



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 12:40 PM UTC

PDB ID : 3WG7 / pdb_00003wg7
Title : A 1.9 angstrom radiation damage free X-ray structure of large (420KDa) protein by femtosecond crystallography
Authors : Hirata, K.; Shinzawa-Itoh, K.; Yano, N.; Takemura, S.; Kato, K.; Hatanaka, M.; Muramoto, K.; Kawahara, T.; Tsukihara, T.; Yamashita, E.; Tono, K.; Ueno, G.; Hikima, T.; Murakami, H.; Inubushi, Y.; Yabashi, M.; Ishikawa, T.; Yamamoto, M.; Ogura, T.; Sugimoto, H.; Shen, J.R.; Yoshikawa, S.; Ago, H.
Deposited on : 2013-07-29
Resolution : 1.90 Å(reported)

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

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

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	:	2022.3.0, CSD as543be (2022)
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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)

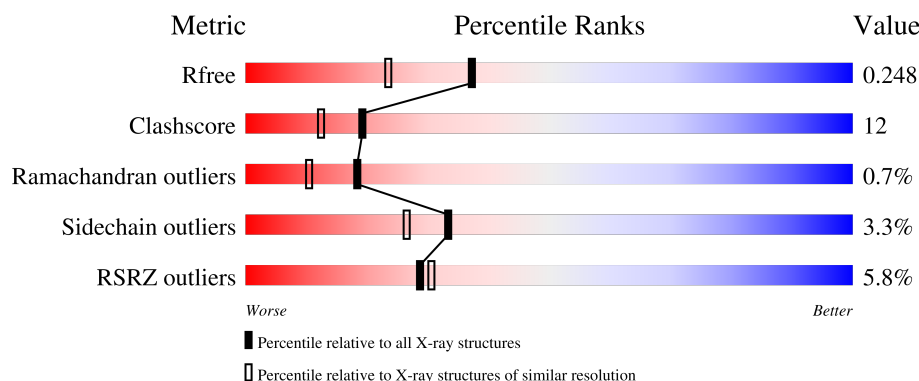
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
2	O	227	
3	C	261	
3	P	261	
4	D	147	
4	Q	147	
5	E	109	
5	R	109	
6	F	98	
6	S	98	
7	G	85	
7	T	85	
8	H	85	
8	U	85	
9	I	73	
9	V	73	
10	J	59	
10	W	59	
11	K	56	
11	X	56	
12	L	47	
12	Y	47	
13	M	46	
13	Z	46	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FME	O	1	-	-	X	-
23	PSC	N	610	-	-	X	-
25	CDL	C	304	-	-	X	-
25	CDL	G	101	-	-	X	-
25	CDL	T	102	-	-	X	-
27	DMU	M	101	X	-	-	-
27	DMU	Z	101	X	-	-	-

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 33302 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	6	0
			4074	2725	629	684	36			
1	N	514	Total	C	N	O	S	0	6	0
			4074	2725	629	684	36			

- 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	1	0
			1832	1189	282	343	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	3	0
			2134	1427	339	353	15			
3	P	259	Total	C	N	O	S	0	3	0
			2134	1427	339	353	15			

- 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			

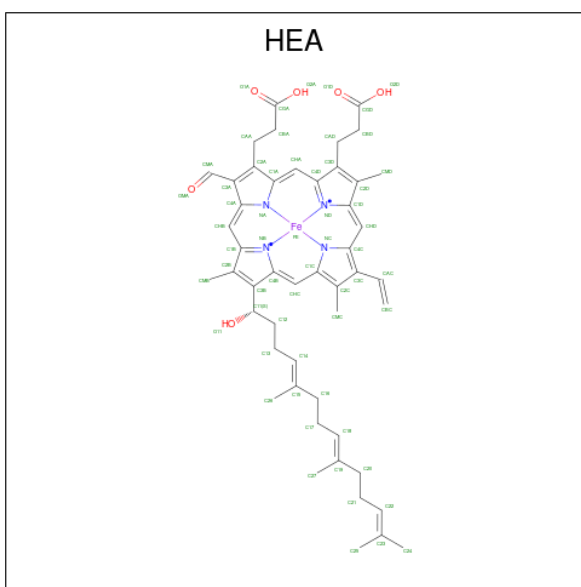
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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		

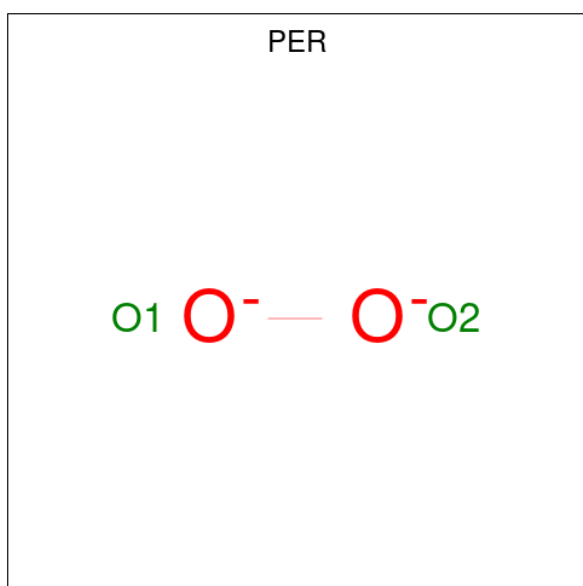
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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).

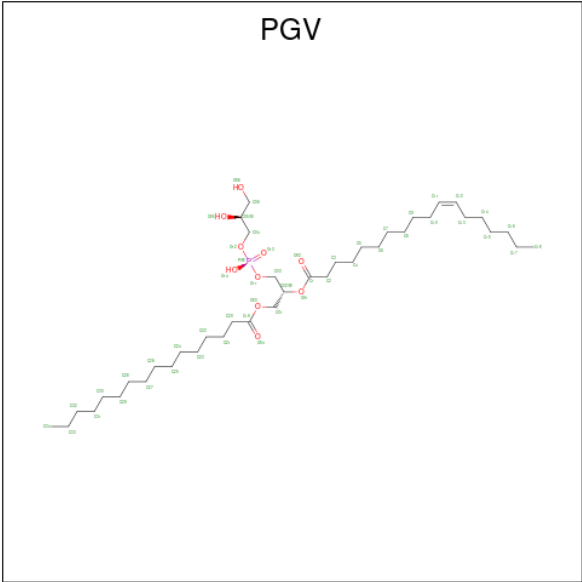
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Na 1 1	0	0
17	C	1	Total Na 1 1	0	0
17	N	1	Total Na 1 1	0	0
17	P	1	Total Na 1 1	0	0

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



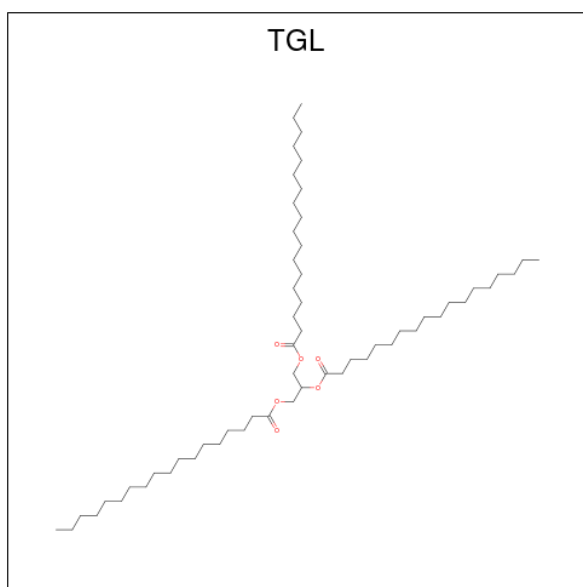
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total O 4 4	0	1
18	N	1	Total O 4 4	0	1

- 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).



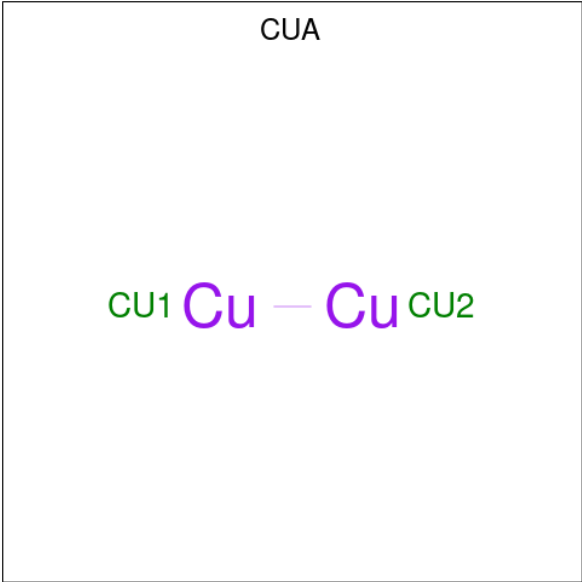
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	P	1	Total	C	O	P	0	0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



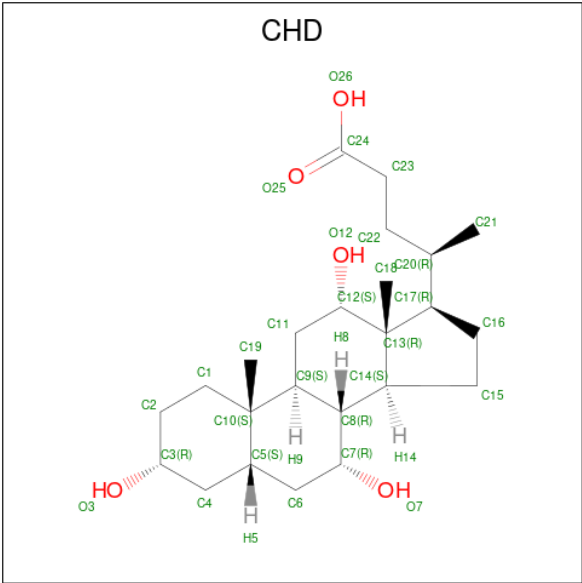
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	B	1	Total	C	O	0	0
			63	57	6		
20	D	1	Total	C	O	0	0
			63	57	6		
20	L	1	Total	C	O	0	0
			63	57	6		
20	N	1	Total	C	O	0	0
			63	57	6		
20	Q	1	Total	C	O	0	0
			63	57	6		
20	Y	1	Total	C	O	0	0
			63	57	6		

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



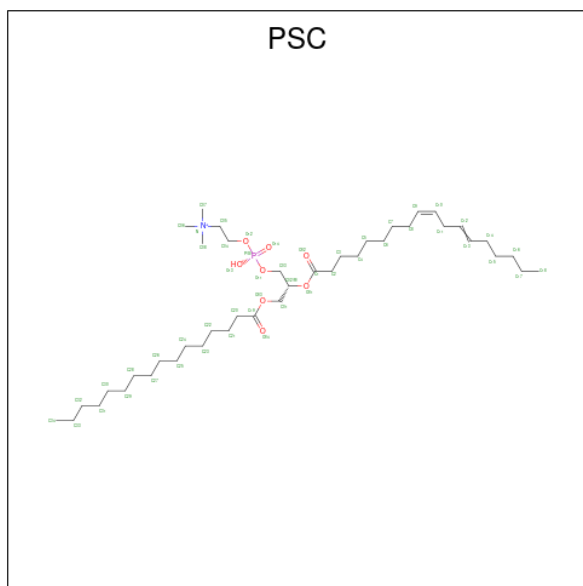
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	B	1	Total	C	O	0	0
			29	24	5		
22	C	1	Total	C	O	0	0
			29	24	5		

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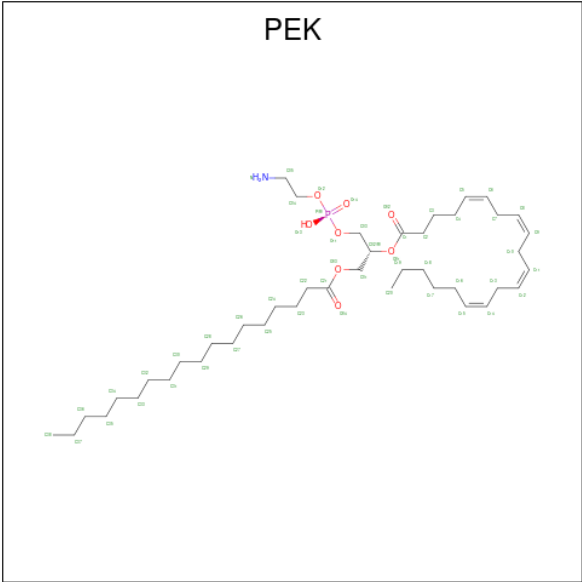
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	C	1	Total	C	O	0	0
			29	24	5		
22	G	1	Total	C	O	0	0
			29	24	5		
22	J	1	Total	C	O	0	0
			29	24	5		
22	P	1	Total	C	O	0	0
			29	24	5		
22	P	1	Total	C	O	0	0
			29	24	5		
22	W	1	Total	C	O	0	0
			29	24	5		

- Molecule 23 is (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: $C_{42}H_{81}NO_8P$).



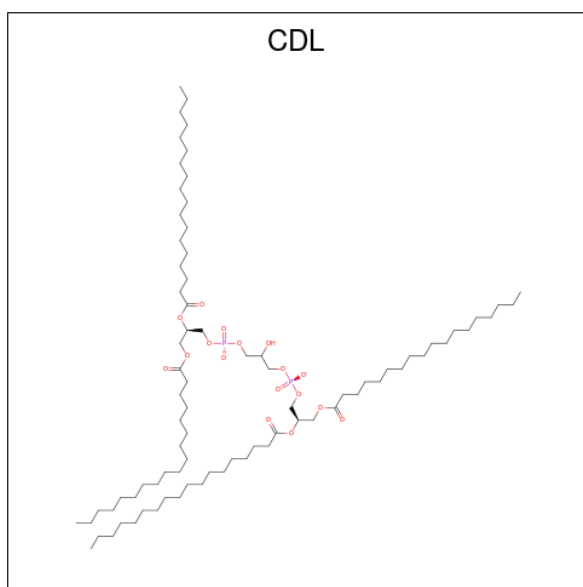
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
23	N	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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

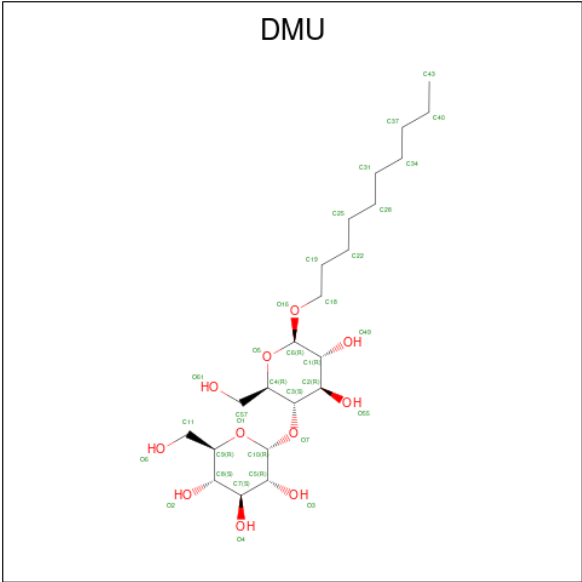


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	C	1	Total	C	O	P	0	0
			100	81	17	2		
25	G	1	Total	C	O	P	0	0
			100	81	17	2		
25	P	1	Total	C	O	P	0	0
			100	81	17	2		
25	T	1	Total	C	O	P	0	0
			100	81	17	2		

- 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	M	1	Total	C	O	0	0
			33	22	11		
27	Z	1	Total	C	O	0	0
			33	22	11		

- Molecule 28 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	265	Total	O	0	0
			265	265		
28	B	194	Total	O	0	0
			194	194		
28	C	141	Total	O	0	0
			141	141		
28	D	160	Total	O	0	0
			160	160		
28	E	125	Total	O	0	0
			125	125		
28	F	112	Total	O	0	0
			112	112		
28	G	70	Total	O	0	0
			70	70		
28	H	70	Total	O	0	0
			70	70		
28	I	52	Total	O	0	0
			52	52		
28	J	31	Total	O	0	0
			31	31		

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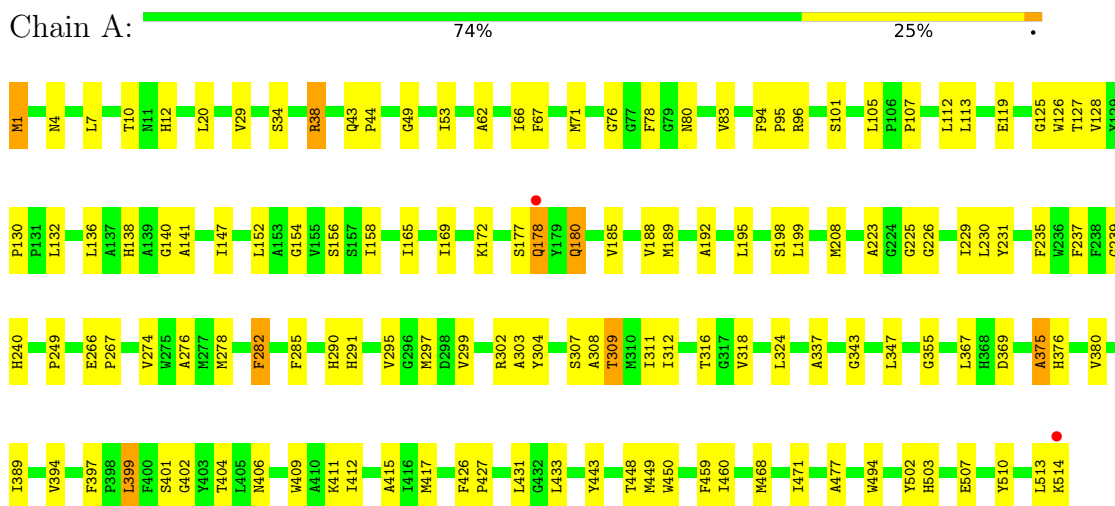
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	K	40	Total 40	O 40	0	0
28	L	31	Total 31	O 31	0	0
28	M	31	Total 31	O 31	0	0
28	N	259	Total 259	O 259	0	0
28	O	157	Total 157	O 157	0	0
28	P	143	Total 143	O 143	0	0
28	Q	90	Total 90	O 90	0	0
28	R	103	Total 103	O 103	0	0
28	S	122	Total 122	O 122	0	0
28	T	56	Total 56	O 56	0	0
28	U	51	Total 51	O 51	0	0
28	V	42	Total 42	O 42	0	0
28	W	38	Total 38	O 38	0	0
28	X	34	Total 34	O 34	0	0
28	Y	37	Total 37	O 37	0	0
28	Z	24	Total 24	O 24	0	0

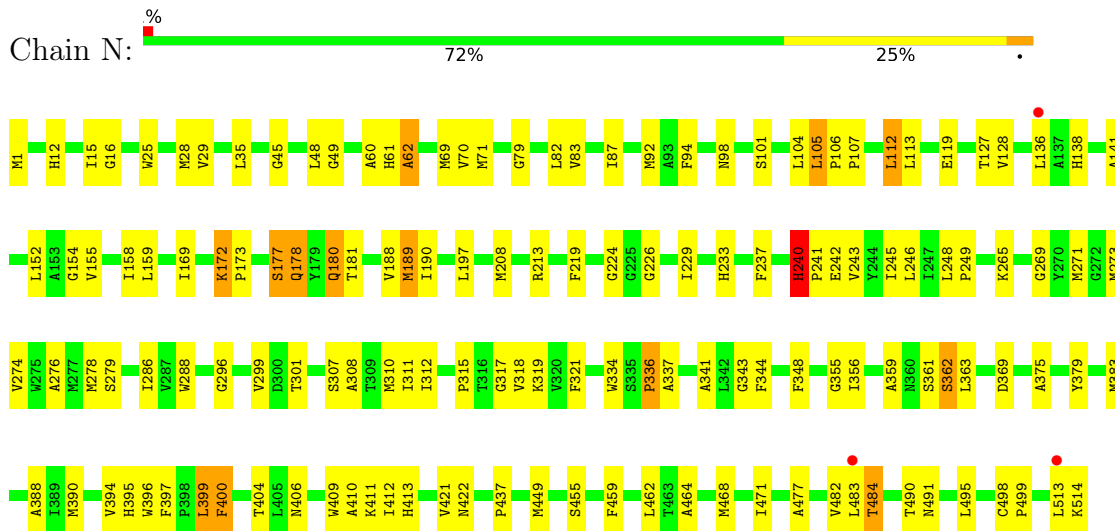
3 Residue-property plots

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

• Molecule 1: Cytochrome c oxidase subunit 1

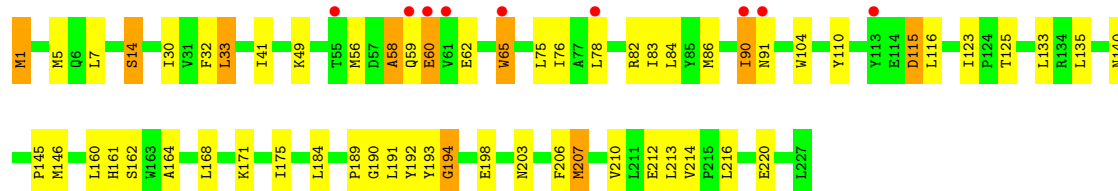


• Molecule 1: Cytochrome c oxidase subunit 1

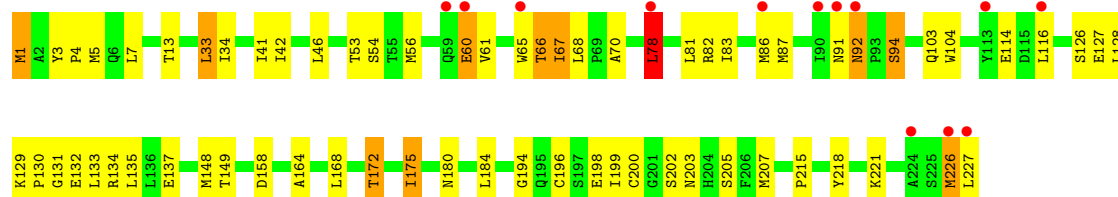


• Molecule 2: Cytochrome c oxidase subunit 2

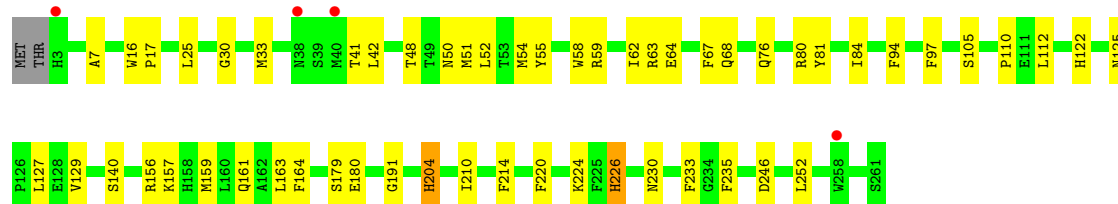
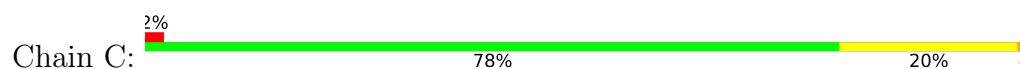




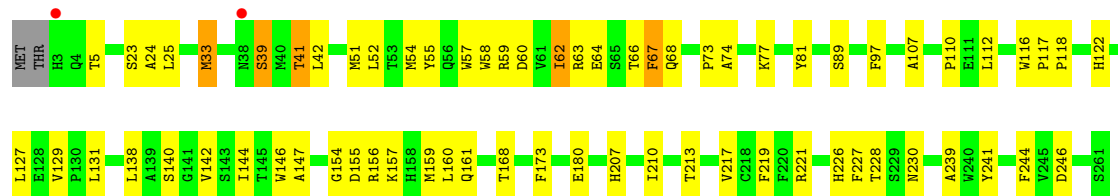
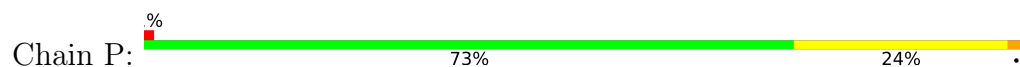
• Molecule 2: Cytochrome c oxidase subunit 2



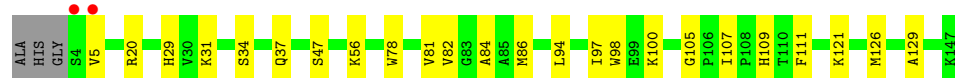
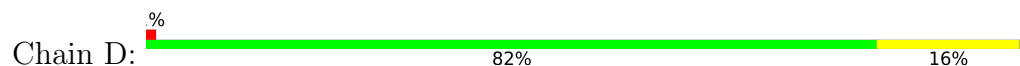
• Molecule 3: Cytochrome c oxidase subunit 3



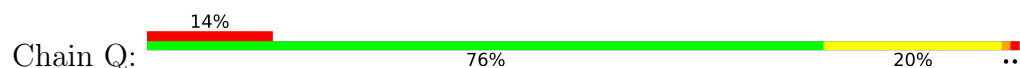
• Molecule 3: Cytochrome c oxidase subunit 3

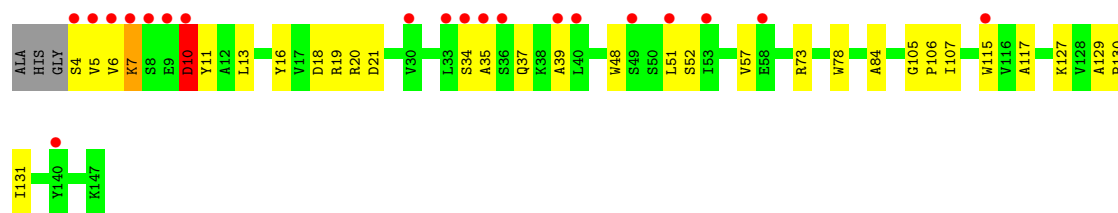


• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

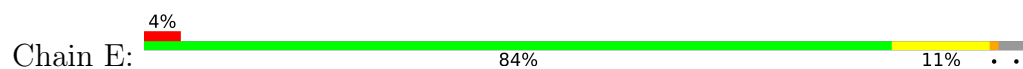


• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

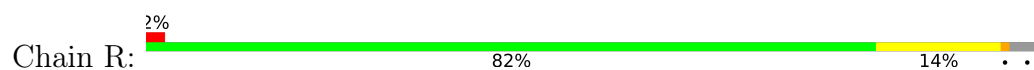




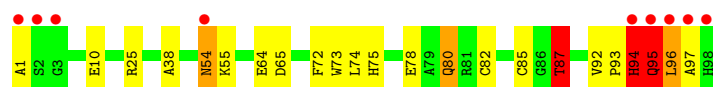
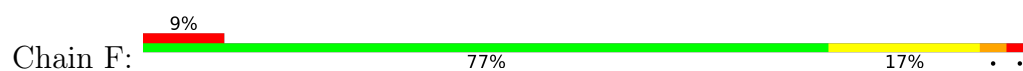
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



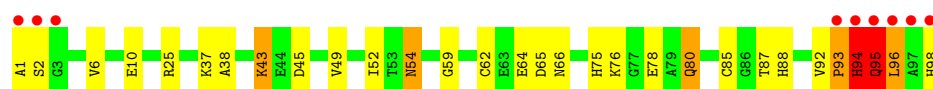
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



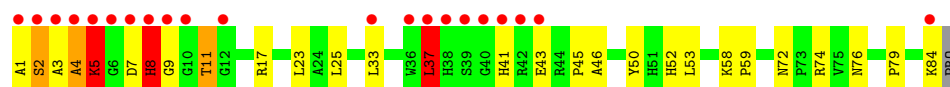
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



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

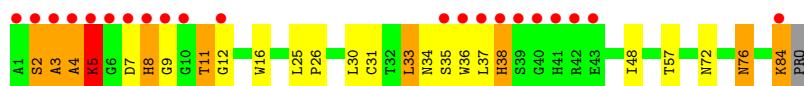


- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

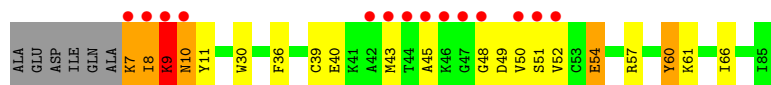


- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

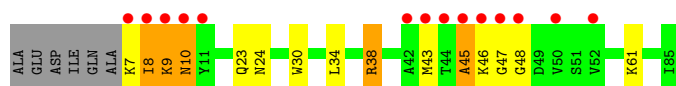
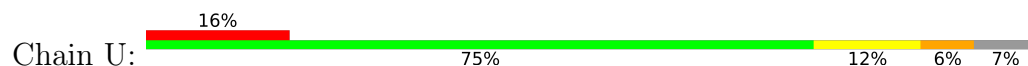




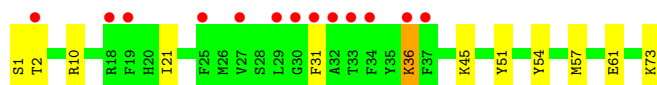
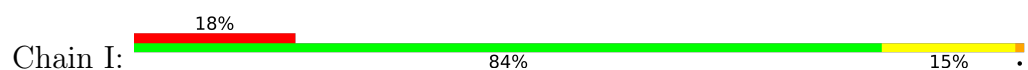
• Molecule 8: Cytochrome c oxidase subunit 6B1



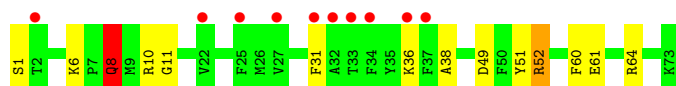
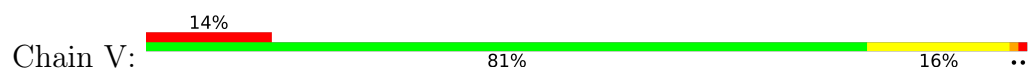
• Molecule 8: Cytochrome c oxidase subunit 6B1



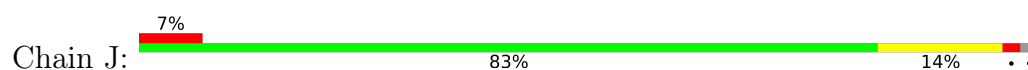
• Molecule 9: Cytochrome c oxidase subunit 6C



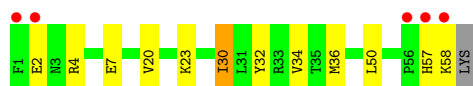
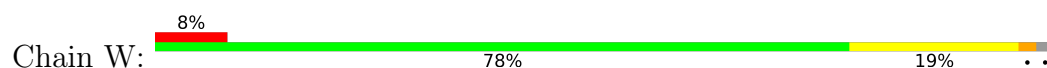
• Molecule 9: Cytochrome c oxidase subunit 6C



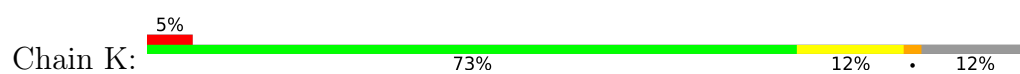
• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



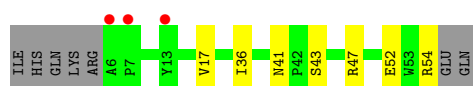
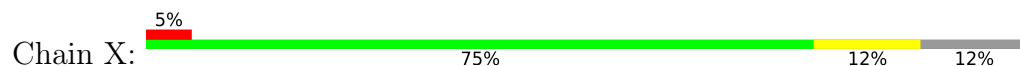
• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



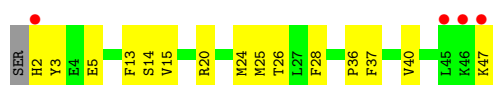
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



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



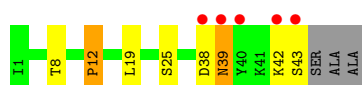
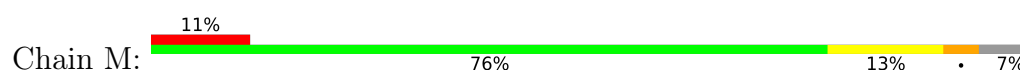
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



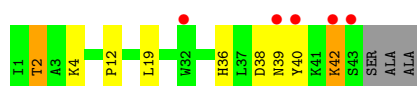
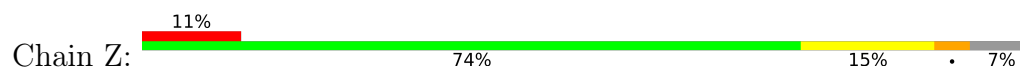
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	182.60Å 204.51Å 178.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.90 40.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.0 (40.00-1.90) 96.0 (40.00-1.90)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.8.0048	Depositor
R, R_{free}	0.195 , 0.230 0.218 , 0.248	Depositor DCC
R_{free} test set	25229 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å ²)	24.9	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 66.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.011 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	33302	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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: PGV, TGL, HEA, PEK, CUA, PSC, CU, TPO, DMU, CDL, PER, NA, CHD, MG, SAC, ZN, FME

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	1.84	57/4203 (1.4%)	1.44	35/5742 (0.6%)
1	N	1.76	62/4203 (1.5%)	1.43	38/5742 (0.7%)
2	B	1.56	10/1868 (0.5%)	1.37	6/2545 (0.2%)
2	O	1.45	16/1860 (0.9%)	1.28	9/2534 (0.4%)
3	C	1.63	15/2221 (0.7%)	1.28	10/3035 (0.3%)
3	P	1.62	21/2221 (0.9%)	1.28	7/3035 (0.2%)
4	D	1.50	6/1229 (0.5%)	1.32	10/1658 (0.6%)
4	Q	1.21	2/1229 (0.2%)	1.21	8/1658 (0.5%)
5	E	1.53	2/871 (0.2%)	1.23	2/1182 (0.2%)
5	R	1.25	1/871 (0.1%)	1.19	0/1182
6	F	1.47	2/765 (0.3%)	1.33	2/1038 (0.2%)
6	S	1.57	3/765 (0.4%)	1.34	3/1038 (0.3%)
7	G	1.46	4/690 (0.6%)	1.32	6/937 (0.6%)
7	T	1.44	3/690 (0.4%)	1.32	5/937 (0.5%)
8	H	1.40	0/682	1.27	3/921 (0.3%)
8	U	1.26	1/682 (0.1%)	1.21	1/921 (0.1%)
9	I	1.20	0/605	1.26	1/802 (0.1%)
9	V	1.12	1/605 (0.2%)	1.31	2/802 (0.2%)
10	J	1.31	0/471	1.26	1/636 (0.2%)
10	W	1.30	1/471 (0.2%)	1.29	1/636 (0.2%)
11	K	1.43	0/398	1.30	2/546 (0.4%)
11	X	1.27	3/398 (0.8%)	1.23	1/546 (0.2%)
12	L	1.56	5/393 (1.3%)	1.43	3/526 (0.6%)
12	Y	1.45	3/393 (0.8%)	1.27	4/526 (0.8%)
13	M	1.50	1/345 (0.3%)	1.26	0/470
13	Z	1.36	0/345	1.16	0/470
All	All	1.57	219/29474 (0.7%)	1.33	160/40065 (0.4%)

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
1	N	0	1
6	F	0	1
6	S	0	1
8	H	0	1
10	J	0	1
10	W	0	1
All	All	0	6

The worst 5 of 219 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	83	VAL	CA-CB	9.91	1.59	1.54
1	N	337	ALA	N-CA	9.89	1.58	1.46
1	A	404	THR	C-O	9.76	1.35	1.23
1	A	154	GLY	N-CA	9.64	1.57	1.45
1	N	288	TRP	N-CA	9.30	1.58	1.46

The worst 5 of 160 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	240	HIS	N-CA-CB	8.84	120.85	110.42
1	N	319	LYS	N-CA-C	-8.36	102.11	111.14
1	N	105	LEU	CA-C-N	-8.19	111.95	120.38
1	N	105	LEU	C-N-CA	-8.19	111.95	120.38
1	N	141	ALA	N-CA-C	8.14	122.47	112.54

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	F	93	PRO	Peptide
8	H	9	LYS	Peptide
10	J	57	HIS	Peptide
1	N	240	HIS	Sidechain
6	S	93	PRO	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4074	0	4058	60	0
1	N	4074	0	4058	80	0
2	B	1832	0	1836	38	0
2	O	1824	0	1833	53	2
3	C	2134	0	2051	41	0
3	P	2134	0	2051	52	0
4	D	1195	0	1183	16	0
4	Q	1195	0	1183	31	0
5	E	852	0	845	7	0
5	R	852	0	845	11	2
6	F	748	0	728	16	1
6	S	748	0	728	37	7
7	G	675	0	643	30	0
7	T	675	0	643	34	0
8	H	662	0	623	22	0
8	U	662	0	623	11	0
9	I	601	0	613	8	2
9	V	601	0	613	9	0
10	J	460	0	459	9	0
10	W	460	0	459	8	0
11	K	384	0	366	7	0
11	X	384	0	366	4	0
12	L	380	0	380	14	0
12	Y	380	0	380	17	0
13	M	335	0	352	10	0
13	Z	335	0	352	11	0
14	A	120	0	108	10	0
14	N	120	0	108	8	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	C	1	0	0	1	0
17	N	1	0	0	0	0
17	P	1	0	0	0	0
18	A	4	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	N	4	0	0	1	0
19	A	102	0	152	10	0
19	C	102	0	152	6	0
19	N	102	0	152	16	0
19	P	102	0	152	11	0
20	B	63	0	110	3	0
20	D	63	0	110	13	0
20	L	63	0	110	12	0
20	N	63	0	110	4	0
20	Q	63	0	110	11	0
20	Y	63	0	110	17	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	29	0	39	1	0
22	C	58	0	78	4	0
22	G	29	0	39	0	0
22	J	29	0	39	5	0
22	P	58	0	78	5	0
22	W	29	0	38	5	0
23	B	52	0	80	13	0
23	N	52	0	80	21	0
24	C	106	0	154	23	0
24	G	53	0	77	6	0
24	P	106	0	154	22	0
24	T	53	0	77	12	0
25	C	100	0	156	23	0
25	G	100	0	156	37	0
25	P	100	0	156	18	0
25	T	100	0	156	29	0
26	F	1	0	0	0	0
26	S	1	0	0	0	0
27	M	33	0	42	1	0
27	Z	33	0	42	0	0
28	A	265	0	0	10	0
28	B	194	0	0	10	2
28	C	141	0	0	8	0
28	D	160	0	0	1	1
28	E	125	0	0	3	0
28	F	112	0	0	2	1
28	G	70	0	0	7	0
28	H	70	0	0	5	0
28	I	52	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	J	31	0	0	2	0
28	K	40	0	0	3	1
28	L	31	0	0	1	0
28	M	31	0	0	1	2
28	N	259	0	0	12	0
28	O	157	0	0	11	6
28	P	143	0	0	8	0
28	Q	90	0	0	5	0
28	R	103	0	0	3	0
28	S	122	0	0	7	1
28	T	56	0	0	2	0
28	U	51	0	0	2	0
28	V	42	0	0	5	0
28	W	38	0	0	2	0
28	X	34	0	0	3	0
28	Y	37	0	0	4	0
28	Z	24	0	0	1	0
All	All	33302	0	31396	727	14

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 12.

The worst 5 of 727 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)
6:S:76:LYS:CE	6:S:93:PRO:HG2	1.47	1.41
6:S:43:LYS:H	6:S:43:LYS:CD	1.28	1.39
6:S:43:LYS:HD3	6:S:43:LYS:N	1.33	1.29
6:S:76:LYS:HD3	28:S:271:HOH:O	1.36	1.25
18:A:606[A]:PER:O2	18:A:606[A]:PER:O1	1.55	1.22

The worst 5 of 14 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:F:294:HOH:O	28:K:114:HOH:O[2_585]	1.63	0.57
9:I:2:THR:CG2	5:R:80:GLU:OE1[3_647]	1.83	0.37
28:B:586:HOH:O	28:M:2318:HOH:O[2_584]	1.90	0.30
2:O:126:SER:O	6:S:94:HIS:CB[2_684]	1.93	0.27
6:S:95:GLN:N	28:O:535:HOH:O[2_685]	1.95	0.25

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	518/514 (101%)	500 (96%)	18 (4%)	0	100	100
1	N	518/514 (101%)	501 (97%)	17 (3%)	0	100	100
2	B	226/227 (100%)	213 (94%)	13 (6%)	0	100	100
2	O	225/227 (99%)	214 (95%)	10 (4%)	1 (0%)	30	22
3	C	260/261 (100%)	254 (98%)	6 (2%)	0	100	100
3	P	260/261 (100%)	255 (98%)	5 (2%)	0	100	100
4	D	142/147 (97%)	138 (97%)	4 (3%)	0	100	100
4	Q	142/147 (97%)	136 (96%)	5 (4%)	1 (1%)	18	10
5	E	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
5	R	103/109 (94%)	103 (100%)	0	0	100	100
6	F	96/98 (98%)	91 (95%)	2 (2%)	3 (3%)	3	0
6	S	96/98 (98%)	90 (94%)	3 (3%)	3 (3%)	3	0
7	G	81/85 (95%)	69 (85%)	7 (9%)	5 (6%)	1	0
7	T	81/85 (95%)	68 (84%)	8 (10%)	5 (6%)	1	0
8	H	77/85 (91%)	71 (92%)	3 (4%)	3 (4%)	2	0
8	U	77/85 (91%)	70 (91%)	4 (5%)	3 (4%)	2	0
9	I	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
9	V	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
10	J	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
10	W	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
11	K	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
11	X	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
12	L	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
12	Y	44/47 (94%)	41 (93%)	3 (7%)	0	100	100
13	M	41/46 (89%)	38 (93%)	3 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	Z	41/46 (89%)	39 (95%)	2 (5%)	0	100	100
All	All	3523/3614 (98%)	3376 (96%)	123 (4%)	24 (1%)	18	10

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	94	HIS
6	F	96	LEU
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	432/426 (101%)	425 (98%)	7 (2%)	55	54
1	N	432/426 (101%)	423 (98%)	9 (2%)	47	44
2	B	211/210 (100%)	198 (94%)	13 (6%)	16	9
2	O	210/210 (100%)	203 (97%)	7 (3%)	33	26
3	C	227/226 (100%)	223 (98%)	4 (2%)	51	50
3	P	227/226 (100%)	222 (98%)	5 (2%)	45	42
4	D	128/129 (99%)	127 (99%)	1 (1%)	73	75
4	Q	128/129 (99%)	123 (96%)	5 (4%)	28	21
5	E	92/95 (97%)	89 (97%)	3 (3%)	33	26
5	R	92/95 (97%)	88 (96%)	4 (4%)	26	18
6	F	81/81 (100%)	75 (93%)	6 (7%)	13	6
6	S	81/81 (100%)	76 (94%)	5 (6%)	16	9
7	G	67/68 (98%)	63 (94%)	4 (6%)	17	9
7	T	67/68 (98%)	60 (90%)	7 (10%)	7	2
8	H	71/75 (95%)	66 (93%)	5 (7%)	14	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	U	71/75 (95%)	69 (97%)	2 (3%)	38	32
9	I	57/57 (100%)	56 (98%)	1 (2%)	51	50
9	V	57/57 (100%)	54 (95%)	3 (5%)	20	12
10	J	49/50 (98%)	49 (100%)	0	100	100
10	W	49/50 (98%)	48 (98%)	1 (2%)	48	46
11	K	39/46 (85%)	38 (97%)	1 (3%)	40	35
11	X	39/46 (85%)	39 (100%)	0	100	100
12	L	39/40 (98%)	38 (97%)	1 (3%)	40	35
12	Y	39/40 (98%)	36 (92%)	3 (8%)	12	5
13	M	37/38 (97%)	34 (92%)	3 (8%)	11	5
13	Z	37/38 (97%)	34 (92%)	3 (8%)	11	5
All	All	3059/3082 (99%)	2956 (97%)	103 (3%)	33	25

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

Mol	Chain	Res	Type
1	N	495	LEU
4	Q	5	VAL
12	Y	26	THR
2	O	60	GLU
3	P	33[A]	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
10	J	29	ASN
2	O	91	ASN
8	U	37	HIS
10	J	57	HIS
1	N	180	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FME	B	1	2	8,9,10	1.39	1 (12%)	8,9,11	7.58	4 (50%)
7	TPO	G	11	7	8,10,11	1.67	2 (25%)	10,14,16	1.56	2 (20%)
7	TPO	T	11	7	8,10,11	1.77	1 (12%)	10,14,16	1.33	1 (10%)
1	FME	A	1	1	8,9,10	0.50	0	8,9,11	1.39	1 (12%)
9	SAC	V	1	9	7,8,9	2.22	2 (28%)	7,9,11	1.40	1 (14%)
1	FME	N	1	1	8,9,10	0.88	0	8,9,11	1.48	2 (25%)
2	FME	O	1	2	8,9,10	0.97	0	8,9,11	1.92	3 (37%)
9	SAC	I	1	9	7,8,9	2.29	2 (28%)	7,9,11	1.31	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FME	B	1	2	-	2/7/9/11	-
7	TPO	G	11	7	-	7/9/11/13	-
7	TPO	T	11	7	-	3/9/11/13	-
1	FME	A	1	1	-	2/7/9/11	-
9	SAC	V	1	9	-	5/7/8/10	-
1	FME	N	1	1	-	2/7/9/11	-
2	FME	O	1	2	-	2/7/9/11	-
9	SAC	I	1	9	-	1/7/8/10	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	1	SAC	OAC-C1A	5.14	1.34	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	V	1	SAC	OAC-C1A	4.87	1.34	1.23
7	T	11	TPO	P-O1P	3.48	1.61	1.50
9	V	1	SAC	CA-N	3.04	1.51	1.46
7	G	11	TPO	P-O1P	2.82	1.59	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CA-N-CN	-20.41	91.43	122.82
2	B	1	FME	O1-CN-N	4.73	137.52	125.32
7	T	11	TPO	CG2-CB-CA	3.19	119.47	113.26
2	O	1	FME	O1-CN-N	-3.02	117.51	125.32
2	B	1	FME	O-C-CA	-2.95	117.18	124.77

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

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

There are no ring outliers.

5 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	FME	2	0
7	G	11	TPO	1	0
7	T	11	TPO	3	0
1	A	1	FME	3	0
2	O	1	FME	9	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 56 ligands modelled in this entry, 10 are monoatomic - leaving 46 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
24	PEK	P	303	-	52,52,52	1.09	3 (5%)	55,57,57	1.39	6 (10%)
23	PSC	N	610	-	51,51,51	1.25	3 (5%)	57,59,59	1.27	4 (7%)
19	PGV	P	301	-	50,50,50	1.07	2 (4%)	53,56,56	1.21	5 (9%)
24	PEK	C	302	-	52,52,52	1.00	2 (3%)	55,57,57	1.10	6 (10%)
27	DMU	Z	101	-	34,34,34	0.74	1 (2%)	45,45,45	1.83	12 (26%)
14	HEA	N	602	18,1	67,67,67	2.12	22 (32%)	81,103,103	1.76	28 (34%)
14	HEA	A	602	18,1	67,67,67	2.44	26 (38%)	81,103,103	2.23	25 (30%)
20	TGL	Q	201	-	62,62,62	1.60	7 (11%)	65,65,65	1.33	11 (16%)
18	PER	A	606[B]	15	1,1,1	0.88	0	-		
21	CUA	B	302	2	0,1,1	-	-	-		
19	PGV	N	607	-	50,50,50	1.03	2 (4%)	53,56,56	1.32	8 (15%)
14	HEA	N	601	1	67,67,67	2.11	19 (28%)	81,103,103	1.81	22 (27%)
24	PEK	T	101	-	52,52,52	1.05	2 (3%)	55,57,57	1.24	4 (7%)
22	CHD	W	101	-	32,32,32	0.83	0	51,51,51	3.06	17 (33%)
18	PER	A	606[A]	15,14	1,1,1	0.90	0	-		
19	PGV	A	608	-	50,50,50	1.23	2 (4%)	53,56,56	1.44	6 (11%)
19	PGV	C	308	-	50,50,50	1.19	2 (4%)	53,56,56	1.22	4 (7%)
19	PGV	C	303	-	50,50,50	0.96	2 (4%)	53,56,56	1.40	7 (13%)
20	TGL	B	301	-	62,62,62	1.36	6 (9%)	65,65,65	1.68	11 (16%)
22	CHD	B	303	-	32,32,32	1.45	4 (12%)	51,51,51	1.92	13 (25%)
27	DMU	M	101	-	34,34,34	0.67	0	45,45,45	2.38	14 (31%)
24	PEK	C	307	-	52,52,52	1.10	2 (3%)	55,57,57	1.20	4 (7%)
20	TGL	L	101	-	62,62,62	1.47	6 (9%)	65,65,65	1.48	10 (15%)
22	CHD	C	306	-	32,32,32	1.20	3 (9%)	51,51,51	1.77	12 (23%)
25	CDL	P	305	-	99,99,99	1.49	15 (15%)	105,111,111	1.40	13 (12%)
19	PGV	P	304	-	50,50,50	0.98	2 (4%)	53,56,56	1.05	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	TGL	N	609	-	62,62,62	1.39	6 (9%)	65,65,65	1.62	9 (13%)
22	CHD	J	101	-	32,32,32	0.71	0	51,51,51	2.59	25 (49%)
25	CDL	G	101	-	99,99,99	1.45	12 (12%)	105,111,111	1.30	9 (8%)
21	CUA	O	301	2	0,1,1	-	-	-	-	-
20	TGL	Y	101	-	62,62,62	1.44	6 (9%)	65,65,65	1.56	11 (16%)
18	PER	N	606[B]	15	1,1,1	0.90	0	-	-	-
24	PEK	G	102	-	52,52,52	1.13	2 (3%)	55,57,57	1.25	6 (10%)
22	CHD	P	307	-	32,32,32	1.33	4 (12%)	51,51,51	1.40	8 (15%)
25	CDL	C	304	-	99,99,99	1.53	16 (16%)	105,111,111	1.51	13 (12%)
19	PGV	A	607	-	50,50,50	1.16	5 (10%)	53,56,56	1.31	5 (9%)
22	CHD	C	305	-	32,32,32	0.81	0	51,51,51	1.99	18 (35%)
22	CHD	G	103	-	32,32,32	1.56	7 (21%)	51,51,51	2.47	18 (35%)
20	TGL	D	201	-	62,62,62	1.60	7 (11%)	65,65,65	1.64	13 (20%)
19	PGV	N	608	-	50,50,50	1.06	2 (4%)	53,56,56	1.51	6 (11%)
24	PEK	P	308	-	52,52,52	1.15	2 (3%)	55,57,57	1.10	4 (7%)
25	CDL	T	102	-	99,99,99	1.45	12 (12%)	105,111,111	1.35	12 (11%)
18	PER	N	606[A]	15,14	1,1,1	0.91	0	-	-	-
23	PSC	B	304	-	51,51,51	1.21	3 (5%)	57,59,59	1.17	4 (7%)
14	HEA	A	601	1	67,67,67	2.54	25 (37%)	81,103,103	2.32	30 (37%)
22	CHD	P	306	-	32,32,32	0.90	1 (3%)	51,51,51	2.45	19 (37%)

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
24	PEK	P	303	-	-	25/56/56/56	-
23	PSC	N	610	-	-	25/55/55/55	-
27	DMU	Z	101	-	2/2/10/10	7/19/59/59	0/2/2/2
19	PGV	P	301	-	-	30/55/55/55	-
24	PEK	C	302	-	-	17/56/56/56	-
14	HEA	N	602	18,1	-	5/36/76/76	-
14	HEA	A	602	18,1	-	7/36/76/76	-
20	TGL	Q	201	-	-	41/65/65/65	-
19	PGV	N	607	-	-	28/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	HEA	N	601	1	-	7/36/76/76	-
24	PEK	T	101	-	-	25/56/56/56	-
22	CHD	W	101	-	-	7/9/74/74	0/4/4/4
19	PGV	A	608	-	-	32/55/55/55	-
19	PGV	C	308	-	-	32/55/55/55	-
19	PGV	C	303	-	-	19/55/55/55	-
20	TGL	B	301	-	-	32/65/65/65	-
22	CHD	B	303	-	-	2/9/74/74	0/4/4/4
27	DMU	M	101	-	2/2/10/10	7/19/59/59	0/2/2/2
24	PEK	C	307	-	-	36/56/56/56	-
20	TGL	L	101	-	-	33/65/65/65	-
22	CHD	C	306	-	-	1/9/74/74	0/4/4/4
25	CDL	P	305	-	-	58/110/110/110	-
19	PGV	P	304	-	-	12/55/55/55	-
20	TGL	N	609	-	-	37/65/65/65	-
22	CHD	J	101	-	-	7/9/74/74	0/4/4/4
25	CDL	G	101	-	-	77/110/110/110	-
20	TGL	Y	101	-	-	39/65/65/65	-
24	PEK	G	102	-	-	29/56/56/56	-
22	CHD	P	307	-	-	2/9/74/74	0/4/4/4
25	CDL	C	304	-	-	62/110/110/110	-
19	PGV	A	607	-	-	9/55/55/55	-
22	CHD	C	305	-	-	6/9/74/74	0/4/4/4
22	CHD	G	103	-	-	2/9/74/74	0/4/4/4
20	TGL	D	201	-	-	38/65/65/65	-
19	PGV	N	608	-	-	12/55/55/55	-
24	PEK	P	308	-	-	36/56/56/56	-
25	CDL	T	102	-	-	65/110/110/110	-
23	PSC	B	304	-	-	34/55/55/55	-
14	HEA	A	601	1	-	8/36/76/76	-
22	CHD	P	306	-	-	8/9/74/74	0/4/4/4

The worst 5 of 243 bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	601	HEA	FE-NA	9.36	2.26	1.95
14	A	602	HEA	FE-NA	6.84	2.17	1.95
14	N	601	HEA	FE-NC	6.57	2.16	1.95
14	A	601	HEA	CHA-C1A	6.29	1.50	1.38
14	A	601	HEA	FE-NC	6.22	2.15	1.95

The worst 5 of 454 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	W	101	CHD	C17-C13-C12	9.82	126.50	117.67
22	G	103	CHD	C1-C2-C3	-9.55	97.84	110.48
22	W	101	CHD	C13-C17-C20	8.62	129.93	119.48
22	W	101	CHD	C18-C13-C12	-7.92	101.13	109.06
22	W	101	CHD	C17-C13-C14	-7.30	92.79	100.11

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
27	M	101	DMU	C9
27	M	101	DMU	C5
27	Z	101	DMU	C9
27	Z	101	DMU	C5

5 of 959 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	A	608	PGV	C04-O12-P-O11
19	A	608	PGV	C04-O12-P-O13
19	A	608	PGV	C04-O12-P-O14
19	A	608	PGV	C02-C03-O11-P
19	A	608	PGV	C05-C04-O12-P

There are no ring outliers.

40 monomers are involved in 325 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	P	303	PEK	9	0
23	N	610	PSC	21	0
19	P	301	PGV	7	0

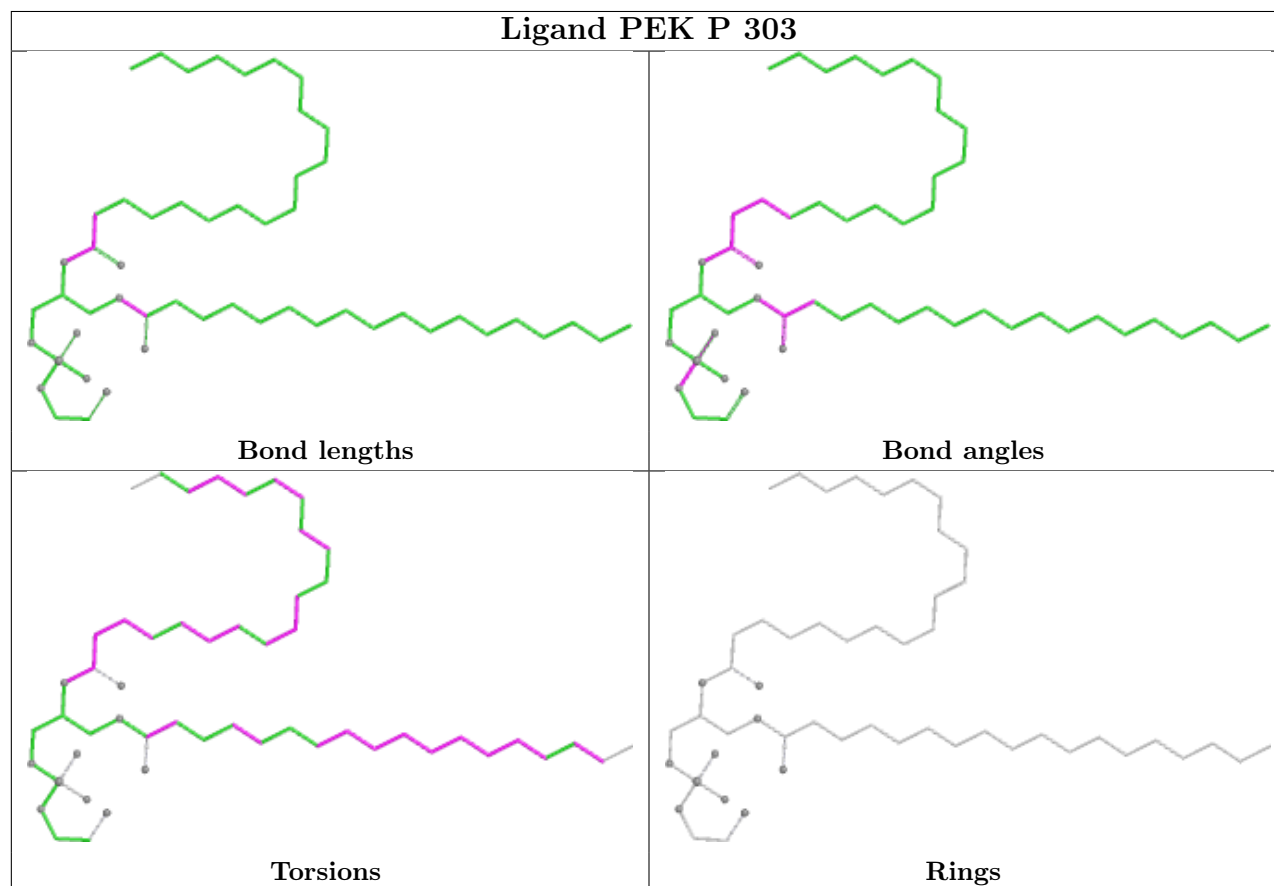
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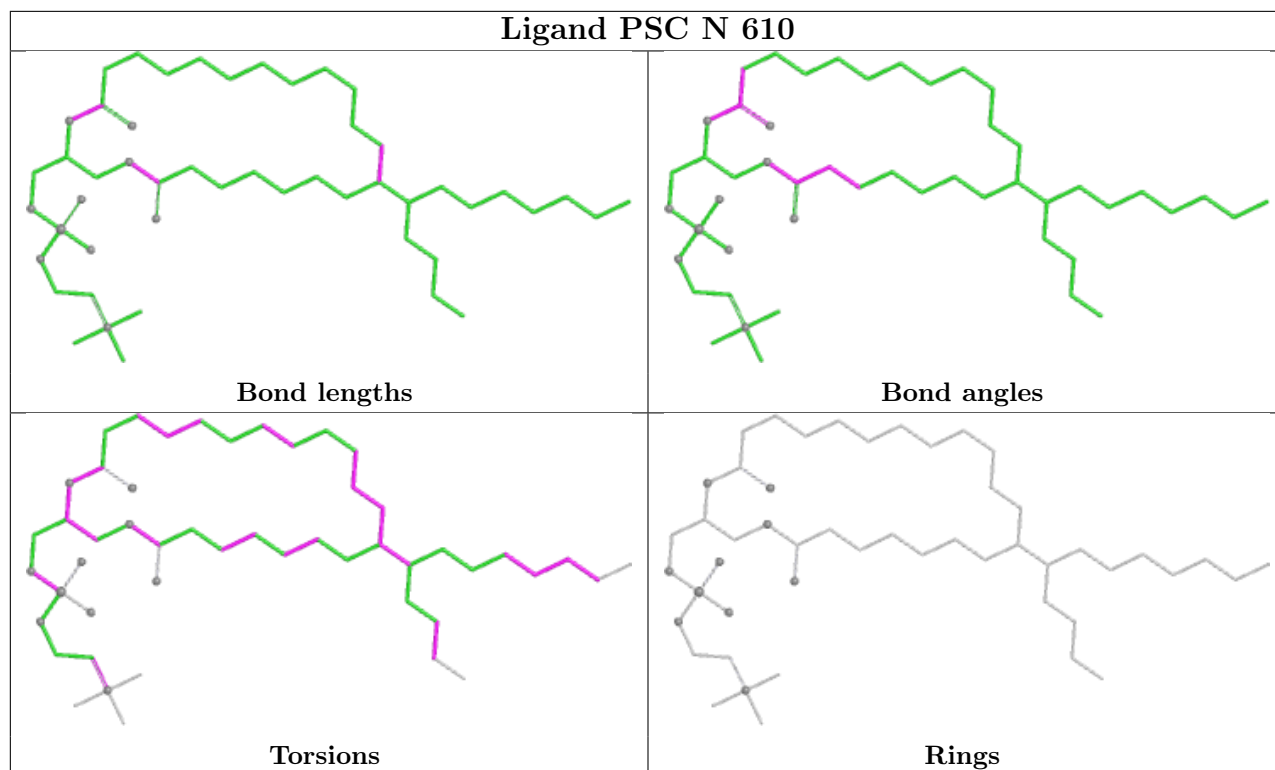
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	C	302	PEK	6	0
14	N	602	HEA	2	0
14	A	602	HEA	2	0
20	Q	201	TGL	11	0
19	N	607	PGV	10	0
14	N	601	HEA	6	0
24	T	101	PEK	12	0
22	W	101	CHD	5	0
18	A	606[A]	PER	1	0
19	A	608	PGV	8	0
19	C	308	PGV	1	0
19	C	303	PGV	5	0
20	B	301	TGL	3	0
22	B	303	CHD	1	0
27	M	101	DMU	1	0
24	C	307	PEK	17	0
20	L	101	TGL	12	0
22	C	306	CHD	1	0
25	P	305	CDL	18	0
19	P	304	PGV	4	0
20	N	609	TGL	4	0
22	J	101	CHD	5	0
25	G	101	CDL	37	0
20	Y	101	TGL	17	0
24	G	102	PEK	6	0
22	P	307	CHD	3	0
25	C	304	CDL	23	0
19	A	607	PGV	2	0
22	C	305	CHD	3	0
20	D	201	TGL	13	0
19	N	608	PGV	6	0
24	P	308	PEK	13	0
25	T	102	CDL	29	0
18	N	606[A]	PER	1	0
23	B	304	PSC	13	0
14	A	601	HEA	8	0
22	P	306	CHD	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

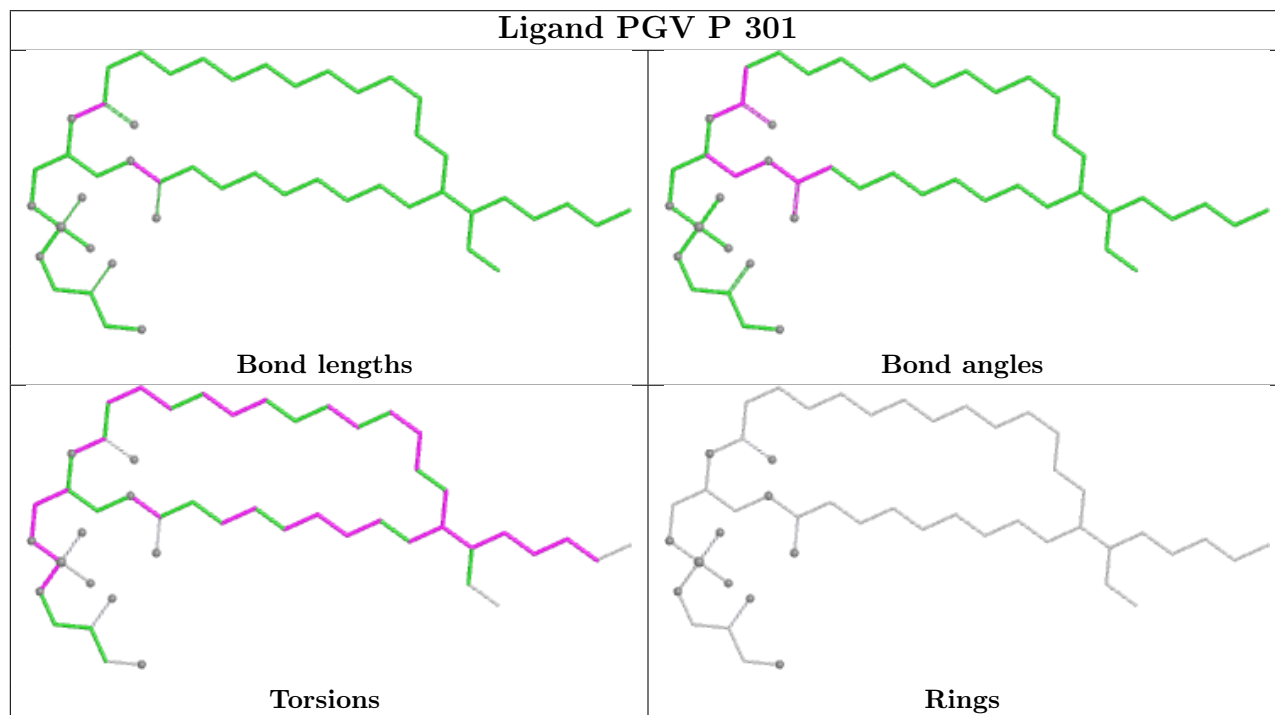
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

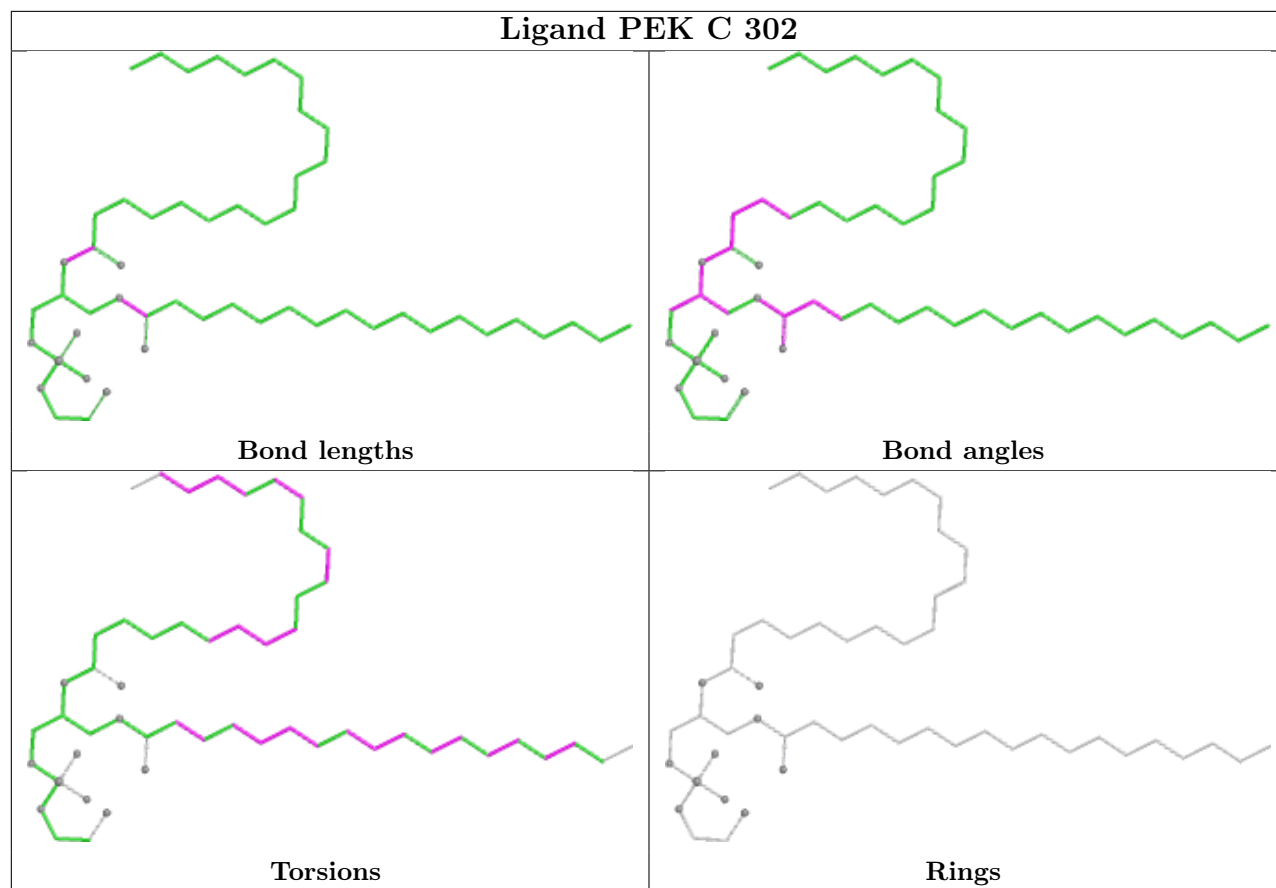


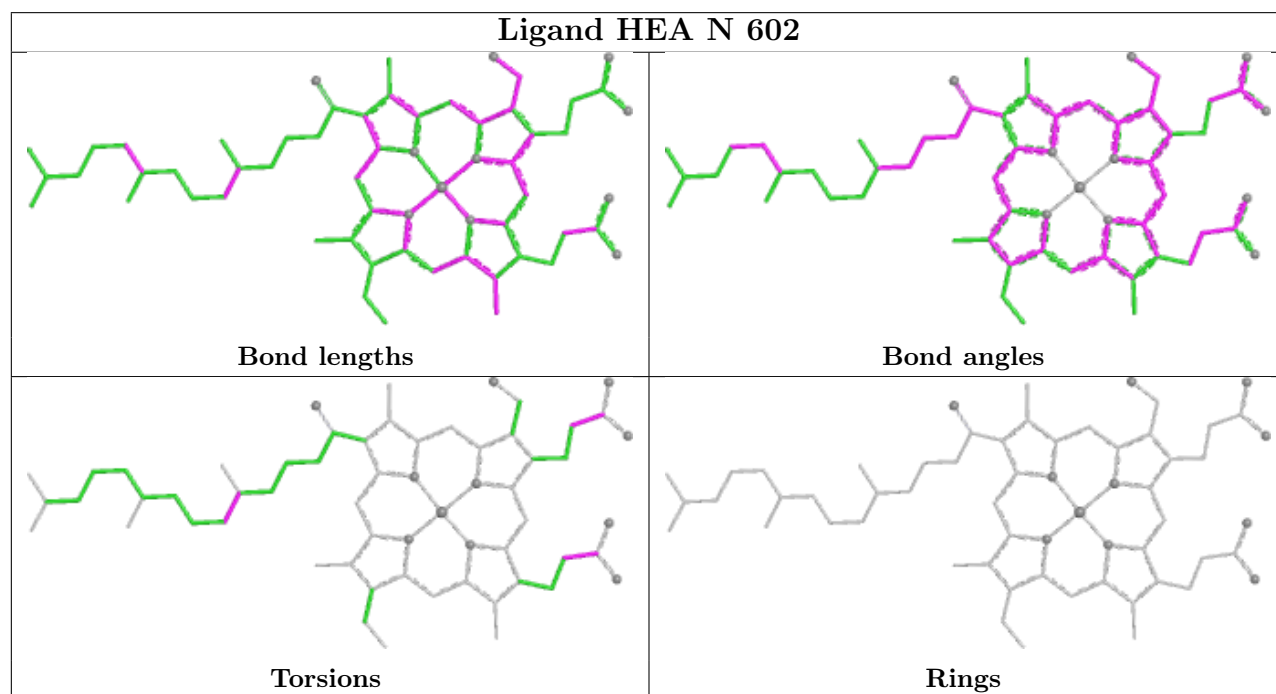
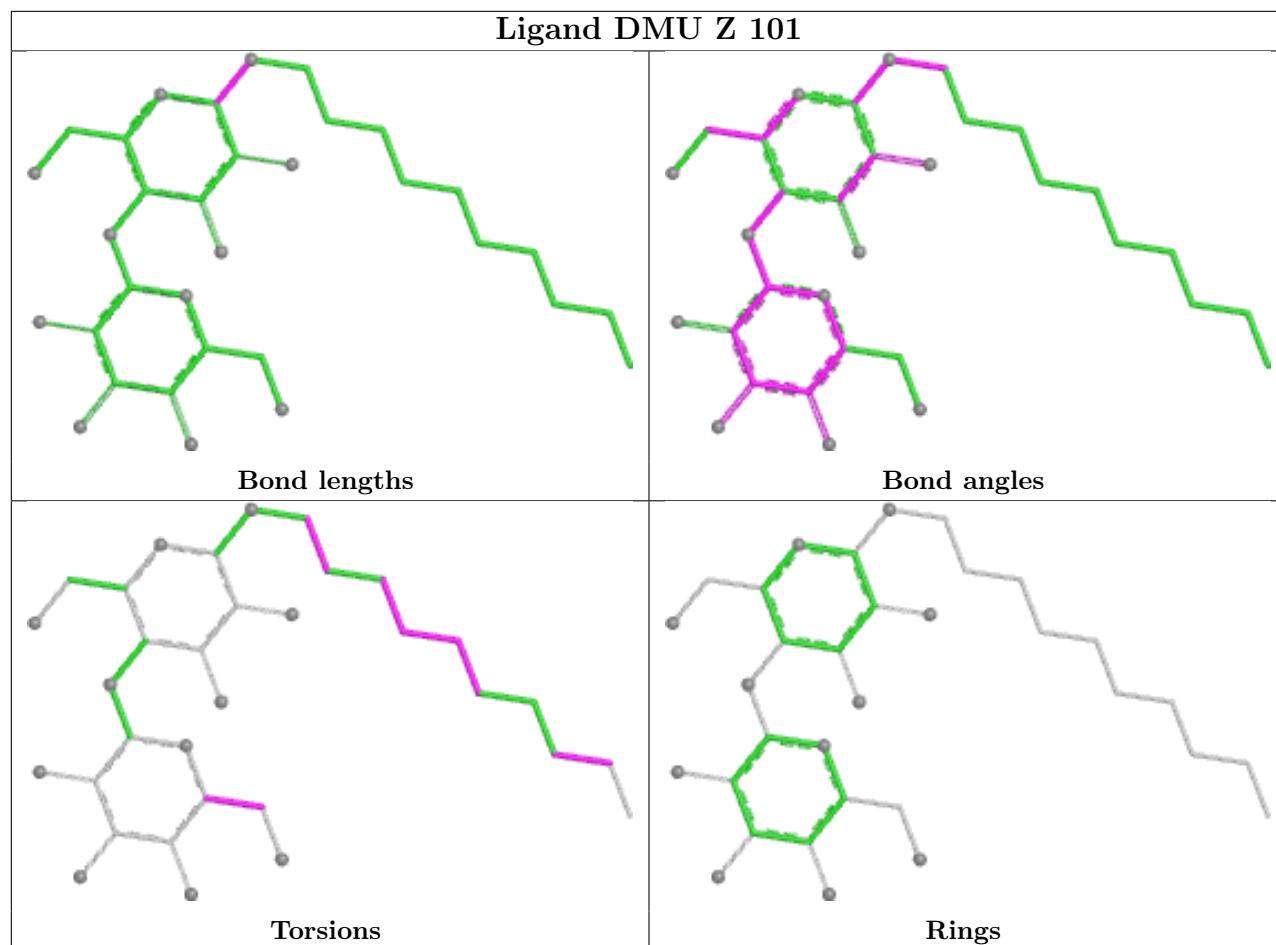
Ligand PSC N 610

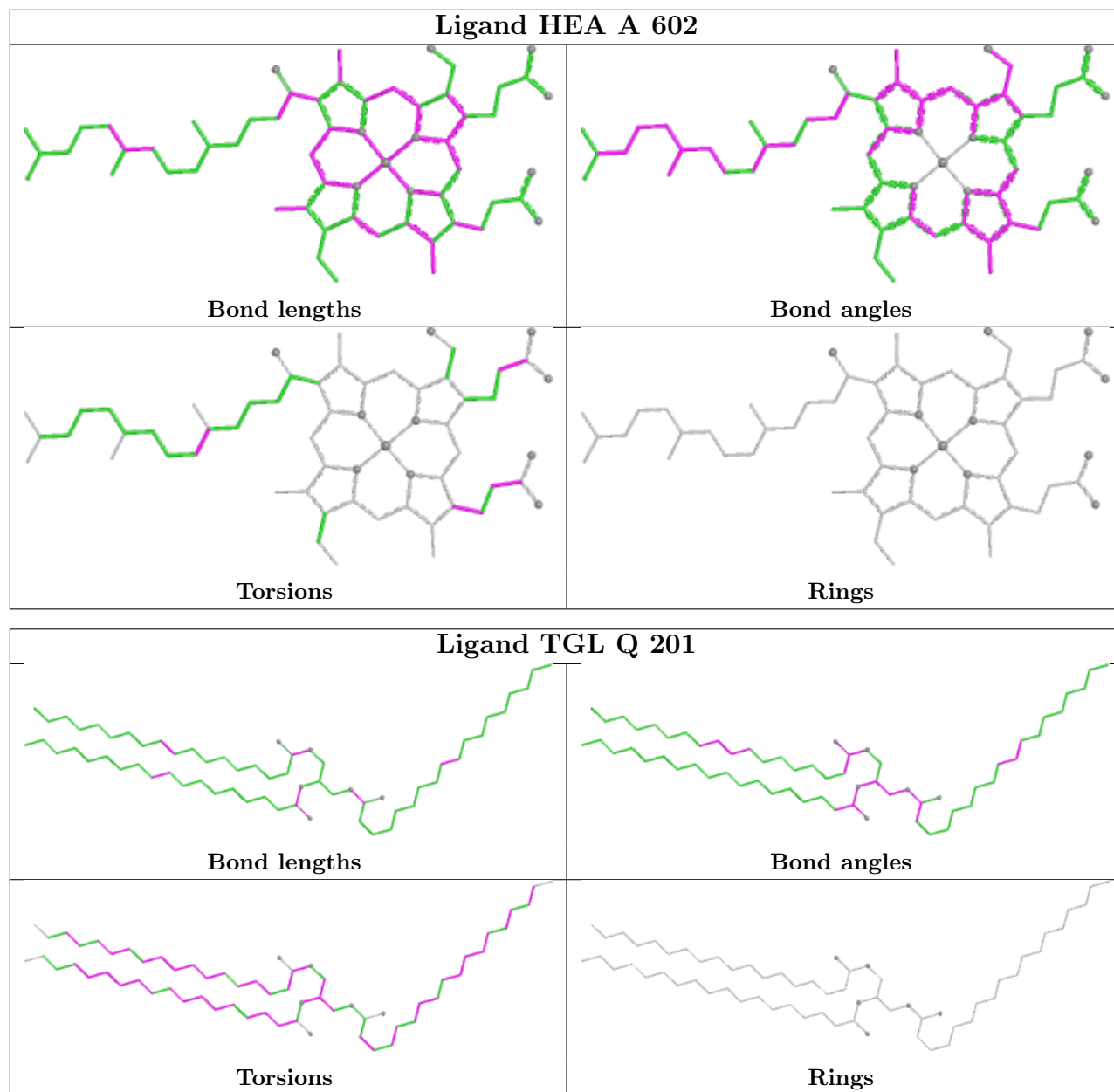


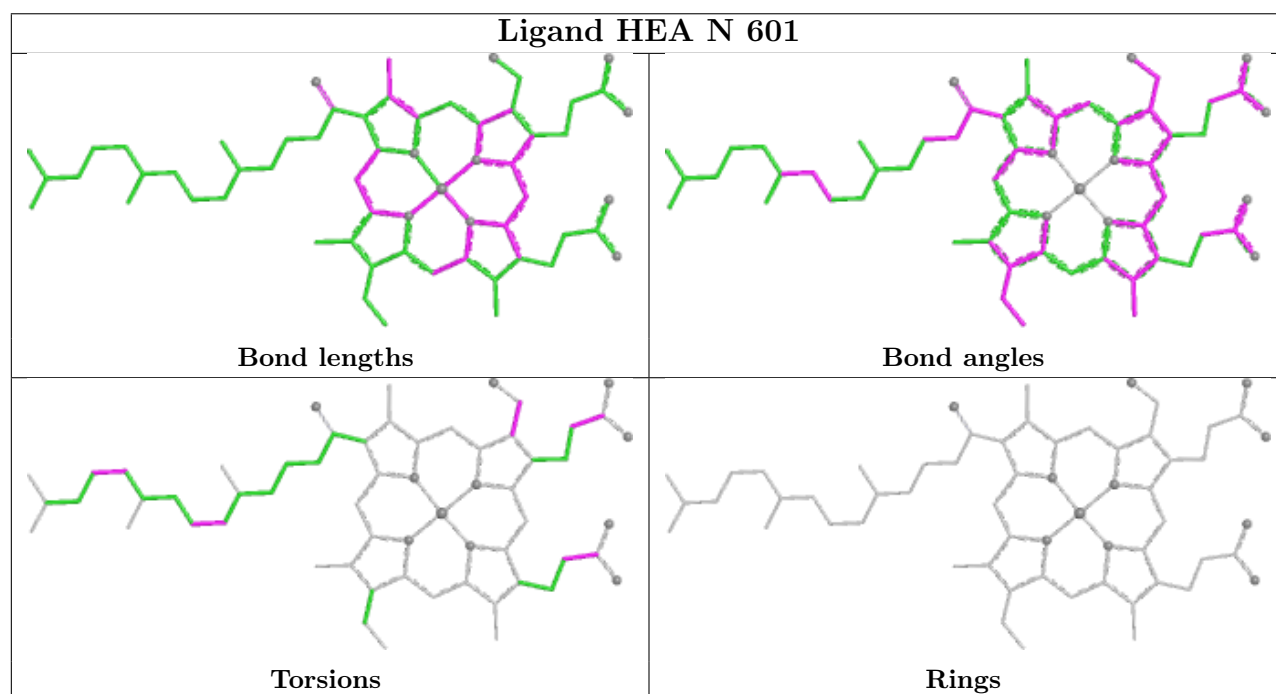
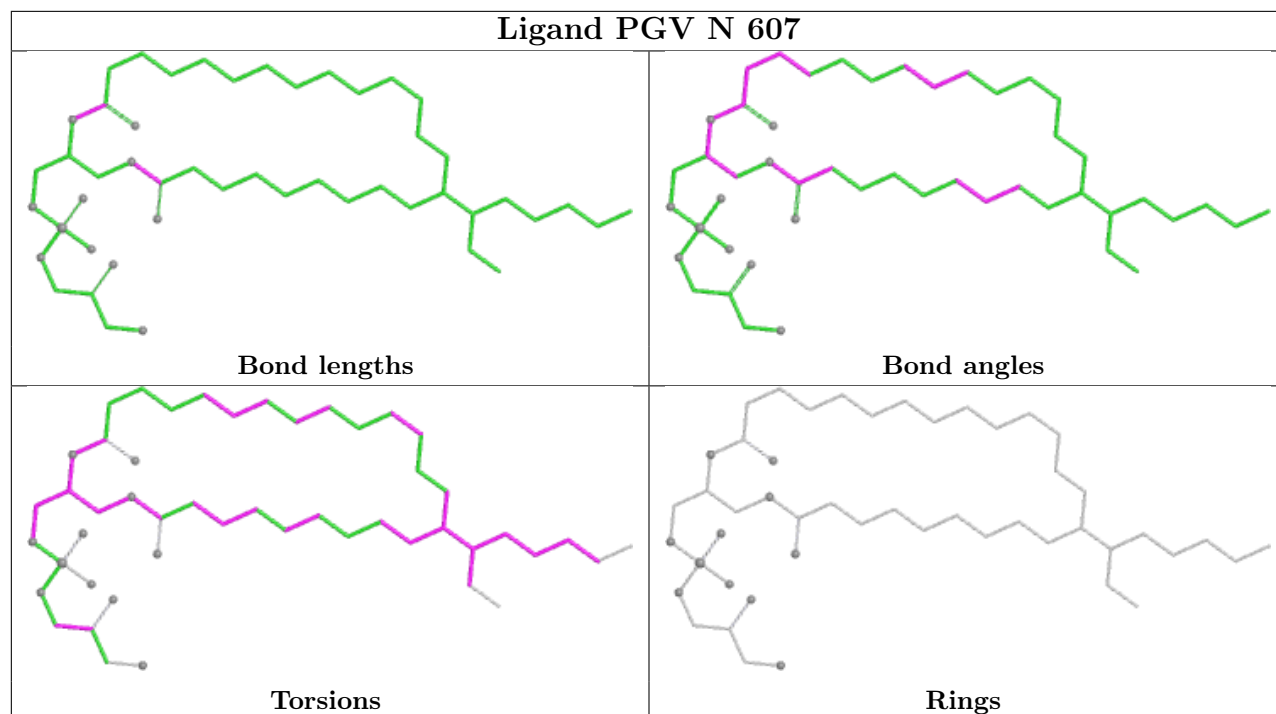
Ligand PGV P 301



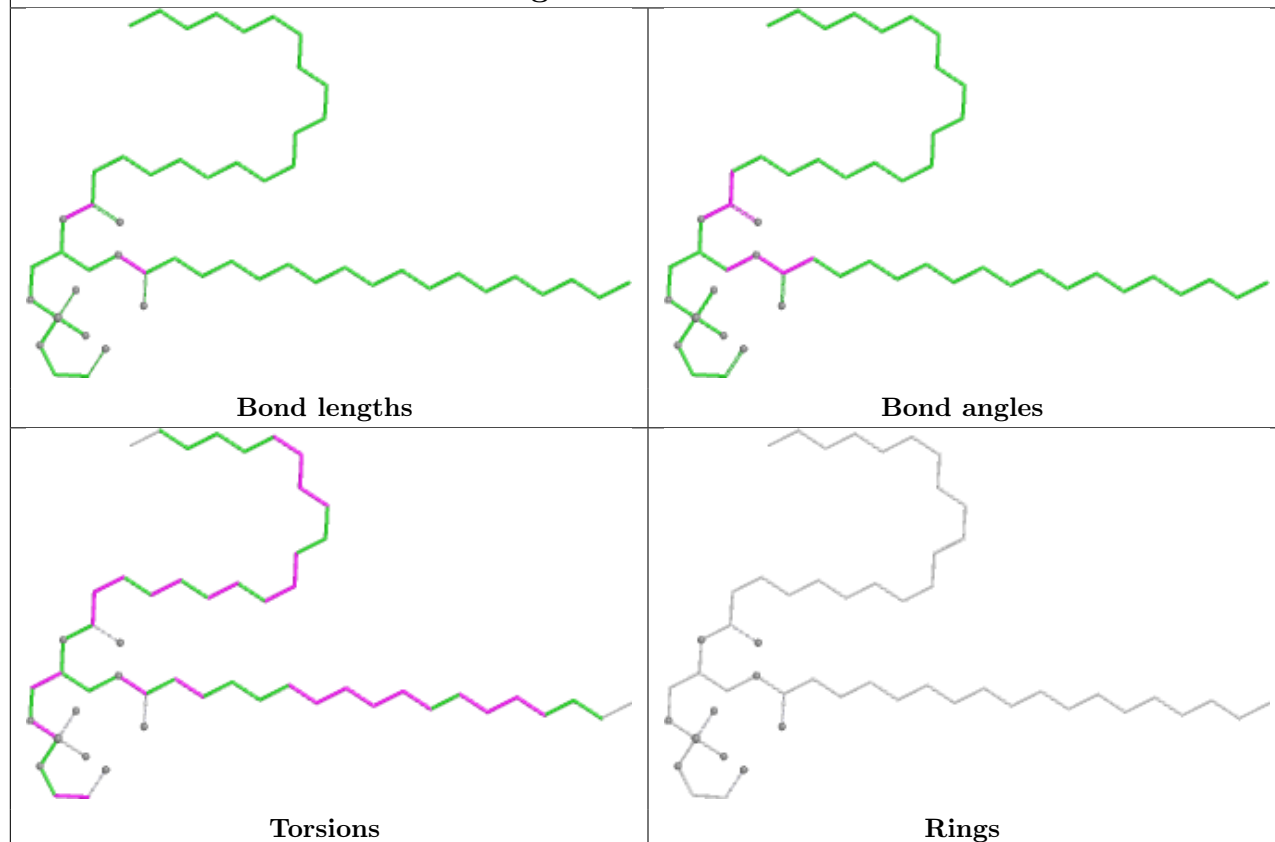




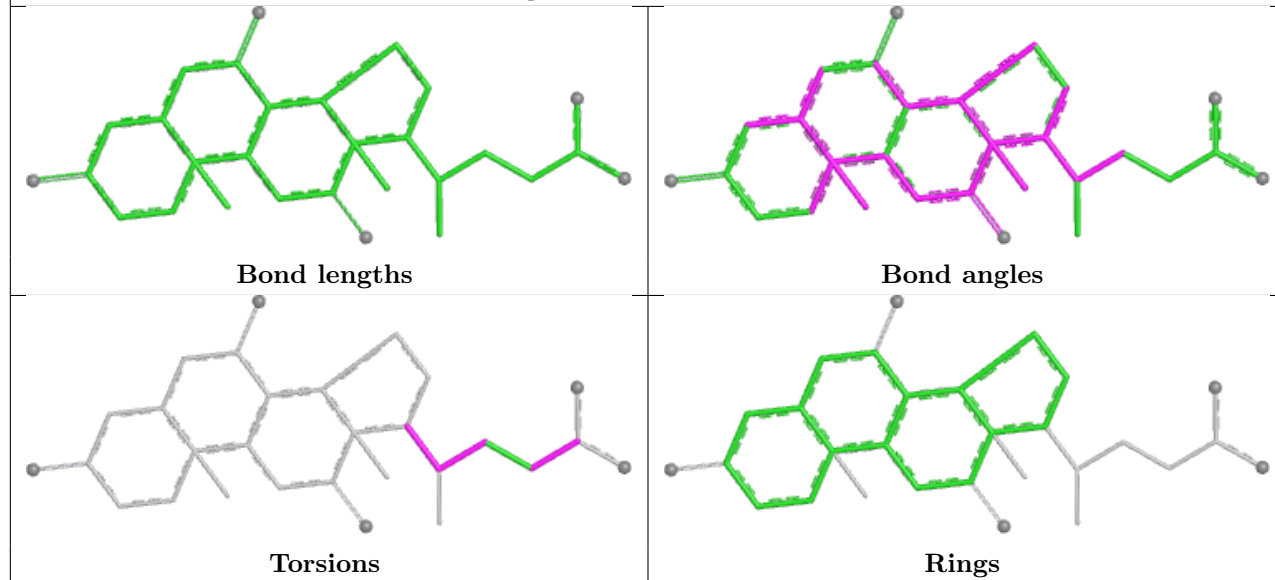


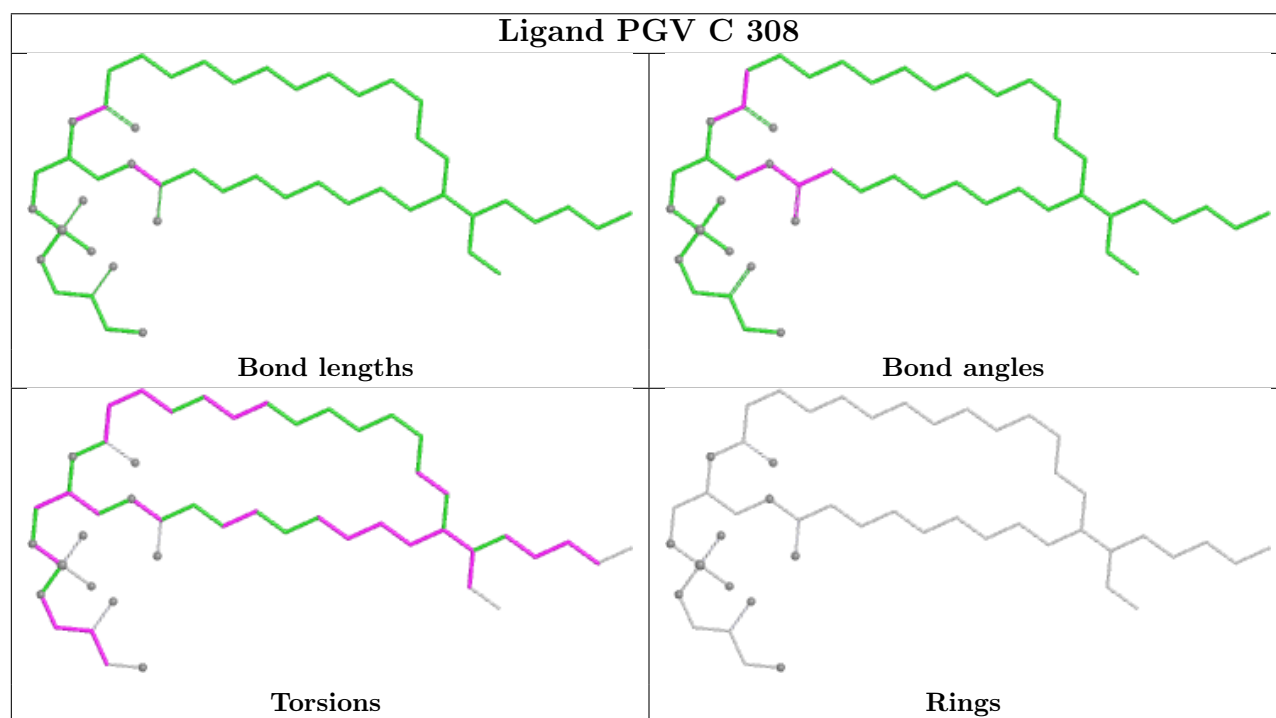
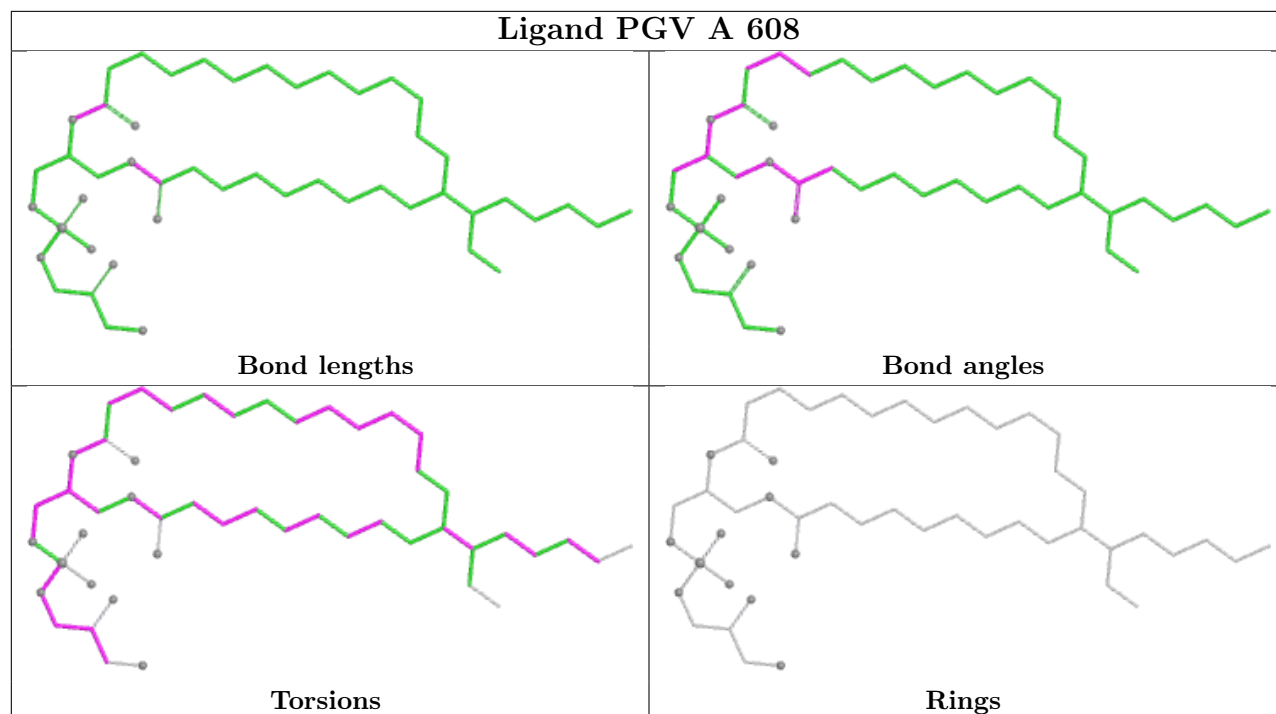


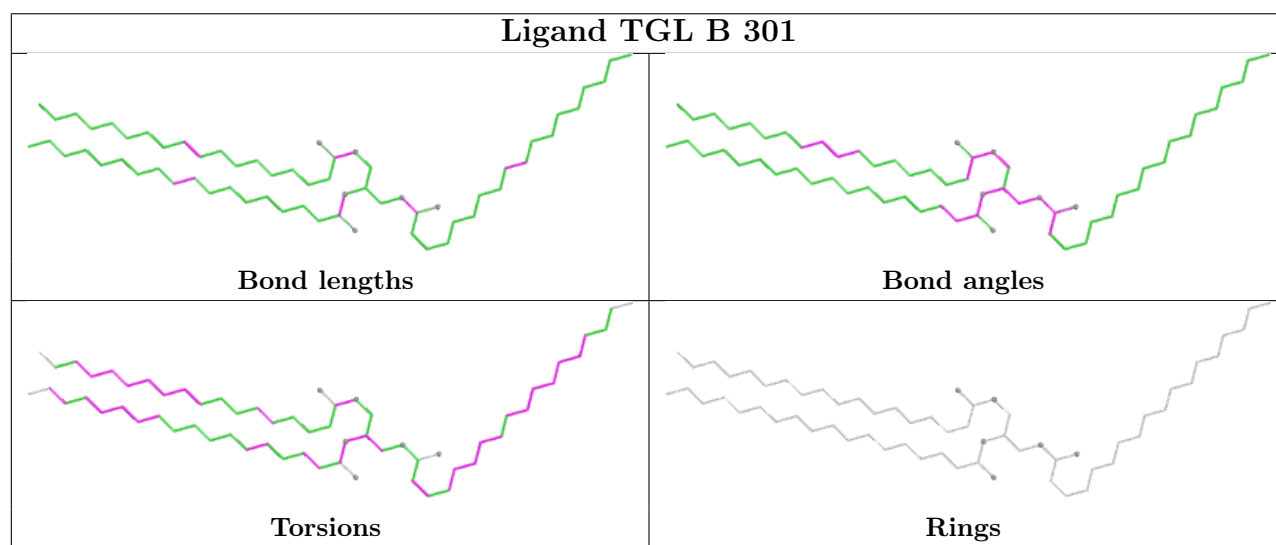
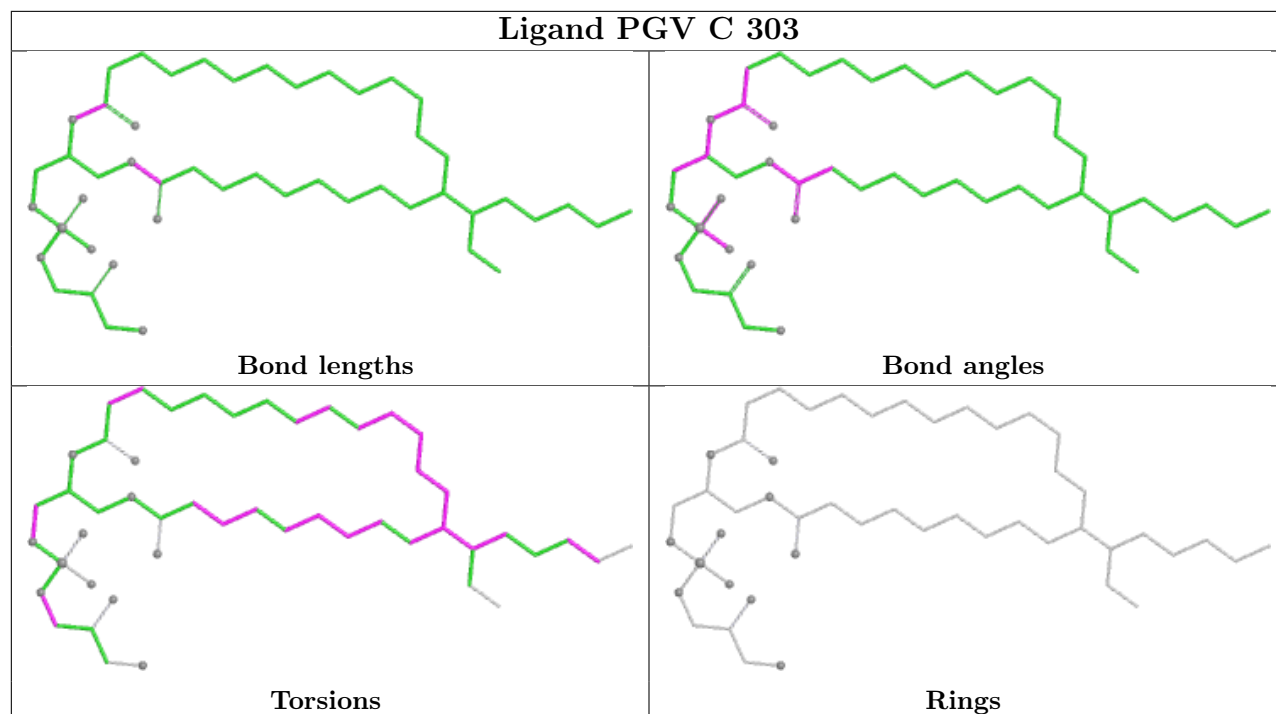
Ligand PEK T 101

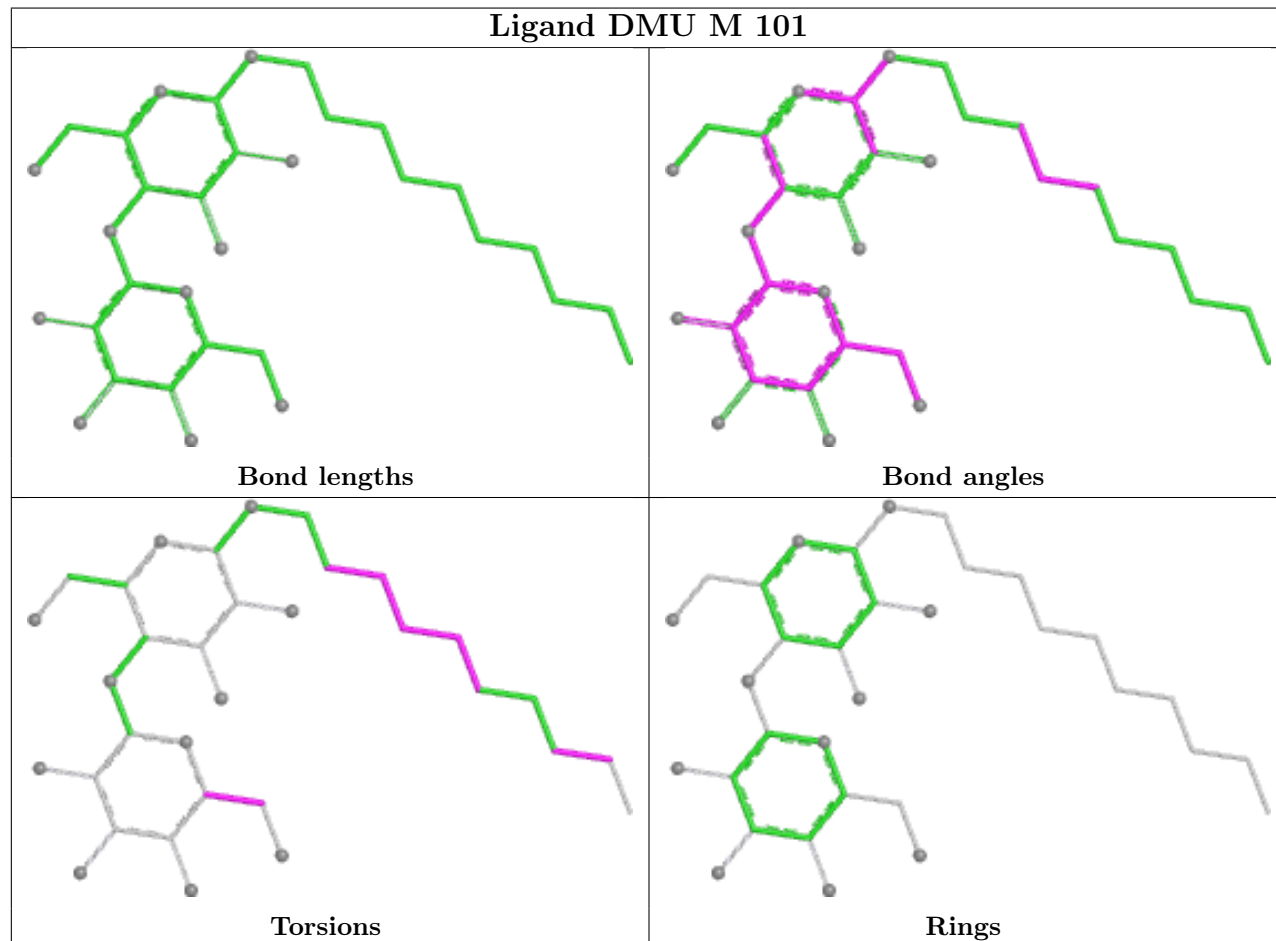
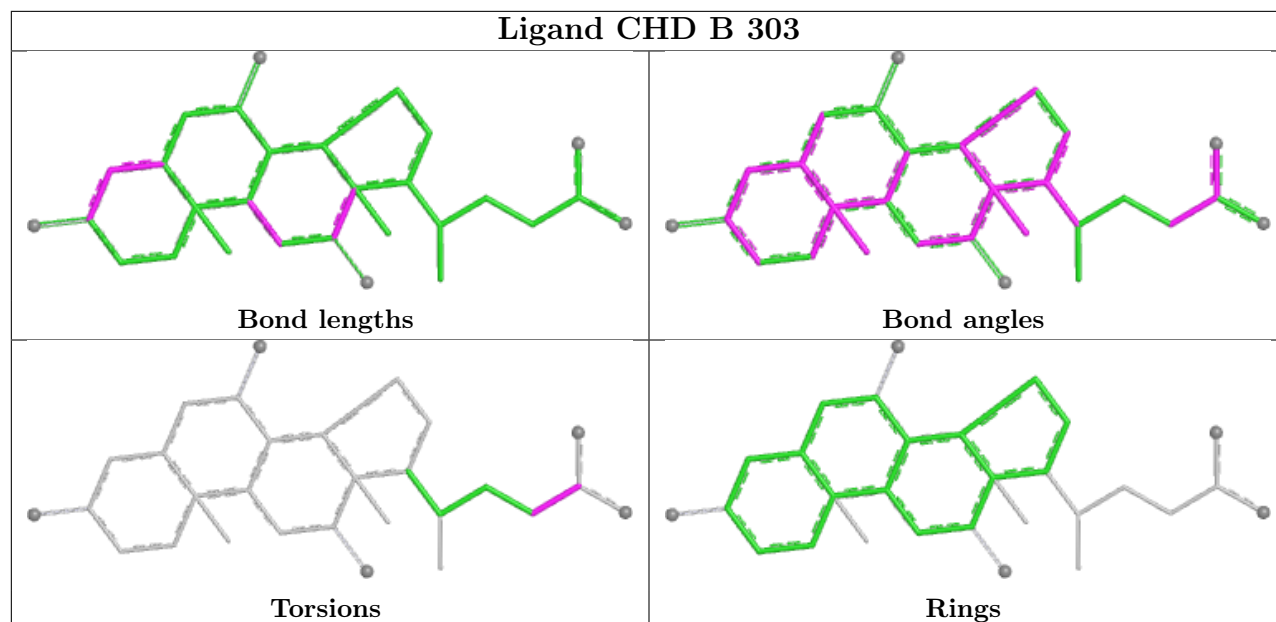


Ligand CHD W 101

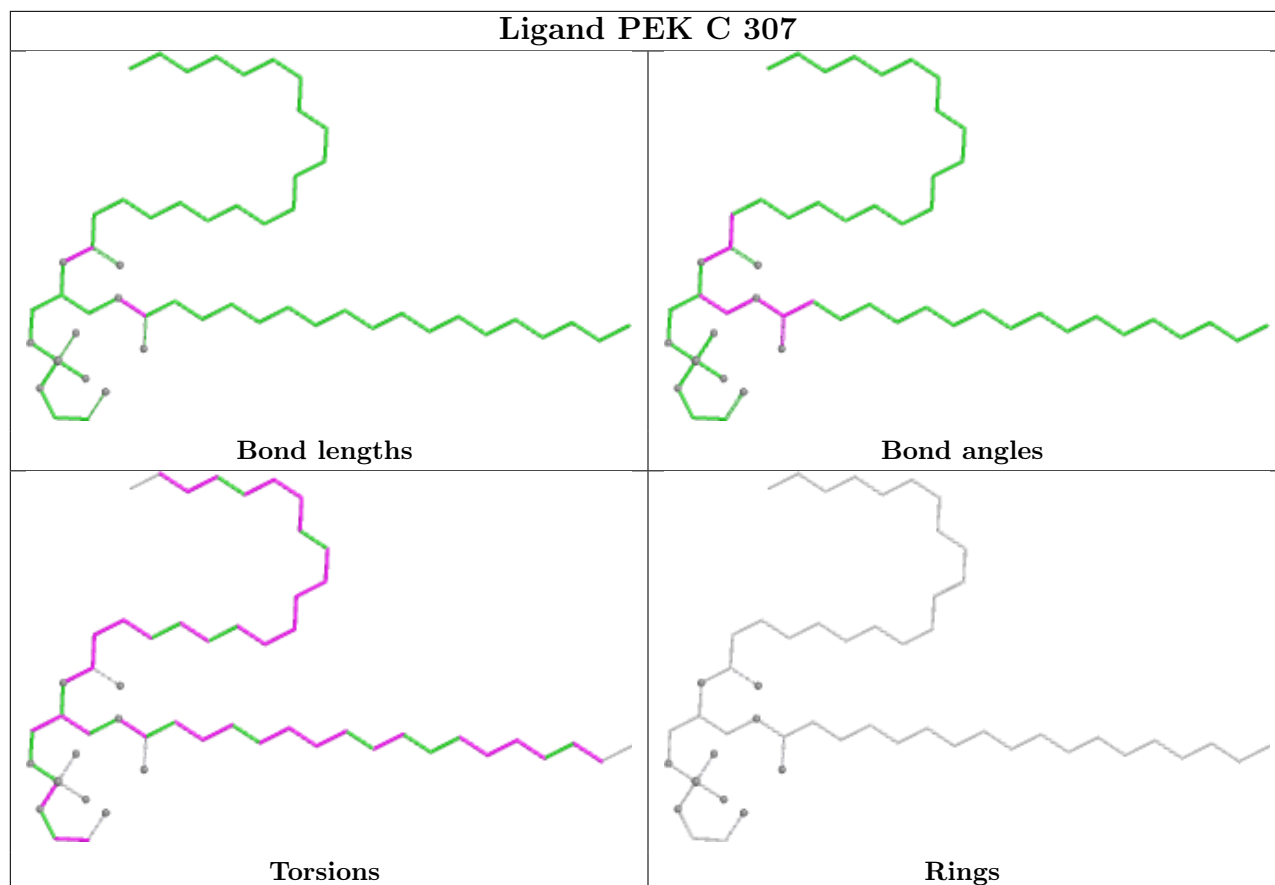




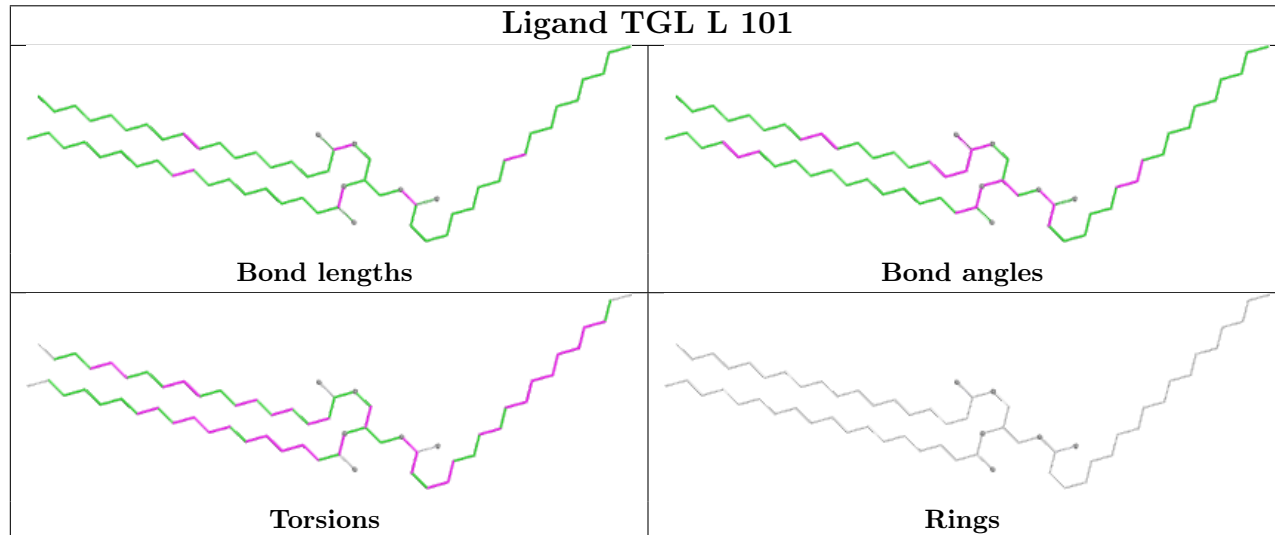


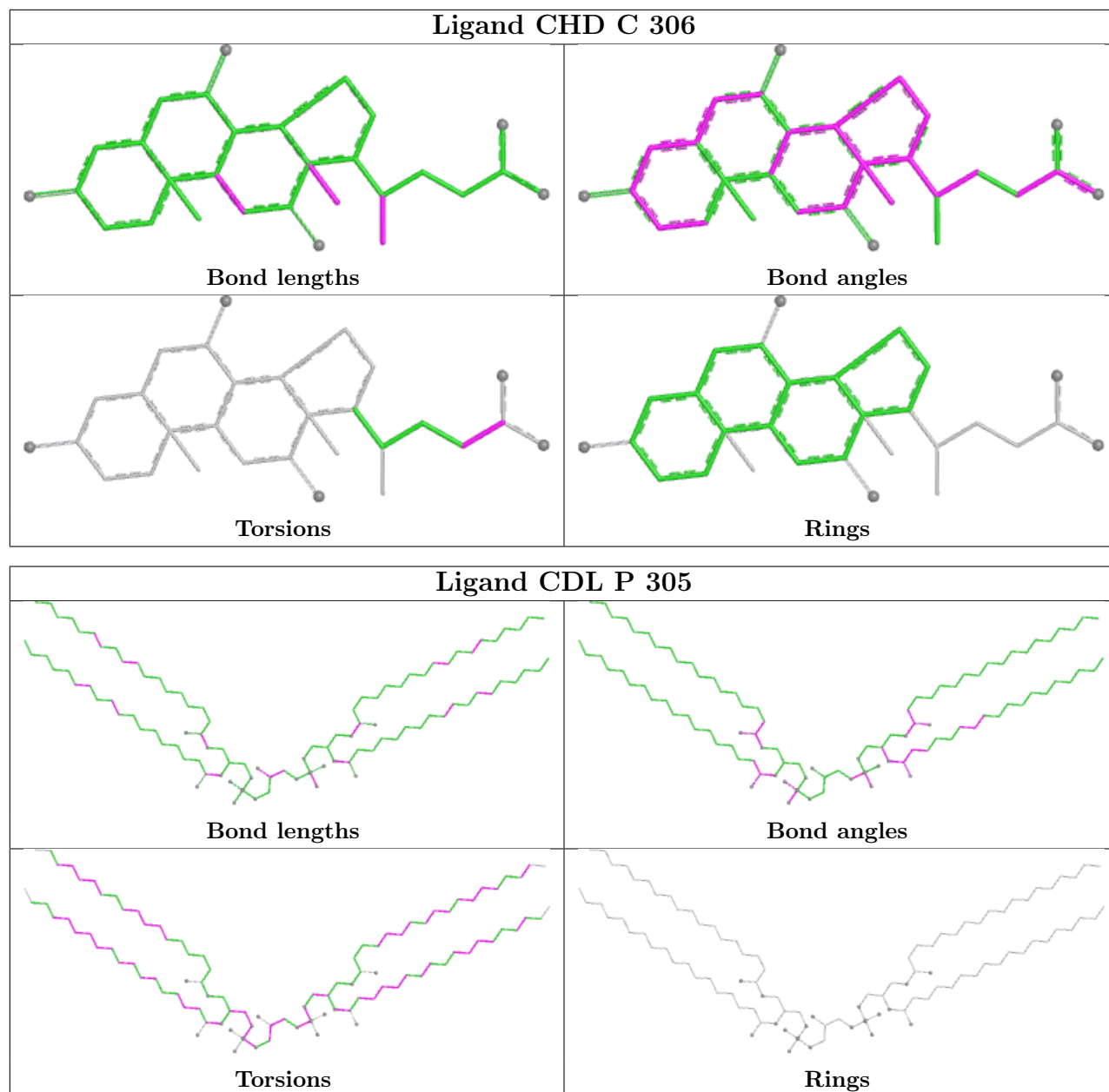


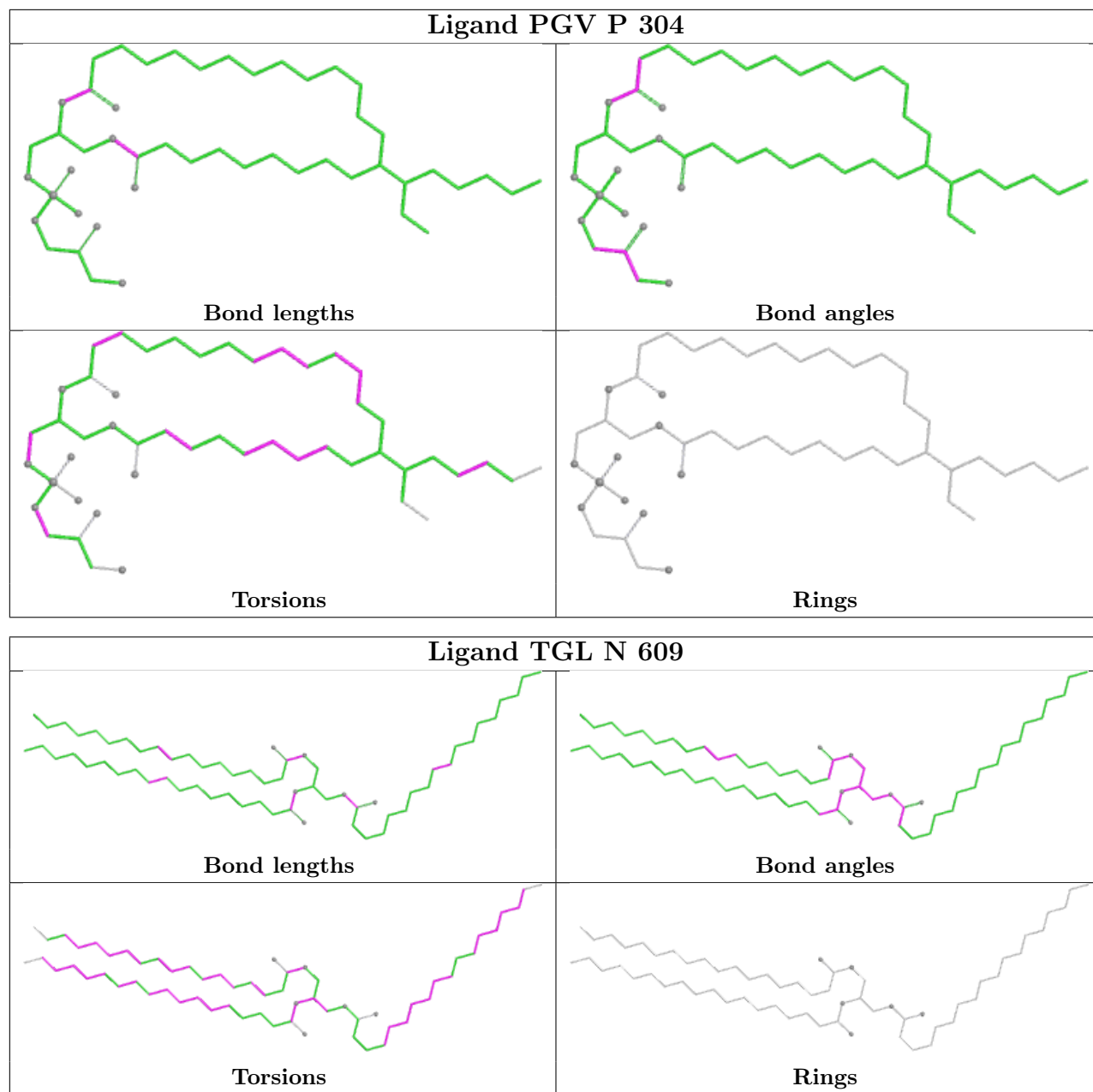
Ligand PEK C 307

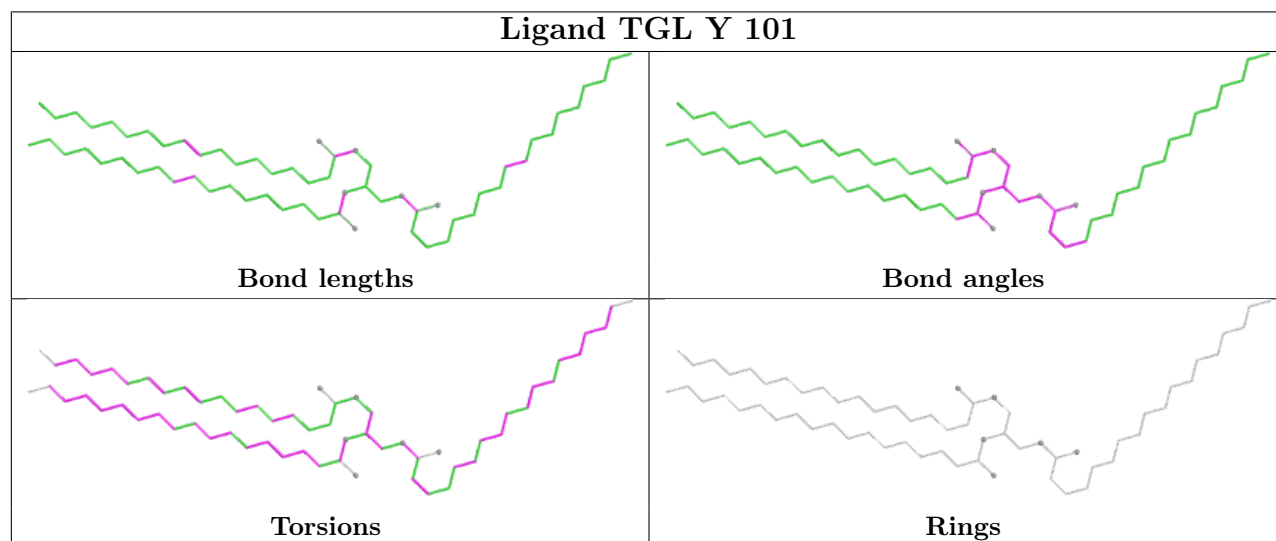
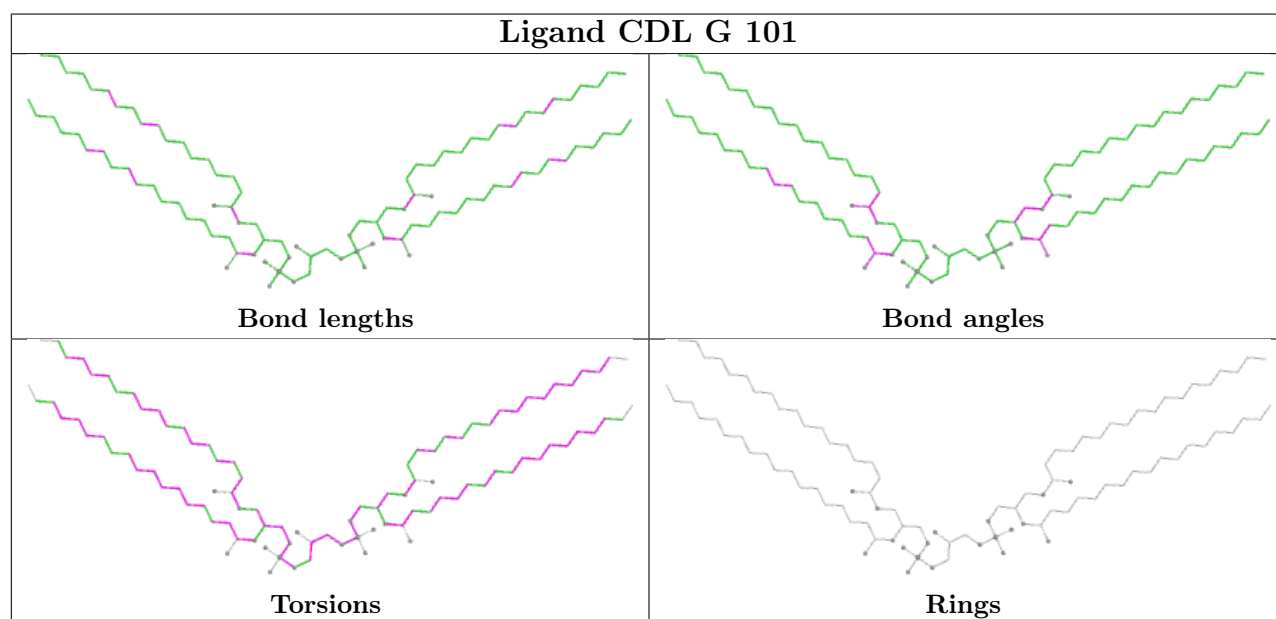
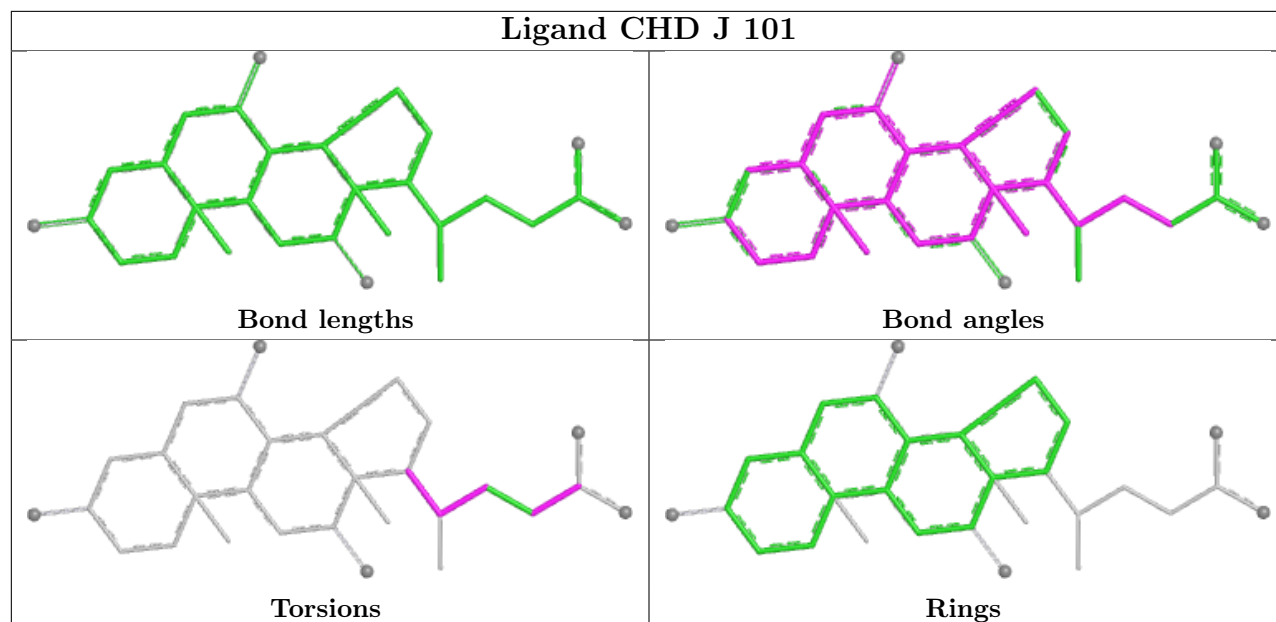


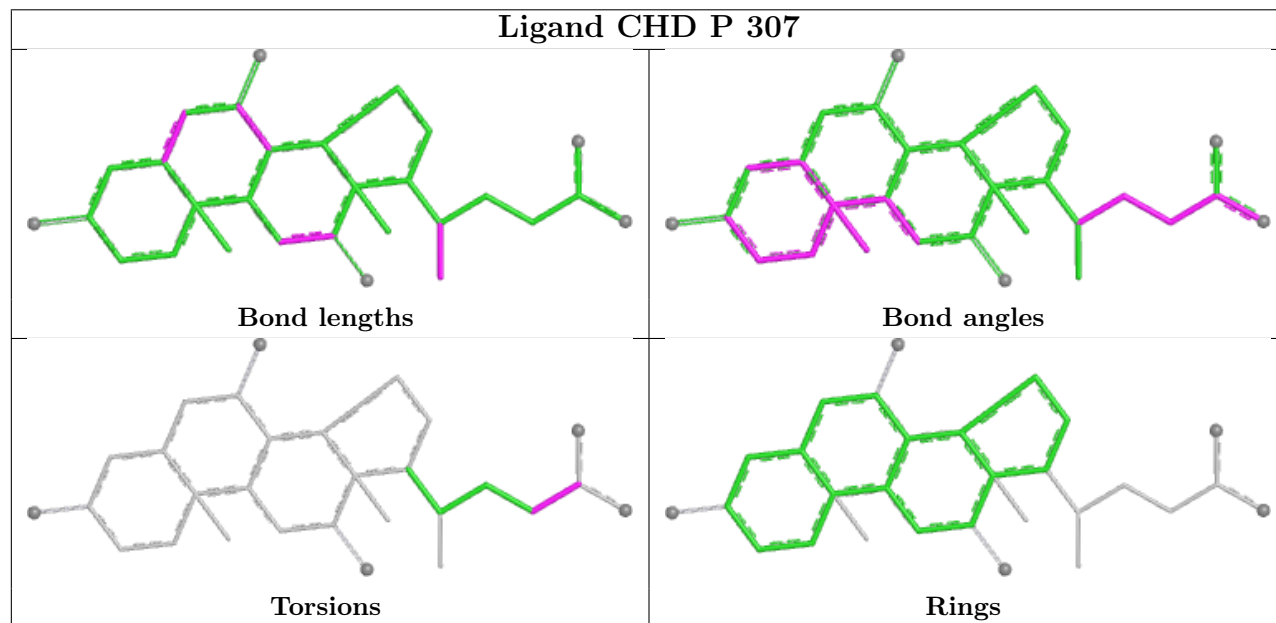
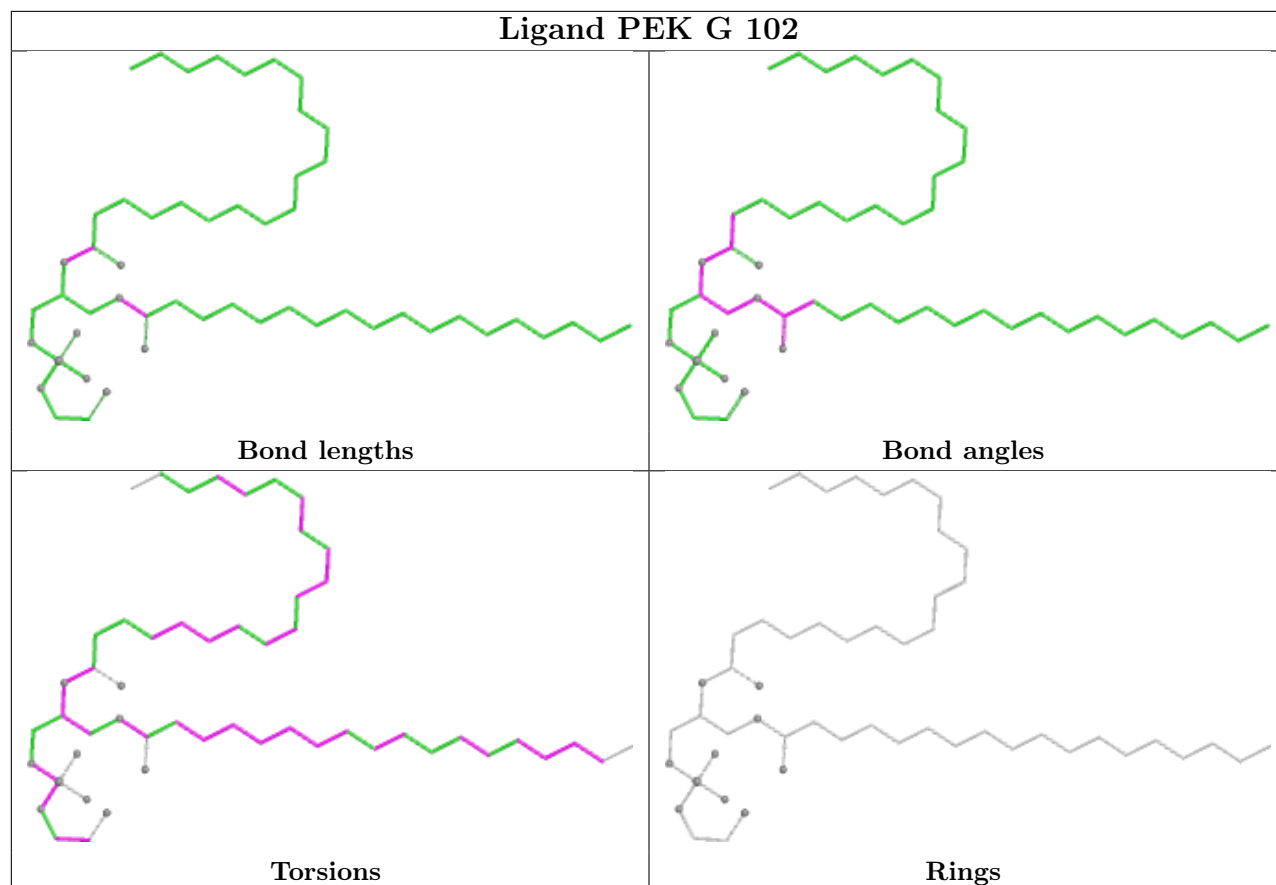
Ligand TGL L 101

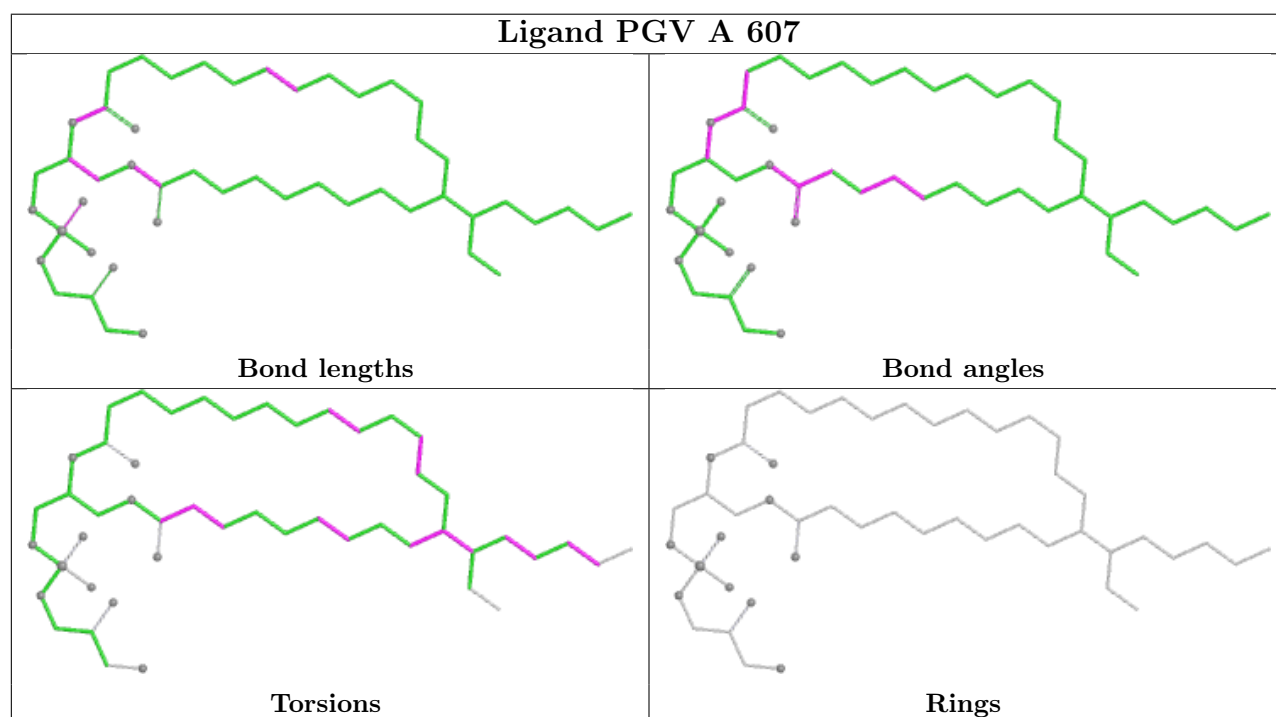
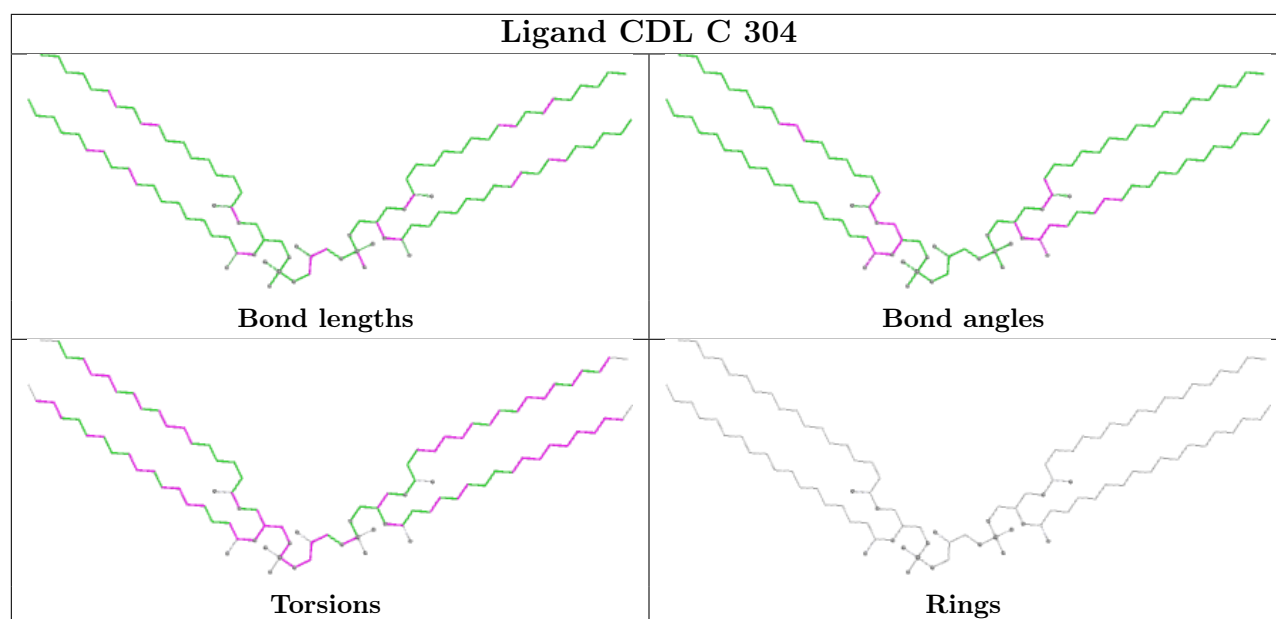


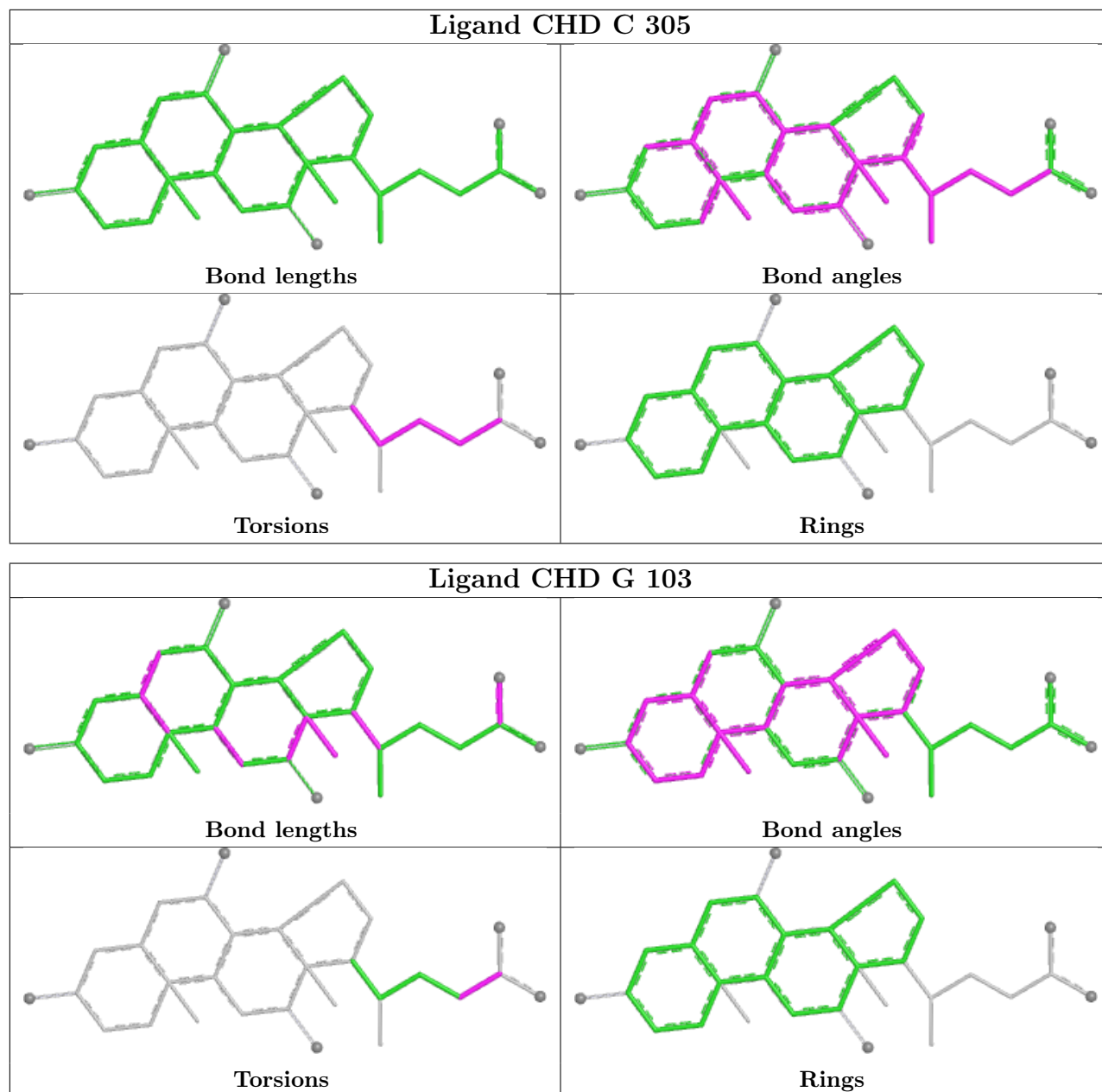


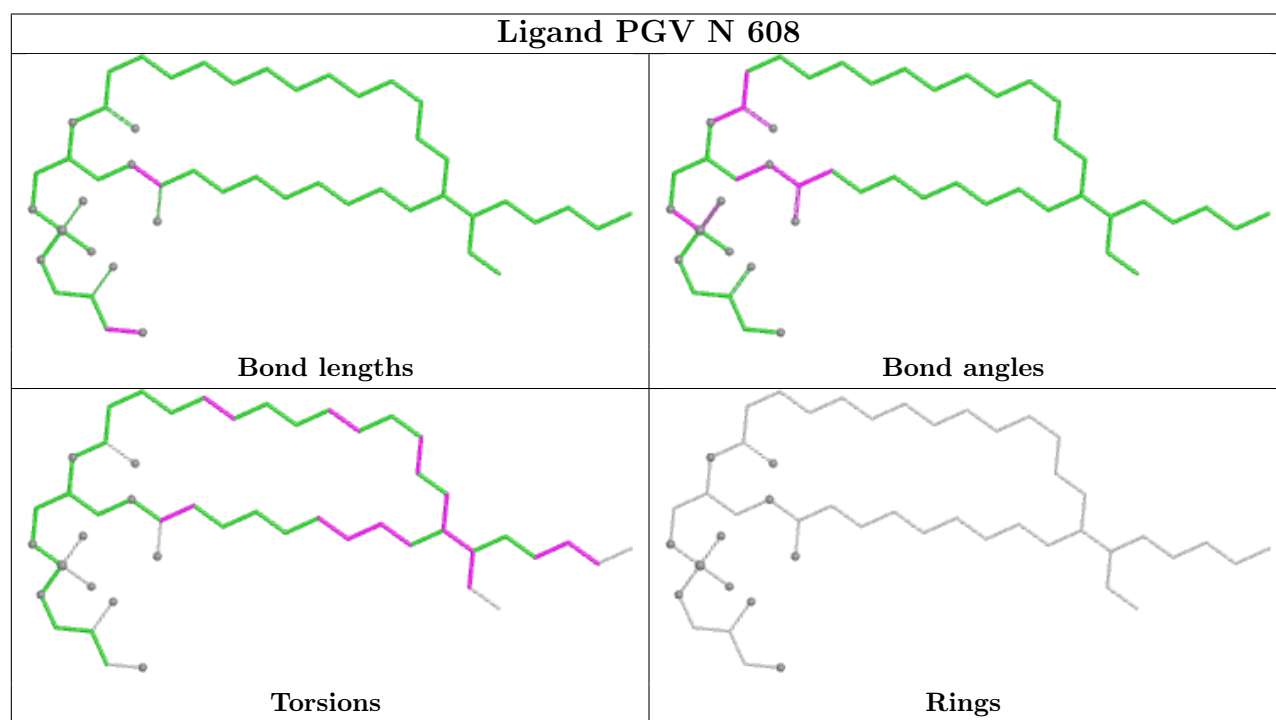
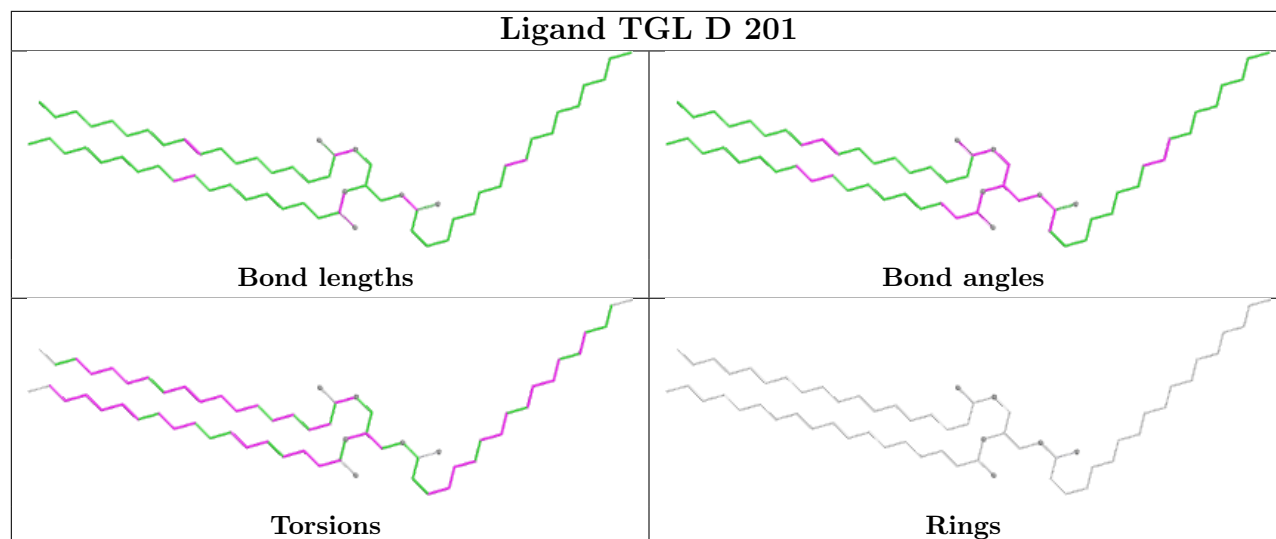


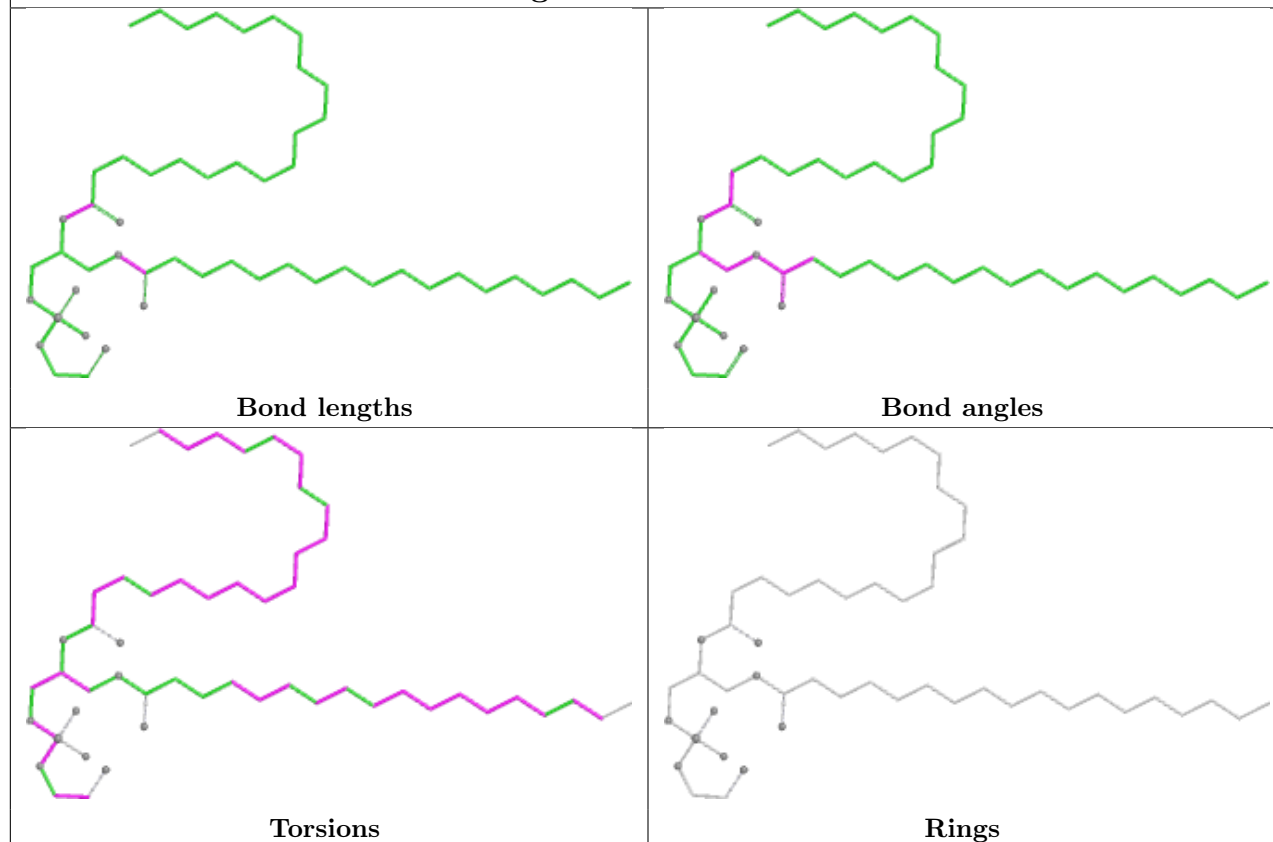
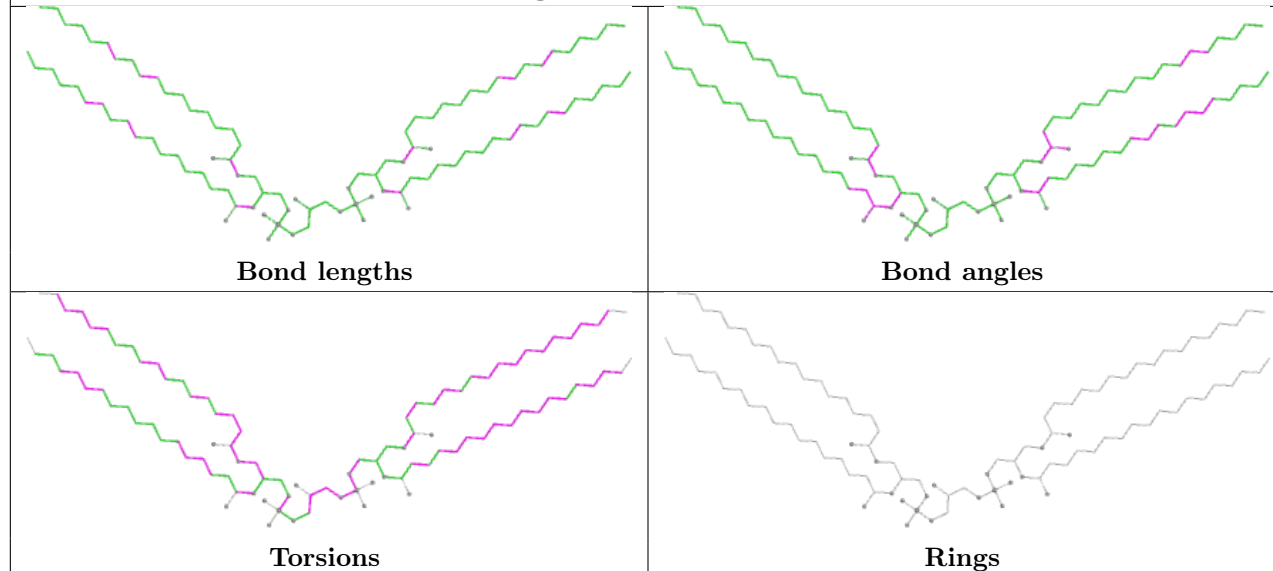




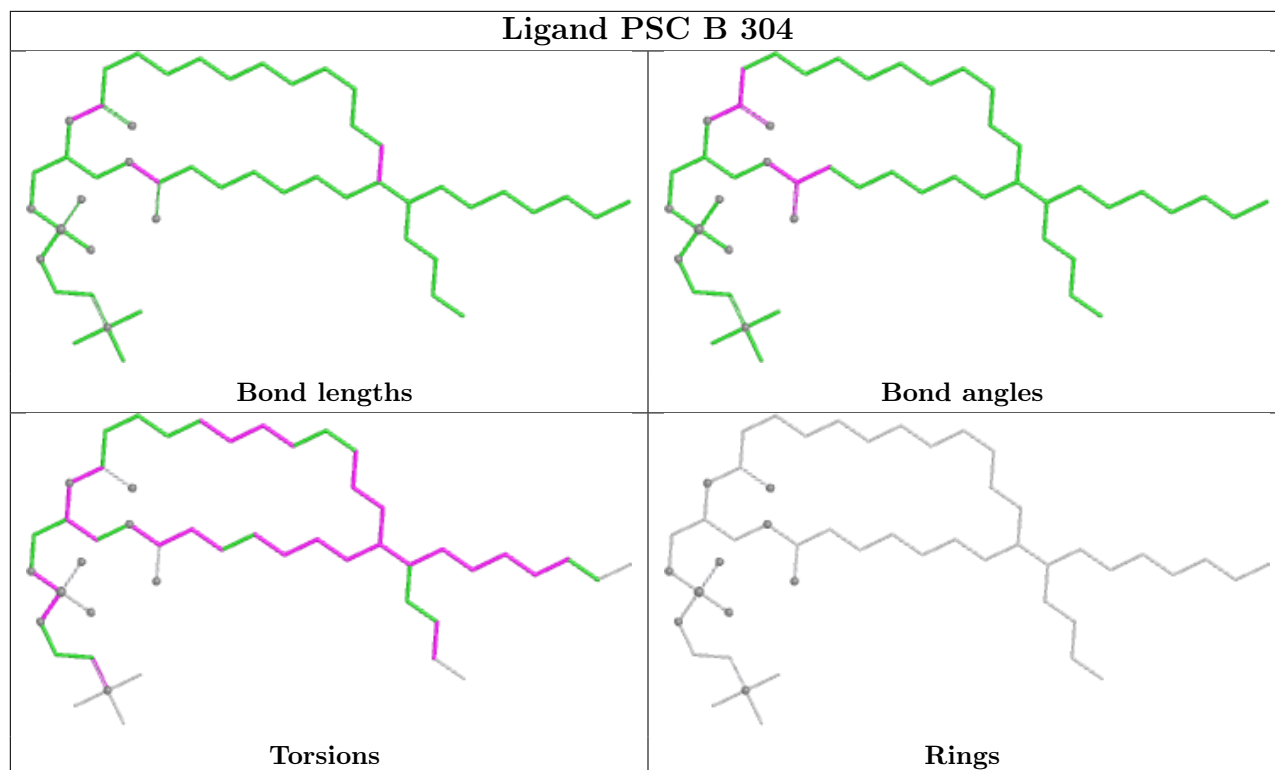




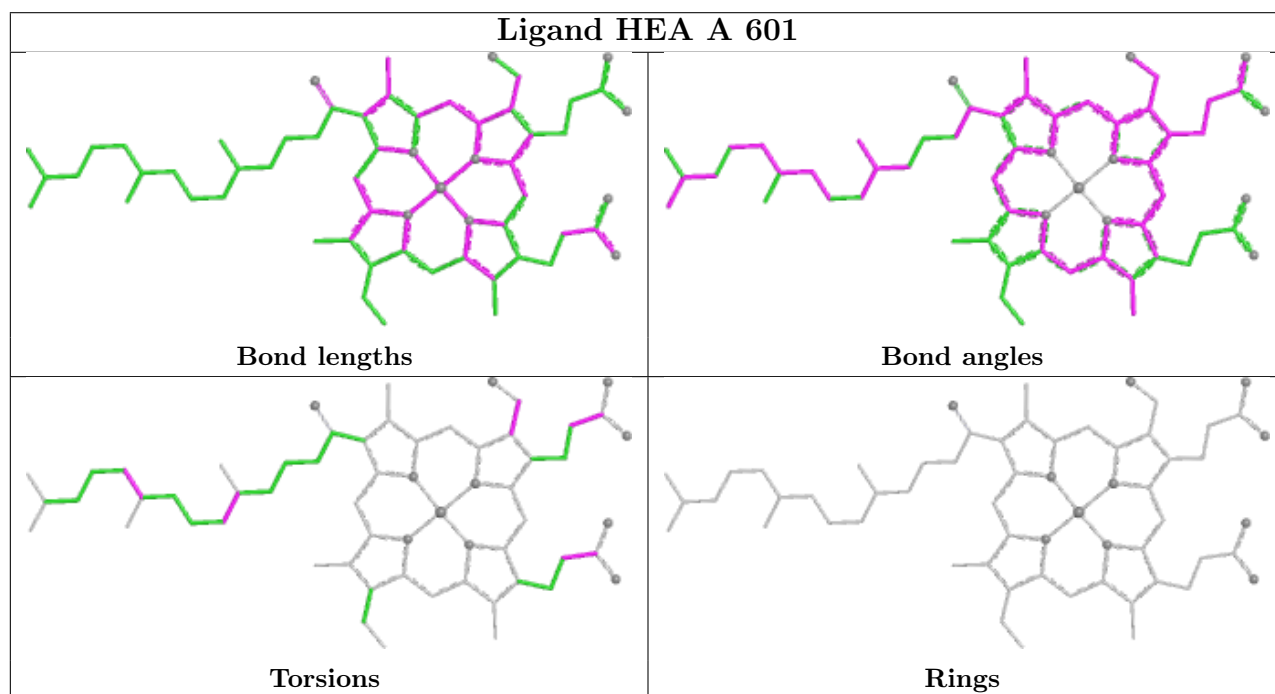


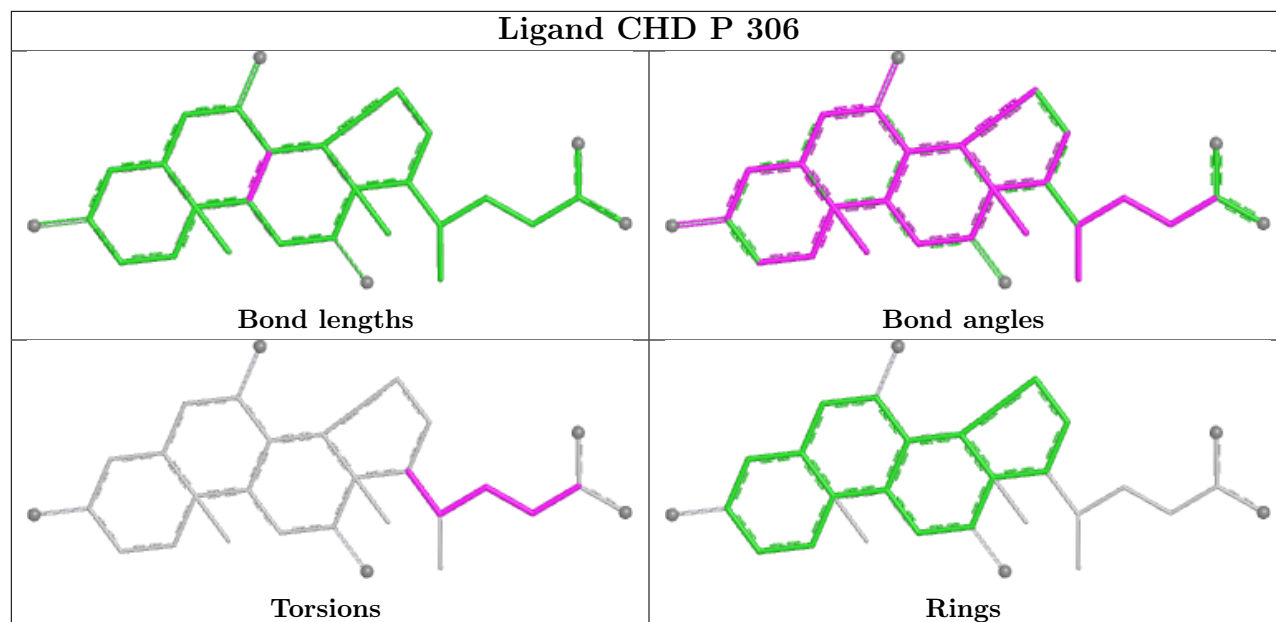
Ligand PEK P 308**Ligand CDL T 102**

Ligand PSC B 304



Ligand HEA A 601





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%)	-0.21	2 (0%) 88 90	6, 15, 22, 51	6 (1%)
1	N	513/514 (99%)	-0.21	3 (0%) 85 87	6, 14, 20, 51	6 (1%)
2	B	226/227 (99%)	0.16	9 (3%) 42 45	9, 18, 39, 65	1 (0%)
2	O	226/227 (99%)	0.31	13 (5%) 29 30	11, 17, 41, 62	0
3	C	259/261 (99%)	-0.10	4 (1%) 72 75	11, 17, 26, 59	3 (1%)
3	P	259/261 (99%)	-0.08	2 (0%) 82 85	9, 16, 26, 46	3 (1%)
4	D	144/147 (97%)	0.14	2 (1%) 73 76	12, 18, 35, 57	0
4	Q	144/147 (97%)	0.96	20 (13%) 6 6	13, 23, 48, 106	0
5	E	105/109 (96%)	0.08	4 (3%) 44 47	11, 17, 41, 88	0
5	R	105/109 (96%)	0.41	2 (1%) 66 70	13, 18, 36, 89	0
6	F	98/98 (100%)	0.79	9 (9%) 14 15	15, 23, 68, 118	0
6	S	98/98 (100%)	0.67	9 (9%) 14 15	13, 20, 61, 97	0
7	G	83/85 (97%)	0.98	21 (25%) 1 1	11, 20, 73, 90	0
7	T	83/85 (97%)	1.15	21 (25%) 1 1	10, 20, 77, 101	0
8	H	79/85 (92%)	0.83	14 (17%) 4 3	16, 24, 62, 76	0
8	U	79/85 (92%)	0.78	14 (17%) 4 3	14, 21, 63, 76	0
9	I	72/73 (98%)	0.90	13 (18%) 3 3	15, 26, 53, 63	0
9	V	72/73 (98%)	1.02	10 (13%) 6 6	13, 26, 47, 58	0
10	J	58/59 (98%)	0.67	4 (6%) 23 24	17, 25, 45, 86	0
10	W	58/59 (98%)	0.72	5 (8%) 16 17	13, 22, 51, 91	0
11	K	49/56 (87%)	0.54	3 (6%) 27 29	16, 22, 36, 42	0
11	X	49/56 (87%)	0.93	3 (6%) 27 29	16, 21, 37, 43	0
12	L	46/47 (97%)	0.28	4 (8%) 16 17	15, 19, 37, 64	0
12	Y	46/47 (97%)	0.44	4 (8%) 16 17	12, 19, 38, 70	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	0.31	5 (11%) 9 10	14, 18, 44, 77	0
13	Z	43/46 (93%)	0.64	5 (11%) 9 10	12, 18, 48, 66	0
All	All	3550/3614 (98%)	0.24	205 (5%) 29 30	6, 17, 43, 118	19 (0%)

The worst 5 of 205 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	F	1	ALA	12.6
6	F	97	ALA	10.6
6	S	97	ALA	10.6
6	F	96	LEU	8.8
6	S	1	ALA	8.7

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	0.42	0.23	63,69,72,74	0
9	SAC	I	1	9/10	0.62	0.25	43,49,64,67	0
7	TPO	T	11	11/12	0.65	0.26	52,69,96,97	0
7	TPO	G	11	11/12	0.68	0.26	65,74,106,115	0
1	FME	A	1	10/11	0.89	0.12	25,33,52,71	0
1	FME	N	1	10/11	0.90	0.12	18,28,48,58	0
2	FME	B	1	10/11	0.94	0.09	15,16,24,33	0
2	FME	O	1	10/11	0.96	0.08	15,16,24,24	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.

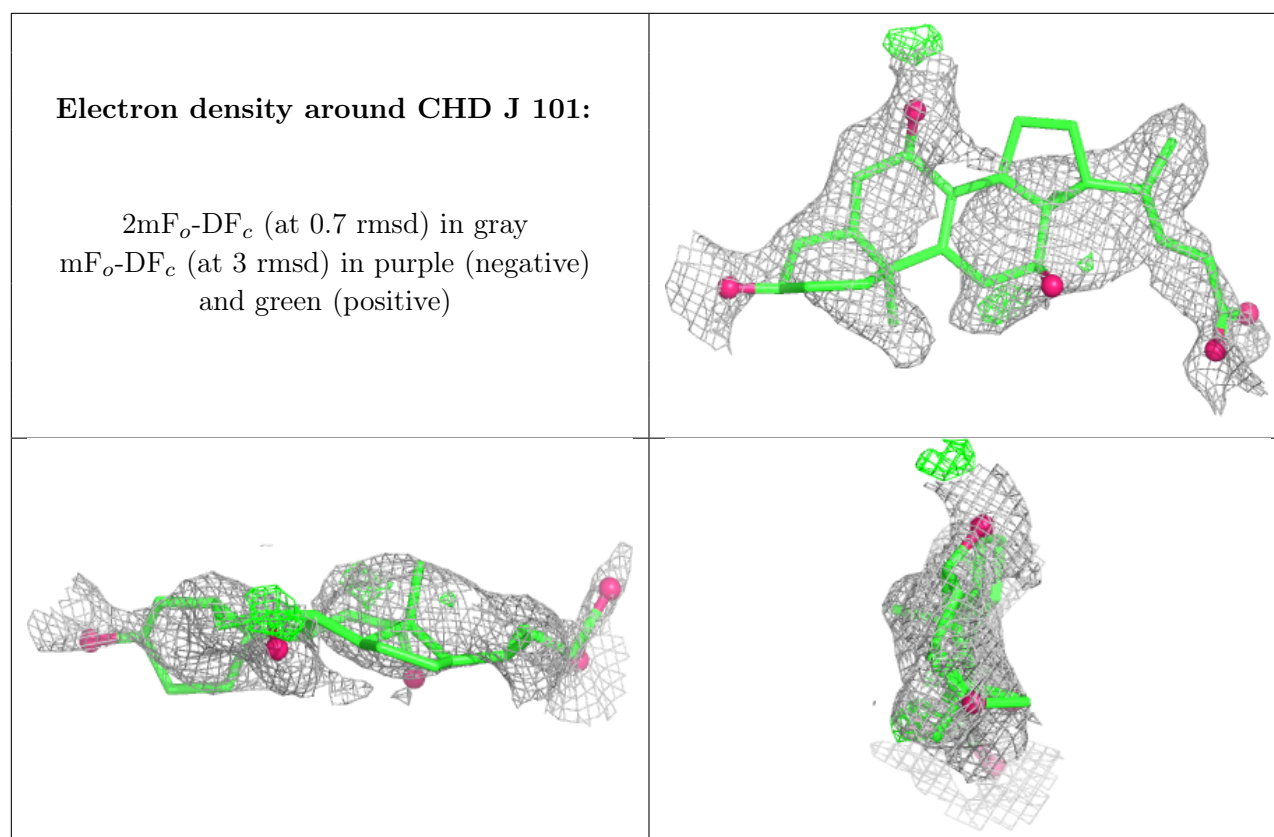
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	CHD	J	101	29/29	0.62	0.27	56,93,101,102	0
22	CHD	W	101	29/29	0.62	0.26	52,82,95,101	0
20	TGL	Q	201	63/63	0.71	0.20	30,47,66,71	0
19	PGV	P	301	51/51	0.73	0.22	45,70,102,114	0
24	PEK	C	307	53/53	0.74	0.22	34,59,94,103	0
19	PGV	C	308	51/51	0.75	0.21	34,64,99,101	0
24	PEK	G	102	53/53	0.75	0.23	37,71,111,121	0
25	CDL	T	102	100/100	0.75	0.22	31,67,118,128	0
24	PEK	T	101	53/53	0.76	0.26	36,76,114,118	0
25	CDL	G	101	100/100	0.77	0.20	34,66,99,138	0
20	TGL	Y	101	63/63	0.78	0.20	33,49,76,81	0
19	PGV	N	607	51/51	0.78	0.20	27,49,103,114	0
23	PSC	B	304	52/52	0.79	0.22	36,84,130,137	0
22	CHD	P	306	29/29	0.79	0.15	34,44,49,56	0
24	PEK	P	308	53/53	0.80	0.20	25,55,100,118	0
20	TGL	L	101	63/63	0.80	0.19	28,44,70,80	0
19	PGV	A	608	51/51	0.80	0.19	24,51,72,84	0
25	CDL	P	305	100/100	0.80	0.20	28,60,102,116	0
20	TGL	D	201	63/63	0.80	0.18	23,45,66,74	0
23	PSC	N	610	52/52	0.81	0.21	24,61,117,126	0
22	CHD	C	305	29/29	0.81	0.14	41,47,53,59	0
25	CDL	C	304	100/100	0.82	0.19	26,59,88,108	0
20	TGL	N	609	63/63	0.83	0.17	31,54,73,76	0
20	TGL	B	301	63/63	0.84	0.17	28,51,75,84	0
17	NA	P	302	1/1	0.88	0.09	29,29,29,29	0
27	DMU	M	101	33/33	0.88	0.11	25,29,39,40	0
27	DMU	Z	101	33/33	0.88	0.10	18,31,34,39	0
16	MG	N	604	1/1	0.91	0.07	17,17,17,17	0
17	NA	C	301	1/1	0.93	0.22	37,37,37,37	0
22	CHD	B	303	29/29	0.93	0.07	8,10,13,19	0
24	PEK	P	303	53/53	0.94	0.11	13,29,70,77	0
22	CHD	P	307	29/29	0.94	0.07	12,19,23,26	0
24	PEK	C	302	53/53	0.94	0.12	13,33,60,65	0
22	CHD	C	306	29/29	0.95	0.07	17,21,25,29	0
22	CHD	G	103	29/29	0.95	0.06	8,10,12,16	0
17	NA	N	605	1/1	0.95	0.06	12,12,12,12	0
19	PGV	C	303	51/51	0.95	0.10	13,22,55,63	0
19	PGV	N	608	51/51	0.95	0.10	12,30,49,58	0
19	PGV	A	607	51/51	0.96	0.10	13,26,49,57	0
19	PGV	P	304	51/51	0.96	0.09	12,27,51,54	0
14	HEA	A	601	60/60	0.97	0.08	10,12,37,46	0
14	HEA	A	602	60/60	0.97	0.06	9,12,18,19	0

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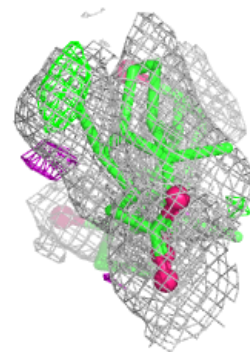
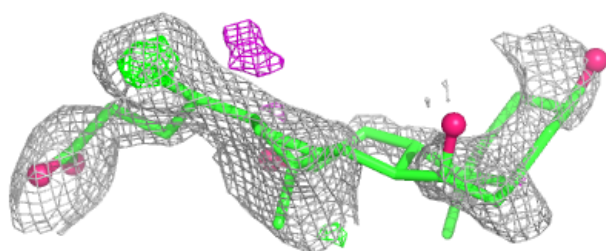
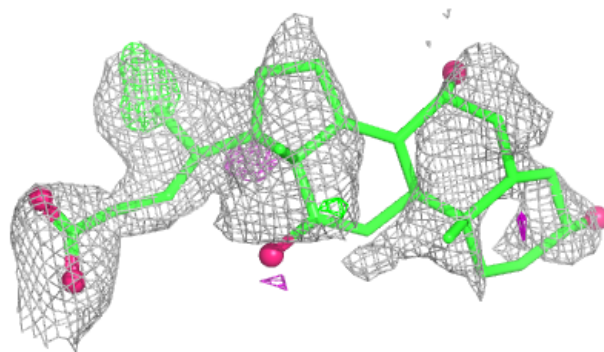
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
21	CUA	O	301	2/2	0.97	0.04	14,14,14,15	0
14	HEA	N	601	60/60	0.97	0.07	10,13,32,39	0
16	MG	A	604	1/1	0.97	0.06	14,14,14,14	0
14	HEA	N	602	60/60	0.98	0.06	9,12,18,21	0
18	PER	A	606[A]	2/2	0.98	0.18	10,10,10,12	0
18	PER	A	606[B]	2/2	0.98	0.18	11,11,11,11	2
18	PER	N	606[A]	2/2	0.98	0.08	10,10,10,12	0
18	PER	N	606[B]	2/2	0.98	0.08	11,11,11,11	2
17	NA	A	605	1/1	0.98	0.04	14,14,14,14	0
26	ZN	F	101	1/1	0.99	0.02	19,19,19,19	0
26	ZN	S	101	1/1	0.99	0.02	18,18,18,18	0
21	CUA	B	302	2/2	0.99	0.03	14,14,14,15	0
15	CU	N	603	1/1	0.99	0.04	14,14,14,14	0
15	CU	A	603	1/1	1.00	0.07	15,15,15,15	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.

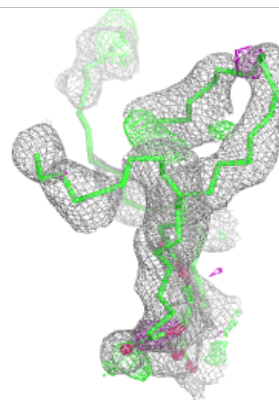
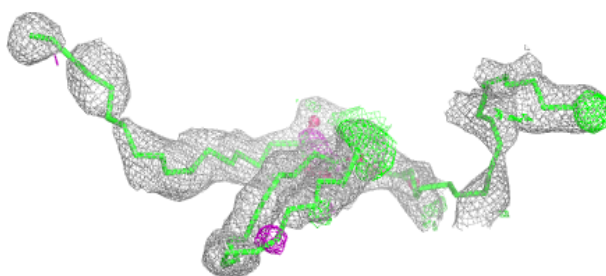
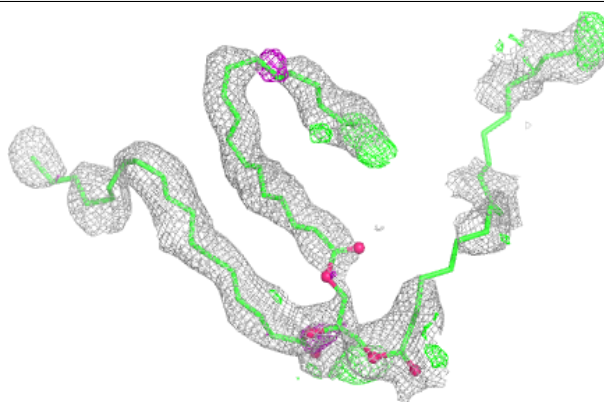


Electron density around CHD W 101:

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

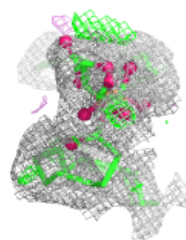
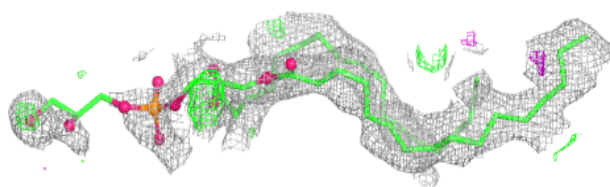
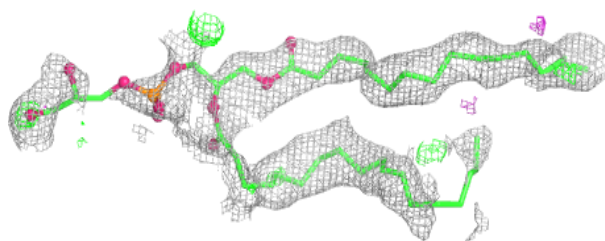
**Electron density around TGL Q 201:**

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



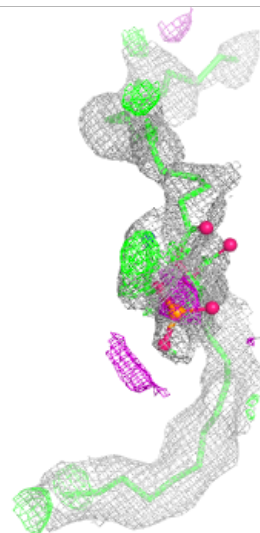
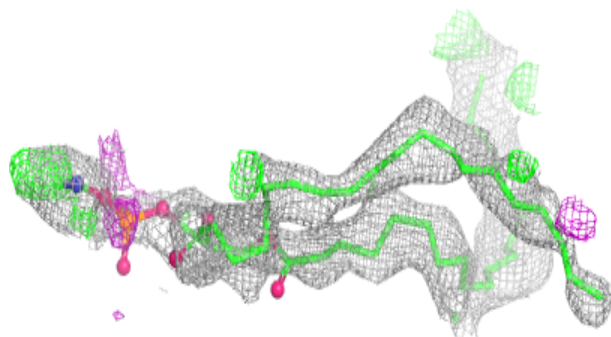
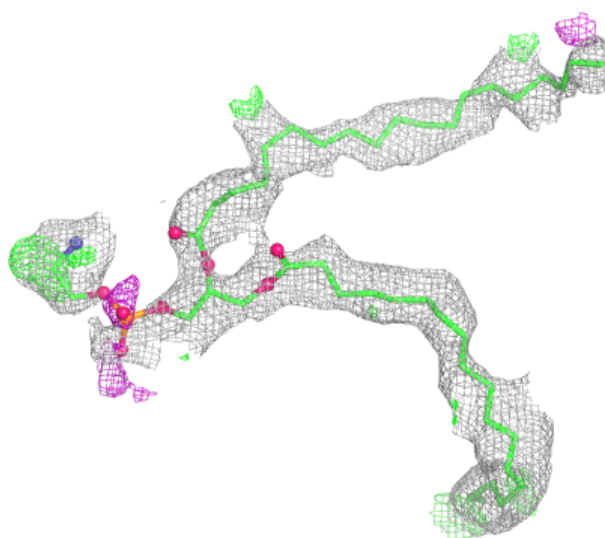
Electron density around PGV P 301:

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



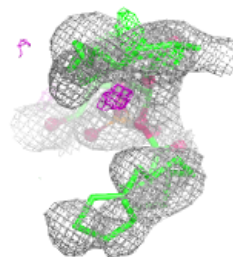
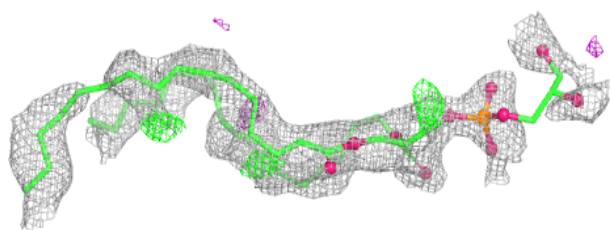
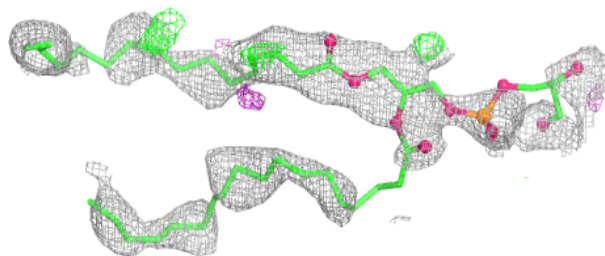
Electron density around PEK C 307:

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



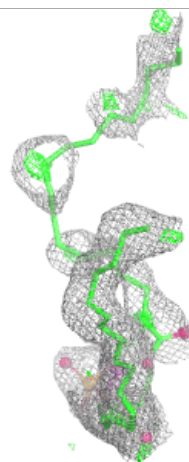
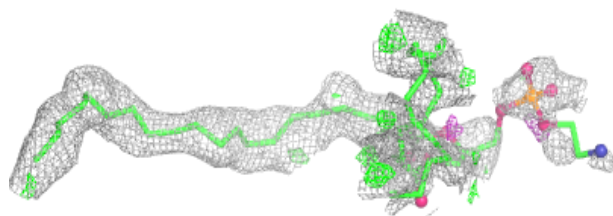
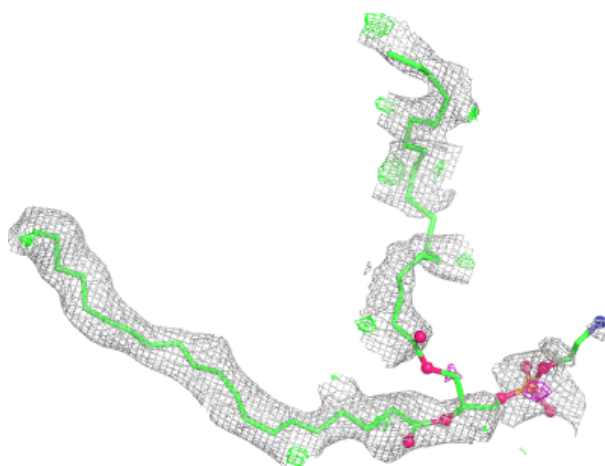
Electron density around PGV C 308:

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



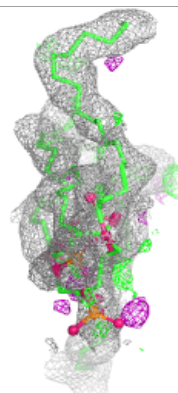
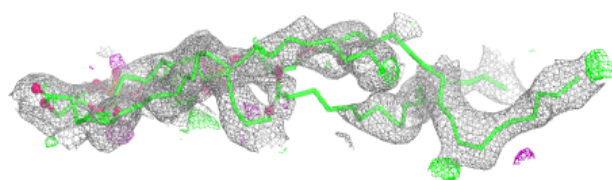
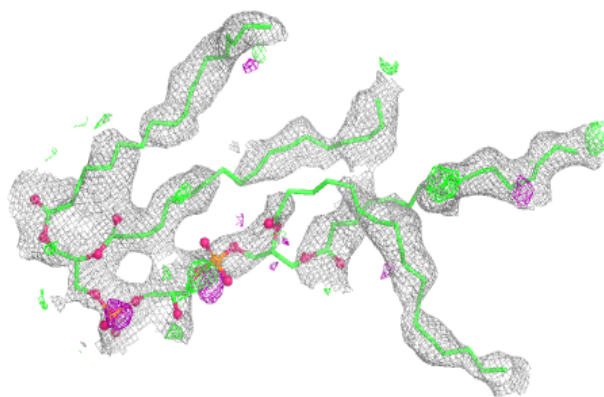
Electron density around PEK G 102:

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

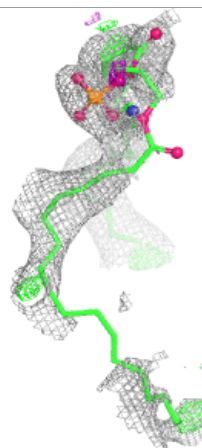
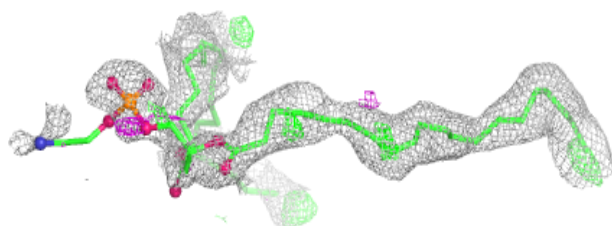
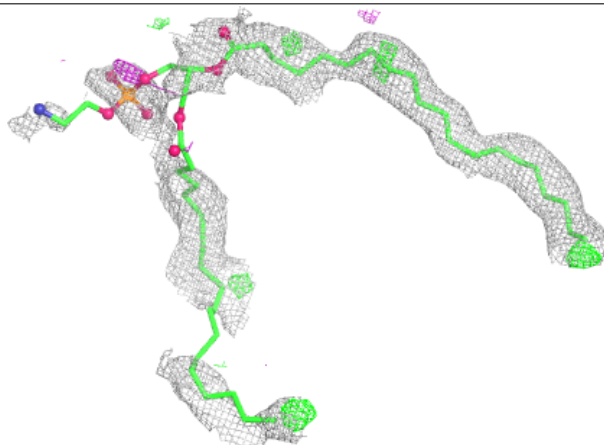


Electron density around CDL T 102:

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

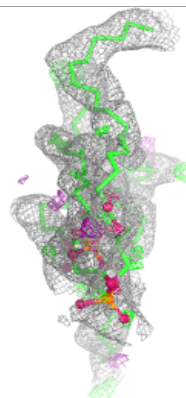
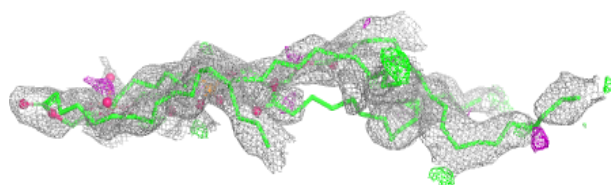
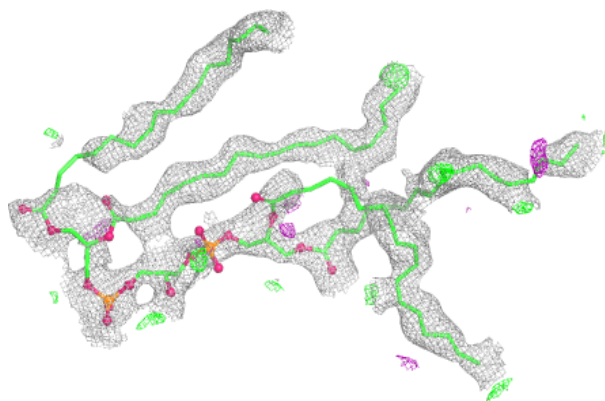
**Electron density around PEK T 101:**

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

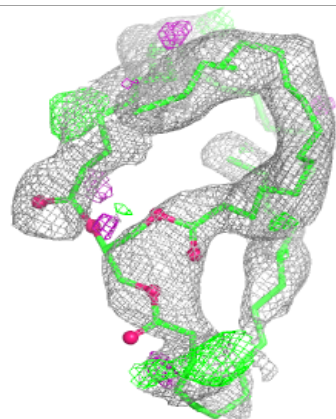
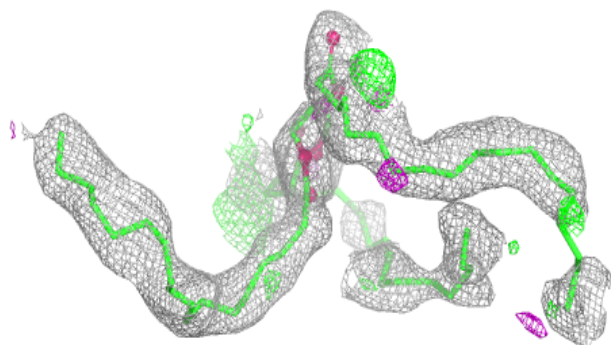
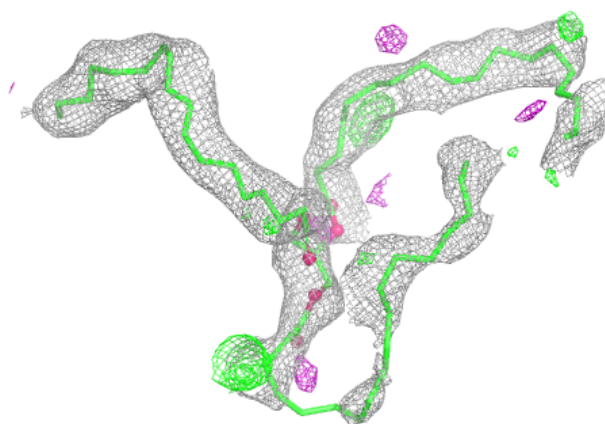


Electron density around CDL G 101:

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

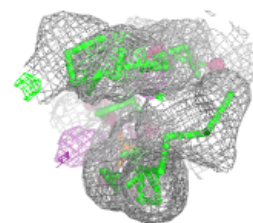
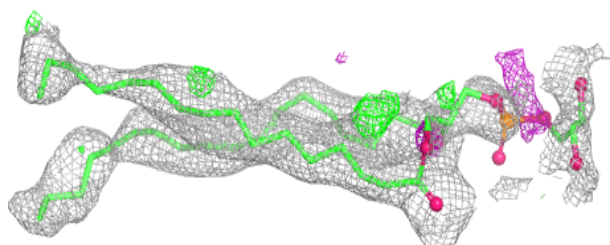
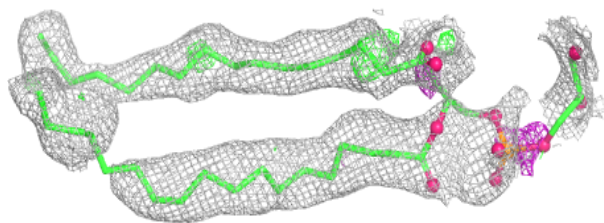
**Electron density around TGL Y 101:**

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

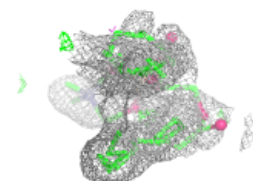
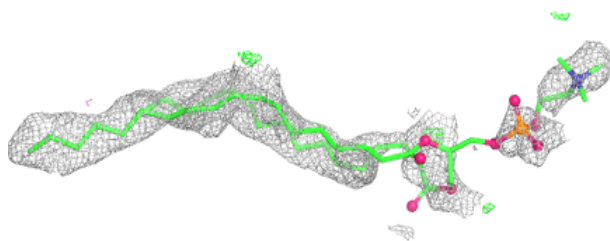
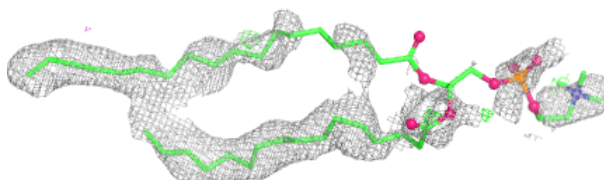


Electron density around PGV N 607:

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

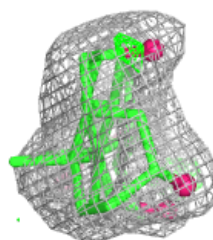
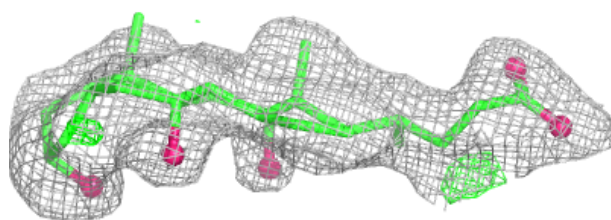
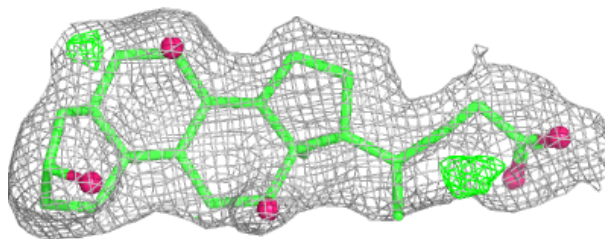
**Electron density around PSC B 304:**

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



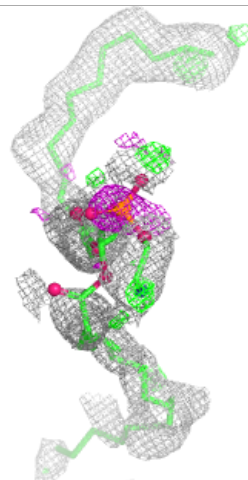
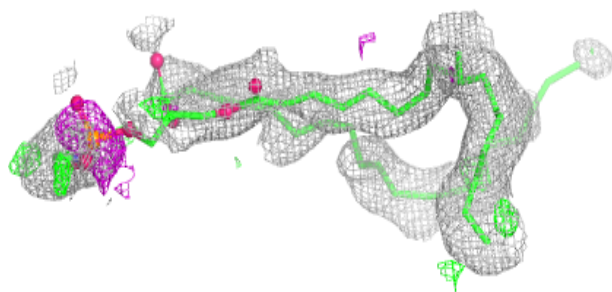
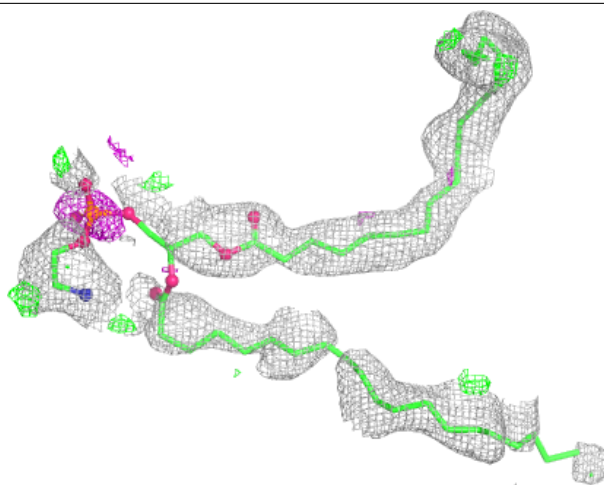
Electron density around CHD P 306:

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



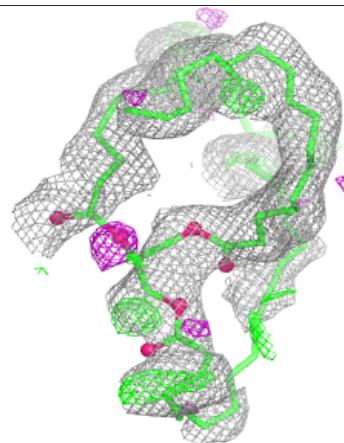
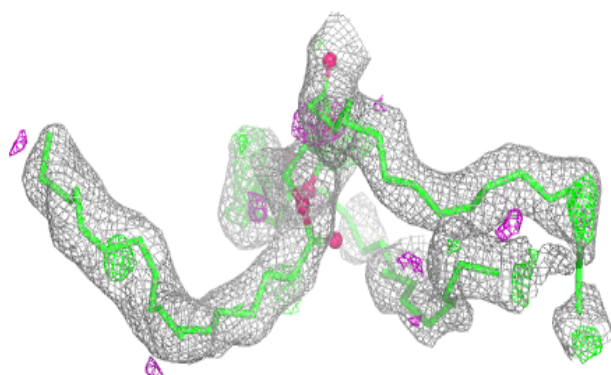
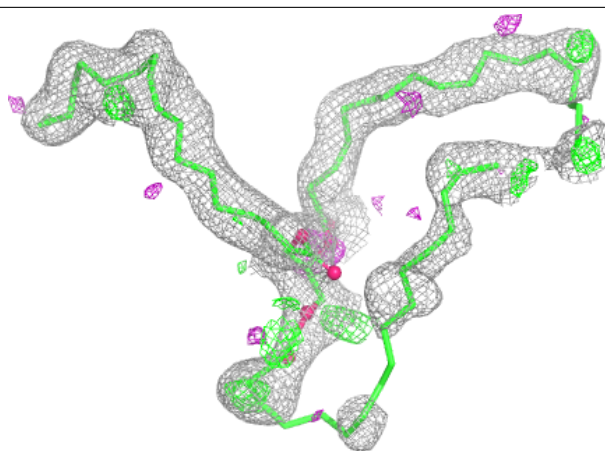
Electron density around PEK P 308:

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

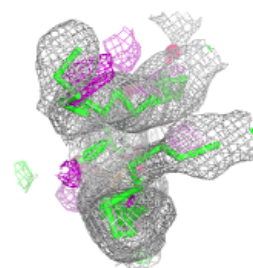
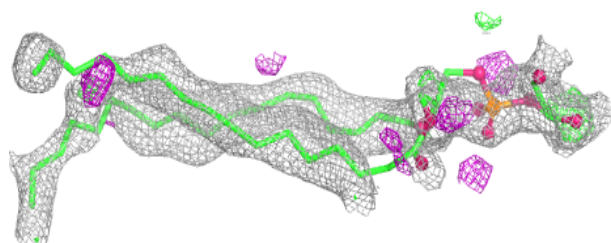
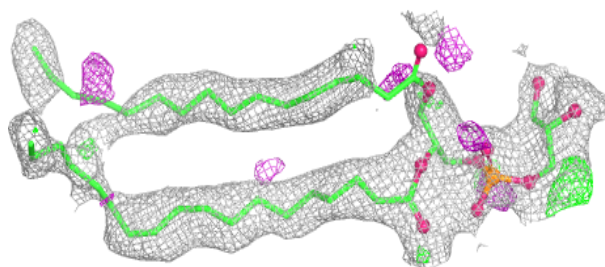


Electron density around TGL L 101:

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

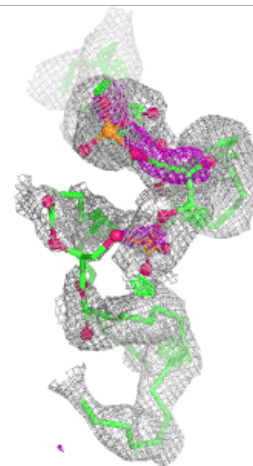
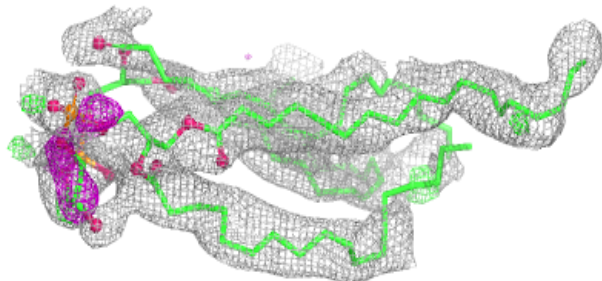
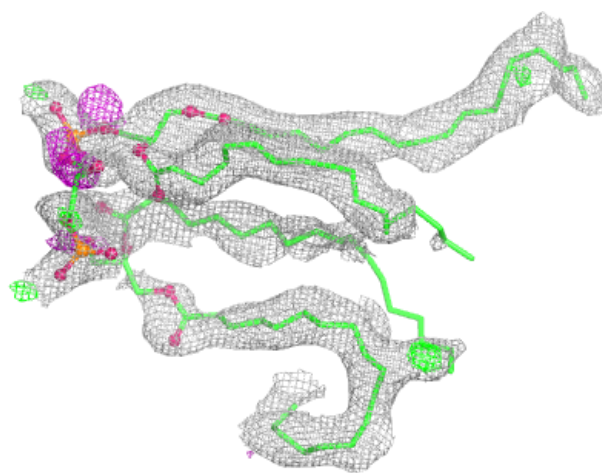
**Electron density around PGV A 608:**

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



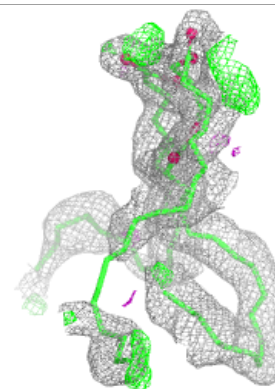
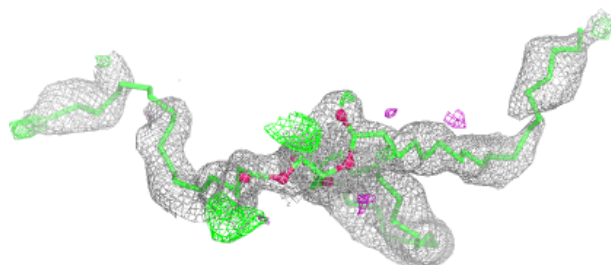
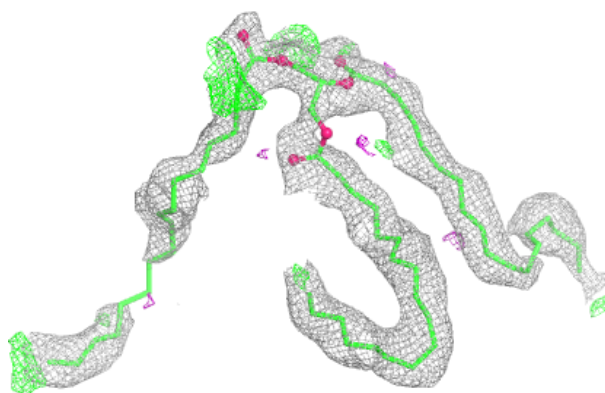
Electron density around CDL P 305:

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

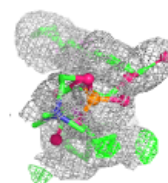
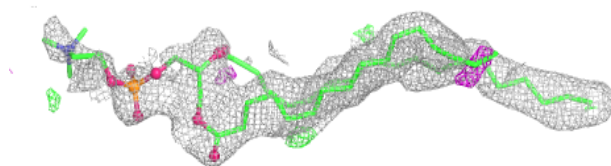
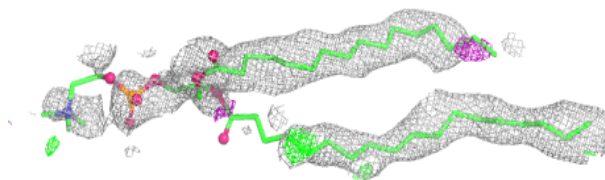


Electron density around TGL D 201:

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

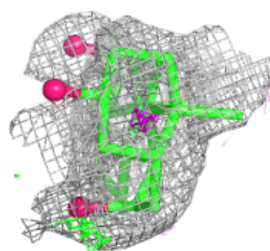
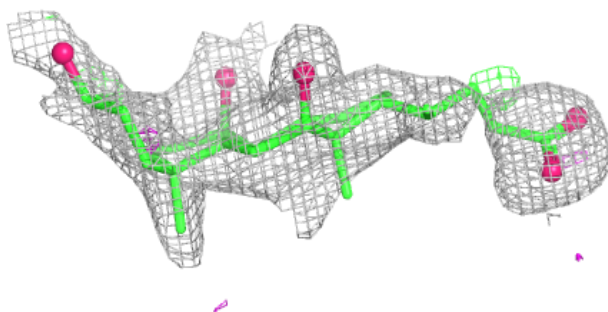
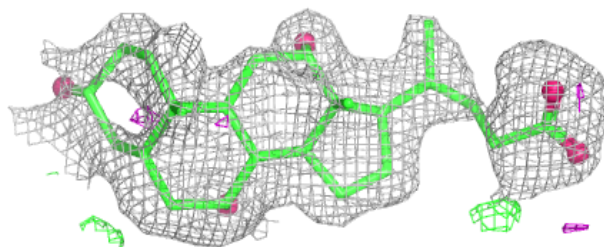
**Electron density around PSC N 610:**

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



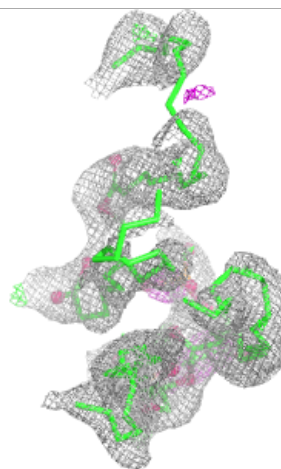
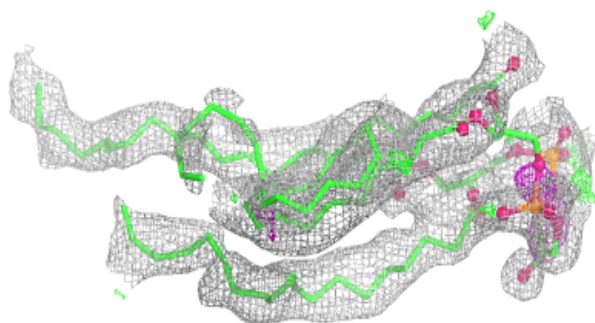
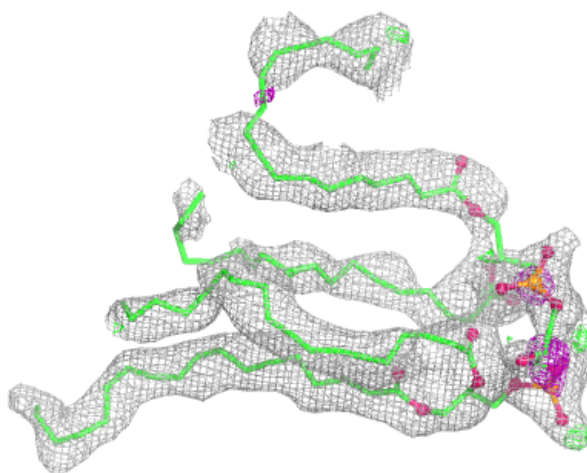
Electron density around CHD C 305:

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



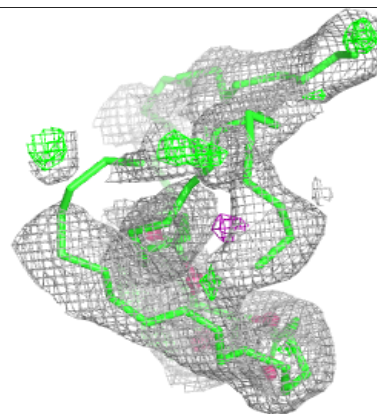
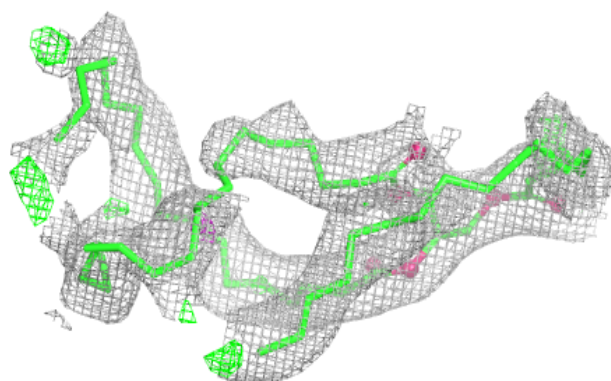
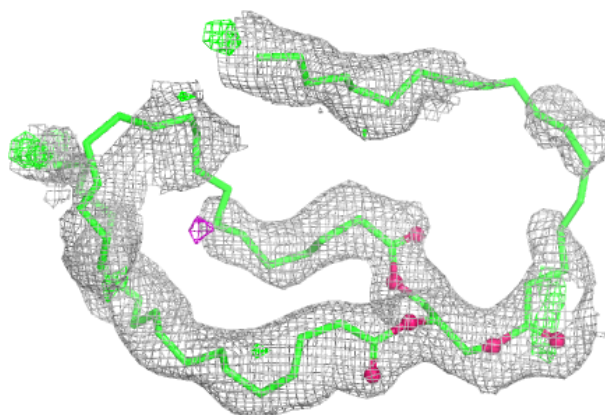
Electron density around CDL C 304:

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

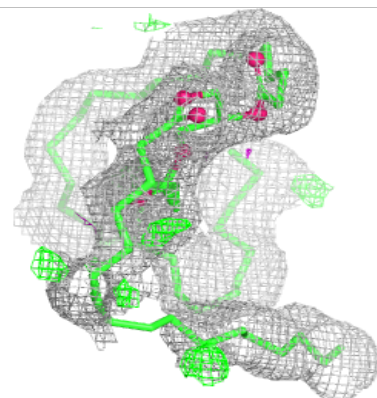
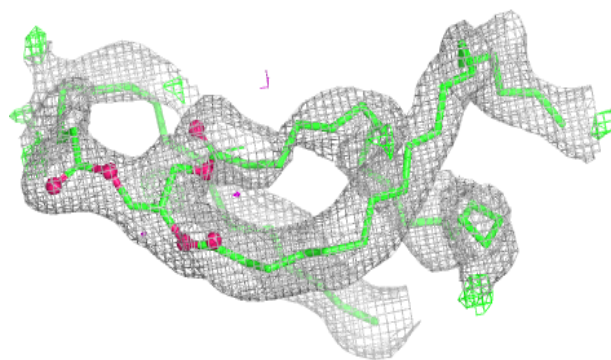
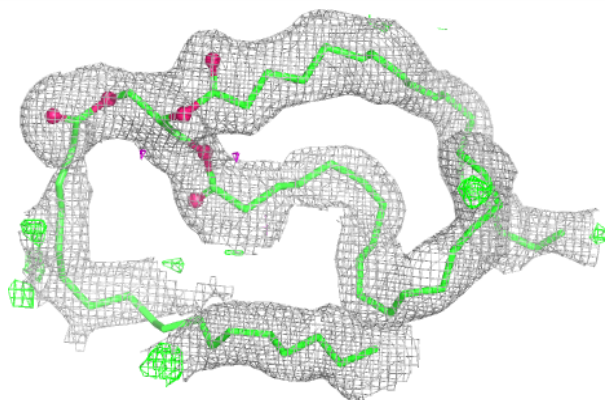


Electron density around TGL N 609:

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

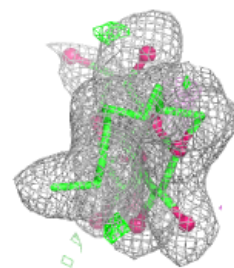
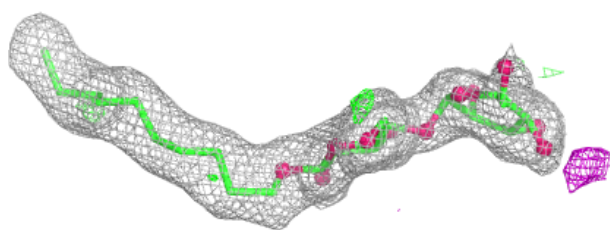
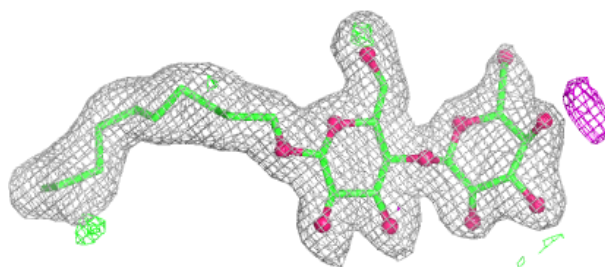
**Electron density around TGL B 301:**

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

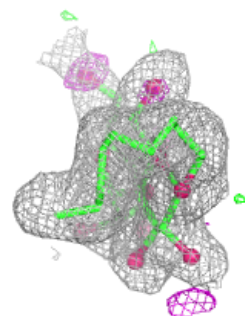
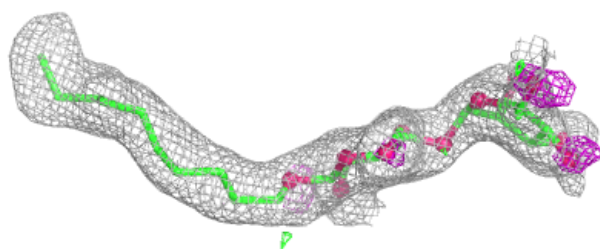
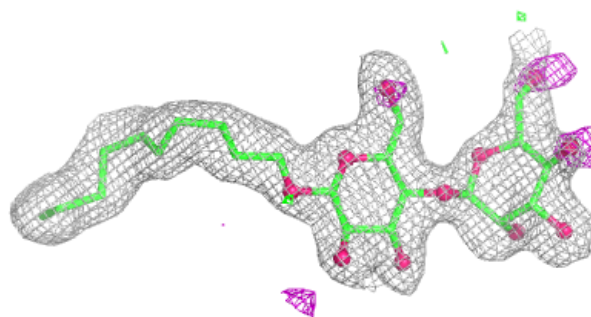


Electron density around DMU M 101:

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

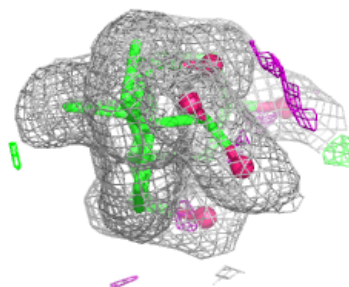
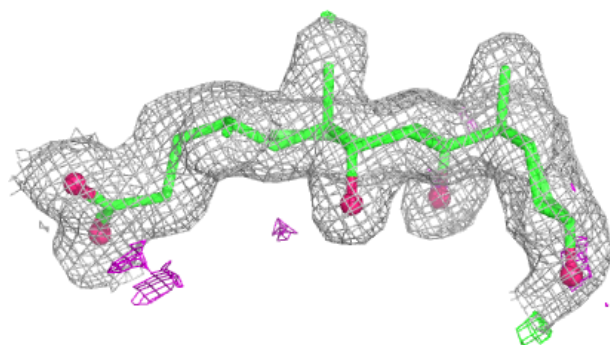
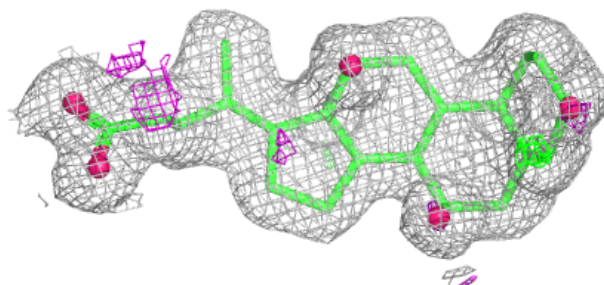
**Electron density around DMU Z 101:**

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

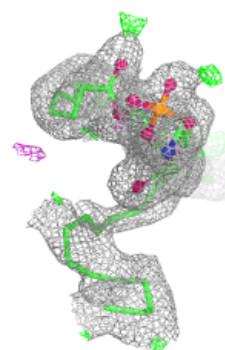
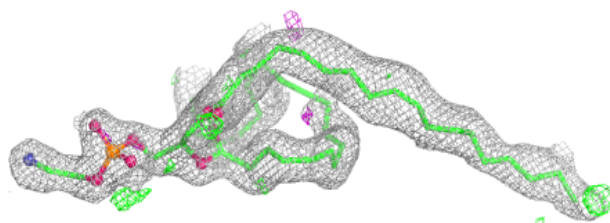
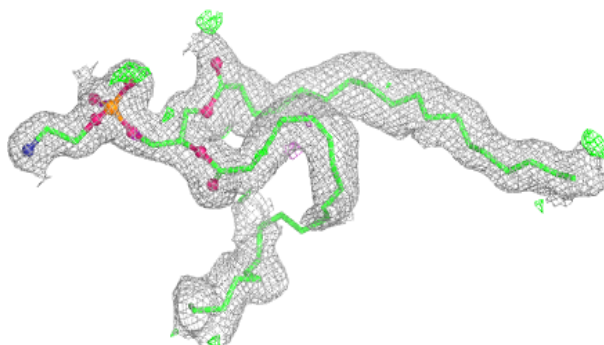


Electron density around CHD B 303:

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

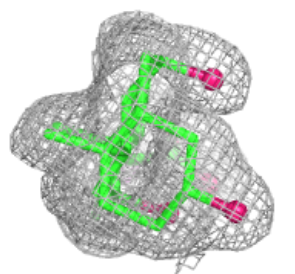
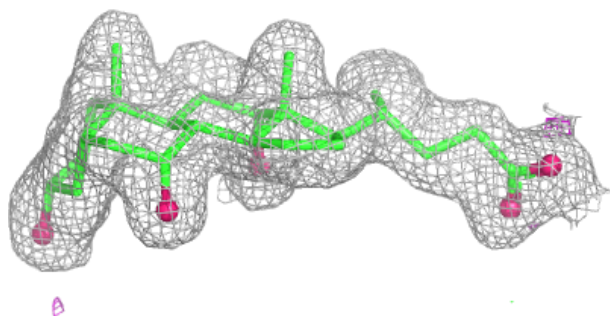
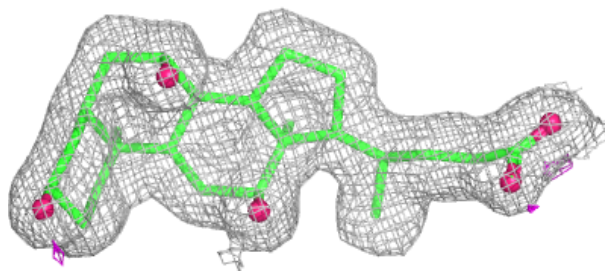
**Electron density around PEK P 303:**

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

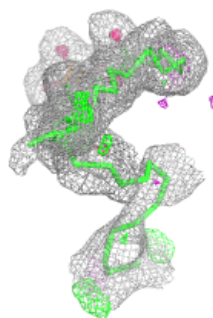
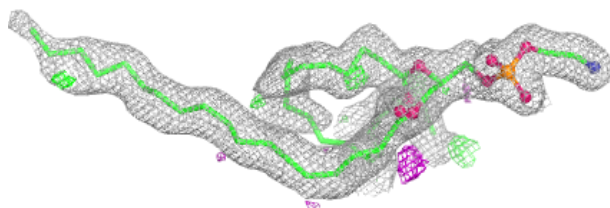
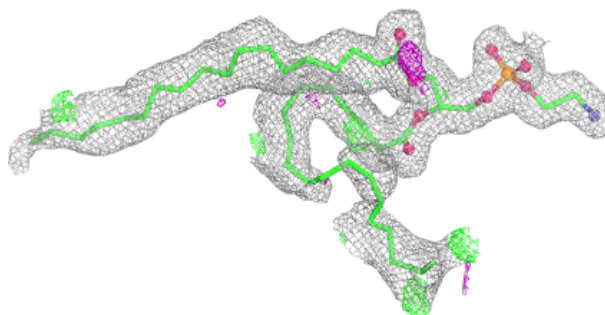


Electron density around CHD P 307:

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

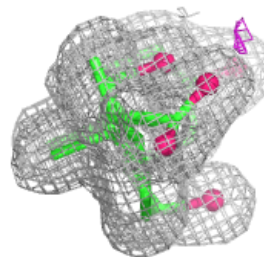
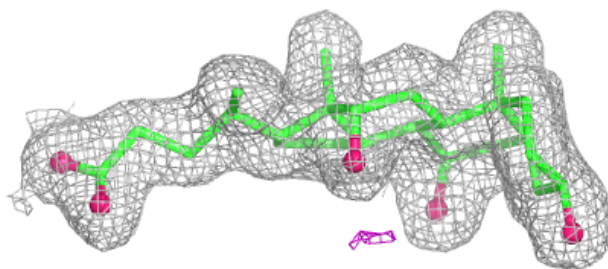
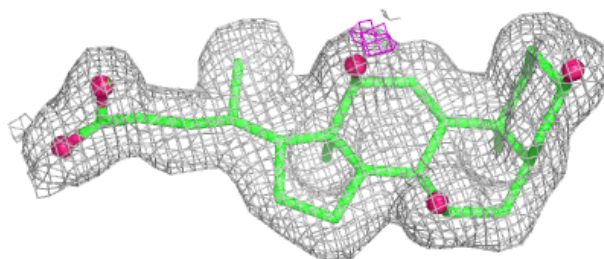
**Electron density around PEK C 302:**

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

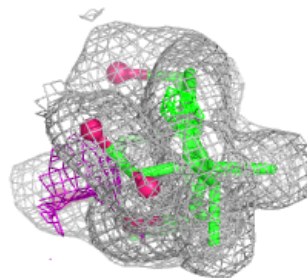
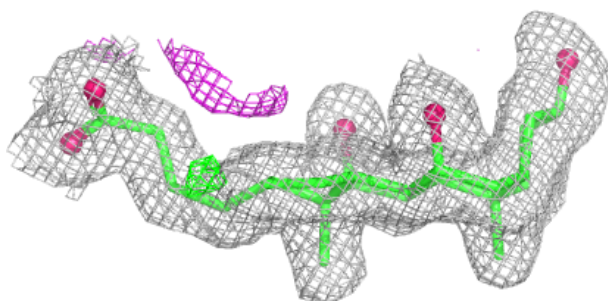
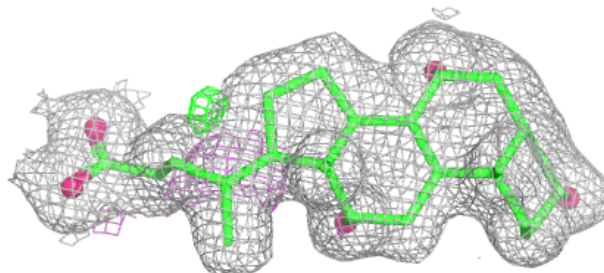


Electron density around CHD C 306:

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

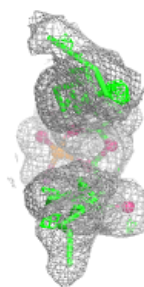
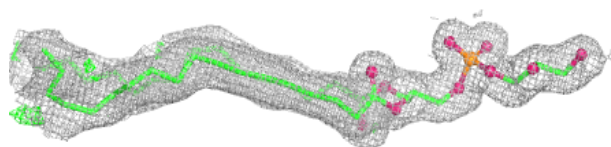
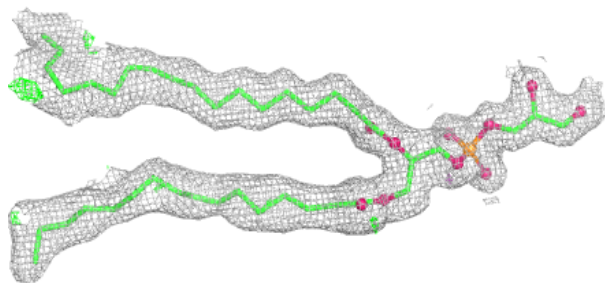
**Electron density around CHD G 103:**

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

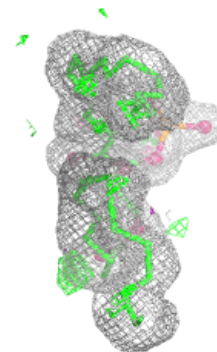
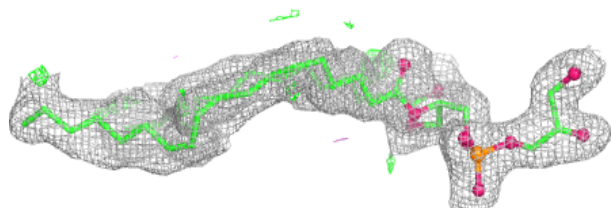
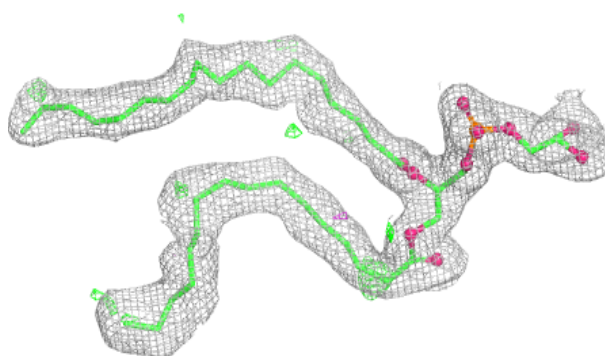


Electron density around PGV C 303:

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

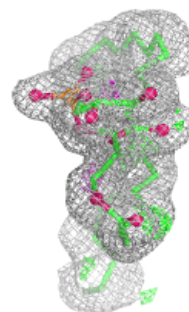
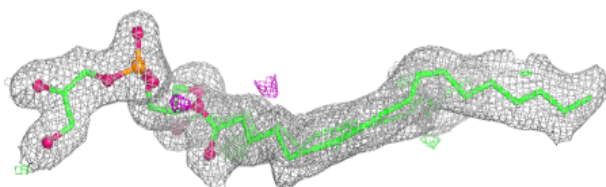
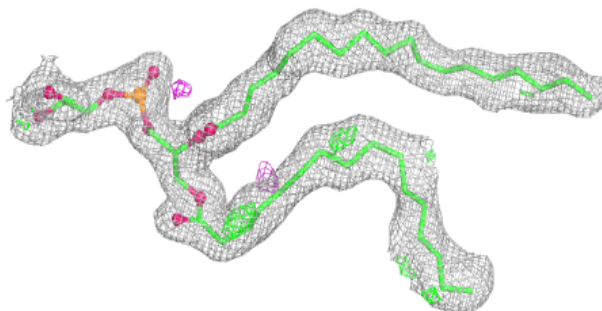
**Electron density around PGV N 608:**

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

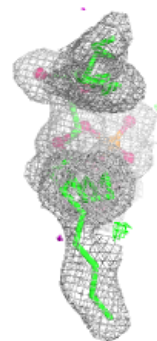
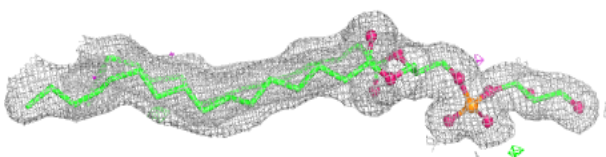
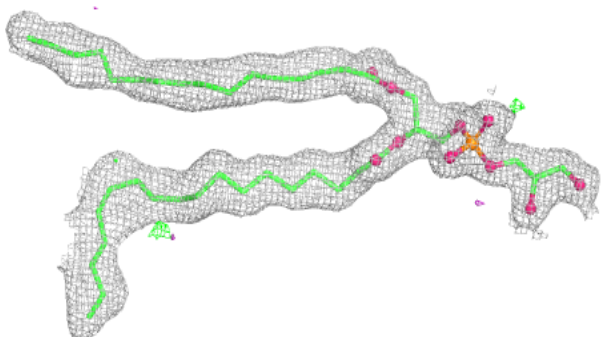


Electron density around PGV A 607:

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

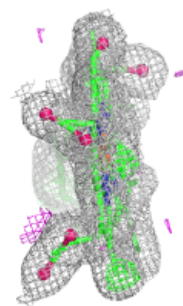
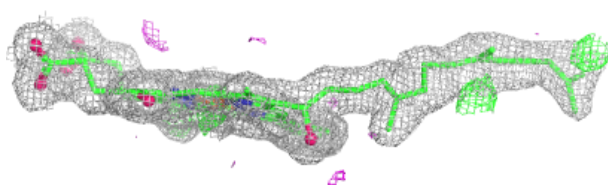
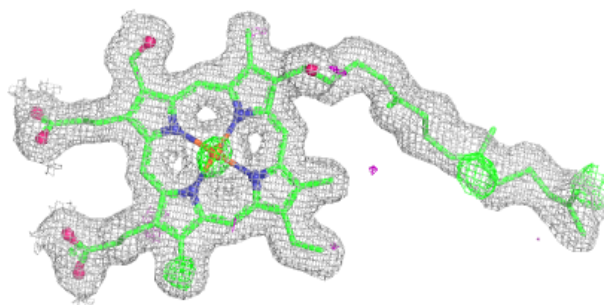
**Electron density around PGV P 304:**

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

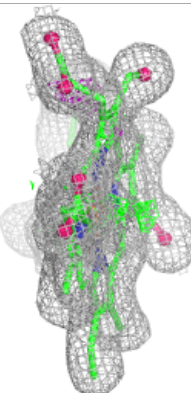
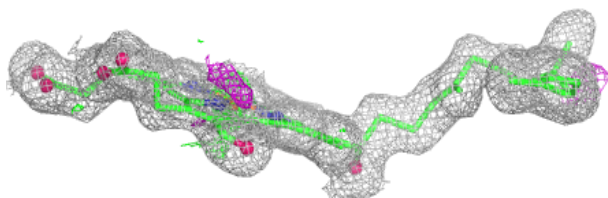
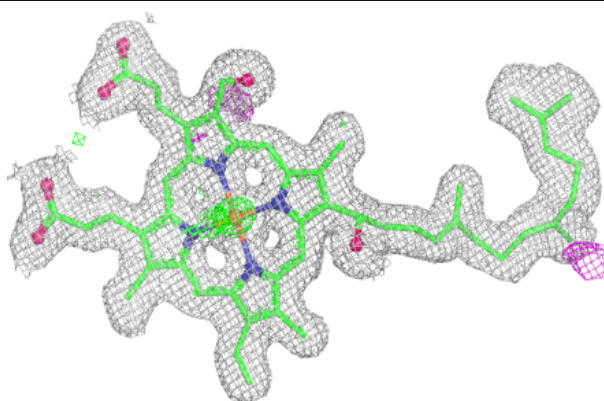


Electron density around HEA A 601:

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

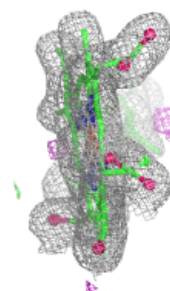
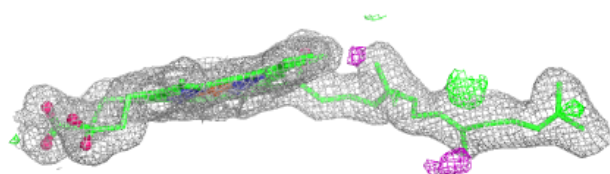
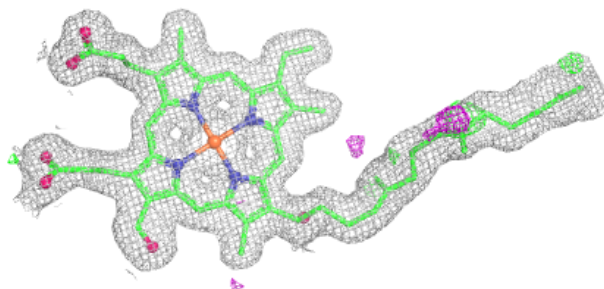
**Electron density around HEA A 602:**

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

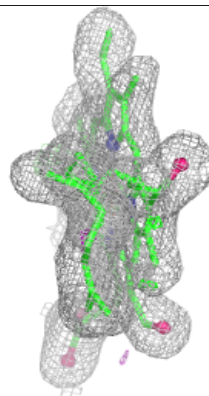
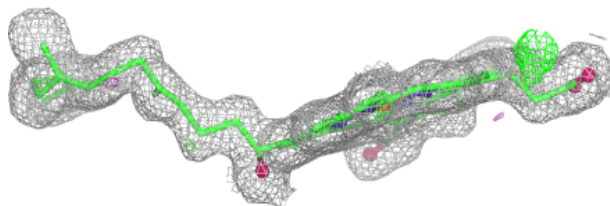
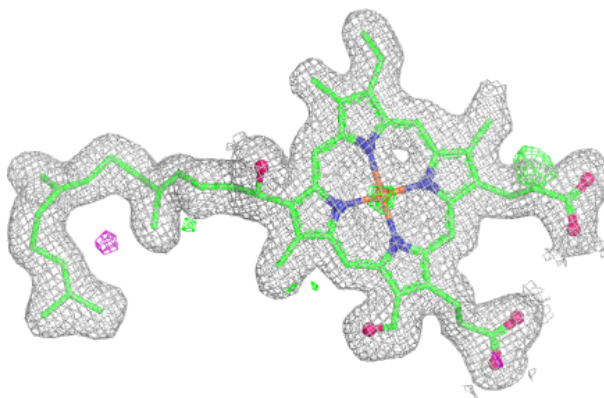


Electron density around HEA N 601:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.