



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 1, 2026 – 07:47 AM UTC

PDB ID : 6NMF / pdb_00006nmf
Title : SFX structure of reduced cytochrome c oxidase at room temperature
Authors : Rousseau, D.L.; Yeh, S.-R.; Ishigami, I.
Deposited on : 2019-01-10
Resolution : 2.80 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)
Xtrriage (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)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

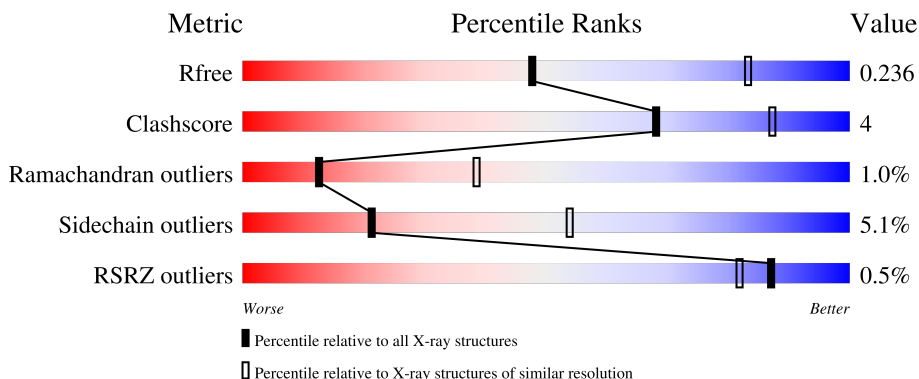
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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.
















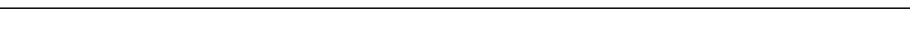




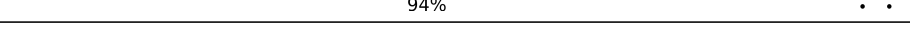


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	
2	O	227	
3	C	261	

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Mol	Chain	Length	Quality of chain
3	P	261	 87% 11% ..
4	D	147	 88% 9% ..
4	Q	147	 86% 12% .
5	E	109	 87% 9% .
5	R	109	 92% 5% .
6	F	98	 82% 13% 5%
6	S	98	 88% 7% 5%
7	G	85	 80% 14% 5% .
7	T	85	 81% 12% 6% .
8	H	85	 85% 8% 7%
8	U	85	 81% 12% 7%
9	I	73	 88% 11% .
9	V	73	 78% 16% ..
10	J	59	 93% 5% .
10	W	59	 83% 15% .
11	K	56	 82% 5% 12%
11	X	56	 66% 21% 12%
12	L	47	 94% ..
12	Y	47	 72% 19% 6% .
13	M	46	 85% 9% 7%
13	Z	46	 78% 15% 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
20	CDL	P	305	-	-	X	-

2 Entry composition [i](#)

There are 27 unique types of molecules in this entry. The entry contains 32083 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	514	Total	C	N	O	S	0	12	0
			4124	2753	638	693	40			
1	N	514	Total	C	N	O	S	0	13	0
			4131	2757	639	694	41			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	227	Total	C	N	O	S	0	6	0
			1874	1216	289	350	19			
2	O	227	Total	C	N	O	S	0	5	0
			1870	1215	289	348	18			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	105	Total	C	N	O	S	0	1	0
			863	550	148	163	2			
5	R	105	Total	C	N	O	S	0	0	0
			852	544	144	162	2			

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

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

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

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

- Molecule 8 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	79	Total	C	N	O	S	0	0	0
			662	417	121	119	5			
8	U	79	Total	C	N	O	S	0	0	0
			662	417	121	119	5			

- Molecule 9 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			
9	V	73	Total	C	N	O	S	0	1	0
			609	395	108	101	5			

- 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	1	0
			391	255	66	68	2			
11	X	49	Total	C	N	O	S	0	1	0
			391	255	66	68	2			

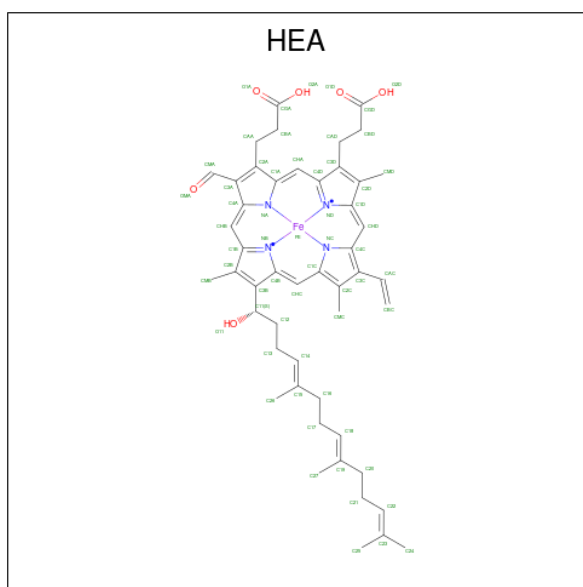
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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: C₄₉H₅₆FeN₄O₆).



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

- Molecule 15 is COPPER (II) ION (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		

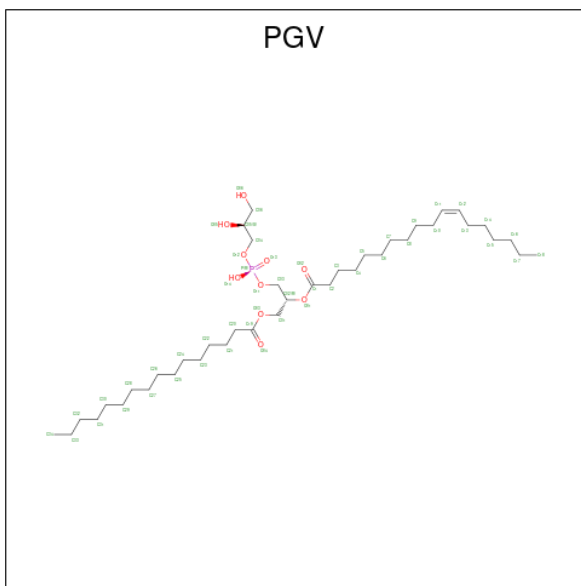
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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).

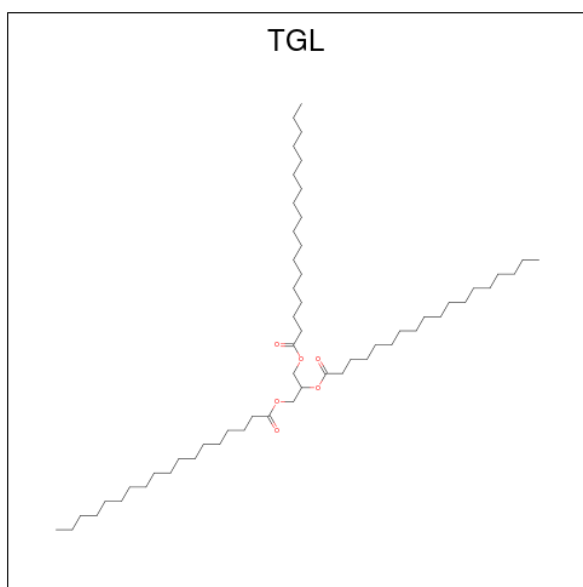
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Na 1 1	0	0
17	N	1	Total Na 1 1	0	0

- Molecule 18 is (1R)-2-{{[[[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P).



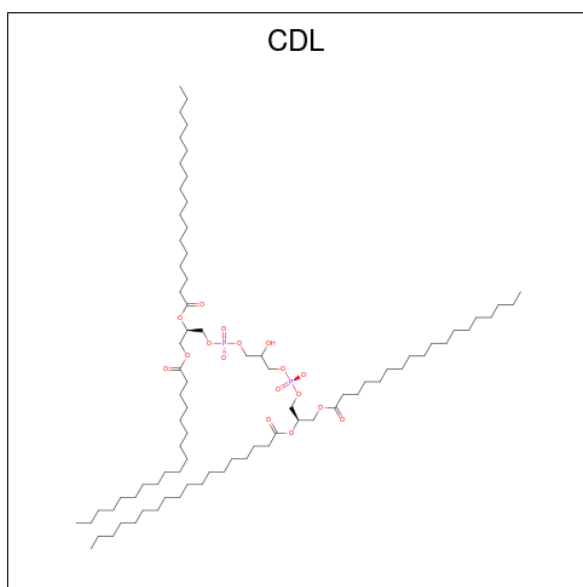
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total C O P 51 40 10 1	0	0
18	A	1	Total C O P 51 40 10 1	0	0
18	C	1	Total C O P 51 40 10 1	0	0
18	C	1	Total C O P 51 40 10 1	0	0
18	N	1	Total C O P 51 40 10 1	0	0
18	P	1	Total C O P 51 40 10 1	0	0
18	P	1	Total C O P 51 40 10 1	0	0
18	P	1	Total C O P 51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

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



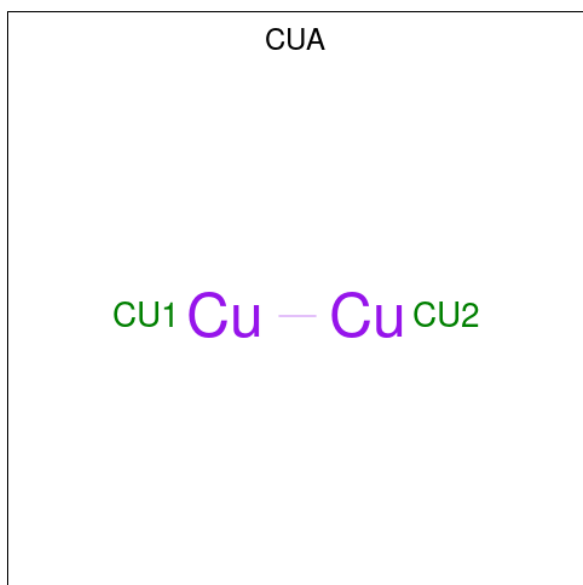
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	C	O	0	0
			63	57	6		
19	B	1	Total	C	O	0	0
			63	57	6		
19	D	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		
19	V	1	Total	C	O	0	0
			63	57	6		
19	Y	1	Total	C	O	0	0
			63	57	6		

- Molecule 20 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



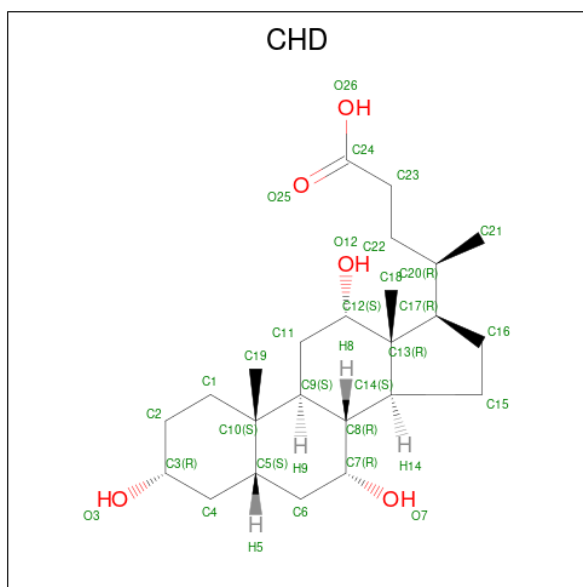
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
20	A	1	100	81	17	2	0	0
20	C	1	100	81	17	2	0	0
20	G	1	100	81	17	2	0	0
20	P	1	100	81	17	2	0	0

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



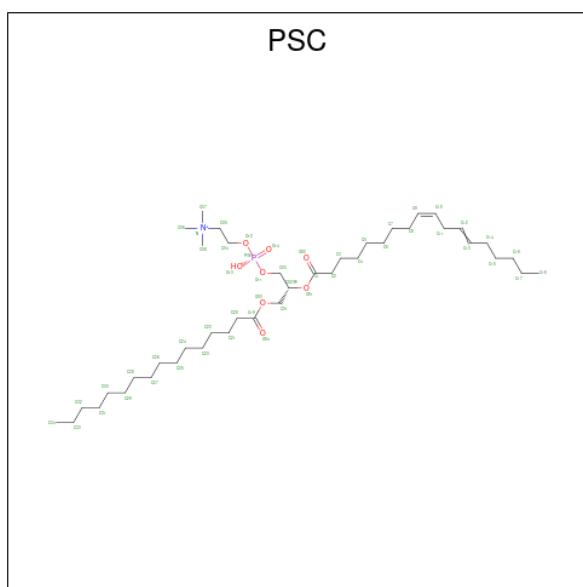
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	B	1	Total Cu 2 2	0	0
21	O	1	Total Cu 2 2	0	0

- Molecule 22 is CHOLIC ACID (CCD ID: CHD) (formula: $C_{24}H_{40}O_5$).



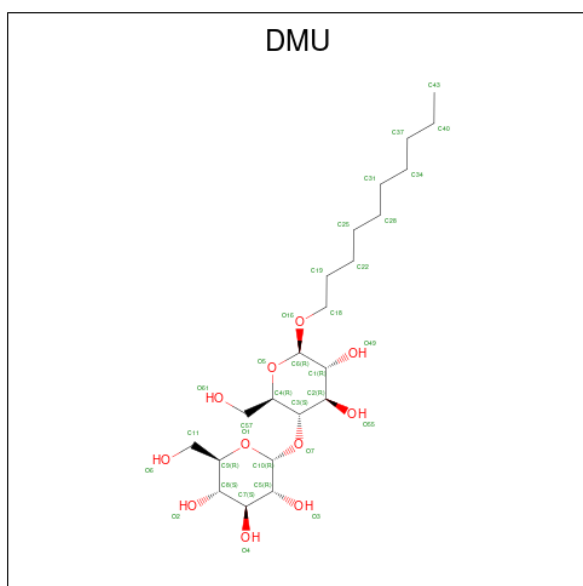
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	B	1	Total C O 29 24 5	0	0
22	C	1	Total C O 29 24 5	0	0
22	C	1	Total C O 29 24 5	0	0
22	G	1	Total C O 29 24 5	0	0
22	J	1	Total C O 29 24 5	0	0
22	P	1	Total C O 29 24 5	0	0
22	P	1	Total C O 29 24 5	0	0
22	W	1	Total C O 29 24 5	0	0

- 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 DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: $C_{22}H_{42}O_{11}$).



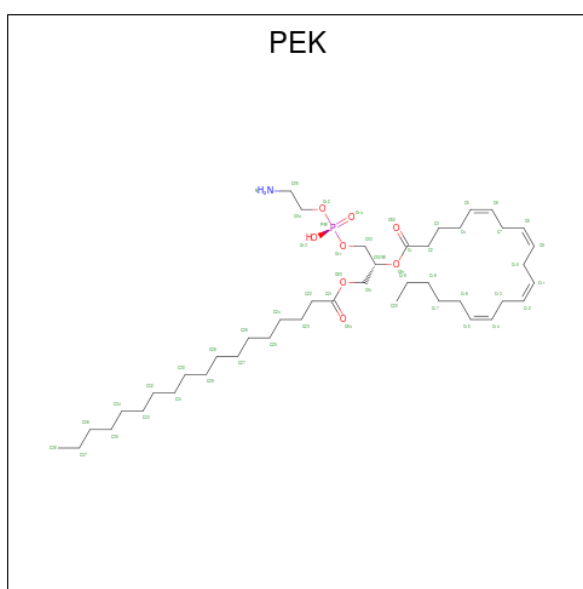
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	C	1	Total	C	O	0	0
			33	22	11		

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

- Molecule 25 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
			Total	C	N	O	P		
25	C	1	53	43	1	8	1	0	0
25	G	1	53	43	1	8	1	0	0
25	G	1	53	43	1	8	1	0	0
25	P	1	53	43	1	8	1	0	0
25	P	1	53	43	1	8	1	0	0
25	T	1	53	43	1	8	1	0	0

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

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

- Molecule 27 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	A	123	Total 123	O 123	0	0
27	B	74	Total 74	O 74	0	0
27	C	57	Total 57	O 57	0	0
27	D	32	Total 32	O 32	0	0
27	E	28	Total 28	O 28	0	0
27	F	28	Total 28	O 28	0	0
27	G	24	Total 24	O 24	0	0
27	H	21	Total 21	O 21	0	0
27	I	20	Total 20	O 20	0	0
27	J	11	Total 11	O 11	0	0
27	K	2	Total 2	O 2	0	0
27	L	24	Total 24	O 24	0	0
27	M	4	Total 4	O 4	0	0
27	N	83	Total 83	O 83	0	0
27	O	52	Total 52	O 52	0	0
27	P	39	Total 39	O 39	0	0
27	Q	22	Total 22	O 22	0	0
27	R	14	Total 14	O 14	0	0

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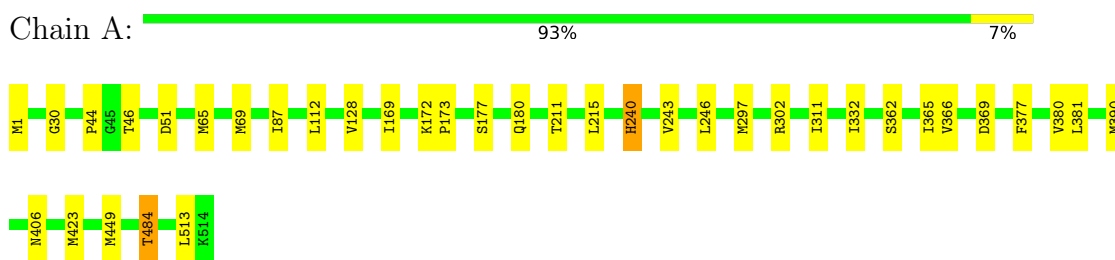
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	S	21	Total O 21 21	0	0
27	T	20	Total O 20 20	0	0
27	U	13	Total O 13 13	0	0
27	V	16	Total O 16 16	0	0
27	W	5	Total O 5 5	0	0
27	X	5	Total O 5 5	0	0
27	Y	2	Total O 2 2	0	0
27	Z	4	Total O 4 4	0	0

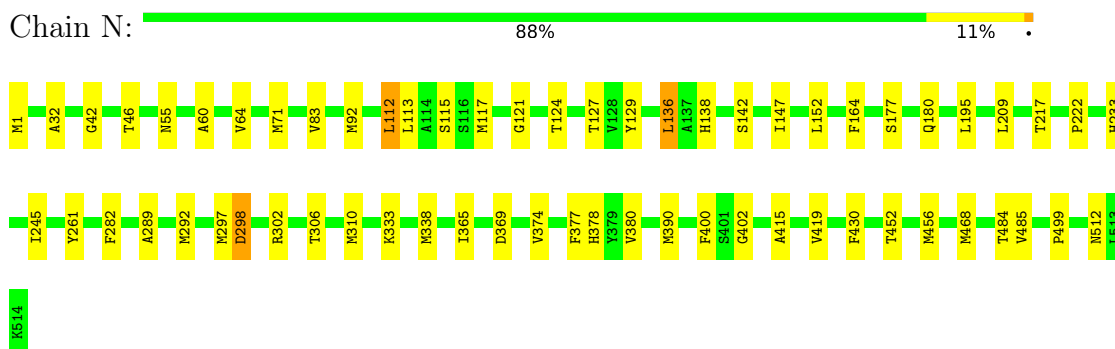
3 Residue-property plots [i](#)

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

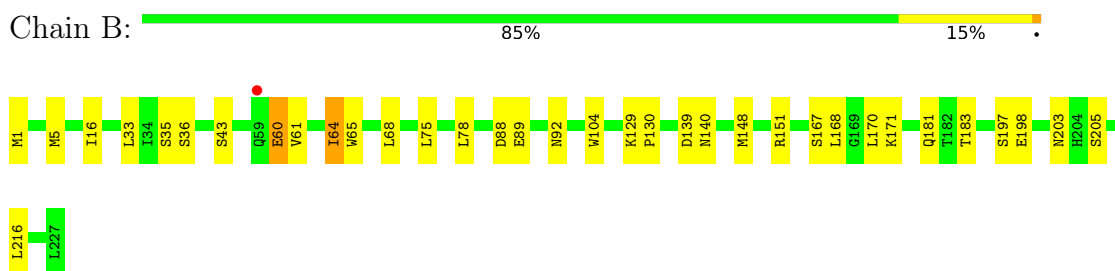
- Molecule 1: Cytochrome c oxidase subunit 1



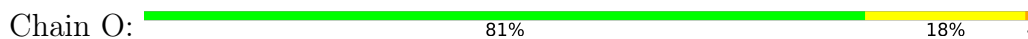
- Molecule 1: Cytochrome c oxidase subunit 1

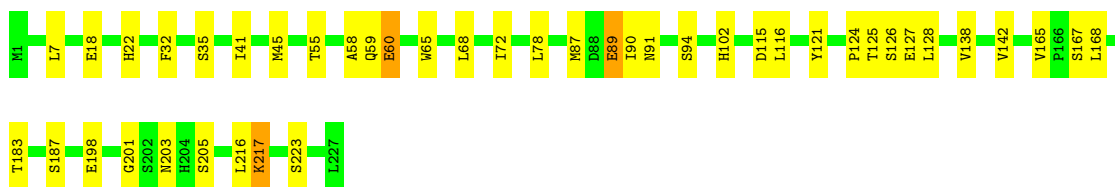


- Molecule 2: Cytochrome c oxidase subunit 2



- Molecule 2: Cytochrome c oxidase subunit 2





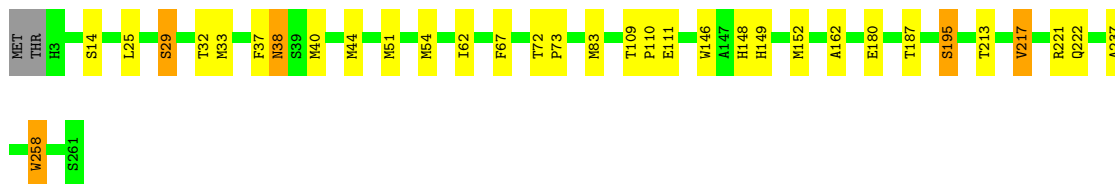
- Molecule 3: Cytochrome c oxidase subunit 3

Chain C: 94% 5%



- Molecule 3: Cytochrome c oxidase subunit 3

Chain P: 87% 11% ..



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

Chain D: 88% 9% ..



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

Chain Q: 86% 12% .



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

Chain E: 87% 9% .

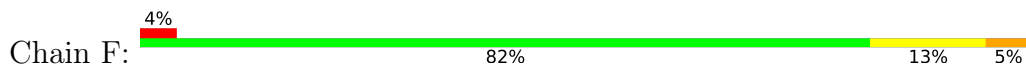


- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

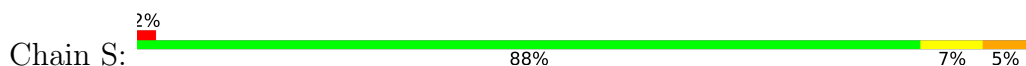
Chain R: 92% 5% .



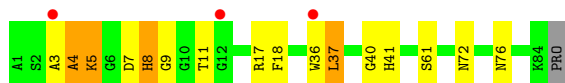
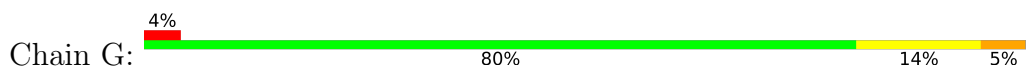
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



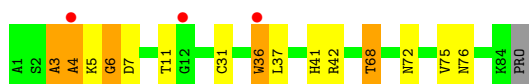
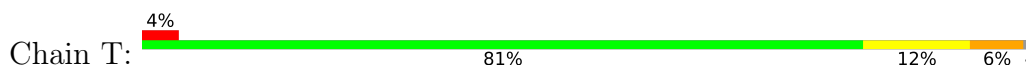
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



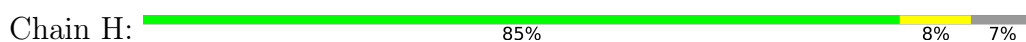
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



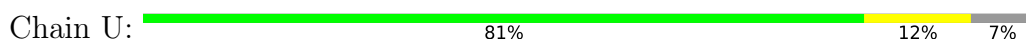
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



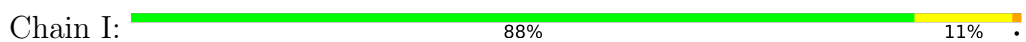
- Molecule 8: Cytochrome c oxidase subunit 6B1



- Molecule 8: Cytochrome c oxidase subunit 6B1

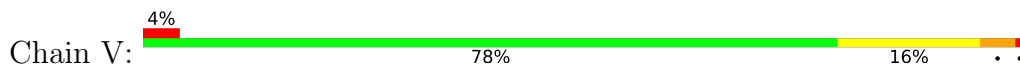


- Molecule 9: Cytochrome c oxidase subunit 6C





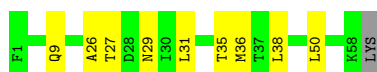
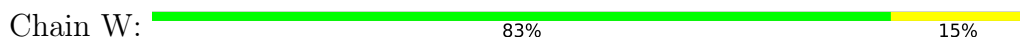
- Molecule 9: Cytochrome c oxidase subunit 6C



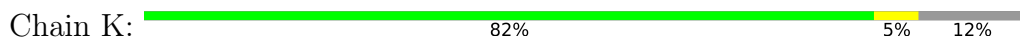
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



- 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

Chain M: 85% 9% 7%

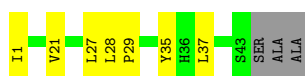
The validation bar for Chain M shows 85% green (good), 9% yellow (outliers), and 7% grey (not modeled).



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

Chain Z: 78% 15% 7%

The validation bar for Chain Z shows 78% green (good), 15% yellow (outliers), and 7% grey (not modeled).



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	178.70Å 189.80Å 211.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 15.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.3 (15.00-2.80) 99.3 (15.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 2.81Å)	Xtrriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.176 , 0.232 0.186 , 0.236	Depositor DCC
R_{free} test set	8641 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	68.0	Xtrriage
Anisotropy	0.092	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 81.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	32083	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% 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: DMU, FME, HEA, CDL, ZN, NA, CUA, TPO, MG, PGV, CHD, PSC, TGL, SAC, PEK, CU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.77	0/4253	0.98	1/5805 (0.0%)
1	N	0.76	1/4260 (0.0%)	1.03	1/5814 (0.0%)
2	B	0.83	1/1912 (0.1%)	1.03	1/2603 (0.0%)
2	O	0.80	1/1908 (0.1%)	0.99	1/2599 (0.0%)
3	C	0.73	0/2261	0.93	0/3090
3	P	0.73	0/2260	0.99	1/3088 (0.0%)
4	D	0.70	0/1284	0.95	2/1730 (0.1%)
4	Q	0.73	0/1237	0.98	1/1668 (0.1%)
5	E	0.72	0/882	0.93	0/1196
5	R	0.69	0/871	0.92	0/1182
6	F	0.84	0/806	1.04	1/1093 (0.1%)
6	S	0.75	0/772	0.95	1/1048 (0.1%)
7	G	0.82	0/702	0.89	0/953
7	T	0.78	1/724 (0.1%)	0.99	4/984 (0.4%)
8	H	0.79	0/682	0.97	0/921
8	U	0.75	0/682	0.94	0/921
9	I	0.78	0/605	0.98	0/802
9	V	0.80	0/613	1.08	1/812 (0.1%)
10	J	0.70	0/471	0.95	0/636
10	W	0.69	0/471	0.96	0/636
11	K	0.81	0/405	0.92	0/556
11	X	0.86	0/405	1.00	0/556
12	L	0.76	0/393	0.93	0/526
12	Y	0.76	0/393	0.96	0/526
13	M	0.79	0/345	1.00	0/470
13	Z	0.71	0/345	1.00	0/470
All	All	0.76	4/29942 (0.0%)	0.98	15/40685 (0.0%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	O	0	1
6	F	0	1
6	S	0	1
7	T	0	1
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	198	GLU	C-O	8.81	1.35	1.23
2	O	198	GLU	C-O	6.67	1.31	1.23
1	N	83	VAL	CA-CB	5.47	1.56	1.54
7	T	75	VAL	N-CA	5.10	1.50	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	T	6	GLY	N-CA-C	6.81	116.41	110.21
9	V	31	PHE	N-CA-C	-6.46	103.51	111.33
4	Q	108	PRO	N-CA-C	6.16	120.90	111.11
3	P	38	ASN	N-CA-C	6.10	123.79	110.80
1	A	240	HIS	N-CA-CB	6.07	117.58	110.42

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	F	93	PRO	Peptide
2	O	91	ASN	Peptide
6	S	94	HIS	Peptide
7	T	6	GLY	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4124	0	4102	19	0
1	N	4131	0	4107	39	0
2	B	1874	0	1869	13	0
2	O	1870	0	1867	15	0
3	C	2174	0	2082	7	0
3	P	2173	0	2083	28	0
4	D	1249	0	1242	9	0
4	Q	1203	0	1191	9	0
5	E	863	0	857	3	0
5	R	852	0	845	1	0
6	F	789	0	769	8	0
6	S	755	0	734	7	0
7	G	686	0	651	8	0
7	T	706	0	665	9	0
8	H	662	0	623	2	0
8	U	662	0	623	4	0
9	I	601	0	613	5	0
9	V	609	0	621	7	0
10	J	460	0	459	1	0
10	W	460	0	459	4	0
11	K	391	0	374	2	0
11	X	391	0	374	4	0
12	L	380	0	380	0	0
12	Y	380	0	380	6	0
13	M	335	0	352	2	0
13	Z	335	0	352	5	0
14	A	120	0	108	1	0
14	N	120	0	108	4	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	102	0	152	1	0
18	C	102	0	152	0	0
18	N	51	0	76	0	0
18	P	153	0	228	6	0
19	A	63	0	110	2	0
19	B	63	0	110	0	0
19	D	63	0	110	0	0
19	N	63	0	110	0	0
19	V	63	0	110	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	Y	63	0	110	1	0
20	A	100	0	156	5	0
20	C	100	0	156	0	0
20	G	100	0	156	4	0
20	P	100	0	156	22	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	29	0	39	0	0
22	C	58	0	78	0	0
22	G	29	0	39	1	0
22	J	29	0	39	2	0
22	P	58	0	78	0	0
22	W	29	0	38	1	0
23	B	52	0	80	0	0
23	N	52	0	80	0	0
24	C	33	0	42	2	0
24	M	33	0	42	0	0
24	P	33	0	42	1	0
24	Q	33	0	42	3	0
25	C	53	0	77	1	0
25	G	106	0	154	1	0
25	P	106	0	154	3	0
25	T	53	0	77	0	0
26	F	1	0	0	0	0
26	S	1	0	0	0	0
27	A	123	0	0	5	0
27	B	74	0	0	2	0
27	C	57	0	0	3	0
27	D	32	0	0	1	0
27	E	28	0	0	0	0
27	F	28	0	0	1	0
27	G	24	0	0	1	0
27	H	21	0	0	1	0
27	I	20	0	0	1	0
27	J	11	0	0	2	0
27	K	2	0	0	0	0
27	L	24	0	0	2	0
27	M	4	0	0	1	0
27	N	83	0	0	0	0
27	O	52	0	0	4	0
27	P	39	0	0	6	0
27	Q	22	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	R	14	0	0	0	0
27	S	21	0	0	1	0
27	T	20	0	0	0	0
27	U	13	0	0	1	0
27	V	16	0	0	6	0
27	W	5	0	0	2	0
27	X	5	0	0	0	0
27	Y	2	0	0	0	0
27	Z	4	0	0	0	0
All	All	32083	0	31883	227	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 4.

The worst 5 of 227 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)
20:P:305:CDL:H531	20:P:305:CDL:H641	1.21	1.14
1:A:65:MET:SD	27:A:811:HOH:O	2.24	0.95
3:P:258:TRP:CG	27:P:424:HOH:O	2.26	0.89
20:P:305:CDL:H531	20:P:305:CDL:C64	2.02	0.88
1:A:423:MET:SD	27:A:804:HOH:O	2.30	0.87

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	524/514 (102%)	504 (96%)	20 (4%)	0	100 100
1	N	525/514 (102%)	499 (95%)	26 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	231/227 (102%)	215 (93%)	13 (6%)	3 (1%)	9	31
2	O	230/227 (101%)	209 (91%)	17 (7%)	4 (2%)	7	25
3	C	265/261 (102%)	258 (97%)	5 (2%)	2 (1%)	16	44
3	P	265/261 (102%)	256 (97%)	8 (3%)	1 (0%)	30	60
4	D	148/147 (101%)	143 (97%)	5 (3%)	0	100	100
4	Q	143/147 (97%)	134 (94%)	8 (6%)	1 (1%)	18	47
5	E	104/109 (95%)	99 (95%)	5 (5%)	0	100	100
5	R	103/109 (94%)	100 (97%)	3 (3%)	0	100	100
6	F	101/98 (103%)	87 (86%)	11 (11%)	3 (3%)	3	12
6	S	97/98 (99%)	91 (94%)	4 (4%)	2 (2%)	5	20
7	G	82/85 (96%)	68 (83%)	7 (8%)	7 (8%)	0	1
7	T	84/85 (99%)	70 (83%)	10 (12%)	4 (5%)	2	6
8	H	77/85 (91%)	72 (94%)	4 (5%)	1 (1%)	9	31
8	U	77/85 (91%)	72 (94%)	4 (5%)	1 (1%)	9	31
9	I	71/73 (97%)	64 (90%)	7 (10%)	0	100	100
9	V	72/73 (99%)	59 (82%)	10 (14%)	3 (4%)	2	7
10	J	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
10	W	56/59 (95%)	51 (91%)	5 (9%)	0	100	100
11	K	48/56 (86%)	43 (90%)	5 (10%)	0	100	100
11	X	48/56 (86%)	43 (90%)	4 (8%)	1 (2%)	5	20
12	L	44/47 (94%)	40 (91%)	4 (9%)	0	100	100
12	Y	44/47 (94%)	42 (96%)	1 (2%)	1 (2%)	5	18
13	M	41/46 (89%)	40 (98%)	0	1 (2%)	4	17
13	Z	41/46 (89%)	37 (90%)	4 (10%)	0	100	100
All	All	3577/3614 (99%)	3351 (94%)	191 (5%)	35 (1%)	12	38

5 of 35 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	94	HIS
7	G	4	ALA
7	G	8	HIS
2	O	59	GLN
2	O	89	GLU

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	438/426 (103%)	425 (97%)	13 (3%)	36	72
1	N	439/426 (103%)	420 (96%)	19 (4%)	26	60
2	B	216/210 (103%)	202 (94%)	14 (6%)	15	43
2	O	215/210 (102%)	197 (92%)	18 (8%)	10	32
3	C	232/226 (103%)	228 (98%)	4 (2%)	53	83
3	P	232/226 (103%)	222 (96%)	10 (4%)	26	60
4	D	134/129 (104%)	125 (93%)	9 (7%)	15	42
4	Q	129/129 (100%)	123 (95%)	6 (5%)	23	57
5	E	93/95 (98%)	87 (94%)	6 (6%)	15	43
5	R	92/95 (97%)	89 (97%)	3 (3%)	33	69
6	F	86/81 (106%)	77 (90%)	9 (10%)	6	22
6	S	82/81 (101%)	76 (93%)	6 (7%)	13	38
7	G	68/68 (100%)	64 (94%)	4 (6%)	18	48
7	T	70/68 (103%)	64 (91%)	6 (9%)	10	31
8	H	71/75 (95%)	68 (96%)	3 (4%)	26	61
8	U	71/75 (95%)	66 (93%)	5 (7%)	14	40
9	I	57/57 (100%)	53 (93%)	4 (7%)	14	40
9	V	58/57 (102%)	51 (88%)	7 (12%)	5	16
10	J	49/50 (98%)	47 (96%)	2 (4%)	27	62
10	W	49/50 (98%)	46 (94%)	3 (6%)	17	46
11	K	40/46 (87%)	40 (100%)	0	100	100
11	X	40/46 (87%)	36 (90%)	4 (10%)	7	24
12	L	39/40 (98%)	37 (95%)	2 (5%)	21	54
12	Y	39/40 (98%)	33 (85%)	6 (15%)	2	10
13	M	37/38 (97%)	36 (97%)	1 (3%)	39	74
13	Z	37/38 (97%)	36 (97%)	1 (3%)	39	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	3113/3082 (101%)	2948 (95%)	165 (5%)	21	52

5 of 165 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	P	195	SER
8	U	84	LYS
4	Q	9	GLU
6	S	87[A]	THR
9	V	73	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
1	N	135	ASN
2	O	140	ASN
8	U	31	GLN
1	N	178	GLN
1	N	512	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	FME	N	1	1	8,9,10	0.62	0	8,9,11	1.98	3 (37%)
9	SAC	V	1	9	7,8,9	1.77	1 (14%)	7,9,11	1.83	3 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	TPO	T	11	7	8,10,11	1.30	1 (12%)	10,14,16	1.40	2 (20%)
2	FME	B	1	2	8,9,10	0.72	0	8,9,11	2.58	4 (50%)
1	FME	A	1	1	8,9,10	0.51	0	8,9,11	1.72	2 (25%)
2	FME	O	1	2	8,9,10	0.64	0	8,9,11	0.98	0
9	SAC	I	1	9	7,8,9	1.95	1 (14%)	7,9,11	2.33	3 (42%)
7	TPO	G	11	7	8,10,11	1.38	2 (25%)	10,14,16	1.63	2 (20%)

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

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	1	SAC	CA-N	4.46	1.53	1.46
9	V	1	SAC	CA-N	4.10	1.52	1.46
7	T	11	TPO	P-OG1	2.79	1.64	1.59
7	G	11	TPO	P-OG1	2.38	1.63	1.59
7	G	11	TPO	CB-CA	2.06	1.58	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CA-N-CN	-5.64	114.15	122.82
1	N	1	FME	CA-N-CN	4.11	129.15	122.82
9	I	1	SAC	OAC-C1A-C2A	-3.68	115.51	122.05
9	I	1	SAC	C-CA-N	3.39	116.05	109.50
7	G	11	TPO	P-OG1-CB	-3.39	114.12	123.33

There are no chirality outliers.

5 of 19 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
2	B	1	FME	O1-CN-N-CA
7	G	11	TPO	N-CA-CB-CG2
7	G	11	TPO	N-CA-CB-OG1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	TGL	A	608	-	62,62,62	1.21	3 (4%)	65,65,65	1.15	5 (7%)
22	CHD	W	101	-	32,32,32	0.82	1 (3%)	51,51,51	2.08	15 (29%)
14	HEA	N	602	1	67,67,67	2.30	25 (37%)	81,103,103	2.53	32 (39%)
19	TGL	D	201	-	62,62,62	1.22	3 (4%)	65,65,65	1.19	6 (9%)
19	TGL	Y	101	-	62,62,62	1.14	3 (4%)	65,65,65	1.04	5 (7%)
22	CHD	G	104	-	32,32,32	0.84	0	51,51,51	1.53	11 (21%)
25	PEK	G	101	-	52,52,52	1.04	2 (3%)	55,57,57	1.21	4 (7%)
19	TGL	N	607	-	62,62,62	1.19	3 (4%)	65,65,65	1.16	8 (12%)
20	CDL	G	102	-	99,99,99	1.09	4 (4%)	105,111,111	1.09	8 (7%)
21	CUA	O	301	2	0,1,1	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CHD	P	306	-	32,32,32	0.58	0	51,51,51	1.69	15 (29%)
18	PGV	C	303	-	50,50,50	0.90	2 (4%)	53,56,56	0.91	3 (5%)
20	CDL	C	304	-	99,99,99	1.10	4 (4%)	105,111,111	1.04	6 (5%)
22	CHD	J	101	-	32,32,32	0.83	0	51,51,51	1.60	6 (11%)
21	CUA	B	302	2	0,1,1	-	-	-	-	-
22	CHD	P	307	-	32,32,32	0.73	0	51,51,51	1.28	5 (9%)
25	PEK	C	302	-	52,52,52	0.86	2 (3%)	55,57,57	1.07	3 (5%)
18	PGV	P	304	-	50,50,50	0.97	2 (4%)	53,56,56	0.94	2 (3%)
22	CHD	C	305	-	32,32,32	0.64	0	51,51,51	1.55	8 (15%)
14	HEA	A	601	1	67,67,67	2.31	26 (38%)	81,103,103	2.18	23 (28%)
18	PGV	C	307	-	50,50,50	1.13	2 (4%)	53,56,56	0.92	3 (5%)
25	PEK	T	101	-	52,52,52	1.13	2 (3%)	55,57,57	1.11	5 (9%)
24	DMU	Q	201	-	34,34,34	0.84	1 (2%)	45,45,45	1.04	2 (4%)
24	DMU	M	101	-	34,34,34	1.08	1 (2%)	45,45,45	1.18	4 (8%)
14	HEA	A	602	1	67,67,67	2.40	24 (35%)	81,103,103	2.49	32 (39%)
24	DMU	P	303	-	34,34,34	1.71	1 (2%)	45,45,45	1.48	5 (11%)
18	PGV	A	607	-	50,50,50	1.08	2 (4%)	53,56,56	1.10	5 (9%)
18	PGV	P	302	-	50,50,50	1.11	2 (4%)	53,56,56	1.18	5 (9%)
24	DMU	C	301	-	34,34,34	1.91	6 (17%)	45,45,45	2.26	9 (20%)
25	PEK	P	308	-	52,52,52	0.88	2 (3%)	55,57,57	1.02	2 (3%)
20	CDL	P	305	-	99,99,99	1.10	4 (4%)	105,111,111	1.22	10 (9%)
22	CHD	B	303	-	32,32,32	0.72	1 (3%)	51,51,51	1.48	7 (13%)
14	HEA	N	601	1	67,67,67	2.45	26 (38%)	81,103,103	2.39	29 (35%)
18	PGV	N	606	-	50,50,50	1.00	2 (4%)	53,56,56	0.98	4 (7%)
22	CHD	C	306	-	32,32,32	0.92	1 (3%)	51,51,51	1.20	8 (15%)
25	PEK	G	103	-	52,52,52	1.10	2 (3%)	55,57,57	1.52	6 (10%)
23	PSC	N	608	-	51,51,51	1.09	2 (3%)	57,59,59	1.78	10 (17%)
18	PGV	P	301	-	50,50,50	0.91	2 (4%)	53,56,56	1.07	3 (5%)
19	TGL	B	301	-	62,62,62	1.18	3 (4%)	65,65,65	1.22	6 (9%)
19	TGL	V	101	-	62,62,62	1.14	3 (4%)	65,65,65	1.26	8 (12%)
25	PEK	P	309	-	52,52,52	1.13	2 (3%)	55,57,57	1.41	6 (10%)
23	PSC	B	304	-	51,51,51	0.99	2 (3%)	57,59,59	1.74	9 (15%)
20	CDL	A	609	-	99,99,99	1.12	4 (4%)	105,111,111	1.16	8 (7%)
18	PGV	A	606	-	50,50,50	0.93	2 (4%)	53,56,56	0.92	3 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	TGL	A	608	-	-	33/65/65/65	-
22	CHD	W	101	-	-	7/9/74/74	0/4/4/4
14	HEA	N	602	1	-	3/36/76/76	-
19	TGL	D	201	-	-	35/65/65/65	-
19	TGL	Y	101	-	-	34/65/65/65	-
22	CHD	G	104	-	-	2/9/74/74	0/4/4/4
25	PEK	G	101	-	-	24/56/56/56	-
19	TGL	N	607	-	-	36/65/65/65	-
20	CDL	G	102	-	-	55/110/110/110	-
22	CHD	P	306	-	-	3/9/74/74	0/4/4/4
18	PGV	C	303	-	-	14/55/55/55	-
20	CDL	C	304	-	-	65/110/110/110	-
22	CHD	J	101	-	-	6/9/74/74	0/4/4/4
22	CHD	P	307	-	-	0/9/74/74	0/4/4/4
25	PEK	C	302	-	-	18/56/56/56	-
18	PGV	P	304	-	-	15/55/55/55	-
22	CHD	C	305	-	-	8/9/74/74	0/4/4/4
14	HEA	A	601	1	-	4/36/76/76	-
18	PGV	C	307	-	-	29/55/55/55	-
25	PEK	T	101	-	-	20/56/56/56	-
24	DMU	Q	201	-	-	7/19/59/59	0/2/2/2
24	DMU	M	101	-	-	8/19/59/59	0/2/2/2
14	HEA	A	602	1	-	6/36/76/76	-
24	DMU	P	303	-	-	6/19/59/59	0/2/2/2
18	PGV	A	607	-	-	30/55/55/55	-
18	PGV	P	302	-	-	32/55/55/55	-
24	DMU	C	301	-	-	12/19/59/59	0/2/2/2
25	PEK	P	308	-	-	16/56/56/56	-
20	CDL	P	305	-	-	51/110/110/110	-
22	CHD	B	303	-	-	2/9/74/74	0/4/4/4
14	HEA	N	601	1	-	4/36/76/76	-
18	PGV	N	606	-	-	27/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CHD	C	306	-	-	2/9/74/74	0/4/4/4
25	PEK	G	103	-	-	29/56/56/56	-
23	PSC	N	608	-	-	28/55/55/55	-
18	PGV	P	301	-	-	13/55/55/55	-
19	TGL	B	301	-	-	35/65/65/65	-
19	TGL	V	101	-	-	32/65/65/65	-
25	PEK	P	309	-	-	22/56/56/56	-
23	PSC	B	304	-	-	24/55/55/55	-
20	CDL	A	609	-	-	58/110/110/110	-
18	PGV	A	606	-	-	9/55/55/55	-

The worst 5 of 179 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	301	DMU	O16-C6	8.51	1.54	1.40
24	P	303	DMU	O16-C6	8.35	1.54	1.40
14	N	601	HEA	C3B-C2B	5.78	1.47	1.34
25	P	309	PEK	O01-C1	5.48	1.49	1.34
14	A	601	HEA	C3B-C2B	5.39	1.47	1.34

The worst 5 of 354 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	301	DMU	C18-O16-C6	9.91	130.61	113.68
14	N	601	HEA	C3A-C2A-C1A	-8.44	99.06	107.05
25	G	103	PEK	O01-C1-C2	7.16	126.96	111.48
14	N	602	HEA	C3A-C2A-C1A	-6.99	100.44	107.05
14	A	602	HEA	C3A-C2A-C1A	-6.94	100.48	107.05

There are no chirality outliers.

5 of 864 torsion outliers are listed below:

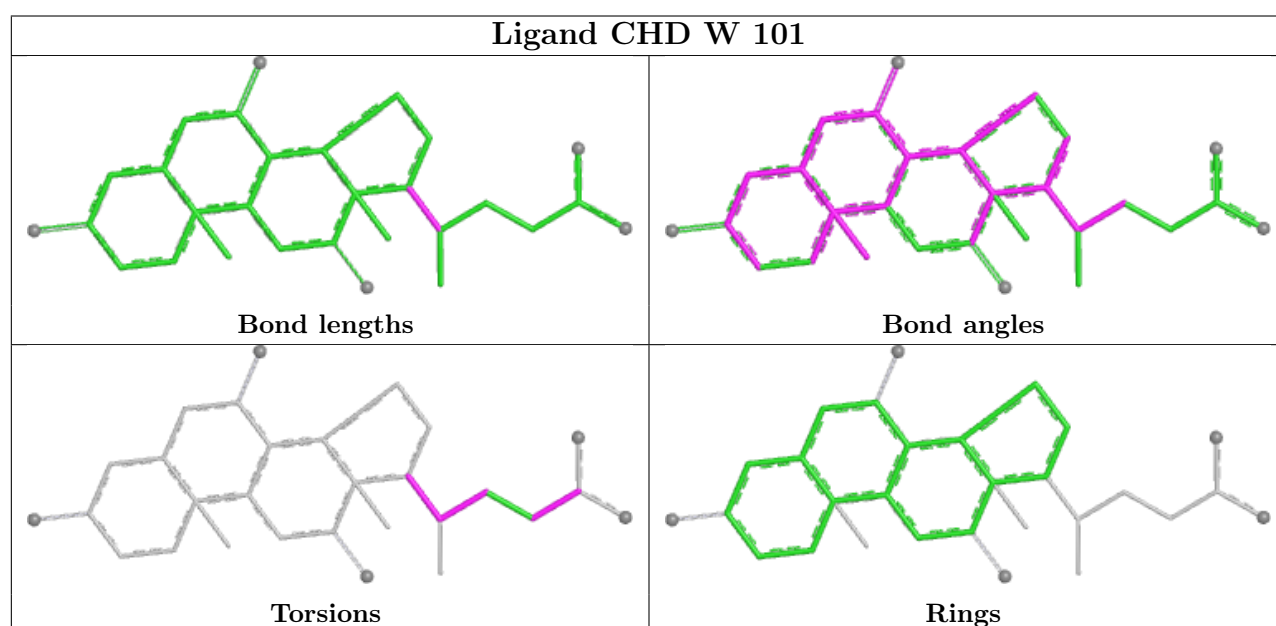
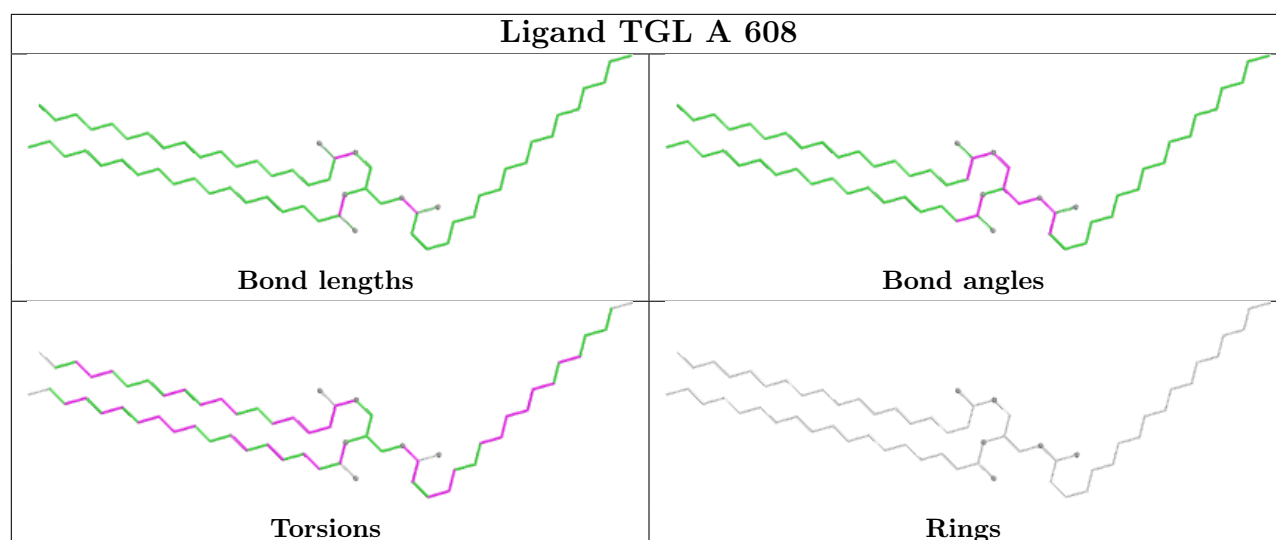
Mol	Chain	Res	Type	Atoms
18	A	607	PGV	C03-O11-P-O12
18	A	607	PGV	C03-O11-P-O14
18	A	607	PGV	C04-O12-P-O11
18	A	607	PGV	C02-C03-O11-P
18	A	607	PGV	C04-C05-C06-O06

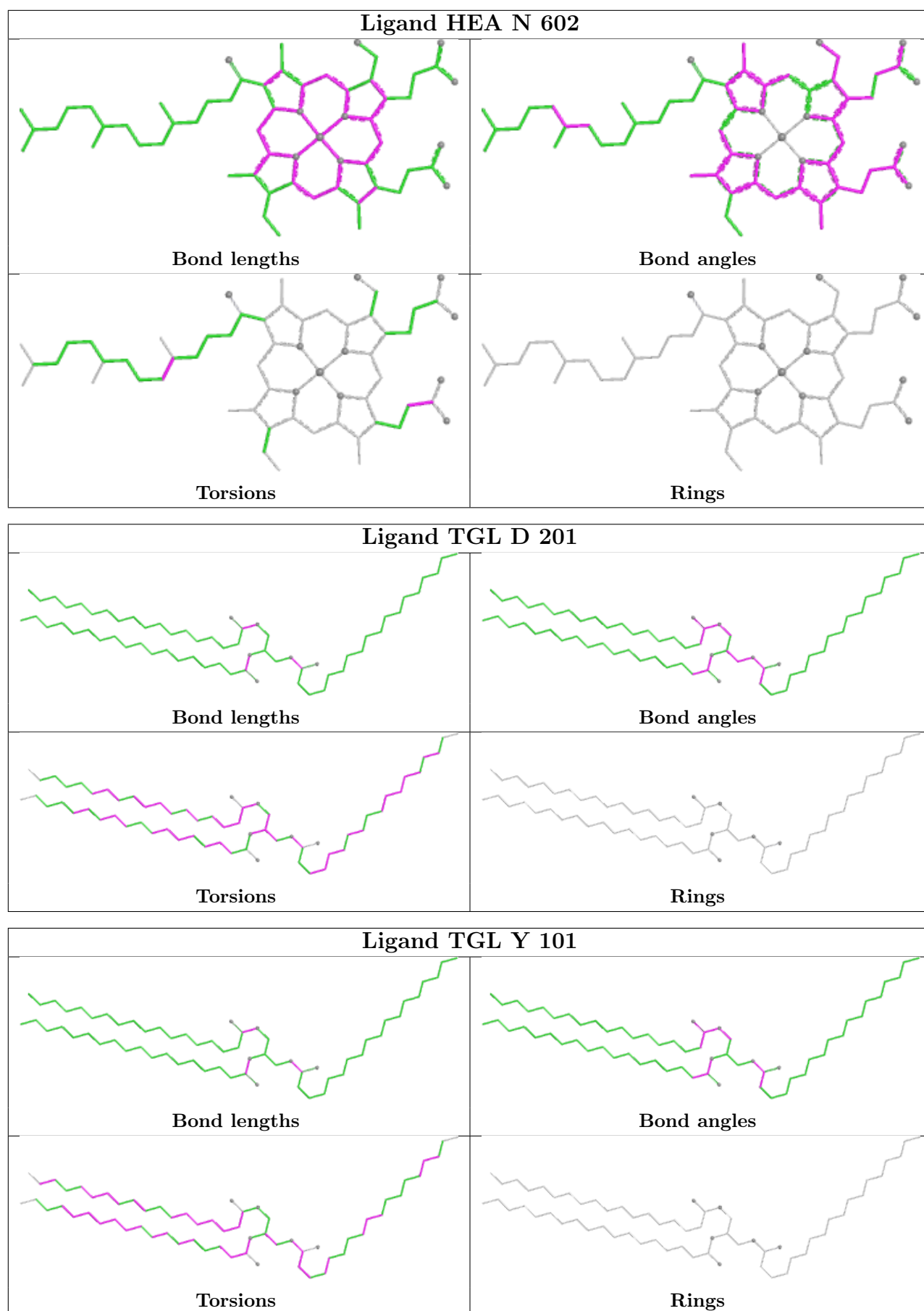
There are no ring outliers.

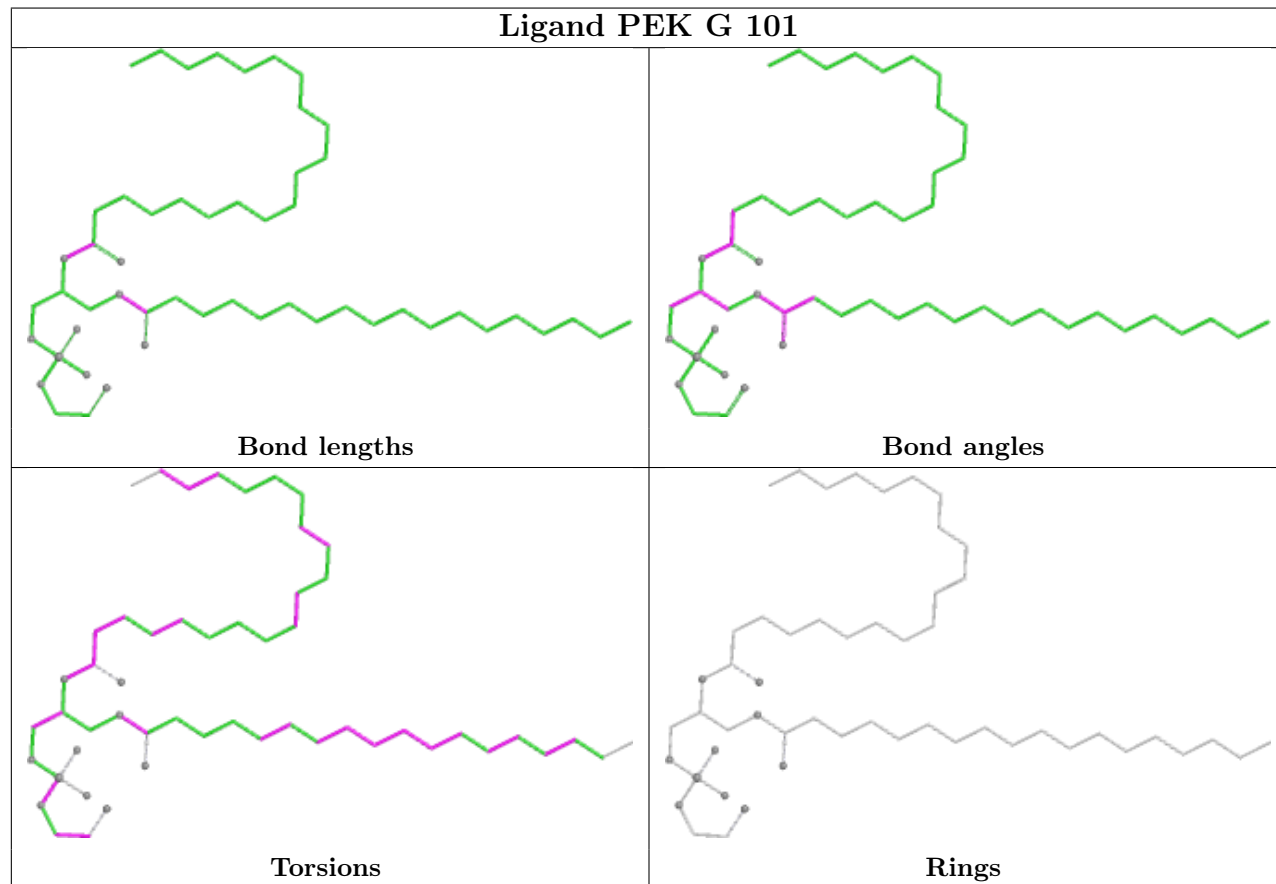
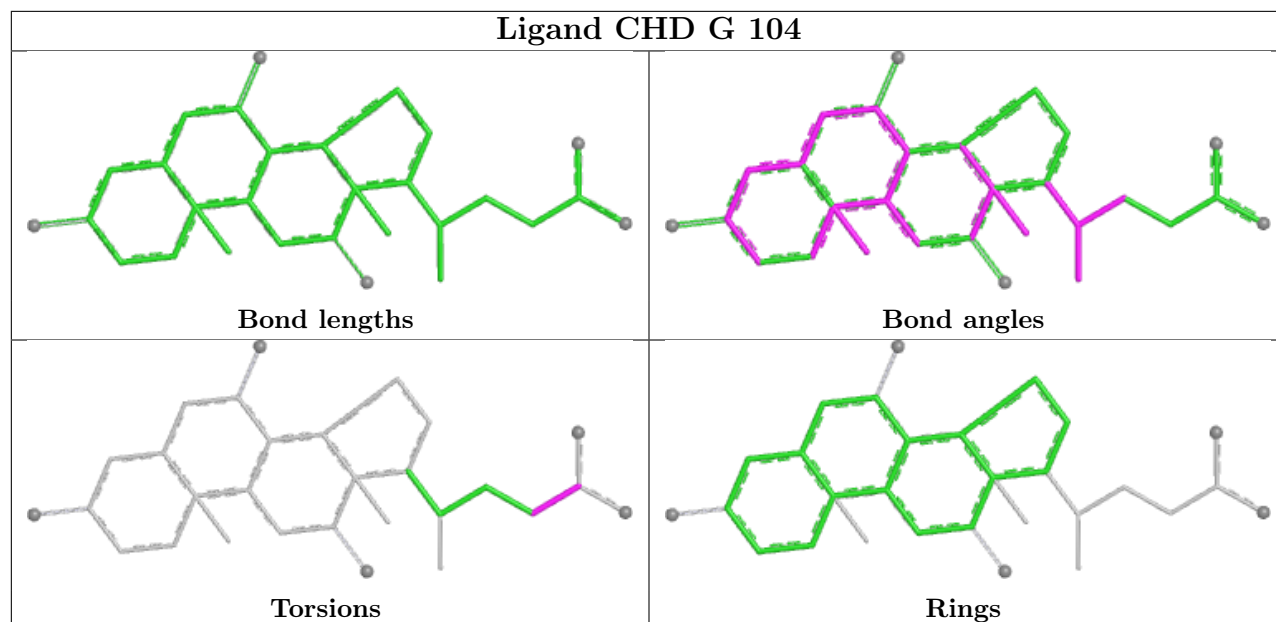
20 monomers are involved in 58 short contacts:

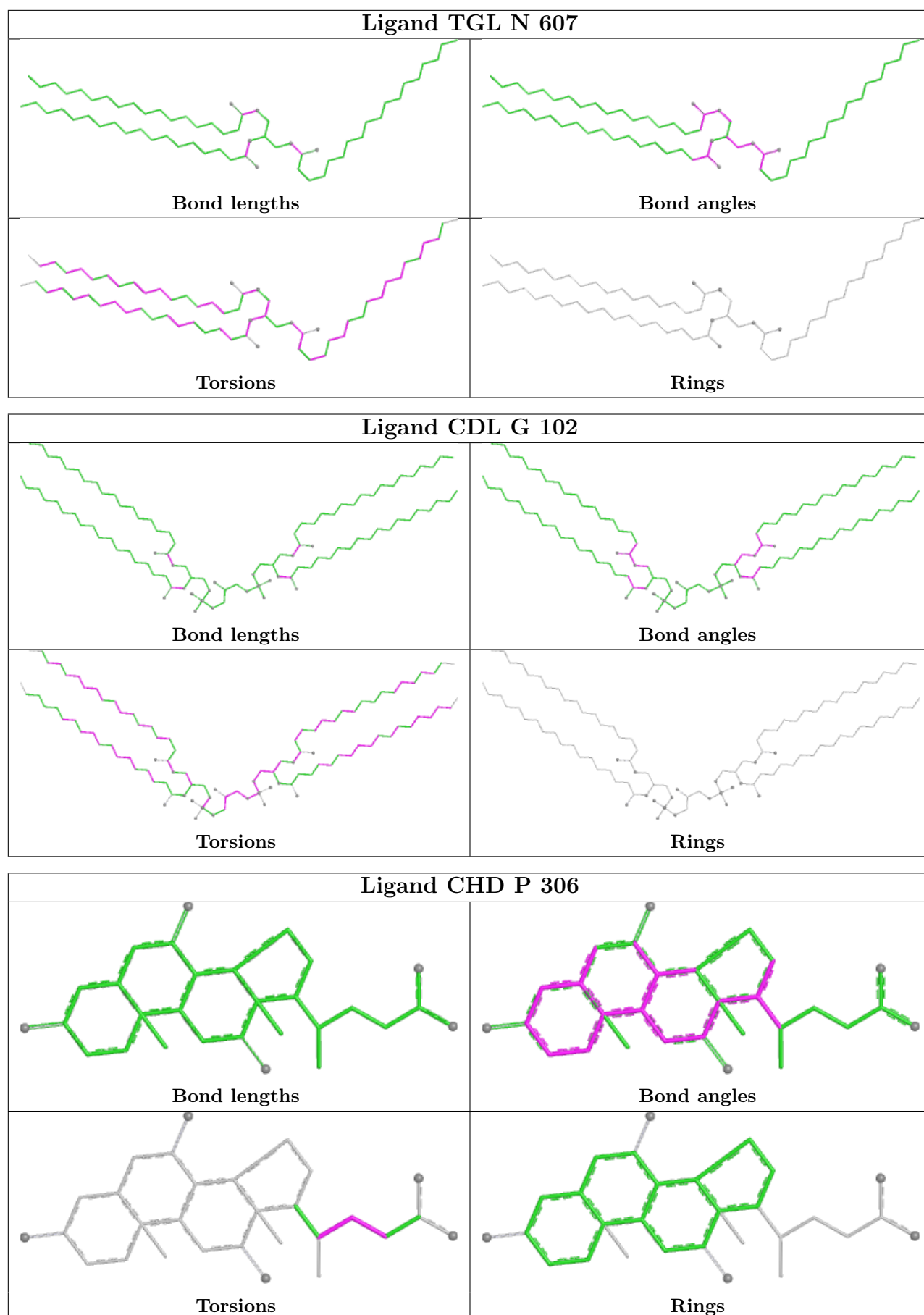
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	608	TGL	2	0
22	W	101	CHD	1	0
14	N	602	HEA	2	0
19	Y	101	TGL	1	0
22	G	104	CHD	1	0
20	G	102	CDL	4	0
22	J	101	CHD	2	0
25	C	302	PEK	1	0
18	P	304	PGV	6	0
24	Q	201	DMU	3	0
14	A	602	HEA	1	0
24	P	303	DMU	1	0
18	A	607	PGV	1	0
24	C	301	DMU	2	0
25	P	308	PEK	3	0
20	P	305	CDL	22	0
14	N	601	HEA	2	0
25	G	103	PEK	1	0
19	V	101	TGL	3	0
20	A	609	CDL	5	0

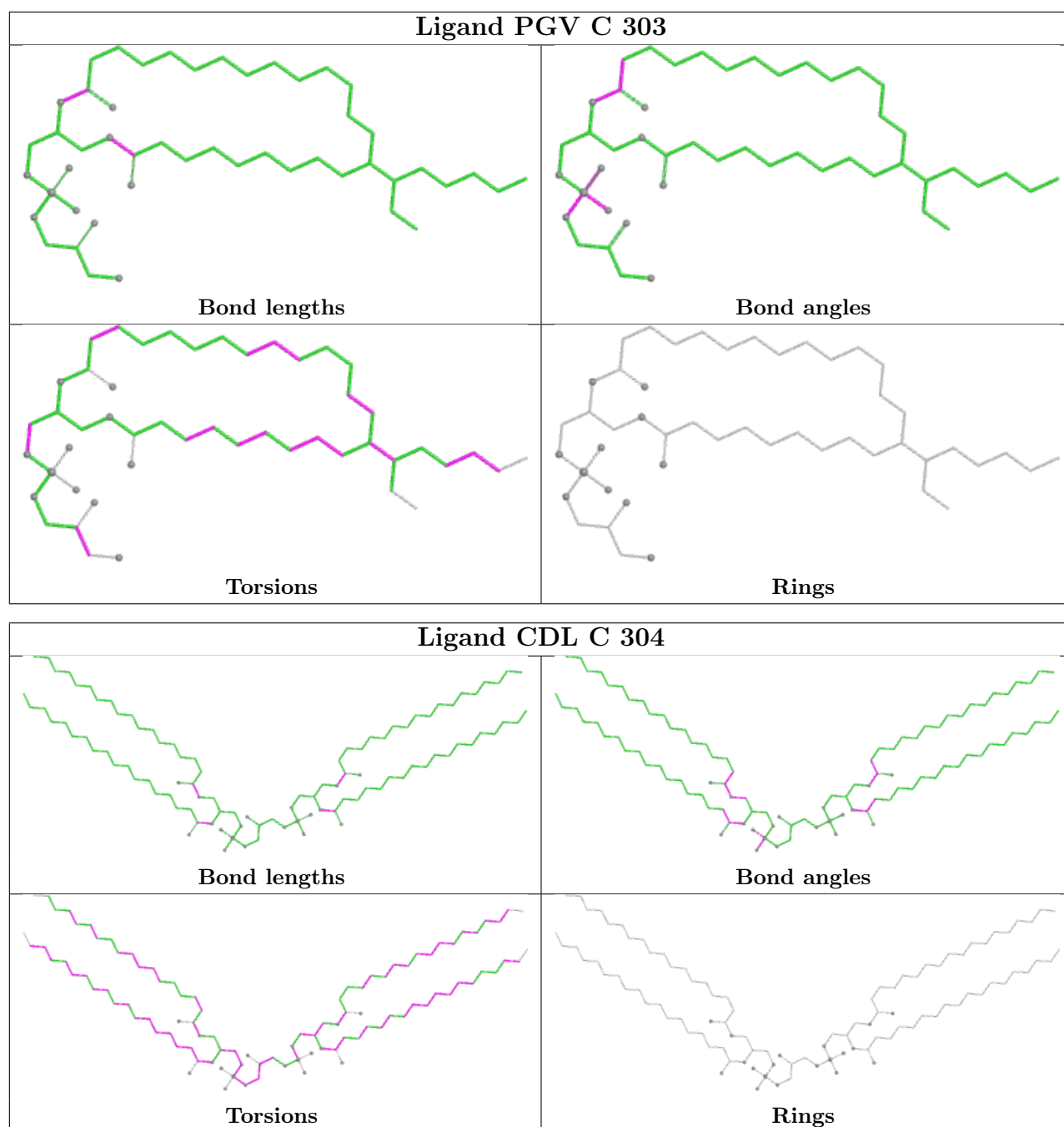
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

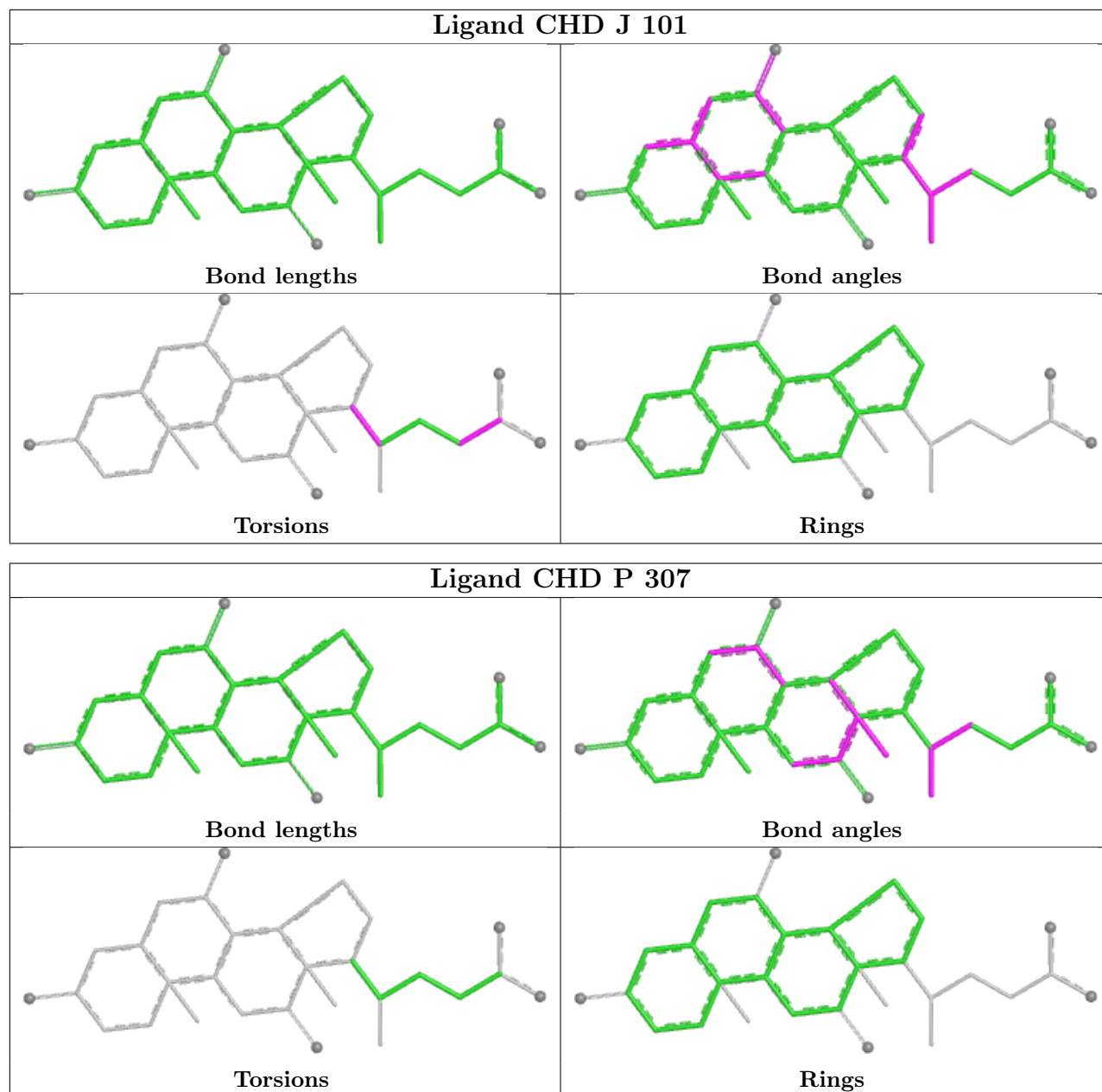


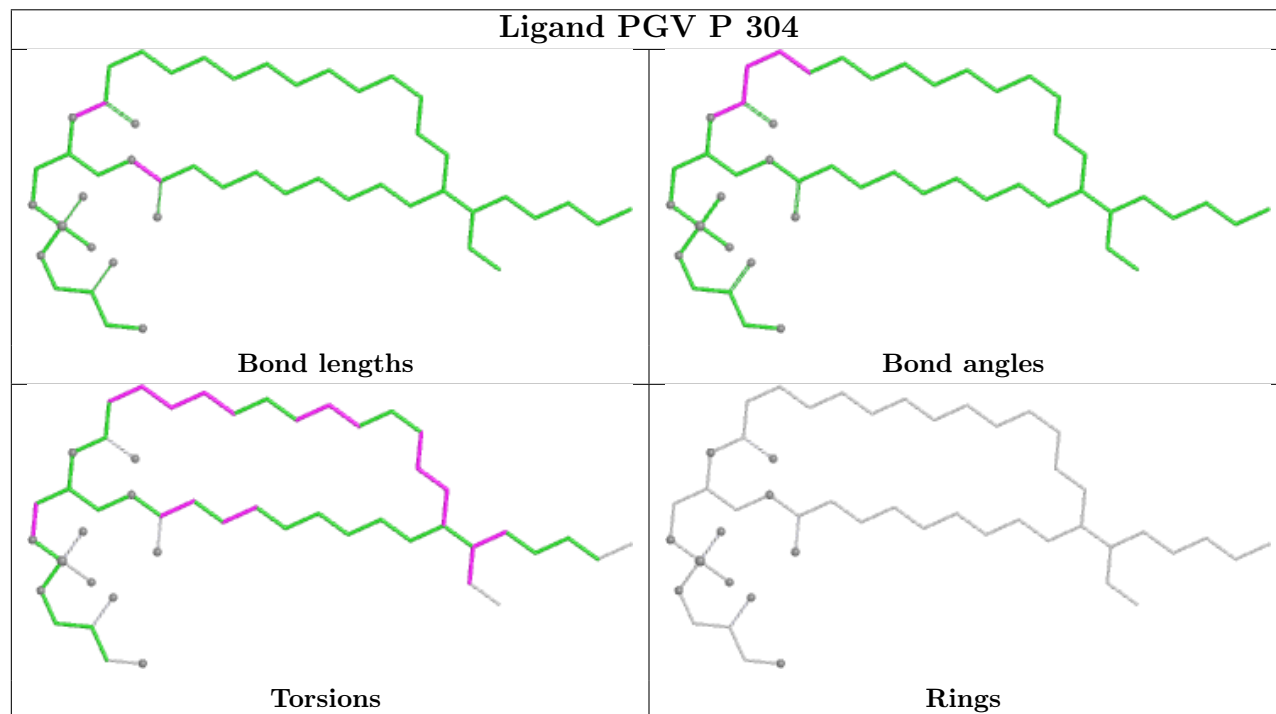
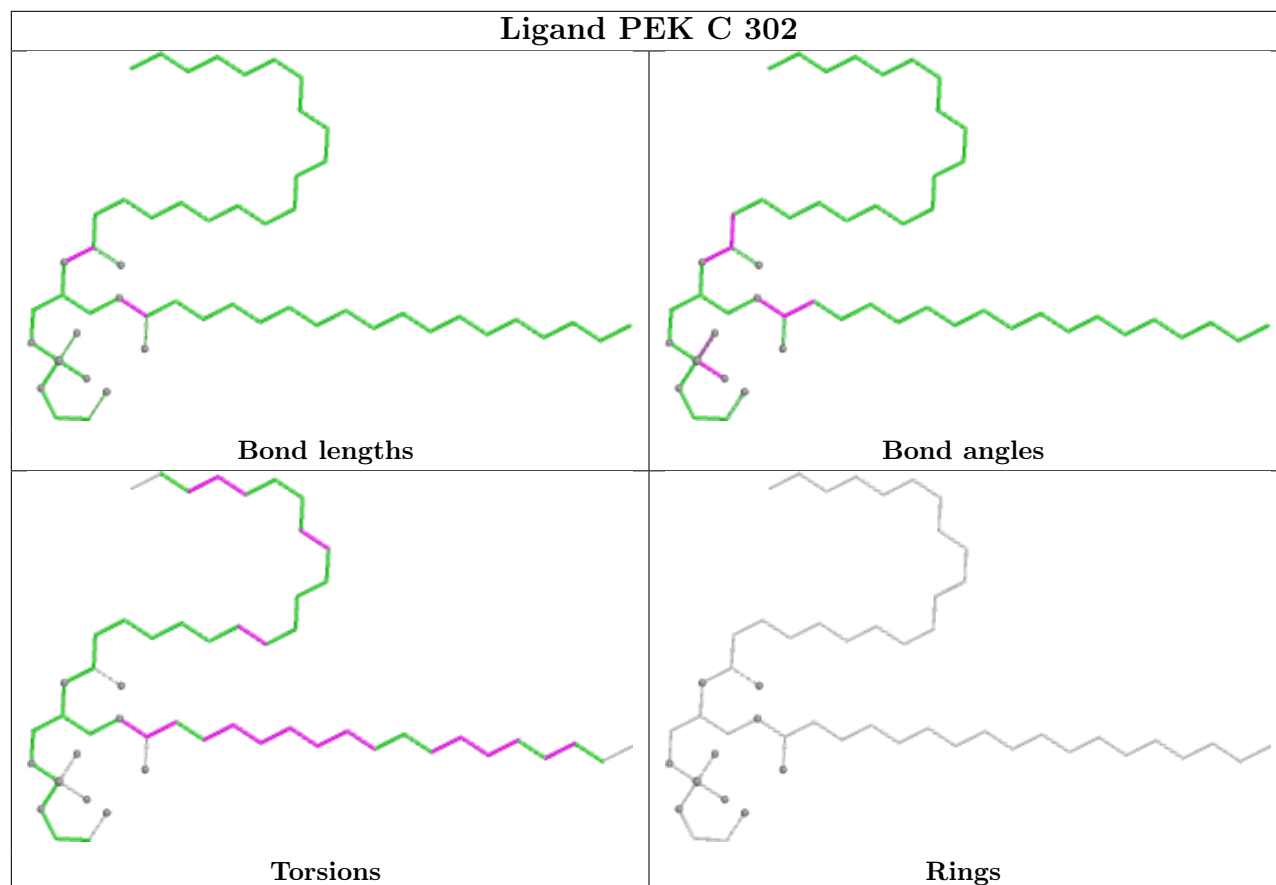


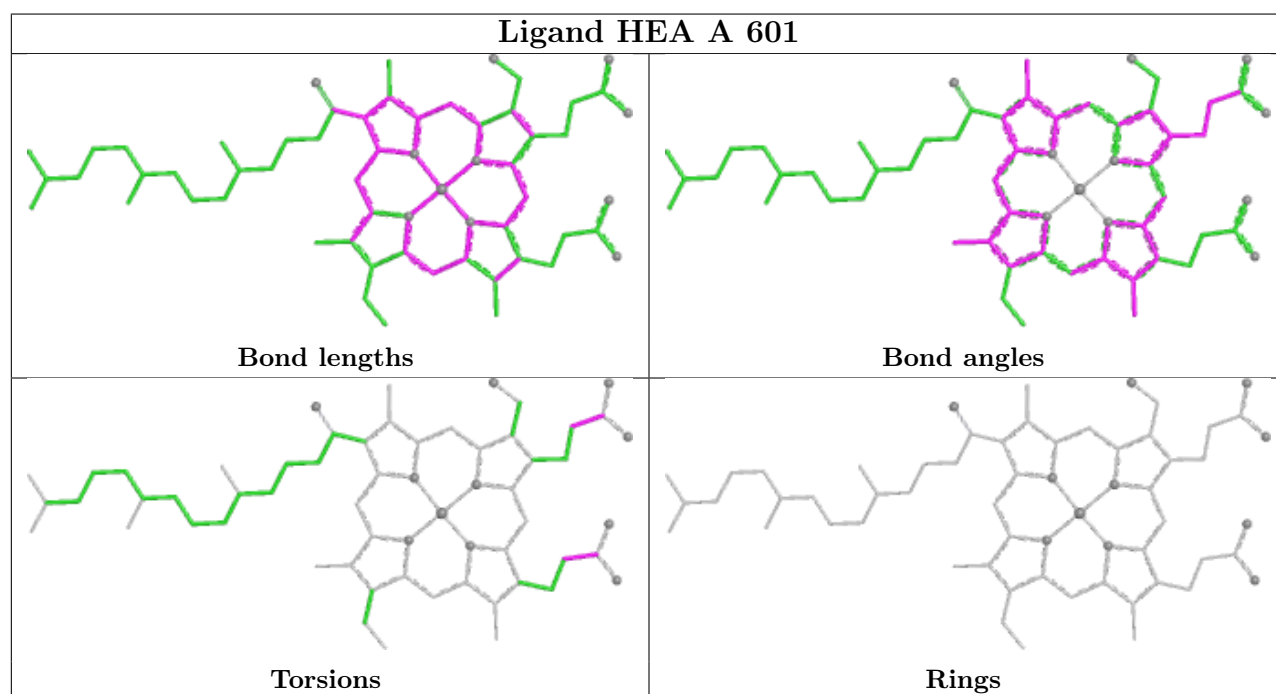
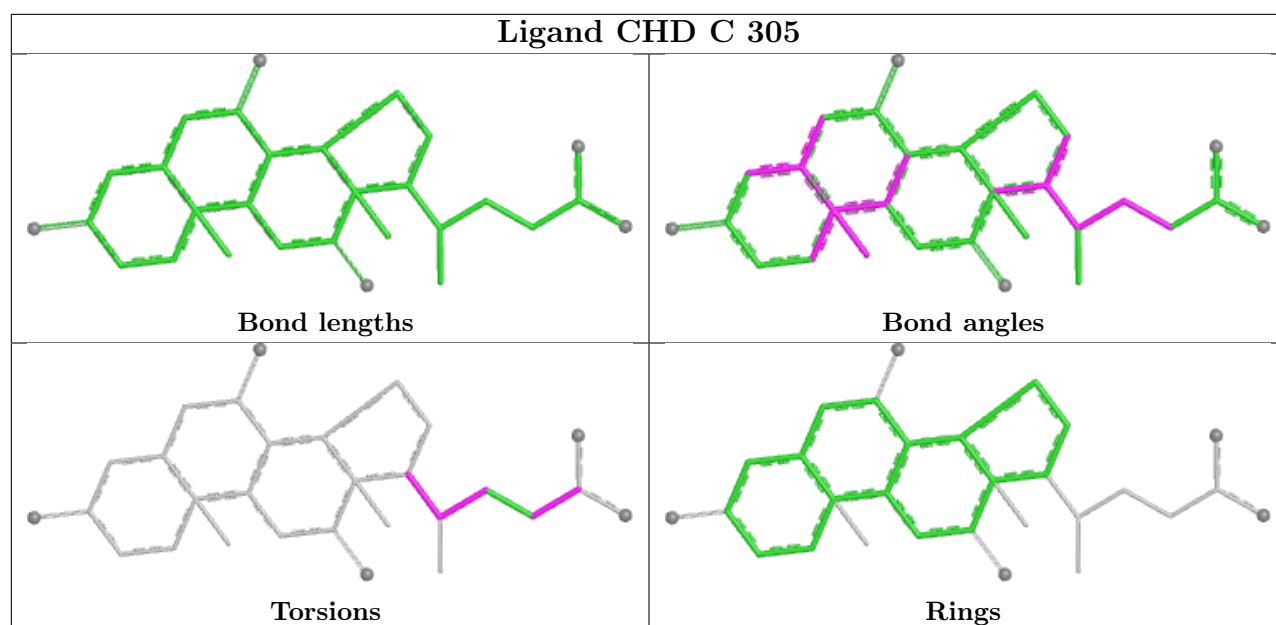


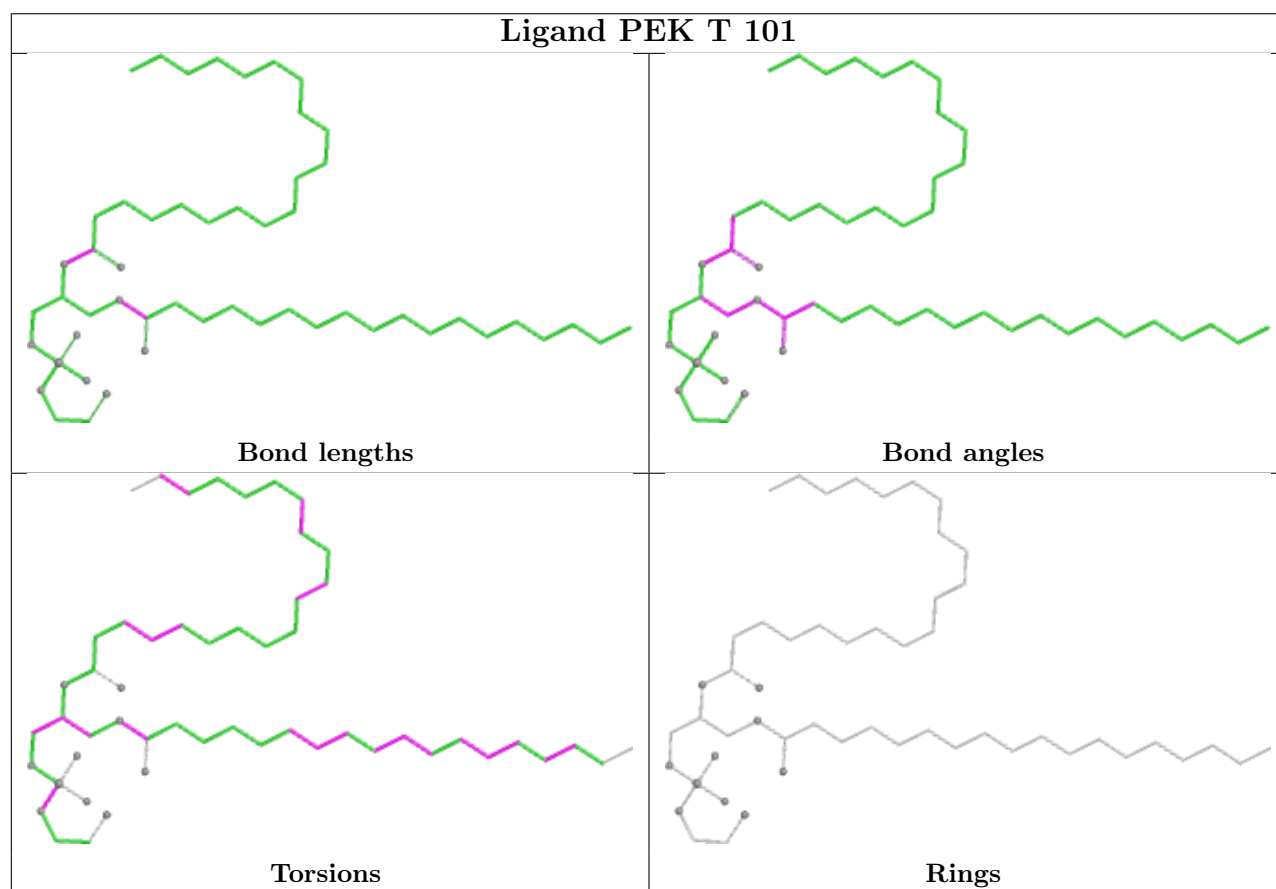
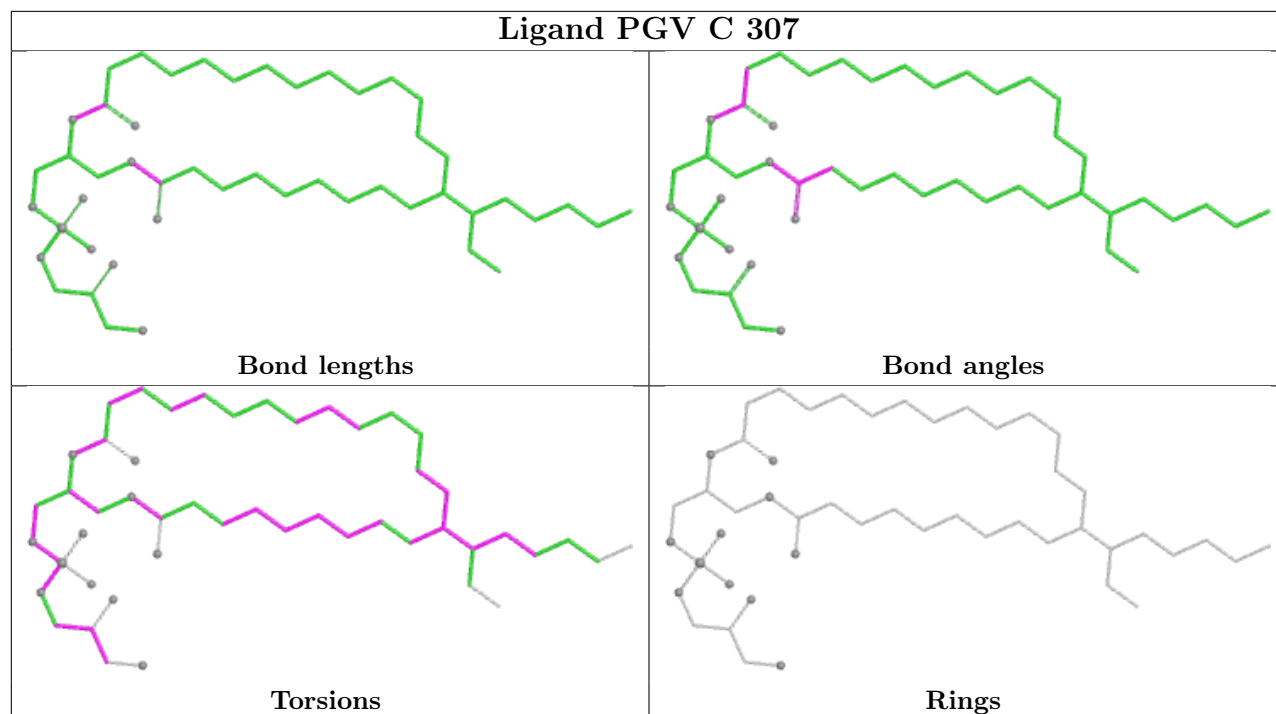


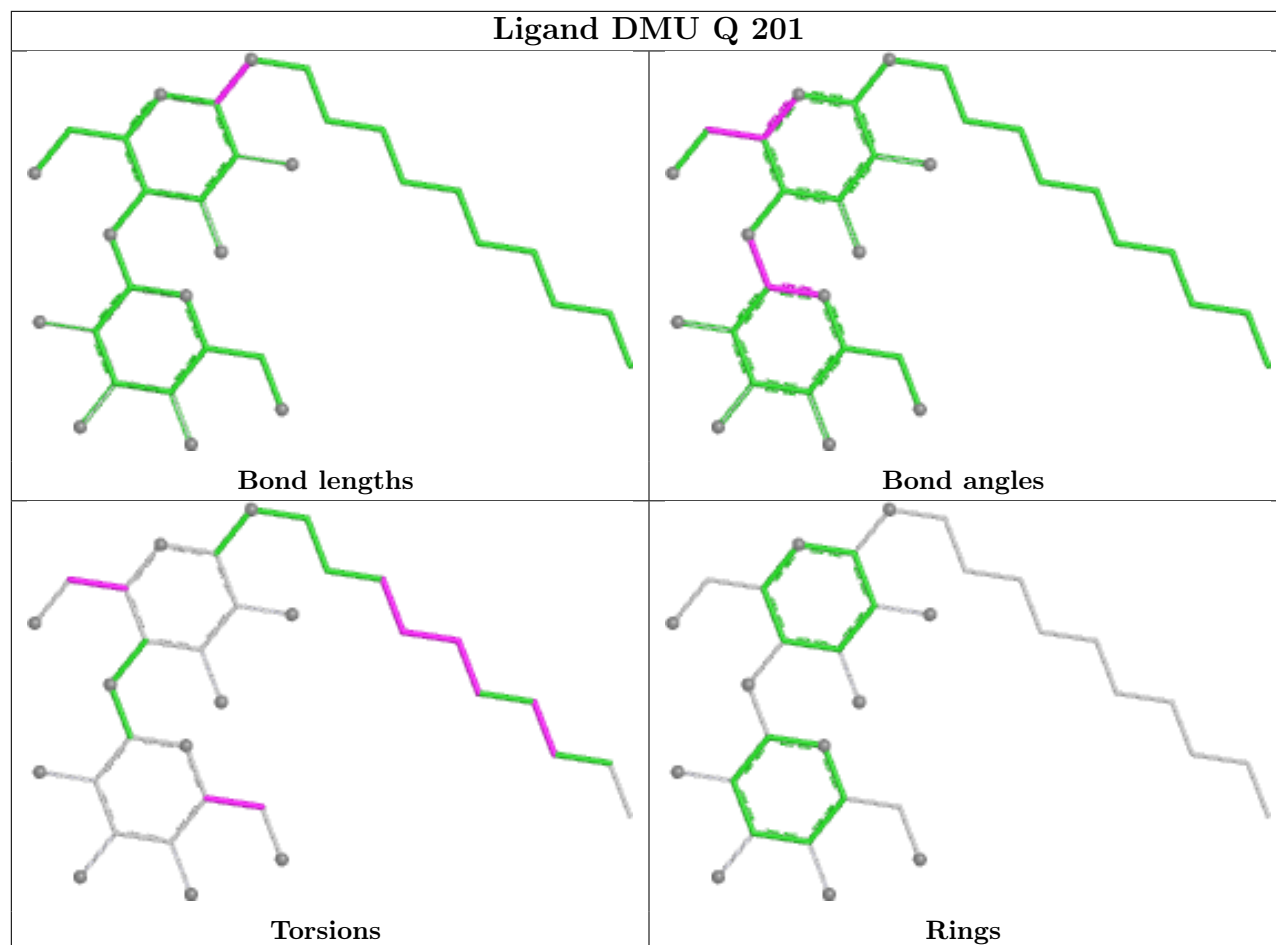


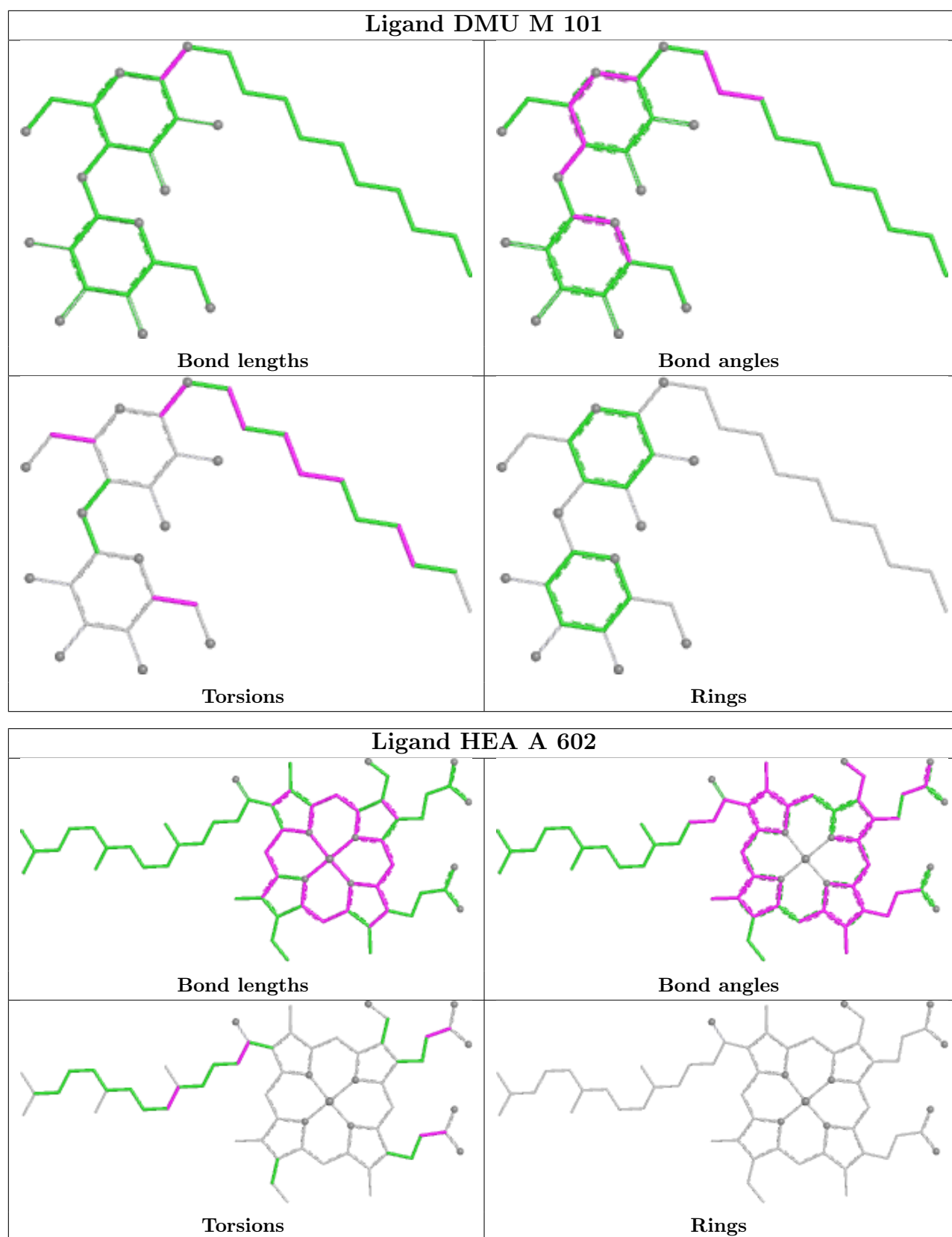


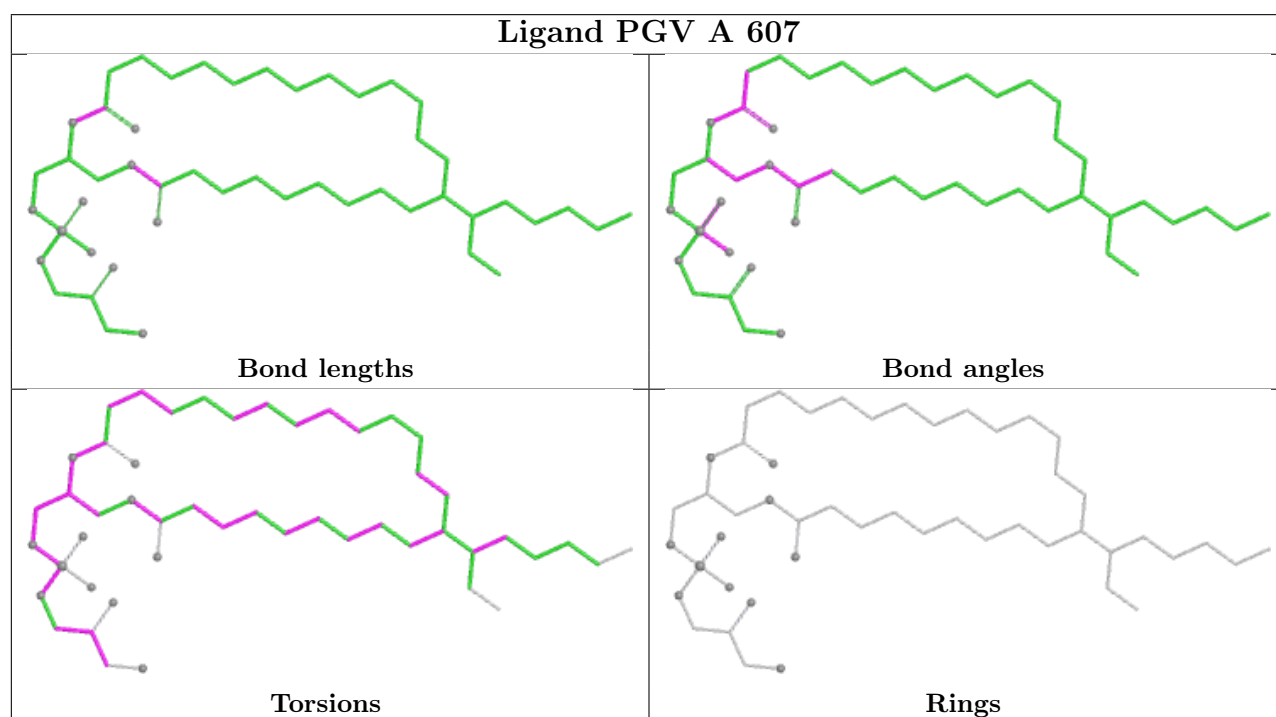
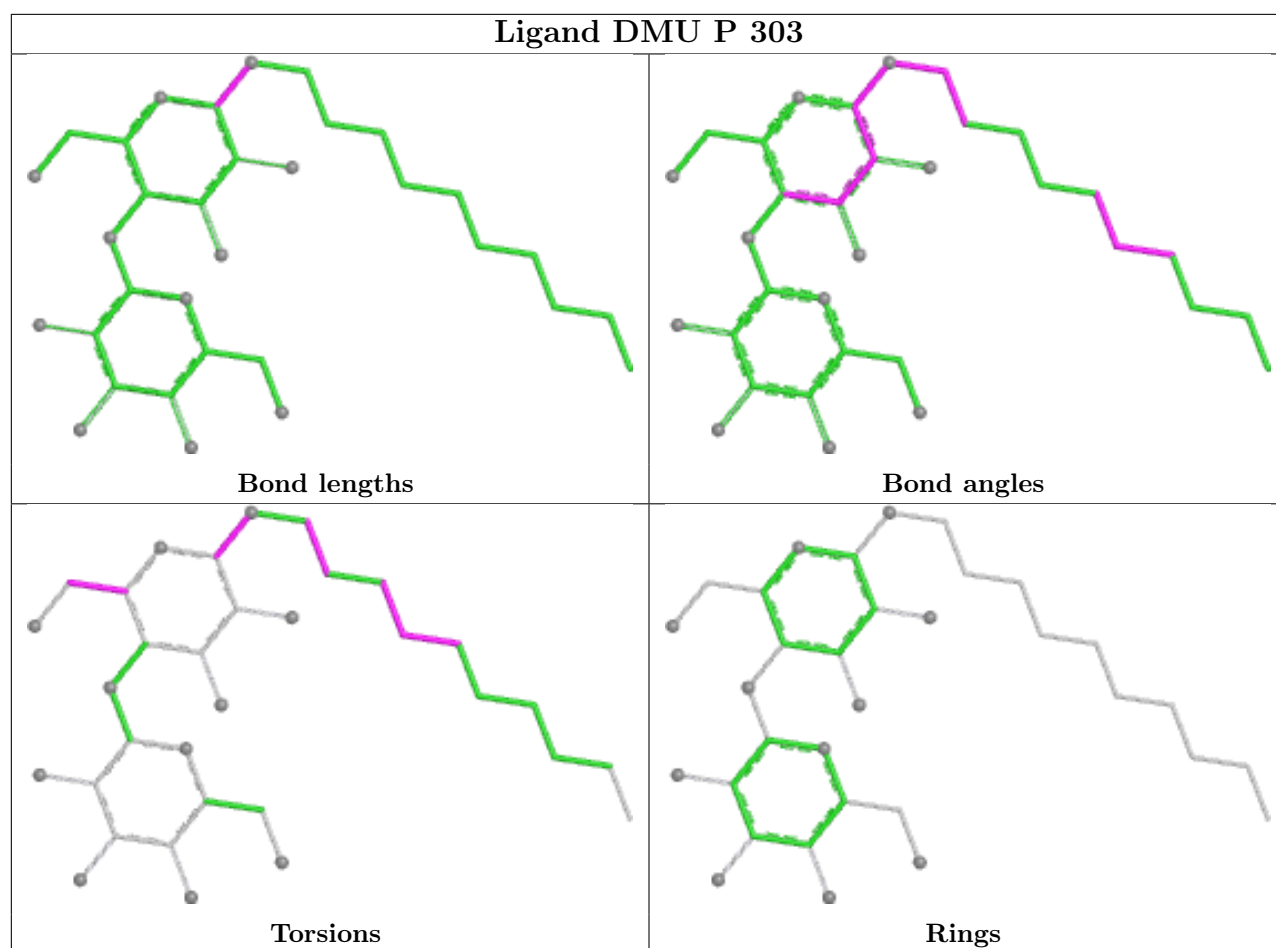


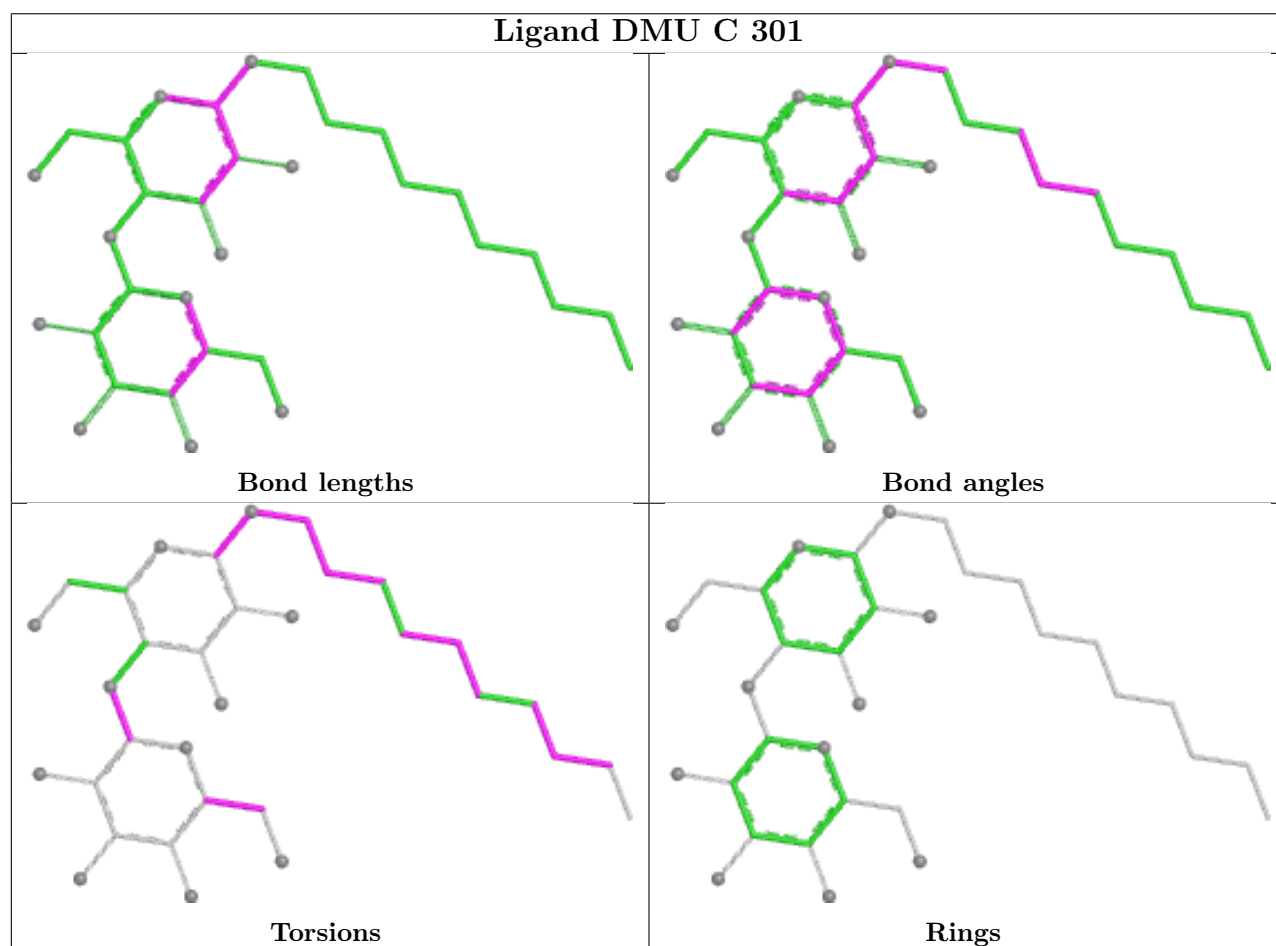
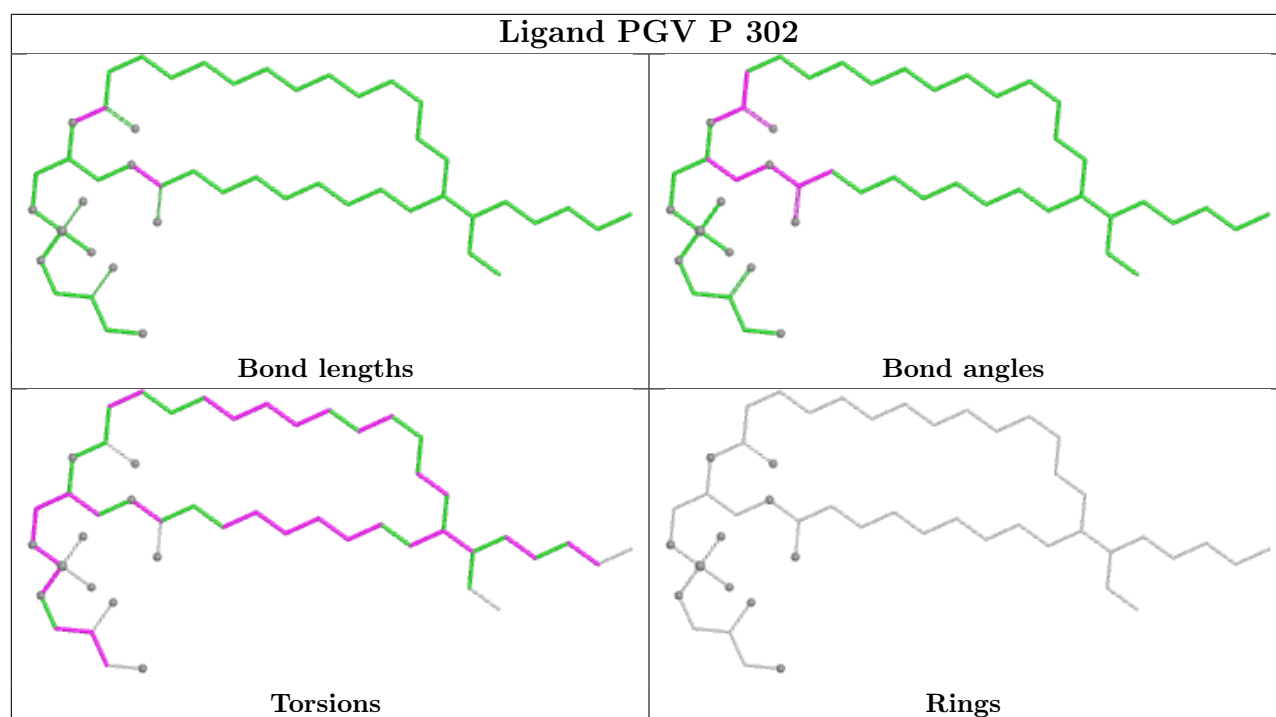


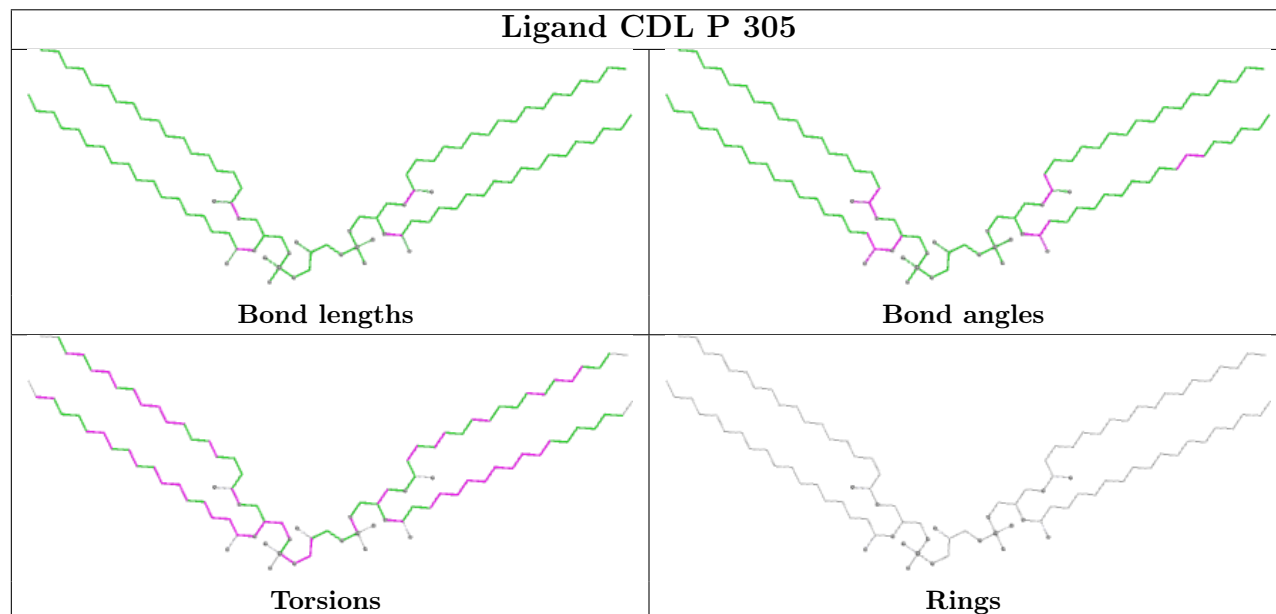
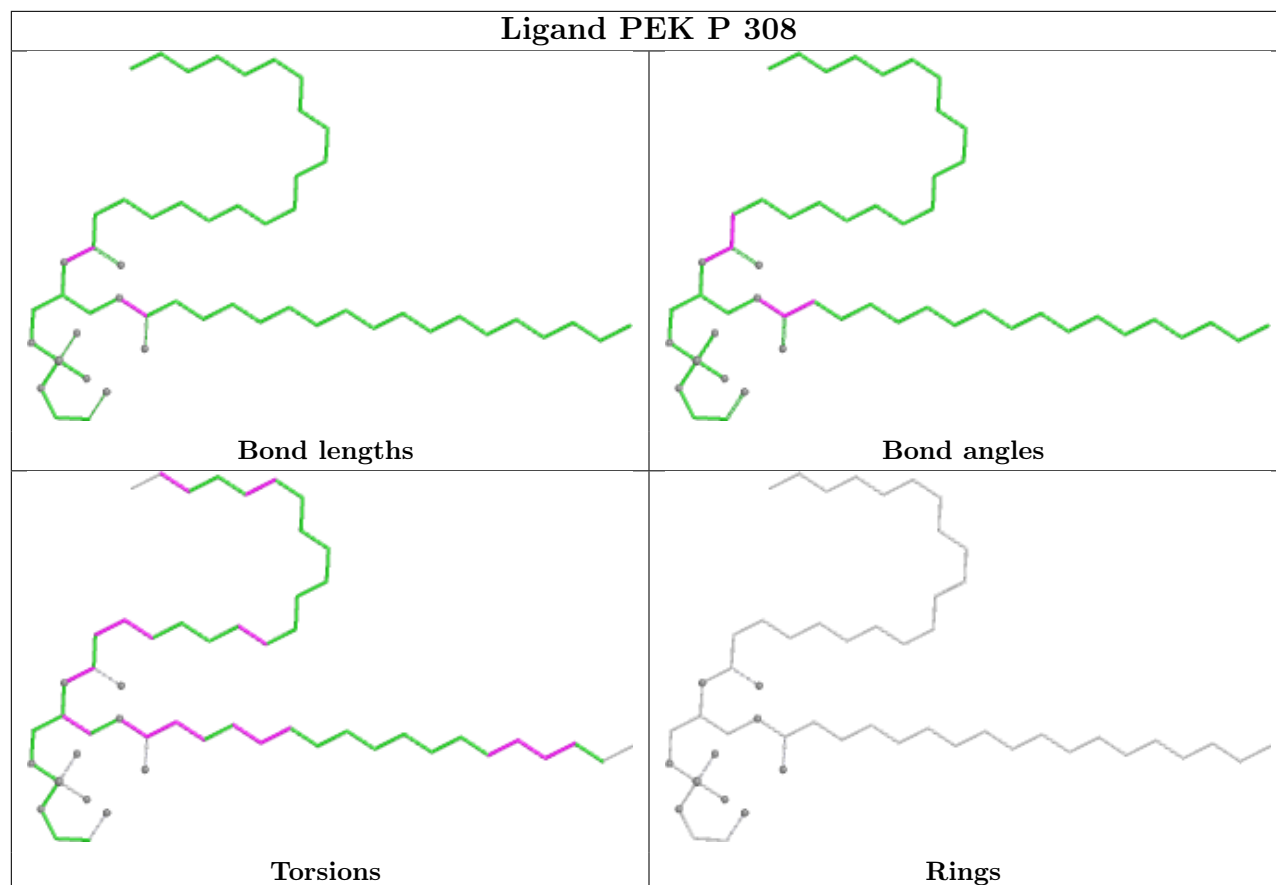


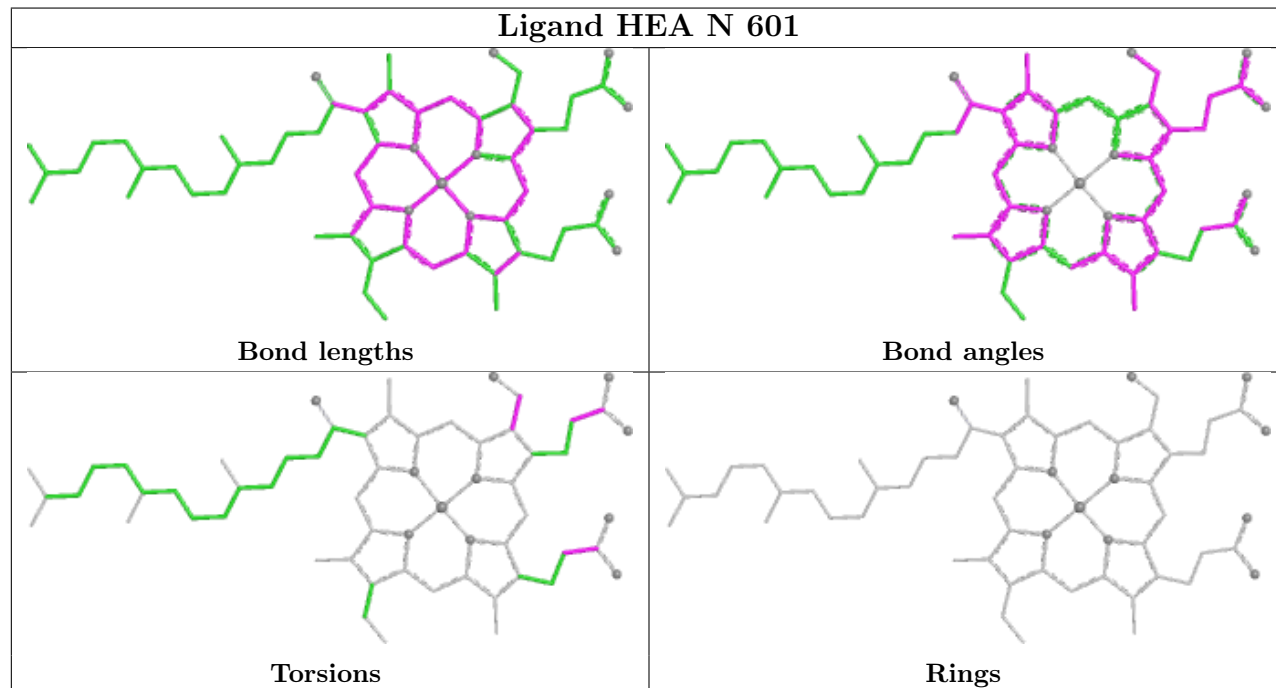
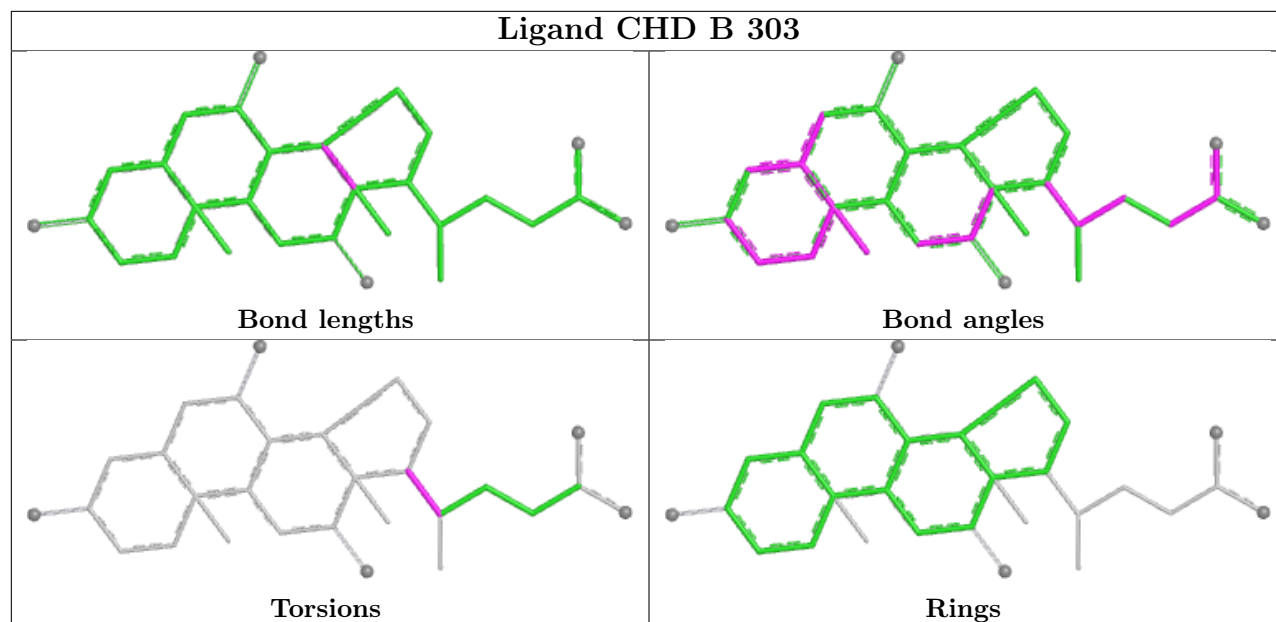


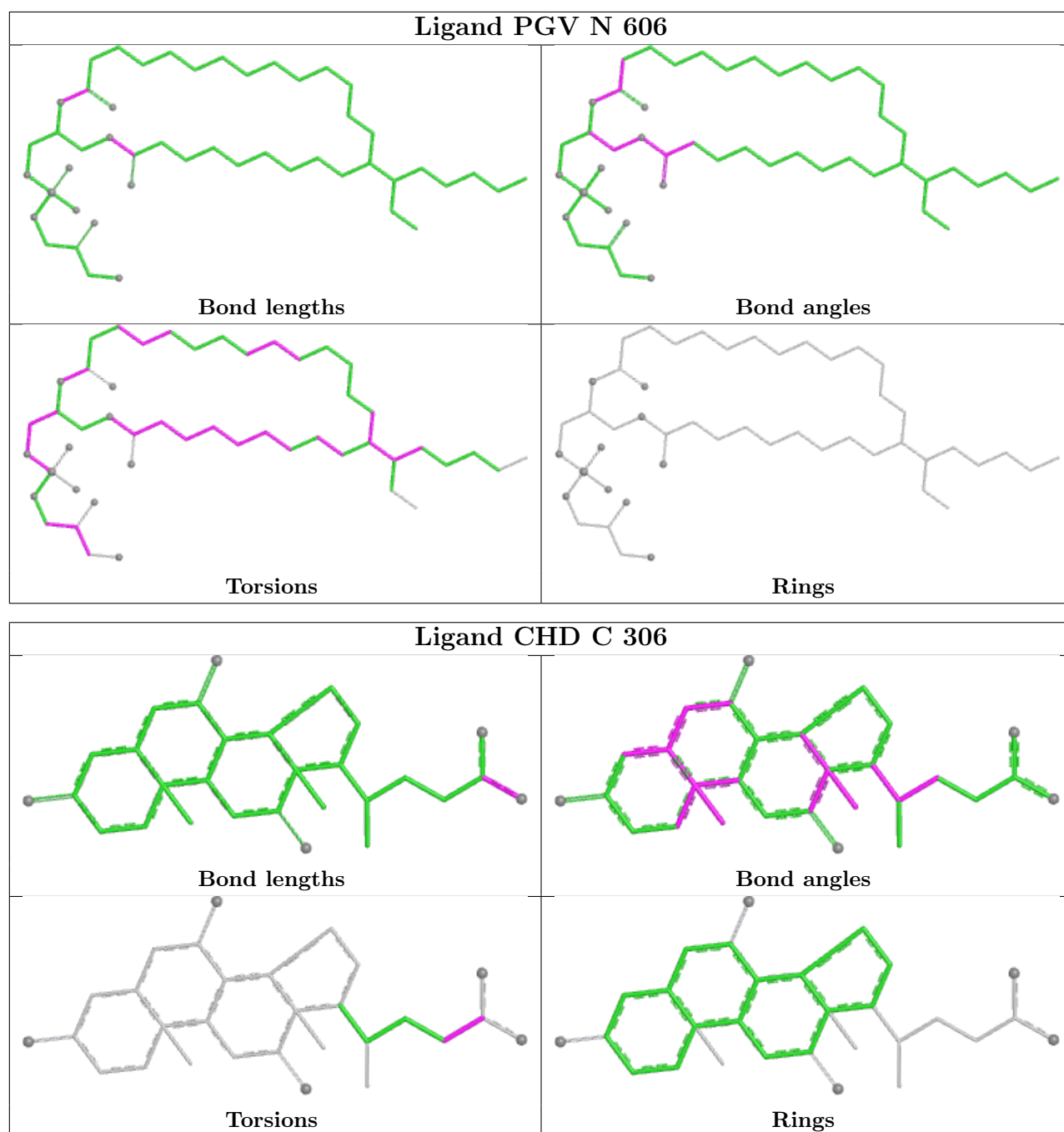


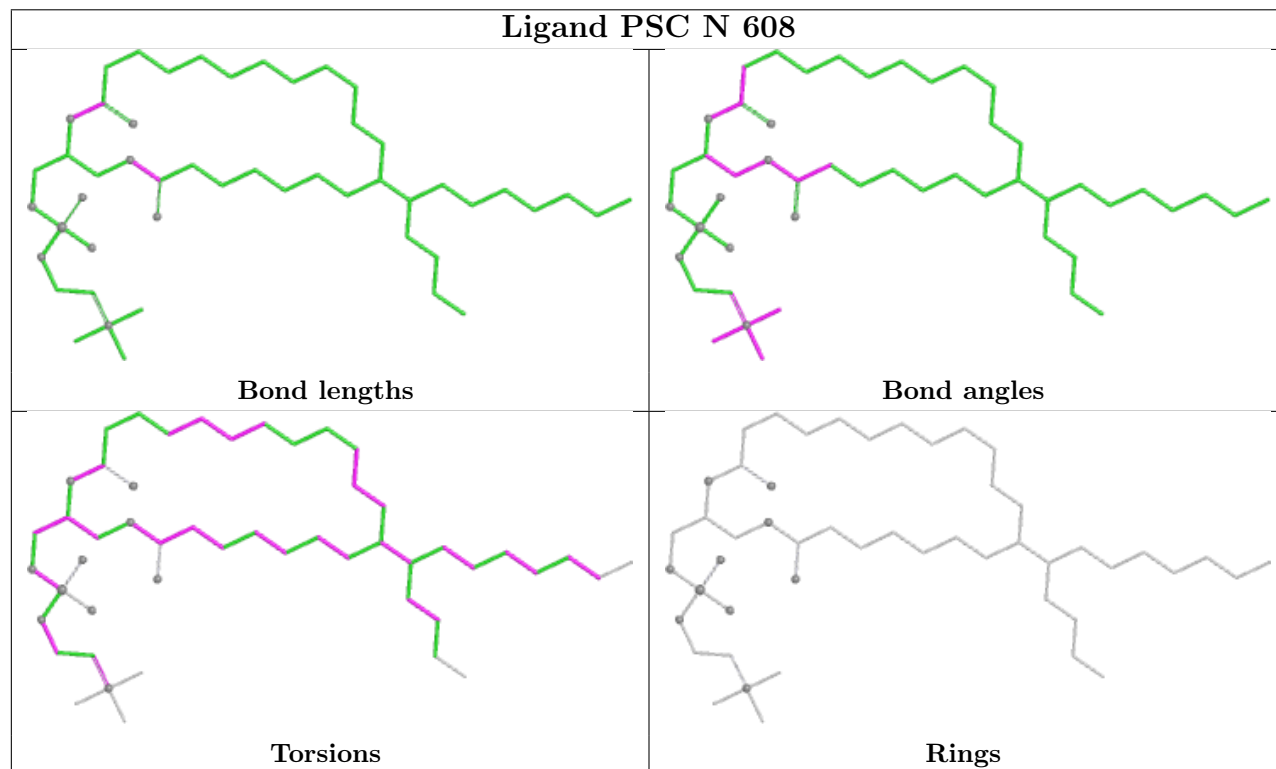
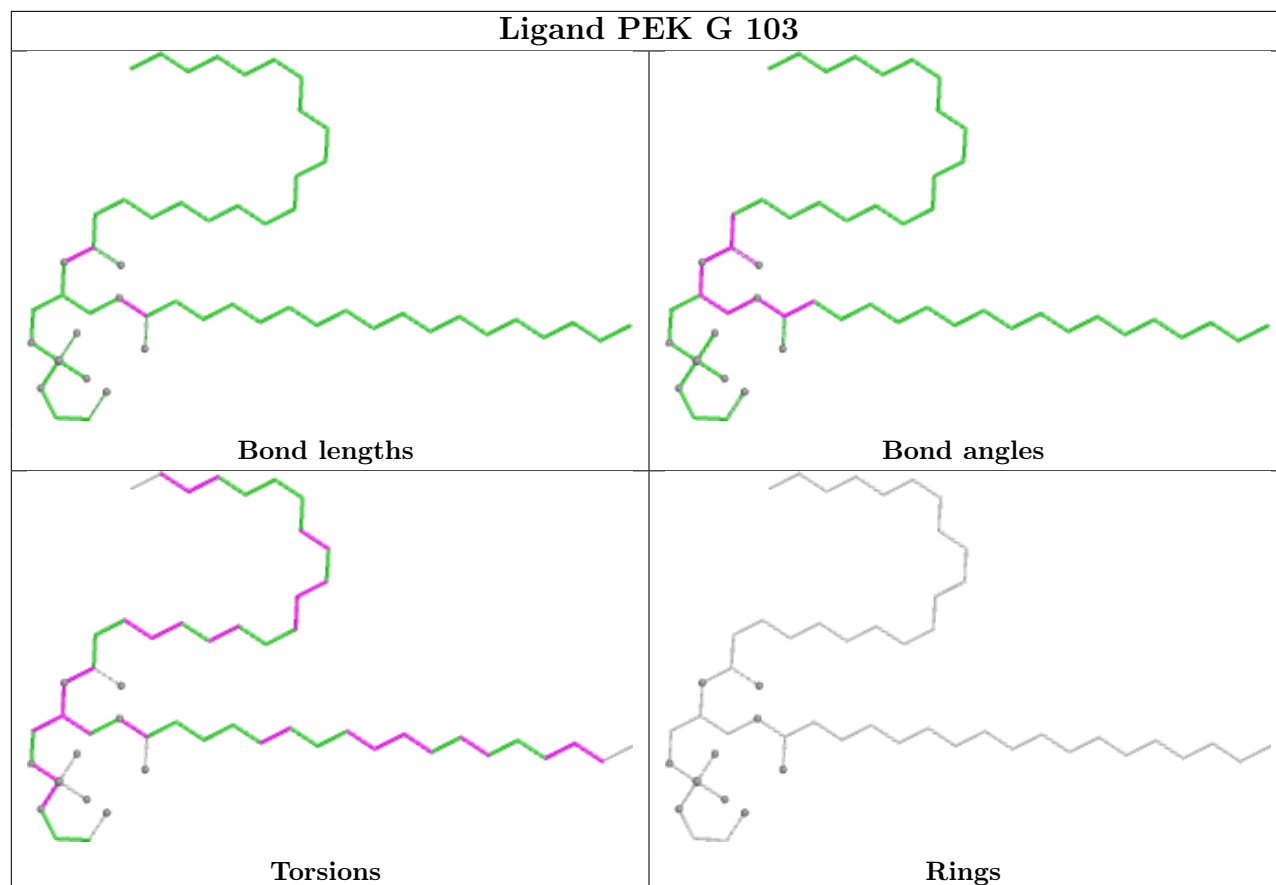


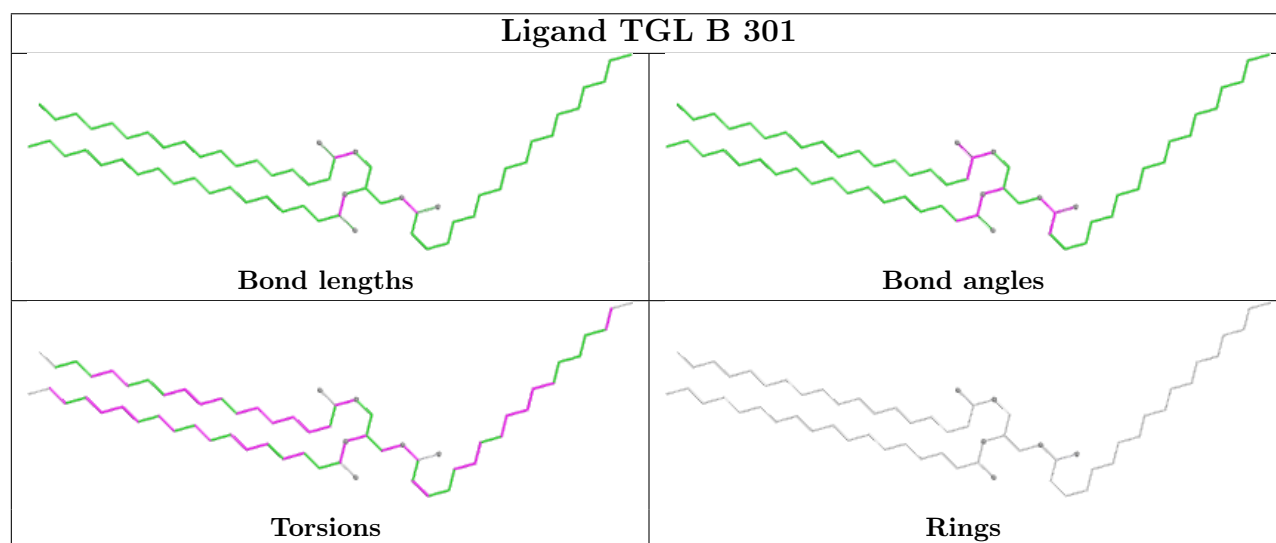
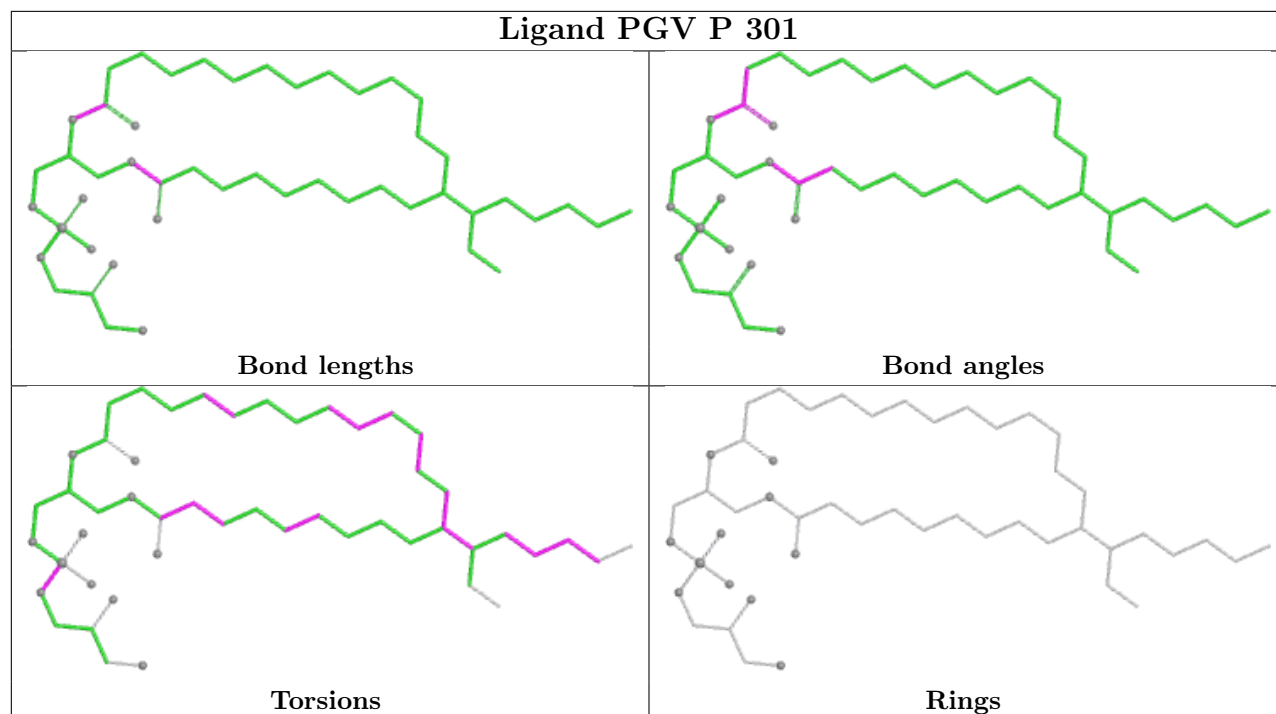


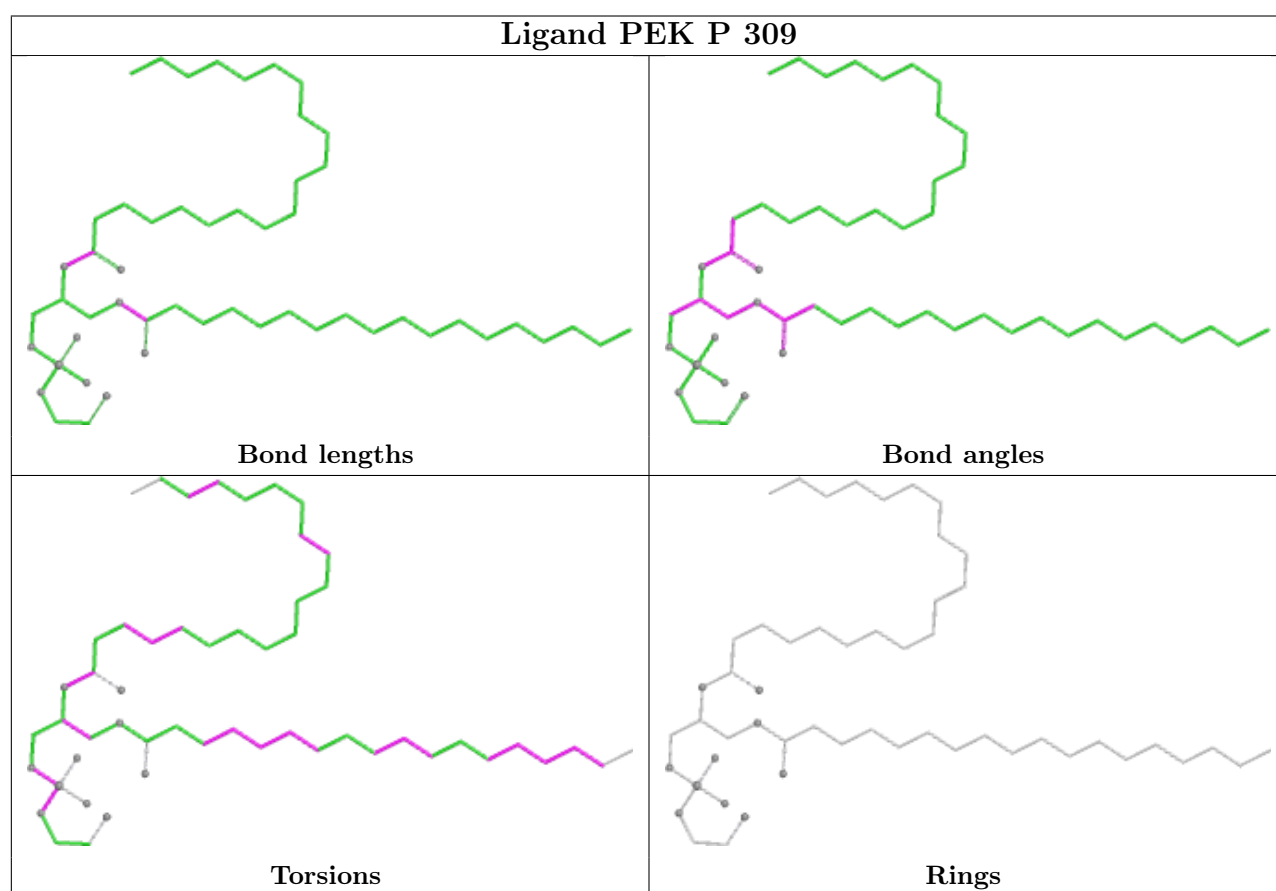
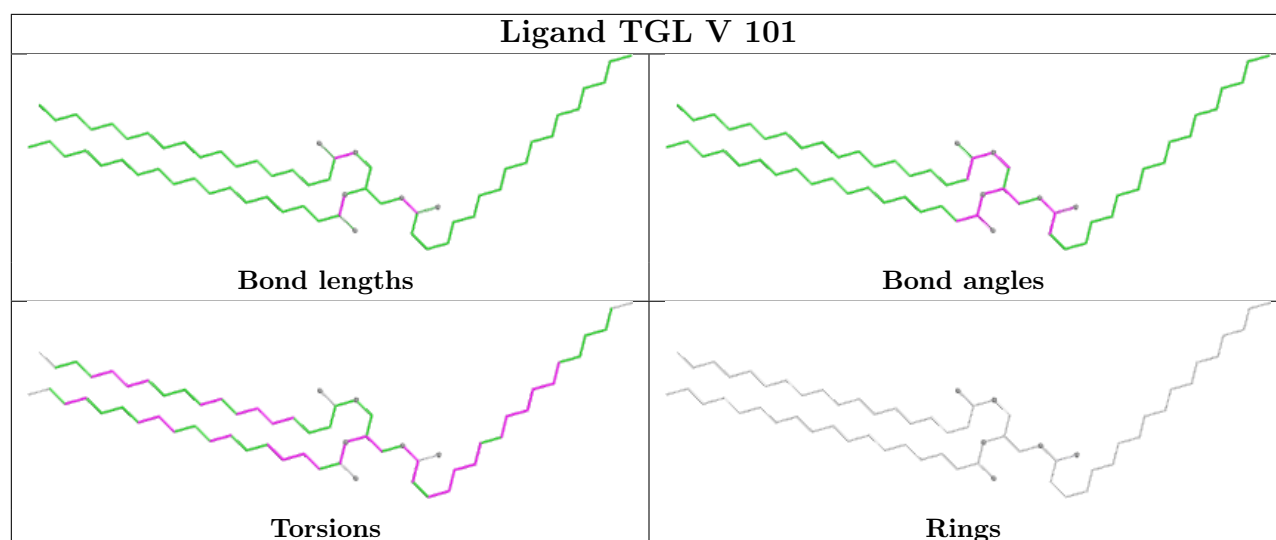


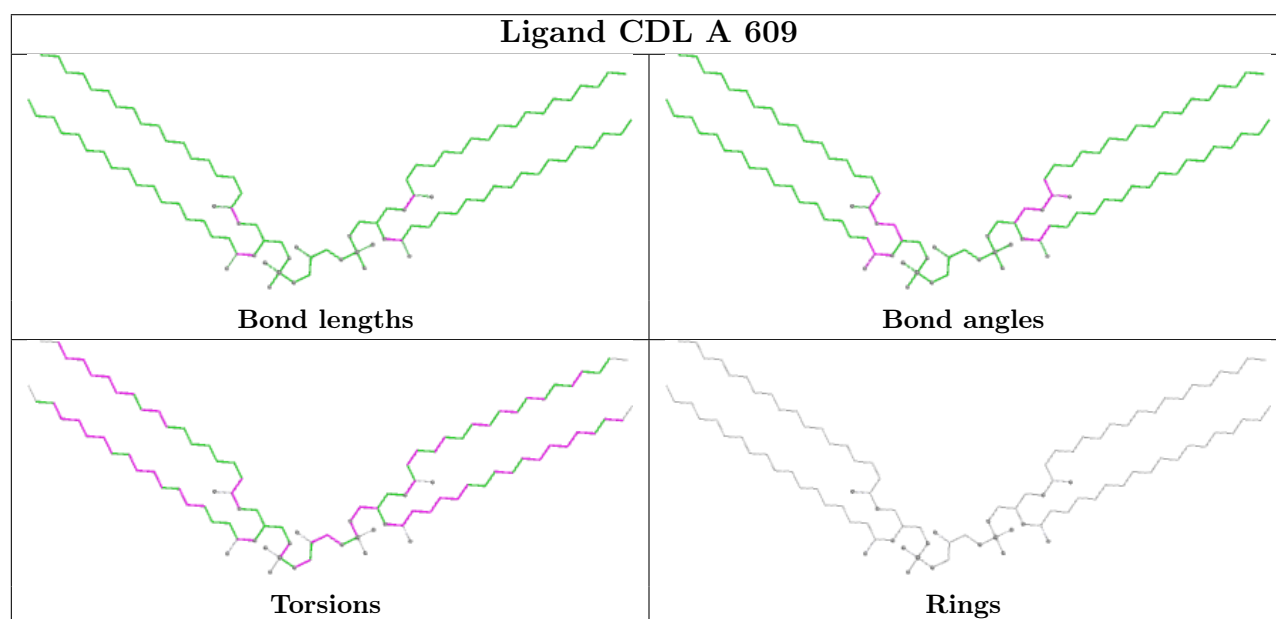
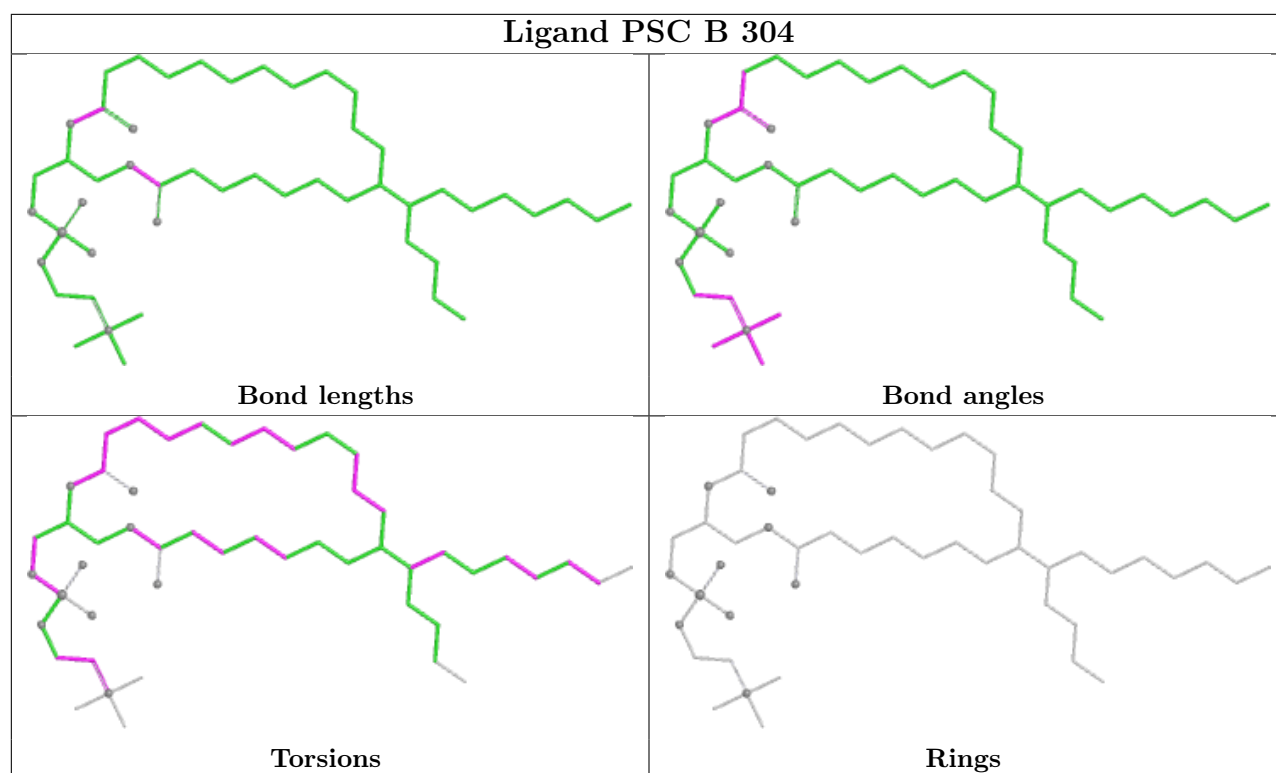


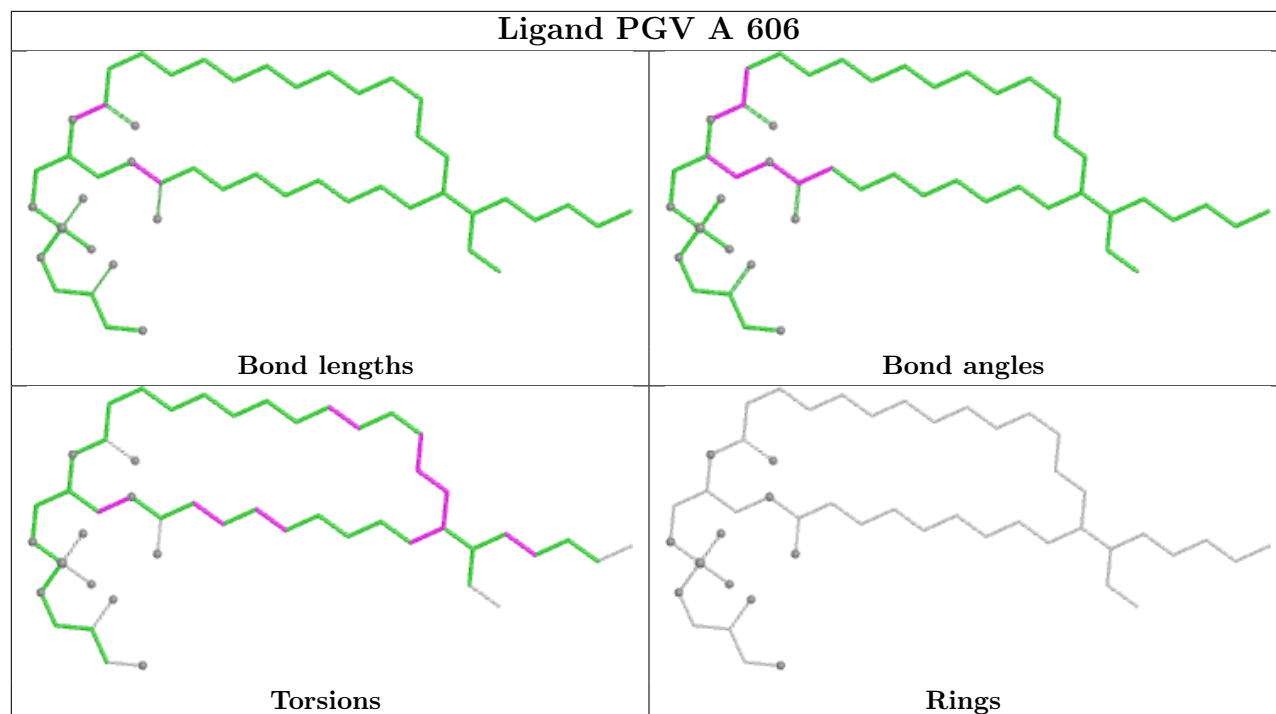












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-1.08	0 100 100	23, 49, 63, 102	12 (2%)
1	N	513/514 (99%)	-0.81	0 100 100	26, 64, 86, 108	13 (2%)
2	B	226/227 (99%)	-0.91	1 (0%) 88 84	27, 57, 86, 152	6 (2%)
2	O	226/227 (99%)	-0.59	0 100 100	33, 76, 115, 162	5 (2%)
3	C	259/261 (99%)	-1.01	0 100 100	26, 54, 75, 111	8 (3%)
3	P	259/261 (99%)	-0.83	0 100 100	24, 66, 89, 144	8 (3%)
4	D	144/147 (97%)	-0.89	0 100 100	27, 61, 91, 127	6 (4%)
4	Q	144/147 (97%)	-0.47	1 (0%) 84 77	38, 91, 136, 199	1 (0%)
5	E	105/109 (96%)	-1.01	0 100 100	34, 61, 98, 151	1 (0%)
5	R	105/109 (96%)	-0.80	0 100 100	57, 80, 102, 148	0
6	F	98/98 (100%)	-0.61	4 (4%) 41 33	27, 63, 144, 210	5 (5%)
6	S	98/98 (100%)	-0.57	2 (2%) 65 56	34, 77, 156, 217	1 (1%)
7	G	83/85 (97%)	-0.42	3 (3%) 46 37	26, 65, 155, 192	1 (1%)
7	T	83/85 (97%)	-0.34	3 (3%) 46 37	30, 81, 152, 230	3 (3%)
8	H	79/85 (92%)	-0.68	0 100 100	49, 70, 142, 155	0
8	U	79/85 (92%)	-0.54	0 100 100	66, 87, 145, 161	0
9	I	72/73 (98%)	-0.70	0 100 100	52, 70, 99, 126	0
9	V	72/73 (98%)	-0.23	3 (4%) 40 32	50, 93, 136, 155	1 (1%)
10	J	58/59 (98%)	-0.74	0 100 100	55, 68, 132, 159	0
10	W	58/59 (98%)	-0.37	0 100 100	75, 90, 131, 176	0
11	K	49/56 (87%)	-0.69	0 100 100	27, 66, 90, 132	1 (2%)
11	X	49/56 (87%)	-0.38	0 100 100	39, 92, 116, 129	1 (2%)
12	L	46/47 (97%)	-0.89	0 100 100	44, 57, 83, 137	0
12	Y	46/47 (97%)	-0.41	0 100 100	68, 86, 109, 139	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	-0.91	0 100 100	49, 57, 102, 141	0
13	Z	43/46 (93%)	-0.34	0 100 100	71, 86, 133, 165	0
All	All	3550/3614 (98%)	-0.77	17 (0%) 87 82	23, 65, 113, 230	73 (2%)

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	V	33	THR	4.6
4	Q	6	VAL	3.8
9	V	30	GLY	3.8
6	S	1	ALA	3.7
9	V	37	PHE	3.3

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	I	1	9/10	0.63	0.14	121,144,159,160	0
7	TPO	G	11	11/12	0.69	0.23	121,154,184,184	0
9	SAC	V	1	9/10	0.69	0.10	135,147,156,162	0
7	TPO	T	11	11/12	0.77	0.18	115,155,185,188	0
1	FME	N	1	10/11	0.85	0.14	101,115,136,144	0
1	FME	A	1	10/11	0.90	0.10	78,86,113,125	0
2	FME	O	1	10/11	0.95	0.08	67,85,98,100	0
2	FME	B	1	10/11	0.97	0.07	49,56,61,63	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.

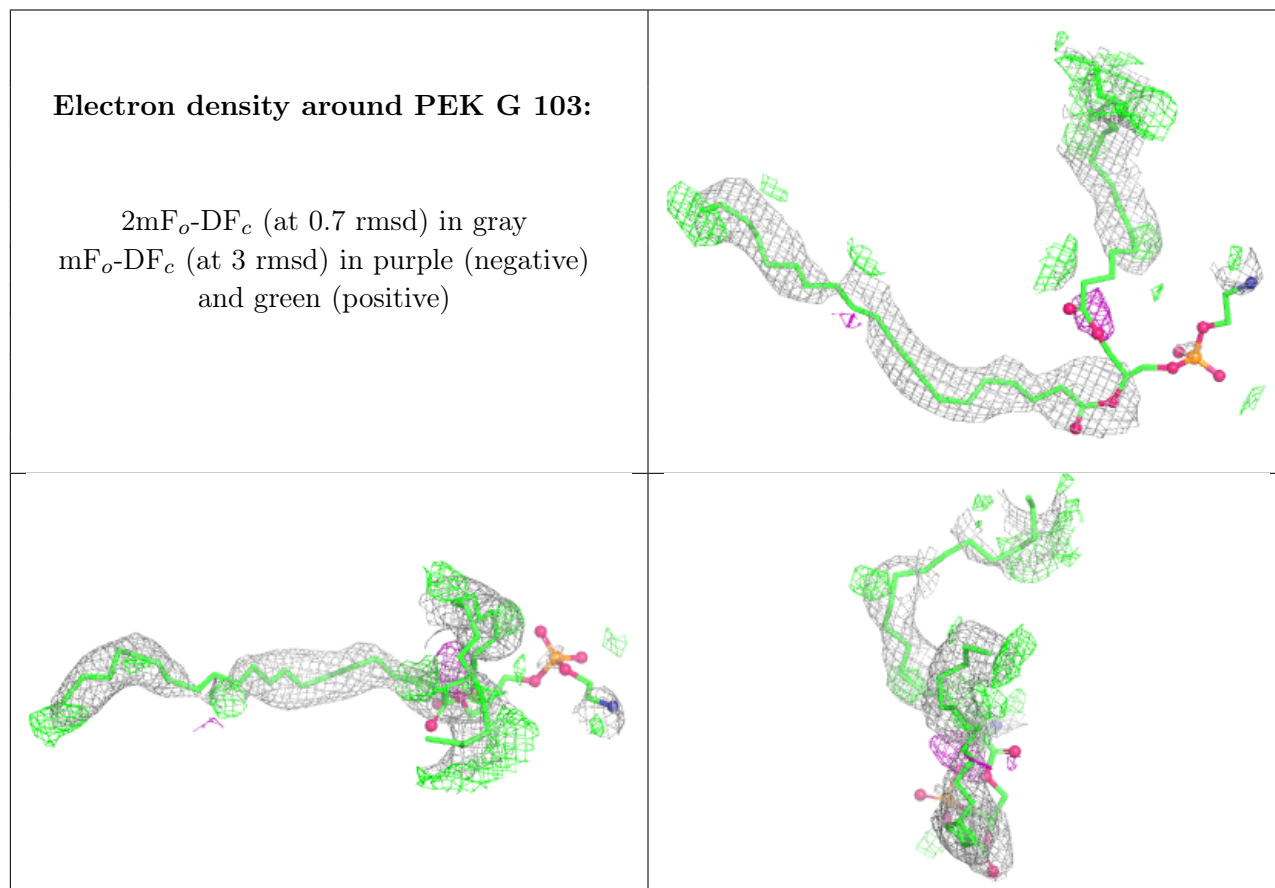
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
25	PEK	G	103	53/53	0.74	0.18	74,142,205,215	0
25	PEK	T	101	53/53	0.79	0.17	87,156,204,213	0
18	PGV	N	606	51/51	0.80	0.12	79,110,191,215	0
19	TGL	N	607	63/63	0.80	0.14	84,123,138,143	0
18	PGV	P	302	51/51	0.82	0.12	74,117,160,166	0
25	PEK	P	309	53/53	0.82	0.12	78,122,173,183	0
22	CHD	W	101	29/29	0.82	0.13	110,149,184,190	0
25	PEK	G	101	53/53	0.83	0.13	74,117,202,210	0
20	CDL	C	304	100/100	0.83	0.14	68,127,168,183	0
18	PGV	C	307	51/51	0.84	0.12	81,118,146,150	0
20	CDL	A	609	100/100	0.84	0.15	96,129,187,213	0
23	PSC	N	608	52/52	0.84	0.15	83,137,241,271	0
24	DMU	P	303	33/33	0.84	0.16	96,163,206,222	0
19	TGL	V	101	63/63	0.85	0.12	53,114,164,179	0
20	CDL	G	102	100/100	0.85	0.14	105,135,187,207	0
20	CDL	P	305	100/100	0.85	0.15	84,133,190,254	0
19	TGL	Y	101	63/63	0.85	0.14	83,122,160,163	0
19	TGL	D	201	63/63	0.85	0.12	72,109,128,135	0
24	DMU	C	301	33/33	0.86	0.16	86,191,206,210	0
23	PSC	B	304	52/52	0.86	0.15	81,130,210,219	0
18	PGV	A	607	51/51	0.87	0.11	72,120,163,176	0
17	NA	N	605	1/1	0.87	0.14	81,81,81,81	0
22	CHD	J	101	29/29	0.87	0.11	87,116,136,140	0
19	TGL	B	301	63/63	0.87	0.12	47,103,141,146	0
22	CHD	C	305	29/29	0.89	0.11	99,115,136,140	0
24	DMU	Q	201	33/33	0.89	0.10	86,110,126,137	0
19	TGL	A	608	63/63	0.89	0.14	56,105,138,148	0
22	CHD	P	306	29/29	0.90	0.10	102,113,124,126	0
24	DMU	M	101	33/33	0.95	0.07	62,69,85,91	0
25	PEK	P	308	53/53	0.95	0.09	65,94,152,173	0
18	PGV	P	304	51/51	0.96	0.08	55,67,117,123	0
18	PGV	P	301	51/51	0.96	0.08	47,71,94,108	0
22	CHD	P	307	29/29	0.96	0.06	55,60,67,69	0
22	CHD	G	104	29/29	0.97	0.06	49,54,62,73	0
22	CHD	B	303	29/29	0.97	0.05	52,55,64,72	0
25	PEK	C	302	53/53	0.97	0.07	49,72,125,132	0
22	CHD	C	306	29/29	0.97	0.06	41,52,60,68	0
18	PGV	C	303	51/51	0.98	0.06	45,60,107,114	0
14	HEA	N	601	60/60	0.98	0.06	42,62,77,82	0
17	NA	A	605	1/1	0.98	0.04	55,55,55,55	0
14	HEA	A	601	60/60	0.98	0.06	40,47,65,75	0
18	PGV	A	606	51/51	0.98	0.06	40,69,89,93	0

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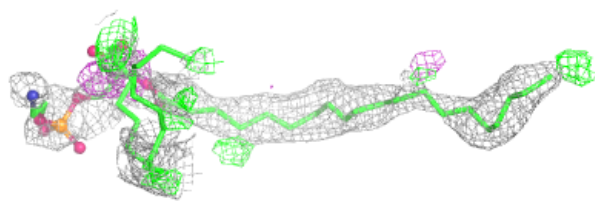
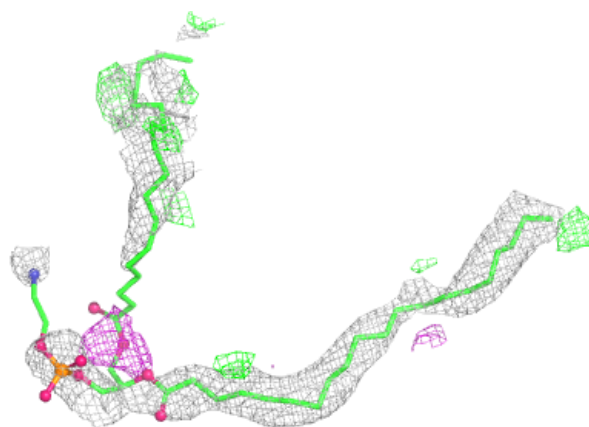
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
14	HEA	A	602	60/60	0.98	0.05	34,43,60,70	0
14	HEA	N	602	60/60	0.99	0.05	43,52,61,64	0
16	MG	N	604	1/1	0.99	0.03	60,60,60,60	0
21	CUA	B	302	2/2	0.99	0.02	53,53,53,57	0
21	CUA	O	301	2/2	0.99	0.03	76,76,76,76	0
26	ZN	S	101	1/1	0.99	0.02	72,72,72,72	0
16	MG	A	604	1/1	1.00	0.01	43,43,43,43	0
15	CU	A	603	1/1	1.00	0.04	53,53,53,53	0
26	ZN	F	101	1/1	1.00	0.02	65,65,65,65	0
15	CU	N	603	1/1	1.00	0.05	64,64,64,64	0

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

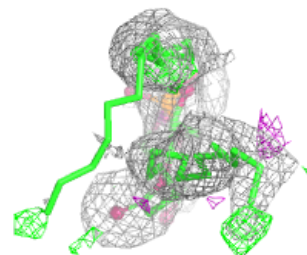
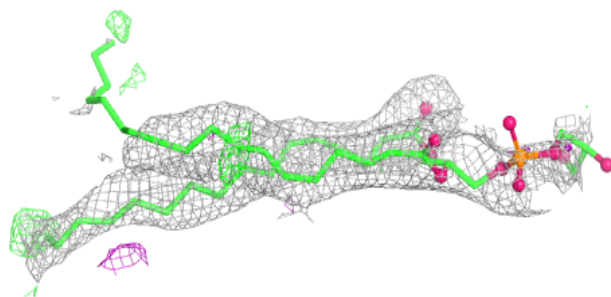
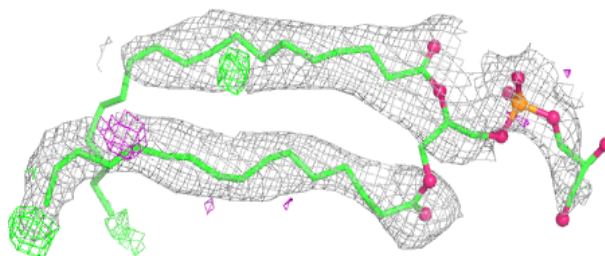


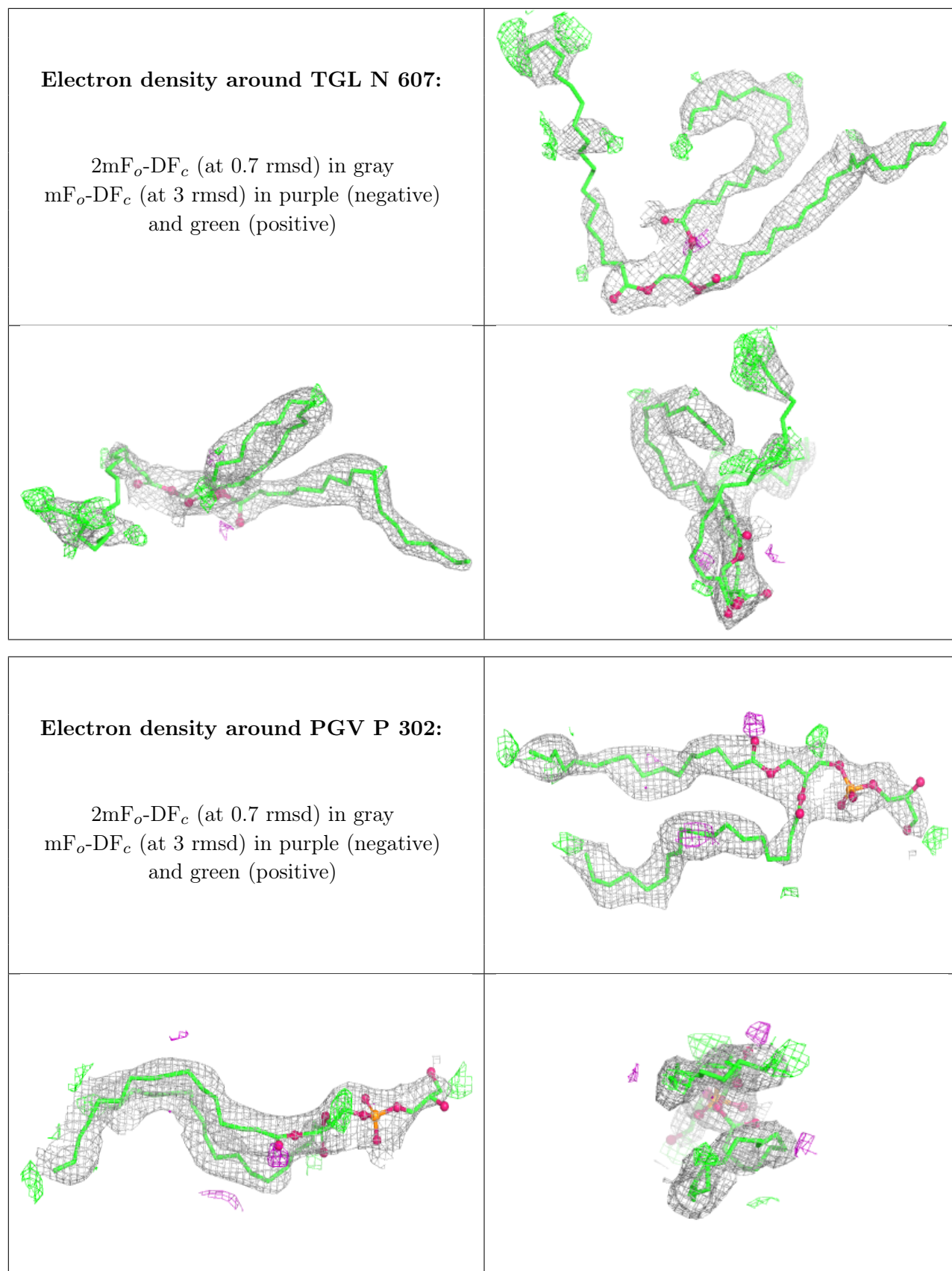
Electron density around PEK T 101:

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

**Electron density around PGV N 606:**

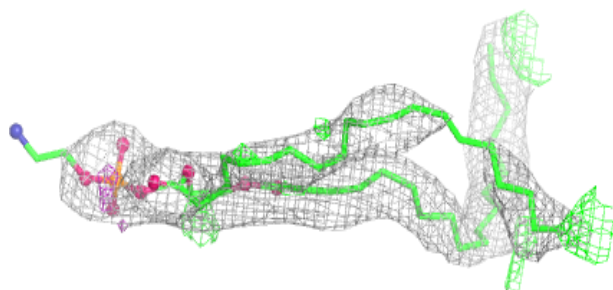
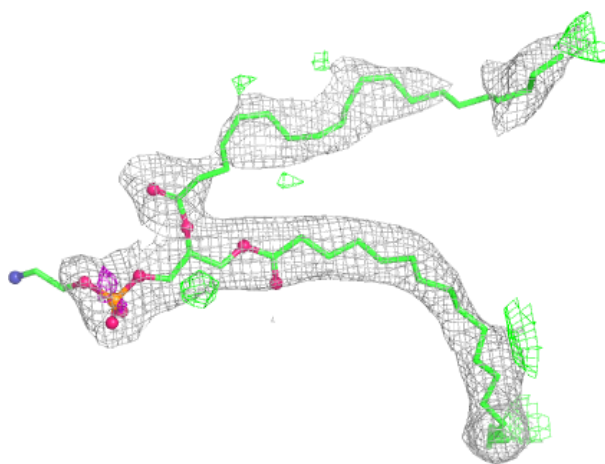
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

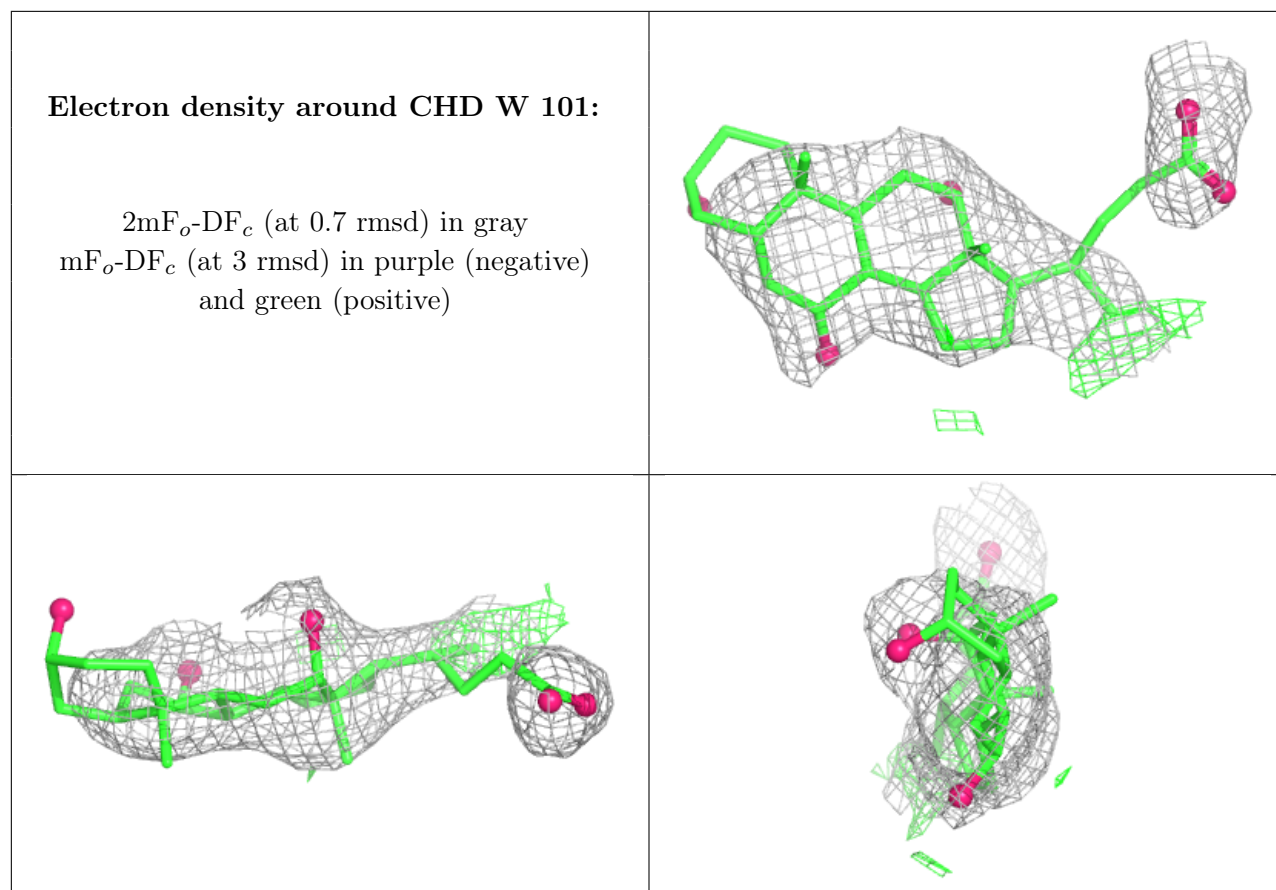




Electron density around PEK P 309:

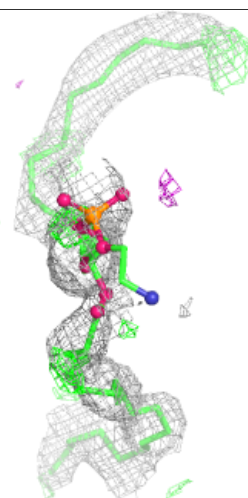
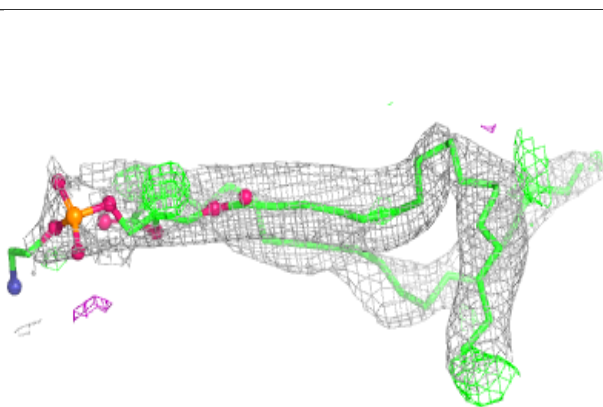
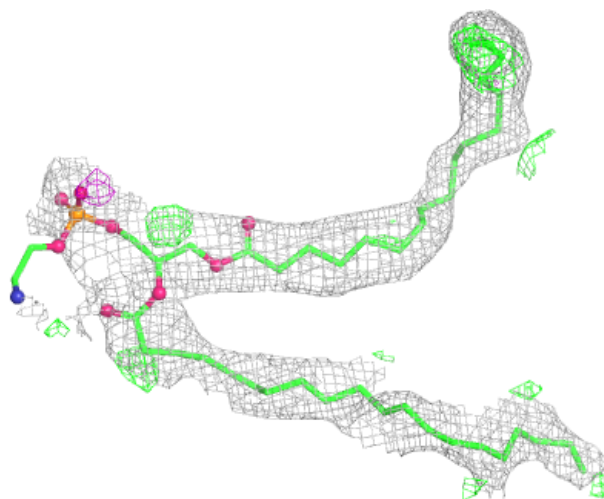
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





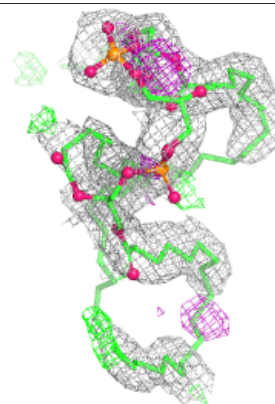
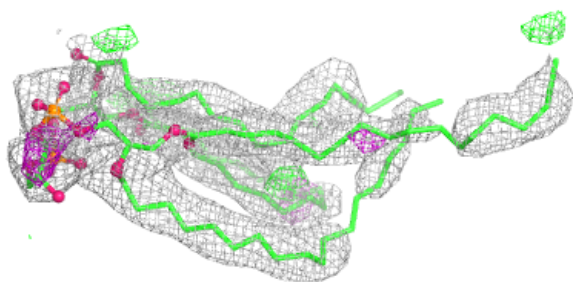
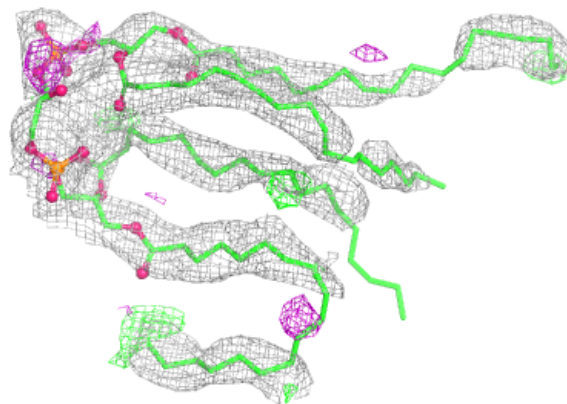
Electron density around PEK G 101:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

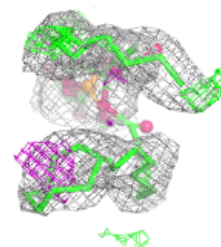
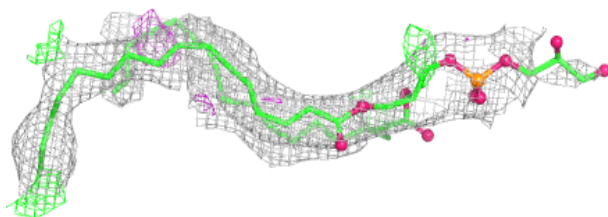
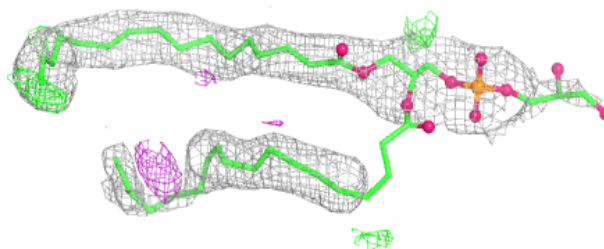


Electron density around CDL C 304:

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

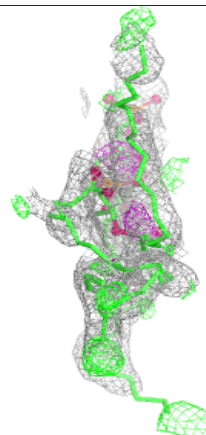
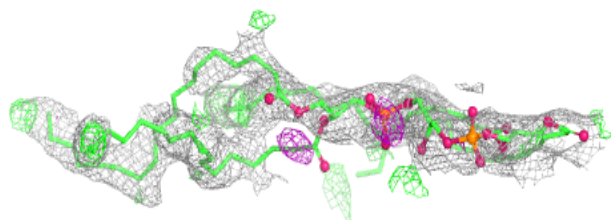
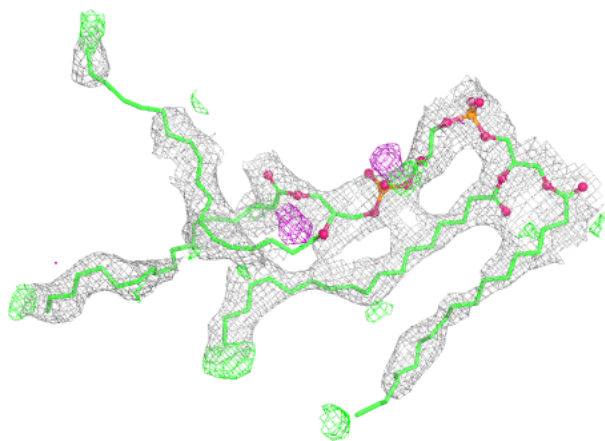
**Electron density around PGV C 307:**

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

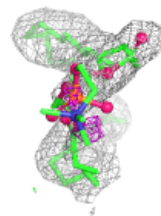
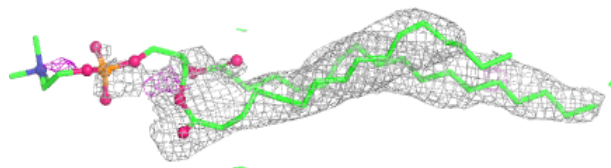
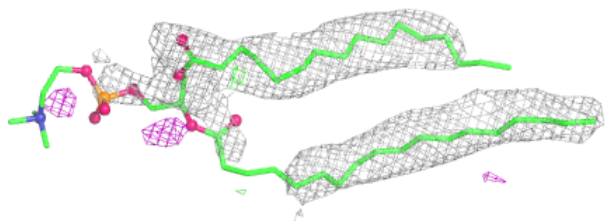


Electron density around CDL A 609:

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

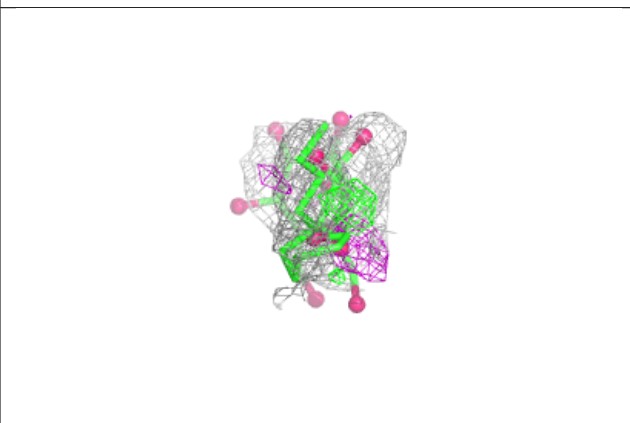
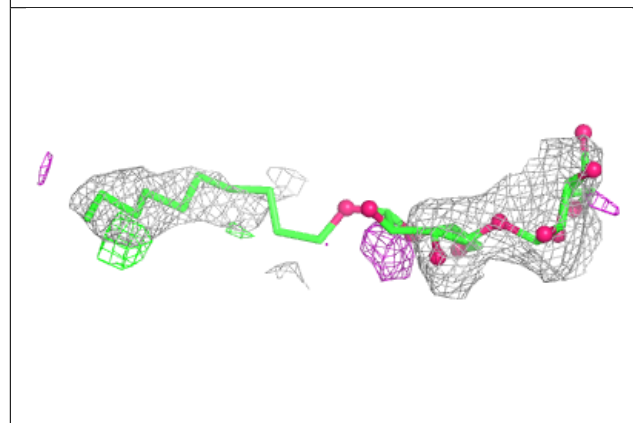
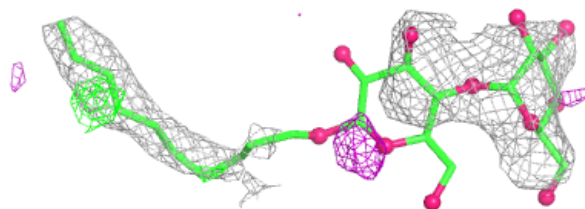
**Electron density around PSC N 608:**

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

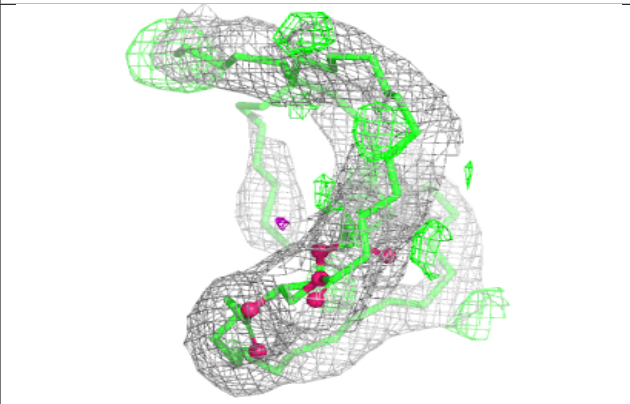
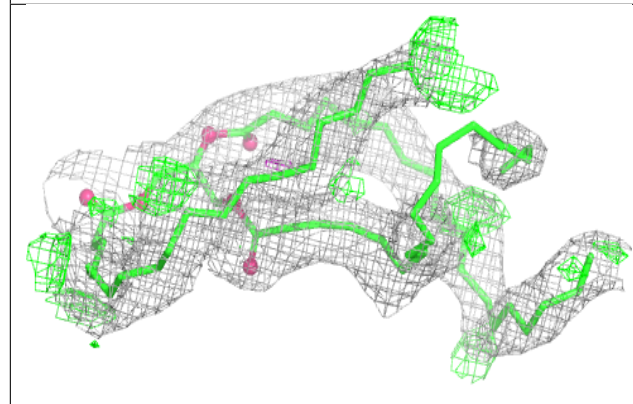
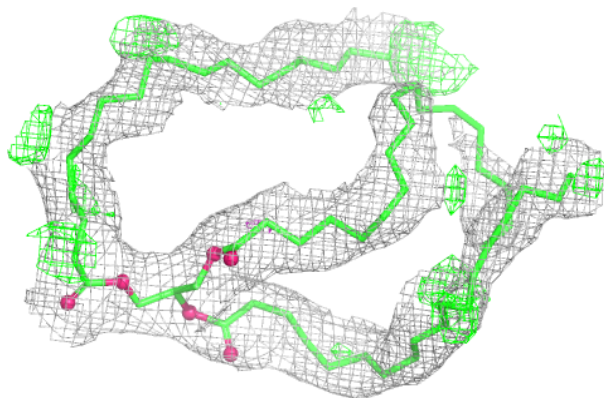


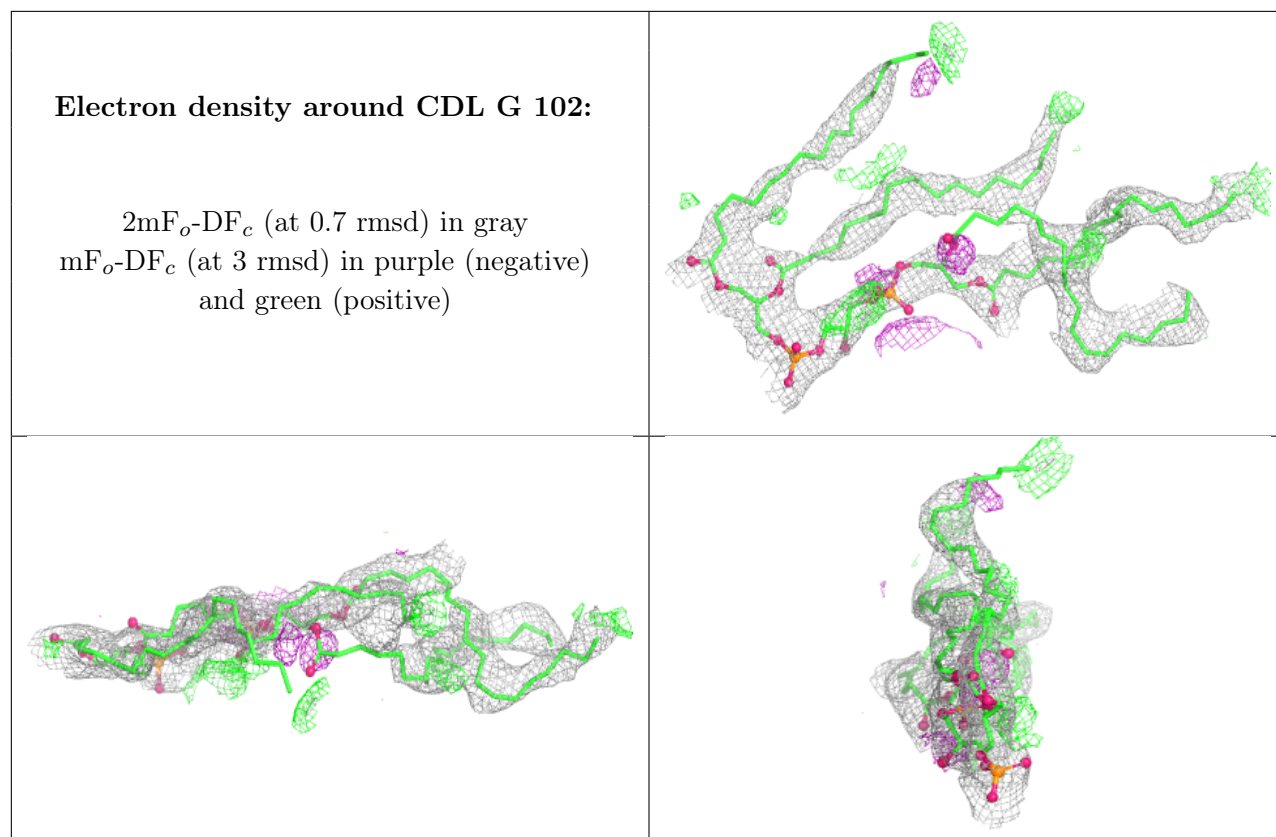
Electron density around DMU P 303:

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

**Electron density around TGL V 101:**

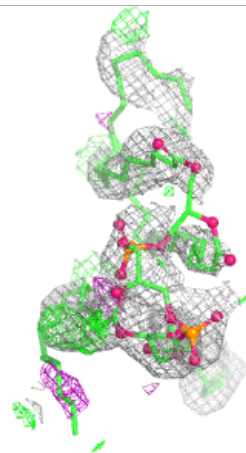
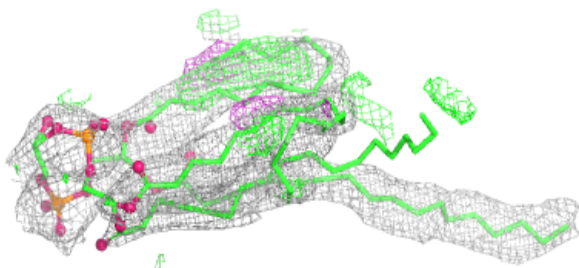
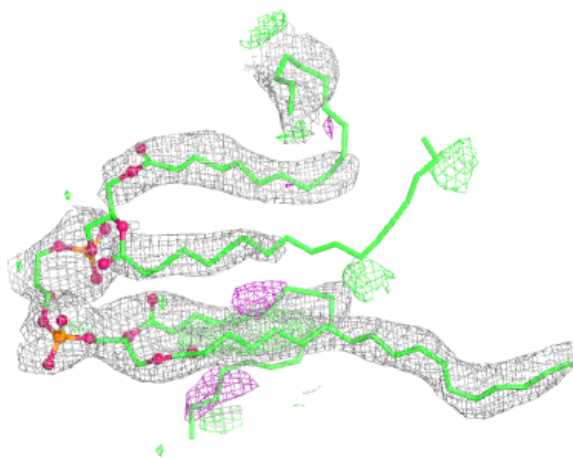
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

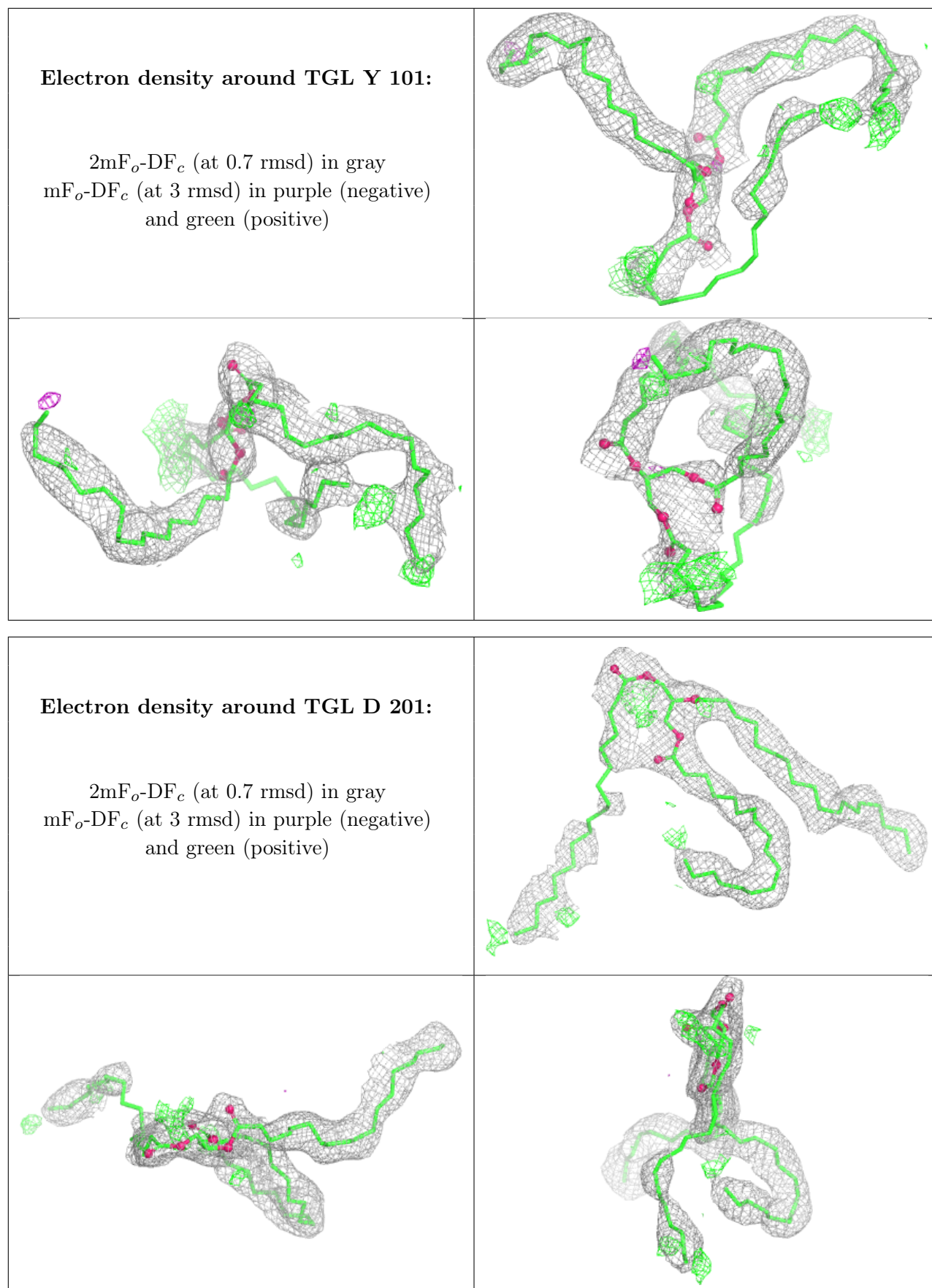




Electron density around CDL P 305:

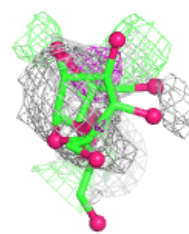
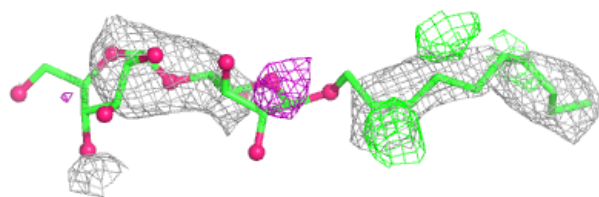
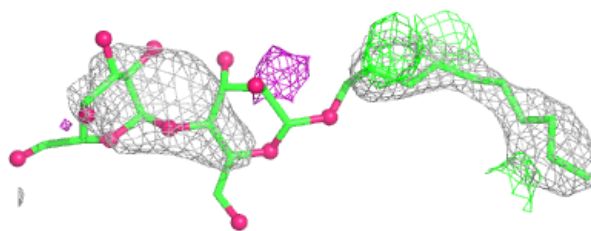
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



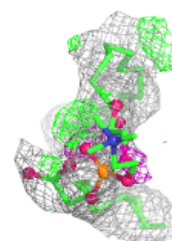
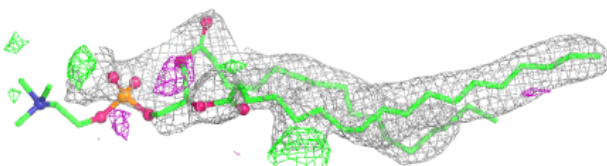
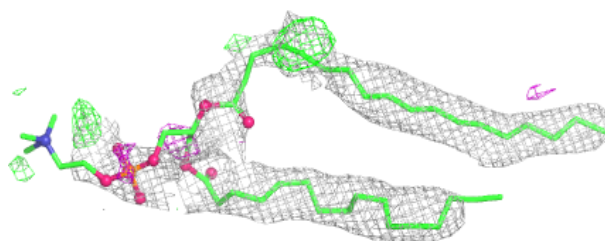


Electron density around DMU C 301:

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and green (positive)

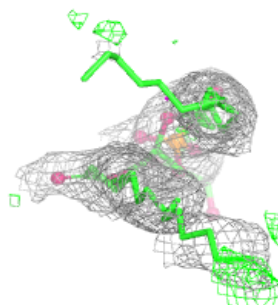
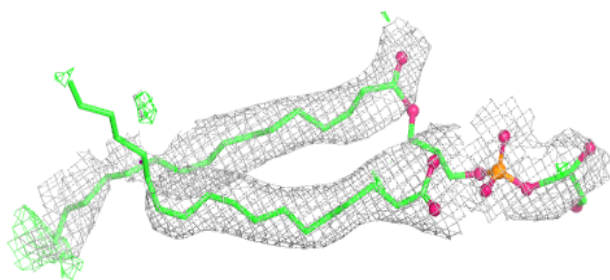
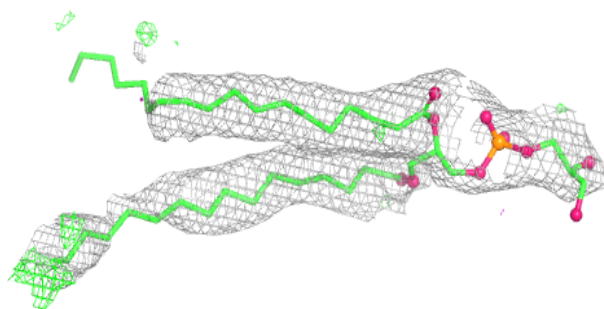
**Electron density around PSC B 304:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

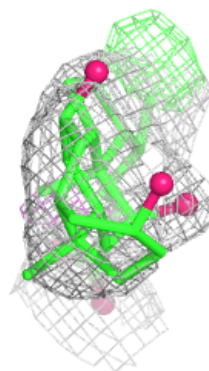
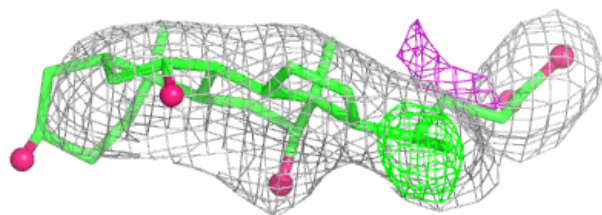
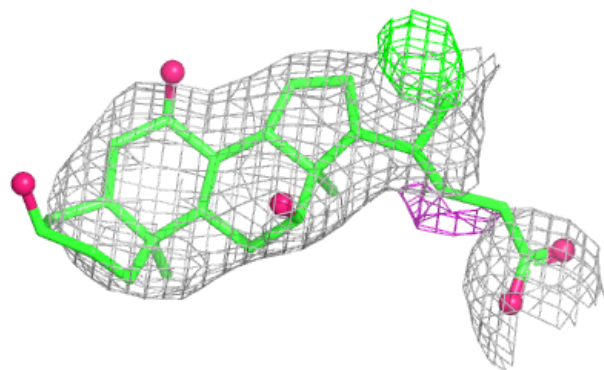


Electron density around PGV A 607:

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and green (positive)

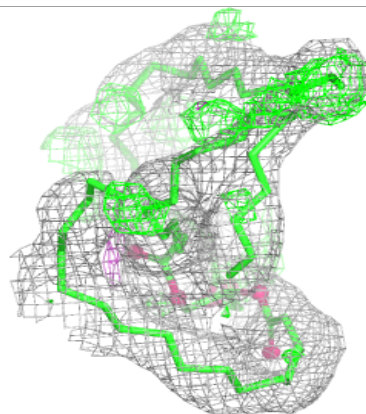
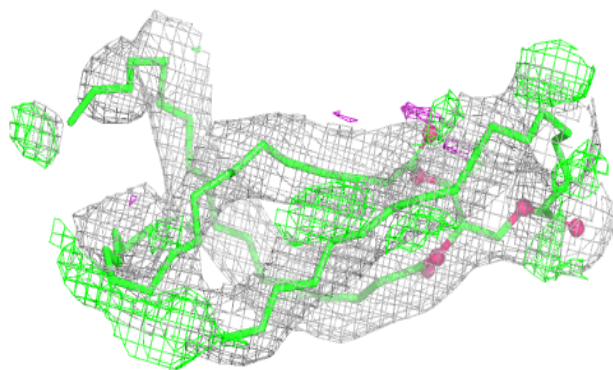
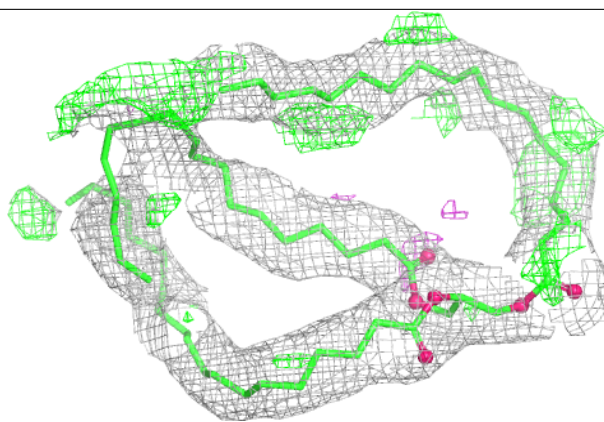
**Electron density around CHD J 101:**

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

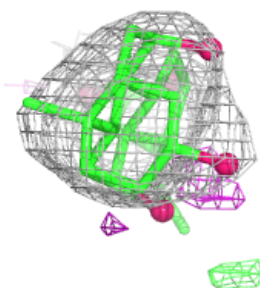
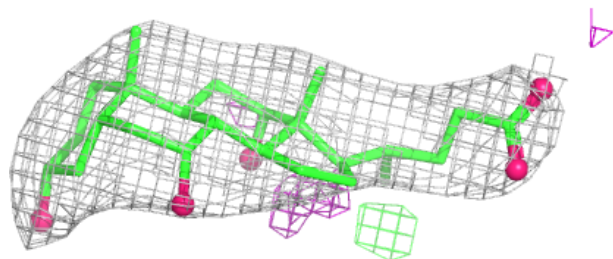
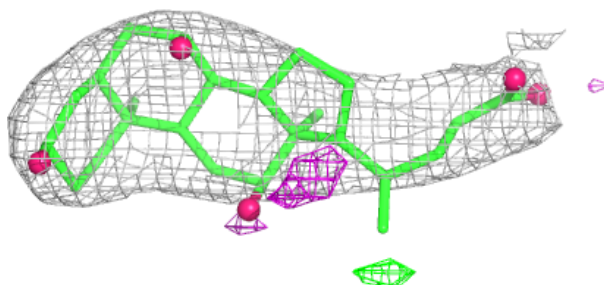


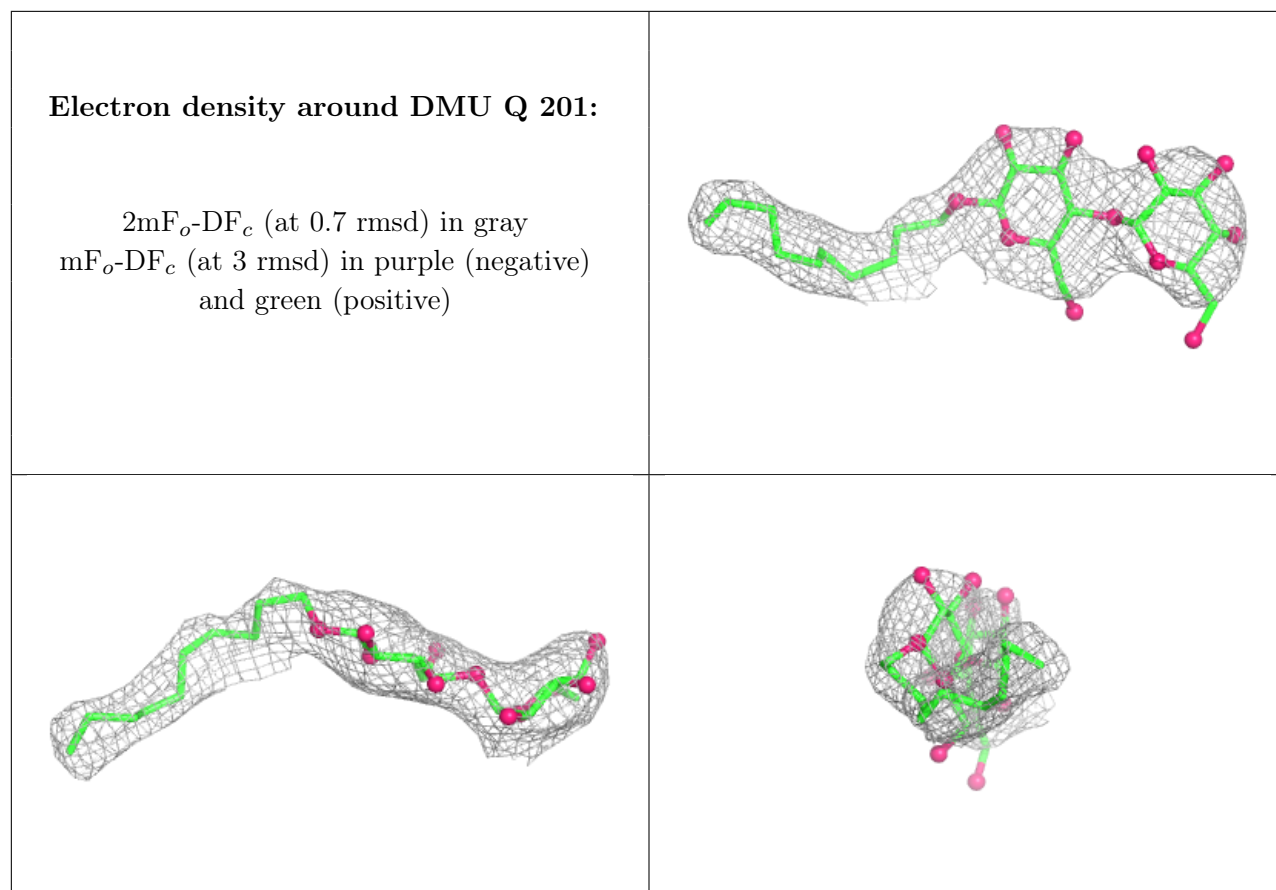
Electron density around TGL B 301:

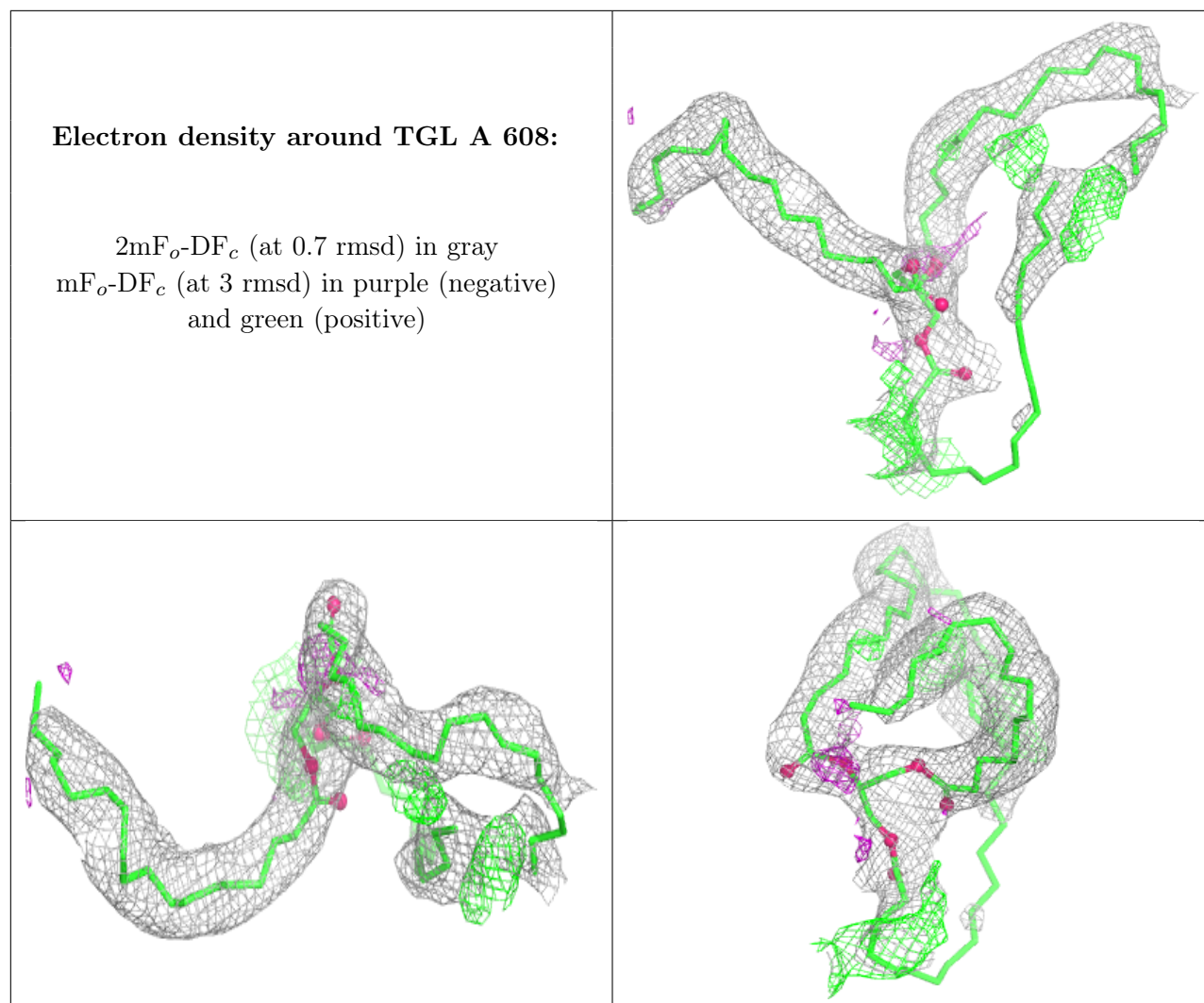
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around 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)

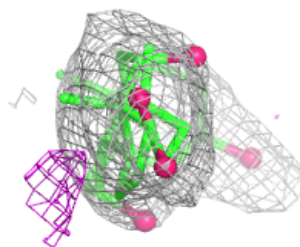
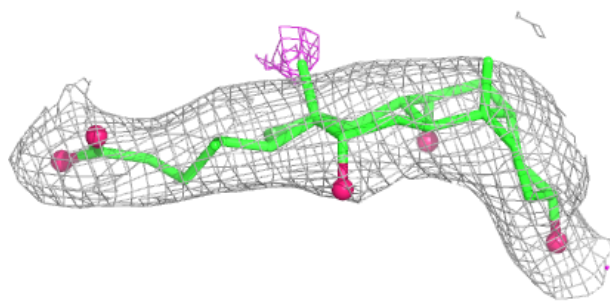
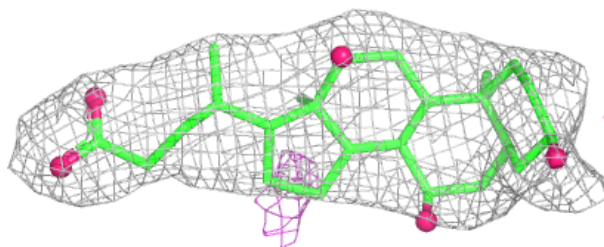




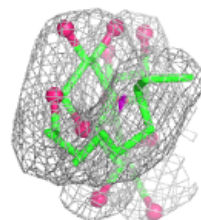
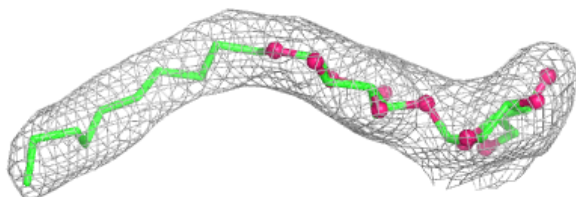
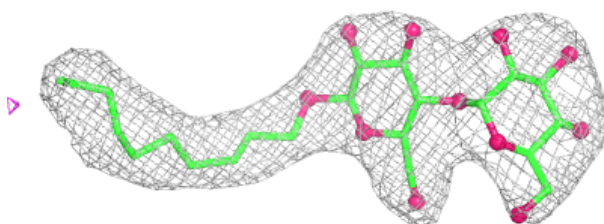


Electron density around CHD P 306:

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

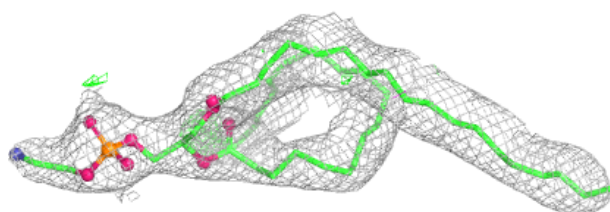
**Electron density around DMU M 101:**

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

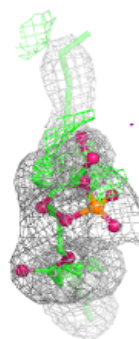
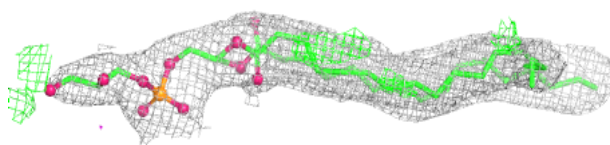
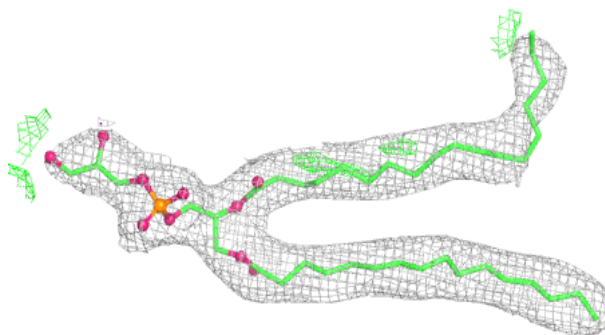


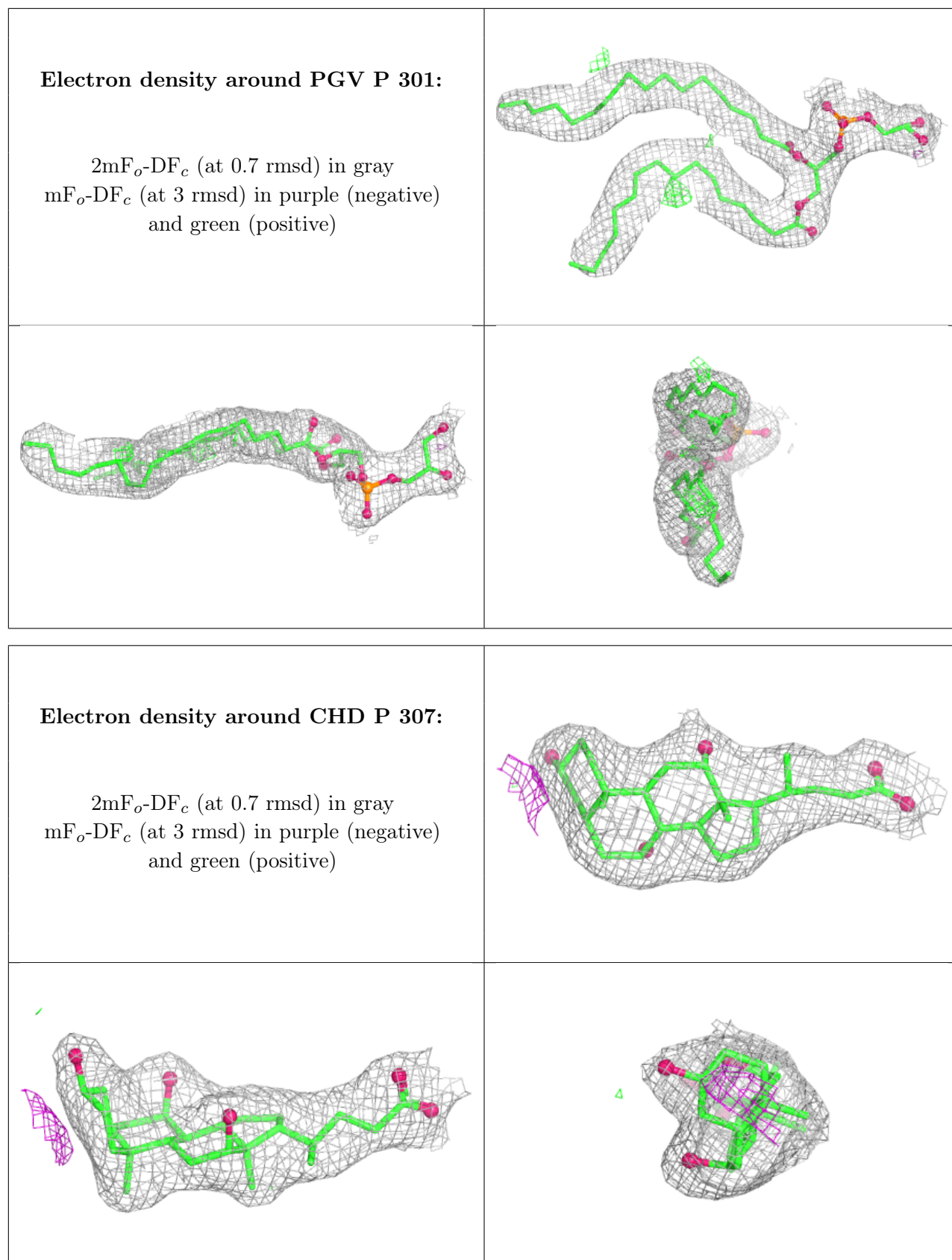
Electron density around PEK P 308:

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

**Electron density around PGV P 304:**

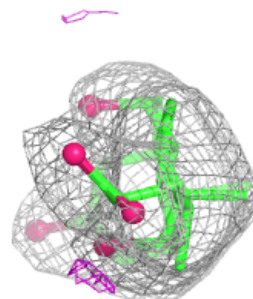
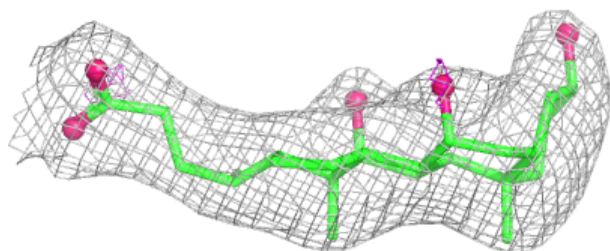
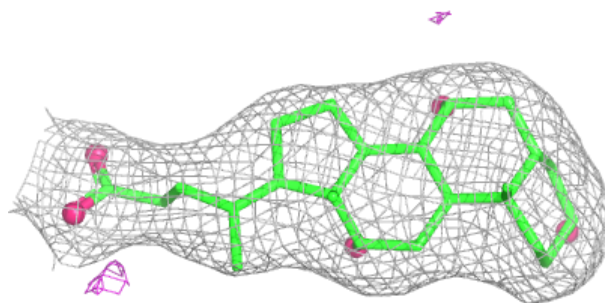
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



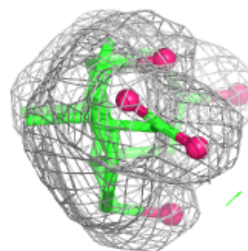
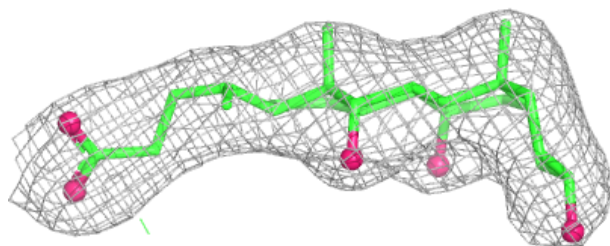
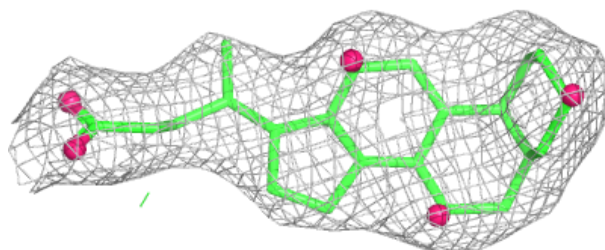


Electron density around CHD G 104:

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

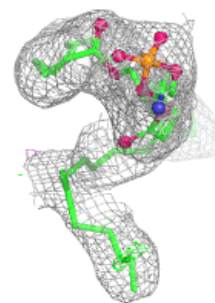
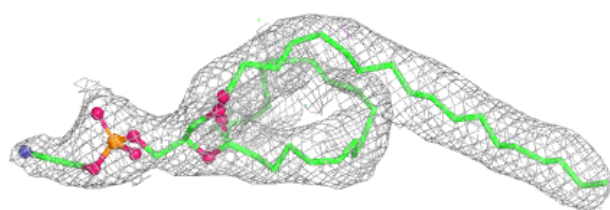
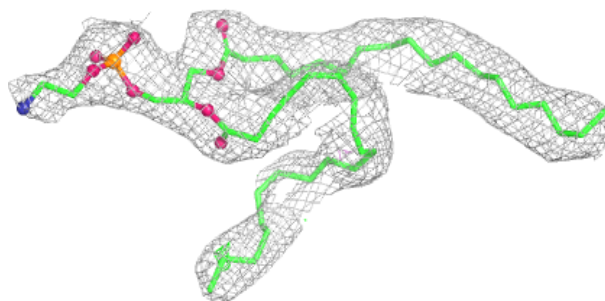
**Electron density around CHD B 303:**

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

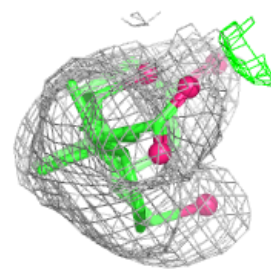
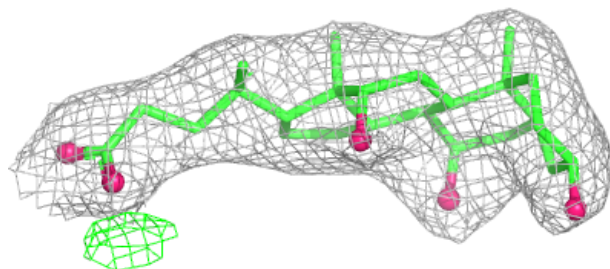
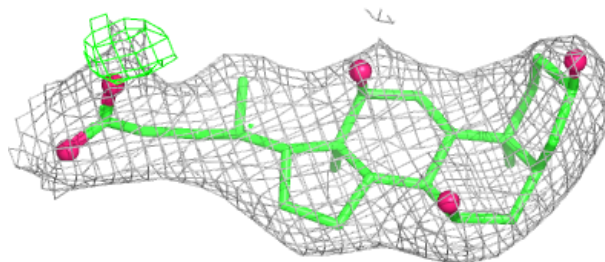


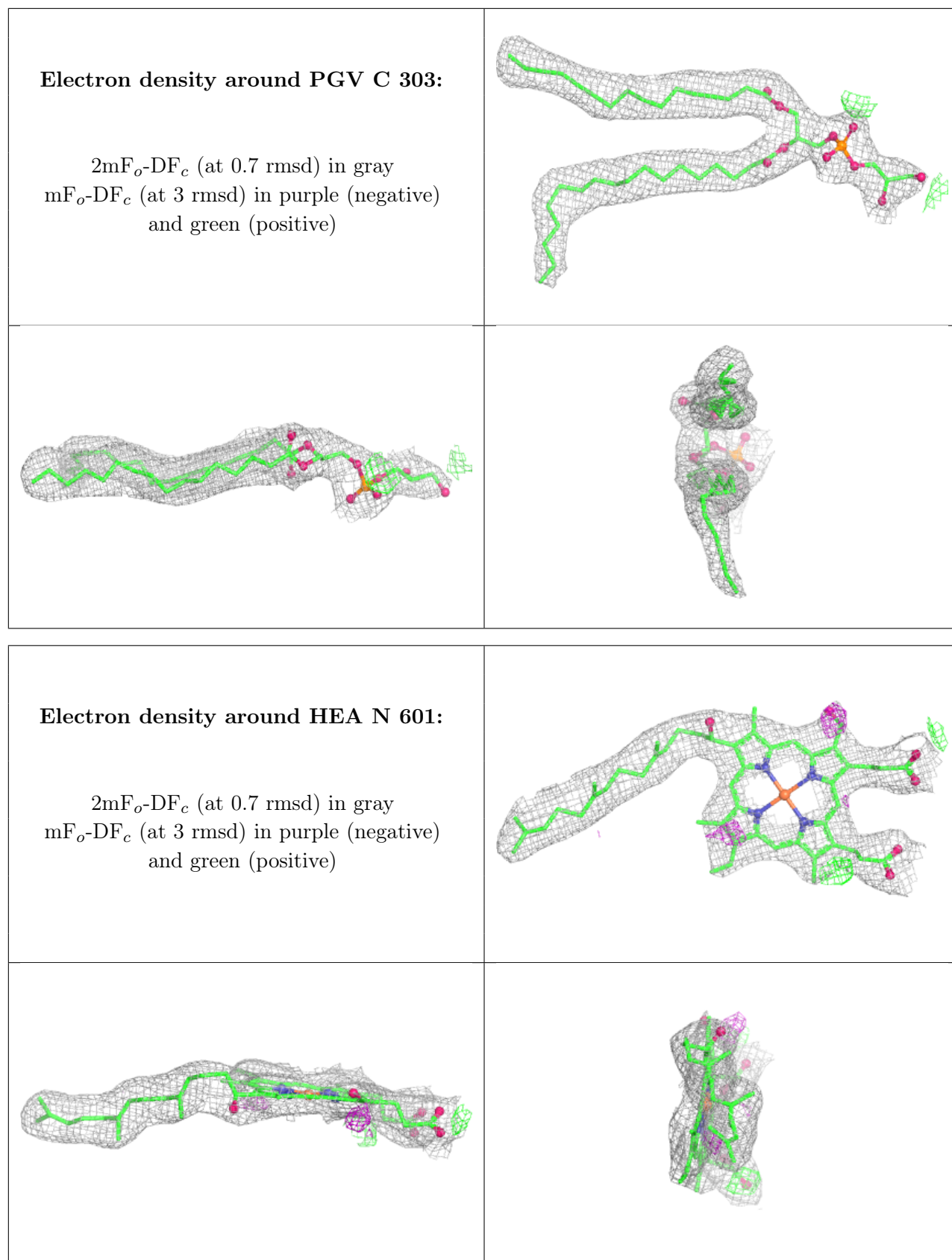
Electron density around PEK C 302:

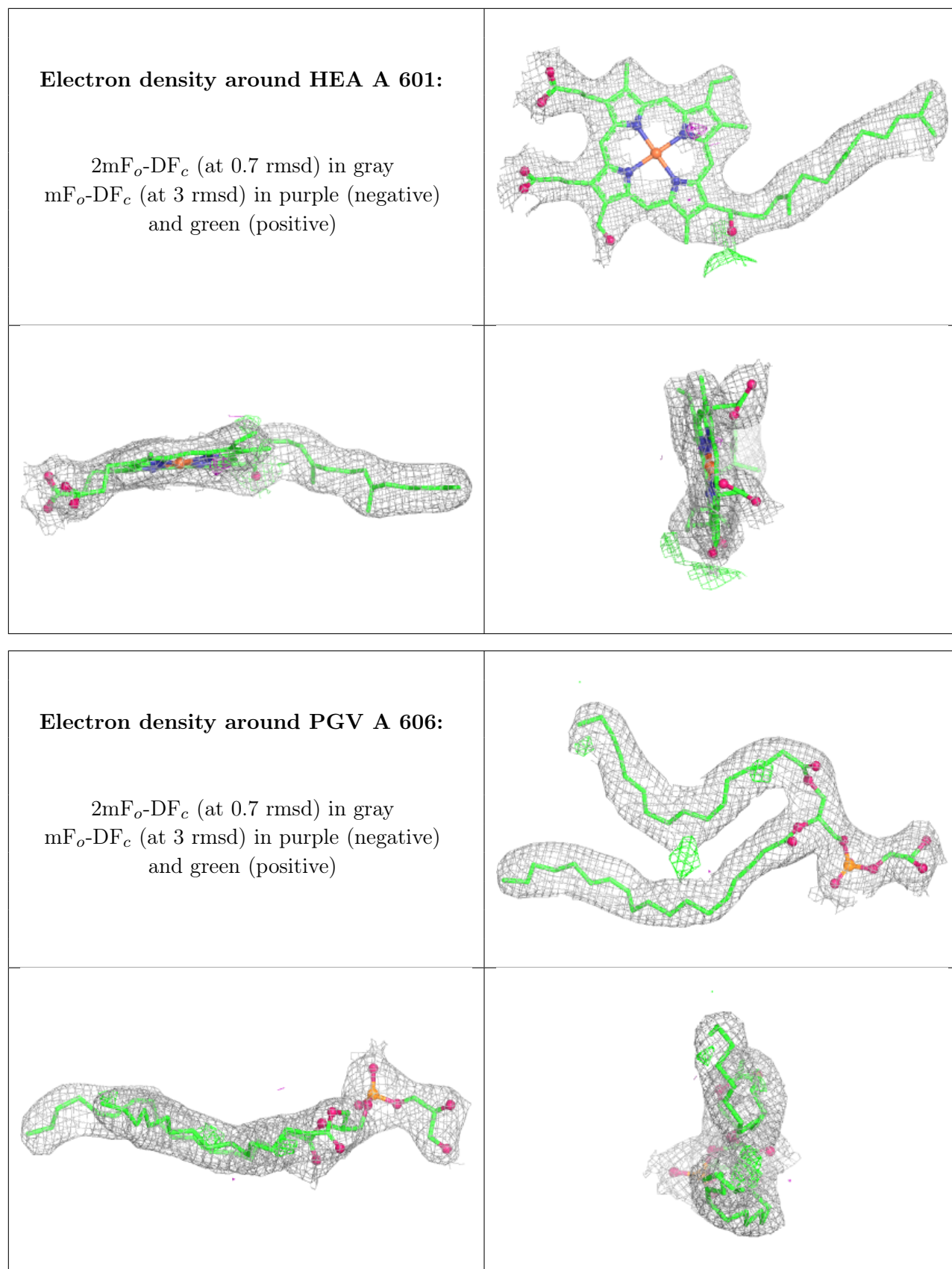
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

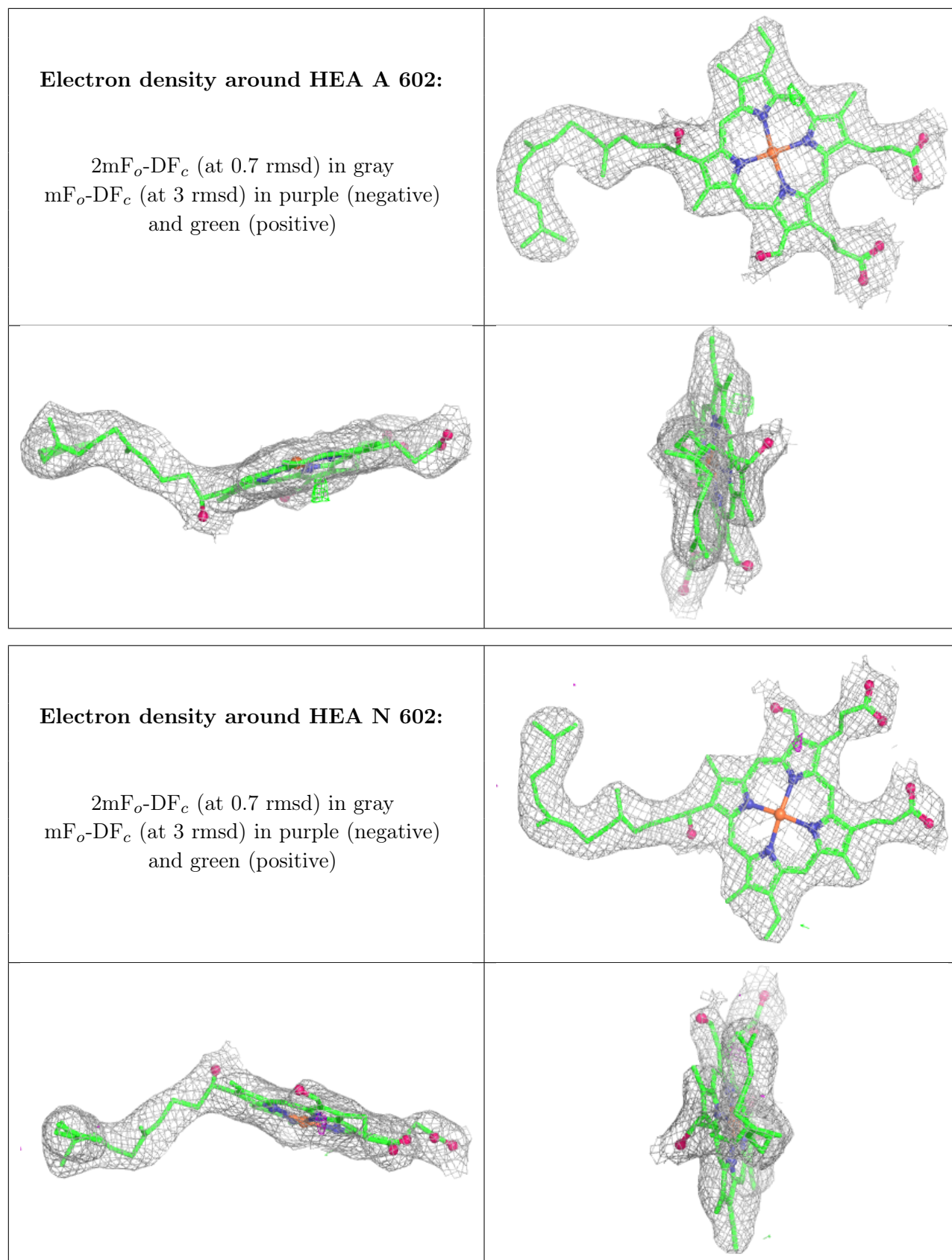
**Electron density around CHD C 306:**

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









6.5 Other polymers [i](#)

There are no such residues in this entry.