



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 01:09 PM UTC

PDB ID : 3ABM / pdb_00003abm
Title : Bovine heart cytochrome c oxidase at the fully oxidized state (200-s X-ray exposure dataset)
Authors : Aoyama, H.; Muramoto, K.; Shinzawa-Itoh, K.; Yamashita, E.; Tsukihara, T.; Ogura, T.; Yoshikawa, S.
Deposited on : 2009-12-16
Resolution : 1.95 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

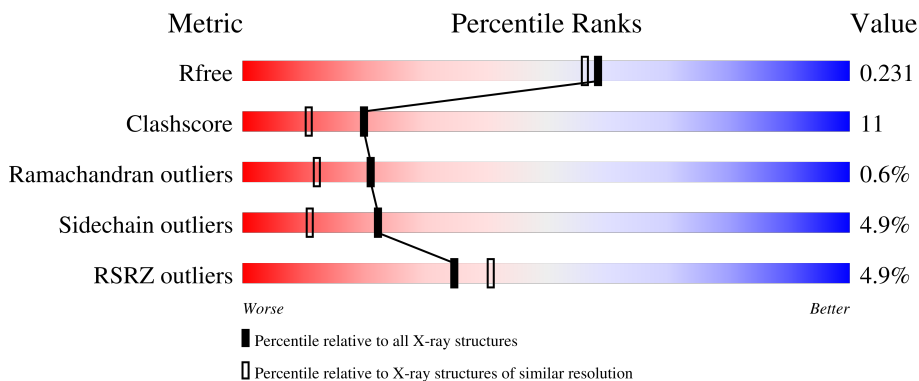
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	

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Mol	Chain	Length	Quality of chain
3	C	261	77% 21% ..
3	P	261	80% 16% ..
4	D	147	78% 18% ..
4	Q	147	69% 24% . . .
5	E	109	84% 10% . 5%
5	R	109	78% 17% . 5%
6	F	98	72% 16% 5% . 5%
6	S	98	59% 31% . . 5%
7	G	85	69% 18% 9% ..
7	T	85	68% 18% 9% . .
8	H	85	66% 18% 5% 12%
8	U	85	68% 18% . 12%
9	I	73	73% 22% . .
9	V	73	68% 25% . .
10	J	59	88% 7% . .
10	W	59	85% 12% .
11	K	56	80% 7% 12%
11	X	56	79% 7% . 12%
12	L	47	74% 21% . .
12	Y	47	74% 17% 6% .
13	M	46	63% 26% . . 7%
13	Z	46	59% 35% 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
22	CHD	B	1086	X	-	-	-
22	CHD	C	271	X	-	-	-
22	CHD	J	60	X	-	-	-
22	CHD	P	1271	X	-	-	-
22	CHD	W	1060	X	-	-	-
24	PEK	T	263	-	-	X	-
25	CDL	G	269	-	-	X	-
25	CDL	P	1270	-	-	X	-
26	PSC	E	230	-	-	X	-
28	DMU	G	272	X	-	-	-
28	DMU	M	526	X	-	-	-
28	DMU	P	1272	X	-	-	-
28	DMU	Z	1526	X	-	-	-

2 Entry composition [i](#)

There are 29 unique types of molecules in this entry. The entry contains 32113 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	4027	2691	623	678	35	0	0	0
1	N	514	4027	2691	623	678	35	0	0	0

- 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	1824	1185	281	340	18	0	0	0
2	O	227	1824	1185	281	340	18	0	0	0

- 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	2110	1412	336	350	12	0	0	0
3	P	259	2110	1412	336	350	12	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	104	Total	C	N	O	S	0	0	0
			842	538	141	161	2			
5	R	104	Total	C	N	O	S	0	0	0
			842	538	141	161	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	93	Total	C	N	O	S	0	0	0
			717	447	127	138	5			
6	S	93	Total	C	N	O	S	0	0	0
			717	447	127	138	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
7	G	84	Total	C	N	O	P	S	0	0	0
			675	431	129	113	1	1			
7	T	84	Total	C	N	O	P	S	0	0	0
			675	431	129	113	1	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	75	Total	C	N	O	S	0	0	0
			628	395	114	114	5			
8	U	75	Total	C	N	O	S	0	0	0
			628	395	114	114	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	71	Total	C	N	O	S	0	0	0
			585	381	105	95	4			
9	V	71	Total	C	N	O	S	0	0	0
			585	381	105	95	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	57	Total	C	N	O	S	0	0	0
			451	291	76	81	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	W	57	Total	C	N	O	S	0	0	0
			451	291	76	81	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	49	Total	C	N	O	S	0	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.

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

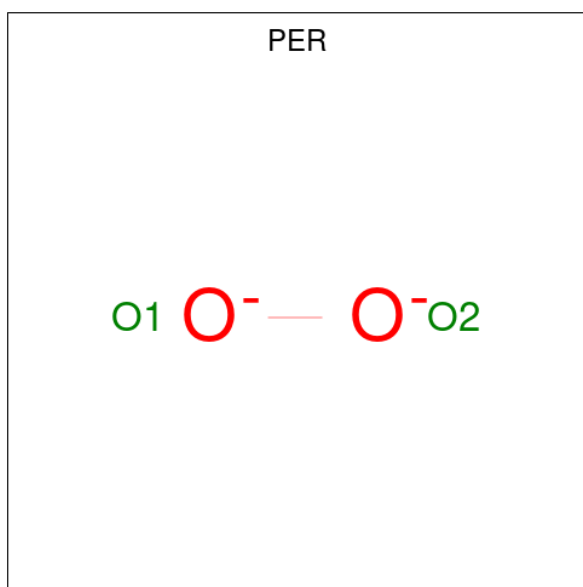
- Molecule 13 is a protein called Cytochrome c oxidase subunit 8B.

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

- Molecule 14 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

- Molecule 15 is PEROXIDE ION (CCD ID: PER) (formula: O₂).



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

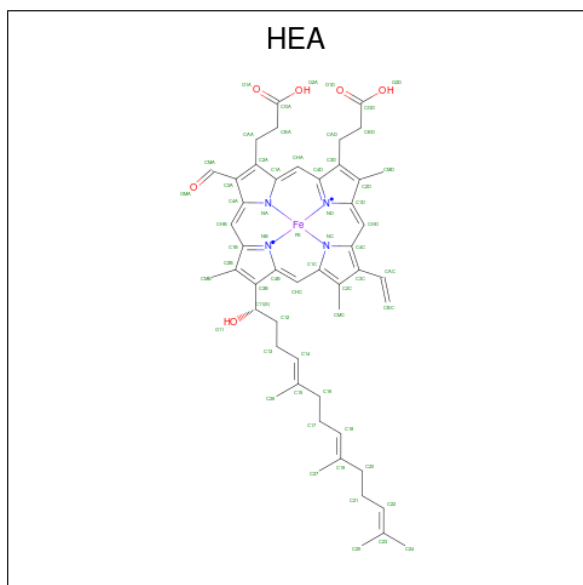
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

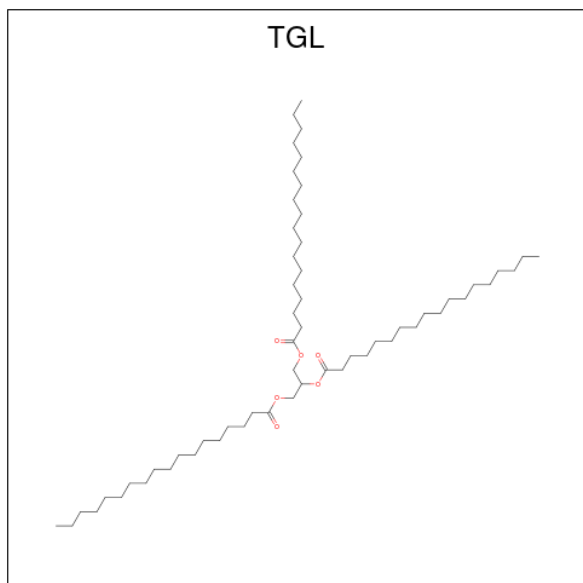
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Na 1 1	0	0
17	N	1	Total Na 1 1	0	0

- Molecule 18 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆).



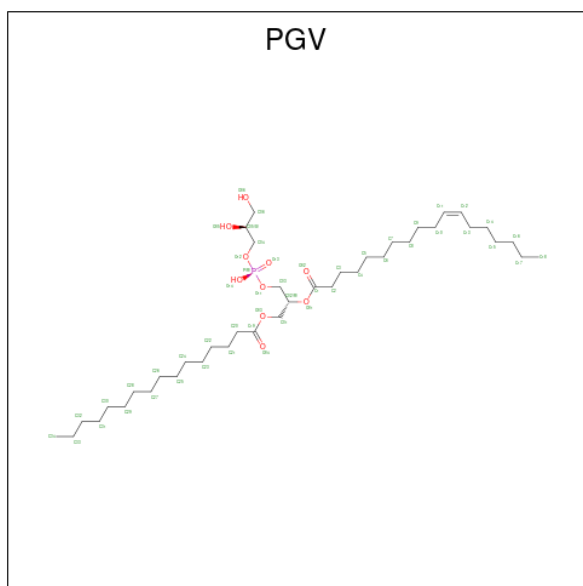
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
			Total	C	Fe	N			O	
18	A	1	Total	60	49	1	4	6	0	0
18	A	1	Total	60	49	1	4	6	0	0
18	N	1	Total	60	49	1	4	6	0	0
18	N	1	Total	60	49	1	4	6	0	0

- Molecule 19 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: $C_{57}H_{110}O_6$).



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

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



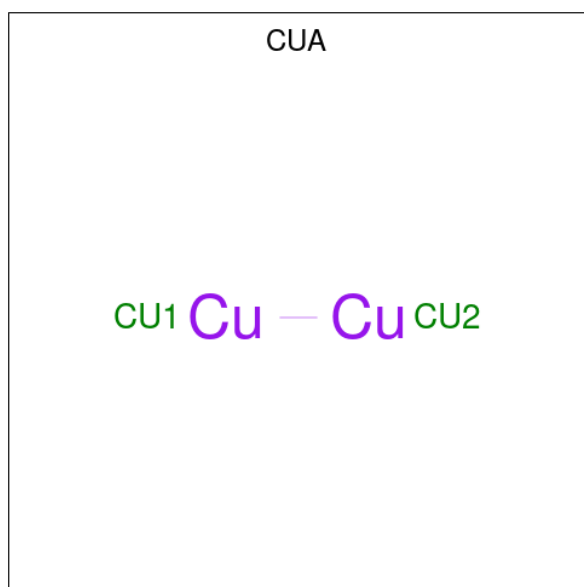
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	H	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		

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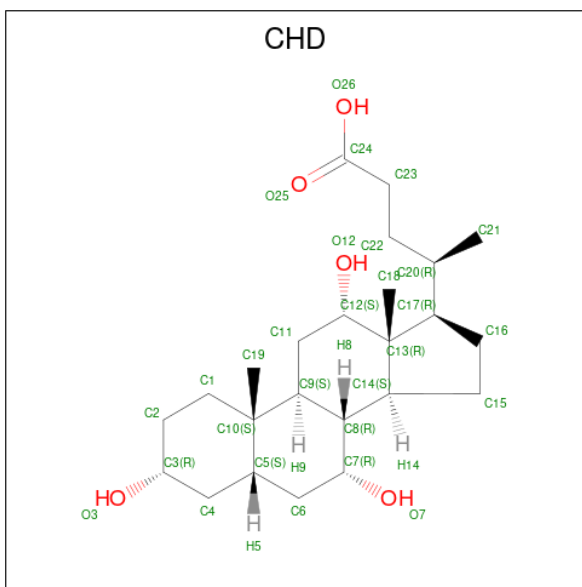
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
20	N	1	51	40	10	1	0	0
20	N	1	51	40	10	1	0	0
20	P	1	51	40	10	1	0	0

- 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).

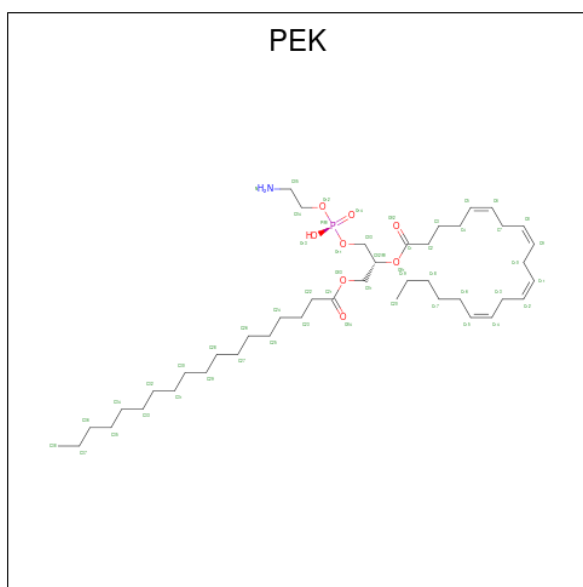


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	B	1	Total C O 29 24 5	0	0
22	C	1	Total C O 29 24 5	0	0
22	C	1	Total C O 29 24 5	0	0
22	J	1	Total C O 29 24 5	0	0
22	O	1	Total C O 29 24 5	0	0
22	P	1	Total C O 29 24 5	0	0
22	P	1	Total C O 29 24 5	0	0
22	W	1	Total C O 29 24 5	0	0

- Molecule 23 is UNKNOWN ATOM OR ION (CCD ID: UNX) (formula: X).

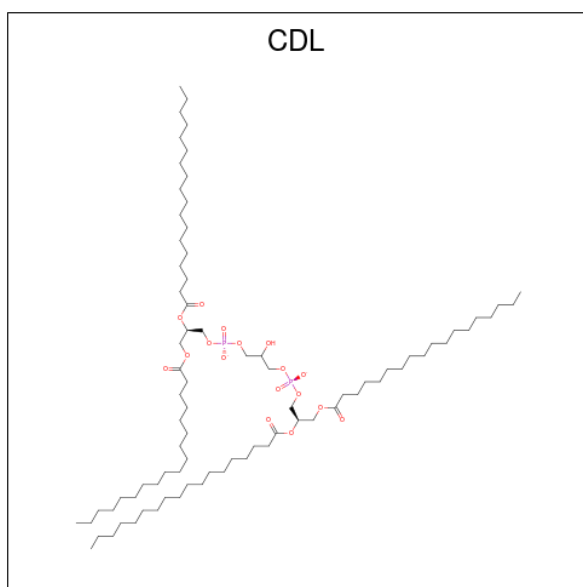
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	C	1	Total X 1 1	0	0
23	P	1	Total X 1 1	0	0

- 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: C₄₃H₇₈NO₈P).



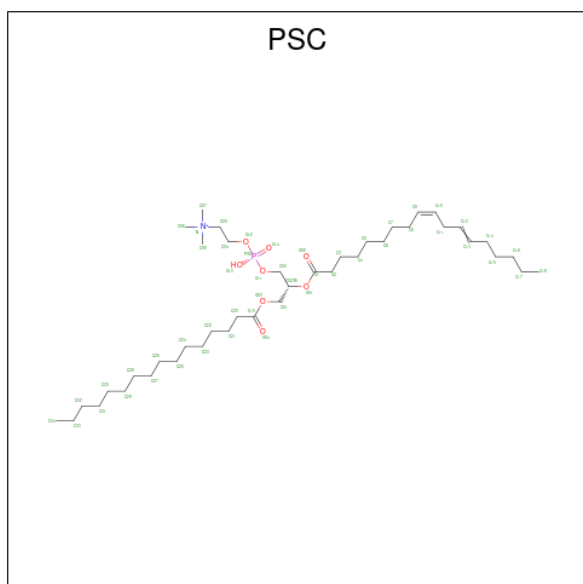
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
24	C	1	53	43	1	8	1	0	0
24	G	1	53	43	1	8	1	0	0
24	G	1	53	43	1	8	1	0	0
24	P	1	53	43	1	8	1	0	0
24	T	1	53	43	1	8	1	0	0
24	T	1	53	43	1	8	1	0	0

- Molecule 25 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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

- Molecule 26 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (CCD ID: PSC) (formula: C₄₂H₈₁NO₈P).

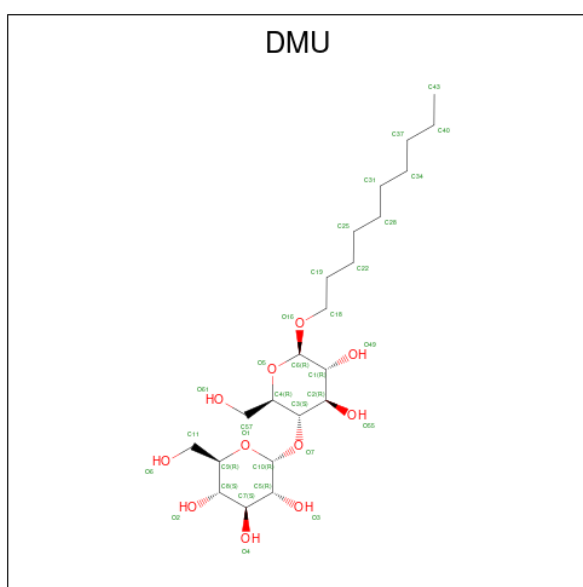


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	E	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
26	R	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 27 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 28 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: C₂₂H₄₂O₁₁).



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

- Molecule 29 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	203	Total O 203 203	0	0
29	B	131	Total O 131 131	0	0
29	C	90	Total O 90 90	0	0
29	D	96	Total O 96 96	0	0
29	E	62	Total O 62 62	0	0
29	F	70	Total O 70 70	0	0
29	G	41	Total O 41 41	0	0
29	H	46	Total O 46 46	0	0
29	I	44	Total O 44 44	0	0
29	J	17	Total O 17 17	0	0
29	K	22	Total O 22 22	0	0
29	L	23	Total O 23 23	0	0
29	M	19	Total O 19 19	0	0
29	N	196	Total O 196 196	0	0
29	O	106	Total O 106 106	0	0
29	P	89	Total O 89 89	0	0
29	Q	54	Total O 54 54	0	0
29	R	52	Total O 52 52	0	0
29	S	62	Total O 62 62	0	0
29	T	39	Total O 39 39	0	0
29	U	39	Total O 39 39	0	0
29	V	16	Total O 16 16	0	0

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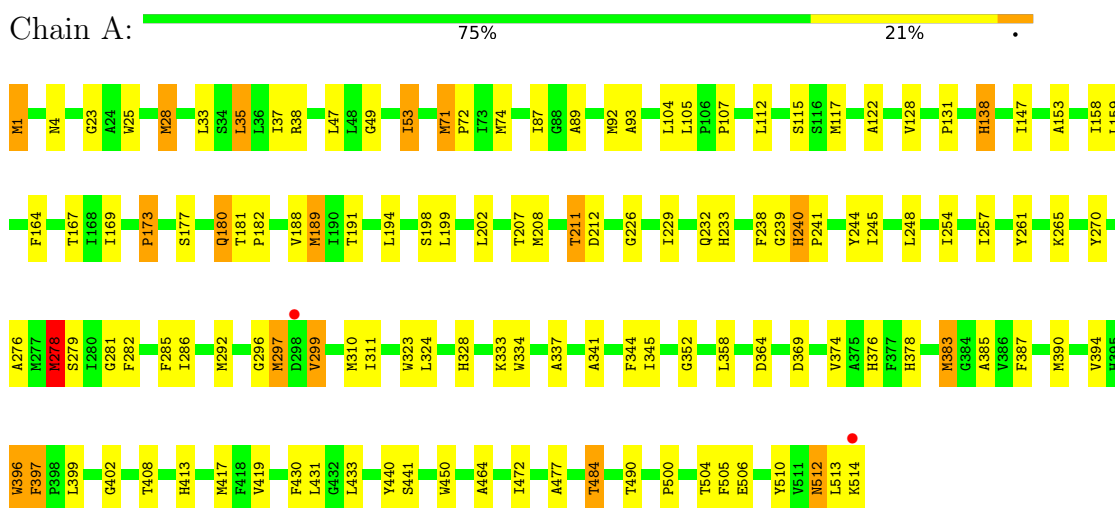
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	W	15	Total 15	O 15	0	0
29	X	16	Total 16	O 16	0	0
29	Y	19	Total 19	O 19	0	0
29	Z	10	Total 10	O 10	0	0

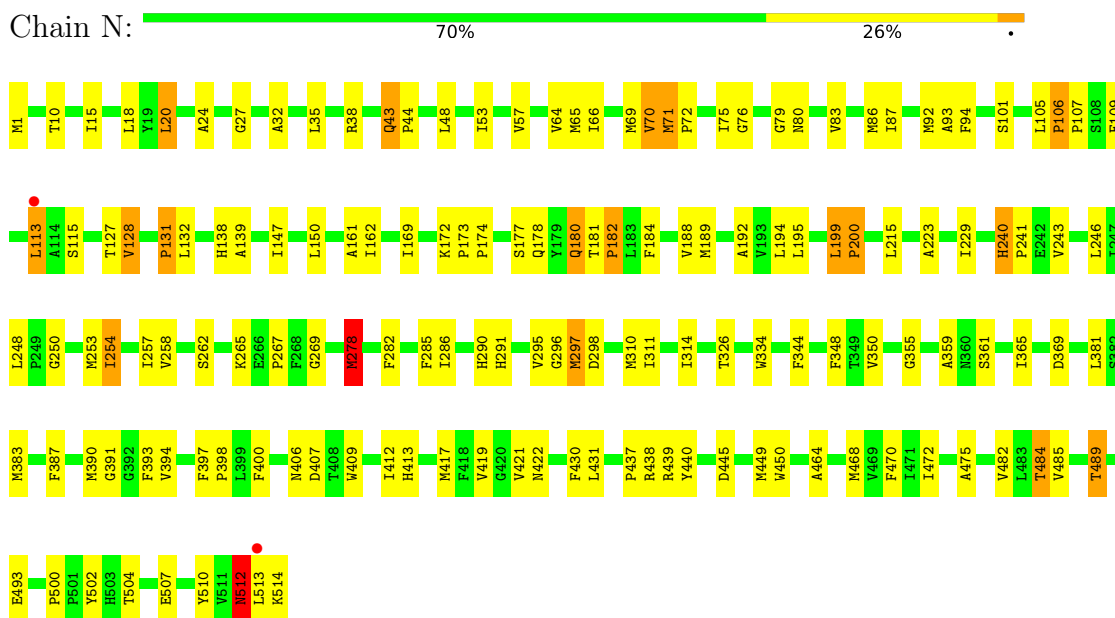
3 Residue-property plots

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.

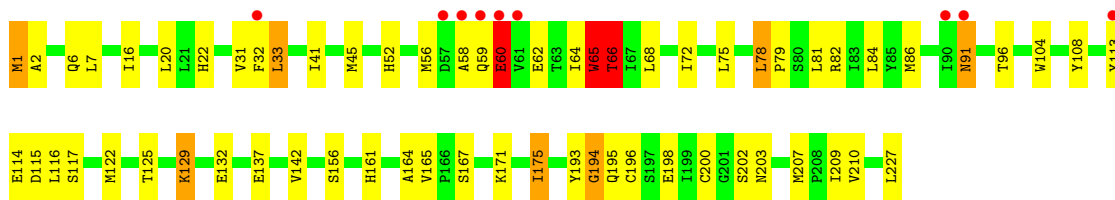
- Molecule 1: Cytochrome c oxidase subunit 1



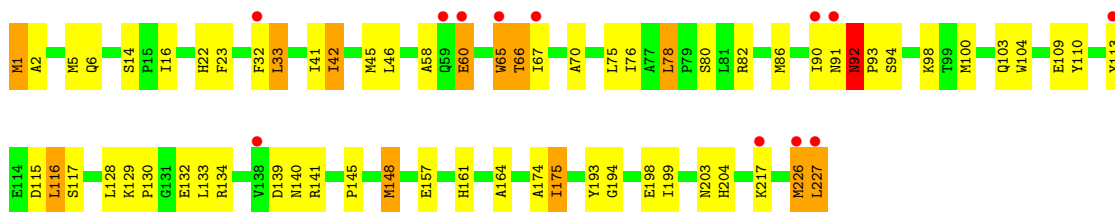
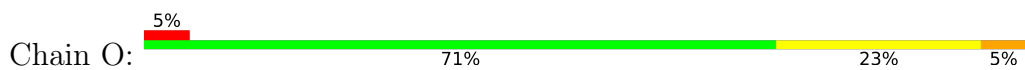
- Molecule 1: Cytochrome c oxidase subunit 1



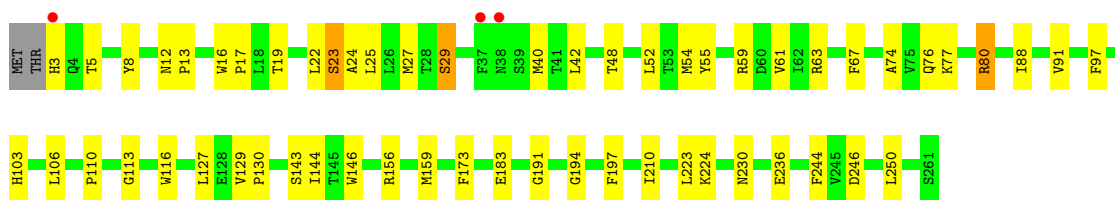
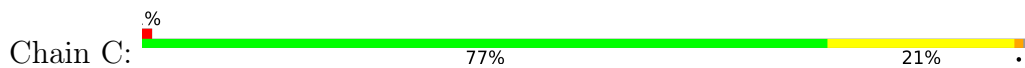
- Molecule 2: Cytochrome c oxidase subunit 2



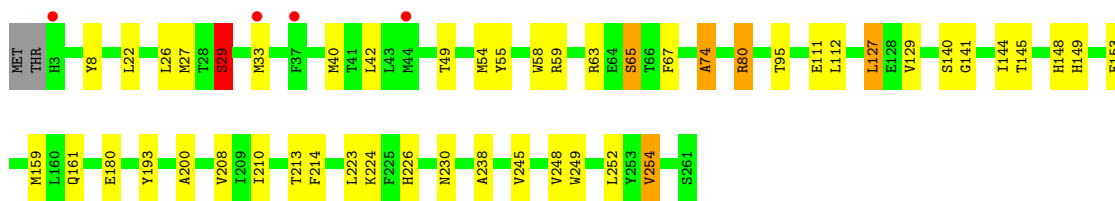
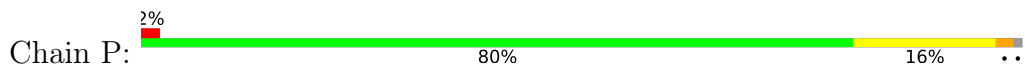
• Molecule 2: Cytochrome c oxidase subunit 2



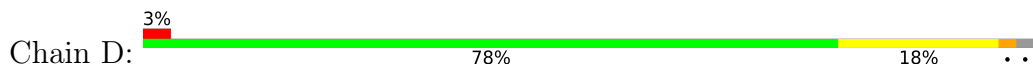
• Molecule 3: Cytochrome c oxidase subunit 3



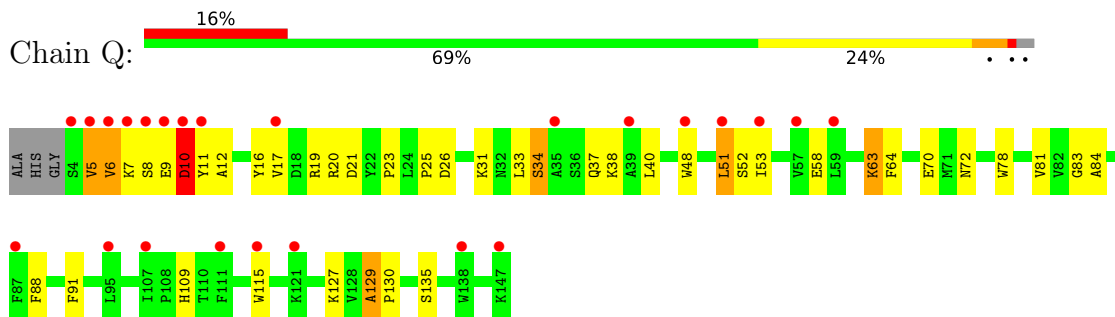
• Molecule 3: Cytochrome c oxidase subunit 3



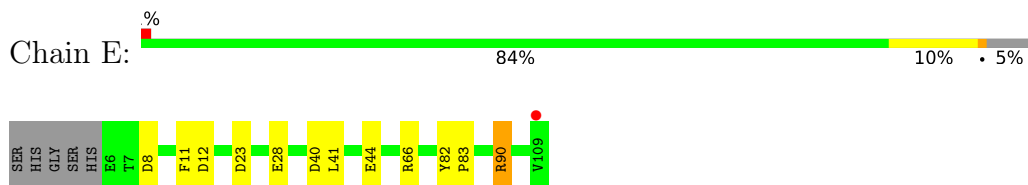
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



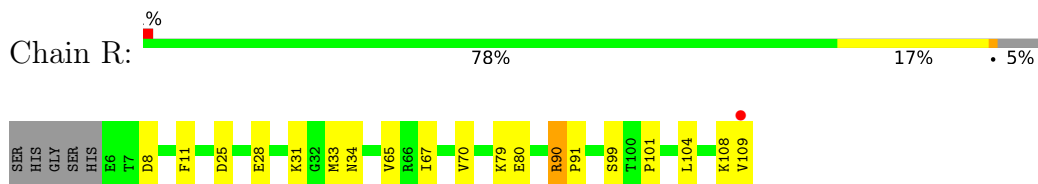
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



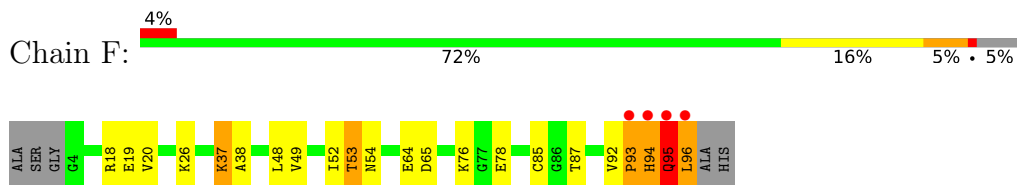
• Molecule 5: Cytochrome c oxidase subunit 5A



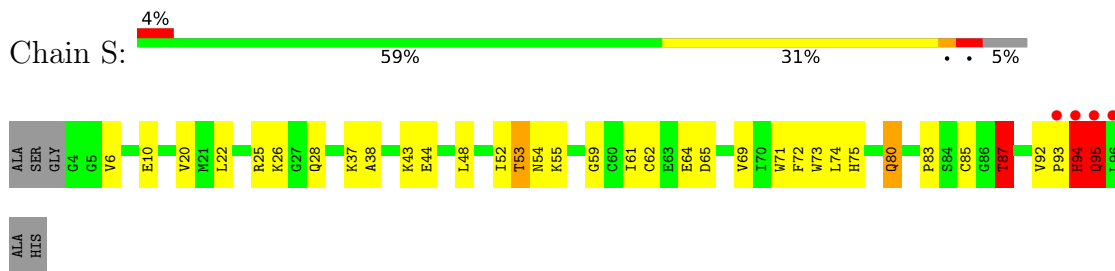
• Molecule 5: Cytochrome c oxidase subunit 5A



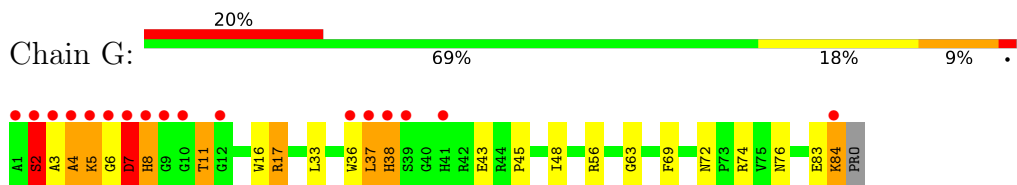
• Molecule 6: Cytochrome c oxidase subunit 5B



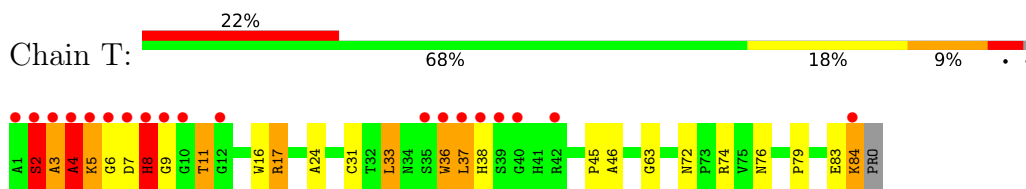
• Molecule 6: Cytochrome c oxidase subunit 5B



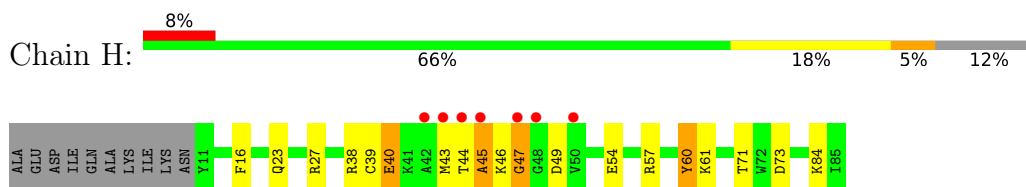
• Molecule 7: Cytochrome c oxidase subunit 6A2



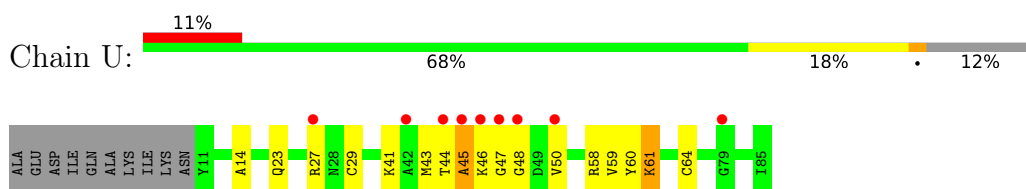
- Molecule 7: Cytochrome c oxidase subunit 6A2



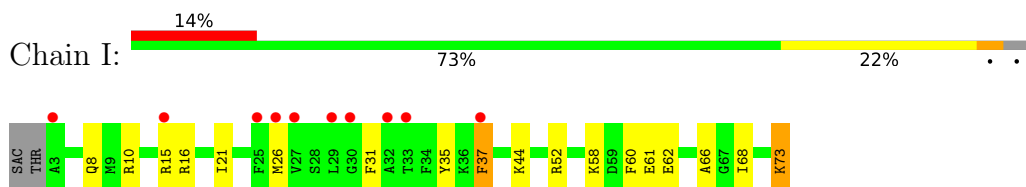
- Molecule 8: Cytochrome c oxidase subunit 6B1



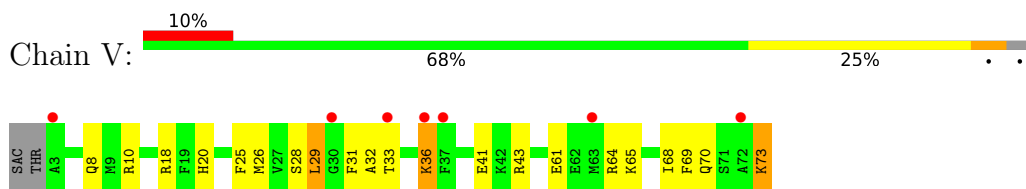
- Molecule 8: Cytochrome c oxidase subunit 6B1



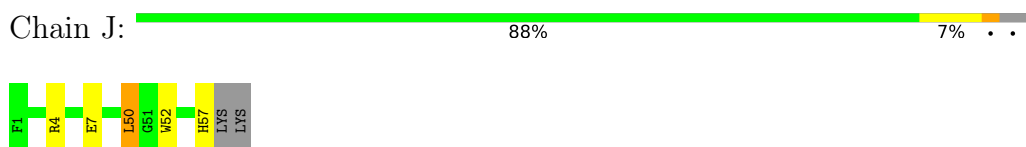
- Molecule 9: Cytochrome c oxidase subunit 6C



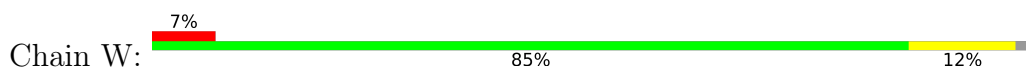
- Molecule 9: Cytochrome c oxidase subunit 6C

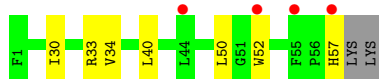


- Molecule 10: Cytochrome c oxidase polypeptide 7A1

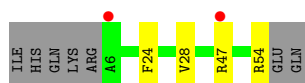
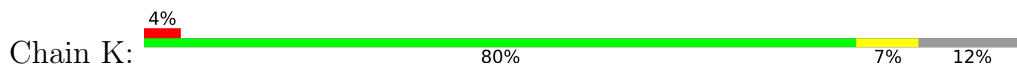


- Molecule 10: Cytochrome c oxidase polypeptide 7A1

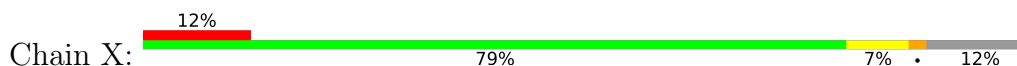




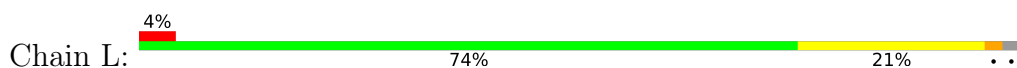
- Molecule 11: Cytochrome c oxidase subunit 7B



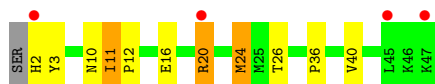
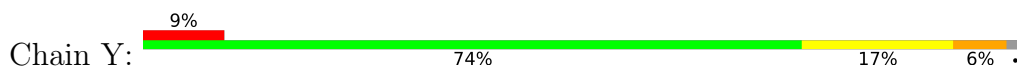
- Molecule 11: Cytochrome c oxidase subunit 7B



- Molecule 12: Cytochrome c oxidase subunit 7C



- Molecule 12: Cytochrome c oxidase subunit 7C



- Molecule 13: Cytochrome c oxidase subunit 8B



- Molecule 13: Cytochrome c oxidase subunit 8B



4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	183.70Å 206.99Å 178.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.95 40.00 – 1.95	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-1.95) 96.4 (40.00-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 1.95Å)	Xtrriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.181 , 0.214 (Not available) , 0.231	Depositor DCC
R_{free} test set	16433 reflections (3.48%)	wwPDB-VP
Wilson B-factor (Å ²)	33.1	Xtrriage
Anisotropy	0.394	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 54.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.007 for l,-k,h	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	32113	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% 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: CUA, CU, CHD, PER, TPO, PGV, PEK, CDL, UNX, TGL, NA, HEA, DMU, ZN, PSC, MG, 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	1.82	47/4156 (1.1%)	1.57	47/5678 (0.8%)
1	N	1.67	44/4156 (1.1%)	1.53	62/5678 (1.1%)
2	B	1.68	17/1860 (0.9%)	1.50	9/2534 (0.4%)
2	O	1.44	5/1860 (0.3%)	1.40	11/2534 (0.4%)
3	C	1.52	8/2197 (0.4%)	1.39	15/3005 (0.5%)
3	P	1.53	6/2197 (0.3%)	1.39	15/3005 (0.5%)
4	D	1.56	6/1229 (0.5%)	1.48	19/1658 (1.1%)
4	Q	1.27	5/1229 (0.4%)	1.31	11/1658 (0.7%)
5	E	1.46	0/860	1.26	4/1167 (0.3%)
5	R	1.24	0/860	1.19	1/1167 (0.1%)
6	F	1.63	6/733 (0.8%)	1.51	7/996 (0.7%)
6	S	1.65	9/733 (1.2%)	1.59	9/996 (0.9%)
7	G	1.56	4/690 (0.6%)	1.36	2/937 (0.2%)
7	T	1.53	6/690 (0.9%)	1.45	8/937 (0.9%)
8	H	1.47	2/648 (0.3%)	1.41	3/877 (0.3%)
8	U	1.24	1/648 (0.2%)	1.30	4/877 (0.5%)
9	I	1.38	0/598	1.32	4/792 (0.5%)
9	V	1.23	0/598	1.20	1/792 (0.1%)
10	J	1.42	0/462	1.30	0/625
10	W	1.21	0/462	1.18	0/625
11	K	1.53	0/398	1.37	0/546
11	X	1.19	0/398	1.31	2/546 (0.4%)
12	L	1.62	2/393 (0.5%)	1.45	3/526 (0.6%)
12	Y	1.35	1/393 (0.3%)	1.35	4/526 (0.8%)
13	M	1.60	3/345 (0.9%)	1.34	0/470
13	Z	1.17	0/345	1.43	5/470 (1.1%)
All	All	1.56	172/29138 (0.6%)	1.43	246/39622 (0.6%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	S	0	2

The worst 5 of 172 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	S	54	ASN	CB-CG	-10.47	1.25	1.52
2	O	198	GLU	C-O	10.33	1.35	1.23
1	N	297	MET	SD-CE	9.78	2.04	1.79
12	L	35	ALA	CA-CB	9.53	1.65	1.53
2	O	175	ILE	CA-CB	9.36	1.61	1.54

The worst 5 of 246 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	240	HIS	N-CA-CB	10.68	120.53	110.39
4	Q	10	ASP	N-CA-C	-9.97	101.90	114.56
6	S	20	VAL	N-CA-C	-9.70	100.93	110.72
2	O	226	MET	N-CA-C	-9.09	102.19	113.28
1	N	169	ILE	CB-CA-C	-8.99	100.19	112.24

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	S	93	PRO	Peptide
6	S	95	GLN	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4027	0	4001	57	0
1	N	4027	0	4001	77	0
2	B	1824	0	1833	33	0
2	O	1824	0	1833	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2110	0	2027	40	0
3	P	2110	0	2027	33	0
4	D	1195	0	1183	24	0
4	Q	1195	0	1183	31	0
5	E	842	0	838	5	0
5	R	842	0	838	11	0
6	F	717	0	700	16	0
6	S	717	0	700	29	0
7	G	675	0	643	38	0
7	T	675	0	644	45	0
8	H	628	0	580	10	0
8	U	628	0	580	9	0
9	I	585	0	597	13	0
9	V	585	0	597	16	0
10	J	451	0	446	5	0
10	W	451	0	446	5	0
11	K	384	0	366	1	0
11	X	384	0	366	5	0
12	L	380	0	380	12	0
12	Y	380	0	380	10	0
13	M	335	0	352	6	0
13	Z	335	0	352	11	0
14	A	1	0	0	0	0
14	N	1	0	0	0	0
15	A	2	0	0	1	0
15	N	2	0	0	1	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	1	0
17	N	1	0	0	0	0
18	A	120	0	108	8	0
18	N	120	0	108	13	0
19	A	63	0	110	13	0
19	D	63	0	110	9	0
19	L	63	0	110	15	0
19	O	126	0	220	23	0
19	Y	63	0	110	18	0
20	A	102	0	152	8	0
20	C	51	0	76	5	0
20	H	51	0	76	3	0
20	N	153	0	228	12	0
20	P	51	0	76	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	29	0	36	2	0
22	C	58	0	70	5	0
22	J	29	0	36	1	0
22	O	29	0	36	0	0
22	P	58	0	71	1	0
22	W	29	0	36	4	0
23	C	1	0	0	0	0
23	P	1	0	0	0	0
24	C	53	0	77	7	0
24	G	106	0	154	31	0
24	P	53	0	77	7	0
24	T	106	0	154	30	0
25	C	100	0	156	19	0
25	G	100	0	156	27	0
25	P	100	0	156	24	0
25	T	100	0	156	19	0
26	E	52	0	80	22	0
26	R	52	0	80	15	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	G	33	0	38	5	0
28	M	33	0	39	0	0
28	P	33	0	40	1	0
28	Z	33	0	38	3	0
29	A	203	0	0	3	0
29	B	131	0	0	2	0
29	C	90	0	0	4	0
29	D	96	0	0	8	0
29	E	62	0	0	0	0
29	F	70	0	0	1	0
29	G	41	0	0	6	0
29	H	46	0	0	2	0
29	I	44	0	0	3	0
29	J	17	0	0	1	0
29	K	22	0	0	2	0
29	L	23	0	0	1	0
29	M	19	0	0	0	0
29	N	196	0	0	4	0
29	O	106	0	0	2	0
29	P	89	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	Q	54	0	0	4	0
29	R	52	0	0	0	0
29	S	62	0	0	6	0
29	T	39	0	0	7	0
29	U	39	0	0	2	0
29	V	16	0	0	3	0
29	W	15	0	0	0	0
29	X	16	0	0	0	0
29	Y	19	0	0	1	0
29	Z	10	0	0	1	0
All	All	32113	0	31063	702	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 702 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)
24:G:265:PEK:C8	24:G:265:PEK:C7	1.75	1.56
24:G:265:PEK:C8	24:G:265:PEK:C9	1.77	1.55
24:G:265:PEK:C9	24:G:265:PEK:C10	1.81	1.50
1:A:297:MET:SD	1:A:297:MET:CE	2.02	1.48
24:G:265:PEK:H383	25:G:269:CDL:C27	1.46	1.44

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	512/514 (100%)	495 (97%)	17 (3%)	0	100	100
1	N	512/514 (100%)	490 (96%)	22 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	225/227 (99%)	216 (96%)	8 (4%)	1 (0%)	30	21
2	O	225/227 (99%)	214 (95%)	10 (4%)	1 (0%)	30	21
3	C	257/261 (98%)	252 (98%)	5 (2%)	0	100	100
3	P	257/261 (98%)	252 (98%)	5 (2%)	0	100	100
4	D	142/147 (97%)	137 (96%)	5 (4%)	0	100	100
4	Q	142/147 (97%)	129 (91%)	12 (8%)	1 (1%)	18	10
5	E	102/109 (94%)	101 (99%)	1 (1%)	0	100	100
5	R	102/109 (94%)	102 (100%)	0	0	100	100
6	F	91/98 (93%)	87 (96%)	2 (2%)	2 (2%)	5	1
6	S	91/98 (93%)	85 (93%)	5 (6%)	1 (1%)	11	4
7	G	81/85 (95%)	69 (85%)	7 (9%)	5 (6%)	1	0
7	T	81/85 (95%)	66 (82%)	10 (12%)	5 (6%)	1	0
8	H	73/85 (86%)	69 (94%)	1 (1%)	3 (4%)	2	0
8	U	73/85 (86%)	66 (90%)	5 (7%)	2 (3%)	4	1
9	I	69/73 (94%)	66 (96%)	3 (4%)	0	100	100
9	V	69/73 (94%)	67 (97%)	2 (3%)	0	100	100
10	J	55/59 (93%)	55 (100%)	0	0	100	100
10	W	55/59 (93%)	55 (100%)	0	0	100	100
11	K	47/56 (84%)	47 (100%)	0	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%)	42 (96%)	2 (4%)	0	100	100
13	M	41/46 (89%)	38 (93%)	3 (7%)	0	100	100
13	Z	41/46 (89%)	40 (98%)	0	1 (2%)	4	1
All	All	3478/3614 (96%)	3328 (96%)	128 (4%)	22 (1%)	21	12

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	60	GLU
6	F	95	GLN
7	G	4	ALA
7	G	7	ASP
7	G	8	HIS

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	426/426 (100%)	415 (97%)	11 (3%)	40	33
1	N	426/426 (100%)	413 (97%)	13 (3%)	35	26
2	B	210/210 (100%)	198 (94%)	12 (6%)	18	8
2	O	210/210 (100%)	196 (93%)	14 (7%)	15	5
3	C	224/226 (99%)	216 (96%)	8 (4%)	31	21
3	P	224/226 (99%)	216 (96%)	8 (4%)	31	21
4	D	128/129 (99%)	126 (98%)	2 (2%)	55	52
4	Q	128/129 (99%)	121 (94%)	7 (6%)	19	8
5	E	91/95 (96%)	89 (98%)	2 (2%)	45	40
5	R	91/95 (96%)	87 (96%)	4 (4%)	25	15
6	F	79/81 (98%)	73 (92%)	6 (8%)	12	4
6	S	79/81 (98%)	73 (92%)	6 (8%)	12	4
7	G	67/68 (98%)	59 (88%)	8 (12%)	5	1
7	T	67/68 (98%)	61 (91%)	6 (9%)	9	2
8	H	67/75 (89%)	63 (94%)	4 (6%)	17	7
8	U	67/75 (89%)	62 (92%)	5 (8%)	12	4
9	I	56/57 (98%)	50 (89%)	6 (11%)	6	1
9	V	56/57 (98%)	49 (88%)	7 (12%)	4	1
10	J	48/50 (96%)	47 (98%)	1 (2%)	47	41
10	W	48/50 (96%)	47 (98%)	1 (2%)	47	41
11	K	39/46 (85%)	37 (95%)	2 (5%)	21	10
11	X	39/46 (85%)	36 (92%)	3 (8%)	12	3
12	L	39/40 (98%)	38 (97%)	1 (3%)	40	33
12	Y	39/40 (98%)	36 (92%)	3 (8%)	12	3
13	M	37/38 (97%)	31 (84%)	6 (16%)	2	0
13	Z	37/38 (97%)	34 (92%)	3 (8%)	11	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	3022/3082 (98%)	2873 (95%)	149 (5%)	22	11

5 of 149 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	S	37	LYS
12	Y	11	ILE
6	S	87	THR
8	U	60	TYR
7	G	84	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
11	K	35	GLN
7	T	76	ASN
1	N	413	HIS
6	S	95	GLN
4	Q	119	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FME	O	1	2	8,9,10	0.80	0	8,9,11	5.26	3 (37%)
7	TPO	T	11	7	8,10,11	2.08	6 (75%)	10,14,16	1.98	2 (20%)

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	1.65	3 (37%)	8,9,11	6.37	4 (50%)
1	FME	A	1	1	8,9,10	0.80	0	8,9,11	4.56	3 (37%)
1	FME	N	1	1	8,9,10	0.74	0	8,9,11	5.91	5 (62%)
7	TPO	G	11	7	8,10,11	2.23	4 (50%)	10,14,16	2.37	4 (40%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FME	O	1	2	-	2/7/9/11	-
7	TPO	T	11	7	-	5/9/11/13	-
2	FME	B	1	2	-	1/7/9/11	-
1	FME	A	1	1	-	3/7/9/11	-
1	FME	N	1	1	-	4/7/9/11	-
7	TPO	G	11	7	-	4/9/11/13	-

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	11	TPO	P-O1P	4.18	1.63	1.50
7	T	11	TPO	P-O1P	3.48	1.61	1.50
2	B	1	FME	O1-CN	-2.65	1.11	1.22
7	G	11	TPO	P-O2P	2.44	1.63	1.54
2	B	1	FME	CG-SD	-2.38	1.69	1.81

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CA-N-CN	-16.38	97.64	122.82
1	N	1	FME	CA-N-CN	-15.33	99.25	122.82
2	O	1	FME	CA-N-CN	-13.71	101.73	122.82
1	A	1	FME	CA-N-CN	-12.21	104.05	122.82
2	B	1	FME	O1-CN-N	5.35	139.14	125.32

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O1-CN-N-CA
1	A	1	FME	N-CA-CB-CG
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.

5 monomers are involved in 8 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 56 ligands modelled in this entry, 8 are monoatomic and 2 are unknown - 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
18	HEA	N	515	1	67,67,67	1.96	17 (25%)	81,103,103	2.43	28 (34%)
24	PEK	T	1265	-	52,52,52	1.24	2 (3%)	55,57,57	1.39	7 (12%)
24	PEK	G	1263	-	52,52,52	1.18	2 (3%)	55,57,57	1.35	5 (9%)
15	PER	N	520	18,14	1,1,1	1.97	0	-	-	-
20	PGV	H	268	-	50,50,50	1.35	2 (4%)	53,56,56	1.52	8 (15%)
26	PSC	E	230	-	51,51,51	1.33	3 (5%)	57,59,59	1.17	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CHD	W	1060	-	32,32,32	0.86	0	51,51,51	5.01	35 (68%)
26	PSC	R	1230	-	51,51,51	1.22	3 (5%)	57,59,59	1.20	5 (8%)
28	DMU	P	1272	-	34,34,34	1.33	3 (8%)	45,45,45	3.12	22 (48%)
22	CHD	O	229	-	32,32,32	1.41	5 (15%)	51,51,51	5.54	36 (70%)
24	PEK	G	265	-	52,52,52	1.81	5 (9%)	55,57,57	1.39	6 (10%)
19	TGL	O	1521	-	62,62,62	1.39	6 (9%)	65,65,65	1.59	12 (18%)
18	HEA	N	516	1,15	67,67,67	1.91	17 (25%)	81,103,103	2.43	32 (39%)
20	PGV	A	522	-	50,50,50	1.10	3 (6%)	53,56,56	1.52	7 (13%)
24	PEK	C	264	-	52,52,52	0.99	3 (5%)	55,57,57	1.50	11 (20%)
19	TGL	L	522	-	62,62,62	1.66	7 (11%)	65,65,65	1.97	18 (27%)
21	CUA	B	228	2	0,1,1	-	-	-	-	-
22	CHD	B	1086	-	32,32,32	1.33	4 (12%)	51,51,51	5.69	35 (68%)
28	DMU	Z	1526	-	34,34,34	1.10	3 (8%)	45,45,45	3.38	23 (51%)
24	PEK	P	1264	-	52,52,52	1.04	4 (7%)	55,57,57	1.70	10 (18%)
25	CDL	T	1269	-	99,99,99	1.47	12 (12%)	105,111,111	1.43	18 (17%)
18	HEA	A	516	1,15	67,67,67	2.07	23 (34%)	81,103,103	2.59	36 (44%)
22	CHD	J	60	-	32,32,32	0.94	1 (3%)	51,51,51	4.88	37 (72%)
28	DMU	G	272	-	34,34,34	1.33	3 (8%)	45,45,45	3.51	24 (53%)
24	PEK	T	263	-	52,52,52	1.21	2 (3%)	55,57,57	1.39	6 (10%)
20	PGV	N	1266	-	50,50,50	0.90	2 (4%)	53,56,56	1.62	7 (13%)
22	CHD	C	271	-	32,32,32	1.31	3 (9%)	51,51,51	5.28	36 (70%)
28	DMU	M	526	-	34,34,34	0.94	1 (2%)	45,45,45	3.24	23 (51%)
20	PGV	N	1268	-	50,50,50	1.24	3 (6%)	53,56,56	1.48	6 (11%)
25	CDL	P	1270	-	99,99,99	1.50	14 (14%)	105,111,111	1.49	14 (13%)
25	CDL	C	270	-	99,99,99	1.48	15 (15%)	105,111,111	1.60	16 (15%)
22	CHD	P	1271	-	32,32,32	0.92	2 (6%)	51,51,51	5.25	30 (58%)
18	HEA	A	515	1	67,67,67	1.96	20 (29%)	81,103,103	2.70	38 (46%)
22	CHD	C	525	-	32,32,32	1.67	8 (25%)	51,51,51	5.48	38 (74%)
15	PER	A	520	18,14	1,1,1	1.97	0	-	-	-
20	PGV	P	1267	-	50,50,50	0.91	2 (4%)	53,56,56	1.46	10 (18%)
19	TGL	A	521	-	62,62,62	1.28	7 (11%)	65,65,65	2.04	12 (18%)
19	TGL	Y	1522	-	62,62,62	1.60	6 (9%)	65,65,65	1.63	16 (24%)
21	CUA	O	228	2	0,1,1	-	-	-	-	-
19	TGL	D	523	-	62,62,62	1.65	7 (11%)	65,65,65	1.63	16 (24%)
20	PGV	N	1524	-	50,50,50	1.07	2 (4%)	53,56,56	1.55	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	PGV	C	267	-	50,50,50	0.98	2 (4%)	53,56,56	1.31	5 (9%)
19	TGL	O	1523	-	62,62,62	1.47	6 (9%)	65,65,65	1.46	10 (15%)
22	CHD	P	1525	-	32,32,32	1.47	4 (12%)	51,51,51	5.58	37 (72%)
25	CDL	G	269	-	99,99,99	1.57	13 (13%)	105,111,111	1.53	17 (16%)
20	PGV	A	524	-	50,50,50	1.24	3 (6%)	53,56,56	1.61	10 (18%)

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
18	HEA	N	515	1	-	7/36/76/76	-
24	PEK	T	1265	-	-	32/56/56/56	-
24	PEK	G	1263	-	-	31/56/56/56	-
20	PGV	H	268	-	-	34/55/55/55	-
26	PSC	E	230	-	-	39/55/55/55	-
22	CHD	W	1060	-	2/2/12/12	6/9/74/74	0/4/4/4
28	DMU	P	1272	-	4/4/10/10	10/19/59/59	0/2/2/2
26	PSC	R	1230	-	-	29/55/55/55	-
22	CHD	O	229	-	-	2/9/74/74	0/4/4/4
24	PEK	G	265	-	-	29/56/56/56	-
19	TGL	O	1521	-	-	32/65/65/65	-
18	HEA	N	516	1,15	-	7/36/76/76	-
20	PGV	A	522	-	-	16/55/55/55	-
28	DMU	Z	1526	-	5/5/10/10	10/19/59/59	0/2/2/2
22	CHD	B	1086	-	1/1/12/12	2/9/74/74	0/4/4/4
19	TGL	L	522	-	-	34/65/65/65	-
24	PEK	C	264	-	-	21/56/56/56	-
24	PEK	P	1264	-	-	19/56/56/56	-
28	DMU	G	272	-	5/5/10/10	10/19/59/59	0/2/2/2
18	HEA	A	516	1,15	-	7/36/76/76	-
22	CHD	J	60	-	2/2/12/12	6/9/74/74	0/4/4/4
25	CDL	T	1269	-	-	58/110/110/110	-
24	PEK	T	263	-	-	28/56/56/56	-
20	PGV	N	1266	-	-	15/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CHD	C	271	-	1/1/12/12	6/9/74/74	0/4/4/4
28	DMU	M	526	-	4/4/10/10	10/19/59/59	0/2/2/2
20	PGV	N	1268	-	-	26/55/55/55	-
25	CDL	P	1270	-	-	61/110/110/110	-
25	CDL	C	270	-	-	65/110/110/110	-
22	CHD	P	1271	-	1/1/12/12	4/9/74/74	0/4/4/4
18	HEA	A	515	1	-	10/36/76/76	-
22	CHD	C	525	-	-	2/9/74/74	0/4/4/4
20	PGV	P	1267	-	-	15/55/55/55	-
19	TGL	A	521	-	-	31/65/65/65	-
19	TGL	Y	1522	-	-	40/65/65/65	-
19	TGL	D	523	-	-	34/65/65/65	-
20	PGV	N	1524	-	-	32/55/55/55	-
20	PGV	C	267	-	-	13/55/55/55	-
19	TGL	O	1523	-	-	31/65/65/65	-
22	CHD	P	1525	-	-	4/9/74/74	0/4/4/4
25	CDL	G	269	-	-	66/110/110/110	-
20	PGV	A	524	-	-	27/55/55/55	-

The worst 5 of 250 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	G	265	PEK	C9-C8	7.99	1.77	1.31
19	L	522	TGL	OG2-CB1	6.61	1.52	1.34
19	Y	1522	TGL	OG2-CB1	6.56	1.52	1.34
19	D	523	TGL	OG1-CA1	6.47	1.52	1.33
20	H	268	PGV	O01-C1	6.43	1.52	1.34

The worst 5 of 773 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1086	CHD	C18-C13-C12	-15.39	93.65	109.06
22	O	229	CHD	C6-C5-C10	14.15	127.72	112.66
22	B	1086	CHD	C6-C5-C10	13.87	127.42	112.66
22	C	525	CHD	C1-C10-C5	13.84	127.62	107.75
22	P	1271	CHD	C10-C9-C8	13.66	127.07	111.84

5 of 25 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	B	1086	CHD	C9
22	C	271	CHD	C9
22	J	60	CHD	C9
22	J	60	CHD	C17
22	P	1271	CHD	C9

5 of 961 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	515	HEA	C2A-C3A-CMA-OMA
18	A	515	HEA	C4A-C3A-CMA-OMA
18	A	516	HEA	C2A-C3A-CMA-OMA
18	N	515	HEA	C16-C17-C18-C19
18	N	516	HEA	C2A-C3A-CMA-OMA

There are no ring outliers.

38 monomers are involved in 342 short contacts:

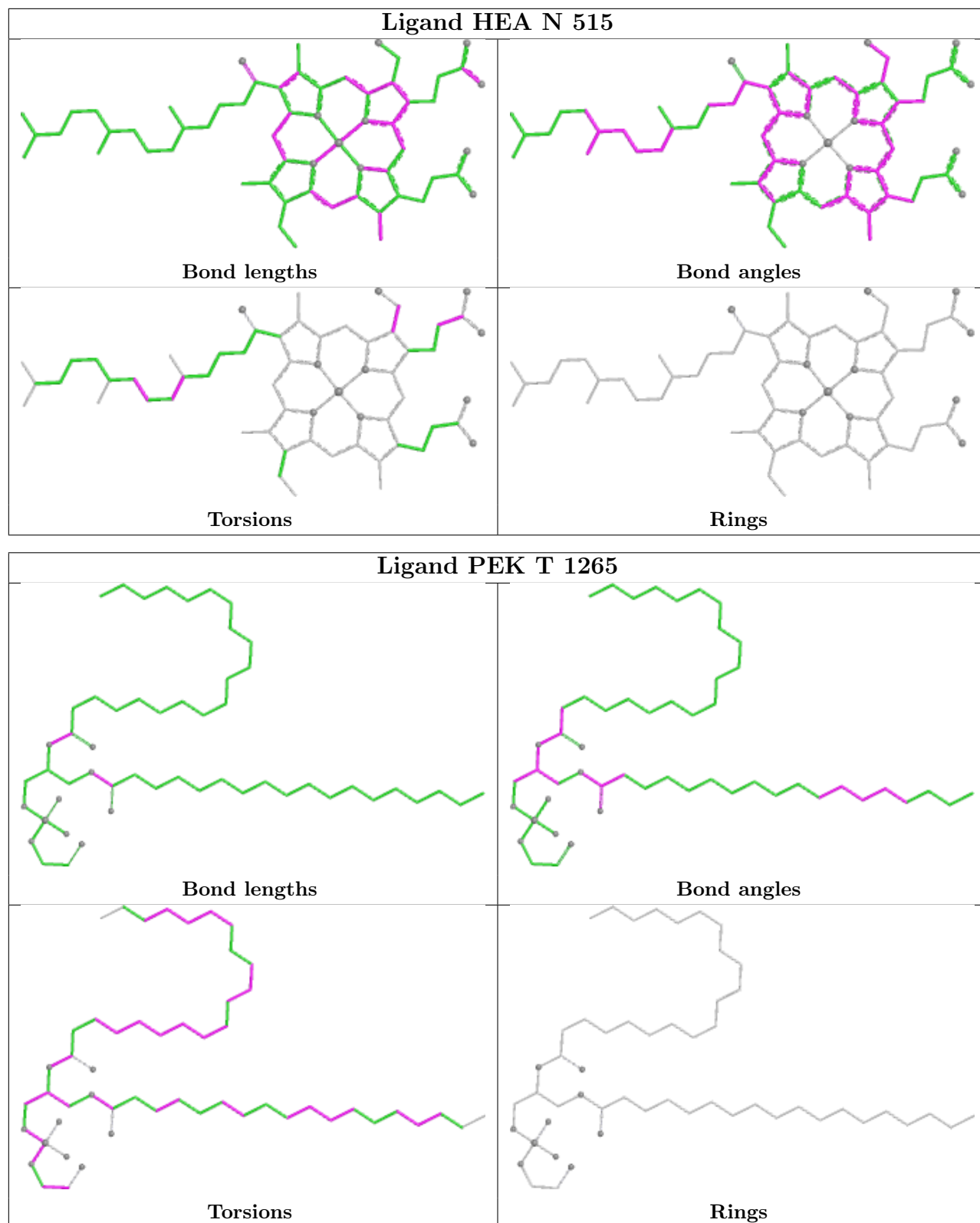
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	N	515	HEA	13	0
24	T	1265	PEK	8	0
24	G	1263	PEK	15	0
15	N	520	PER	1	0
20	H	268	PGV	3	0
26	E	230	PSC	22	0
22	W	1060	CHD	4	0
26	R	1230	PSC	15	0
28	P	1272	DMU	1	0
24	G	265	PEK	16	0
19	O	1521	TGL	14	0
20	A	522	PGV	2	0
24	C	264	PEK	7	0
19	L	522	TGL	15	0
22	B	1086	CHD	2	0
28	Z	1526	DMU	3	0
24	P	1264	PEK	7	0
25	T	1269	CDL	19	0
22	J	60	CHD	1	0
28	G	272	DMU	5	0
24	T	263	PEK	22	0
22	C	271	CHD	2	0
20	N	1268	PGV	1	0
25	P	1270	CDL	24	0

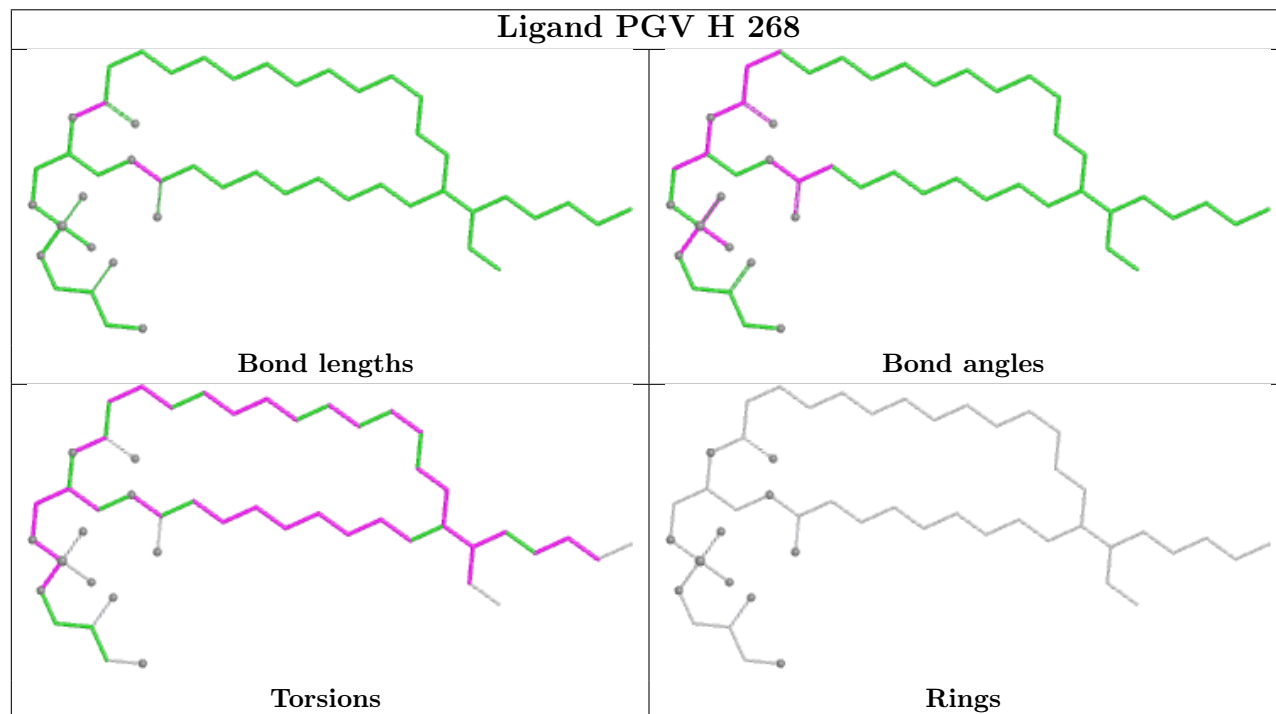
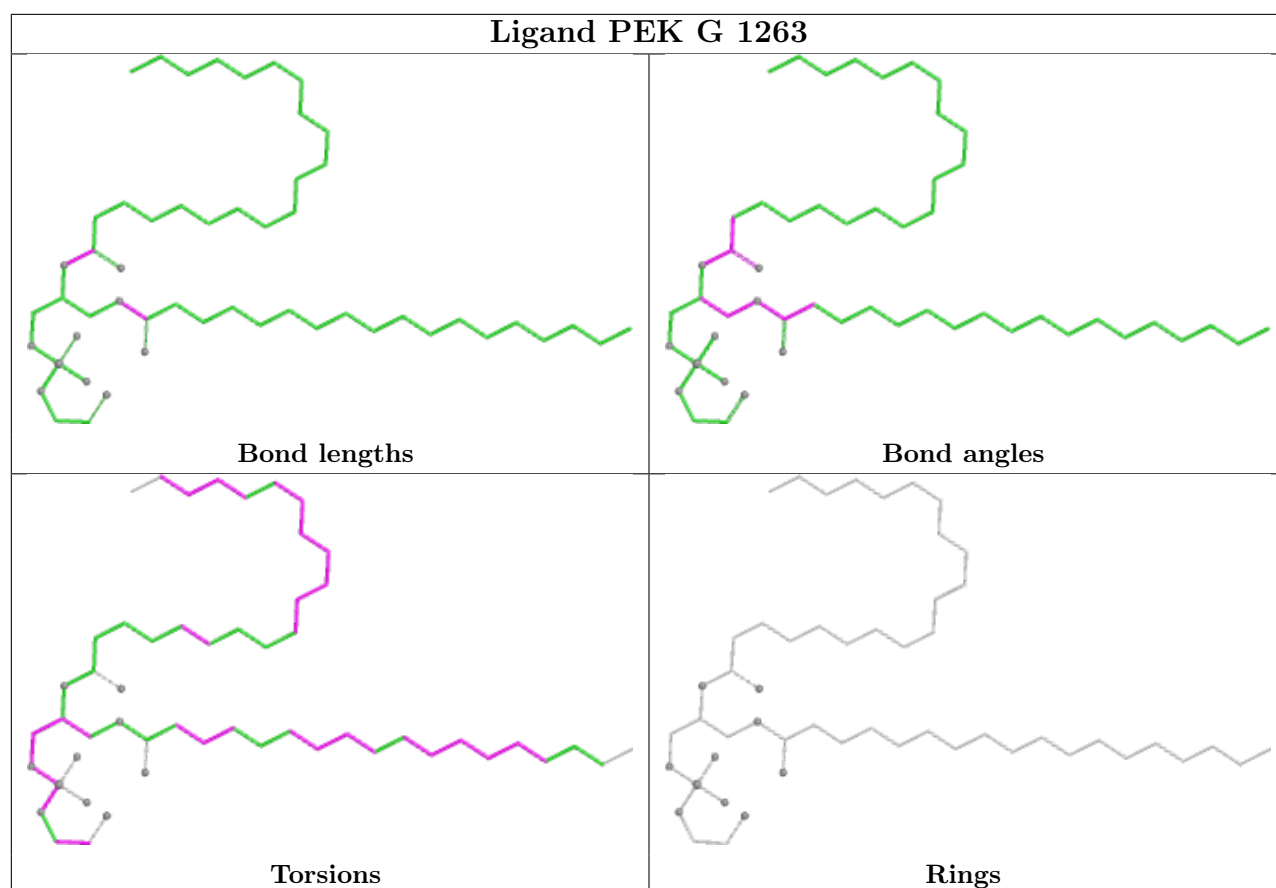
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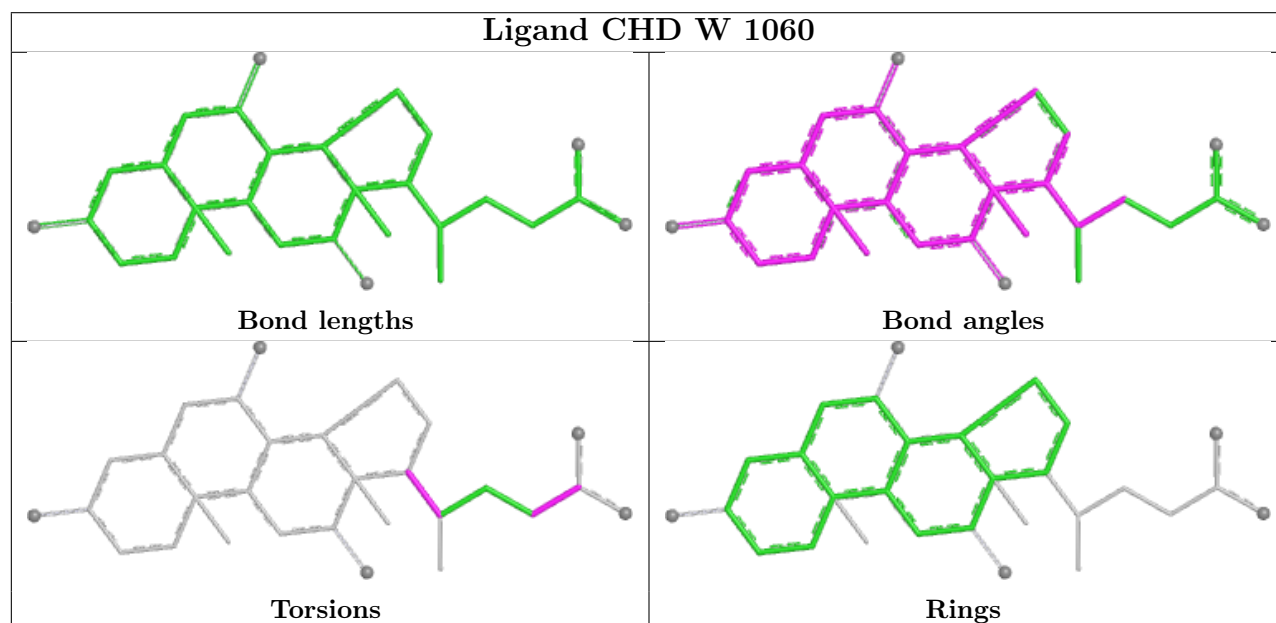
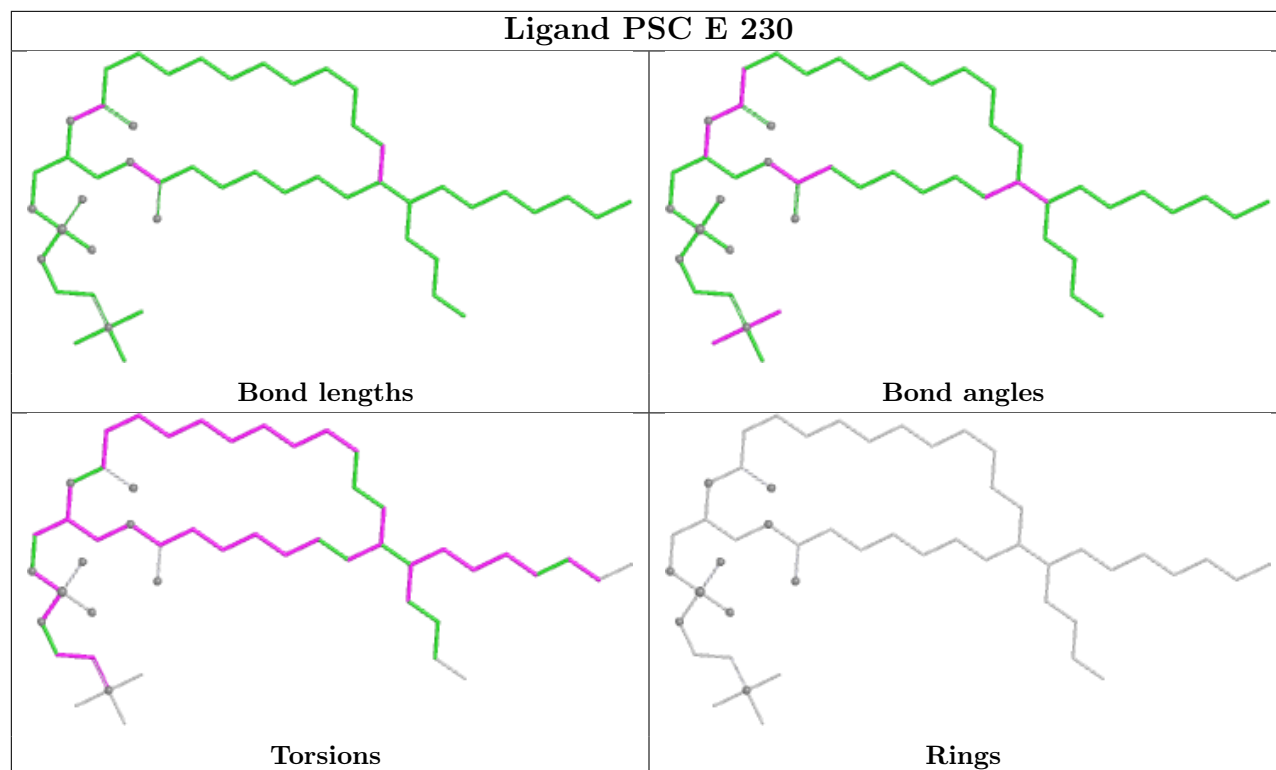
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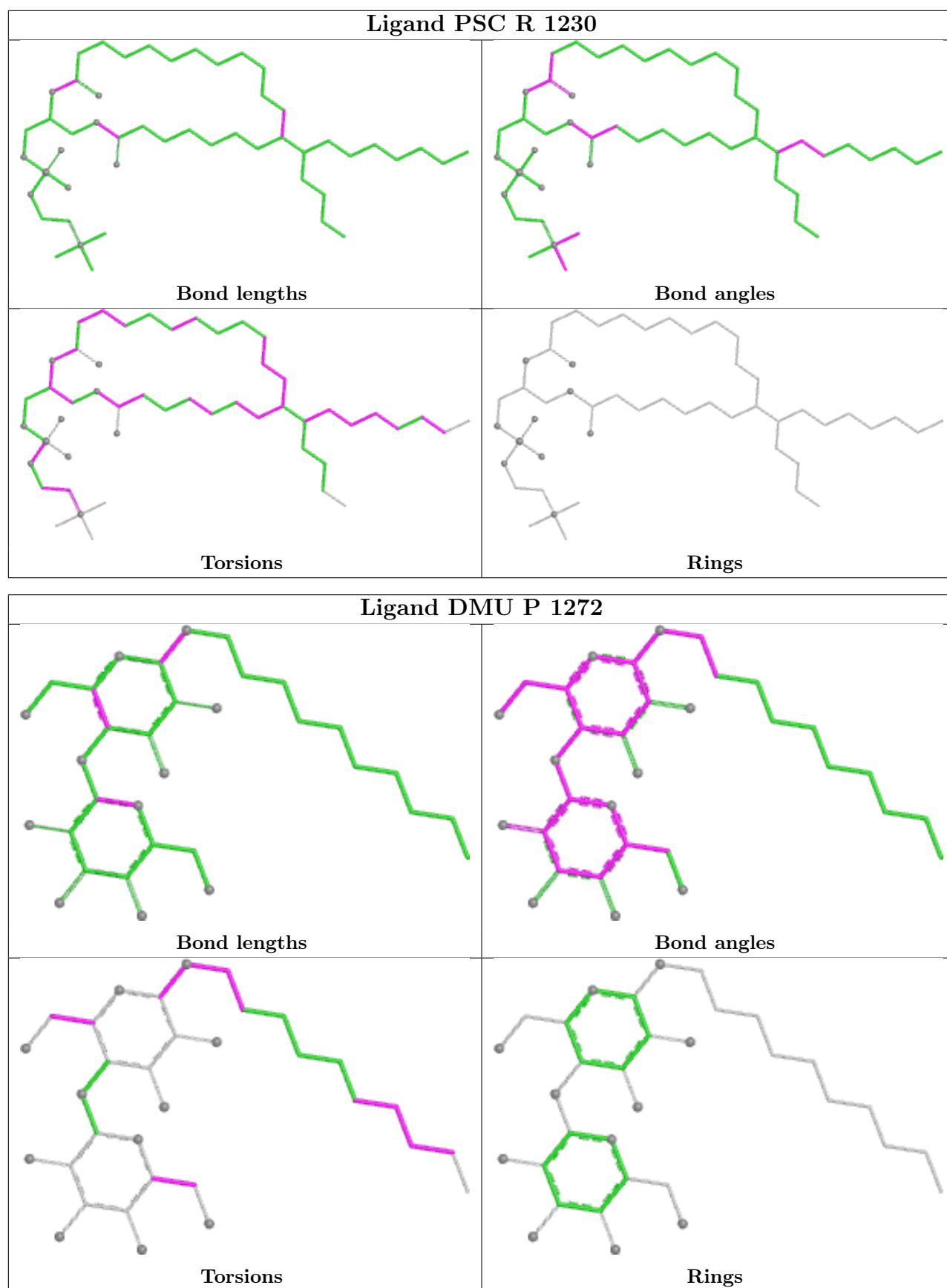
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	C	270	CDL	19	0
22	P	1271	CHD	1	0
18	A	515	HEA	8	0
22	C	525	CHD	3	0
15	A	520	PER	1	0
20	P	1267	PGV	12	0
19	A	521	TGL	13	0
19	Y	1522	TGL	18	0
19	D	523	TGL	9	0
20	N	1524	PGV	11	0
20	C	267	PGV	5	0
19	O	1523	TGL	9	0
25	G	269	CDL	27	0
20	A	524	PGV	6	0

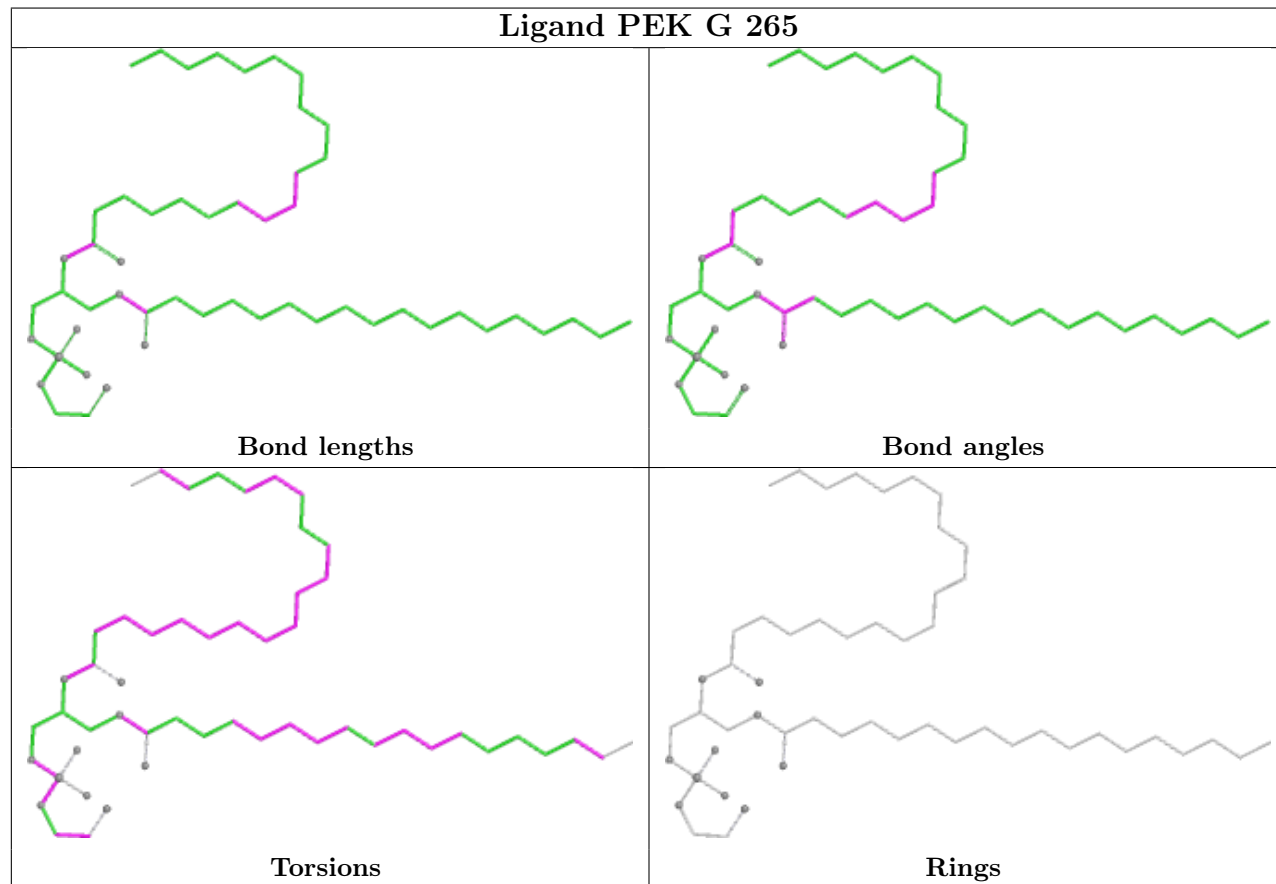
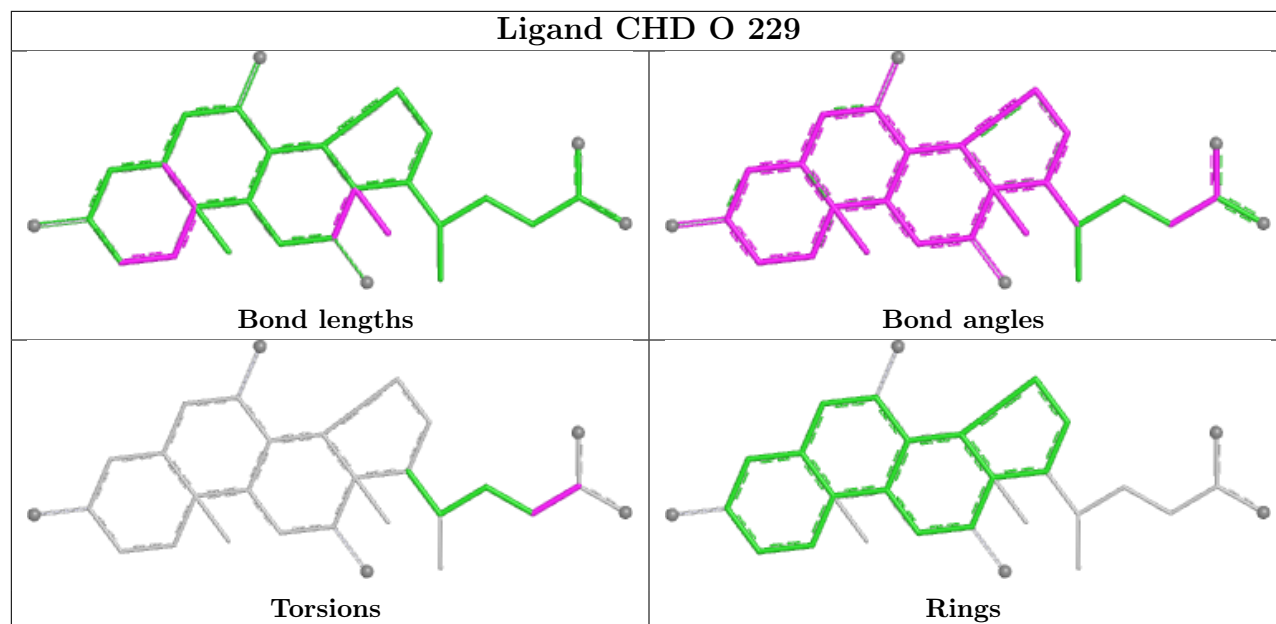
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

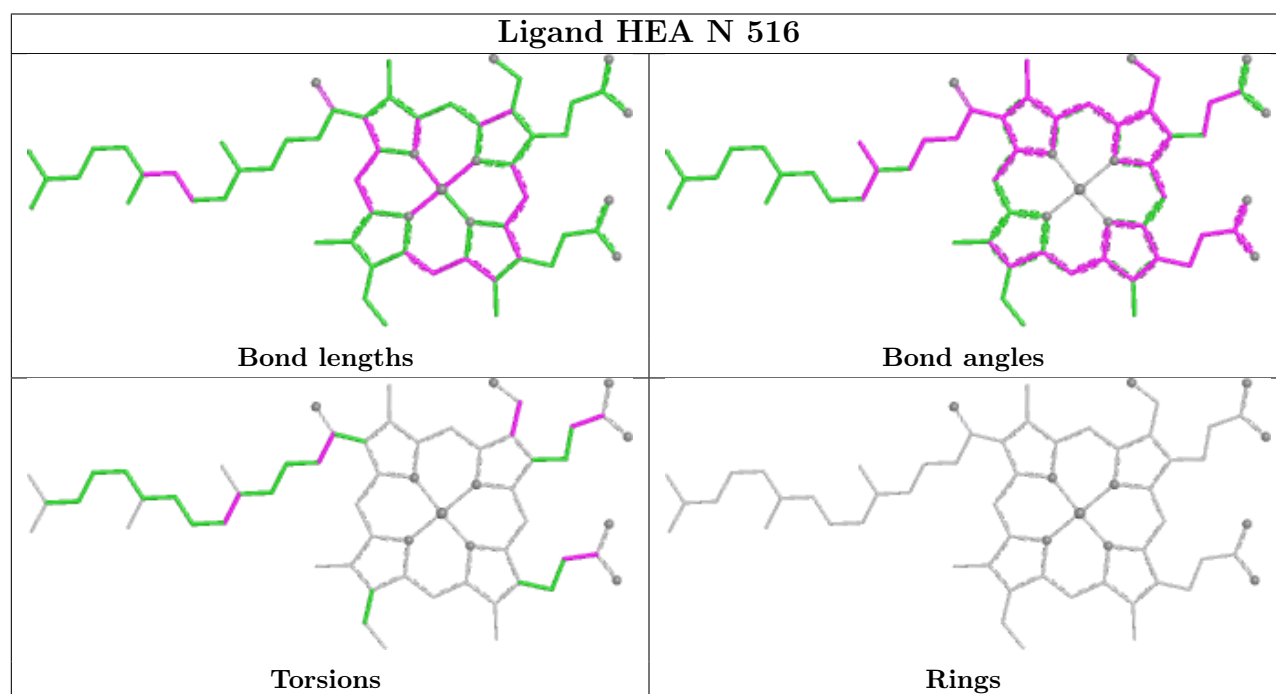
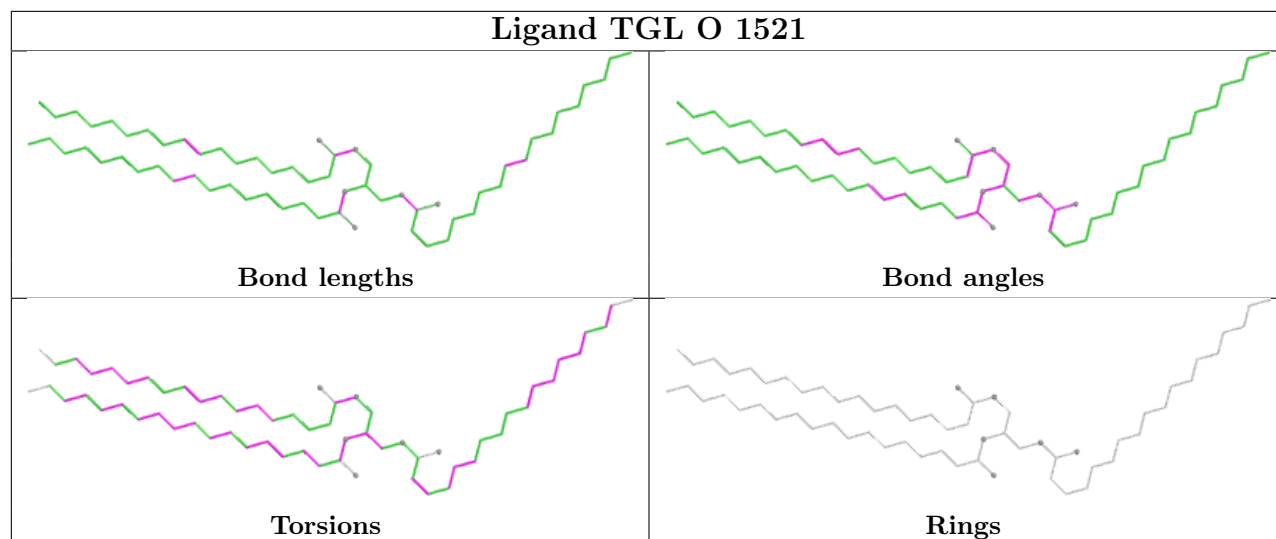


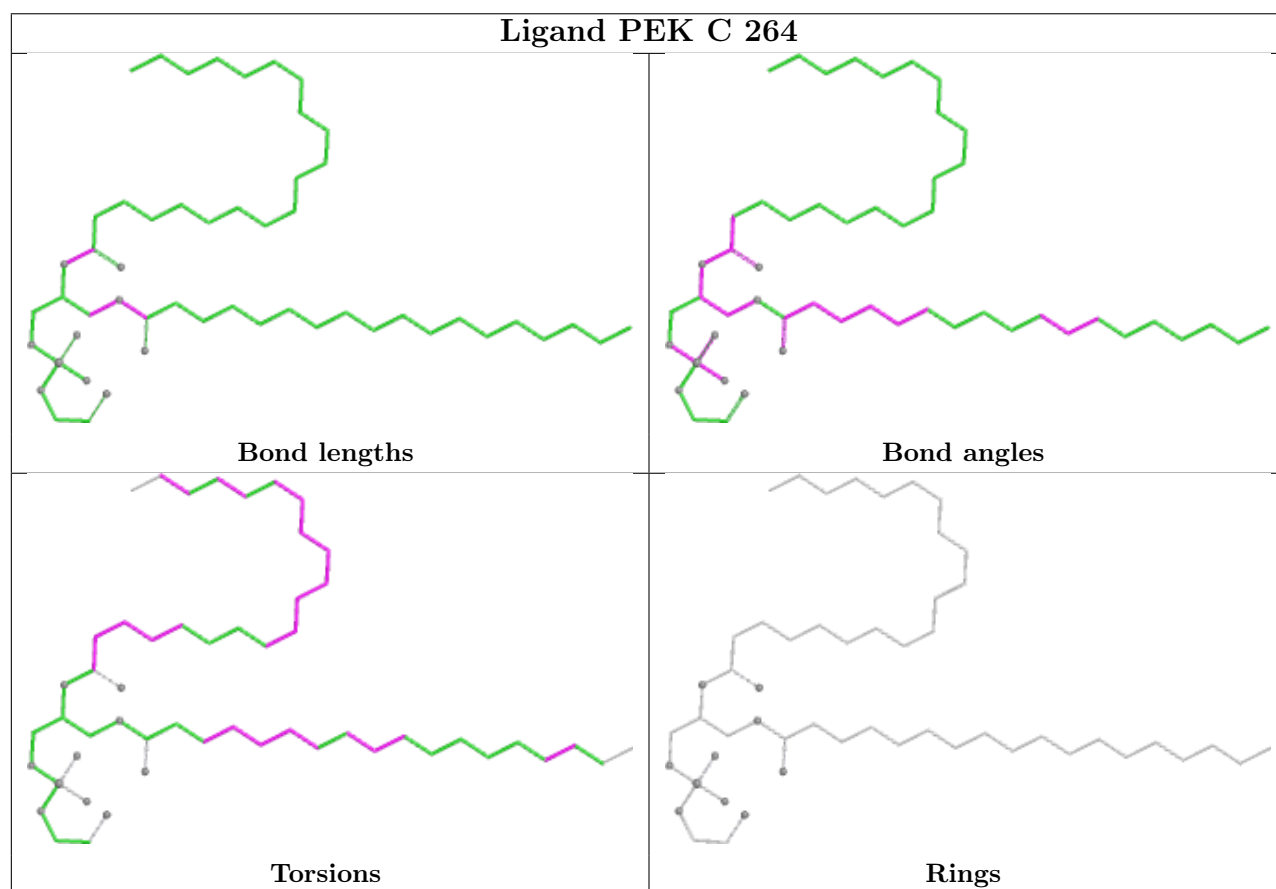
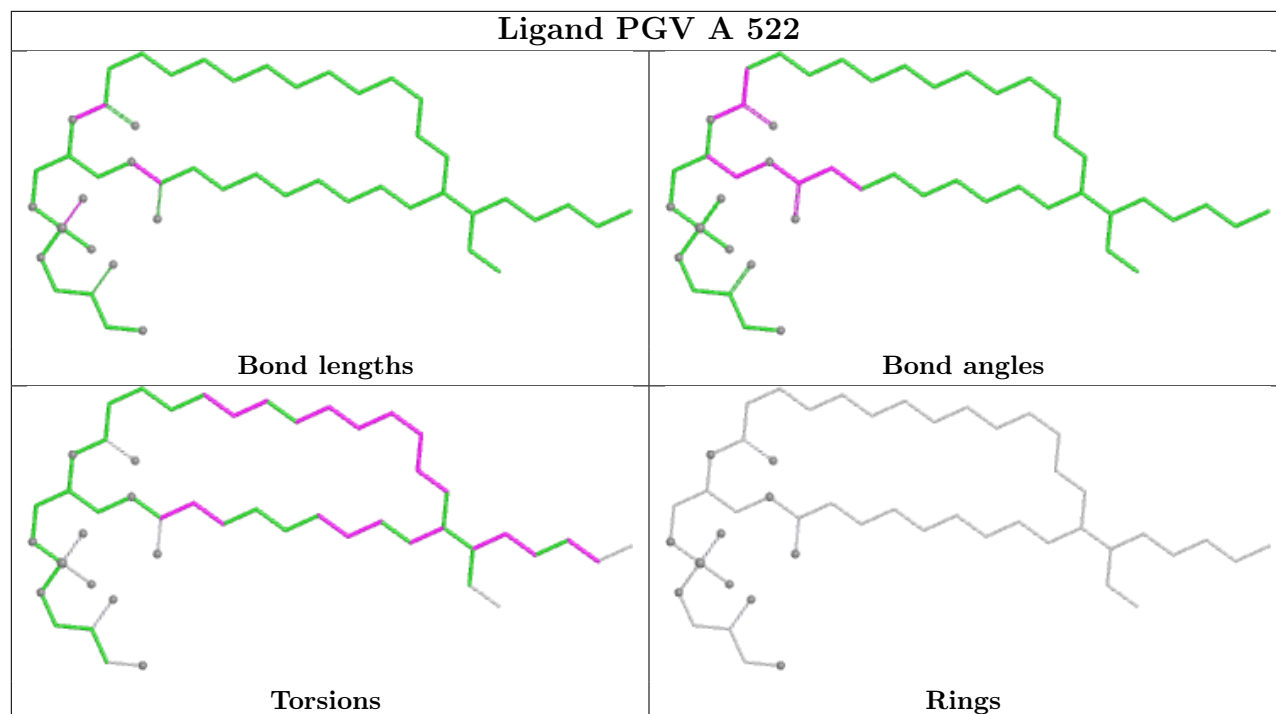


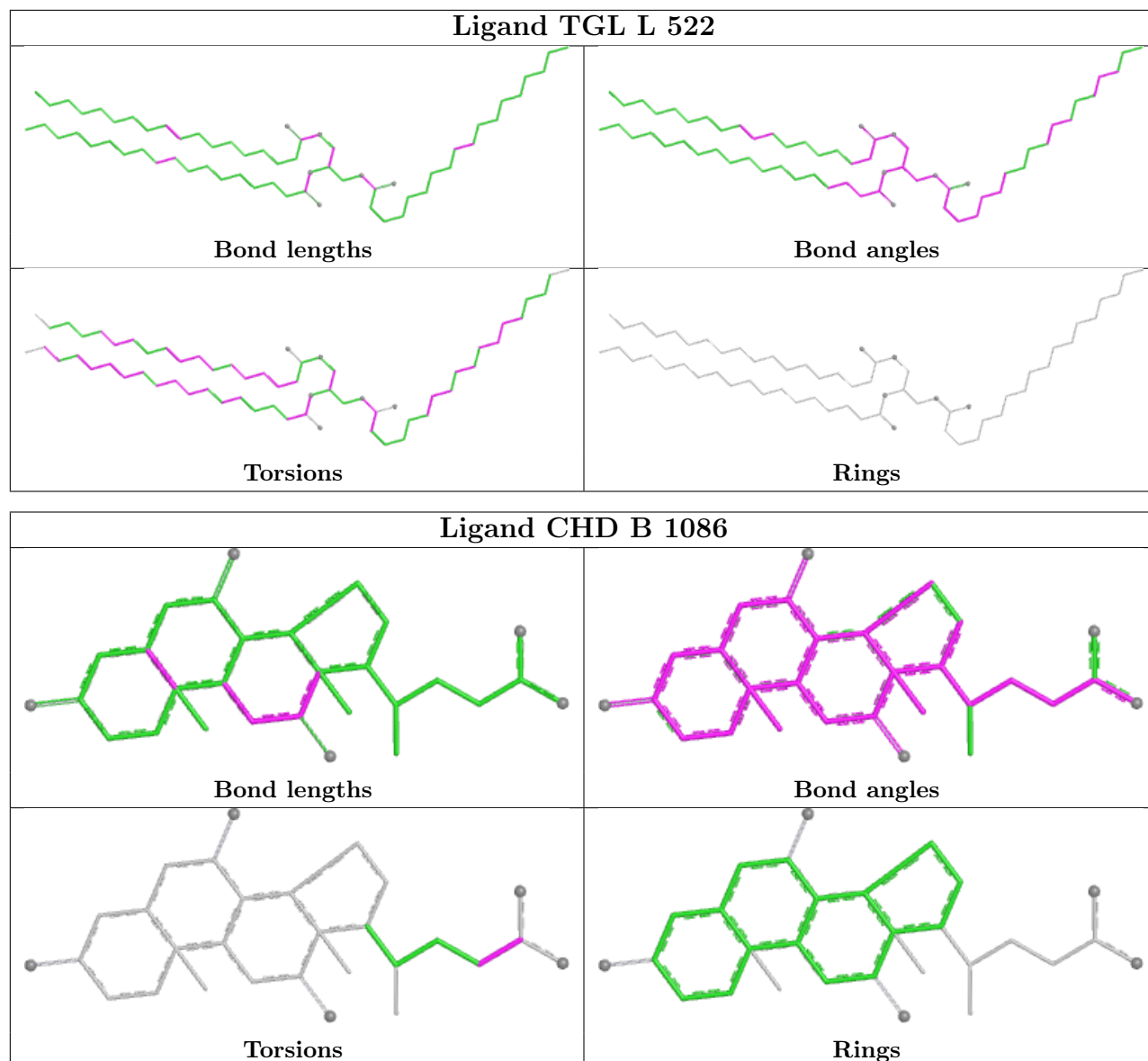


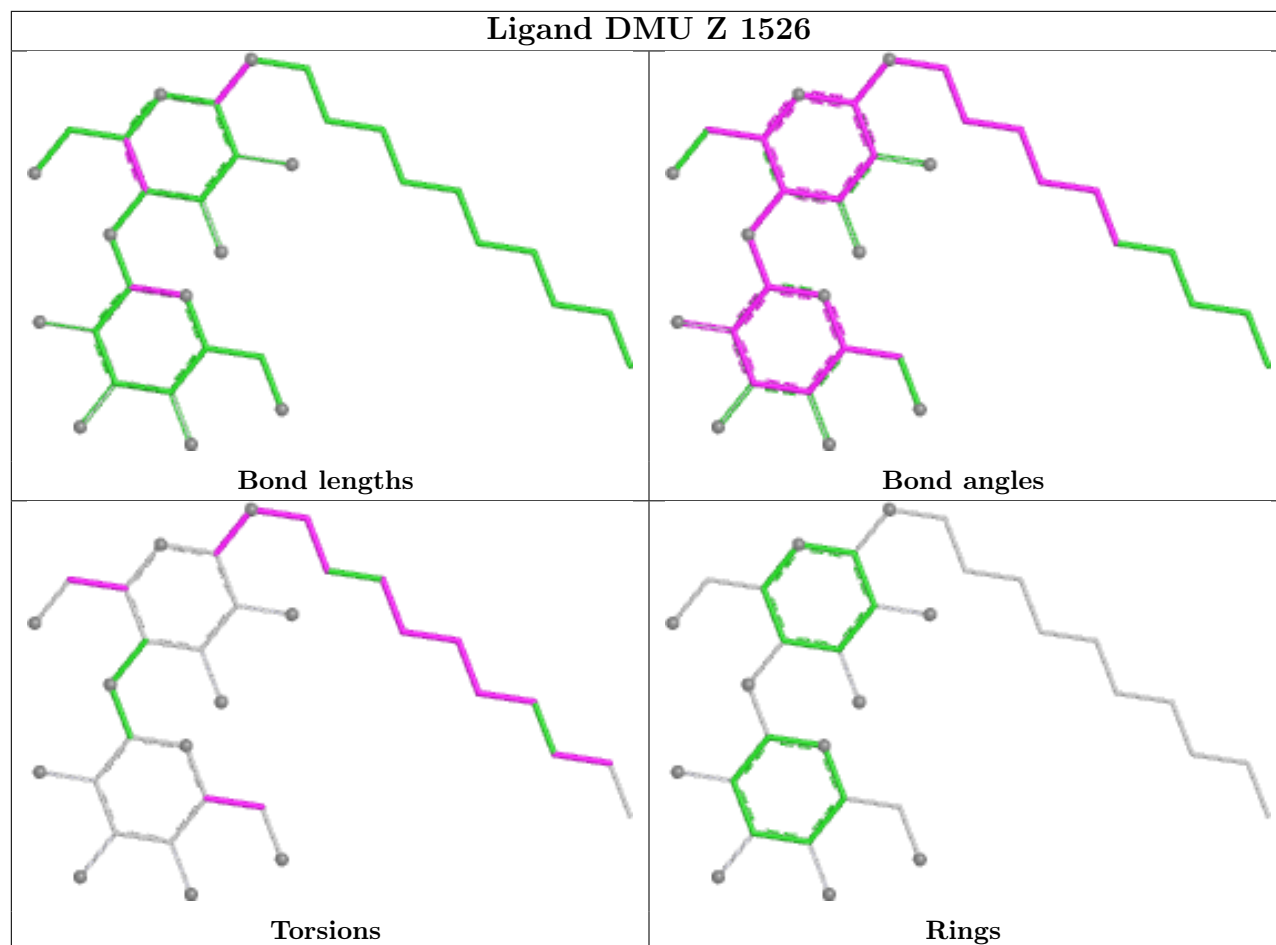


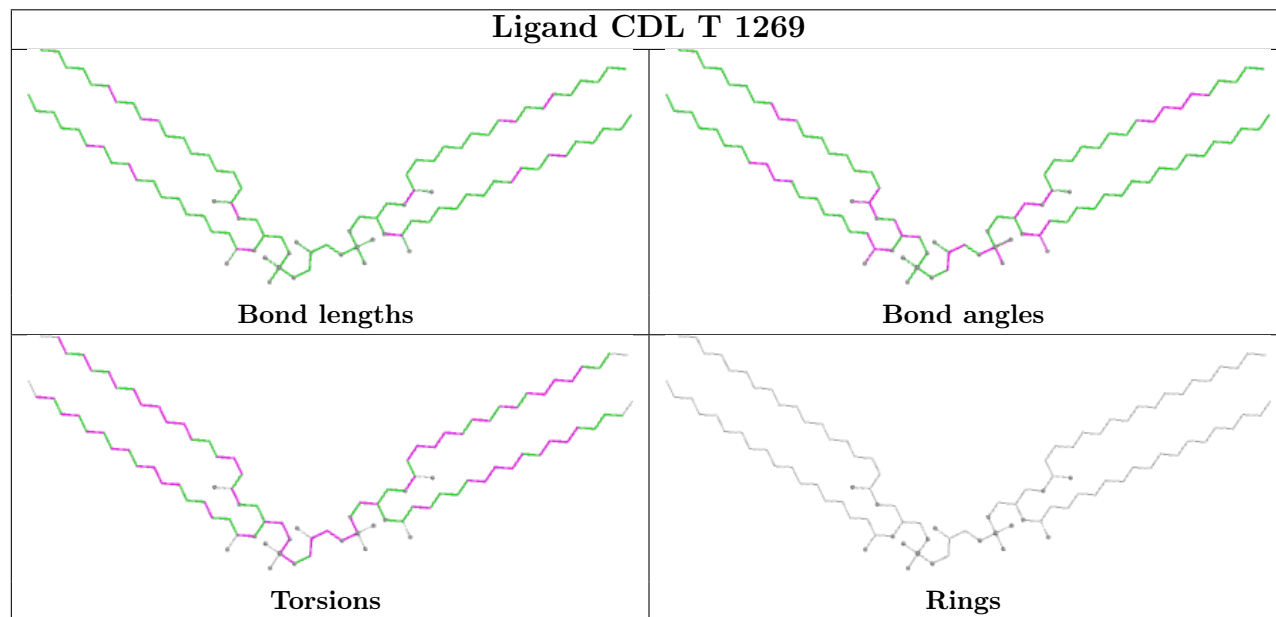
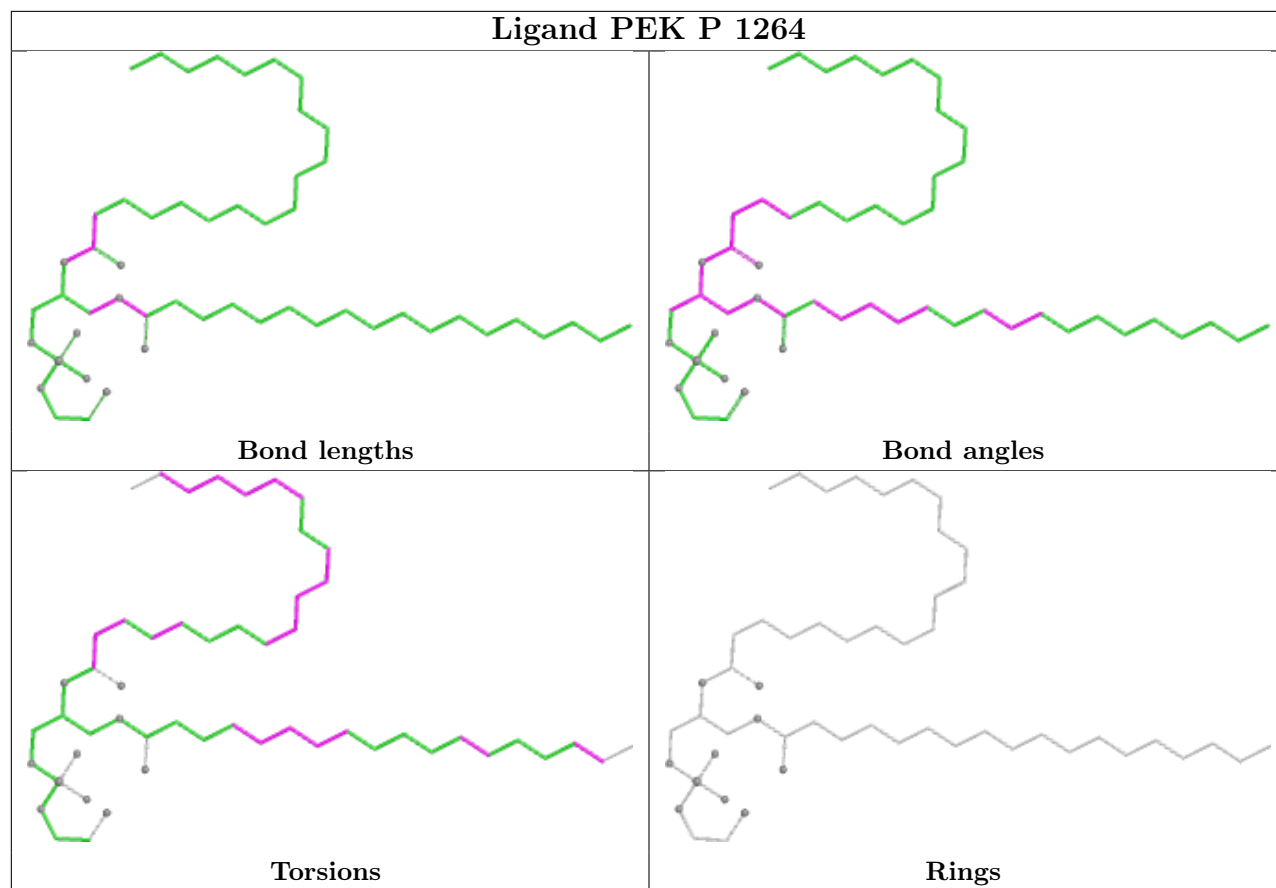


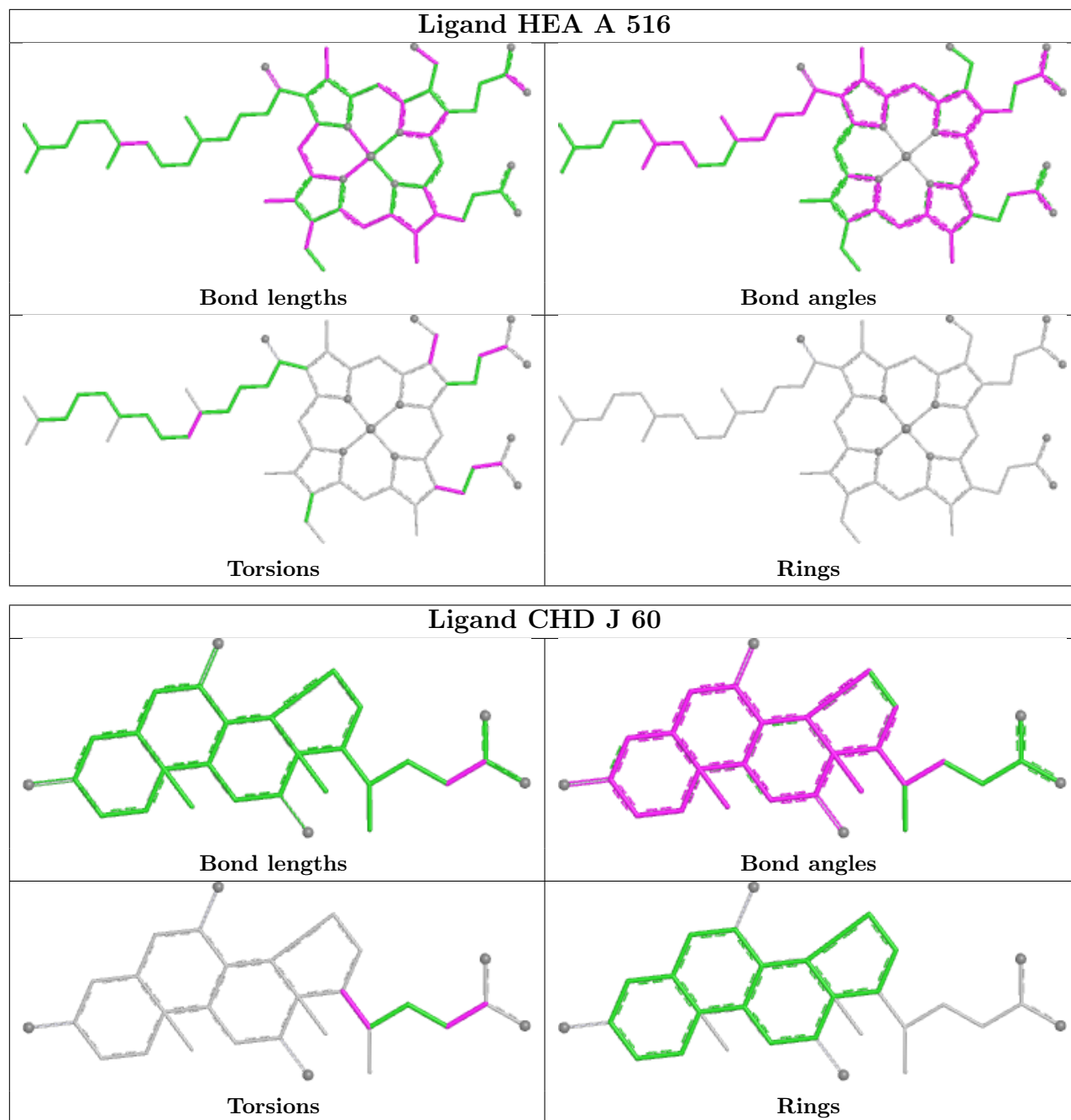


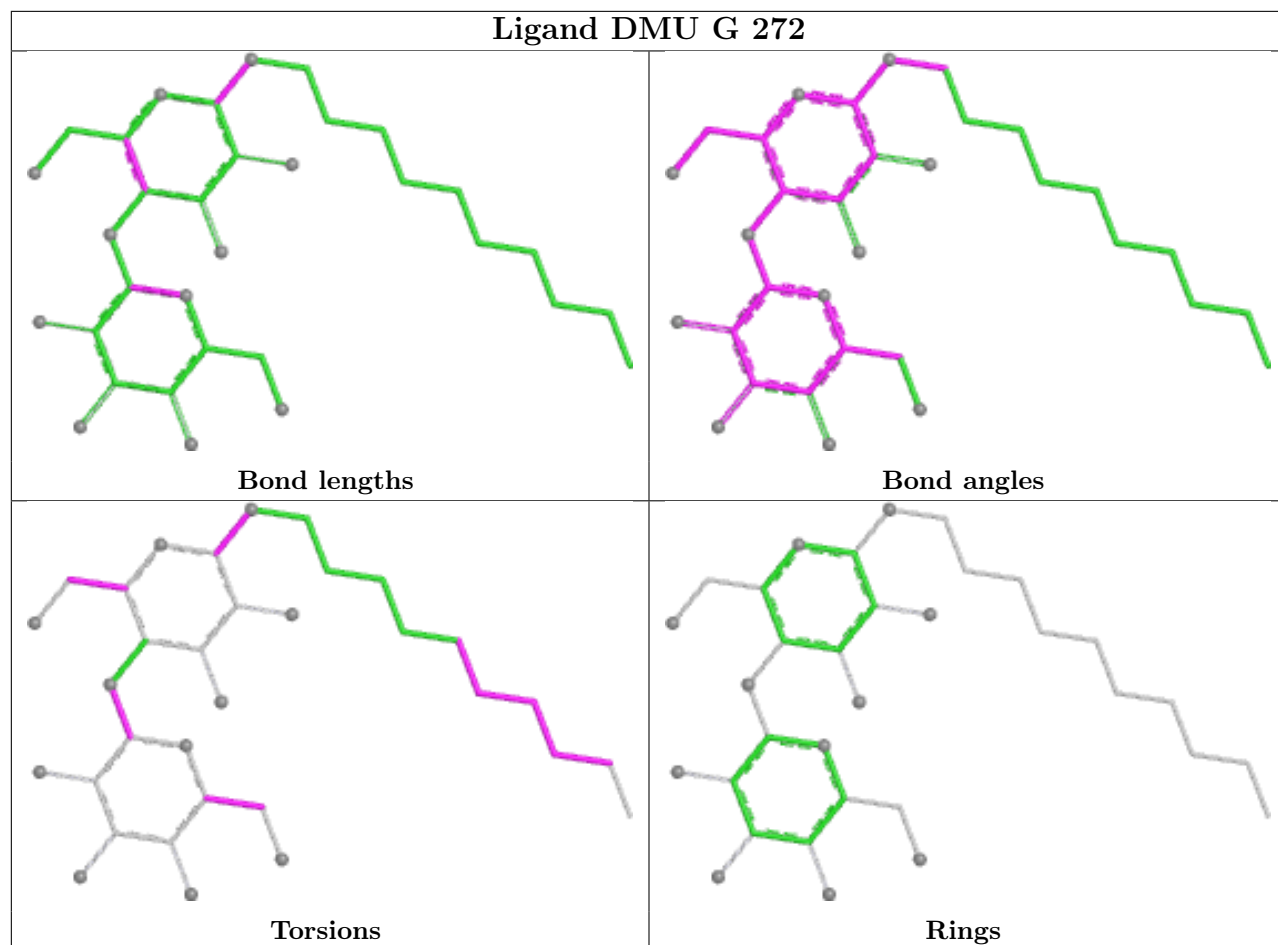


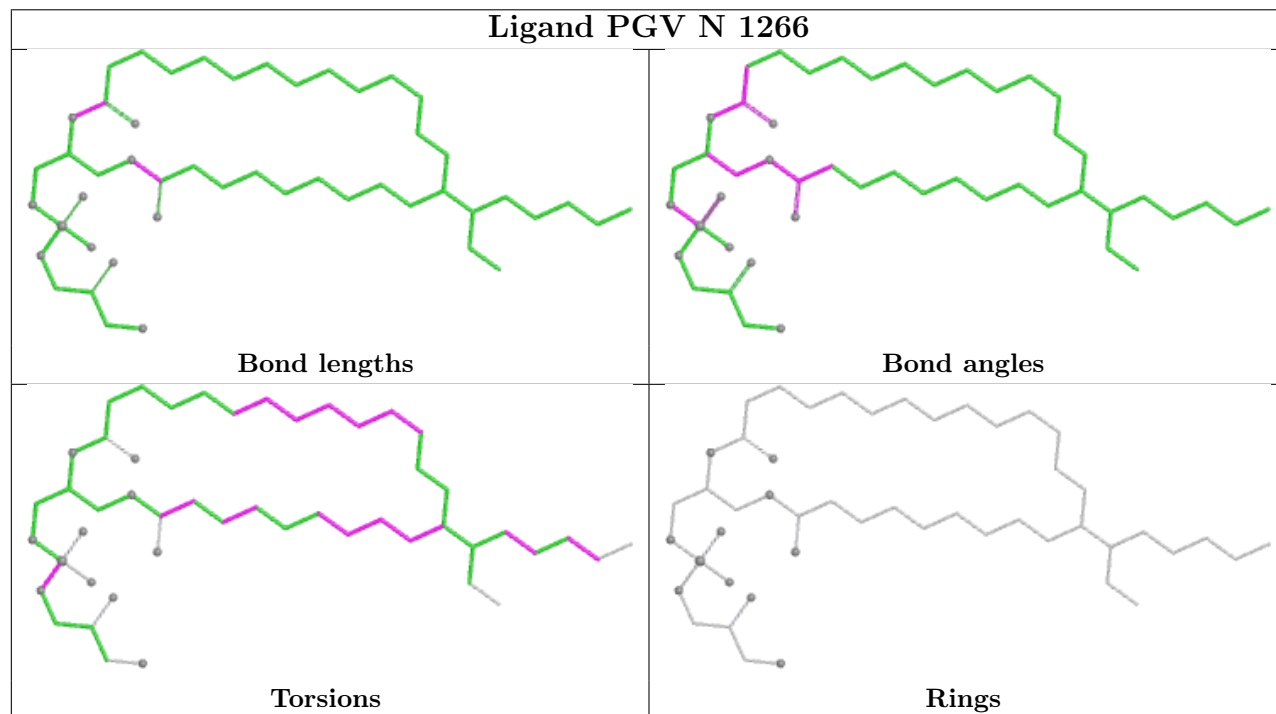
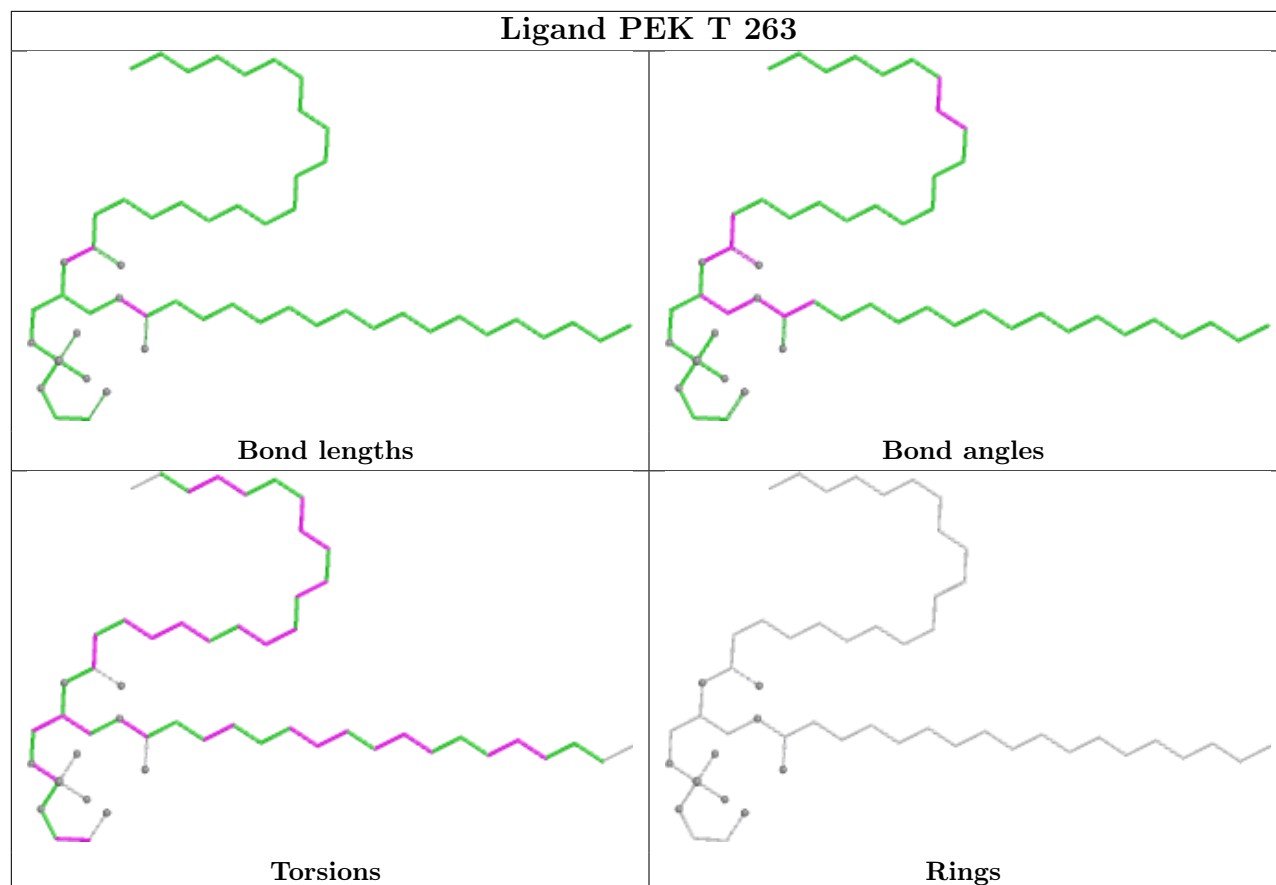


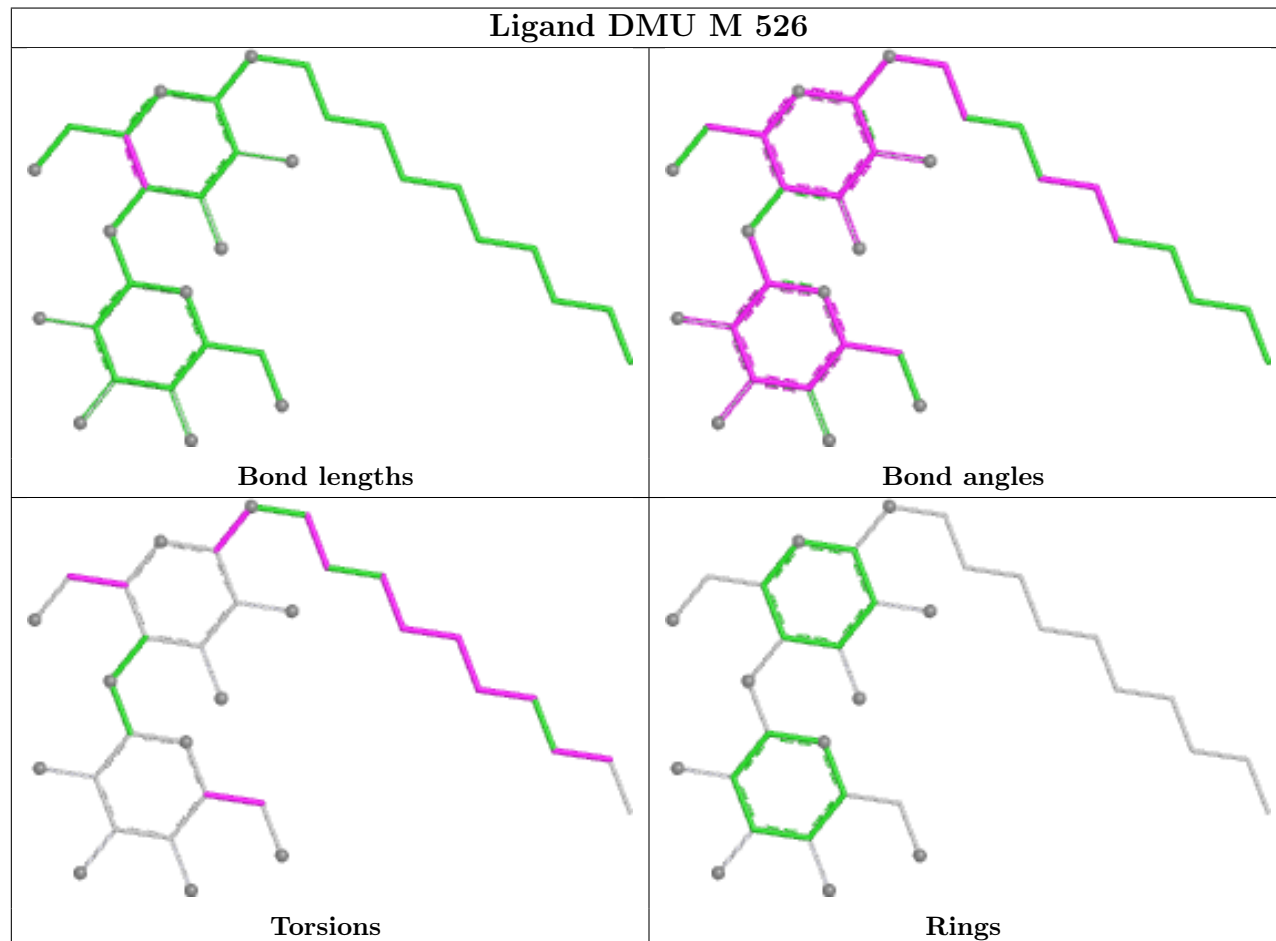
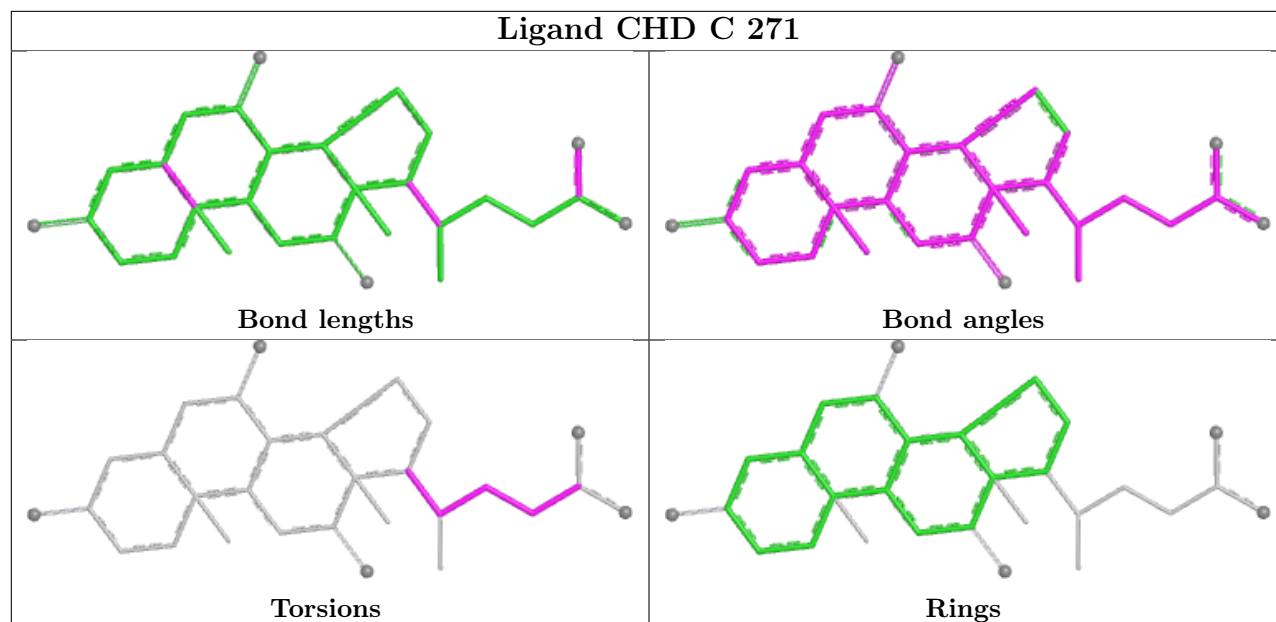


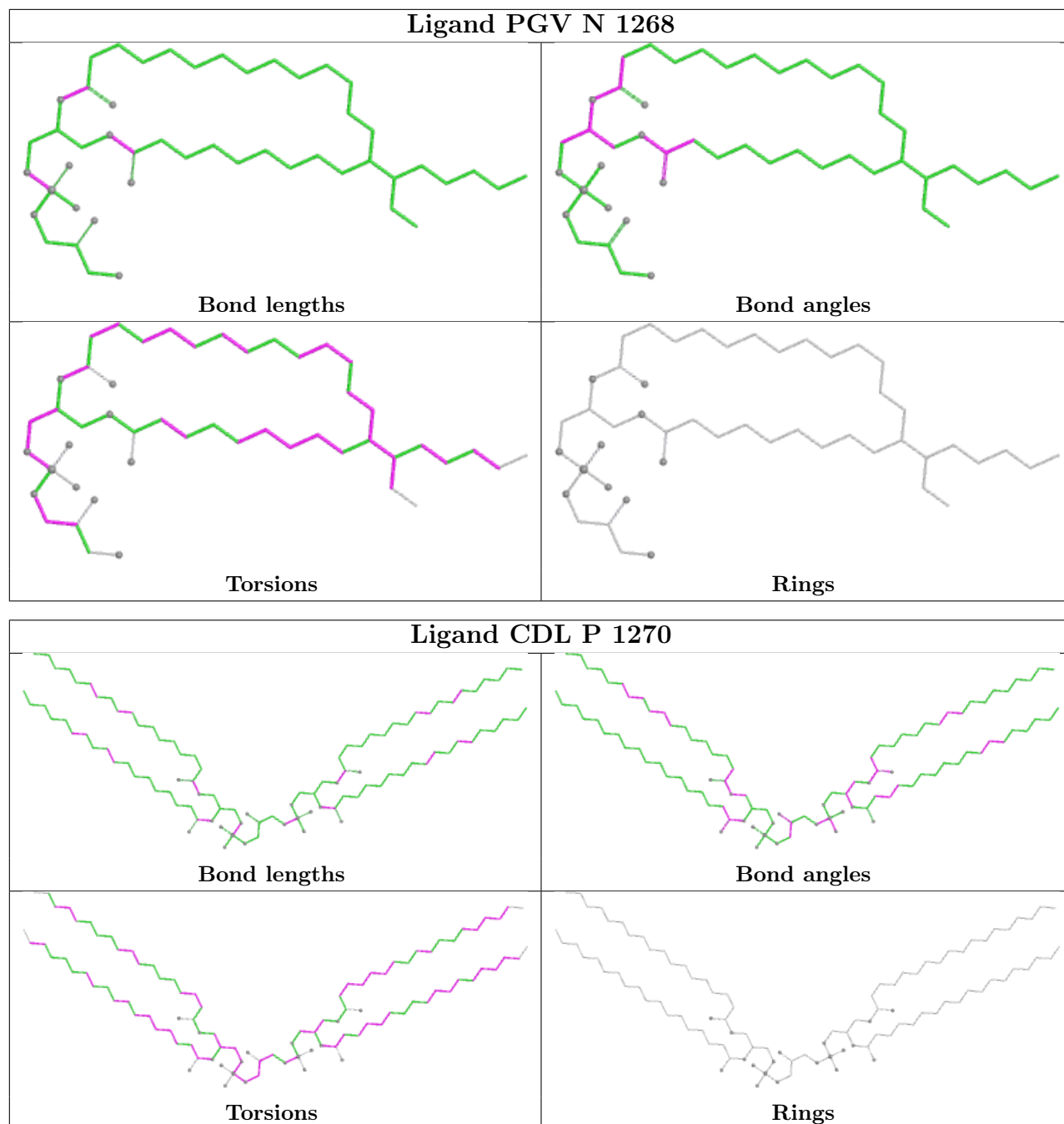


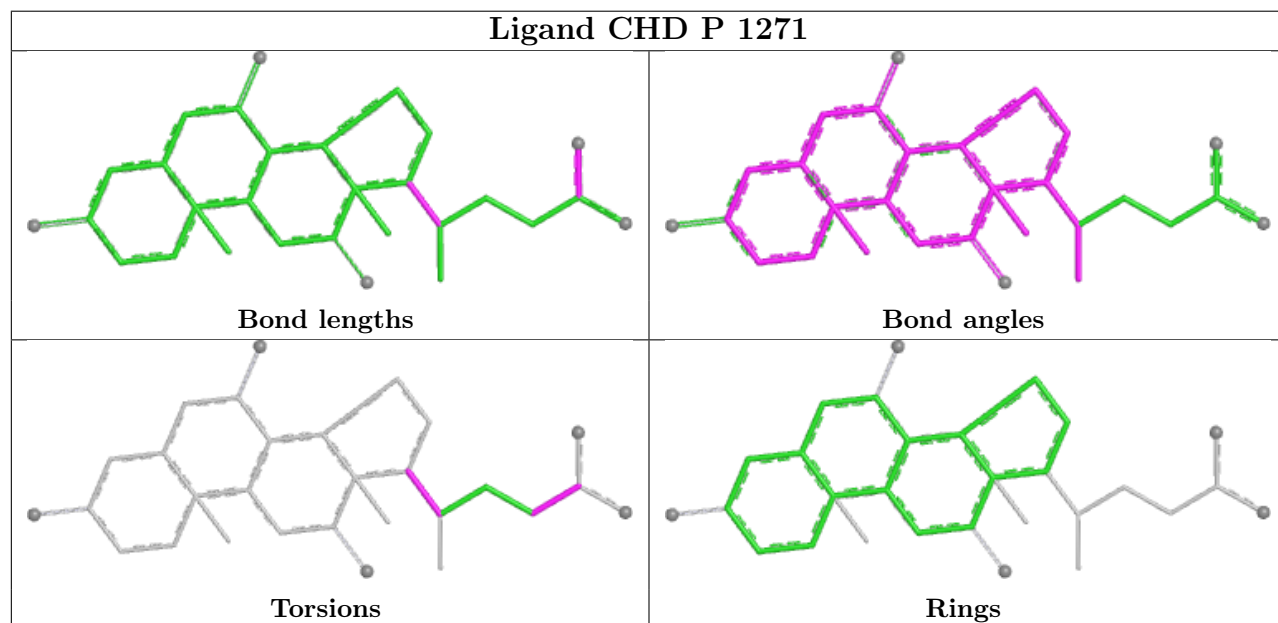
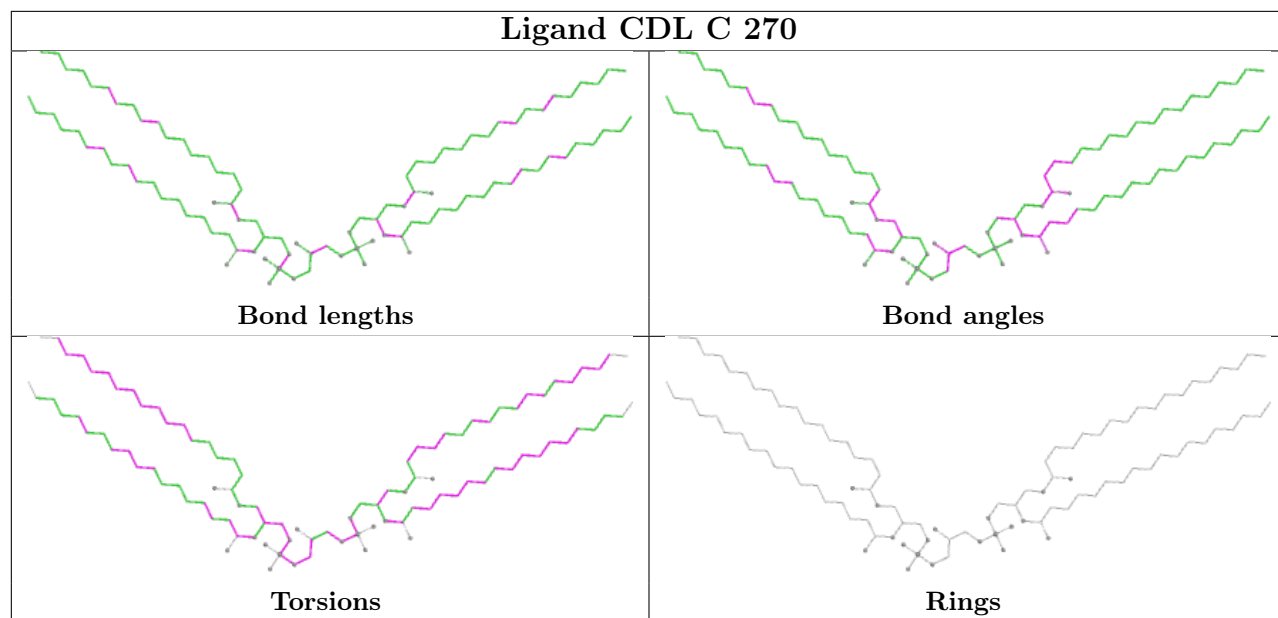


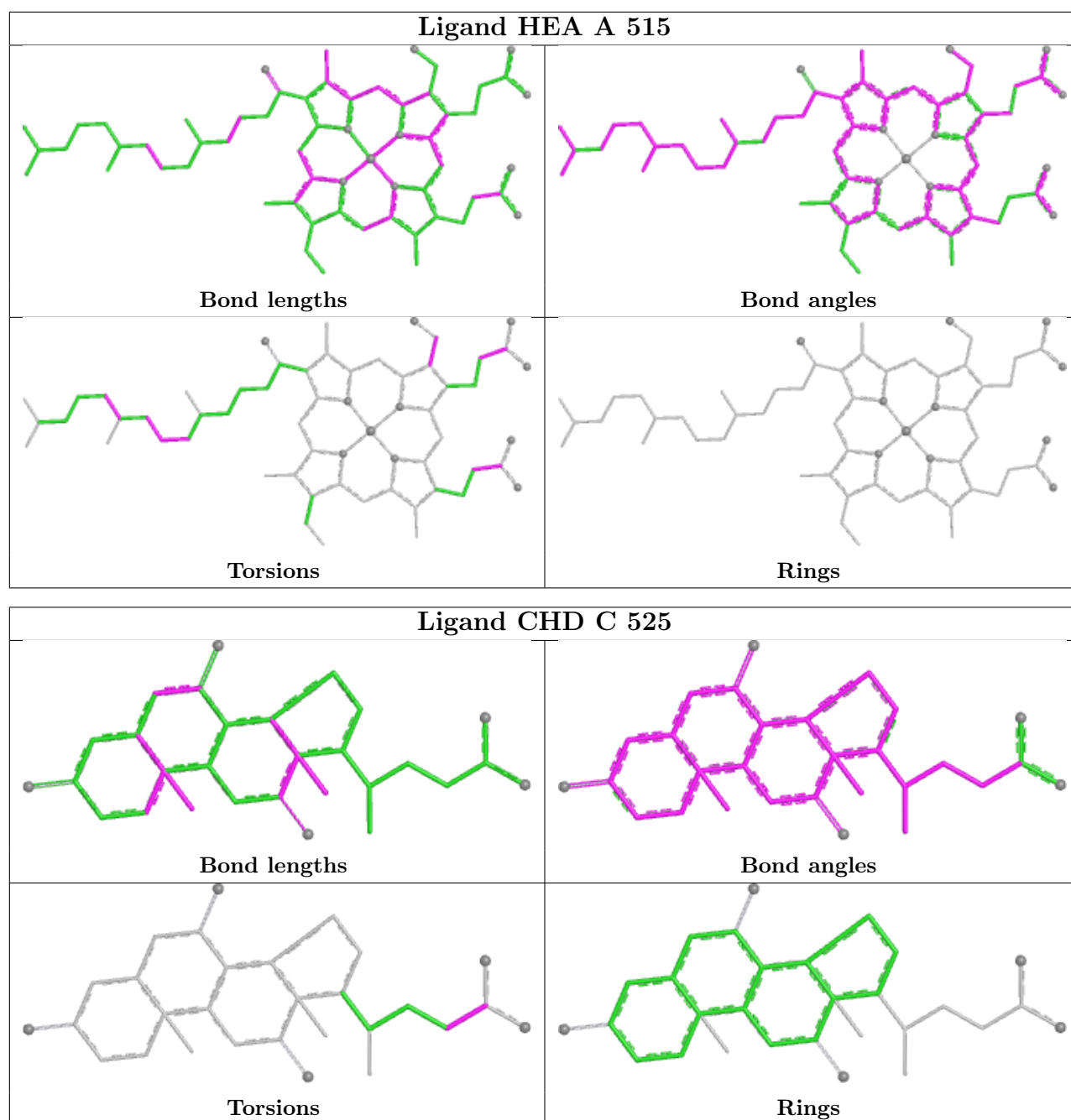


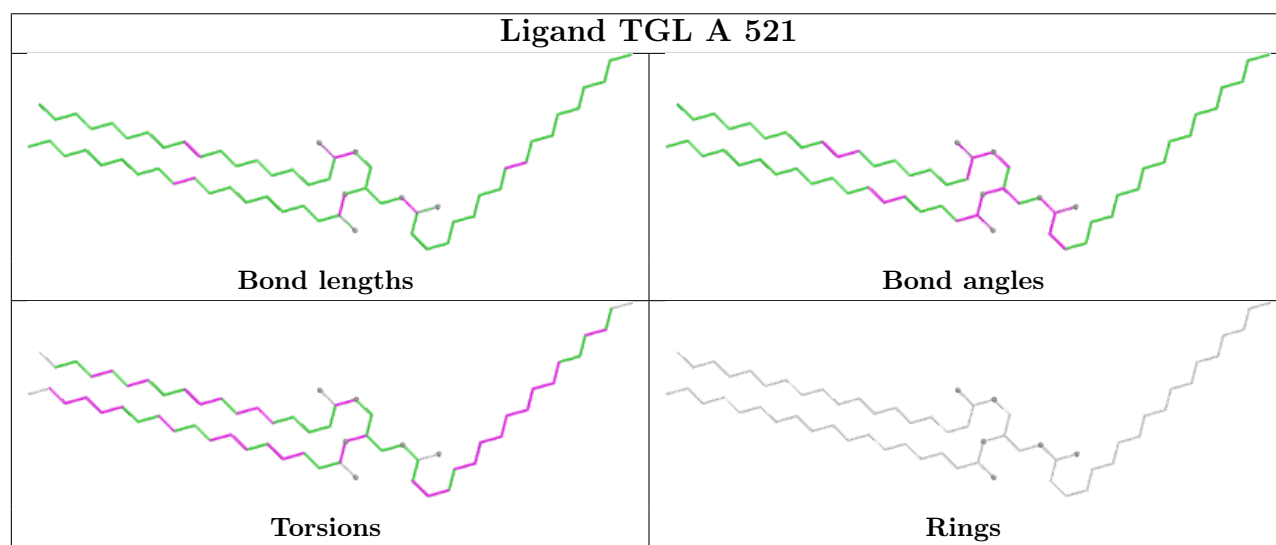
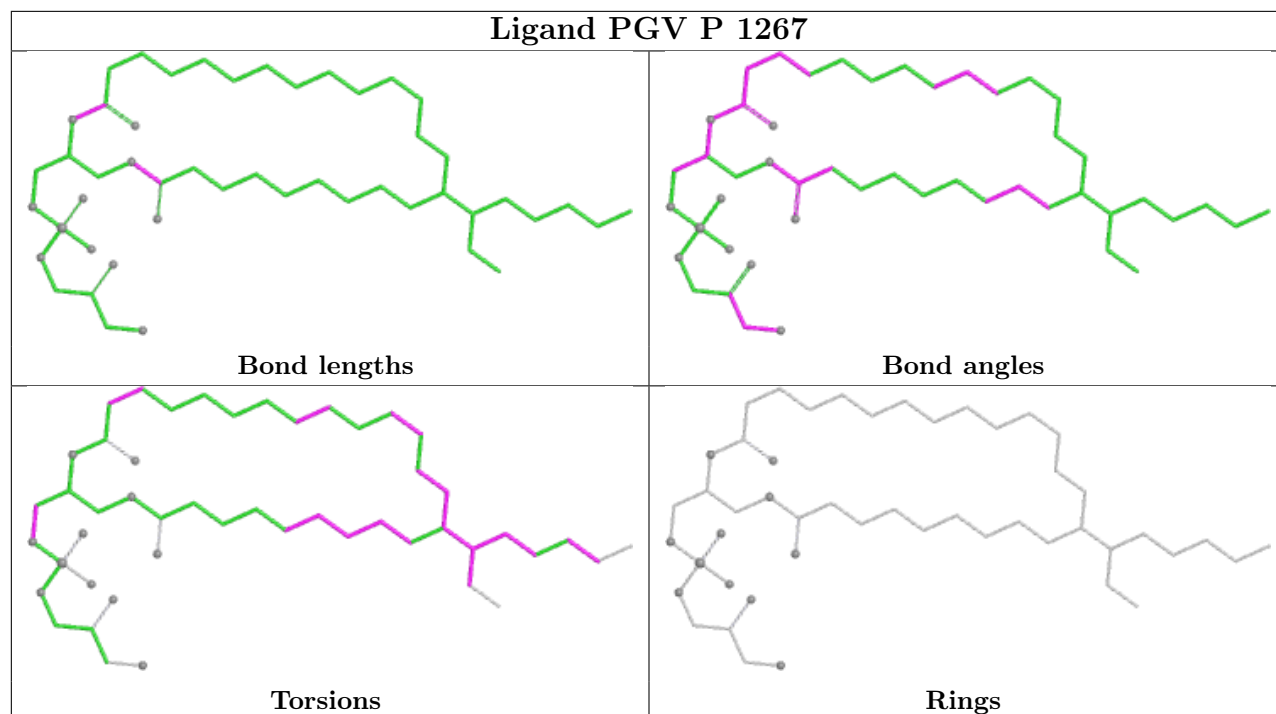


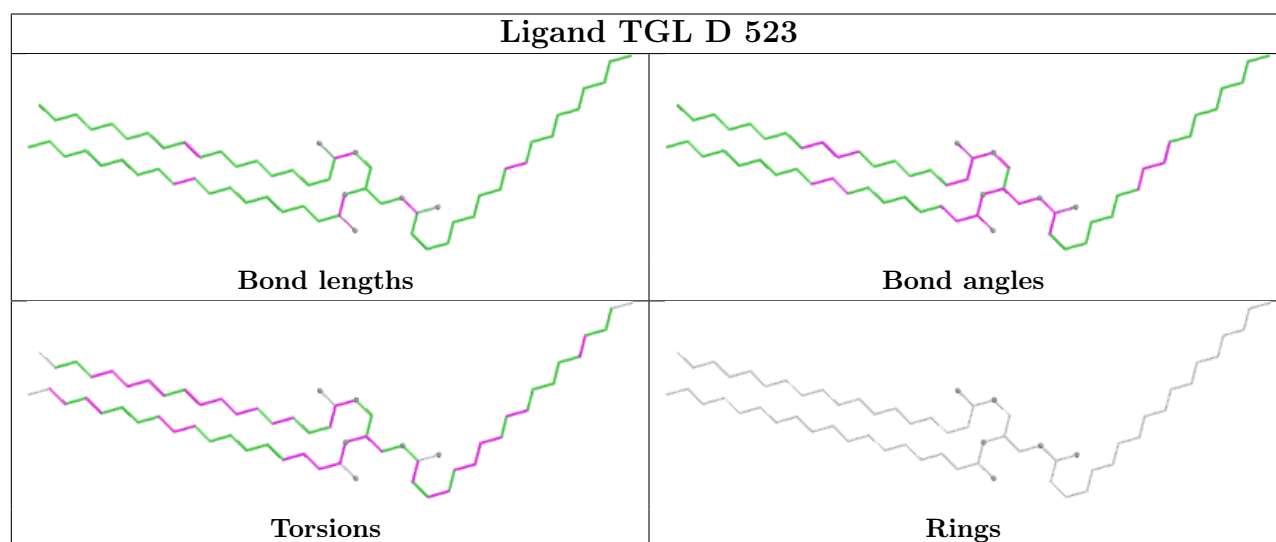
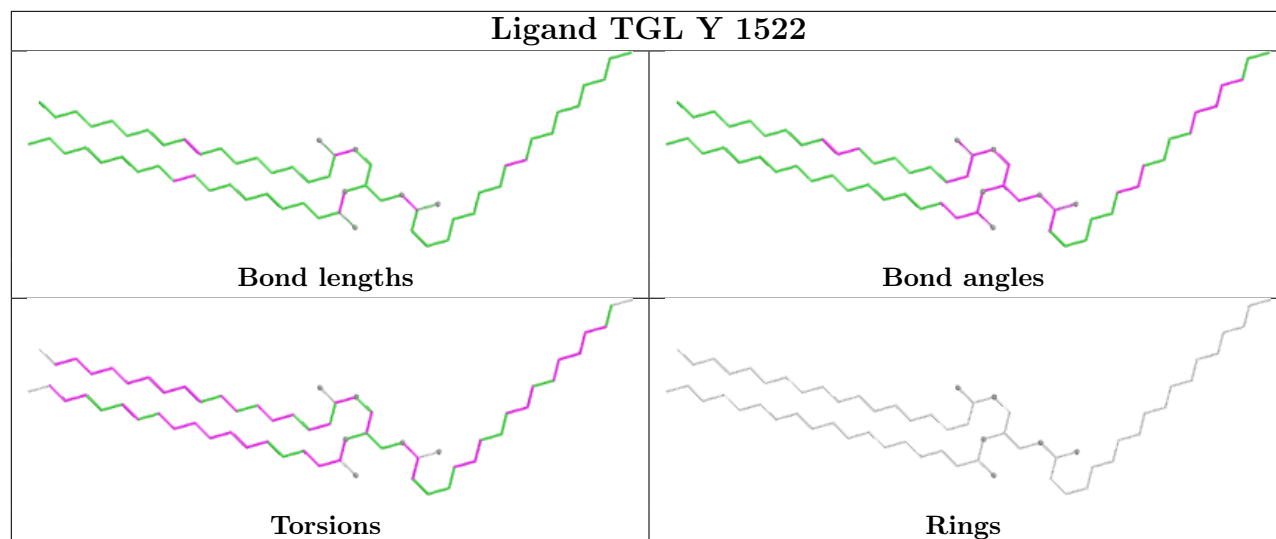


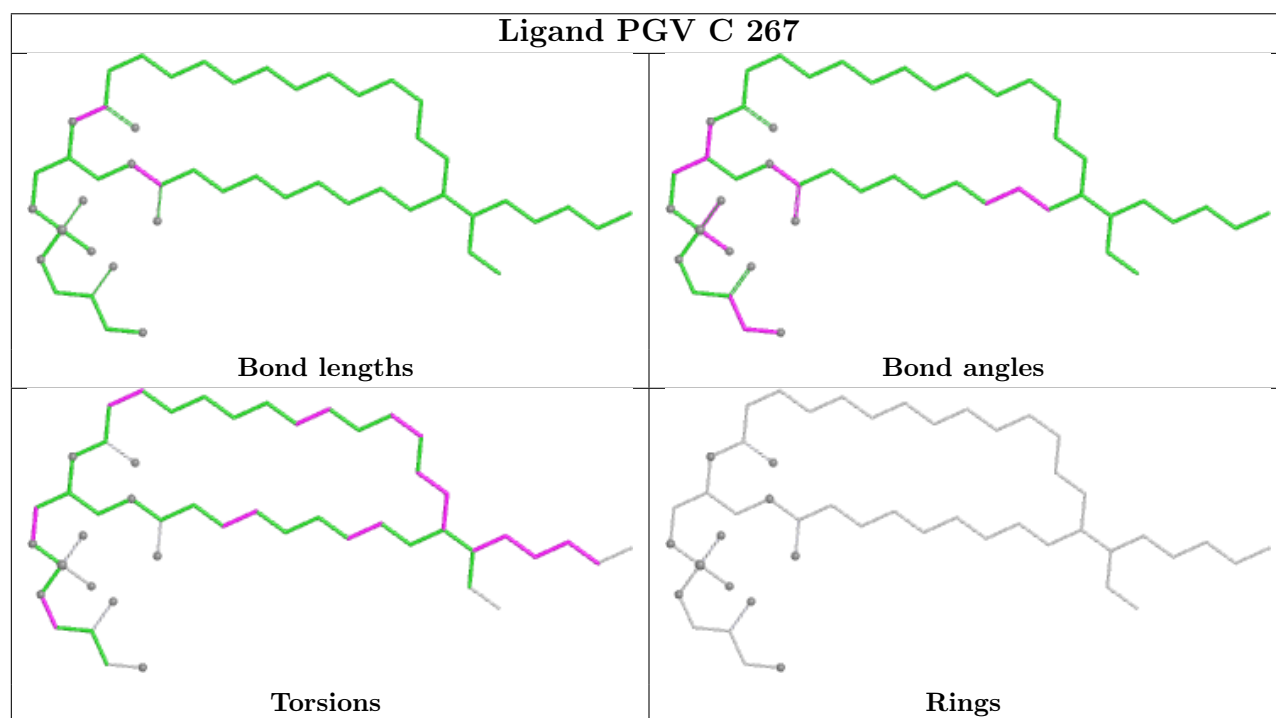
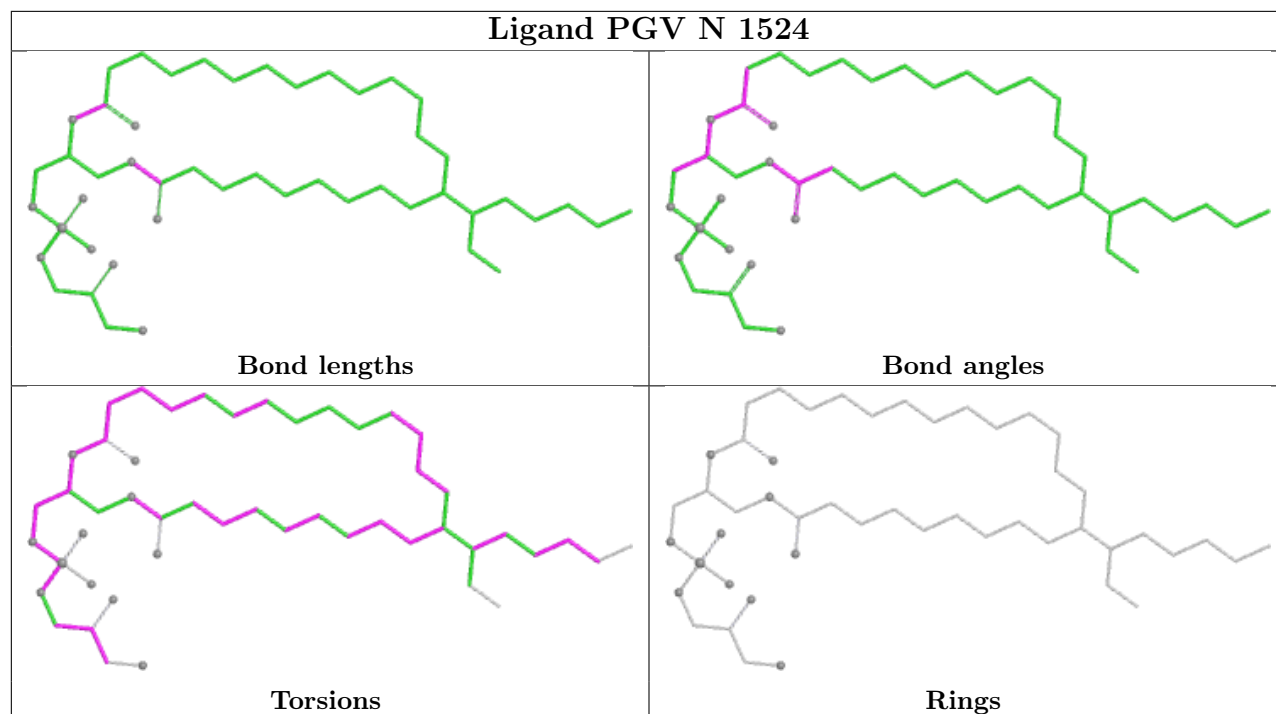


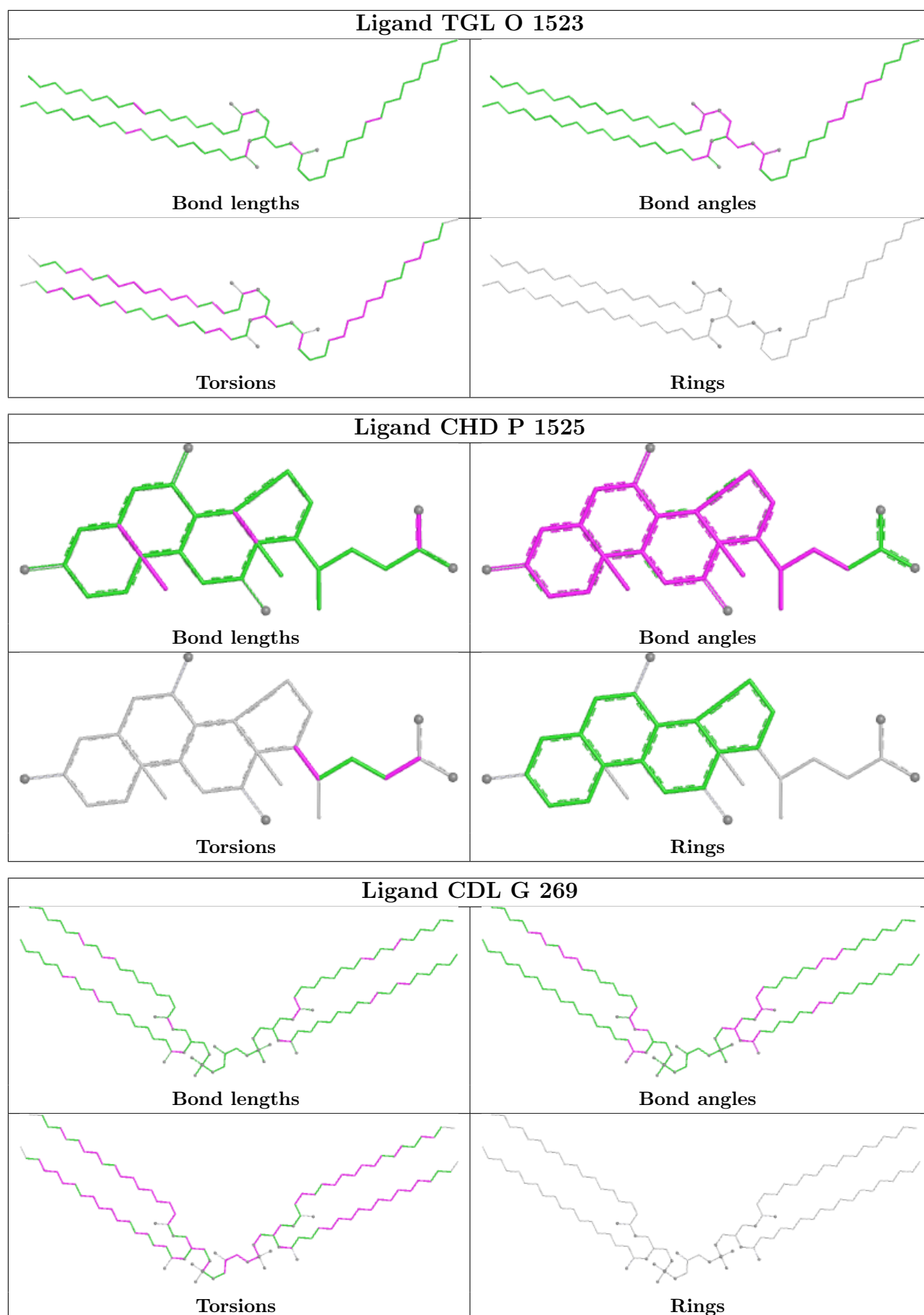


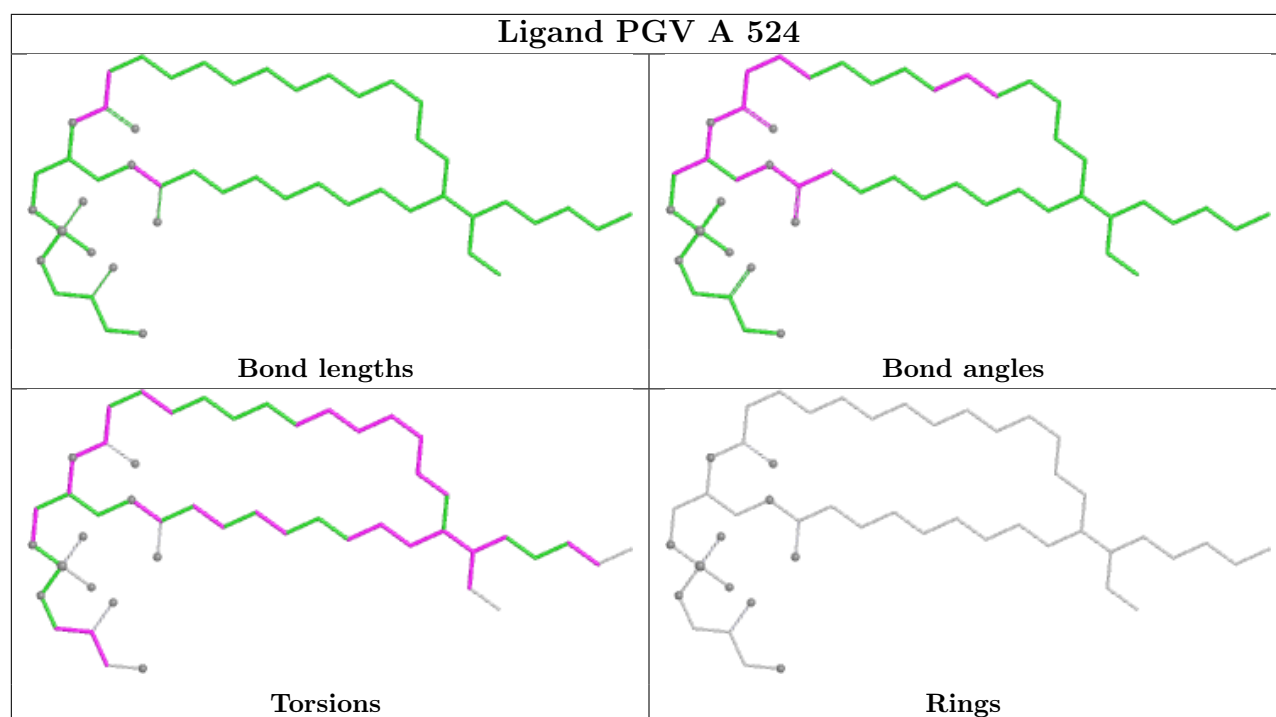












5.7 Other polymers [i](#)

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%)	-0.42	2 (0%) 88 91	23, 29, 37, 63	0
1	N	513/514 (99%)	0.07	2 (0%) 88 91	27, 34, 43, 64	0
2	B	226/227 (99%)	0.04	9 (3%) 42 49	24, 34, 56, 82	0
2	O	226/227 (99%)	0.60	12 (5%) 32 37	30, 40, 62, 82	0
3	C	259/261 (99%)	-0.12	3 (1%) 76 82	25, 32, 44, 61	0
3	P	259/261 (99%)	0.22	4 (1%) 72 78	28, 35, 47, 64	0
4	D	144/147 (97%)	0.10	4 (2%) 55 62	29, 35, 50, 65	0
4	Q	144/147 (97%)	1.22	24 (16%) 4 4	36, 50, 70, 109	0
5	E	104/109 (95%)	-0.10	1 (0%) 79 84	29, 35, 54, 70	0
5	R	104/109 (95%)	0.54	1 (0%) 79 84	32, 41, 57, 75	0
6	F	93/98 (94%)	0.28	4 (4%) 40 46	29, 38, 56, 93	0
6	S	93/98 (94%)	0.62	4 (4%) 40 46	32, 40, 62, 87	0
7	G	83/85 (97%)	0.95	17 (20%) 2 2	29, 38, 93, 99	0
7	T	83/85 (97%)	1.30	19 (22%) 2 2	30, 42, 90, 104	0
8	H	75/85 (88%)	0.45	7 (9%) 14 16	30, 41, 77, 83	0
8	U	75/85 (88%)	0.81	9 (12%) 9 10	36, 46, 80, 86	0
9	I	71/73 (97%)	0.71	10 (14%) 6 7	31, 41, 65, 71	0
9	V	71/73 (97%)	1.11	7 (9%) 13 14	36, 51, 66, 75	0
10	J	57/59 (96%)	0.38	0 100 100	32, 41, 58, 73	0
10	W	57/59 (96%)	0.97	4 (7%) 22 26	36, 45, 62, 78	0
11	K	49/56 (87%)	0.38	2 (4%) 41 48	32, 38, 49, 58	0
11	X	49/56 (87%)	1.30	7 (14%) 6 7	42, 47, 62, 69	0
12	L	46/47 (97%)	0.14	2 (4%) 40 46	30, 35, 54, 79	0
12	Y	46/47 (97%)	0.80	4 (8%) 16 18	34, 42, 62, 82	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	0.62	5 (11%) 9 11	29, 35, 87, 107	0
13	Z	43/46 (93%)	1.30	9 (20%) 2 2	37, 44, 96, 112	0
All	All	3526/3614 (97%)	0.28	172 (4%) 35 41	23, 36, 61, 112	0

The worst 5 of 172 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	6	VAL	9.4
6	S	96	LEU	8.0
4	Q	4	SER	6.8
7	T	4	ALA	6.4
6	S	94	HIS	6.2

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	TPO	T	11	11/12	0.56	0.22	71,78,95,96	0
7	TPO	G	11	11/12	0.60	0.27	71,78,96,97	0
1	FME	A	1	10/11	0.88	0.13	48,51,72,78	0
1	FME	N	1	10/11	0.89	0.16	47,49,70,71	0
2	FME	O	1	10/11	0.94	0.11	39,40,48,52	0
2	FME	B	1	10/11	0.94	0.09	32,33,40,58	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.

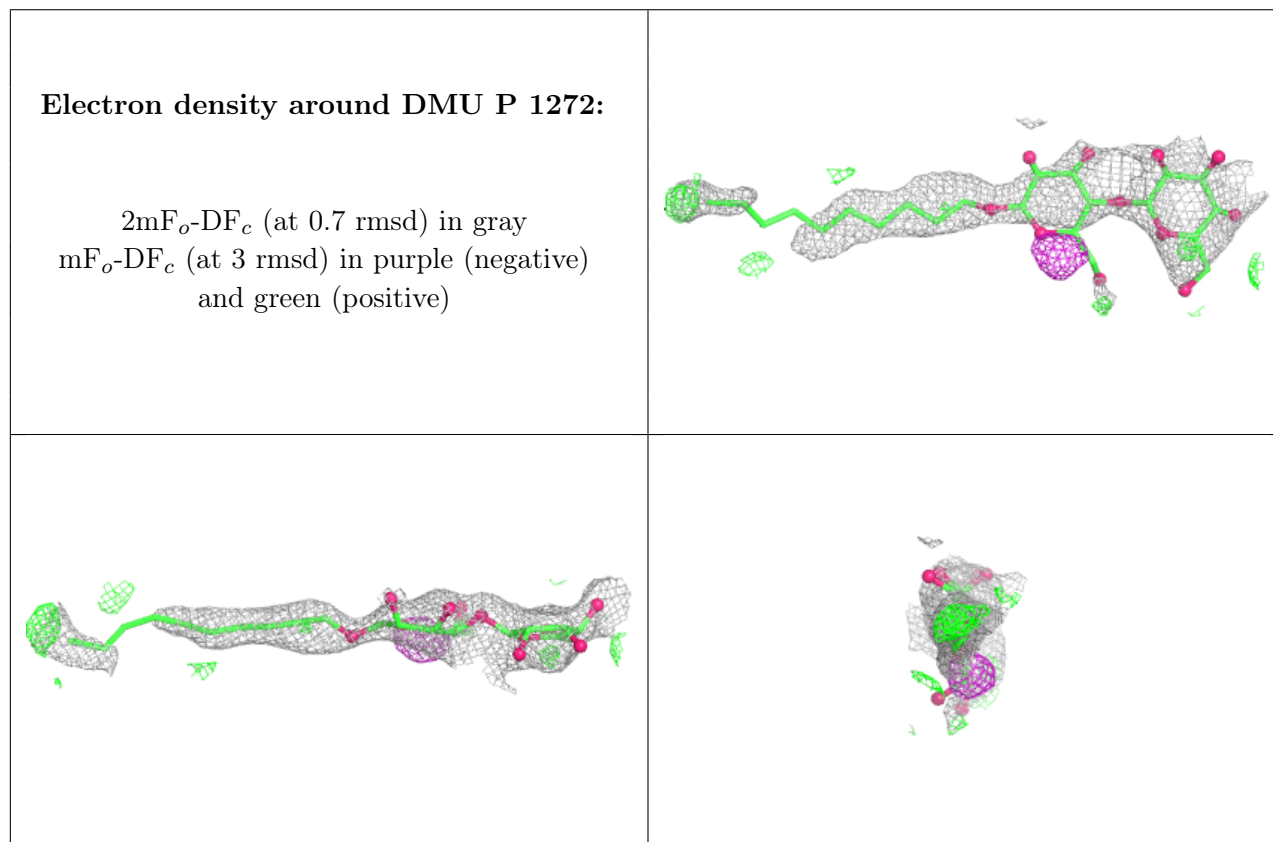
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
28	DMU	P	1272	33/33	0.72	0.21	80,103,111,112	0
22	CHD	W	1060	29/29	0.73	0.21	87,91,96,97	0
24	PEK	T	263	53/53	0.74	0.26	55,95,117,119	0
25	CDL	G	269	100/100	0.75	0.23	64,87,115,118	0
28	DMU	G	272	33/33	0.75	0.18	65,94,105,105	0
24	PEK	G	265	53/53	0.75	0.24	45,82,114,116	0
25	CDL	T	1269	100/100	0.77	0.21	61,84,108,111	0
26	PSC	R	1230	52/52	0.77	0.26	43,96,122,124	0
20	PGV	H	268	51/51	0.77	0.25	59,84,110,112	0
24	PEK	G	1263	53/53	0.77	0.25	60,95,118,119	0
19	TGL	O	1523	63/63	0.78	0.25	54,76,89,94	0
19	TGL	Y	1522	63/63	0.78	0.23	45,72,86,88	0
24	PEK	T	1265	53/53	0.78	0.23	44,79,110,112	0
20	PGV	A	524	51/51	0.78	0.22	33,74,105,108	0
25	CDL	P	1270	100/100	0.80	0.23	41,85,115,120	0
22	CHD	J	60	29/29	0.81	0.21	77,83,93,94	0
19	TGL	D	523	63/63	0.81	0.21	44,63,81,82	0
20	PGV	N	1268	51/51	0.81	0.23	67,91,112,114	0
19	TGL	L	522	63/63	0.82	0.19	38,59,77,79	0
19	TGL	O	1521	63/63	0.82	0.19	53,77,88,89	0
26	PSC	E	230	52/52	0.82	0.22	58,99,125,127	0
19	TGL	A	521	63/63	0.82	0.20	48,69,84,89	0
25	CDL	C	270	100/100	0.82	0.21	41,84,118,119	0
20	PGV	N	1524	51/51	0.82	0.19	41,75,113,114	0
23	UNX	C	262	1/1	0.86	0.49	28,28,28,28	0
28	DMU	Z	1526	33/33	0.86	0.12	39,54,67,69	0
17	NA	A	519	1/1	0.89	0.17	42,42,42,42	0
23	UNX	P	1262	1/1	0.91	0.48	22,22,22,22	0
22	CHD	C	271	29/29	0.91	0.11	46,51,53,55	0
17	NA	N	1519	1/1	0.92	0.20	45,45,45,45	0
22	CHD	P	1271	29/29	0.93	0.10	48,53,56,58	0
28	DMU	M	526	33/33	0.93	0.10	39,47,65,67	0
22	CHD	C	525	29/29	0.94	0.08	28,33,40,45	0
24	PEK	C	264	53/53	0.95	0.11	29,47,73,75	0
22	CHD	O	229	29/29	0.95	0.08	23,31,37,37	0
22	CHD	P	1525	29/29	0.95	0.08	29,36,42,44	0
24	PEK	P	1264	53/53	0.95	0.12	29,48,75,78	0
20	PGV	C	267	51/51	0.96	0.10	25,36,67,70	0
22	CHD	B	1086	29/29	0.96	0.06	26,30,37,47	0
20	PGV	N	1266	51/51	0.96	0.10	31,42,67,71	0
20	PGV	P	1267	51/51	0.97	0.09	28,40,72,79	0
20	PGV	A	522	51/51	0.97	0.09	25,39,65,66	0
15	PER	N	520	2/2	0.97	0.08	31,31,31,34	0

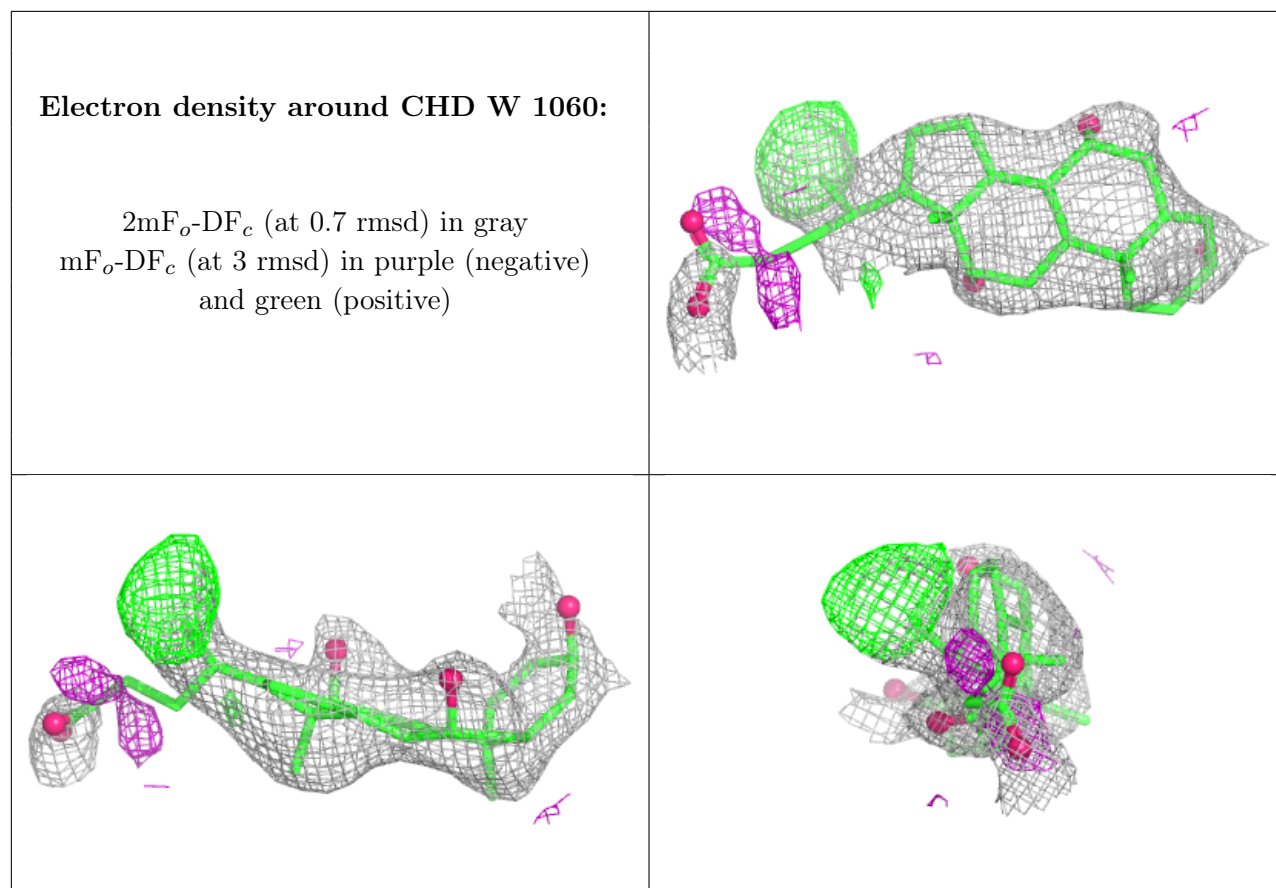
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
18	HEA	N	516	60/60	0.98	0.07	26,32,39,41	0
15	PER	A	520	2/2	0.98	0.05	25,25,25,32	0
16	MG	N	1518	1/1	0.98	0.04	34,34,34,34	0
21	CUA	O	228	2/2	0.98	0.04	36,36,36,37	0
18	HEA	N	515	60/60	0.98	0.07	23,32,51,54	0
18	HEA	A	515	60/60	0.99	0.06	19,26,50,53	0
27	ZN	S	99	1/1	0.99	0.03	38,38,38,38	0
18	HEA	A	516	60/60	0.99	0.05	20,26,33,36	0
21	CUA	B	228	2/2	0.99	0.03	27,27,27,30	0
16	MG	A	518	1/1	0.99	0.03	27,27,27,27	0
14	CU	N	517	1/1	0.99	0.04	32,32,32,32	0
27	ZN	F	99	1/1	1.00	0.01	34,34,34,34	0
14	CU	A	517	1/1	1.00	0.02	29,29,29,29	0

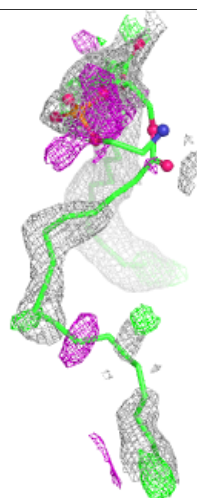
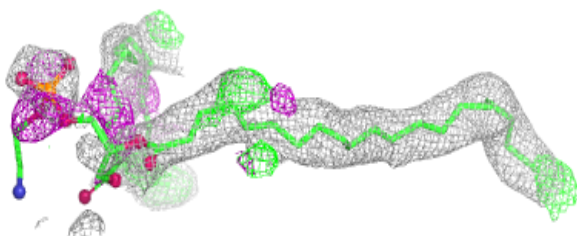
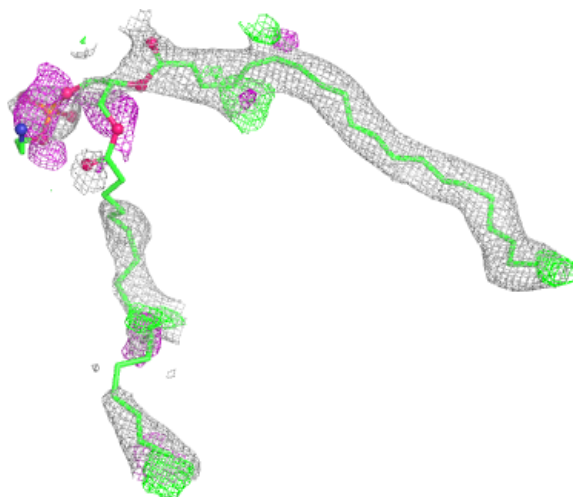
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

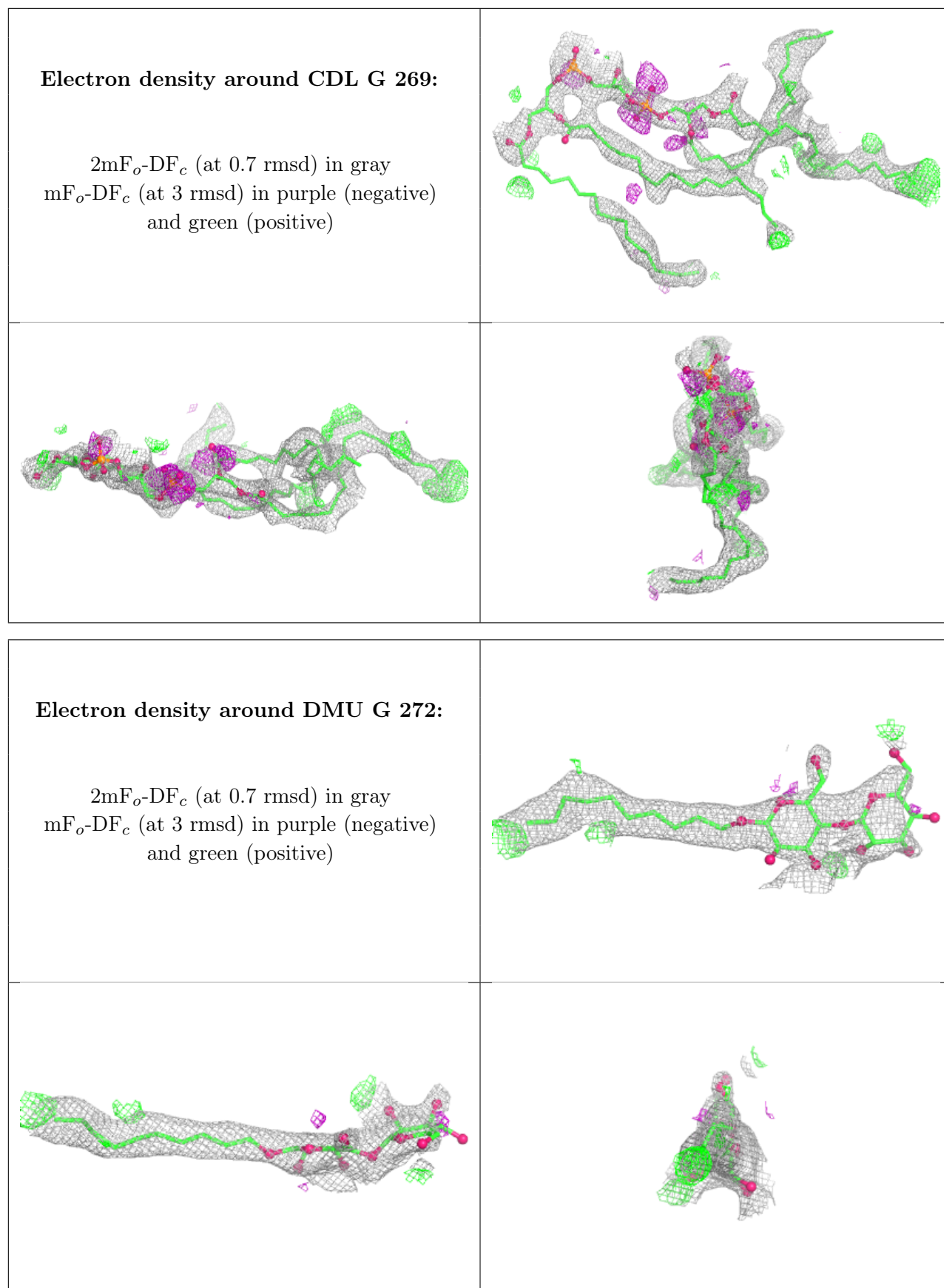


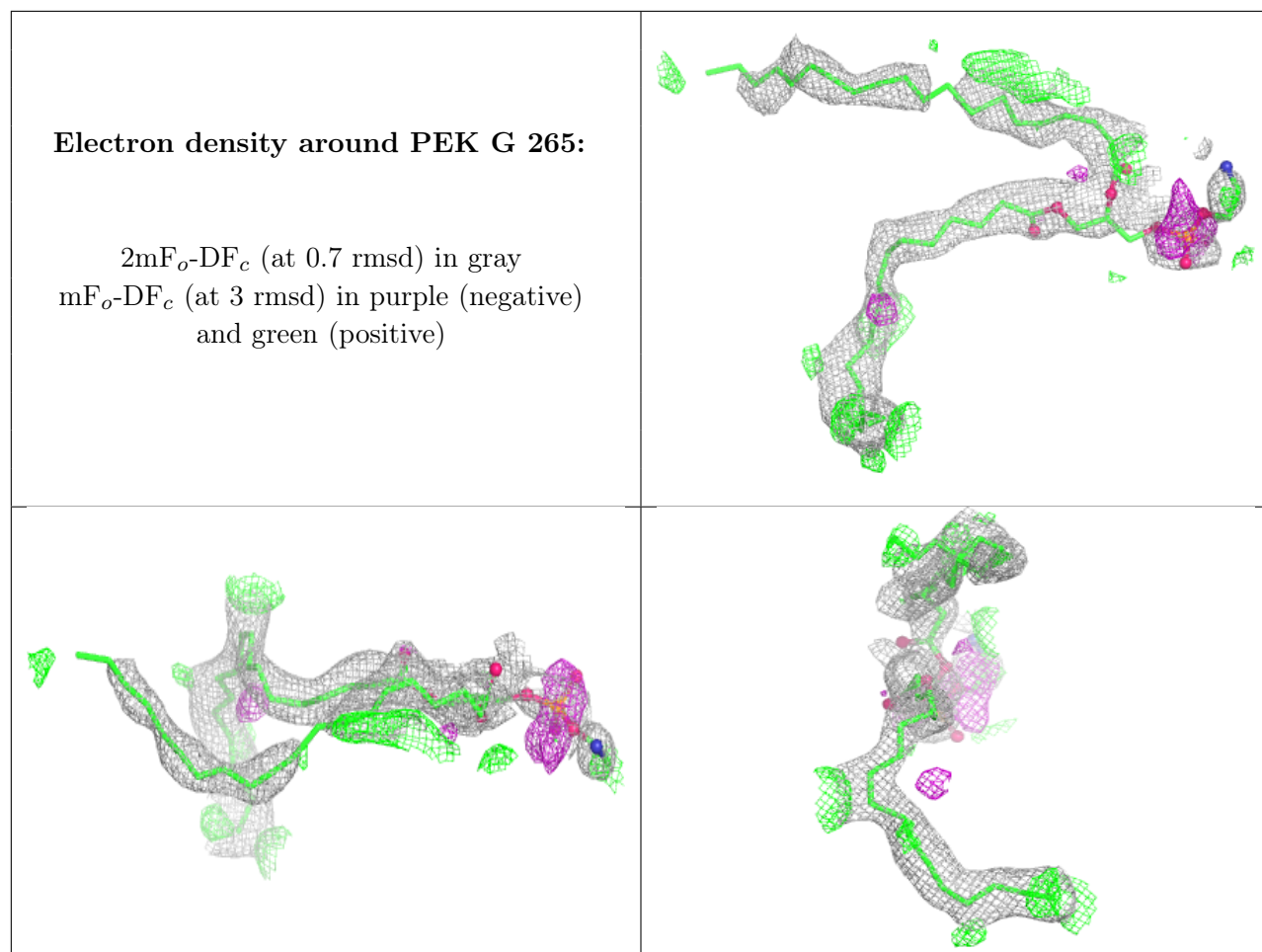


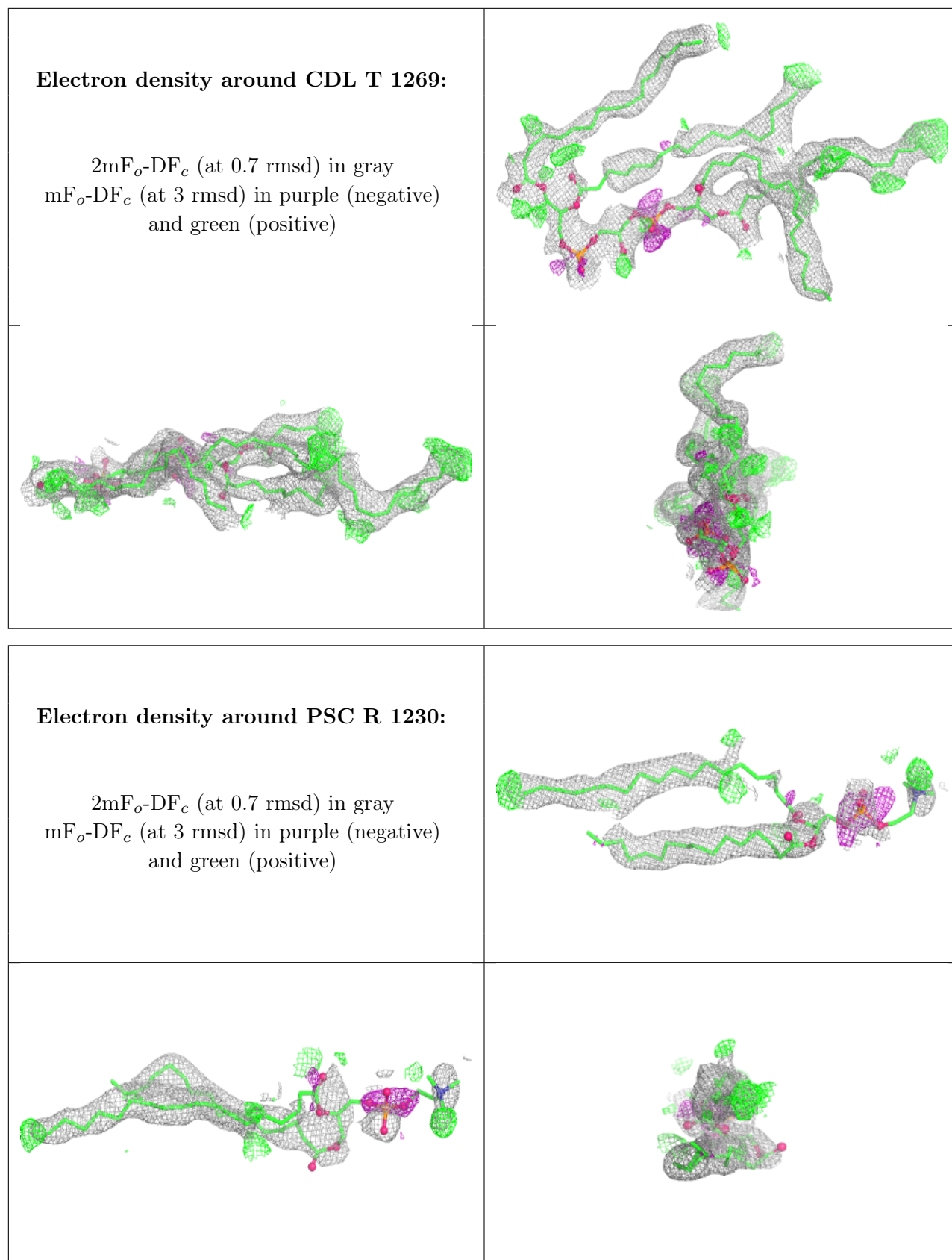
Electron density around PEK T 263:

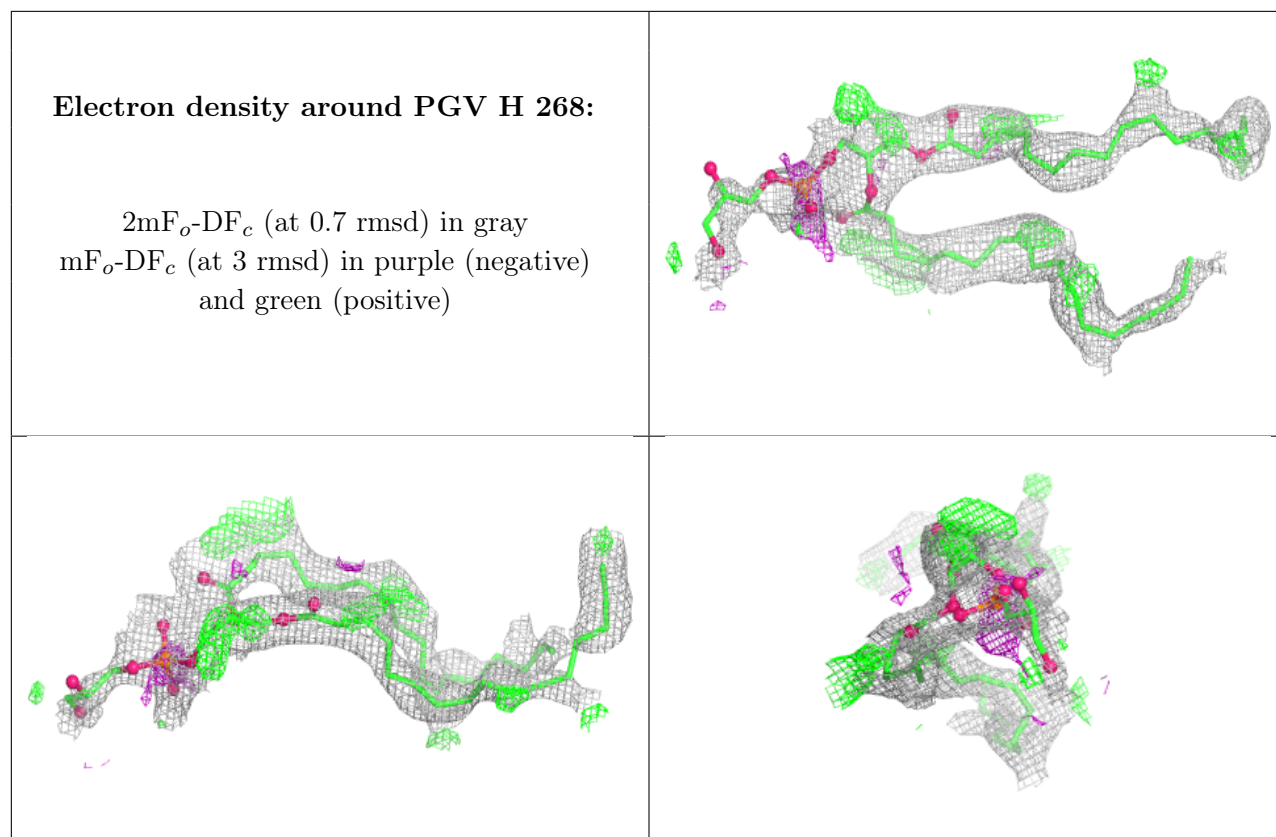
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





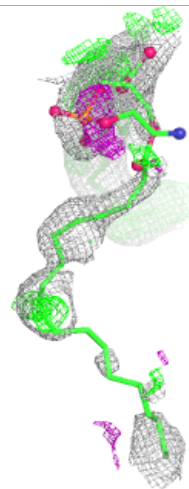
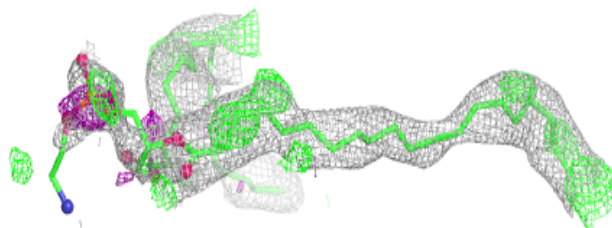
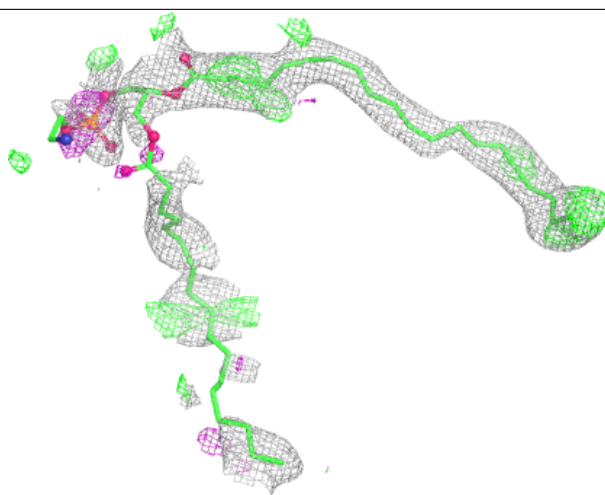


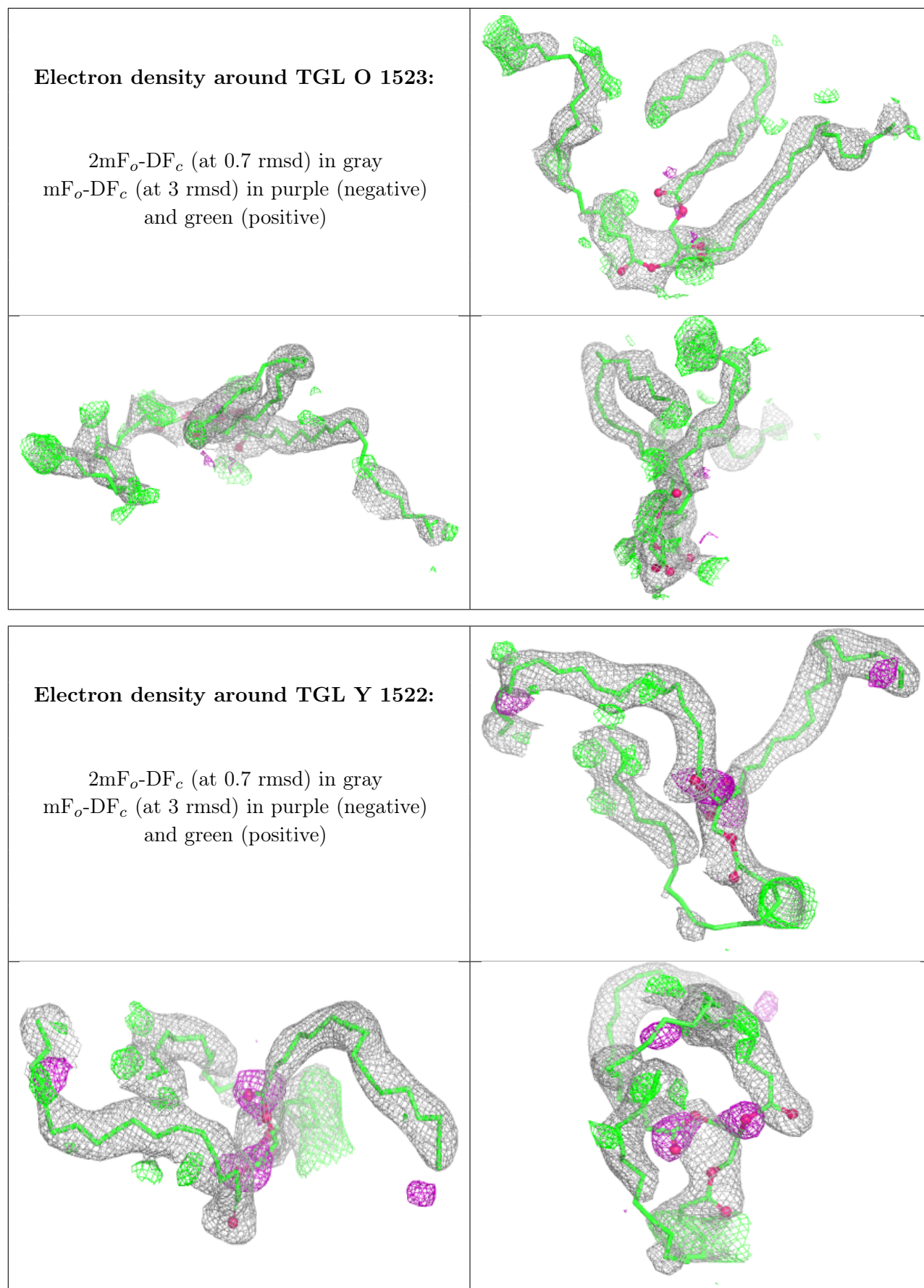


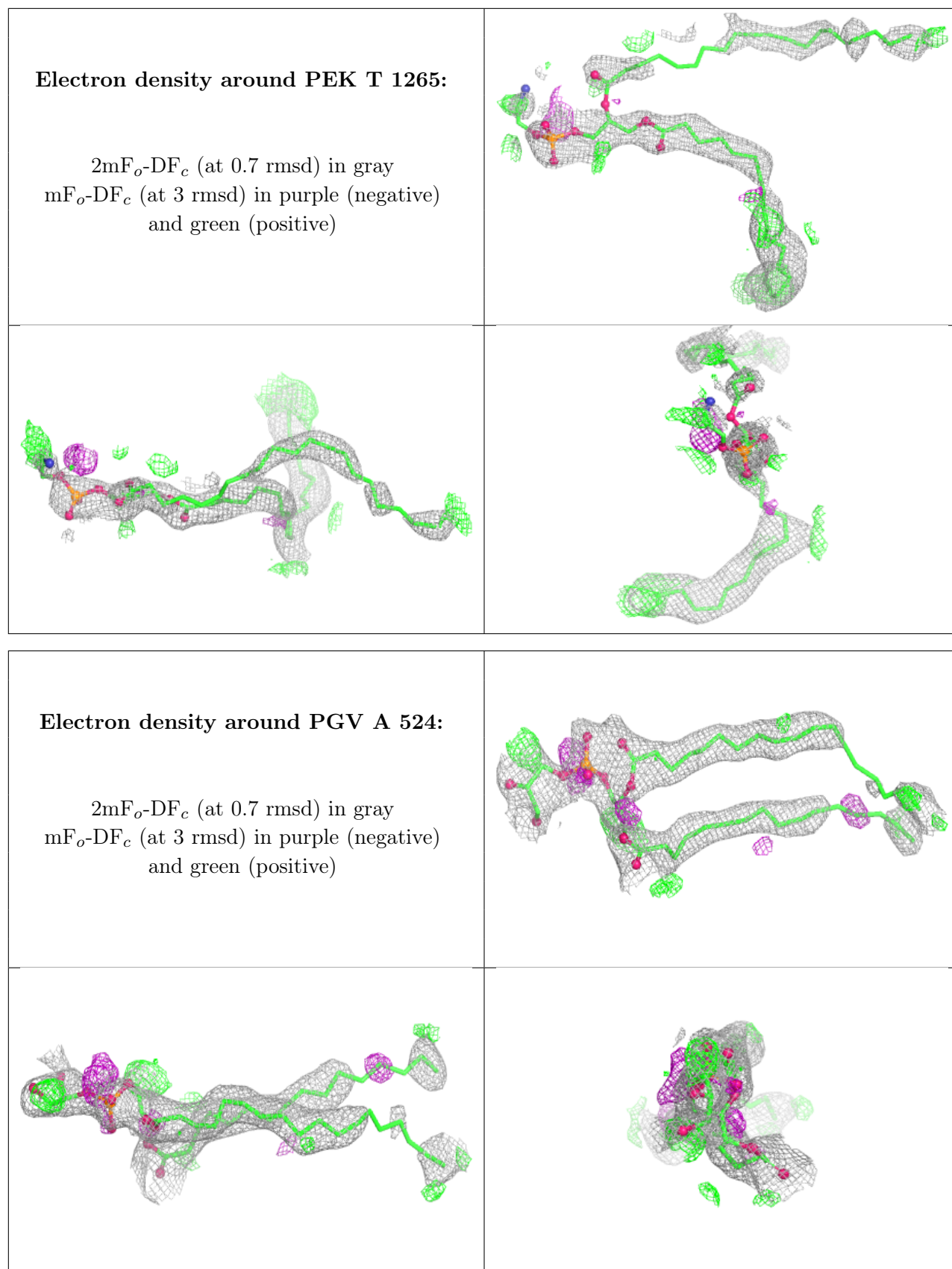


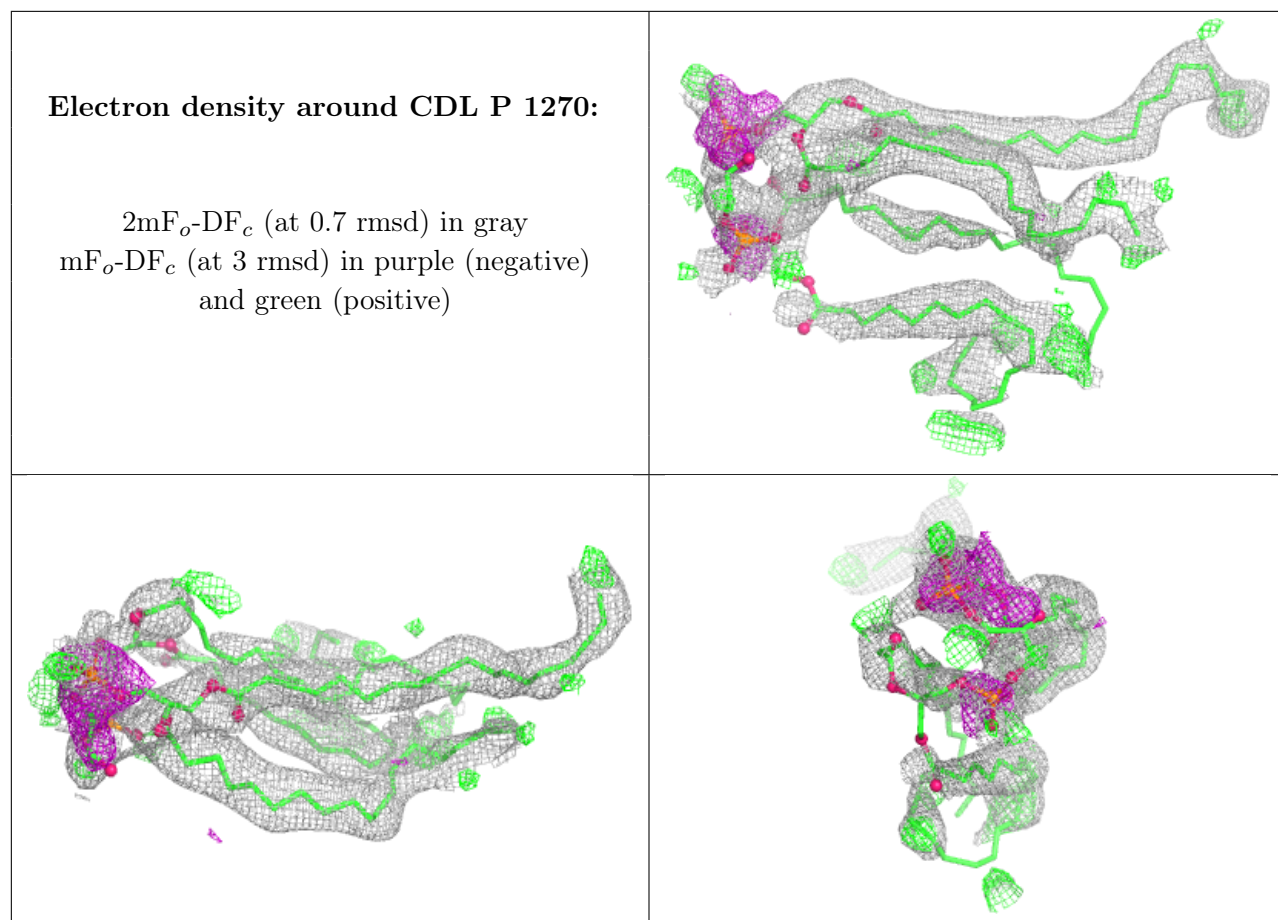
Electron density around PEK G 1263:

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



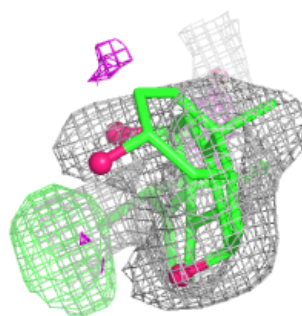
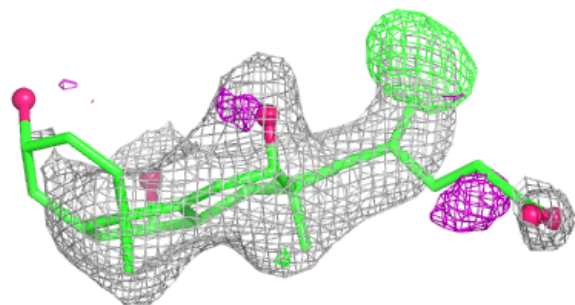
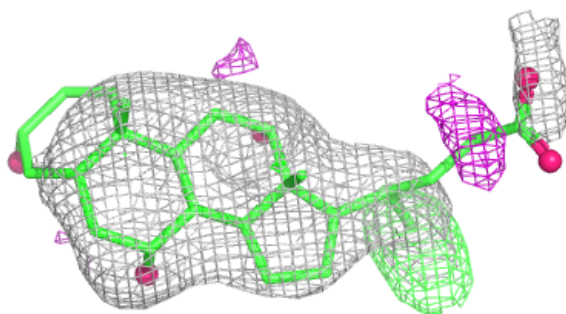




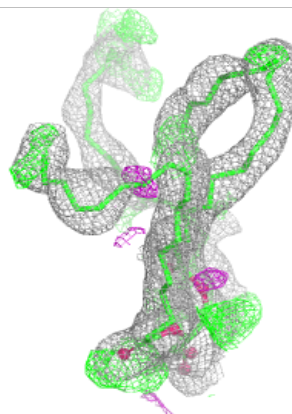
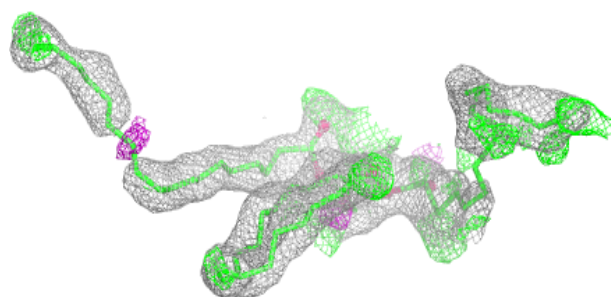
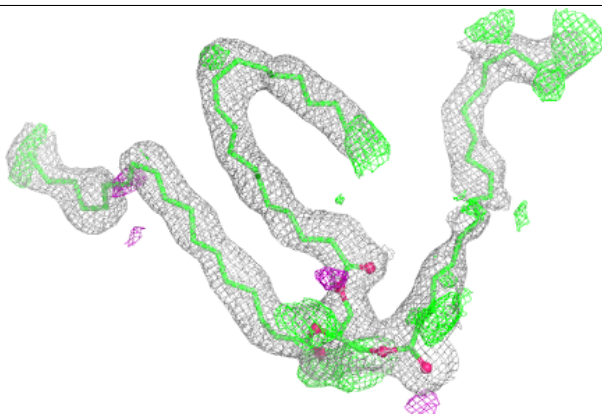


Electron density around CHD J 60:

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and green (positive)

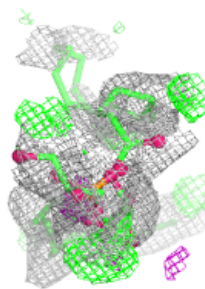
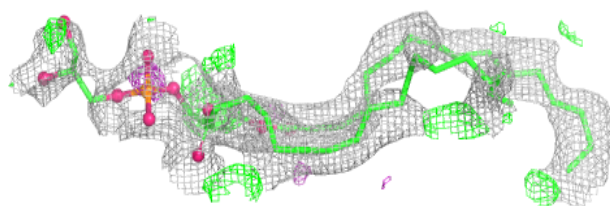
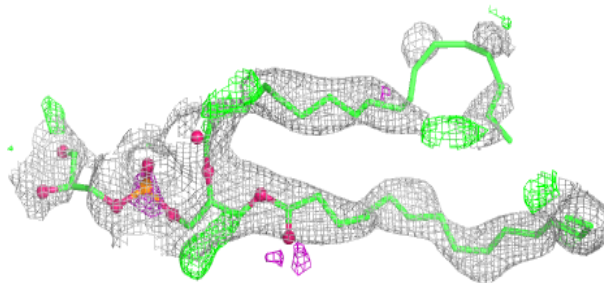
**Electron density around TGL D 523:**

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



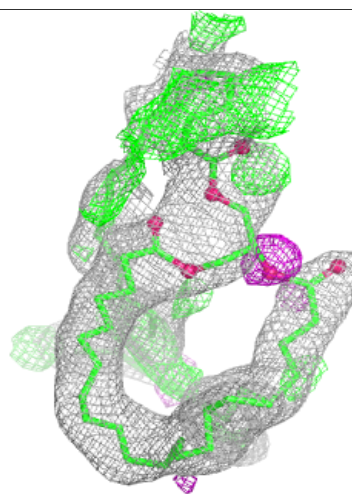
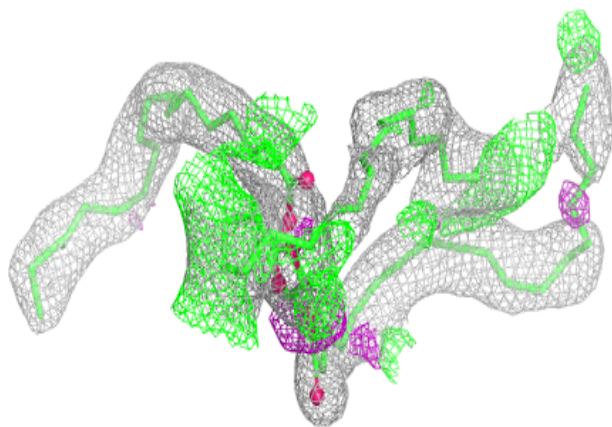
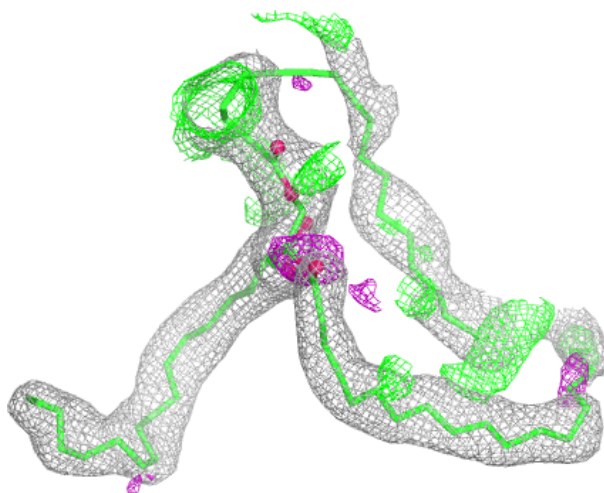
Electron density around PGV N 1268:

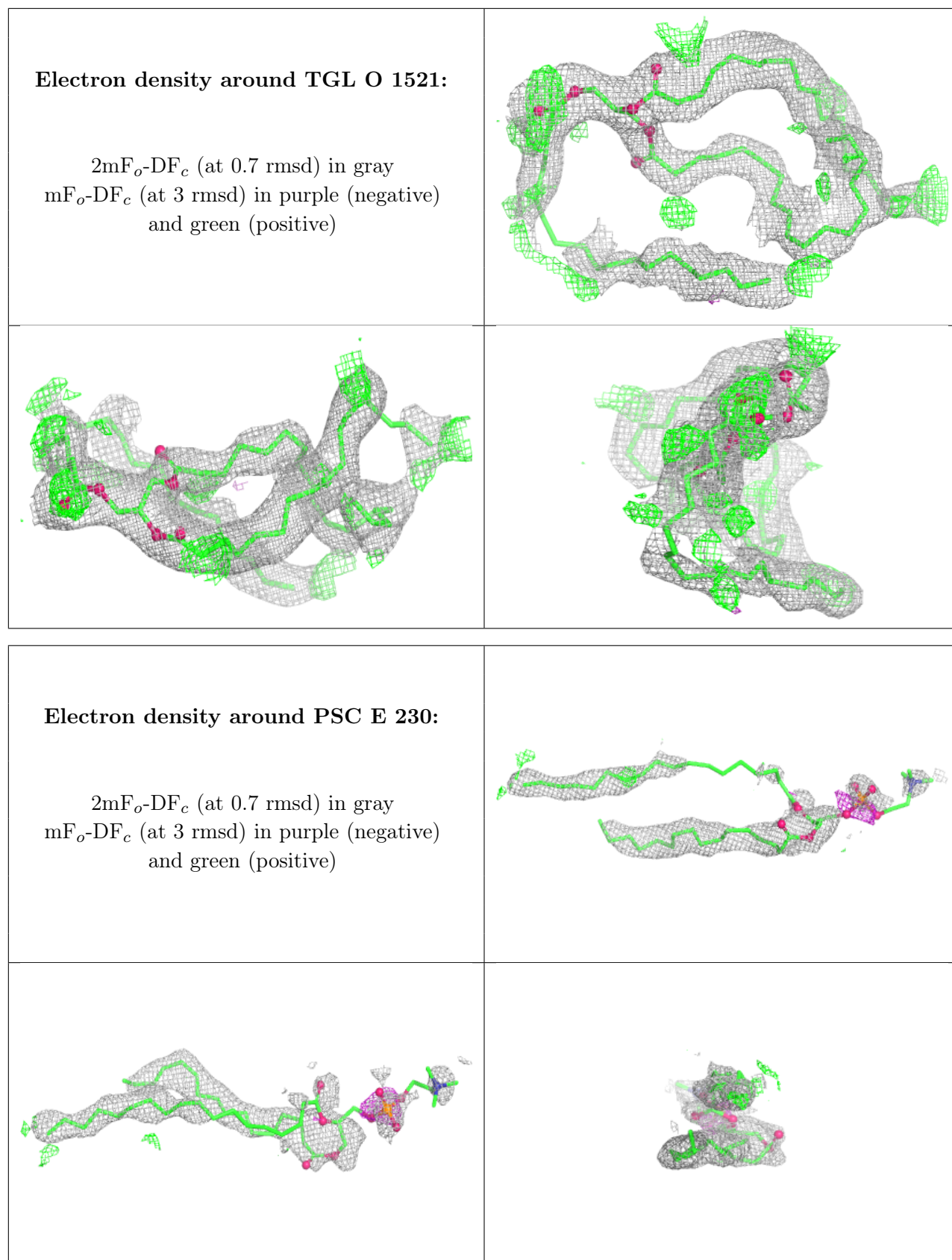
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

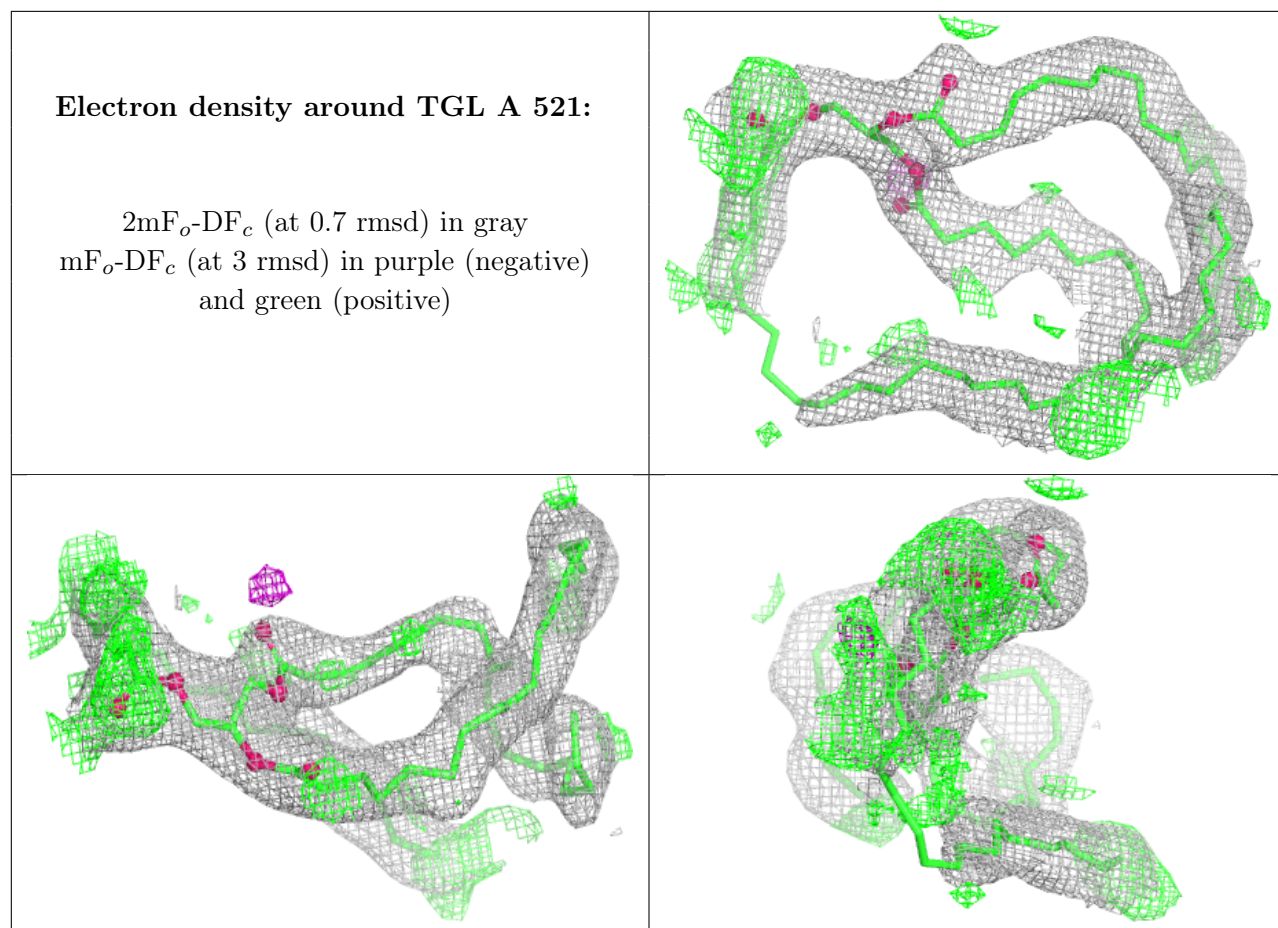


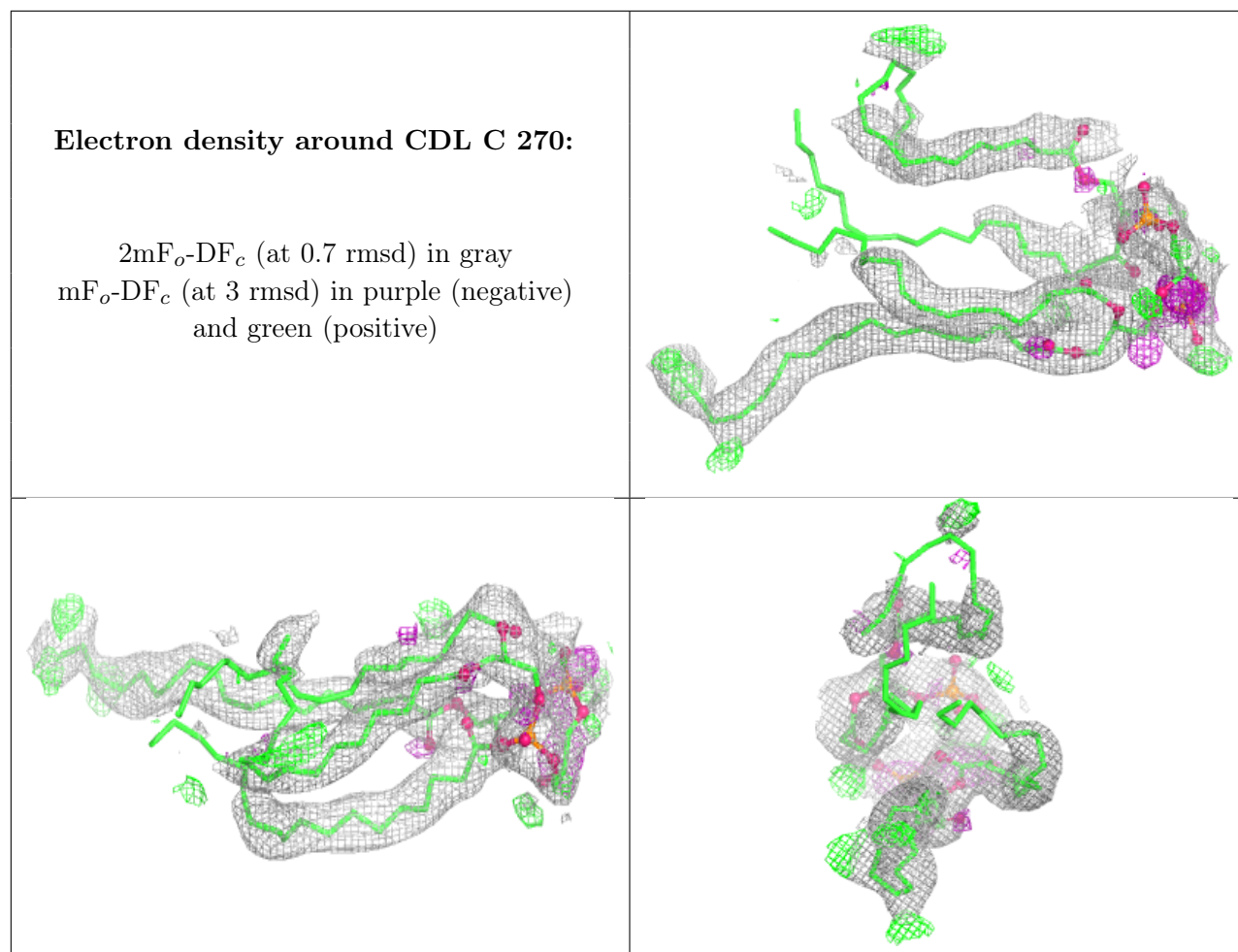
Electron density around TGL L 522:

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



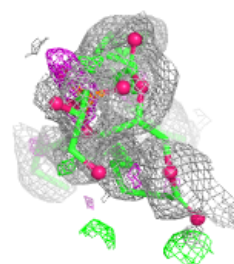
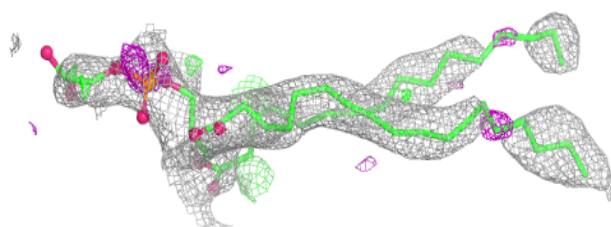
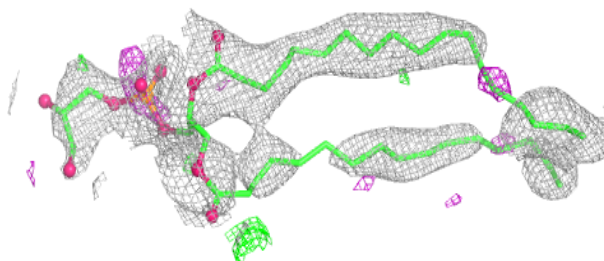




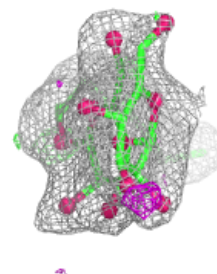
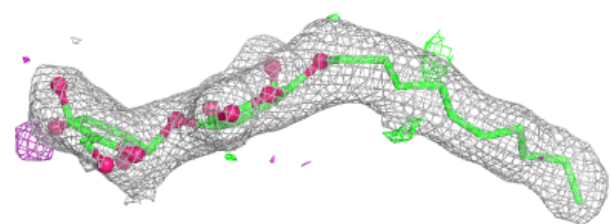
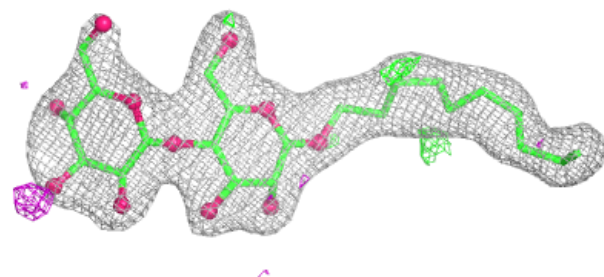


Electron density around PGV N 1524:

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

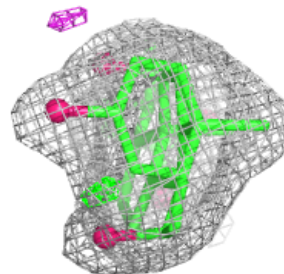
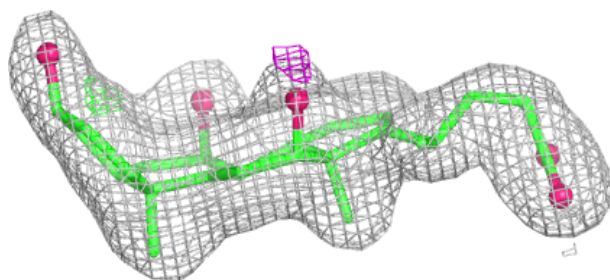
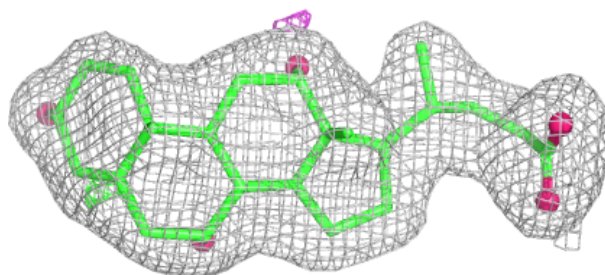
**Electron density around DMU Z 1526:**

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

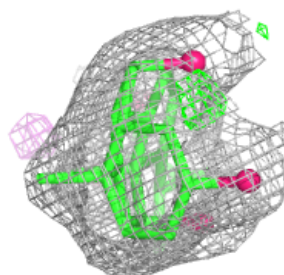
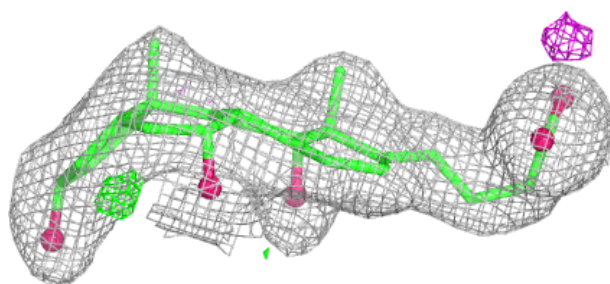
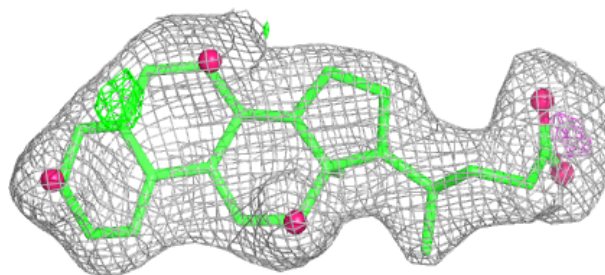


Electron density around CHD C 271:

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

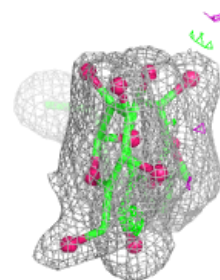
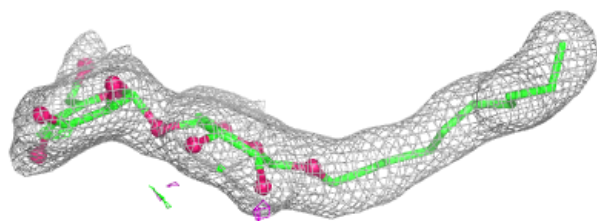
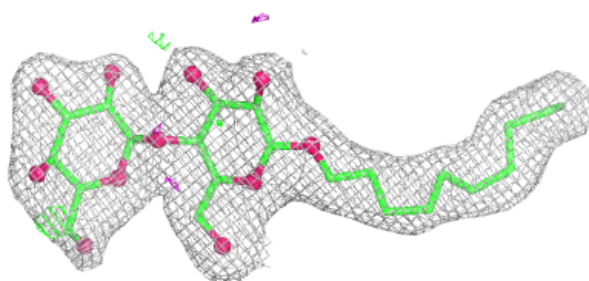
**Electron density around CHD P 1271:**

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

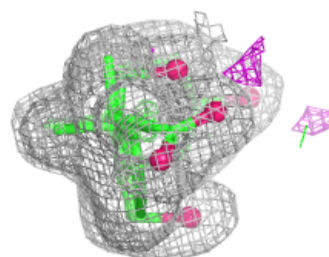
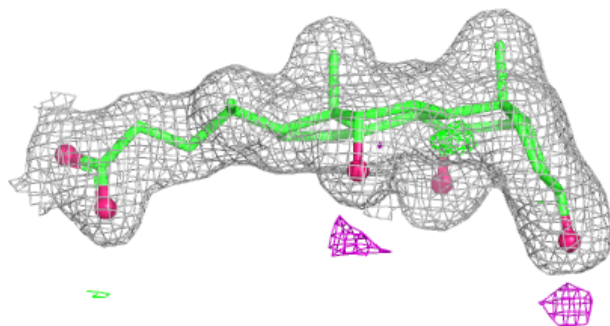
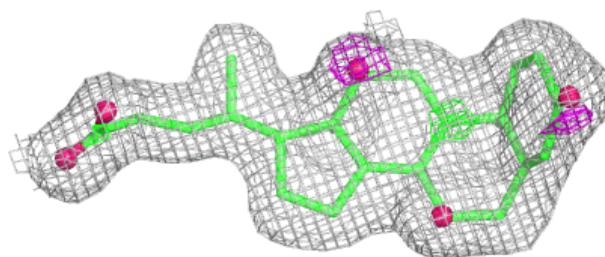


Electron density around DMU M 526:

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

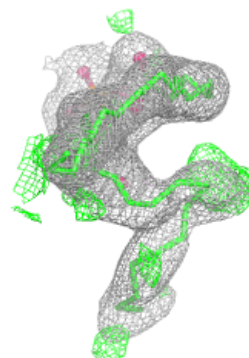
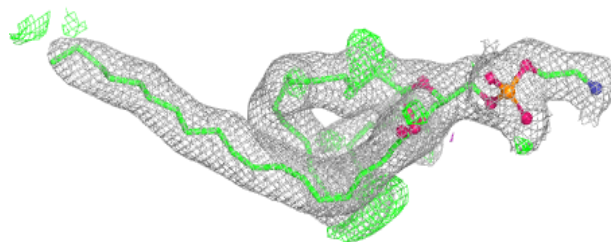
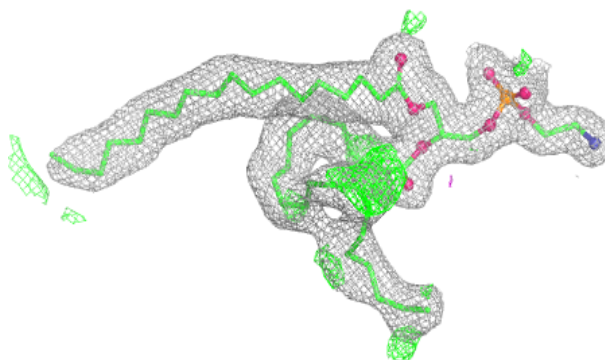
**Electron density around CHD C 525:**

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

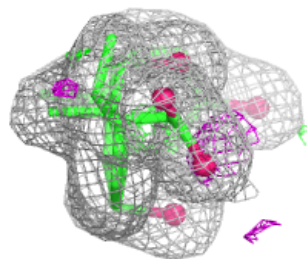
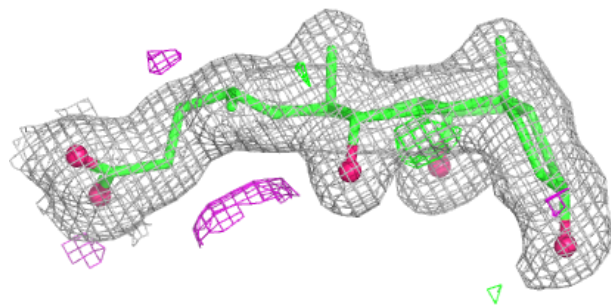
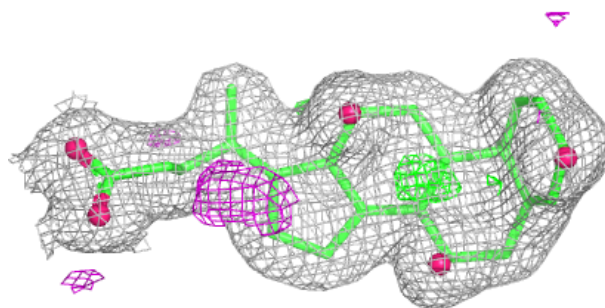


Electron density around PEK C 264:

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

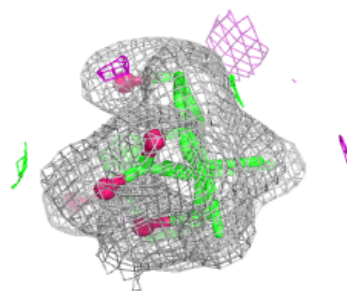
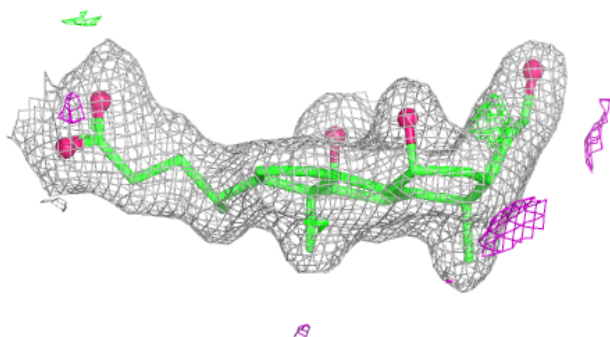
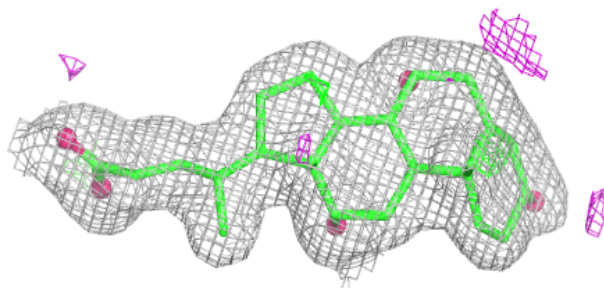
**Electron density around CHD O 229:**

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

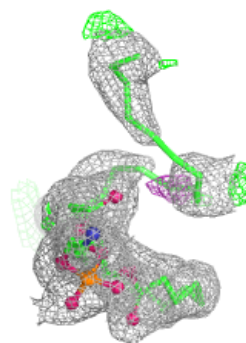
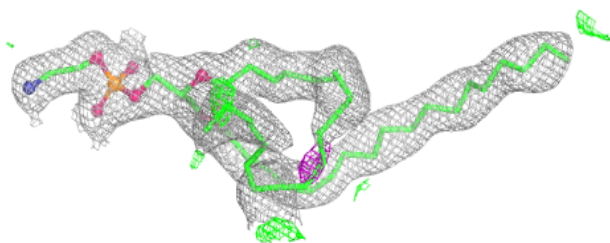
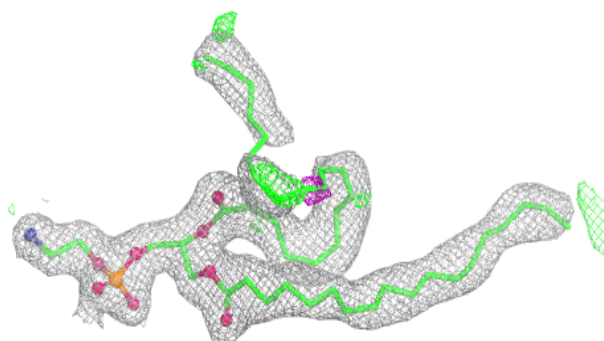


Electron density around CHD P 1525:

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

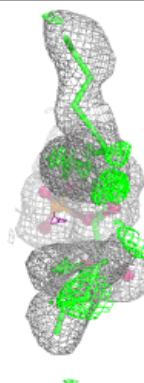
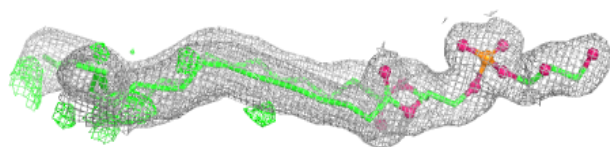
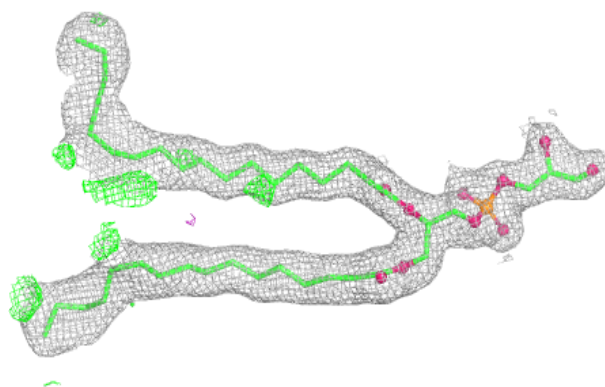
**Electron density around PEK P 1264:**

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

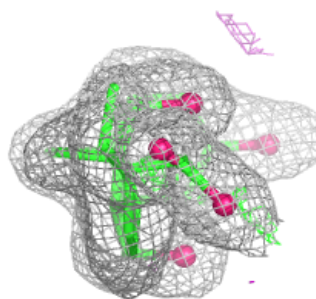
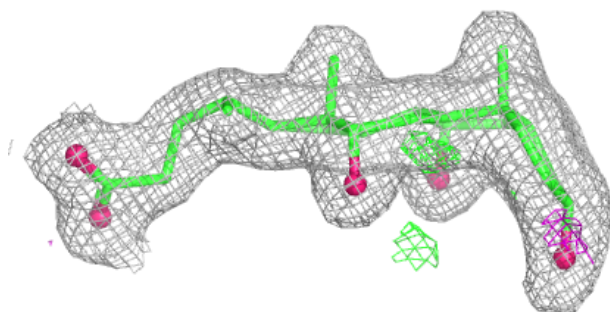
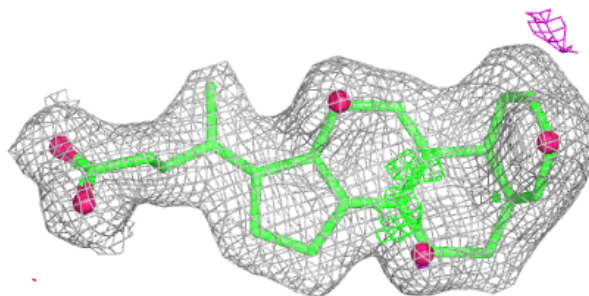


Electron density around PGV C 267:

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

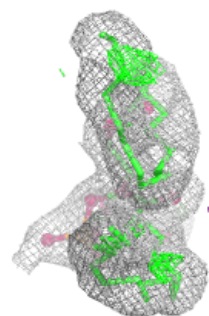
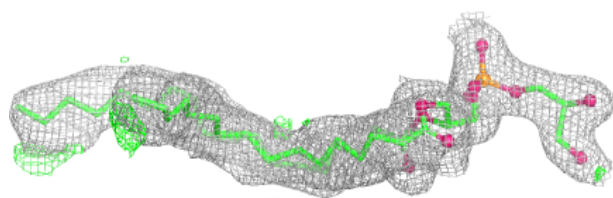
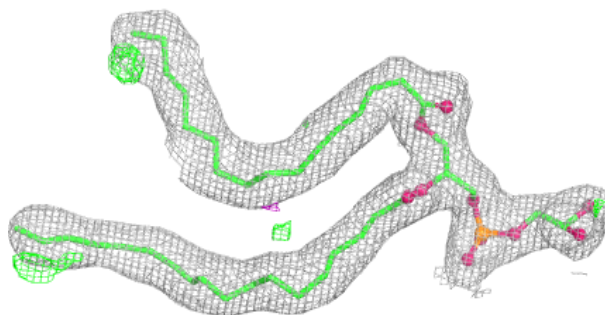
**Electron density around CHD B 1086:**

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

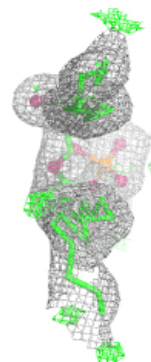
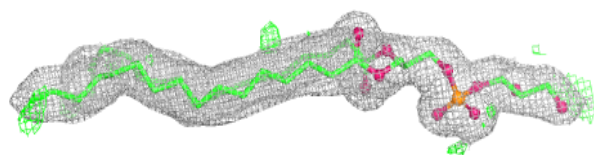
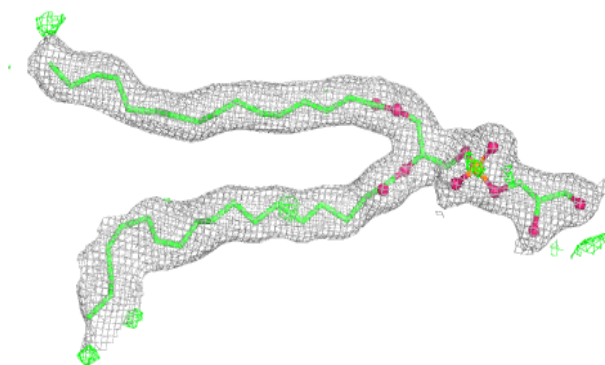


Electron density around PGV N 1266:

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

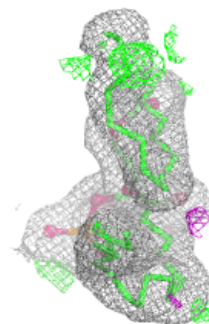
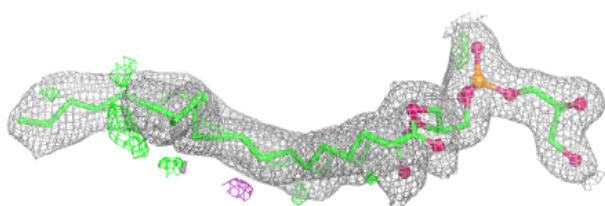
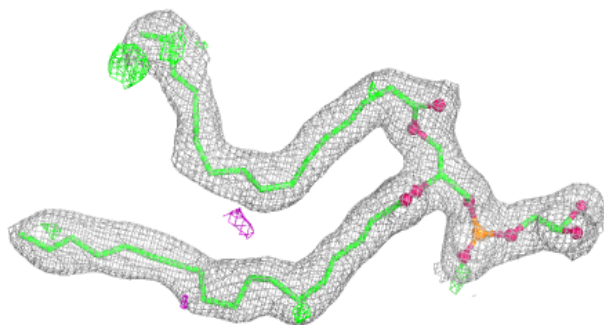
**Electron density around PGV P 1267:**

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

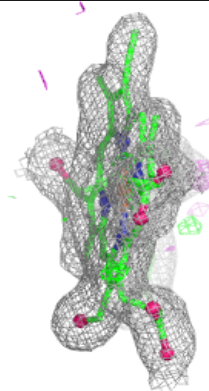
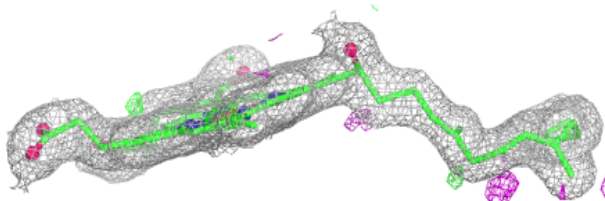
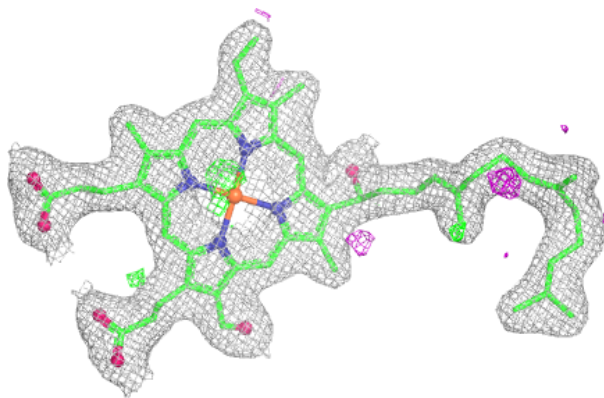


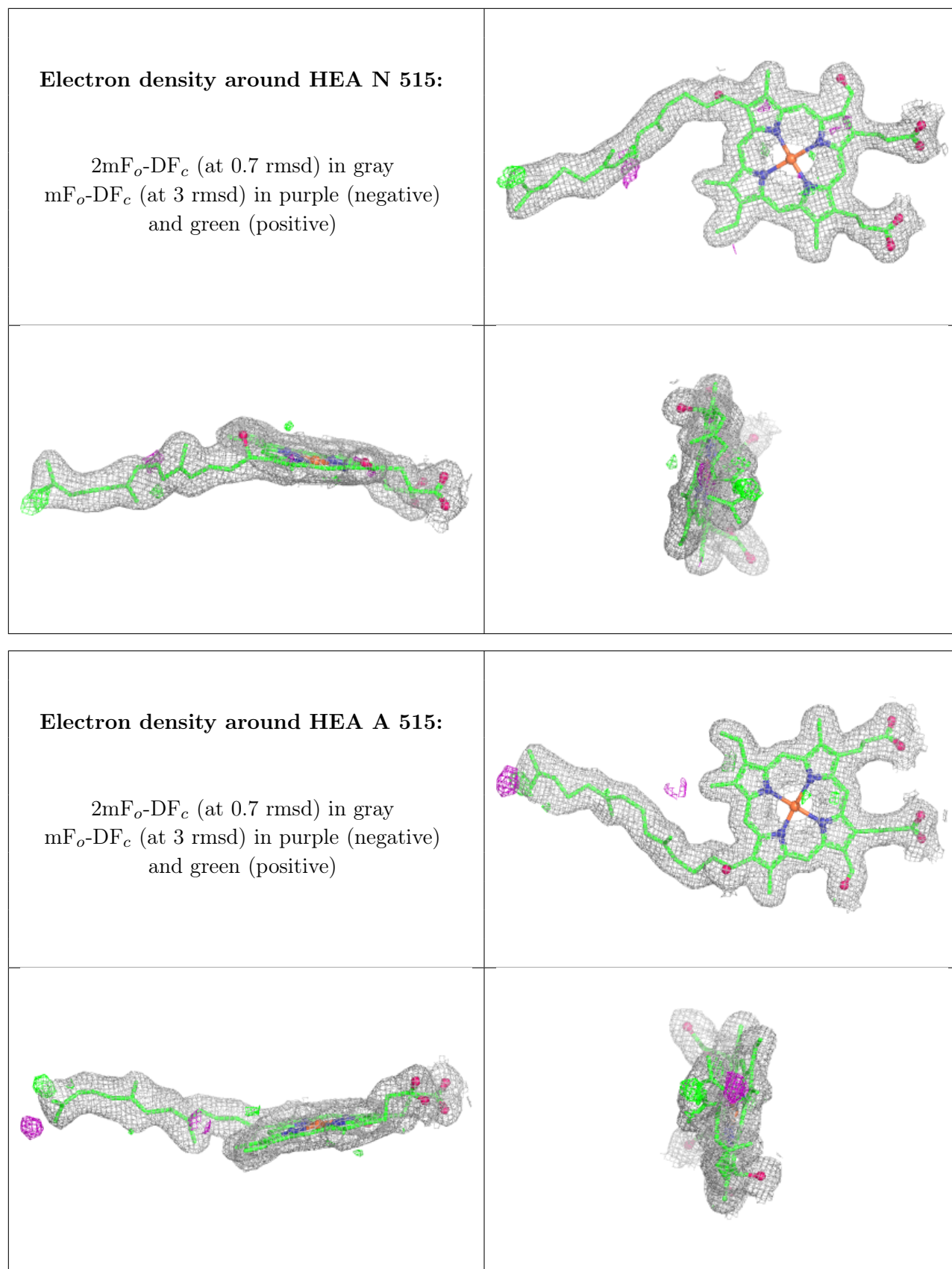
Electron density around PGV A 522:

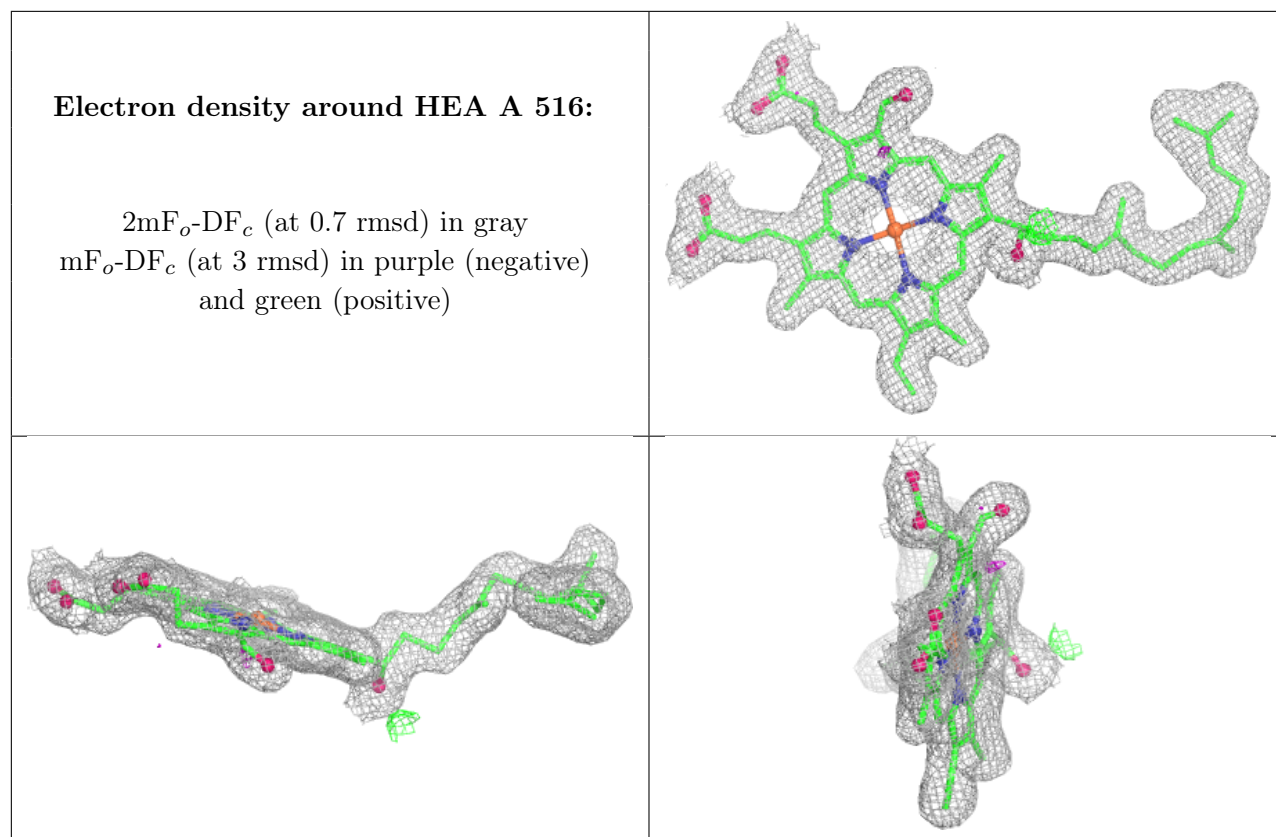
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around HEA N 516:**

$2mF_o-DF_c$ (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.