



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 07:54 PM EDT

PDB ID : 3AG1 / pdb_00003ag1
Title : Bovine Heart Cytochrome c Oxidase in the Carbon Monoxide-bound Fully Reduced State at 280 K
Authors : Muramoto, K.; Ohta, K.; Shinzawa-Itoh, K.; Kanda, K.; Taniguchi, M.; Nabekura, H.; Yamashita, E.; Tsukihara, T.; Yoshikawa, S.
Deposited on : 2010-03-19
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

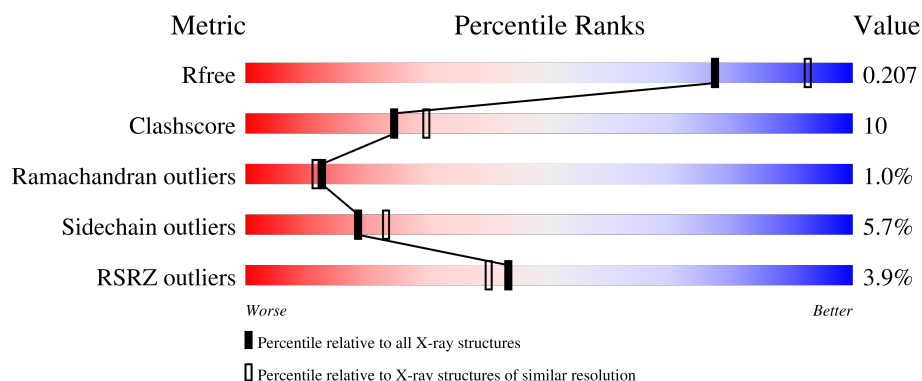
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



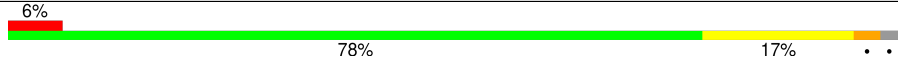
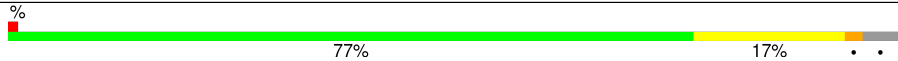
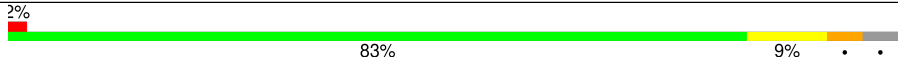
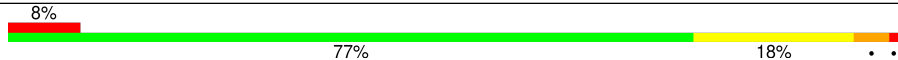
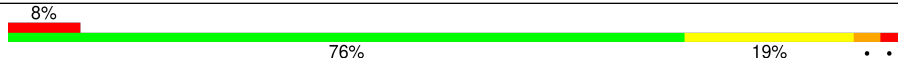
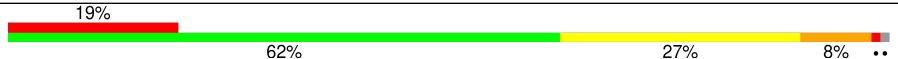
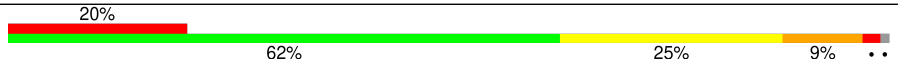
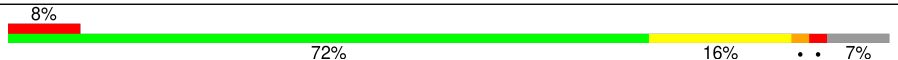
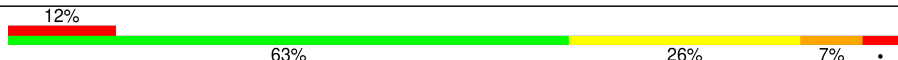
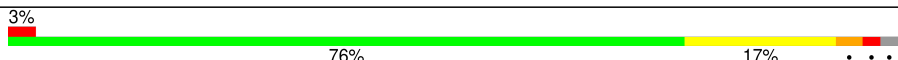
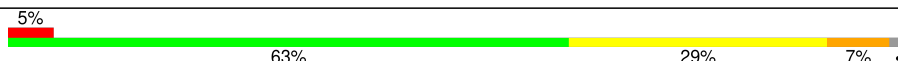
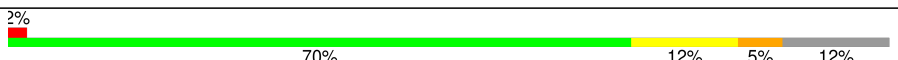
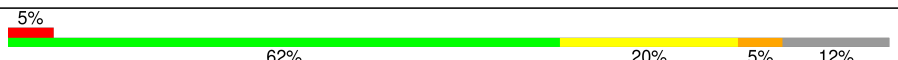
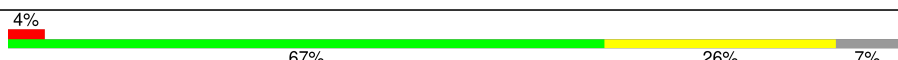
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	514	
1	N	514	
2	B	227	
2	O	227	

Continued on next page...

Continued from previous page...

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CHD	B	1085	X	-	-	-
23	CHD	C	271	X	-	-	-
23	CHD	J	60	X	-	-	-
23	CHD	O	229	X	-	-	-
23	CHD	P	1271	X	-	-	-
23	CHD	W	1059	X	-	-	-
24	UNX	C	262	-	-	-	X
24	UNX	P	262	-	-	-	X
25	CDL	C	270	-	-	X	-
25	CDL	G	269	-	-	X	-
25	CDL	T	1269	-	-	X	-
26	DMU	C	272	X	-	-	-
26	DMU	M	526	X	-	-	-
26	DMU	T	1272	X	-	-	-
26	DMU	Z	1526	X	-	-	-

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 32105 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			
9	V	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			

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

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

Continued on next page...

Continued from previous page...

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.

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			

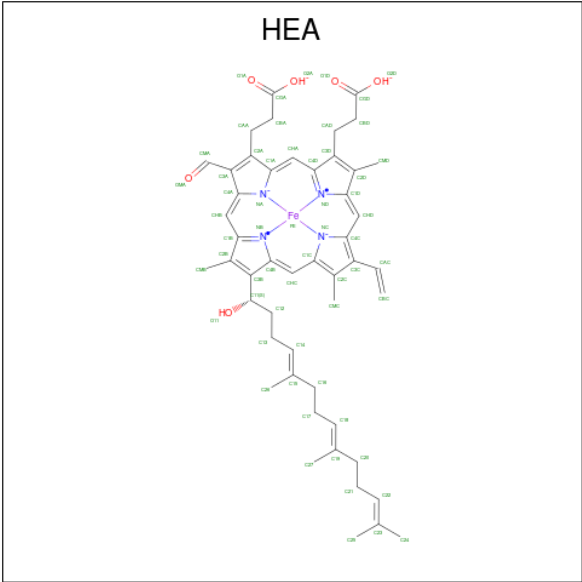
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C.

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.

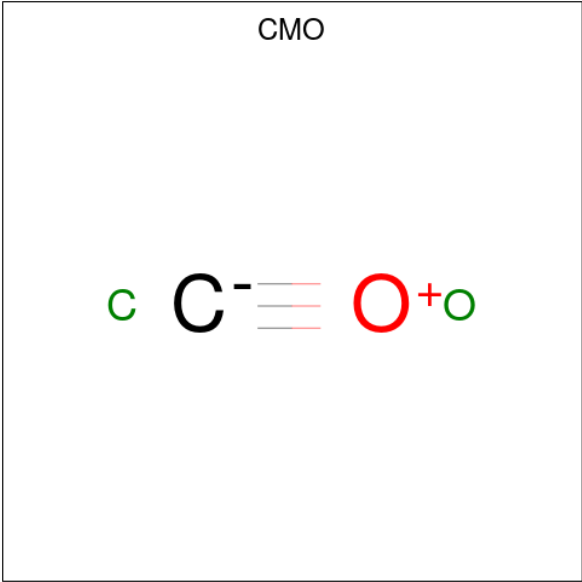
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	0	0
			335	223	53	59			
13	Z	43	Total	C	N	O	0	0	0
			335	223	53	59			

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



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 CARBON MONOXIDE (CCD ID: CMO) (formula: CO).



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

- Molecule 16 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

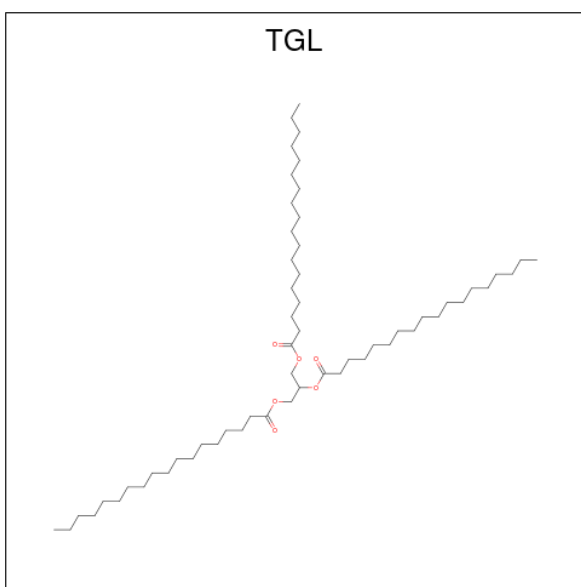
- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 18 is SODIUM ION (CCD ID: NA) (formula: Na).

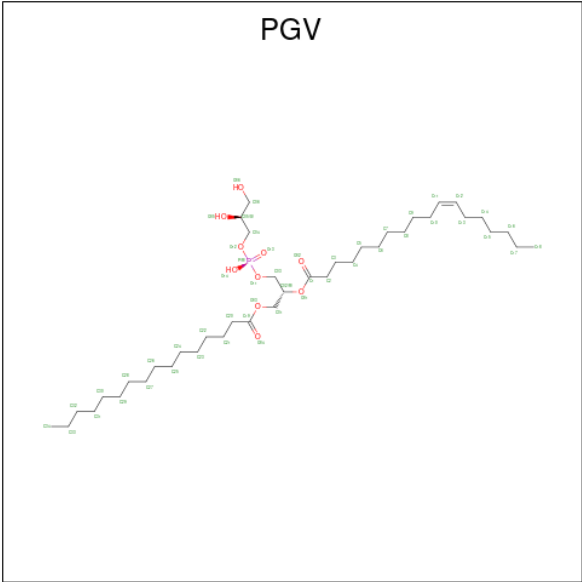
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total Na 1 1	0	0
18	N	1	Total Na 1 1	0	0

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



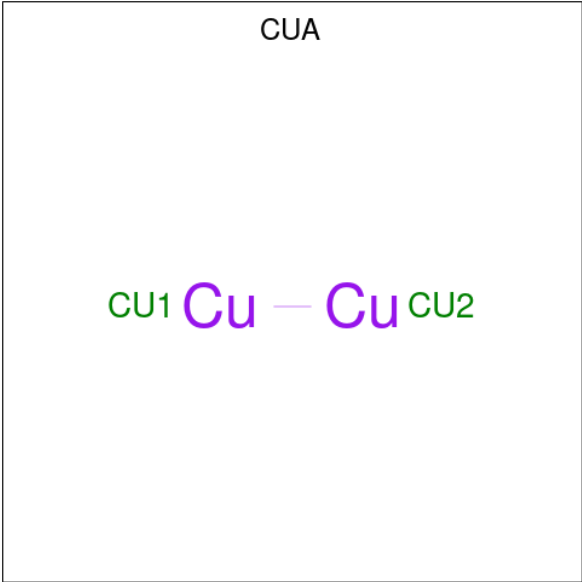
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	C	O	0	0
			63	57	6		
19	B	1	Total	C	O	0	0
			63	57	6		
19	L	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		

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



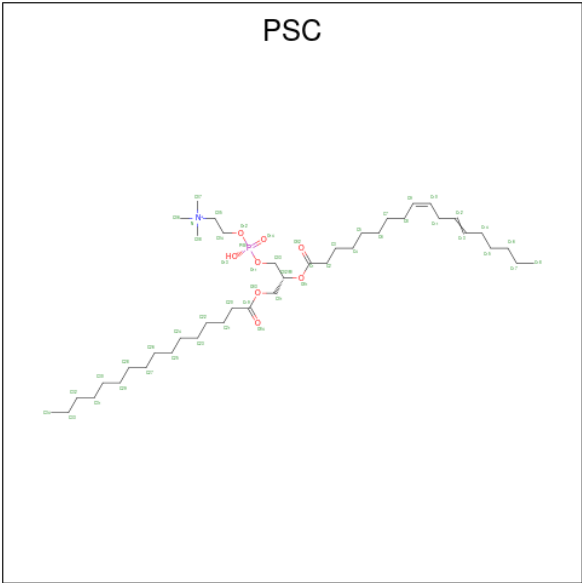
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0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

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



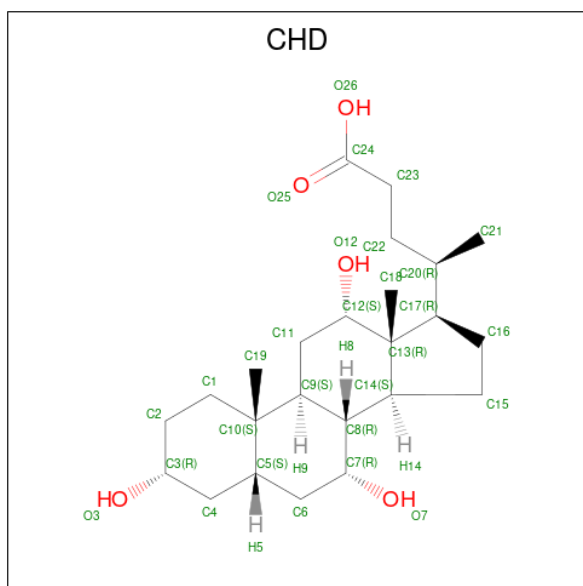
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

Continued on next page...

Continued from previous page...

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

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

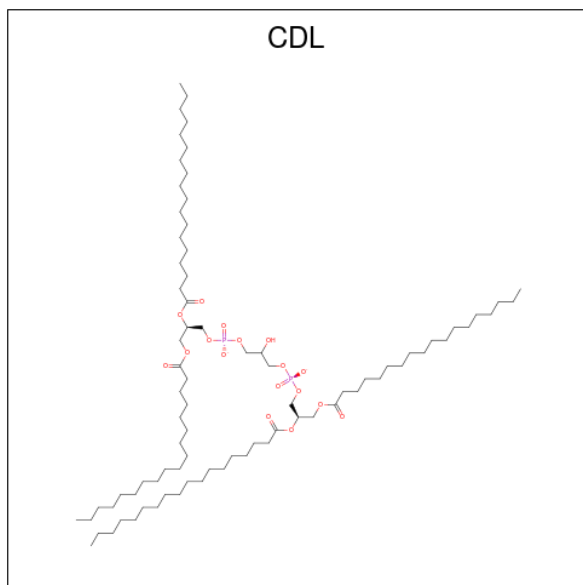


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	B	1	Total	C	O	0	0
			29	24	5		
23	C	1	Total	C	O	0	0
			29	24	5		
23	C	1	Total	C	O	0	0
			29	24	5		
23	J	1	Total	C	O	0	0
			29	24	5		
23	O	1	Total	C	O	0	0
			29	24	5		
23	P	1	Total	C	O	0	0
			29	24	5		
23	P	1	Total	C	O	0	0
			29	24	5		
23	W	1	Total	C	O	0	0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

- Molecule 24 is UNKNOWN LIGAND (CCD ID: UNX) (formula: X).

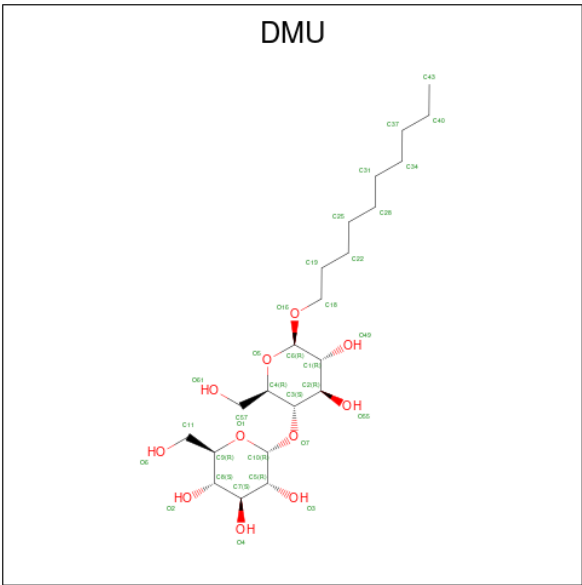
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	C	1	Total X 1 1	0	0
24	P	1	Total X 1 1	0	0

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



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

- Molecule 26 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: $C_{22}H_{42}O_{11}$).

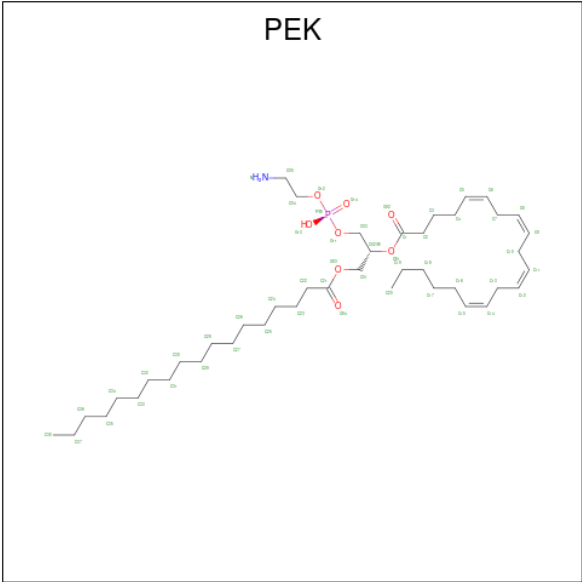


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	C	1	Total	C	O	0	0
			33	22	11		
26	M	1	Total	C	O	0	0
			33	22	11		
26	T	1	Total	C	O	0	0
			33	22	11		
26	Z	1	Total	C	O	0	0
			33	22	11		

- 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 (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
28	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	S	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 29 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	A	205	Total	O	0	0
			205	205		
29	B	121	Total	O	0	0
			121	121		
29	C	80	Total	O	0	0
			80	80		
29	D	75	Total	O	0	0
			75	75		
29	E	39	Total	O	0	0
			39	39		
29	F	70	Total	O	0	0
			70	70		

Continued on next page...

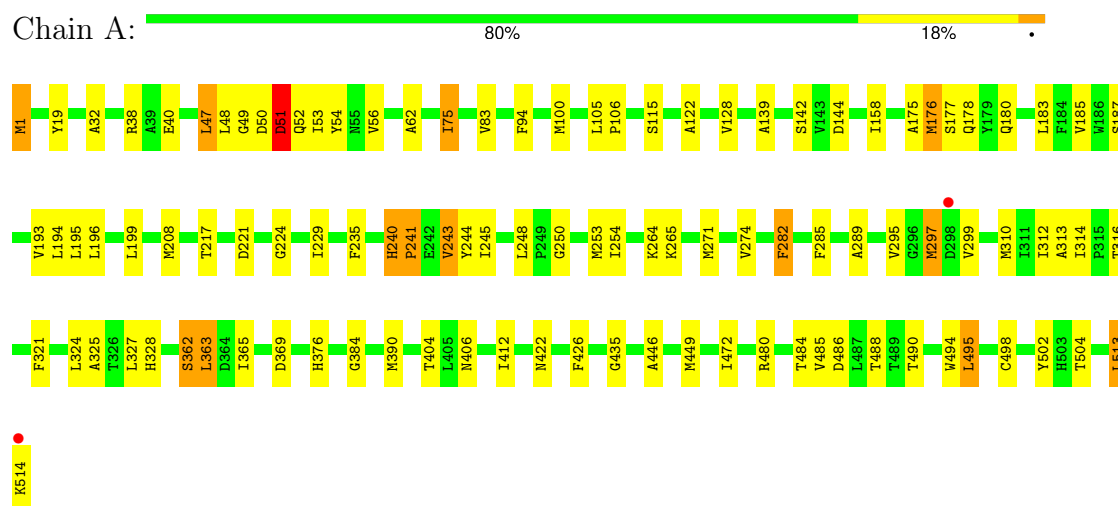
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	G	42	Total 42	O 42	0	0
29	H	33	Total 33	O 33	0	0
29	I	24	Total 24	O 24	0	0
29	J	9	Total 9	O 9	0	0
29	K	17	Total 17	O 17	0	0
29	L	20	Total 20	O 20	0	0
29	M	15	Total 15	O 15	0	0
29	N	184	Total 184	O 184	0	0
29	O	97	Total 97	O 97	0	0
29	P	81	Total 81	O 81	0	0
29	Q	47	Total 47	O 47	0	0
29	R	27	Total 27	O 27	0	0
29	S	52	Total 52	O 52	0	0
29	T	37	Total 37	O 37	0	0
29	U	28	Total 28	O 28	0	0
29	V	17	Total 17	O 17	0	0
29	W	12	Total 12	O 12	0	0
29	X	12	Total 12	O 12	0	0
29	Y	16	Total 16	O 16	0	0
29	Z	9	Total 9	O 9	0	0

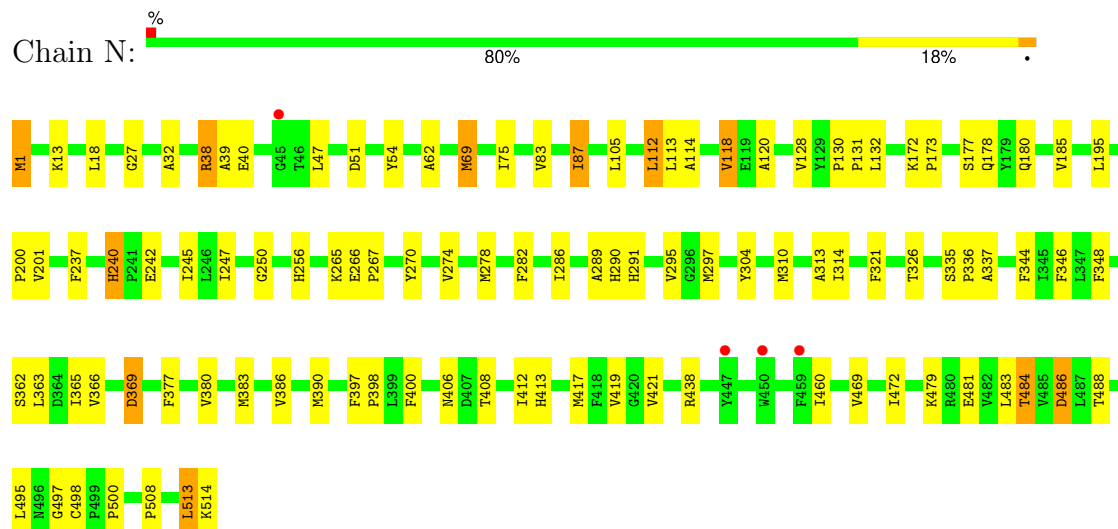
3 Residue-property plots

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

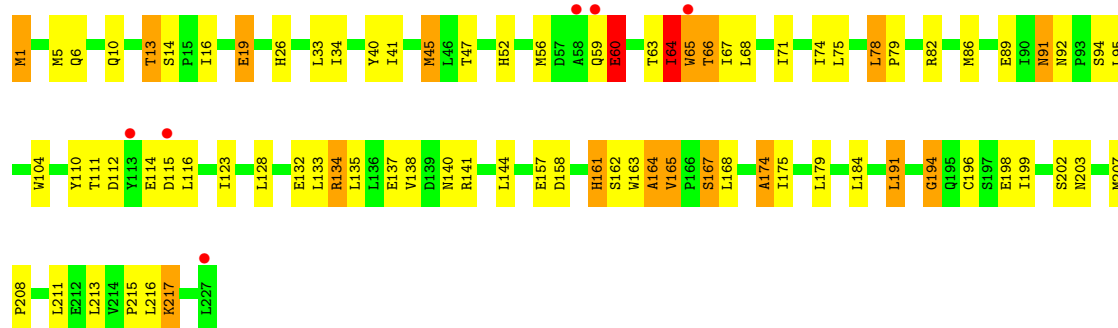


• Molecule 1: Cytochrome c oxidase subunit 1

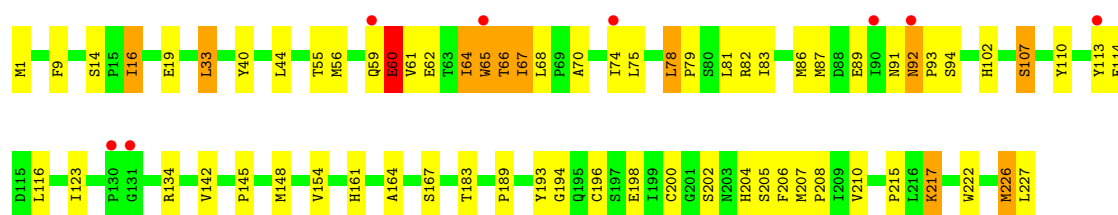


• Molecule 2: Cytochrome c oxidase subunit 2

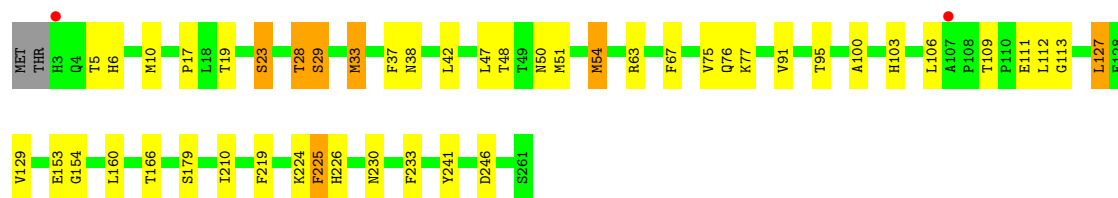
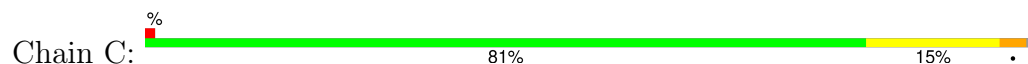




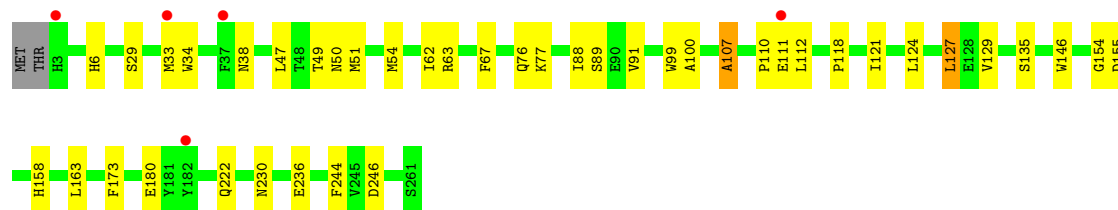
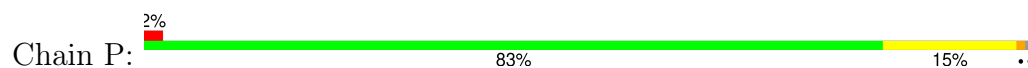
• Molecule 2: Cytochrome c oxidase subunit 2



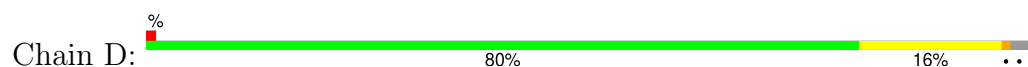
• Molecule 3: Cytochrome c oxidase subunit 3



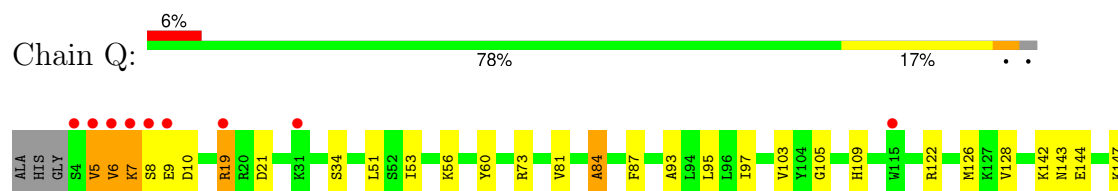
• Molecule 3: Cytochrome c oxidase subunit 3



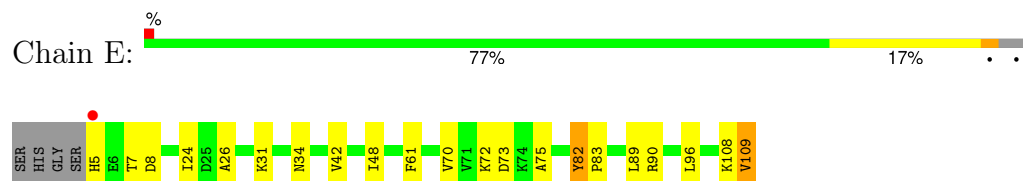
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



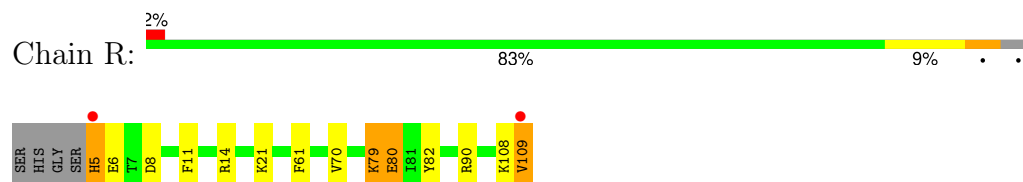
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



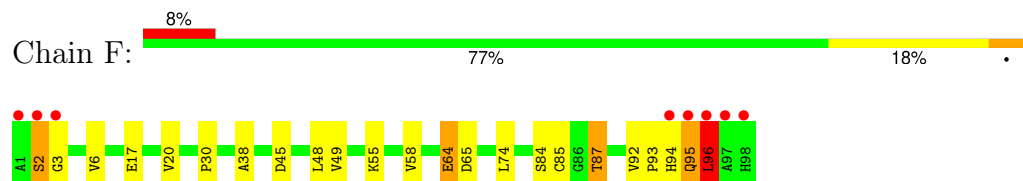
- Molecule 5: Cytochrome c oxidase subunit 5A



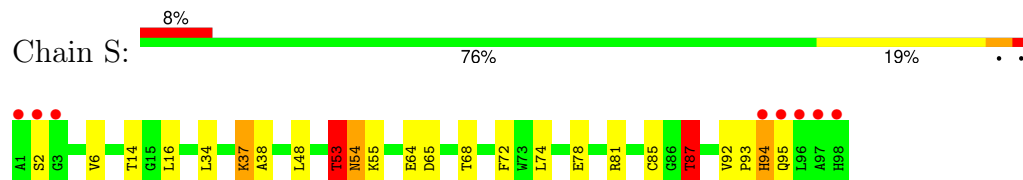
- Molecule 5: Cytochrome c oxidase subunit 5A



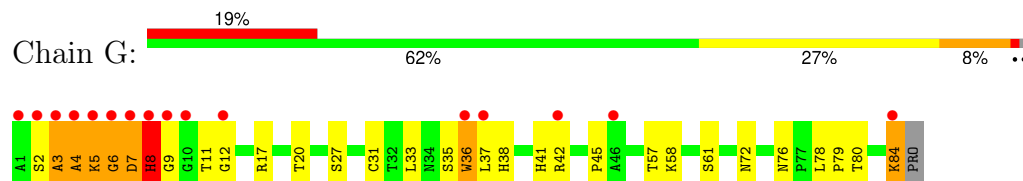
- Molecule 6: Cytochrome c oxidase subunit 5B



- Molecule 6: Cytochrome c oxidase subunit 5B

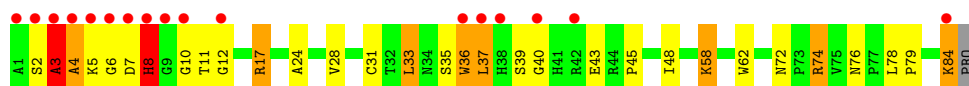


- Molecule 7: Cytochrome c oxidase subunit 6A2

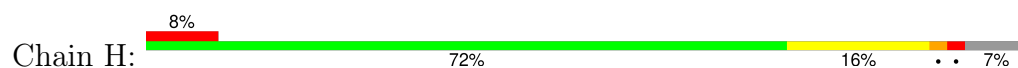


- Molecule 7: Cytochrome c oxidase subunit 6A2

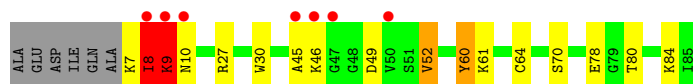




- Molecule 8: Cytochrome c oxidase subunit 6B1



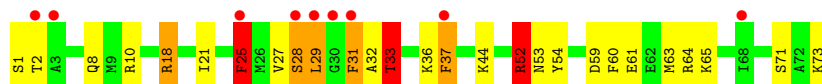
- Molecule 8: Cytochrome c oxidase subunit 6B1



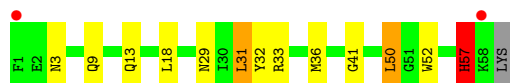
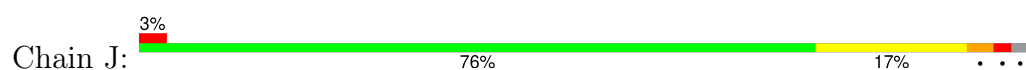
- Molecule 9: Cytochrome c oxidase subunit 6C



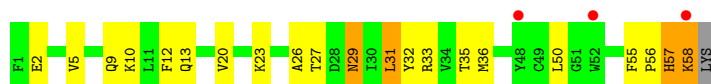
- Molecule 9: Cytochrome c oxidase subunit 6C



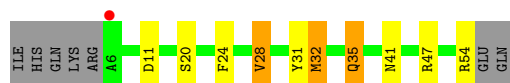
- Molecule 10: Cytochrome c oxidase polypeptide 7A1



- Molecule 10: Cytochrome c oxidase polypeptide 7A1



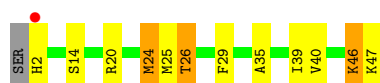
- Molecule 11: Cytochrome c oxidase subunit 7B



- Molecule 11: Cytochrome c oxidase subunit 7B



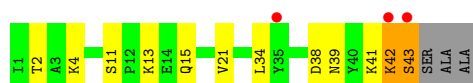
- Molecule 12: Cytochrome c oxidase subunit 7C



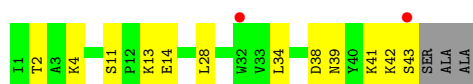
- Molecule 12: Cytochrome c oxidase subunit 7C



- Molecule 13: Cytochrome c oxidase subunit 8B



- Molecule 13: Cytochrome c oxidase subunit 8B



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	189.49Å 210.89Å 178.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.20 40.00 – 2.21	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.20) 99.2 (40.00-2.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.3	Depositor
R, R_{free}	0.162 , 0.192 0.180 , 0.207	Depositor DCC
R_{free} test set	17414 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	51.1	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 48.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	32105	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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: SAC, UNX, PEK, CDL, CUA, FME, CU, HEA, PGV, DMU, TGL, CMO, MG, ZN, NA, PSC, TPO, CHD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.84	45/4156 (1.1%)	1.44	27/5678 (0.5%)
1	N	1.54	24/4156 (0.6%)	1.31	20/5678 (0.4%)
2	B	1.83	28/1860 (1.5%)	1.50	19/2534 (0.7%)
2	O	1.46	9/1860 (0.5%)	1.35	14/2534 (0.6%)
3	C	1.68	14/2197 (0.6%)	1.30	14/3005 (0.5%)
3	P	1.47	9/2197 (0.4%)	1.26	10/3005 (0.3%)
4	D	1.65	8/1229 (0.7%)	1.39	5/1658 (0.3%)
4	Q	1.38	11/1229 (0.9%)	1.25	7/1658 (0.4%)
5	E	1.54	7/871 (0.8%)	1.33	4/1182 (0.3%)
5	R	1.25	1/871 (0.1%)	1.14	1/1182 (0.1%)
6	F	1.78	8/765 (1.0%)	1.50	7/1038 (0.7%)
6	S	1.53	5/765 (0.7%)	1.36	3/1038 (0.3%)
7	G	1.64	7/690 (1.0%)	1.43	10/937 (1.1%)
7	T	1.63	10/690 (1.4%)	1.37	5/937 (0.5%)
8	H	1.53	6/682 (0.9%)	1.28	2/921 (0.2%)
8	U	1.28	2/682 (0.3%)	1.23	3/921 (0.3%)
9	I	1.65	5/605 (0.8%)	1.38	4/802 (0.5%)
9	V	1.43	2/605 (0.3%)	1.35	5/802 (0.6%)
10	J	1.57	1/471 (0.2%)	1.37	5/636 (0.8%)
10	W	1.30	3/471 (0.6%)	1.22	3/636 (0.5%)
11	K	1.62	4/398 (1.0%)	1.37	2/546 (0.4%)
11	X	1.17	0/398	1.42	7/546 (1.3%)
12	L	1.70	4/393 (1.0%)	1.42	1/526 (0.2%)
12	Y	1.24	0/393	1.29	2/526 (0.4%)
13	M	1.54	0/345	1.49	3/470 (0.6%)
13	Z	1.19	0/345	1.19	0/470
All	All	1.59	213/29324 (0.7%)	1.35	183/39866 (0.5%)

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	F	0	1
6	S	0	1
10	J	0	1
10	W	0	1
All	All	0	4

The worst 5 of 213 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	129	ALA	CA-CB	15.72	1.63	1.52
1	N	83	VAL	CA-CB	14.65	1.62	1.54
4	Q	5	VAL	CA-CB	12.07	1.66	1.53
2	B	198	GLU	C-O	11.90	1.38	1.23
2	O	198	GLU	C-O	11.90	1.38	1.23

The worst 5 of 183 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	65	TRP	N-CA-C	10.38	125.15	113.21
9	V	29	LEU	N-CA-C	9.65	123.01	111.33
7	T	8	HIS	N-CA-C	8.87	129.69	110.80
7	T	7	ASP	N-CA-C	8.71	129.35	110.80
2	B	64	ILE	N-CA-C	-8.58	102.18	110.42

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	F	93	PRO	Peptide
10	J	57	HIS	Peptide
6	S	93	PRO	Peptide
10	W	57	HIS	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	4027	0	4001	44	0
1	N	4027	0	4001	55	0
2	B	1824	0	1833	39	0
2	O	1824	0	1833	44	0
3	C	2110	0	2027	22	0
3	P	2110	0	2027	24	0
4	D	1195	0	1183	9	0
4	Q	1195	0	1183	16	0
5	E	852	0	845	11	0
5	R	852	0	845	10	0
6	F	748	0	728	10	0
6	S	748	0	728	14	0
7	G	675	0	644	26	0
7	T	675	0	644	42	0
8	H	662	0	623	8	0
8	U	662	0	623	12	0
9	I	601	0	613	23	0
9	V	601	0	613	26	0
10	J	460	0	459	7	0
10	W	460	0	459	12	0
11	K	384	0	366	3	0
11	X	384	0	366	7	0
12	L	380	0	380	14	0
12	Y	380	0	380	11	0
13	M	335	0	352	7	0
13	Z	335	0	352	4	0
14	A	120	0	108	3	0
14	N	120	0	108	7	0
15	A	2	0	0	0	0
15	N	2	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	1	0	0	0	0
18	N	1	0	0	0	0
19	A	63	0	110	3	0
19	B	63	0	109	9	0
19	L	63	0	110	19	0
19	N	189	0	330	22	0
20	A	102	0	152	14	0
20	C	102	0	152	7	0
20	N	102	0	152	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	P	102	0	152	7	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	52	0	80	17	0
22	R	52	0	80	16	0
23	B	29	0	37	3	0
23	C	58	0	71	3	0
23	J	29	0	36	2	0
23	O	29	0	37	1	0
23	P	58	0	72	4	0
23	W	29	0	36	3	0
24	C	1	0	0	0	0
24	P	1	0	0	0	0
25	C	100	0	156	21	0
25	G	100	0	156	24	0
25	P	100	0	156	16	0
25	T	100	0	156	23	0
26	C	33	0	38	2	0
26	M	33	0	38	0	0
26	T	33	0	39	6	0
26	Z	33	0	39	1	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	G	159	0	231	22	0
28	S	53	0	77	6	0
28	T	106	0	154	19	0
29	A	205	0	0	3	0
29	B	121	0	0	3	0
29	C	80	0	0	2	0
29	D	75	0	0	1	0
29	E	39	0	0	1	0
29	F	70	0	0	2	0
29	G	42	0	0	5	0
29	H	33	0	0	5	0
29	I	24	0	0	1	0
29	J	9	0	0	0	0
29	K	17	0	0	0	0
29	L	20	0	0	2	0
29	M	15	0	0	0	0
29	N	184	0	0	6	0
29	O	97	0	0	2	0
29	P	81	0	0	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	Q	47	0	0	2	0
29	R	27	0	0	0	0
29	S	52	0	0	1	0
29	T	37	0	0	8	0
29	U	28	0	0	4	0
29	V	17	0	0	4	0
29	W	12	0	0	2	0
29	X	12	0	0	1	0
29	Y	16	0	0	0	0
29	Z	9	0	0	0	0
All	All	32105	0	31280	613	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 10.

The worst 5 of 613 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ILE:CD1	1:A:75:ILE:CG1	1.76	1.62
28:G:265:PEK:C7	28:G:265:PEK:C6	1.81	1.53
7:T:58:LYS:CE	7:T:58:LYS:NZ	1.72	1.47
12:L:20:ARG:NH2	19:L:522:TGL:HC32	1.40	1.36
7:T:45:PRO:CD	29:T:3099:HOH:O	1.75	1.35

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%)	500 (98%)	12 (2%)	0	100	100
1	N	512/514 (100%)	495 (97%)	17 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	225/227 (99%)	213 (95%)	11 (5%)	1 (0%)	30	34
2	O	225/227 (99%)	212 (94%)	12 (5%)	1 (0%)	30	34
3	C	257/261 (98%)	253 (98%)	3 (1%)	1 (0%)	30	34
3	P	257/261 (98%)	252 (98%)	4 (2%)	1 (0%)	30	34
4	D	142/147 (97%)	139 (98%)	3 (2%)	0	100	100
4	Q	142/147 (97%)	132 (93%)	9 (6%)	1 (1%)	18	19
5	E	103/109 (94%)	103 (100%)	0	0	100	100
5	R	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
6	F	96/98 (98%)	88 (92%)	5 (5%)	3 (3%)	3	1
6	S	96/98 (98%)	91 (95%)	3 (3%)	2 (2%)	5	3
7	G	81/85 (95%)	67 (83%)	9 (11%)	5 (6%)	1	0
7	T	81/85 (95%)	65 (80%)	11 (14%)	5 (6%)	1	0
8	H	77/85 (91%)	66 (86%)	5 (6%)	6 (8%)	1	0
8	U	77/85 (91%)	69 (90%)	4 (5%)	4 (5%)	1	0
9	I	71/73 (97%)	63 (89%)	6 (8%)	2 (3%)	4	2
9	V	71/73 (97%)	64 (90%)	4 (6%)	3 (4%)	2	1
10	J	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
10	W	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
11	K	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
11	X	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
12	L	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
12	Y	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
13	M	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
13	Z	41/46 (89%)	39 (95%)	1 (2%)	1 (2%)	4	3
All	All	3504/3614 (97%)	3339 (95%)	129 (4%)	36 (1%)	12	11

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	94	HIS
7	G	3	ALA
7	G	4	ALA
7	G	7	ASP
7	G	8	HIS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	426/426 (100%)	413 (97%)	13 (3%)	35	48
1	N	426/426 (100%)	415 (97%)	11 (3%)	40	55
2	B	210/210 (100%)	201 (96%)	9 (4%)	26	35
2	O	210/210 (100%)	194 (92%)	16 (8%)	12	14
3	C	224/226 (99%)	218 (97%)	6 (3%)	39	53
3	P	224/226 (99%)	222 (99%)	2 (1%)	70	84
4	D	128/129 (99%)	120 (94%)	8 (6%)	16	19
4	Q	128/129 (99%)	121 (94%)	7 (6%)	19	24
5	E	92/95 (97%)	88 (96%)	4 (4%)	26	35
5	R	92/95 (97%)	84 (91%)	8 (9%)	9	10
6	F	81/81 (100%)	75 (93%)	6 (7%)	13	14
6	S	81/81 (100%)	75 (93%)	6 (7%)	13	14
7	G	67/68 (98%)	61 (91%)	6 (9%)	9	9
7	T	67/68 (98%)	61 (91%)	6 (9%)	9	9
8	H	71/75 (95%)	66 (93%)	5 (7%)	14	16
8	U	71/75 (95%)	64 (90%)	7 (10%)	7	8
9	I	57/57 (100%)	47 (82%)	10 (18%)	2	1
9	V	57/57 (100%)	46 (81%)	11 (19%)	1	1
10	J	49/50 (98%)	47 (96%)	2 (4%)	27	37
10	W	49/50 (98%)	42 (86%)	7 (14%)	3	3
11	K	39/46 (85%)	36 (92%)	3 (8%)	12	13
11	X	39/46 (85%)	35 (90%)	4 (10%)	7	7
12	L	39/40 (98%)	36 (92%)	3 (8%)	12	13
12	Y	39/40 (98%)	36 (92%)	3 (8%)	12	13
13	M	37/38 (97%)	31 (84%)	6 (16%)	2	2
13	Z	37/38 (97%)	32 (86%)	5 (14%)	4	3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	3040/3082 (99%)	2866 (94%)	174 (6%)	18	23

5 of 174 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	Q	53	ILE
8	U	84	LYS
5	R	70	VAL
6	S	87	THR
9	V	33	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
3	P	50	ASN
7	T	76	ASN
3	P	68	GLN
4	Q	37	GLN
10	W	29	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	FME	N	1	1	8,9,10	0.85	0	8,9,11	4.38	4 (50%)
1	FME	A	1	1	8,9,10	0.66	0	8,9,11	4.94	5 (62%)

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	1.16	1 (12%)	8,9,11	6.17	4 (50%)
7	TPO	G	11	7	8,10,11	2.56	6 (75%)	10,14,16	2.21	3 (30%)
7	TPO	T	11	7	8,10,11	2.70	5 (62%)	10,14,16	2.30	4 (40%)
9	SAC	I	1	9	7,8,9	3.73	2 (28%)	7,9,11	3.64	2 (28%)
2	FME	O	1	2	8,9,10	0.90	0	8,9,11	3.72	4 (50%)
9	SAC	V	1	9	7,8,9	3.67	2 (28%)	7,9,11	2.71	4 (57%)

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

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

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	V	1	SAC	CA-N	7.29	1.57	1.46
9	I	1	SAC	CA-N	6.68	1.56	1.46
9	I	1	SAC	OAC-C1A	6.52	1.37	1.23
9	V	1	SAC	OAC-C1A	5.55	1.35	1.23
7	T	11	TPO	P-OG1	4.47	1.67	1.59

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CA-N-CN	-16.81	96.98	122.82
1	A	1	FME	CA-N-CN	-12.33	103.86	122.82
1	N	1	FME	CA-N-CN	-10.28	107.00	122.82
2	O	1	FME	CA-N-CN	-9.32	108.49	122.82
9	I	1	SAC	C-CA-N	8.94	126.74	109.50

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

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

3 monomers are involved in 3 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	$\# Z > 2$
25	CDL	C	270	-	99,99,99	1.55	15 (15%)	105,111,111	1.48	15 (14%)
21	CUA	B	228	2	0,1,1	-	-	-	-	-
14	HEA	A	515	1	67,67,67	2.06	22 (32%)	81,103,103	2.24	24 (29%)
19	TGL	N	1523	-	62,62,62	1.51	8 (12%)	65,65,65	1.44	11 (16%)
20	PGV	P	1267	-	50,50,50	1.03	2 (4%)	53,56,56	1.03	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	HEA	N	515	1	67,67,67	2.06	21 (31%)	81,103,103	1.88	27 (33%)
19	TGL	A	523	-	62,62,62	1.48	6 (9%)	65,65,65	1.71	14 (21%)
26	DMU	M	526	-	34,34,34	1.28	2 (5%)	45,45,45	3.46	22 (48%)
21	CUA	O	228	2	0,1,1	-	-	-	-	-
20	PGV	A	524	-	50,50,50	1.34	3 (6%)	53,56,56	1.42	8 (15%)
28	PEK	T	1264	-	52,52,52	0.92	4 (7%)	55,57,57	1.42	11 (20%)
22	PSC	R	1229	-	51,51,51	1.38	3 (5%)	57,59,59	1.27	6 (10%)
25	CDL	T	1269	-	99,99,99	1.60	12 (12%)	105,111,111	1.51	14 (13%)
26	DMU	Z	1526	-	34,34,34	1.01	3 (8%)	45,45,45	3.15	21 (46%)
23	CHD	P	1271	-	32,32,32	0.91	1 (3%)	51,51,51	5.16	35 (68%)
22	PSC	B	229	-	51,51,51	1.42	3 (5%)	57,59,59	1.31	7 (12%)
26	DMU	T	1272	-	34,34,34	1.38	3 (8%)	45,45,45	3.16	22 (48%)
25	CDL	P	1270	-	99,99,99	1.55	13 (13%)	105,111,111	1.43	12 (11%)
23	CHD	W	1059	-	32,32,32	0.80	1 (3%)	51,51,51	5.03	34 (66%)
20	PGV	N	1524	-	50,50,50	1.28	2 (4%)	53,56,56	1.23	6 (11%)
15	CMO	N	520	14	0,1,1	-	-	-	-	-
20	PGV	P	1268	-	50,50,50	1.44	2 (4%)	53,56,56	1.63	8 (15%)
23	CHD	B	1085	-	32,32,32	1.63	4 (12%)	51,51,51	5.54	37 (72%)
26	DMU	C	272	-	34,34,34	1.34	5 (14%)	45,45,45	3.38	21 (46%)
28	PEK	G	1263	-	52,52,52	1.42	5 (9%)	55,57,57	1.50	8 (14%)
19	TGL	N	1522	-	62,62,62	1.70	7 (11%)	65,65,65	1.81	16 (24%)
28	PEK	G	265	-	52,52,52	1.63	6 (11%)	55,57,57	1.54	11 (20%)
28	PEK	G	264	-	52,52,52	1.06	5 (9%)	55,57,57	1.58	10 (18%)
25	CDL	G	269	-	99,99,99	1.53	13 (13%)	105,111,111	1.45	17 (16%)
23	CHD	C	271	-	32,32,32	0.94	3 (9%)	51,51,51	4.96	34 (66%)
28	PEK	T	263	-	52,52,52	1.42	4 (7%)	55,57,57	1.22	5 (9%)
23	CHD	O	229	-	32,32,32	1.54	6 (18%)	51,51,51	5.49	37 (72%)
20	PGV	C	268	-	50,50,50	1.48	3 (6%)	53,56,56	1.72	7 (13%)
28	PEK	S	1265	-	52,52,52	1.30	3 (5%)	55,57,57	1.33	5 (9%)
19	TGL	L	522	-	62,62,62	1.77	9 (14%)	65,65,65	2.01	16 (24%)
23	CHD	J	60	-	32,32,32	1.11	2 (6%)	51,51,51	5.28	37 (72%)
14	HEA	A	516	1	67,67,67	2.08	23 (34%)	81,103,103	2.19	29 (35%)
20	PGV	C	267	-	50,50,50	0.91	2 (4%)	53,56,56	1.20	6 (11%)
23	CHD	C	525	-	32,32,32	1.46	4 (12%)	51,51,51	4.99	39 (76%)
15	CMO	A	520	-	0,1,1	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	PGV	N	1266	-	50,50,50	0.87	3 (6%)	53,56,56	1.39	5 (9%)
20	PGV	A	521	-	50,50,50	0.83	2 (4%)	53,56,56	1.75	7 (13%)
19	TGL	B	521	-	62,62,62	1.55	8 (12%)	65,65,65	2.51	18 (27%)
19	TGL	N	1521	-	62,62,62	1.50	9 (14%)	65,65,65	2.24	15 (23%)
14	HEA	N	516	15,1	67,67,67	1.95	25 (37%)	81,103,103	2.21	27 (33%)
23	CHD	P	1525	-	32,32,32	1.11	3 (9%)	51,51,51	5.41	38 (74%)

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
25	CDL	C	270	-	-	68/110/110/110	-
14	HEA	A	515	1	-	6/36/76/76	-
19	TGL	N	1523	-	-	32/65/65/65	-
20	PGV	P	1267	-	-	14/55/55/55	-
26	DMU	M	526	-	5/5/10/10	8/19/59/59	0/2/2/2
14	HEA	N	515	1	-	6/36/76/76	-
19	TGL	A	523	-	-	33/65/65/65	-
20	PGV	A	524	-	-	32/55/55/55	-
28	PEK	T	1264	-	-	21/56/56/56	-
22	PSC	R	1229	-	-	28/55/55/55	-
25	CDL	T	1269	-	-	59/110/110/110	-
26	DMU	Z	1526	-	5/5/10/10	10/19/59/59	0/2/2/2
23	CHD	P	1271	-	1/1/12/12	6/9/74/74	0/4/4/4
22	PSC	B	229	-	-	33/55/55/55	-
26	DMU	T	1272	-	6/6/10/10	12/19/59/59	0/2/2/2
25	CDL	P	1270	-	-	78/110/110/110	-
23	CHD	W	1059	-	2/2/12/12	6/9/74/74	0/4/4/4
20	PGV	N	1524	-	-	29/55/55/55	-
23	CHD	B	1085	-	1/1/12/12	2/9/74/74	0/4/4/4
20	PGV	P	1268	-	-	35/55/55/55	-
26	DMU	C	272	-	5/5/10/10	11/19/59/59	0/2/2/2
28	PEK	G	1263	-	-	32/56/56/56	-
19	TGL	N	1522	-	-	36/65/65/65	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	PEK	G	265	-	-	24/56/56/56	-
28	PEK	G	264	-	-	23/56/56/56	-
25	CDL	G	269	-	-	58/110/110/110	-
23	CHD	C	271	-	1/1/12/12	7/9/74/74	0/4/4/4
28	PEK	T	263	-	-	26/56/56/56	-
23	CHD	O	229	-	1/1/12/12	5/9/74/74	0/4/4/4
20	PGV	C	268	-	-	29/55/55/55	-
28	PEK	S	1265	-	-	27/56/56/56	-
19	TGL	L	522	-	-	42/65/65/65	-
23	CHD	J	60	-	1/1/12/12	7/9/74/74	0/4/4/4
14	HEA	A	516	1	-	6/36/76/76	-
20	PGV	C	267	-	-	13/55/55/55	-
23	CHD	C	525	-	-	1/9/74/74	0/4/4/4
20	PGV	N	1266	-	-	14/55/55/55	-
20	PGV	A	521	-	-	14/55/55/55	-
19	TGL	B	521	-	-	36/65/65/65	-
19	TGL	N	1521	-	-	36/65/65/65	-
14	HEA	N	516	15,1	-	9/36/76/76	-
23	CHD	P	1525	-	-	4/9/74/74	0/4/4/4

The worst 5 of 280 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	L	522	TGL	OG2-CB1	7.62	1.55	1.34
19	N	1522	TGL	OG2-CB1	7.47	1.55	1.34
20	C	268	PGV	O01-C1	7.20	1.54	1.34
20	P	1268	PGV	O01-C1	7.09	1.54	1.34
14	A	516	HEA	FE-NA	6.76	2.17	1.95

The worst 5 of 745 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	P	1525	CHD	C6-C5-C10	14.73	128.34	112.66
23	J	60	CHD	C10-C9-C8	13.45	126.83	111.84
23	B	1085	CHD	C6-C5-C10	13.38	126.90	112.66
23	C	271	CHD	C10-C9-C8	13.15	126.50	111.84
23	P	1525	CHD	C1-C10-C5	12.99	126.39	107.75

5 of 28 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	B	1085	CHD	C9
23	C	271	CHD	C9
23	J	60	CHD	C9
23	O	229	CHD	C9
23	P	1271	CHD	C9

5 of 978 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	516	HEA	C2A-C3A-CMA-OMA
14	A	516	HEA	C4A-C3A-CMA-OMA
14	N	515	HEA	C2A-C3A-CMA-OMA
14	N	515	HEA	C4A-C3A-CMA-OMA
14	N	516	HEA	C2A-C3A-CMA-OMA

There are no ring outliers.

40 monomers are involved in 272 short contacts:

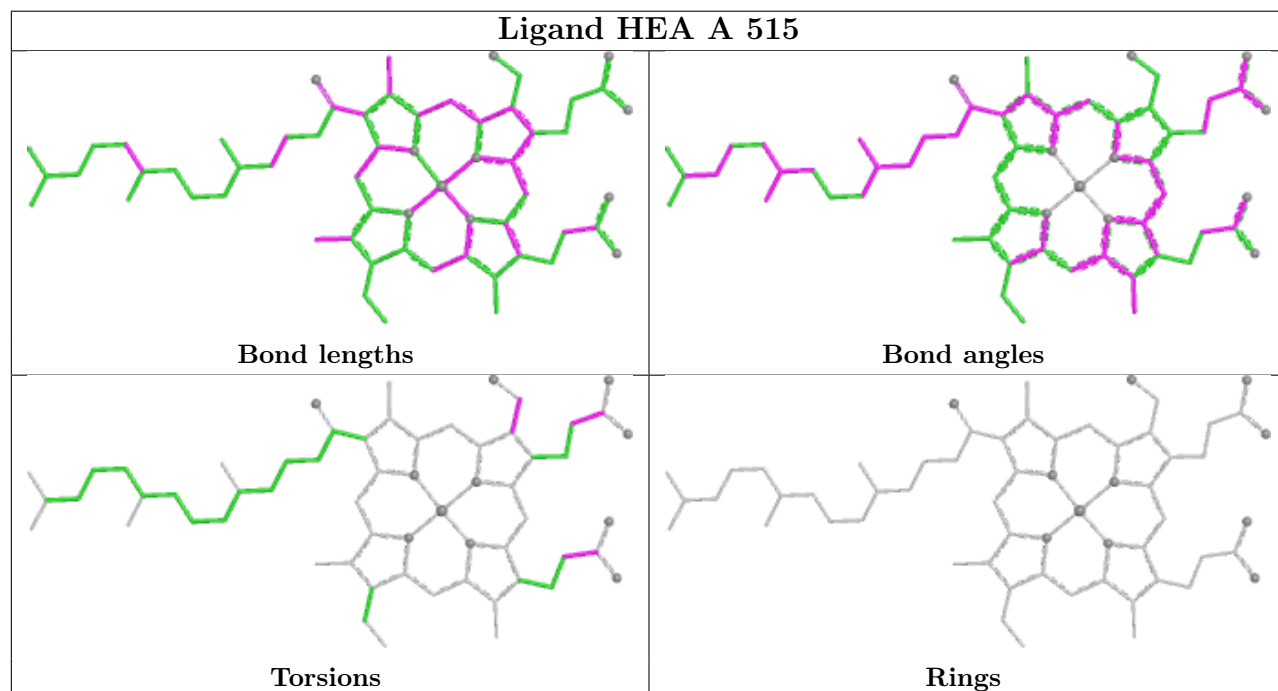
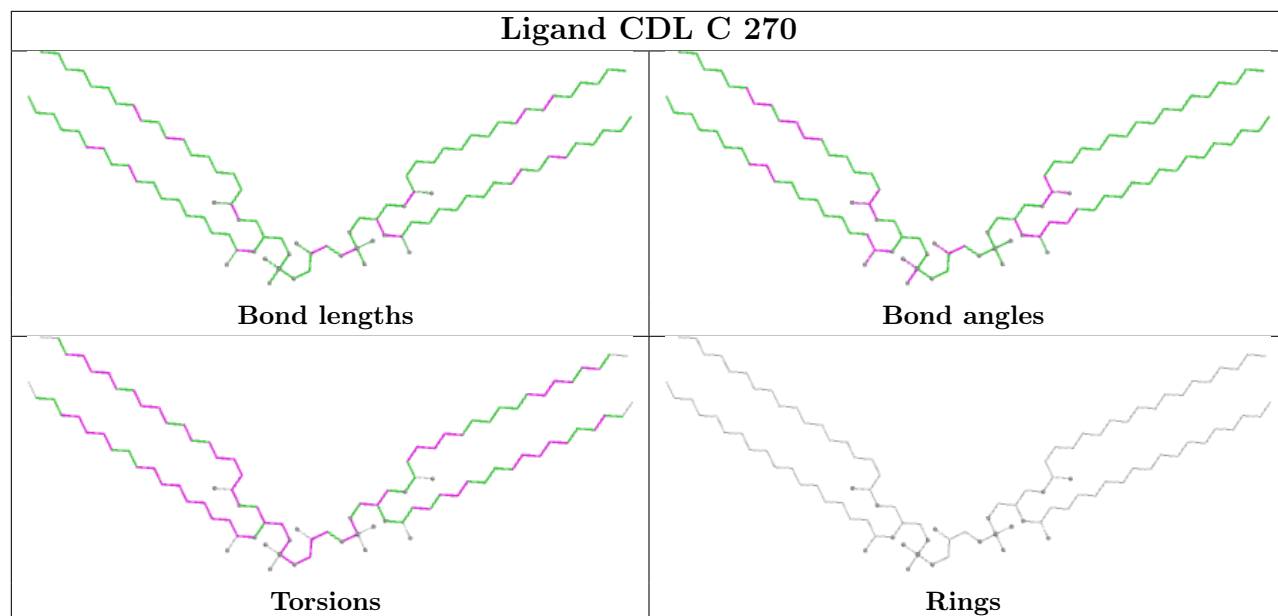
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	C	270	CDL	21	0
14	A	515	HEA	2	0
19	N	1523	TGL	5	0
20	P	1267	PGV	5	0
14	N	515	HEA	5	0
19	A	523	TGL	3	0
20	A	524	PGV	12	0
28	T	1264	PEK	4	0
22	R	1229	PSC	16	0
25	T	1269	CDL	23	0
26	Z	1526	DMU	1	0
23	P	1271	CHD	3	0
22	B	229	PSC	17	0
26	T	1272	DMU	6	0
25	P	1270	CDL	16	0
23	W	1059	CHD	3	0
20	N	1524	PGV	8	0
20	P	1268	PGV	2	0
23	B	1085	CHD	3	0
26	C	272	DMU	2	0
28	G	1263	PEK	10	0
19	N	1522	TGL	7	0

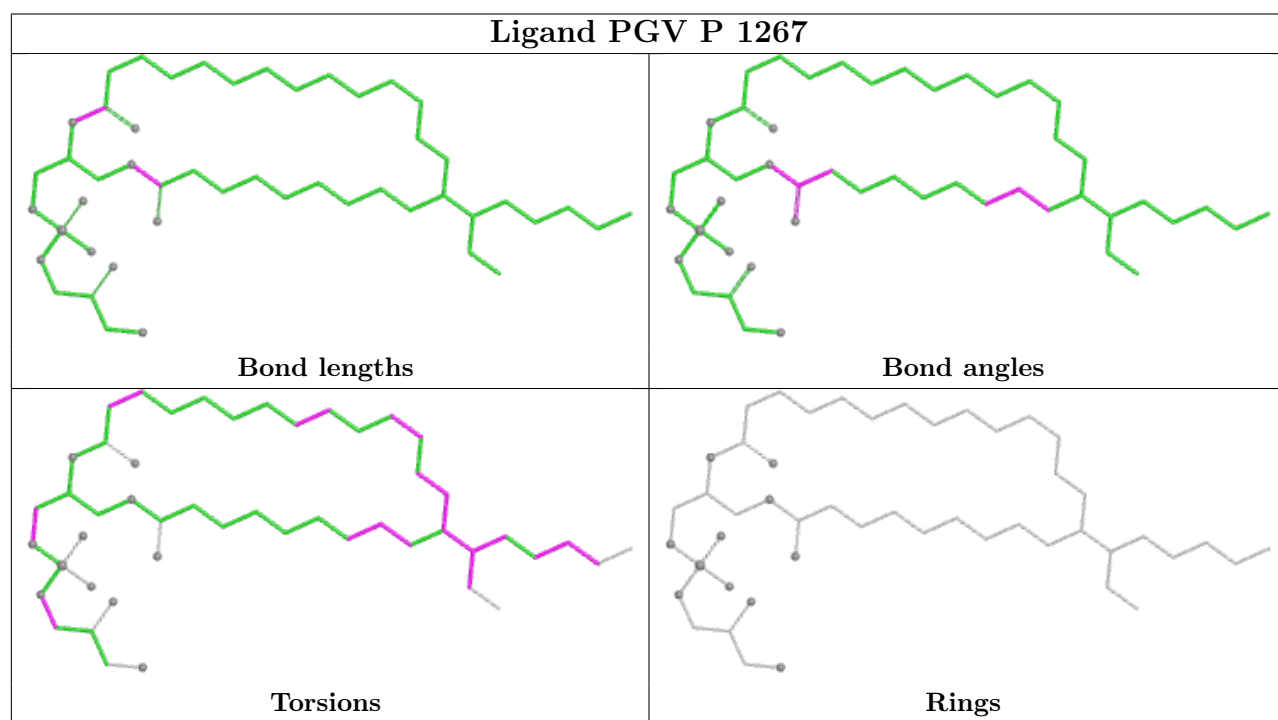
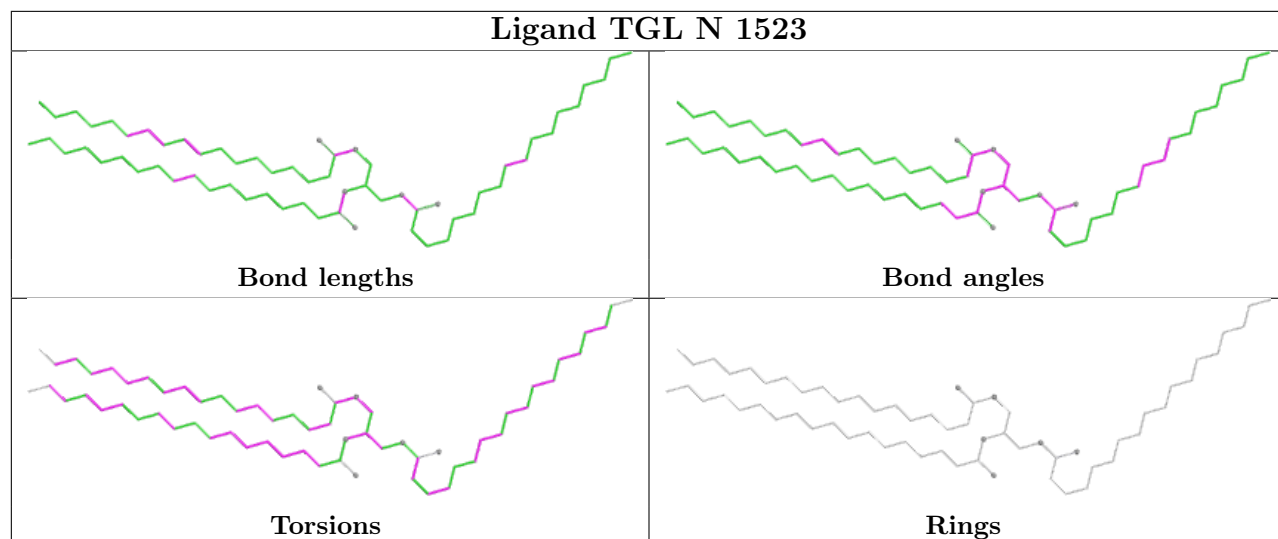
Continued on next page...

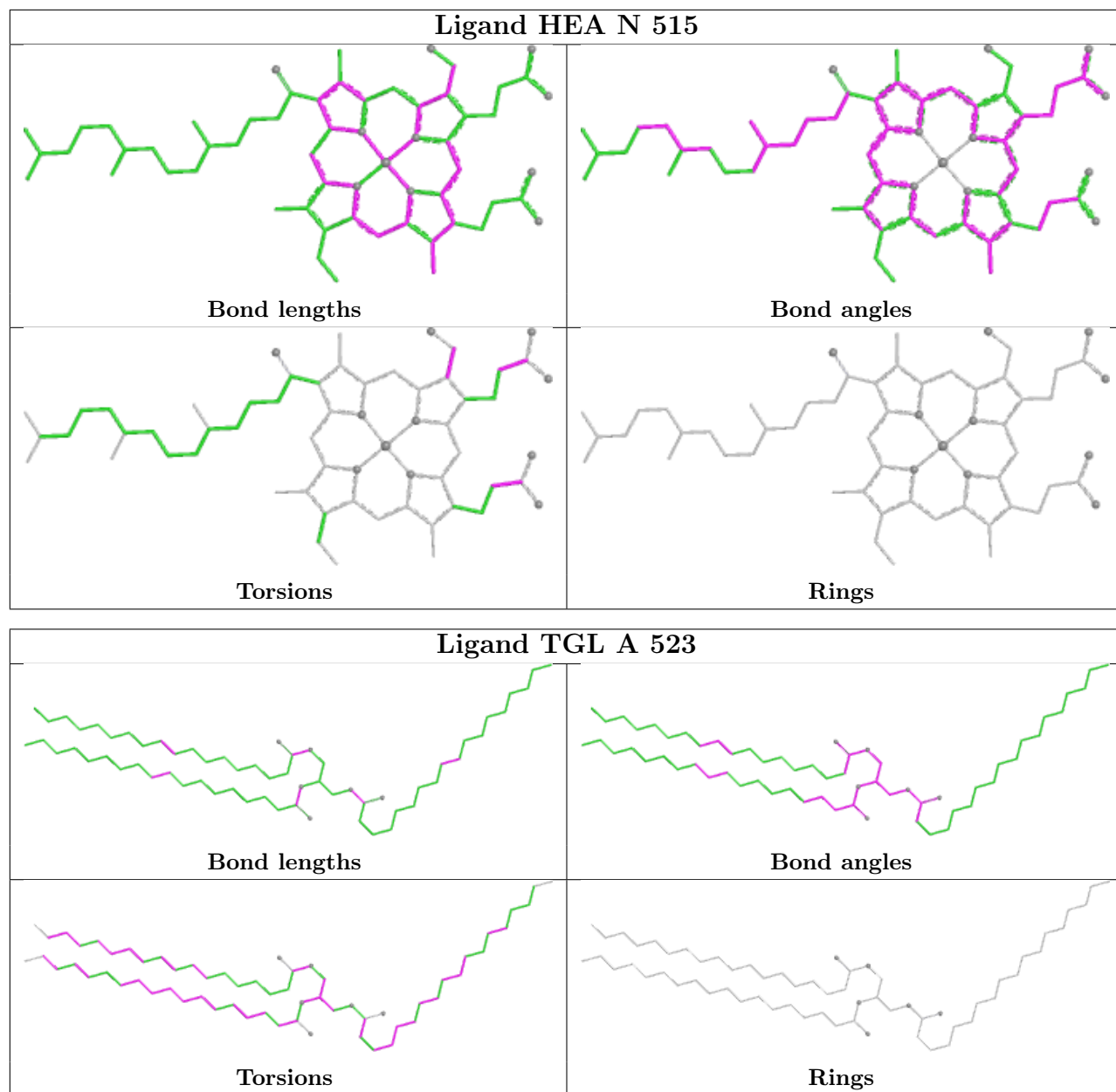
Continued from previous page...

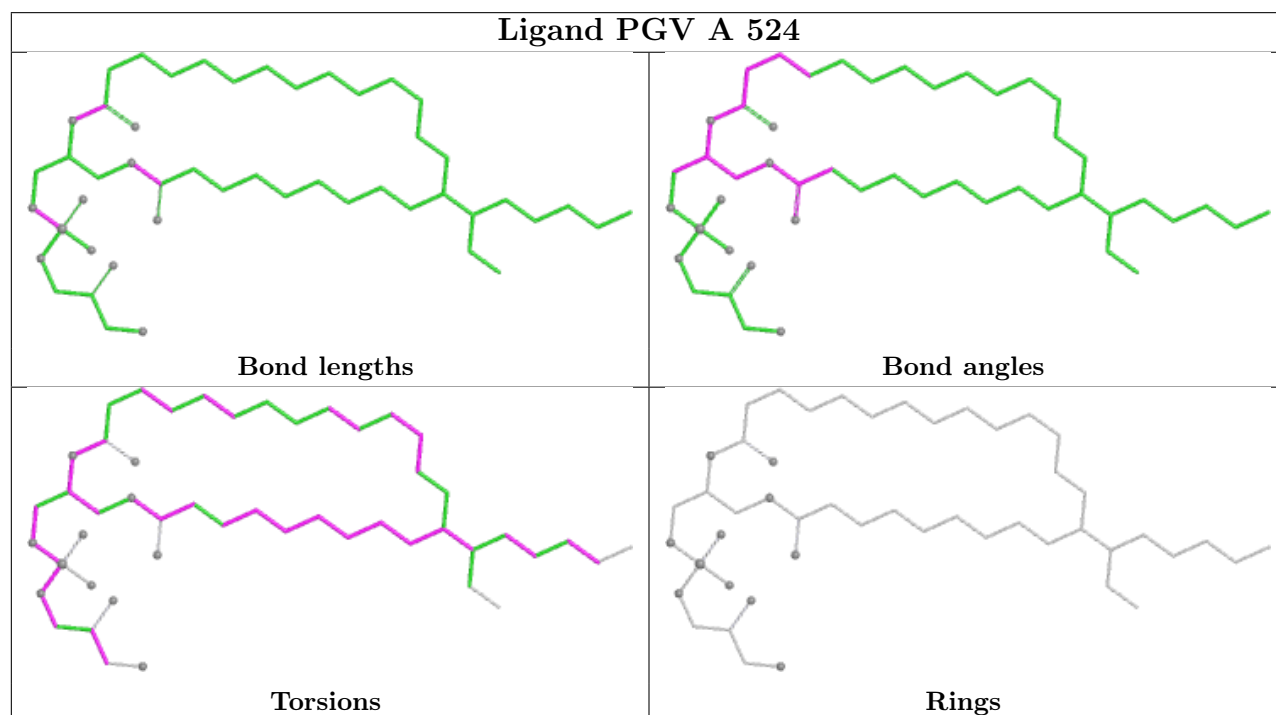
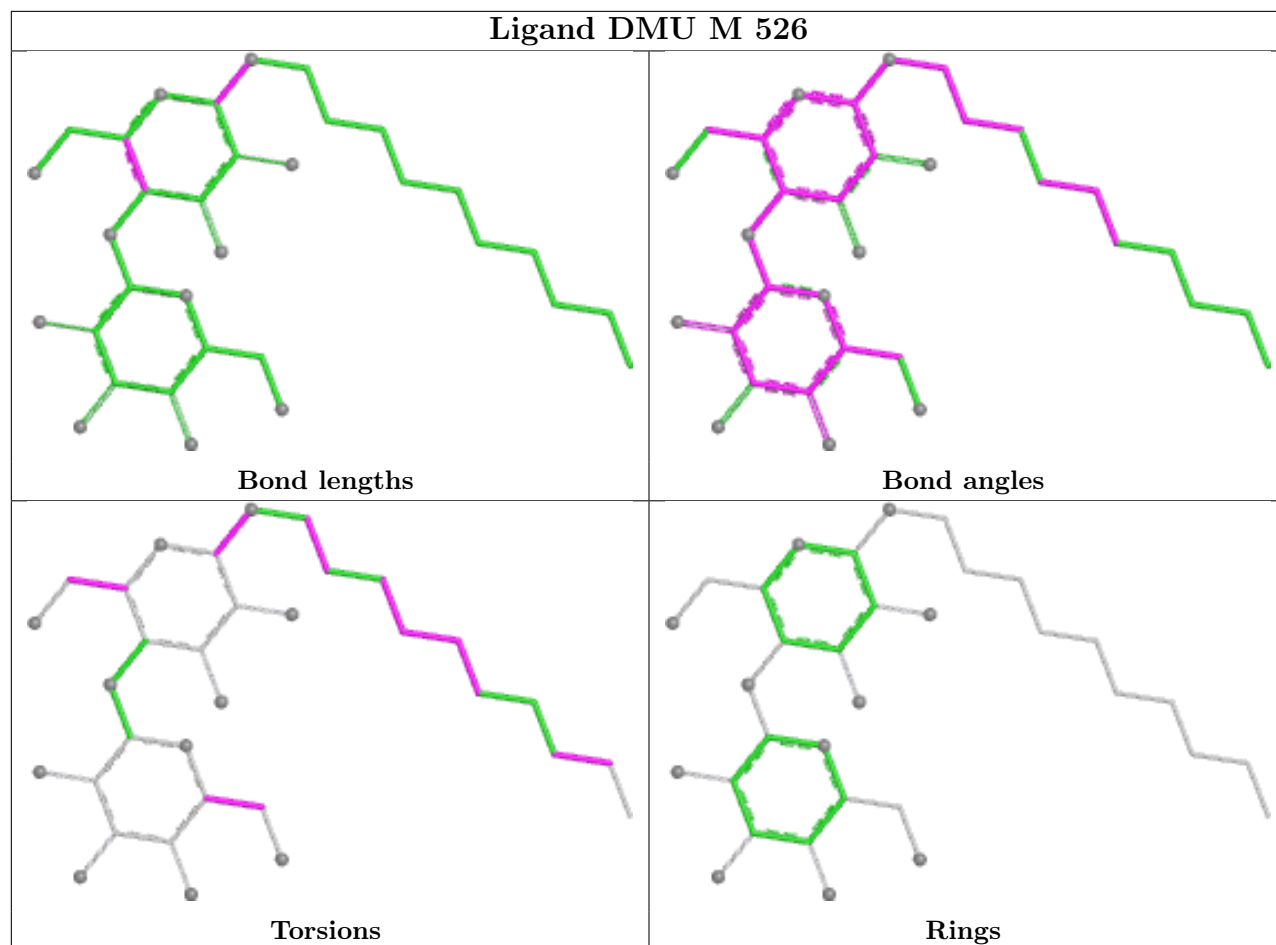
Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	G	265	PEK	8	0
28	G	264	PEK	4	0
25	G	269	CDL	24	0
23	C	271	CHD	2	0
28	T	263	PEK	15	0
23	O	229	CHD	1	0
28	S	1265	PEK	6	0
19	L	522	TGL	19	0
23	J	60	CHD	2	0
14	A	516	HEA	1	0
20	C	267	PGV	7	0
23	C	525	CHD	1	0
20	N	1266	PGV	1	0
20	A	521	PGV	2	0
19	B	521	TGL	9	0
19	N	1521	TGL	10	0
14	N	516	HEA	2	0
23	P	1525	CHD	1	0

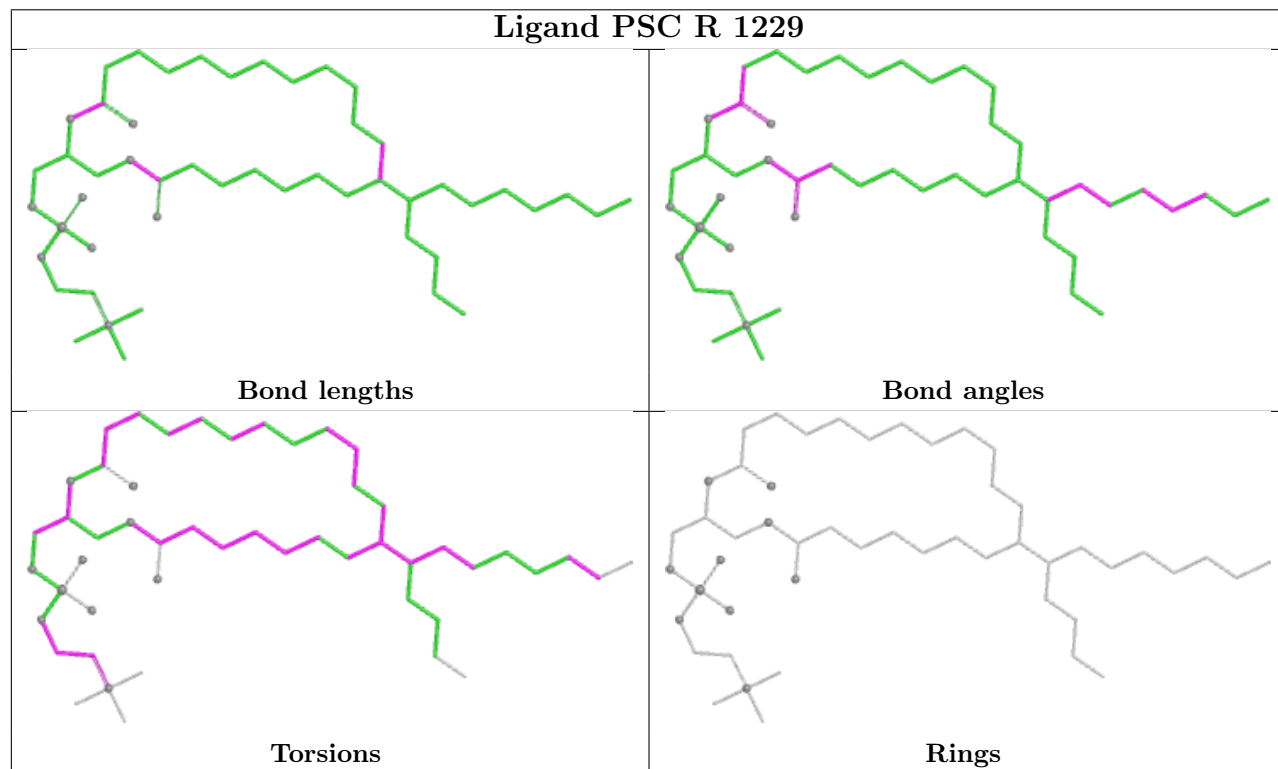
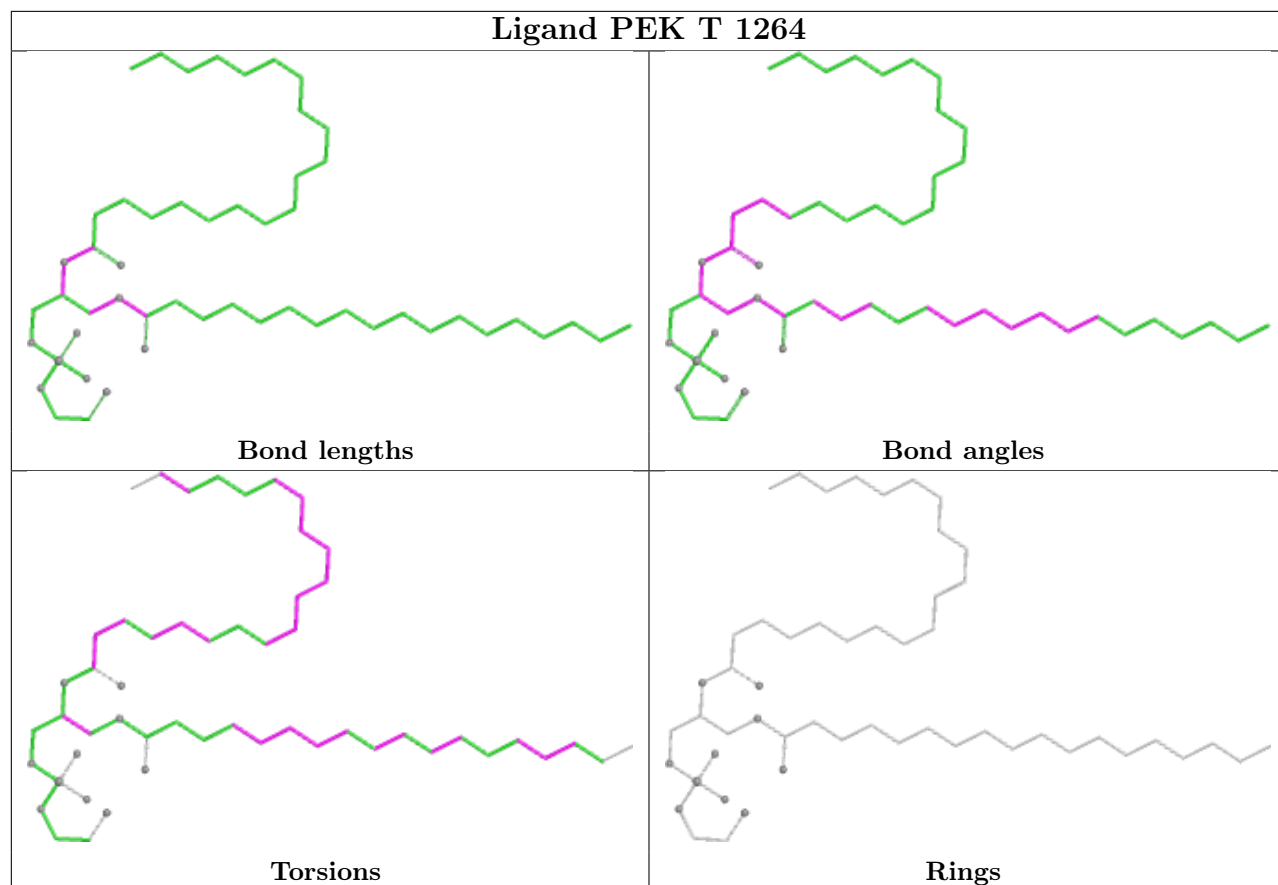
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

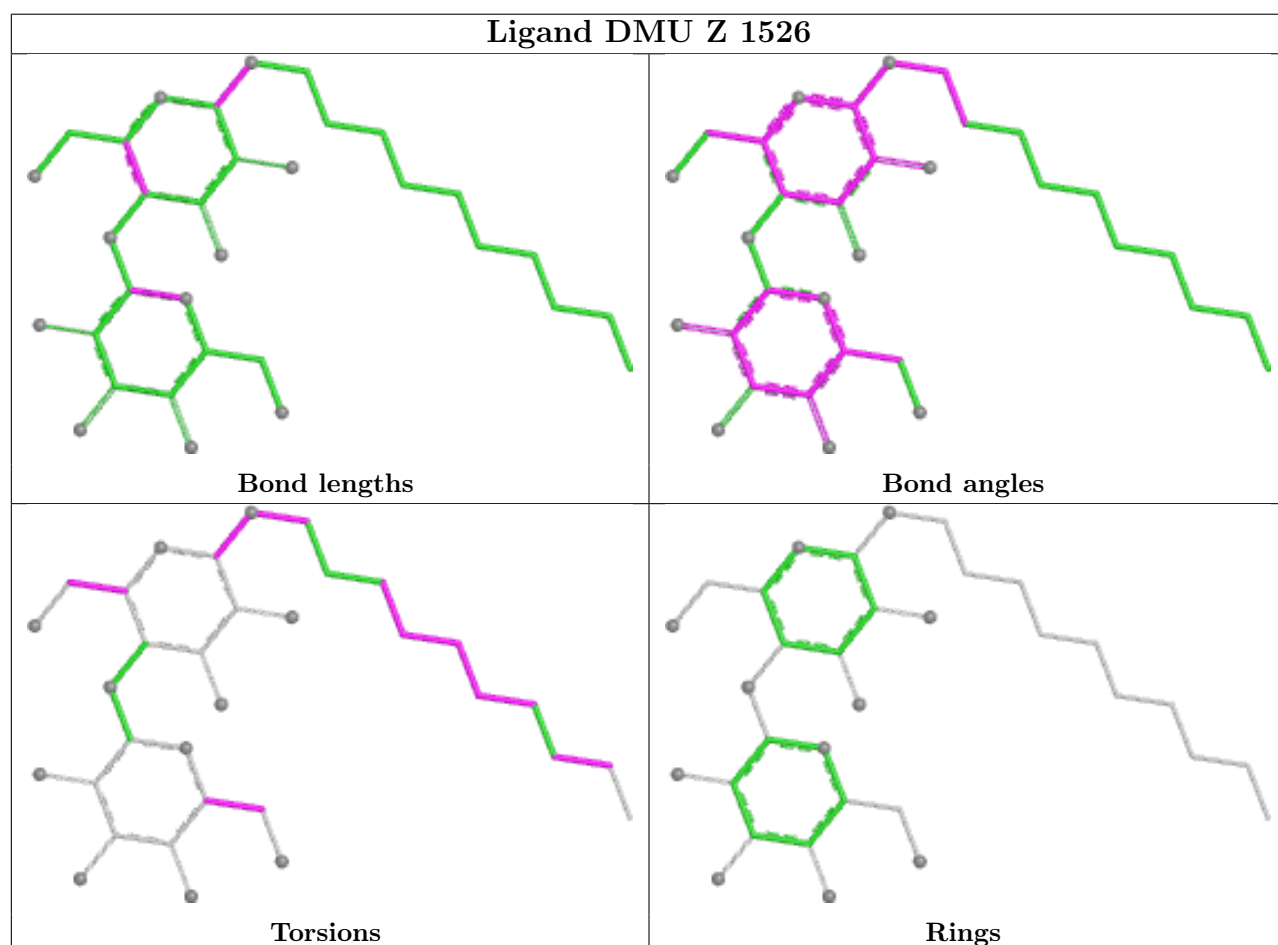
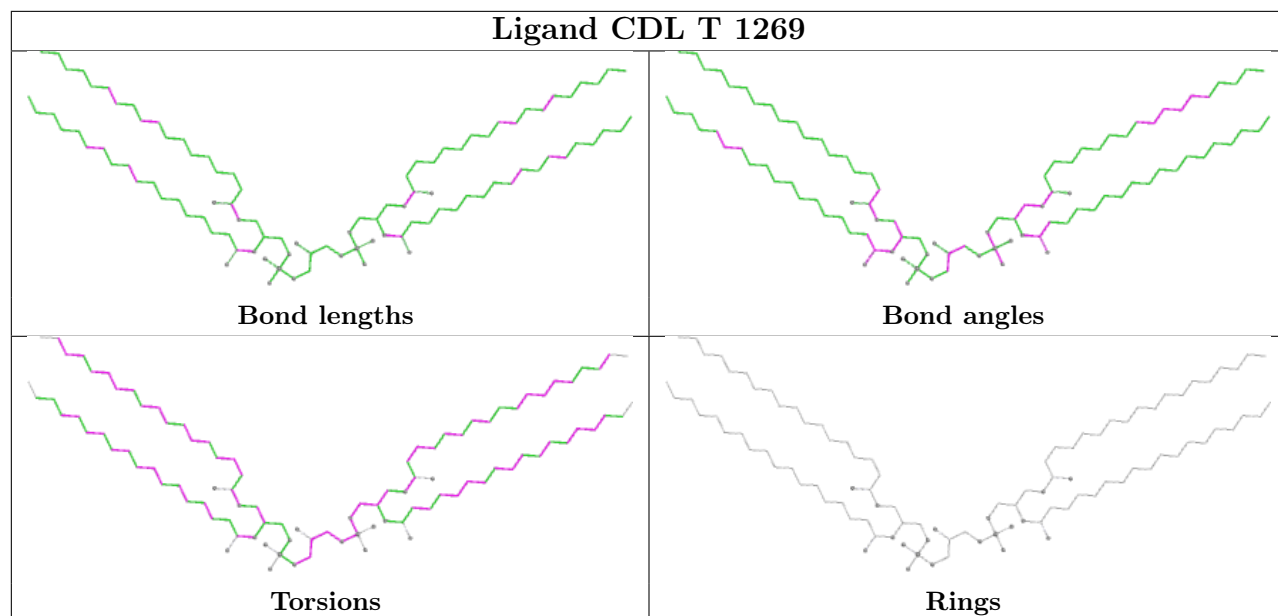




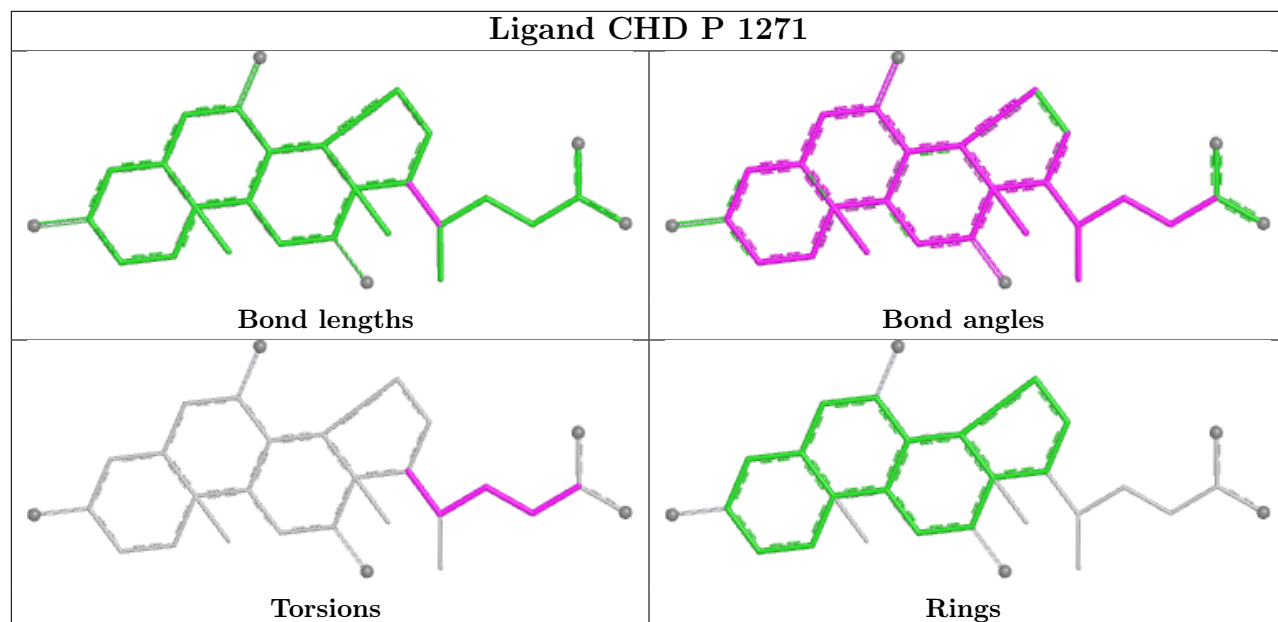




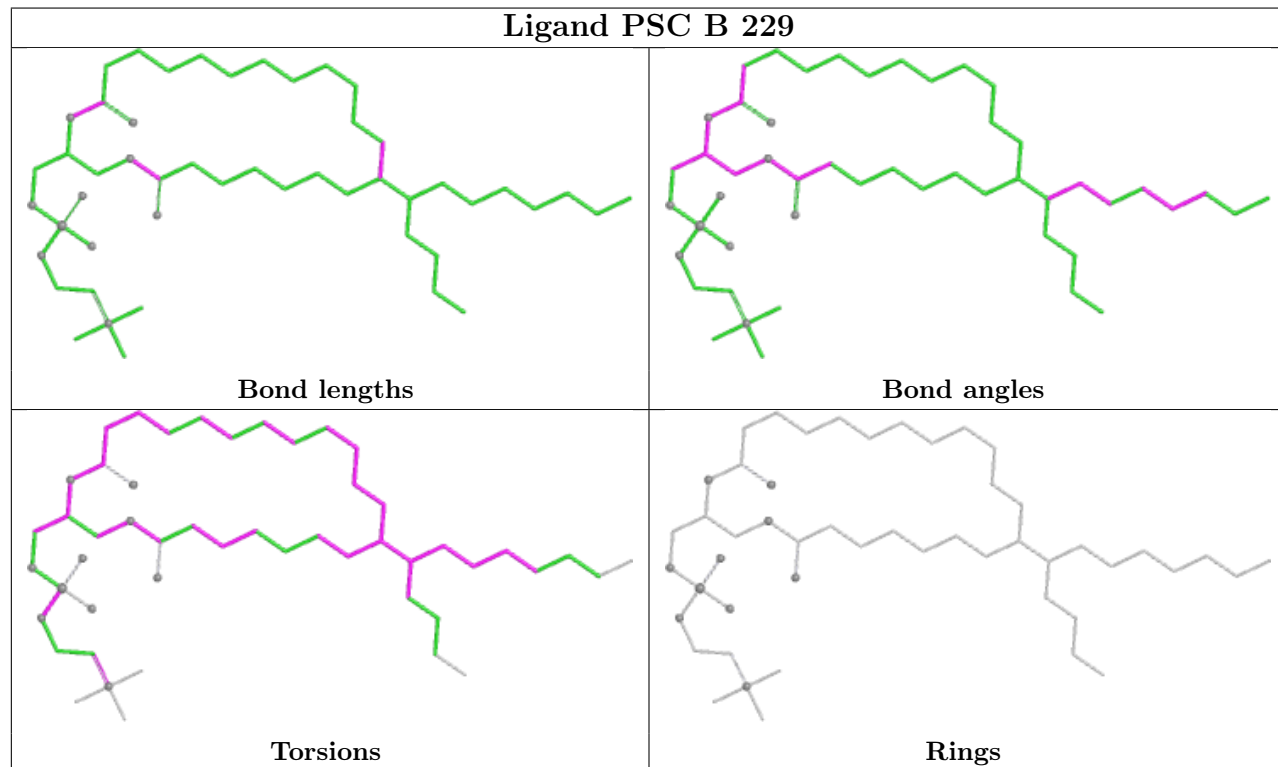


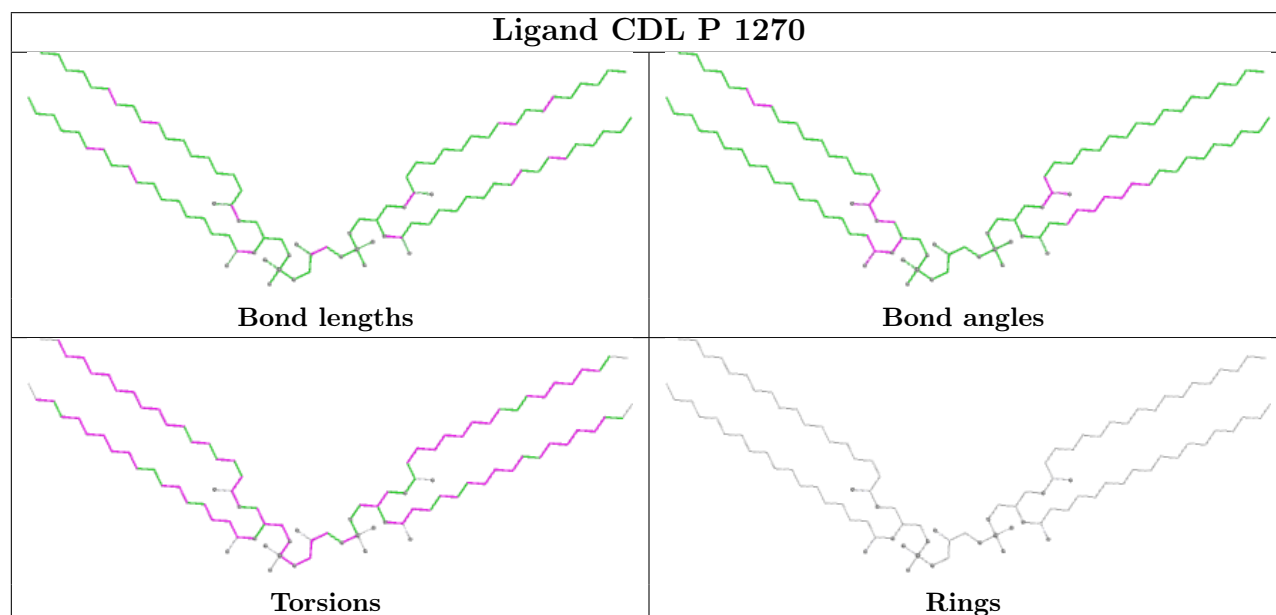
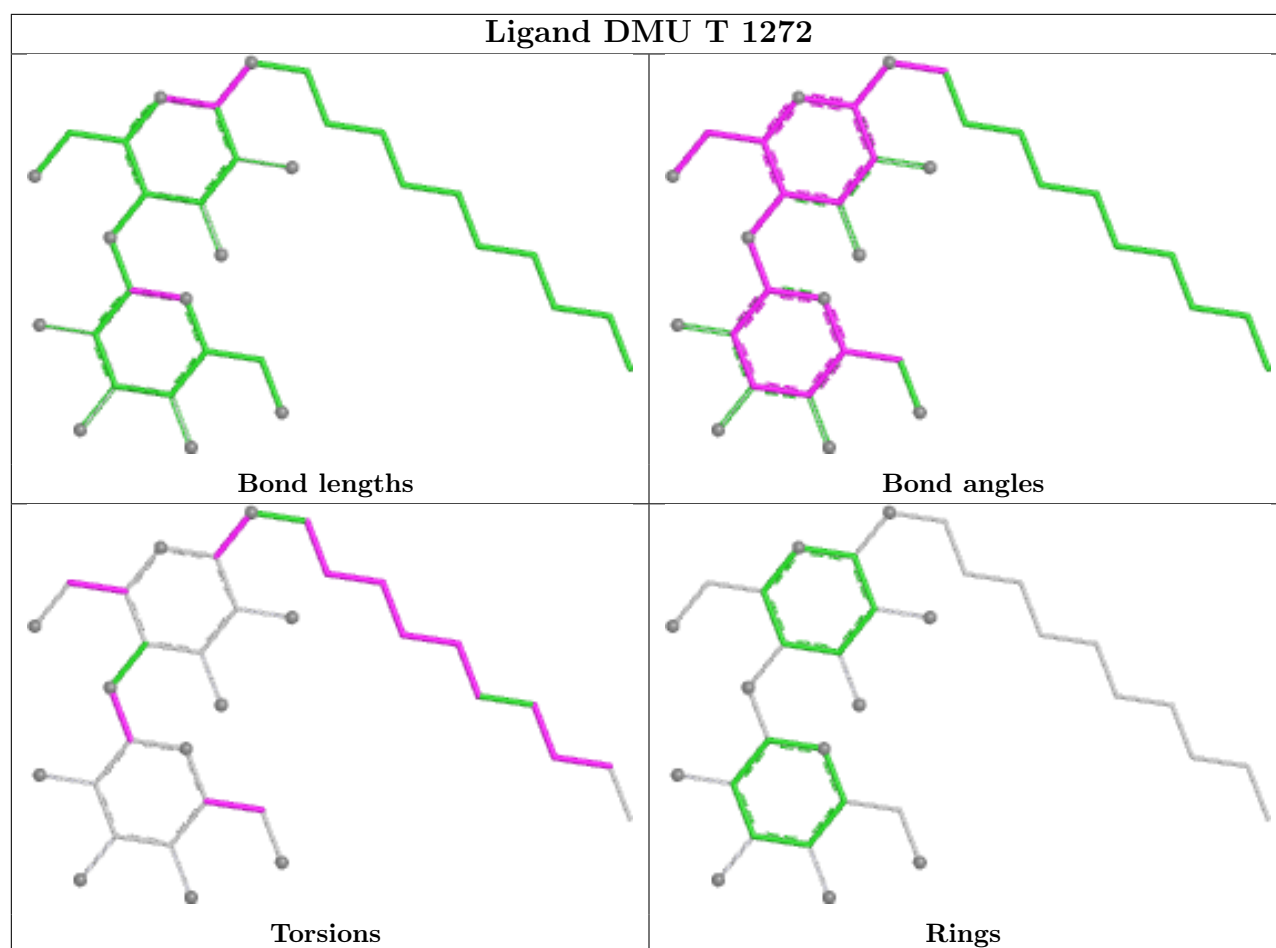


Ligand CHD P 1271

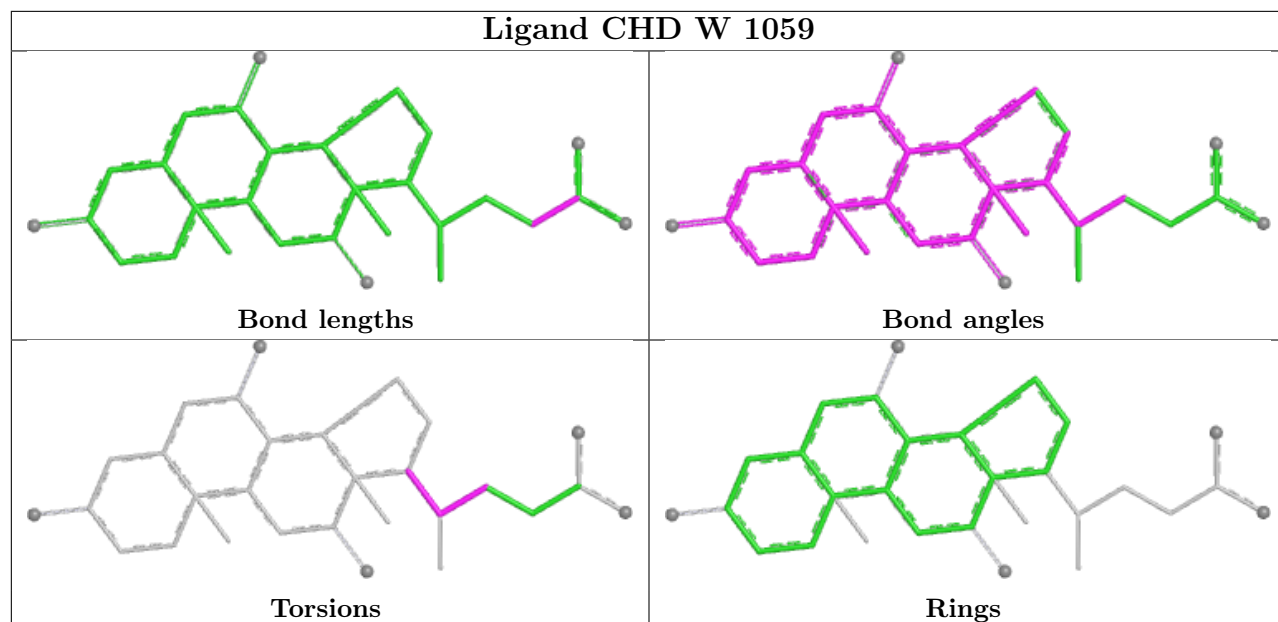


Ligand PSC B 229

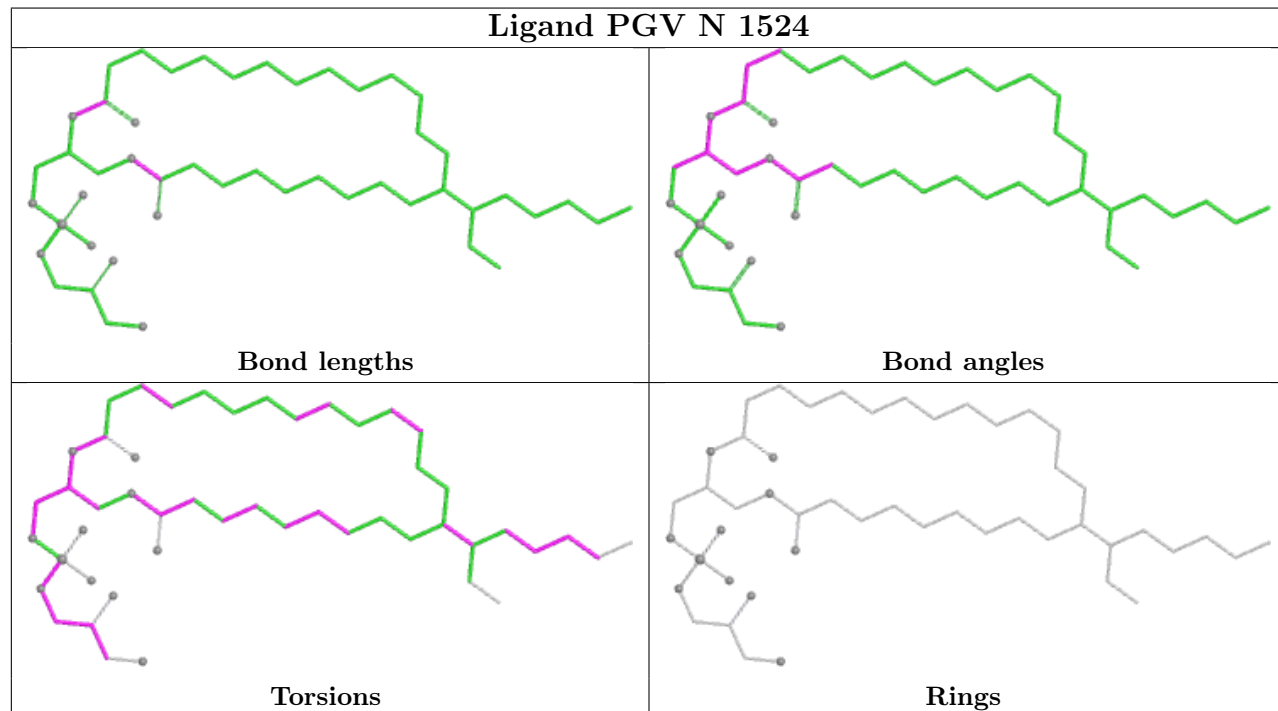


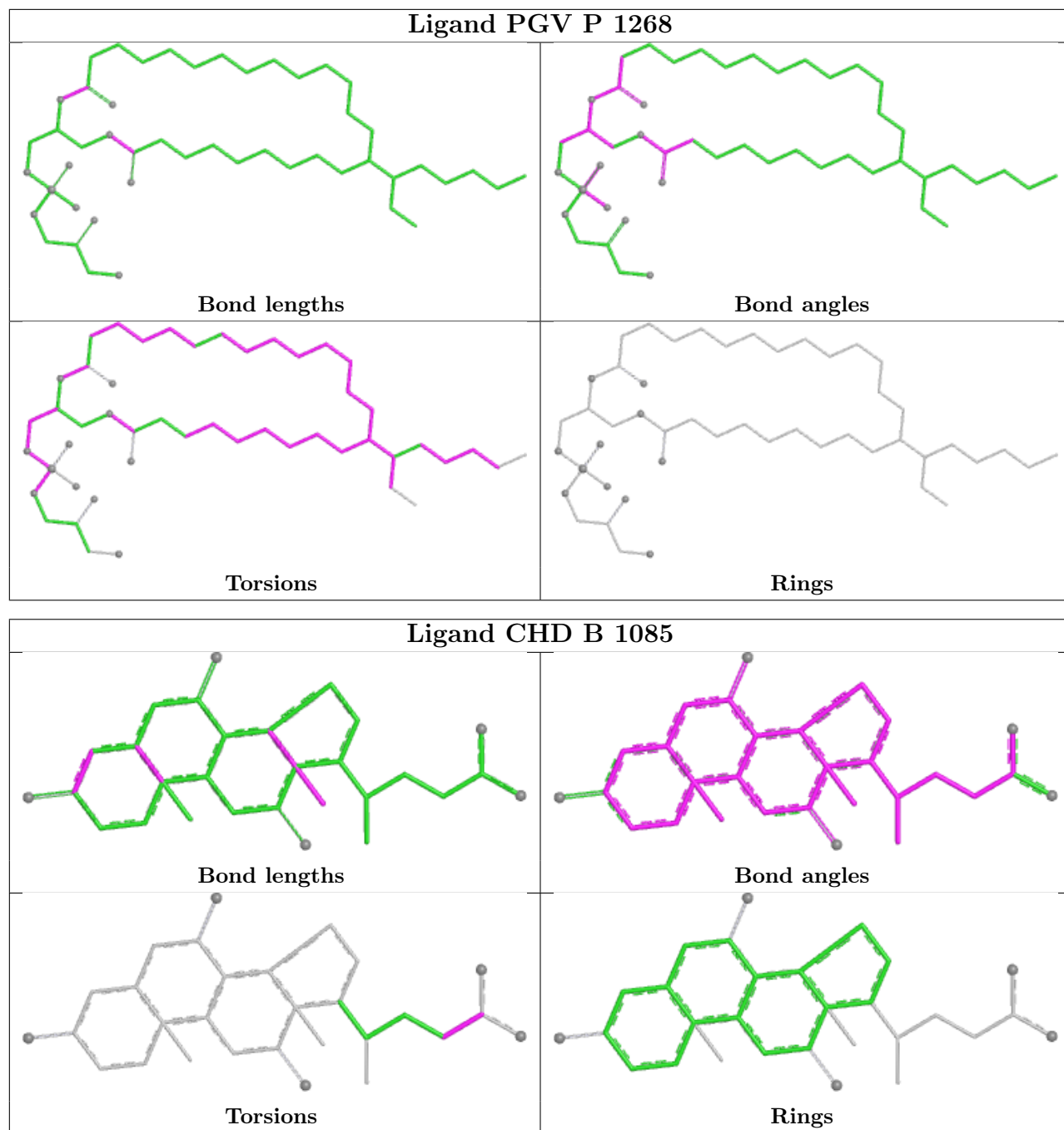


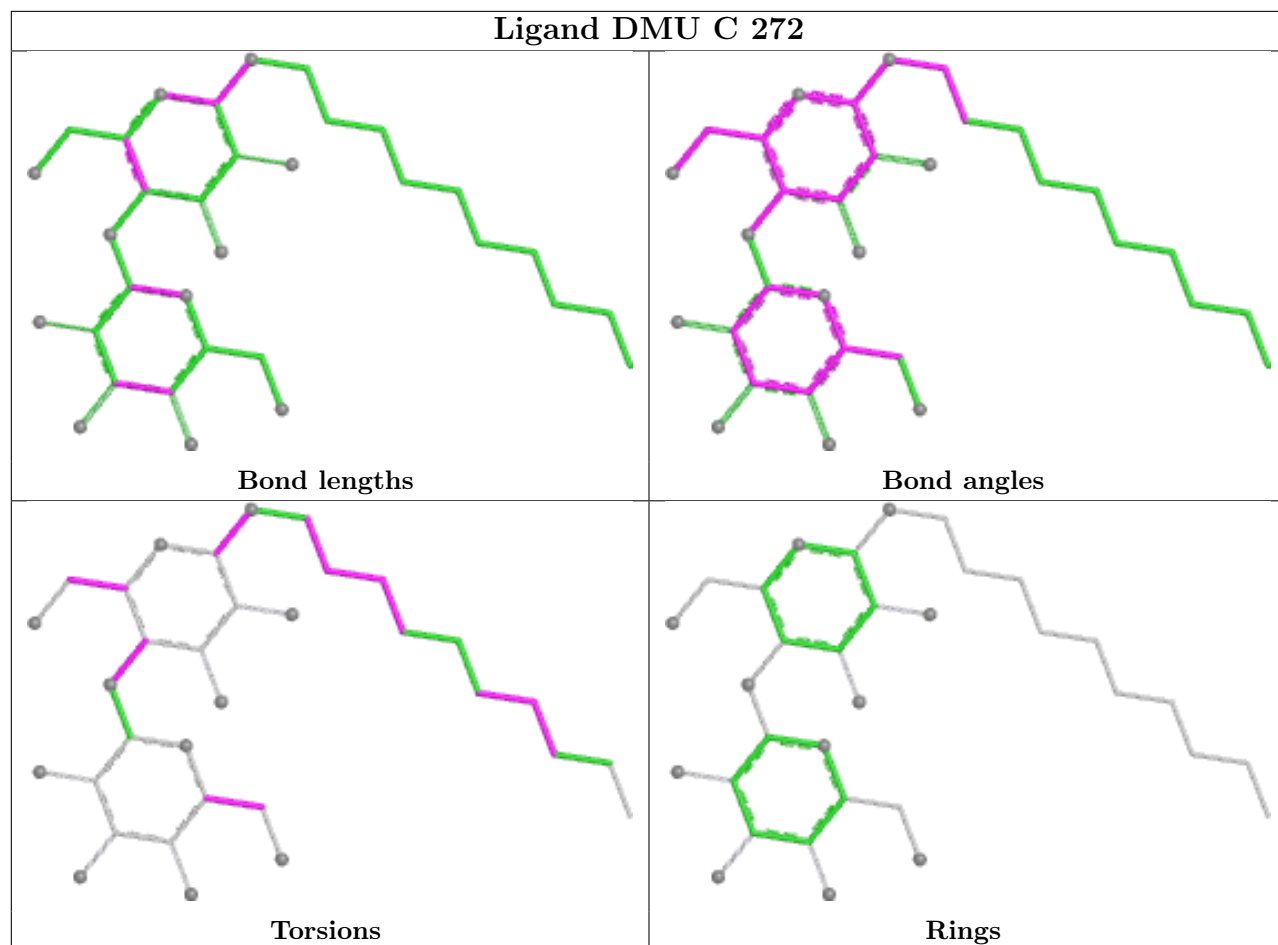
Ligand CHD W 1059

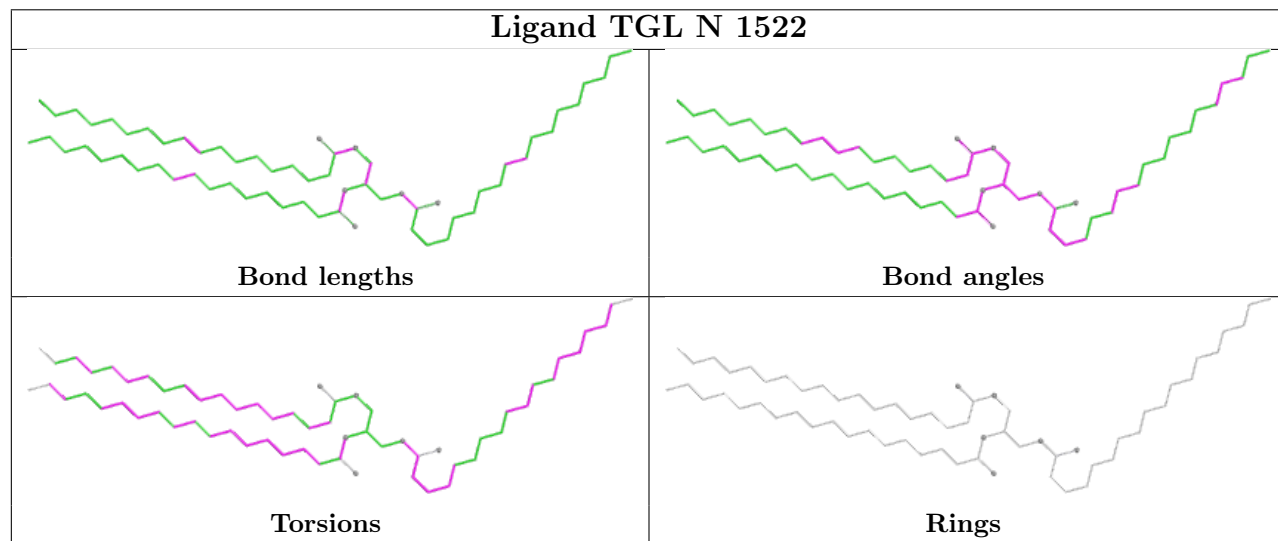
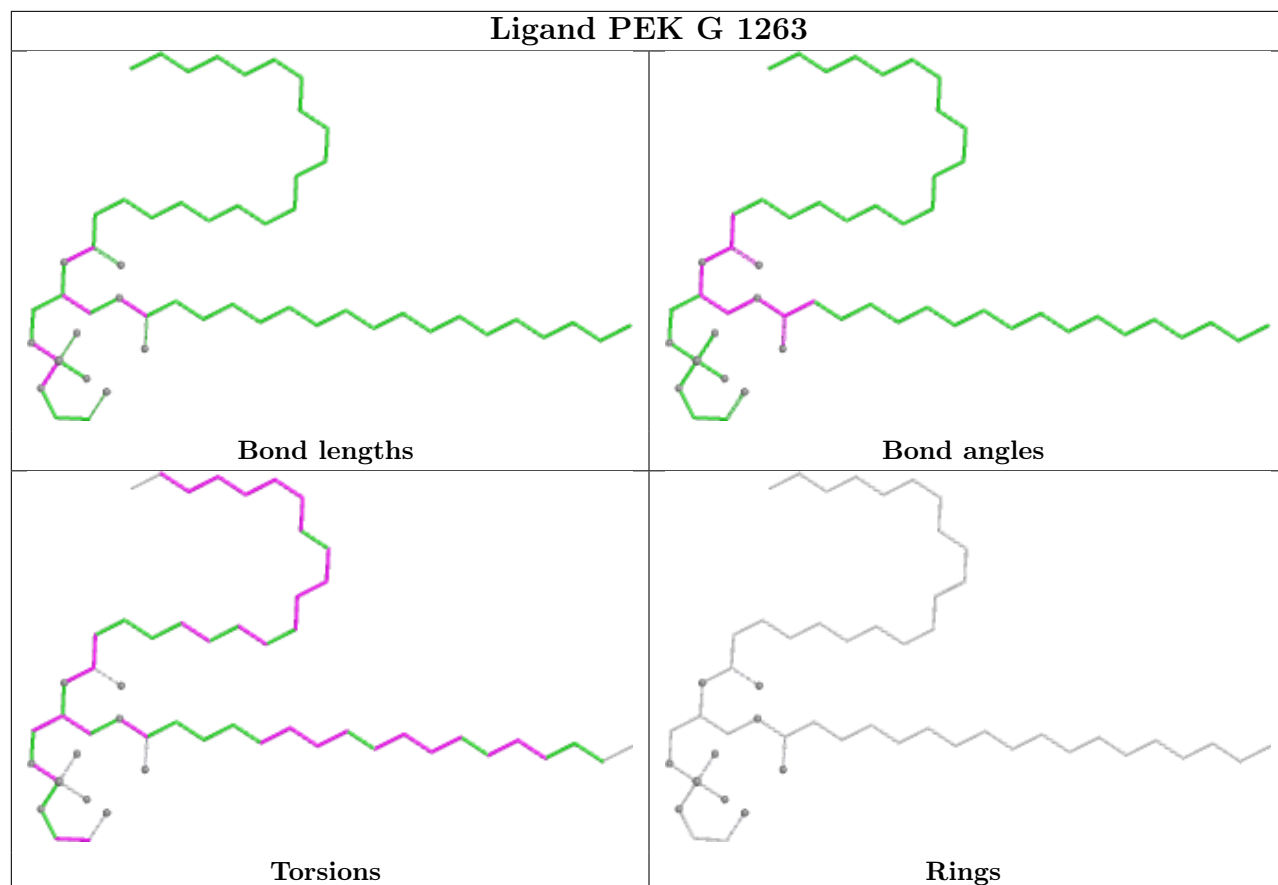


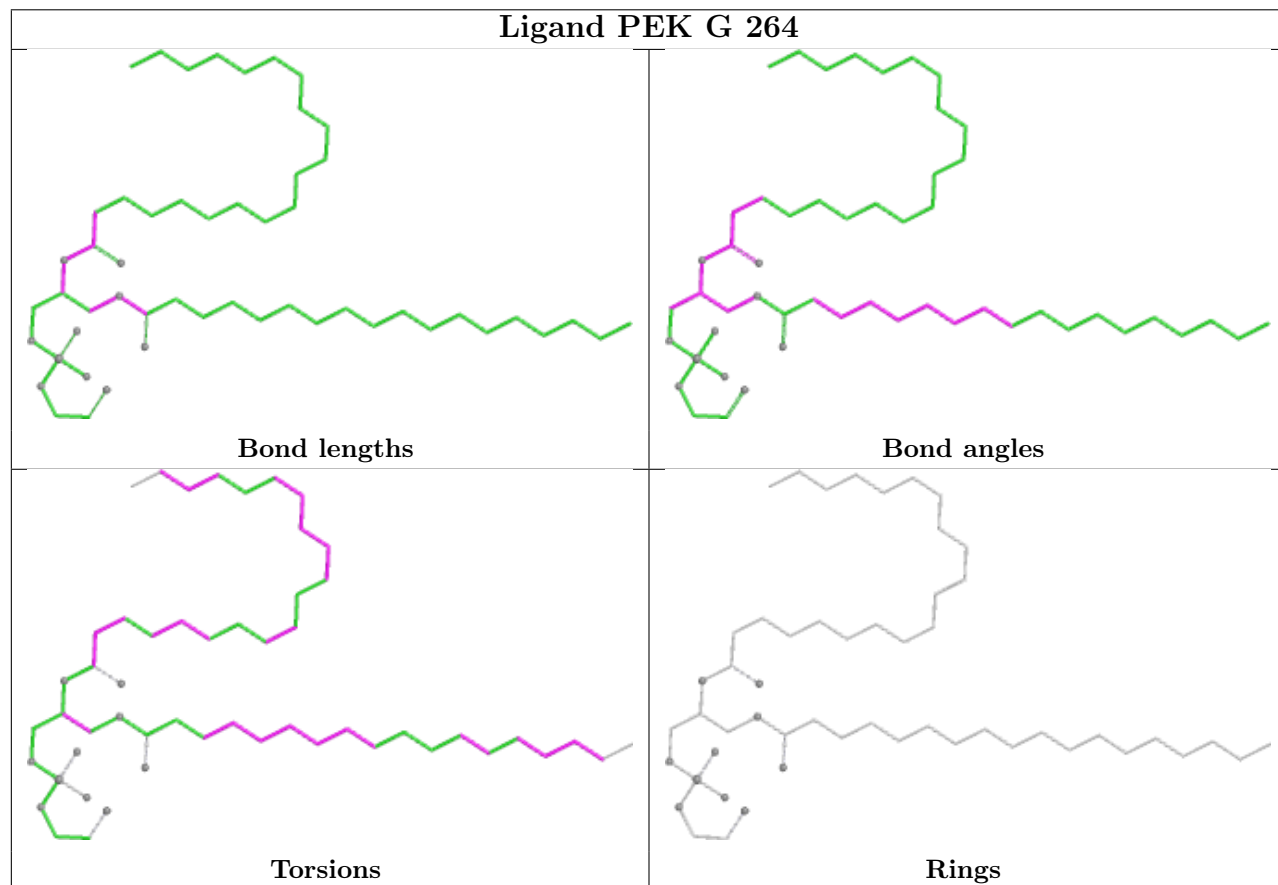
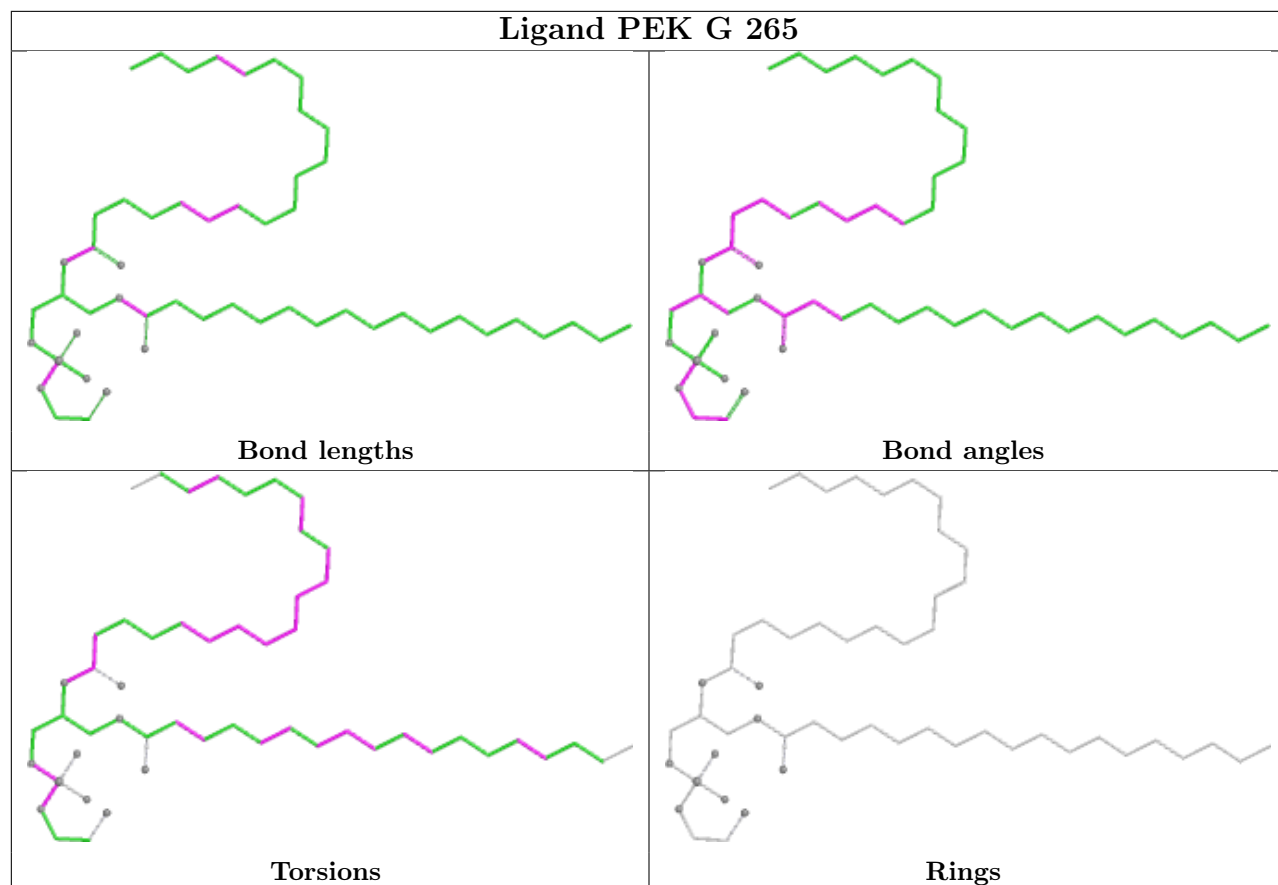
Ligand PGV N 1524

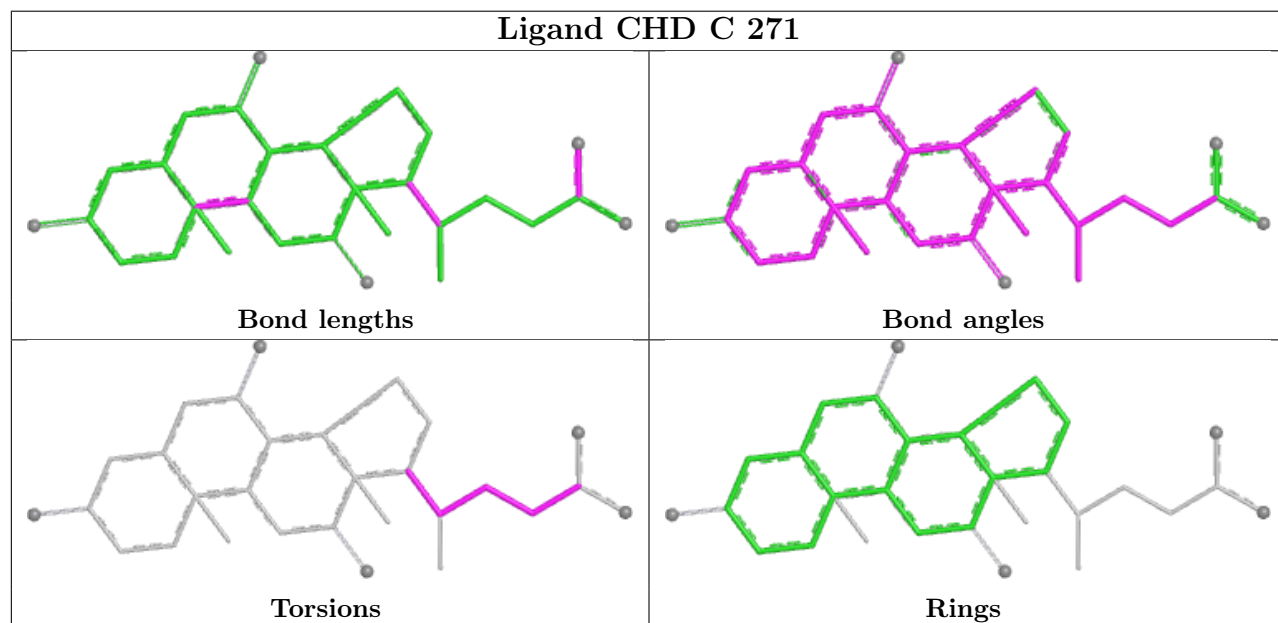
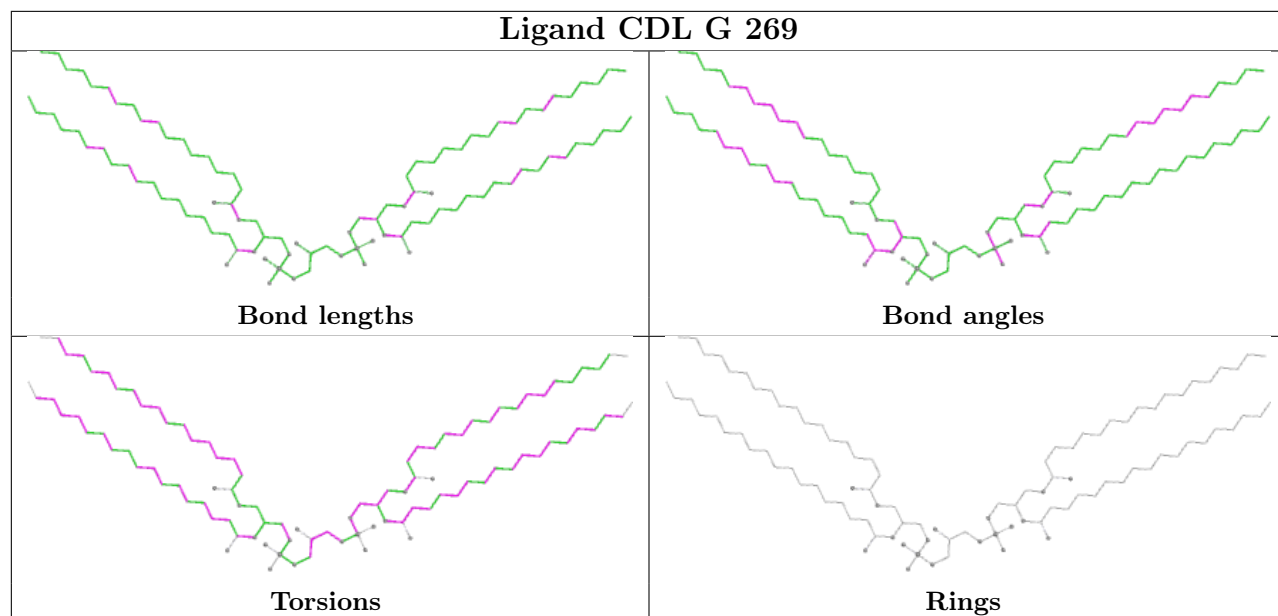




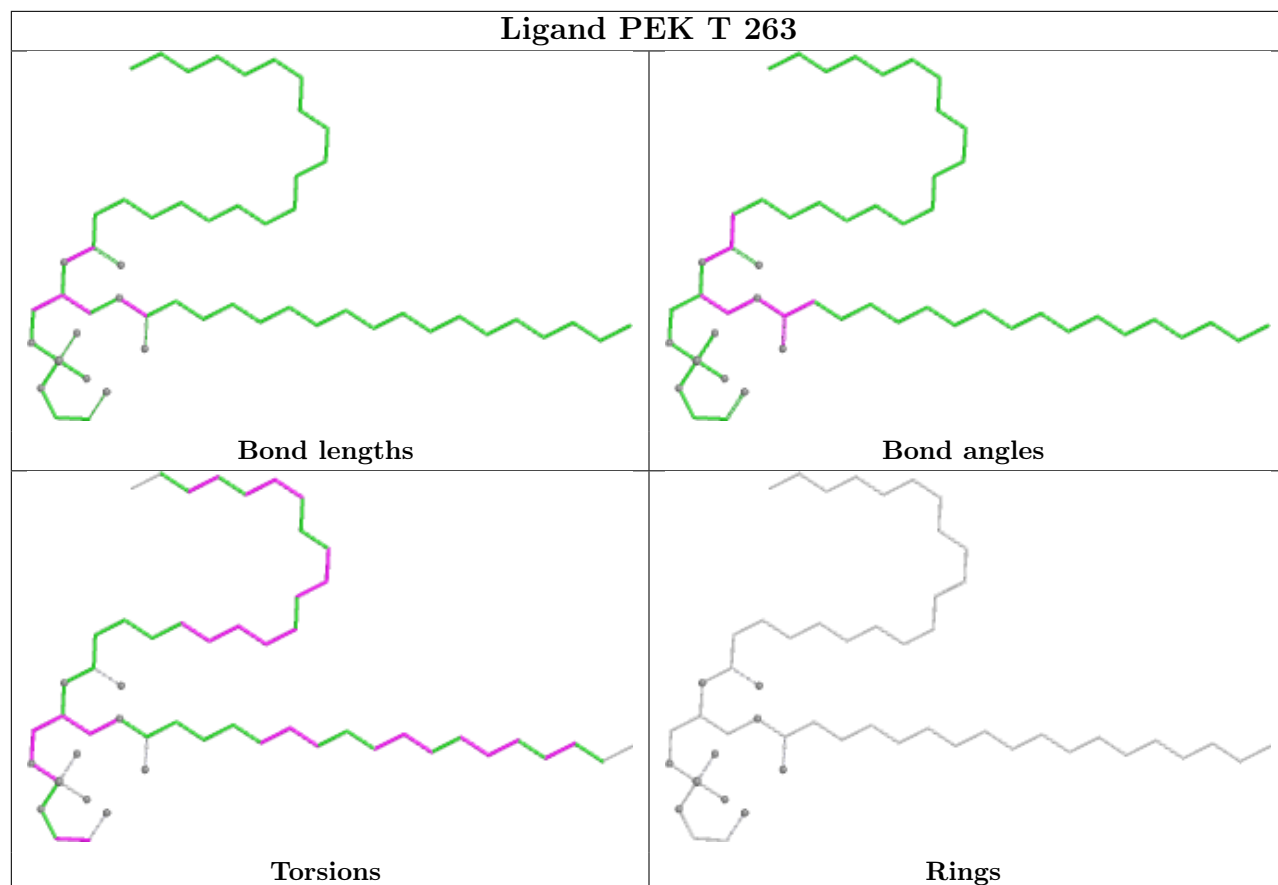




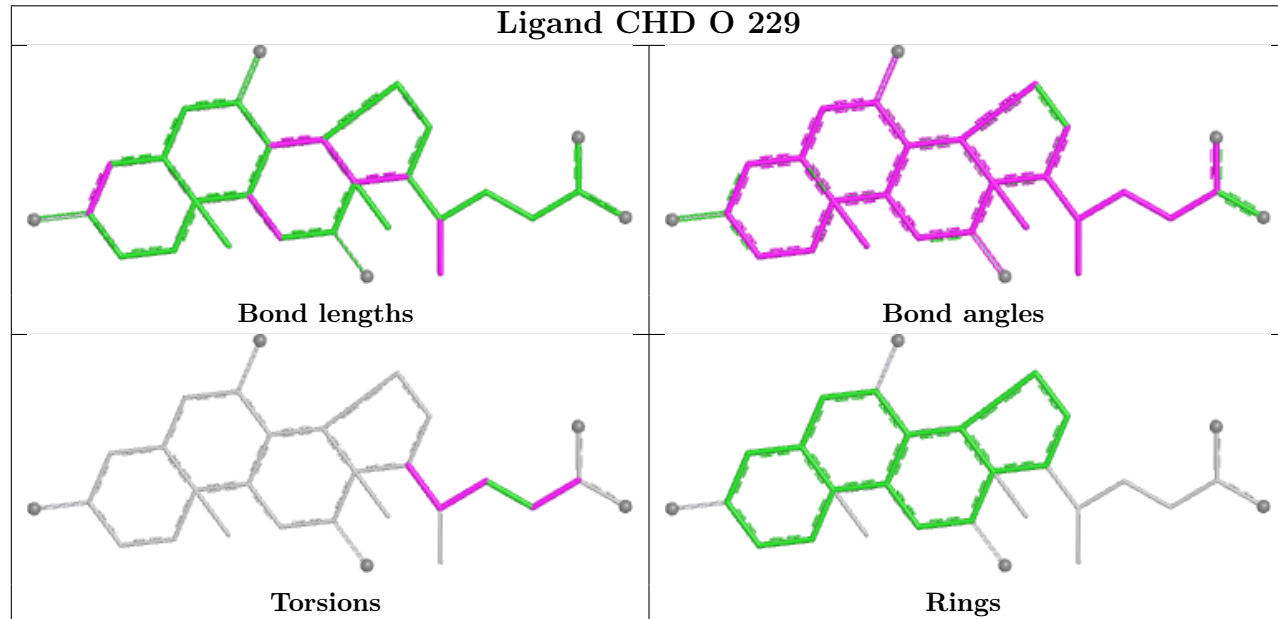


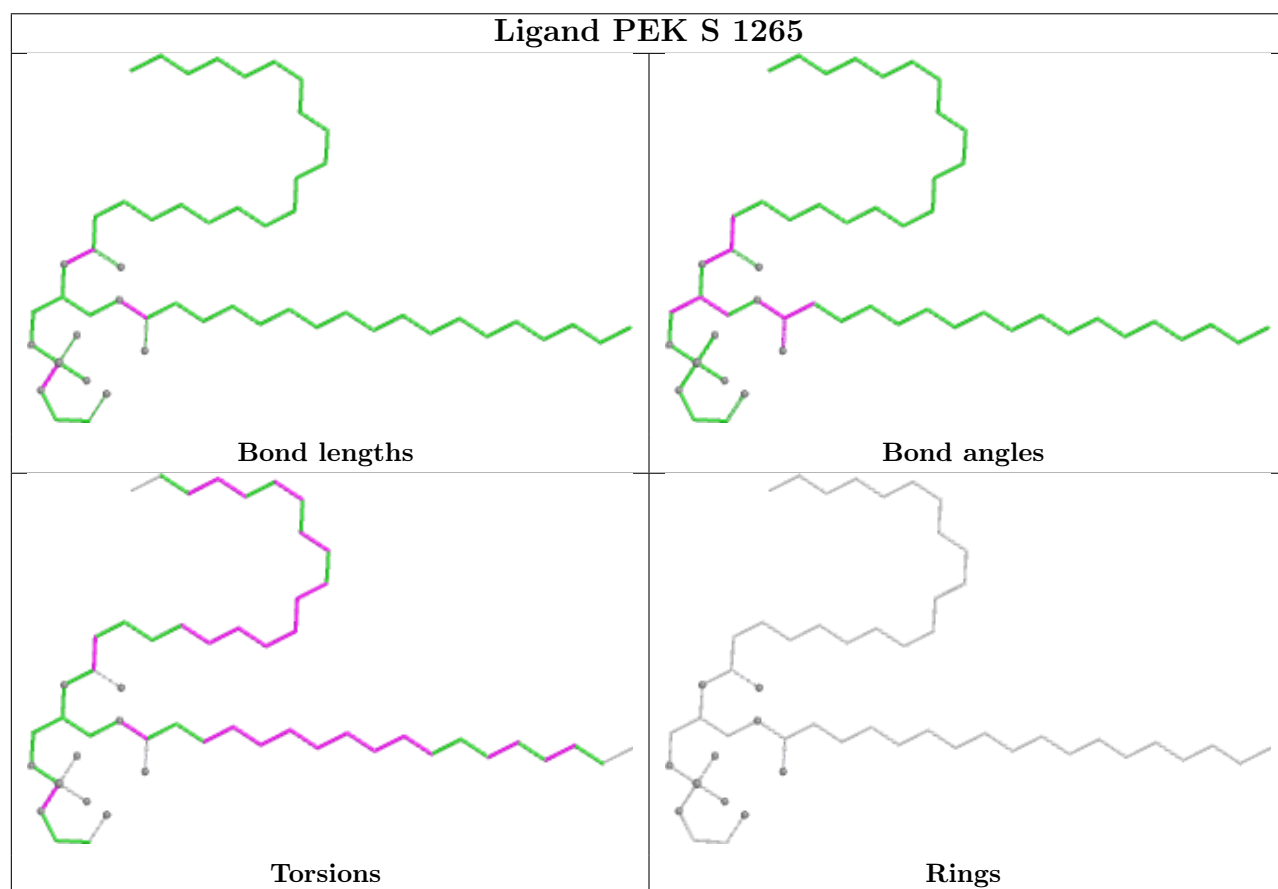
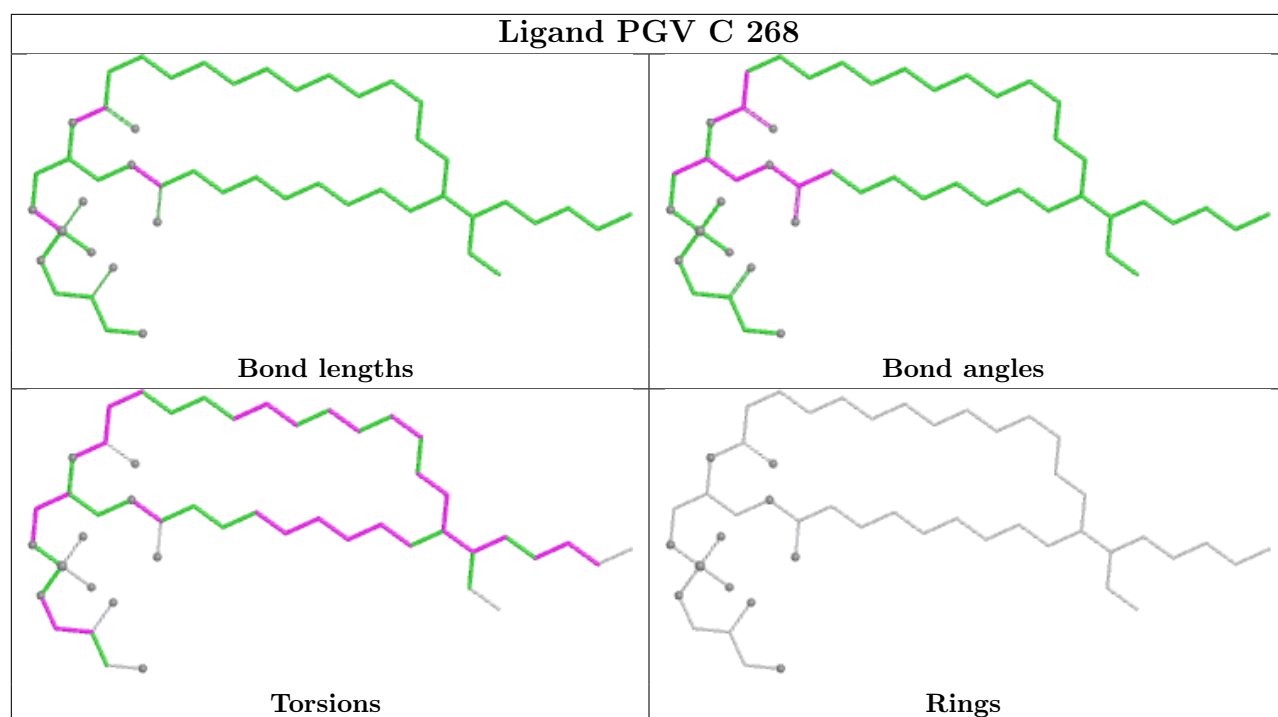


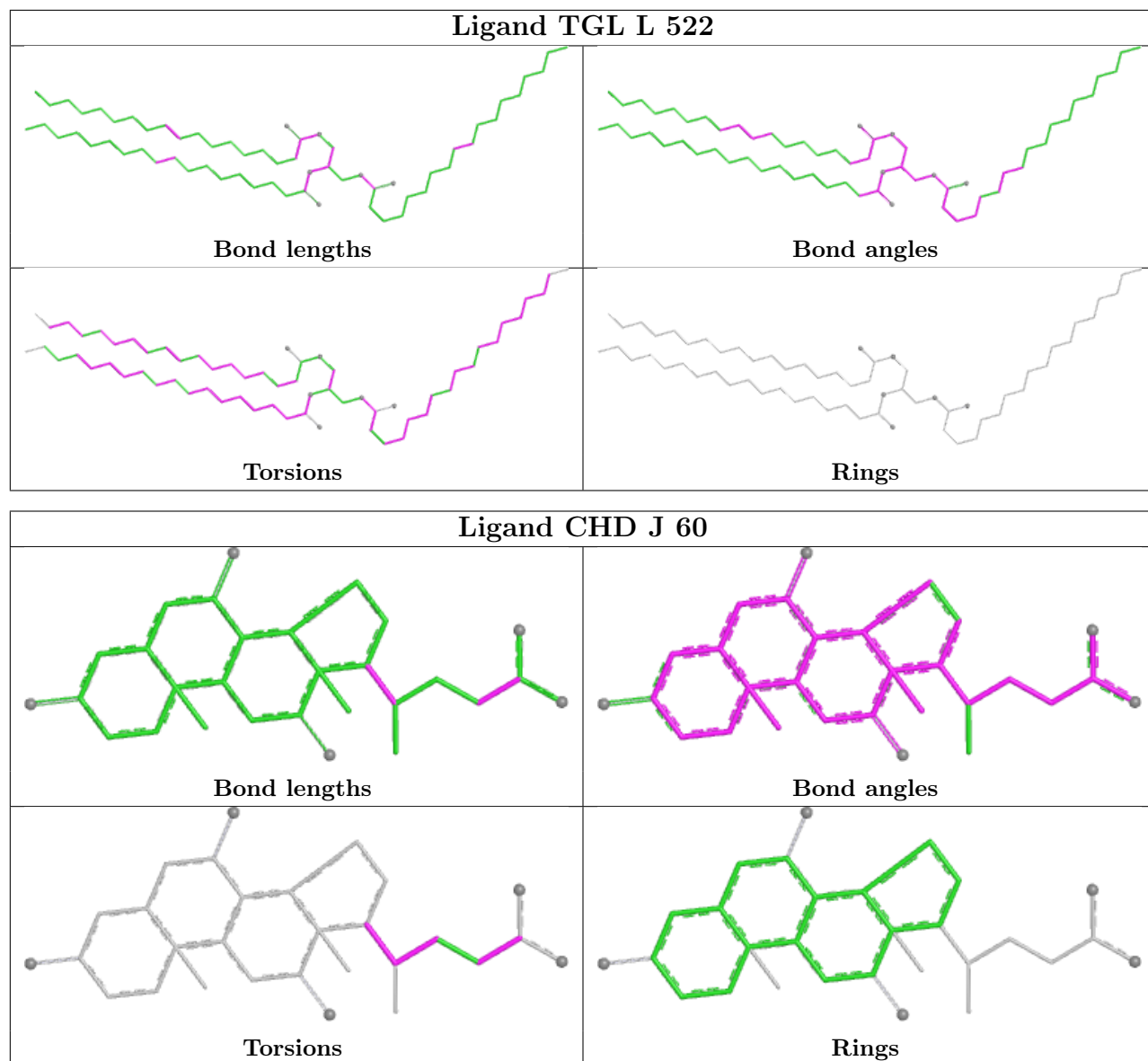
Ligand PEK T 263

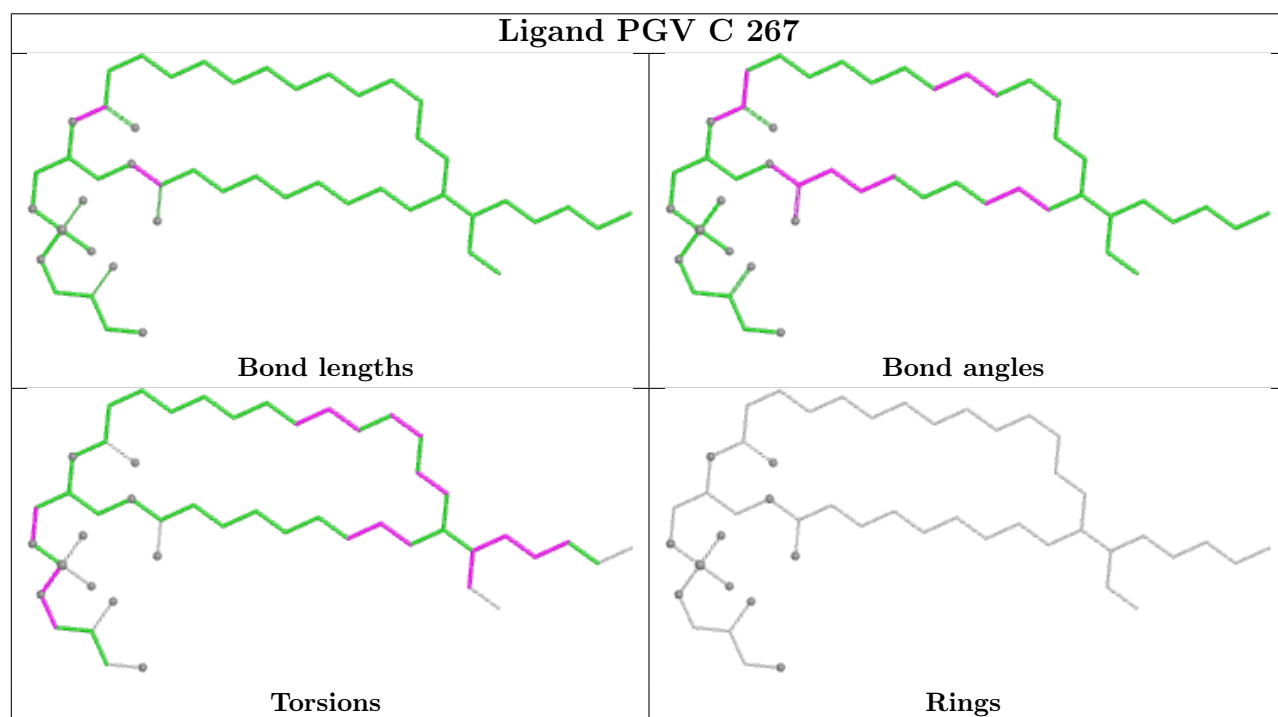
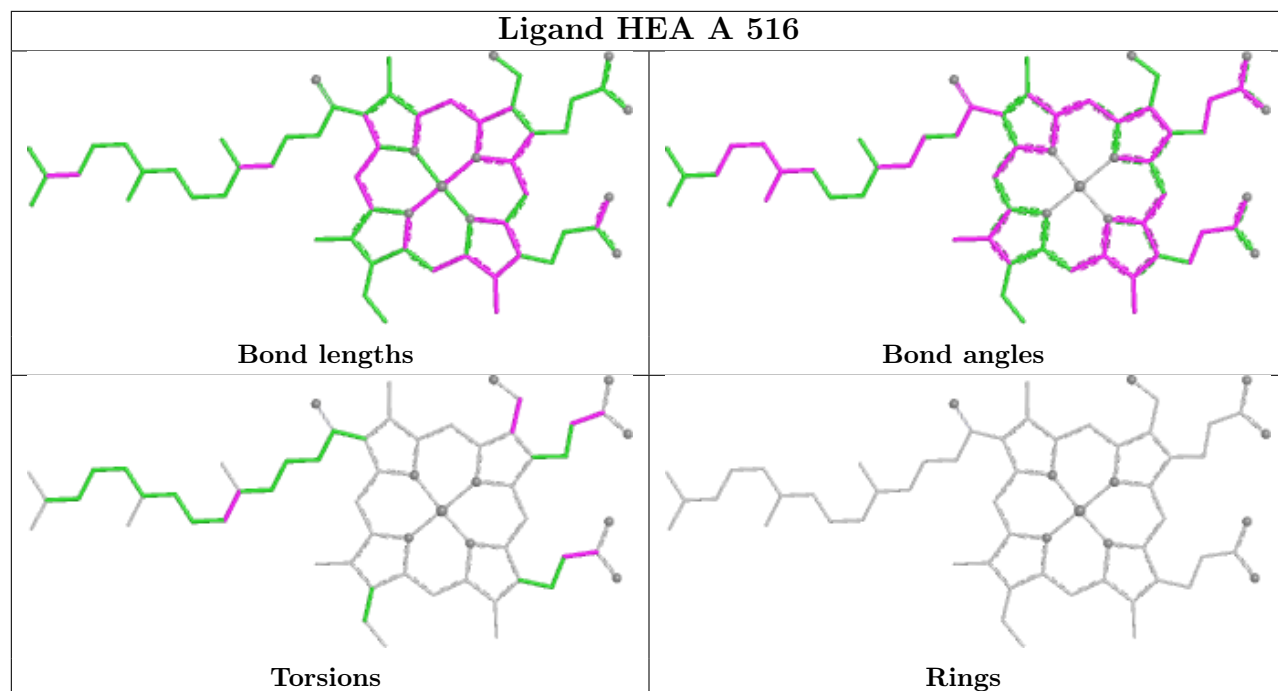


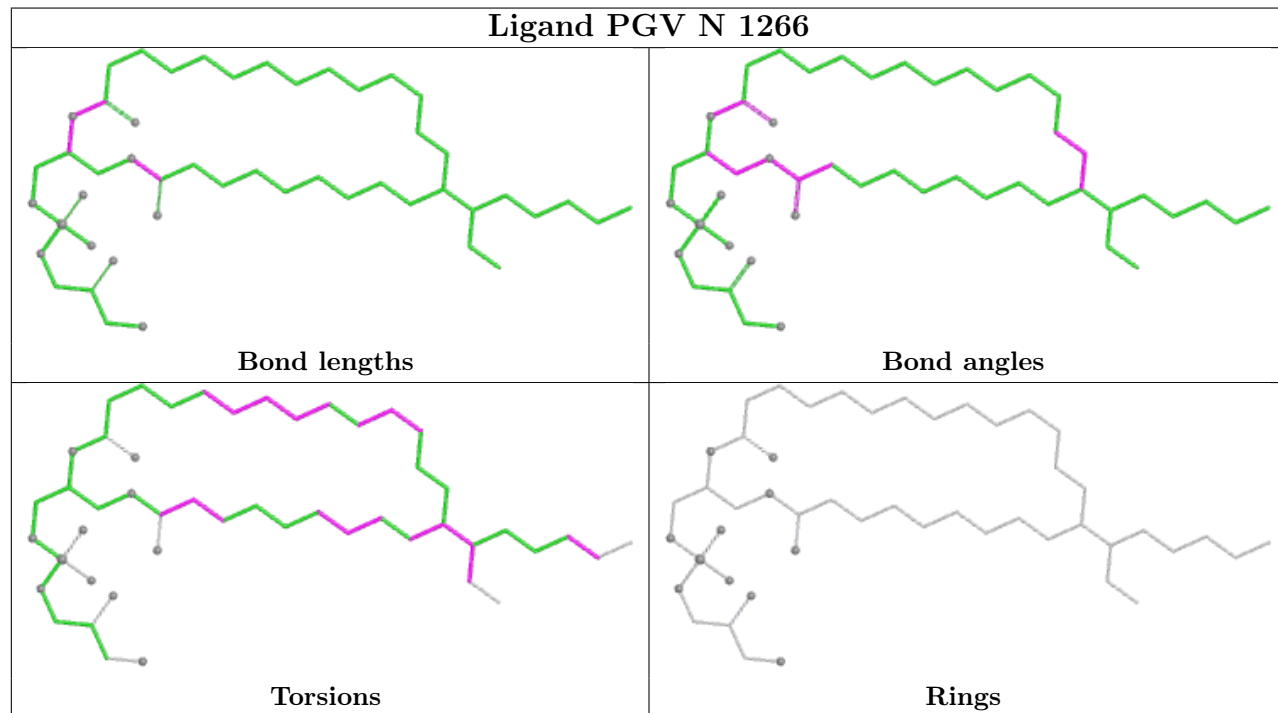
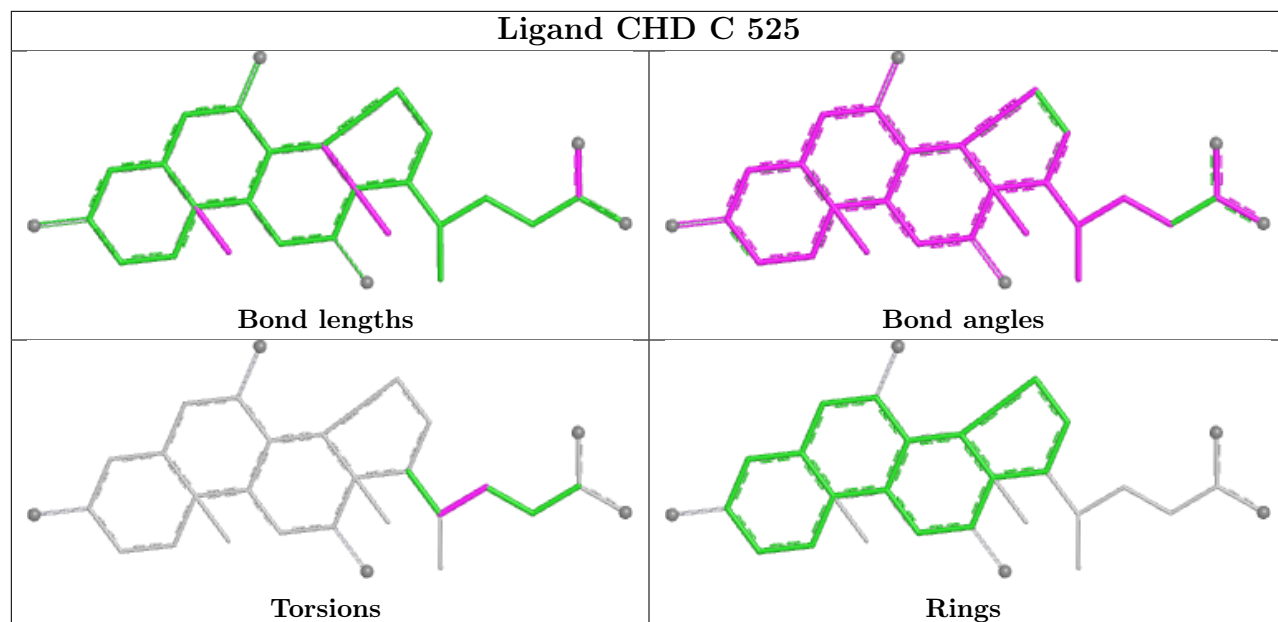
Ligand CHD O 229

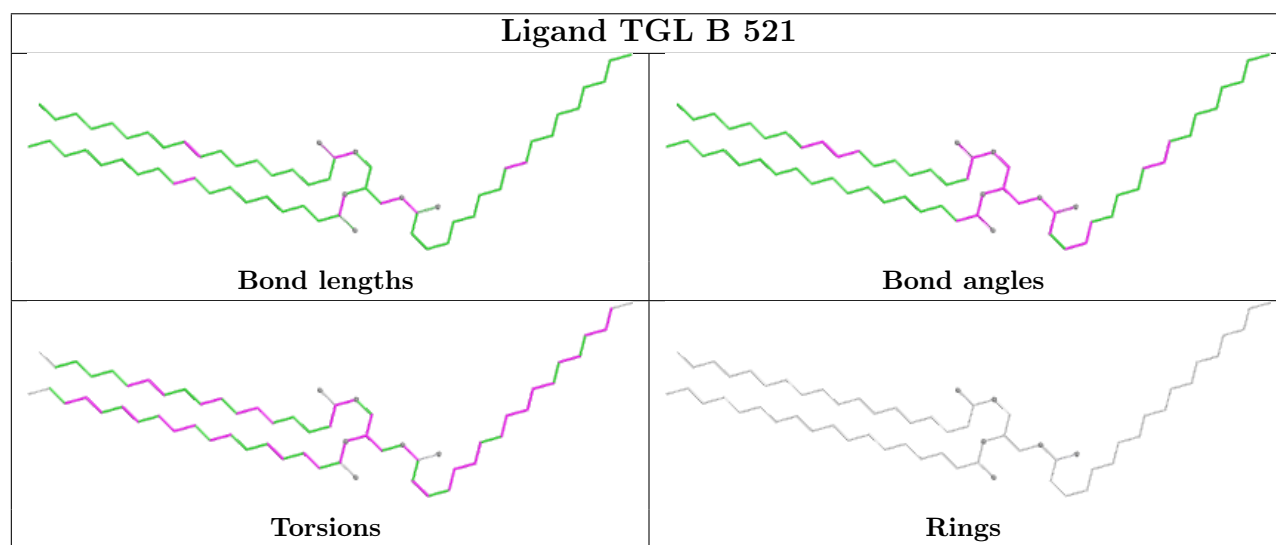
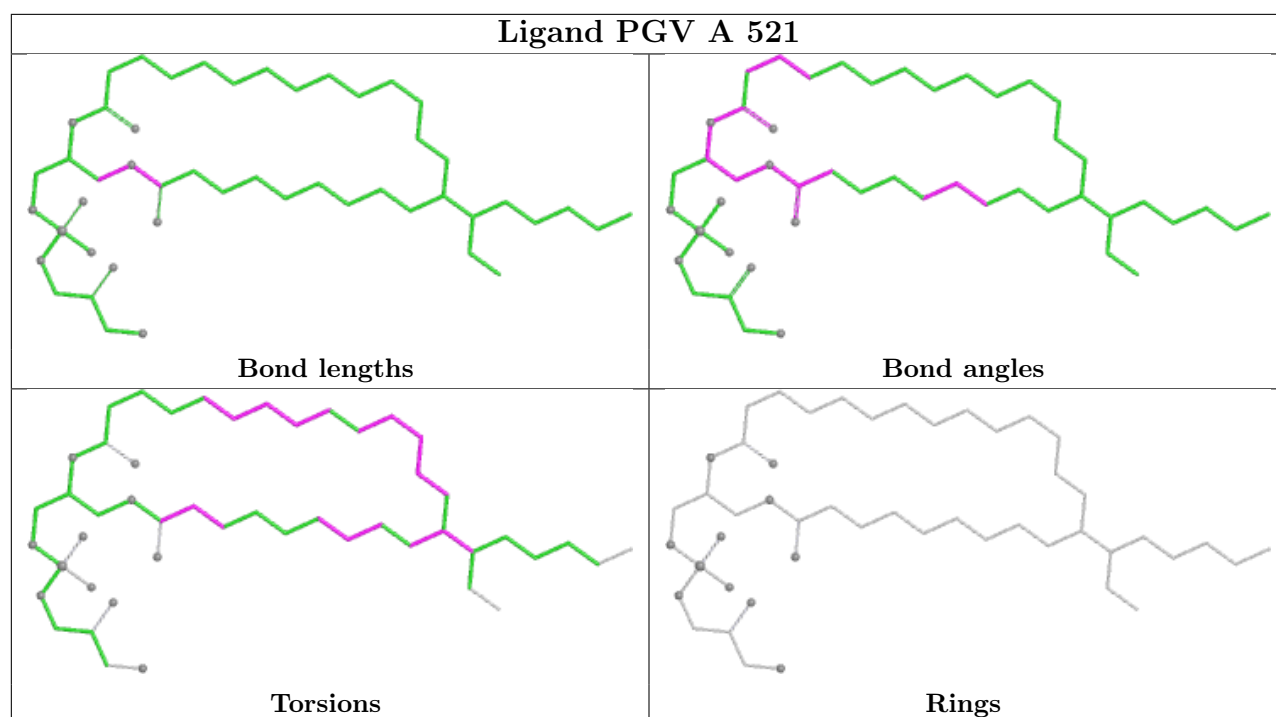


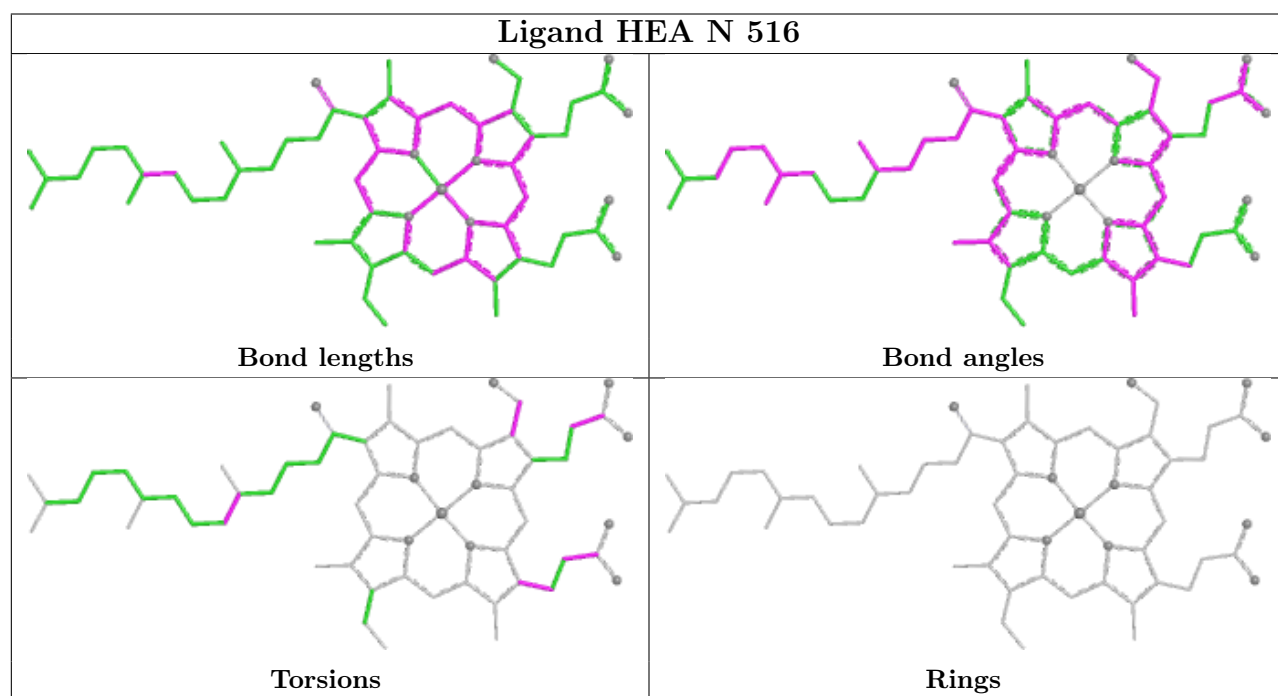
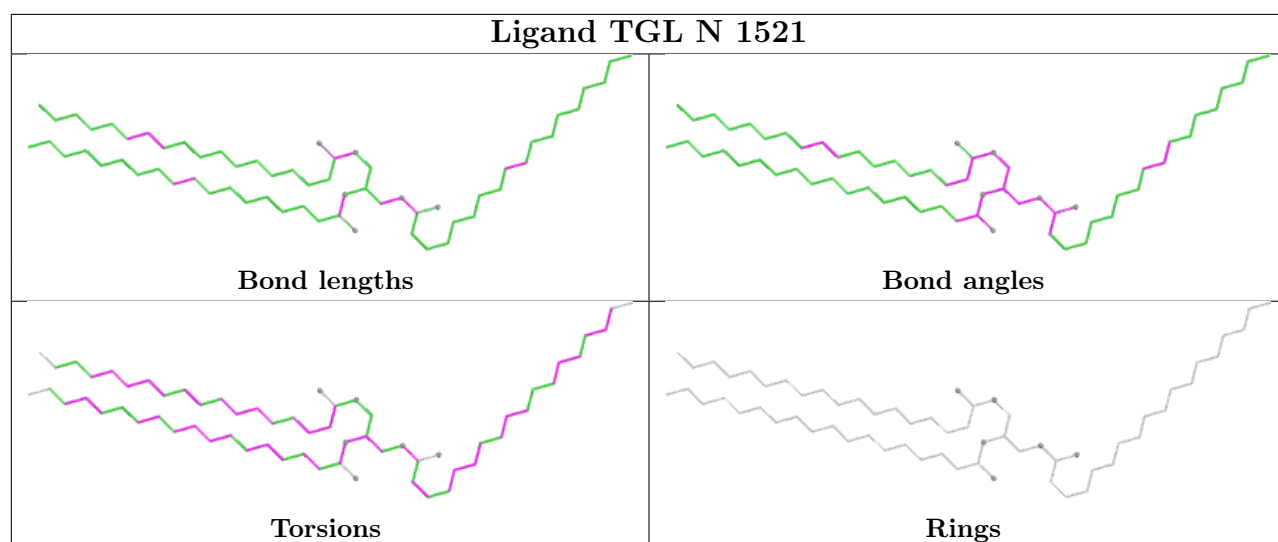


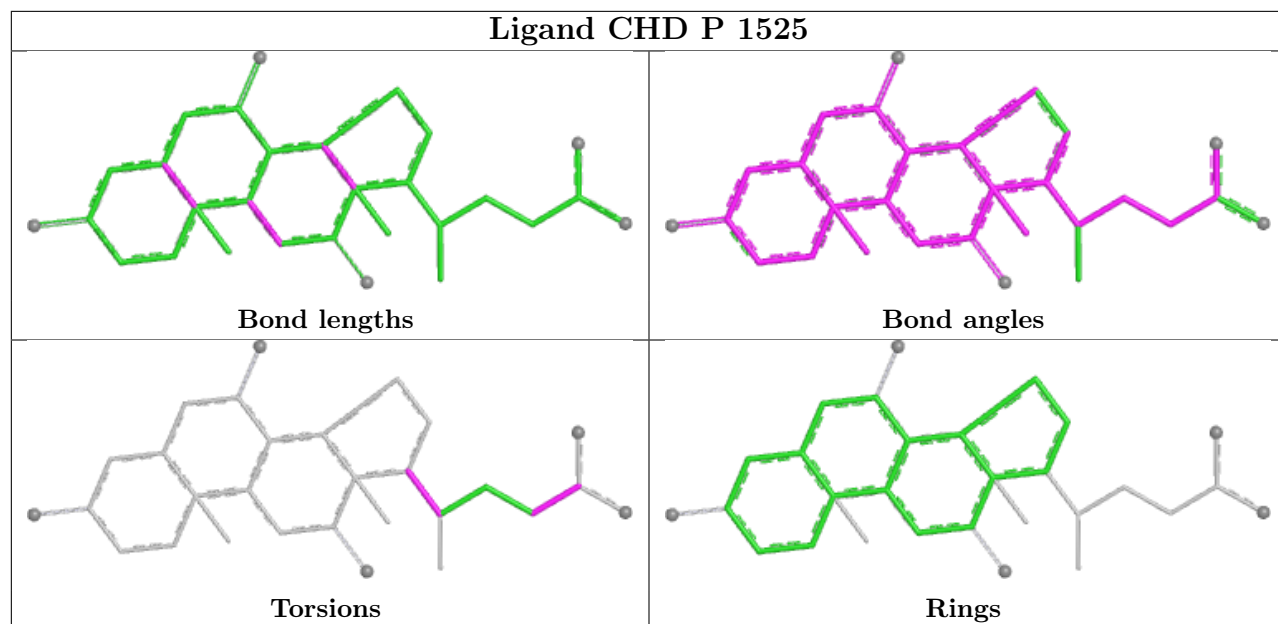












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	513/514 (99%)	-0.41	2 (0%) 88 87	36, 42, 52, 84	0
1	N	513/514 (99%)	0.08	4 (0%) 82 80	43, 51, 63, 92	0
2	B	226/227 (99%)	-0.07	6 (2%) 56 53	36, 48, 78, 111	0
2	O	226/227 (99%)	0.51	8 (3%) 47 44	49, 61, 93, 120	0
3	C	259/261 (99%)	-0.43	2 (0%) 82 80	38, 45, 59, 86	0
3	P	259/261 (99%)	-0.02	5 (1%) 66 63	44, 51, 68, 88	0
4	D	144/147 (97%)	-0.19	2 (1%) 73 71	43, 51, 75, 91	0
4	Q	144/147 (97%)	0.70	9 (6%) 26 23	55, 69, 96, 132	0
5	E	105/109 (96%)	-0.26	1 (0%) 79 77	43, 51, 83, 118	0
5	R	105/109 (96%)	0.05	2 (1%) 66 63	51, 63, 92, 123	0
6	F	98/98 (100%)	0.09	8 (8%) 17 15	40, 53, 112, 143	0
6	S	98/98 (100%)	0.24	8 (8%) 17 15	49, 61, 113, 144	0
7	G	83/85 (97%)	0.69	16 (19%) 3 2	42, 55, 123, 129	0
7	T	83/85 (97%)	0.79	17 (20%) 2 2	46, 62, 121, 133	0
8	H	79/85 (92%)	0.21	7 (8%) 15 13	46, 58, 119, 129	0
8	U	79/85 (92%)	0.45	7 (8%) 15 13	54, 69, 120, 127	0
9	I	72/73 (98%)	0.30	8 (11%) 10 8	48, 60, 105, 112	0
9	V	72/73 (98%)	0.74	9 (12%) 8 6	52, 74, 109, 112	0
10	J	58/59 (98%)	0.21	2 (3%) 48 45	45, 58, 86, 119	0
10	W	58/59 (98%)	0.68	3 (5%) 33 29	54, 66, 88, 120	0
11	K	49/56 (87%)	0.07	1 (2%) 65 62	45, 57, 75, 83	0
11	X	49/56 (87%)	0.66	3 (6%) 27 24	62, 69, 85, 99	0
12	L	46/47 (97%)	-0.09	1 (2%) 62 59	43, 48, 70, 100	0
12	Y	46/47 (97%)	0.72	3 (6%) 25 22	53, 61, 82, 100	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	-0.04	3 (6%) 22 19	44, 51, 88, 120	0
13	Z	43/46 (93%)	0.76	2 (4%) 36 33	57, 65, 96, 121	0
All	All	3550/3614 (98%)	0.08	139 (3%) 43 40	36, 53, 92, 144	0

The worst 5 of 139 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	6	VAL	8.2
6	F	1	ALA	8.1
8	H	8	ILE	7.8
6	S	1	ALA	7.2
7	G	3	ALA	7.2

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
9	SAC	V	1	9/10	0.34	0.21	110,112,114,115	0
7	TPO	T	11	11/12	0.39	0.28	97,105,129,130	0
9	SAC	I	1	9/10	0.45	0.22	99,103,106,106	0
7	TPO	G	11	11/12	0.48	0.34	93,102,125,127	0
1	FME	N	1	10/11	0.77	0.28	77,82,105,107	0
1	FME	A	1	10/11	0.83	0.20	63,70,93,102	0
2	FME	O	1	10/11	0.93	0.15	59,59,64,64	0
2	FME	B	1	10/11	0.98	0.07	46,48,51,61	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column

labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	UNX	C	262	1/1	0.56	0.52	75,75,75,75	0
24	UNX	P	262	1/1	0.70	0.45	75,75,75,75	0
28	PEK	G	1263	53/53	0.75	0.29	83,126,150,150	0
28	PEK	T	263	53/53	0.76	0.27	78,123,145,149	0
23	CHD	W	1059	29/29	0.77	0.20	110,117,120,122	0
22	PSC	B	229	52/52	0.78	0.24	70,117,150,150	0
23	CHD	J	60	29/29	0.80	0.18	103,112,119,120	0
26	DMU	C	272	33/33	0.80	0.20	96,129,132,134	0
20	PGV	C	268	51/51	0.81	0.26	78,103,119,120	0
26	DMU	T	1272	33/33	0.81	0.21	111,140,141,141	0
22	PSC	R	1229	52/52	0.81	0.26	73,120,150,150	0
20	PGV	P	1268	51/51	0.81	0.26	78,108,125,126	0
19	TGL	A	523	63/63	0.82	0.31	78,102,131,132	0
19	TGL	N	1523	63/63	0.82	0.29	84,111,131,133	0
19	TGL	N	1522	63/63	0.83	0.27	72,95,111,112	0
28	PEK	G	265	53/53	0.83	0.23	70,109,135,138	0
25	CDL	G	269	100/100	0.83	0.28	89,118,138,141	0
20	PGV	N	1524	51/51	0.83	0.24	67,106,139,140	0
25	CDL	T	1269	100/100	0.85	0.26	92,117,138,143	0
28	PEK	S	1265	53/53	0.85	0.25	75,112,133,136	0
19	TGL	B	521	63/63	0.85	0.25	54,96,118,120	0
20	PGV	A	524	51/51	0.86	0.22	62,101,132,135	0
19	TGL	N	1521	63/63	0.86	0.24	69,101,120,123	0
25	CDL	C	270	100/100	0.87	0.22	56,112,137,139	0
19	TGL	L	522	63/63	0.87	0.25	57,89,109,113	0
25	CDL	P	1270	100/100	0.87	0.23	69,119,136,137	0
26	DMU	Z	1526	33/33	0.87	0.15	73,80,94,96	0
18	NA	N	519	1/1	0.91	0.22	58,58,58,58	0
23	CHD	C	271	29/29	0.92	0.15	86,97,99,99	0
26	DMU	M	526	33/33	0.92	0.10	52,63,87,91	0
23	CHD	P	1271	29/29	0.94	0.12	98,101,103,104	0
23	CHD	P	1525	29/29	0.95	0.09	48,54,57,59	0
28	PEK	G	264	53/53	0.95	0.14	44,65,107,109	0
23	CHD	B	1085	29/29	0.96	0.07	46,50,53,59	0
23	CHD	O	229	29/29	0.96	0.07	45,49,56,62	0
28	PEK	T	1264	53/53	0.96	0.14	49,70,109,111	0
20	PGV	N	1266	51/51	0.97	0.11	45,60,81,84	0
23	CHD	C	525	29/29	0.97	0.07	38,50,57,65	0
20	PGV	P	1267	51/51	0.97	0.12	45,56,102,106	0
20	PGV	A	521	51/51	0.97	0.10	36,53,77,79	0
15	CMO	N	520	2/2	0.97	0.06	47,47,47,48	0
17	MG	N	518	1/1	0.97	0.04	50,50,50,50	0

Continued on next page...

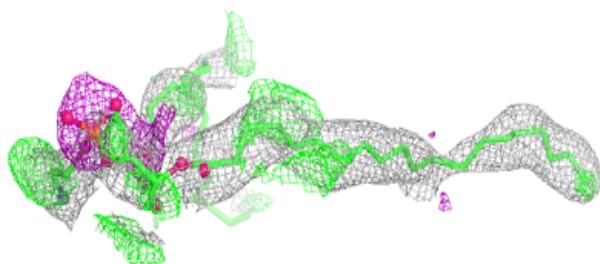
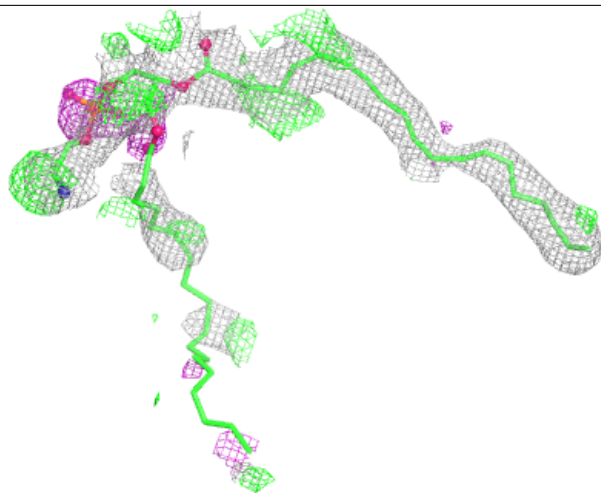
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
17	MG	A	518	1/1	0.98	0.07	40,40,40,40	0
21	CUA	O	228	2/2	0.98	0.04	52,52,52,54	0
20	PGV	C	267	51/51	0.98	0.10	38,52,95,97	0
14	HEA	N	515	60/60	0.98	0.09	47,52,65,66	0
14	HEA	N	516	60/60	0.98	0.07	42,48,69,74	0
15	CMO	A	520	2/2	0.98	0.05	39,39,39,41	0
14	HEA	A	516	60/60	0.98	0.06	32,40,56,64	0
21	CUA	B	228	2/2	0.99	0.03	41,41,41,42	0
27	ZN	F	99	1/1	0.99	0.02	48,48,48,48	0
18	NA	A	519	1/1	0.99	0.06	47,47,47,47	0
14	HEA	A	515	60/60	0.99	0.06	33,40,54,68	0
16	CU	N	517	1/1	1.00	0.02	49,49,49,49	0
16	CU	A	517	1/1	1.00	0.04	40,40,40,40	0
27	ZN	S	99	1/1	1.00	0.01	56,56,56,56	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.

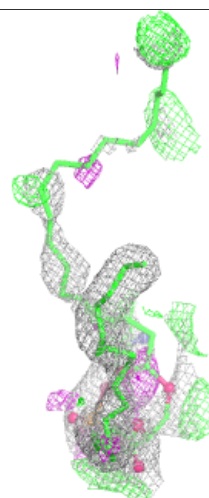
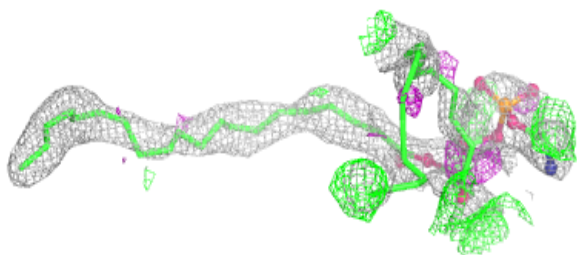
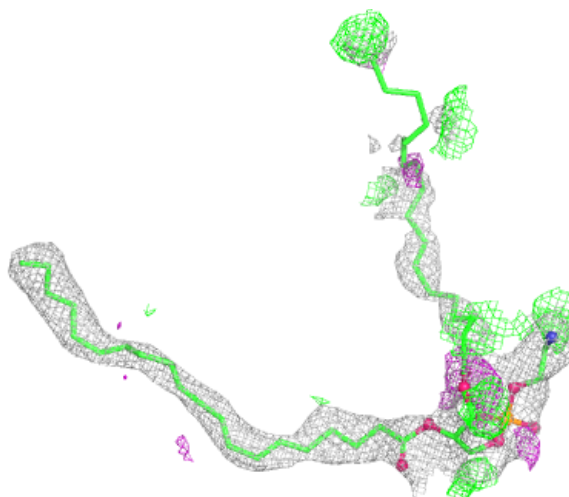
Electron density around PEK G 1263:

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



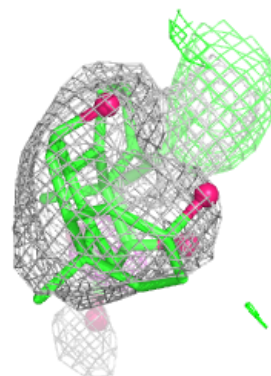
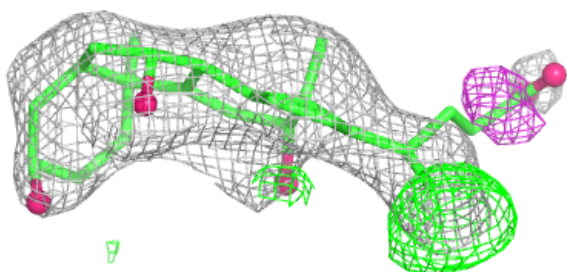
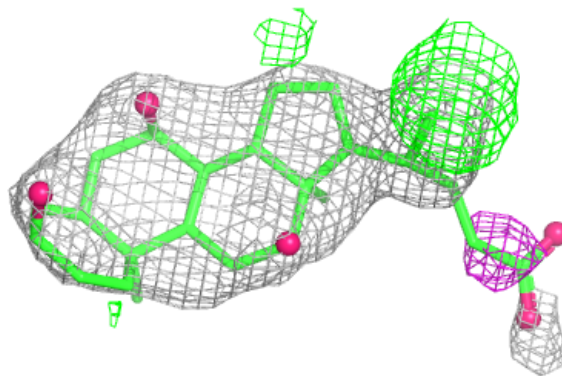
Electron density around PEK T 263:

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

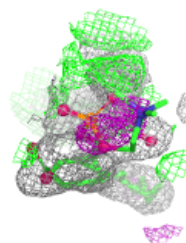
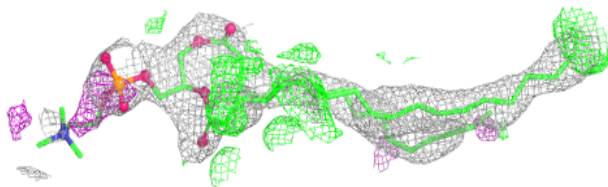
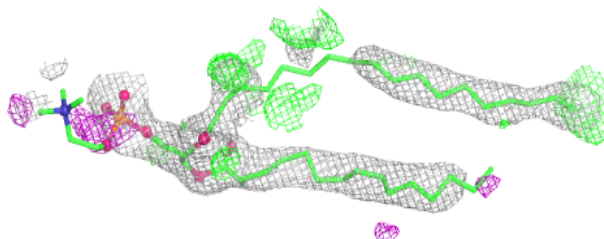


Electron density around CHD W 1059:

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

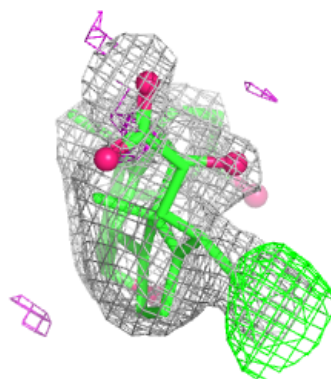
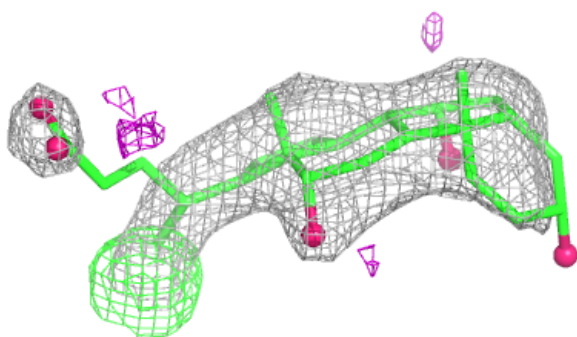
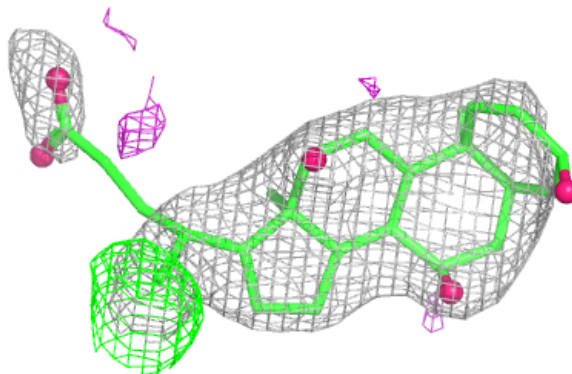
**Electron density around PSC B 229:**

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

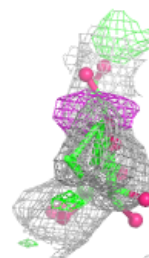
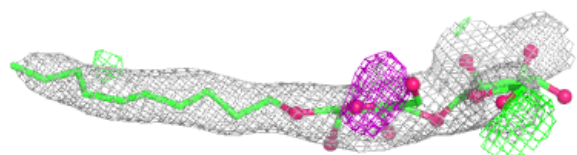
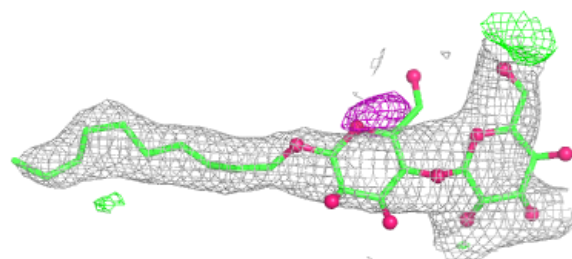


Electron density around CHD J 60:

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

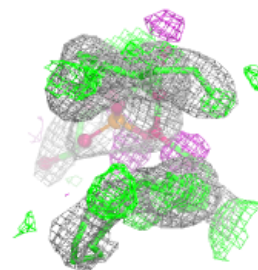
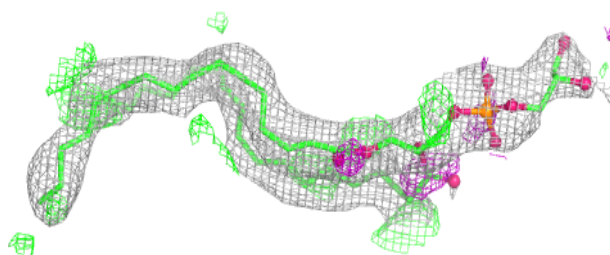
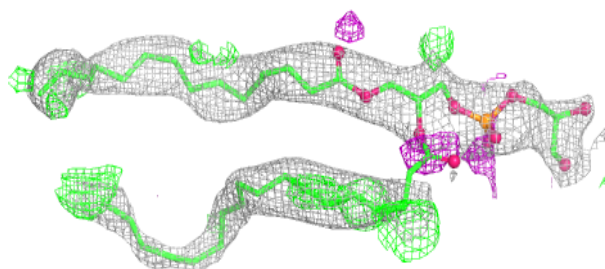
**Electron density around DMU C 272:**

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

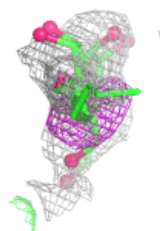
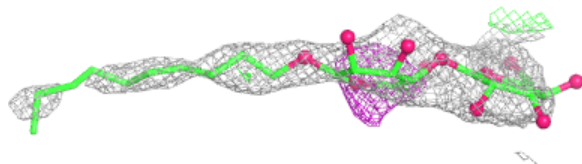
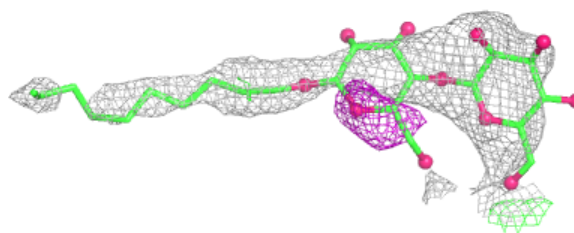


Electron density around PGV C 268:

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

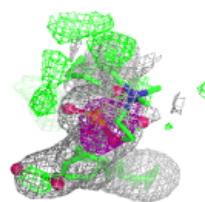
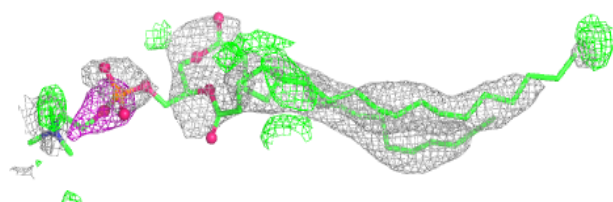
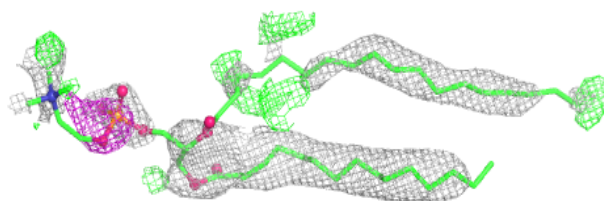
**Electron density around DMU T 1272:**

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

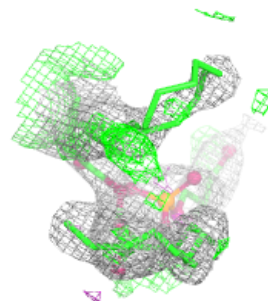
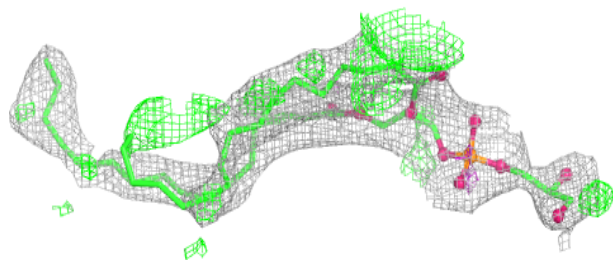
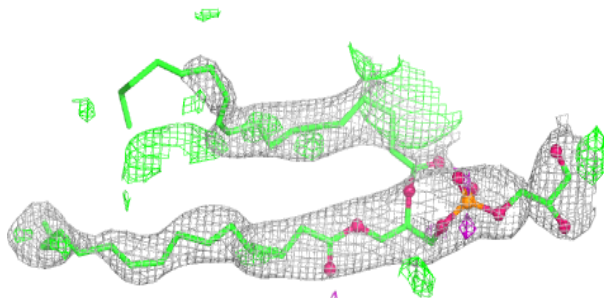


Electron density around PSC R 1229:

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

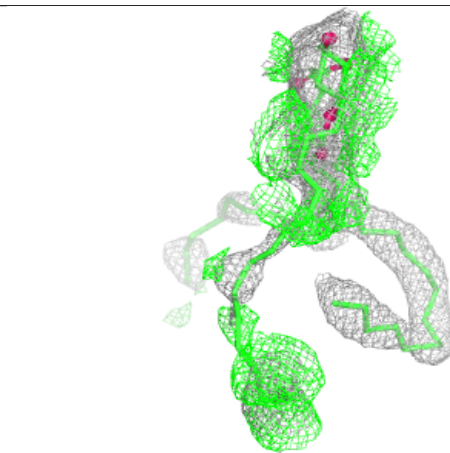
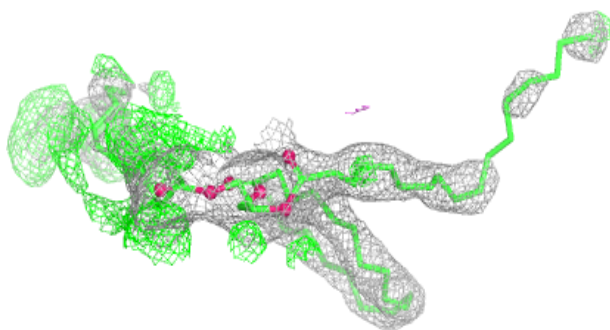
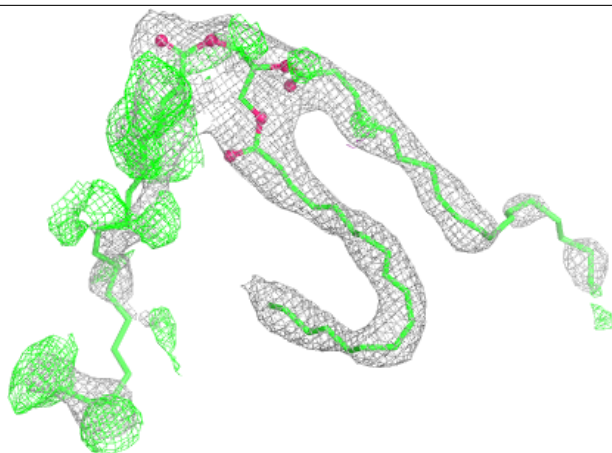
**Electron density around PGV P 1268:**

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

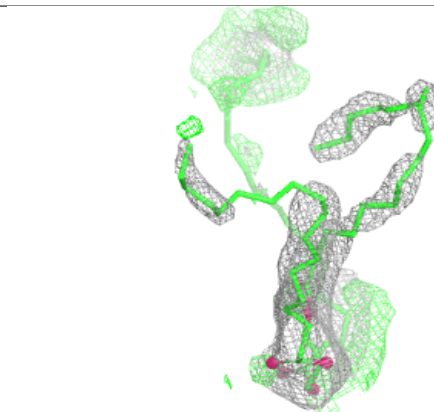
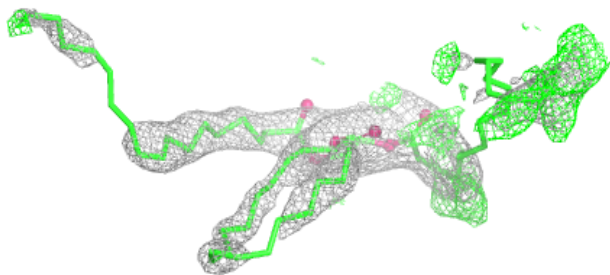
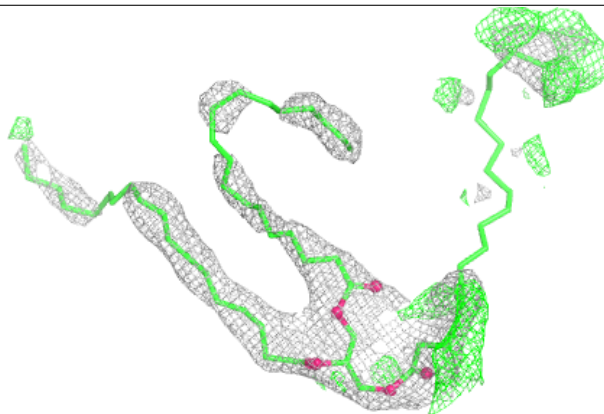


Electron density around TGL A 523:

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

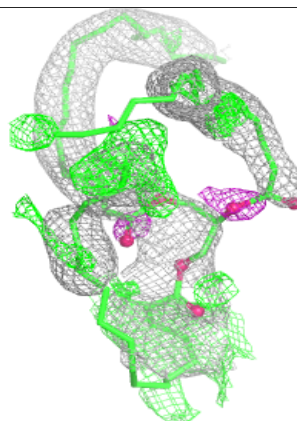
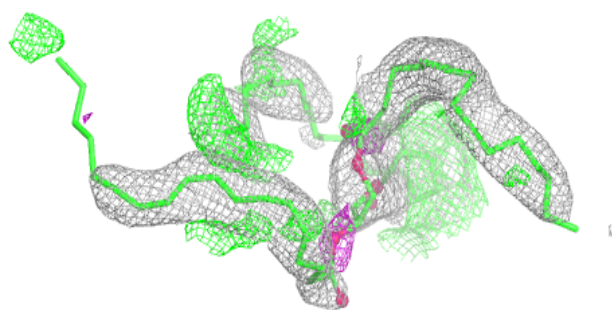
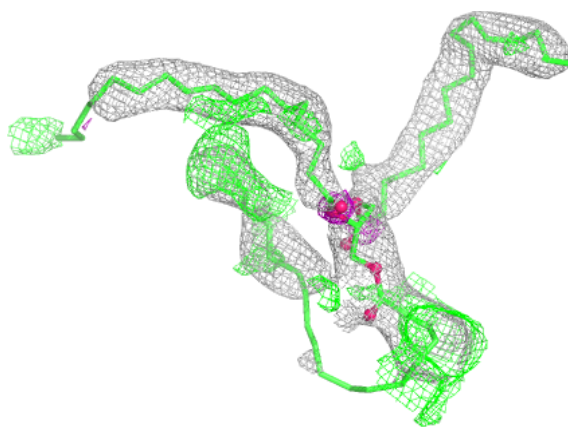
**Electron density around TGL N 1523:**

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



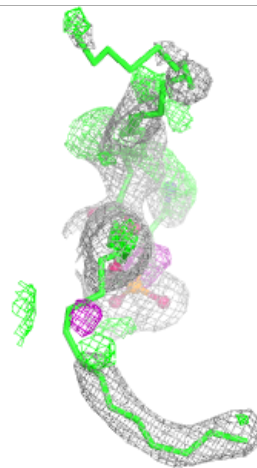
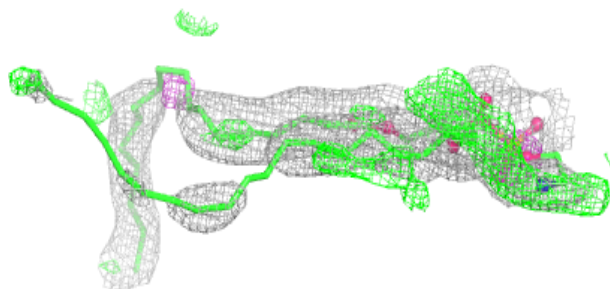
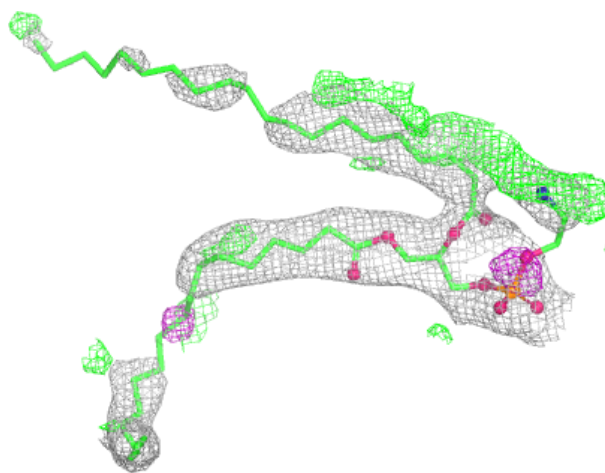
Electron density around TGL N 1522:

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



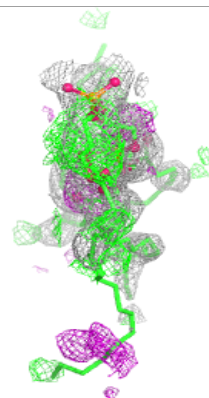
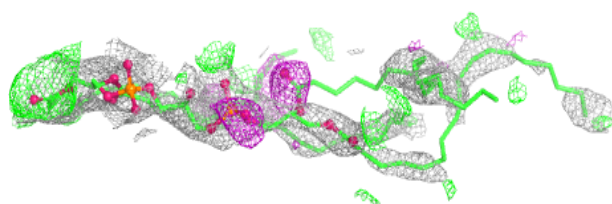
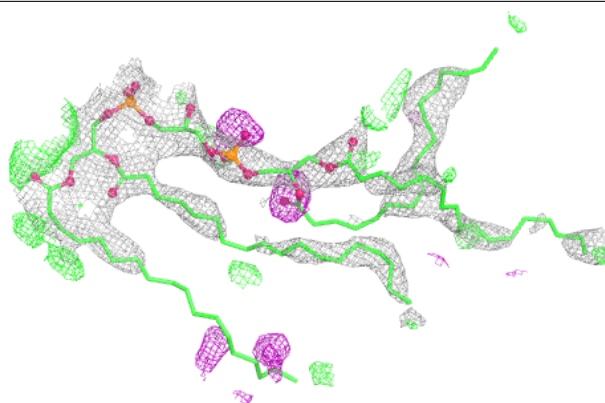
Electron density around PEK G 265:

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

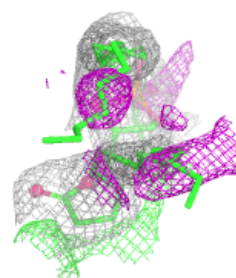
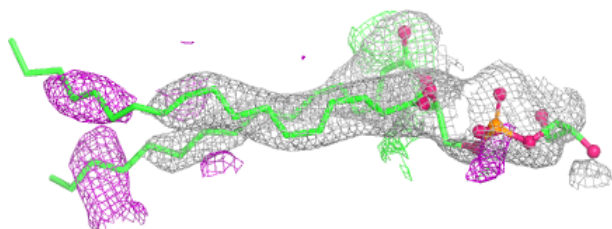
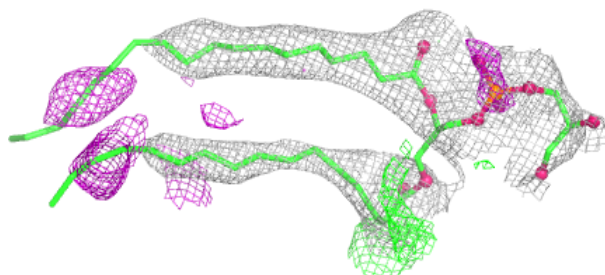


Electron density around CDL G 269:

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

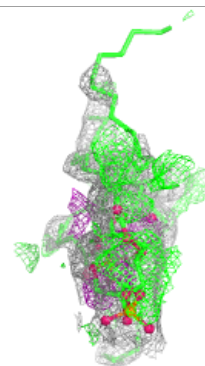
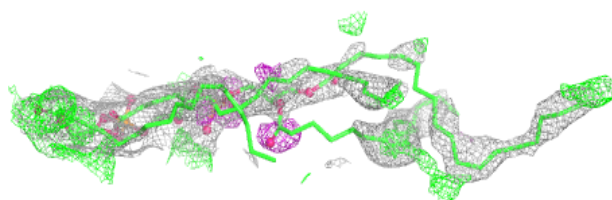
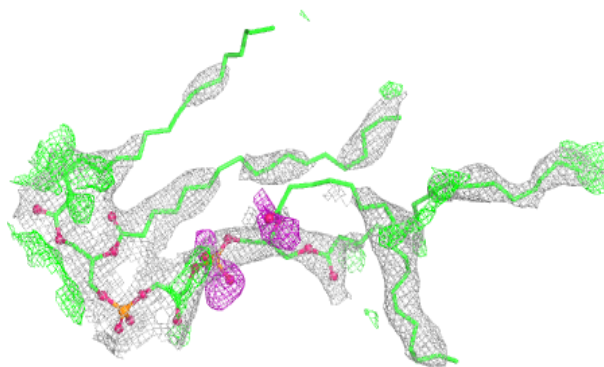
**Electron density around PGV N 1524:**

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

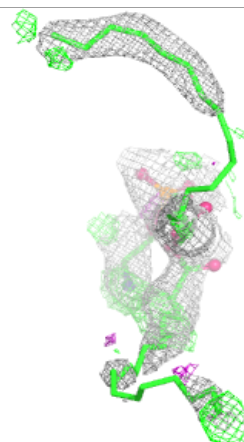
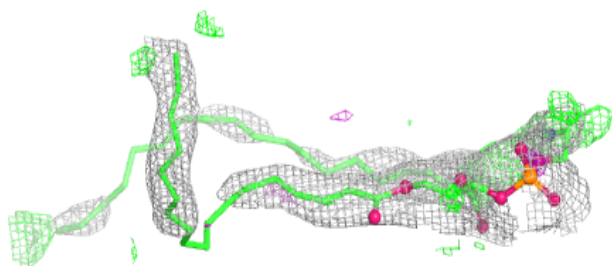
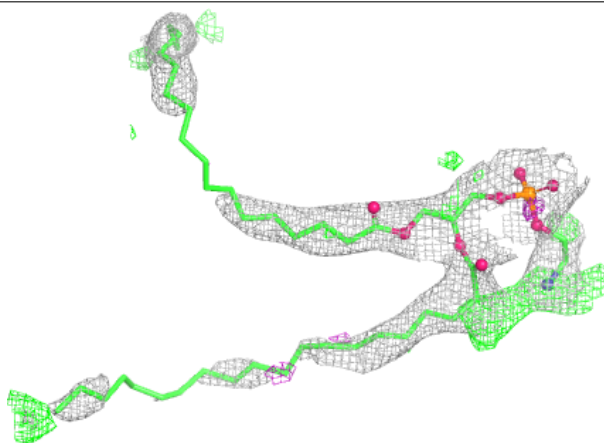


Electron density around CDL T 1269:

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

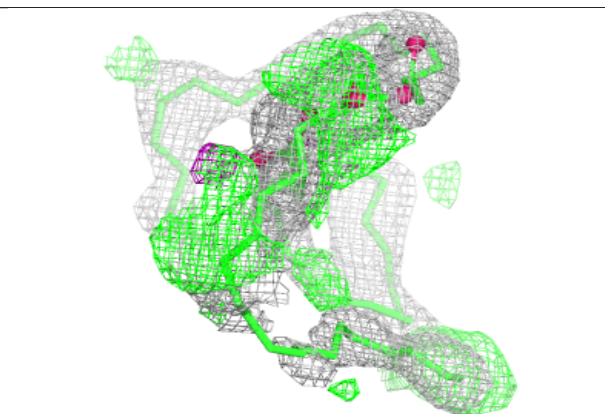
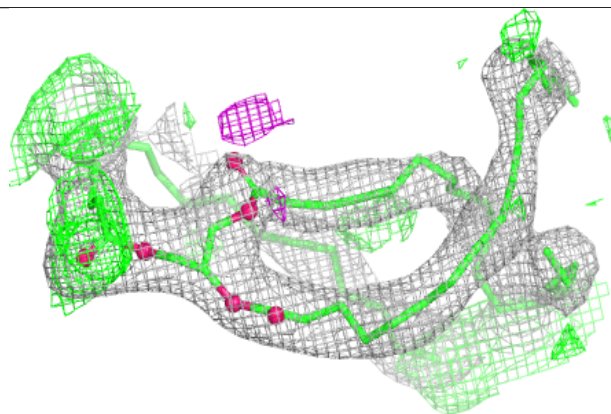
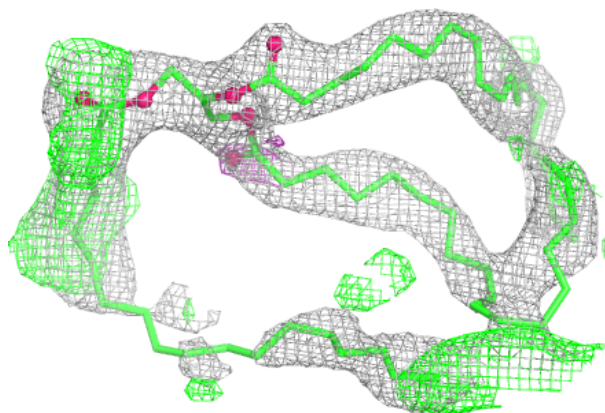
**Electron density around PEK S 1265:**

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

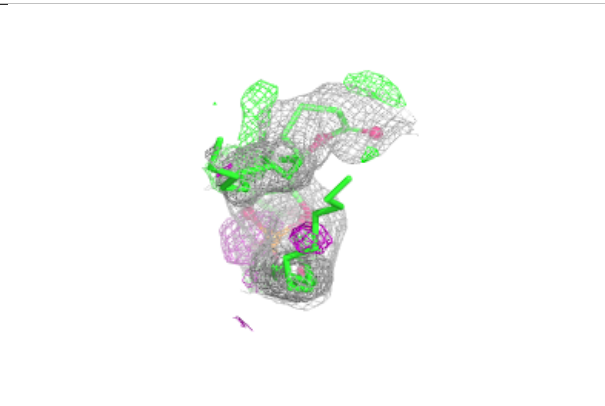
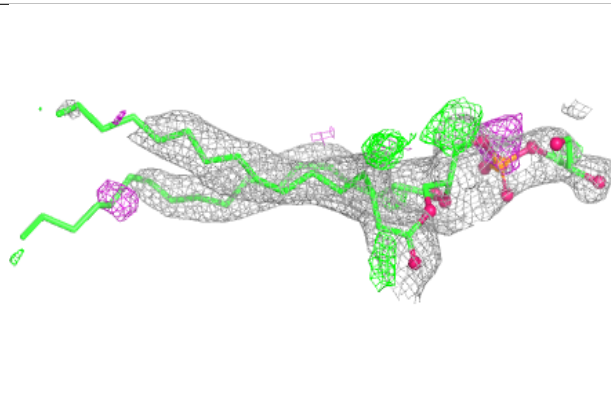
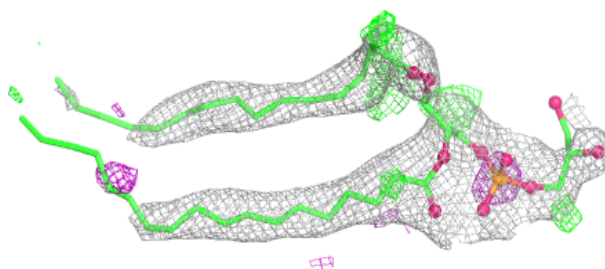


Electron density around TGL B 521:

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

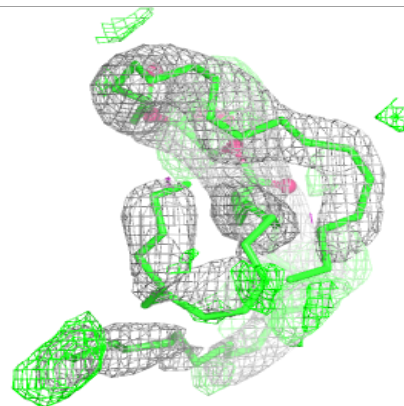
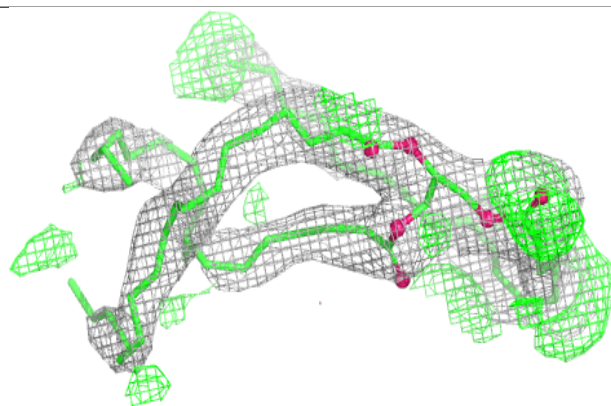
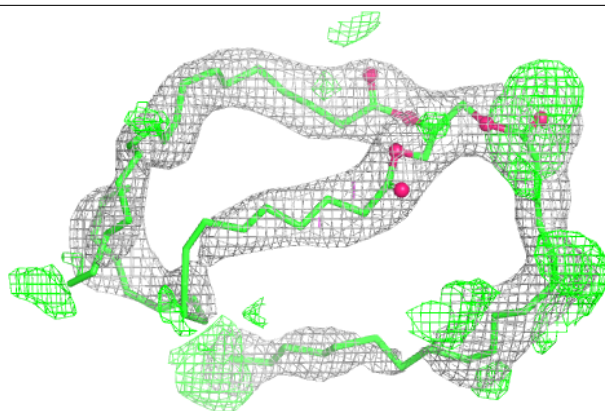
**Electron density around PGV A 524:**

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

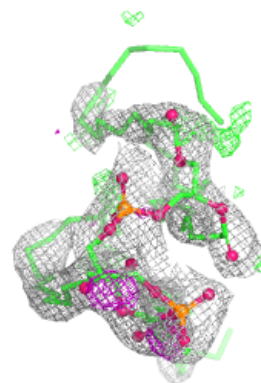
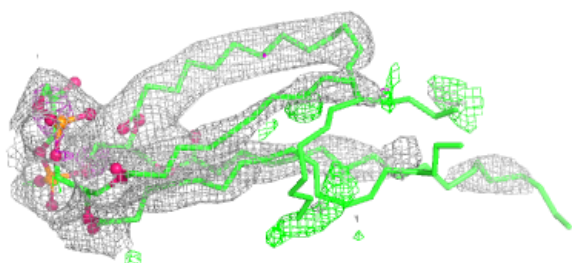
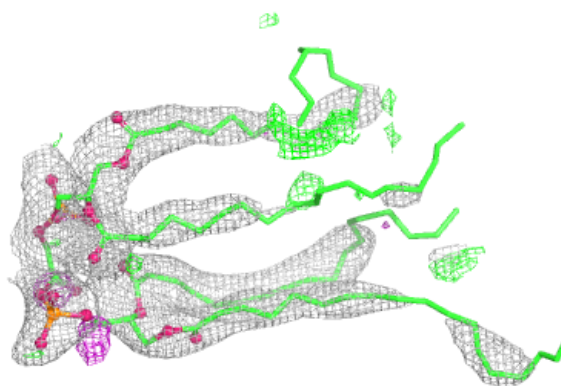


Electron density around TGL N 1521:

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

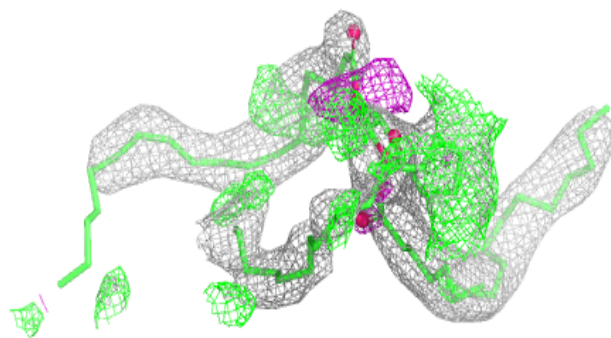
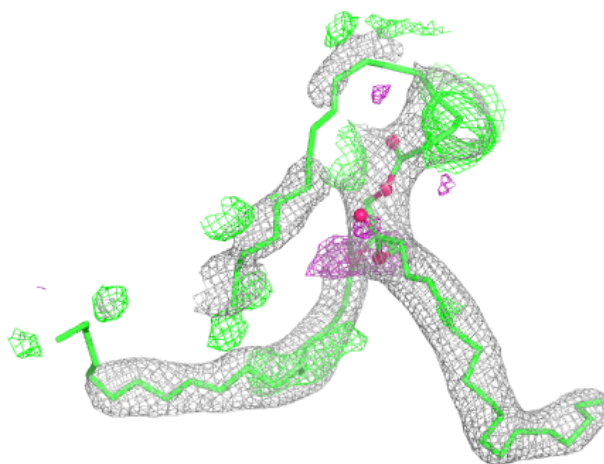
**Electron density around CDL C 270:**

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



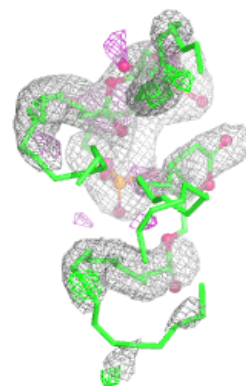
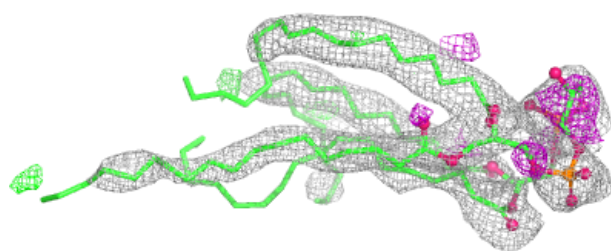
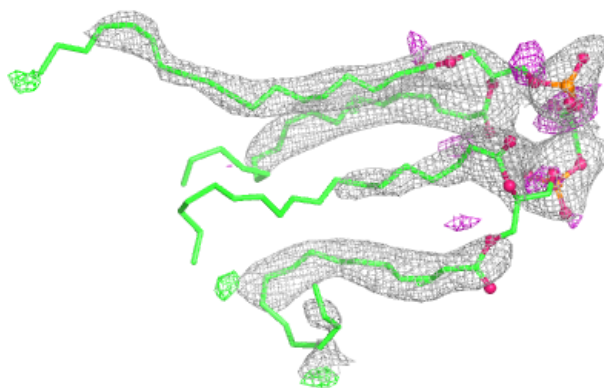
Electron density around TGL L 522:

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

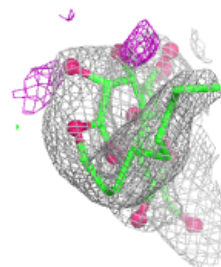
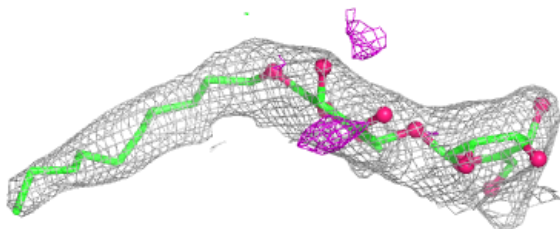
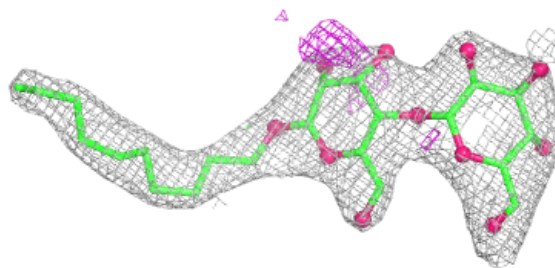


Electron density around CDL P 1270:

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

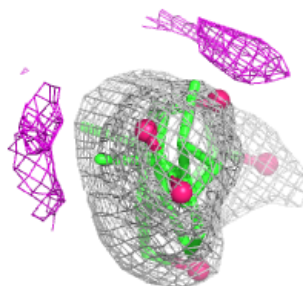
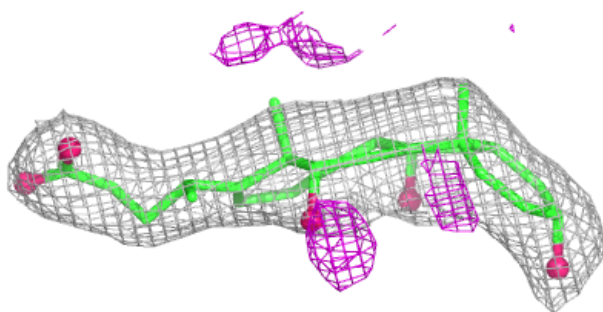
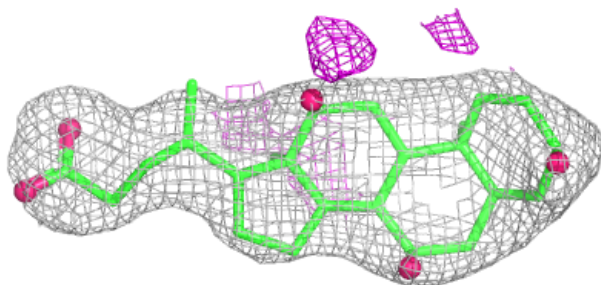
**Electron density around DMU Z 1526:**

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

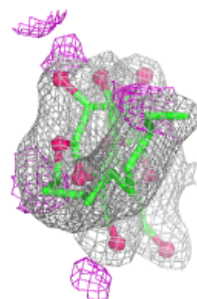
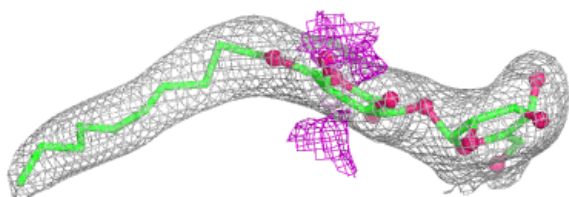
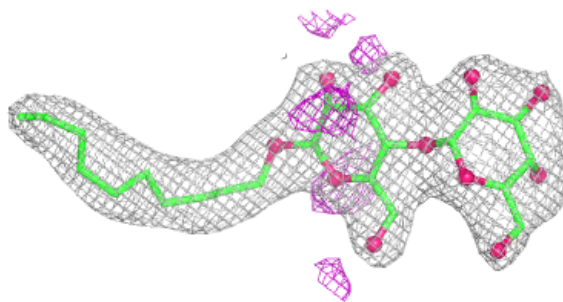


Electron density around CHD C 271:

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

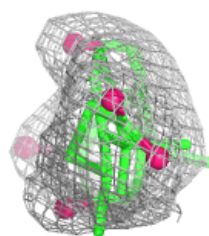
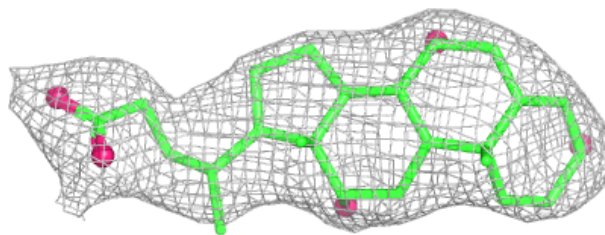
**Electron density around DMU M 526:**

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

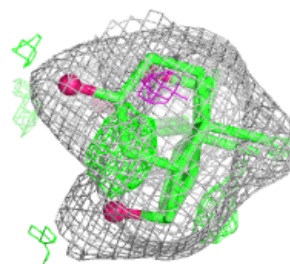
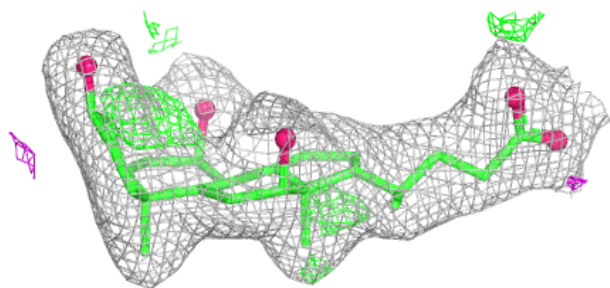
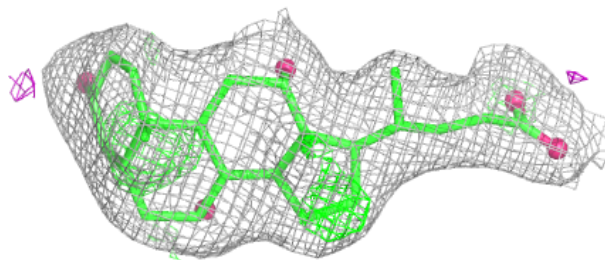


Electron density around CHD P 1271:

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

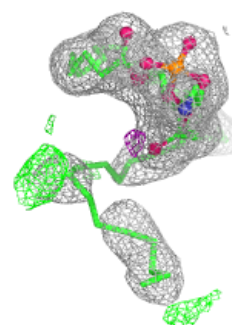
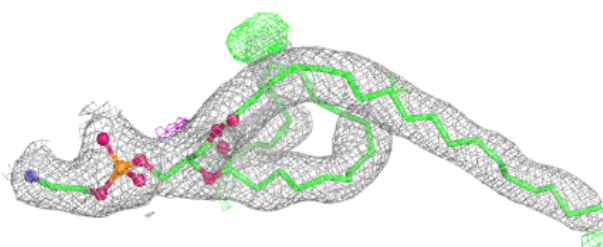
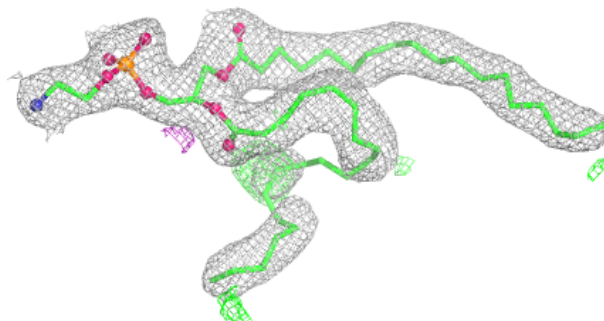
**Electron density around CHD P 1525:**

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

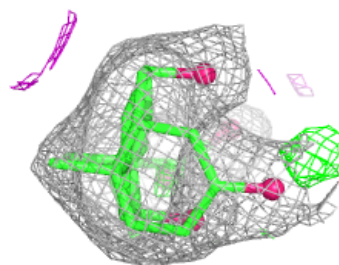
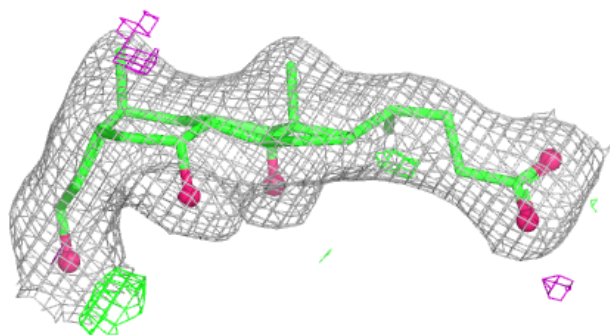
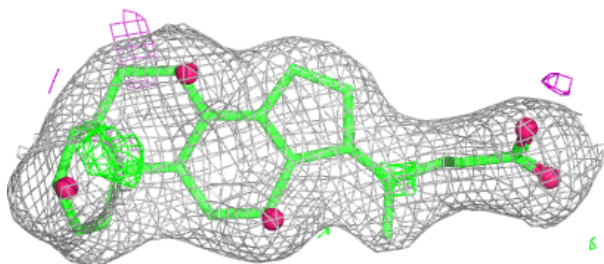


Electron density around PEK G 264:

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

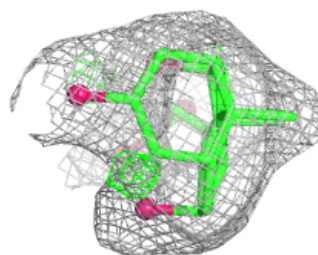
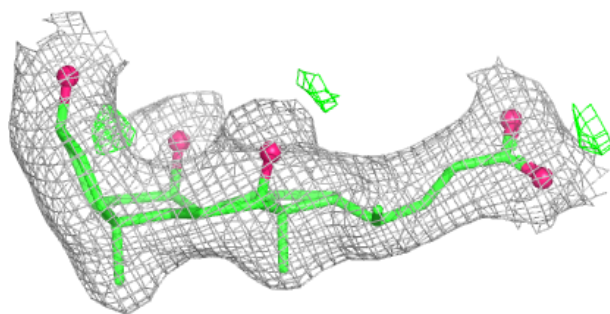
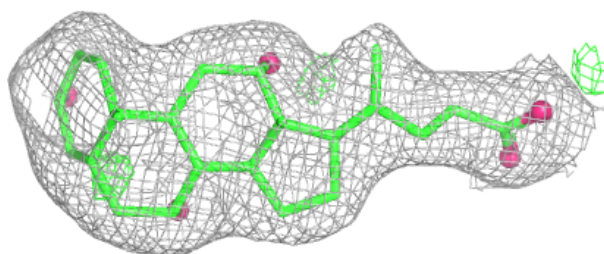
**Electron density around CHD B 1085:**

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

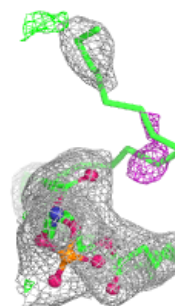
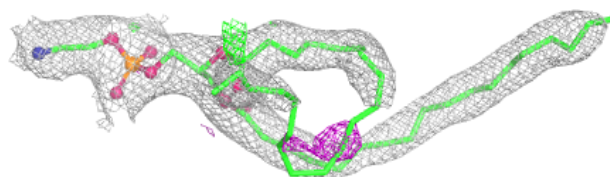
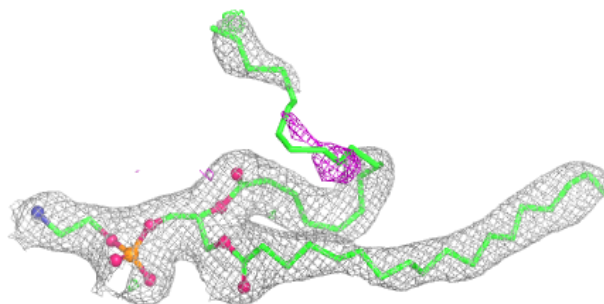


Electron density around CHD O 229:

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

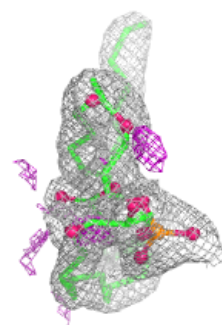
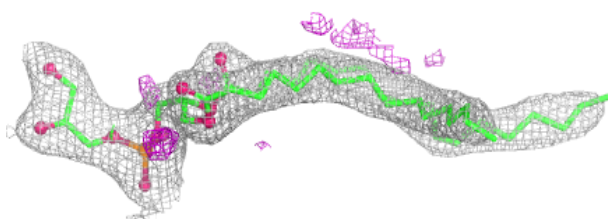
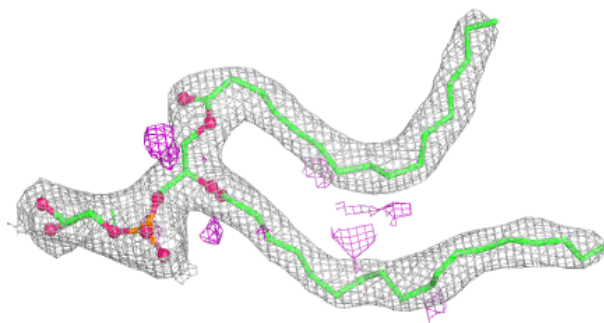
**Electron density around PEK T 1264:**

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

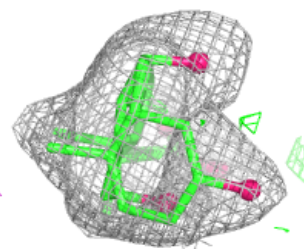
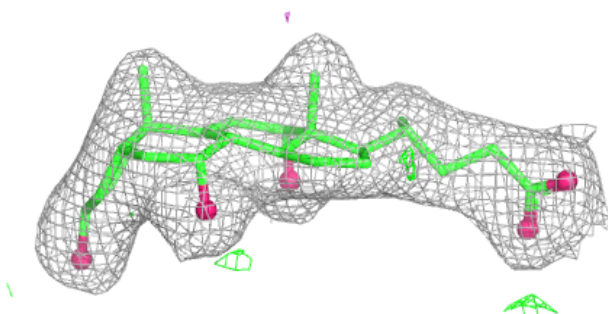
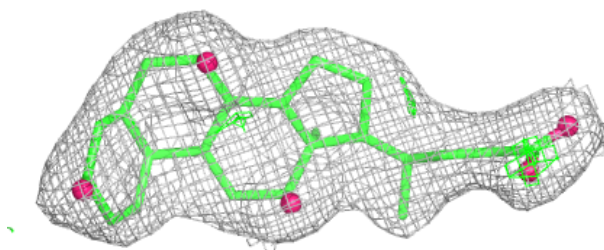


Electron density around PGV N 1266:

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

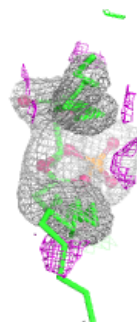
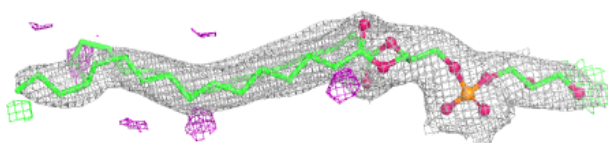
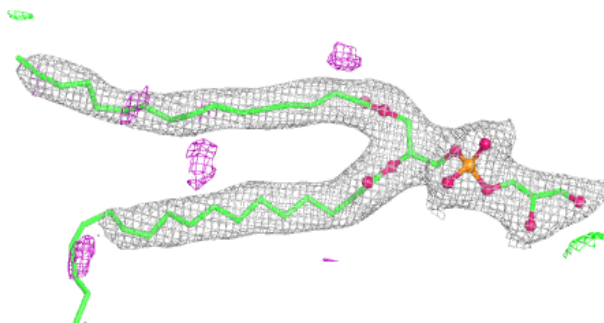
**Electron density around CHD C 525:**

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

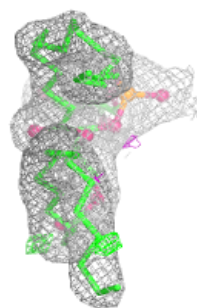
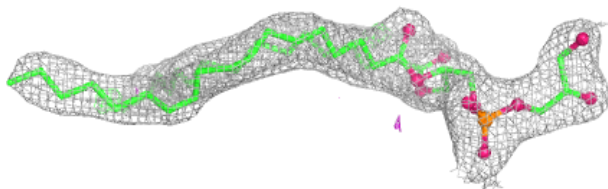
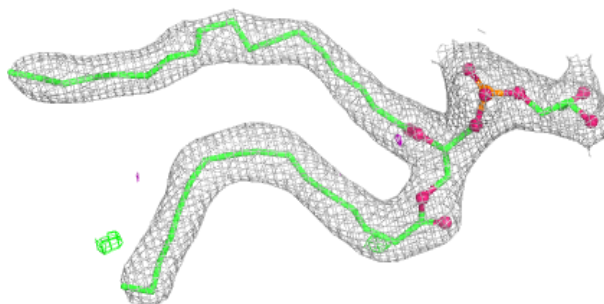


Electron density around PGV P 1267:

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

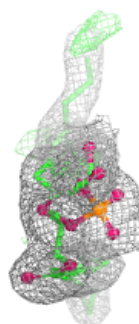
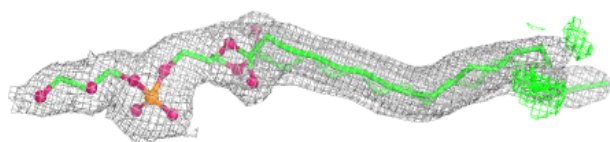
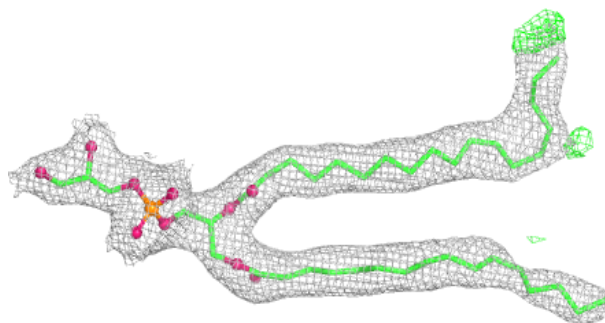
**Electron density around PGV A 521:**

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

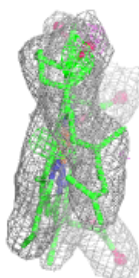
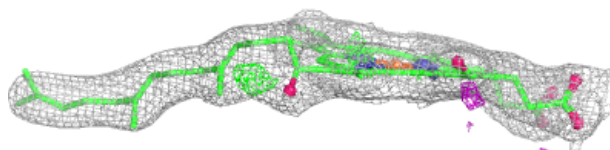
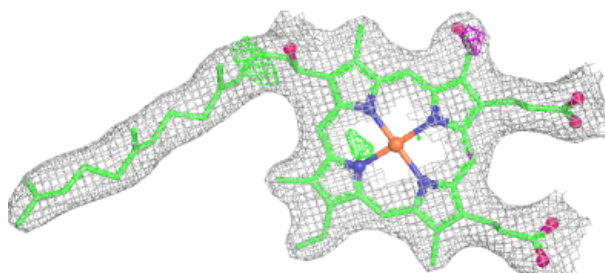


Electron density around PGV C 267:

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

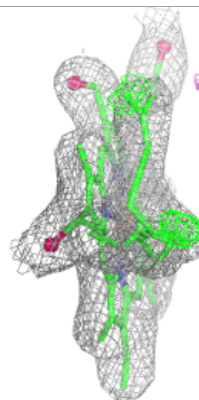
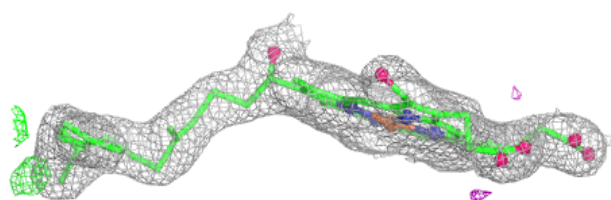
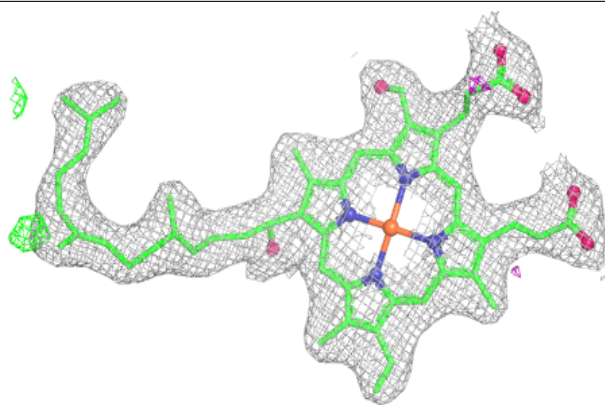
**Electron density around HEA N 515:**

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

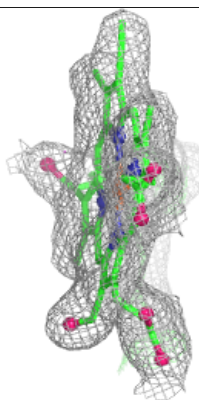
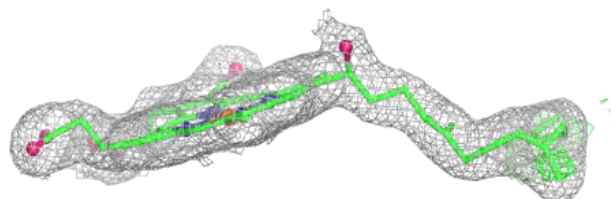
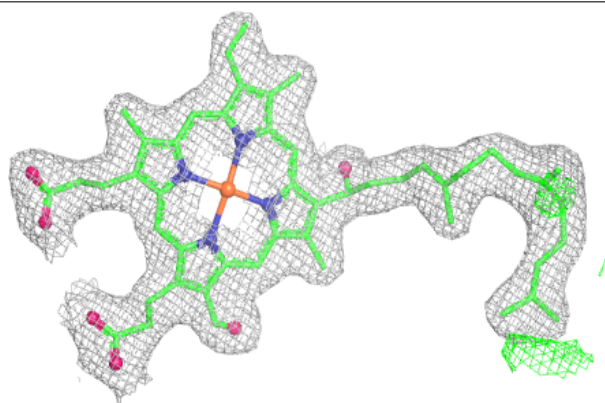


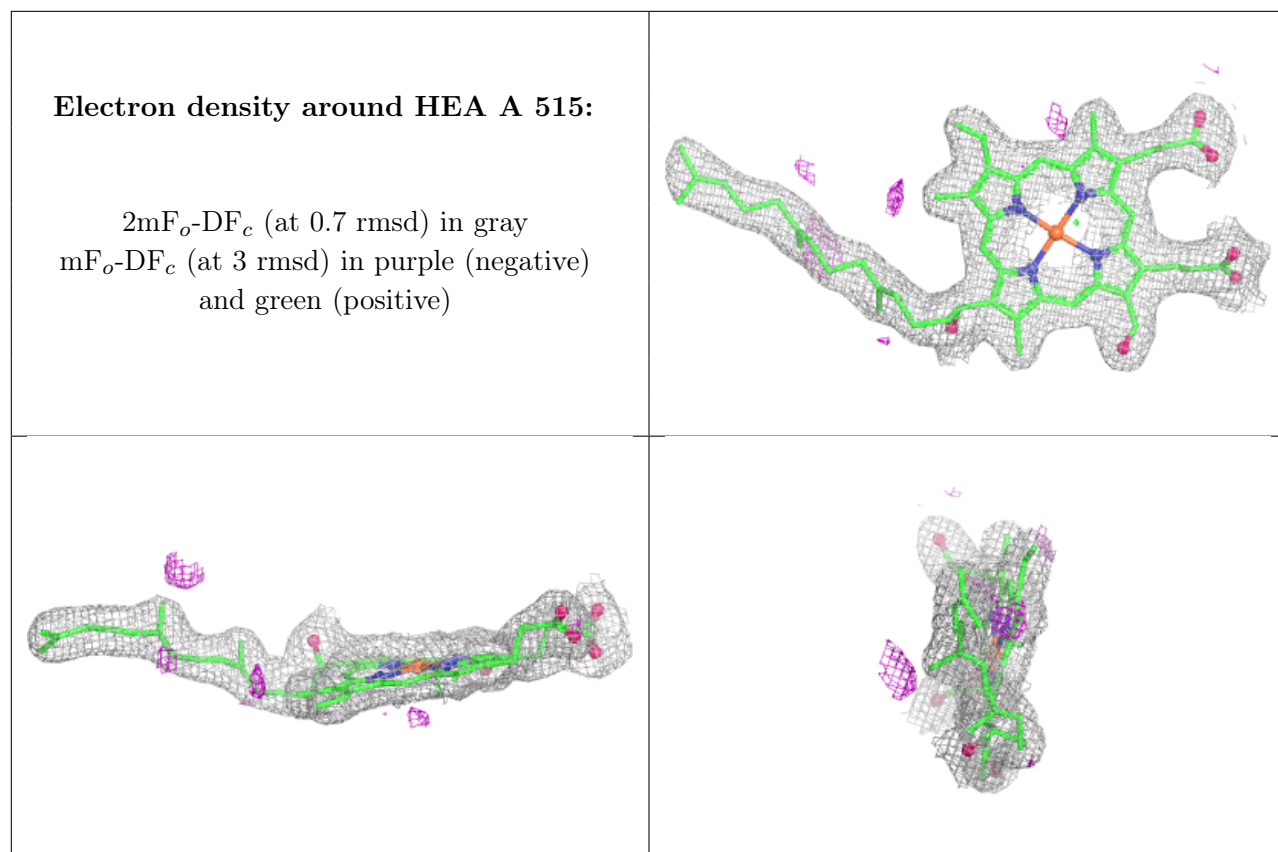
Electron density around HEA N 516:

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

**Electron density around HEA A 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.