



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 10:01 PM EDT

PDB ID : 2DYR / pdb_00002dyr
Title : Bovine heart cytochrome C oxidase at the fully oxidized state
Authors : Shinzawa-Itoh, K.; Aoyama, H.; Muramoto, K.; Kurauchi, T.; Mizushima, T.; Yamashita, E.; Tsukihara, T.; Yoshikawa, S.
Deposited on : 2006-09-16
Resolution : 1.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
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

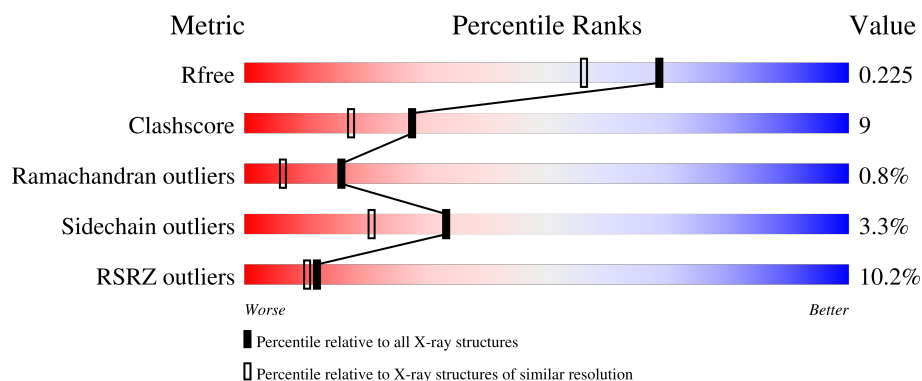
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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

Mol	Chain	Length	Quality of chain
1	A	514	 81% 17% •
1	N	514	 79% 19% •
2	B	227	 78% 19% •
2	O	227	 73% 25% •
3	C	261	 87% 12% •

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Mol	Chain	Length	Quality of chain
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
20	TGL	L	522	-	-	X	-
22	CHD	C	271	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CHD	J	60	X	-	-	-
22	CHD	P	1271	X	-	-	-
22	CHD	W	1060	X	-	-	-
23	DMU	C	272	X	-	-	-
23	DMU	M	526	X	-	-	-
23	DMU	P	1272	X	-	-	-
23	DMU	Z	1526	X	-	-	-
26	CDL	G	269	-	-	X	-
26	CDL	T	1269	-	-	X	-

2 Entry composition [i](#)

There are 28 unique types of molecules in this entry. The entry contains 32735 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 polypeptide Va.

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 polypeptide Vb.

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 polypeptide VIa-heart.

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

- Molecule 8 is a protein called Cytochrome c oxidase subunit VIb isoform 1.

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 polypeptide VIc.

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 VIIa-heart.

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

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

- Molecule 11 is a protein called Cytochrome c oxidase polypeptide VIIb.

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 polypeptide VIIc.

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 polypeptide VIII-heart.

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		

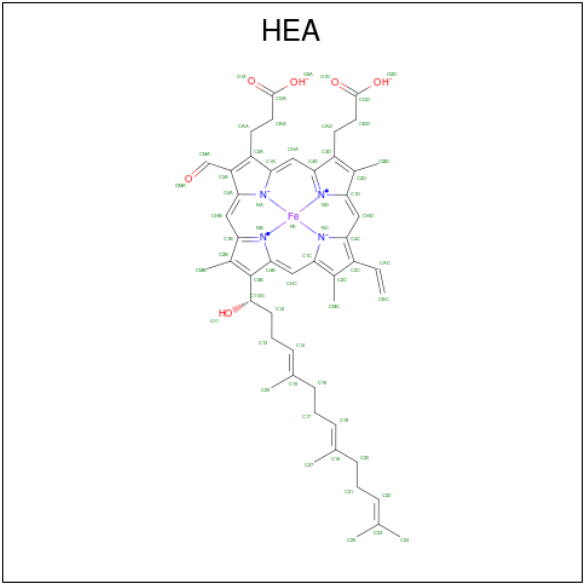
- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 16 is SODIUM ION (CCD ID: NA) (formula: Na).

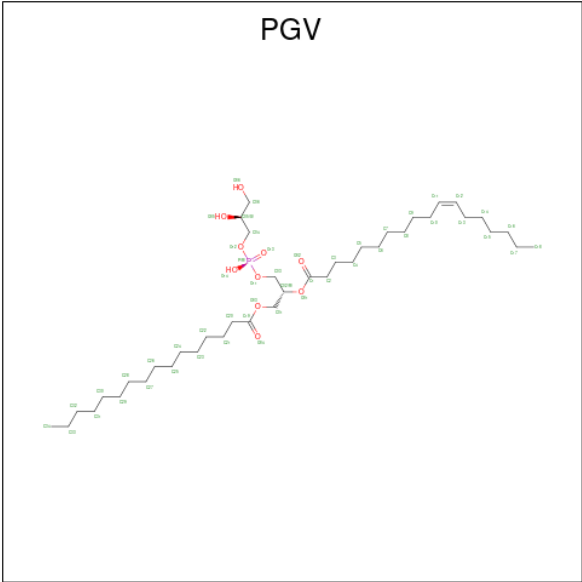
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Na	0	0
			1	1		
16	N	1	Total	Na	0	0
			1	1		

- Molecule 17 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆).



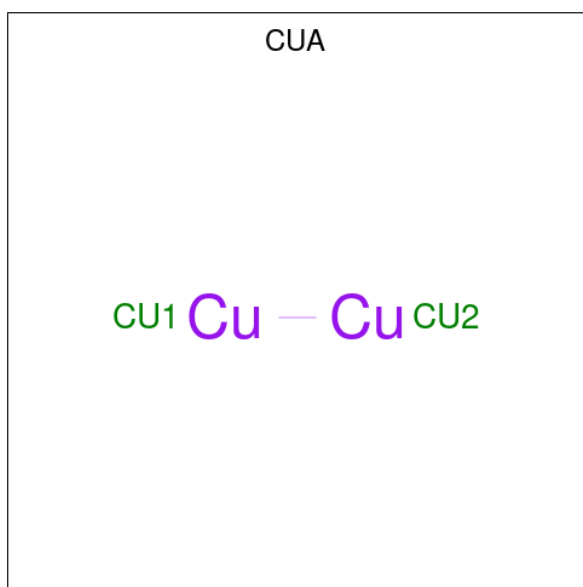
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
17	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
17	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
17	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

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



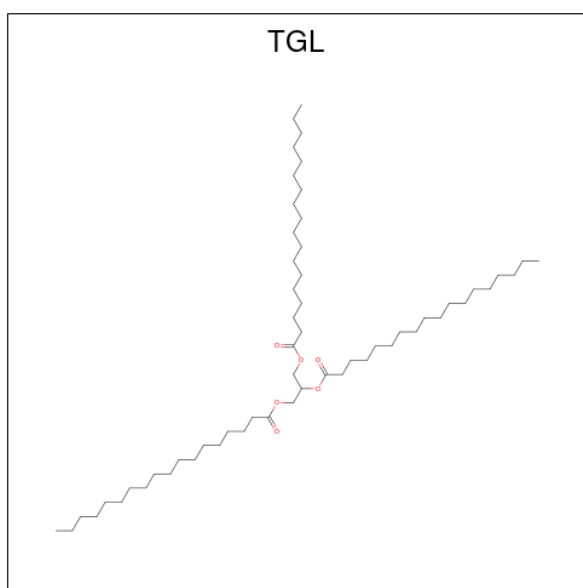
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	A	1	Total	C	O	P	0	0
			51	40	10	1		
18	A	1	Total	C	O	P	0	0
			51	40	10	1		
18	C	1	Total	C	O	P	0	0
			51	40	10	1		
18	C	1	Total	C	O	P	0	0
			51	40	10	1		
18	N	1	Total	C	O	P	0	0
			51	40	10	1		
18	P	1	Total	C	O	P	0	0
			51	40	10	1		
18	P	1	Total	C	O	P	0	0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

- Molecule 19 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



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

- Molecule 20 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: $C_{57}H_{110}O_6$).



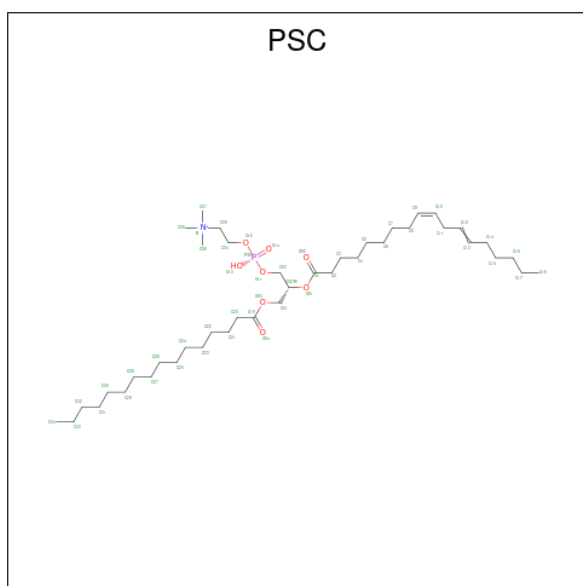
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	B	1	Total	C	O	0	0
			63	57	6		
20	D	1	Total	C	O	0	0
			63	57	6		

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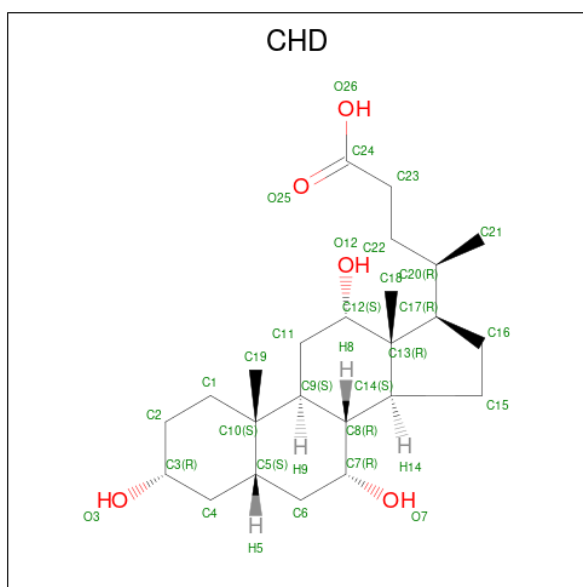
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	L	1	Total	C	O	0	0
			63	57	6		
20	N	1	Total	C	O	0	0
			63	57	6		
20	N	1	Total	C	O	0	0
			63	57	6		
20	Q	1	Total	C	O	0	0
			63	57	6		

- Molecule 21 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (CCD ID: PSC) (formula: $C_{42}H_{81}NO_8P$).



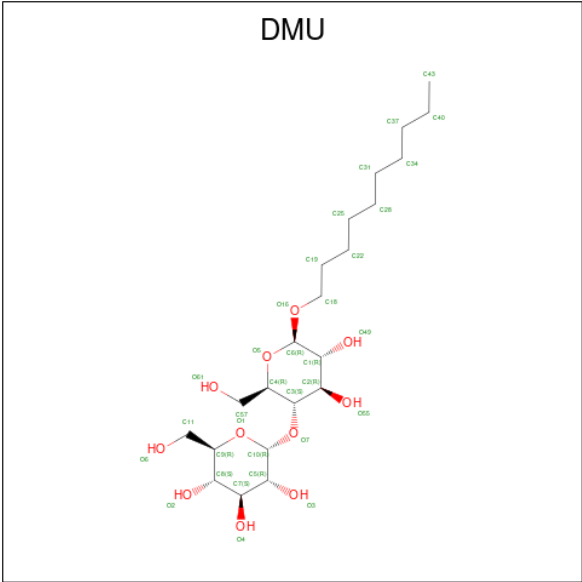
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
21	O	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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



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

- Molecule 23 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: $C_{22}H_{42}O_{11}$).

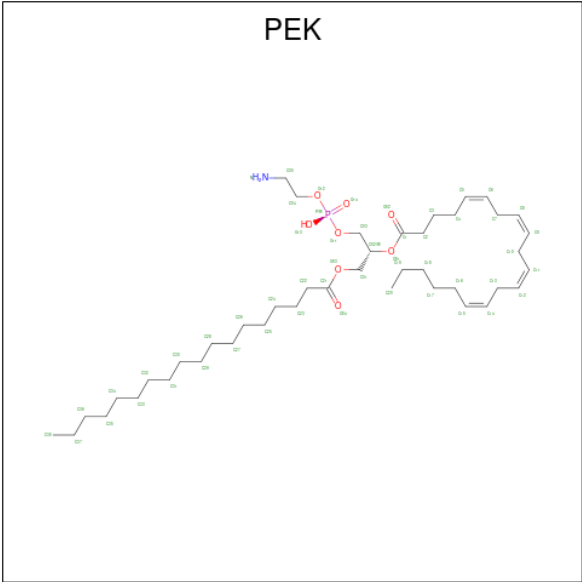


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	C	1	Total	C	O	0	0
			33	22	11		
23	M	1	Total	C	O	0	0
			33	22	11		
23	P	1	Total	C	O	0	0
			33	22	11		
23	Z	1	Total	C	O	0	0
			33	22	11		

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

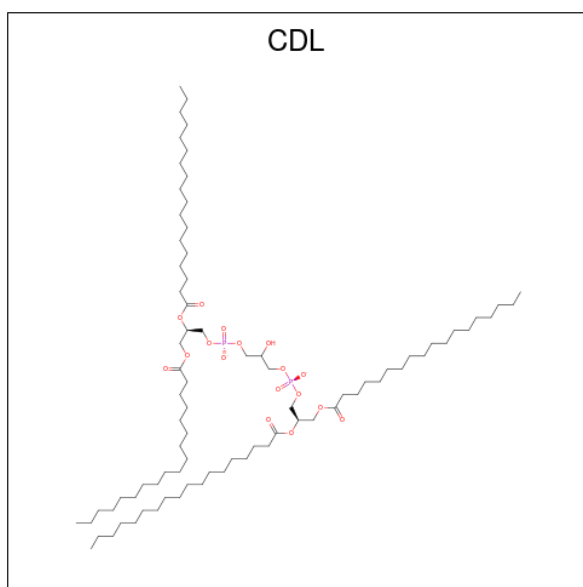
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	C	1	Total	X	0	0
			1	1		
24	P	1	Total	X	0	0
			1	1		

- Molecule 25 is (1S)-2-[[[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (CCD ID: PEK) (formula: C₄₃H₇₈NO₈P).



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

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



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

- Molecule 27 is 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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	243	Total	O	0	0
			243	243		
28	B	186	Total	O	0	0
			186	186		
28	C	127	Total	O	0	0
			127	127		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	D	109	Total 109	O 109	0	0
28	E	67	Total 67	O 67	0	0
28	F	85	Total 85	O 85	0	0
28	G	57	Total 57	O 57	0	0
28	H	66	Total 66	O 66	0	0
28	I	58	Total 58	O 58	0	0
28	J	21	Total 21	O 21	0	0
28	K	38	Total 38	O 38	0	0
28	L	22	Total 22	O 22	0	0
28	M	27	Total 27	O 27	0	0
28	N	212	Total 212	O 212	0	0
28	O	152	Total 152	O 152	0	0
28	P	120	Total 120	O 120	0	0
28	Q	75	Total 75	O 75	0	0
28	R	32	Total 32	O 32	0	0
28	S	53	Total 53	O 53	0	0
28	T	59	Total 59	O 59	0	0
28	U	62	Total 62	O 62	0	0
28	V	33	Total 33	O 33	0	0
28	W	18	Total 18	O 18	0	0
28	X	29	Total 29	O 29	0	0

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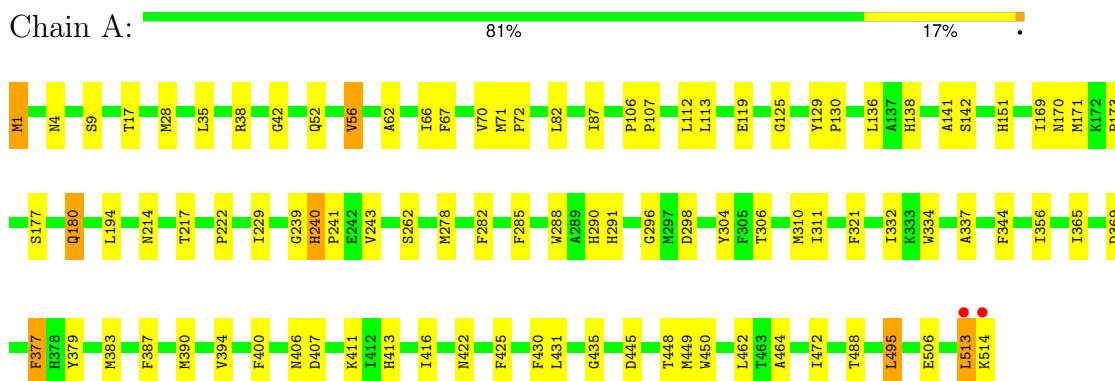
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	Y	31	Total	O	0	0
			31	31		
28	Z	21	Total	O	0	0
			21	21		

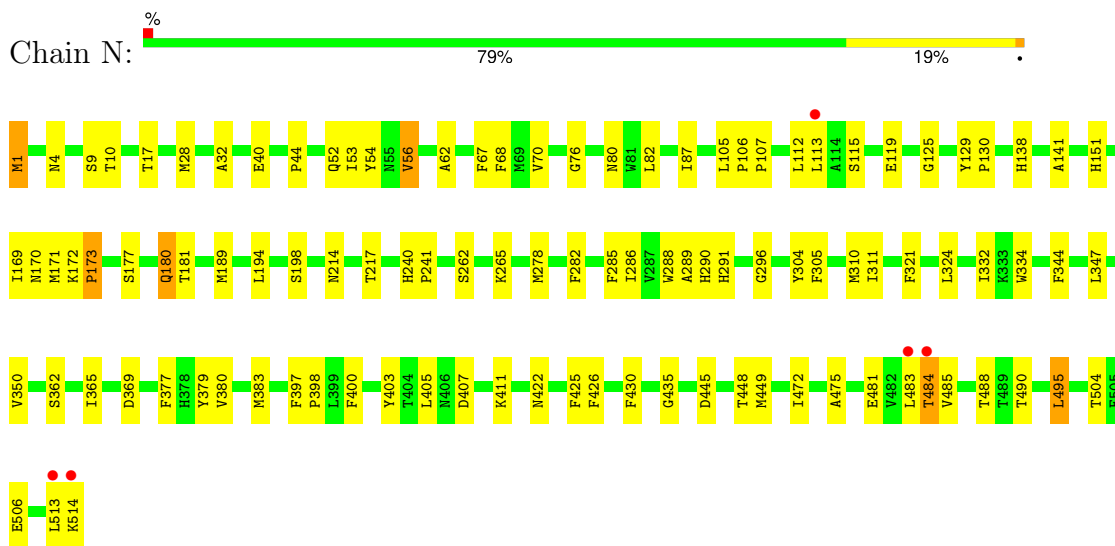
3 Residue-property plots

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.

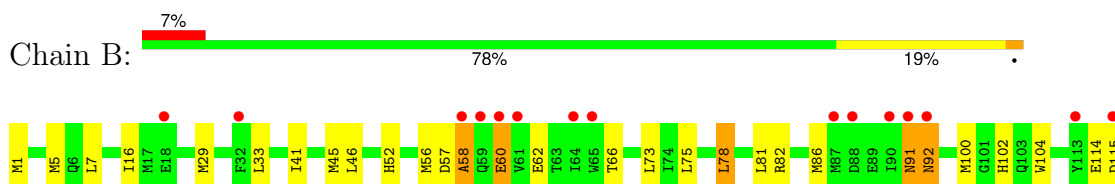
• Molecule 1: Cytochrome c oxidase subunit 1



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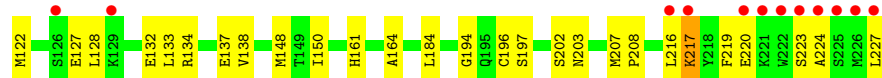


• Molecule 2: Cytochrome c oxidase subunit 2

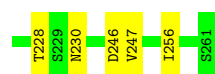
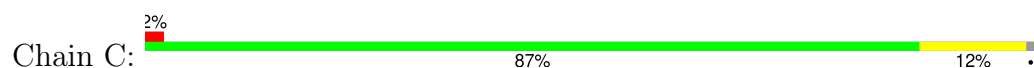




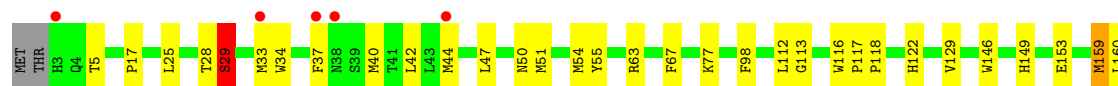
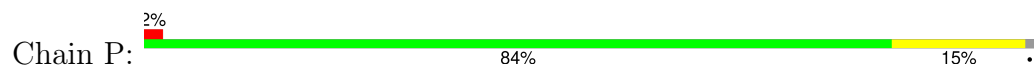
• Molecule 2: Cytochrome c oxidase subunit 2



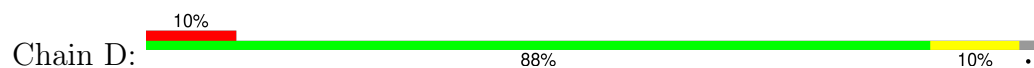
• Molecule 3: Cytochrome c oxidase subunit 3



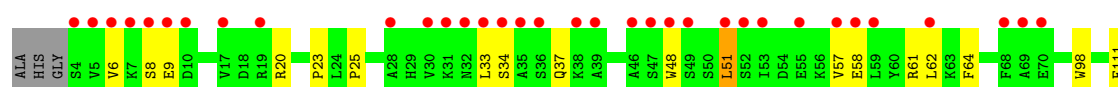
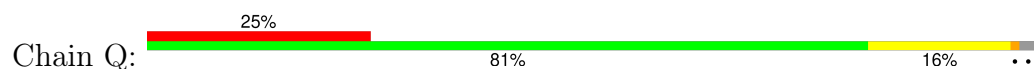
• Molecule 3: Cytochrome c oxidase subunit 3

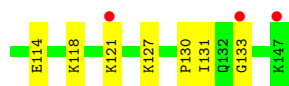


• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

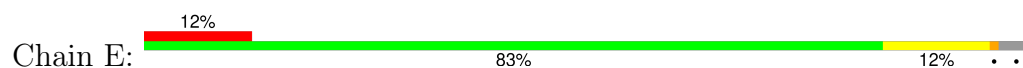


• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

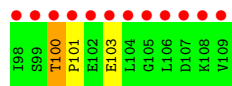
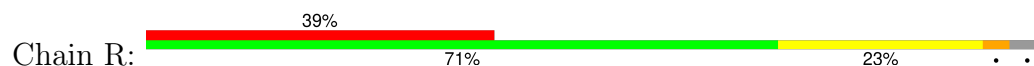




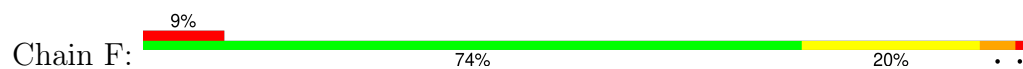
• Molecule 5: Cytochrome c oxidase polypeptide Va



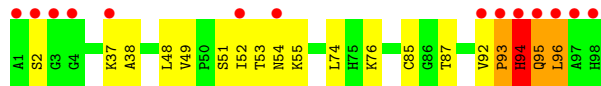
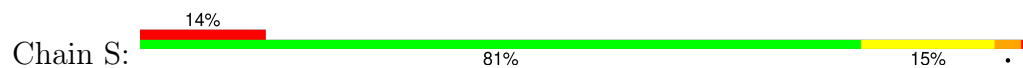
• Molecule 5: Cytochrome c oxidase polypeptide Va



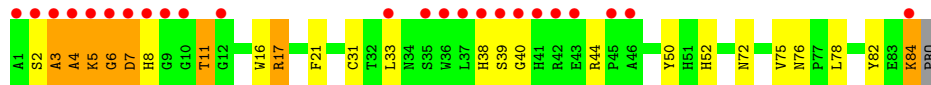
• Molecule 6: Cytochrome c oxidase polypeptide Vb



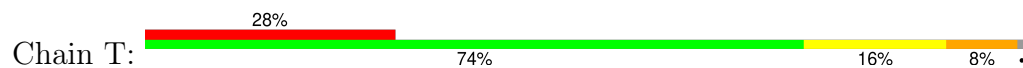
• Molecule 6: Cytochrome c oxidase polypeptide Vb

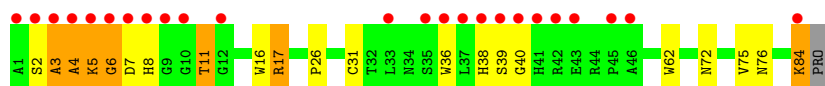


• Molecule 7: Cytochrome c oxidase polypeptide VIa-heart

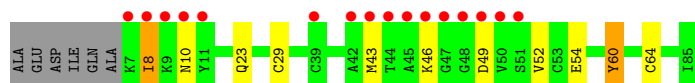
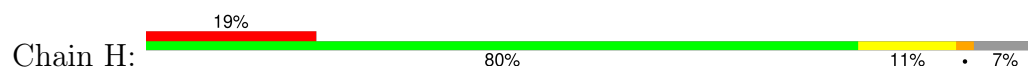


• Molecule 7: Cytochrome c oxidase polypeptide VIa-heart

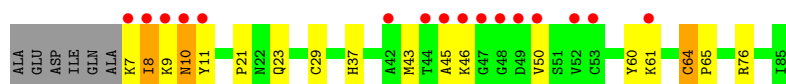




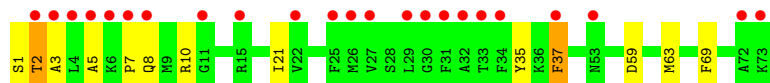
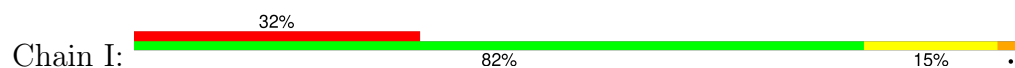
- Molecule 8: Cytochrome c oxidase subunit VIb isoform 1



- Molecule 8: Cytochrome c oxidase subunit VIb isoform 1



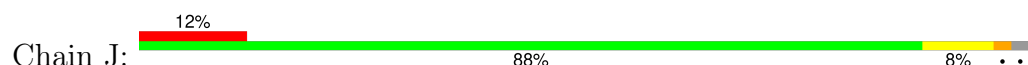
- Molecule 9: Cytochrome c oxidase polypeptide VIc



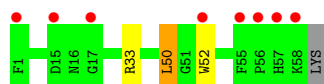
- Molecule 9: Cytochrome c oxidase polypeptide VIc



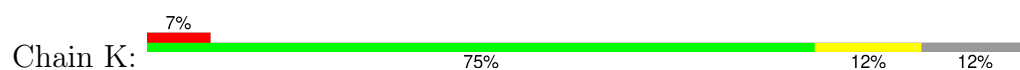
- Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart



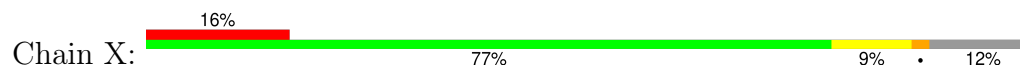
- Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart



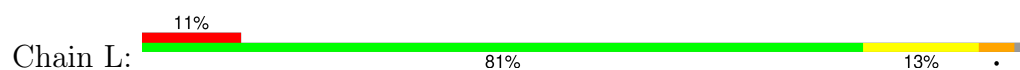
- Molecule 11: Cytochrome c oxidase polypeptide VIIb



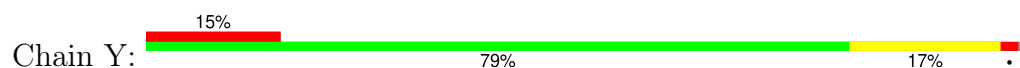
- Molecule 11: Cytochrome c oxidase polypeptide VIIb



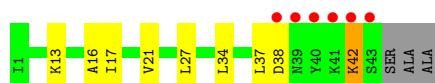
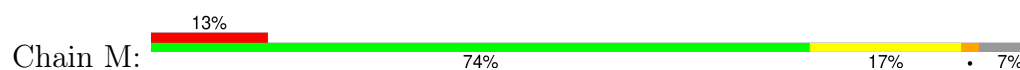
- Molecule 12: Cytochrome c oxidase polypeptide VIIc



- Molecule 12: Cytochrome c oxidase polypeptide VIIc



- Molecule 13: Cytochrome c oxidase polypeptide VIII-heart



- Molecule 13: Cytochrome c oxidase polypeptide VIII-heart



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	182.59Å 205.14Å 178.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.80 40.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-1.80) 99.2 (40.00-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.09 (at 1.80Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.202 , 0.227 0.203 , 0.225	Depositor DCC
R_{free} test set	22992 reflections (3.78%)	wwPDB-VP
Wilson B-factor (Å ²)	25.2	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.009 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	32735	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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: ZN, TPO, NA, SAC, FME, PEK, MG, UNX, CDL, DMU, PGV, HEA, PSC, CU, CUA, TGL, 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	0.63	1/4156 (0.0%)	1.05	28/5678 (0.5%)
1	N	0.60	1/4156 (0.0%)	1.03	25/5678 (0.4%)
2	B	0.59	0/1860	1.02	3/2534 (0.1%)
2	O	0.61	0/1860	1.06	7/2534 (0.3%)
3	C	0.56	0/2197	0.90	4/3005 (0.1%)
3	P	0.55	0/2197	0.93	8/3005 (0.3%)
4	D	0.54	0/1229	1.00	1/1658 (0.1%)
4	Q	0.57	0/1229	1.02	1/1658 (0.1%)
5	E	0.59	0/871	0.97	1/1182 (0.1%)
5	R	0.55	0/871	1.07	6/1182 (0.5%)
6	F	0.60	0/765	1.20	12/1038 (1.2%)
6	S	0.62	0/765	1.22	7/1038 (0.7%)
7	G	0.61	1/690 (0.1%)	1.01	3/937 (0.3%)
7	T	0.63	1/690 (0.1%)	1.02	2/937 (0.2%)
8	H	0.56	0/682	1.01	4/921 (0.4%)
8	U	0.56	0/682	1.04	3/921 (0.3%)
9	I	0.55	0/605	0.89	1/802 (0.1%)
9	V	0.54	0/605	0.85	1/802 (0.1%)
10	J	0.52	0/471	0.91	0/636
10	W	0.51	0/471	0.97	0/636
11	K	0.59	0/398	1.13	4/546 (0.7%)
11	X	0.54	0/398	1.05	2/546 (0.4%)
12	L	0.51	0/393	0.87	2/526 (0.4%)
12	Y	0.54	0/393	0.90	1/526 (0.2%)
13	M	0.54	0/345	0.96	1/470 (0.2%)
13	Z	0.52	0/345	0.98	1/470 (0.2%)
All	All	0.58	4/29324 (0.0%)	1.01	128/39866 (0.3%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	N	0	1
8	U	0	1
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	5	LYS	CA-C	5.40	1.56	1.53
1	A	130	PRO	CA-C	5.21	1.57	1.52
1	N	173	PRO	CA-C	5.21	1.54	1.51
7	T	5	LYS	CA-C	5.03	1.56	1.53

The worst 5 of 128 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	133	GLY	N-CA-C	12.74	127.28	112.50
4	Q	133	GLY	N-CA-C	12.61	127.12	112.50
6	S	94	HIS	N-CA-C	9.91	131.91	110.80
6	F	93	PRO	N-CA-C	9.66	126.31	111.34
6	F	94	HIS	N-CA-C	9.15	130.29	110.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	N	240	HIS	Sidechain
8	U	11	TYR	Sidechain

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	69	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	4027	0	4001	77	0
2	B	1824	0	1833	32	0
2	O	1824	0	1833	42	0
3	C	2110	0	2027	30	0
3	P	2110	0	2027	34	0
4	D	1195	0	1183	10	0
4	Q	1195	0	1183	18	0
5	E	852	0	845	6	0
5	R	852	0	845	15	0
6	F	748	0	728	12	0
6	S	748	0	728	15	0
7	G	675	0	644	26	0
7	T	675	0	644	28	0
8	H	662	0	623	5	0
8	U	662	0	623	10	0
9	I	601	0	613	8	0
9	V	601	0	613	9	0
10	J	460	0	459	5	0
10	W	460	0	459	3	0
11	K	384	0	366	3	0
11	X	384	0	366	6	0
12	L	380	0	380	15	0
12	Y	380	0	380	10	0
13	M	335	0	352	5	0
13	Z	335	0	352	6	0
14	A	1	0	0	0	0
14	N	1	0	0	0	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	120	0	108	3	0
17	N	120	0	108	3	0
18	A	102	0	152	7	0
18	C	102	0	152	8	0
18	N	51	0	76	2	0
18	P	102	0	152	8	0
18	Z	51	0	76	4	0
19	B	2	0	0	0	0
19	O	2	0	0	0	0
20	B	63	0	110	10	0
20	D	63	0	110	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	L	63	0	110	23	0
20	N	126	0	220	30	0
20	Q	63	0	110	6	0
21	B	52	0	80	13	0
21	O	52	0	80	12	0
22	B	29	0	39	0	0
22	C	58	0	78	2	0
22	J	29	0	39	2	0
22	O	29	0	39	1	0
22	P	58	0	78	2	0
22	W	29	0	39	2	0
23	C	33	0	36	2	0
23	M	33	0	36	0	0
23	P	33	0	36	7	0
23	Z	33	0	36	1	0
24	C	1	0	0	0	0
24	P	1	0	0	0	0
25	C	106	0	154	11	0
25	G	53	0	77	7	0
25	P	106	0	154	12	0
25	T	53	0	77	8	0
26	C	100	0	156	17	0
26	G	100	0	156	21	0
26	P	100	0	156	15	0
26	T	100	0	156	21	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	A	243	0	0	4	0
28	B	186	0	0	4	0
28	C	127	0	0	2	0
28	D	109	0	0	4	0
28	E	67	0	0	0	0
28	F	85	0	0	1	0
28	G	57	0	0	2	0
28	H	66	0	0	1	0
28	I	58	0	0	3	0
28	J	21	0	0	1	0
28	K	38	0	0	0	0
28	L	22	0	0	2	0
28	M	27	0	0	1	0
28	N	212	0	0	3	0
28	O	152	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	P	120	0	0	3	0
28	Q	75	0	0	3	0
28	R	32	0	0	0	0
28	S	53	0	0	1	0
28	T	59	0	0	2	0
28	U	62	0	0	3	0
28	V	33	0	0	2	0
28	W	18	0	0	0	0
28	X	29	0	0	1	0
28	Y	31	0	0	2	0
28	Z	21	0	0	2	0
All	All	32735	0	31294	557	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 9.

The worst 5 of 557 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)
7:G:84:LYS:H	7:G:84:LYS:HD2	1.17	1.05
7:T:84:LYS:HD2	7:T:84:LYS:H	1.19	1.02
3:C:63:ARG:HE	26:C:270:CDL:HA22	1.24	1.01
21:O:1230:PSC:H142	21:O:1230:PSC:H343	1.42	1.01
21:B:230:PSC:H343	21:B:230:PSC:H142	1.42	1.01

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%)	497 (97%)	15 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	512/514 (100%)	497 (97%)	15 (3%)	0	100	100
2	B	225/227 (99%)	211 (94%)	12 (5%)	2 (1%)	14	5
2	O	225/227 (99%)	208 (92%)	15 (7%)	2 (1%)	14	5
3	C	257/261 (98%)	252 (98%)	5 (2%)	0	100	100
3	P	257/261 (98%)	251 (98%)	6 (2%)	0	100	100
4	D	142/147 (97%)	138 (97%)	4 (3%)	0	100	100
4	Q	142/147 (97%)	138 (97%)	4 (3%)	0	100	100
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%)	89 (93%)	5 (5%)	2 (2%)	5	1
6	S	96/98 (98%)	90 (94%)	3 (3%)	3 (3%)	3	0
7	G	81/85 (95%)	67 (83%)	7 (9%)	7 (9%)	0	0
7	T	81/85 (95%)	65 (80%)	9 (11%)	7 (9%)	0	0
8	H	77/85 (91%)	70 (91%)	5 (6%)	2 (3%)	4	0
8	U	77/85 (91%)	70 (91%)	5 (6%)	2 (3%)	4	0
9	I	71/73 (97%)	67 (94%)	4 (6%)	0	100	100
9	V	71/73 (97%)	66 (93%)	5 (7%)	0	100	100
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%)	43 (98%)	1 (2%)	0	100	100
13	M	41/46 (89%)	41 (100%)	0	0	100	100
13	Z	41/46 (89%)	41 (100%)	0	0	100	100
All	All	3504/3614 (97%)	3350 (96%)	127 (4%)	27 (1%)	16	6

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	4	ALA
7	G	7	ASP
7	G	8	HIS

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Mol	Chain	Res	Type
7	G	39	SER
6	S	94	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%)	420 (99%)	6 (1%)	59	52
1	N	426/426 (100%)	417 (98%)	9 (2%)	47	36
2	B	210/210 (100%)	201 (96%)	9 (4%)	26	13
2	O	210/210 (100%)	198 (94%)	12 (6%)	18	8
3	C	224/226 (99%)	220 (98%)	4 (2%)	51	43
3	P	224/226 (99%)	218 (97%)	6 (3%)	39	27
4	D	128/129 (99%)	126 (98%)	2 (2%)	55	47
4	Q	128/129 (99%)	124 (97%)	4 (3%)	35	23
5	E	92/95 (97%)	89 (97%)	3 (3%)	33	21
5	R	92/95 (97%)	89 (97%)	3 (3%)	33	21
6	F	81/81 (100%)	78 (96%)	3 (4%)	30	18
6	S	81/81 (100%)	78 (96%)	3 (4%)	30	18
7	G	67/68 (98%)	64 (96%)	3 (4%)	24	12
7	T	67/68 (98%)	63 (94%)	4 (6%)	17	7
8	H	71/75 (95%)	68 (96%)	3 (4%)	26	14
8	U	71/75 (95%)	68 (96%)	3 (4%)	26	14
9	I	57/57 (100%)	53 (93%)	4 (7%)	14	4
9	V	57/57 (100%)	53 (93%)	4 (7%)	14	4
10	J	49/50 (98%)	48 (98%)	1 (2%)	48	38
10	W	49/50 (98%)	48 (98%)	1 (2%)	48	38
11	K	39/46 (85%)	39 (100%)	0	100	100
11	X	39/46 (85%)	38 (97%)	1 (3%)	40	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	39/40 (98%)	38 (97%)	1 (3%)	40	28
12	Y	39/40 (98%)	37 (95%)	2 (5%)	21	9
13	M	37/38 (97%)	33 (89%)	4 (11%)	6	1
13	Z	37/38 (97%)	33 (89%)	4 (11%)	6	1
All	All	3040/3082 (99%)	2941 (97%)	99 (3%)	33	21

5 of 99 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	O	75	LEU
4	Q	9	GLU
2	O	91	ASN
3	P	29	SER
5	R	87	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
1	N	503	HIS
5	R	94	ASN
1	N	512	ASN
3	P	68	GLN
7	T	76	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
2	FME	O	1	2	8,9,10	0.69	0	8,9,11	1.67	2 (25%)
7	TPO	G	11	7	8,10,11	1.59	1 (12%)	10,14,16	1.12	1 (10%)
1	FME	A	1	1	8,9,10	0.68	0	8,9,11	1.12	1 (12%)
7	TPO	T	11	7	8,10,11	1.35	1 (12%)	10,14,16	1.13	0
2	FME	B	1	2	8,9,10	0.77	0	8,9,11	2.23	2 (25%)
1	FME	N	1	1	8,9,10	0.74	0	8,9,11	1.62	2 (25%)
9	SAC	V	1	9	7,8,9	2.68	2 (28%)	7,9,11	1.97	3 (42%)
9	SAC	I	1	9	7,8,9	2.50	2 (28%)	7,9,11	1.77	2 (28%)

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
2	FME	O	1	2	-	1/7/9/11	-
7	TPO	G	11	7	-	5/9/11/13	-
1	FME	A	1	1	-	3/7/9/11	-
7	TPO	T	11	7	-	4/9/11/13	-
2	FME	B	1	2	-	1/7/9/11	-
1	FME	N	1	1	-	4/7/9/11	-
9	SAC	V	1	9	-	3/7/8/10	-
9	SAC	I	1	9	-	3/7/8/10	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	V	1	SAC	OAC-C1A	5.32	1.35	1.23
9	I	1	SAC	OAC-C1A	5.17	1.34	1.23
9	V	1	SAC	CA-N	4.28	1.52	1.46
9	I	1	SAC	CA-N	3.83	1.52	1.46
7	G	11	TPO	CB-CA	3.11	1.60	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CA-N-CN	-4.41	116.05	122.82
2	B	1	FME	C-CA-N	4.24	117.69	109.50
1	N	1	FME	CA-N-CN	-3.73	117.09	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	1	FME	C-CA-N	3.56	116.37	109.50
9	I	1	SAC	C-CA-N	-3.28	103.16	109.50

There are no chirality outliers.

5 of 24 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 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	1	FME	4	0
7	G	11	TPO	1	0
1	A	1	FME	4	0
7	T	11	TPO	1	0
1	N	1	FME	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 54 ligands modelled in this entry, 8 are monoatomic and 2 are unknown - leaving 44 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	PEK	G	1263	-	52,52,52	1.83	12 (23%)	55,57,57	1.22	4 (7%)
19	CUA	B	228	2	0,1,1	-	-	-		
22	CHD	W	1060	-	32,32,32	0.98	2 (6%)	51,51,51	3.17	26 (50%)
20	TGL	B	521	-	62,62,62	0.70	0	65,65,65	1.43	11 (16%)
25	PEK	C	265	-	52,52,52	1.62	10 (19%)	55,57,57	1.10	5 (9%)
23	DMU	Z	1526	-	34,34,34	3.20	8 (23%)	45,45,45	4.22	19 (42%)
18	PGV	Z	1524	-	50,50,50	1.05	3 (6%)	53,56,56	0.92	2 (3%)
20	TGL	Q	1523	-	62,62,62	0.82	2 (3%)	65,65,65	1.27	9 (13%)
20	TGL	N	1521	-	62,62,62	0.74	1 (1%)	65,65,65	1.42	10 (15%)
25	PEK	P	1265	-	52,52,52	1.66	11 (21%)	55,57,57	1.08	5 (9%)
22	CHD	J	60	-	32,32,32	0.91	1 (3%)	51,51,51	3.19	25 (49%)
18	PGV	P	1267	-	50,50,50	0.85	1 (2%)	53,56,56	0.83	1 (1%)
21	PSC	O	1230	-	51,51,51	1.16	3 (5%)	57,59,59	0.88	1 (1%)
22	CHD	P	1525	-	32,32,32	0.88	0	51,51,51	1.59	9 (17%)
18	PGV	C	268	-	50,50,50	1.25	3 (6%)	53,56,56	0.82	1 (1%)
26	CDL	G	269	-	99,99,99	0.93	6 (6%)	105,111,111	0.97	7 (6%)
17	HEA	A	516	1	67,67,67	1.13	4 (5%)	81,103,103	1.15	4 (4%)
20	TGL	L	522	-	62,62,62	1.14	4 (6%)	65,65,65	1.73	13 (20%)
26	CDL	C	270	-	99,99,99	0.80	3 (3%)	105,111,111	0.99	6 (5%)
23	DMU	M	526	-	34,34,34	3.25	8 (23%)	45,45,45	4.27	19 (42%)
18	PGV	A	525	-	50,50,50	0.90	2 (4%)	53,56,56	0.75	2 (3%)
23	DMU	P	1272	-	34,34,34	3.03	8 (23%)	45,45,45	4.07	19 (42%)
21	PSC	B	230	-	51,51,51	1.19	3 (5%)	57,59,59	0.87	1 (1%)
22	CHD	P	1271	-	32,32,32	0.82	0	51,51,51	3.54	22 (43%)
18	PGV	N	1266	-	50,50,50	0.93	2 (4%)	53,56,56	0.78	3 (5%)
17	HEA	N	516	1	67,67,67	1.13	6 (8%)	81,103,103	1.24	9 (11%)
25	PEK	P	1264	-	52,52,52	1.43	4 (7%)	55,57,57	1.05	3 (5%)
22	CHD	C	271	-	32,32,32	0.84	0	51,51,51	3.60	22 (43%)
26	CDL	P	1270	-	99,99,99	0.83	3 (3%)	105,111,111	0.97	6 (5%)
25	PEK	C	264	-	52,52,52	1.44	4 (7%)	55,57,57	1.02	3 (5%)
26	CDL	T	1269	-	99,99,99	0.89	4 (4%)	105,111,111	0.98	7 (6%)
18	PGV	A	524	-	50,50,50	1.08	3 (6%)	53,56,56	0.95	2 (3%)
19	CUA	O	228	2	0,1,1	-	-	-		
25	PEK	T	263	-	52,52,52	1.85	12 (23%)	55,57,57	1.22	4 (7%)
18	PGV	P	1268	-	50,50,50	1.28	4 (8%)	53,56,56	0.84	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	TGL	N	1522	-	62,62,62	1.17	4 (6%)	65,65,65	1.71	13 (20%)
22	CHD	C	525	-	32,32,32	0.87	1 (3%)	51,51,51	1.65	12 (23%)
18	PGV	C	267	-	50,50,50	0.84	1 (2%)	53,56,56	0.85	2 (3%)
17	HEA	A	515	1	67,67,67	1.09	4 (5%)	81,103,103	1.11	6 (7%)
22	CHD	B	1086	-	32,32,32	0.75	0	51,51,51	1.80	14 (27%)
23	DMU	C	272	-	34,34,34	3.03	8 (23%)	45,45,45	4.07	19 (42%)
20	TGL	D	523	-	62,62,62	0.79	1 (1%)	65,65,65	1.30	9 (13%)
17	HEA	N	515	1	67,67,67	1.04	3 (4%)	81,103,103	1.11	6 (7%)
22	CHD	O	229	-	32,32,32	0.85	0	51,51,51	1.83	13 (25%)

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	PEK	G	1263	-	-	28/56/56/56	-
22	CHD	W	1060	-	5/5/12/12	8/9/74/74	0/4/4/4
20	TGL	B	521	-	-	14/65/65/65	-
25	PEK	C	265	-	-	20/56/56/56	-
23	DMU	Z	1526	-	5/5/10/10	8/19/59/59	0/2/2/2
18	PGV	Z	1524	-	-	30/55/55/55	-
20	TGL	Q	1523	-	-	14/65/65/65	-
20	TGL	N	1521	-	-	14/65/65/65	-
25	PEK	P	1265	-	-	21/56/56/56	-
22	CHD	J	60	-	5/5/12/12	8/9/74/74	0/4/4/4
18	PGV	P	1267	-	-	17/55/55/55	-
21	PSC	O	1230	-	-	39/55/55/55	-
22	CHD	P	1525	-	-	2/9/74/74	0/4/4/4
18	PGV	C	268	-	-	34/55/55/55	-
26	CDL	G	269	-	-	61/110/110/110	-
17	HEA	A	516	1	-	6/36/76/76	-
20	TGL	L	522	-	-	16/65/65/65	-
26	CDL	C	270	-	-	68/110/110/110	-
23	DMU	M	526	-	5/5/10/10	8/19/59/59	0/2/2/2
18	PGV	A	525	-	-	13/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	DMU	P	1272	-	6/6/10/10	9/19/59/59	0/2/2/2
21	PSC	B	230	-	-	39/55/55/55	-
22	CHD	P	1271	-	5/5/12/12	8/9/74/74	0/4/4/4
18	PGV	N	1266	-	-	14/55/55/55	-
17	HEA	N	516	1	-	5/36/76/76	-
25	PEK	P	1264	-	-	21/56/56/56	-
22	CHD	C	271	-	5/5/12/12	8/9/74/74	0/4/4/4
26	CDL	P	1270	-	-	69/110/110/110	-
25	PEK	C	264	-	-	21/56/56/56	-
26	CDL	T	1269	-	-	61/110/110/110	-
18	PGV	A	524	-	-	31/55/55/55	-
25	PEK	T	263	-	-	28/56/56/56	-
18	PGV	P	1268	-	-	34/55/55/55	-
20	TGL	N	1522	-	-	16/65/65/65	-
22	CHD	C	525	-	-	2/9/74/74	0/4/4/4
18	PGV	C	267	-	-	17/55/55/55	-
17	HEA	A	515	1	-	8/36/76/76	-
22	CHD	B	1086	-	-	2/9/74/74	0/4/4/4
23	DMU	C	272	-	6/6/10/10	9/19/59/59	0/2/2/2
20	TGL	D	523	-	-	14/65/65/65	-
17	HEA	N	515	1	-	7/36/76/76	-
22	CHD	O	229	-	-	2/9/74/74	0/4/4/4

The worst 5 of 159 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	Z	1526	DMU	O7-C3	-8.20	1.23	1.43
23	M	526	DMU	O7-C3	-8.15	1.23	1.43
23	M	526	DMU	O16-C6	-7.56	1.27	1.40
23	Z	1526	DMU	O16-C6	-7.49	1.27	1.40
23	M	526	DMU	O1-C9	-7.19	1.26	1.44

The worst 5 of 375 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	271	CHD	C17-C13-C14	10.49	110.64	100.11
23	C	272	DMU	C1-C2-C3	10.11	132.62	109.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	P	1272	DMU	C1-C2-C3	9.99	132.34	109.68
22	P	1271	CHD	C17-C13-C14	9.97	110.12	100.11
22	P	1271	CHD	C10-C9-C8	9.84	122.80	111.84

5 of 42 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	C	271	CHD	C14
22	C	271	CHD	C12
22	C	271	CHD	C8
22	C	271	CHD	C3
22	C	271	CHD	C9

5 of 854 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	524	PGV	C04-O12-P-O11
18	A	524	PGV	C04-O12-P-O13
18	A	524	PGV	C04-O12-P-O14
18	A	524	PGV	C02-C03-O11-P
18	A	524	PGV	C05-C04-O12-P

There are no ring outliers.

37 monomers are involved in 252 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	G	1263	PEK	7	0
22	W	1060	CHD	2	0
20	B	521	TGL	10	0
25	C	265	PEK	6	0
23	Z	1526	DMU	1	0
18	Z	1524	PGV	4	0
20	Q	1523	TGL	6	0
20	N	1521	TGL	14	0
25	P	1265	PEK	6	0
22	J	60	CHD	2	0
18	P	1267	PGV	5	0
21	O	1230	PSC	12	0
18	C	268	PGV	1	0
26	G	269	CDL	21	0
17	A	516	HEA	1	0
20	L	522	TGL	23	0

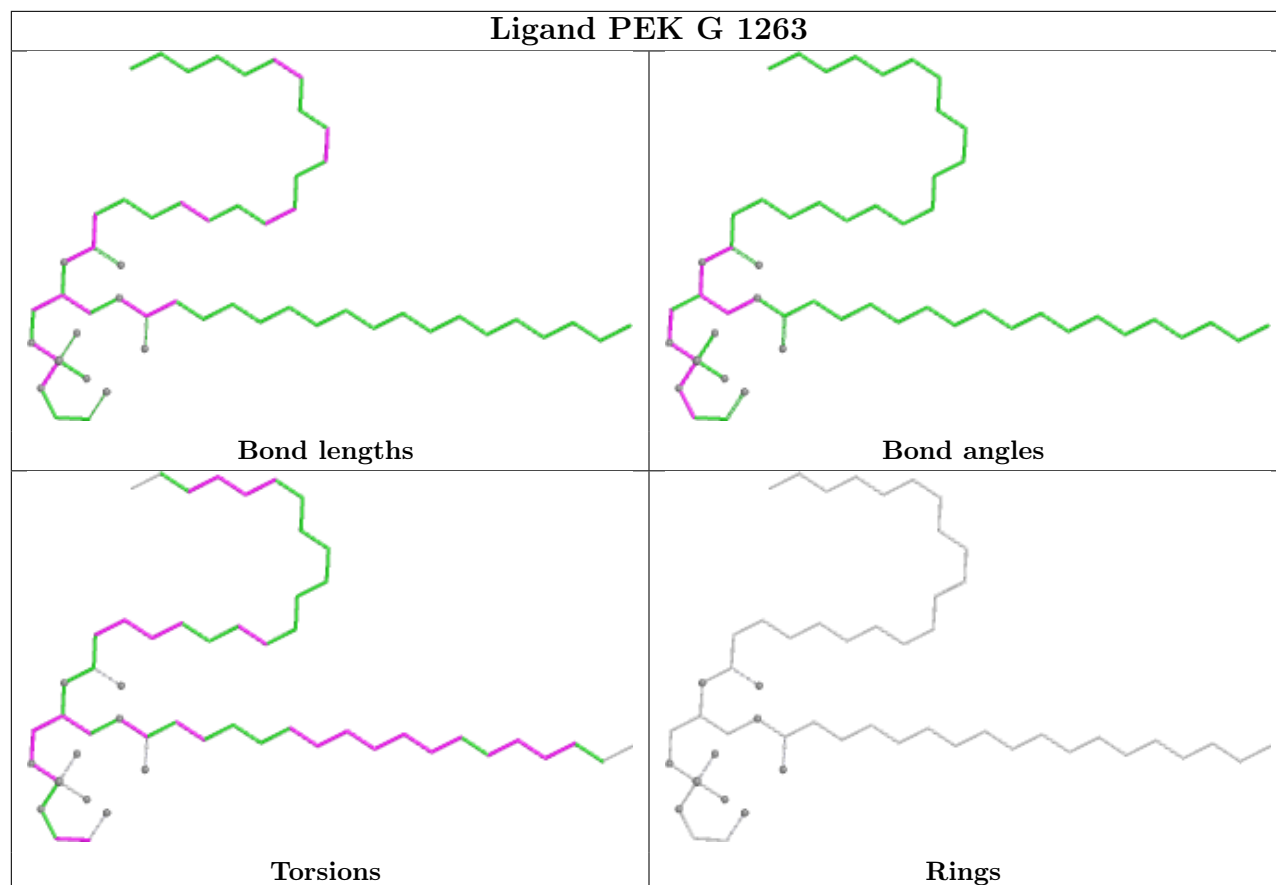
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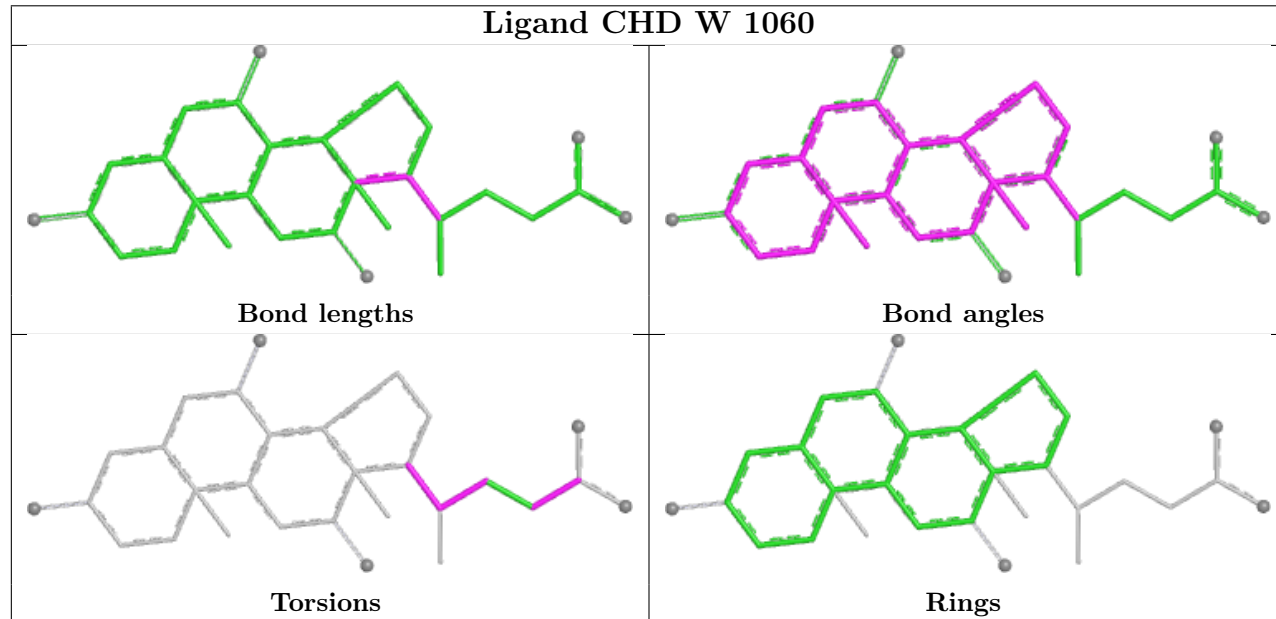
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	C	270	CDL	17	0
18	A	525	PGV	1	0
23	P	1272	DMU	7	0
21	B	230	PSC	13	0
22	P	1271	CHD	2	0
18	N	1266	PGV	2	0
25	P	1264	PEK	6	0
22	C	271	CHD	2	0
26	P	1270	CDL	15	0
25	C	264	PEK	5	0
26	T	1269	CDL	21	0
18	A	524	PGV	6	0
25	T	263	PEK	8	0
18	P	1268	PGV	3	0
20	N	1522	TGL	16	0
18	C	267	PGV	7	0
17	A	515	HEA	2	0
23	C	272	DMU	2	0
20	D	523	TGL	5	0
17	N	515	HEA	3	0
22	O	229	CHD	1	0

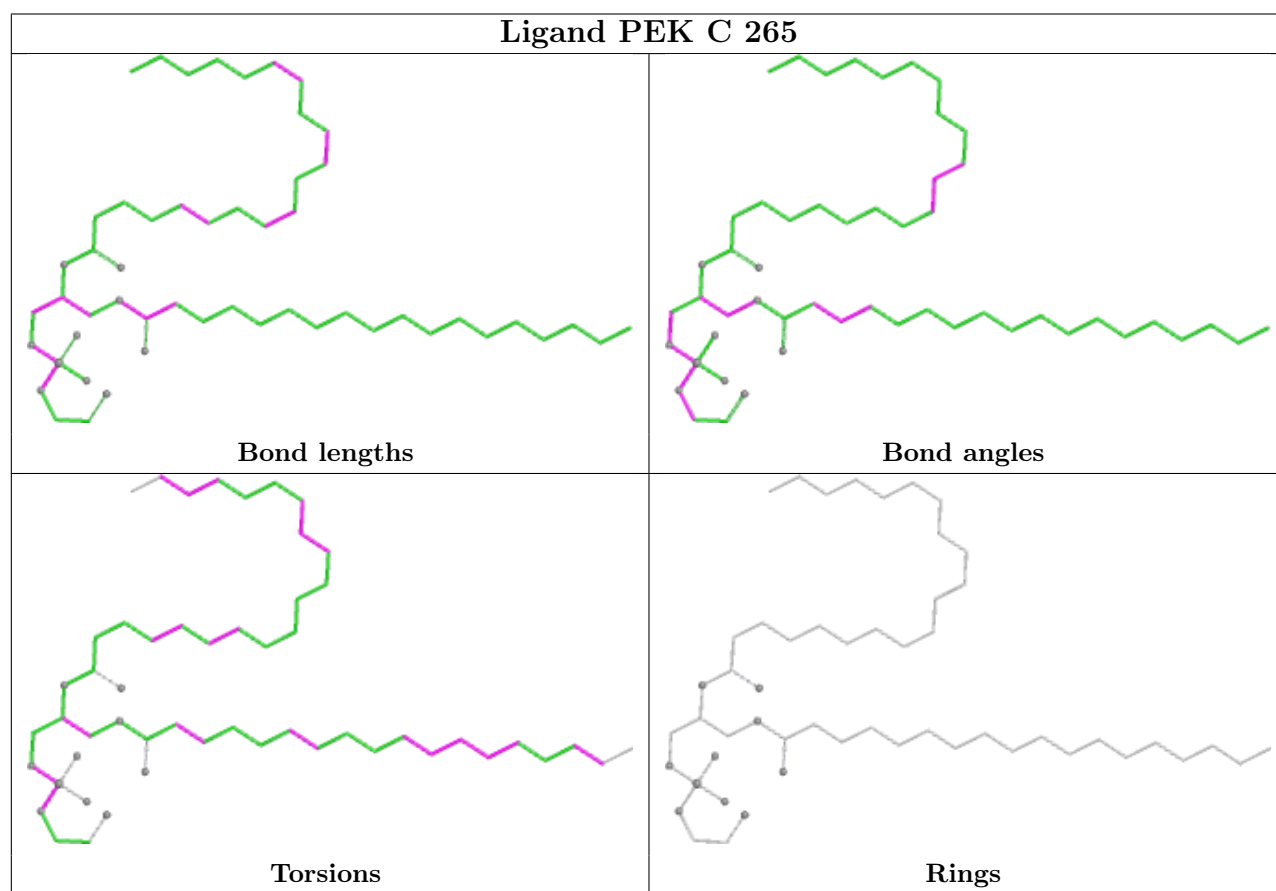
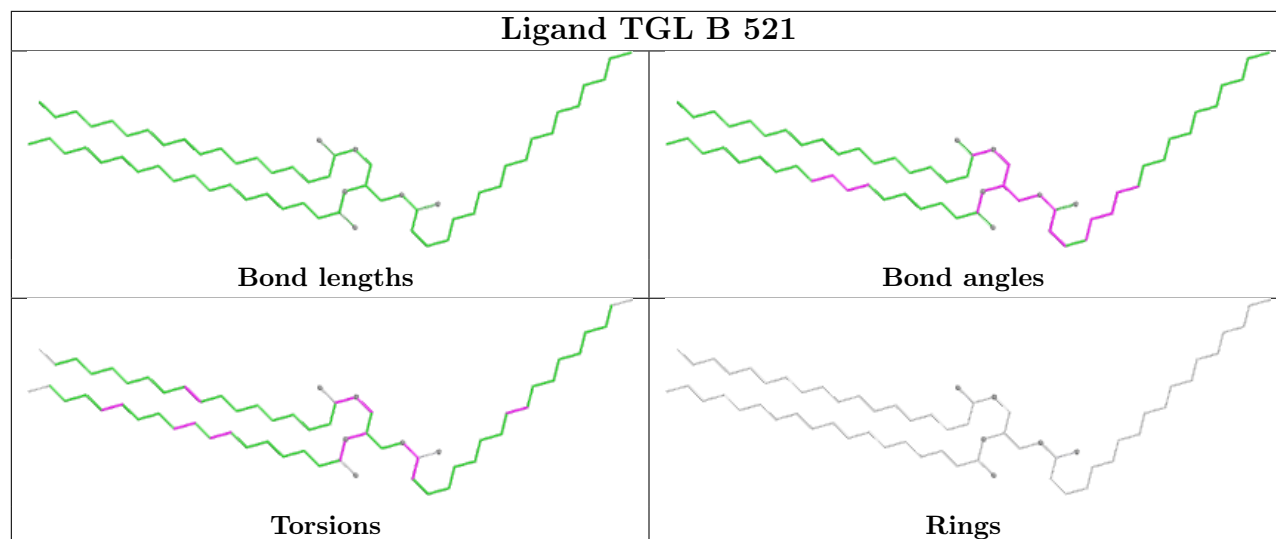
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

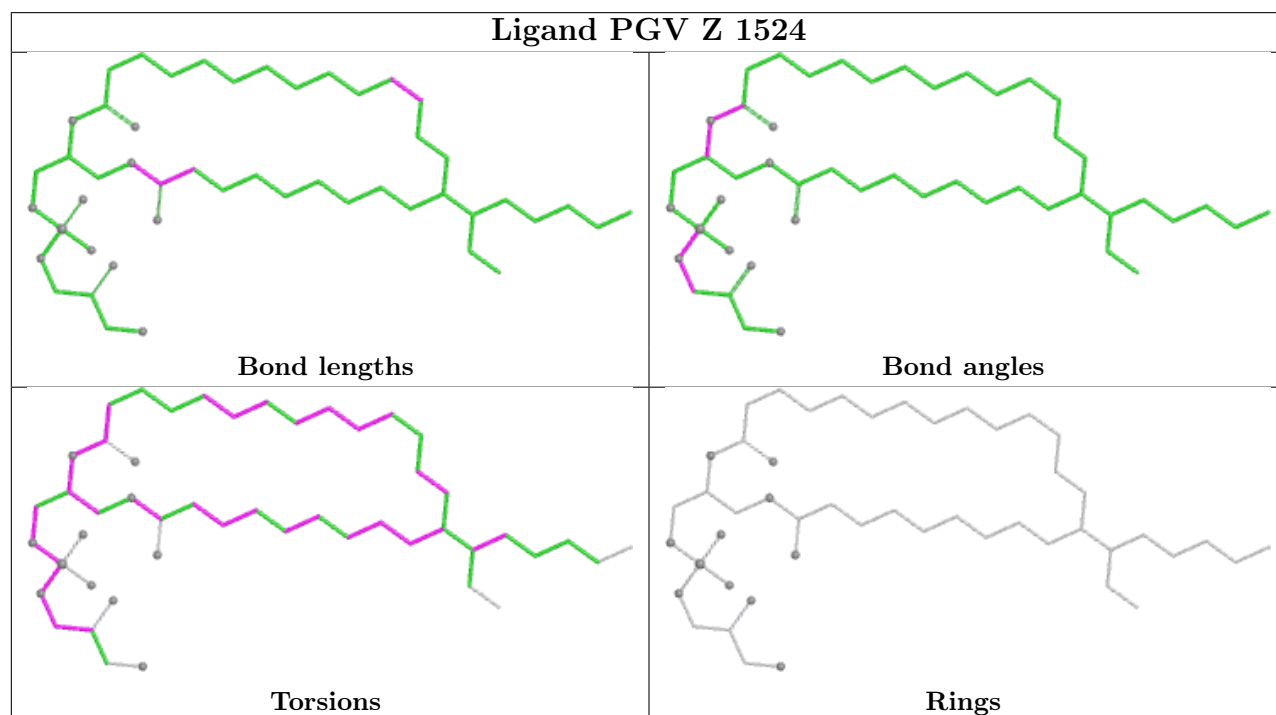
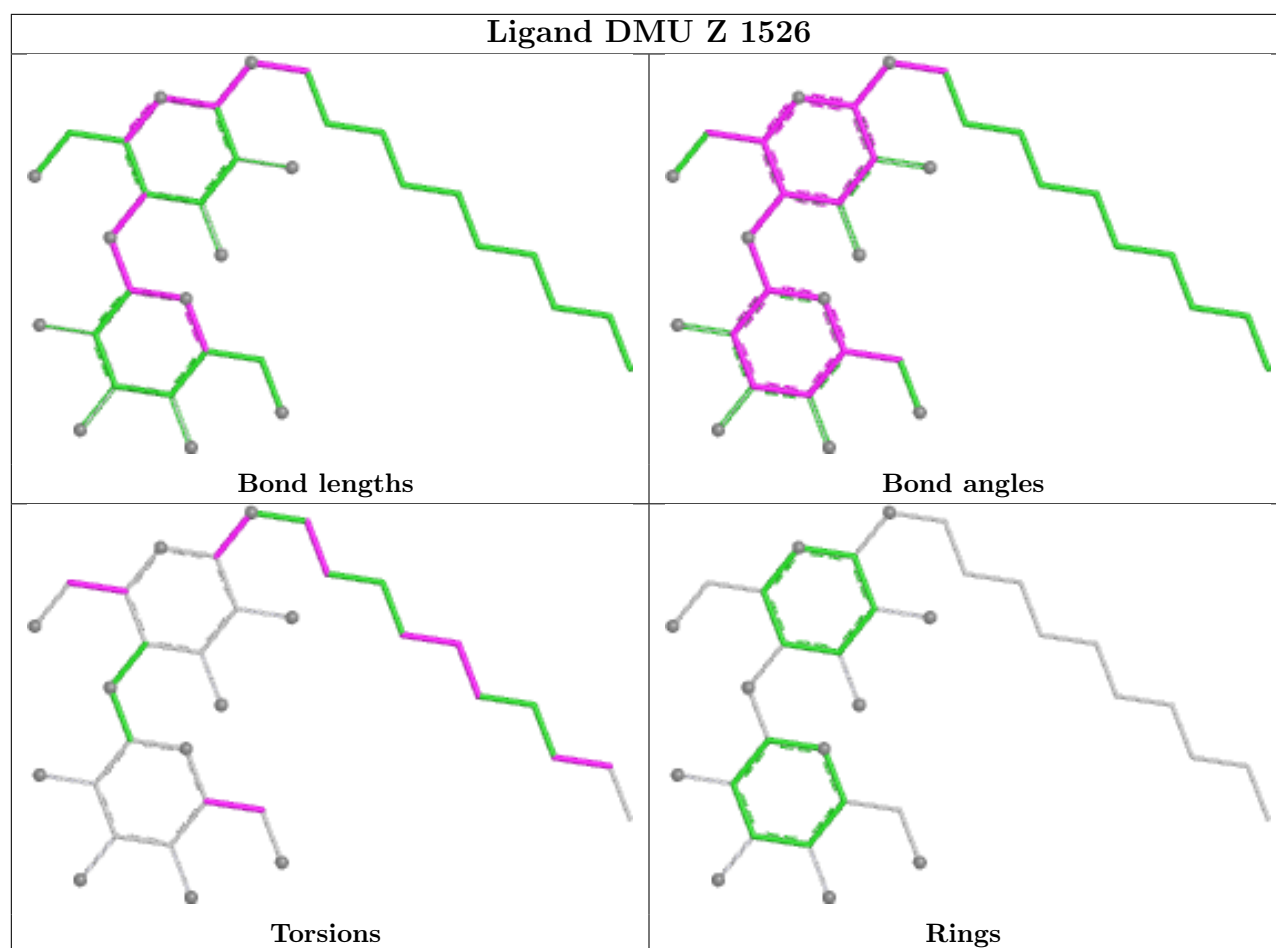
Ligand PEK G 1263

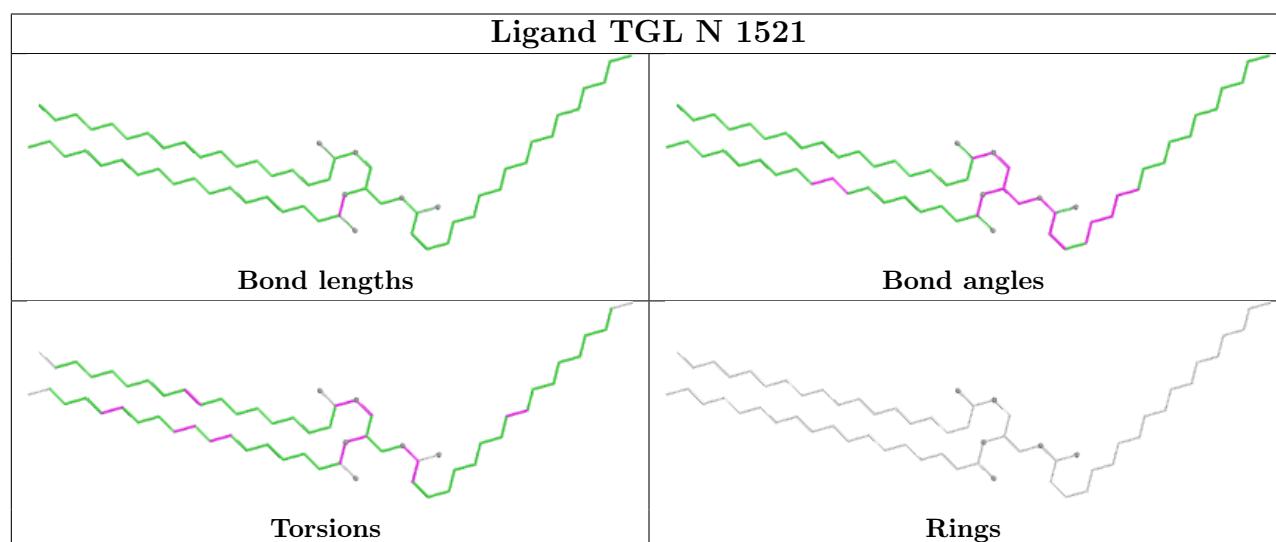
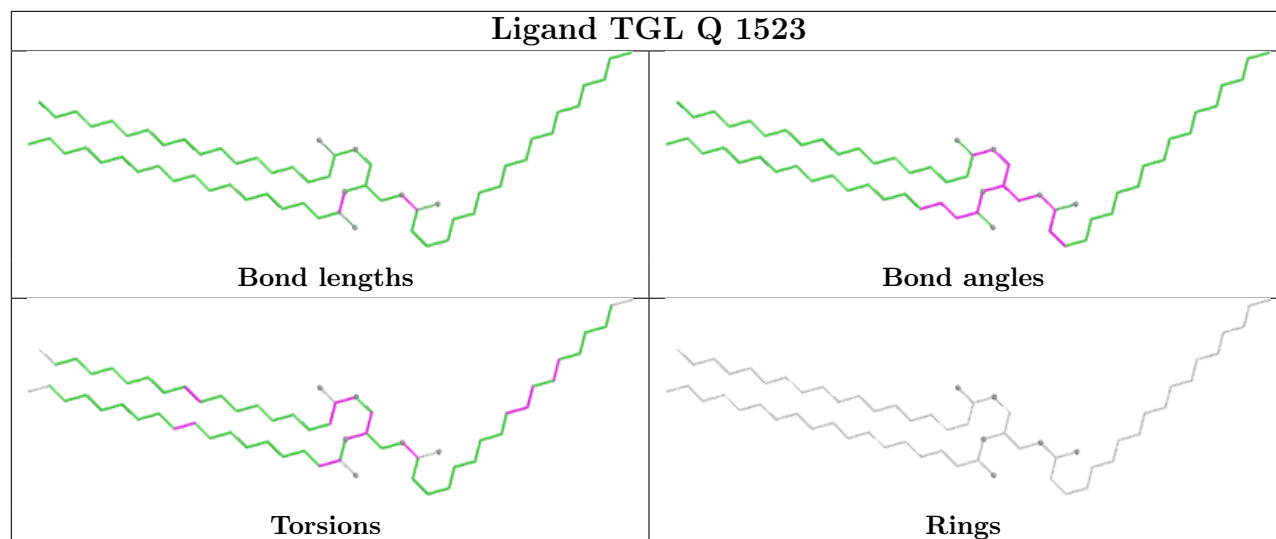


Ligand CHD W 1060

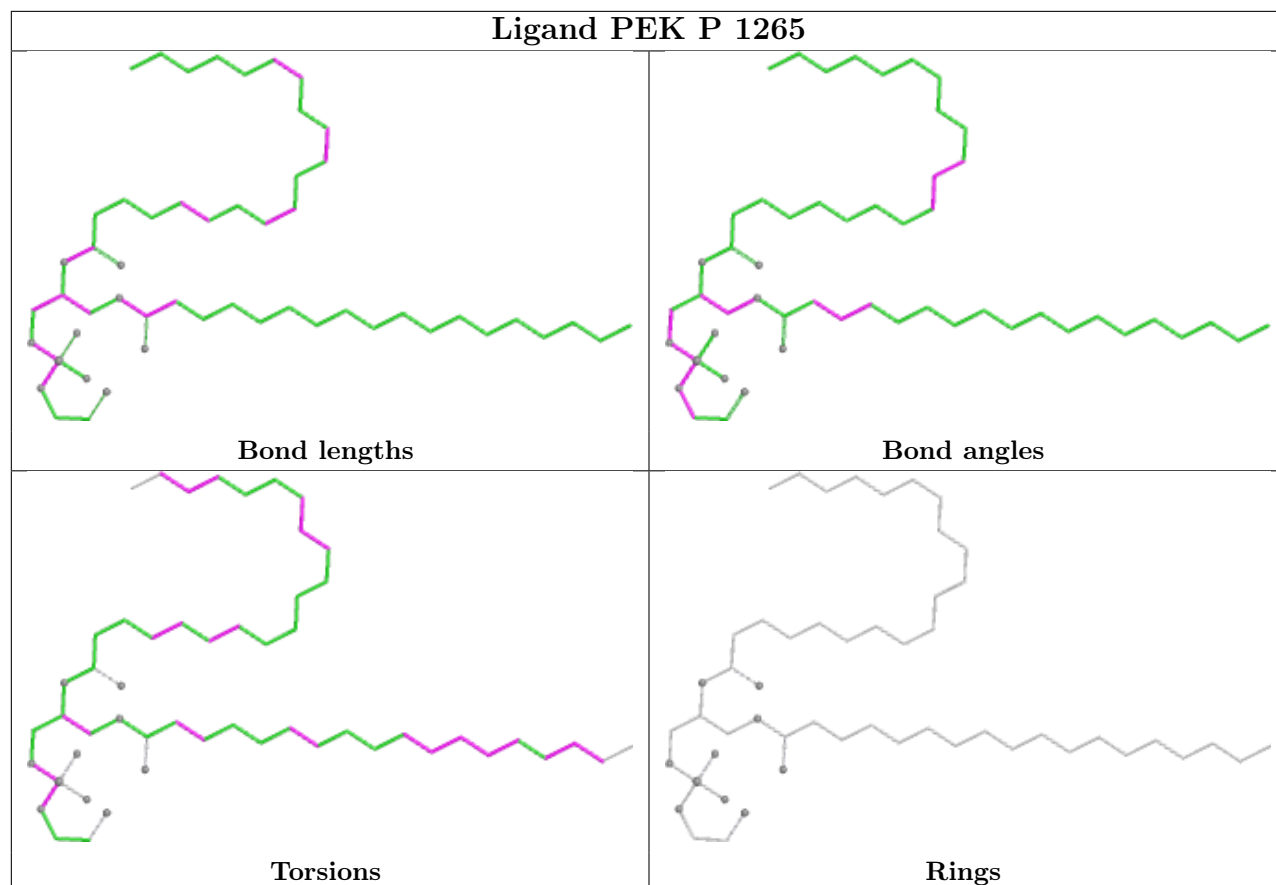




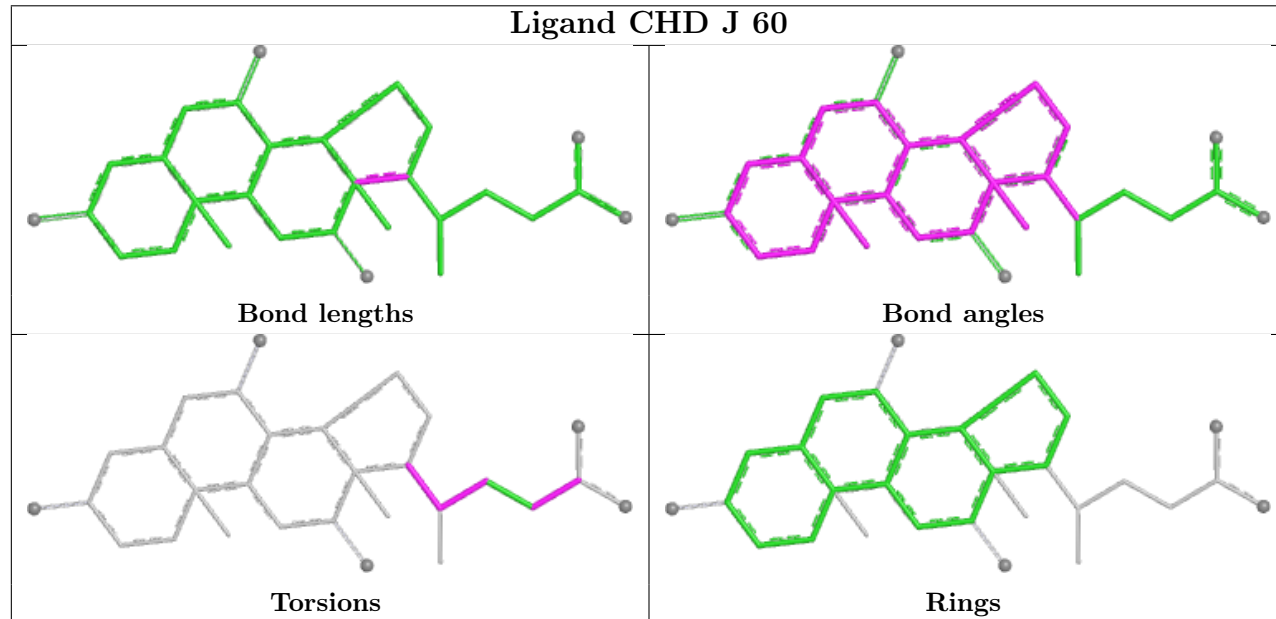


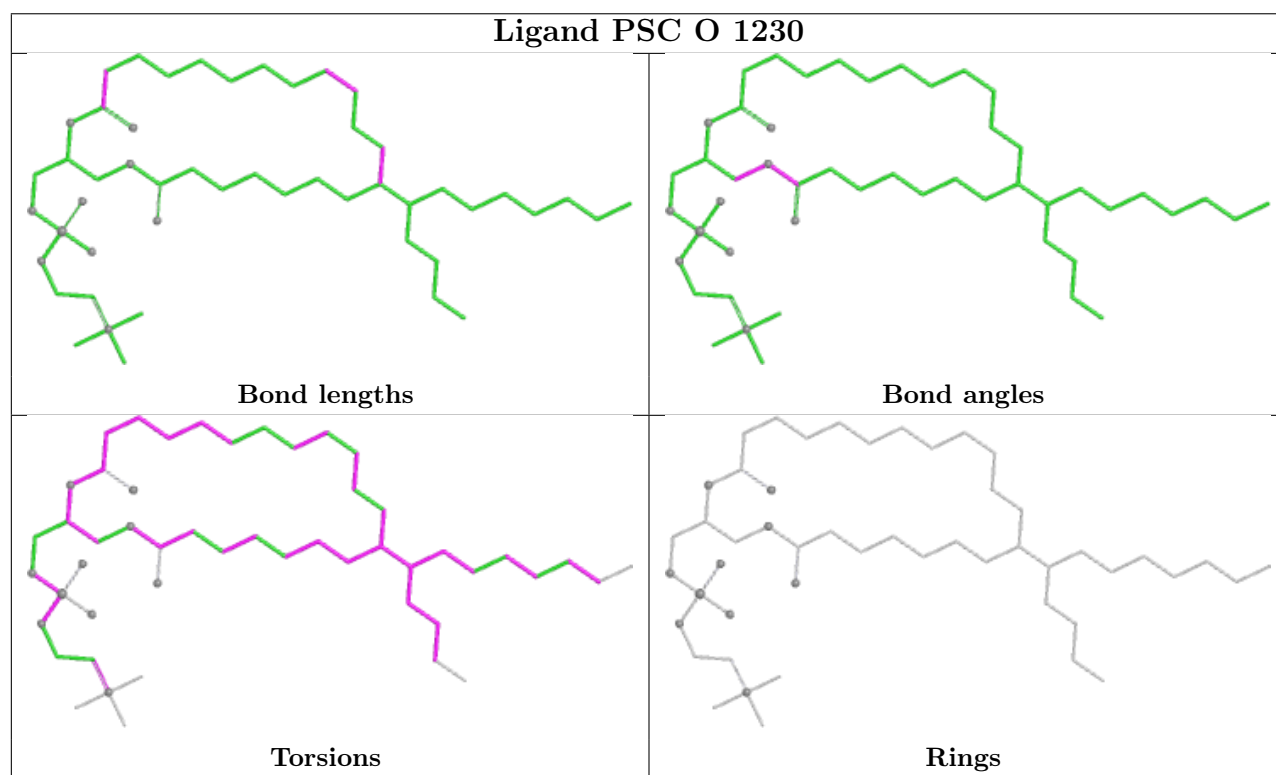
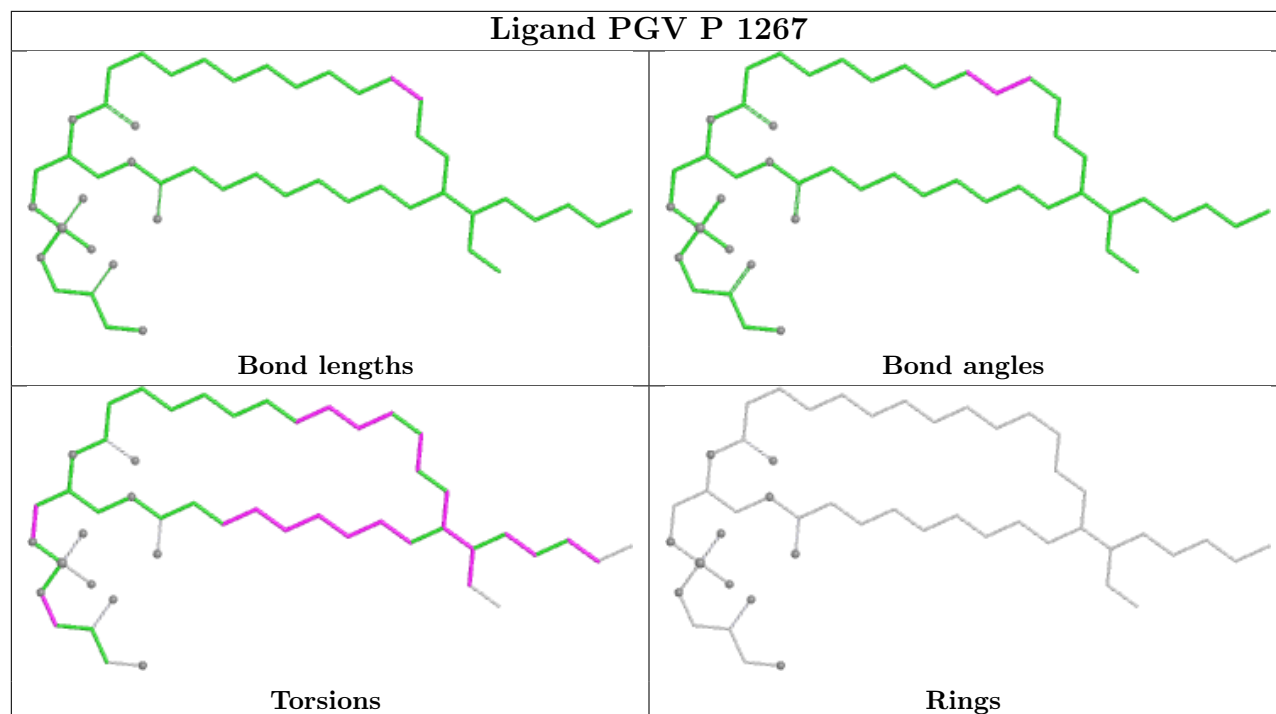


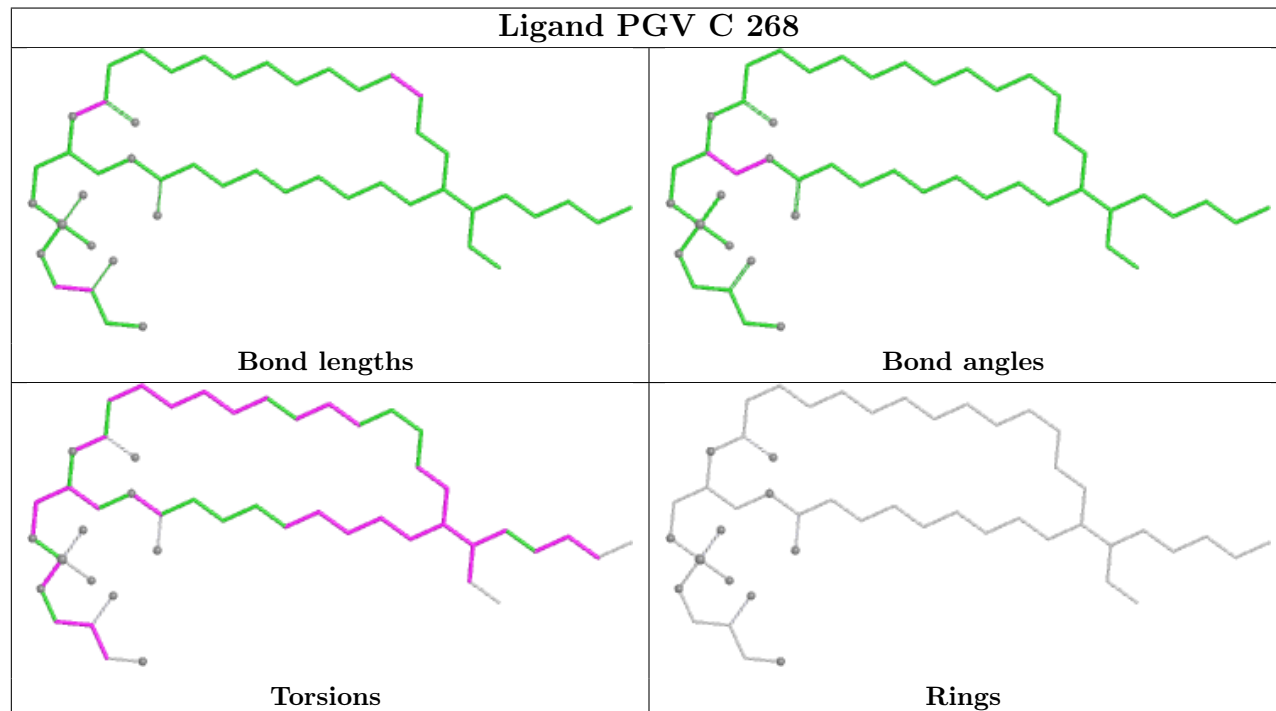
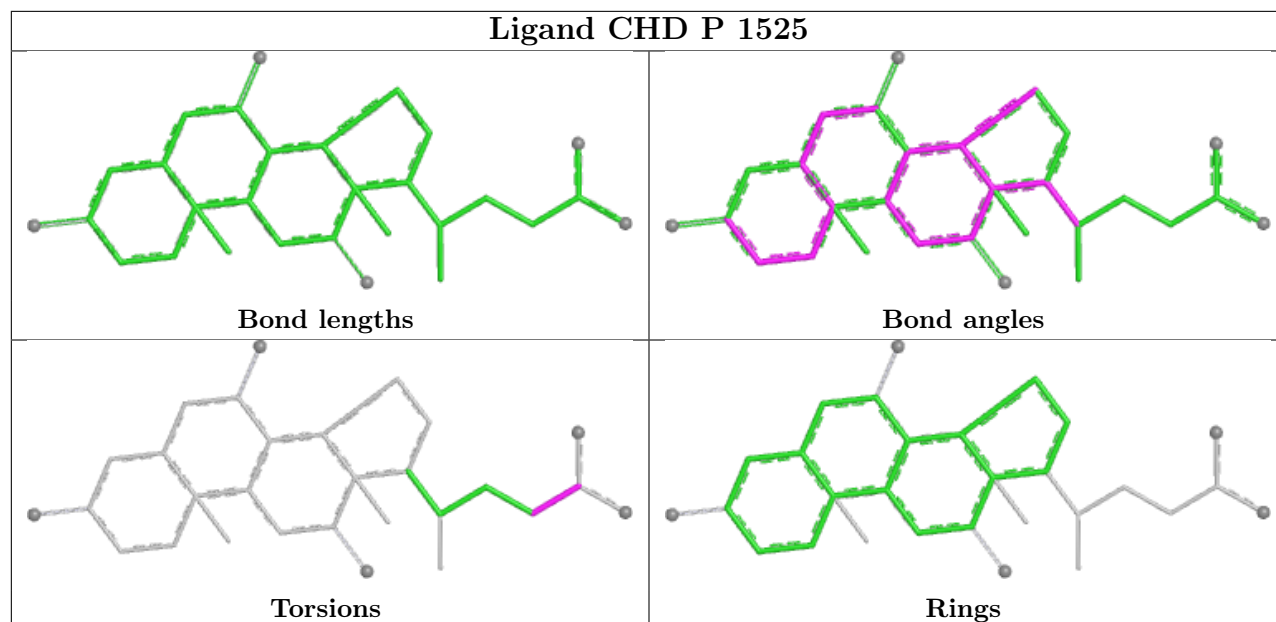
Ligand PEK P 1265

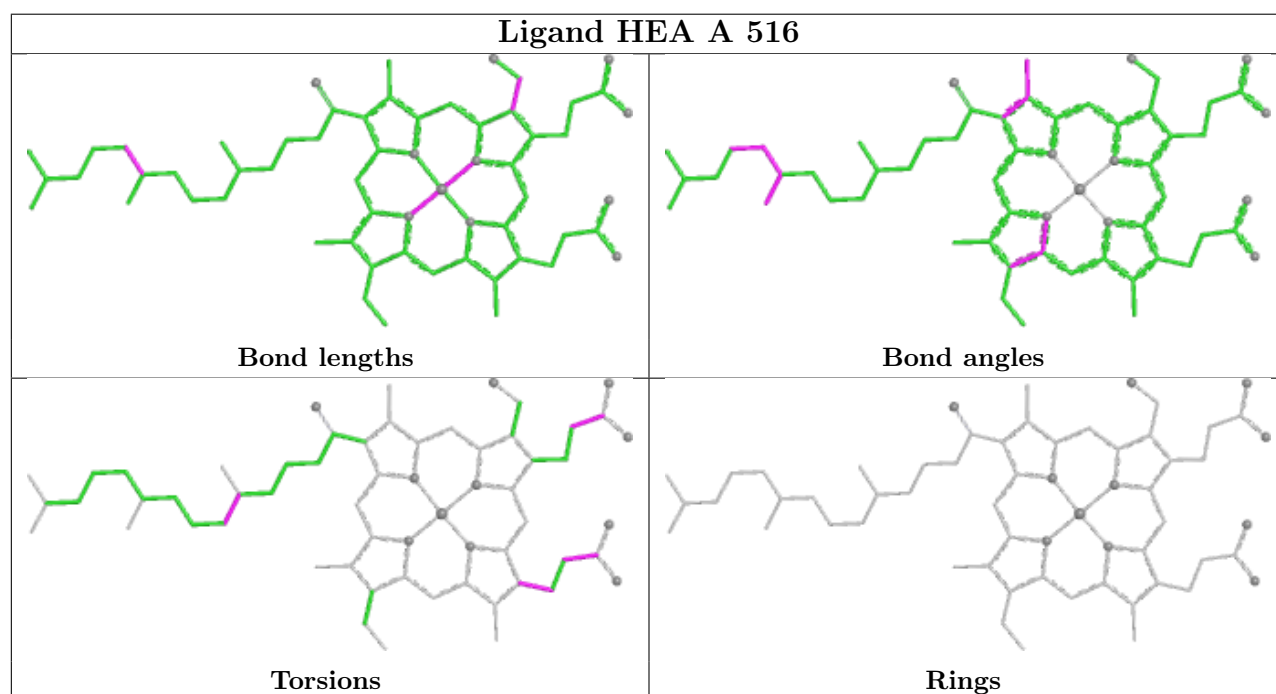
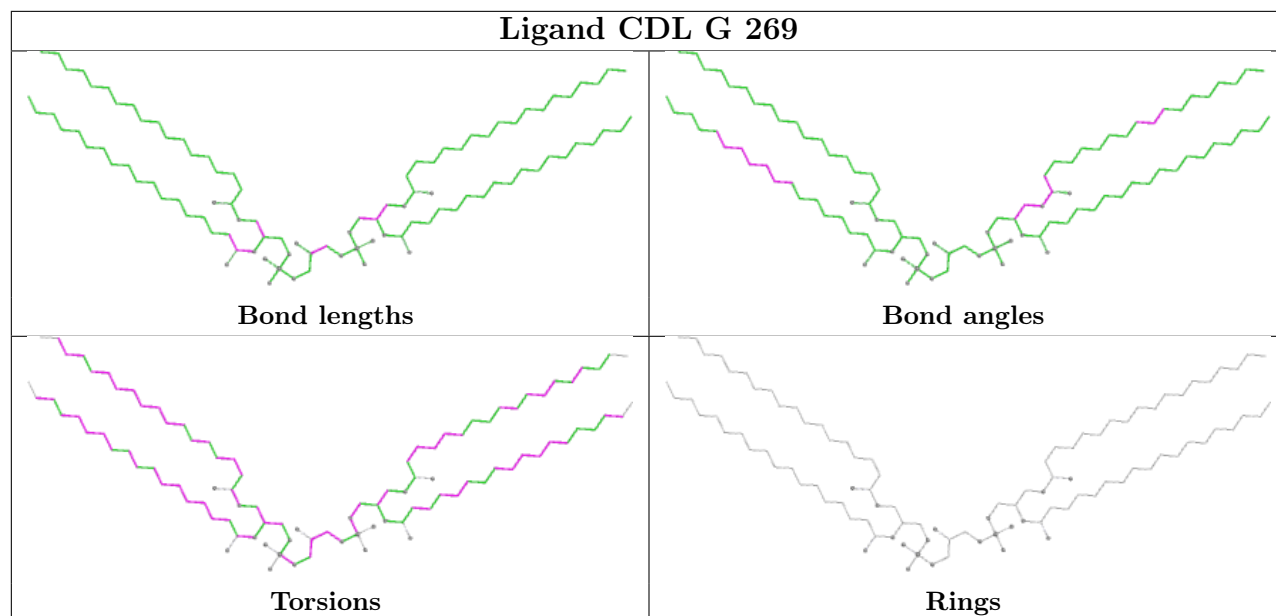


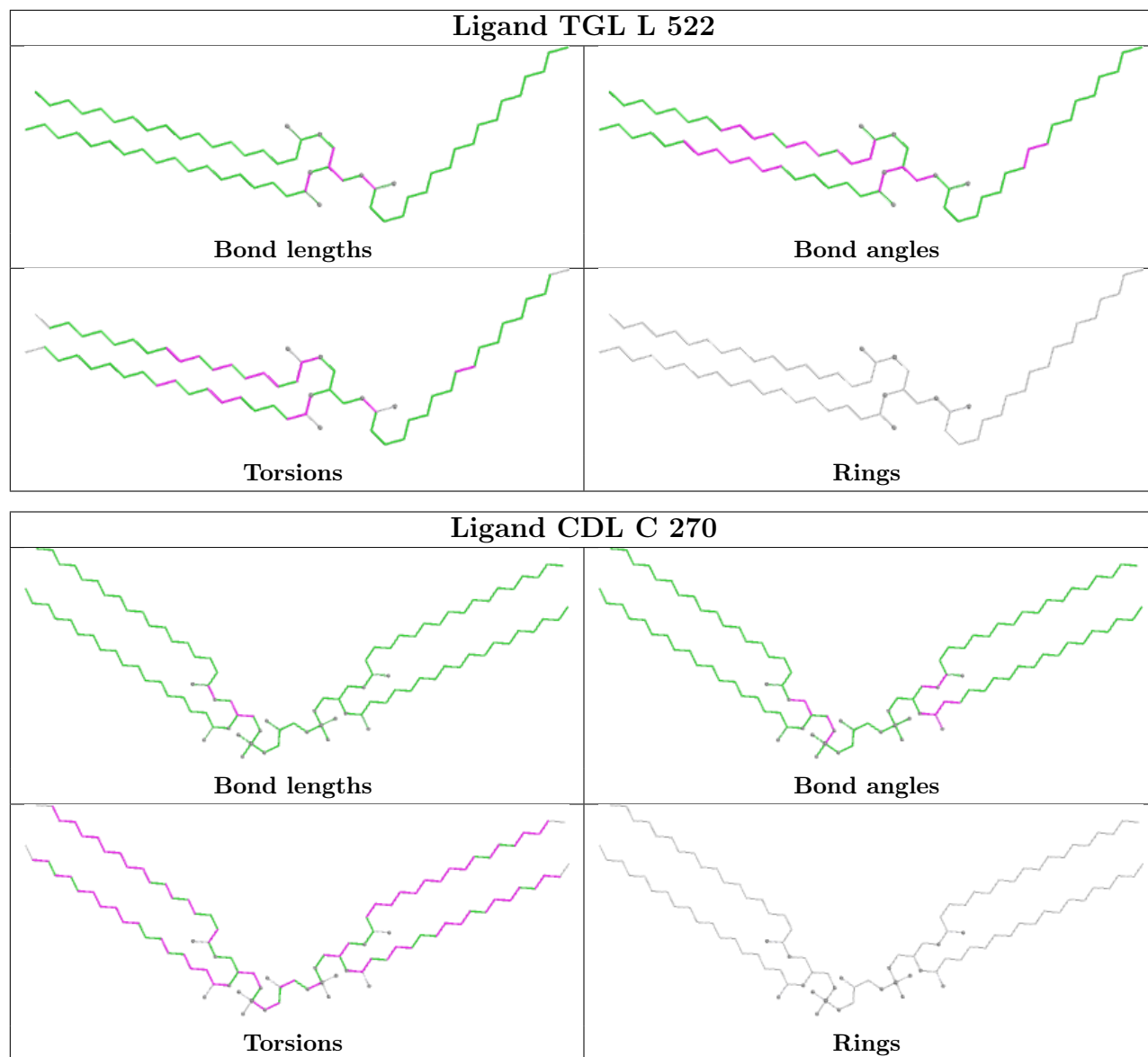
Ligand CHD J 60

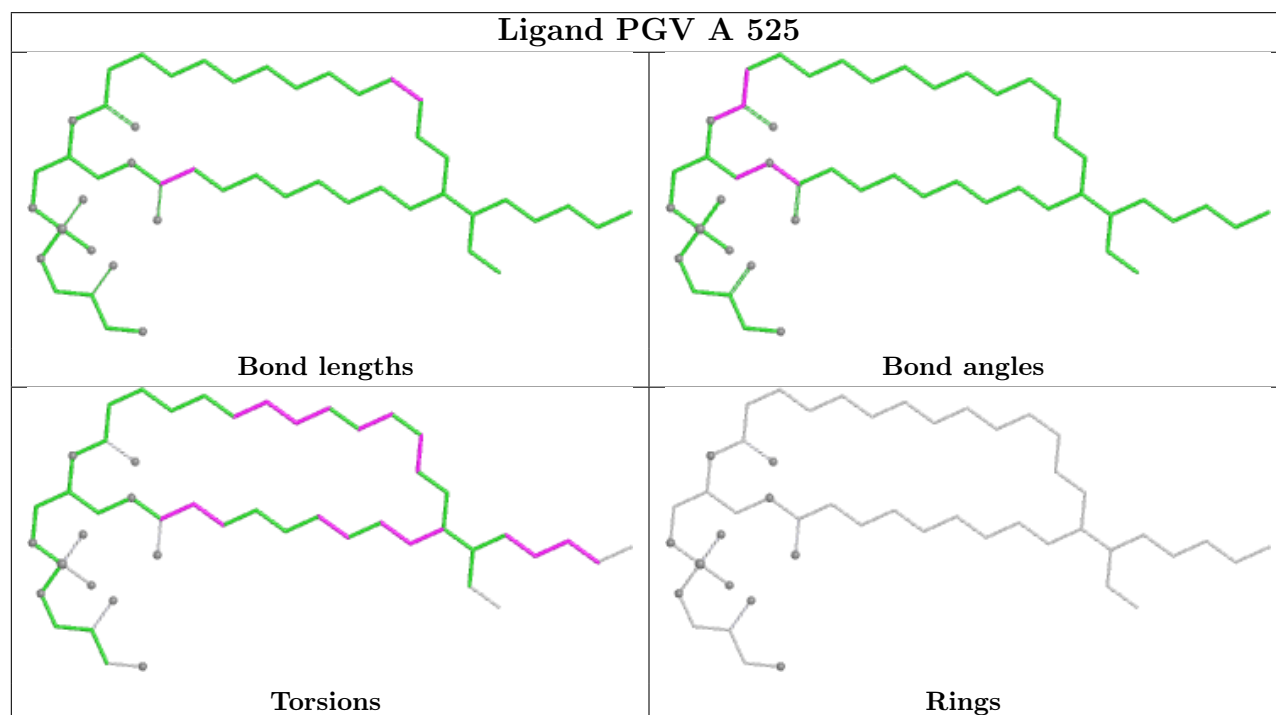
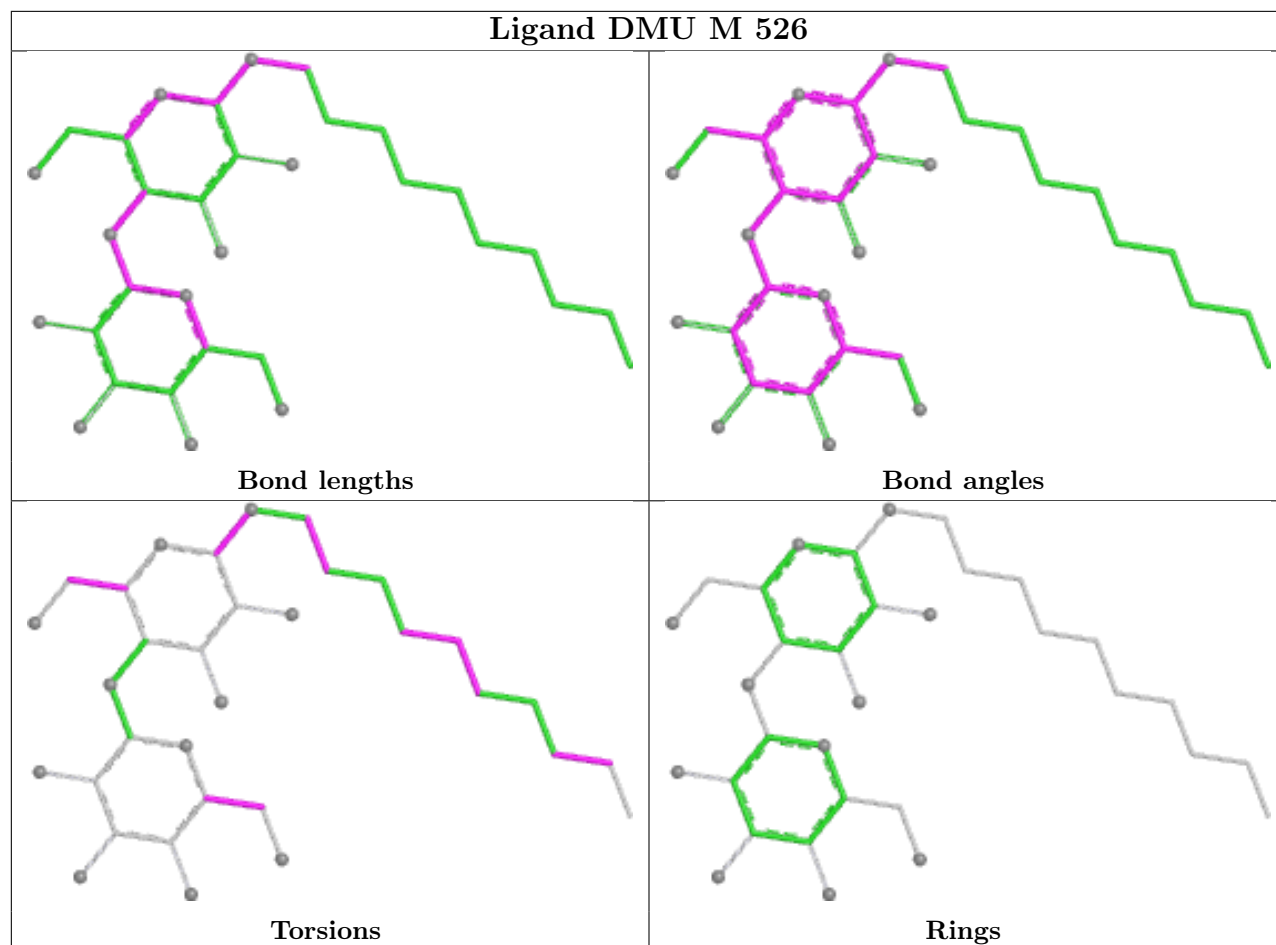




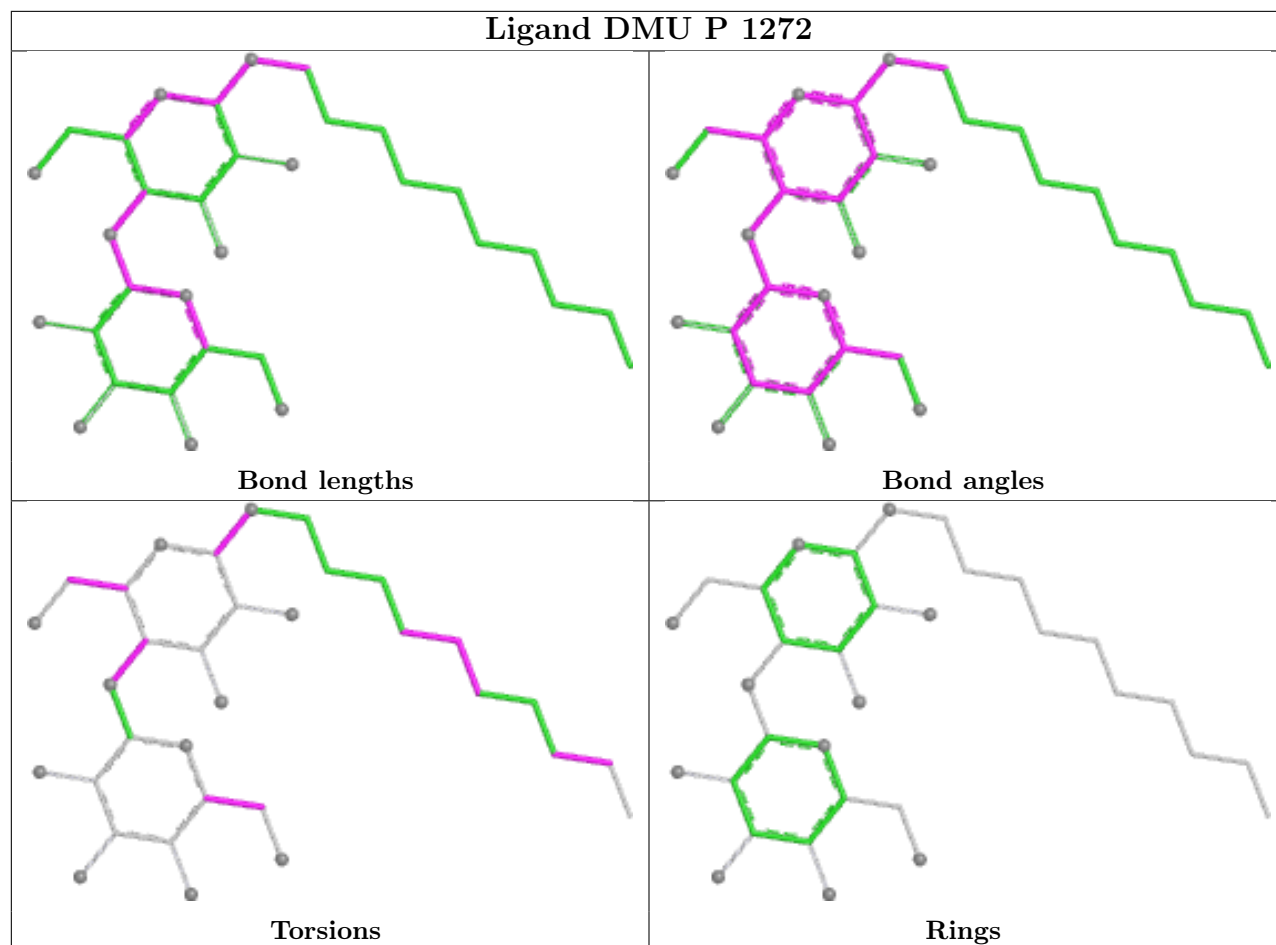




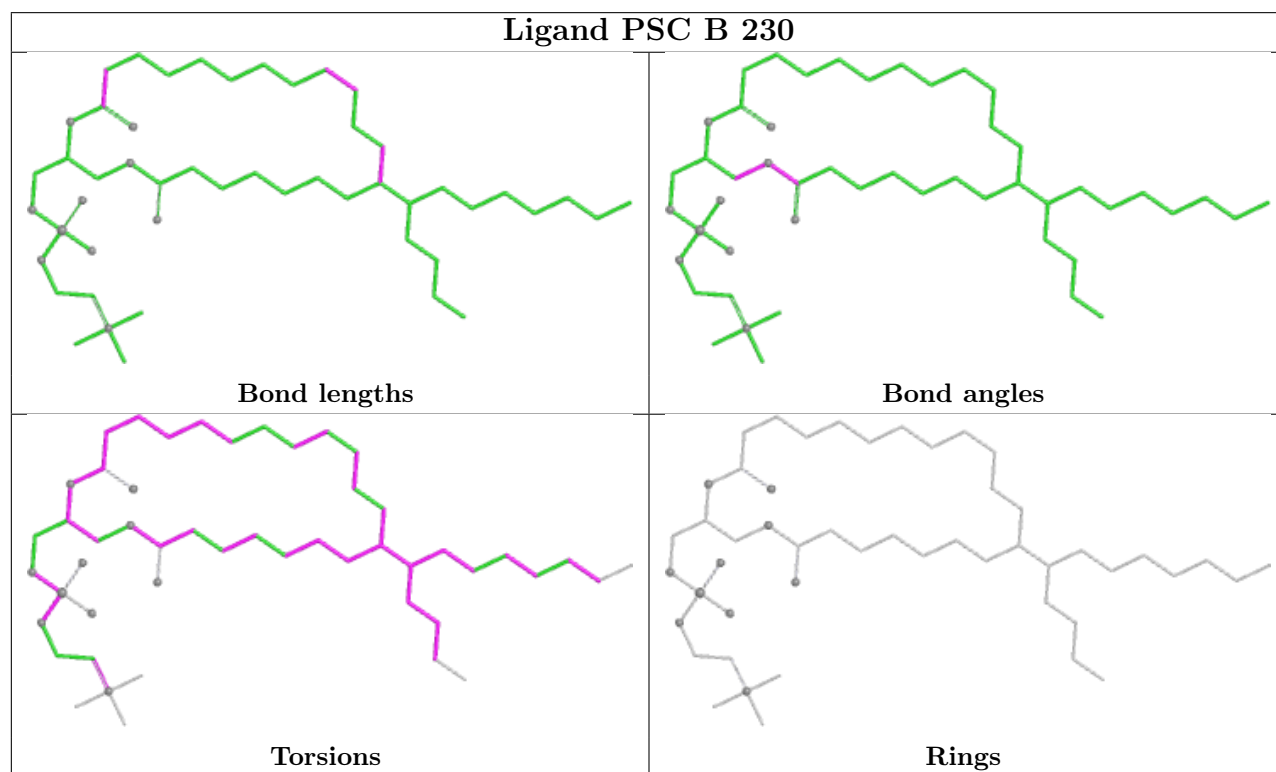


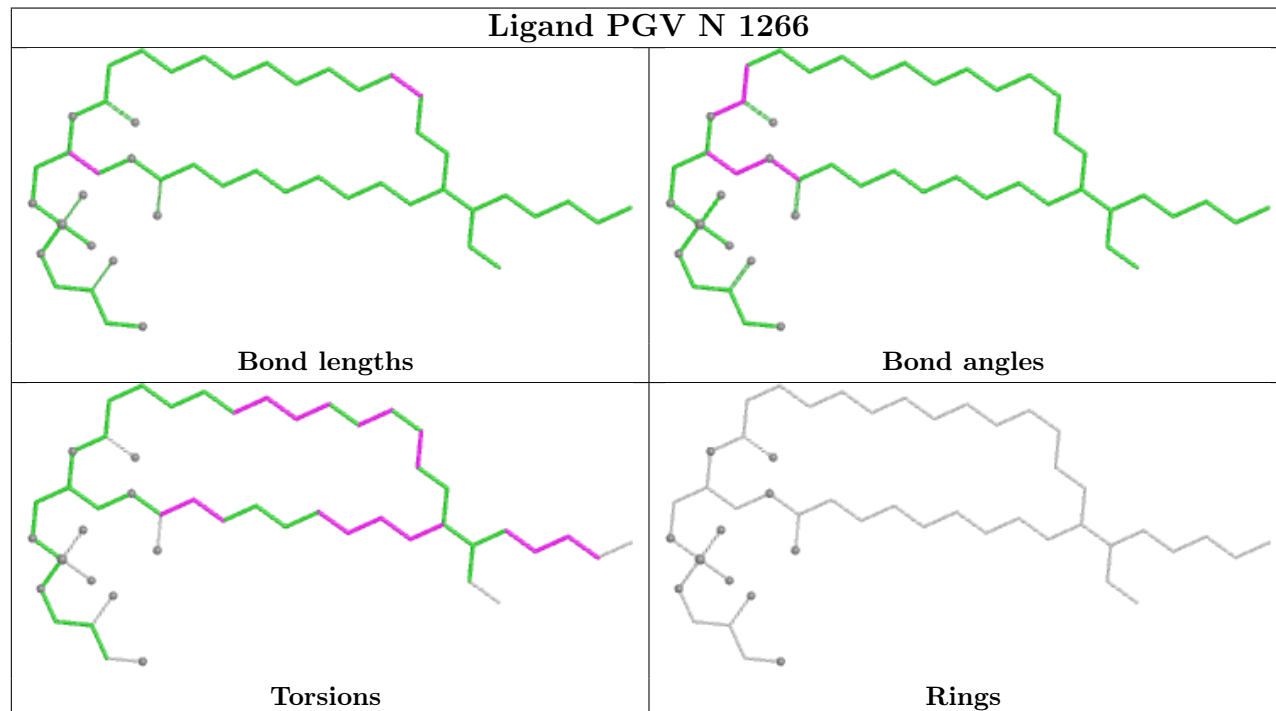
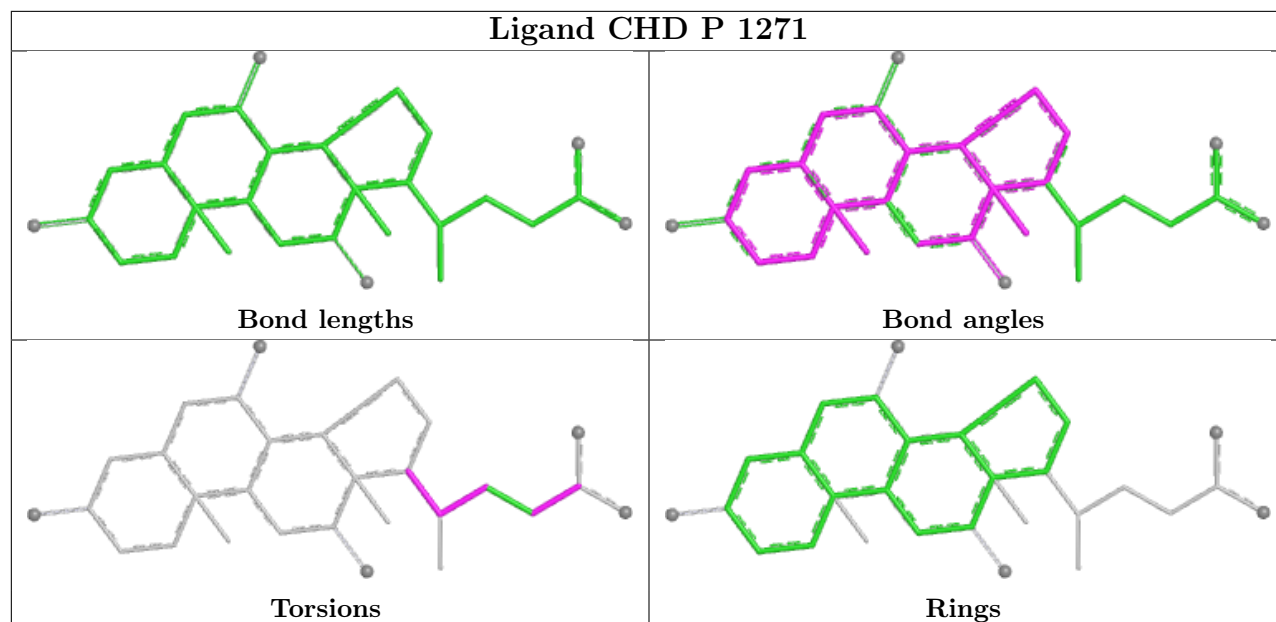


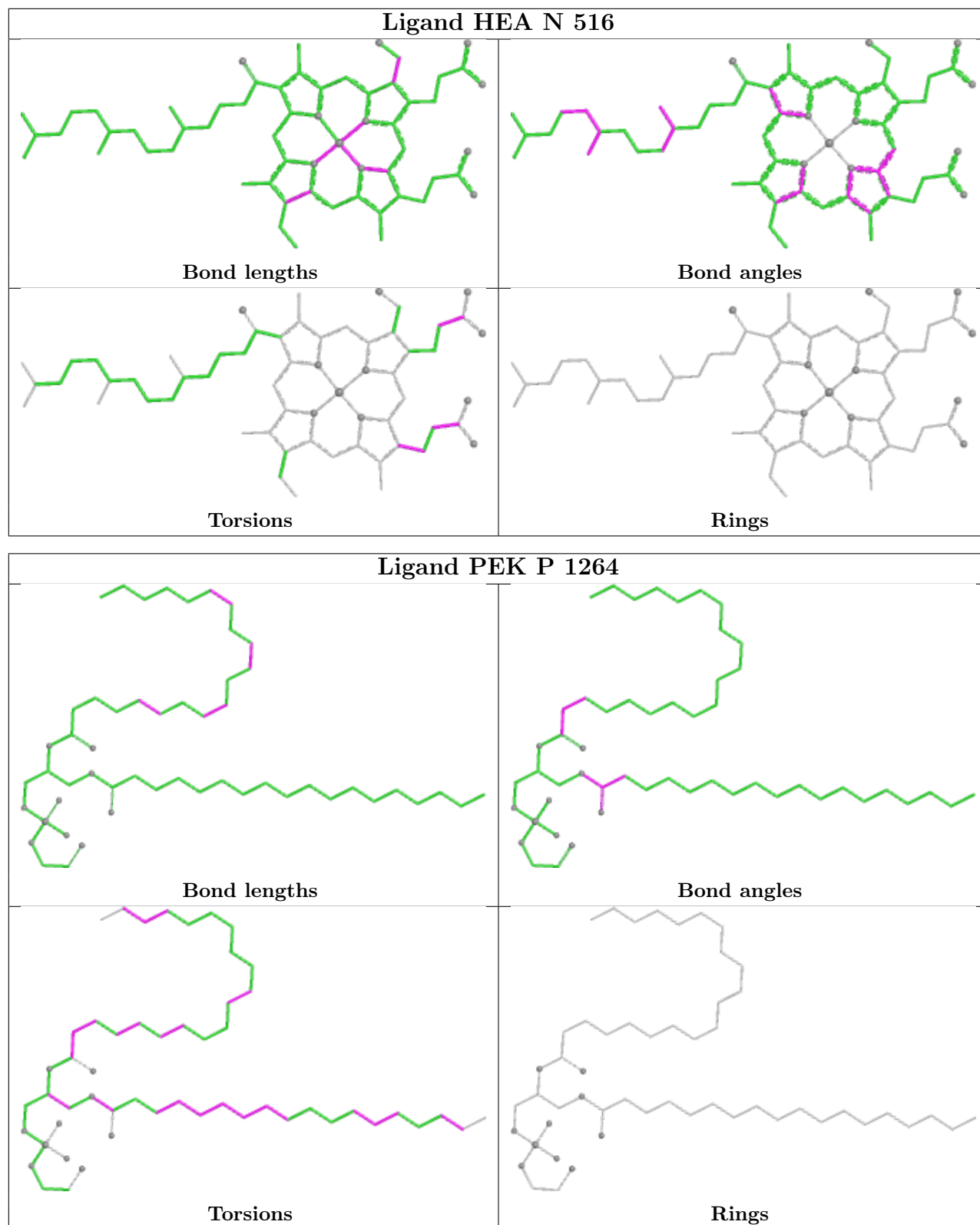
Ligand DMU P 1272

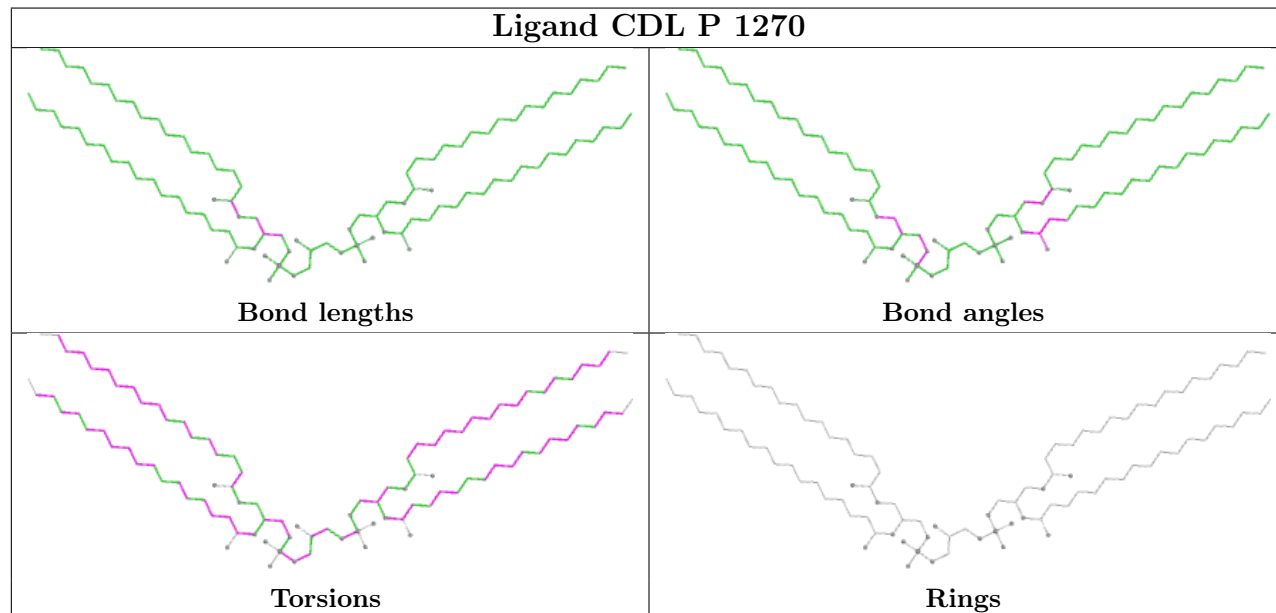
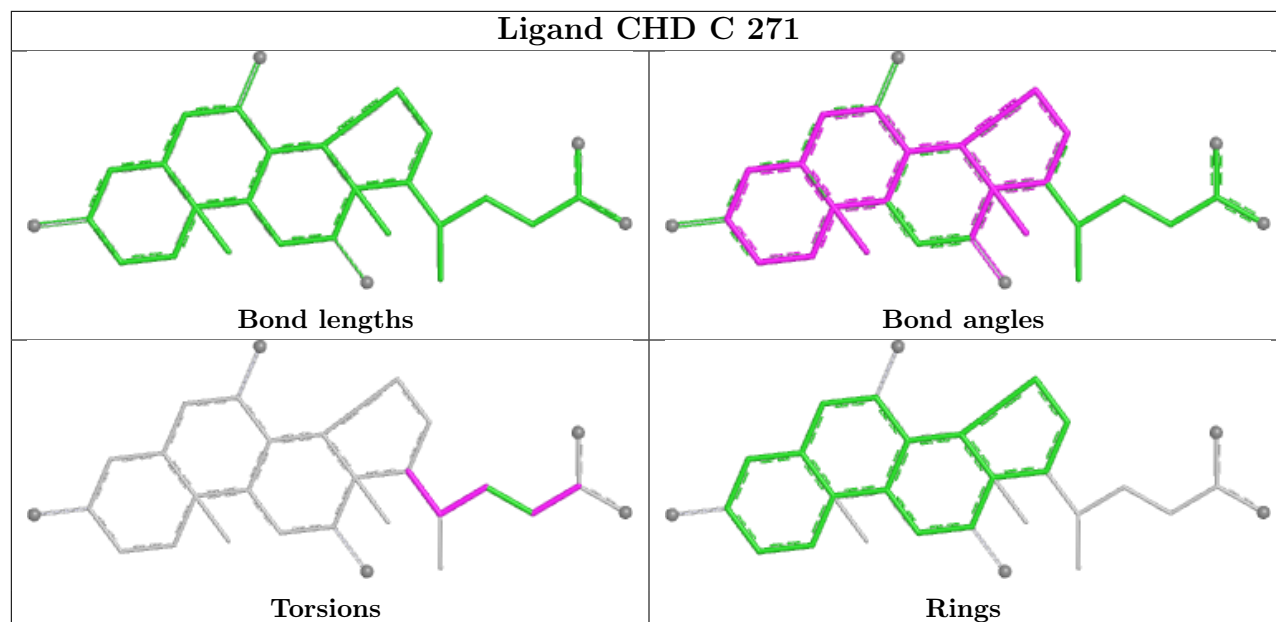


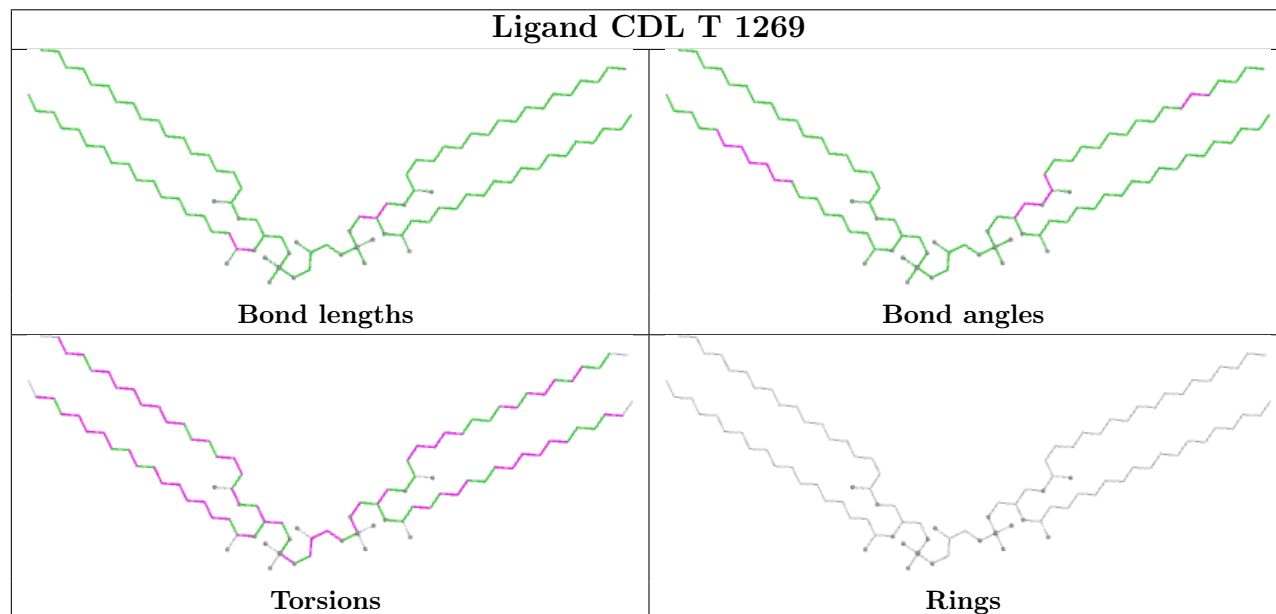
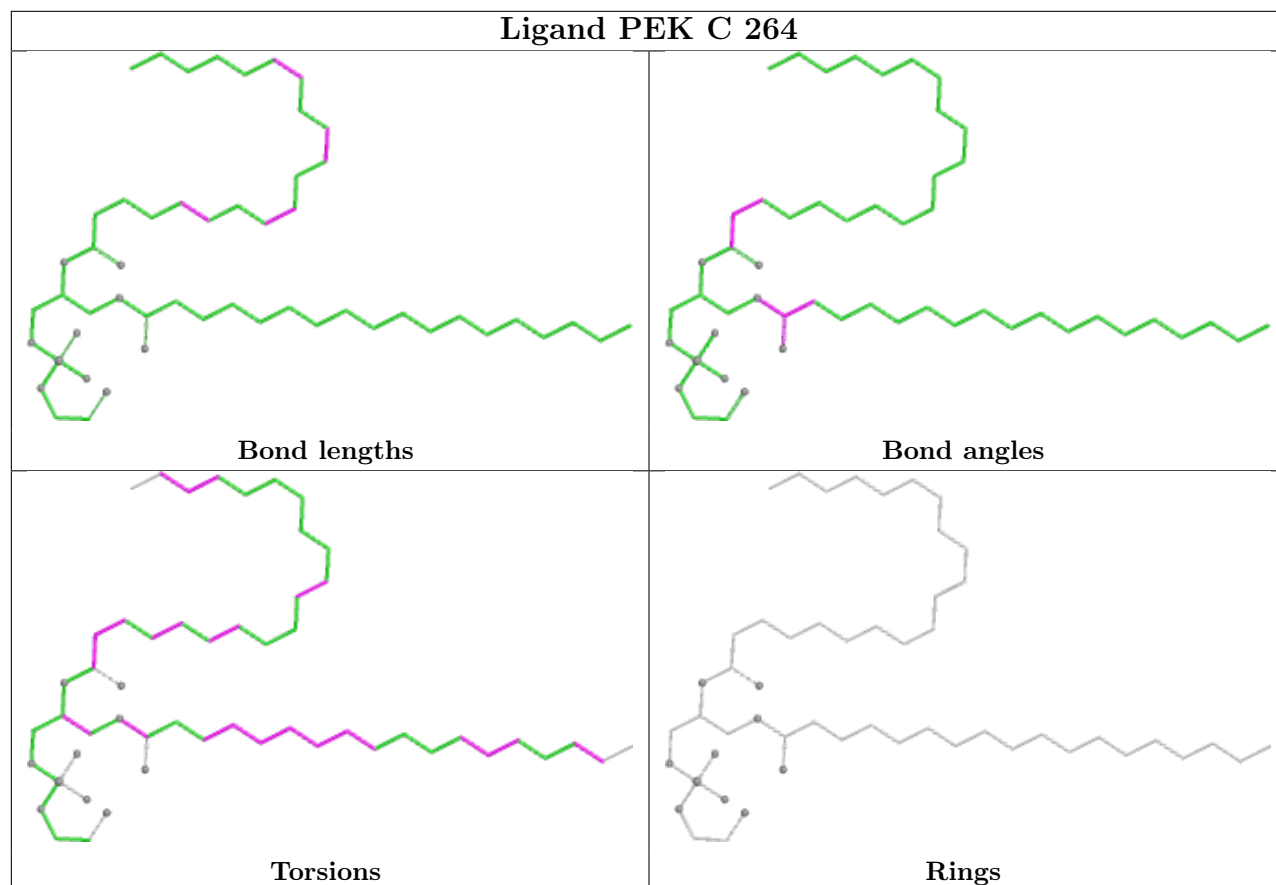
Ligand PSC B 230

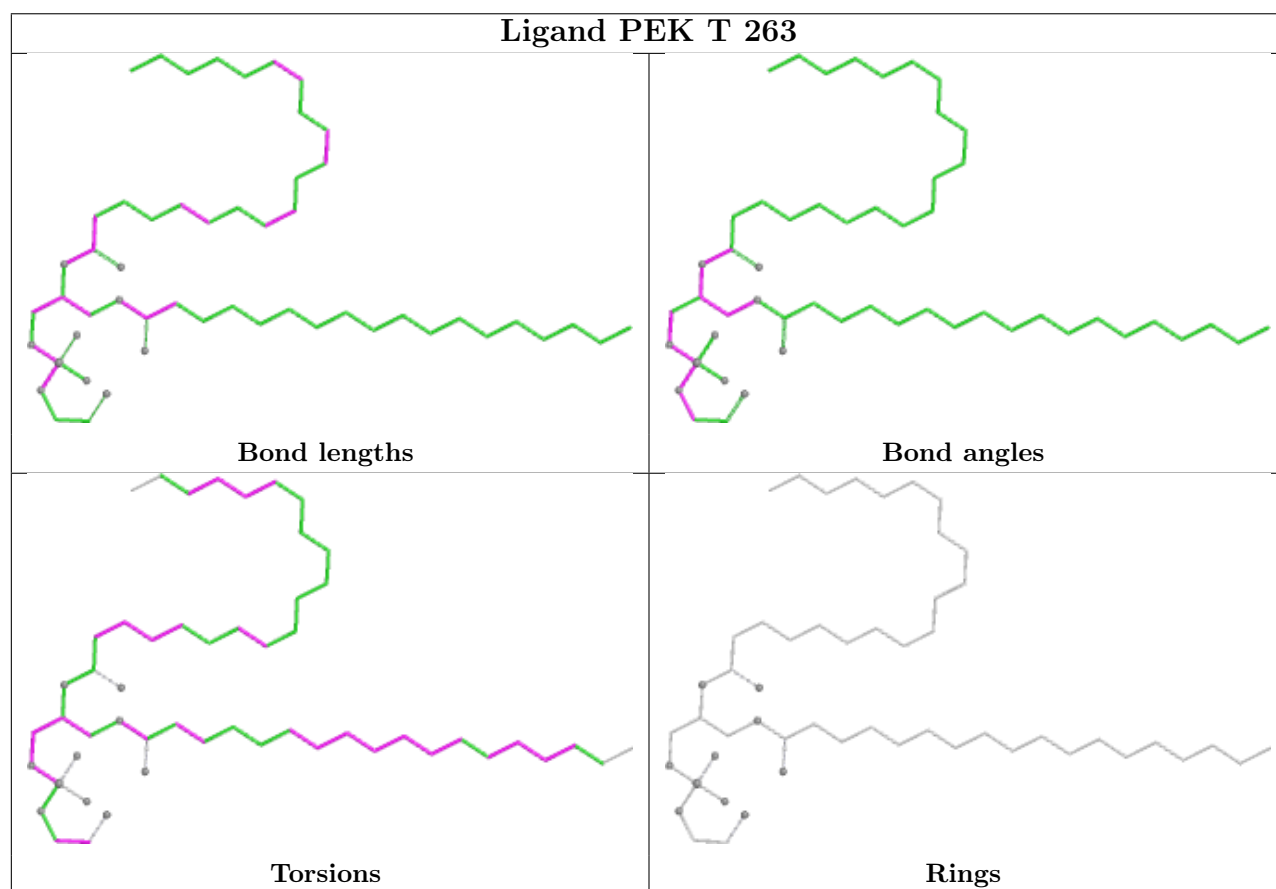
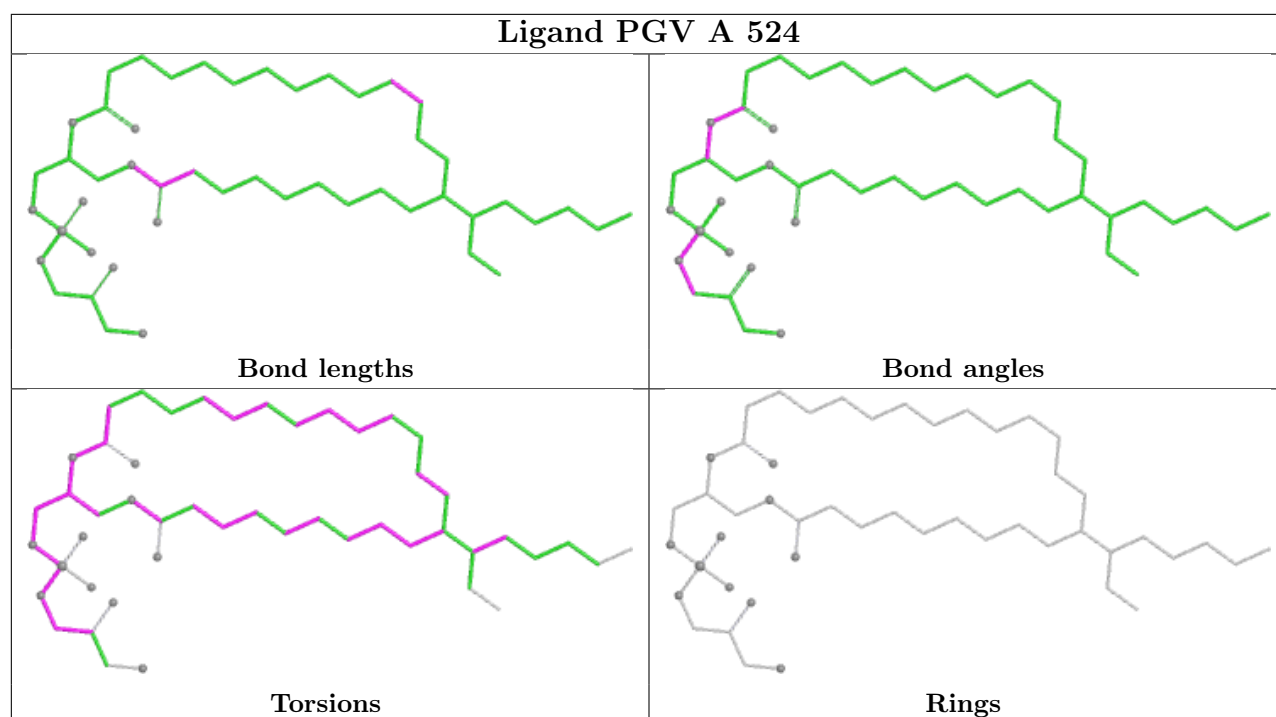


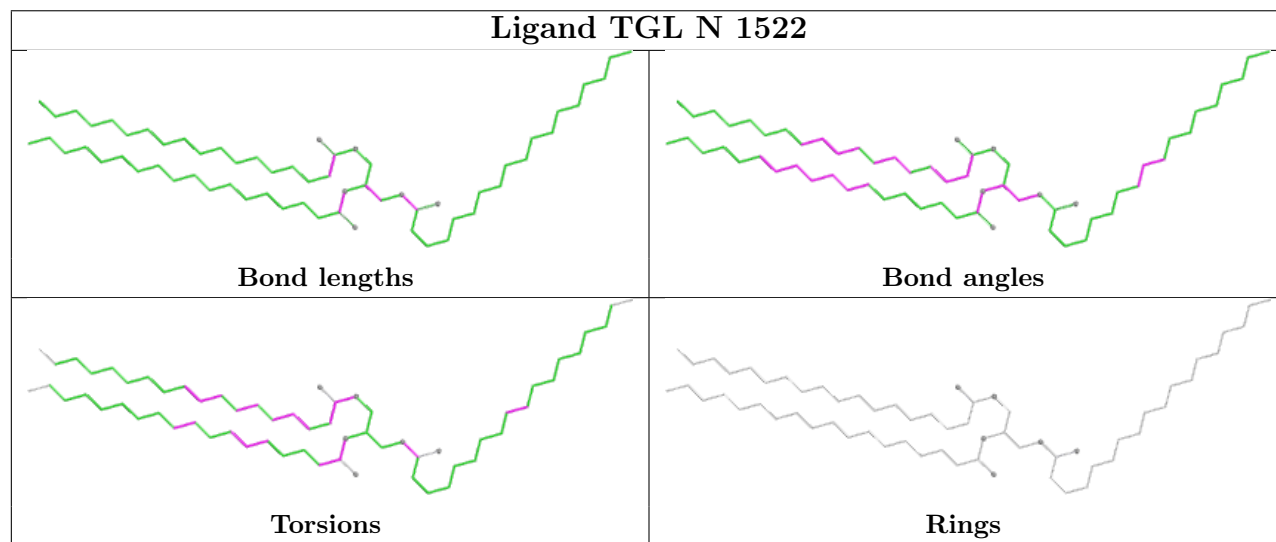
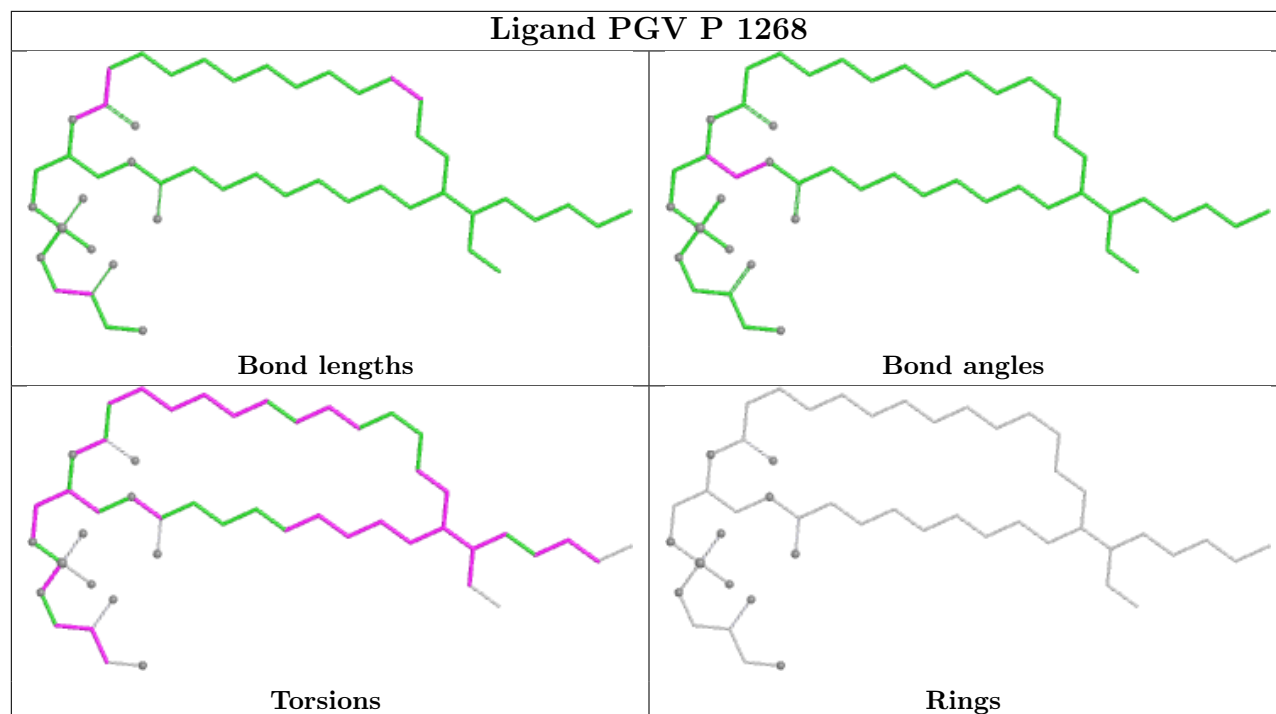


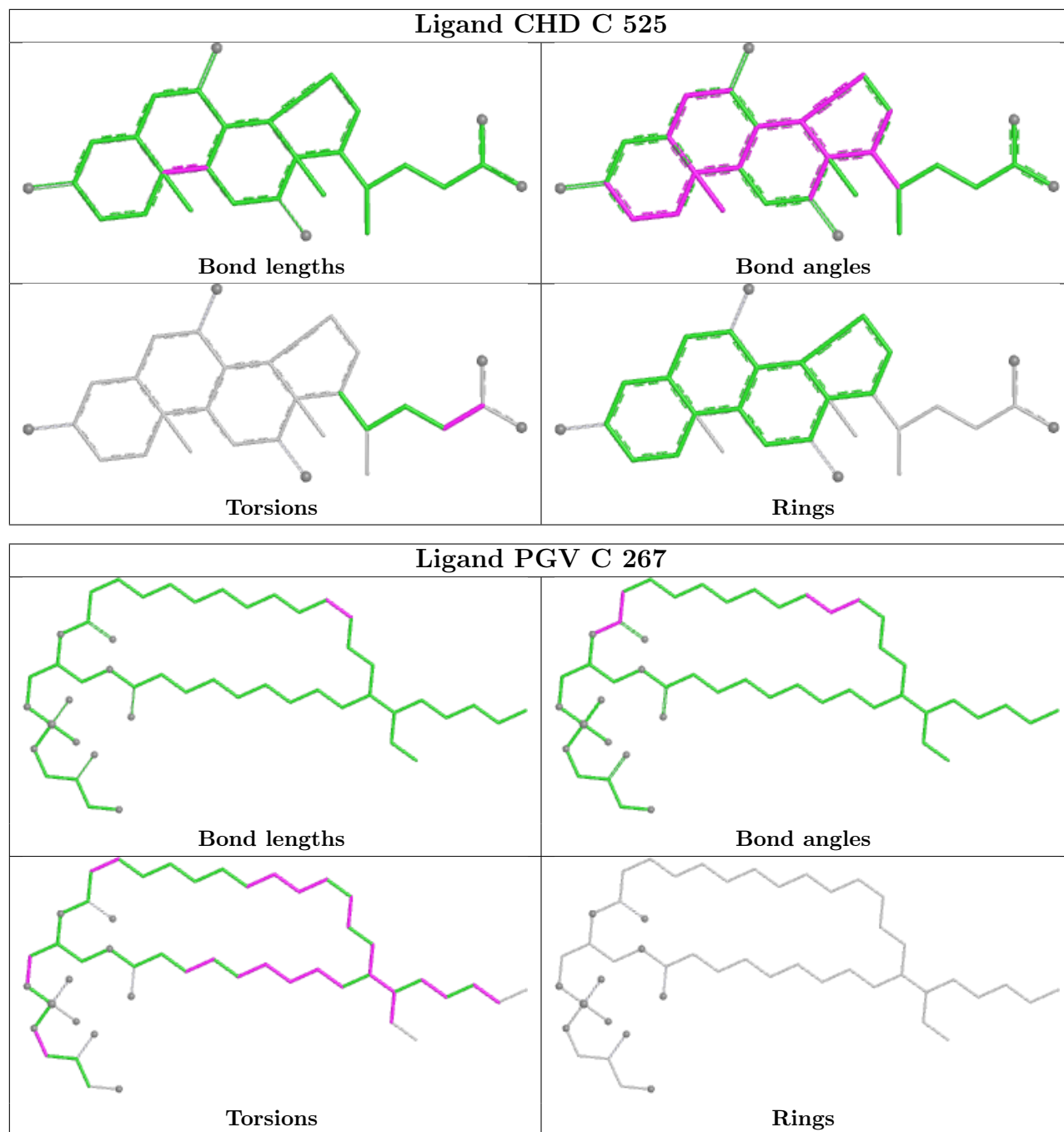


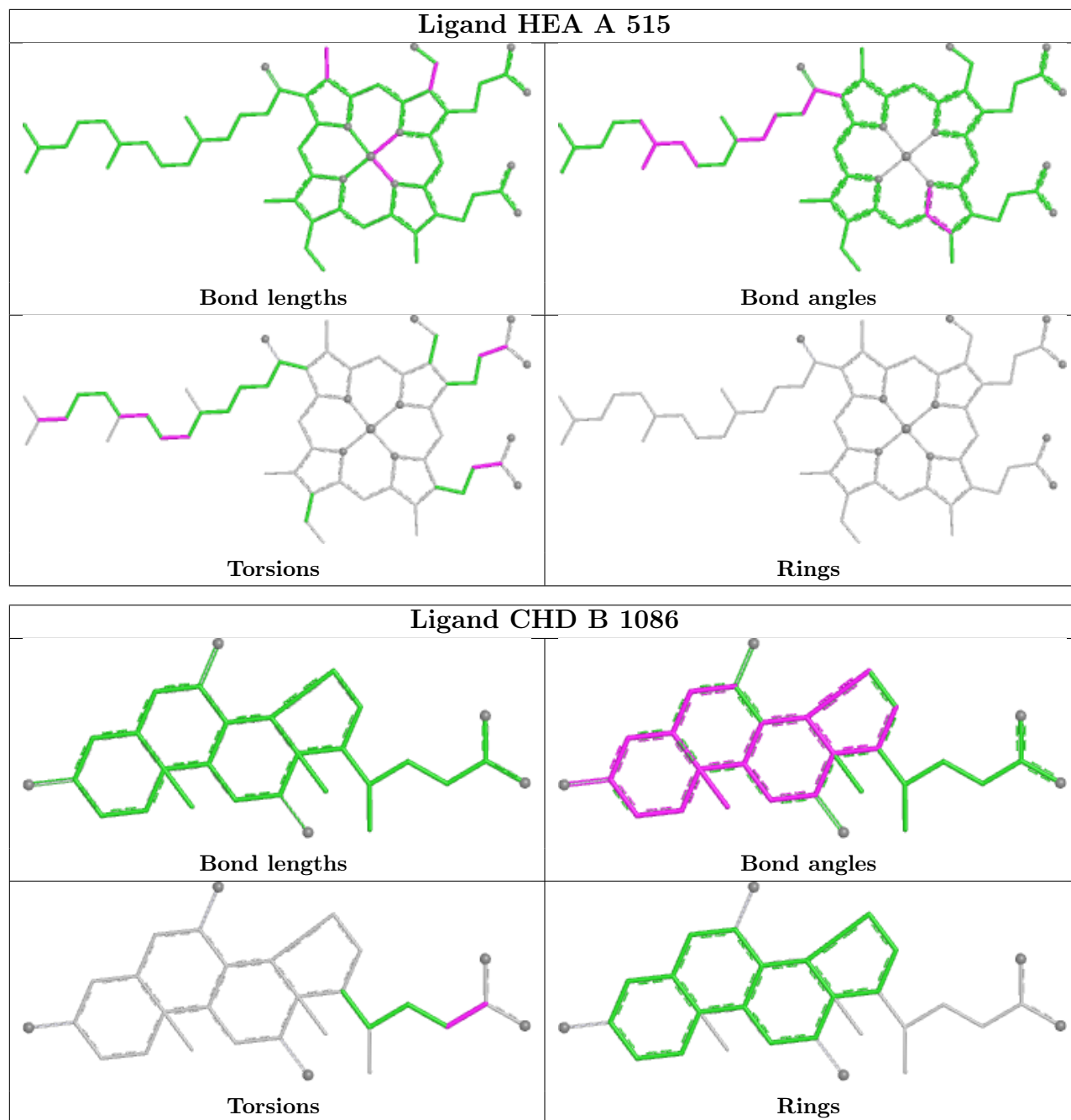


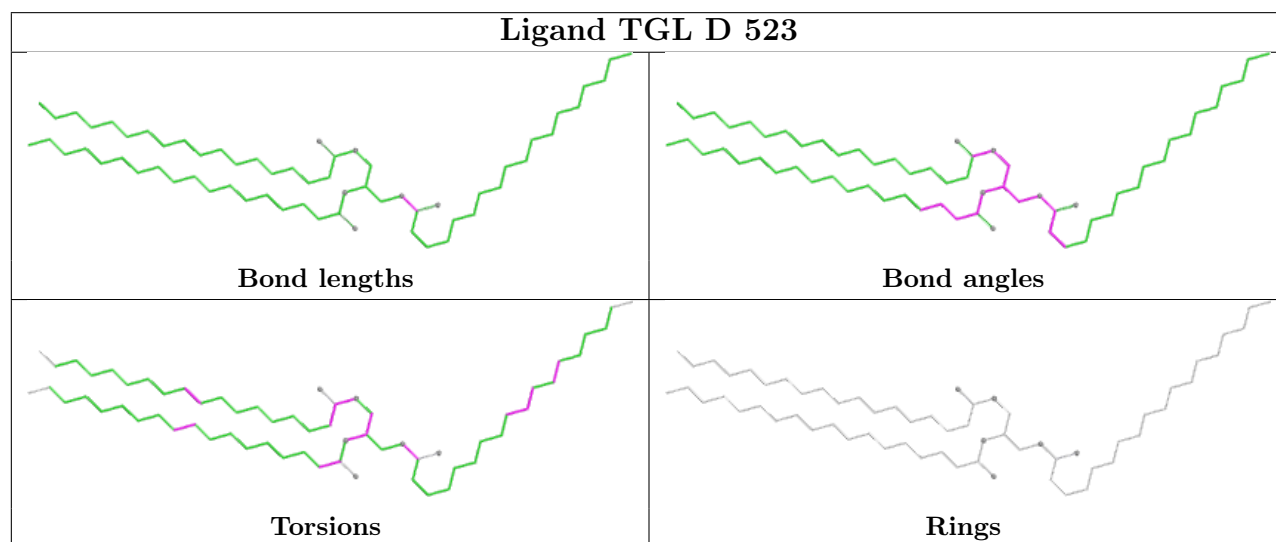
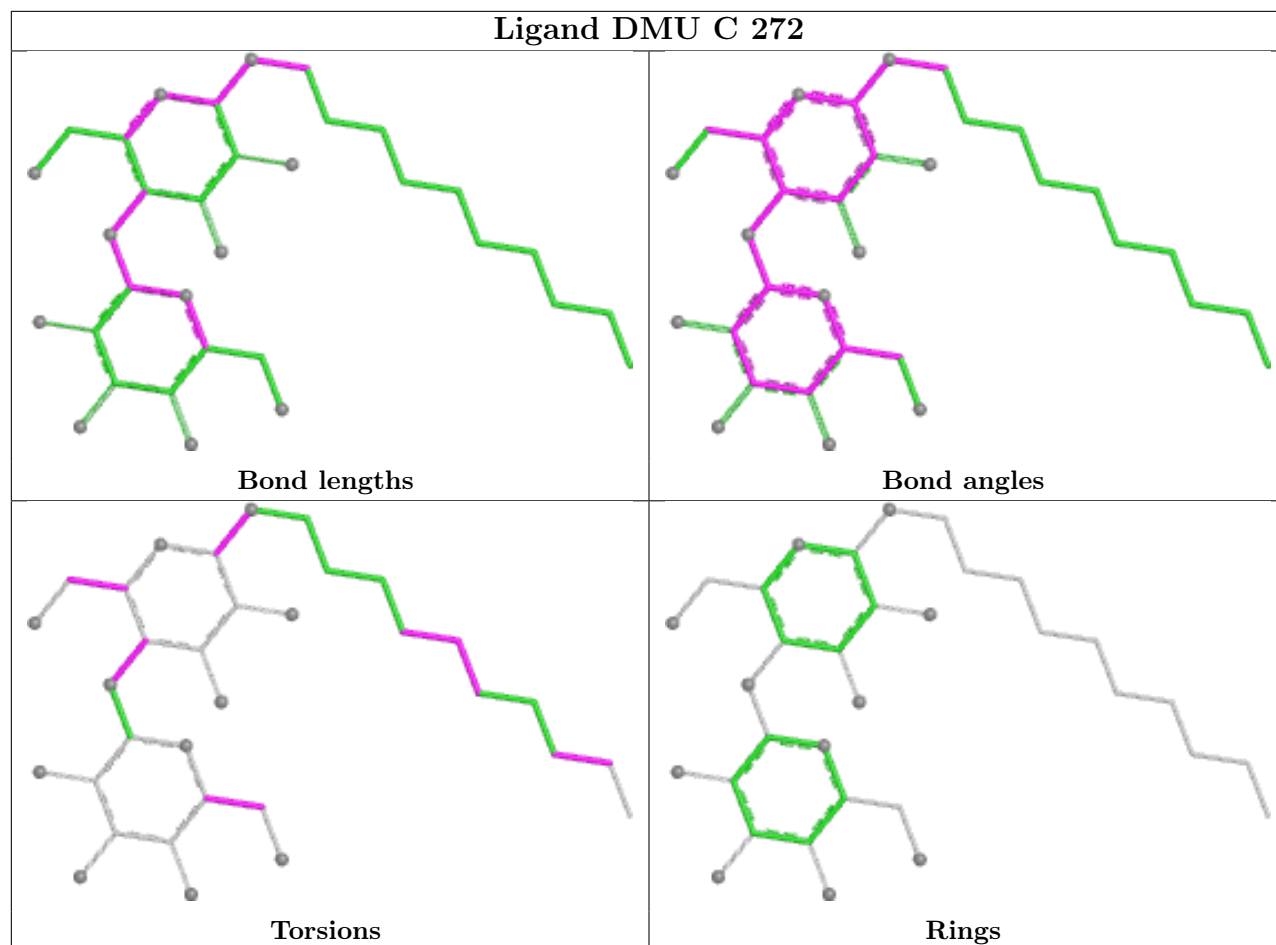


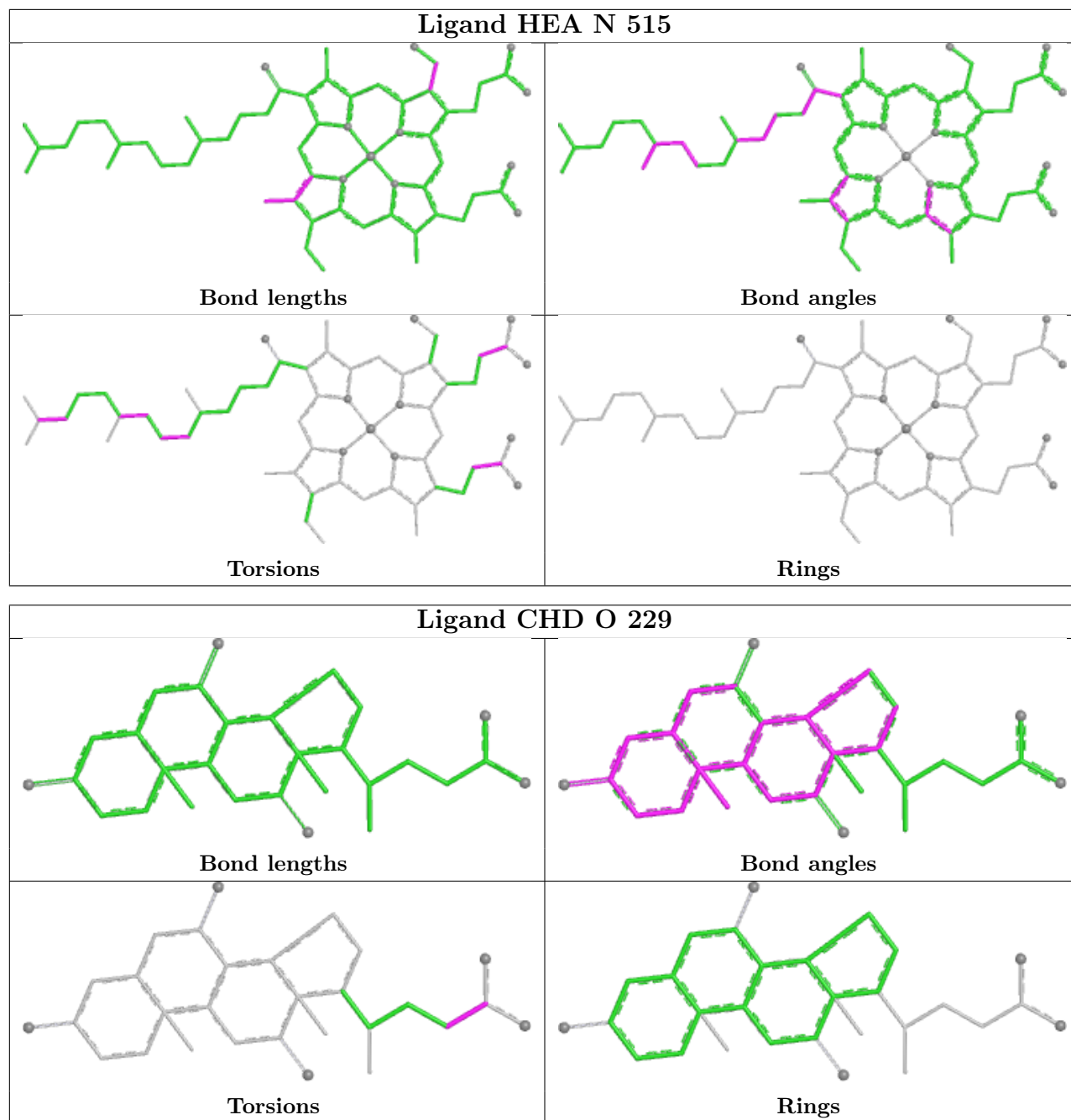












5.7 Other polymers [i](#)

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%)	-0.56	2 (0%) 88 89	16, 22, 31, 72	0
1	N	513/514 (99%)	-0.33	5 (0%) 79 80	17, 24, 34, 66	0
2	B	226/227 (99%)	0.18	15 (6%) 24 23	18, 29, 52, 90	0
2	O	226/227 (99%)	0.64	24 (10%) 11 9	22, 32, 61, 84	0
3	C	259/261 (99%)	-0.26	4 (1%) 72 72	19, 25, 39, 70	0
3	P	259/261 (99%)	-0.13	5 (1%) 66 66	19, 26, 40, 74	0
4	D	144/147 (97%)	0.58	14 (9%) 13 11	21, 31, 57, 86	0
4	Q	144/147 (97%)	1.62	37 (25%) 1 1	28, 42, 65, 100	0
5	E	105/109 (96%)	0.70	13 (12%) 8 6	22, 31, 59, 101	0
5	R	105/109 (96%)	1.87	42 (40%) 1 0	25, 39, 71, 102	0
6	F	98/98 (100%)	0.63	9 (9%) 14 12	20, 32, 88, 110	0
6	S	98/98 (100%)	0.99	14 (14%) 6 5	20, 31, 93, 106	0
7	G	83/85 (97%)	1.45	24 (28%) 1 1	23, 34, 99, 107	0
7	T	83/85 (97%)	1.66	24 (28%) 1 1	23, 36, 102, 109	0
8	H	79/85 (92%)	0.97	16 (20%) 3 2	23, 35, 90, 108	0
8	U	79/85 (92%)	1.22	16 (20%) 3 2	27, 39, 91, 110	0
9	I	72/73 (98%)	1.46	23 (31%) 1 1	25, 44, 65, 85	0
9	V	72/73 (98%)	1.76	20 (27%) 1 1	24, 49, 68, 94	0
10	J	58/59 (98%)	0.84	7 (12%) 8 7	26, 36, 72, 99	0
10	W	58/59 (98%)	1.24	8 (13%) 6 5	26, 38, 75, 106	0
11	K	49/56 (87%)	0.89	4 (8%) 17 15	26, 36, 50, 66	0
11	X	49/56 (87%)	1.30	9 (18%) 3 2	35, 41, 60, 76	0
12	L	46/47 (97%)	0.31	5 (10%) 10 9	22, 28, 52, 87	0
12	Y	46/47 (97%)	0.79	7 (15%) 5 4	26, 34, 65, 88	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	0.55	6 (13%)	23, 28, 75, 103	0
13	Z	43/46 (93%)	1.11	8 (18%)	31, 36, 80, 106	0
All	All	3550/3614 (98%)	0.39	361 (10%)	16, 29, 64, 110	0

The worst 5 of 361 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	S	1	ALA	17.3
6	F	1	ALA	15.7
4	Q	6	VAL	12.8
9	V	3	ALA	12.7
6	S	97	ALA	11.3

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	SAC	V	1	9/10	0.18	0.23	99,100,104,104	0
7	TPO	G	11	11/12	0.46	0.31	77,85,107,108	0
7	TPO	T	11	11/12	0.55	0.31	76,84,110,112	0
9	SAC	I	1	9/10	0.60	0.27	93,97,99,99	0
1	FME	A	1	10/11	0.84	0.15	40,45,66,72	0
1	FME	N	1	10/11	0.84	0.18	39,43,65,69	0
2	FME	O	1	10/11	0.90	0.15	37,38,47,53	0
2	FME	B	1	10/11	0.93	0.13	23,31,39,50	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
23	DMU	P	1272	33/33	0.66	0.23	73,96,104,105	0
25	PEK	T	263	53/53	0.66	0.28	45,83,100,103	0
22	CHD	W	1060	29/29	0.69	0.28	98,104,106,108	0
23	DMU	C	272	33/33	0.70	0.22	71,97,102,104	0
25	PEK	G	1263	53/53	0.71	0.27	46,83,99,101	0
18	PGV	P	1268	51/51	0.71	0.27	65,84,104,106	0
26	CDL	T	1269	100/100	0.71	0.26	54,84,97,105	0
22	CHD	J	60	29/29	0.72	0.28	98,104,107,109	0
25	PEK	C	265	53/53	0.74	0.28	44,88,103,104	0
20	TGL	N	1522	63/63	0.74	0.28	42,67,79,82	0
21	PSC	B	230	52/52	0.74	0.25	48,84,113,116	0
26	CDL	G	269	100/100	0.74	0.27	61,83,101,105	0
20	TGL	D	523	63/63	0.74	0.26	47,65,79,82	0
20	TGL	B	521	63/63	0.75	0.26	49,64,85,90	0
25	PEK	P	1265	53/53	0.75	0.29	46,89,107,109	0
20	TGL	Q	1523	63/63	0.75	0.26	45,70,80,84	0
18	PGV	C	268	51/51	0.75	0.28	65,84,103,106	0
26	CDL	P	1270	100/100	0.75	0.27	42,88,101,105	0
20	TGL	N	1521	63/63	0.75	0.24	49,67,84,86	0
22	CHD	C	271	29/29	0.76	0.23	87,95,96,97	0
18	PGV	A	524	51/51	0.76	0.26	35,71,101,104	0
21	PSC	O	1230	52/52	0.76	0.28	48,80,111,116	0
26	CDL	C	270	100/100	0.77	0.25	44,87,100,106	0
18	PGV	Z	1524	51/51	0.77	0.23	38,71,101,104	0
22	CHD	P	1271	29/29	0.78	0.22	89,95,98,101	0
20	TGL	L	522	63/63	0.78	0.27	34,65,79,81	0
24	UNX	P	1262	1/1	0.87	0.42	43,43,43,43	0
23	DMU	Z	1526	33/33	0.88	0.12	40,49,61,64	0
24	UNX	C	262	1/1	0.92	0.31	47,47,47,47	0
23	DMU	M	526	33/33	0.92	0.11	32,42,55,58	0
16	NA	N	1519	1/1	0.93	0.08	30,30,30,30	0
25	PEK	P	1264	53/53	0.94	0.13	25,44,68,72	0
25	PEK	C	264	53/53	0.95	0.12	10,44,70,73	0
18	PGV	C	267	51/51	0.96	0.10	20,34,58,62	0
15	MG	N	1518	1/1	0.96	0.06	26,26,26,26	0
22	CHD	C	525	29/29	0.96	0.06	21,27,30,33	0
18	PGV	N	1266	51/51	0.96	0.11	20,38,55,64	0
18	PGV	P	1267	51/51	0.96	0.11	23,34,59,61	0
22	CHD	P	1525	29/29	0.96	0.06	20,27,31,34	0
16	NA	A	519	1/1	0.96	0.08	27,27,27,27	0
18	PGV	A	525	51/51	0.96	0.11	21,36,56,63	0
22	CHD	O	229	29/29	0.97	0.05	19,22,28,32	0

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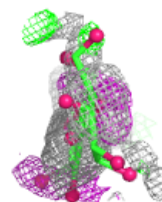
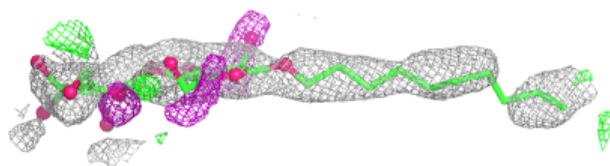
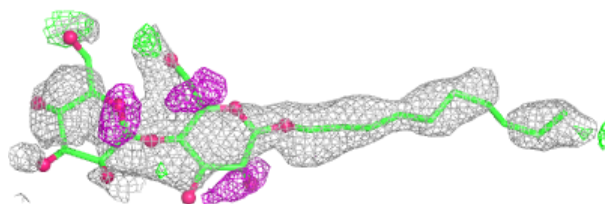
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	CHD	B	1086	29/29	0.97	0.06	20,24,30,37	0
19	CUA	O	228	2/2	0.98	0.04	26,26,26,27	0
15	MG	A	518	1/1	0.98	0.03	20,20,20,20	0
17	HEA	N	515	60/60	0.98	0.06	18,24,41,43	0
17	HEA	A	516	60/60	0.99	0.05	15,18,29,29	0
17	HEA	A	515	60/60	0.99	0.06	12,20,44,45	0
19	CUA	B	228	2/2	0.99	0.02	19,19,19,22	0
17	HEA	N	516	60/60	0.99	0.05	17,20,29,31	0
27	ZN	F	99	1/1	0.99	0.02	25,25,25,25	0
27	ZN	S	99	1/1	0.99	0.02	27,27,27,27	0
14	CU	A	517	1/1	1.00	0.01	20,20,20,20	0
14	CU	N	517	1/1	1.00	0.01	21,21,21,21	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.

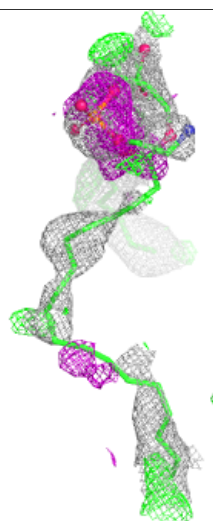
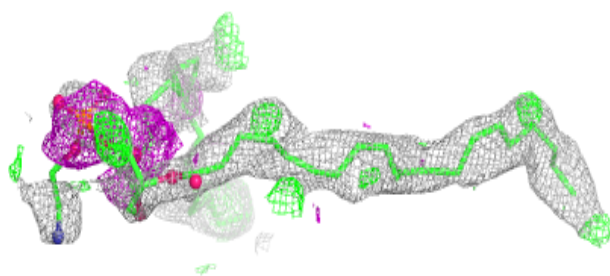
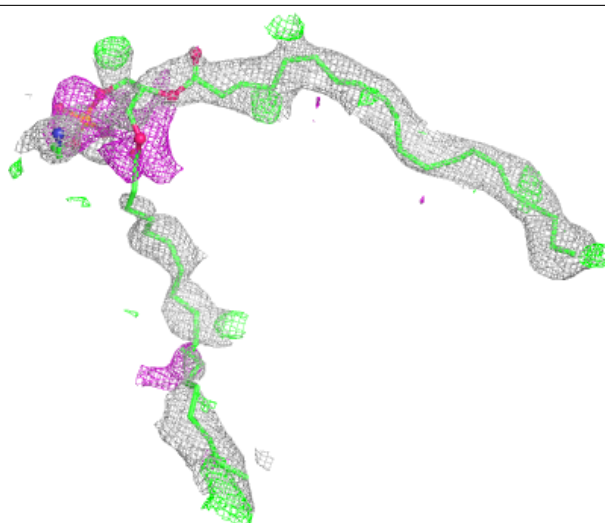
Electron density around DMU P 1272:

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



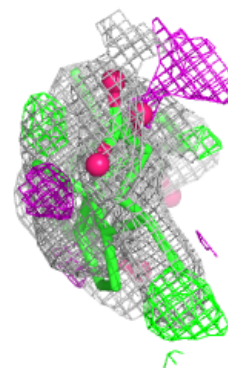
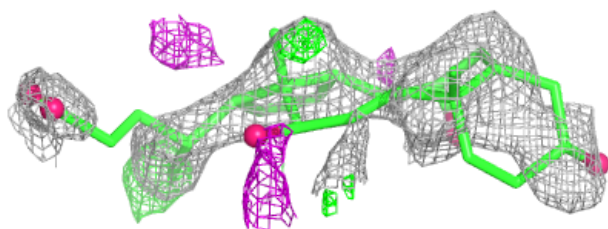
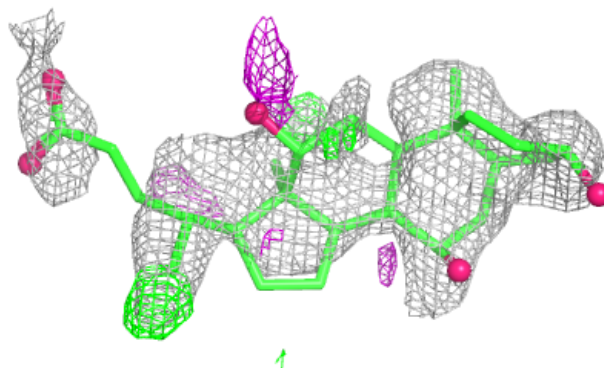
Electron density around PEK T 263:

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

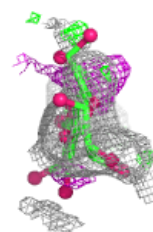
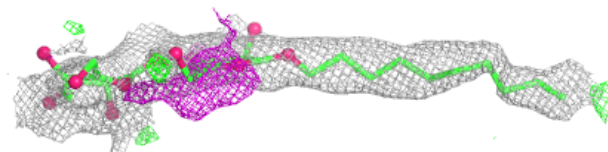
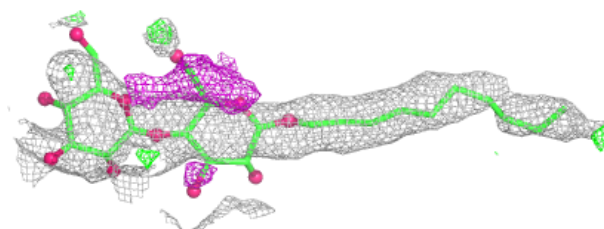


Electron density around CHD W 1060:

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

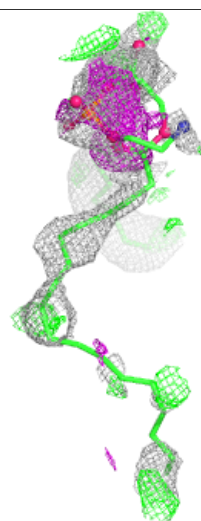
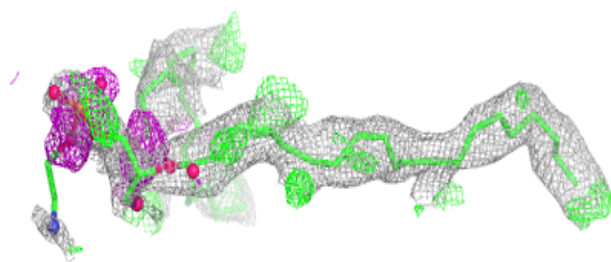
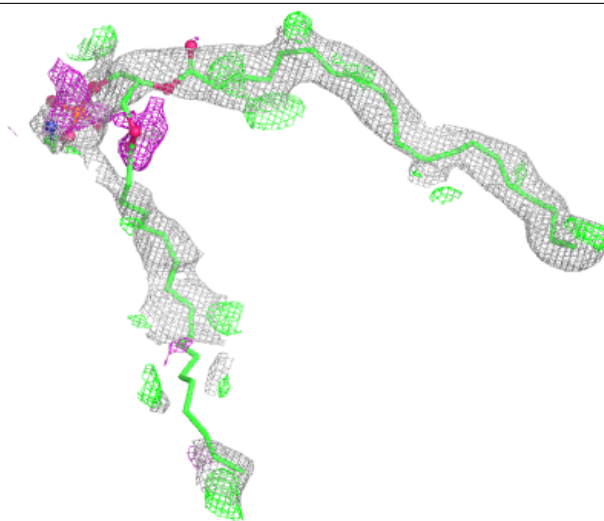
**Electron density around DMU C 272:**

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



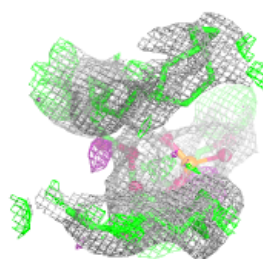
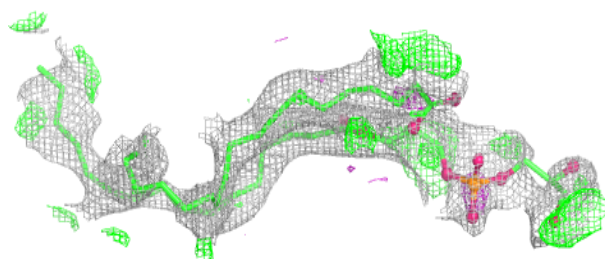
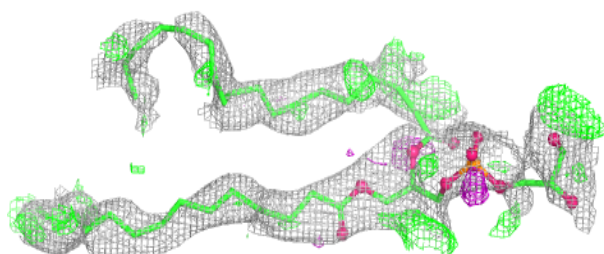
Electron density around PEK G 1263:

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

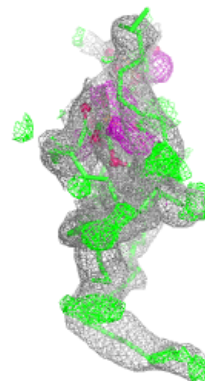
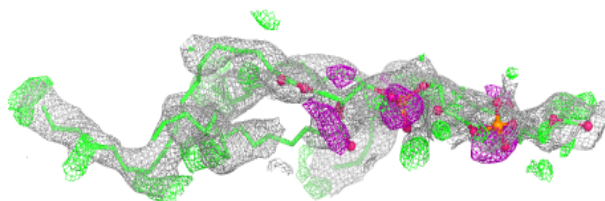
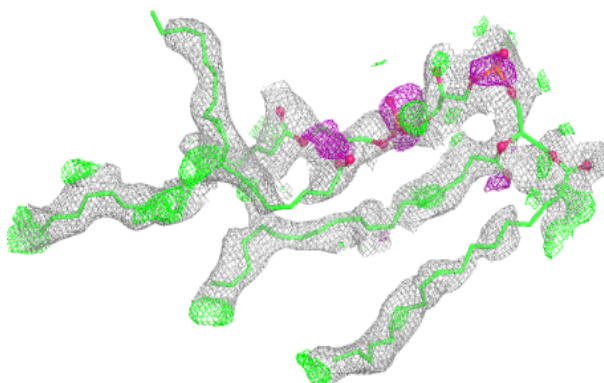


Electron density around PGV P 1268:

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

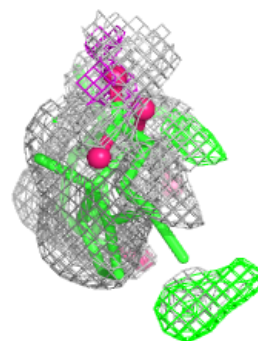
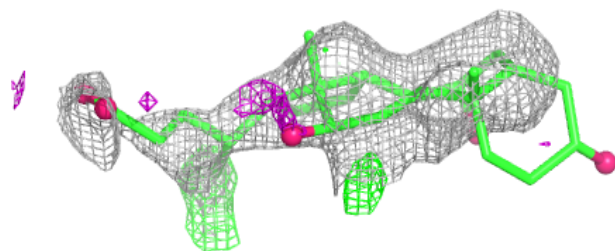
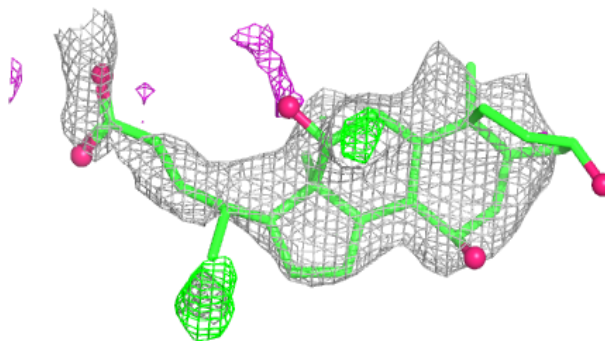
**Electron density around CDL T 1269:**

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



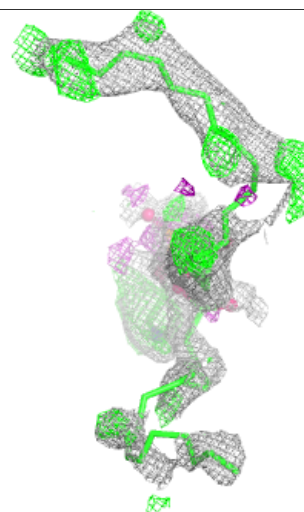
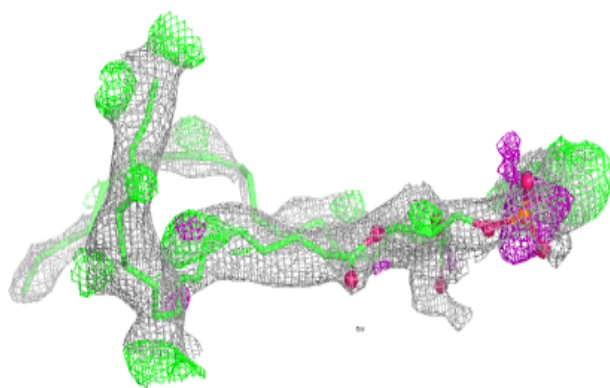
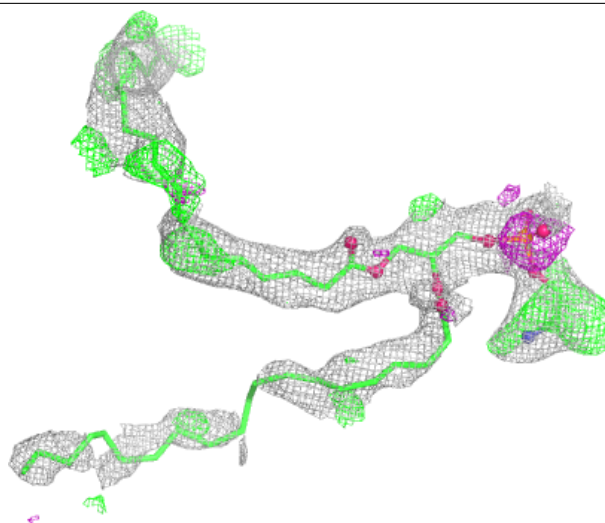
Electron density around CHD J 60:

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



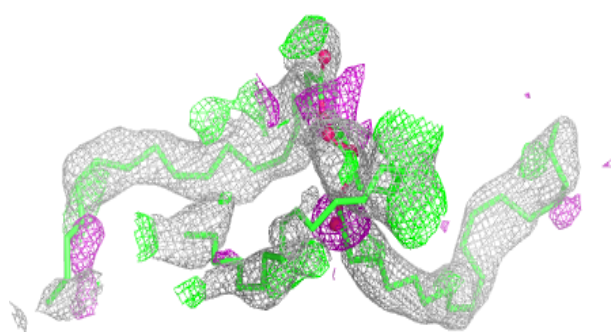
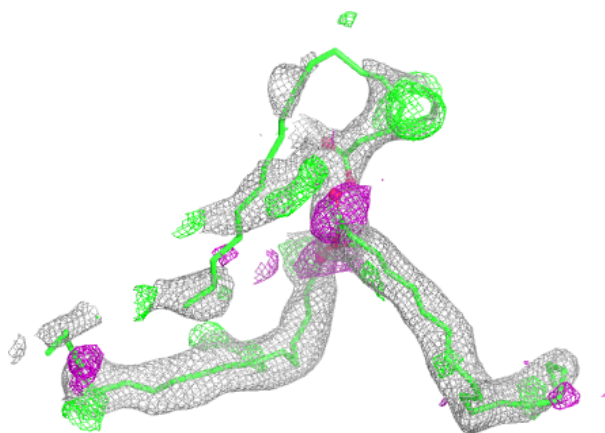
Electron density around PEK C 265:

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

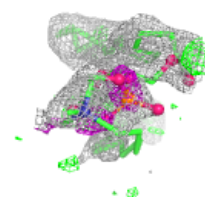
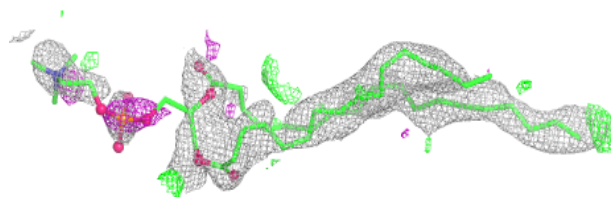
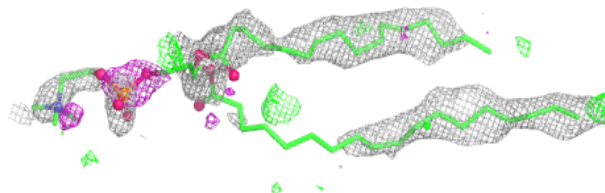


Electron density around TGL N 1522:

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

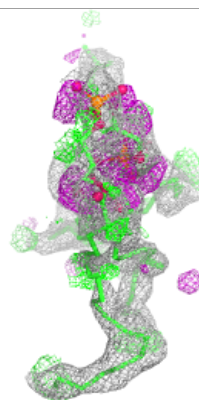
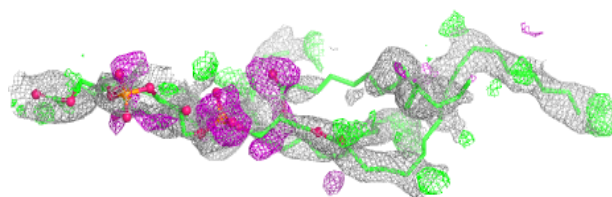
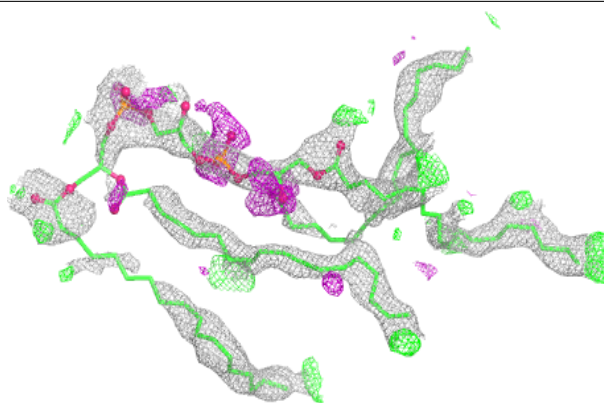
**Electron density around PSC B 230:**

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

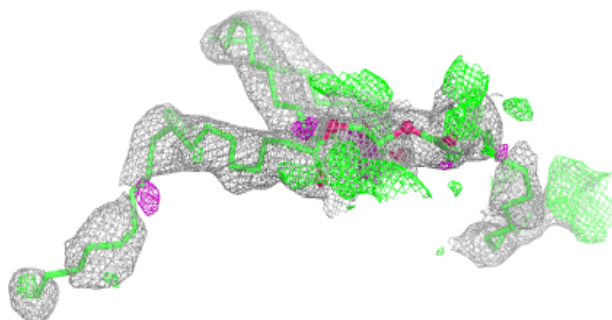
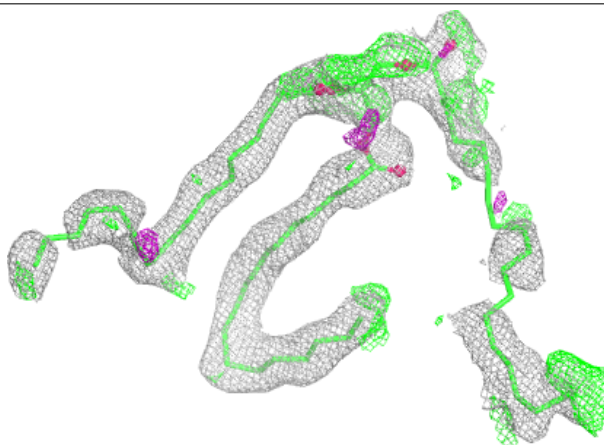


Electron density around CDL G 269:

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

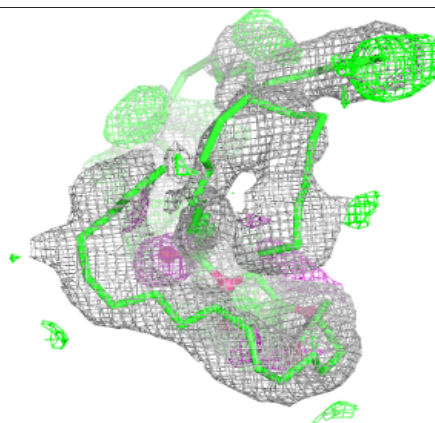
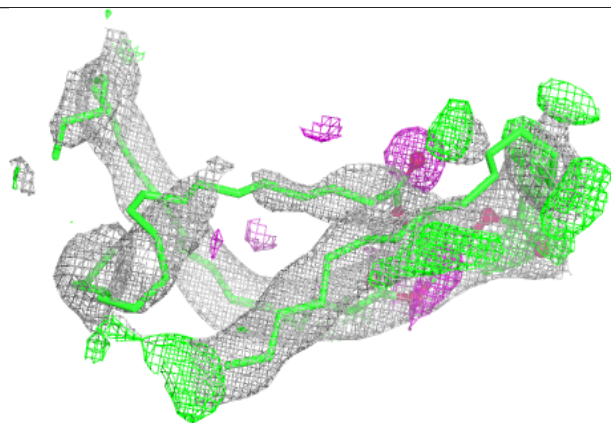
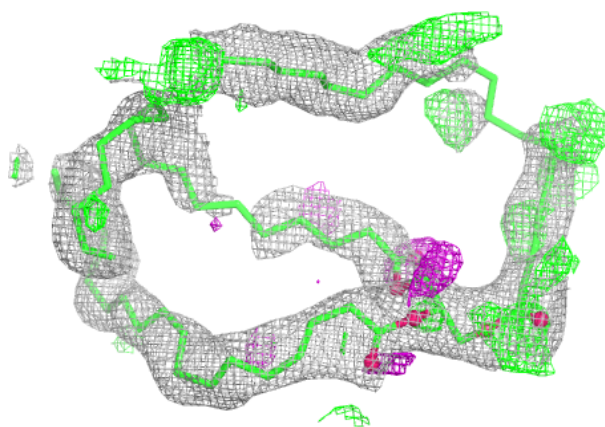
**Electron density around TGL D 523:**

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



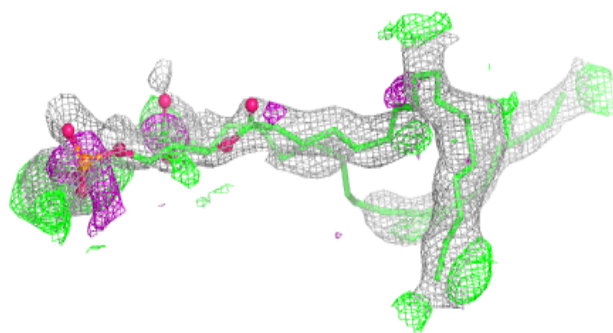
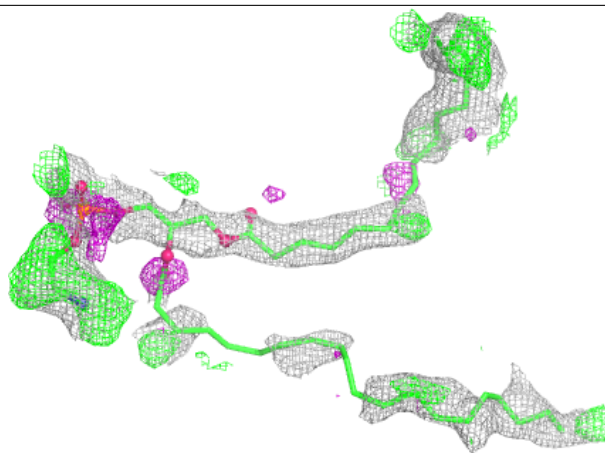
Electron density around TGL B 521:

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



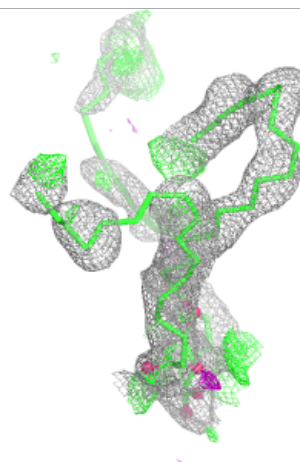
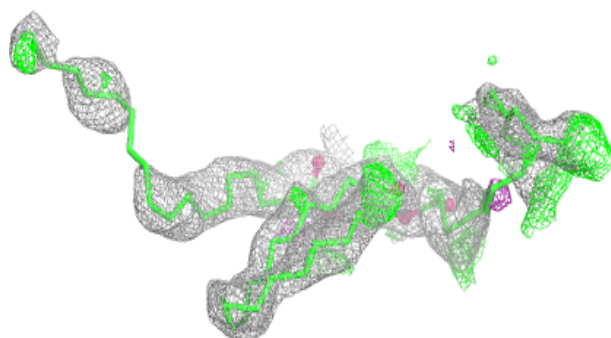
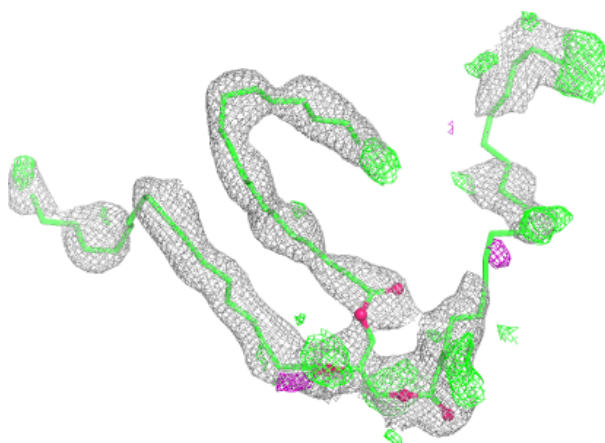
Electron density around PEK P 1265:

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



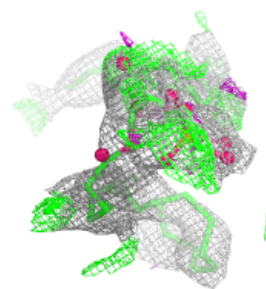
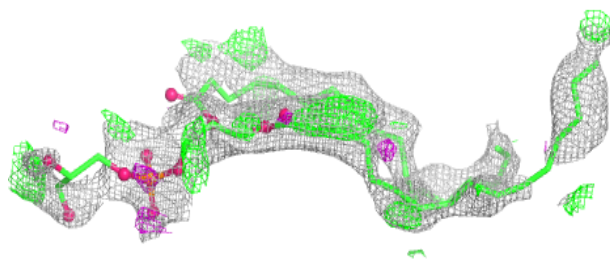
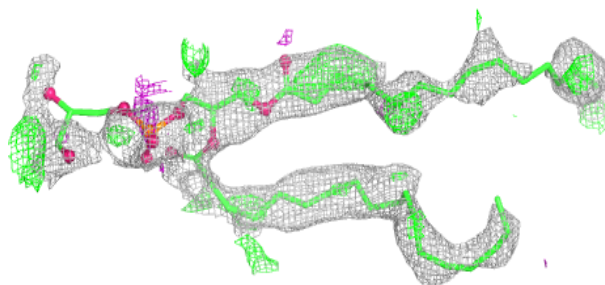
Electron density around TGL Q 1523:

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

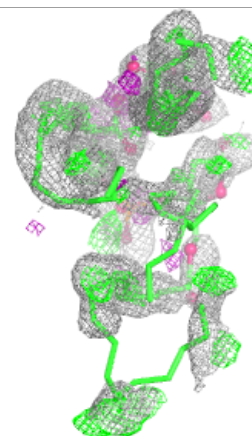
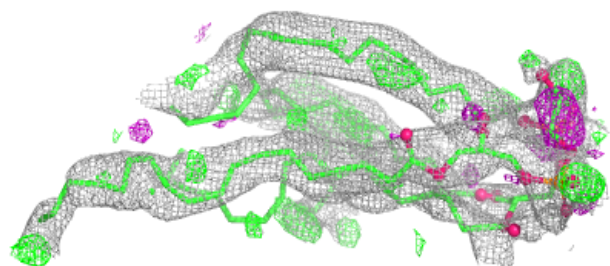
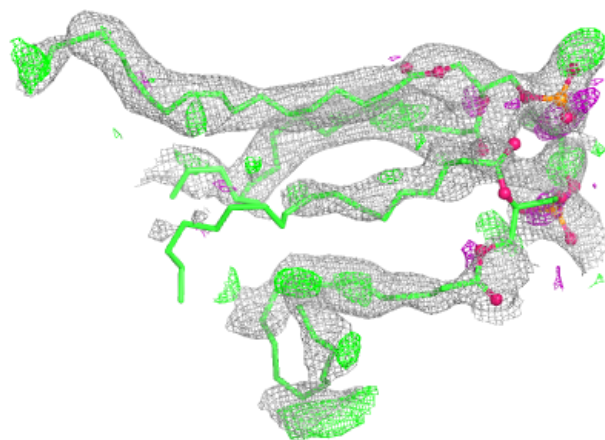


Electron density around PGV C 268:

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

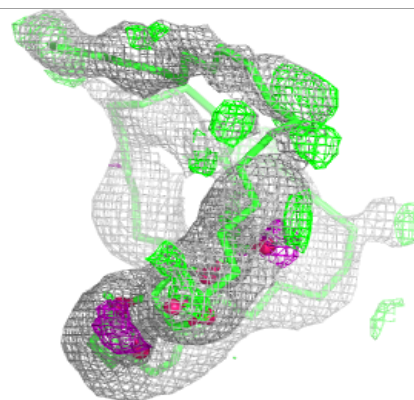
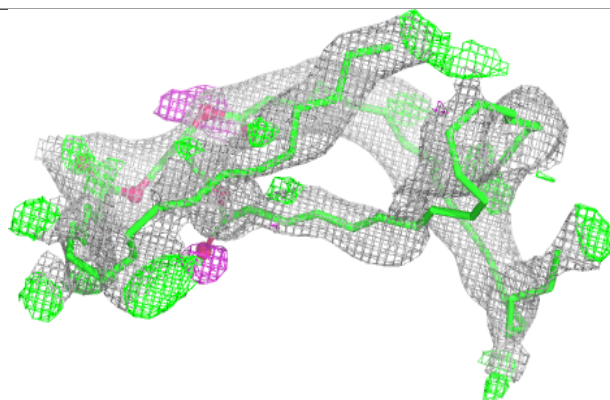
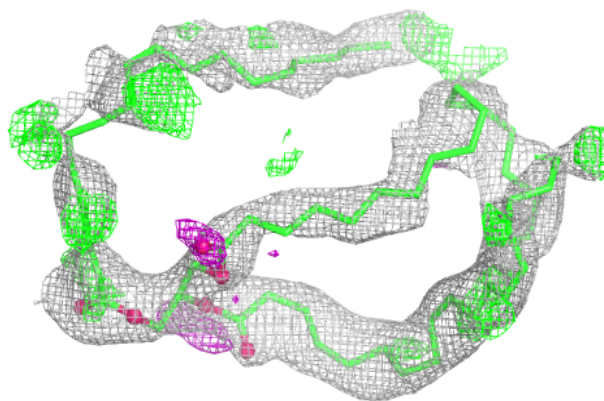
**Electron density around CDL P 1270:**

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

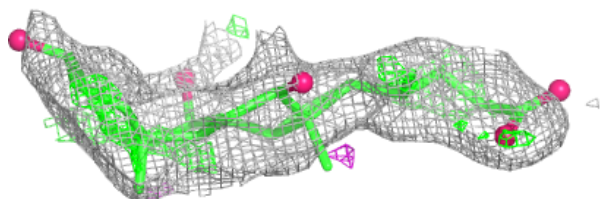
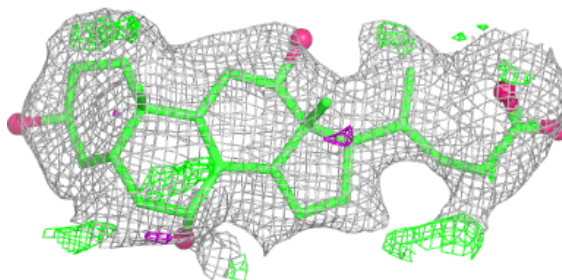


Electron density around TGL N 1521:

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

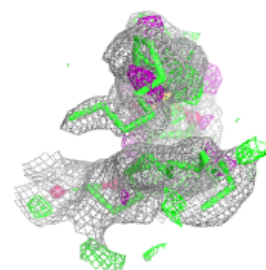
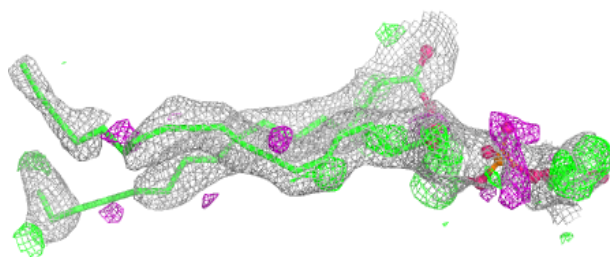
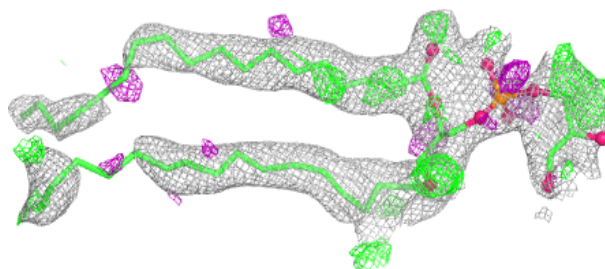
**Electron density around CHD C 271:**

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

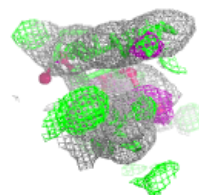
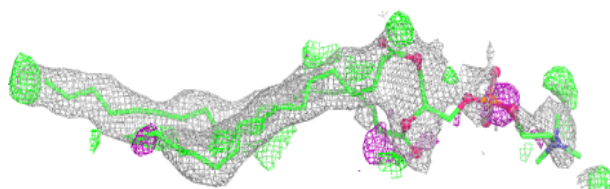
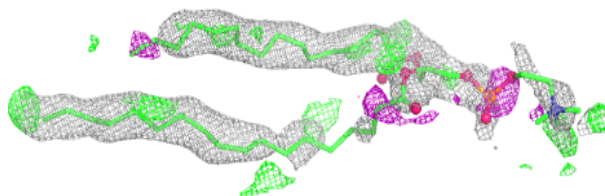


Electron density around PGV A 524:

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

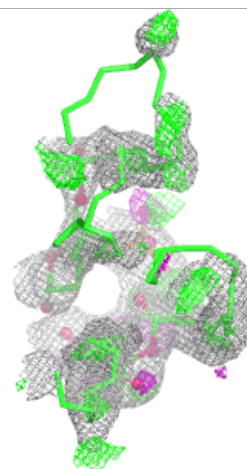
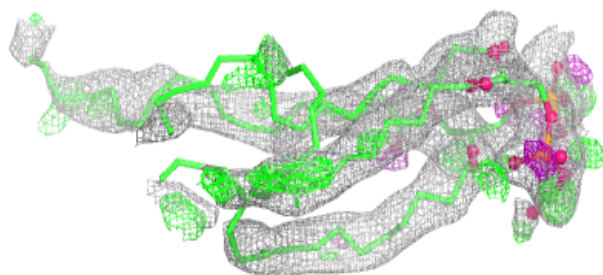
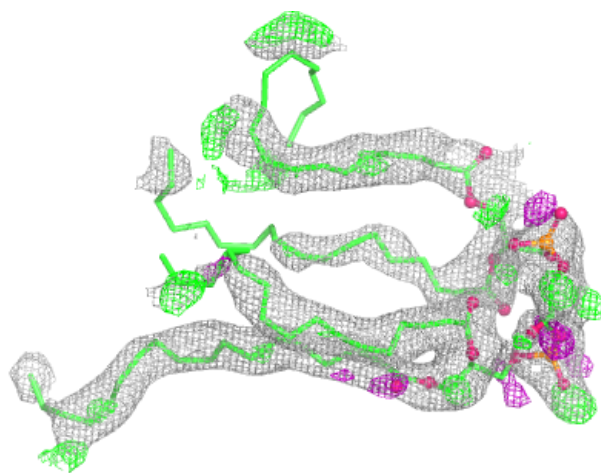
**Electron density around PSC O 1230:**

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



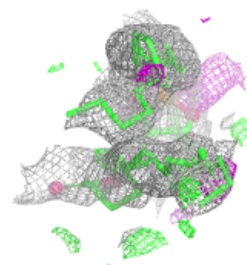
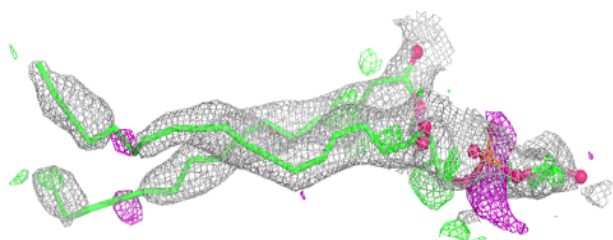
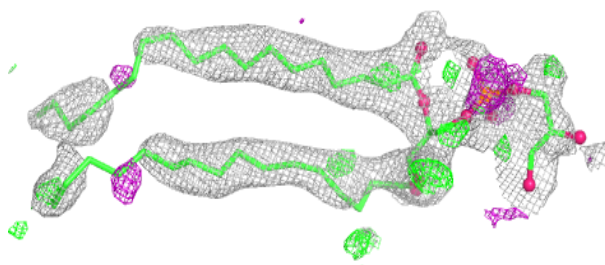
Electron density around CDL C 270:

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

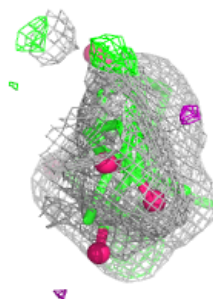
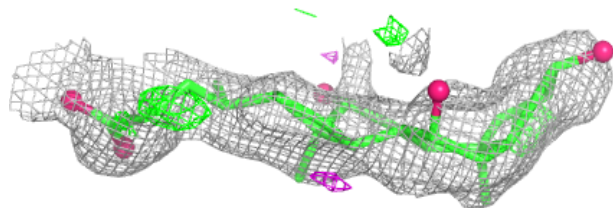
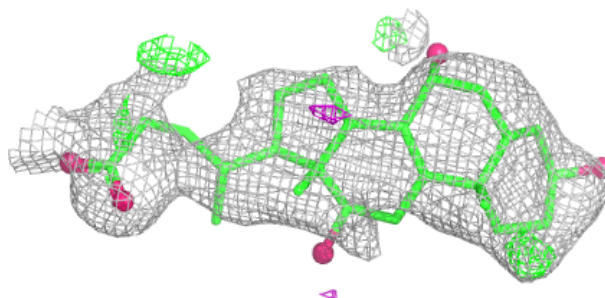


Electron density around PGV Z 1524:

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

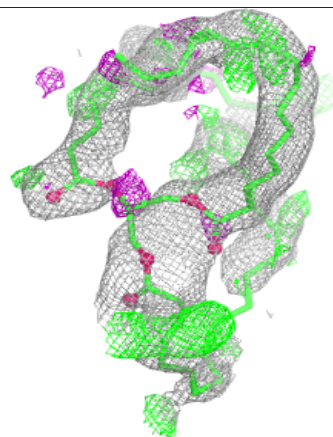
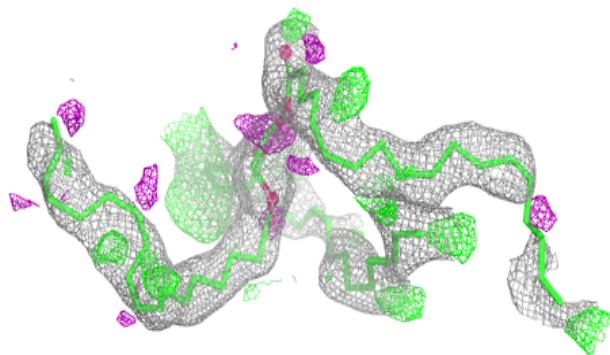
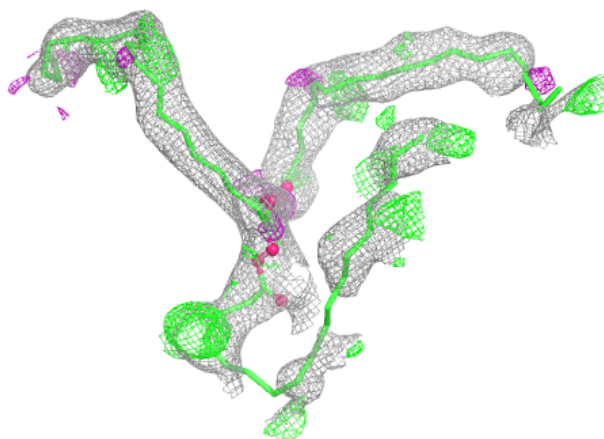
**Electron density around CHD P 1271:**

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



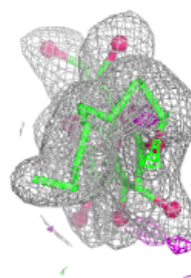
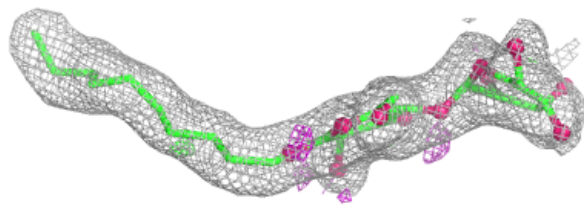
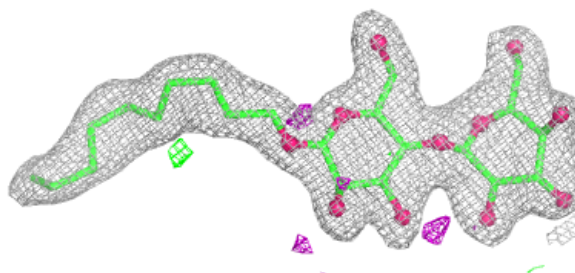
Electron density around TGL L 522:

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

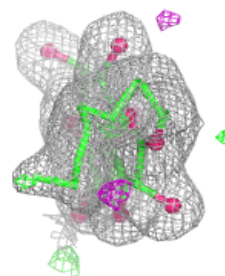
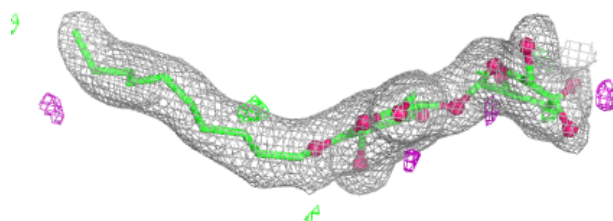
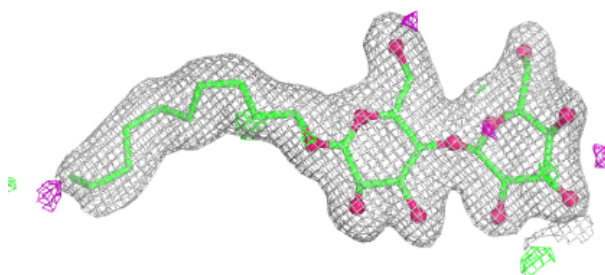


Electron density around DMU Z 1526:

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

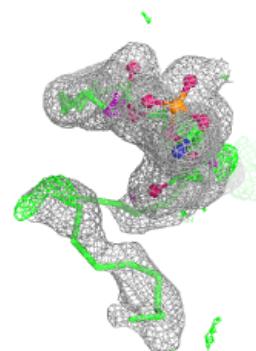
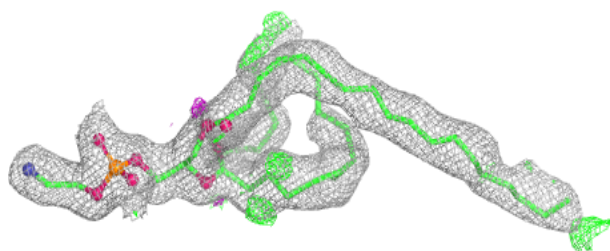
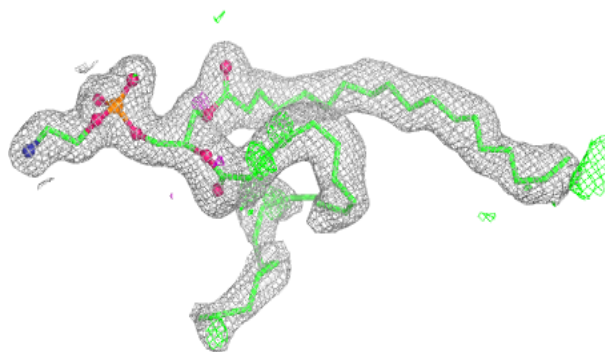
**Electron density around DMU M 526:**

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

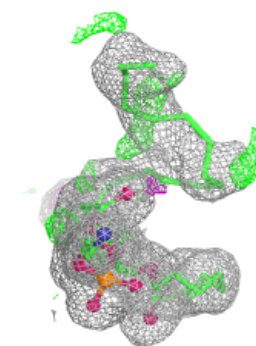
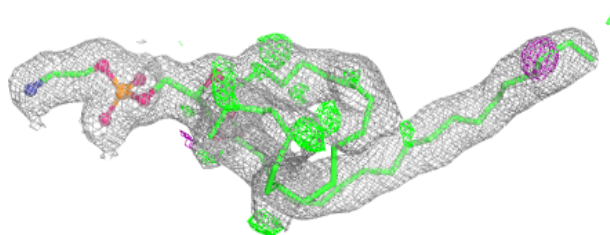
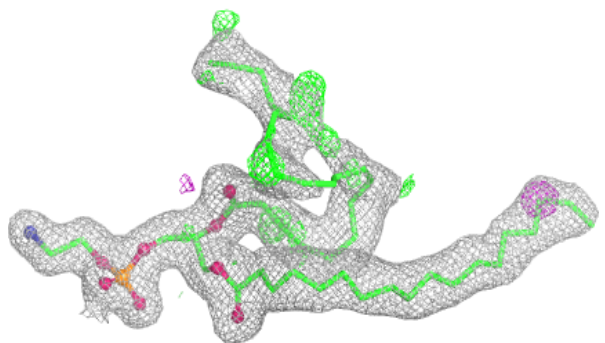


Electron density around PEK P 1264:

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

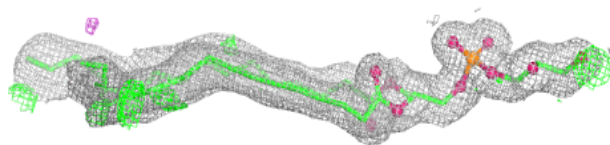
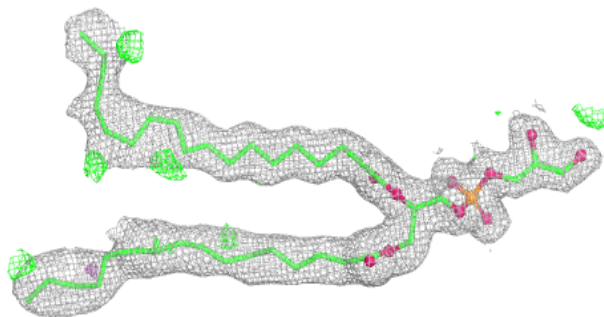
**Electron density around PEK C 264:**

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

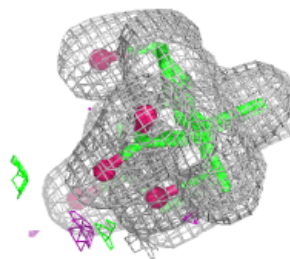
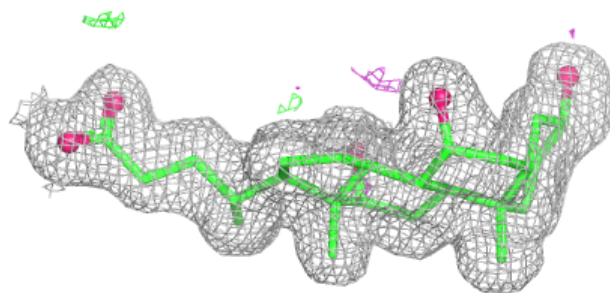
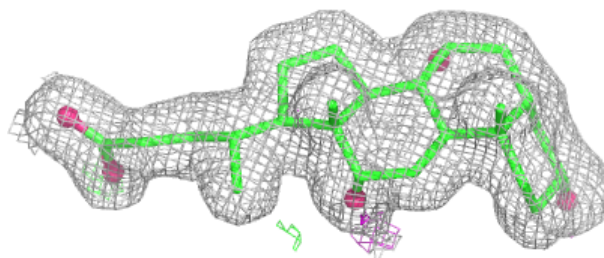


Electron density around PGV C 267:

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

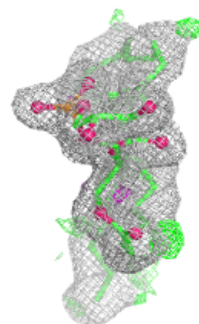
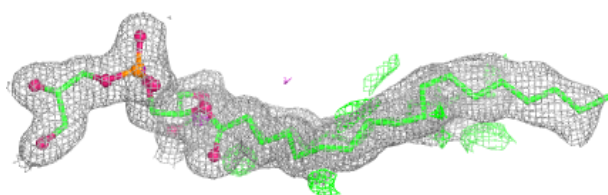
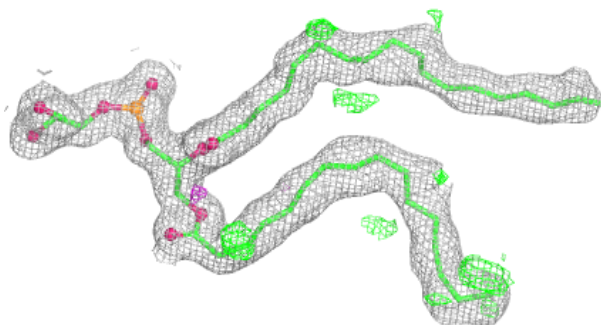
**Electron density around CHD C 525:**

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

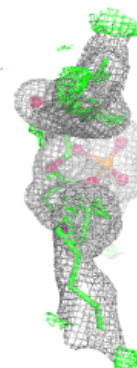
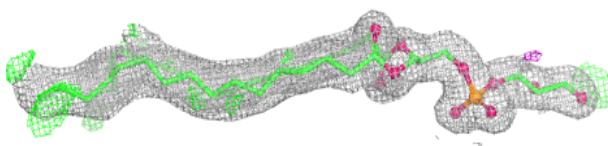
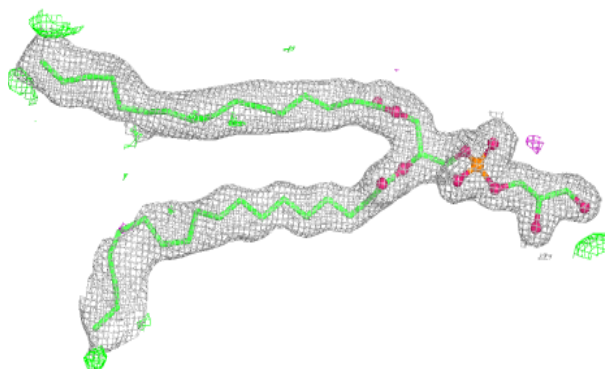


Electron density around PGV N 1266:

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

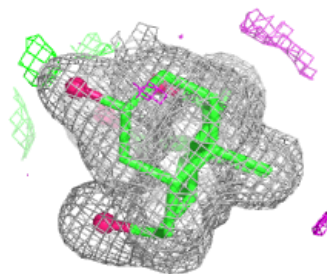
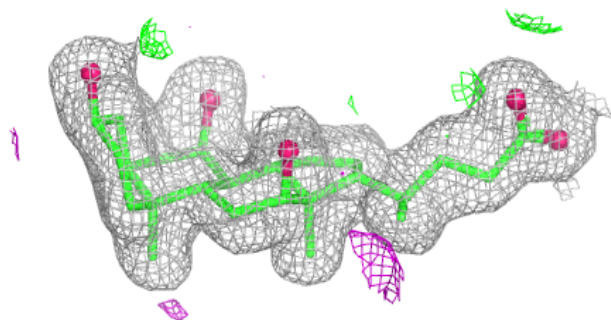
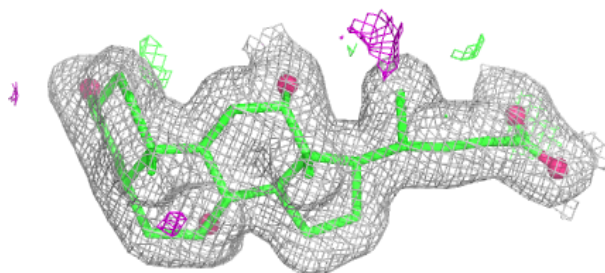
**Electron density around PGV P 1267:**

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

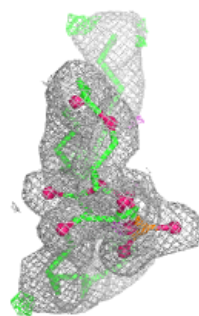
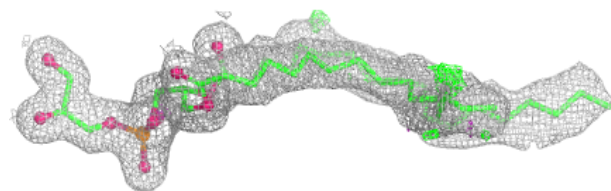
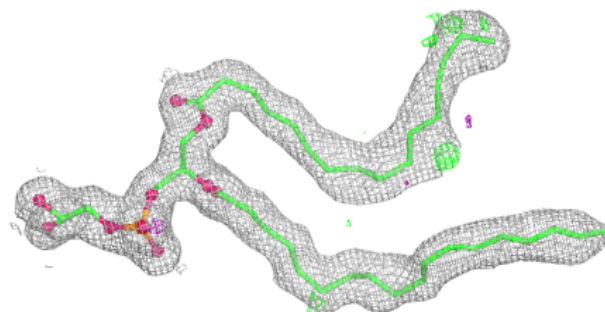


Electron density around CHD P 1525:

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

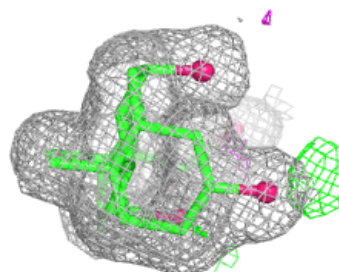
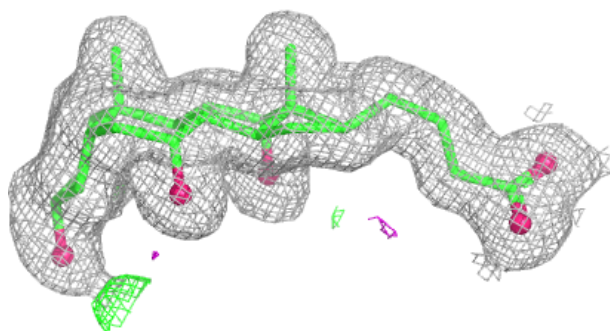
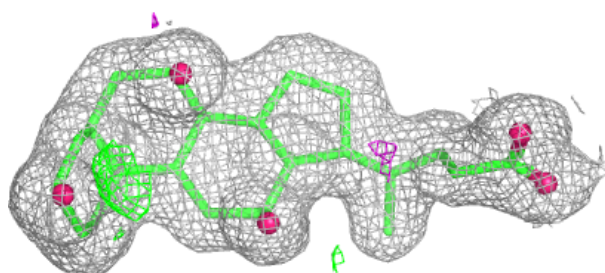
**Electron density around PGV A 525:**

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

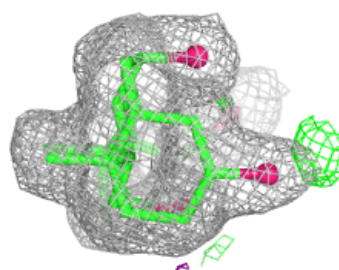
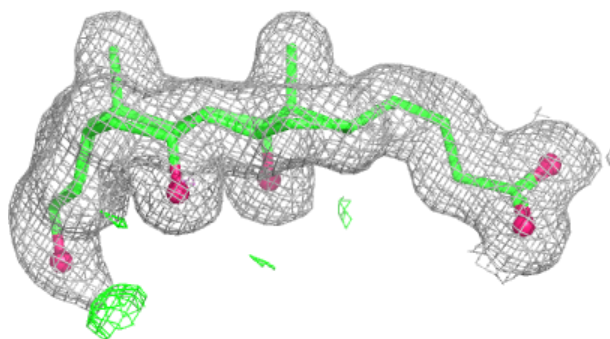
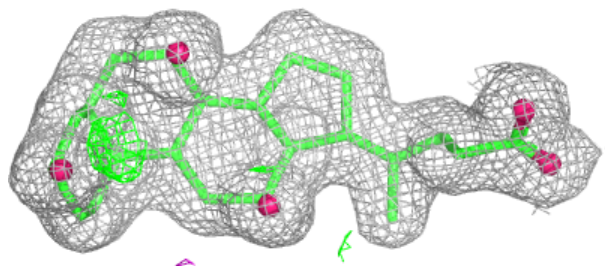


Electron density around CHD O 229:

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

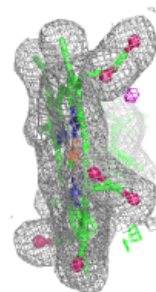
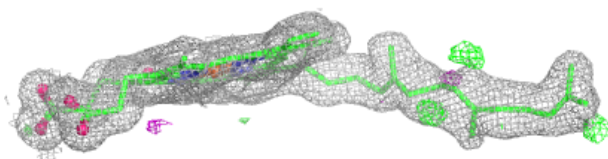
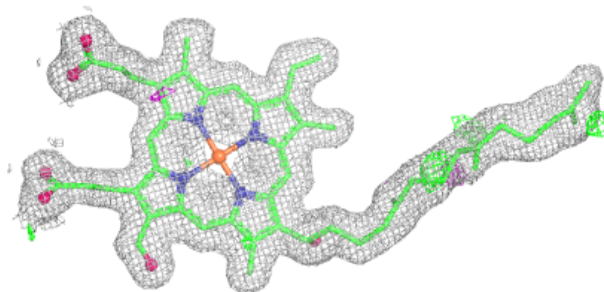
**Electron density around CHD B 1086:**

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

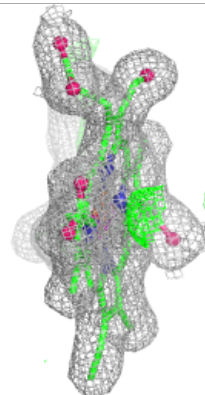
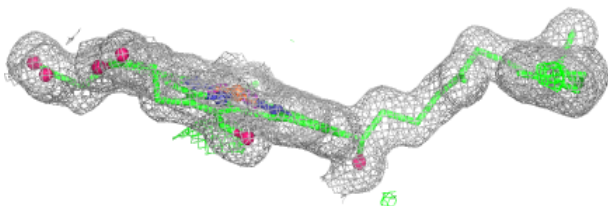
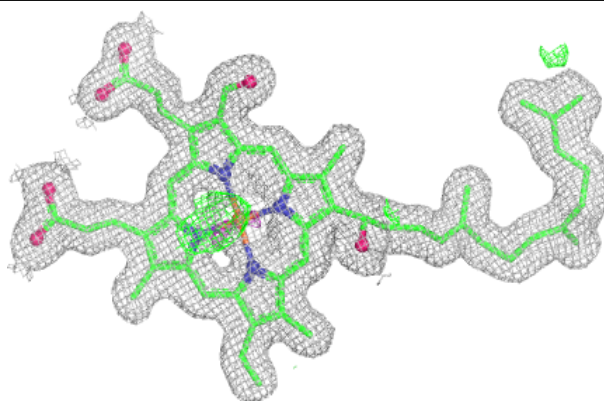


Electron density around HEA N 515:

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

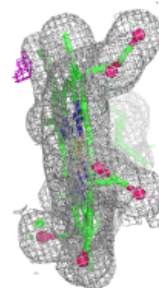
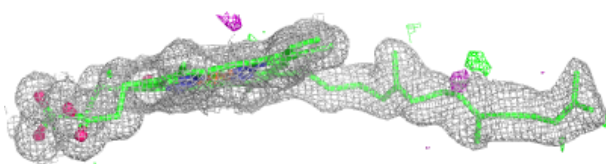
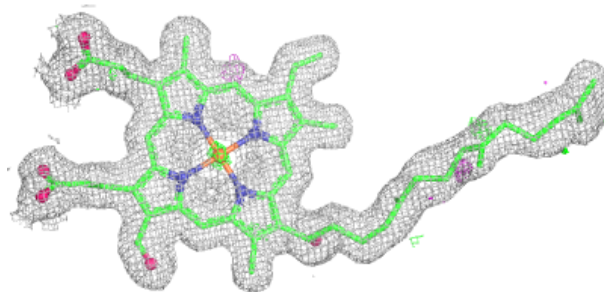
**Electron density around HEA A 516:**

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

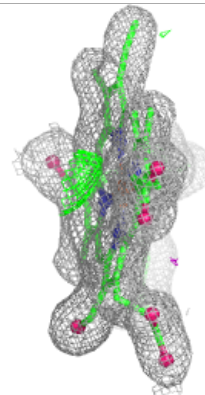
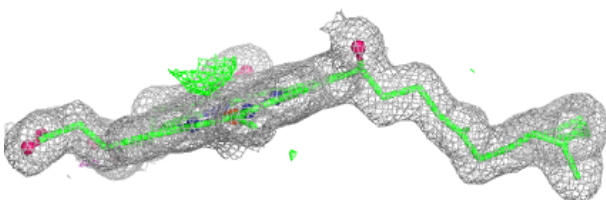
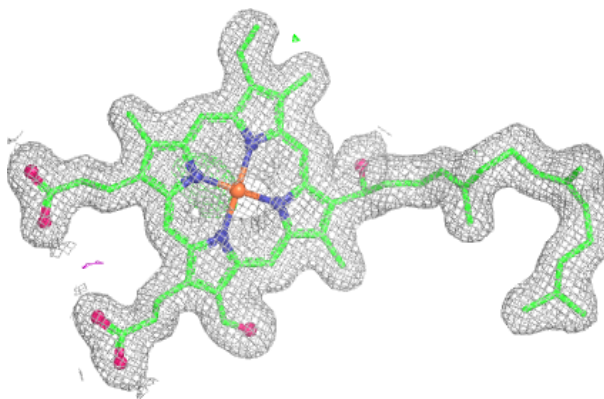


Electron density around HEA A 515:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.