



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 11:26 AM JST

PDB ID : 5X1B / pdb_00005x1b
Title : CO bound cytochrome c oxidase at 20 nsec after pump laser irradiation to release CO from O₂ reduction center
Authors : Shimada, A.; Kubo, M.; Baba, S.; Yamashita, K.; Hirata, K.; Ueno, G.; Nomura, T.; Kimura, T.; Shinzawa-Itoh, K.; Baba, J.; Hatano, K.; Eto, Y.; Miyamoto, A.; Murakami, H.; Kumasaka, T.; Owada, S.; Tono, K.; Yabashi, M.; Yamaguchi, Y.; Yanagisawa, S.; Sakaguchi, M.; Ogura, T.; Komiya, R.; Yan, J.; Yamashita, E.; Yamamoto, M.; Ago, H.; Yoshikawa, S.; Tsukihara, T.
Deposited on : 2017-01-25
Resolution : 2.40 Å(reported)

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

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

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

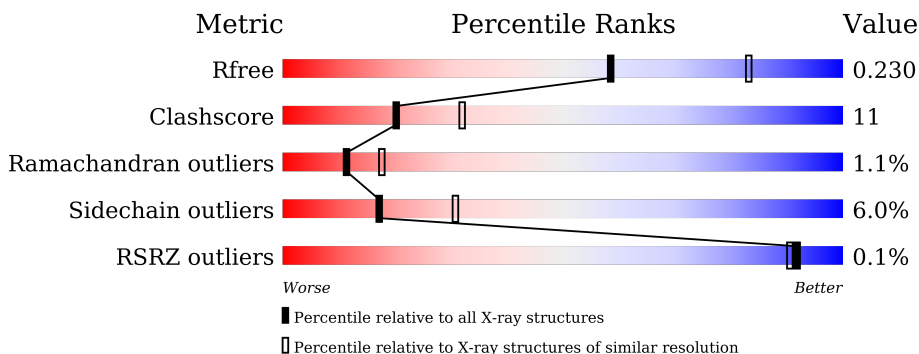
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

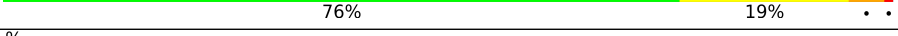
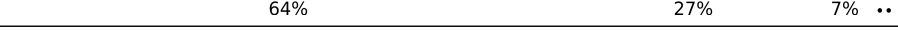
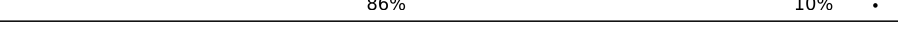
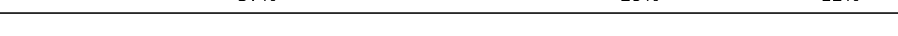
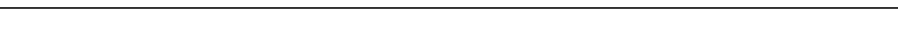
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	227	

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Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.50

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Mol	Chain	Length	Quality of chain
2	O	227	 70% 26% .
3	C	261	 82% 16% ..
3	P	261	 79% 18% ..
4	D	147	 76% 21% ..
4	Q	147	 65% 32% ..
5	E	109	 80% 15% . .
5	R	109	 67% 28% . .
6	F	98	 76% 20% .
6	S	98	 76% 19% . .
7	G	85	 59% 32% 8% .
7	T	85	 64% 27% 7% ..
8	H	85	 73% 15% . . 7%
8	U	85	 68% 20% . . 7%
9	I	73	 86% 10% .
9	V	73	 66% 29% . .
10	J	59	 73% 24% . .
10	W	59	 73% 22% . .
11	K	56	 71% 12% . 12%
11	X	56	 57% 29% . 12%
12	L	47	 66% 30% . .
12	Y	47	 68% 28% . .
13	M	46	 63% 28% . 7%
13	Z	46	 54% 30% 9% 7%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	EDO	A	614	-	-	X	-

2 Entry composition

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	1	0
			4030	2694	623	678	35			
1	N	514	Total	C	N	O	S	0	0	0
			4027	2691	623	678	35			

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
7	G	84	Total 675	C 431	N 129	O 113	P 1	S 1	0	0	0
7	T	84	Total 675	C 431	N 129	O 113	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	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			
9	V	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			

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

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

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

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

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

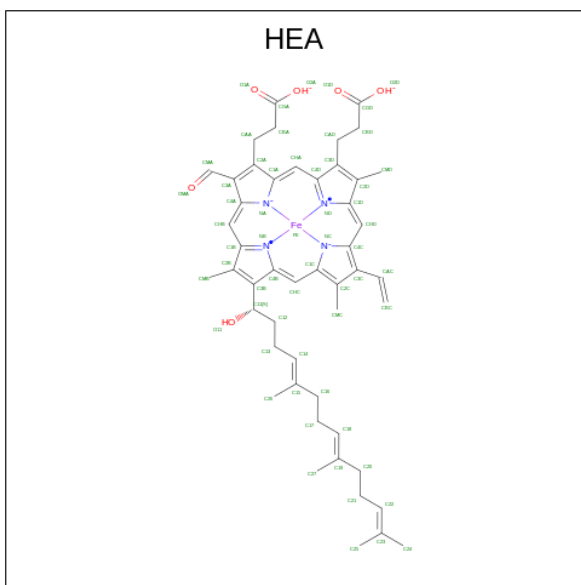
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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

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

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

- Molecule 14 is HEME-A (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		

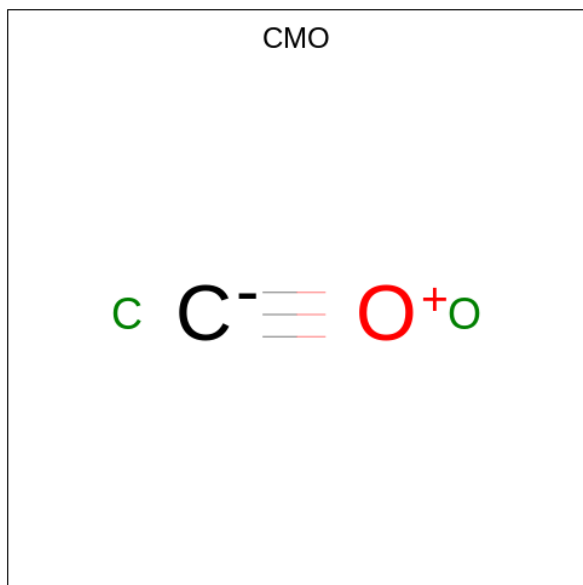
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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).

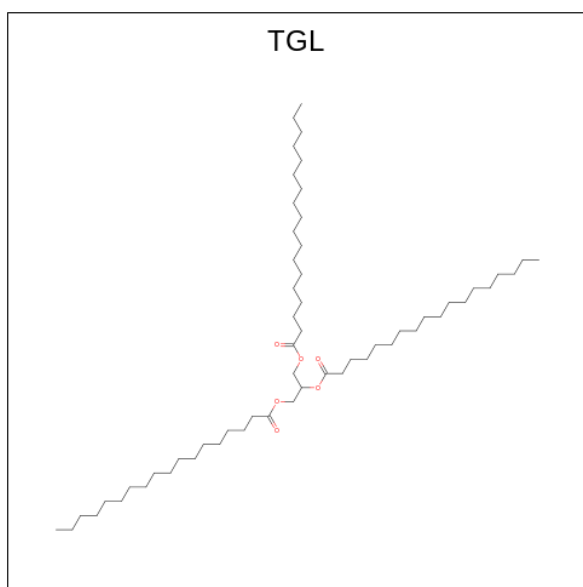
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Na	0	0
			1	1		
17	N	1	Total	Na	0	0
			1	1		

- Molecule 18 is CARBON MONOXIDE (CCD ID: CMO) (formula: CO).



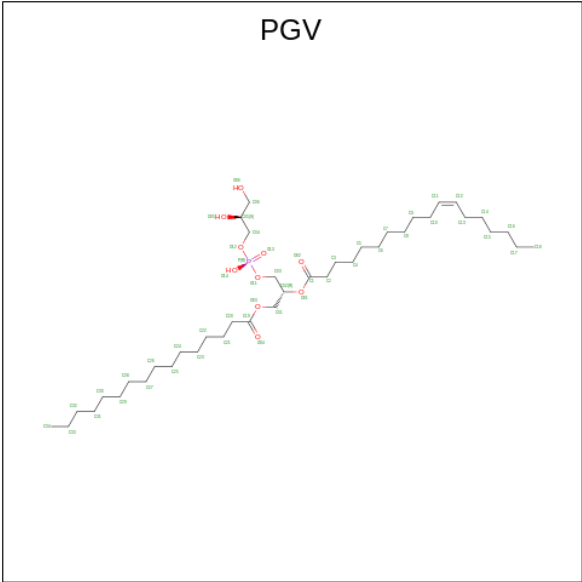
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	A	1	Total	C	O	0	0
			2	1	1		
18	N	1	Total	C	O	0	0
			2	1	1		

- Molecule 19 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: C₅₇H₁₁₀O₆).



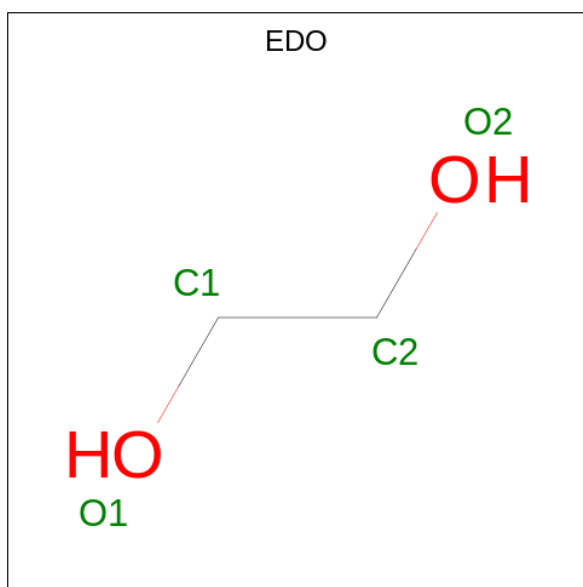
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	C	O	0	0
			63	57	6		
19	D	1	Total	C	O	0	0
			63	57	6		
19	L	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		

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



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

- Molecule 21 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



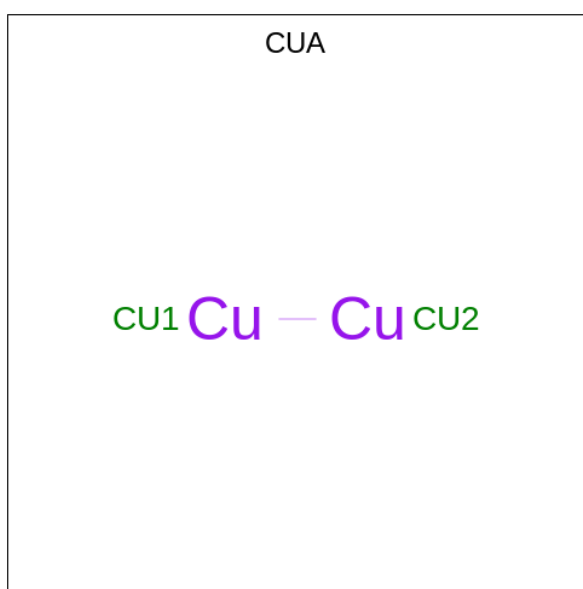
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	B	1	Total	C	O	0	0
			4	2	2		
21	B	1	Total	C	O	0	0
			4	2	2		
21	C	1	Total	C	O	0	0
			4	2	2		
21	C	1	Total	C	O	0	0
			4	2	2		
21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

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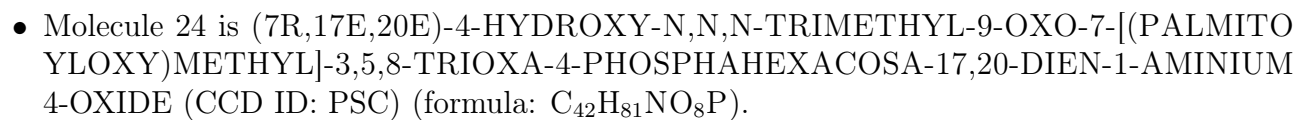
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	K	1	Total	C	O	0	0
			4	2	2		
21	L	1	Total	C	O	0	0
			4	2	2		
21	N	1	Total	C	O	0	0
			4	2	2		
21	T	1	Total	C	O	0	0
			4	2	2		

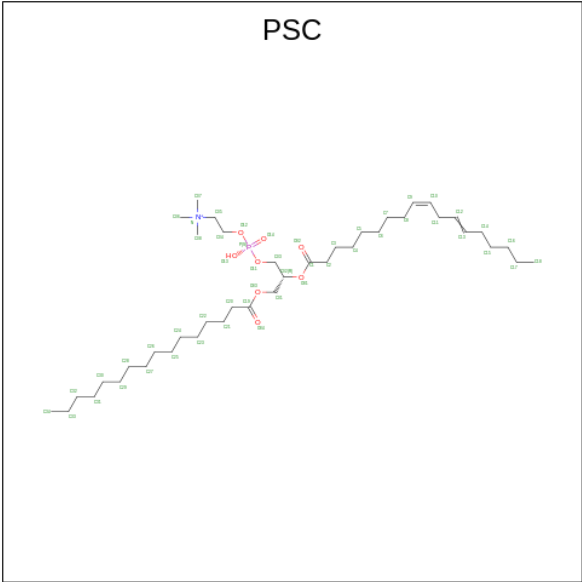
- Molecule 22 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



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

- Molecule 23 is CHOLIC ACID (CCD ID: CHD) (formula: C₂₄H₄₀O₅).



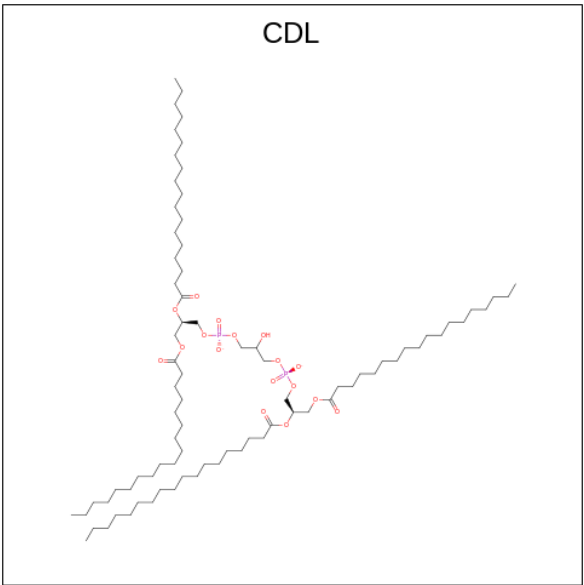


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
24	R	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 25 is UNKNOWN LIGAND (CCD ID: UNX) (formula: X).

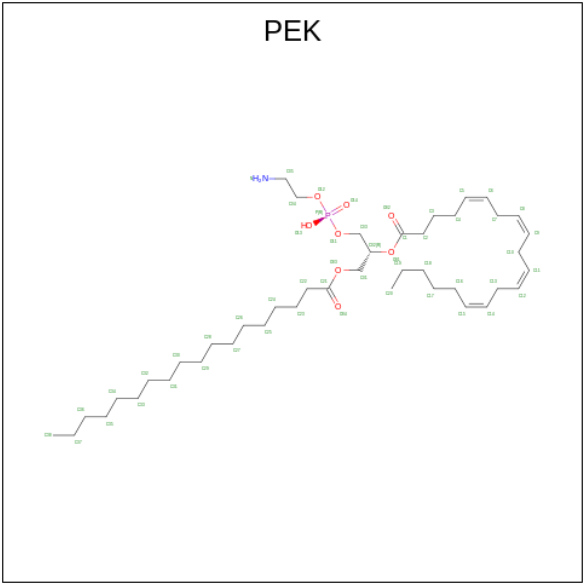
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	C	1	Total	X	0	0
			1	1		
25	P	1	Total	X	0	0
			1	1		

- Molecule 26 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



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

- Molecule 27 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (CCD ID: PEK) (formula: C₄₃H₇₈NO₈P).

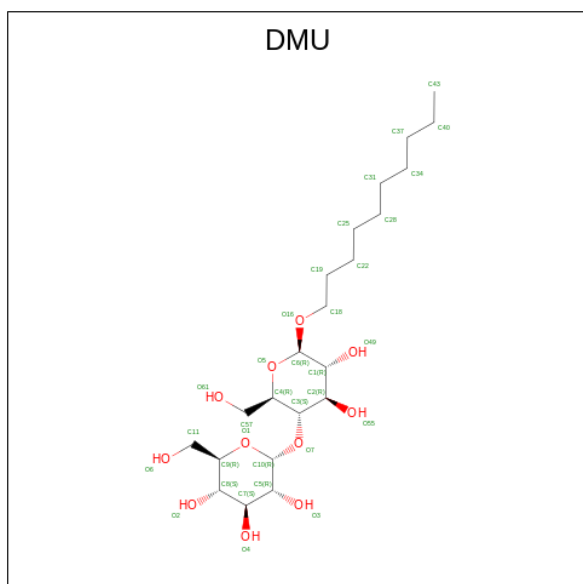


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
27	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 28 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 29 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: C₂₂H₄₂O₁₁).



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

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

- Molecule 30 is water.

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

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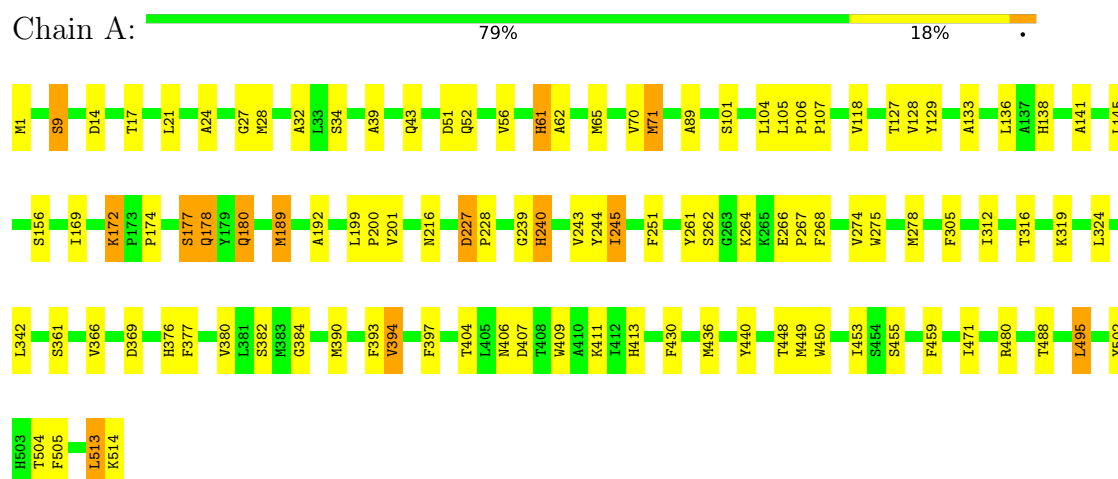
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	S	43	Total 43	O 43	0	0
30	T	20	Total 20	O 20	0	0
30	U	31	Total 31	O 31	0	0
30	V	19	Total 19	O 19	0	0
30	W	17	Total 17	O 17	0	0
30	X	9	Total 9	O 9	0	0
30	Y	6	Total 6	O 6	0	0
30	Z	4	Total 4	O 4	0	0

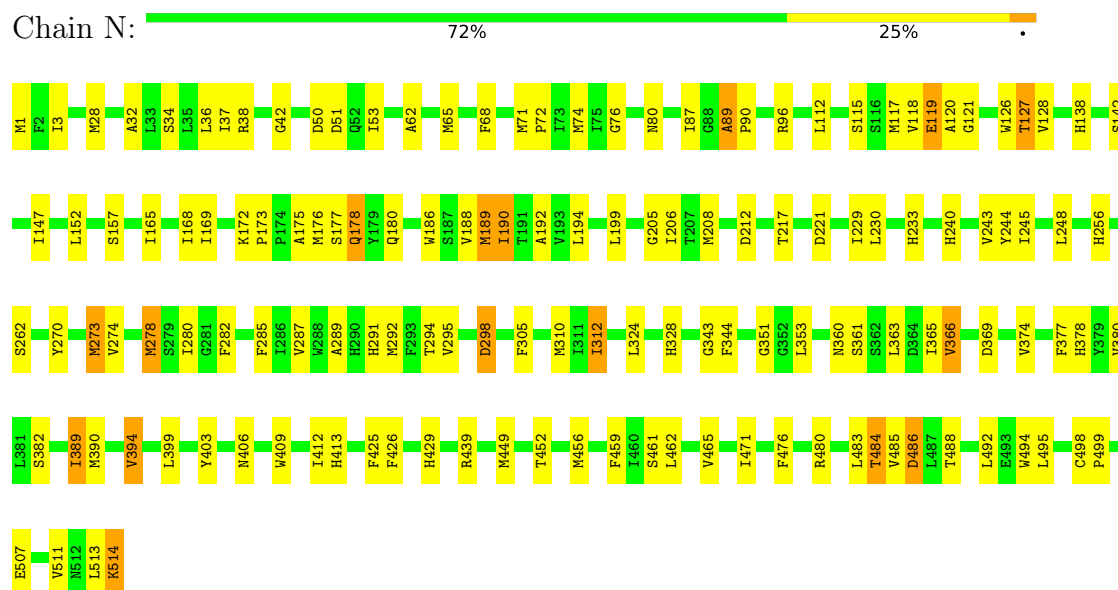
3 Residue-property plots

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

• Molecule 1: Cytochrome c oxidase subunit 1

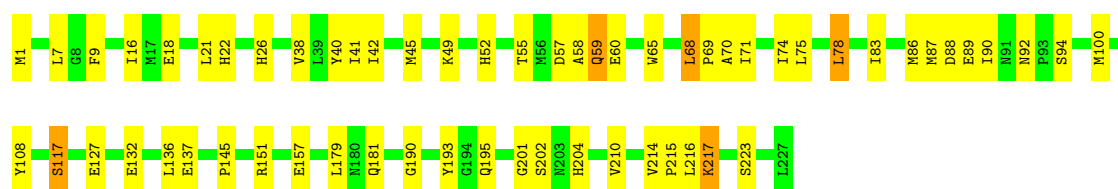


• Molecule 1: Cytochrome c oxidase subunit 1



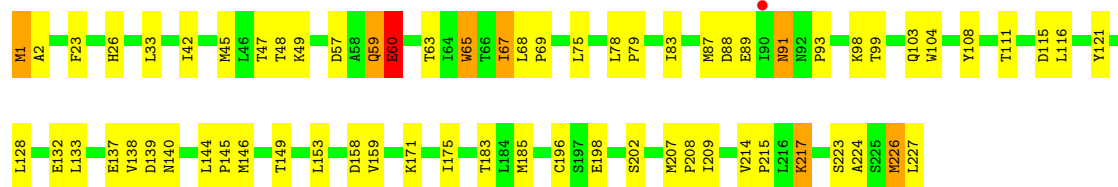
• Molecule 2: Cytochrome c oxidase subunit 2

Chain B: 



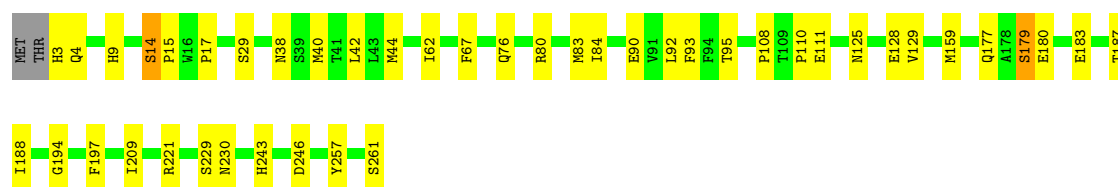
• Molecule 2: Cytochrome c oxidase subunit 2

Chain O: 



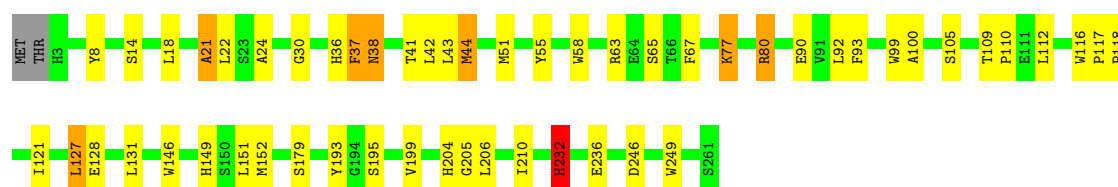
• Molecule 3: Cytochrome c oxidase subunit 3

Chain C: 



• Molecule 3: Cytochrome c oxidase subunit 3

Chain P: 

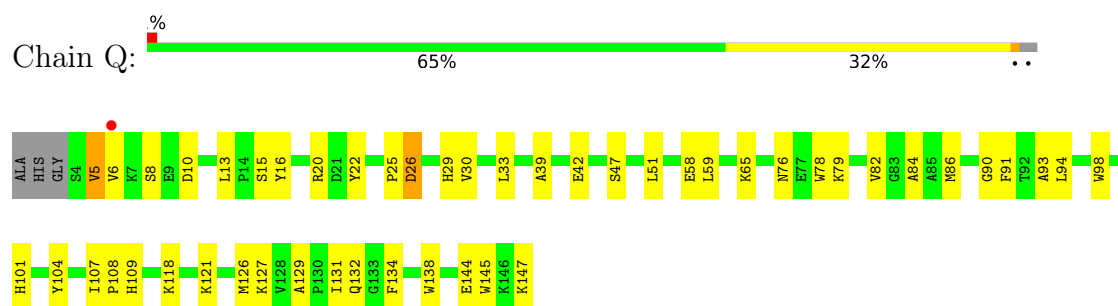


• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

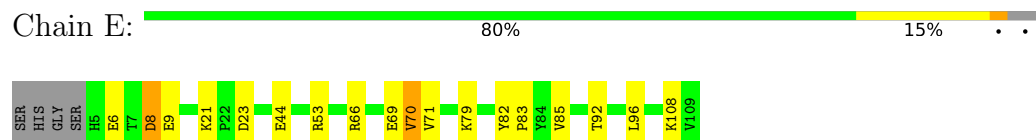
Chain D: 



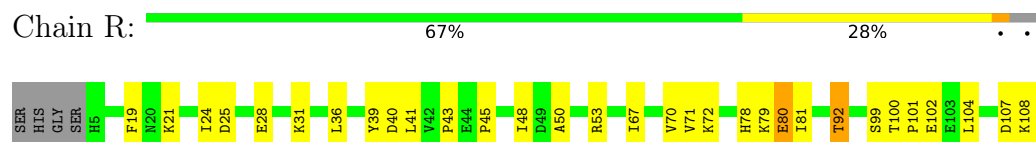
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



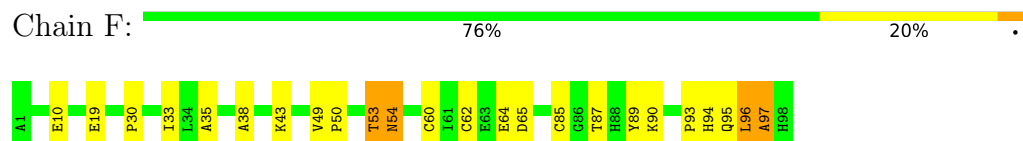
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



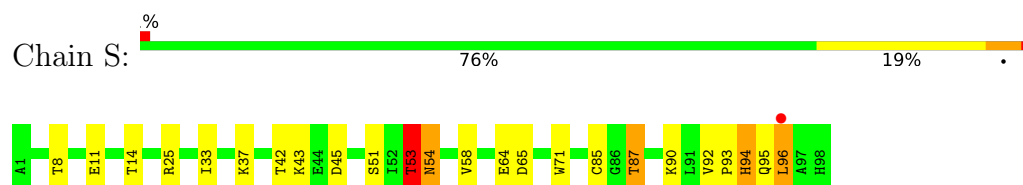
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



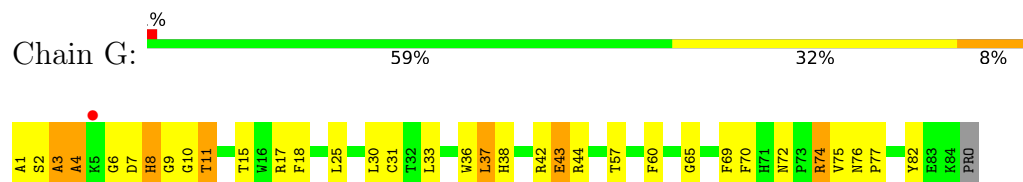
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



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



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



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

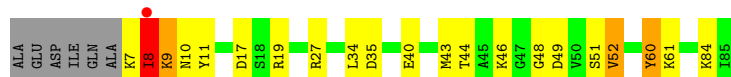




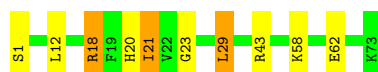
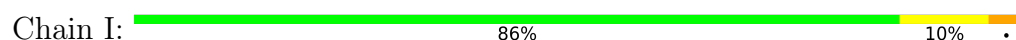
- Molecule 8: Cytochrome c oxidase subunit 6B1



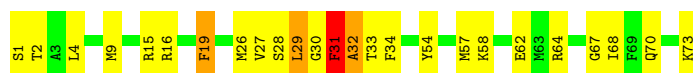
- Molecule 8: Cytochrome c oxidase subunit 6B1



- Molecule 9: Cytochrome c oxidase subunit 6C



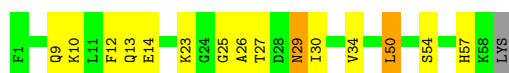
- Molecule 9: Cytochrome c oxidase subunit 6C



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



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



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





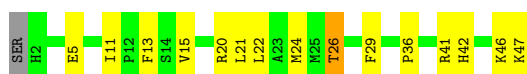
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

Chain X: 57% 29% 12%



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

Chain L: 66% 30% 4%



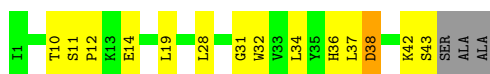
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain Y: 68% 28% 4%



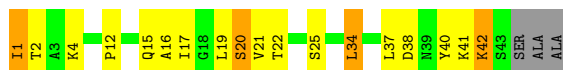
- Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

Chain M: 63% 28% 9%



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

Chain Z: 54% 30% 9% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	185.85Å 209.49Å 179.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.40 15.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.7 (15.00-2.40) 97.7 (15.00-2.40)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0048	Depositor
R, R_{free}	0.182 , 0.230 0.182 , 0.230	Depositor DCC
R_{free} test set	13569 reflections (1.08%)	wwPDB-VP
Wilson B-factor (Å ²)	56.1	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 53.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.045 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	31717	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.16	5/4164 (0.1%)	1.22	21/5689 (0.4%)
1	N	1.09	5/4156 (0.1%)	1.14	12/5678 (0.2%)
2	B	1.07	3/1860 (0.2%)	1.18	5/2534 (0.2%)
2	O	0.97	1/1860 (0.1%)	1.14	4/2534 (0.2%)
3	C	1.12	1/2197 (0.0%)	1.10	7/3005 (0.2%)
3	P	1.12	2/2197 (0.1%)	1.11	5/3005 (0.2%)
4	D	0.96	0/1229	1.05	2/1658 (0.1%)
4	Q	0.88	1/1229 (0.1%)	1.07	5/1658 (0.3%)
5	E	0.87	0/871	1.06	0/1182
5	R	0.84	0/871	1.02	2/1182 (0.2%)
6	F	0.99	0/765	1.09	1/1038 (0.1%)
6	S	1.01	0/765	1.12	1/1038 (0.1%)
7	G	1.18	1/690 (0.1%)	1.07	1/937 (0.1%)
7	T	1.09	0/690	1.08	2/937 (0.2%)
8	H	0.97	0/682	1.18	1/921 (0.1%)
8	U	0.95	0/682	1.05	1/921 (0.1%)
9	I	0.87	0/605	1.09	0/802
9	V	0.77	0/605	1.07	3/802 (0.4%)
10	J	0.92	0/471	1.05	0/636
10	W	0.85	0/471	1.01	0/636
11	K	0.94	0/398	1.07	0/546
11	X	0.89	0/398	1.12	2/546 (0.4%)
12	L	1.01	0/393	1.16	2/526 (0.4%)
12	Y	0.97	0/393	1.11	0/526
13	M	1.08	0/345	1.17	1/470 (0.2%)
13	Z	0.83	0/345	1.08	0/470
All	All	1.04	19/29332 (0.1%)	1.12	78/39877 (0.2%)

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

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

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

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	198	GLU	CA-C	-6.83	1.44	1.52
1	A	133	ALA	CA-C	6.18	1.61	1.52
1	A	376	HIS	CG-CD2	6.16	1.42	1.35
1	A	376	HIS	ND1-CE1	6.12	1.38	1.32
1	N	256	HIS	CG-CD2	5.63	1.42	1.35

The worst 5 of 78 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	MET	CA-C-N	-8.59	110.08	119.19
1	A	71	MET	C-N-CA	-8.59	110.08	119.19
1	N	287	VAL	N-CA-C	7.98	119.77	112.43
2	B	201	GLY	N-CA-C	7.65	122.70	111.76
6	F	96	LEU	N-CA-C	-7.63	100.92	113.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	G	11	TPO	Peptide
7	T	10	GLY	Peptide
7	T	11	TPO	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4030	0	4009	78	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	4027	0	4002	113	0
2	B	1824	0	1833	37	0
2	O	1824	0	1833	45	0
3	C	2110	0	2027	33	0
3	P	2110	0	2027	45	0
4	D	1195	0	1183	22	0
4	Q	1195	0	1183	32	0
5	E	852	0	845	9	0
5	R	852	0	845	22	0
6	F	748	0	728	13	0
6	S	748	0	728	19	0
7	G	675	0	643	30	0
7	T	675	0	643	24	0
8	H	662	0	623	13	0
8	U	662	0	623	11	0
9	I	601	0	613	9	0
9	V	601	0	613	25	0
10	J	460	0	459	9	0
10	W	460	0	459	11	0
11	K	384	0	366	6	0
11	X	384	0	366	14	0
12	L	380	0	380	13	0
12	Y	380	0	380	16	0
13	M	335	0	352	8	0
13	Z	335	0	352	19	0
14	A	120	0	108	12	0
14	N	120	0	108	13	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	2	0	0	1	0
18	N	2	0	0	0	0
19	A	63	0	110	3	0
19	D	63	0	110	1	0
19	L	63	0	110	4	0
19	N	189	0	330	12	0
20	A	102	0	152	3	0
20	C	102	0	152	0	0
20	G	51	0	76	2	0

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	I	12	0	0	0	0
30	J	19	0	0	2	0
30	K	19	0	0	3	0
30	L	14	0	0	2	0
30	M	15	0	0	1	0
30	N	117	0	0	16	0
30	O	77	0	0	8	0
30	P	54	0	0	5	0
30	Q	29	0	0	7	0
30	R	29	0	0	3	0
30	S	43	0	0	4	0
30	T	20	0	0	6	0
30	U	31	0	0	3	0
30	V	19	0	0	4	0
30	W	17	0	0	1	0
30	X	9	0	0	4	0
30	Y	6	0	0	1	0
30	Z	4	0	0	0	0
All	All	31717	0	31348	701	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 11.

The worst 5 of 701 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:240:HIS:NE2	1:N:244:TYR:CE2	1.73	1.45
1:A:240:HIS:NE2	1:A:244:TYR:HE2	1.01	1.42
1:A:240:HIS:NE2	1:A:244:TYR:CE2	1.78	1.30
1:A:240:HIS:CD2	1:A:244:TYR:HE2	1.49	1.29
1:N:240:HIS:NE2	1:N:244:TYR:HE2	0.80	1.28

There are no symmetry-related clashes.

5.3 Torsion angles

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	513/514 (100%)	494 (96%)	19 (4%)	0	100	100
1	N	512/514 (100%)	488 (95%)	23 (4%)	1 (0%)	43	58
2	B	225/227 (99%)	213 (95%)	11 (5%)	1 (0%)	30	43
2	O	225/227 (99%)	211 (94%)	12 (5%)	2 (1%)	14	22
3	C	257/261 (98%)	250 (97%)	7 (3%)	0	100	100
3	P	257/261 (98%)	248 (96%)	6 (2%)	3 (1%)	10	16
4	D	142/147 (97%)	133 (94%)	9 (6%)	0	100	100
4	Q	142/147 (97%)	130 (92%)	9 (6%)	3 (2%)	5	7
5	E	103/109 (94%)	98 (95%)	4 (4%)	1 (1%)	12	20
5	R	103/109 (94%)	99 (96%)	3 (3%)	1 (1%)	12	20
6	F	96/98 (98%)	87 (91%)	7 (7%)	2 (2%)	5	7
6	S	96/98 (98%)	90 (94%)	5 (5%)	1 (1%)	12	20
7	G	81/85 (95%)	69 (85%)	8 (10%)	4 (5%)	1	1
7	T	81/85 (95%)	68 (84%)	5 (6%)	8 (10%)	0	0
8	H	77/85 (91%)	67 (87%)	9 (12%)	1 (1%)	9	14
8	U	77/85 (91%)	69 (90%)	4 (5%)	4 (5%)	1	1
9	I	71/73 (97%)	66 (93%)	5 (7%)	0	100	100
9	V	71/73 (97%)	64 (90%)	6 (8%)	1 (1%)	9	13
10	J	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
10	W	56/59 (95%)	53 (95%)	2 (4%)	1 (2%)	6	9
11	K	47/56 (84%)	47 (100%)	0	0	100	100
11	X	47/56 (84%)	41 (87%)	5 (11%)	1 (2%)	5	7
12	L	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
12	Y	44/47 (94%)	40 (91%)	4 (9%)	0	100	100
13	M	41/46 (89%)	40 (98%)	0	1 (2%)	4	5
13	Z	41/46 (89%)	38 (93%)	2 (5%)	1 (2%)	4	5
All	All	3505/3614 (97%)	3301 (94%)	167 (5%)	37 (1%)	11	18

5 of 37 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	427/426 (100%)	406 (95%)	21 (5%)	22	39
1	N	426/426 (100%)	403 (95%)	23 (5%)	20	35
2	B	210/210 (100%)	198 (94%)	12 (6%)	18	33
2	O	210/210 (100%)	197 (94%)	13 (6%)	16	29
3	C	224/226 (99%)	221 (99%)	3 (1%)	61	80
3	P	224/226 (99%)	217 (97%)	7 (3%)	35	57
4	D	128/129 (99%)	124 (97%)	4 (3%)	35	57
4	Q	128/129 (99%)	118 (92%)	10 (8%)	11	20
5	E	92/95 (97%)	87 (95%)	5 (5%)	20	35
5	R	92/95 (97%)	86 (94%)	6 (6%)	15	27
6	F	81/81 (100%)	74 (91%)	7 (9%)	10	16
6	S	81/81 (100%)	71 (88%)	10 (12%)	4	6
7	G	67/68 (98%)	63 (94%)	4 (6%)	17	31
7	T	67/68 (98%)	64 (96%)	3 (4%)	24	42
8	H	71/75 (95%)	64 (90%)	7 (10%)	7	11
8	U	71/75 (95%)	65 (92%)	6 (8%)	10	16
9	I	57/57 (100%)	54 (95%)	3 (5%)	20	36
9	V	57/57 (100%)	50 (88%)	7 (12%)	4	6
10	J	49/50 (98%)	43 (88%)	6 (12%)	5	7
10	W	49/50 (98%)	44 (90%)	5 (10%)	7	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	39/46 (85%)	35 (90%)	4 (10%)	7	11
11	X	39/46 (85%)	36 (92%)	3 (8%)	12	20
12	L	39/40 (98%)	37 (95%)	2 (5%)	21	37
12	Y	39/40 (98%)	37 (95%)	2 (5%)	21	37
13	M	37/38 (97%)	34 (92%)	3 (8%)	11	18
13	Z	37/38 (97%)	32 (86%)	5 (14%)	4	5
All	All	3041/3082 (99%)	2860 (94%)	181 (6%)	17	31

5 of 181 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	O	226	MET
6	S	37	LYS
3	P	80	ARG
4	Q	58	GLU
7	T	17	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
1	N	178	GLN
9	V	8	GLN
1	N	512	ASN
8	U	23	GLN
6	S	54	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

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

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

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

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

All (5) bond length outliers are listed below:

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

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

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

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 72 ligands modelled in this entry, 8 are monoatomic and 2 are unknown - leaving 62 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
29	DMU	Z	101	-	34,34,34	0.53	0	45,45,45	1.13	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	EDO	B	304	-	3,3,3	0.40	0	2,2,2	0.60	0
20	PGV	C	302	-	50,50,50	0.92	2 (4%)	53,56,56	0.93	4 (7%)
14	HEA	N	602	1	66,67,67	2.18	22 (33%)	78,103,103	1.53	17 (21%)
19	TGL	L	101	-	62,62,62	1.19	3 (4%)	65,65,65	1.25	5 (7%)
20	PGV	C	308	-	50,50,50	1.21	2 (4%)	53,56,56	1.01	3 (5%)
18	CMO	N	606	-	0,1,1	-	-	-	-	-
19	TGL	D	201	-	62,62,62	1.13	3 (4%)	65,65,65	0.99	5 (7%)
23	CHD	W	101	-	32,32,32	0.91	1 (3%)	51,51,51	2.11	17 (33%)
21	EDO	A	612	-	3,3,3	0.52	0	2,2,2	0.10	0
23	CHD	O	302	-	32,32,32	1.04	2 (6%)	51,51,51	1.46	8 (15%)
27	PEK	P	302	-	52,52,52	0.87	2 (3%)	55,57,57	1.35	5 (9%)
27	PEK	T	102	-	52,52,52	1.19	2 (3%)	55,57,57	1.13	4 (7%)
21	EDO	B	305	-	3,3,3	0.39	0	2,2,2	0.49	0
21	EDO	C	310	-	3,3,3	0.53	0	2,2,2	0.33	0
26	CDL	T	103	-	99,99,99	1.37	12 (12%)	105,111,111	1.31	11 (10%)
23	CHD	C	305	-	32,32,32	0.99	1 (3%)	51,51,51	1.25	7 (13%)
20	PGV	A	609	-	50,50,50	1.10	2 (4%)	53,56,56	1.08	5 (9%)
14	HEA	A	602	1	66,67,67	2.20	21 (31%)	78,103,103	1.53	17 (21%)
27	PEK	G	102	-	52,52,52	1.21	2 (3%)	55,57,57	1.06	5 (9%)
21	EDO	A	614	-	3,3,3	0.59	0	2,2,2	0.11	0
21	EDO	F	102	-	3,3,3	0.57	0	2,2,2	0.06	0
21	EDO	G	104	-	3,3,3	0.40	0	2,2,2	0.56	0
20	PGV	A	608	-	50,50,50	0.79	2 (4%)	53,56,56	1.44	5 (9%)
19	TGL	N	609	-	62,62,62	1.12	3 (4%)	65,65,65	1.29	8 (12%)
21	EDO	A	613	-	3,3,3	0.54	0	2,2,2	0.24	0
20	PGV	P	303	-	50,50,50	0.93	2 (4%)	53,56,56	1.08	5 (9%)
21	EDO	K	103	-	3,3,3	0.56	0	2,2,2	0.11	0
19	TGL	A	607	-	62,62,62	1.23	4 (6%)	65,65,65	1.38	10 (15%)
21	EDO	A	610	-	3,3,3	0.52	0	2,2,2	0.57	0
21	EDO	T	104	-	3,3,3	0.45	0	2,2,2	0.26	0
23	CHD	C	304	-	32,32,32	0.62	0	51,51,51	1.97	16 (31%)
23	CHD	P	305	-	32,32,32	0.59	0	51,51,51	1.81	13 (25%)
20	PGV	N	607	-	50,50,50	1.09	2 (4%)	53,56,56	1.07	4 (7%)
20	PGV	N	608	-	50,50,50	0.90	3 (6%)	53,56,56	1.17	4 (7%)
19	TGL	N	610	-	62,62,62	1.13	3 (4%)	65,65,65	1.13	6 (9%)
20	PGV	G	103	-	50,50,50	1.07	2 (4%)	53,56,56	0.95	2 (3%)
27	PEK	C	306	-	52,52,52	1.03	2 (3%)	55,57,57	0.90	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	EDO	K	101	-	3,3,3	0.47	0	2,2,2	0.33	0
23	CHD	B	302	-	32,32,32	0.81	0	51,51,51	1.26	4 (7%)
14	HEA	A	601	1	66,67,67	1.86	19 (28%)	78,103,103	2.34	33 (42%)
23	CHD	P	306	-	32,32,32	0.74	1 (3%)	51,51,51	1.53	12 (23%)
29	DMU	M	101	-	34,34,34	0.53	0	45,45,45	1.14	4 (8%)
19	TGL	N	611	-	62,62,62	1.18	3 (4%)	65,65,65	1.24	7 (10%)
21	EDO	L	102	-	3,3,3	0.46	0	2,2,2	0.40	0
26	CDL	P	304	-	99,99,99	1.39	12 (12%)	105,111,111	1.16	7 (6%)
21	EDO	N	612	-	3,3,3	0.56	0	2,2,2	0.16	0
14	HEA	N	601	1	66,67,67	1.88	21 (31%)	78,103,103	1.52	13 (16%)
26	CDL	C	303	-	99,99,99	1.39	12 (12%)	105,111,111	1.22	7 (6%)
21	EDO	C	311	-	3,3,3	0.53	0	2,2,2	0.30	0
21	EDO	K	102	-	3,3,3	0.50	0	2,2,2	0.26	0
24	PSC	R	201	-	51,51,51	1.22	3 (5%)	57,59,59	0.99	4 (7%)
26	CDL	C	307	-	99,99,99	1.43	13 (13%)	105,111,111	1.23	8 (7%)
22	CUA	O	301	2	0,1,1	-	-	-	-	-
23	CHD	J	101	-	32,32,32	0.66	0	51,51,51	1.54	10 (19%)
27	PEK	G	101	-	52,52,52	0.94	2 (3%)	55,57,57	1.23	4 (7%)
18	CMO	A	606	15	0,1,1	-	-	-	-	-
21	EDO	A	611	-	3,3,3	0.37	0	2,2,2	0.61	0
24	PSC	B	303	-	51,51,51	1.28	3 (5%)	57,59,59	1.07	5 (8%)
21	EDO	C	309	-	3,3,3	0.38	0	2,2,2	0.68	0
27	PEK	T	101	-	52,52,52	1.16	2 (3%)	55,57,57	1.06	4 (7%)
22	CUA	B	301	2	0,1,1	-	-	-	-	-

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
29	DMU	Z	101	-	-	9/19/59/59	0/2/2/2
21	EDO	B	304	-	-	1/1/1/1	-
20	PGV	C	302	-	-	15/55/55/55	-
14	HEA	N	602	1	-	8/36/76/76	-
19	TGL	L	101	-	-	35/65/65/65	-
20	PGV	C	308	-	-	32/55/55/55	-
19	TGL	D	201	-	-	38/65/65/65	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CHD	W	101	-	-	6/9/74/74	0/4/4/4
21	EDO	A	612	-	-	1/1/1/1	-
23	CHD	O	302	-	-	4/9/74/74	0/4/4/4
27	PEK	P	302	-	-	17/56/56/56	-
27	PEK	T	102	-	-	29/56/56/56	-
21	EDO	B	305	-	-	0/1/1/1	-
21	EDO	C	310	-	-	1/1/1/1	-
26	CDL	T	103	-	-	63/110/110/110	-
23	CHD	C	305	-	-	2/9/74/74	0/4/4/4
20	PGV	A	609	-	-	31/55/55/55	-
14	HEA	A	602	1	-	5/36/76/76	-
27	PEK	G	102	-	-	35/56/56/56	-
21	EDO	A	614	-	-	0/1/1/1	-
21	EDO	F	102	-	-	0/1/1/1	-
21	EDO	G	104	-	-	0/1/1/1	-
20	PGV	A	608	-	-	11/55/55/55	-
19	TGL	N	609	-	-	37/65/65/65	-
21	EDO	A	613	-	-	1/1/1/1	-
20	PGV	P	303	-	-	21/55/55/55	-
21	EDO	K	103	-	-	0/1/1/1	-
19	TGL	A	607	-	-	36/65/65/65	-
21	EDO	A	610	-	-	1/1/1/1	-
21	EDO	T	104	-	-	1/1/1/1	-
23	CHD	C	304	-	-	5/9/74/74	0/4/4/4
23	CHD	P	305	-	-	9/9/74/74	0/4/4/4
20	PGV	N	607	-	-	33/55/55/55	-
20	PGV	N	608	-	-	22/55/55/55	-
19	TGL	N	610	-	-	42/65/65/65	-
20	PGV	G	103	-	-	33/55/55/55	-
27	PEK	C	306	-	-	30/56/56/56	-
21	EDO	K	101	-	-	1/1/1/1	-
23	CHD	B	302	-	-	2/9/74/74	0/4/4/4
14	HEA	A	601	1	-	10/36/76/76	-
23	CHD	P	306	-	-	3/9/74/74	0/4/4/4
29	DMU	M	101	-	-	5/19/59/59	0/2/2/2
19	TGL	N	611	-	-	34/65/65/65	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	EDO	L	102	-	-	1/1/1/1	-
26	CDL	P	304	-	-	66/110/110/110	-
21	EDO	N	612	-	-	0/1/1/1	-
14	HEA	N	601	1	-	7/36/76/76	-
26	CDL	C	303	-	-	65/110/110/110	-
21	EDO	C	311	-	-	0/1/1/1	-
21	EDO	K	102	-	-	1/1/1/1	-
24	PSC	R	201	-	-	29/55/55/55	-
26	CDL	C	307	-	-	64/110/110/110	-
23	CHD	J	101	-	-	9/9/74/74	0/4/4/4
27	PEK	G	101	-	-	21/56/56/56	-
21	EDO	A	611	-	-	1/1/1/1	-
24	PSC	B	303	-	-	30/55/55/55	-
21	EDO	C	309	-	-	1/1/1/1	-
27	PEK	T	101	-	-	22/56/56/56	-

The worst 5 of 191 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	602	HEA	FE-ND	7.22	2.17	1.94
14	N	602	HEA	FE-NB	6.39	2.14	1.94
14	N	602	HEA	FE-ND	5.64	2.12	1.94
19	L	101	TGL	OG2-CB1	5.59	1.50	1.34
19	A	607	TGL	OG1-CA1	5.58	1.49	1.33

The worst 5 of 315 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	601	HEA	C3C-C4C-NC	7.18	114.66	110.25
14	A	601	HEA	C3D-C4D-ND	6.48	116.63	110.36
23	W	101	CHD	C13-C17-C20	5.97	126.63	119.50
19	N	611	TGL	OG2-CB1-CB2	5.80	124.01	111.50
19	N	609	TGL	OG2-CB1-CB2	5.64	123.66	111.50

There are no chirality outliers.

5 of 986 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	601	HEA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
14	A	601	HEA	C3A-C2A-CAA-CBA
14	A	602	HEA	C2A-C3A-CMA-OMA
14	A	602	HEA	C4A-C3A-CMA-OMA
14	N	601	HEA	C2A-C3A-CMA-OMA

There are no ring outliers.

46 monomers are involved in 157 short contacts:

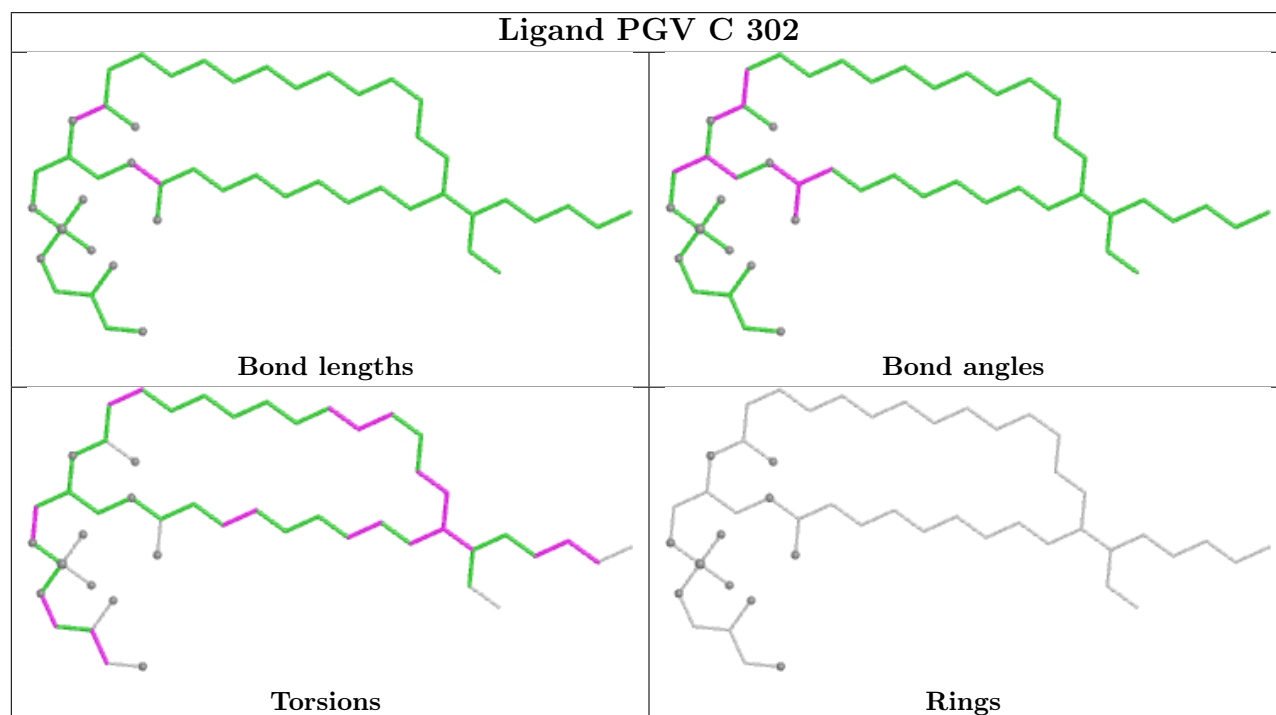
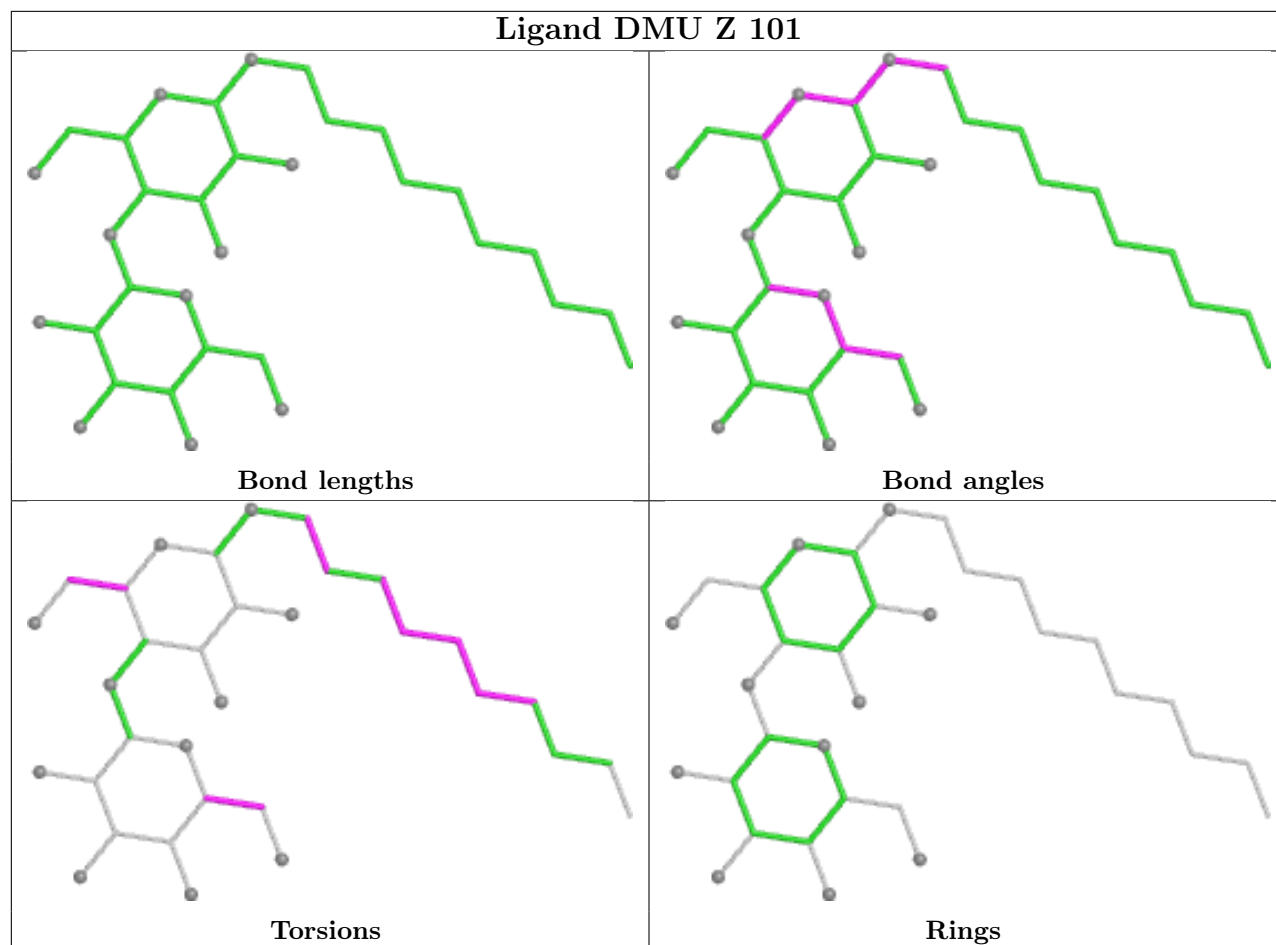
Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	Z	101	DMU	1	0
14	N	602	HEA	3	0
19	L	101	TGL	4	0
19	D	201	TGL	1	0
23	W	101	CHD	1	0
21	A	612	EDO	2	0
23	O	302	CHD	1	0
27	P	302	PEK	4	0
27	T	102	PEK	1	0
21	B	305	EDO	1	0
26	T	103	CDL	13	0
23	C	305	CHD	1	0
20	A	609	PGV	2	0
14	A	602	HEA	6	0
27	G	102	PEK	6	0
21	A	614	EDO	4	0
20	A	608	PGV	1	0
19	N	609	TGL	5	0
21	A	613	EDO	2	0
20	P	303	PGV	3	0
19	A	607	TGL	3	0
21	A	610	EDO	1	0
21	T	104	EDO	2	0
23	C	304	CHD	2	0
23	P	305	CHD	1	0
20	N	607	PGV	6	0
20	N	608	PGV	2	0
19	N	610	TGL	3	0
20	G	103	PGV	2	0
27	C	306	PEK	3	0
23	B	302	CHD	1	0
14	A	601	HEA	6	0
23	P	306	CHD	1	0

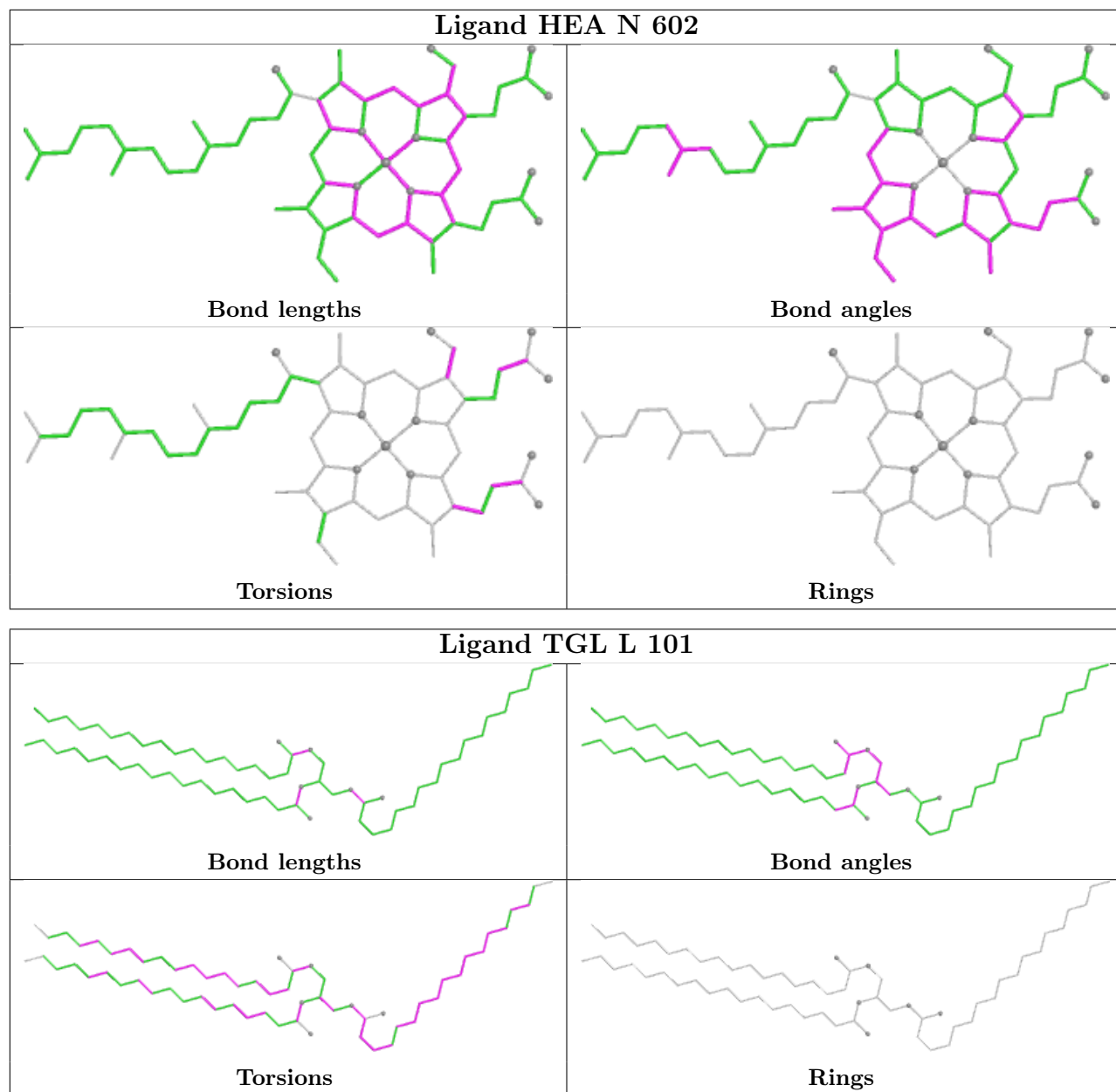
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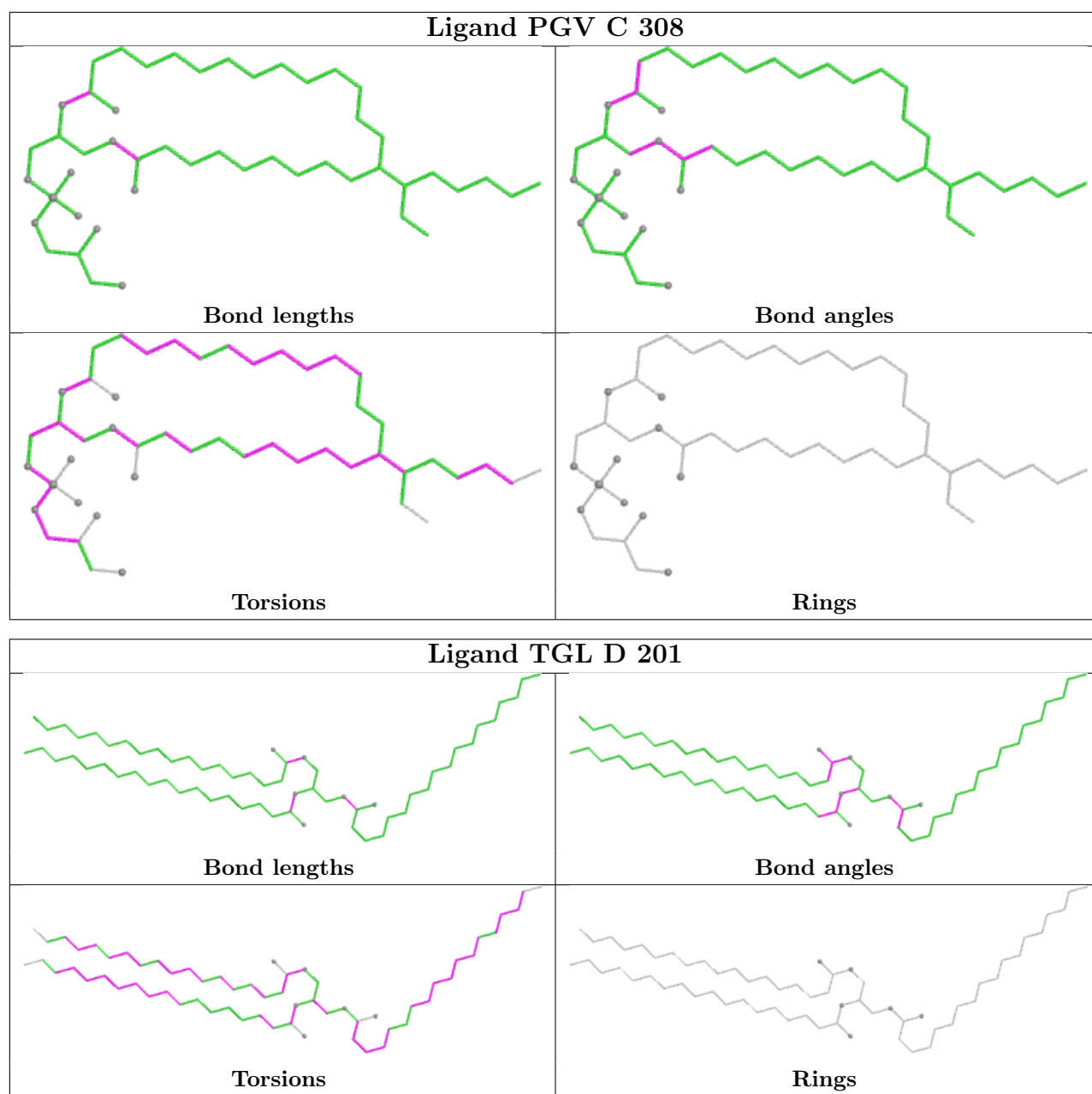
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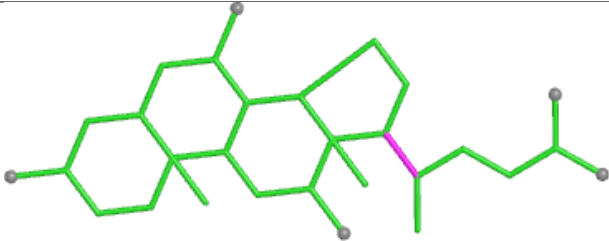
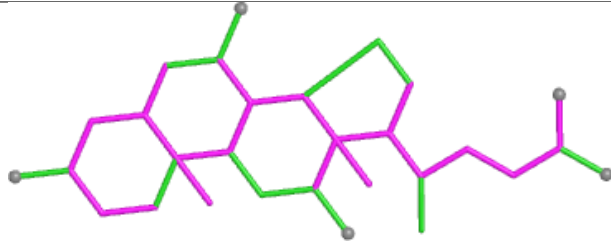
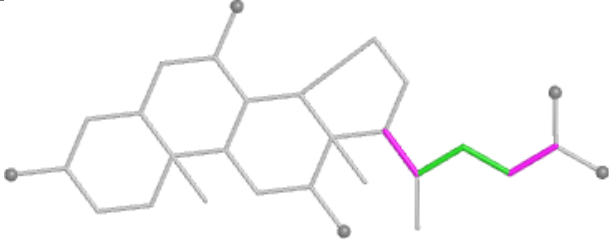
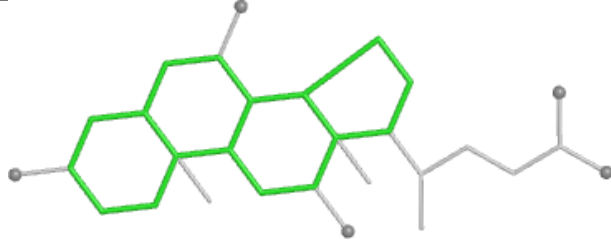
Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	M	101	DMU	1	0
19	N	611	TGL	4	0
26	P	304	CDL	8	0
21	N	612	EDO	1	0
14	N	601	HEA	10	0
26	C	303	CDL	2	0
24	R	201	PSC	6	0
26	C	307	CDL	13	0
23	J	101	CHD	1	0
27	G	101	PEK	4	0
18	A	606	CMO	1	0
24	B	303	PSC	12	0
27	T	101	PEK	3	0

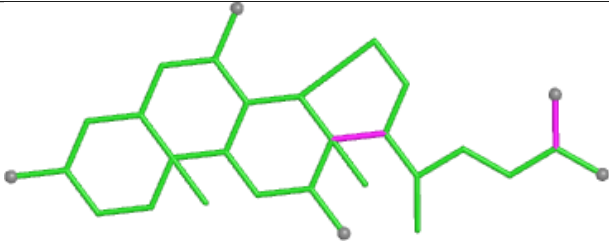
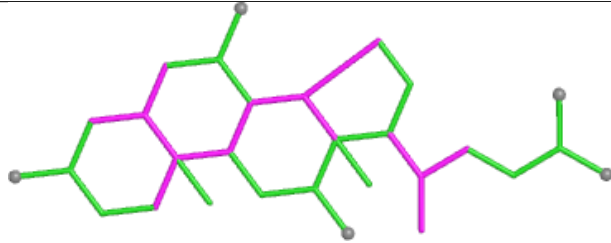
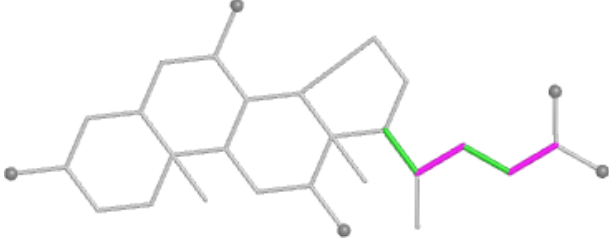
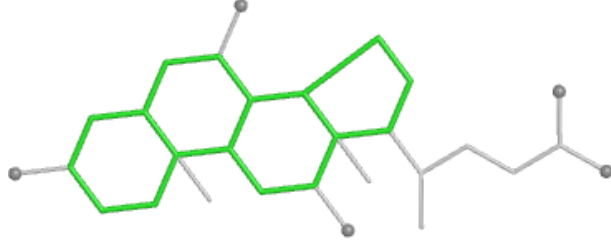
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



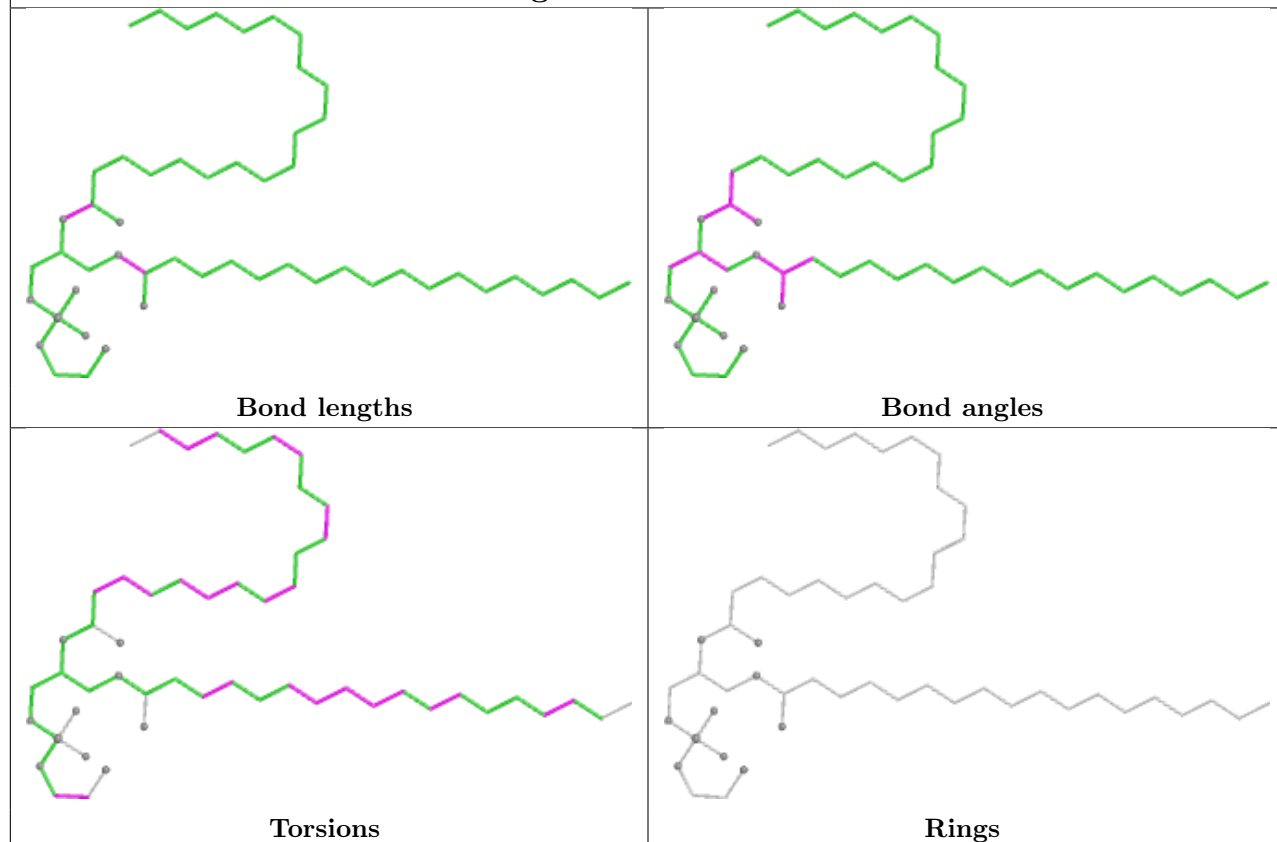




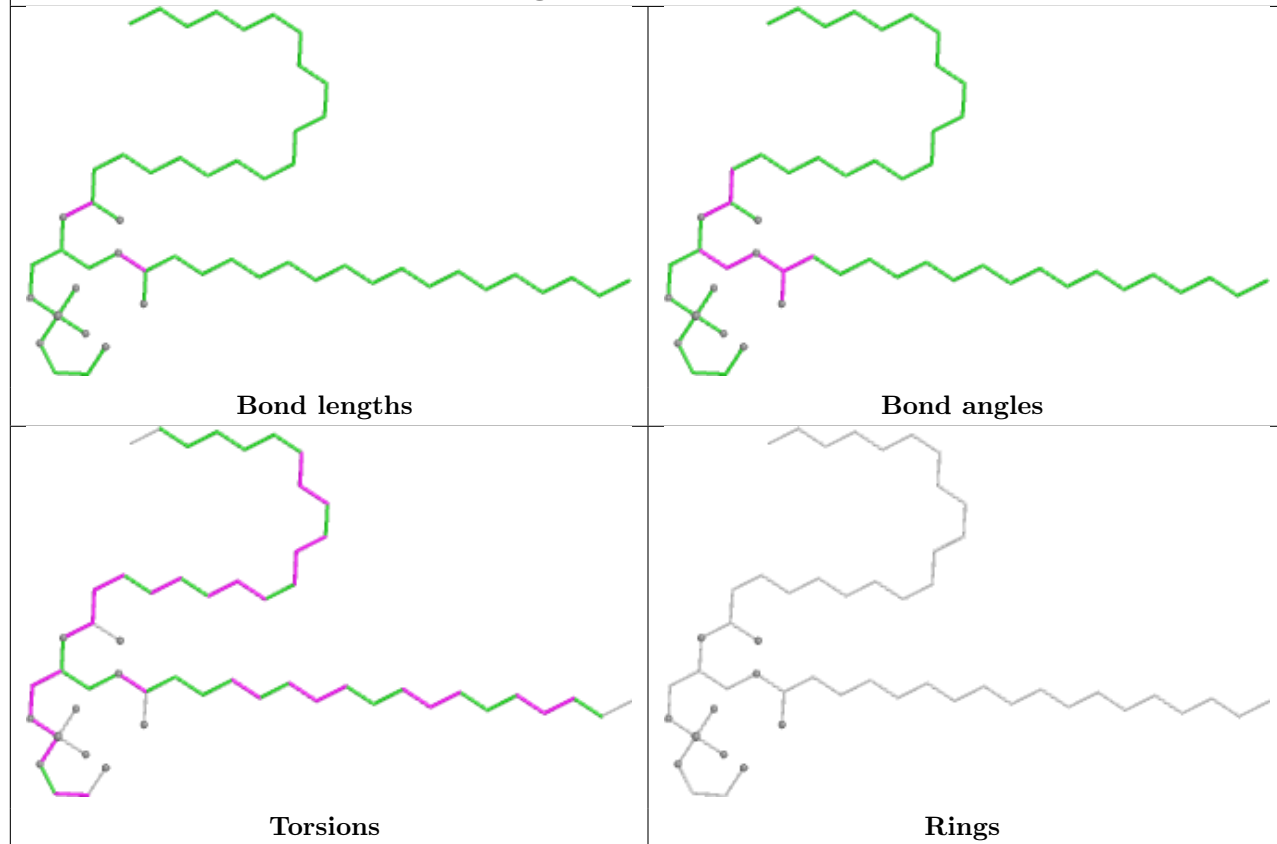
Ligand CHD W 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

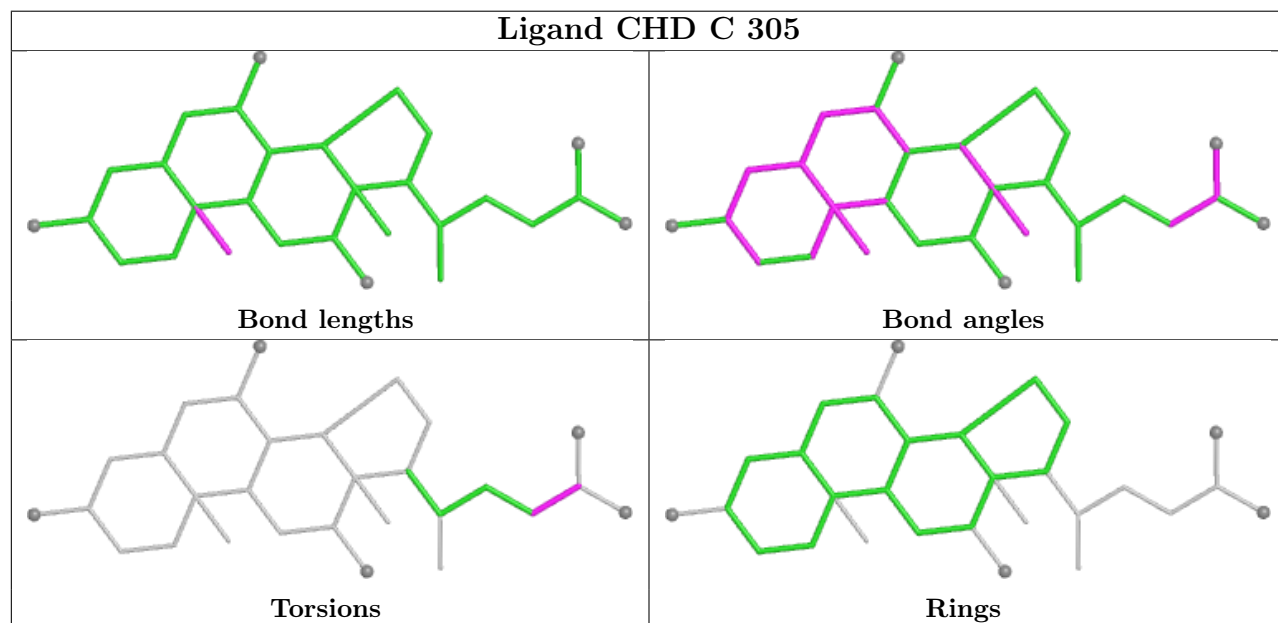
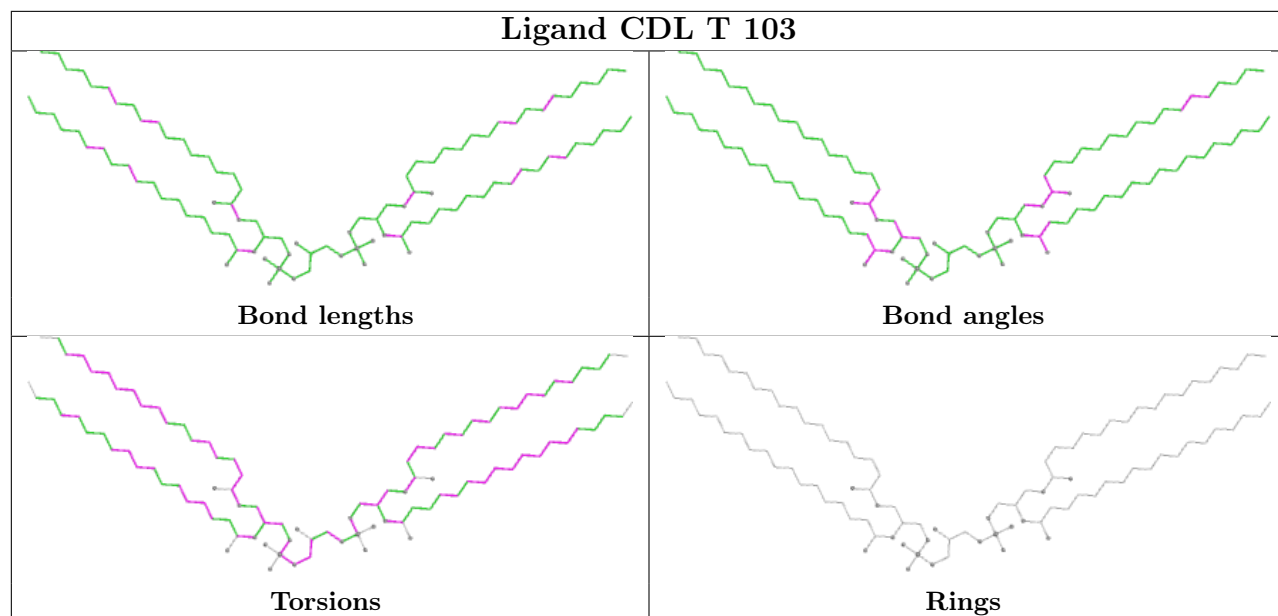
Ligand CHD O 302	
	
Bond lengths	Bond angles
	
Torsions	Rings

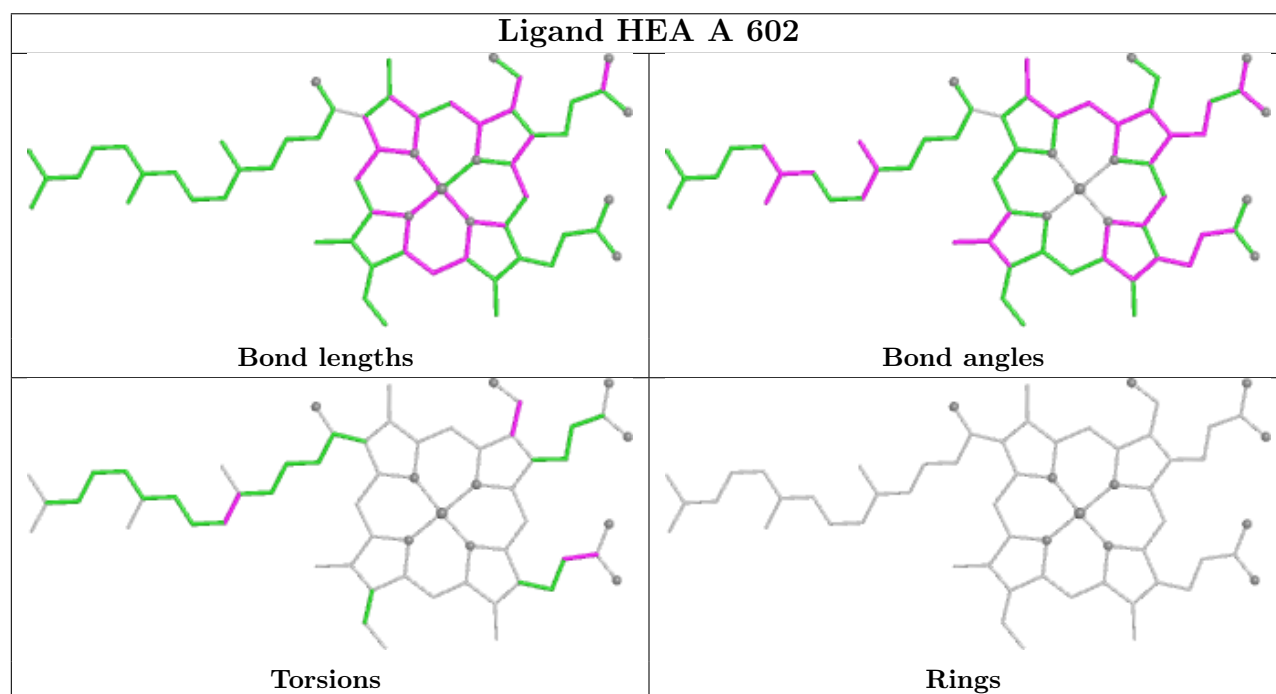
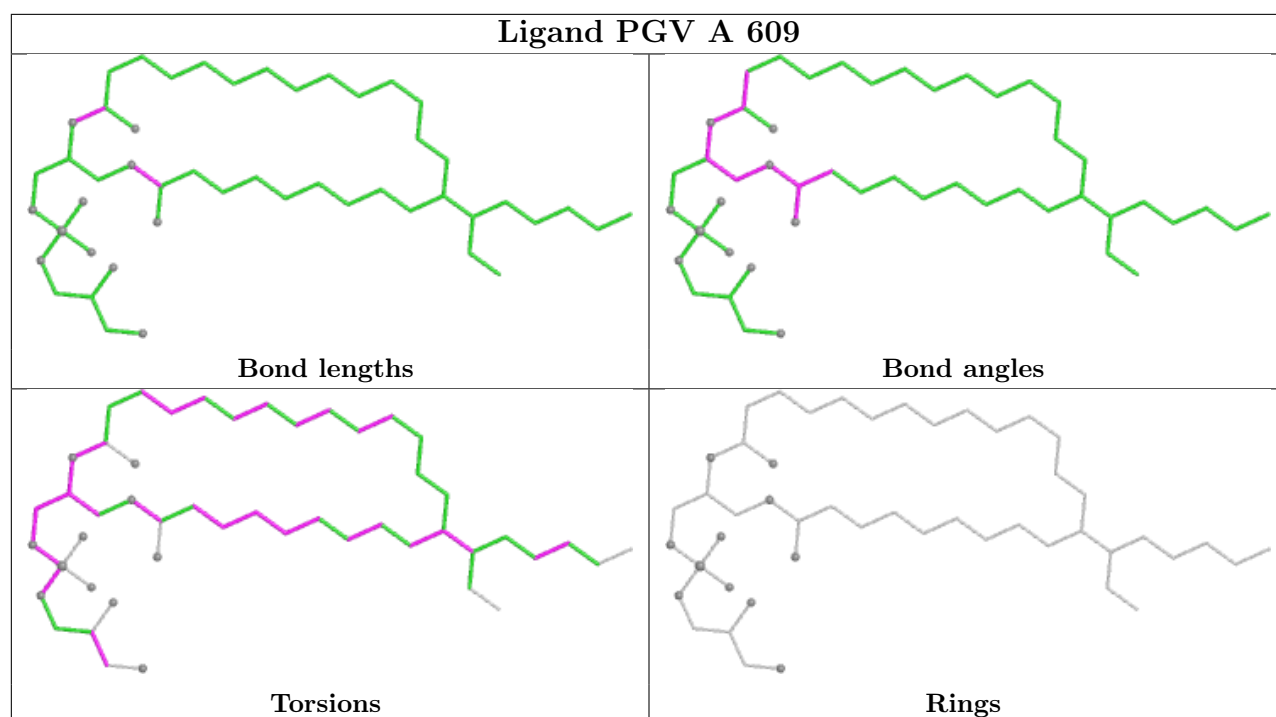
Ligand PEK P 302

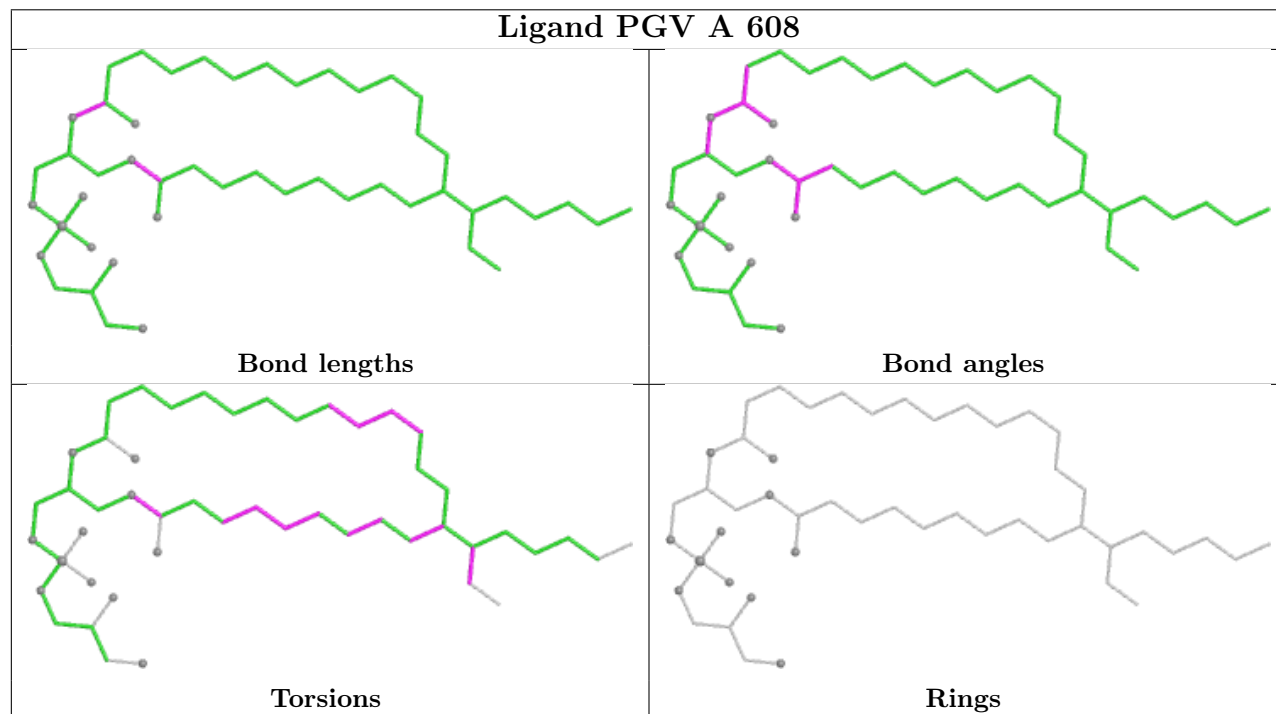
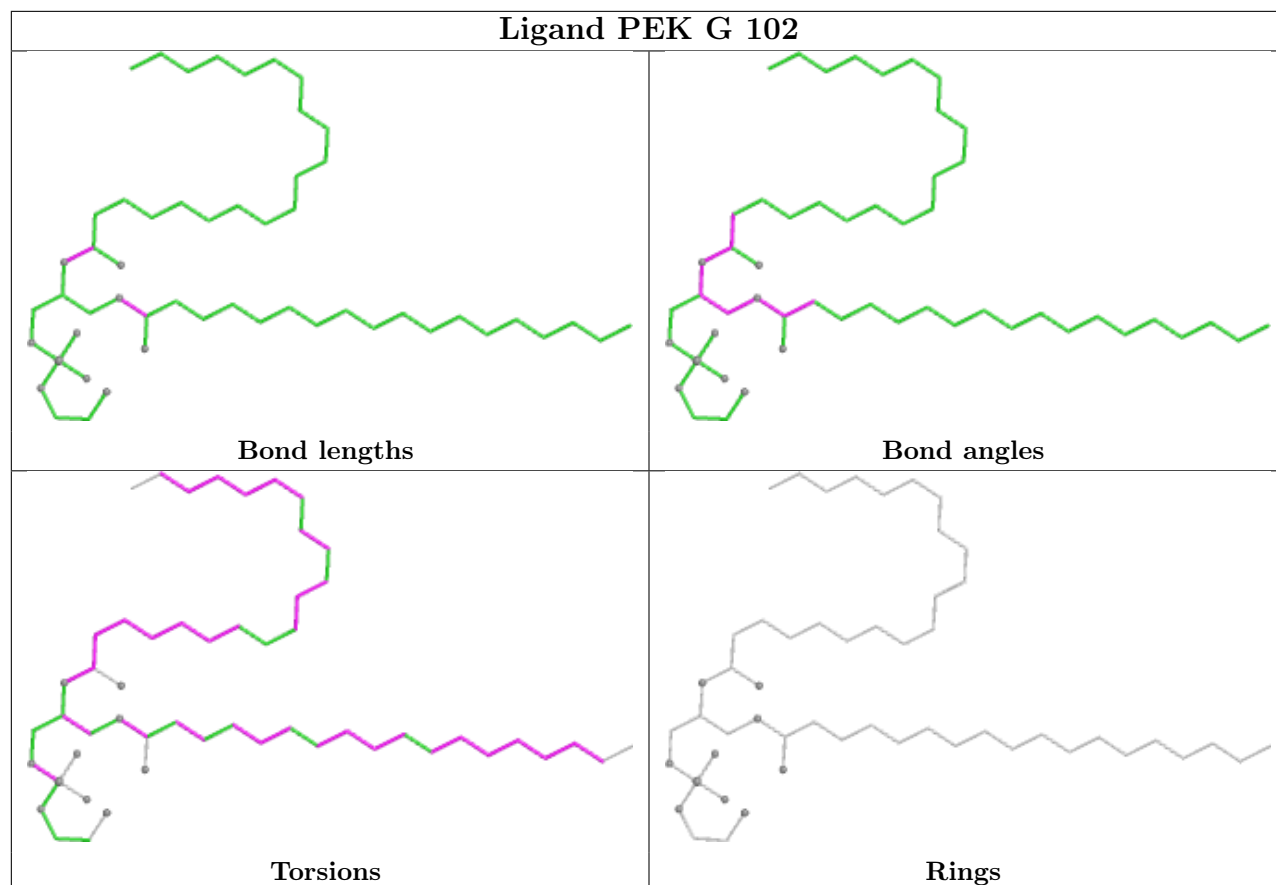


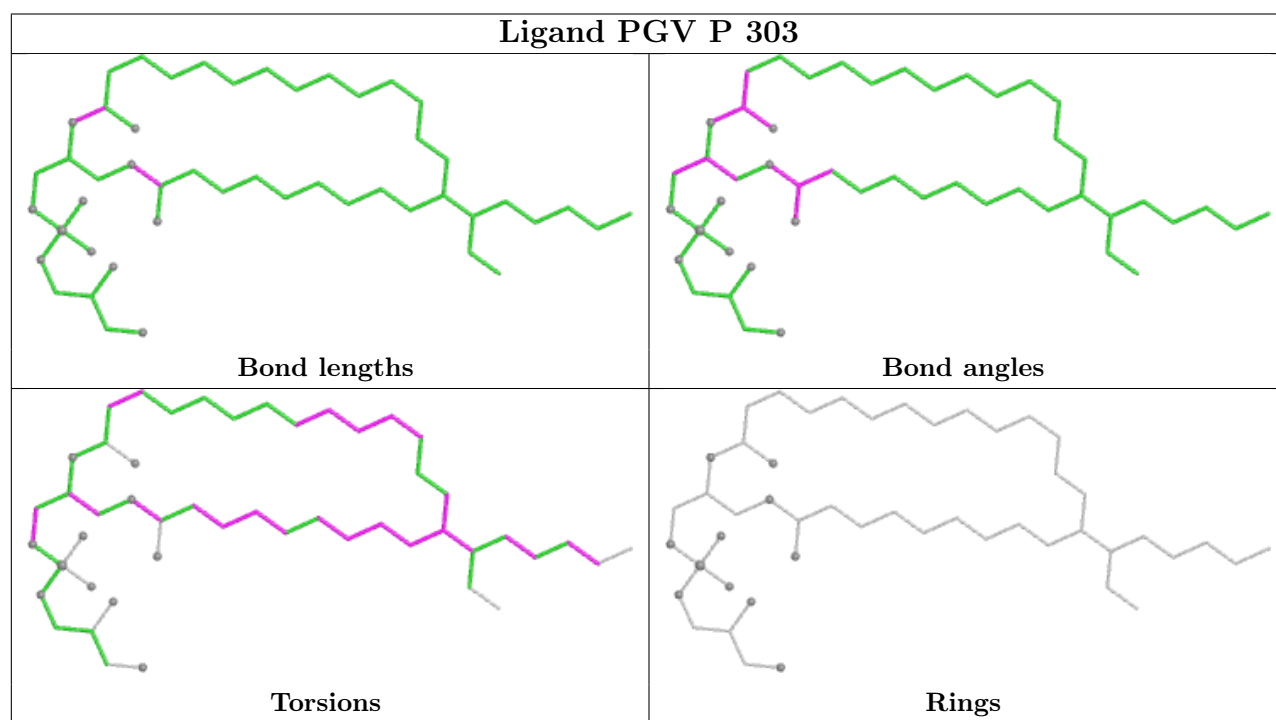
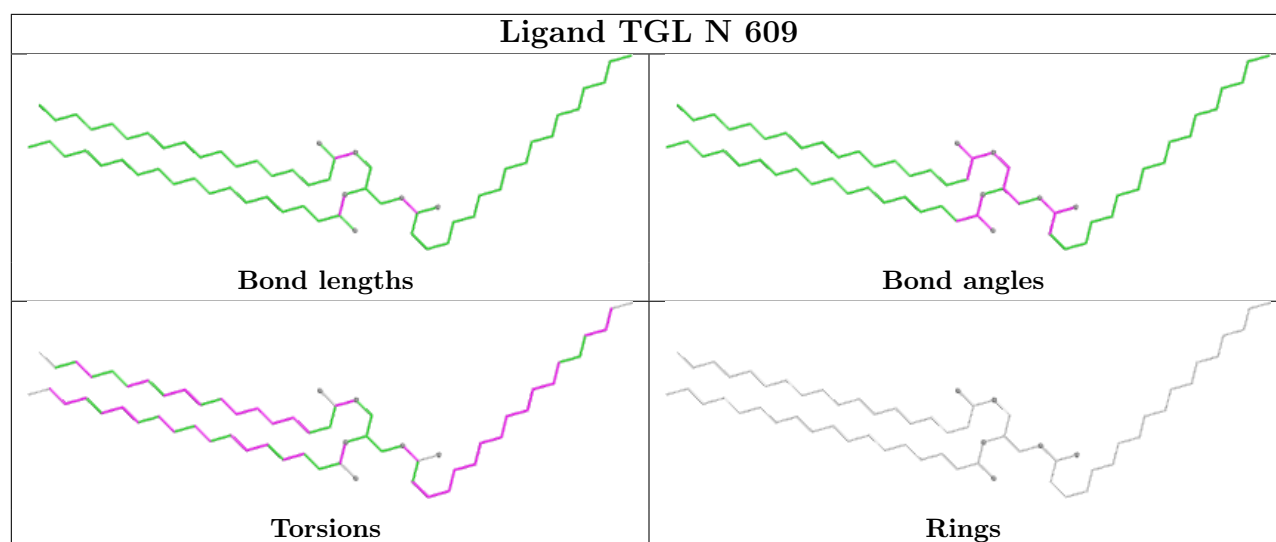
Ligand PEK T 102

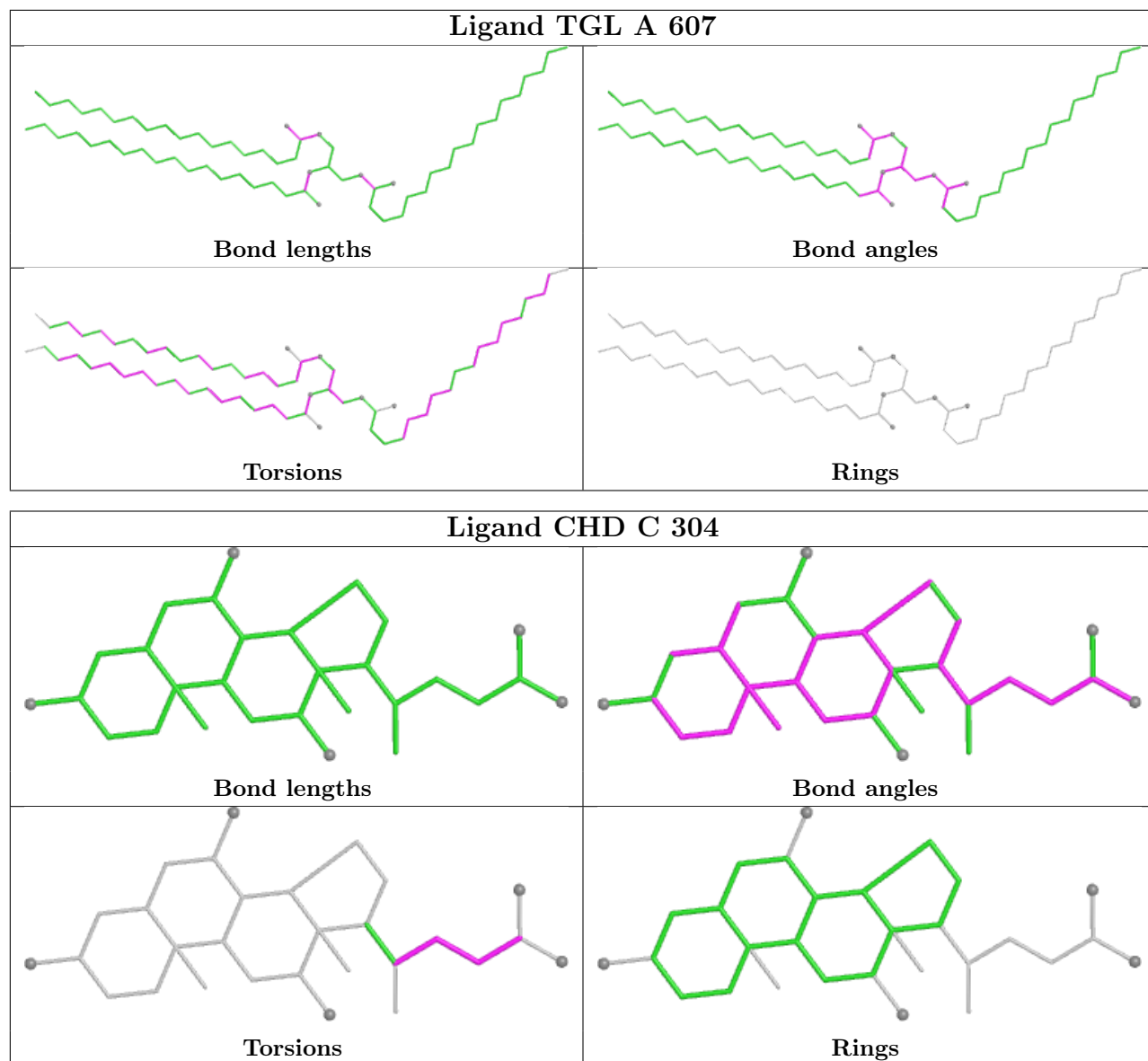


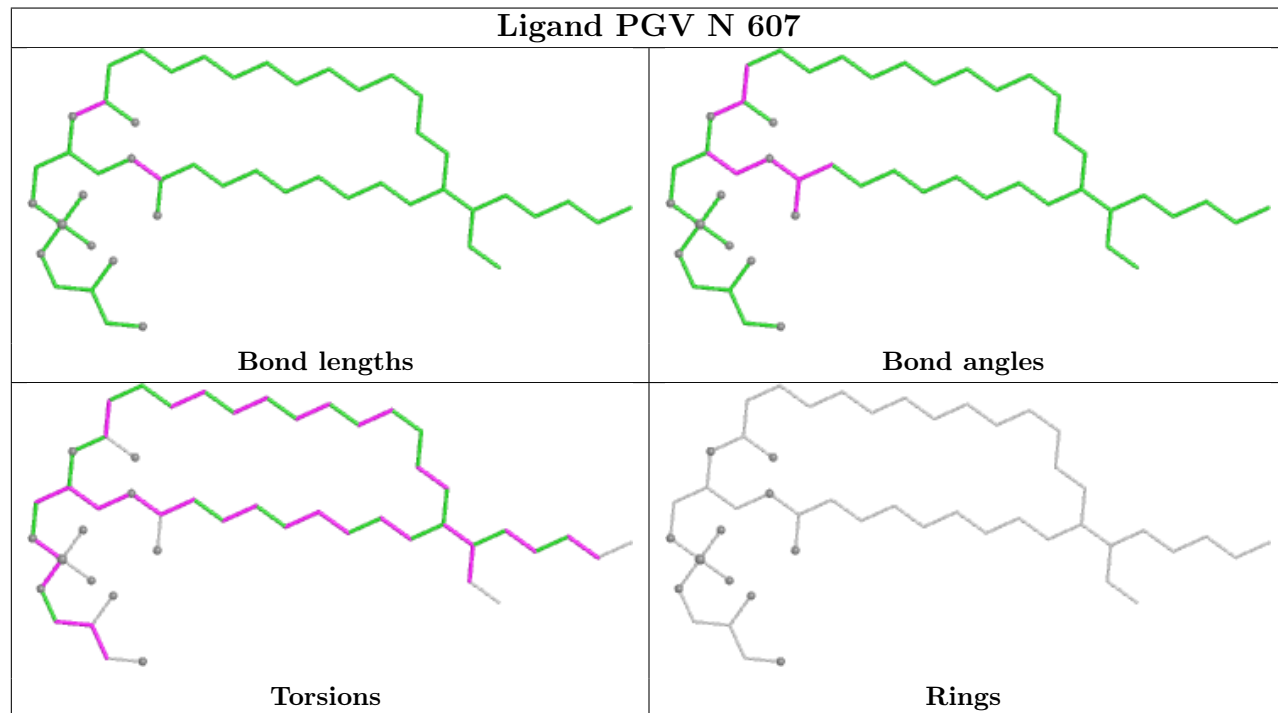
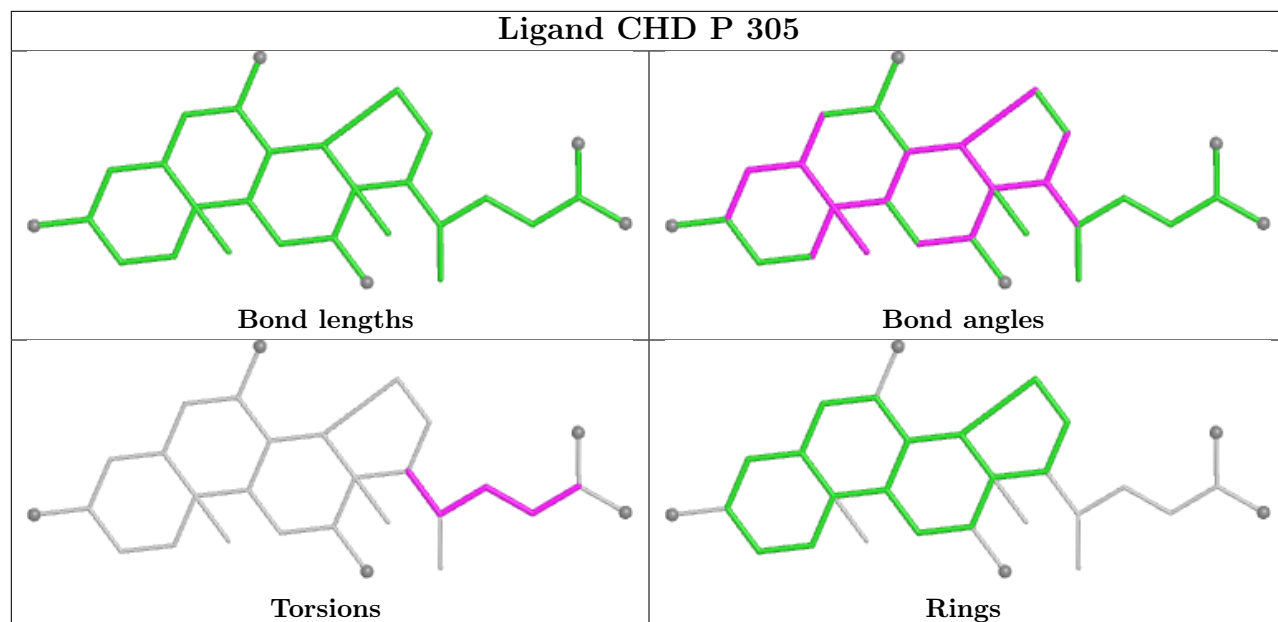


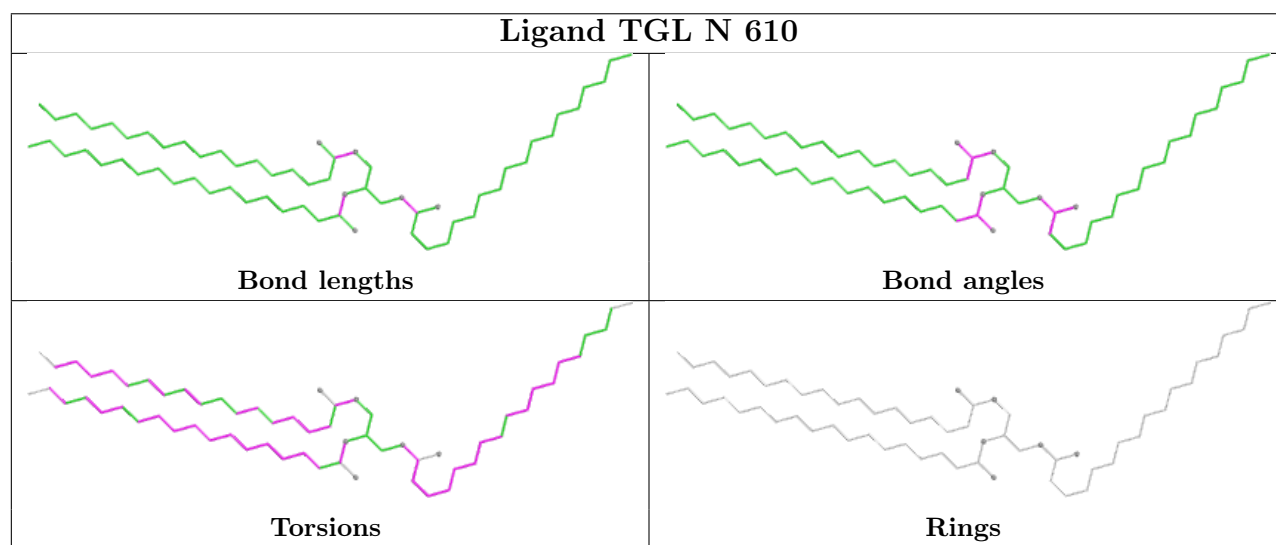
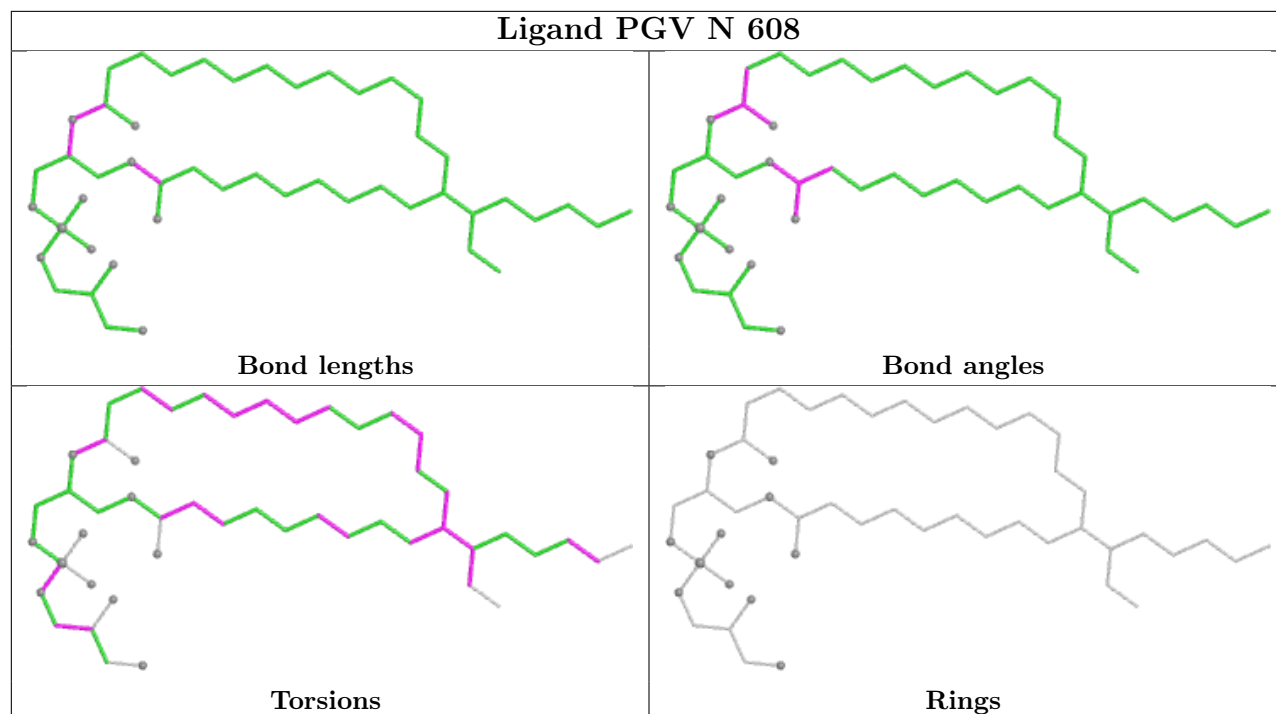


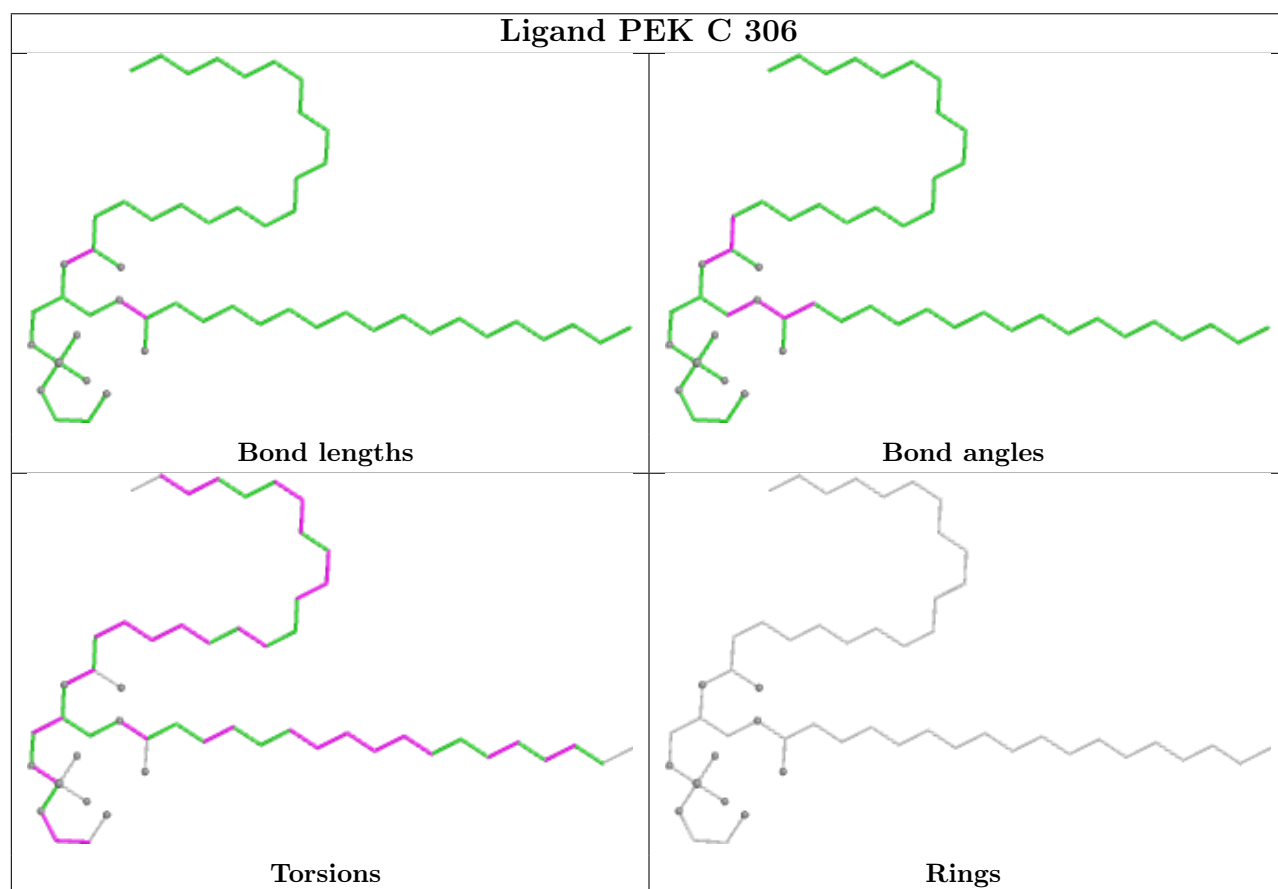
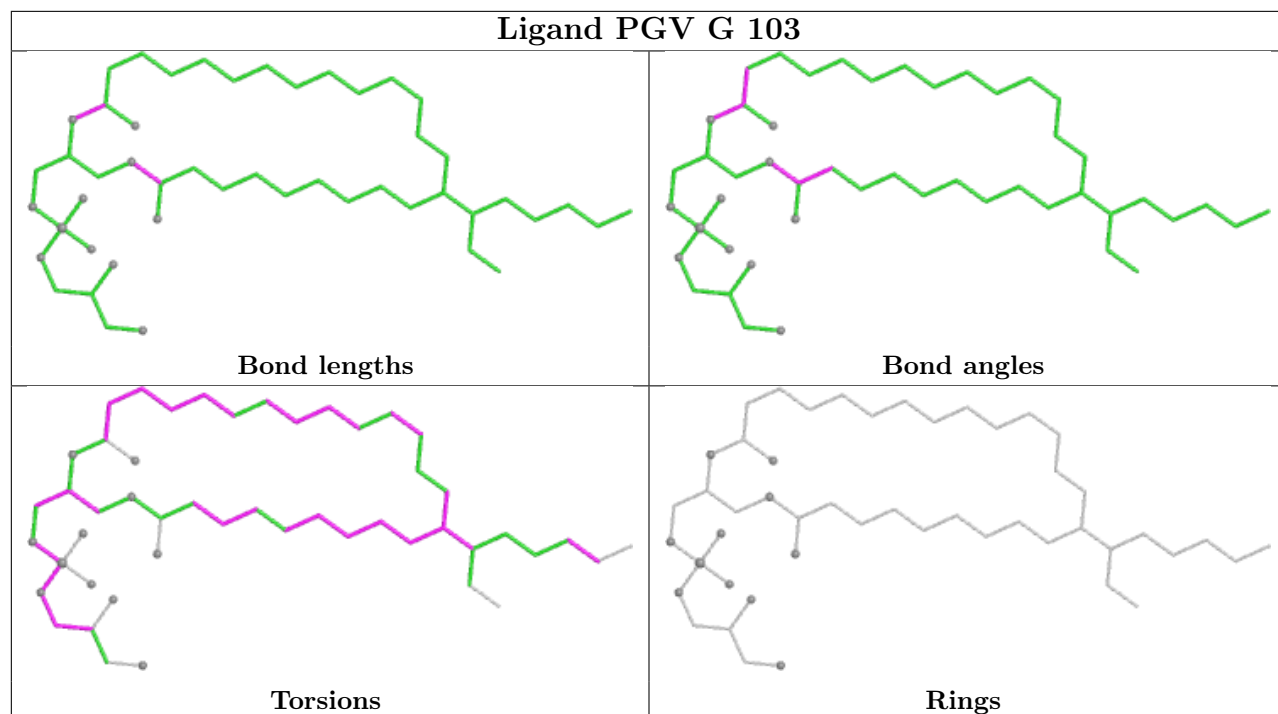


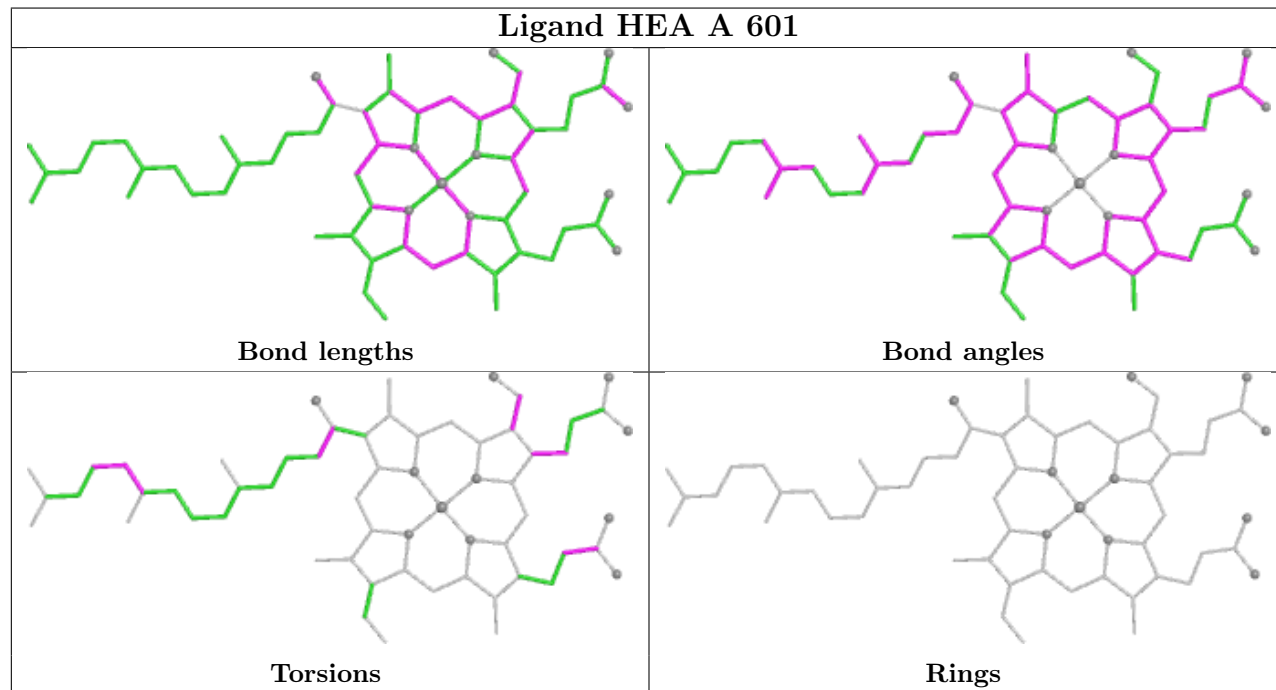
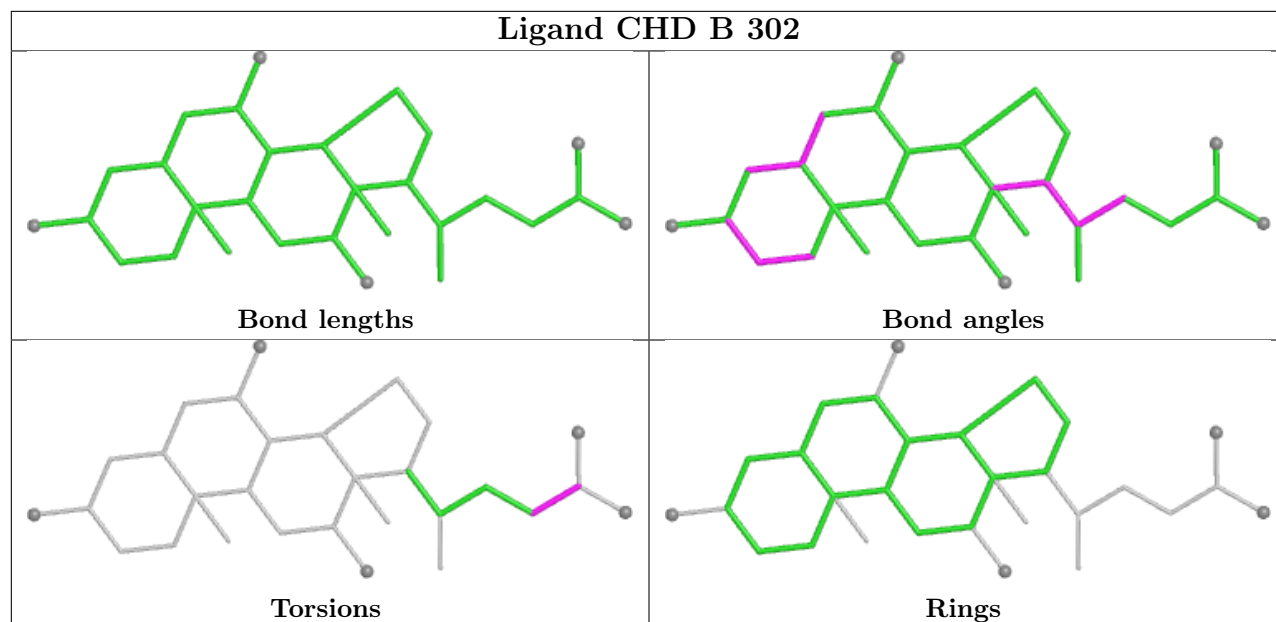


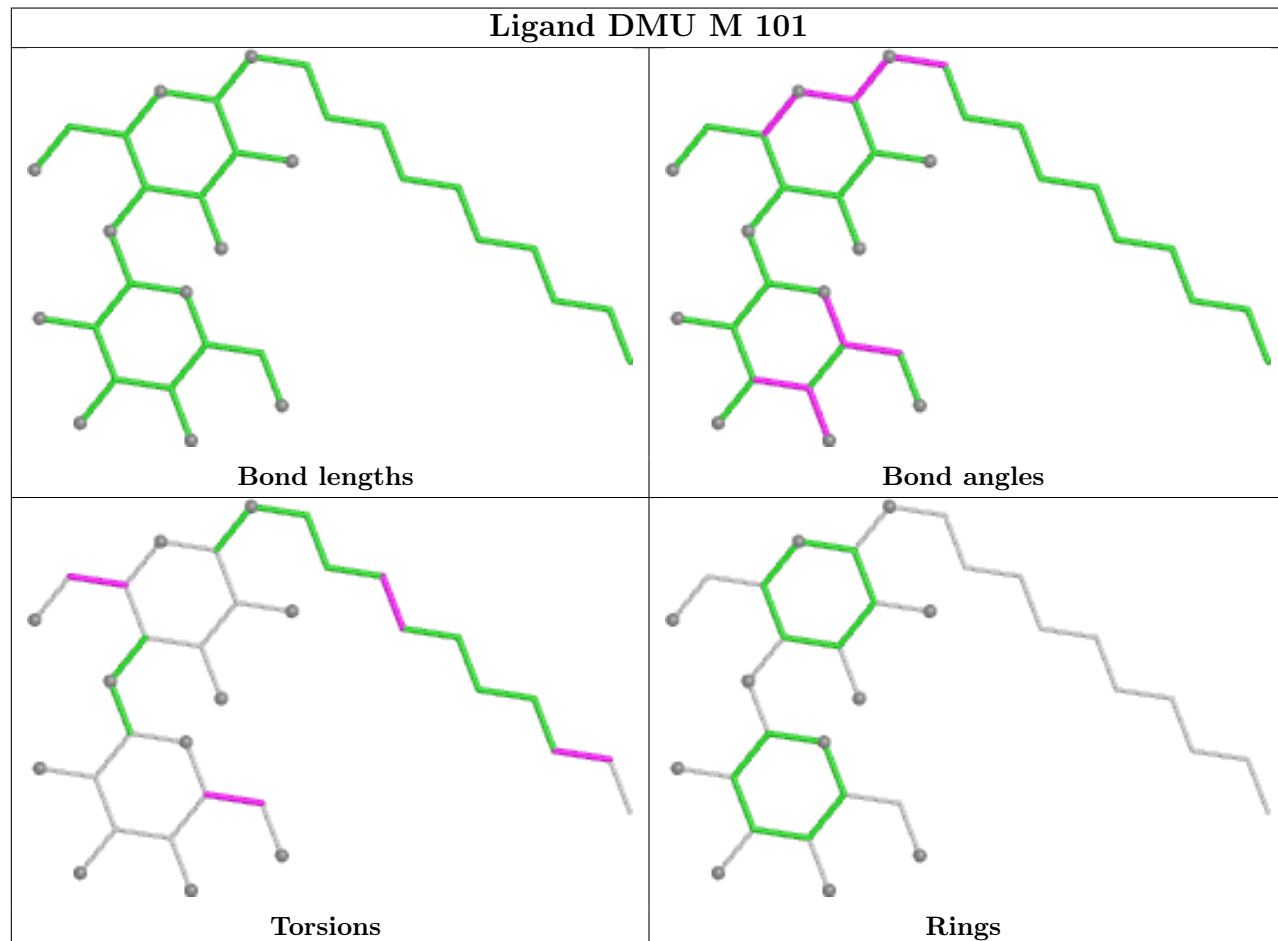
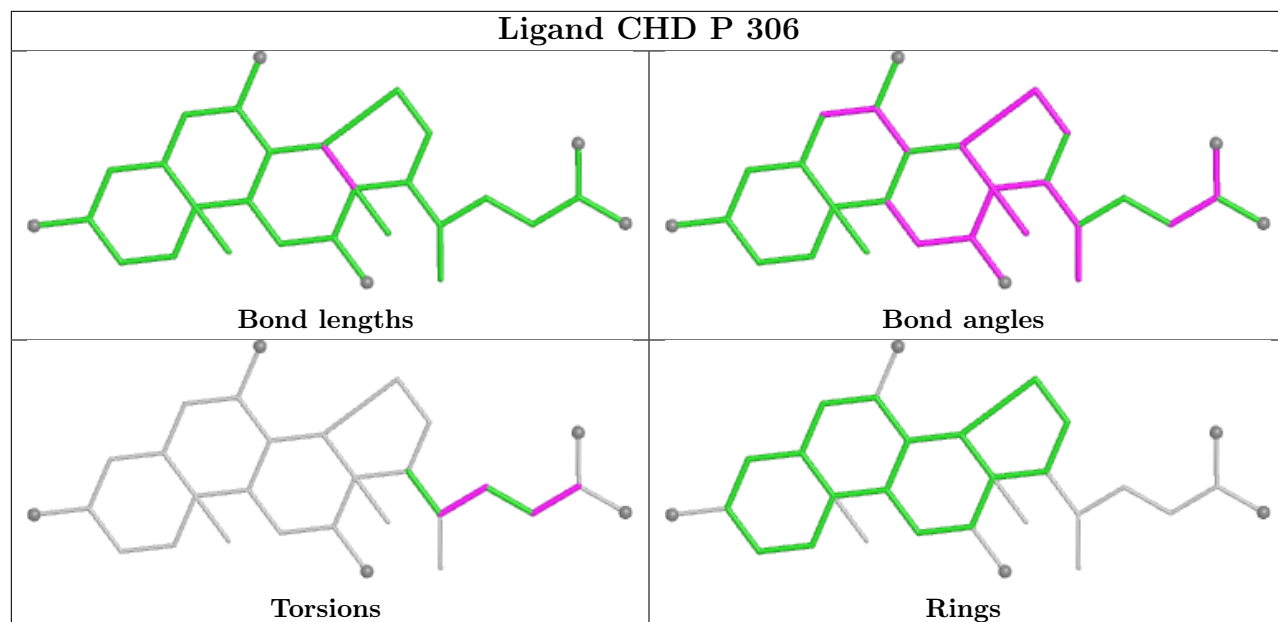


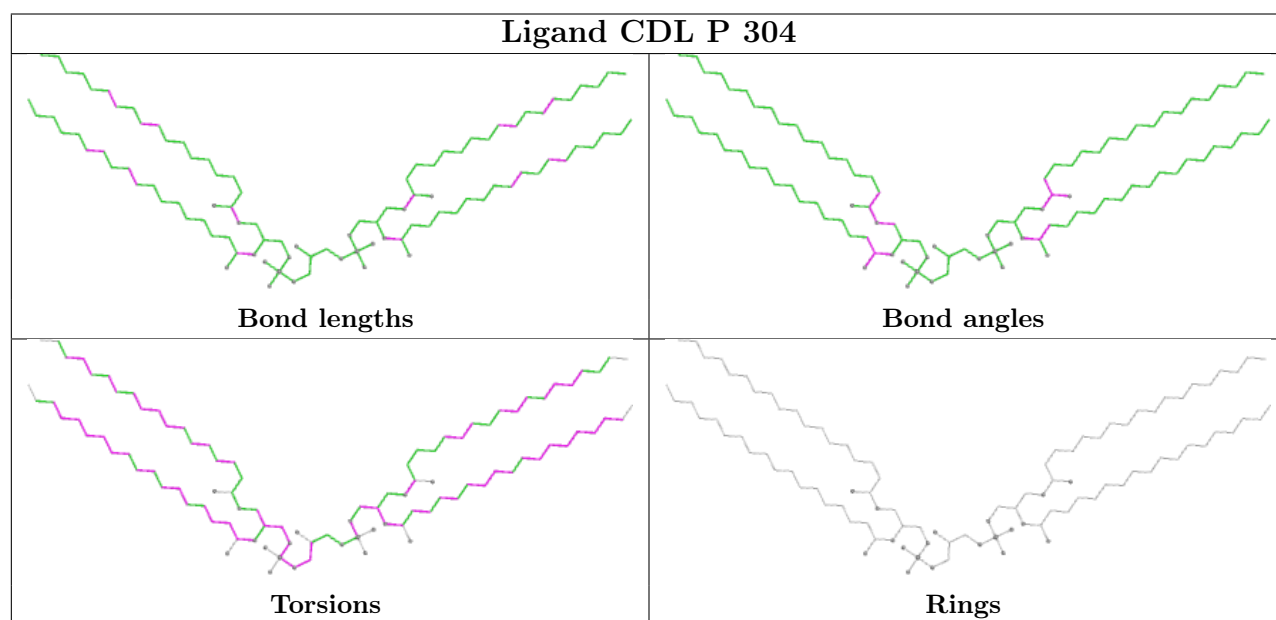
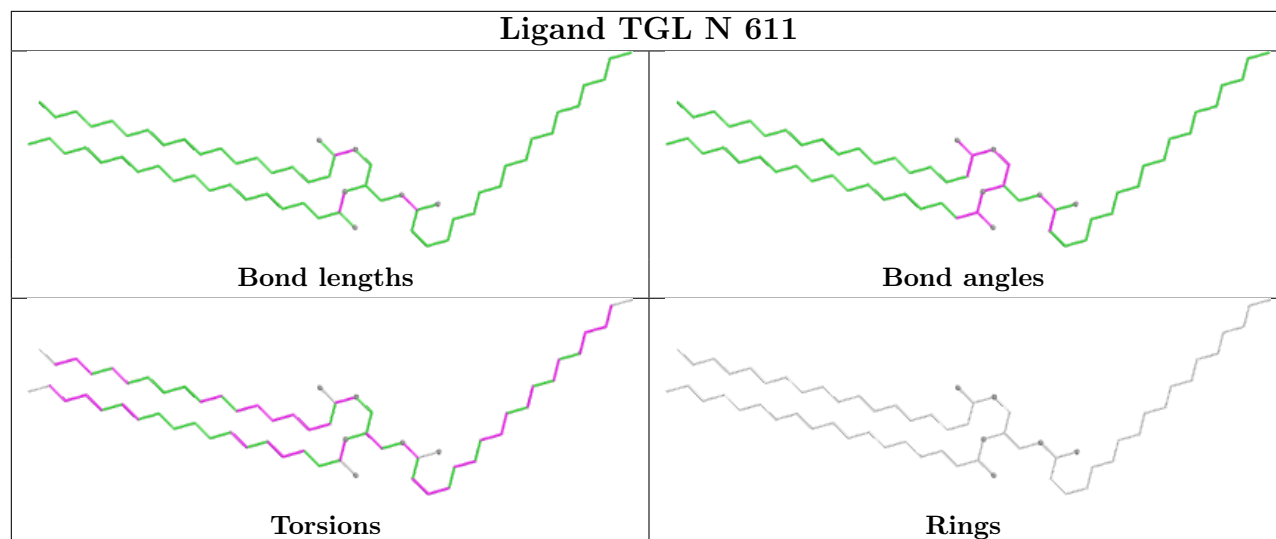


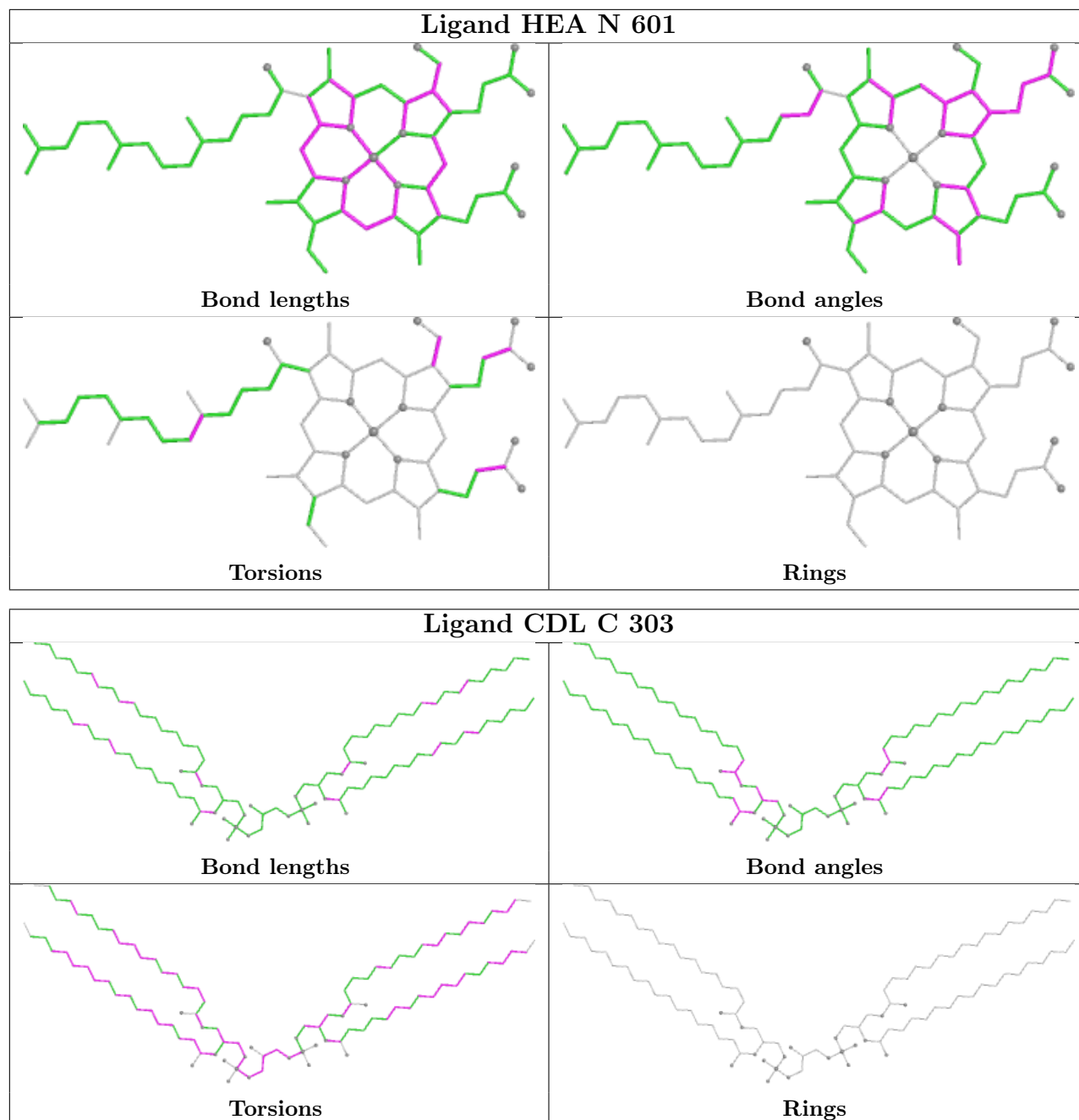




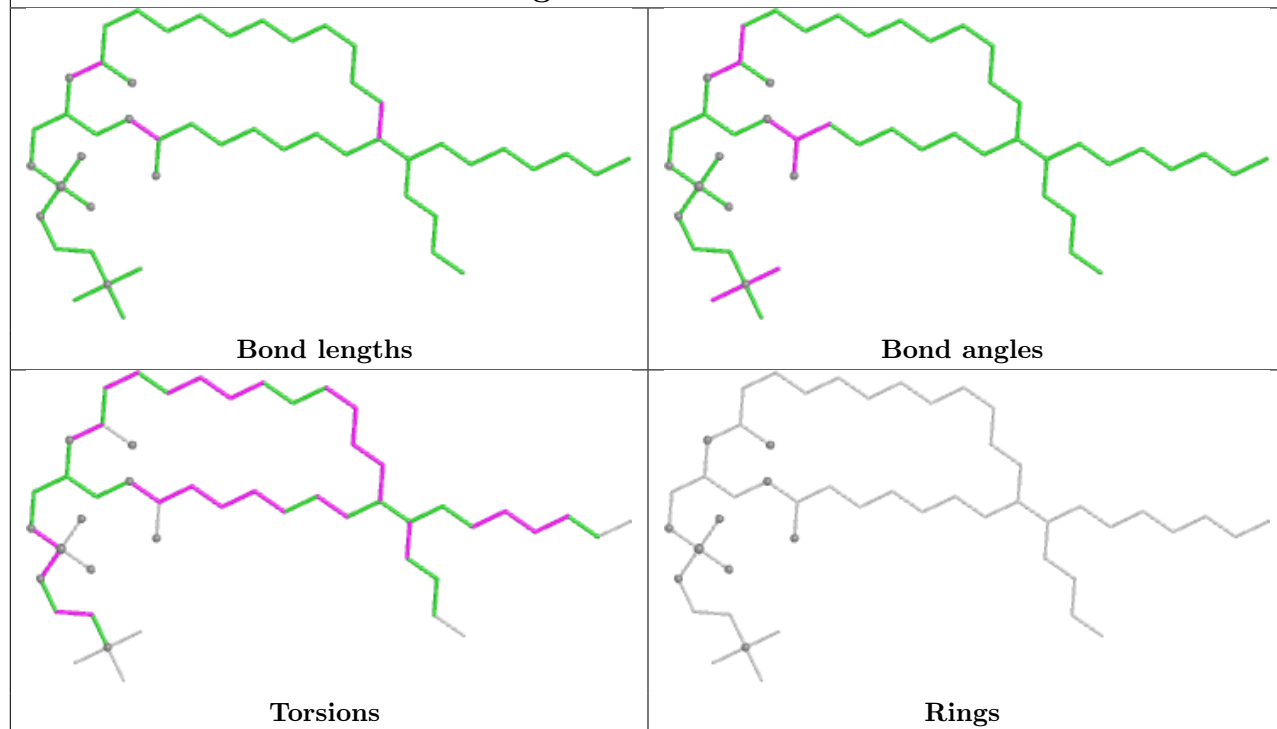




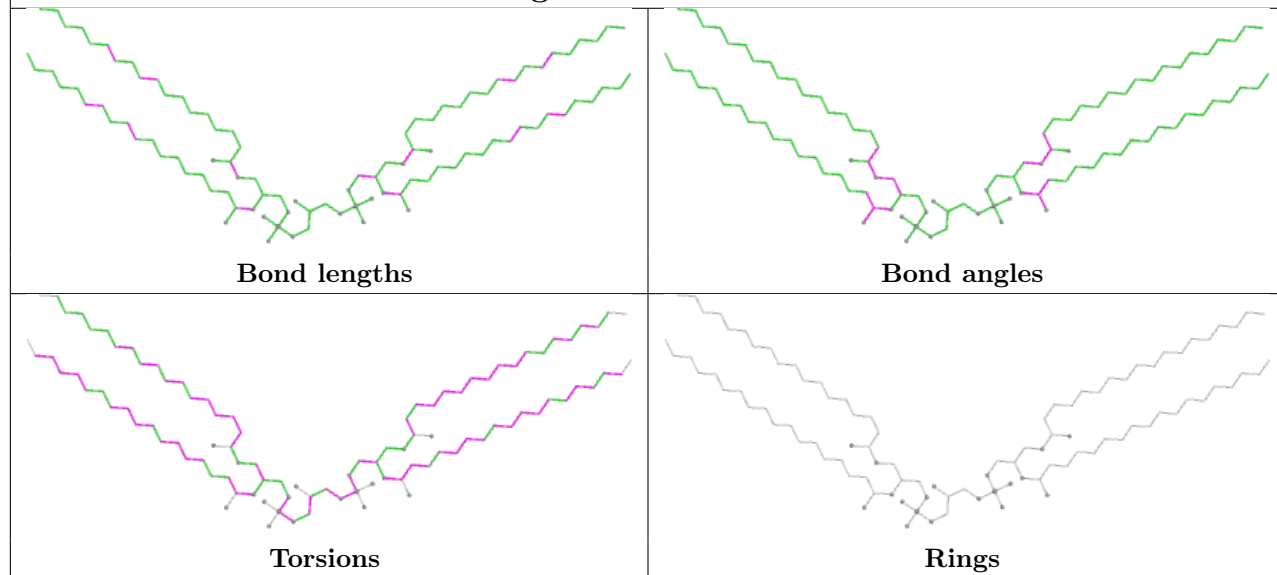


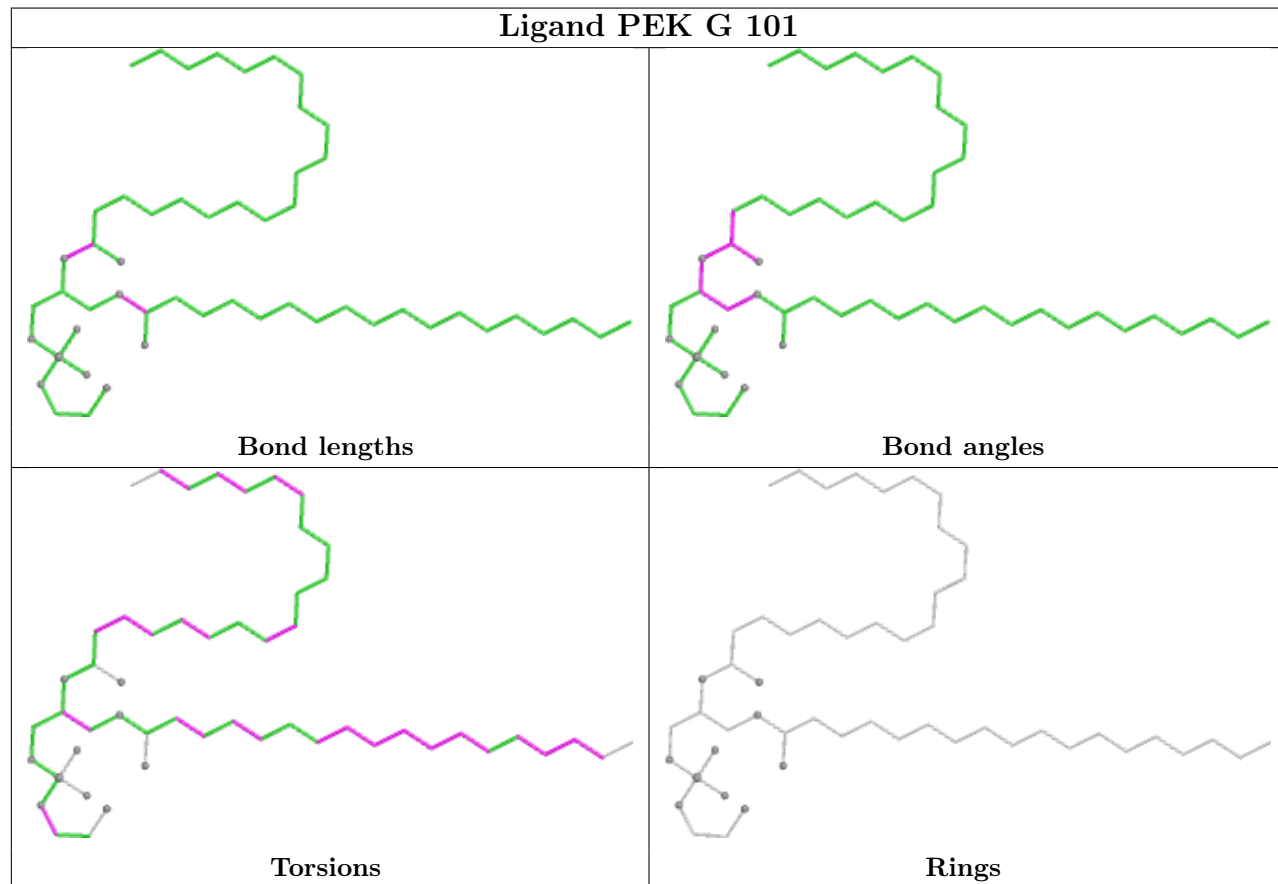
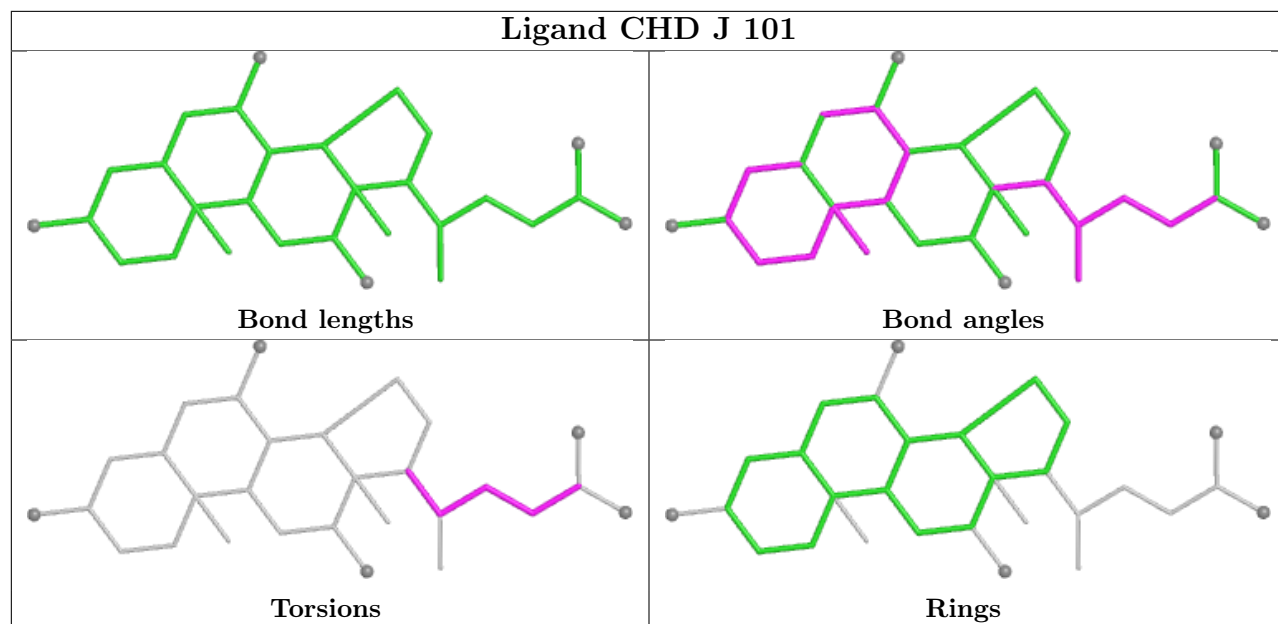


Ligand PSC R 201

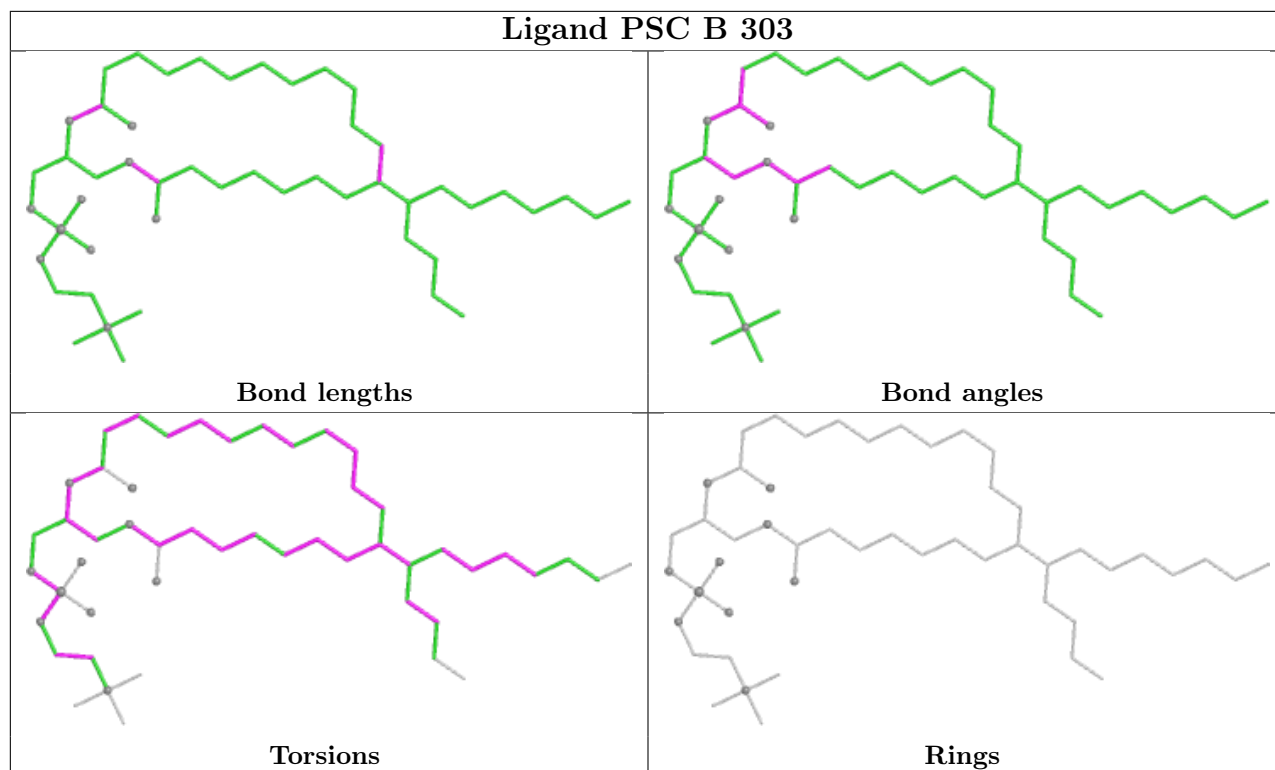


Ligand CDL C 307

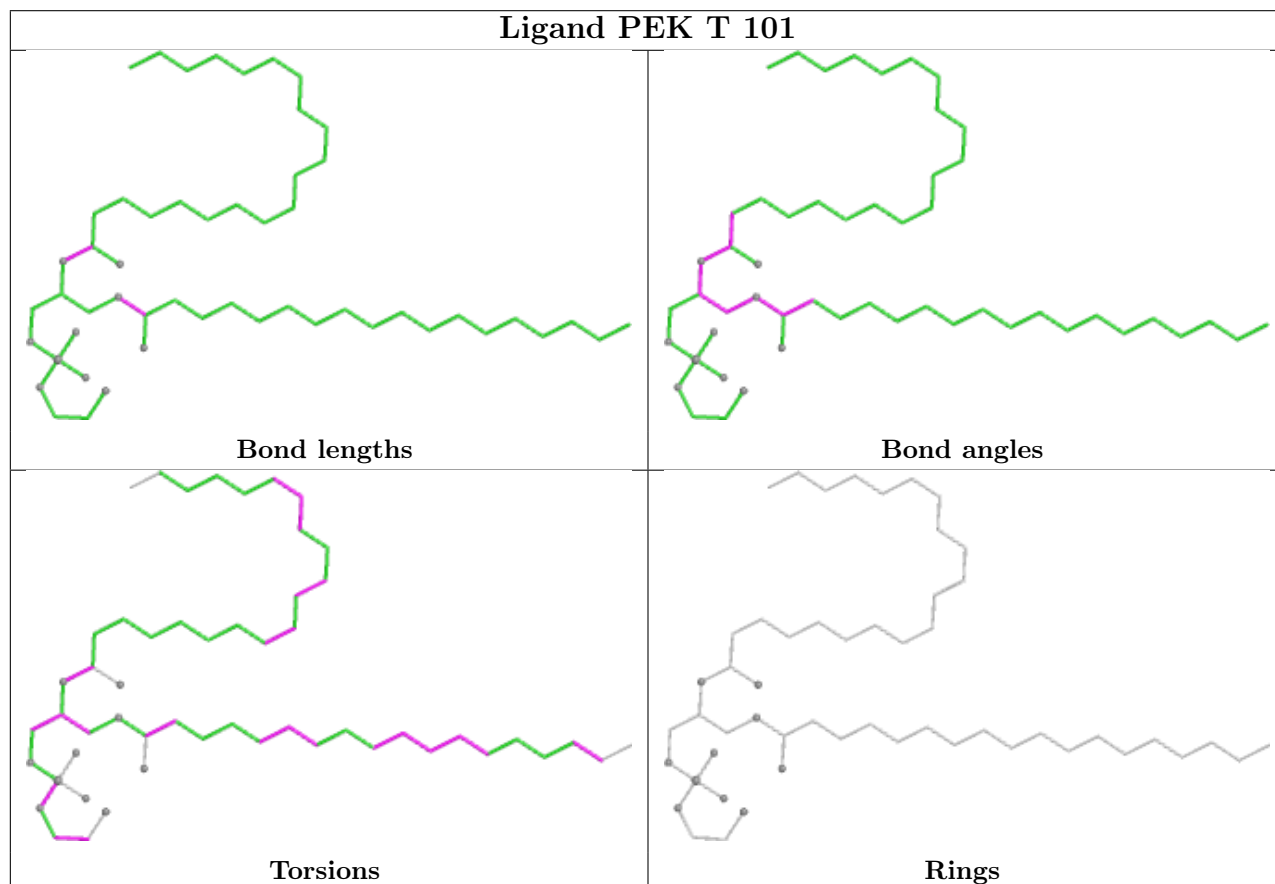




Ligand PSC B 303



Ligand PEK T 101



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%)	-1.16	0 100 100	39, 53, 66, 101	1 (0%)
1	N	513/514 (99%)	-1.09	0 100 100	43, 60, 76, 104	0
2	B	226/227 (99%)	-1.07	0 100 100	46, 59, 91, 128	0
2	O	226/227 (99%)	-0.97	1 (0%) 88 86	54, 69, 104, 150	0
3	C	259/261 (99%)	-1.09	0 100 100	46, 57, 75, 115	0
3	P	259/261 (99%)	-1.02	0 100 100	46, 62, 81, 121	0
4	D	144/147 (97%)	-1.08	0 100 100	52, 66, 89, 117	0
4	Q	144/147 (97%)	-0.78	1 (0%) 84 81	64, 83, 125, 160	0
5	E	105/109 (96%)	-1.19	0 100 100	50, 65, 92, 147	0
5	R	105/109 (96%)	-1.04	0 100 100	62, 79, 105, 154	0
6	F	98/98 (100%)	-0.94	0 100 100	52, 66, 134, 154	0
6	S	98/98 (100%)	-0.84	1 (1%) 79 76	58, 74, 145, 162	0
7	G	83/85 (97%)	-0.72	1 (1%) 76 73	55, 66, 143, 159	0
7	T	83/85 (97%)	-0.65	0 100 100	53, 73, 147, 158	0
8	H	79/85 (92%)	-0.89	0 100 100	54, 69, 141, 156	0
8	U	79/85 (92%)	-0.82	1 (1%) 75 71	61, 80, 139, 153	0
9	I	72/73 (98%)	-0.85	0 100 100	58, 73, 101, 114	0
9	V	72/73 (98%)	-0.79	0 100 100	59, 84, 114, 142	0
10	J	58/59 (98%)	-1.01	0 100 100	57, 70, 111, 144	0
10	W	58/59 (98%)	-0.94	0 100 100	66, 82, 123, 158	0
11	K	49/56 (87%)	-0.89	0 100 100	59, 72, 93, 119	0
11	X	49/56 (87%)	-0.81	0 100 100	70, 84, 119, 127	0
12	L	46/47 (97%)	-1.08	0 100 100	49, 60, 80, 122	0
12	Y	46/47 (97%)	-0.88	0 100 100	60, 75, 102, 119	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	-0.92	0	100 100	50, 63, 99, 147	0
13	Z	43/46 (93%)	-0.74	0	100 100	70, 79, 121, 164	0
All	All	3550/3614 (98%)	-1.00	5 (0%)	92 90	39, 64, 107, 164	1 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	6	VAL	3.0
2	O	90	ILE	2.9
6	S	96	LEU	2.5
7	G	5	LYS	2.4
8	U	8	ILE	2.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	SAC	V	1	9/10	0.63	0.09	138,151,167,167	0
7	TPO	T	11	11/12	0.68	0.15	101,147,160,160	0
7	TPO	G	11	11/12	0.80	0.10	102,140,157,157	0
9	SAC	I	1	9/10	0.84	0.07	116,134,157,165	0
1	FME	N	1	10/11	0.91	0.10	80,86,125,151	0
1	FME	A	1	10/11	0.95	0.11	74,86,128,147	0
2	FME	O	1	10/11	0.97	0.06	64,71,76,79	0
2	FME	B	1	10/11	0.98	0.04	58,65,72,72	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(Å ²)	Q<0.9
23	CHD	W	101	29/29	0.75	0.12	107,145,150,150	0
27	PEK	G	102	53/53	0.76	0.15	100,135,150,150	0
24	PSC	B	303	52/52	0.77	0.15	75,147,150,150	0
27	PEK	T	101	53/53	0.78	0.15	79,136,150,150	0
20	PGV	N	607	51/51	0.79	0.12	99,137,150,150	0
24	PSC	R	201	52/52	0.79	0.15	76,137,150,150	0
21	EDO	C	310	4/4	0.82	0.18	94,105,106,112	0
20	PGV	A	609	51/51	0.82	0.11	69,115,159,161	0
19	TGL	N	611	63/63	0.82	0.15	90,126,148,150	0
27	PEK	T	102	53/53	0.82	0.14	78,133,150,150	0
26	CDL	P	304	100/100	0.83	0.12	71,140,150,150	0
26	CDL	T	103	100/100	0.83	0.15	76,140,150,150	0
19	TGL	A	607	63/63	0.83	0.12	54,97,122,132	0
25	UNX	P	301	1/1	0.83	0.39	15,15,15,15	1
26	CDL	C	307	100/100	0.83	0.15	89,138,150,150	0
19	TGL	L	101	63/63	0.84	0.17	67,113,143,150	0
20	PGV	C	308	51/51	0.84	0.11	75,125,150,150	0
19	TGL	N	610	63/63	0.85	0.13	90,134,149,150	0
25	UNX	C	301	1/1	0.86	0.33	26,26,26,26	1
21	EDO	A	614	4/4	0.87	0.30	133,137,141,148	0
19	TGL	D	201	63/63	0.87	0.13	87,126,147,150	0
27	PEK	C	306	53/53	0.87	0.12	71,132,149,150	0
29	DMU	Z	101	33/33	0.87	0.12	80,128,149,150	0
26	CDL	C	303	100/100	0.88	0.10	66,123,153,155	0
19	TGL	N	609	63/63	0.88	0.10	60,120,149,150	0
20	PGV	G	103	51/51	0.88	0.10	96,127,150,150	0
21	EDO	C	309	4/4	0.90	0.09	76,86,100,122	0
21	EDO	C	311	4/4	0.91	0.10	80,95,109,118	0
23	CHD	C	304	29/29	0.91	0.08	93,117,125,127	0
21	EDO	B	305	4/4	0.92	0.12	105,110,115,123	0
23	CHD	P	305	29/29	0.92	0.09	120,135,145,147	0
21	EDO	K	103	4/4	0.92	0.08	90,92,99,101	0
21	EDO	T	104	4/4	0.92	0.16	124,129,131,132	0
23	CHD	J	101	29/29	0.93	0.07	123,142,150,150	0
21	EDO	L	102	4/4	0.93	0.12	83,84,84,90	0
21	EDO	K	102	4/4	0.93	0.15	101,108,112,116	0
21	EDO	K	101	4/4	0.93	0.14	86,107,118,131	0
21	EDO	A	613	4/4	0.94	0.22	112,112,121,122	0
29	DMU	M	101	33/33	0.94	0.08	70,102,129,136	0
21	EDO	A	610	4/4	0.94	0.08	75,75,78,81	0
21	EDO	N	612	4/4	0.95	0.10	79,80,82,84	0

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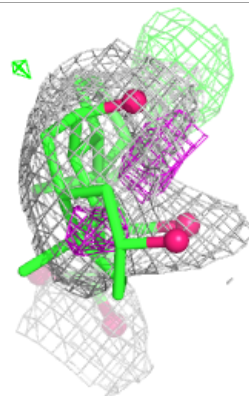
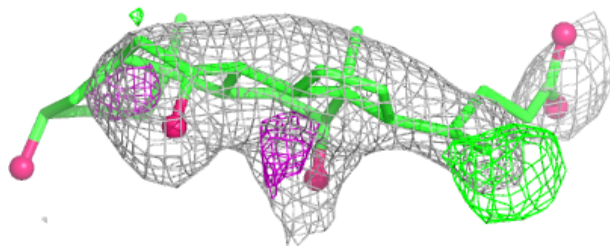
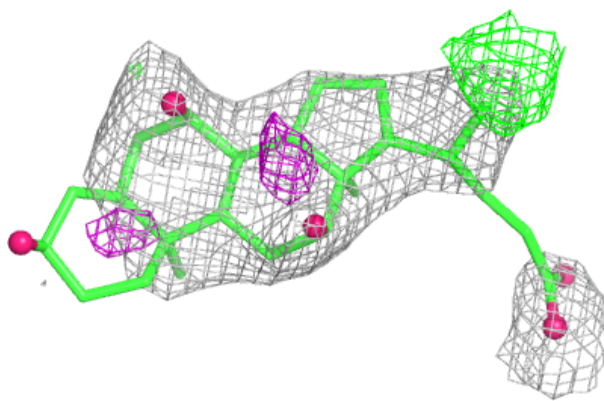
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
21	EDO	A	612	4/4	0.95	0.21	88,115,122,127	0
21	EDO	F	102	4/4	0.96	0.06	80,88,96,96	0
27	PEK	P	302	53/53	0.96	0.07	59,91,150,150	0
27	PEK	G	101	53/53	0.97	0.05	57,72,126,136	0
23	CHD	B	302	29/29	0.97	0.05	48,64,74,77	0
23	CHD	P	306	29/29	0.97	0.04	57,65,72,73	0
21	EDO	A	611	4/4	0.97	0.07	86,94,107,113	0
23	CHD	C	305	29/29	0.97	0.05	47,61,71,81	0
21	EDO	G	104	4/4	0.97	0.10	97,101,102,105	0
23	CHD	O	302	29/29	0.97	0.05	50,57,67,72	0
17	NA	A	605	1/1	0.98	0.05	59,59,59,59	0
20	PGV	N	608	51/51	0.98	0.06	47,76,117,142	0
20	PGV	P	303	51/51	0.98	0.05	51,72,132,148	0
20	PGV	A	608	51/51	0.98	0.05	51,66,79,86	0
18	CMO	A	606	2/2	0.98	0.13	55,55,55,55	0
20	PGV	C	302	51/51	0.98	0.05	49,58,90,99	0
18	CMO	N	606	2/2	0.98	0.14	77,77,77,80	0
14	HEA	N	602	60/60	0.98	0.06	47,57,69,75	0
21	EDO	B	304	4/4	0.98	0.07	71,75,75,75	0
14	HEA	A	602	60/60	0.99	0.05	45,51,60,62	0
17	NA	N	605	1/1	0.99	0.02	70,70,70,70	0
14	HEA	N	601	60/60	0.99	0.05	47,56,78,84	0
28	ZN	F	101	1/1	0.99	0.02	64,64,64,64	0
14	HEA	A	601	60/60	0.99	0.05	34,46,65,70	0
16	MG	N	604	1/1	0.99	0.03	57,57,57,57	0
15	CU	N	603	1/1	1.00	0.01	55,55,55,55	0
16	MG	A	604	1/1	1.00	0.01	51,51,51,51	0
15	CU	A	603	1/1	1.00	0.02	55,55,55,55	0
28	ZN	S	101	1/1	1.00	0.03	70,70,70,70	0
22	CUA	B	301	2/2	1.00	0.03	54,54,54,58	0
22	CUA	O	301	2/2	1.00	0.02	66,66,66,67	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.

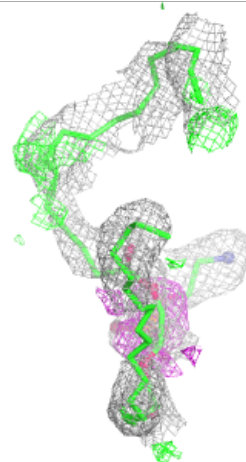
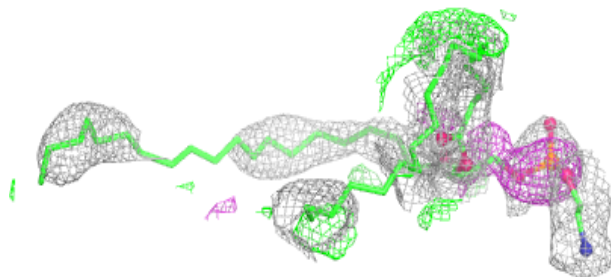
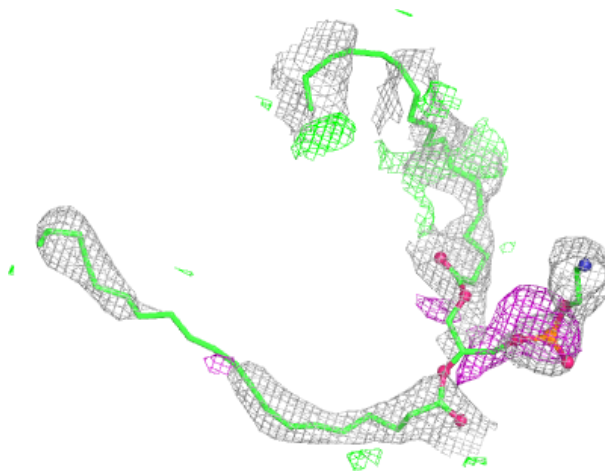
Electron density around CHD W 101:

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



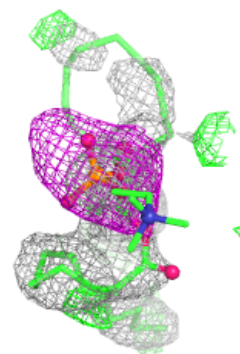
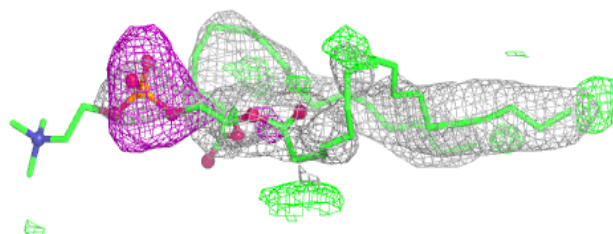
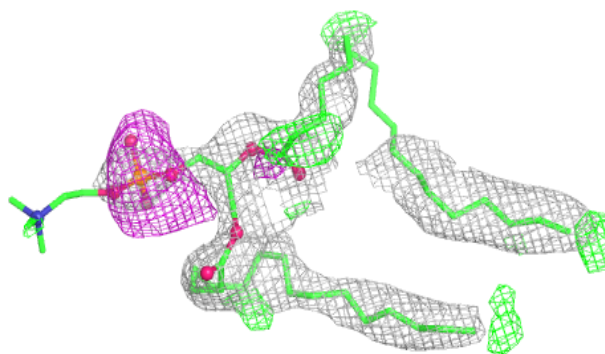
Electron density around PEK G 102:

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

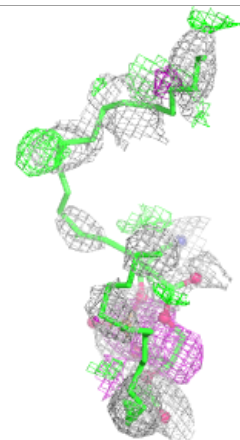
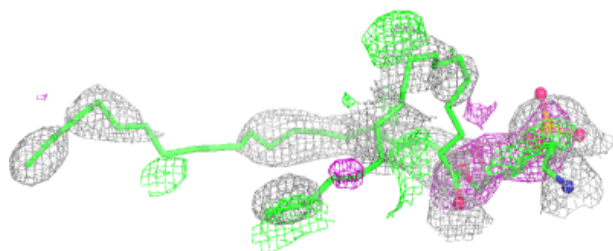
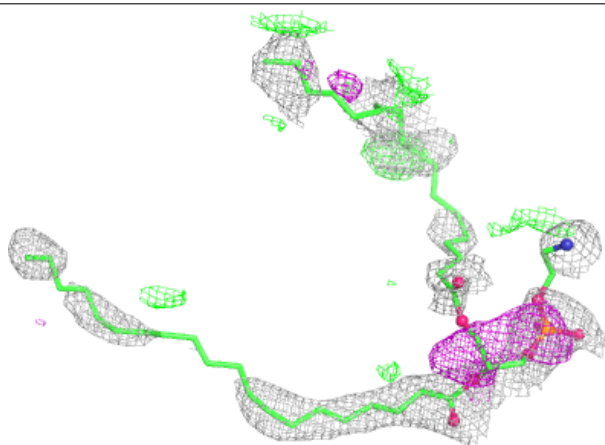


Electron density around PSC B 303:

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

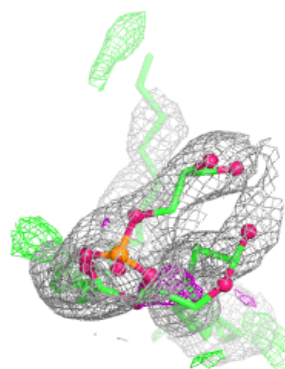
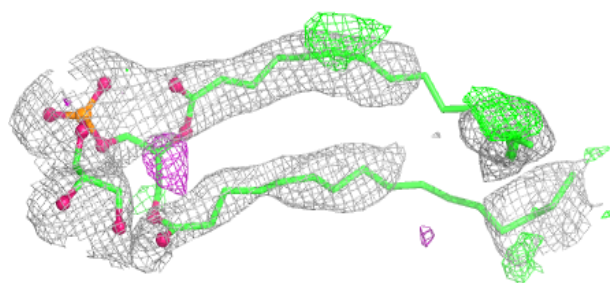
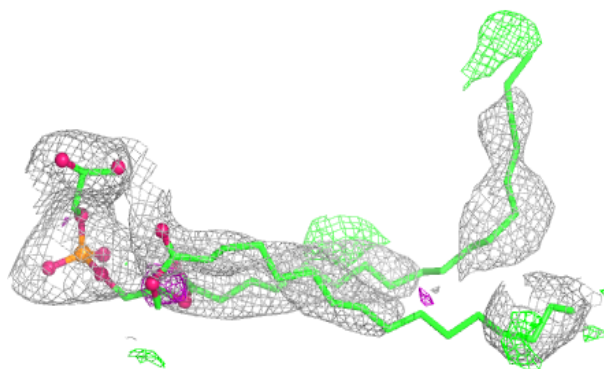
**Electron density around PEK T 101:**

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

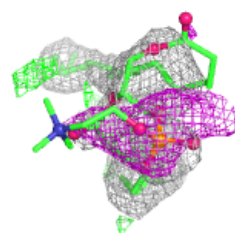
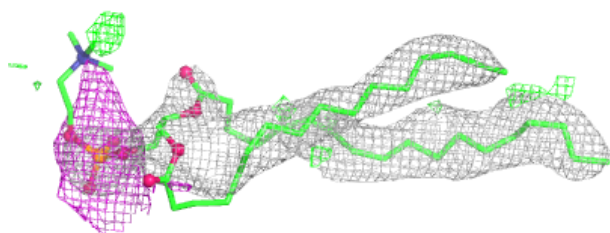
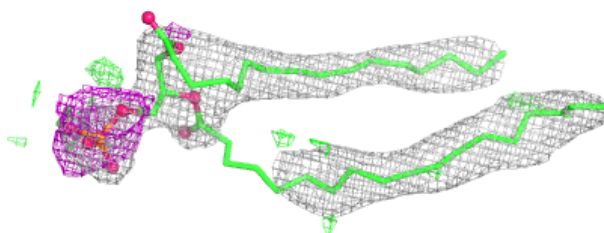


Electron density around PGV N 607:

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

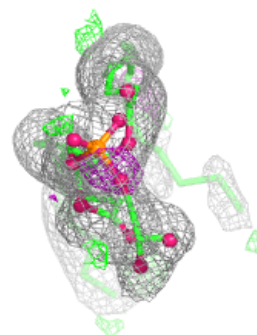
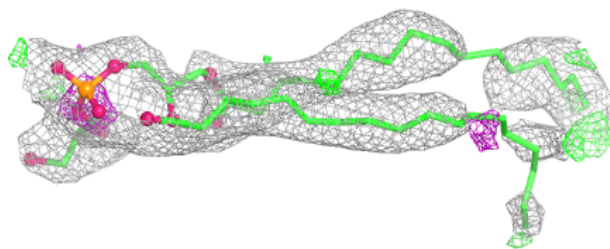
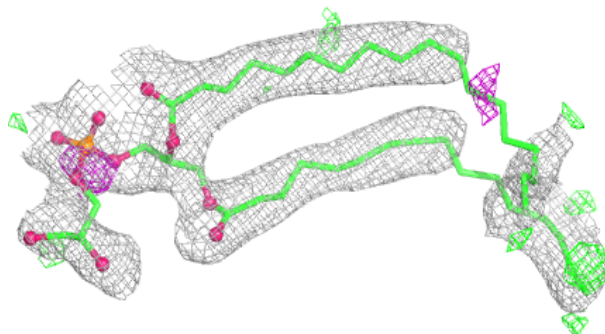
**Electron density around PSC R 201:**

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



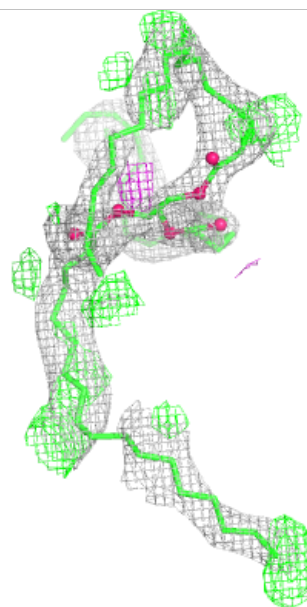
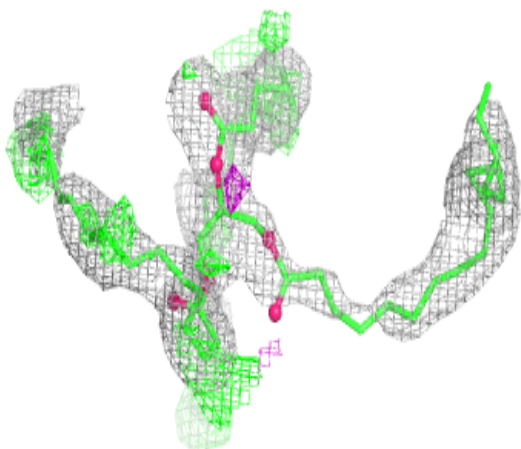
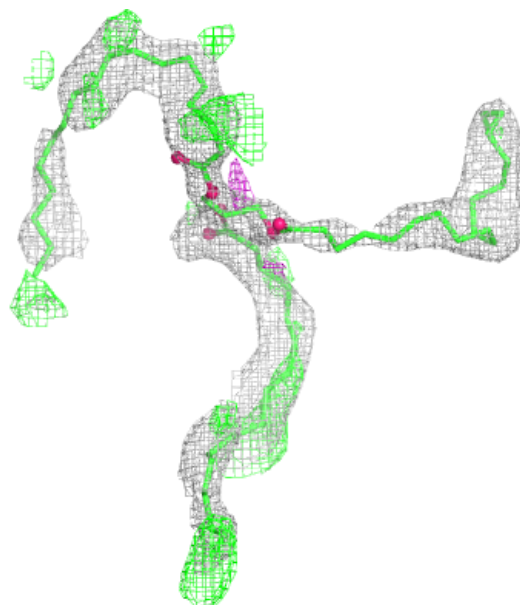
Electron density around PGV A 609:

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



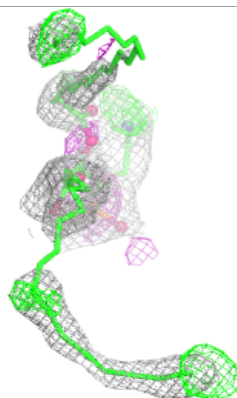
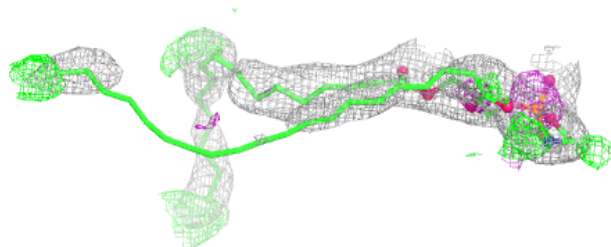
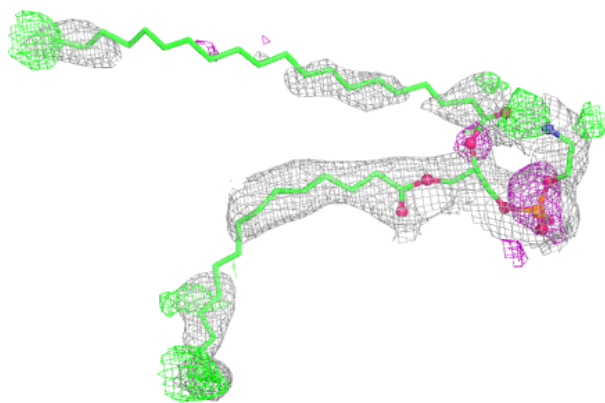
Electron density around TGL N 611:

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

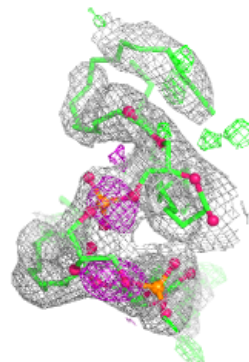
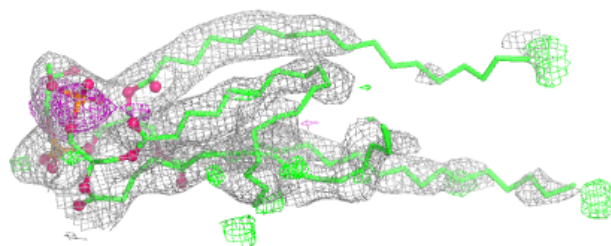
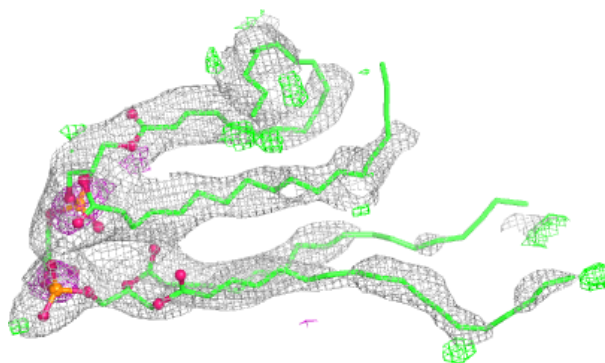


Electron density around PEK T 102:

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

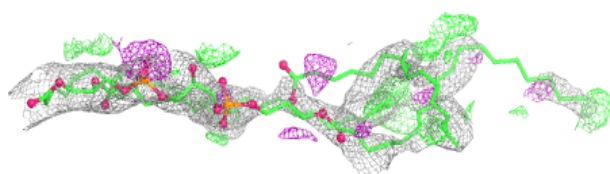
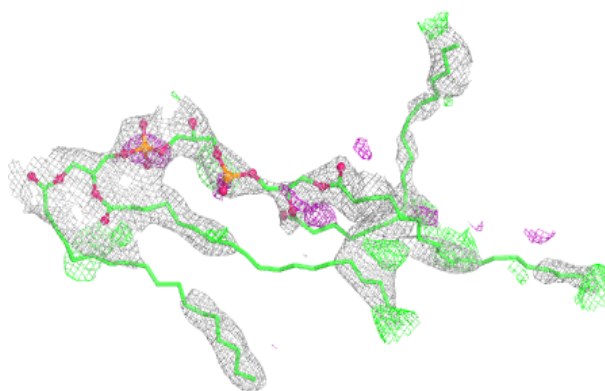
**Electron density around CDL P 304:**

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

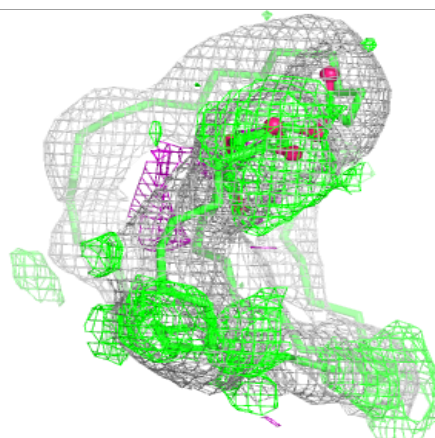
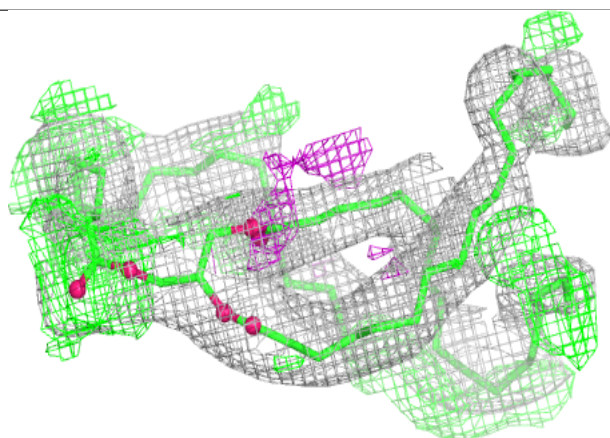
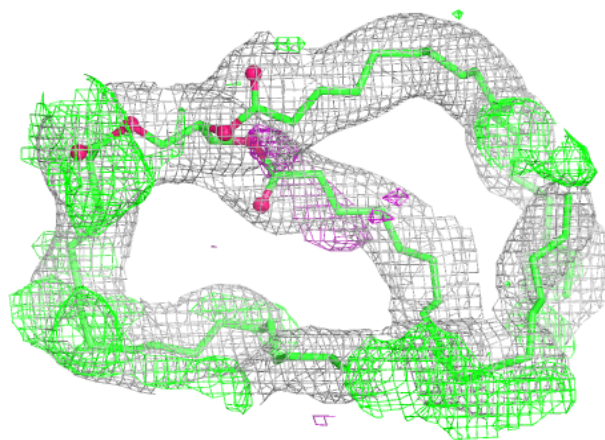


Electron density around CDL T 103:

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

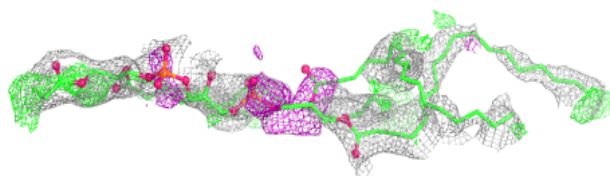
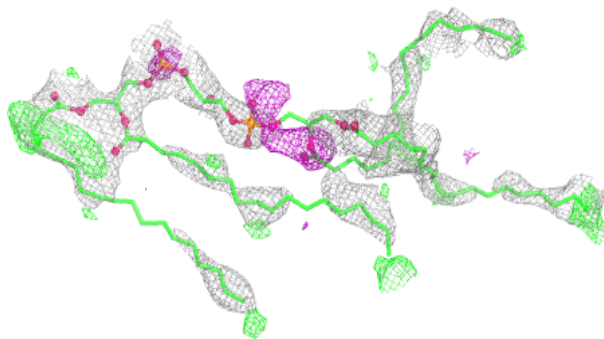
**Electron density around TGL A 607:**

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



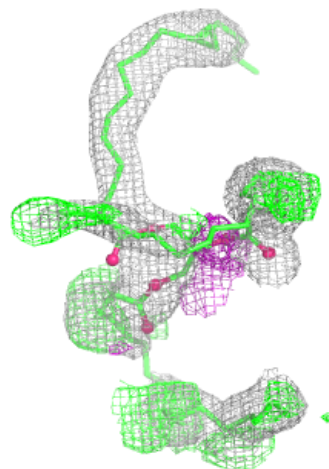
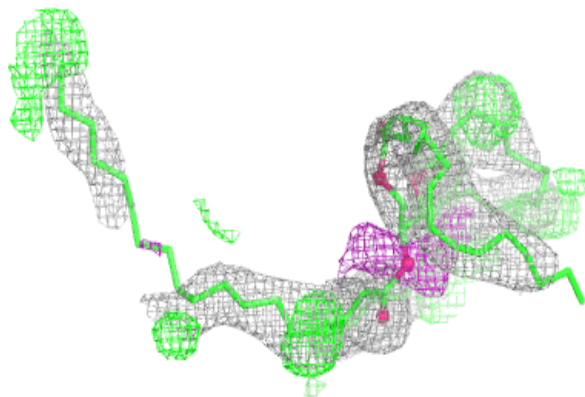
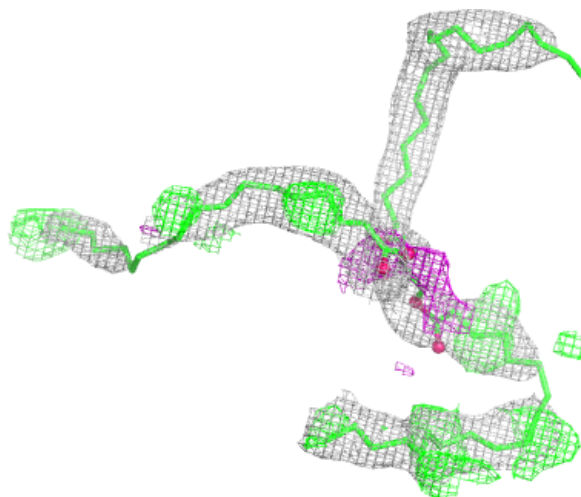
Electron density around CDL C 307:

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



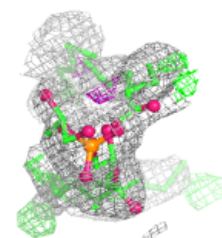
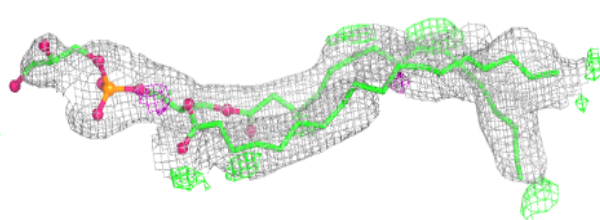
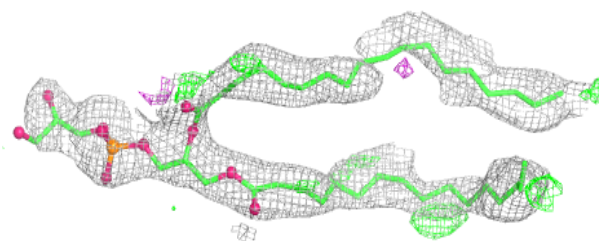
Electron density around TGL L 101:

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

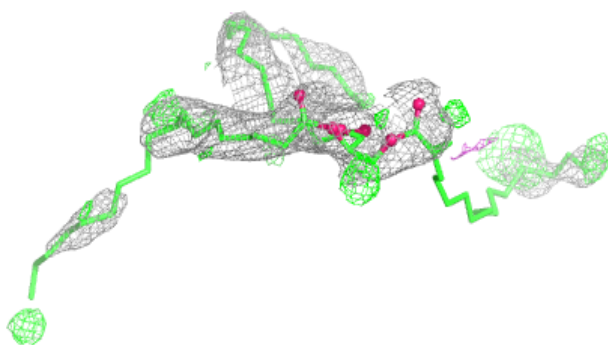
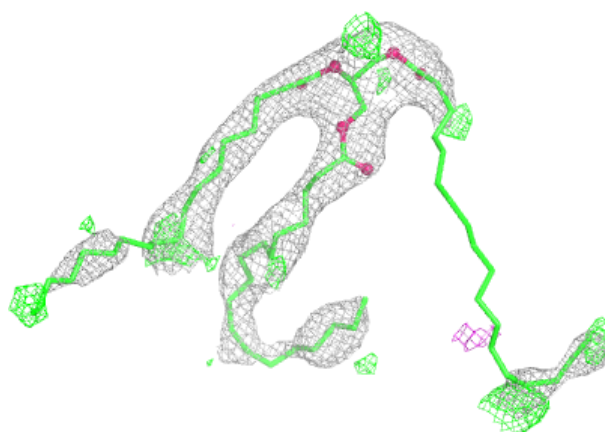


Electron density around PGV C 308:

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

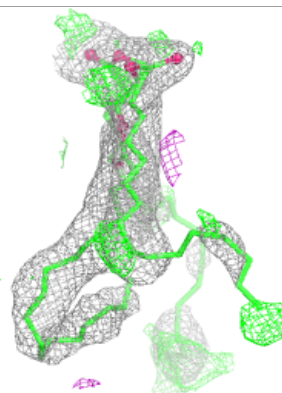
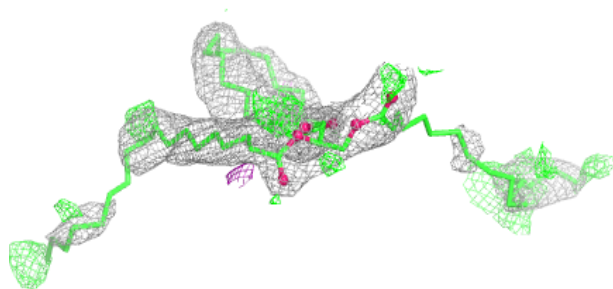
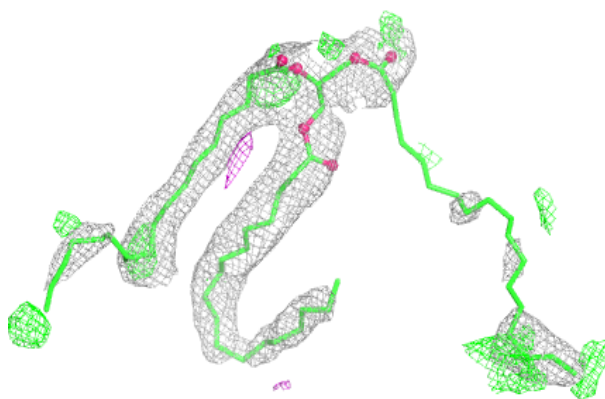
**Electron density around TGL N 610:**

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

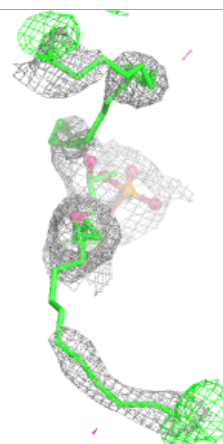
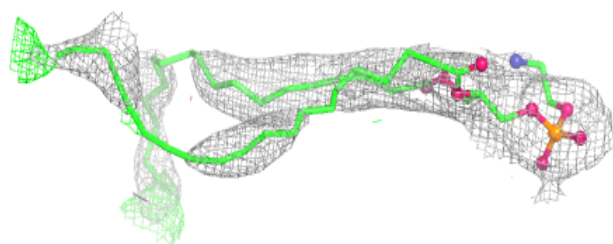
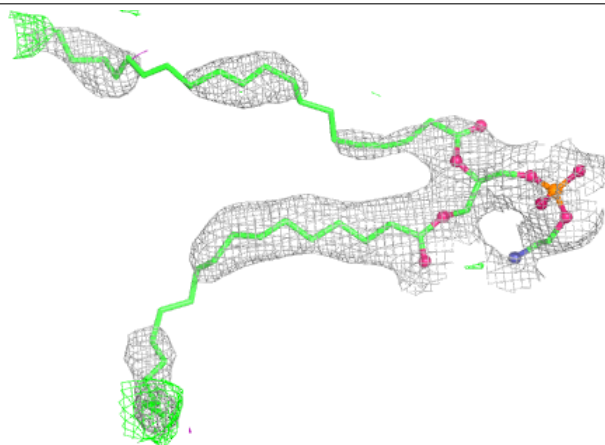


Electron density around TGL D 201:

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

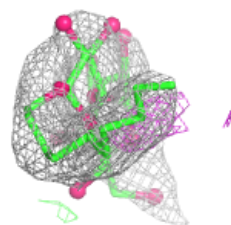
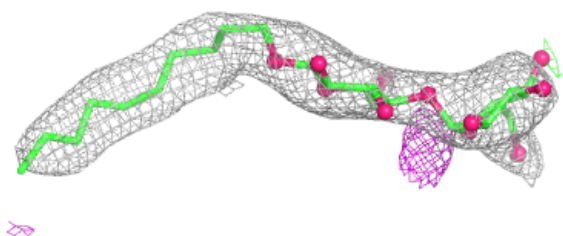
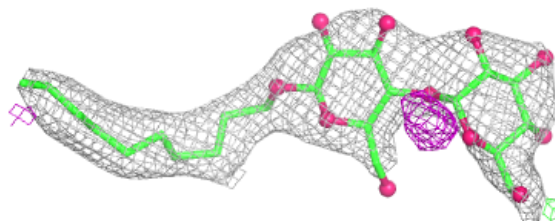
**Electron density around PEK C 306:**

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

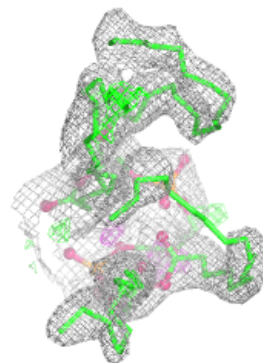
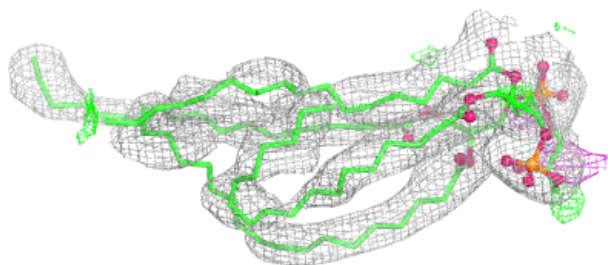
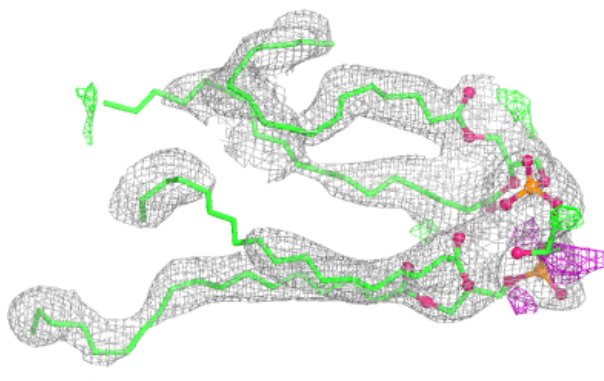


Electron density around DMU Z 101:

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

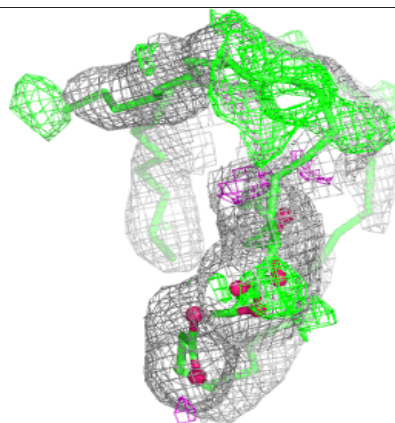
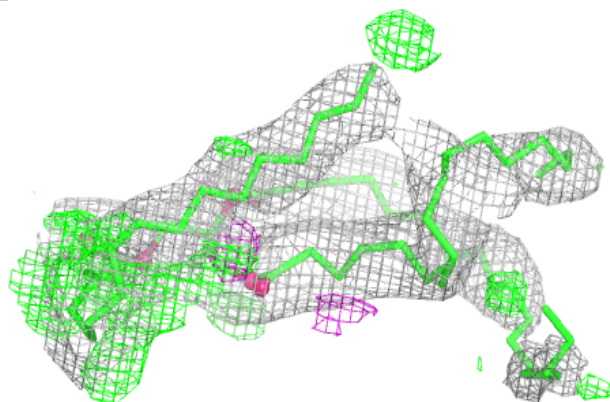
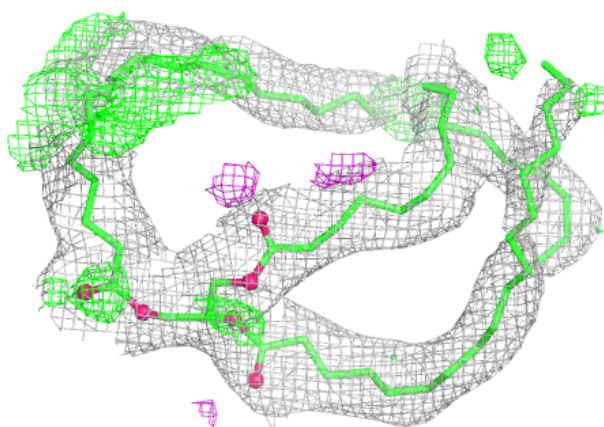
**Electron density around CDL C 303:**

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

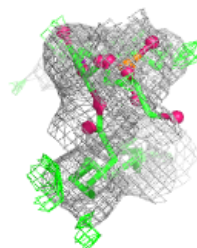
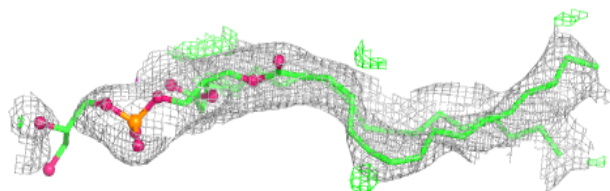
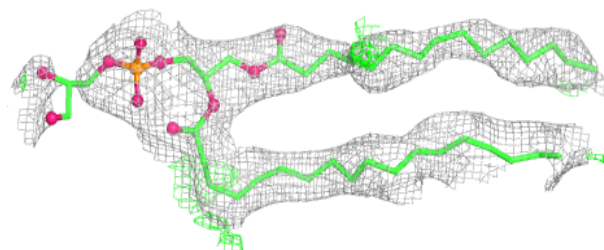


Electron density around TGL N 609:

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

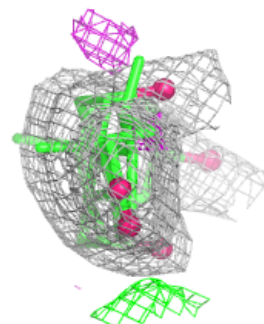
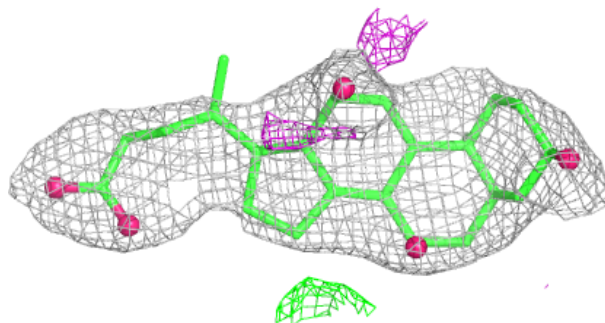
**Electron density around PGV G 103:**

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

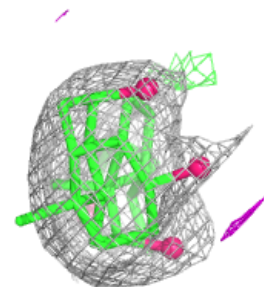
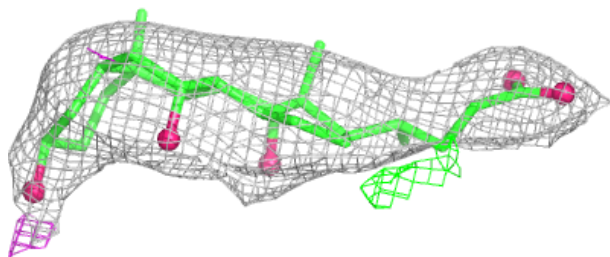
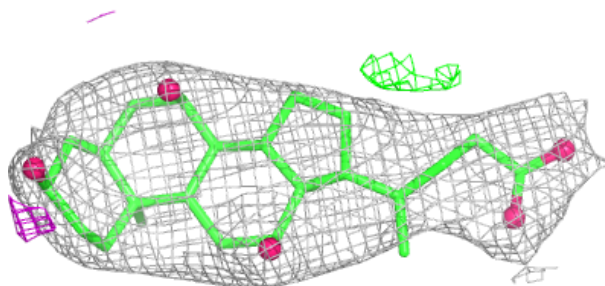


Electron density around CHD C 304:

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

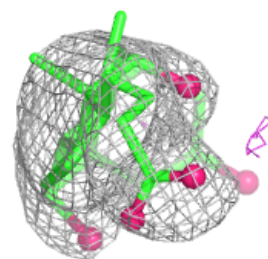
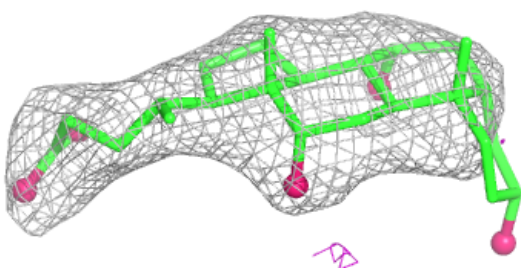
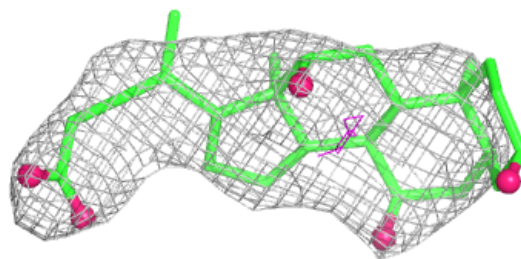
**Electron density around CHD P 305:**

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

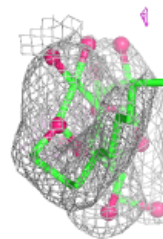
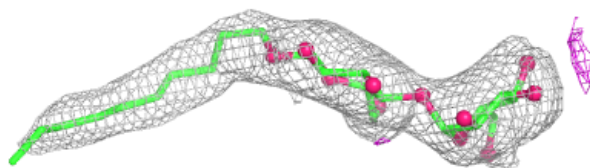


Electron density around CHD J 101:

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

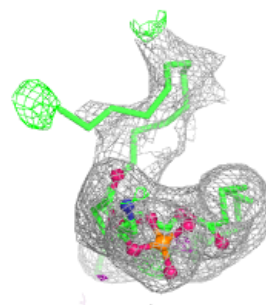
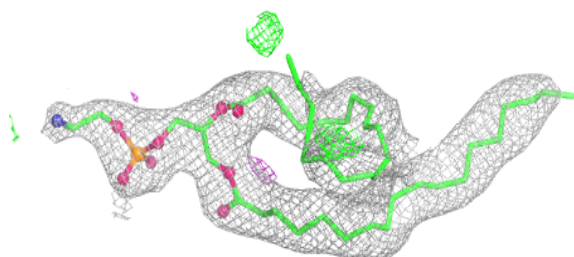
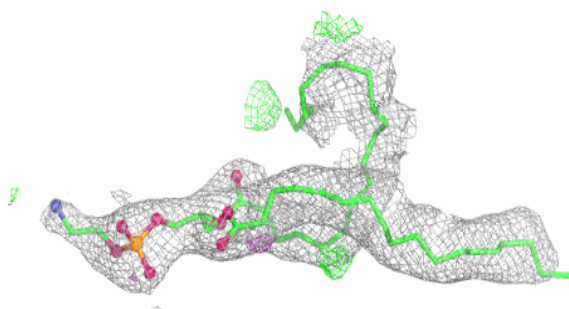
**Electron density around DMU M 101:**

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

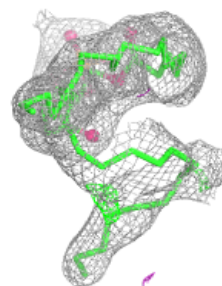
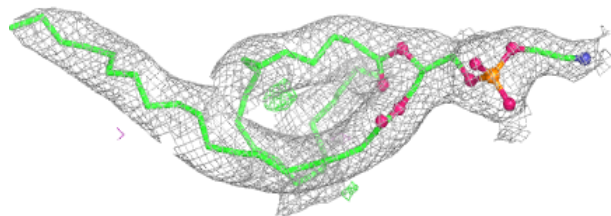
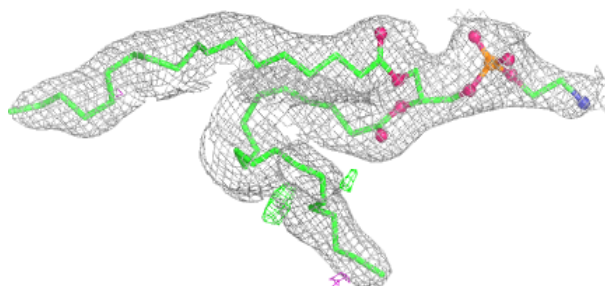


Electron density around PEK P 302:

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

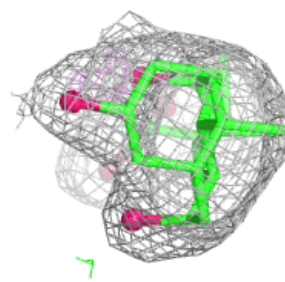
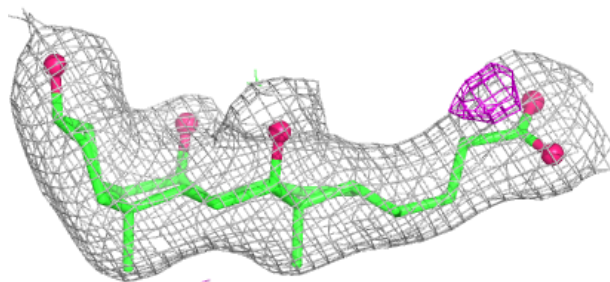
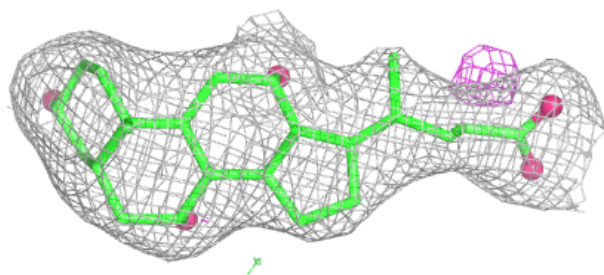
**Electron density around PEK G 101:**

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

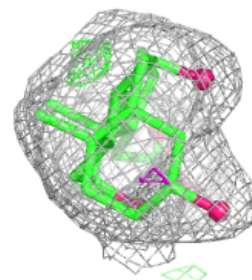
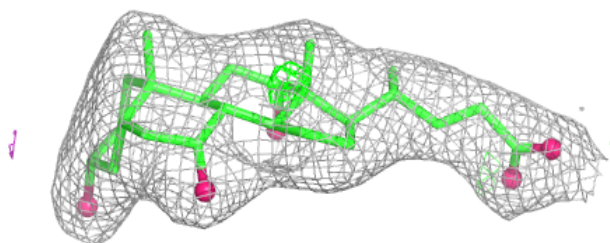
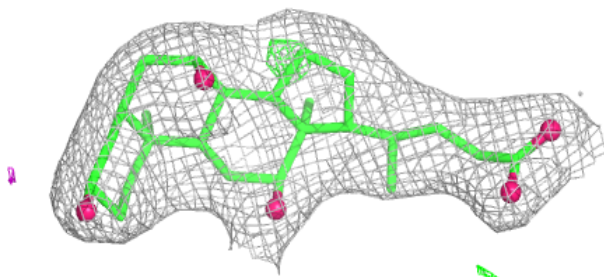


Electron density around CHD B 302:

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

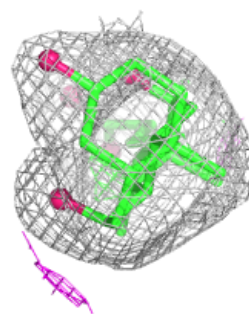
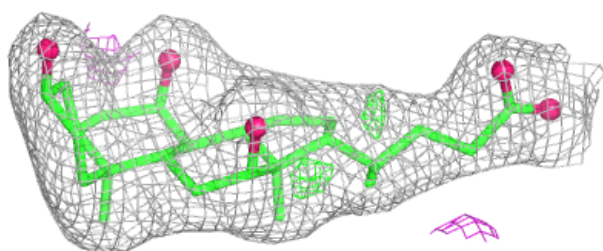
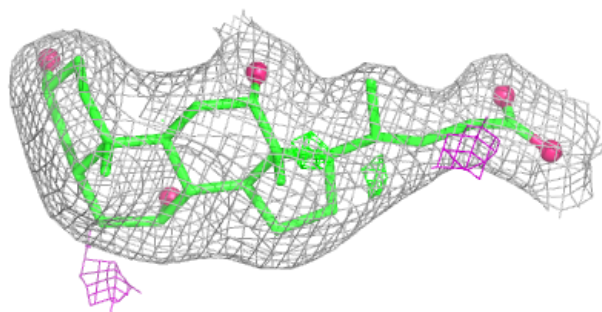
**Electron density around CHD P 306:**

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

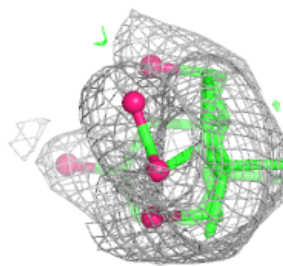
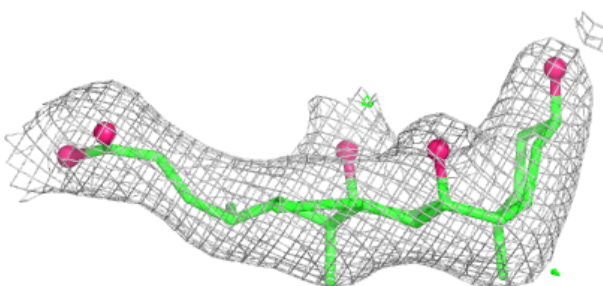
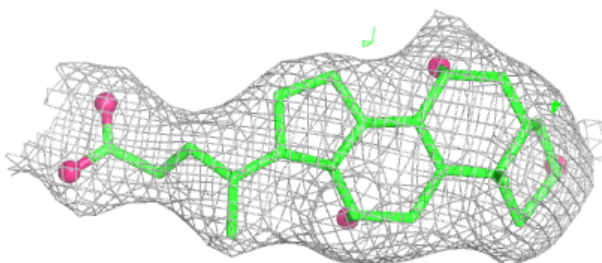


Electron density around CHD C 305:

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

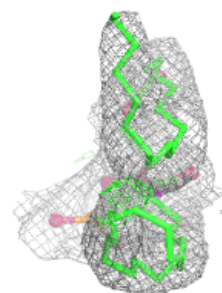
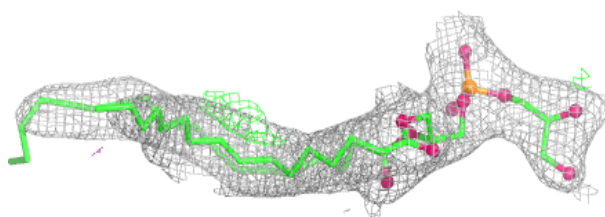
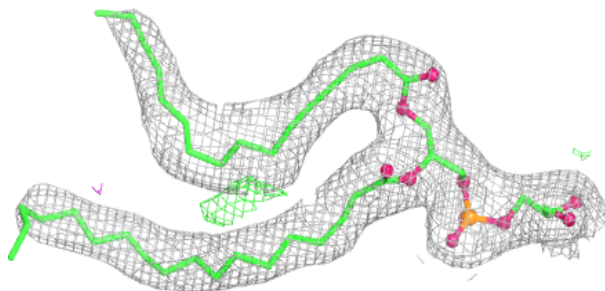
**Electron density around CHD O 302:**

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

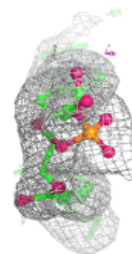
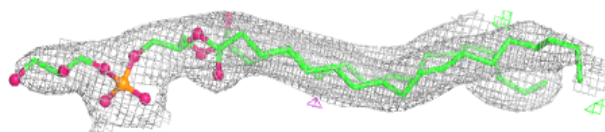
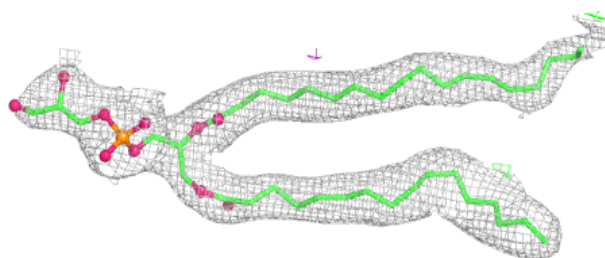


Electron density around PGV N 608:

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

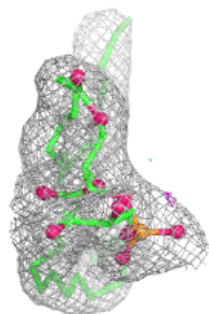
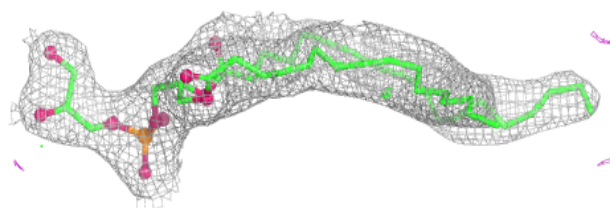
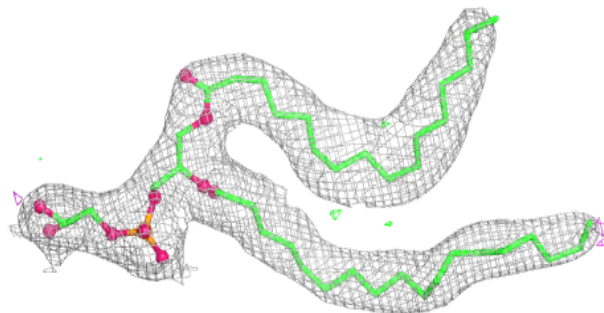
**Electron density around PGV P 303:**

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

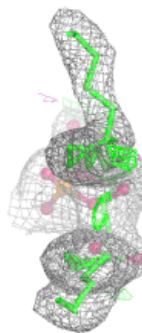
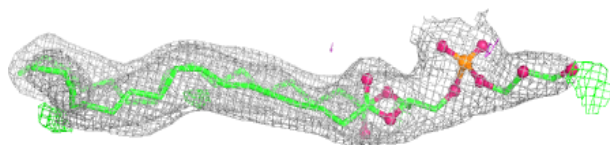
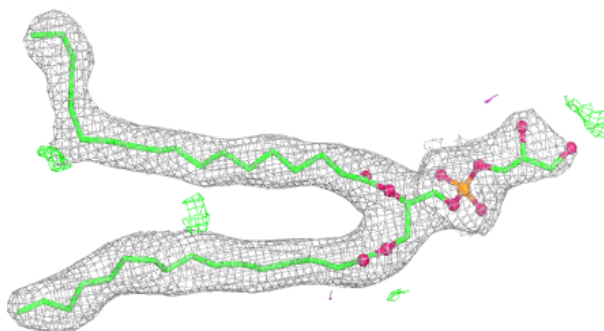


Electron density around PGV A 608:

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

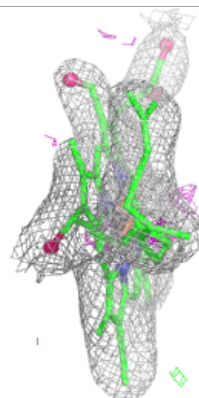
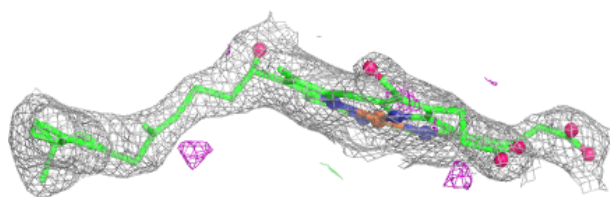
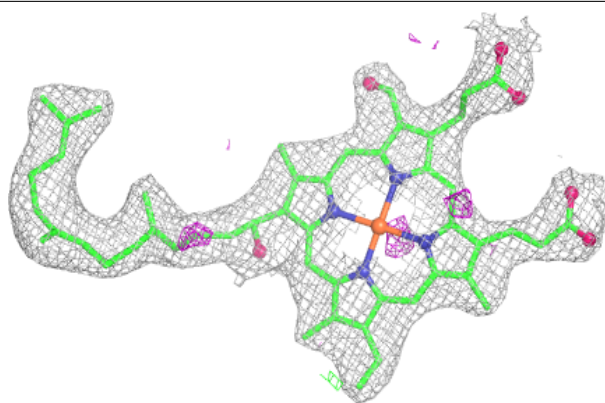
**Electron density around PGV C 302:**

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

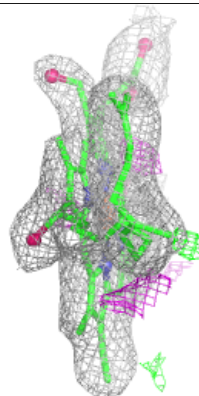
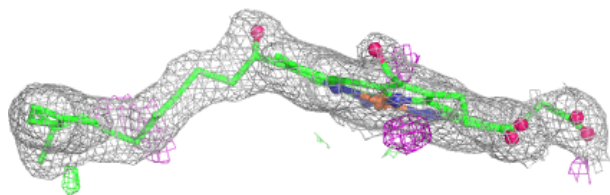
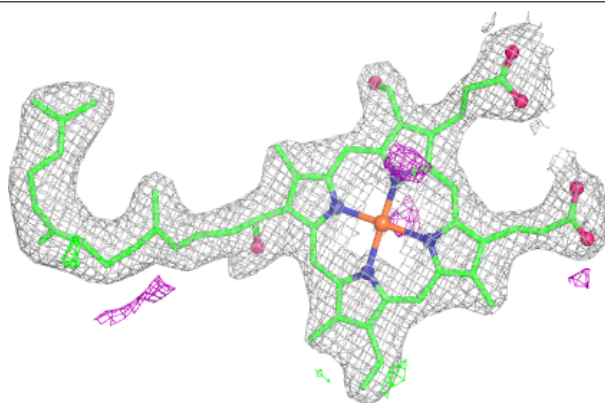


Electron density around HEA N 602:

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

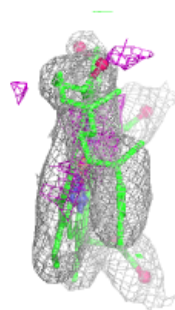
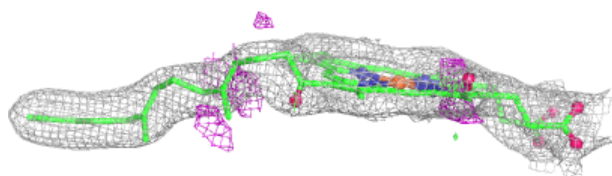
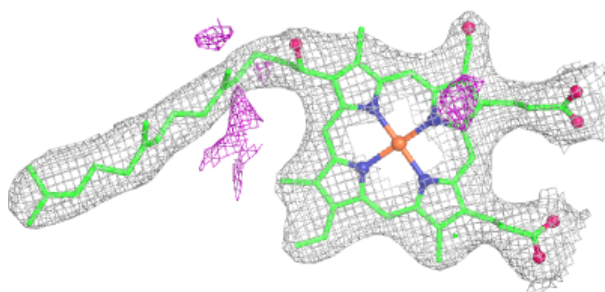
**Electron density around HEA A 602:**

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

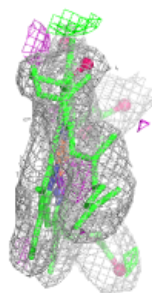
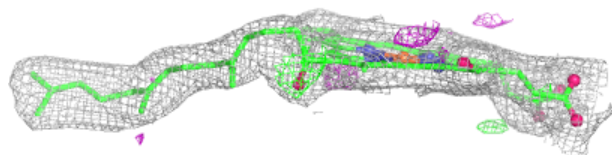
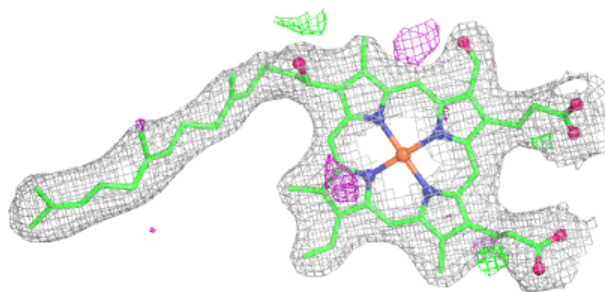


Electron density around HEA N 601:

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

**Electron density around HEA A 601:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.