	 18% 75% 19% . .
8	H	85	 12% 82% 9% 7%
8	U	85	 12% 80% 13% 7%
9	I	73	 11% 95% . .
9	V	73	 14% 95% . .
10	J	59	 5% 93% . .
10	W	59	 5% 88% 7% . .
11	K	56	 7% 80% 7% 9%
11	X	56	 4% 79% 9% 12%
12	L	47	 4% 83% 15% .
12	Y	47	 6% 83% 13% .
13	M	46	 9% 85% 7% 7%
13	Z	46	 9% 83% 7% 11%

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 33571 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	11	0
			4115	2746	637	694	38			
1	N	514	Total	C	N	O	S	8	11	0
			4115	2747	637	692	39			

- Molecule 2 is a protein called Cytochrome c oxidase subunit 2, Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	5	0
			1869	1215	288	346	20			
2	O	227	Total	C	N	O	S	0	6	0
			1877	1220	289	347	21			

- 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
			2181	1455	346	363	17			
3	P	259	Total	C	N	O	S	0	9	0
			2184	1456	349	363	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	238	GLY	ALA	conflict	UNP P00415
P	238	GLY	ALA	conflict	UNP P00415

- 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	3	0
			1222	797	200	221	4			
4	Q	139	Total	C	N	O	S	0	2	0
			1182	770	195	213	4			

- 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	1	0
			863	550	148	163	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	93	Total	C	N	O	S	0	3	0
			737	456	132	144	5			
6	S	96	Total	C	N	O	S	0	1	0
			740	460	131	143	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
7	G	82	Total 678	C 436	N 129	O 111	P 1	S 1	0	1	0
7	T	82	Total 664	C 425	N 127	O 110	P 1	S 1	0	0	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	72	Total	C	N	O	S	0	0	0
			592	385	106	97	4			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	V	72	Total	C	N	O	S	0	0	0
			592	385	106	97	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	57	Total	C	N	O	S	0	0	0
			451	291	76	81	3			
10	W	57	Total	C	N	O	S	0	1	0
			460	296	77	84	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	51	Total	C	N	O	S	0	0	0
			402	260	68	72	2			
11	X	49	Total	C	N	O	S	0	1	0
			391	255	66	68	2			

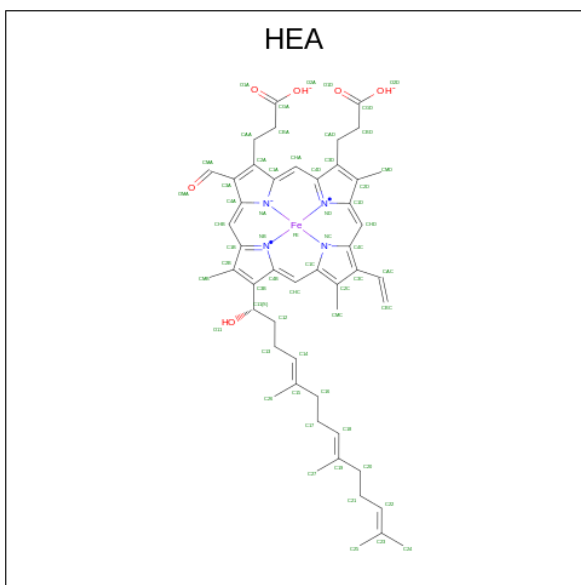
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			380	254	64	60	2			
12	Y	45	Total	C	N	O	S	0	1	0
			378	253	63	59	3			

- 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	41	Total	C	N	O	0	0	0
			320	214	50	56			

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



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

- Molecule 15 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

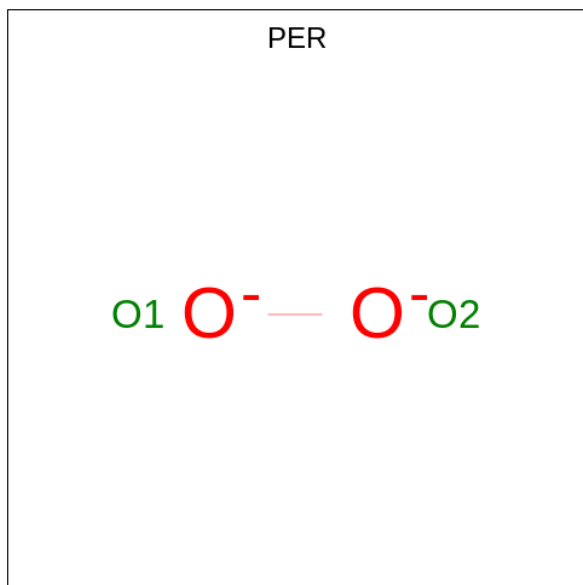
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 17 is SODIUM ION (CCD ID: NA) (formula: Na).

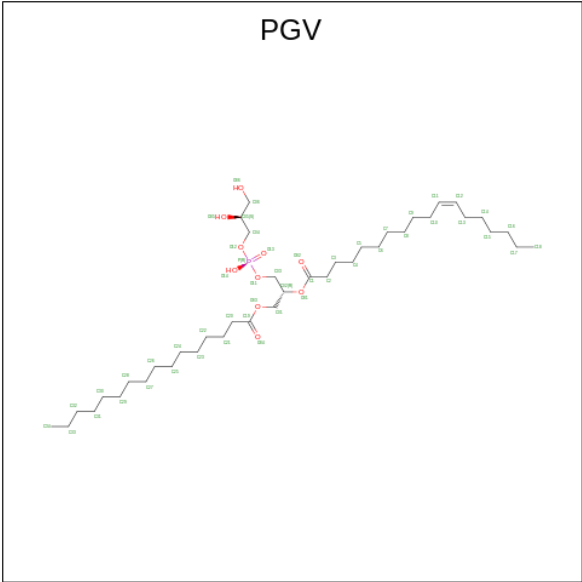
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Na	0	0
			1	1		
17	N	1	Total	Na	0	0
			1	1		

- Molecule 18 is PEROXIDE ION (CCD ID: PER) (formula: O₂).



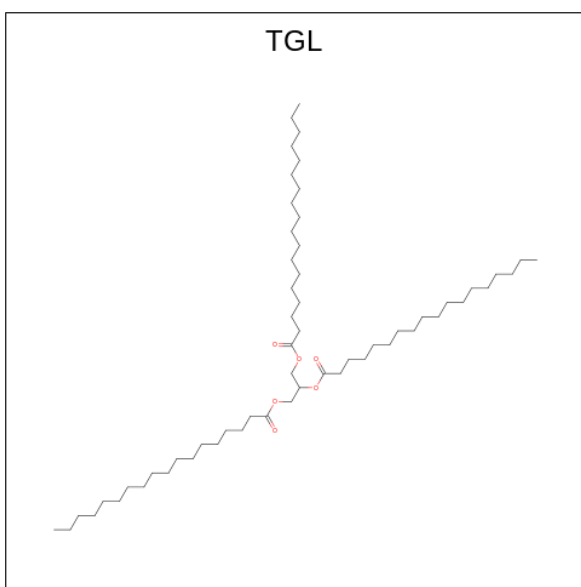
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	1	Total	O	0	0
			2	2		
18	N	1	Total	O	0	0
			2	2		

- Molecule 19 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P).



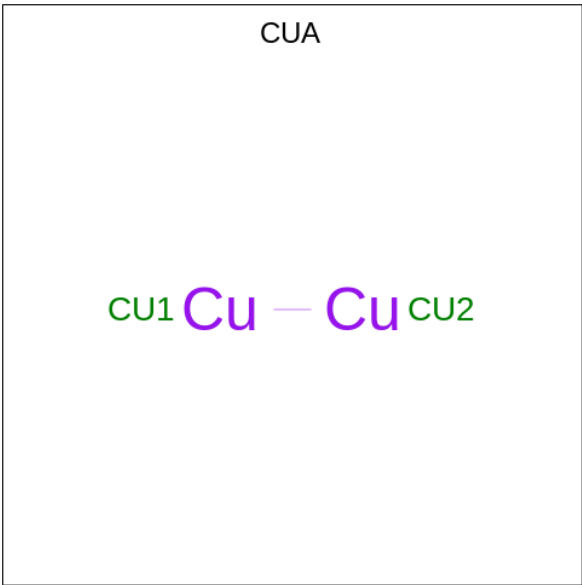
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	D	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	P	1	Total	C	O	P	0	0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

- Molecule 20 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: C₅₇H₁₁₀O₆).



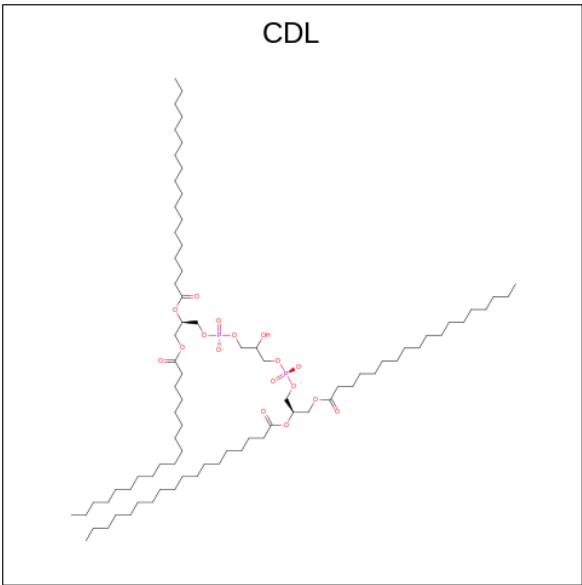
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	A	1	Total	C	O	0	0
			63	57	6		
20	D	1	Total	C	O	0	0
			63	57	6		
20	L	1	Total	C	O	0	0
			63	57	6		
20	N	1	Total	C	O	0	0
			63	57	6		
20	Q	1	Total	C	O	0	0
			63	57	6		
20	Y	1	Total	C	O	0	0
			63	57	6		

- Molecule 21 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



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 CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



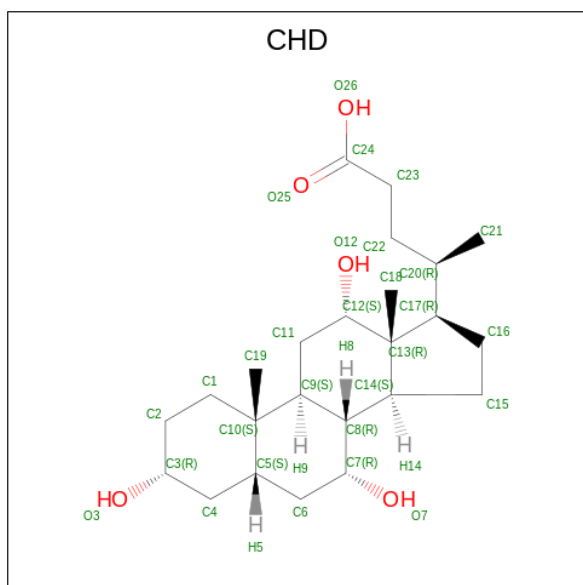
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
22	C	1	Total	C	O	P	0	0
			100	81	17	2		
22	G	1	Total	C	O	P	0	0
			100	81	17	2		

Continued on next page...

Continued from previous page...

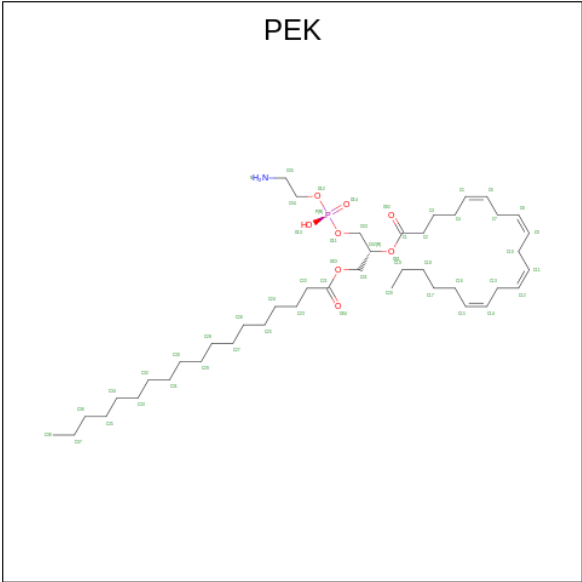
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
22	P	1	Total	C	O	P	0	0
			100	81	17	2		
22	T	1	Total	C	O	P	0	0
			100	81	17	2		

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



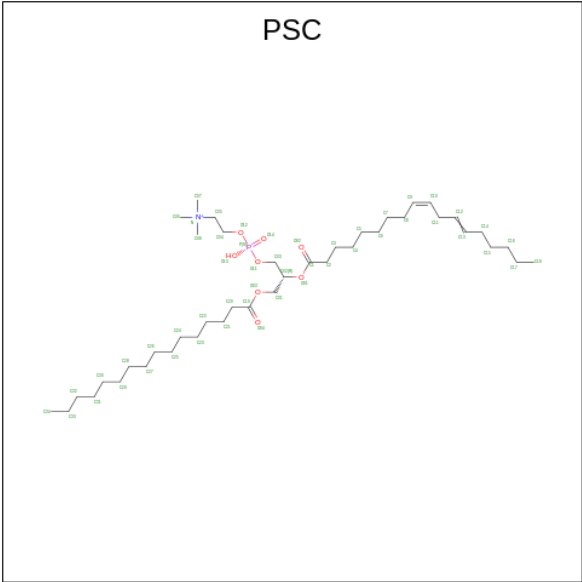
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	C	1	Total	C	O		0	0
			29	24	5			
23	C	1	Total	C	O		0	0
			29	24	5			
23	G	1	Total	C	O		0	0
			29	24	5			
23	P	1	Total	C	O		0	0
			29	24	5			
23	P	1	Total	C	O		0	0
			29	24	5			
23	T	1	Total	C	O		0	0
			29	24	5			

- Molecule 24 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (CCD ID: PEK) (formula: $C_{43}H_{78}NO_8P$).



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

- Molecule 25 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 (CCD ID: PSC) (formula: C₄₂H₈₁NO₈P).

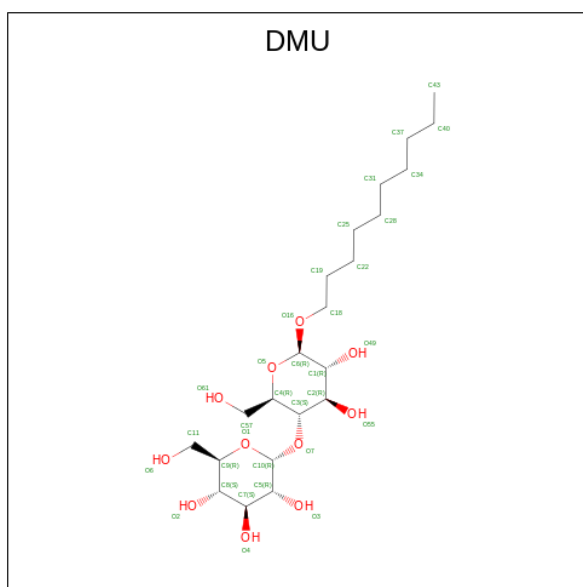


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	E	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
25	O	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 26 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 27 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: C₂₂H₄₂O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	J	1	Total 33	C 22	O 11	0	0
27	M	1	Total 33	C 22	O 11	0	0
27	W	1	Total 33	C 22	O 11	0	0
27	Z	1	Total 33	C 22	O 11	0	0

- Molecule 28 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	276	Total O 276 276	0	0
28	B	180	Total O 180 180	0	0
28	C	149	Total O 149 149	0	0
28	D	179	Total O 179 179	0	0
28	E	128	Total O 128 128	0	0
28	F	119	Total O 119 119	0	0
28	G	65	Total O 65 65	0	0
28	H	76	Total O 76 76	0	0

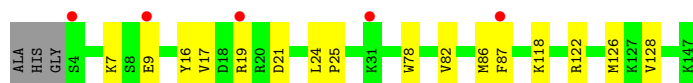
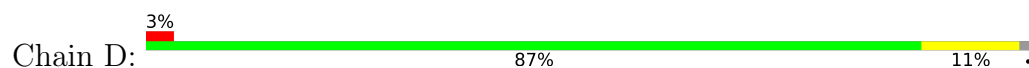
Continued on next page...

Continued from previous page...

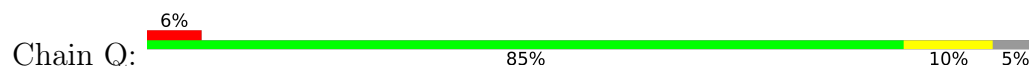
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	I	51	Total 51	O 51	0	0
28	J	41	Total 41	O 41	0	0
28	K	36	Total 36	O 36	0	0
28	L	40	Total 40	O 40	0	0
28	M	36	Total 36	O 36	0	0
28	N	289	Total 289	O 289	0	0
28	O	139	Total 139	O 139	0	0
28	P	144	Total 144	O 144	0	0
28	Q	69	Total 69	O 69	0	0
28	R	81	Total 81	O 81	0	0
28	S	118	Total 118	O 118	0	0
28	T	63	Total 63	O 63	0	0
28	U	61	Total 61	O 61	0	0
28	V	28	Total 28	O 28	0	0
28	W	35	Total 35	O 35	0	0
28	X	25	Total 25	O 25	0	0
28	Y	34	Total 34	O 34	0	0
28	Z	24	Total 24	O 24	0	0



- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



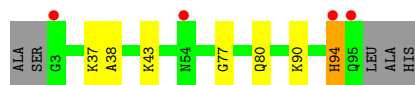
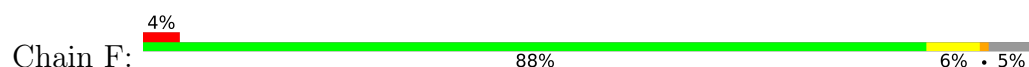
- Molecule 5: Cytochrome c oxidase subunit 5A



- Molecule 5: Cytochrome c oxidase subunit 5A



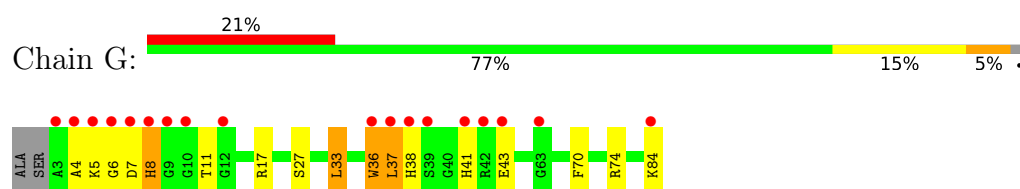
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



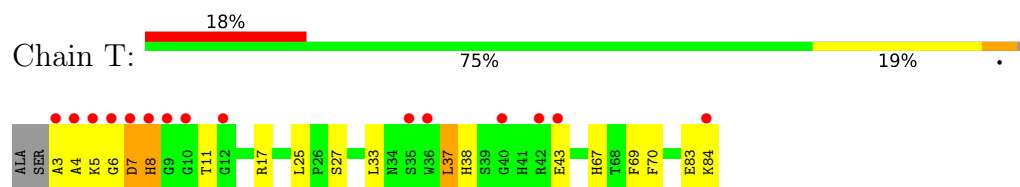
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



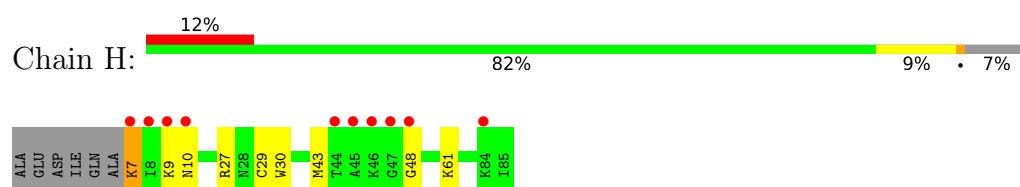
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



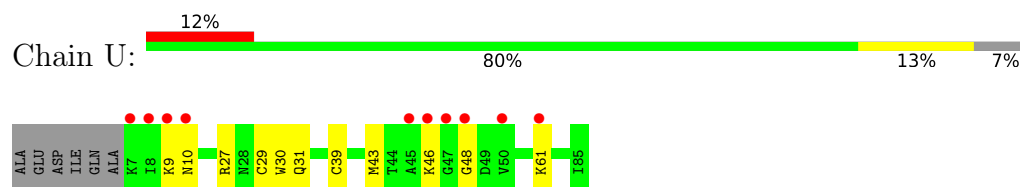
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



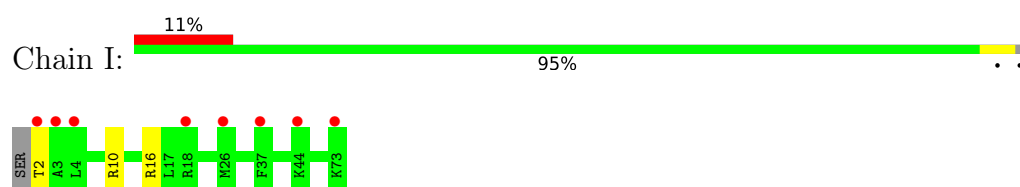
- Molecule 8: Cytochrome c oxidase subunit 6B1



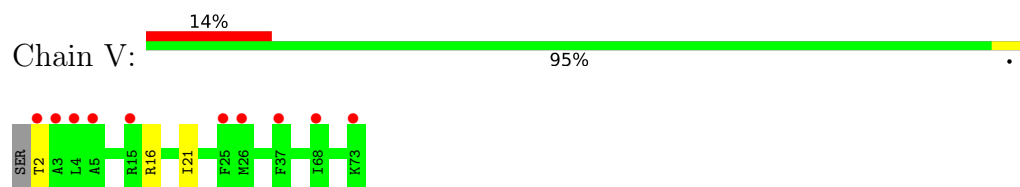
- Molecule 8: Cytochrome c oxidase subunit 6B1



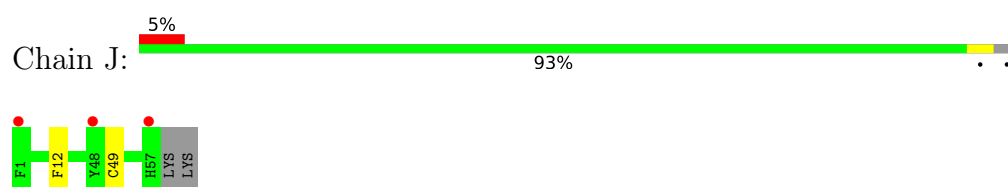
- Molecule 9: Cytochrome c oxidase subunit 6C



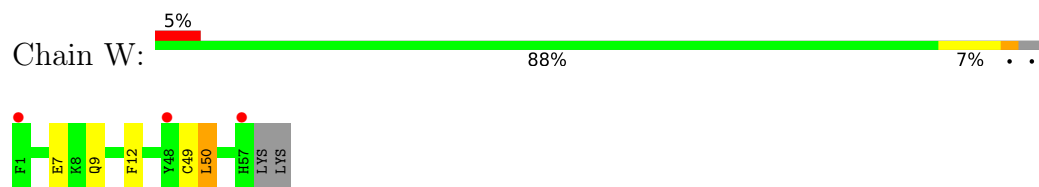
- Molecule 9: Cytochrome c oxidase subunit 6C



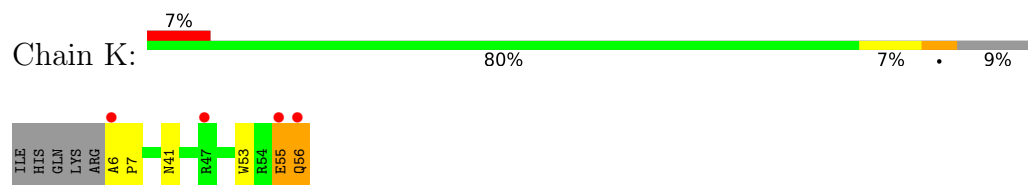
- Molecule 10: Cytochrome c oxidase subunit 7A1



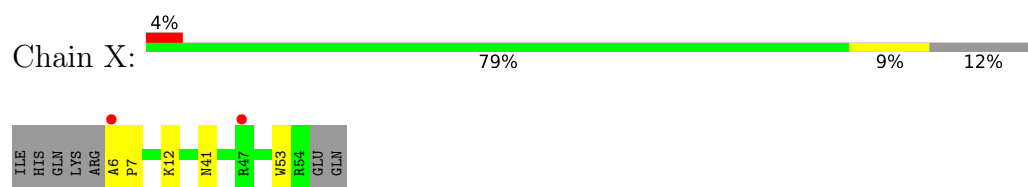
• Molecule 10: Cytochrome c oxidase subunit 7A1



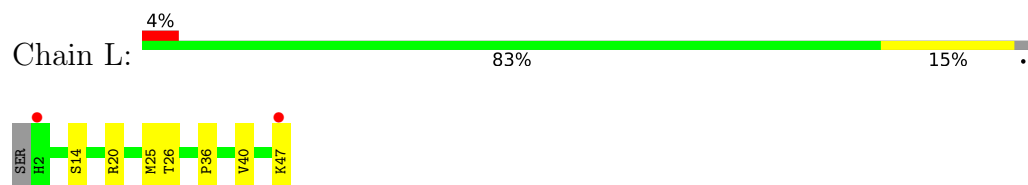
• Molecule 11: Cytochrome c oxidase subunit 7B



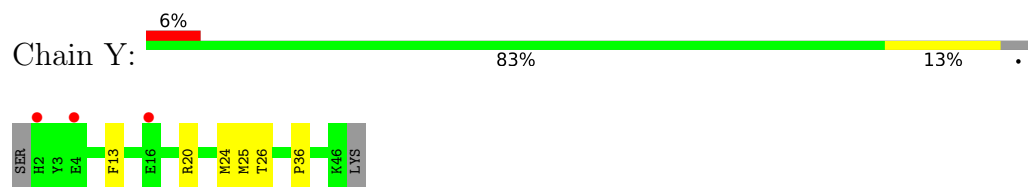
• Molecule 11: Cytochrome c oxidase subunit 7B



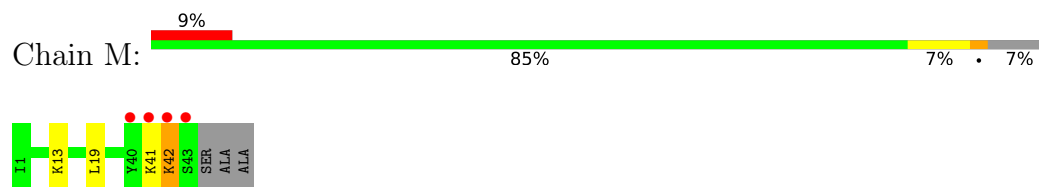
• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



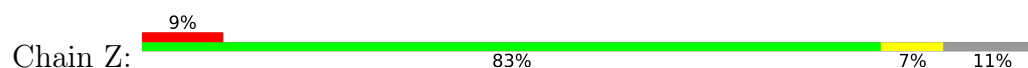
• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

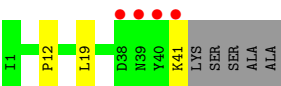


• Molecule 13: Cytochrome c oxidase subunit 8B



• Molecule 13: Cytochrome c oxidase subunit 8B





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	181.80Å 203.58Å 177.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.97 – 2.20 29.97 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.4 (29.97-2.20) 99.8 (29.97-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.92 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5, PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.185 , 0.213 0.191 , 0.217	Depositor DCC
R_{free} test set	16583 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	30.2	Xtriage
Anisotropy	0.867	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 63.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.003 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	33571	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.14	0/4244	0.31	1/5795 (0.0%)
1	N	0.14	1/4244 (0.0%)	0.29	1/5794 (0.0%)
2	B	0.15	0/1907	0.30	0/2597
2	O	0.12	0/1915	0.33	1/2607 (0.0%)
3	C	0.09	0/2268	0.22	0/3096
3	P	0.12	0/2271	0.23	0/3100
4	D	0.09	0/1257	0.23	0/1695
4	Q	0.09	0/1217	0.23	0/1641
5	E	0.10	0/882	0.23	0/1196
5	R	0.14	0/882	0.26	0/1196
6	F	0.22	0/753	0.37	0/1023
6	S	0.13	0/756	0.28	0/1026
7	G	0.11	0/695	0.33	0/945
7	T	0.12	0/679	0.35	0/922
8	H	0.10	0/682	0.34	0/921
8	U	0.10	0/682	0.31	0/921
9	I	0.12	0/605	0.28	0/802
9	V	0.09	0/605	0.23	0/802
10	J	0.08	0/462	0.19	0/625
10	W	0.08	0/471	0.21	0/637
11	K	0.46	1/416 (0.2%)	0.38	0/570
11	X	0.34	1/405 (0.2%)	0.25	0/556
12	L	0.09	0/393	0.24	0/526
12	Y	0.08	0/391	0.23	0/525
13	M	0.10	0/345	0.25	0/470
13	Z	0.09	0/330	0.23	0/451
All	All	0.14	3/29757 (0.0%)	0.28	3/40439 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	41	ASN	C-O	8.07	1.27	1.23
11	X	41	ASN	C-O	6.27	1.26	1.23
1	N	83	VAL	CA-CB	-5.30	1.51	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	119	GLU	CB-CA-C	-8.70	106.53	116.54
1	N	125	GLY	CA-C-O	-6.22	116.61	122.39
2	O	201	GLY	N-CA-C	5.70	117.32	111.56

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4115	0	4087	49	0
1	N	4115	0	4092	50	0
2	B	1869	0	1868	25	0
2	O	1877	0	1876	29	0
3	C	2181	0	2092	32	0
3	P	2184	0	2095	29	0
4	D	1222	0	1211	18	0
4	Q	1182	0	1162	10	0
5	E	863	0	857	5	0
5	R	863	0	857	2	0
6	F	737	0	711	6	0
6	S	740	0	721	3	0
7	G	678	0	640	16	0
7	T	664	0	630	18	0
8	H	662	0	623	5	0
8	U	662	0	623	8	0
9	I	592	0	604	3	0
9	V	592	0	604	2	0
10	J	451	0	446	3	0
10	W	460	0	451	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	K	402	0	380	5	0
11	X	391	0	374	2	0
12	L	380	0	380	5	0
12	Y	378	0	375	8	0
13	M	335	0	352	3	0
13	Z	320	0	334	2	0
14	A	120	0	108	8	0
14	N	120	0	108	7	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	2	0	0	0	0
18	N	2	0	0	0	0
19	A	51	0	76	6	0
19	C	102	0	152	4	0
19	D	51	0	76	11	0
19	N	102	0	152	13	0
19	P	102	0	152	5	0
20	A	63	0	110	2	0
20	D	63	0	110	9	0
20	L	63	0	110	7	0
20	N	63	0	110	4	0
20	Q	63	0	110	6	0
20	Y	63	0	110	8	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	C	100	0	156	14	0
22	G	100	0	156	14	0
22	P	100	0	156	13	0
22	T	100	0	156	20	0
23	C	58	0	78	0	0
23	G	29	0	39	1	0
23	P	58	0	78	0	0
23	T	29	0	39	0	0
24	C	53	0	77	6	0
24	G	106	0	154	12	0
24	P	106	0	154	10	0
24	T	53	0	77	7	0
25	E	52	0	80	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	O	52	0	80	10	0
26	F	1	0	0	0	0
26	S	1	0	0	0	0
27	J	33	0	42	6	0
27	M	33	0	42	0	0
27	W	33	0	42	4	0
27	Z	33	0	42	0	0
28	A	276	0	0	3	0
28	B	180	0	0	0	0
28	C	149	0	0	0	0
28	D	179	0	0	1	0
28	E	128	0	0	0	0
28	F	119	0	0	3	0
28	G	65	0	0	2	0
28	H	76	0	0	1	0
28	I	51	0	0	0	0
28	J	41	0	0	0	0
28	K	36	0	0	2	0
28	L	40	0	0	0	0
28	M	36	0	0	1	0
28	N	289	0	0	5	0
28	O	139	0	0	0	0
28	P	144	0	0	0	0
28	Q	69	0	0	1	0
28	R	81	0	0	1	0
28	S	118	0	0	0	0
28	T	63	0	0	2	0
28	U	61	0	0	2	0
28	V	28	0	0	0	0
28	W	35	0	0	0	0
28	X	25	0	0	0	0
28	Y	34	0	0	0	0
28	Z	24	0	0	0	0
All	All	33571	0	31577	378	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 378 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:N:609:PGV:H011	19:N:609:PGV:H31	1.57	0.87
22:P:304:CDL:H151	22:P:304:CDL:HA61	1.57	0.85
2:O:91:ASN:O	2:O:92:ASN:ND2	2.11	0.83
2:B:70:ALA:HB1	22:T:103:CDL:H451	1.62	0.82
7:G:5:LYS:HB3	1:N:278[B]:MET:HE2	1.64	0.79

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	523/514 (102%)	509 (97%)	14 (3%)	0	100	100
1	N	523/514 (102%)	508 (97%)	15 (3%)	0	100	100
2	B	230/581 (40%)	225 (98%)	5 (2%)	0	100	100
2	O	231/581 (40%)	225 (97%)	5 (2%)	1 (0%)	30	34
3	C	266/261 (102%)	262 (98%)	4 (2%)	0	100	100
3	P	266/261 (102%)	262 (98%)	4 (2%)	0	100	100
4	D	145/147 (99%)	142 (98%)	3 (2%)	0	100	100
4	Q	139/147 (95%)	136 (98%)	3 (2%)	0	100	100
5	E	104/109 (95%)	104 (100%)	0	0	100	100
5	R	104/109 (95%)	104 (100%)	0	0	100	100
6	F	94/98 (96%)	93 (99%)	1 (1%)	0	100	100
6	S	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
7	G	80/84 (95%)	73 (91%)	5 (6%)	2 (2%)	4	2
7	T	79/84 (94%)	74 (94%)	3 (4%)	2 (2%)	4	2
8	H	77/85 (91%)	73 (95%)	3 (4%)	1 (1%)	9	8
8	U	77/85 (91%)	73 (95%)	3 (4%)	1 (1%)	9	8

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	70/73 (96%)	69 (99%)	1 (1%)	0	100	100
9	V	70/73 (96%)	69 (99%)	1 (1%)	0	100	100
10	J	55/59 (93%)	55 (100%)	0	0	100	100
10	W	56/59 (95%)	56 (100%)	0	0	100	100
11	K	49/56 (88%)	48 (98%)	1 (2%)	0	100	100
11	X	48/56 (86%)	47 (98%)	1 (2%)	0	100	100
12	L	44/47 (94%)	44 (100%)	0	0	100	100
12	Y	44/47 (94%)	44 (100%)	0	0	100	100
13	M	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
13	Z	39/46 (85%)	39 (100%)	0	0	100	100
All	All	3549/4320 (82%)	3467 (98%)	75 (2%)	7 (0%)	43	51

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	7	ASP
8	H	10	ASN
7	T	7	ASP
8	U	10	ASN
7	G	4	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	437/426 (103%)	430 (98%)	7 (2%)	55	71
1	N	437/426 (103%)	431 (99%)	6 (1%)	59	75
2	B	215/511 (42%)	208 (97%)	7 (3%)	33	45
2	O	216/511 (42%)	212 (98%)	4 (2%)	50	66
3	C	233/225 (104%)	231 (99%)	2 (1%)	70	84
3	P	233/225 (104%)	232 (100%)	1 (0%)	84	92

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	131/129 (102%)	128 (98%)	3 (2%)	44	59
4	Q	125/129 (97%)	124 (99%)	1 (1%)	73	85
5	E	93/95 (98%)	93 (100%)	0	100	100
5	R	93/95 (98%)	93 (100%)	0	100	100
6	F	81/81 (100%)	79 (98%)	2 (2%)	42	56
6	S	81/81 (100%)	80 (99%)	1 (1%)	63	78
7	G	67/67 (100%)	60 (90%)	7 (10%)	7	7
7	T	66/67 (98%)	61 (92%)	5 (8%)	12	14
8	H	71/75 (95%)	67 (94%)	4 (6%)	19	24
8	U	71/75 (95%)	69 (97%)	2 (3%)	38	52
9	I	57/58 (98%)	56 (98%)	1 (2%)	51	68
9	V	57/58 (98%)	56 (98%)	1 (2%)	51	68
10	J	48/50 (96%)	48 (100%)	0	100	100
10	W	49/50 (98%)	47 (96%)	2 (4%)	27	37
11	K	41/46 (89%)	39 (95%)	2 (5%)	22	29
11	X	40/46 (87%)	39 (98%)	1 (2%)	42	56
12	L	39/40 (98%)	37 (95%)	2 (5%)	21	27
12	Y	39/40 (98%)	38 (97%)	1 (3%)	40	55
13	M	37/38 (97%)	35 (95%)	2 (5%)	20	25
13	Z	35/38 (92%)	34 (97%)	1 (3%)	37	51
All	All	3092/3682 (84%)	3027 (98%)	65 (2%)	48	63

5 of 65 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	U	29	CYS
9	V	2	THR
7	G	36[B]	TRP
7	G	36[A]	TRP
10	W	7	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
4	Q	119	GLN
8	U	31	GLN
8	H	28	ASN
8	H	31	GLN
8	H	32	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	TPO	G	11	7	8,10,11	1.30	1 (12%)	10,14,16	0.99	1 (10%)
1	FME	A	1	1	8,9,10	0.48	0	7,9,11	1.34	0
2	FME	O	1	2	8,9,10	0.46	0	7,9,11	1.26	0
7	TPO	T	11	7	8,10,11	1.29	1 (12%)	10,14,16	0.85	0
2	FME	B	1	2	8,9,10	0.47	0	7,9,11	1.34	0
1	FME	N	1	1	8,9,10	0.46	0	7,9,11	1.30	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	TPO	G	11	7	-	5/9/11/13	-
1	FME	A	1	1	-	5/7/9/11	-
2	FME	O	1	2	-	1/7/9/11	-
7	TPO	T	11	7	-	4/9/11/13	-
2	FME	B	1	2	-	1/7/9/11	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	N	1	1	-	5/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	11	TPO	P-O1P	2.77	1.59	1.50
7	T	11	TPO	P-O1P	2.76	1.59	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	11	TPO	CG2-CB-CA	2.31	117.71	113.16

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O1-CN-N-CA
1	A	1	FME	N-CA-CB-CG
1	A	1	FME	C-CA-CB-CG
7	G	11	TPO	N-CA-CB-CG2
7	G	11	TPO	N-CA-CB-OG1

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	1	FME	1	0
2	B	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 52 ligands modelled in this entry, 8 are monoatomic - leaving 44 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
27	DMU	W	101	-	34,34,34	0.34	0	45,45,45	0.85	1 (2%)
24	PEK	C	306	-	52,52,52	0.94	2 (3%)	55,57,57	1.27	6 (10%)
24	PEK	P	307	-	52,52,52	0.93	2 (3%)	55,57,57	1.41	9 (16%)
20	TGL	Q	201	-	62,62,62	0.99	3 (4%)	65,65,65	1.14	5 (7%)
23	CHD	P	306	-	32,32,32	0.81	1 (3%)	51,51,51	0.95	1 (1%)
22	CDL	C	302	-	99,99,99	1.33	12 (12%)	105,111,111	1.42	13 (12%)
21	CUA	O	601	2	0,1,1	-	-	-	-	-
27	DMU	Z	101	-	34,34,34	0.38	0	45,45,45	0.76	1 (2%)
27	DMU	J	101	-	34,34,34	0.48	1 (2%)	45,45,45	0.99	1 (2%)
14	HEA	N	602	18,1	66,67,67	1.84	26 (39%)	78,103,103	1.66	18 (23%)
27	DMU	M	101	-	34,34,34	0.36	0	45,45,45	0.76	1 (2%)
19	PGV	N	609	-	50,50,50	1.00	2 (4%)	53,56,56	1.31	7 (13%)
18	PER	N	606	14,15	1,1,1	0.27	0	-	-	-
23	CHD	C	304	-	32,32,32	0.83	1 (3%)	51,51,51	1.01	1 (1%)
18	PER	A	606	14,15	1,1,1	0.26	0	-	-	-
20	TGL	L	101	-	62,62,62	1.00	3 (4%)	65,65,65	1.13	5 (7%)
19	PGV	C	301	-	50,50,50	0.37	0	53,56,56	0.49	1 (1%)
22	CDL	T	103	-	99,99,99	1.31	12 (12%)	105,111,111	1.25	7 (6%)
23	CHD	T	101	-	32,32,32	0.82	1 (3%)	51,51,51	1.10	4 (7%)
20	TGL	A	608	-	62,62,62	0.98	3 (4%)	65,65,65	1.15	5 (7%)
25	PSC	O	602	-	51,51,51	1.13	3 (5%)	57,59,59	1.51	4 (7%)
19	PGV	P	303	-	50,50,50	0.33	0	53,56,56	0.53	0
23	CHD	C	303	-	32,32,32	0.87	1 (3%)	51,51,51	1.35	7 (13%)
19	PGV	P	302	-	50,50,50	0.98	2 (4%)	53,56,56	1.35	8 (15%)
24	PEK	G	102	-	52,52,52	0.96	2 (3%)	55,57,57	1.21	5 (9%)
20	TGL	D	202	-	62,62,62	0.97	3 (4%)	65,65,65	1.07	4 (6%)
19	PGV	A	607	-	50,50,50	0.94	2 (4%)	53,56,56	1.11	3 (5%)
22	CDL	P	304	-	99,99,99	1.31	12 (12%)	105,111,111	1.33	13 (12%)
20	TGL	N	608	-	62,62,62	0.99	3 (4%)	65,65,65	1.11	5 (7%)
22	CDL	G	103	-	99,99,99	1.32	12 (12%)	105,111,111	1.36	8 (7%)
14	HEA	A	602	18,1	66,67,67	1.84	25 (37%)	78,103,103	1.67	23 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	PGV	N	607	-	50,50,50	0.94	2 (4%)	53,56,56	1.10	3 (5%)
24	PEK	G	101	-	52,52,52	0.89	2 (3%)	55,57,57	1.36	8 (14%)
23	CHD	G	104	-	32,32,32	0.81	1 (3%)	51,51,51	1.09	3 (5%)
23	CHD	P	305	-	32,32,32	0.78	0	51,51,51	1.76	8 (15%)
14	HEA	A	601	1	66,67,67	1.83	25 (37%)	78,103,103	1.65	16 (20%)
19	PGV	C	305	-	50,50,50	0.96	2 (4%)	53,56,56	1.37	8 (15%)
24	PEK	T	102	-	52,52,52	0.94	2 (3%)	55,57,57	1.22	4 (7%)
21	CUA	B	601	2	0,1,1	-	-	-	-	-
20	TGL	Y	101	-	62,62,62	1.00	3 (4%)	65,65,65	0.96	3 (4%)
25	PSC	E	201	-	51,51,51	1.10	3 (5%)	57,59,59	1.41	5 (8%)
14	HEA	N	601	1	66,67,67	1.84	25 (37%)	78,103,103	1.64	16 (20%)
24	PEK	P	301	-	52,52,52	0.98	2 (3%)	55,57,57	1.18	5 (9%)
19	PGV	D	201	-	50,50,50	0.32	0	53,56,56	0.33	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	DMU	W	101	-	-	8/19/59/59	0/2/2/2
24	PEK	C	306	-	-	19/56/56/56	-
24	PEK	P	307	-	-	20/56/56/56	-
20	TGL	Q	201	-	-	21/65/65/65	-
23	CHD	P	306	-	-	3/9/74/74	0/4/4/4
22	CDL	C	302	-	-	40/110/110/110	-
27	DMU	Z	101	-	-	4/19/59/59	0/2/2/2
27	DMU	J	101	-	-	8/19/59/59	0/2/2/2
14	HEA	N	602	18,1	-	8/36/76/76	-
27	DMU	M	101	-	-	6/19/59/59	0/2/2/2
19	PGV	N	609	-	-	23/55/55/55	-
23	CHD	C	304	-	-	1/9/74/74	0/4/4/4
20	TGL	L	101	-	-	28/65/65/65	-
19	PGV	C	301	-	-	21/55/55/55	-
22	CDL	T	103	-	-	33/110/110/110	-
23	CHD	T	101	-	-	2/9/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	TGL	A	608	-	-	26/65/65/65	-
25	PSC	O	602	-	-	25/55/55/55	-
19	PGV	P	303	-	-	22/55/55/55	-
23	CHD	C	303	-	-	5/9/74/74	0/4/4/4
19	PGV	P	302	-	-	19/55/55/55	-
24	PEK	G	102	-	-	20/56/56/56	-
20	TGL	D	202	-	-	27/65/65/65	-
19	PGV	A	607	-	-	11/55/55/55	-
22	CDL	P	304	-	-	39/110/110/110	-
20	TGL	N	608	-	-	27/65/65/65	-
22	CDL	G	103	-	-	35/110/110/110	-
14	HEA	A	602	18,1	-	9/36/76/76	-
19	PGV	N	607	-	-	7/55/55/55	-
24	PEK	G	101	-	-	21/56/56/56	-
23	CHD	G	104	-	-	2/9/74/74	0/4/4/4
23	CHD	P	305	-	-	5/9/74/74	1/4/4/4
14	HEA	A	601	1	-	11/36/76/76	-
19	PGV	C	305	-	-	14/55/55/55	-
24	PEK	T	102	-	-	13/56/56/56	-
20	TGL	Y	101	-	-	34/65/65/65	-
25	PSC	E	201	-	-	20/55/55/55	-
14	HEA	N	601	1	-	9/36/76/76	-
24	PEK	P	301	-	-	26/56/56/56	-
19	PGV	D	201	-	-	29/55/55/55	-

The worst 5 of 201 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	O	602	PSC	O01-C1	4.93	1.48	1.34
22	C	302	CDL	OA8-CA7	4.86	1.47	1.33
24	P	301	PEK	O03-C21	4.86	1.47	1.33
25	E	201	PSC	O01-C1	4.68	1.47	1.34
19	C	305	PGV	O03-C19	4.64	1.46	1.33

The worst 5 of 245 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	O	602	PSC	O01-C1-C2	6.98	126.54	111.50
23	P	305	CHD	C6-C5-C4	-6.64	103.54	111.19
25	E	201	PSC	O01-C1-C2	5.81	124.02	111.50
22	G	103	CDL	OA6-CA5-C11	5.55	123.45	111.50
24	P	301	PEK	O01-C1-C2	5.36	123.06	111.50

There are no chirality outliers.

5 of 701 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	601	HEA	C2A-C3A-CMA-OMA
14	A	601	HEA	C4A-C3A-CMA-OMA
14	A	601	HEA	C18-C19-C20-C21
14	A	601	HEA	C27-C19-C20-C21
14	A	602	HEA	C2A-C3A-CMA-OMA

All (1) ring outliers are listed below:

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

33 monomers are involved in 214 short contacts:

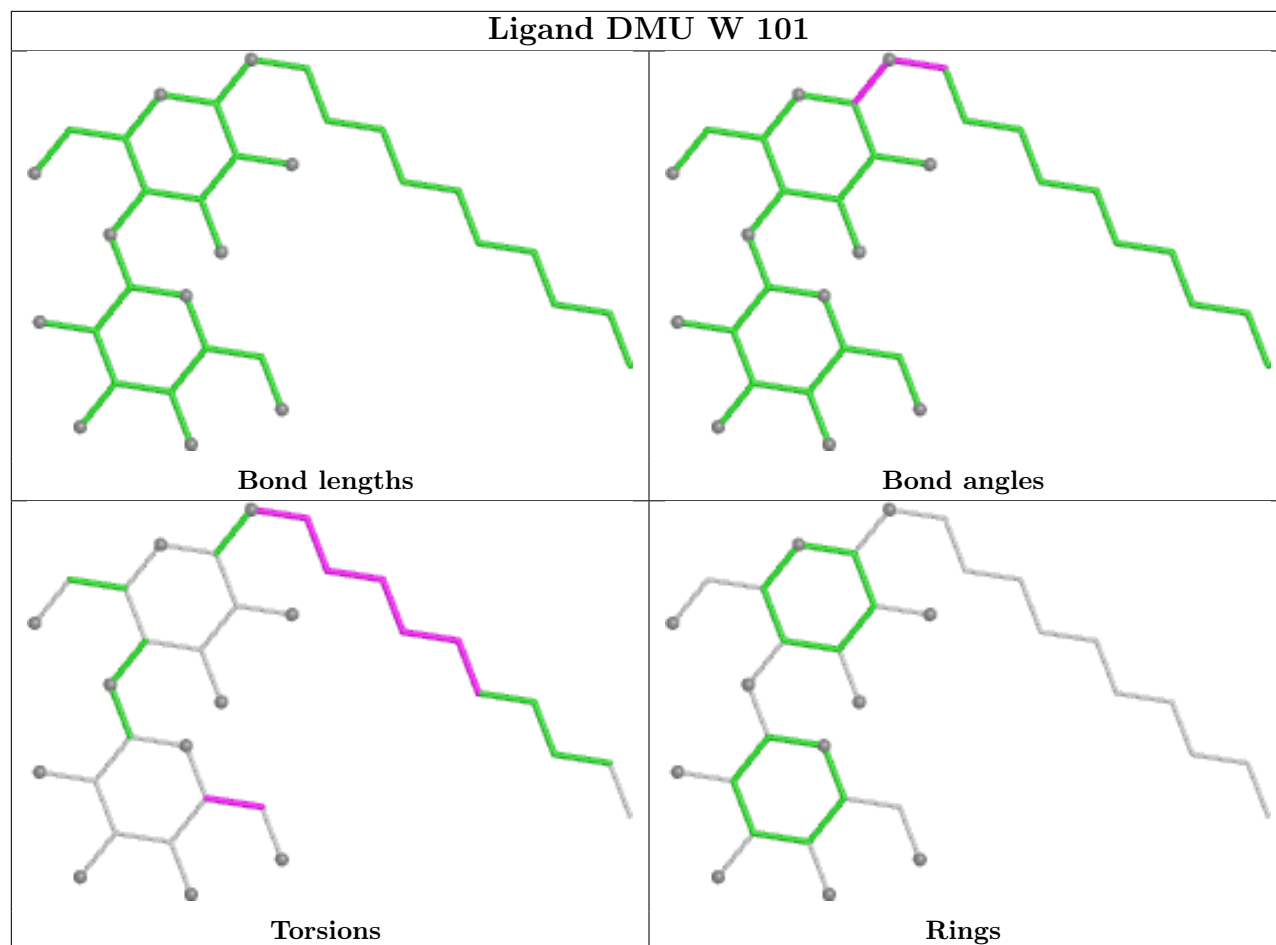
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	W	101	DMU	4	0
24	C	306	PEK	6	0
24	P	307	PEK	4	0
20	Q	201	TGL	6	0
22	C	302	CDL	14	0
27	J	101	DMU	6	0
14	N	602	HEA	3	0
19	N	609	PGV	8	0
20	L	101	TGL	7	0
19	C	301	PGV	3	0
22	T	103	CDL	20	0
20	A	608	TGL	2	0
25	O	602	PSC	10	0
19	P	303	PGV	3	0
19	P	302	PGV	2	0
24	G	102	PEK	8	0
20	D	202	TGL	9	0
19	A	607	PGV	6	0
22	P	304	CDL	13	0

Continued on next page...

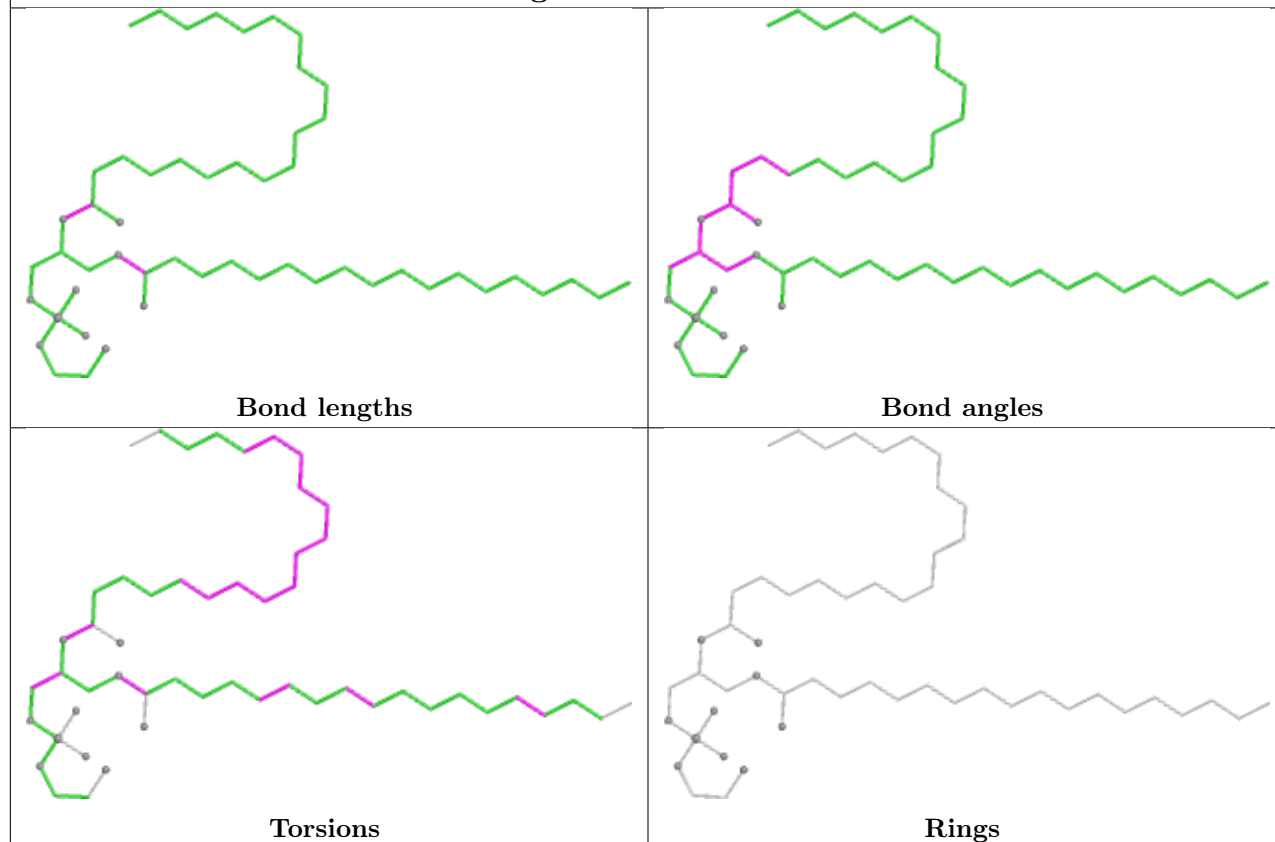
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	N	608	TGL	4	0
22	G	103	CDL	14	0
14	A	602	HEA	3	0
19	N	607	PGV	5	0
24	G	101	PEK	4	0
23	G	104	CHD	1	0
14	A	601	HEA	5	0
19	C	305	PGV	1	0
24	T	102	PEK	7	0
20	Y	101	TGL	8	0
25	E	201	PSC	10	0
14	N	601	HEA	4	0
24	P	301	PEK	6	0
19	D	201	PGV	11	0

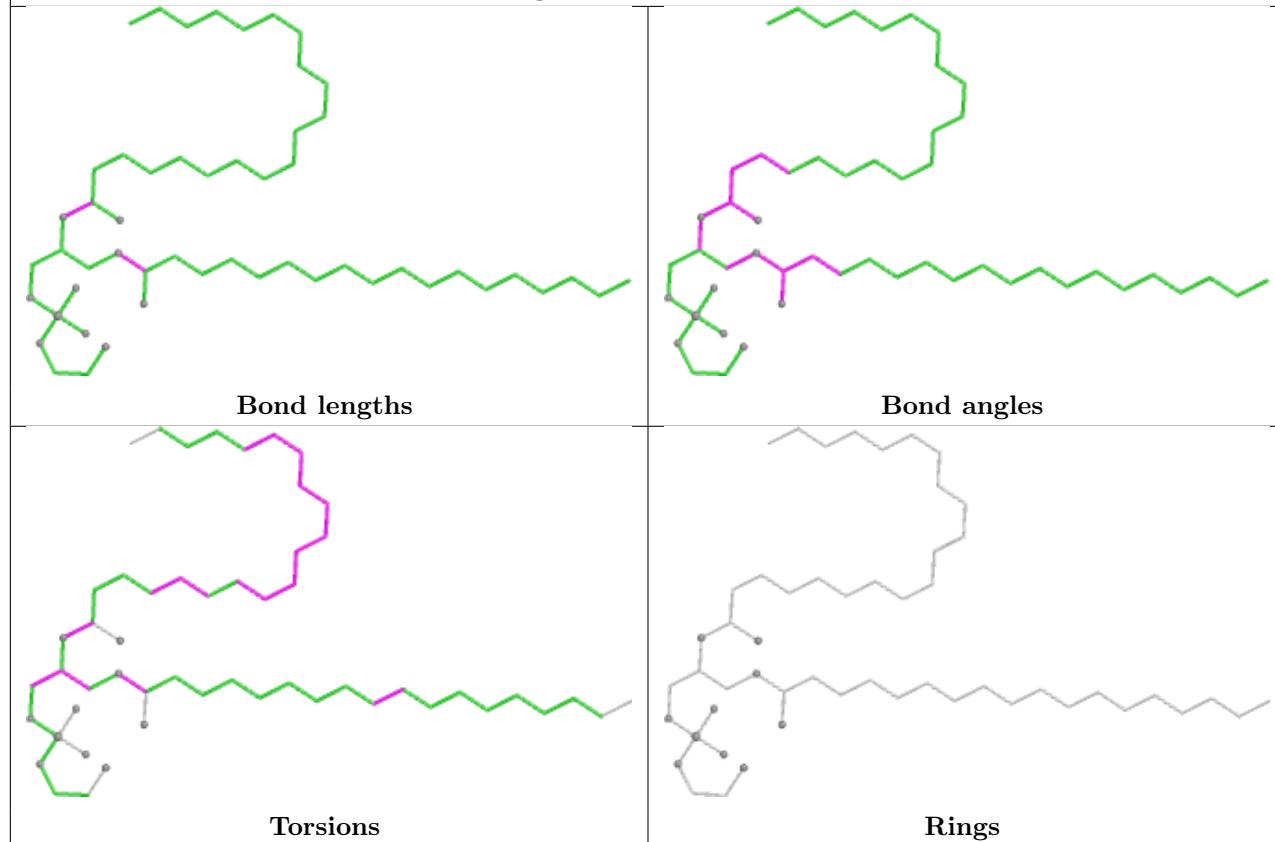
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

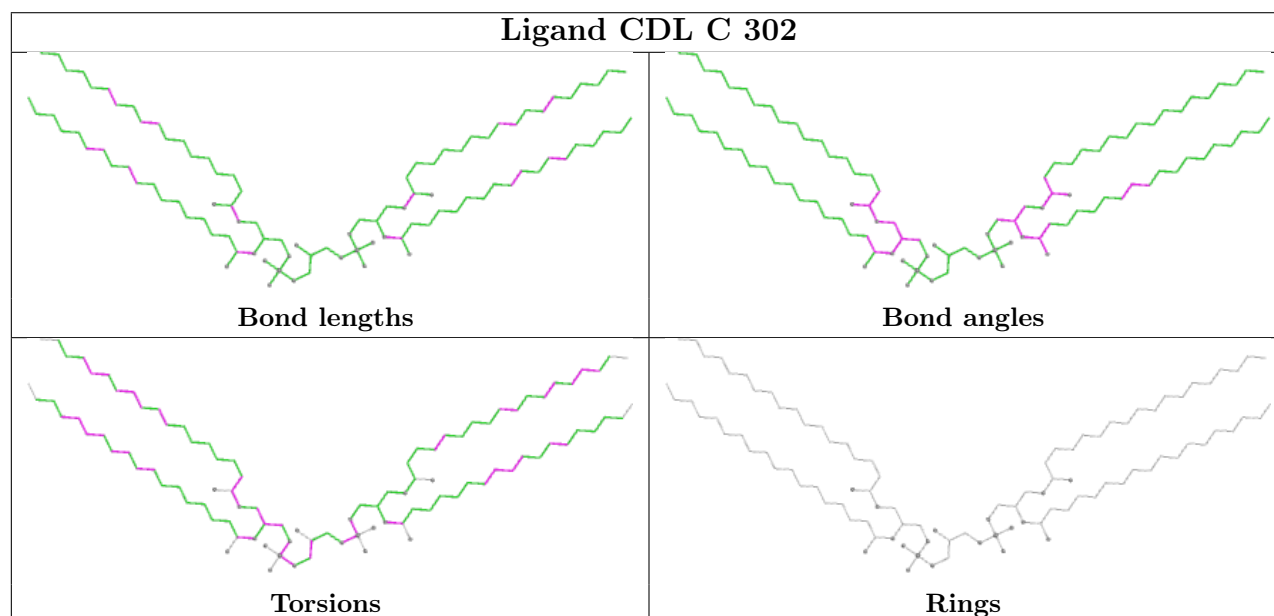
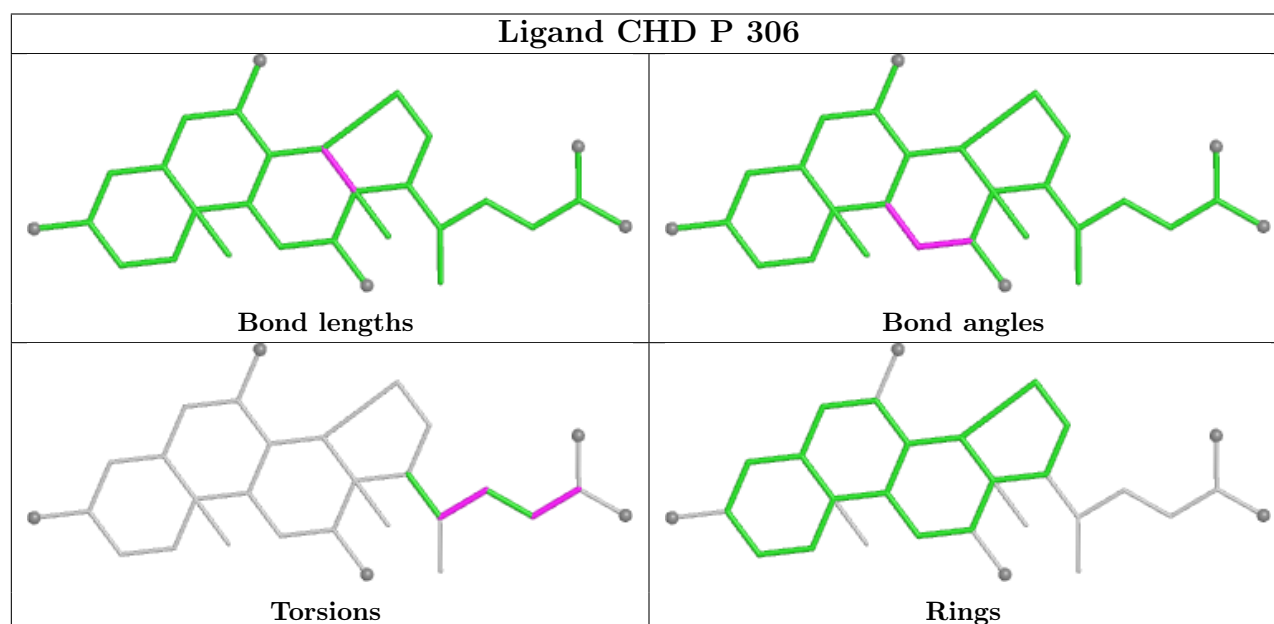
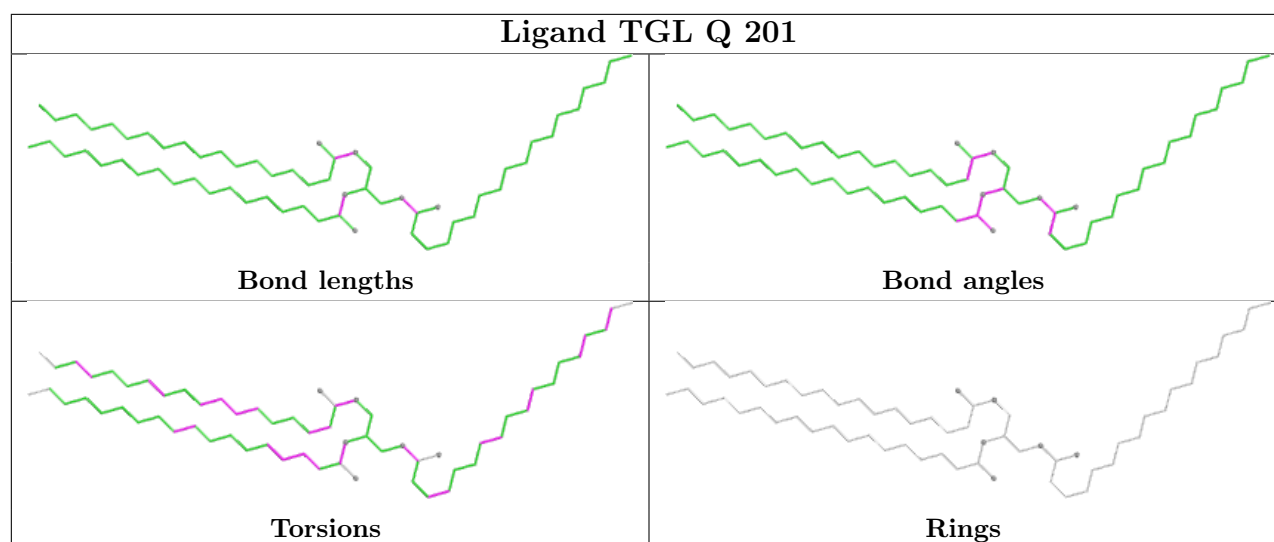


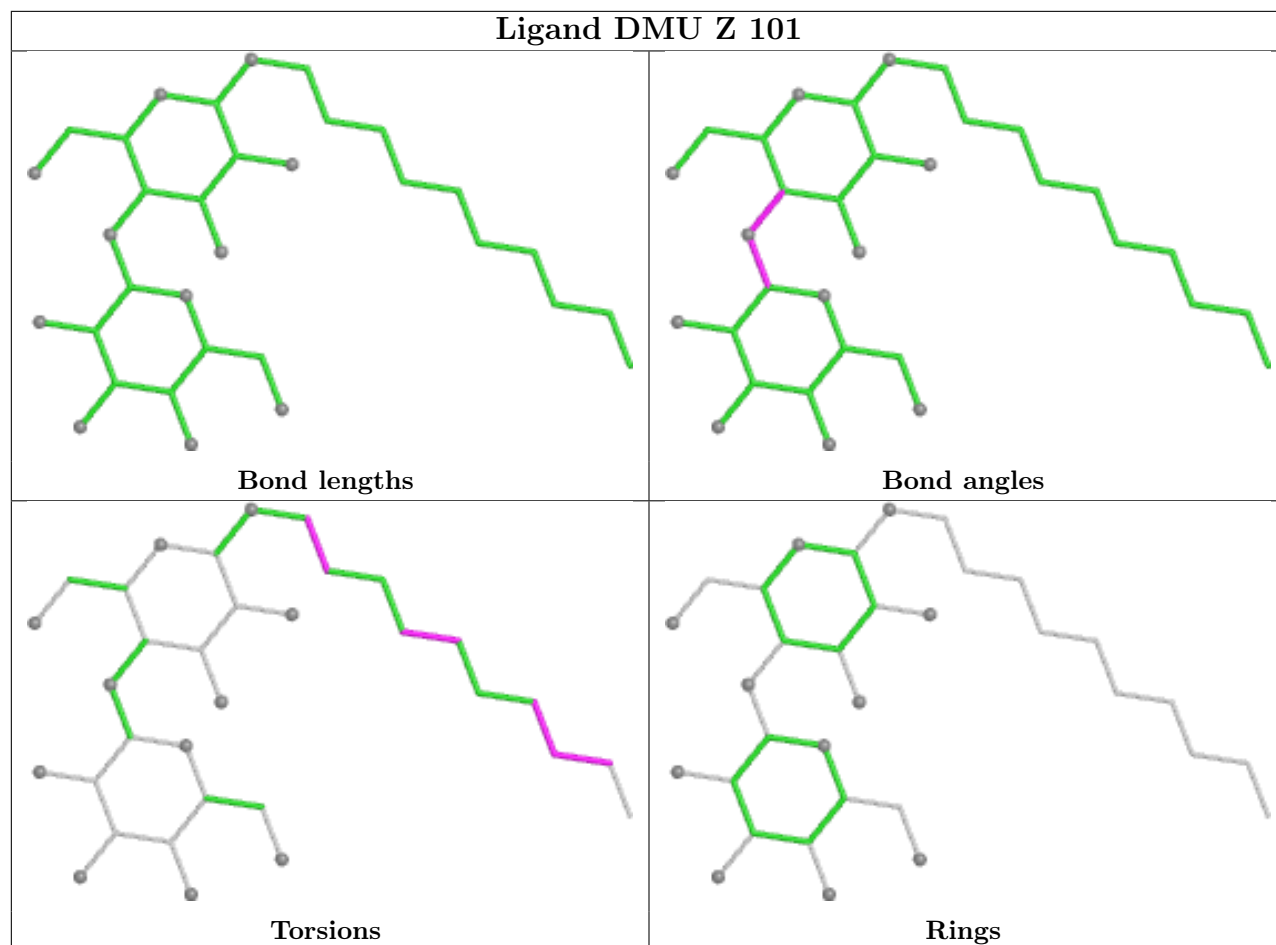
Ligand PEK C 306

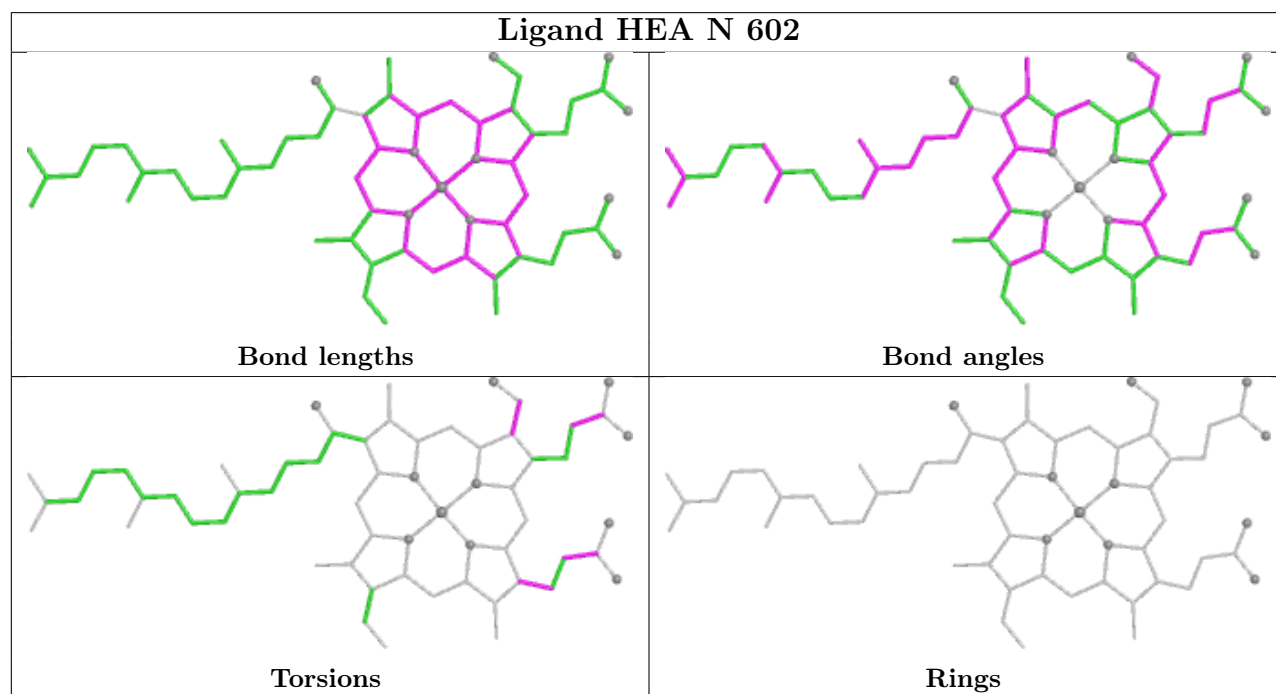
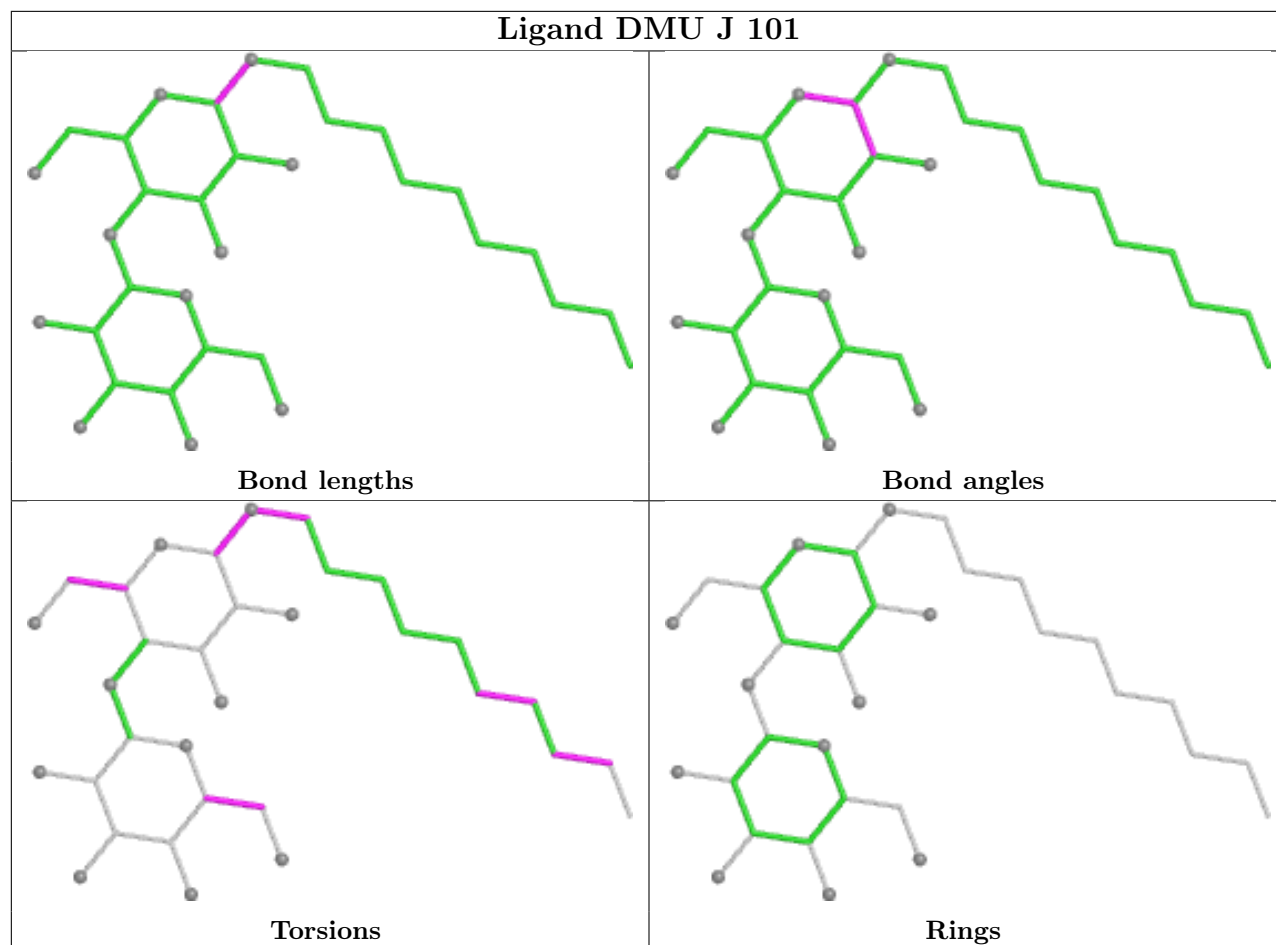


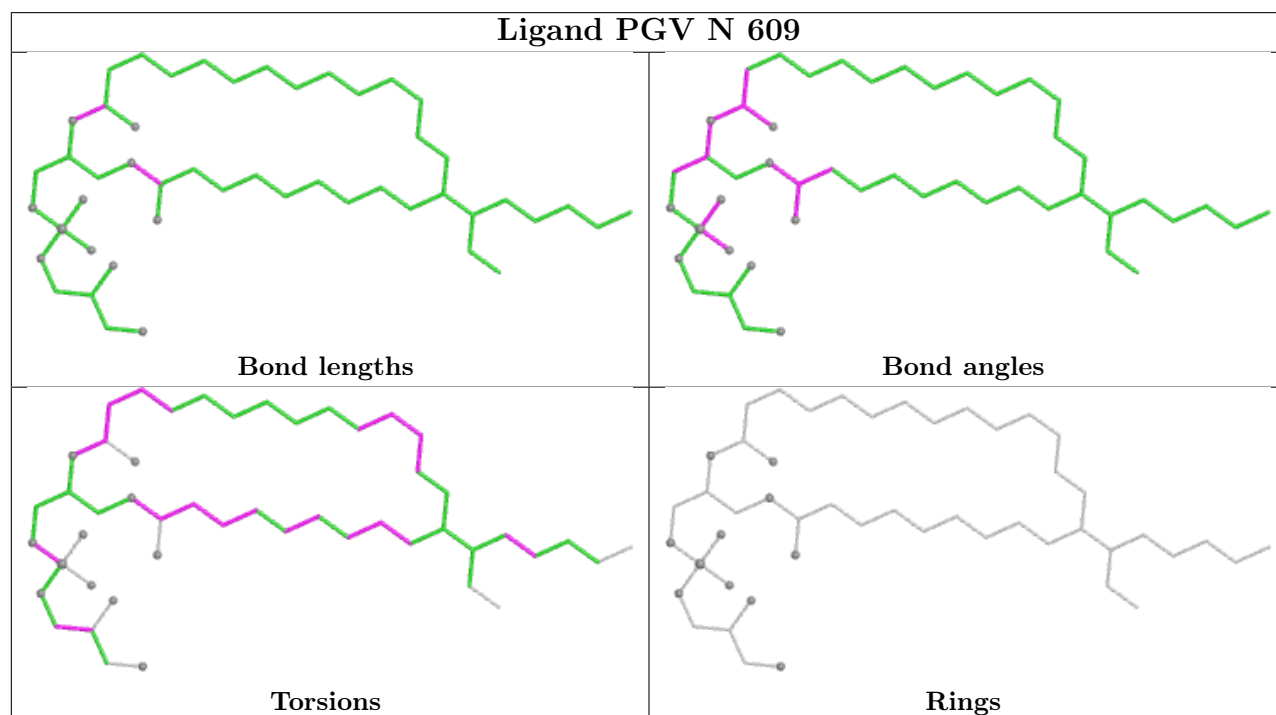
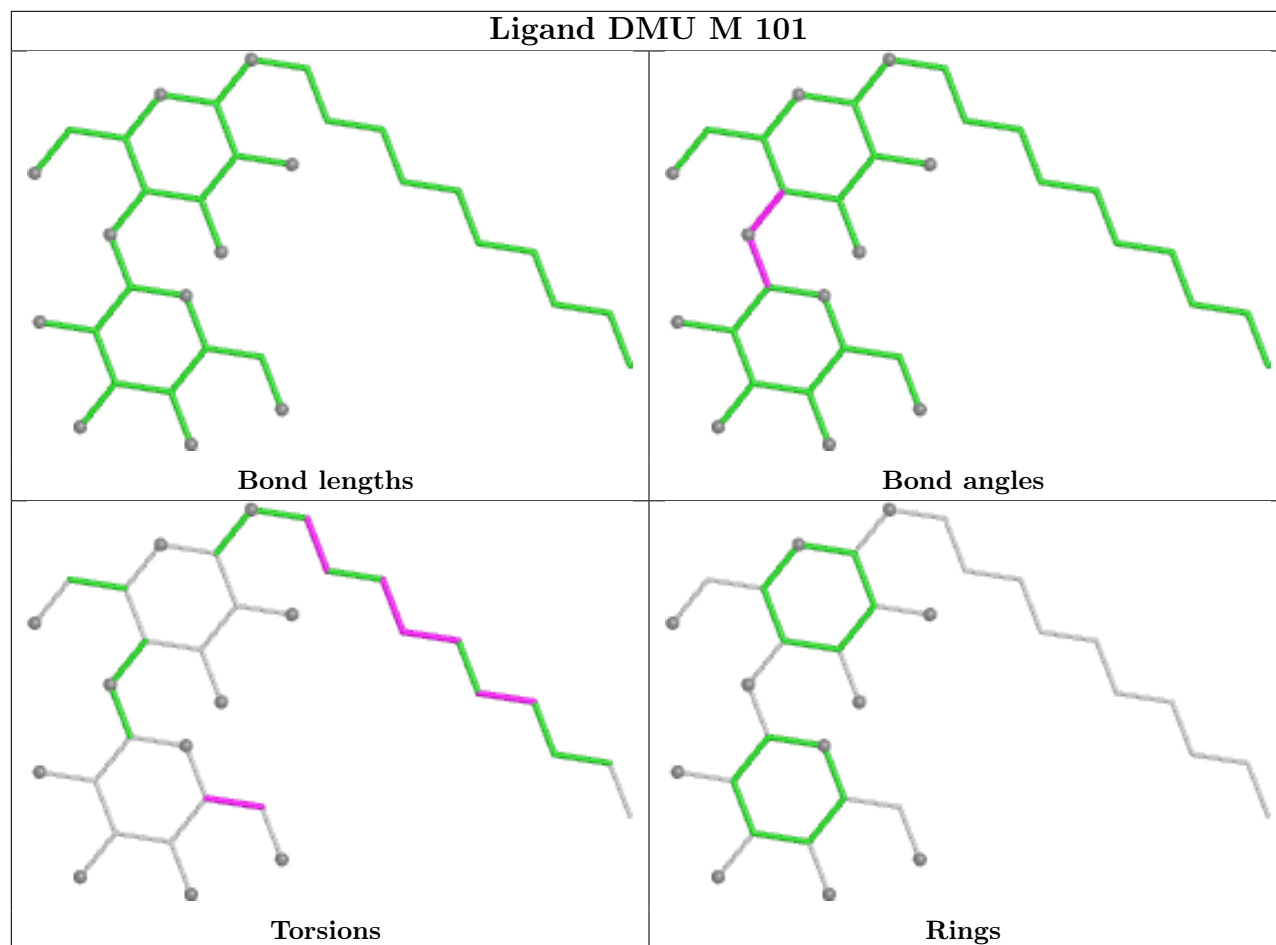
Ligand PEK P 307

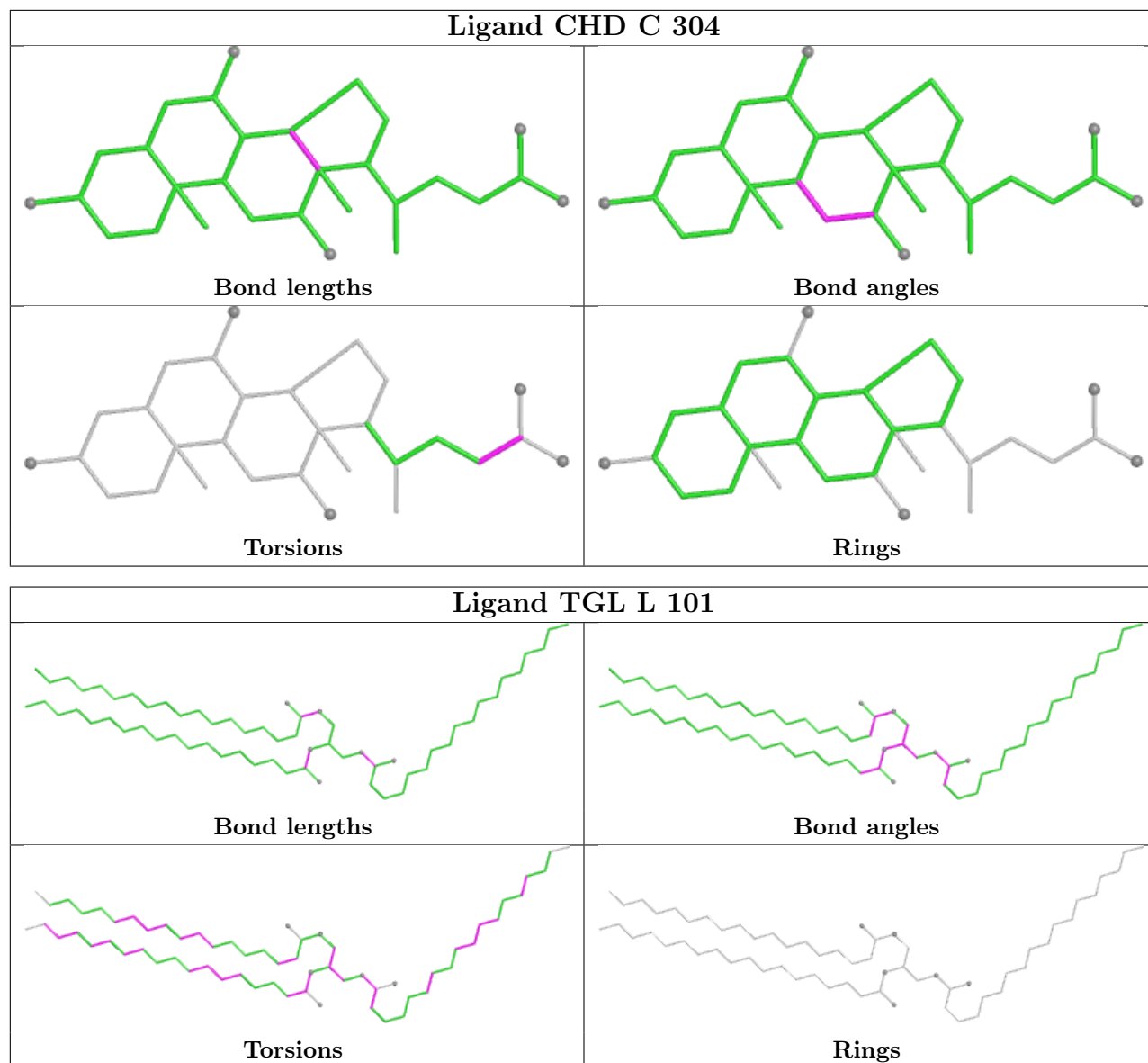


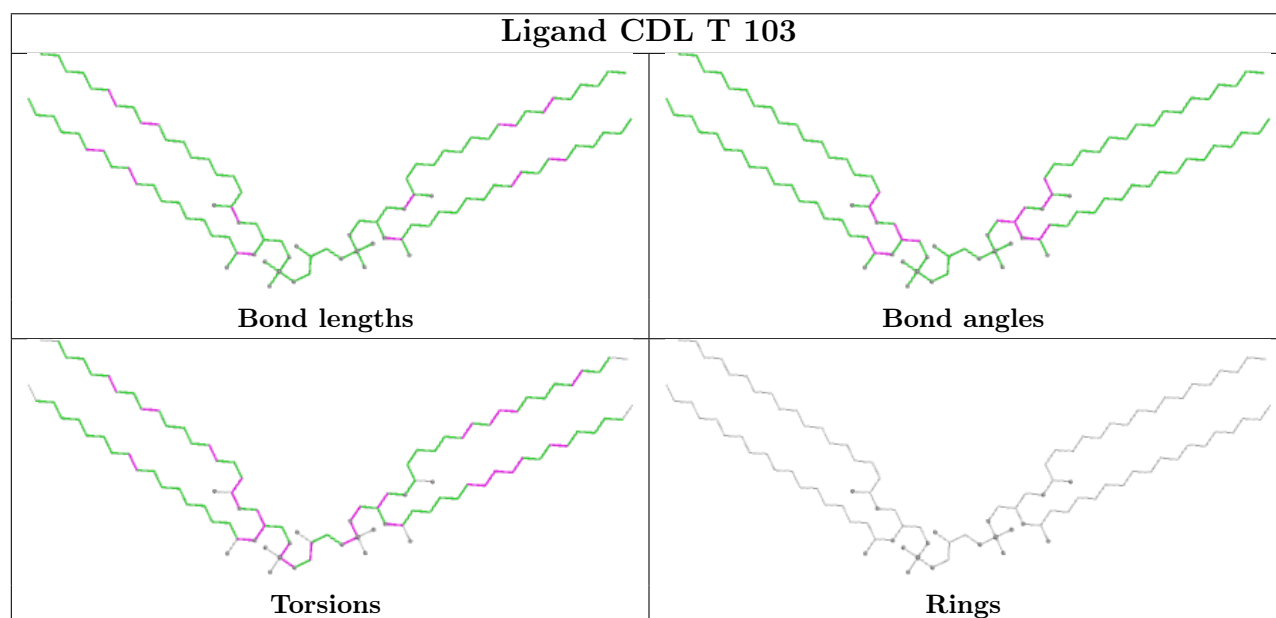
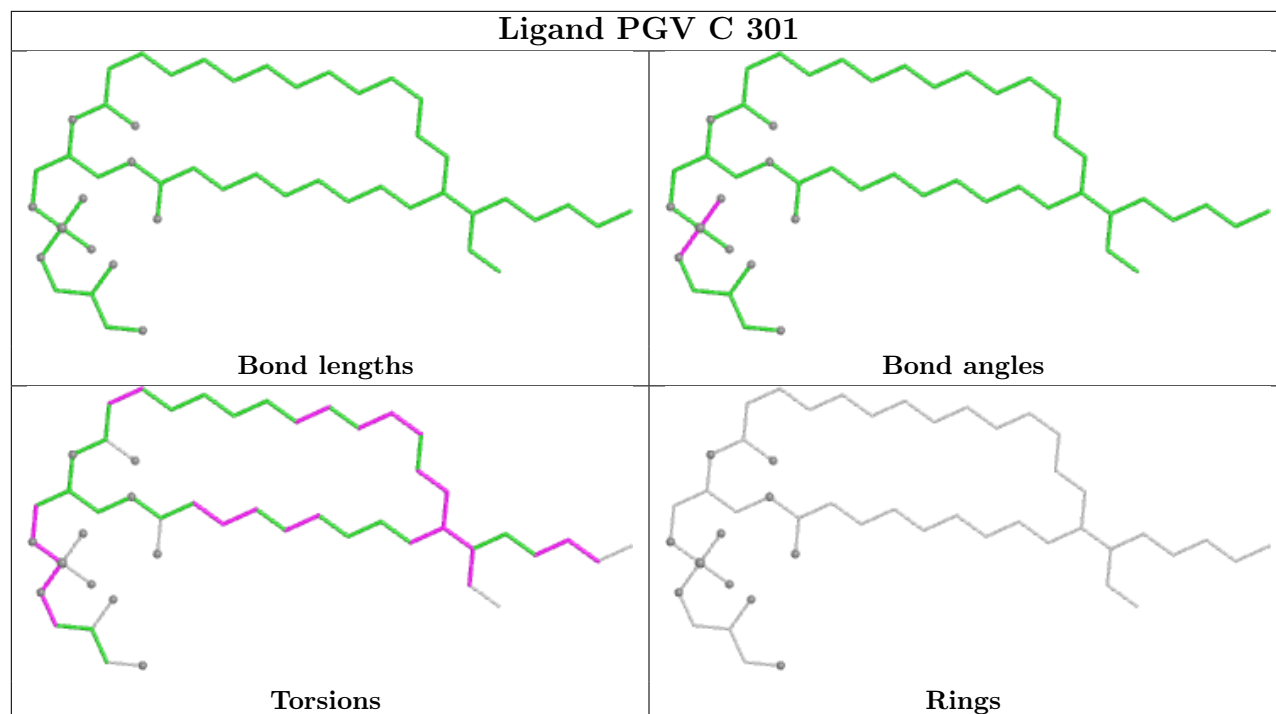


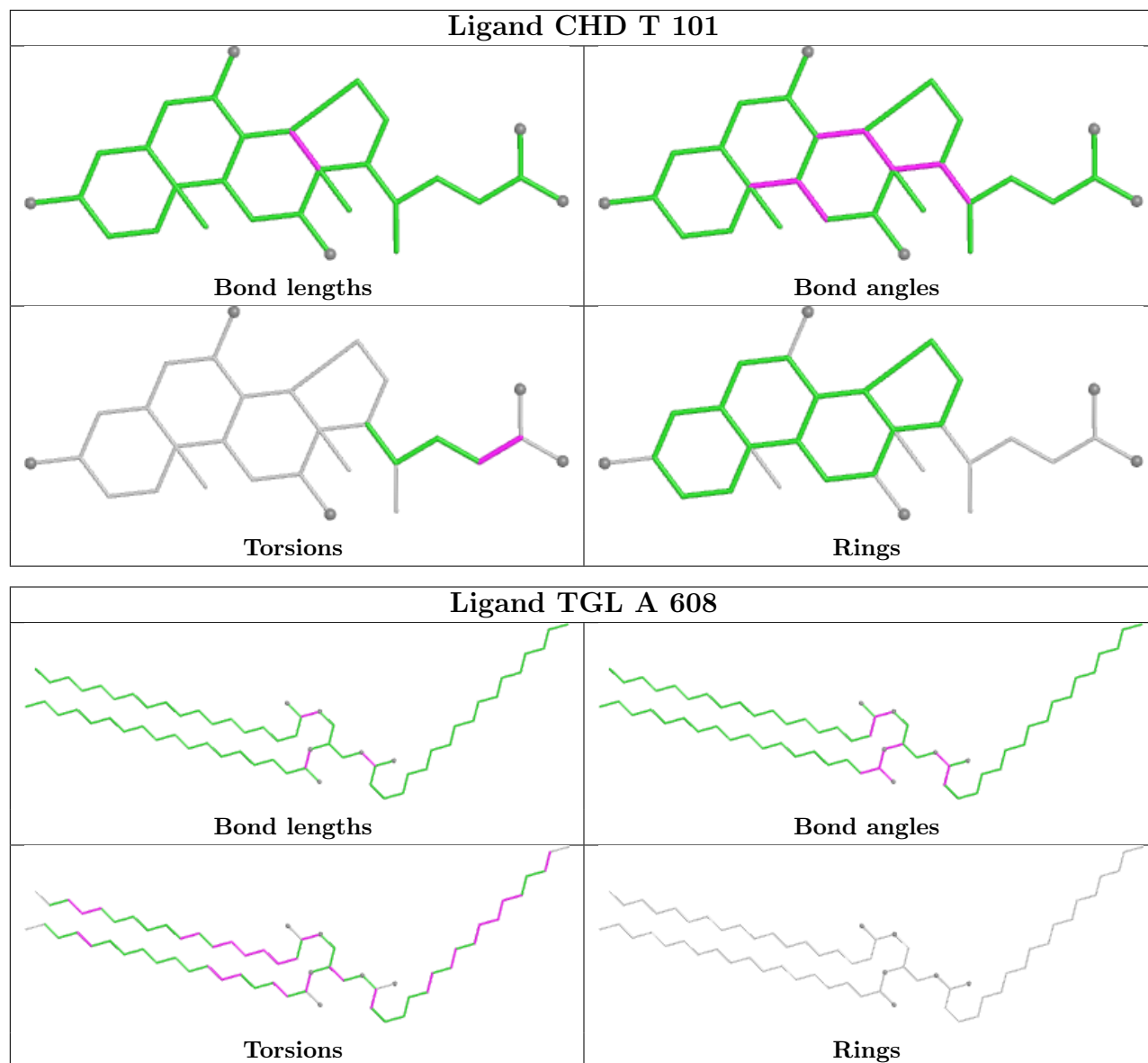




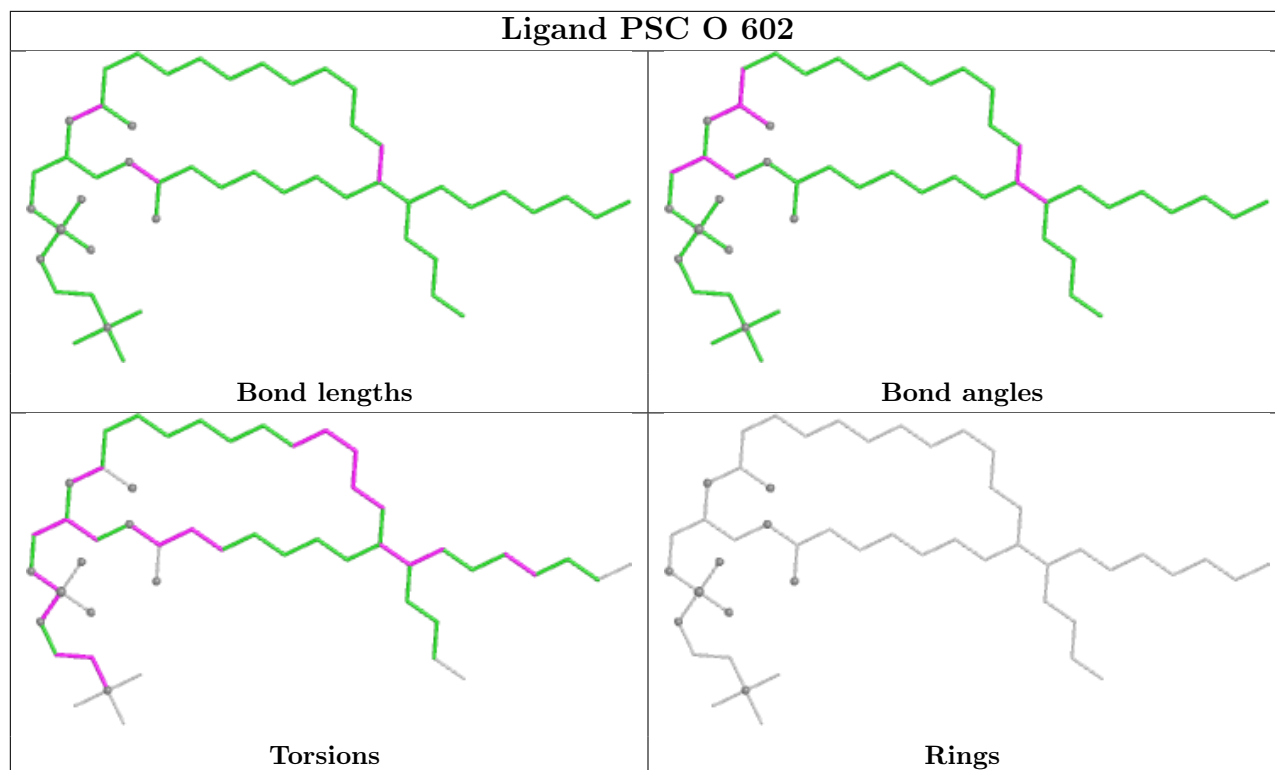




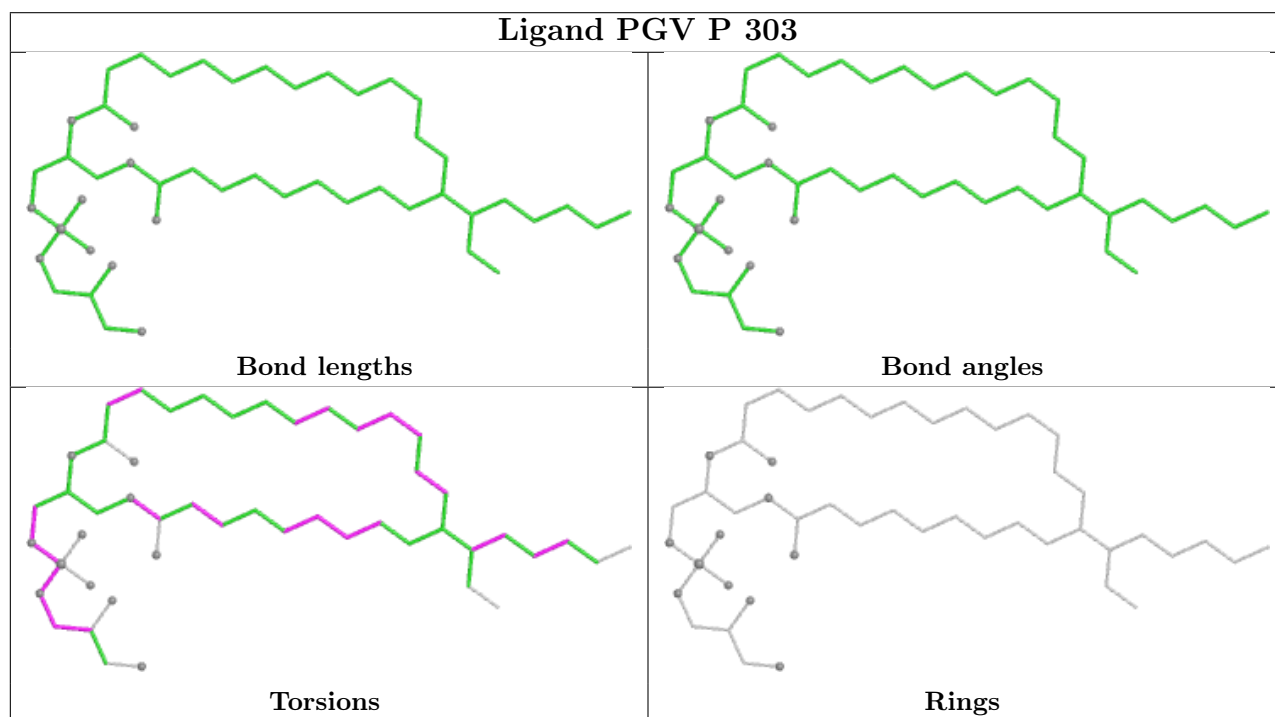


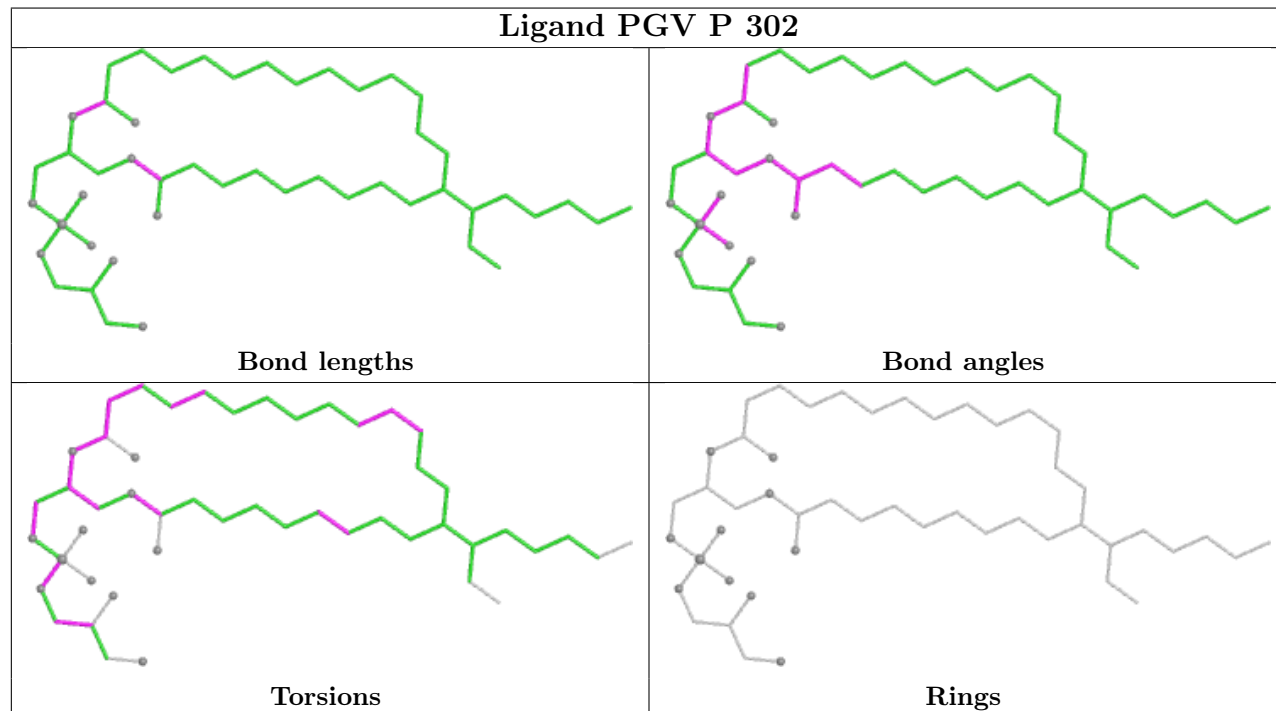
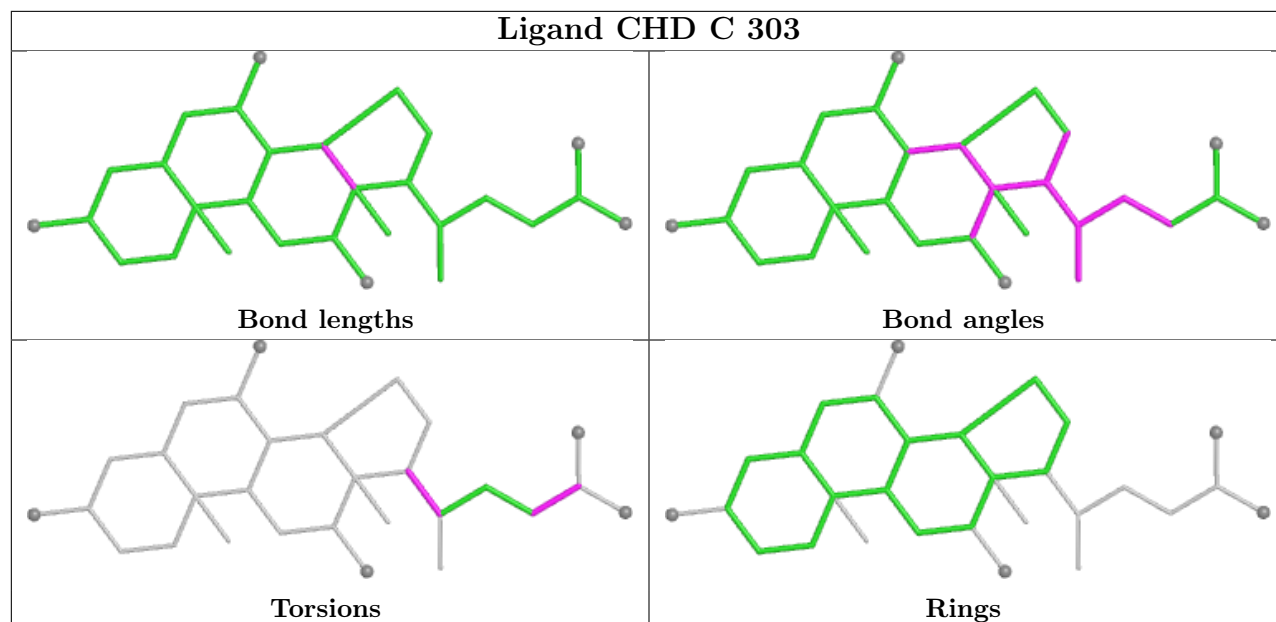


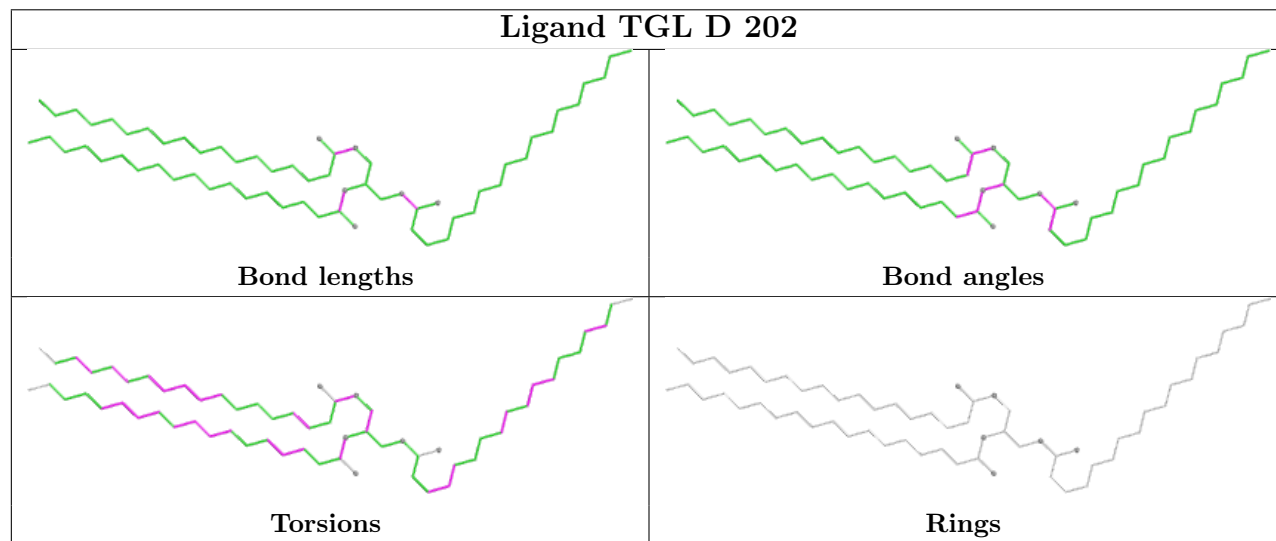
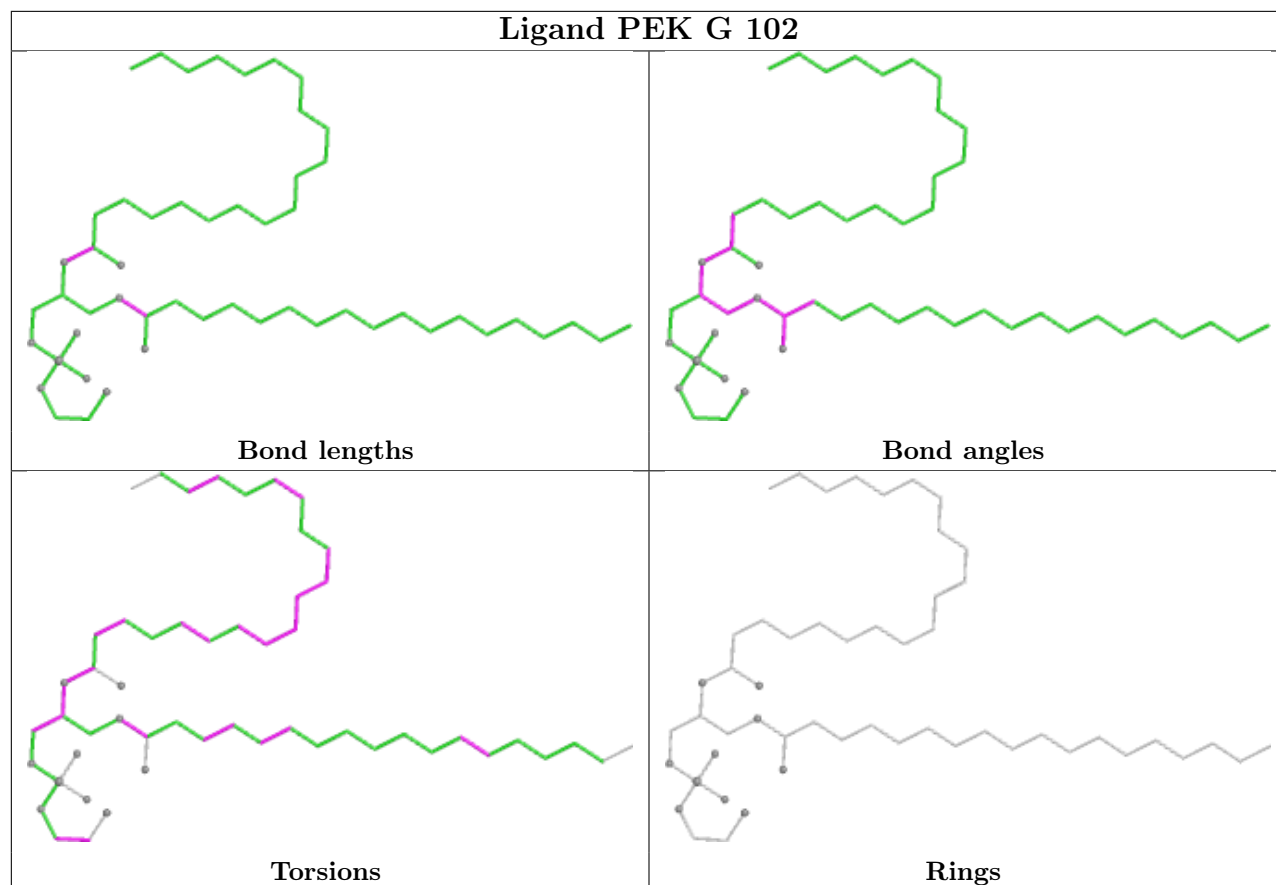
Ligand PSC O 602

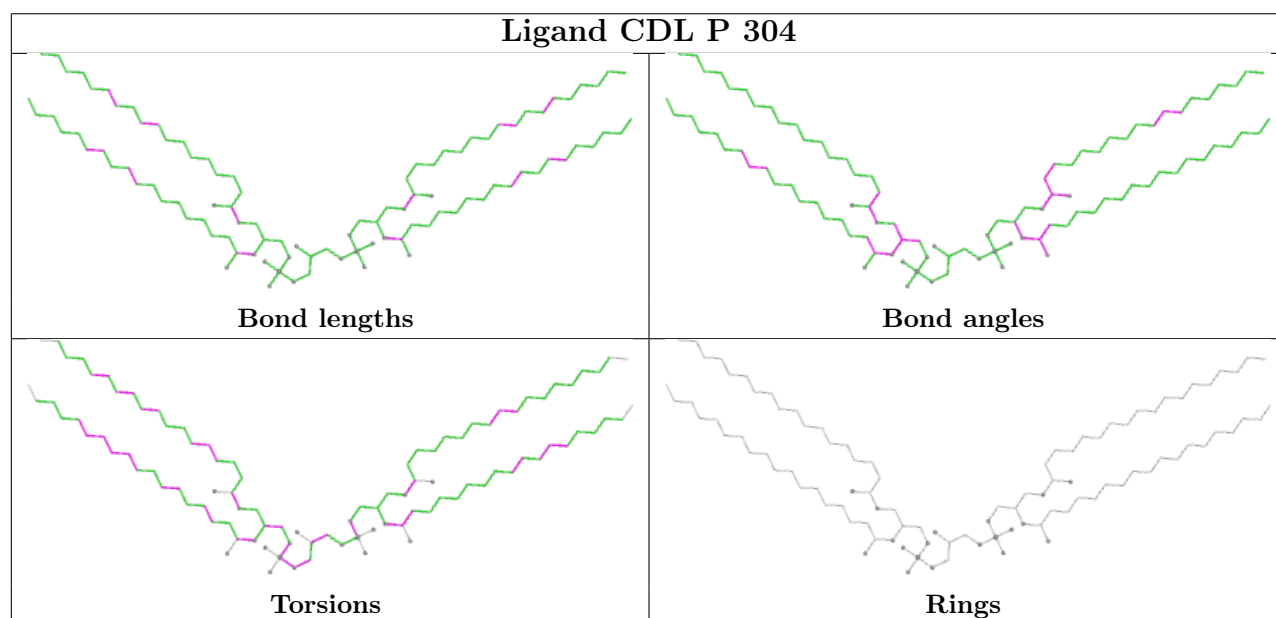
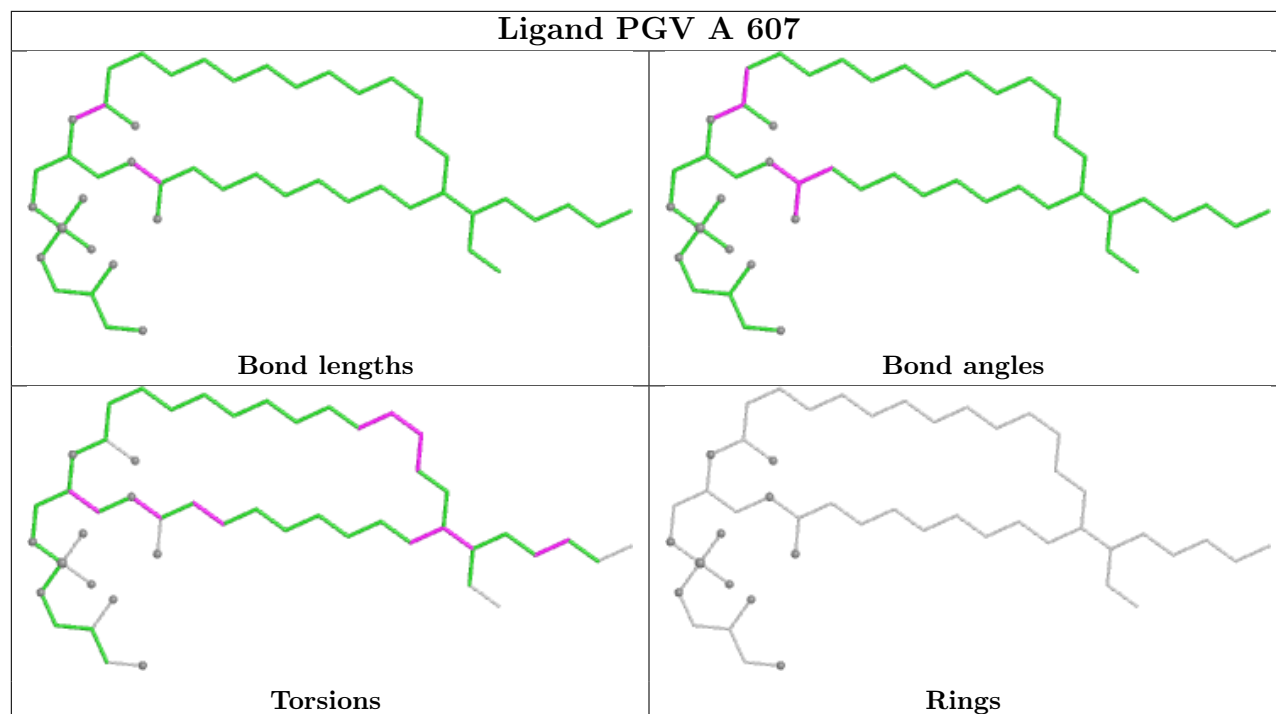


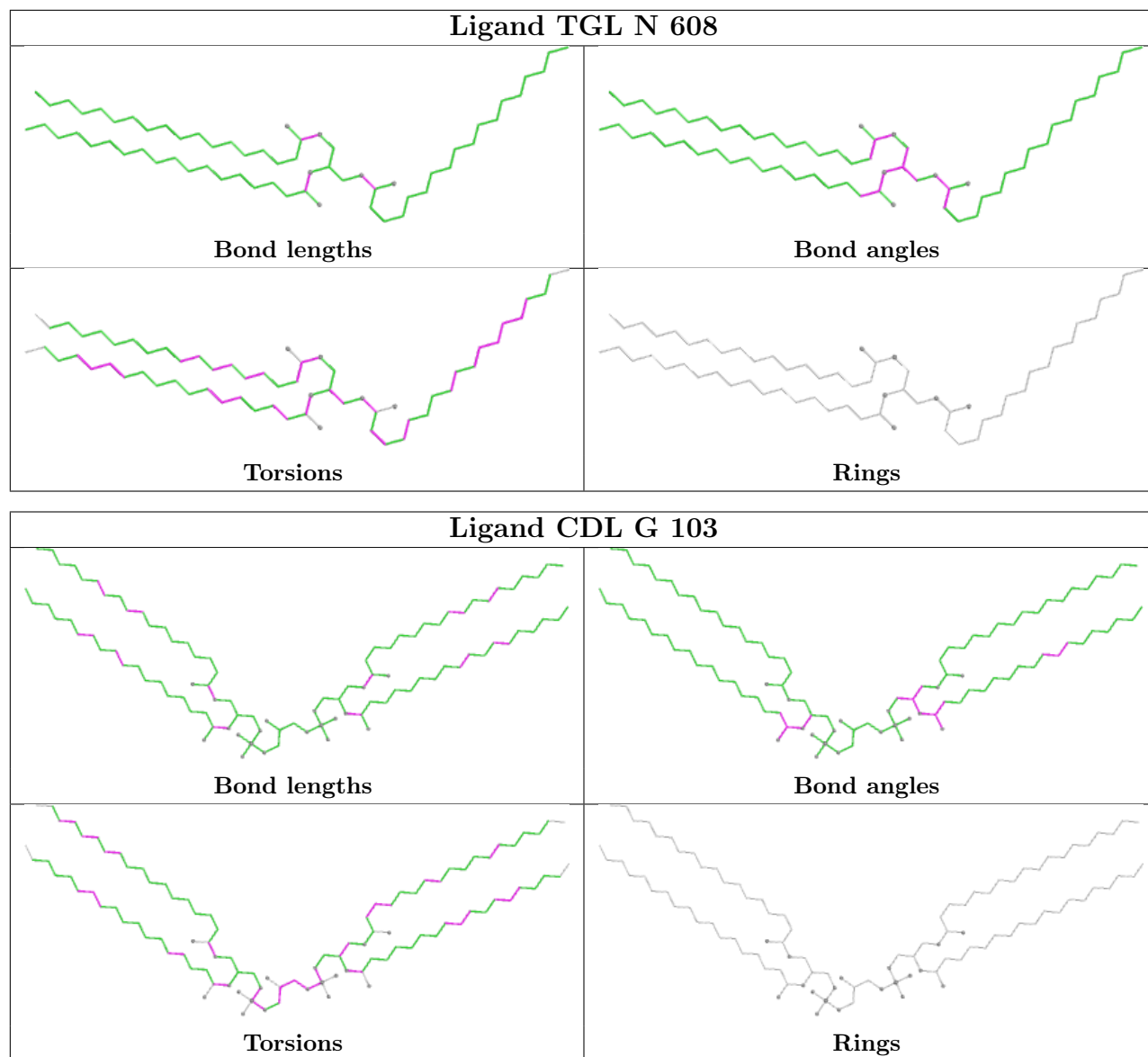
Ligand PGV P 303

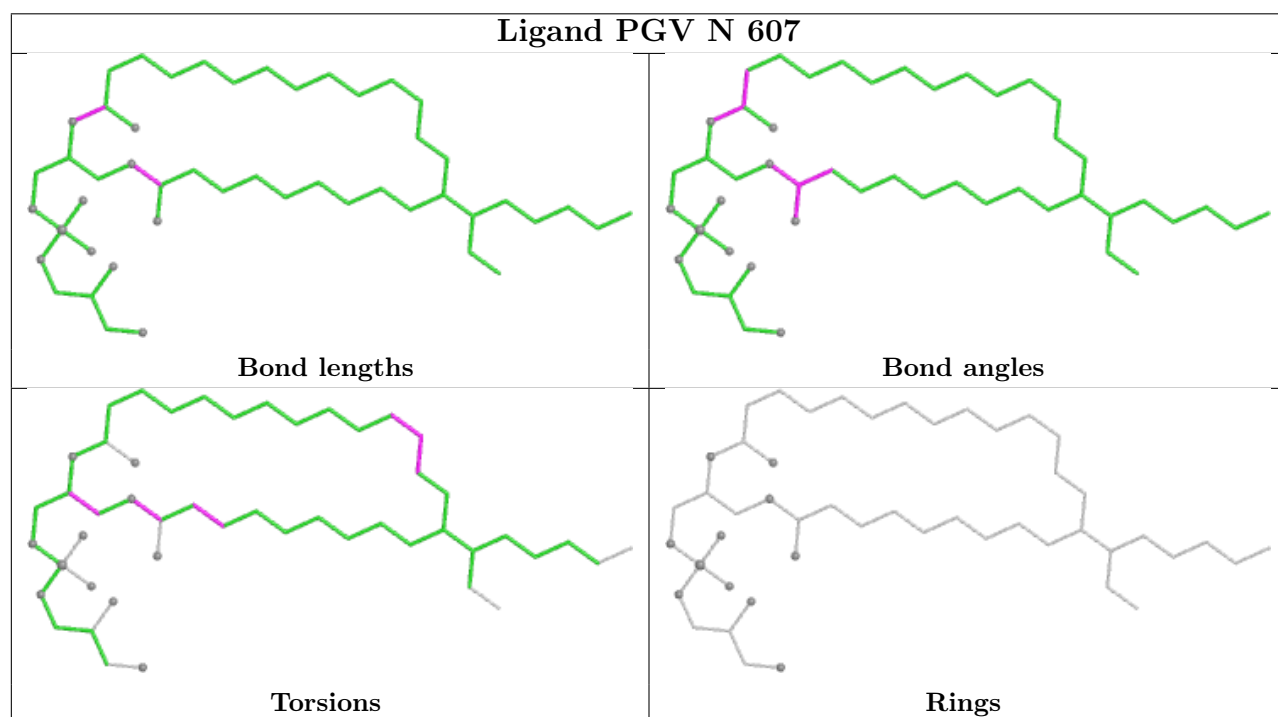
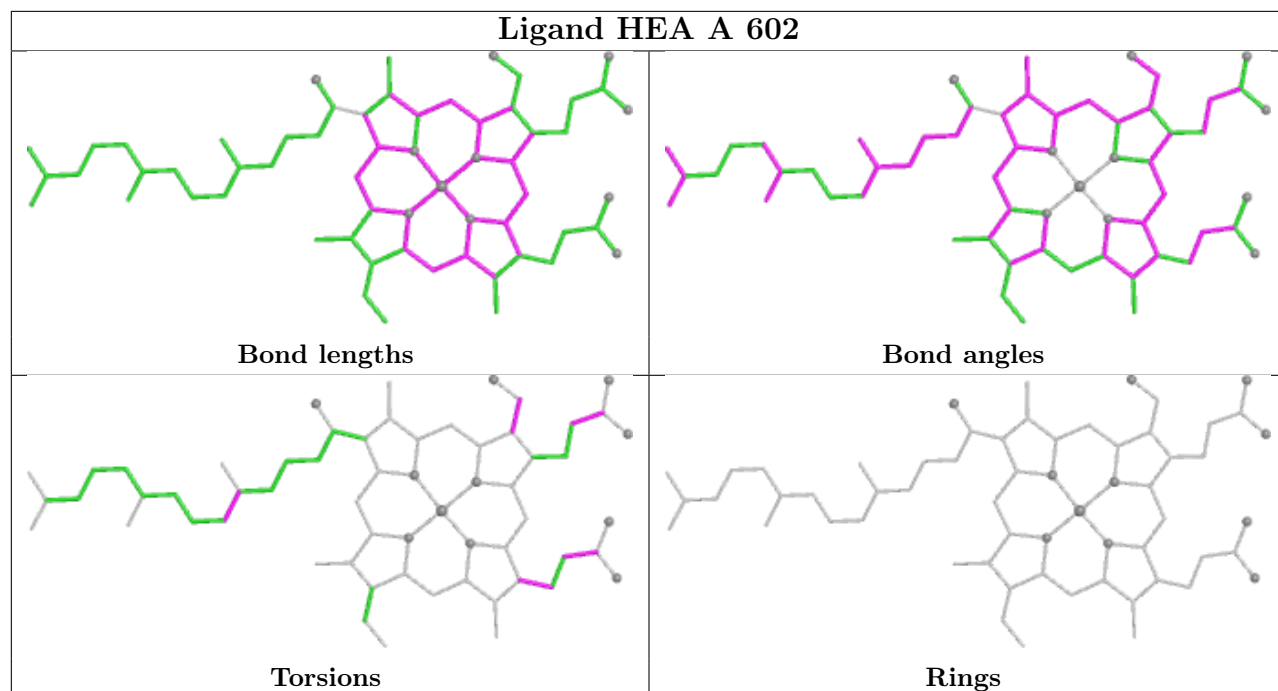




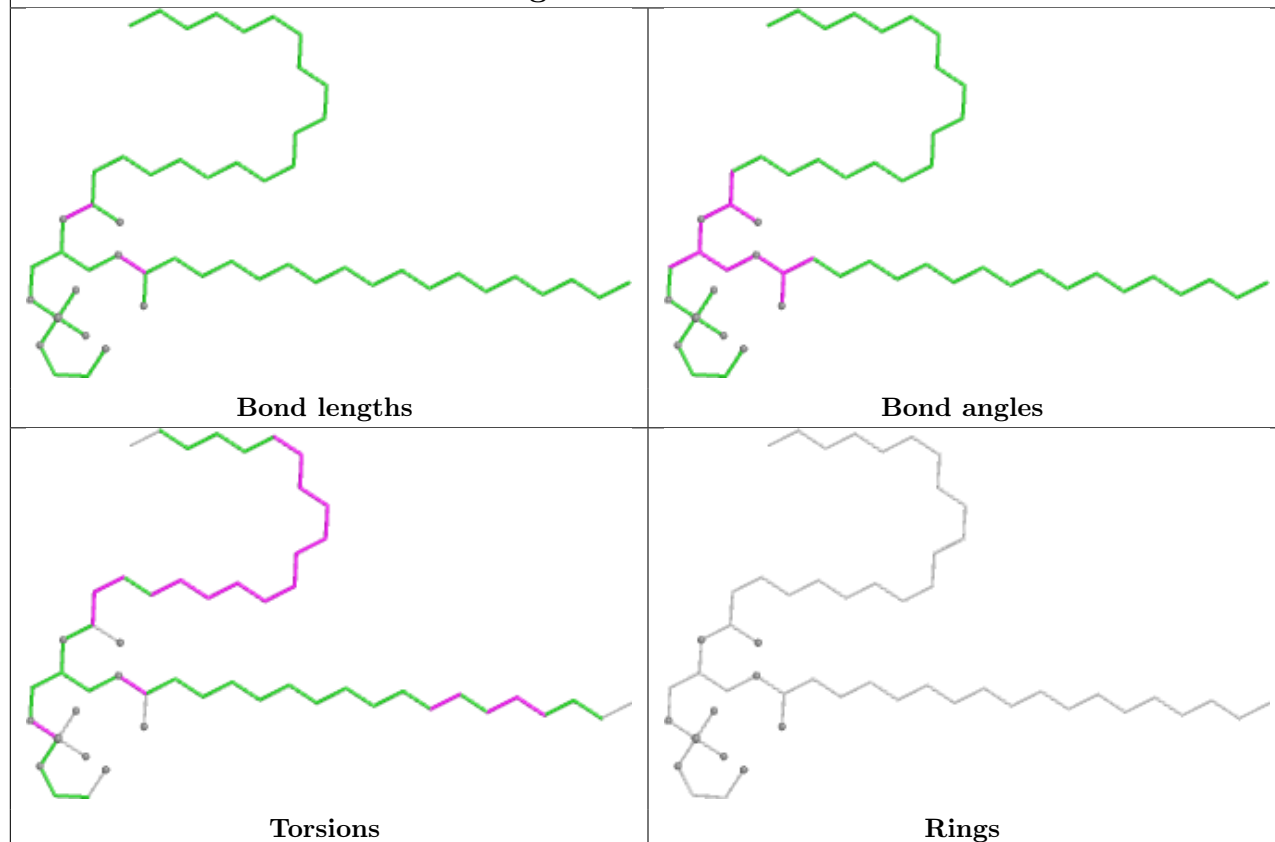




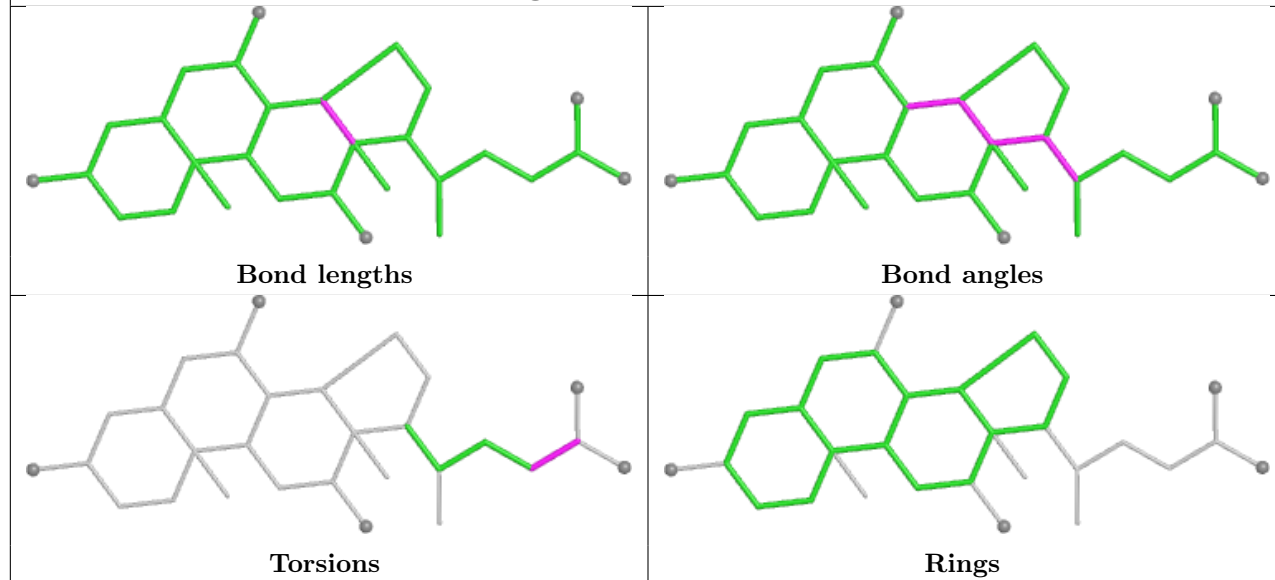


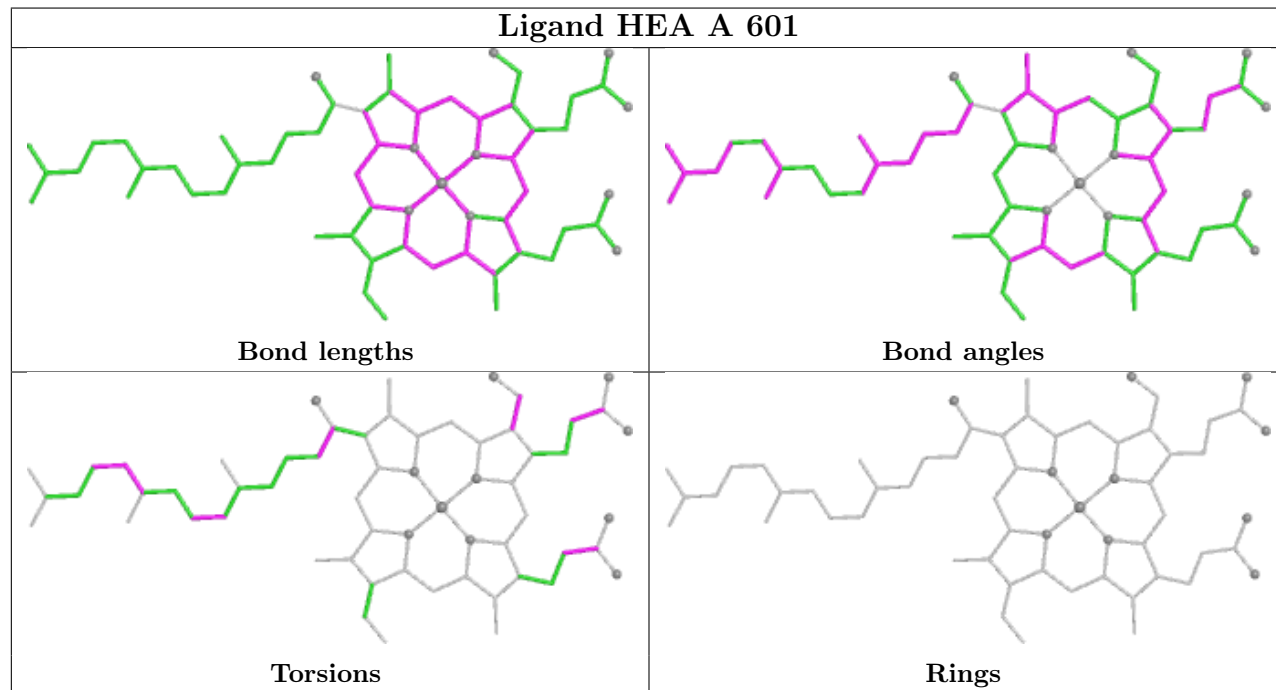
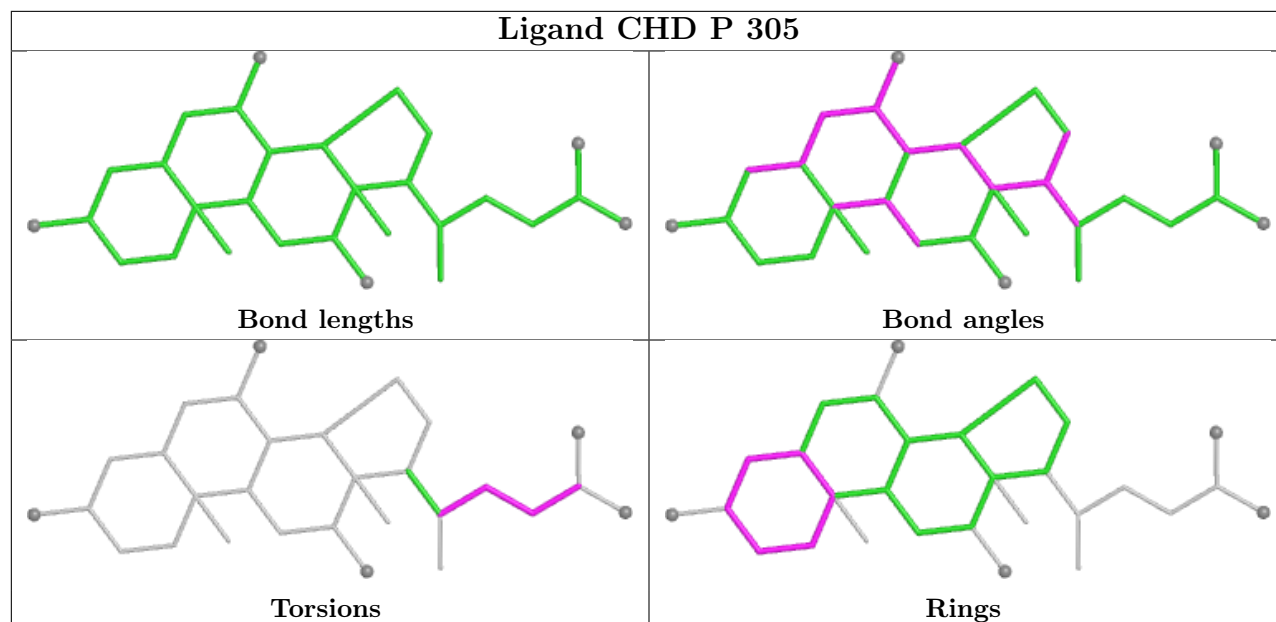


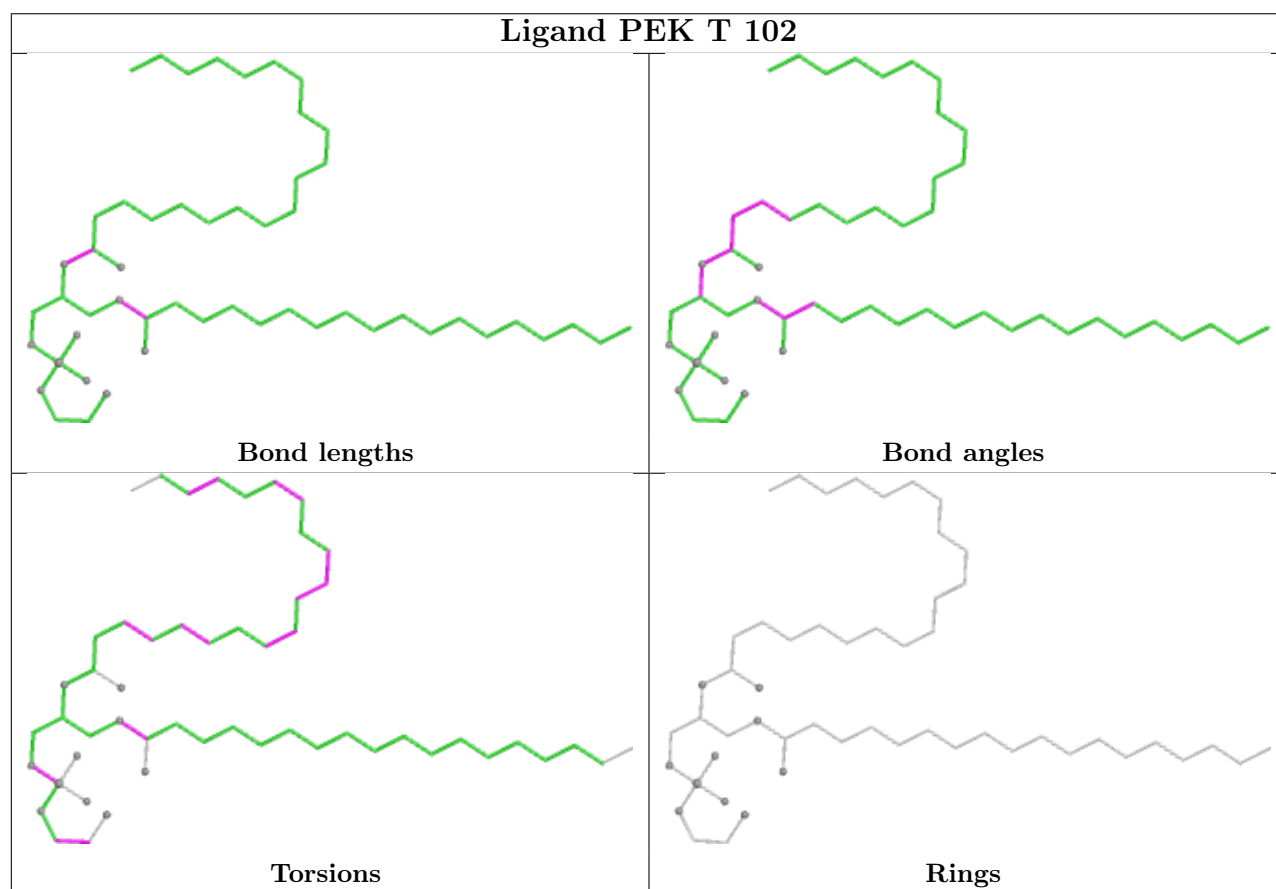
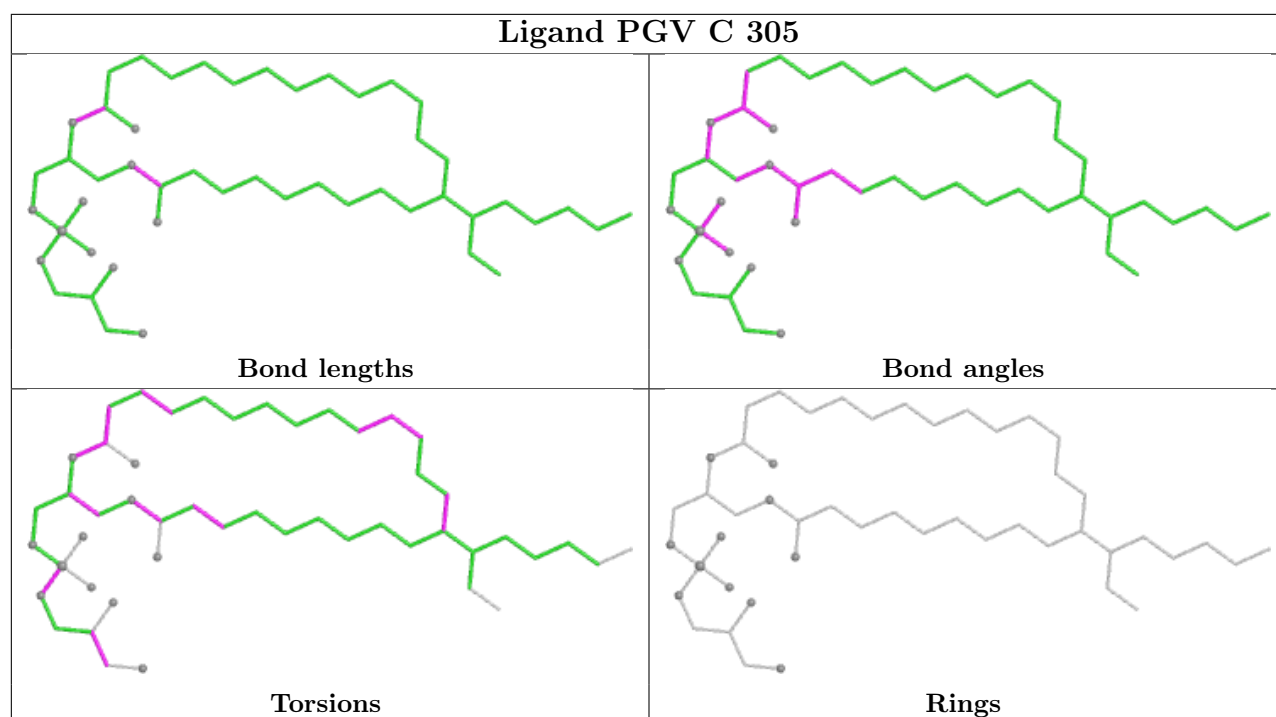
Ligand PEK G 101

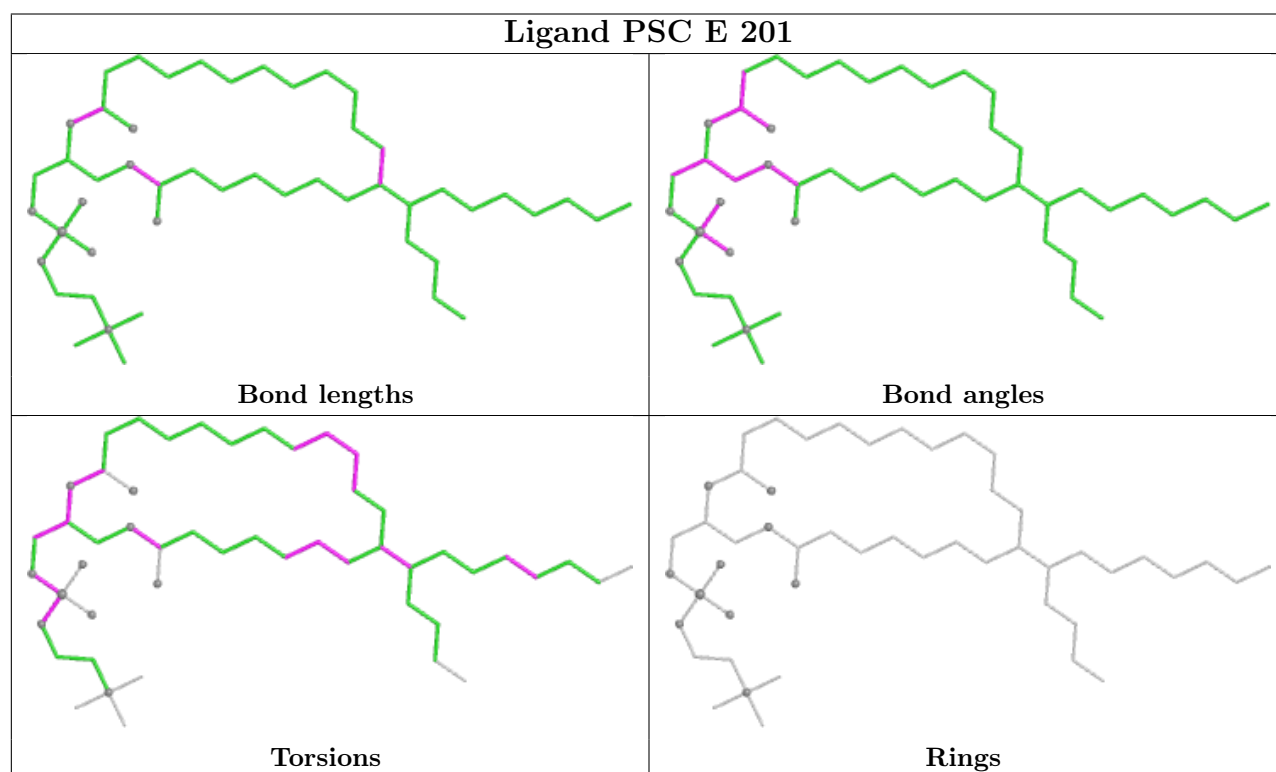
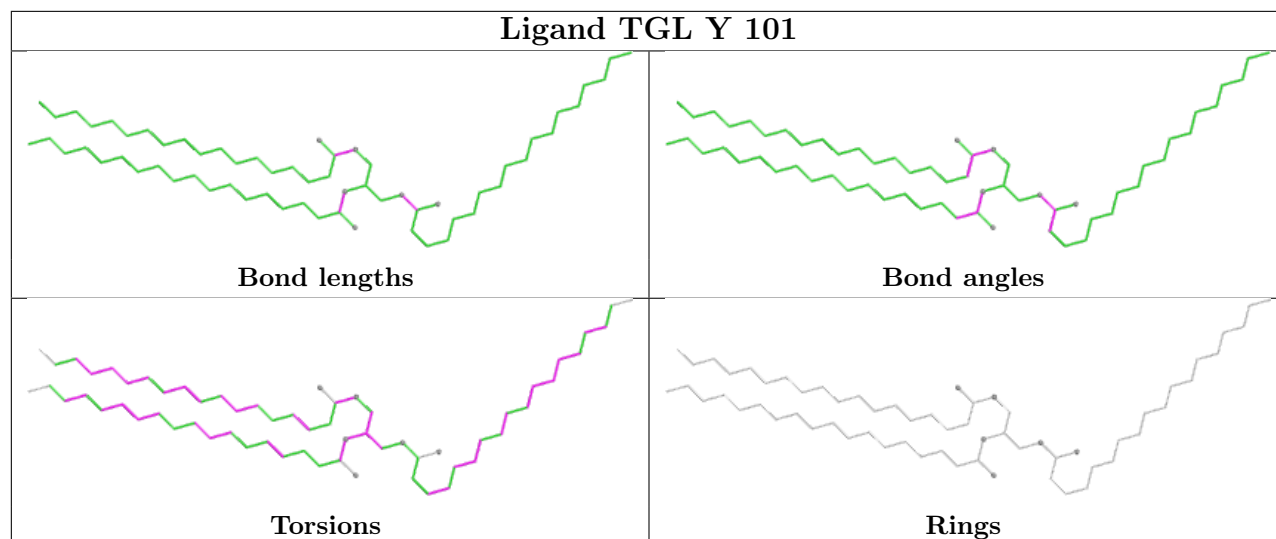


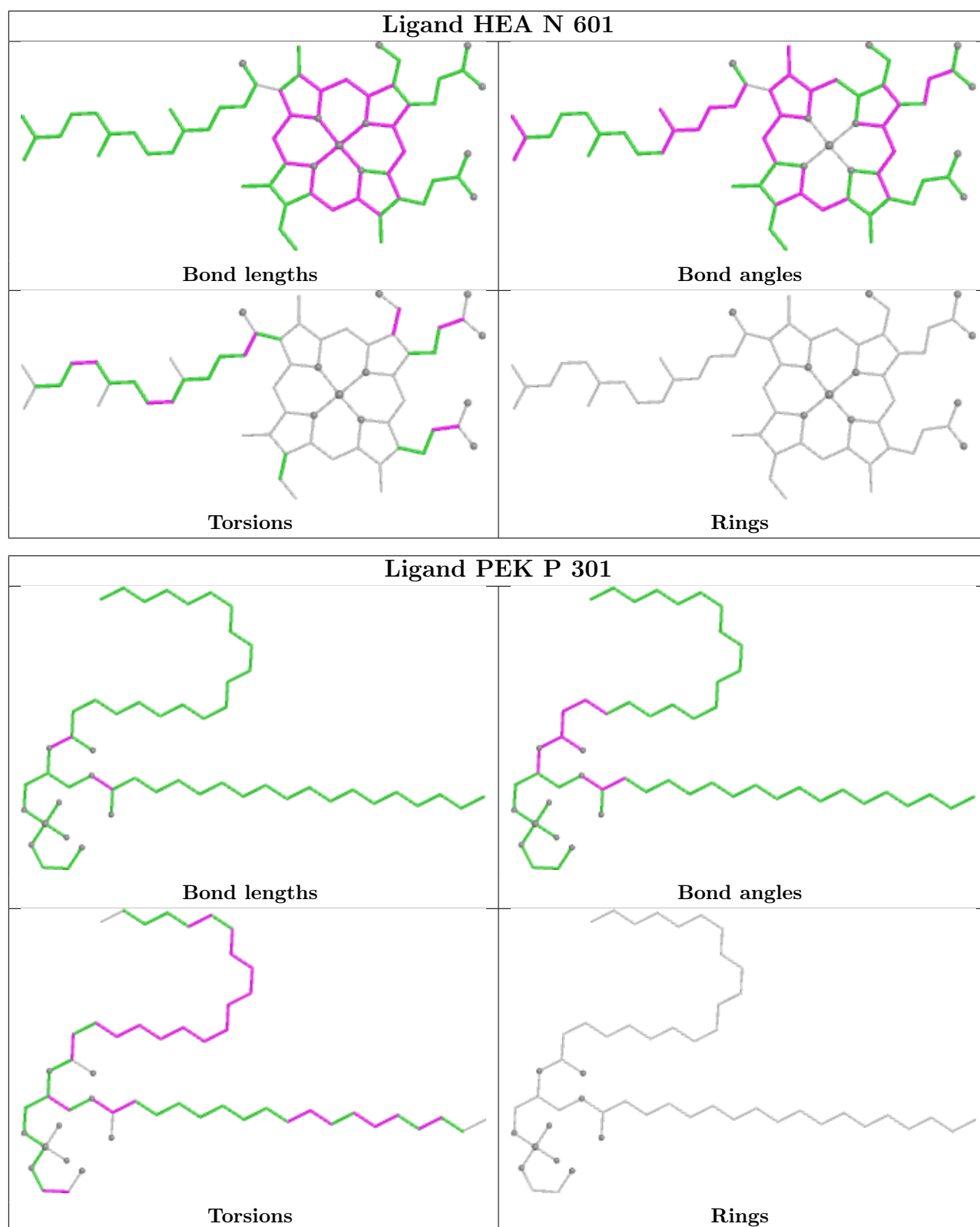
Ligand CHD G 104

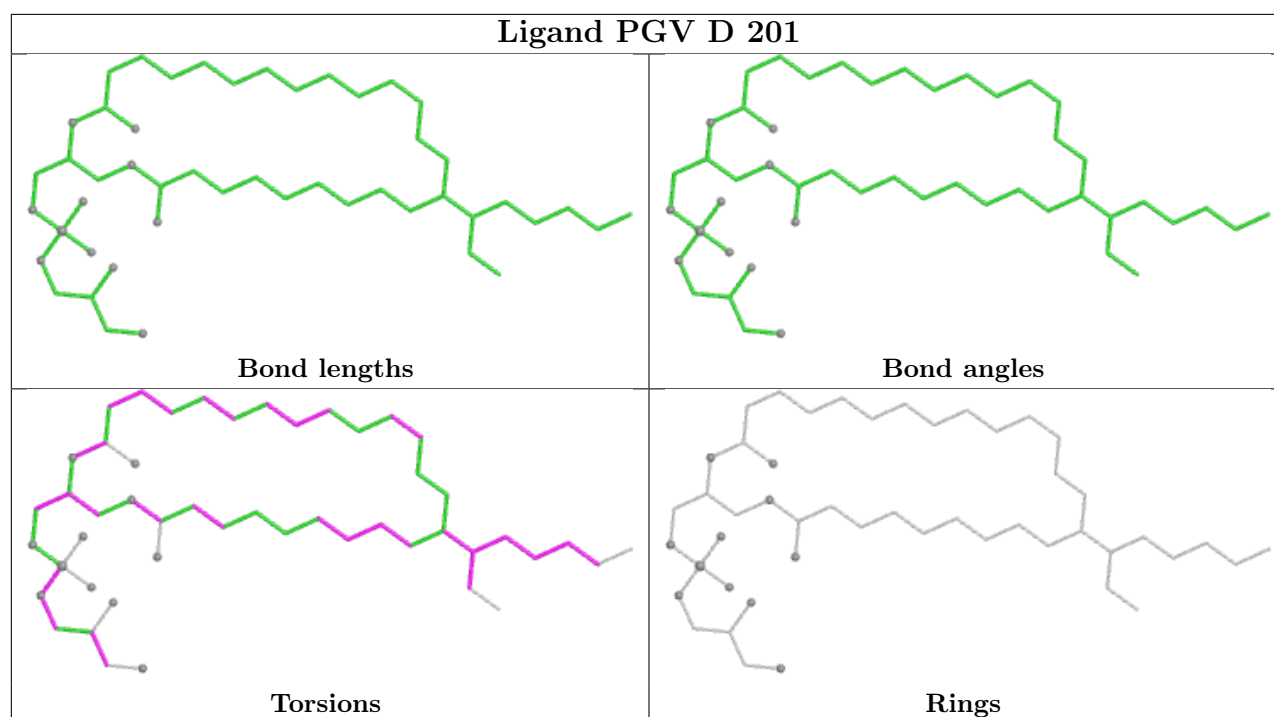












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	513/514 (99%)	-0.13	5 (0%)	79 77	15, 29, 38, 92	11 (2%)
1	N	513/514 (99%)	-0.07	3 (0%)	85 83	15, 32, 44, 79	11 (2%)
2	B	226/581 (38%)	0.35	12 (5%)	32 29	24, 37, 70, 123	5 (2%)
2	O	226/581 (38%)	0.57	18 (7%)	18 16	21, 42, 79, 167	6 (2%)
3	C	259/261 (99%)	-0.05	3 (1%)	76 74	14, 33, 48, 95	8 (3%)
3	P	259/261 (99%)	0.07	3 (1%)	76 74	14, 33, 50, 97	9 (3%)
4	D	144/147 (97%)	0.18	5 (3%)	47 44	17, 39, 61, 99	3 (2%)
4	Q	139/147 (94%)	0.71	9 (6%)	25 22	21, 52, 86, 150	2 (1%)
5	E	105/109 (96%)	0.20	2 (1%)	66 63	30, 40, 69, 146	1 (0%)
5	R	105/109 (96%)	0.61	6 (5%)	29 26	27, 49, 79, 144	1 (0%)
6	F	93/98 (94%)	0.32	4 (4%)	40 36	18, 39, 67, 139	3 (3%)
6	S	96/98 (97%)	0.46	9 (9%)	14 11	21, 38, 76, 113	1 (1%)
7	G	81/84 (96%)	1.19	18 (22%)	2 1	30, 41, 124, 185	1 (1%)
7	T	81/84 (96%)	1.20	15 (18%)	3 2	30, 43, 124, 198	0
8	H	79/85 (92%)	0.74	10 (12%)	8 6	29, 42, 124, 143	0
8	U	79/85 (92%)	0.82	10 (12%)	8 6	34, 47, 138, 151	0
9	I	72/73 (98%)	0.79	8 (11%)	10 8	35, 52, 81, 101	0
9	V	72/73 (98%)	1.13	10 (13%)	6 5	37, 58, 94, 139	0
10	J	57/59 (96%)	0.32	3 (5%)	32 29	32, 44, 79, 96	0
10	W	57/59 (96%)	0.61	3 (5%)	32 29	28, 45, 84, 109	1 (1%)
11	K	51/56 (91%)	0.51	4 (7%)	19 16	34, 45, 71, 97	0
11	X	49/56 (87%)	0.61	2 (4%)	41 38	23, 52, 77, 89	1 (2%)
12	L	46/47 (97%)	0.24	2 (4%)	40 36	28, 36, 62, 111	0
12	Y	45/47 (95%)	0.46	3 (6%)	24 21	28, 42, 78, 91	1 (2%)

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	0.26	4 (9%) 14 12	30, 35, 95, 136	0
13	Z	41/46 (89%)	0.54	4 (9%) 13 10	36, 44, 84, 109	0
All	All	3531/4320 (81%)	0.29	175 (4%) 34 31	14, 36, 76, 198	65 (1%)

The worst 5 of 175 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	G	36[A]	TRP	12.4
2	O	227	LEU	11.4
7	T	4	ALA	9.3
7	G	4	ALA	9.2
7	T	3	ALA	9.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	TPO	G	11	11/12	0.70	0.29	97,139,209,217	0
7	TPO	T	11	11/12	0.74	0.28	86,138,197,210	0
1	FME	N	1	10/11	0.87	0.19	43,50,90,92	0
1	FME	A	1	10/11	0.89	0.16	38,51,75,118	0
2	FME	O	1	10/11	0.95	0.12	35,40,60,89	0
2	FME	B	1	10/11	0.96	0.11	32,36,49,94	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

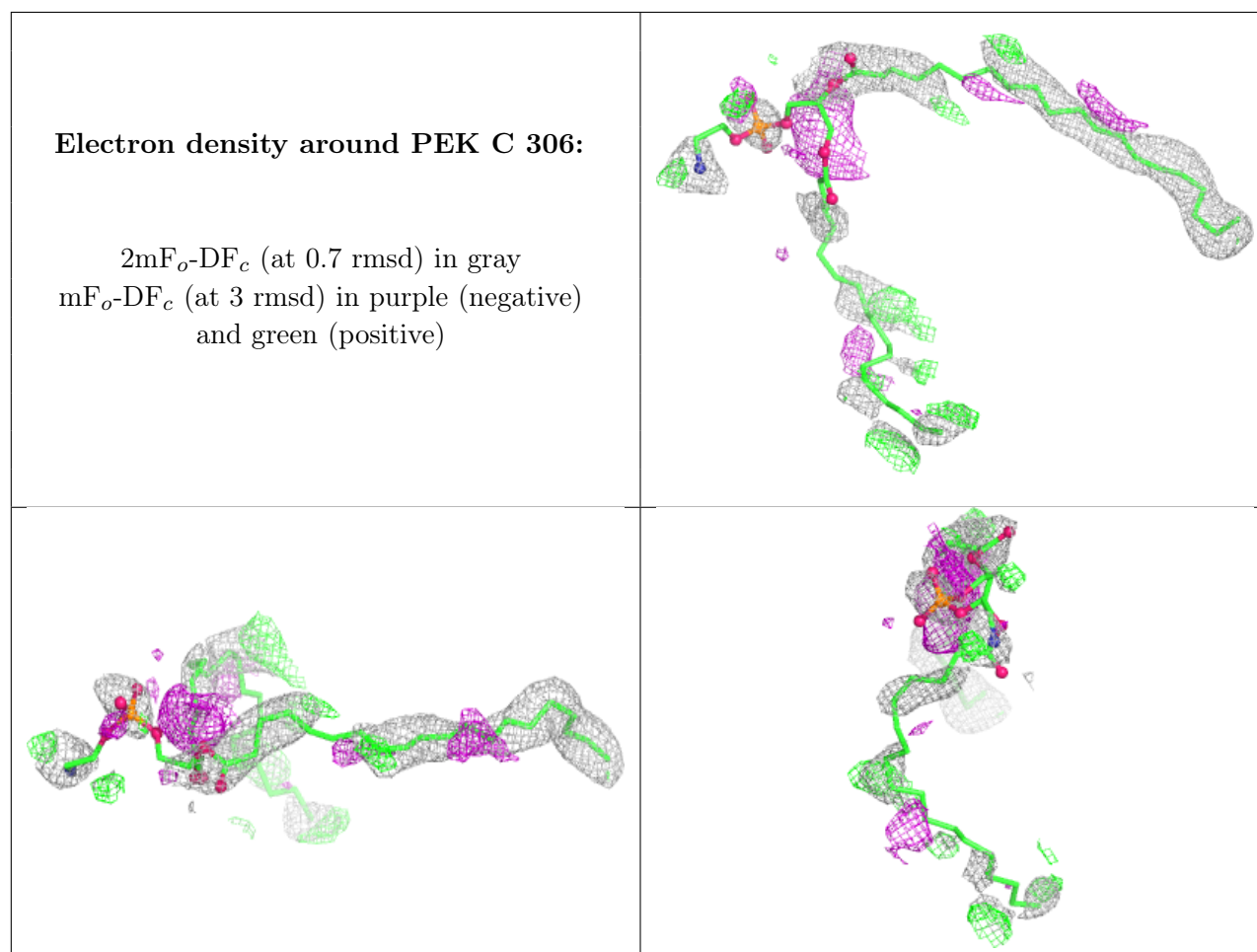
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	PEK	C	306	53/53	0.66	0.28	41,97,176,196	0
19	PGV	P	302	51/51	0.70	0.30	52,93,171,178	0
22	CDL	G	103	100/100	0.72	0.30	51,107,157,207	0
20	TGL	Q	201	63/63	0.72	0.28	44,79,121,133	0
24	PEK	P	301	53/53	0.73	0.26	39,89,173,197	0
22	CDL	T	103	100/100	0.74	0.30	46,97,179,209	0
19	PGV	D	201	51/51	0.75	0.28	34,83,159,180	0
24	PEK	G	101	53/53	0.75	0.24	41,88,171,203	0
23	CHD	C	303	29/29	0.75	0.19	75,97,118,124	0
24	PEK	P	307	53/53	0.75	0.26	43,91,163,188	0
25	PSC	O	602	52/52	0.75	0.27	41,94,202,234	0
22	CDL	P	304	100/100	0.77	0.24	38,95,140,162	0
19	PGV	C	305	51/51	0.77	0.25	34,83,144,188	0
23	CHD	P	305	29/29	0.78	0.20	63,100,124,132	0
19	PGV	N	609	51/51	0.78	0.25	39,91,166,187	0
20	TGL	Y	101	63/63	0.79	0.26	35,70,121,169	0
27	DMU	W	101	33/33	0.79	0.16	41,89,119,122	0
22	CDL	C	302	100/100	0.80	0.22	38,88,143,153	0
25	PSC	E	201	52/52	0.80	0.25	40,114,206,225	0
20	TGL	A	608	63/63	0.80	0.23	33,76,105,138	0
20	TGL	D	202	63/63	0.80	0.24	39,74,102,128	0
27	DMU	J	101	33/33	0.81	0.17	43,89,113,124	0
20	TGL	N	608	63/63	0.81	0.23	33,75,107,121	0
20	TGL	L	101	63/63	0.82	0.23	32,61,108,130	0
24	PEK	G	102	53/53	0.87	0.23	31,54,111,129	0
19	PGV	N	607	51/51	0.88	0.18	17,49,75,89	0
19	PGV	A	607	51/51	0.89	0.18	21,44,73,90	0
24	PEK	T	102	53/53	0.89	0.19	29,54,103,123	0
19	PGV	P	303	51/51	0.89	0.20	28,46,107,120	0
27	DMU	Z	101	33/33	0.90	0.11	40,56,76,89	0
27	DMU	M	101	33/33	0.91	0.11	34,49,62,87	0
23	CHD	C	304	29/29	0.92	0.08	25,35,44,47	0
19	PGV	C	301	51/51	0.92	0.16	22,46,88,101	0
23	CHD	P	306	29/29	0.93	0.08	24,37,45,53	0
23	CHD	G	104	29/29	0.95	0.07	21,29,38,49	0
18	PER	A	606	2/2	0.95	0.17	36,36,36,42	0
18	PER	N	606	2/2	0.95	0.17	38,38,38,46	0
23	CHD	T	101	29/29	0.95	0.07	20,28,43,56	0
14	HEA	N	601	60/60	0.96	0.12	18,34,62,79	0
14	HEA	N	602	60/60	0.96	0.09	18,30,45,54	0
17	NA	A	605	1/1	0.97	0.17	15,15,15,15	0
14	HEA	A	601	60/60	0.97	0.10	11,29,56,88	0
14	HEA	A	602	60/60	0.97	0.09	18,28,46,49	0

Continued on next page...

Continued from previous page...

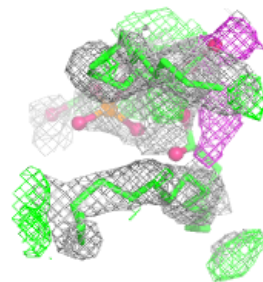
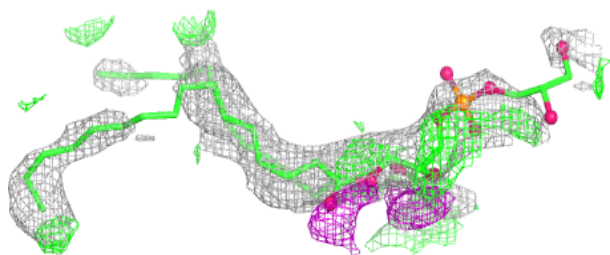
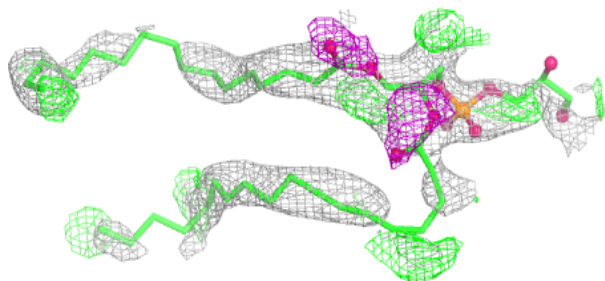
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	ZN	F	101	1/1	0.98	0.16	21,21,21,21	0
26	ZN	S	101	1/1	0.98	0.15	21,21,21,21	0
15	CU	N	603	1/1	0.98	0.08	18,18,18,18	0
21	CUA	O	601	2/2	0.98	0.09	20,20,20,20	0
15	CU	A	603	1/1	0.98	0.08	18,18,18,18	0
17	NA	N	605	1/1	0.98	0.13	17,17,17,17	0
16	MG	N	604	1/1	0.99	0.12	13,13,13,13	0
21	CUA	B	601	2/2	0.99	0.06	17,17,17,20	0
16	MG	A	604	1/1	0.99	0.10	13,13,13,13	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.

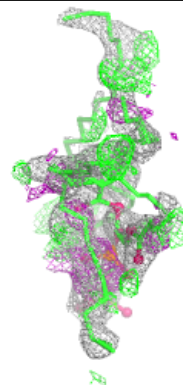
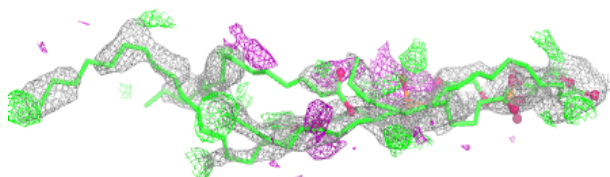
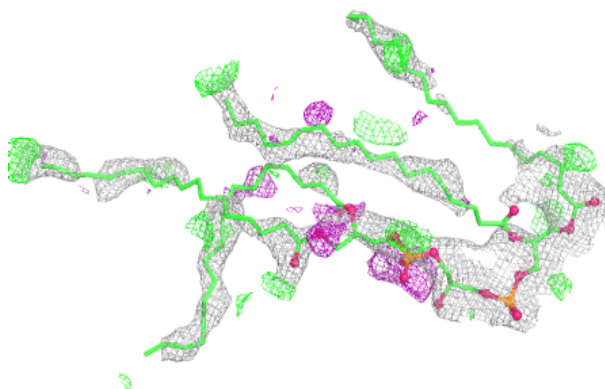


Electron density around PGV P 302:

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

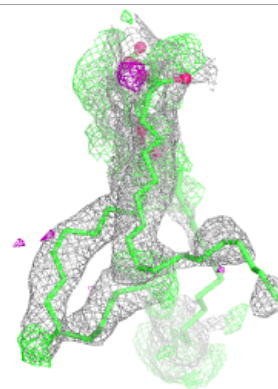
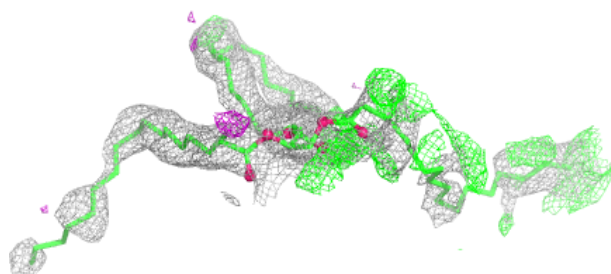
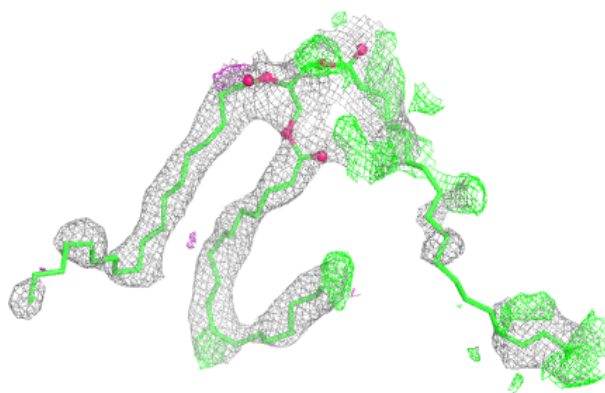
**Electron density around CDL G 103:**

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

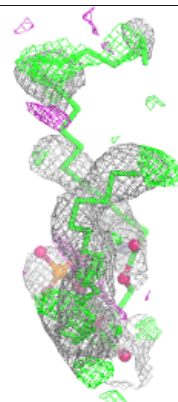
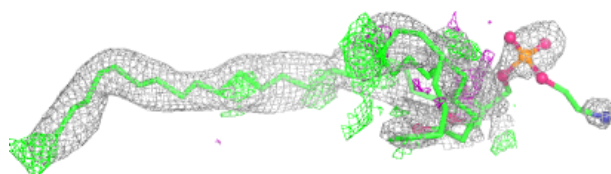
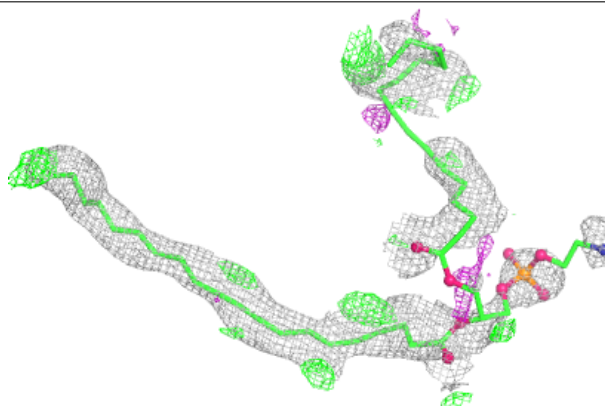


Electron density around TGL Q 201:

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

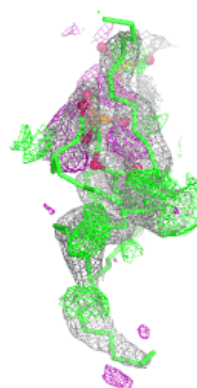
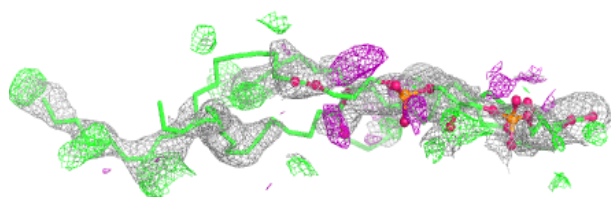
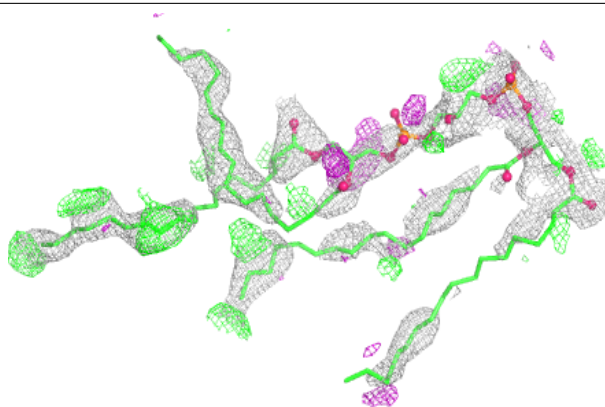
**Electron density around PEK P 301:**

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

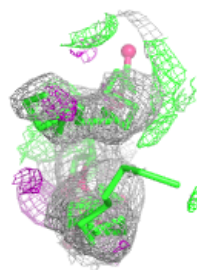
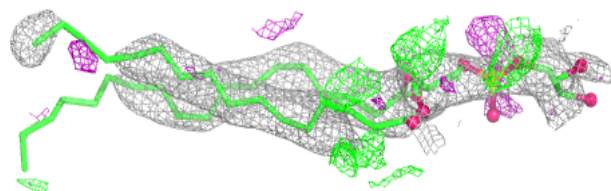
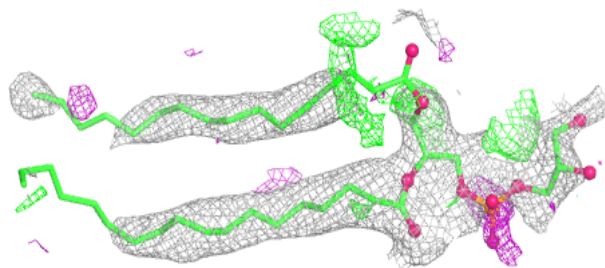


Electron density around CDL T 103:

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

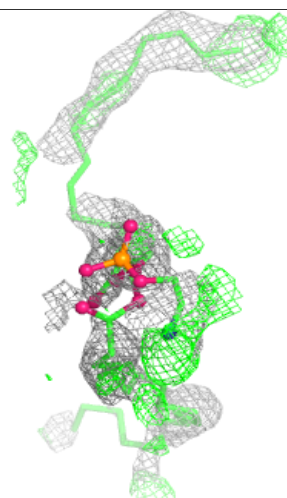
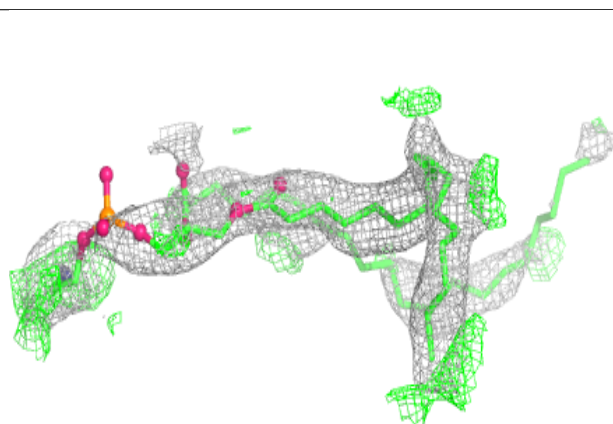
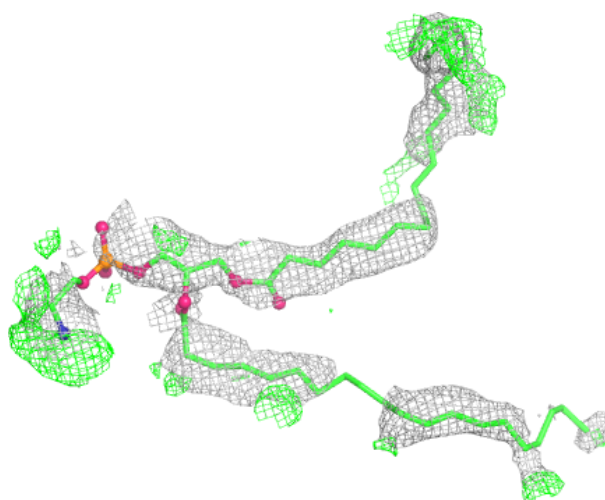
**Electron density around PGV D 201:**

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



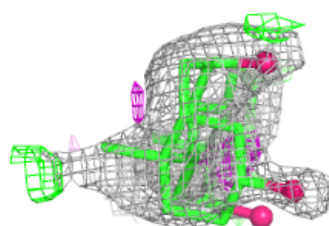
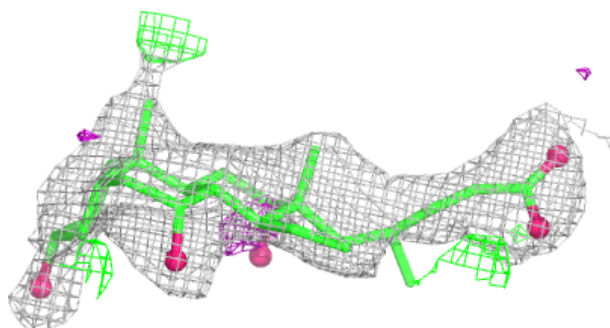
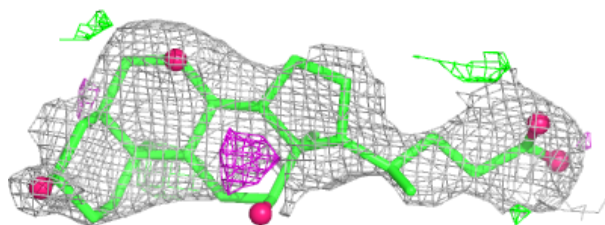
Electron density around PEK G 101:

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

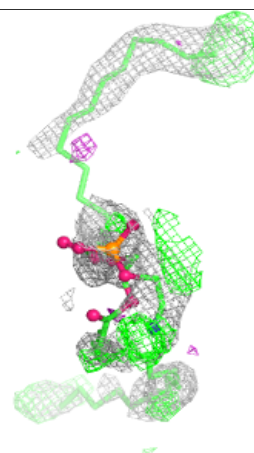
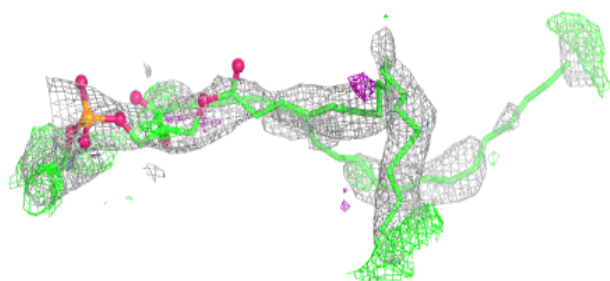
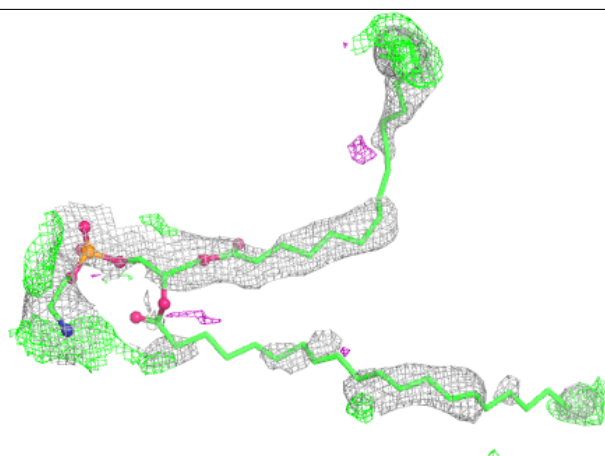


Electron density around CHD C 303:

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

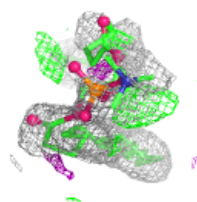
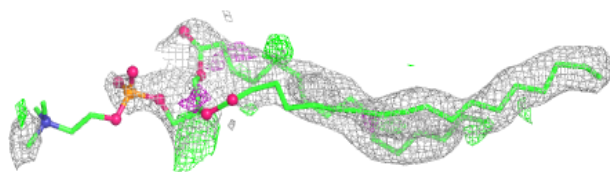
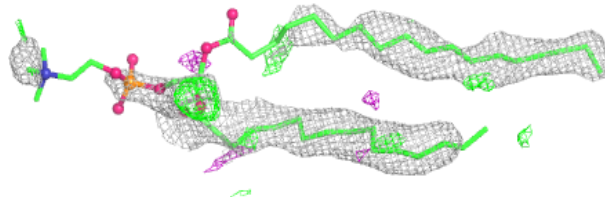
**Electron density around PEK P 307:**

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

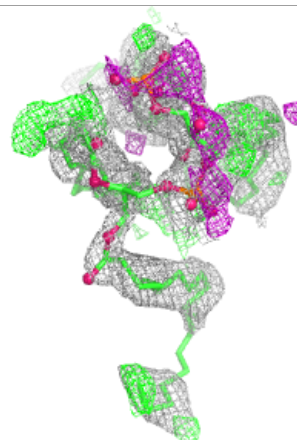
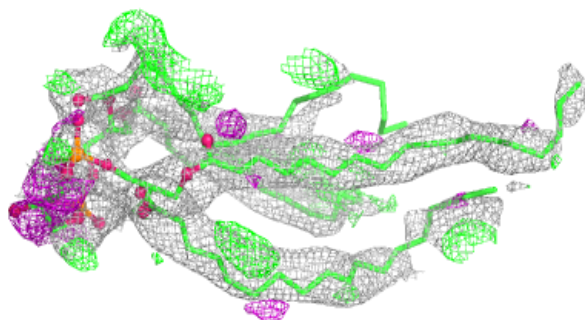
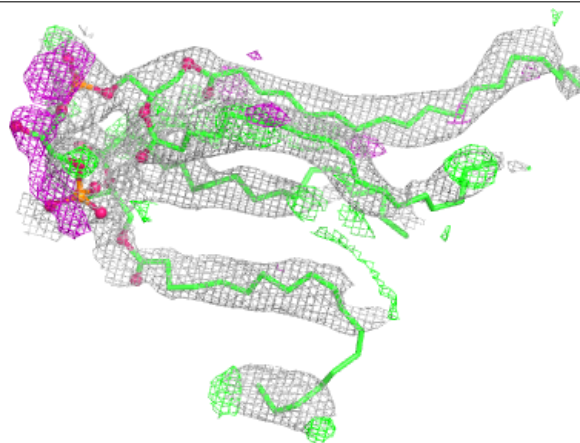


Electron density around PSC O 602:

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

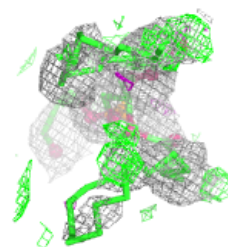
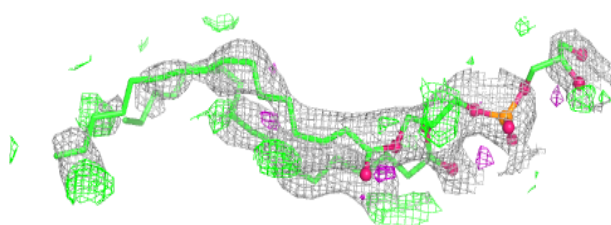
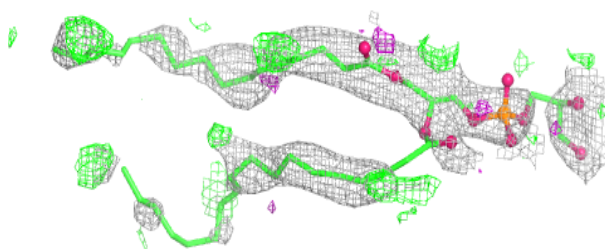
**Electron density around CDL P 304:**

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

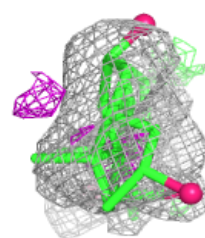
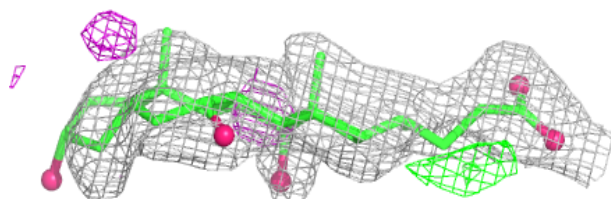
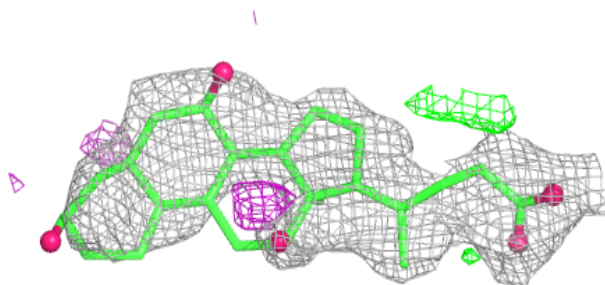


Electron density around PGV C 305:

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

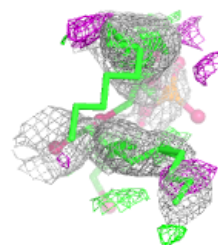
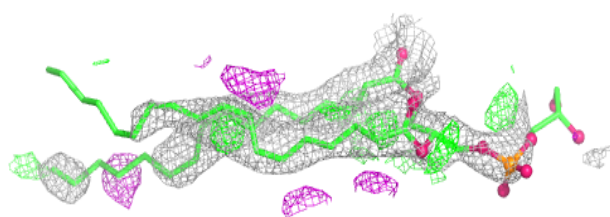
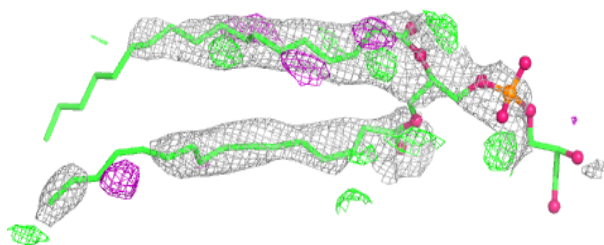
**Electron density around CHD P 305:**

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



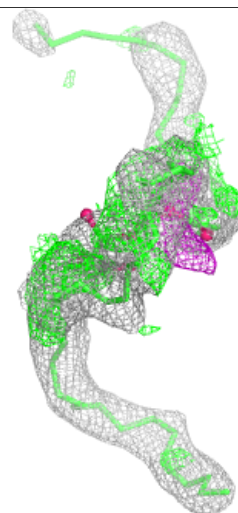
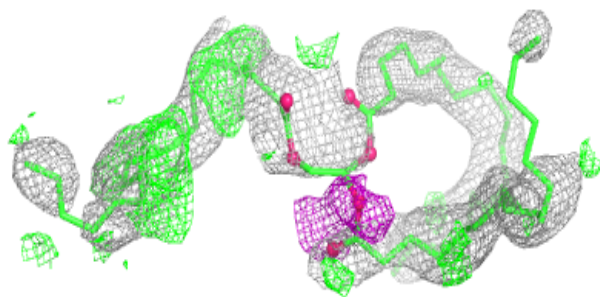
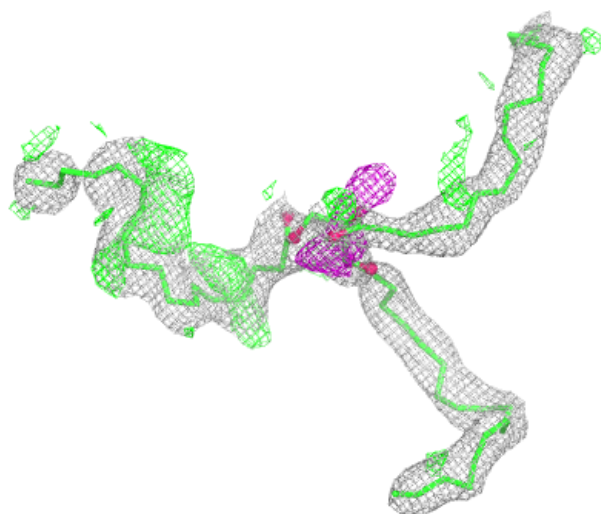
Electron density around PGV N 609:

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



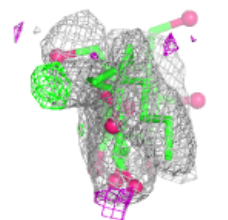
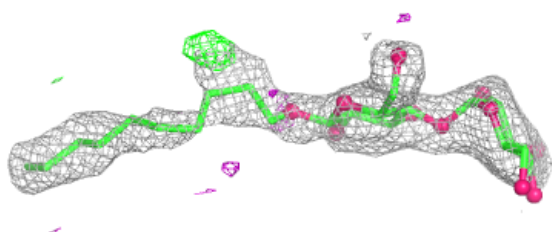
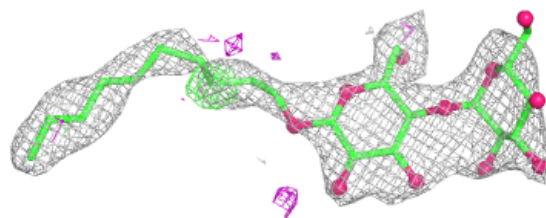
Electron density around TGL Y 101:

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



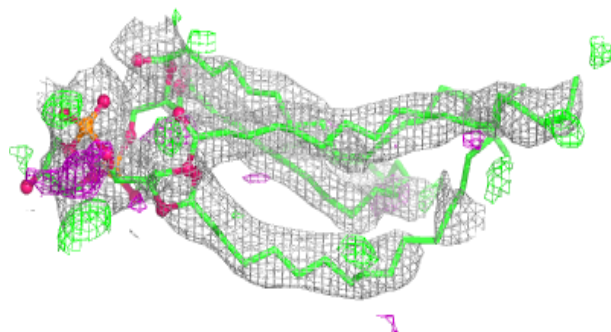
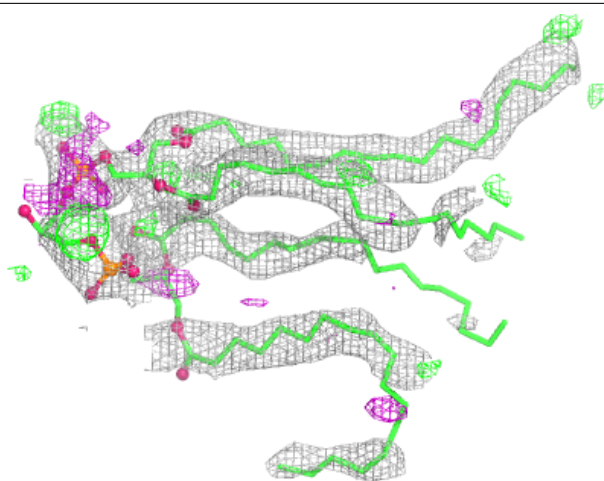
Electron density around DMU W 101:

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



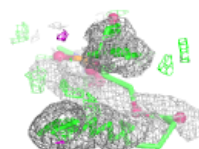
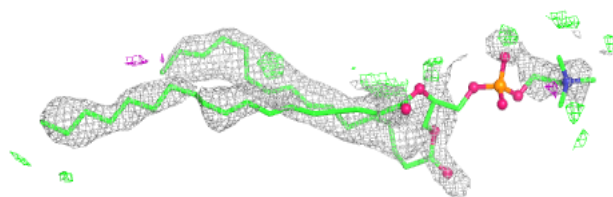
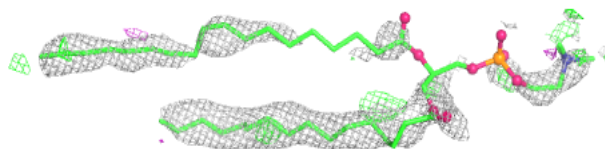
Electron density around CDL C 302:

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

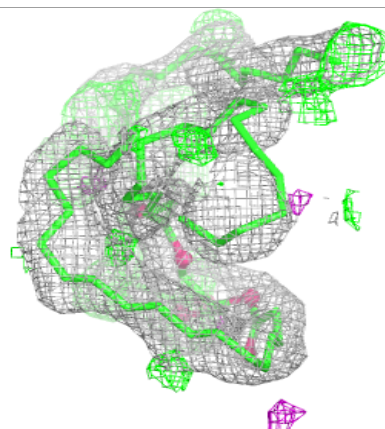
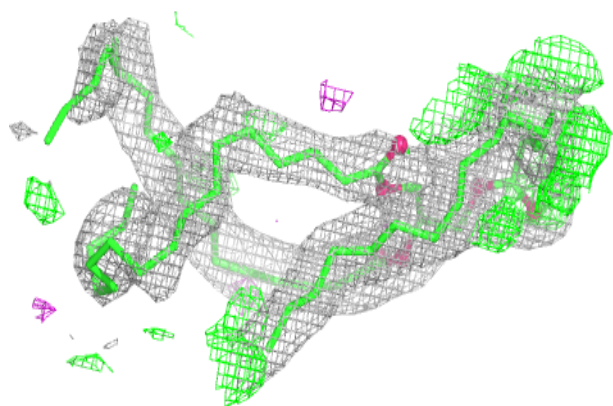
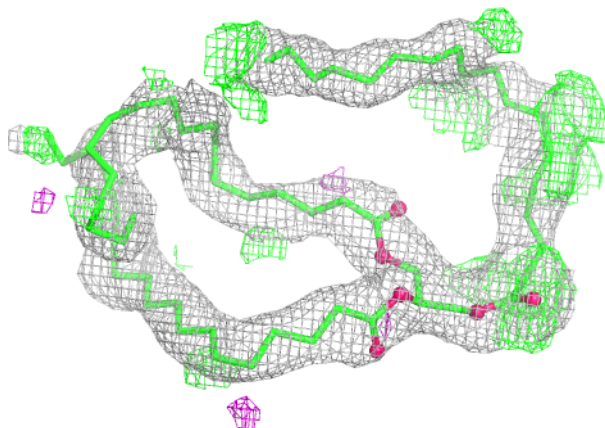


Electron density around PSC E 201:

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

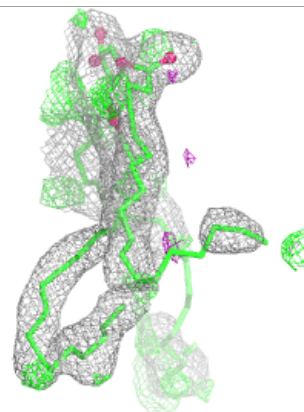
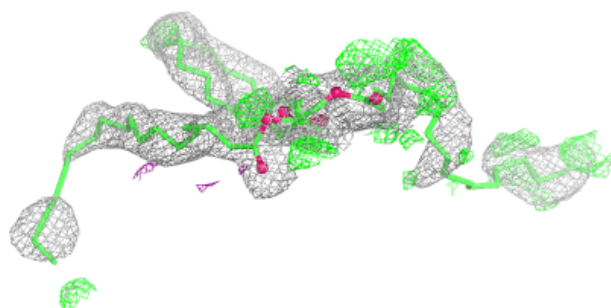
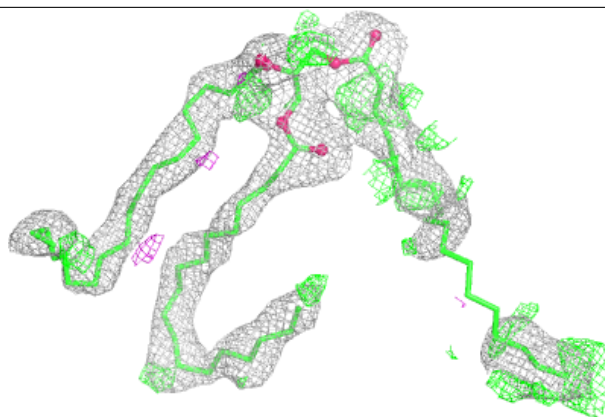
**Electron density around TGL A 608:**

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

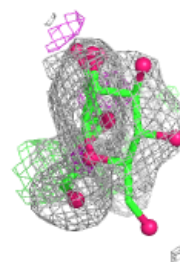
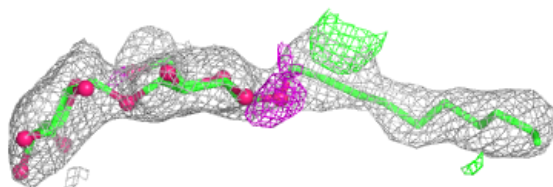
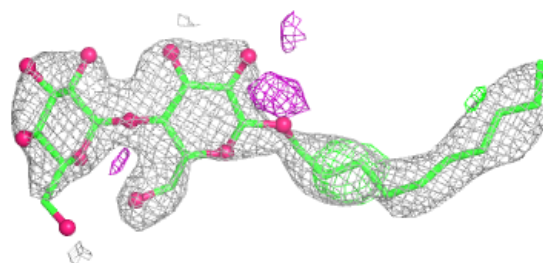


Electron density around TGL D 202:

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

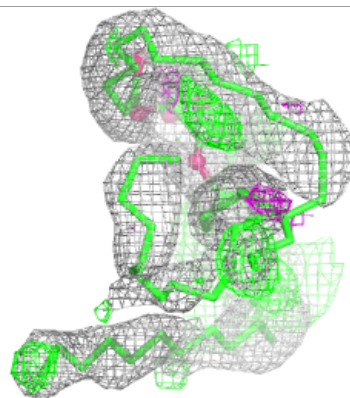
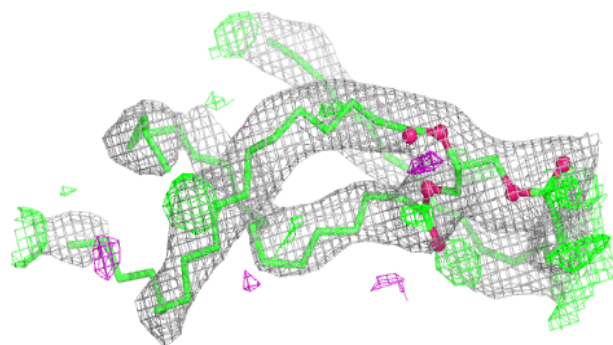
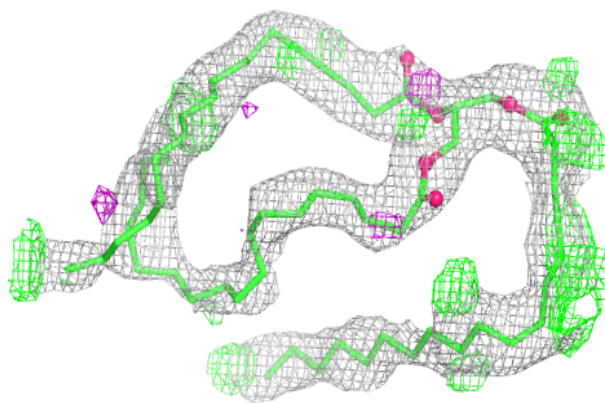
**Electron density around DMU J 101:**

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



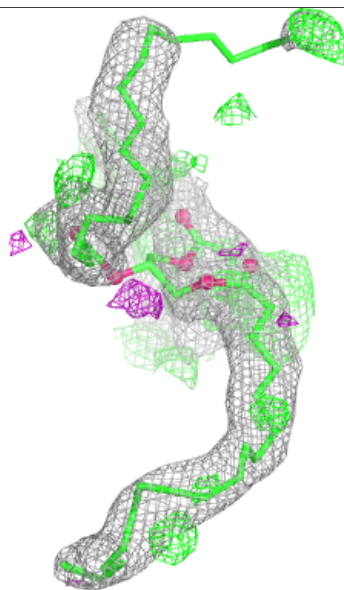
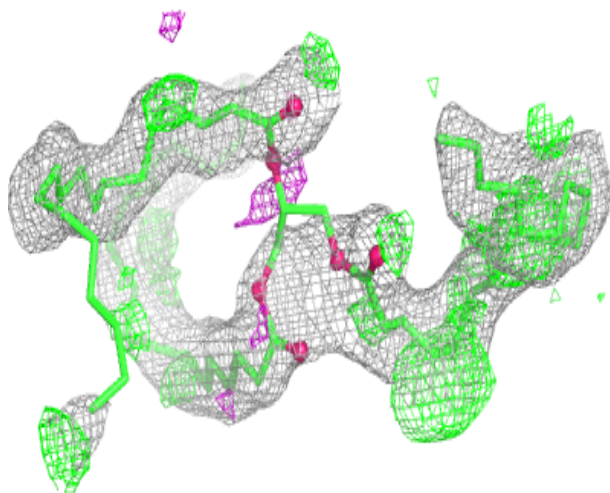
Electron density around TGL N 608:

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



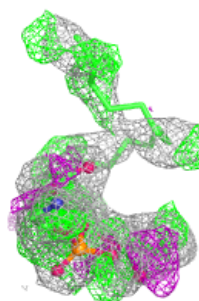
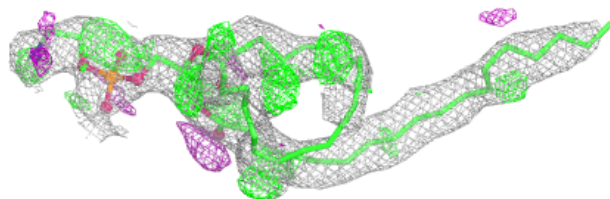
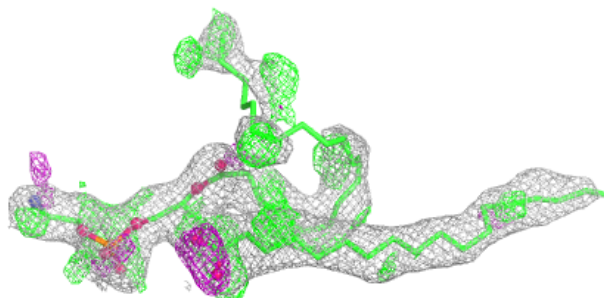
Electron density around TGL L 101:

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

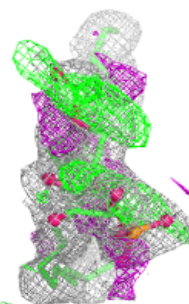
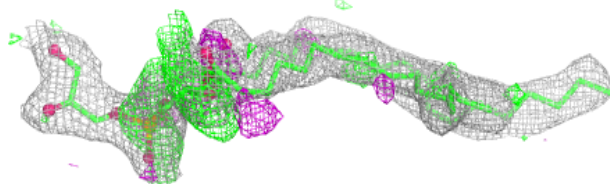
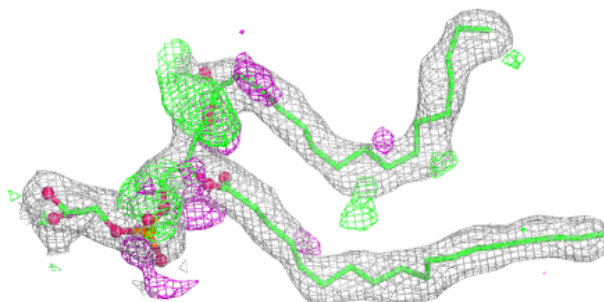


Electron density around PEK G 102:

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

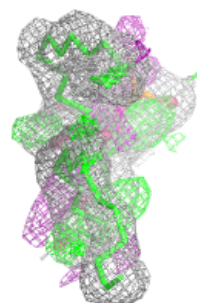
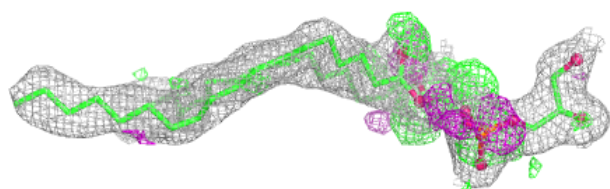
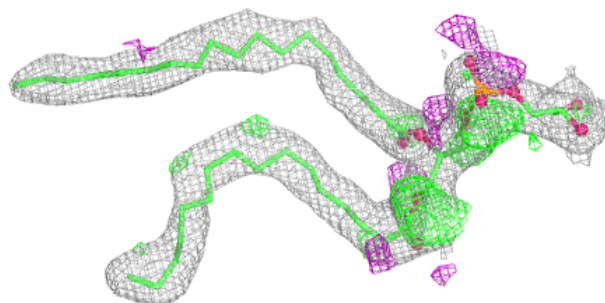
**Electron density around PGV N 607:**

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

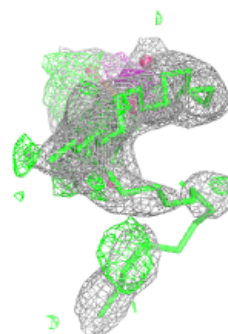
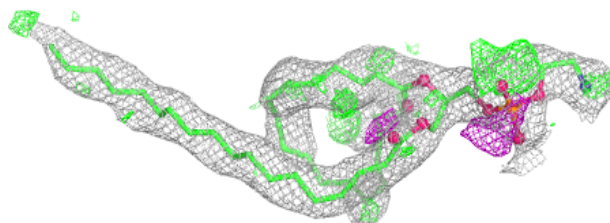
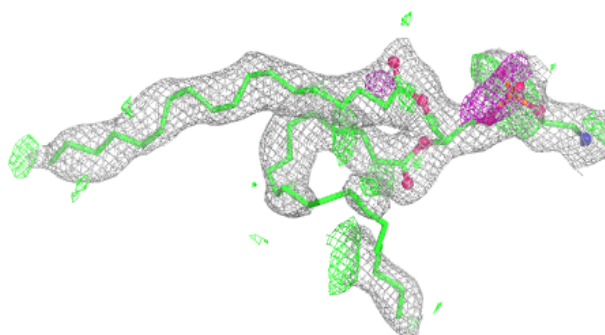


Electron density around PGV A 607:

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

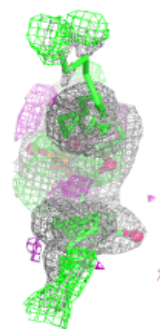
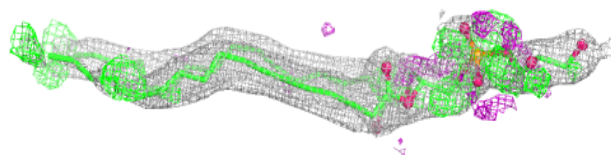
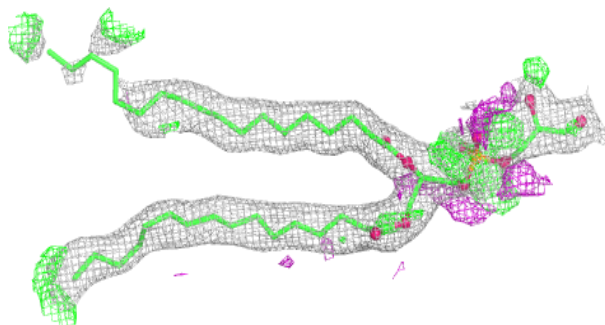
**Electron density around PEK T 102:**

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

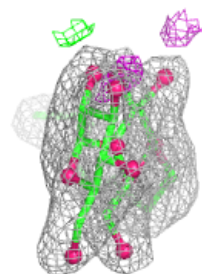
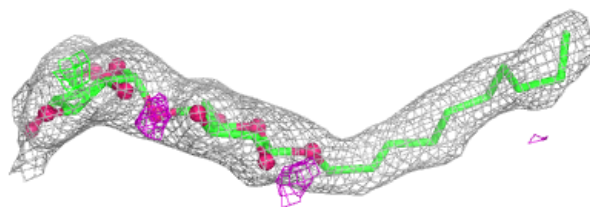
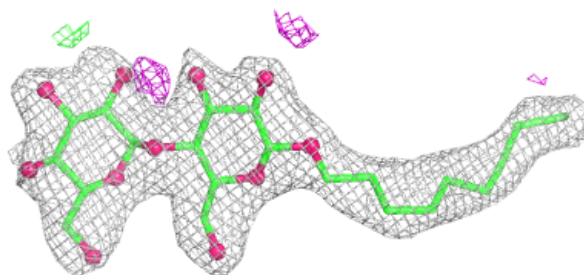


Electron density around PGV P 303:

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

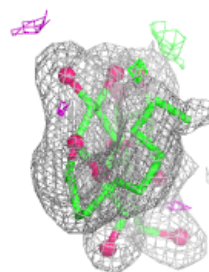
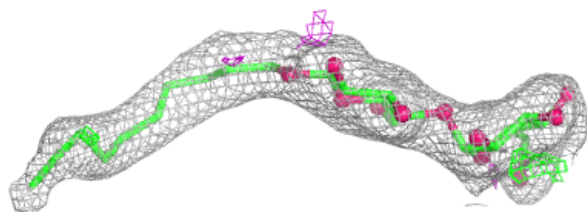
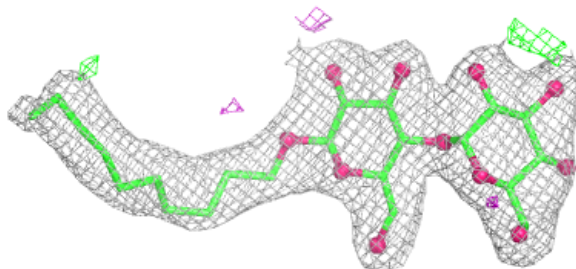
**Electron density around DMU Z 101:**

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

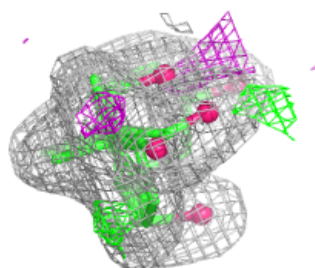
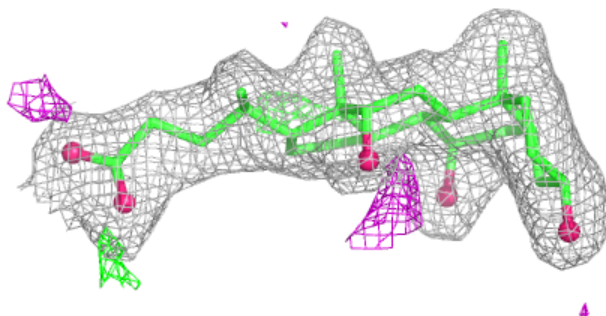
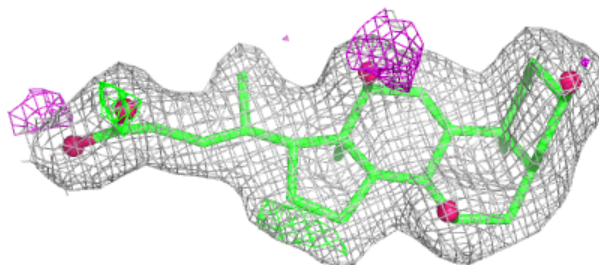


Electron density around DMU M 101:

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

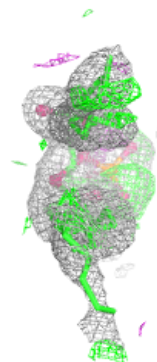
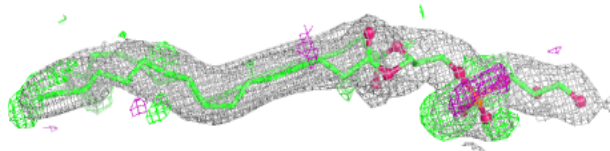
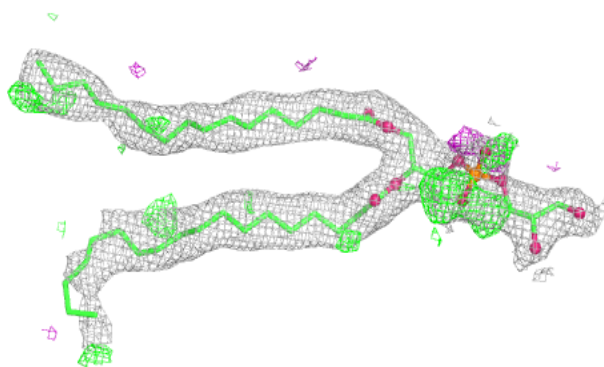
**Electron density around CHD C 304:**

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

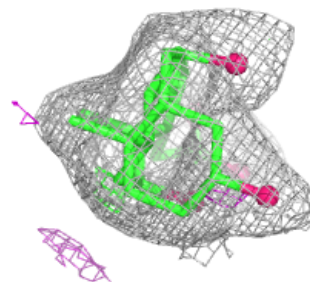
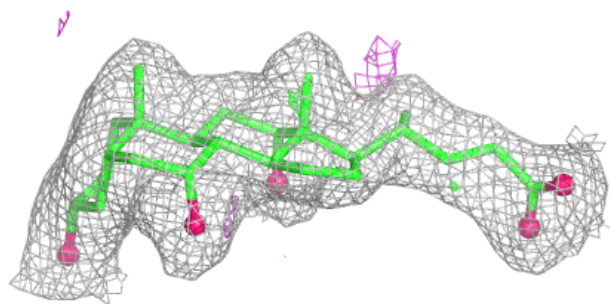
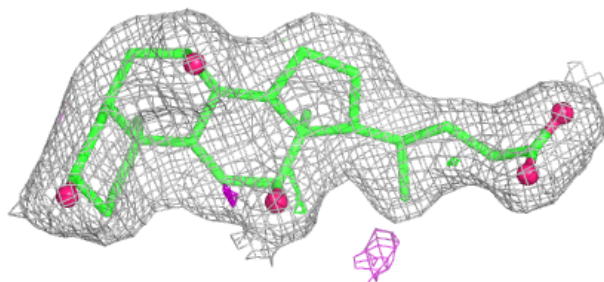


Electron density around PGV C 301:

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

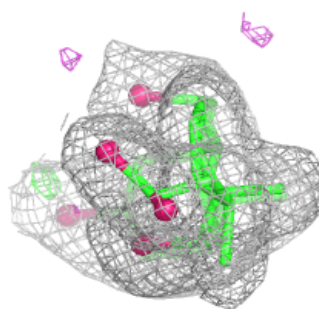
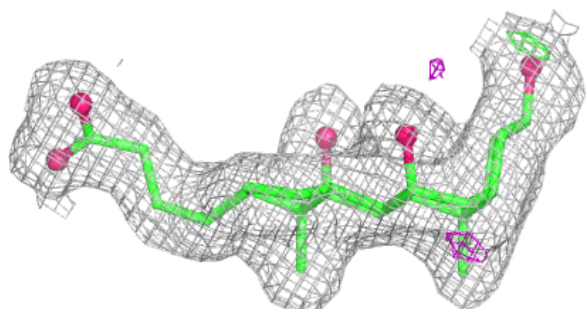
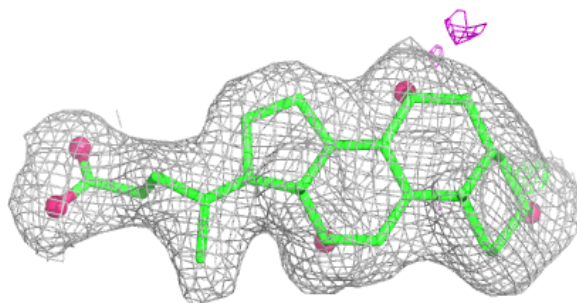
**Electron density around CHD P 306:**

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

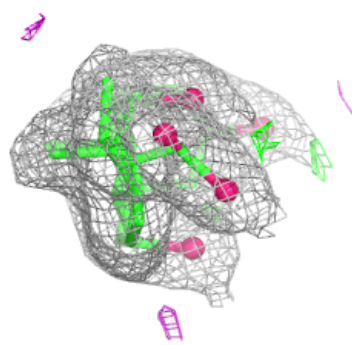
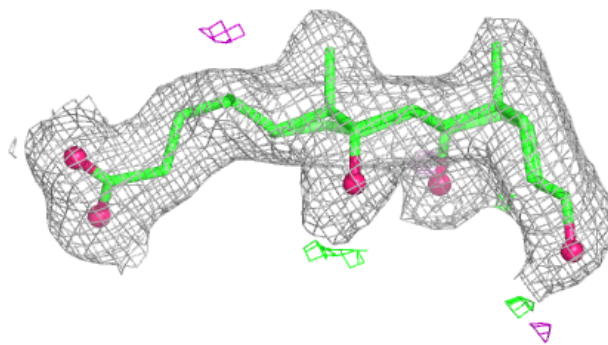
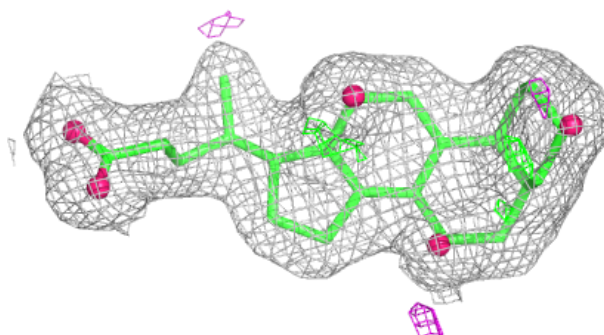


Electron density around CHD G 104:

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

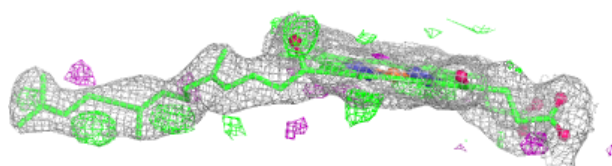
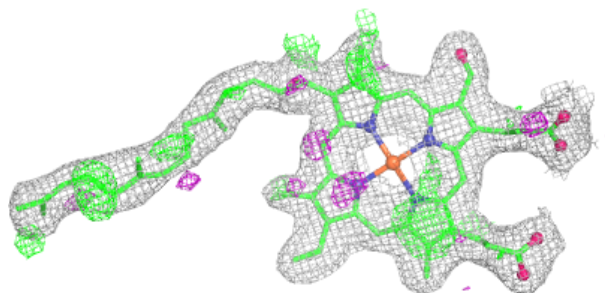
**Electron density around CHD T 101:**

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

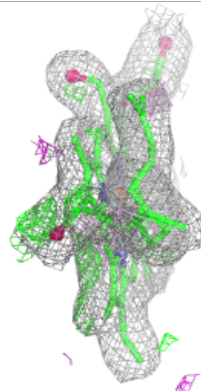
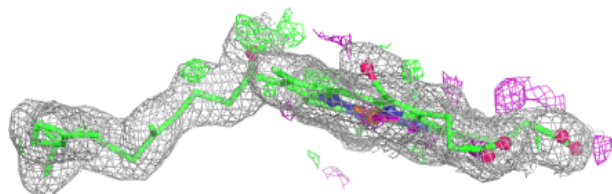
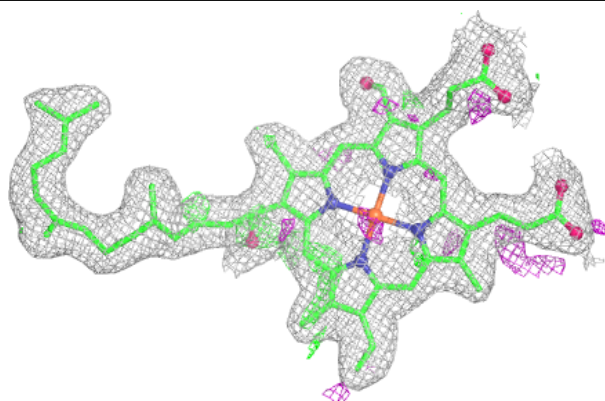


Electron density around HEA N 601:

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

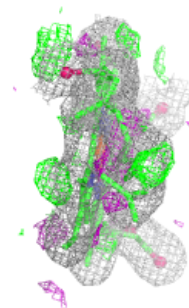
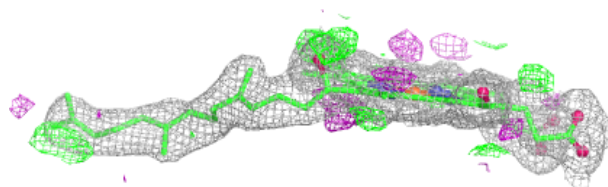
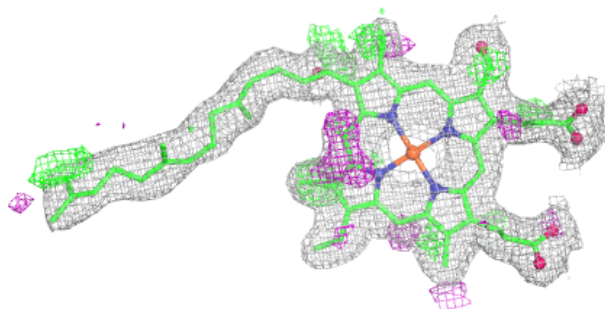
**Electron density around HEA N 602:**

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

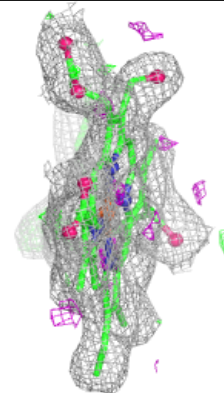
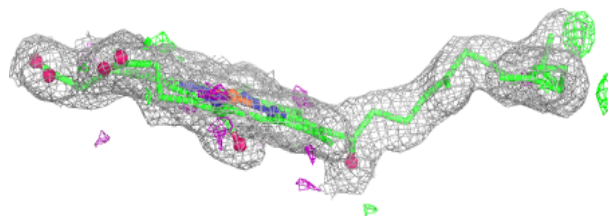
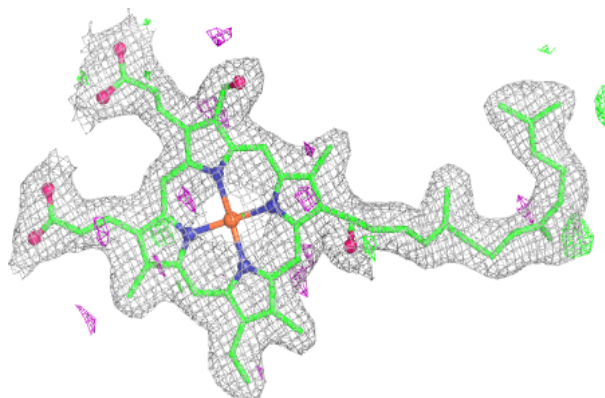


Electron density around HEA A 601:

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

**Electron density around HEA A 602:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.