



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 25, 2023 – 10:54 PM EDT

PDB ID : 3AG4  
Title : Bovine Heart Cytochrome c Oxidase in the Cyanide Ion-bound Fully Reduced State at 100 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 : 2.05 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

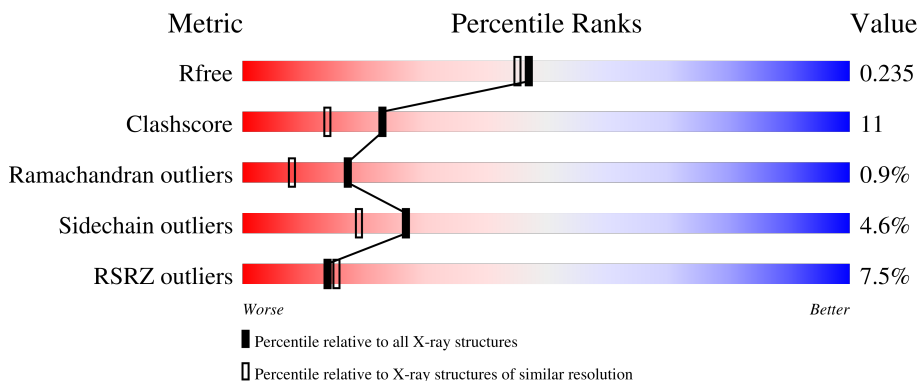
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


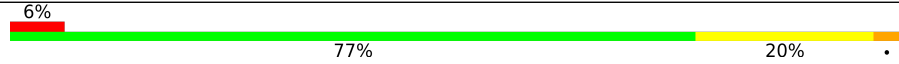
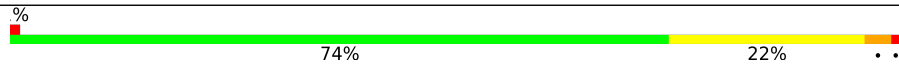

The reported resolution of this entry is 2.05 Å.

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))
$R_{free}$	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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

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Mol	Chain	Length	Quality of chain
3	C	261	80% 16% ..
3	P	261	75% 22% ..
4	D	147	82% 13% ...
4	Q	147	19% 80% 18% ..
5	E	109	2% 85% 10% ..
5	R	109	5% 78% 15% ..
6	F	98	8% 77% 20% .
6	S	98	11% 71% 22% ..
7	G	85	18% 59% 27% 12% ..
7	T	85	21% 61% 21% 14% ..
8	H	85	14% 72% 18% . 7%
8	U	85	19% 71% 20% . 7%
9	I	73	8% 84% 16%
9	V	73	15% 71% 26% .
10	J	59	14% 80% 17% ..
10	W	59	19% 85% 8% 5% .
11	K	56	75% 11% . 12%
11	X	56	21% 80% 5% . 12%
12	L	47	2% 72% 21% ..
12	Y	47	6% 60% 34% ..
13	M	46	7% 70% 13% 11% 7%
13	Z	46	15% 67% 24% . 7%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CYN	N	520	-	-	X	-
22	CHD	C	271	X	-	-	-
22	CHD	J	60	X	-	-	-
22	CHD	P	1271	X	-	-	-
22	CHD	W	1059	X	-	-	X
23	UNX	C	262	-	-	-	X
23	UNX	P	262	-	-	-	X
25	CDL	C	270	-	-	X	-
25	CDL	G	269	-	-	X	-
25	CDL	T	1269	-	-	X	-
28	DMU	G	272	X	-	-	-
28	DMU	M	526	X	-	-	-
28	DMU	P	1272	X	-	-	-
28	DMU	Z	1526	X	-	-	-
9	SAC	V	1	-	-	-	X

## 2 Entry composition [i](#)

There are 29 unique types of molecules in this entry. The entry contains 32324 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	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			

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

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

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			

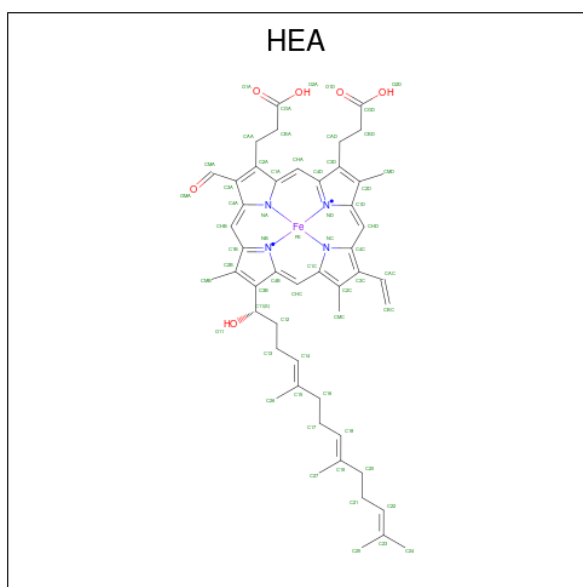
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C.

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.

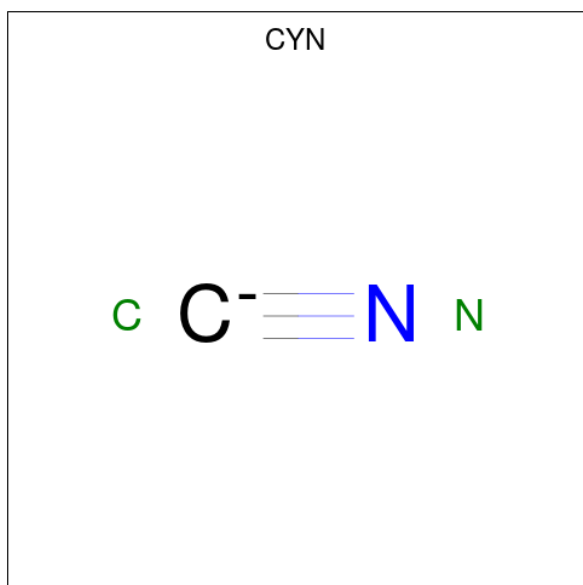
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	0	0
			335	223	53	59			
13	Z	43	Total	C	N	O	0	0	0
			335	223	53	59			

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



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

- Molecule 15 is CYANIDE ION (three-letter code: CYN) (formula: CN).





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

- Molecule 16 is COPPER (II) ION (three-letter code: 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

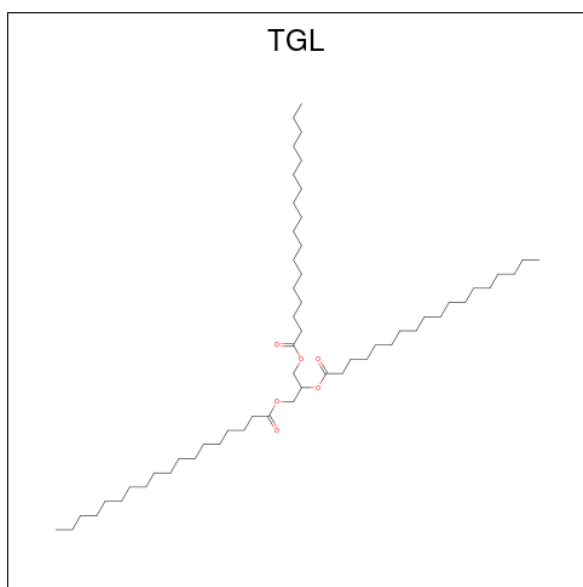
- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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 (three-letter code: NA) (formula: Na).

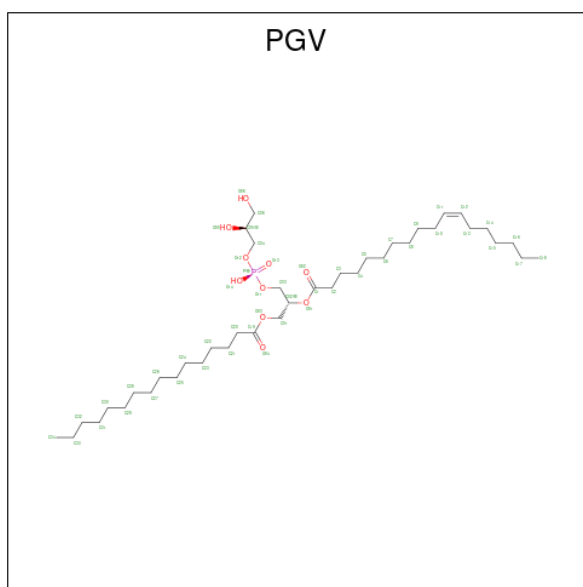
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total Na 1 1	0	0
18	N	1	Total Na 1 1	0	0

- Molecule 19 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C<sub>57</sub>H<sub>110</sub>O<sub>6</sub>).



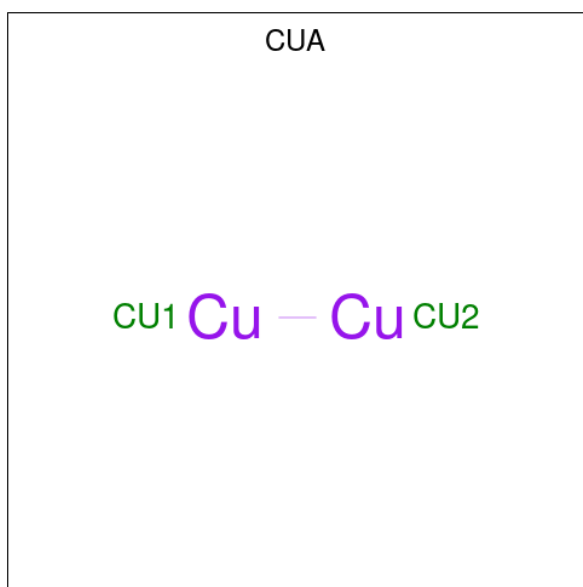
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	C	O	0	0
			63	57	6		
19	D	1	Total	C	O	0	0
			63	57	6		
19	L	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		
19	Q	1	Total	C	O	0	0
			63	57	6		

- Molecule 20 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C<sub>40</sub>H<sub>77</sub>O<sub>10</sub>P).



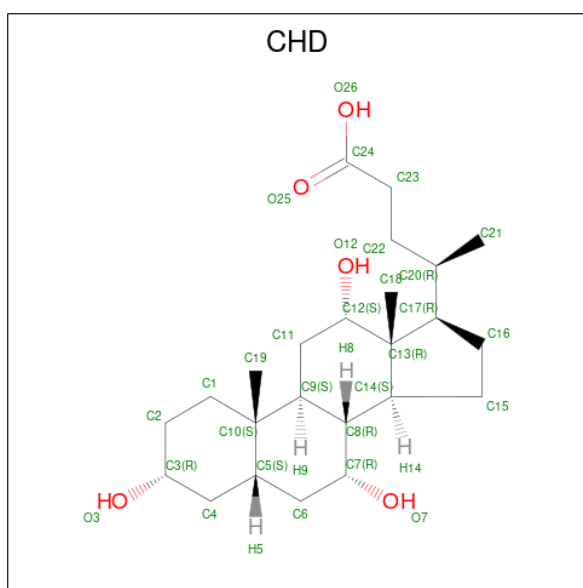
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
20	A	1	51	40	10	1	0	0
20	A	1	51	40	10	1	0	0
20	C	1	51	40	10	1	0	0
20	C	1	51	40	10	1	0	0
20	N	1	51	40	10	1	0	0
20	N	1	51	40	10	1	0	0
20	P	1	51	40	10	1	0	0
20	P	1	51	40	10	1	0	0

- Molecule 21 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu<sub>2</sub>).



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

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



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

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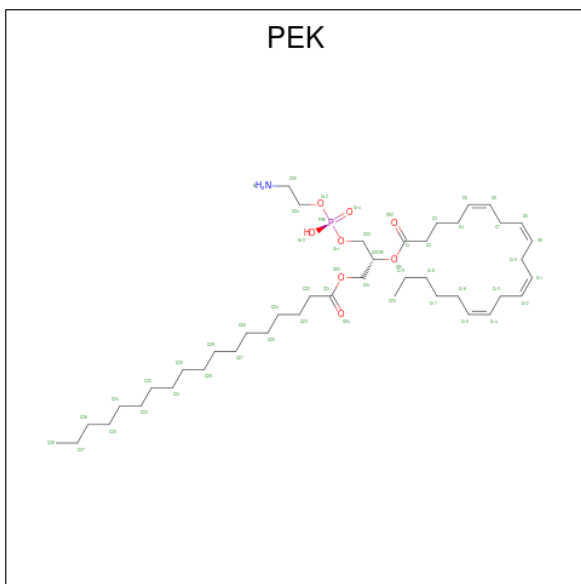
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	C	1	Total	C	O	0	0
			29	24	5		
22	J	1	Total	C	O	0	0
			29	24	5		
22	O	1	Total	C	O	0	0
			29	24	5		
22	P	1	Total	C	O	0	0
			29	24	5		
22	P	1	Total	C	O	0	0
			29	24	5		
22	W	1	Total	C	O	0	0
			29	24	5		

- Molecule 23 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

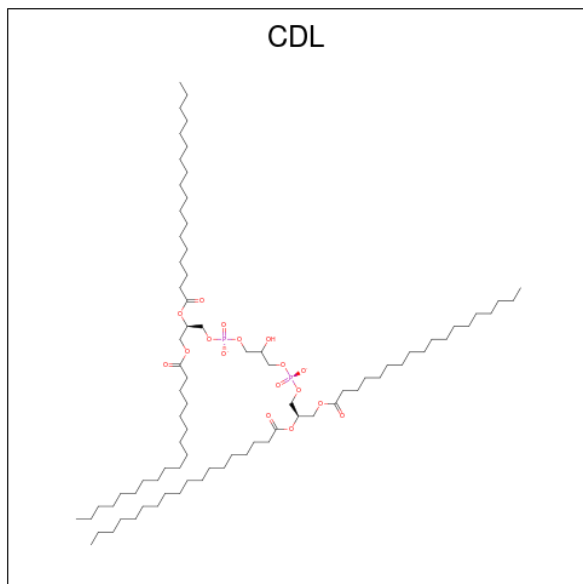
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	C	1	Total	X	0	0
			1	1		
23	P	1	Total	X	0	0
			1	1		

- Molecule 24 is (1S)-2-[[[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY]-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula: C<sub>43</sub>H<sub>78</sub>NO<sub>8</sub>P).



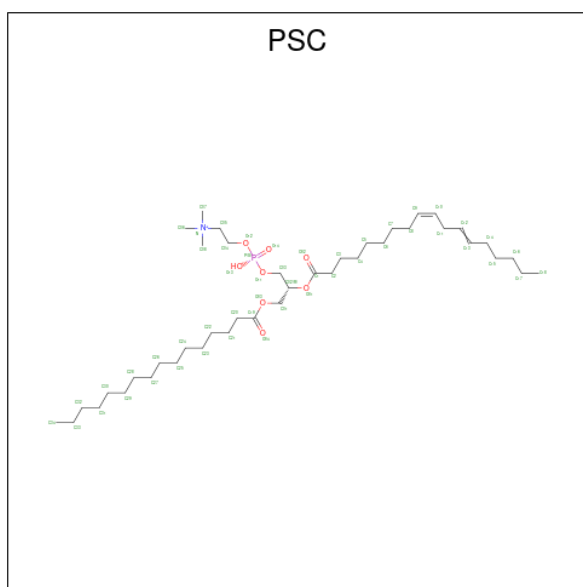
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	S	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

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



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

- Molecule 26 is (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 (three-letter code: PSC) (formula:  $C_{42}H_{81}NO_8P$ ).

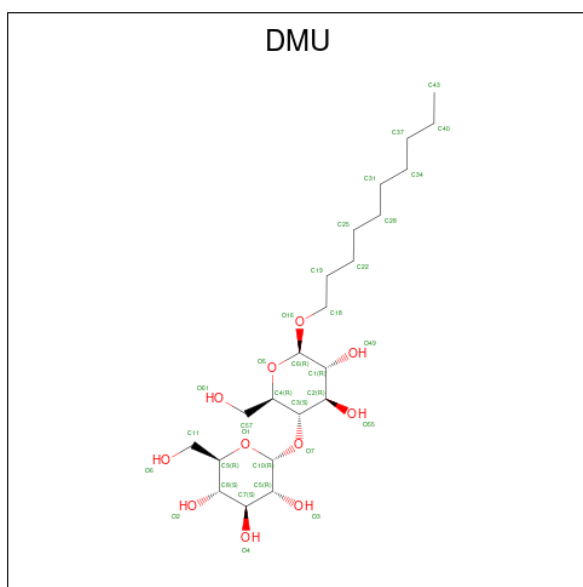


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	E	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
26	R	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 27 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 28 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: C<sub>22</sub>H<sub>42</sub>O<sub>11</sub>).



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

- Molecule 29 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	A	225	Total	O	0	0
			225	225		
29	B	125	Total	O	0	0
			125	125		
29	C	106	Total	O	0	0
			106	106		
29	D	91	Total	O	0	0
			91	91		
29	E	62	Total	O	0	0
			62	62		
29	F	75	Total	O	0	0
			75	75		
29	G	41	Total	O	0	0
			41	41		
29	H	47	Total	O	0	0
			47	47		

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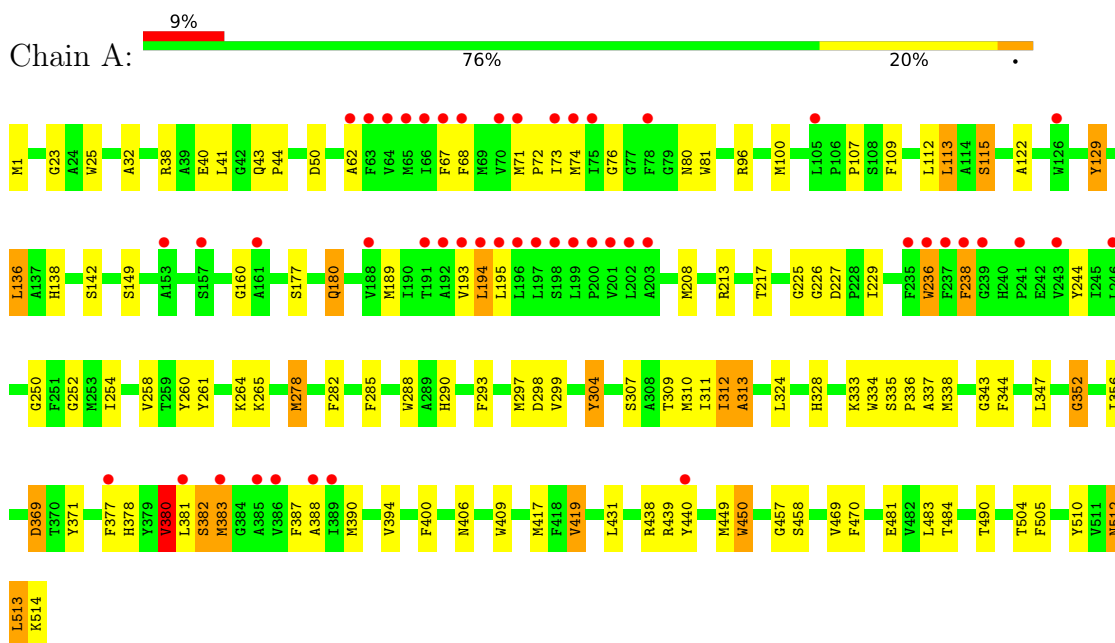
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	I	38	Total O 38 38	0	0
29	J	20	Total O 20 20	0	0
29	K	20	Total O 20 20	0	0
29	L	22	Total O 22 22	0	0
29	M	15	Total O 15 15	0	0
29	N	199	Total O 199 199	0	0
29	O	107	Total O 107 107	0	0
29	P	100	Total O 100 100	0	0
29	Q	55	Total O 55 55	0	0
29	R	40	Total O 40 40	0	0
29	S	56	Total O 56 56	0	0
29	T	36	Total O 36 36	0	0
29	U	41	Total O 41 41	0	0
29	V	18	Total O 18 18	0	0
29	W	12	Total O 12 12	0	0
29	X	14	Total O 14 14	0	0
29	Y	12	Total O 12 12	0	0
29	Z	11	Total O 11 11	0	0

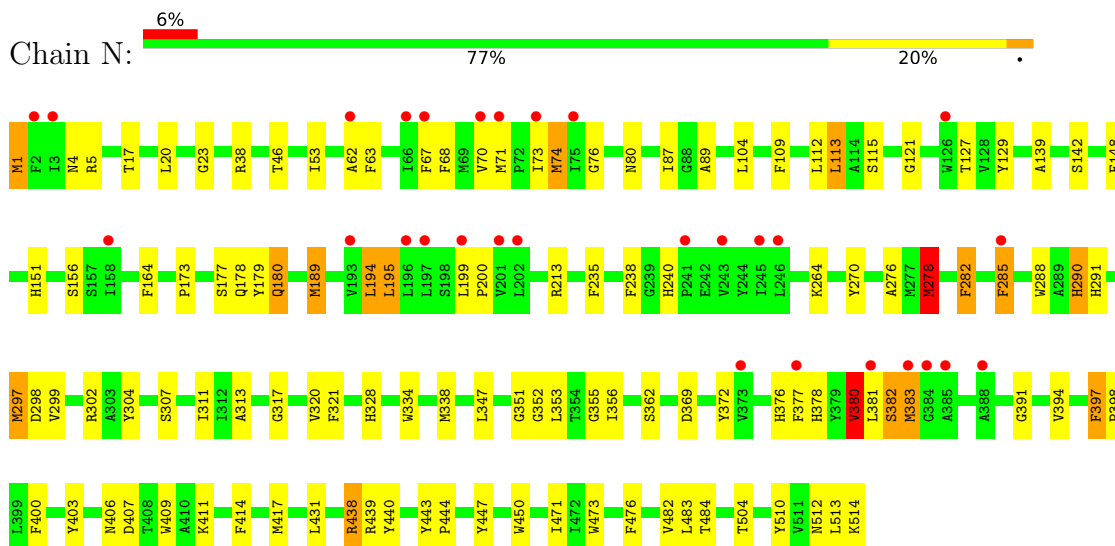
### 3 Residue-property plots [i](#)

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

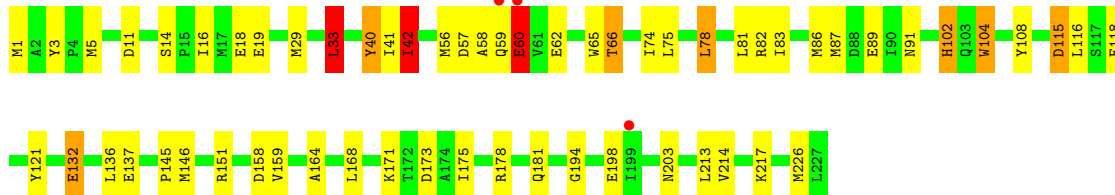
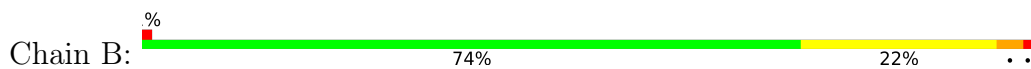
- Molecule 1: Cytochrome c oxidase subunit 1



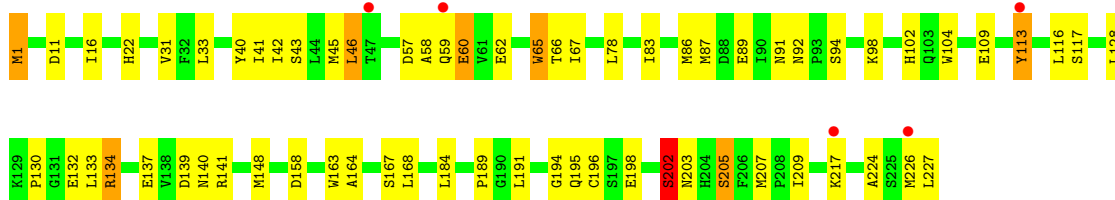
- Molecule 1: Cytochrome c oxidase subunit 1



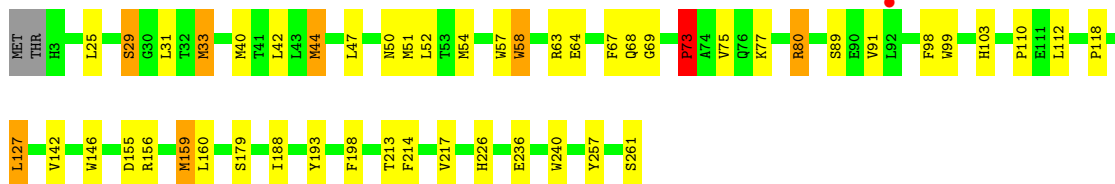
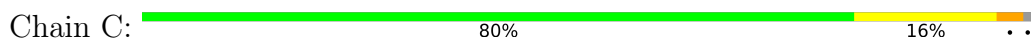
- Molecule 2: Cytochrome c oxidase subunit 2



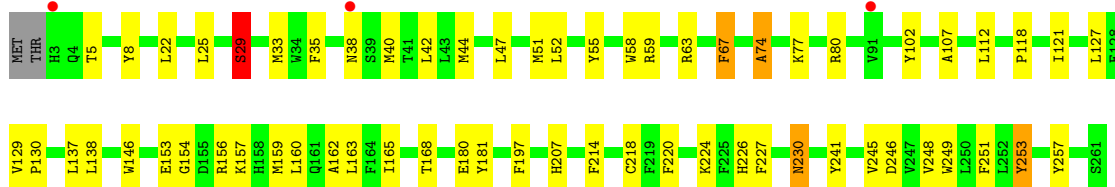
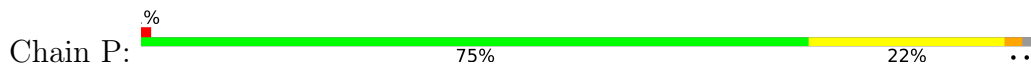
- Molecule 2: Cytochrome c oxidase subunit 2



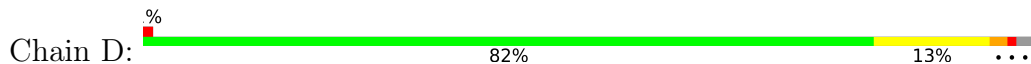
- Molecule 3: Cytochrome c oxidase subunit 3



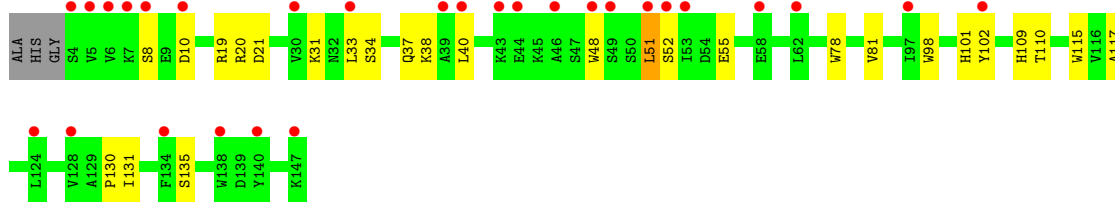
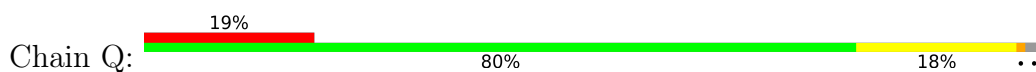
- Molecule 3: Cytochrome c oxidase subunit 3



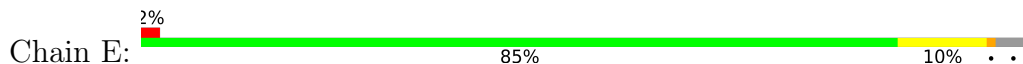
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



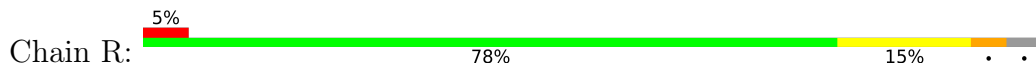
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



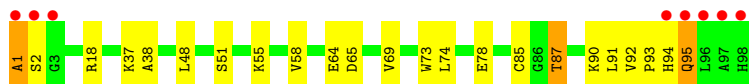
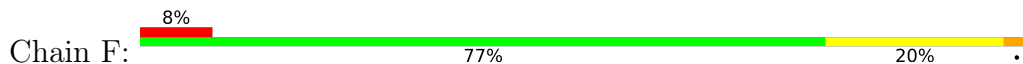
- Molecule 5: Cytochrome c oxidase subunit 5A



- Molecule 5: Cytochrome c oxidase subunit 5A



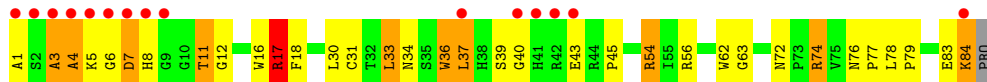
- Molecule 6: Cytochrome c oxidase subunit 5B



- Molecule 6: Cytochrome c oxidase subunit 5B

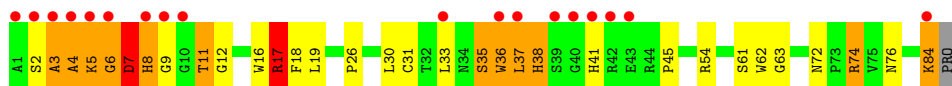


- Molecule 7: Cytochrome c oxidase subunit 6A2

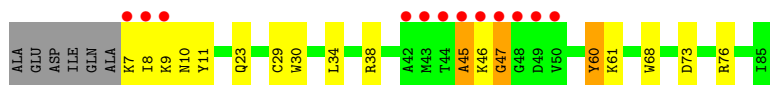


- Molecule 7: Cytochrome c oxidase subunit 6A2

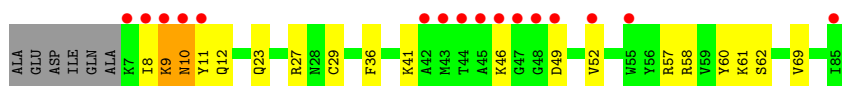




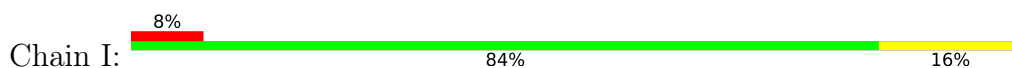
- Molecule 8: Cytochrome c oxidase subunit 6B1



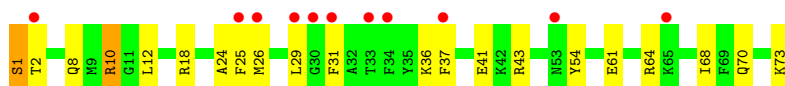
- Molecule 8: Cytochrome c oxidase subunit 6B1



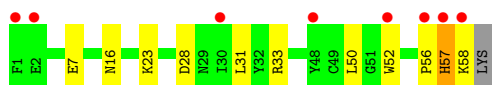
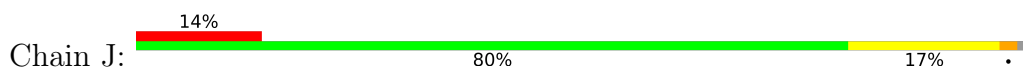
- Molecule 9: Cytochrome c oxidase subunit 6C



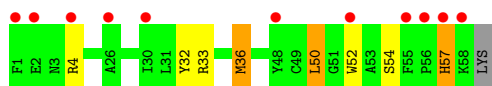
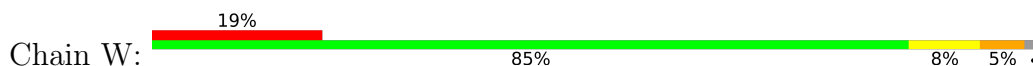
- Molecule 9: Cytochrome c oxidase subunit 6C




- Molecule 10: Cytochrome c oxidase polypeptide 7A1



- Molecule 10: Cytochrome c oxidase polypeptide 7A1




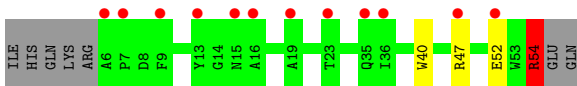
- Molecule 11: Cytochrome c oxidase subunit 7B

Chain K:  75% 11% 12%




• Molecule 11: Cytochrome c oxidase subunit 7B

Chain X:  21% 80% 5% 12%



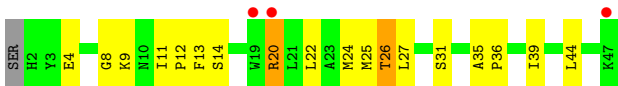
• Molecule 12: Cytochrome c oxidase subunit 7C

Chain L:  2% 72% 21% 3%



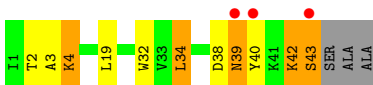
• Molecule 12: Cytochrome c oxidase subunit 7C

Chain Y:  6% 60% 34% 2%



• Molecule 13: Cytochrome c oxidase subunit 8B

Chain M:  7% 70% 13% 11% 7%



• Molecule 13: Cytochrome c oxidase subunit 8B

Chain Z:  15% 67% 24% 7%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	183.36Å 206.65Å 178.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.05 52.61 – 2.05	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.05) 99.8 (52.61-2.05)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.60 (at 2.05Å)	Xtrriage
Refinement program	REFMAC 5.3	Depositor
R, $R_{free}$	0.186 , 0.219 0.204 , 0.235	Depositor DCC
$R_{free}$ test set	21002 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.5	Xtrriage
Anisotropy	0.525	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 63.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.006 for l,-k,h	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	32324	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: HEA, UNX, PEK, CU, NA, CHD, PGV, CDL, CYN, DMU, PSC, TPO, TGL, FME, SAC, CUA, ZN, MG

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	1.69	52/4156 (1.3%)	1.27	32/5678 (0.6%)
1	N	1.51	31/4156 (0.7%)	1.11	14/5678 (0.2%)
2	B	1.53	13/1860 (0.7%)	1.21	11/2534 (0.4%)
2	O	1.24	3/1860 (0.2%)	1.08	5/2534 (0.2%)
3	C	1.52	14/2197 (0.6%)	1.07	6/3005 (0.2%)
3	P	1.51	16/2197 (0.7%)	1.05	3/3005 (0.1%)
4	D	1.55	12/1229 (1.0%)	1.22	7/1658 (0.4%)
4	Q	1.12	2/1229 (0.2%)	0.95	3/1658 (0.2%)
5	E	1.45	1/871 (0.1%)	1.04	2/1182 (0.2%)
5	R	1.20	2/871 (0.2%)	0.96	1/1182 (0.1%)
6	F	1.46	4/765 (0.5%)	1.17	2/1038 (0.2%)
6	S	1.28	1/765 (0.1%)	1.16	4/1038 (0.4%)
7	G	1.35	1/690 (0.1%)	1.10	5/937 (0.5%)
7	T	1.36	3/690 (0.4%)	1.23	5/937 (0.5%)
8	H	1.35	1/682 (0.1%)	1.12	5/921 (0.5%)
8	U	1.13	1/682 (0.1%)	0.95	0/921
9	I	1.34	3/605 (0.5%)	1.03	0/802
9	V	1.18	0/605	0.95	1/802 (0.1%)
10	J	1.25	0/471	1.04	1/636 (0.2%)
10	W	1.16	0/471	1.00	0/636
11	K	1.44	3/398 (0.8%)	1.08	1/546 (0.2%)
11	X	1.18	2/398 (0.5%)	0.96	2/546 (0.4%)
12	L	1.64	4/393 (1.0%)	1.11	2/526 (0.4%)
12	Y	1.42	0/393	1.04	0/526
13	M	1.49	1/345 (0.3%)	1.18	1/470 (0.2%)
13	Z	1.22	0/345	0.97	1/470 (0.2%)
All	All	1.45	170/29324 (0.6%)	1.12	114/39866 (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
6	F	0	1
6	S	0	1
10	J	0	1
10	W	0	1
12	L	0	1
All	All	0	5

The worst 5 of 170 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	181	TYR	CD1-CE1	9.79	1.54	1.39
1	A	438	ARG	CB-CG	-9.36	1.27	1.52
1	A	388	ALA	CA-CB	8.80	1.71	1.52
3	P	29	SER	CB-OG	-8.78	1.30	1.42
1	N	139	ALA	CA-CB	8.50	1.70	1.52

The worst 5 of 114 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	20	ARG	NE-CZ-NH2	-16.98	111.81	120.30
1	A	310	MET	CG-SD-CE	-14.80	76.53	100.20
1	A	278	MET	CG-SD-CE	-14.00	77.80	100.20
1	N	278	MET	CG-SD-CE	-12.95	79.47	100.20
4	D	20	ARG	NE-CZ-NH1	12.84	126.72	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	F	93	PRO	Peptide
10	J	57	HIS	Peptide
12	L	2	HIS	Peptide
6	S	93	PRO	Peptide
10	W	57	HIS	Peptide

## 5.2 Too-close contacts [\(i\)](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4027	0	4001	74	0
1	N	4027	0	4001	84	0
2	B	1824	0	1833	34	0
2	O	1824	0	1833	58	0
3	C	2110	0	2027	36	0
3	P	2110	0	2027	46	0
4	D	1195	0	1183	17	0
4	Q	1195	0	1183	21	0
5	E	852	0	845	5	0
5	R	852	0	845	11	0
6	F	748	0	728	16	0
6	S	748	0	728	25	0
7	G	675	0	643	37	0
7	T	675	0	643	49	0
8	H	662	0	623	6	0
8	U	662	0	623	11	0
9	I	601	0	613	9	0
9	V	601	0	613	17	0
10	J	460	0	459	7	0
10	W	460	0	459	9	0
11	K	384	0	366	2	0
11	X	384	0	366	4	0
12	L	380	0	380	11	0
12	Y	380	0	380	15	0
13	M	335	0	352	9	0
13	Z	335	0	352	8	0
14	A	120	0	108	13	0
14	N	120	0	108	13	0
15	A	2	0	0	0	0
15	N	2	0	0	2	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	7	0
19	D	63	0	110	13	0
19	L	63	0	110	15	0
19	N	126	0	220	22	0
19	Q	63	0	110	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	A	102	0	152	10	0
20	C	102	0	152	6	0
20	N	102	0	152	7	0
20	P	102	0	152	5	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	29	0	36	3	0
22	C	58	0	70	4	0
22	J	29	0	36	2	0
22	O	29	0	36	1	0
22	P	58	0	73	5	0
22	W	29	0	35	6	0
23	C	1	0	0	0	0
23	P	1	0	0	0	0
24	C	53	0	77	3	0
24	G	106	0	154	24	0
24	S	53	0	77	16	0
24	T	106	0	154	28	0
25	C	100	0	156	21	0
25	G	100	0	156	28	0
25	P	100	0	156	19	0
25	T	100	0	156	34	0
26	E	52	0	80	16	0
26	R	52	0	80	14	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	G	33	0	38	3	0
28	M	33	0	38	1	0
28	P	33	0	38	5	0
28	Z	33	0	39	2	0
29	A	225	0	0	8	0
29	B	125	0	0	4	0
29	C	106	0	0	2	0
29	D	91	0	0	1	0
29	E	62	0	0	0	0
29	F	75	0	0	2	0
29	G	41	0	0	3	0
29	H	47	0	0	2	0
29	I	38	0	0	1	0
29	J	20	0	0	1	0
29	K	20	0	0	1	0
29	L	22	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	M	15	0	0	1	0
29	N	199	0	0	4	0
29	O	107	0	0	4	0
29	P	100	0	0	3	0
29	Q	55	0	0	2	0
29	R	40	0	0	1	0
29	S	56	0	0	5	0
29	T	36	0	0	4	0
29	U	41	0	0	4	0
29	V	18	0	0	1	0
29	W	12	0	0	0	0
29	X	14	0	0	0	0
29	Y	12	0	0	1	0
29	Z	11	0	0	0	0
All	All	32324	0	31275	705	0

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

The worst 5 of 705 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:N:74:MET:CB	1:N:74:MET:CG	1.76	1.56
1:A:312:ILE:CG1	1:A:312:ILE:CD1	1.78	1.54
4:D:100:LYS:CE	4:D:100:LYS:NZ	1.69	1.51
3:C:73:PRO:CG	3:C:73:PRO:CB	1.75	1.48
14:A:516:HEA:O11	14:A:516:HEA:C11	1.64	1.45

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	512/514 (100%)	495 (97%)	17 (3%)	0	100	100
1	N	512/514 (100%)	495 (97%)	16 (3%)	1 (0%)	47	39
2	B	225/227 (99%)	212 (94%)	11 (5%)	2 (1%)	17	8
2	O	225/227 (99%)	211 (94%)	12 (5%)	2 (1%)	17	8
3	C	257/261 (98%)	251 (98%)	6 (2%)	0	100	100
3	P	257/261 (98%)	251 (98%)	5 (2%)	1 (0%)	34	24
4	D	142/147 (97%)	137 (96%)	5 (4%)	0	100	100
4	Q	142/147 (97%)	137 (96%)	5 (4%)	0	100	100
5	E	103/109 (94%)	97 (94%)	6 (6%)	0	100	100
5	R	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
6	F	96/98 (98%)	91 (95%)	3 (3%)	2 (2%)	7	1
6	S	96/98 (98%)	89 (93%)	4 (4%)	3 (3%)	4	0
7	G	81/85 (95%)	66 (82%)	7 (9%)	8 (10%)	0	0
7	T	81/85 (95%)	67 (83%)	9 (11%)	5 (6%)	1	0
8	H	77/85 (91%)	67 (87%)	4 (5%)	6 (8%)	1	0
8	U	77/85 (91%)	70 (91%)	5 (6%)	2 (3%)	5	1
9	I	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
9	V	71/73 (97%)	66 (93%)	5 (7%)	0	100	100
10	J	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
10	W	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
11	K	47/56 (84%)	46 (98%)	0	1 (2%)	7	1
11	X	47/56 (84%)	44 (94%)	3 (6%)	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%)	41 (100%)	0	0	100	100
13	Z	41/46 (89%)	38 (93%)	3 (7%)	0	100	100
All	All	3504/3614 (97%)	3336 (95%)	135 (4%)	33 (1%)	17	8

5 of 33 Ramachandran outliers are listed below:

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

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

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	426/426 (100%)	414 (97%)	12 (3%)	43	37
1	N	426/426 (100%)	414 (97%)	12 (3%)	43	37
2	B	210/210 (100%)	200 (95%)	10 (5%)	25	18
2	O	210/210 (100%)	197 (94%)	13 (6%)	18	10
3	C	224/226 (99%)	217 (97%)	7 (3%)	40	33
3	P	224/226 (99%)	218 (97%)	6 (3%)	44	38
4	D	128/129 (99%)	126 (98%)	2 (2%)	62	59
4	Q	128/129 (99%)	125 (98%)	3 (2%)	50	44
5	E	92/95 (97%)	91 (99%)	1 (1%)	73	73
5	R	92/95 (97%)	86 (94%)	6 (6%)	17	9
6	F	81/81 (100%)	76 (94%)	5 (6%)	18	10
6	S	81/81 (100%)	73 (90%)	8 (10%)	8	3
7	G	67/68 (98%)	59 (88%)	8 (12%)	5	1
7	T	67/68 (98%)	57 (85%)	10 (15%)	3	0
8	H	71/75 (95%)	67 (94%)	4 (6%)	21	12
8	U	71/75 (95%)	66 (93%)	5 (7%)	15	7
9	I	57/57 (100%)	53 (93%)	4 (7%)	15	7
9	V	57/57 (100%)	53 (93%)	4 (7%)	15	7
10	J	49/50 (98%)	48 (98%)	1 (2%)	55	50
10	W	49/50 (98%)	46 (94%)	3 (6%)	18	10
11	K	39/46 (85%)	38 (97%)	1 (3%)	46	39
11	X	39/46 (85%)	37 (95%)	2 (5%)	24	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	39/40 (98%)	38 (97%)	1 (3%)	46	39
12	Y	39/40 (98%)	37 (95%)	2 (5%)	24	15
13	M	37/38 (97%)	31 (84%)	6 (16%)	2	0
13	Z	37/38 (97%)	33 (89%)	4 (11%)	6	2
All	All	3040/3082 (99%)	2900 (95%)	140 (5%)	27	19

5 of 140 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	T	38	HIS
7	T	84	LYS
10	W	36	MET
8	H	60	TYR
8	H	29	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
2	O	22	HIS
3	P	149	HIS
9	V	70	GLN
2	O	52	HIS
2	O	195	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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
7	TPO	G	11	7	8,10,11	2.39	3 (37%)	10,14,16	1.75	3 (30%)
7	TPO	T	11	7	8,10,11	2.23	3 (37%)	10,14,16	2.14	2 (20%)
1	FME	N	1	1	8,9,10	1.37	1 (12%)	7,9,11	5.36	4 (57%)
2	FME	B	1	2	8,9,10	2.06	1 (12%)	7,9,11	6.70	4 (57%)
9	SAC	I	1	9	7,8,9	2.37	2 (28%)	8,9,11	1.48	2 (25%)
1	FME	A	1	1	8,9,10	1.04	1 (12%)	7,9,11	5.90	4 (57%)
2	FME	O	1	2	8,9,10	1.17	1 (12%)	7,9,11	6.11	2 (28%)
9	SAC	V	1	9	7,8,9	3.15	2 (28%)	8,9,11	2.22	3 (37%)

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

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

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	V	1	SAC	CA-N	5.80	1.54	1.46
9	V	1	SAC	OAC-C1A	5.52	1.35	1.23
2	B	1	FME	O1-CN	-4.38	1.09	1.22
9	I	1	SAC	CA-N	4.31	1.52	1.46
9	I	1	SAC	OAC-C1A	4.27	1.32	1.23

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CA-N-CN	-16.27	97.80	122.82
2	O	1	FME	CA-N-CN	-15.72	98.64	122.82
1	A	1	FME	CA-N-CN	-14.12	101.11	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	1	FME	CA-N-CN	-13.38	102.24	122.82
7	T	11	TPO	CG2-CB-CA	5.79	124.59	113.16

There are no chirality outliers.

5 of 20 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 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	11	TPO	1	0
7	T	11	TPO	1	0
1	N	1	FME	1	0
2	O	1	FME	1	0
9	V	1	SAC	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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
24	PEK	G	1263	-	52,52,52	1.18	2 (3%)	55,57,57	1.17	5 (9%)
21	CUA	O	228	2	0,1,1	-	-	-	-	-
20	PGV	N	1266	-	50,50,50	0.93	1 (2%)	53,56,56	1.36	6 (11%)
14	HEA	N	516	15,1	57,67,67	2.00	15 (26%)	61,103,103	3.52	30 (49%)
25	CDL	P	1270	-	99,99,99	1.38	12 (12%)	105,111,111	1.38	14 (13%)
26	PSC	E	229	-	51,51,51	1.28	3 (5%)	57,59,59	1.36	6 (10%)
19	TGL	L	522	-	62,62,62	1.58	8 (12%)	65,65,65	1.83	16 (24%)
28	DMU	P	1272	-	34,34,34	1.23	1 (2%)	45,45,45	3.19	23 (51%)
24	PEK	T	263	-	52,52,52	1.23	2 (3%)	55,57,57	1.18	6 (10%)
20	PGV	C	268	-	50,50,50	1.30	3 (6%)	53,56,56	1.46	6 (11%)
22	CHD	B	1085	-	32,32,32	1.53	6 (18%)	51,51,51	5.64	37 (72%)
22	CHD	W	1059	-	32,32,32	1.14	2 (6%)	51,51,51	5.13	34 (66%)
22	CHD	J	60	-	32,32,32	0.79	0	51,51,51	4.89	40 (78%)
26	PSC	R	1229	-	51,51,51	1.22	3 (5%)	57,59,59	1.01	5 (8%)
14	HEA	A	515	1	57,67,67	1.62	11 (19%)	61,103,103	2.13	18 (29%)
19	TGL	D	523	-	62,62,62	1.61	7 (11%)	65,65,65	1.51	12 (18%)
20	PGV	N	1524	-	50,50,50	1.22	2 (4%)	53,56,56	1.27	6 (11%)
20	PGV	P	1267	-	50,50,50	0.85	2 (4%)	53,56,56	1.42	7 (13%)
24	PEK	T	1264	-	52,52,52	0.93	2 (3%)	55,57,57	1.94	8 (14%)
14	HEA	N	515	1	57,67,67	1.49	7 (12%)	61,103,103	2.15	18 (29%)
25	CDL	G	269	-	99,99,99	1.50	14 (14%)	105,111,111	1.50	17 (16%)
21	CUA	B	228	2	0,1,1	-	-	-	-	-
28	DMU	Z	1526	-	34,34,34	0.97	2 (5%)	45,45,45	3.14	21 (46%)
22	CHD	C	271	-	32,32,32	0.94	2 (6%)	51,51,51	5.07	35 (68%)
24	PEK	C	264	-	52,52,52	0.89	2 (3%)	55,57,57	1.78	12 (21%)
25	CDL	C	270	-	99,99,99	1.38	12 (12%)	105,111,111	1.42	15 (14%)
24	PEK	G	265	-	52,52,52	1.21	3 (5%)	55,57,57	1.24	3 (5%)
20	PGV	A	524	-	50,50,50	1.19	2 (4%)	53,56,56	1.34	7 (13%)
19	TGL	N	1522	-	62,62,62	1.59	7 (11%)	65,65,65	1.61	15 (23%)
22	CHD	P	1271	-	32,32,32	0.80	0	51,51,51	4.90	37 (72%)
15	CYN	A	520	14,16	0,1,1	-	-	-	-	-
25	CDL	T	1269	-	99,99,99	1.38	12 (12%)	105,111,111	1.41	16 (15%)
22	CHD	C	525	-	32,32,32	1.84	7 (21%)	51,51,51	5.39	34 (66%)
24	PEK	S	1265	-	52,52,52	1.34	3 (5%)	55,57,57	1.30	5 (9%)
19	TGL	Q	1523	-	62,62,62	1.36	6 (9%)	65,65,65	1.24	9 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	PGV	A	522	-	50,50,50	0.98	2 (4%)	53,56,56	1.28	6 (11%)
28	DMU	M	526	-	34,34,34	0.85	1 (2%)	45,45,45	3.42	27 (60%)
28	DMU	G	272	-	34,34,34	1.27	4 (11%)	45,45,45	3.27	23 (51%)
15	CYN	N	520	14,16	0,1,1	-	-	-	-	-
19	TGL	N	1521	-	62,62,62	1.34	6 (9%)	65,65,65	1.47	12 (18%)
14	HEA	A	516	15,1	57,67,67	2.18	16 (28%)	61,103,103	3.90	33 (54%)
22	CHD	O	229	-	32,32,32	1.25	2 (6%)	51,51,51	5.55	35 (68%)
20	PGV	P	1268	-	50,50,50	1.28	3 (6%)	53,56,56	1.51	7 (13%)
20	PGV	C	267	-	50,50,50	0.88	3 (6%)	53,56,56	1.37	4 (7%)
19	TGL	A	521	-	62,62,62	1.45	7 (11%)	65,65,65	2.37	17 (26%)
22	CHD	P	1525	-	32,32,32	1.52	5 (15%)	51,51,51	5.13	42 (82%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PEK	G	1263	-	-	27/56/56/56	-
20	PGV	N	1266	-	-	13/55/55/55	-
14	HEA	N	516	15,1	-	10/32/76/76	-
25	CDL	P	1270	-	-	69/110/110/110	-
26	PSC	E	229	-	-	32/55/55/55	-
19	TGL	L	522	-	-	35/65/65/65	-
28	DMU	P	1272	-	6/6/10/10	11/19/59/59	0/2/2/2
24	PEK	T	263	-	-	33/56/56/56	-
20	PGV	C	268	-	-	34/55/55/55	-
22	CHD	B	1085	-	-	2/9/74/74	0/4/4/4
22	CHD	W	1059	-	2/2/12/12	7/9/74/74	0/4/4/4
22	CHD	J	60	-	2/2/12/12	6/9/74/74	0/4/4/4
26	PSC	R	1229	-	-	39/55/55/55	-
14	HEA	A	515	1	-	5/32/76/76	-
19	TGL	D	523	-	-	37/65/65/65	-
20	PGV	N	1524	-	-	36/55/55/55	-
20	PGV	P	1267	-	-	14/55/55/55	-
24	PEK	T	1264	-	-	23/56/56/56	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	HEA	N	515	1	-	6/32/76/76	-
25	CDL	G	269	-	-	65/110/110/110	-
28	DMU	Z	1526	-	5/5/10/10	9/19/59/59	0/2/2/2
22	CHD	C	271	-	1/1/12/12	4/9/74/74	0/4/4/4
24	PEK	C	264	-	-	21/56/56/56	-
25	CDL	C	270	-	-	74/110/110/110	-
24	PEK	G	265	-	-	29/56/56/56	-
22	CHD	P	1271	-	1/1/12/12	7/9/74/74	0/4/4/4
19	TGL	N	1522	-	-	39/65/65/65	-
20	PGV	A	524	-	-	33/55/55/55	-
25	CDL	T	1269	-	-	65/110/110/110	-
22	CHD	C	525	-	-	2/9/74/74	0/4/4/4
24	PEK	S	1265	-	-	25/56/56/56	-
19	TGL	Q	1523	-	-	38/65/65/65	-
20	PGV	A	522	-	-	15/55/55/55	-
28	DMU	M	526	-	4/4/10/10	10/19/59/59	0/2/2/2
28	DMU	G	272	-	6/6/10/10	12/19/59/59	0/2/2/2
19	TGL	N	1521	-	-	41/65/65/65	-
14	HEA	A	516	15,1	-	6/32/76/76	-
22	CHD	O	229	-	-	2/9/74/74	0/4/4/4
20	PGV	P	1268	-	-	30/55/55/55	-
20	PGV	C	267	-	-	14/55/55/55	-
19	TGL	A	521	-	-	35/65/65/65	-
22	CHD	P	1525	-	-	2/9/74/74	0/4/4/4

The worst 5 of 210 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	516	HEA	O11-C11	9.88	1.64	1.42
14	N	516	HEA	O11-C11	7.49	1.59	1.42
19	N	1522	TGL	OG2-CB1	6.85	1.53	1.34
19	L	522	TGL	OG2-CB1	6.42	1.52	1.34
20	P	1268	PGV	O01-C1	6.27	1.52	1.34

The worst 5 of 729 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1085	CHD	C18-C13-C12	-16.45	92.32	109.07
22	P	1271	CHD	C10-C9-C8	14.25	127.12	111.82
22	C	271	CHD	C10-C9-C8	13.69	126.52	111.82
22	C	525	CHD	C6-C5-C10	12.69	126.13	112.66
22	B	1085	CHD	C1-C10-C5	12.48	126.22	107.77

5 of 27 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	C	271	CHD	C9
22	J	60	CHD	C9
22	J	60	CHD	C17
22	P	1271	CHD	C9
22	W	1059	CHD	C9

5 of 1017 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	516	HEA	C2D-C3D-CAD-CBD
14	N	515	HEA	C14-C15-C16-C17
14	N	515	HEA	C26-C15-C16-C17
14	N	516	HEA	C2D-C3D-CAD-CBD
14	N	516	HEA	C4D-C3D-CAD-CBD

There are no ring outliers.

42 monomers are involved in 341 short contacts:

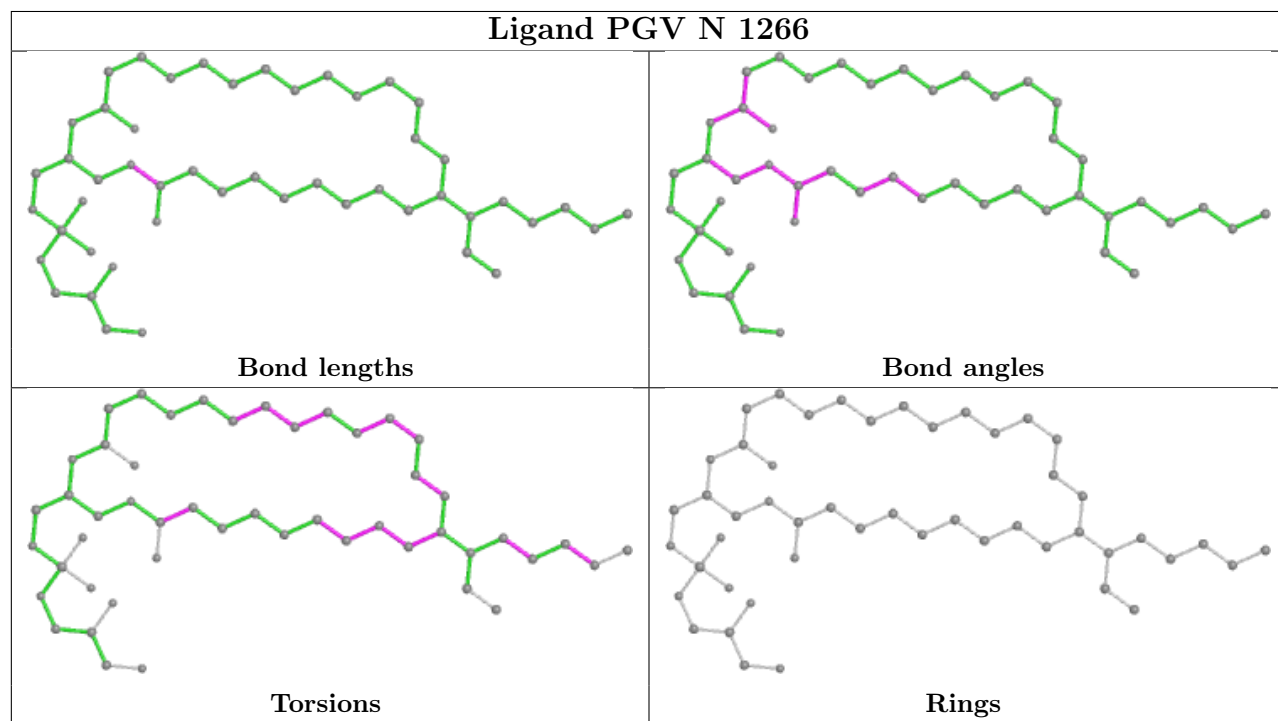
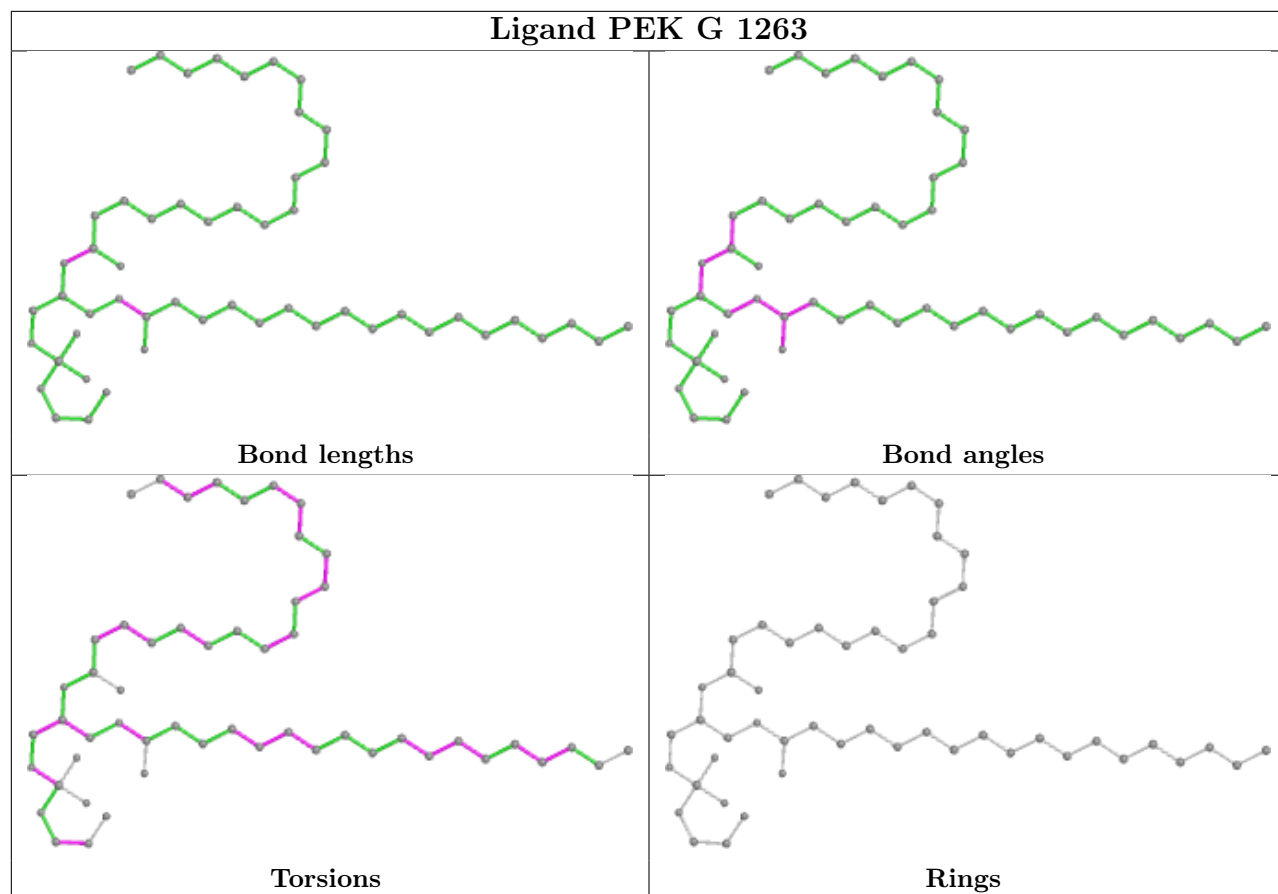
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	G	1263	PEK	11	0
14	N	516	HEA	10	0
25	P	1270	CDL	19	0
26	E	229	PSC	16	0
19	L	522	TGL	15	0
28	P	1272	DMU	5	0
24	T	263	PEK	19	0
20	C	268	PGV	3	0
22	B	1085	CHD	3	0
22	W	1059	CHD	6	0
22	J	60	CHD	2	0
26	R	1229	PSC	14	0
14	A	515	HEA	5	0
19	D	523	TGL	13	0
20	N	1524	PGV	7	0

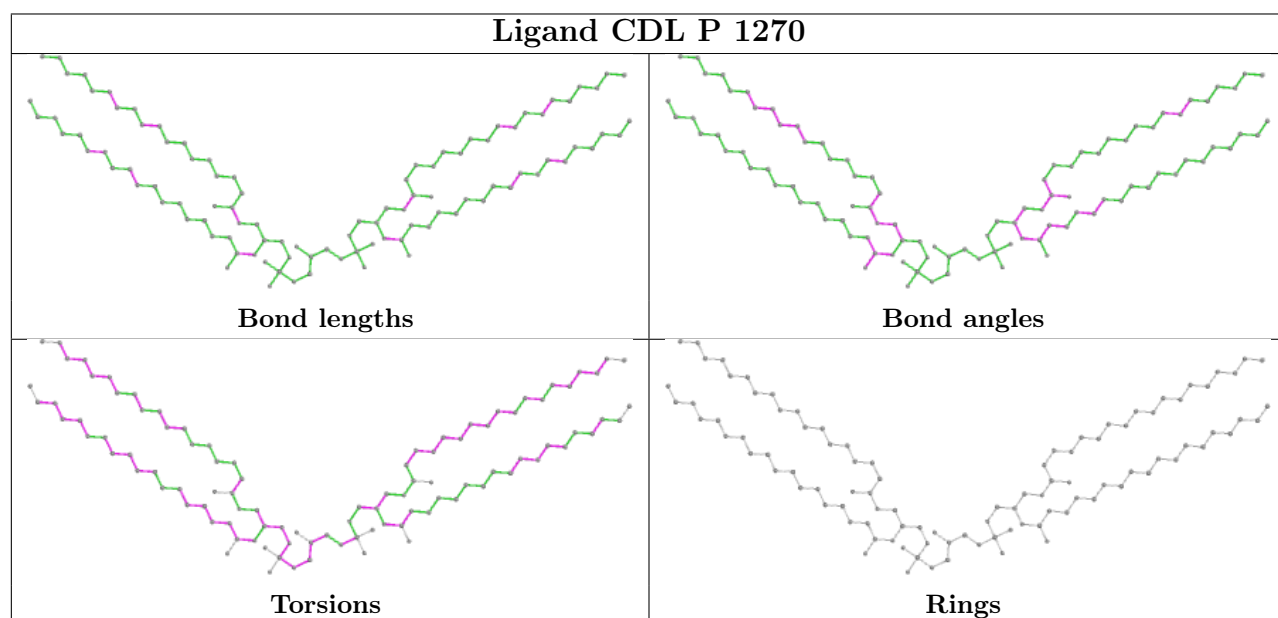
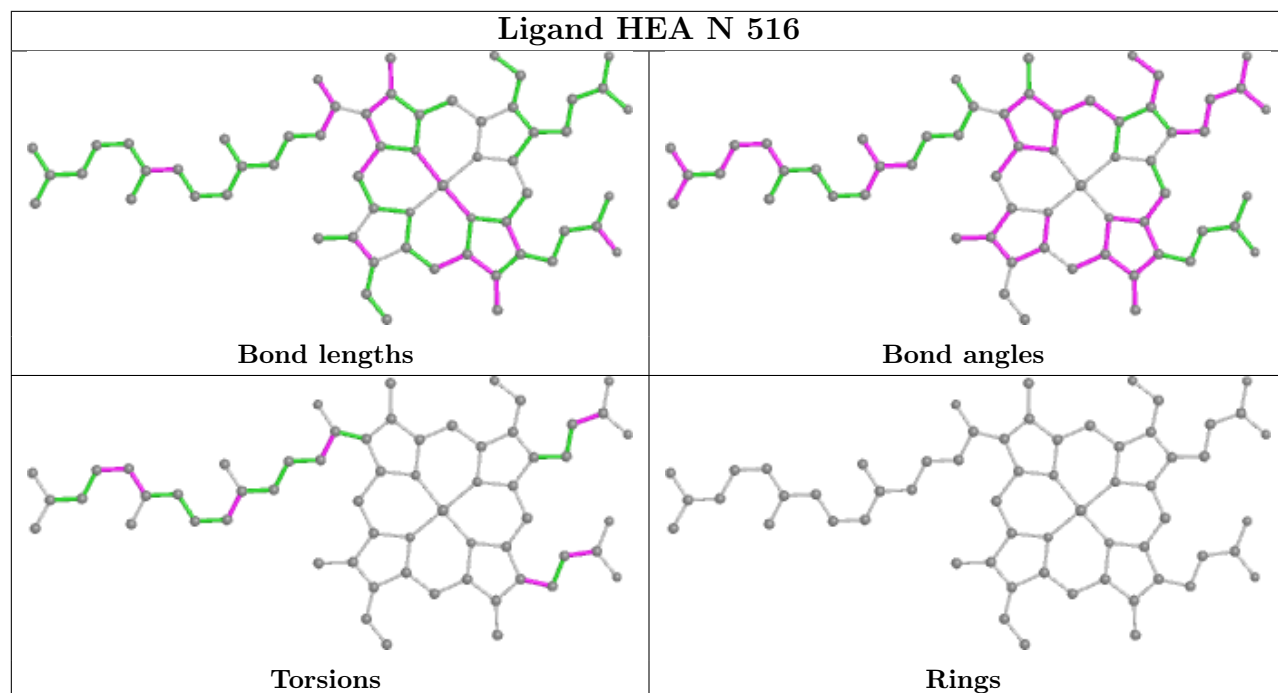
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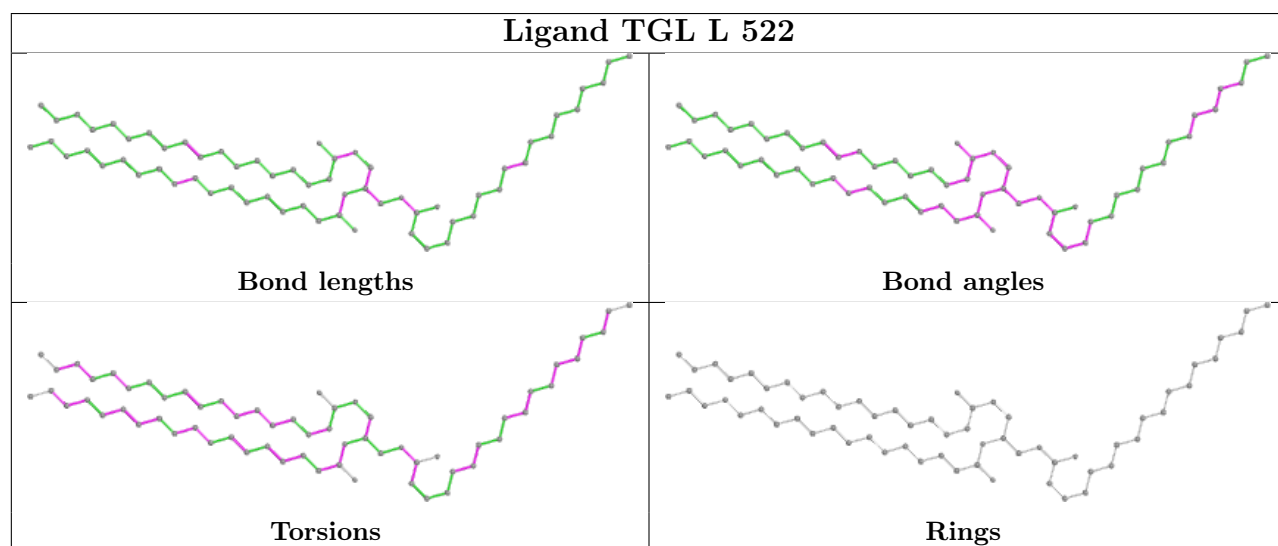
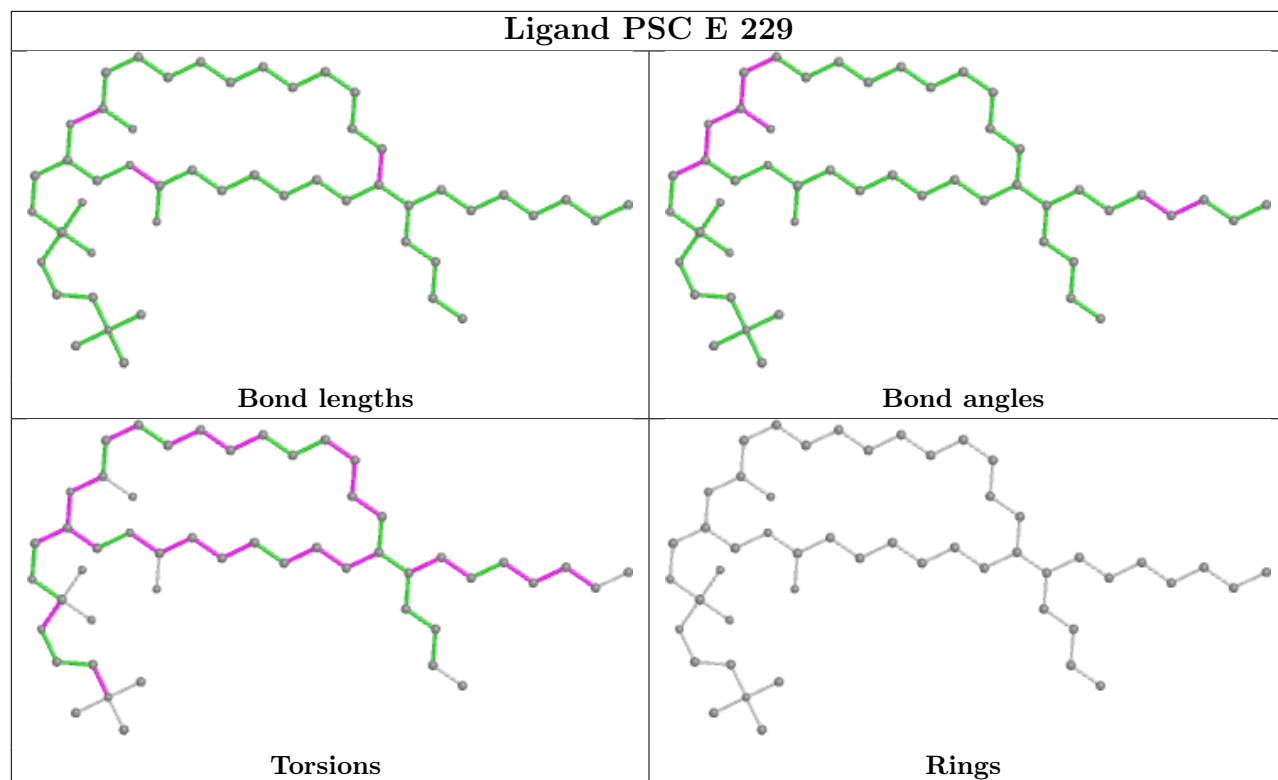
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	P	1267	PGV	3	0
24	T	1264	PEK	9	0
14	N	515	HEA	3	0
25	G	269	CDL	28	0
28	Z	1526	DMU	2	0
22	C	271	CHD	3	0
24	C	264	PEK	3	0
25	C	270	CDL	21	0
24	G	265	PEK	13	0
20	A	524	PGV	8	0
19	N	1522	TGL	15	0
22	P	1271	CHD	4	0
25	T	1269	CDL	34	0
22	C	525	CHD	1	0
24	S	1265	PEK	16	0
19	Q	1523	TGL	10	0
20	A	522	PGV	2	0
28	M	526	DMU	1	0
28	G	272	DMU	3	0
15	N	520	CYN	2	0
19	N	1521	TGL	7	0
14	A	516	HEA	8	0
22	O	229	CHD	1	0
20	P	1268	PGV	2	0
20	C	267	PGV	3	0
19	A	521	TGL	7	0
22	P	1525	CHD	1	0

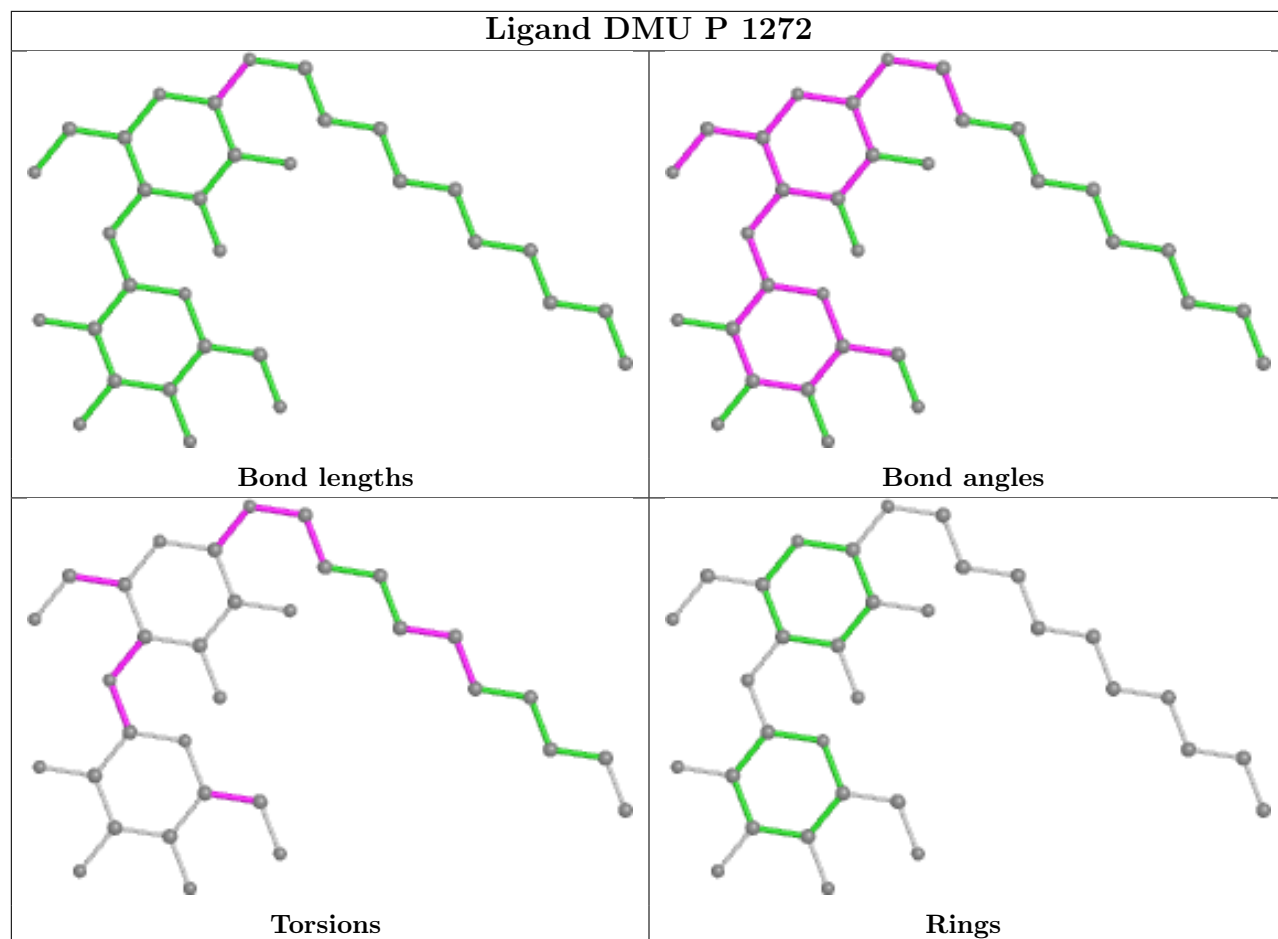
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

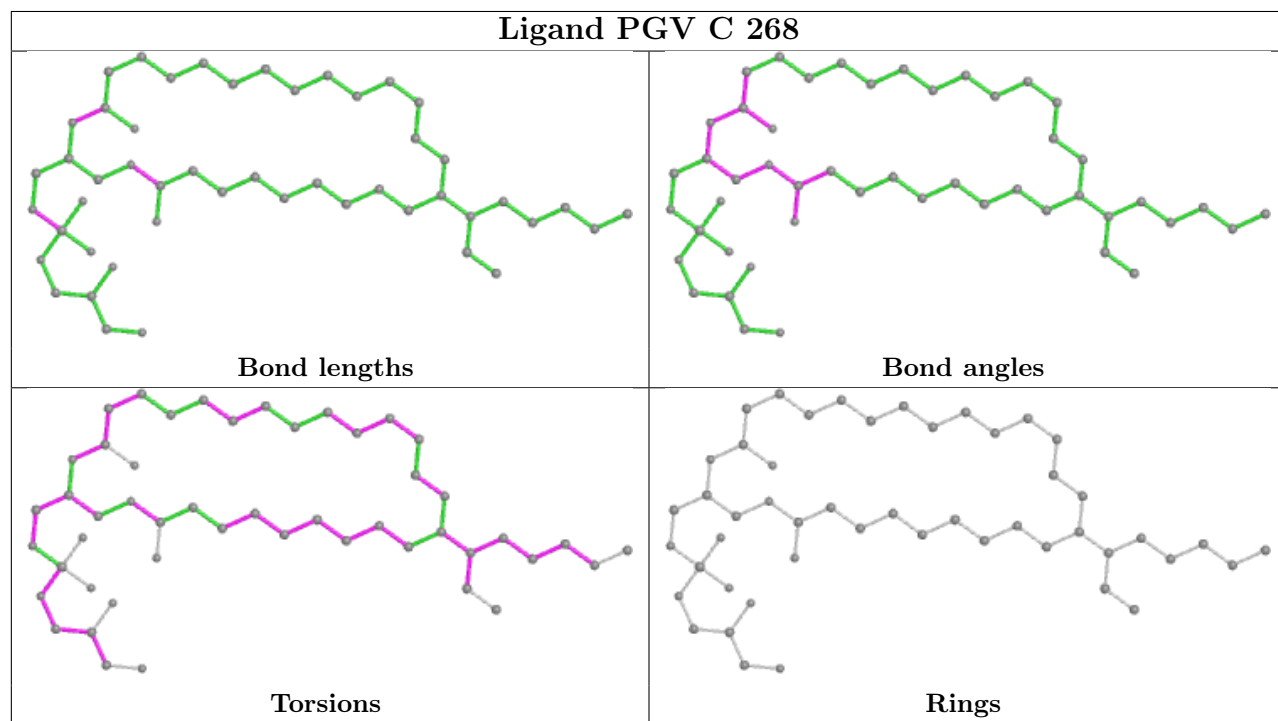
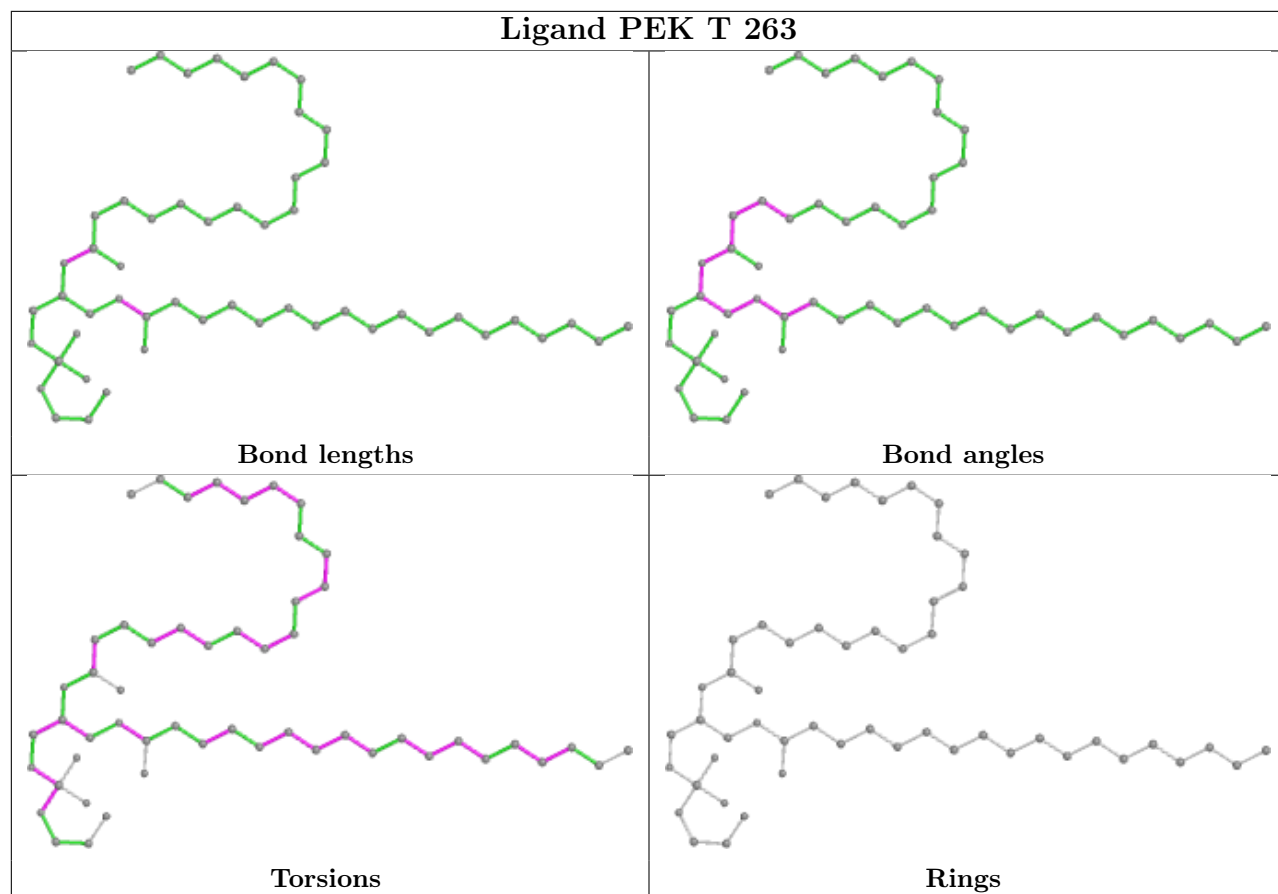


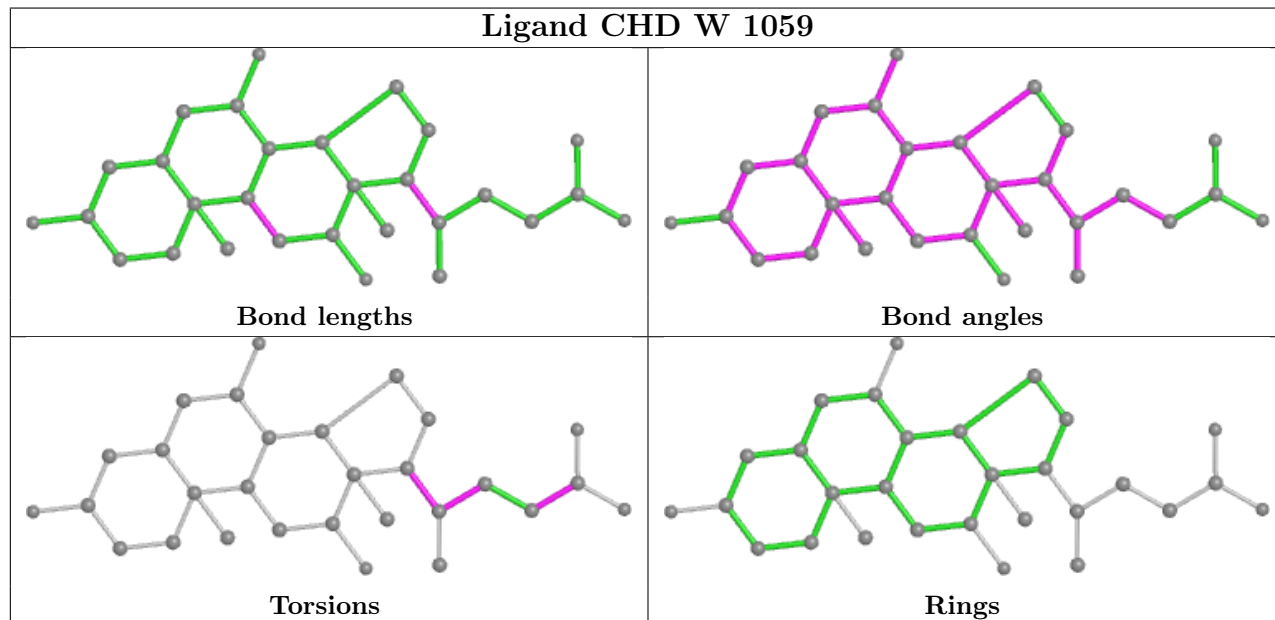
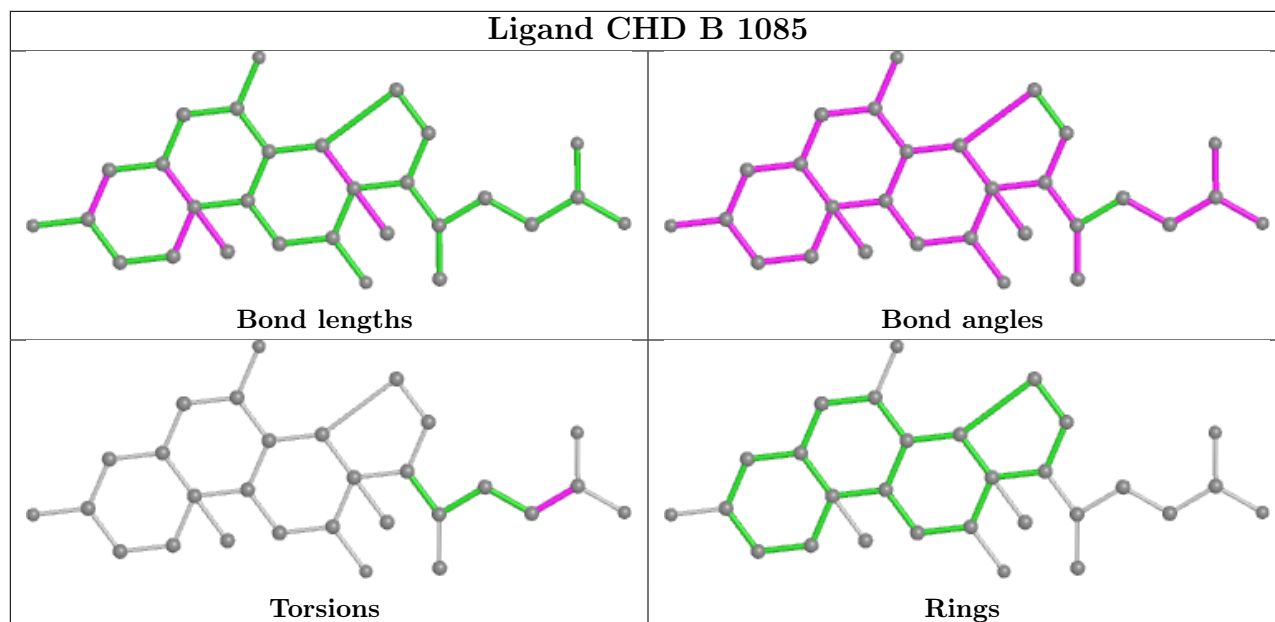


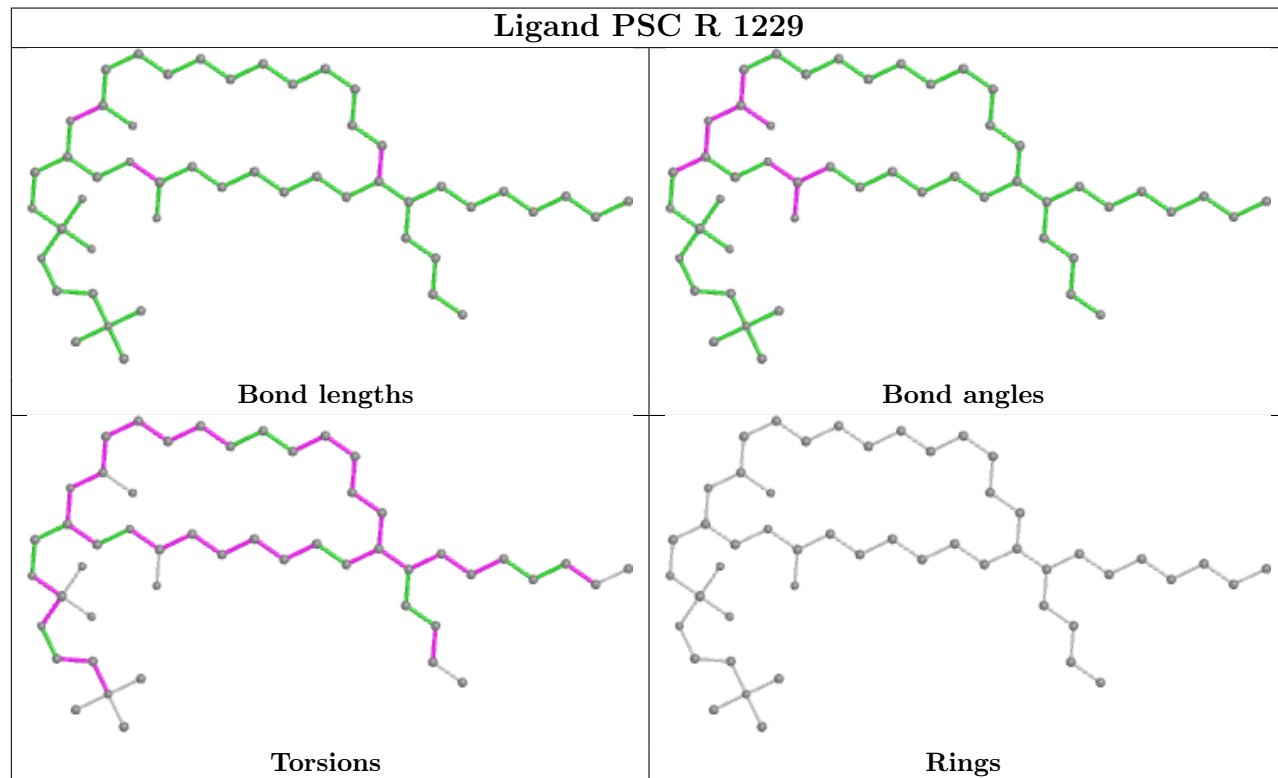
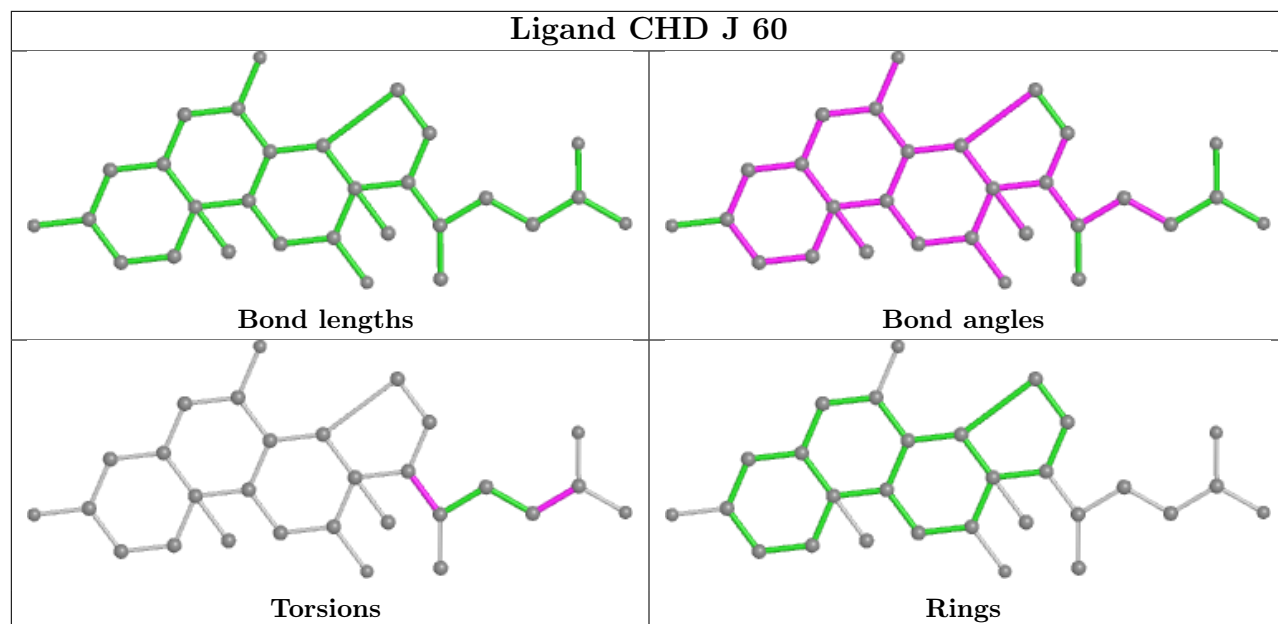


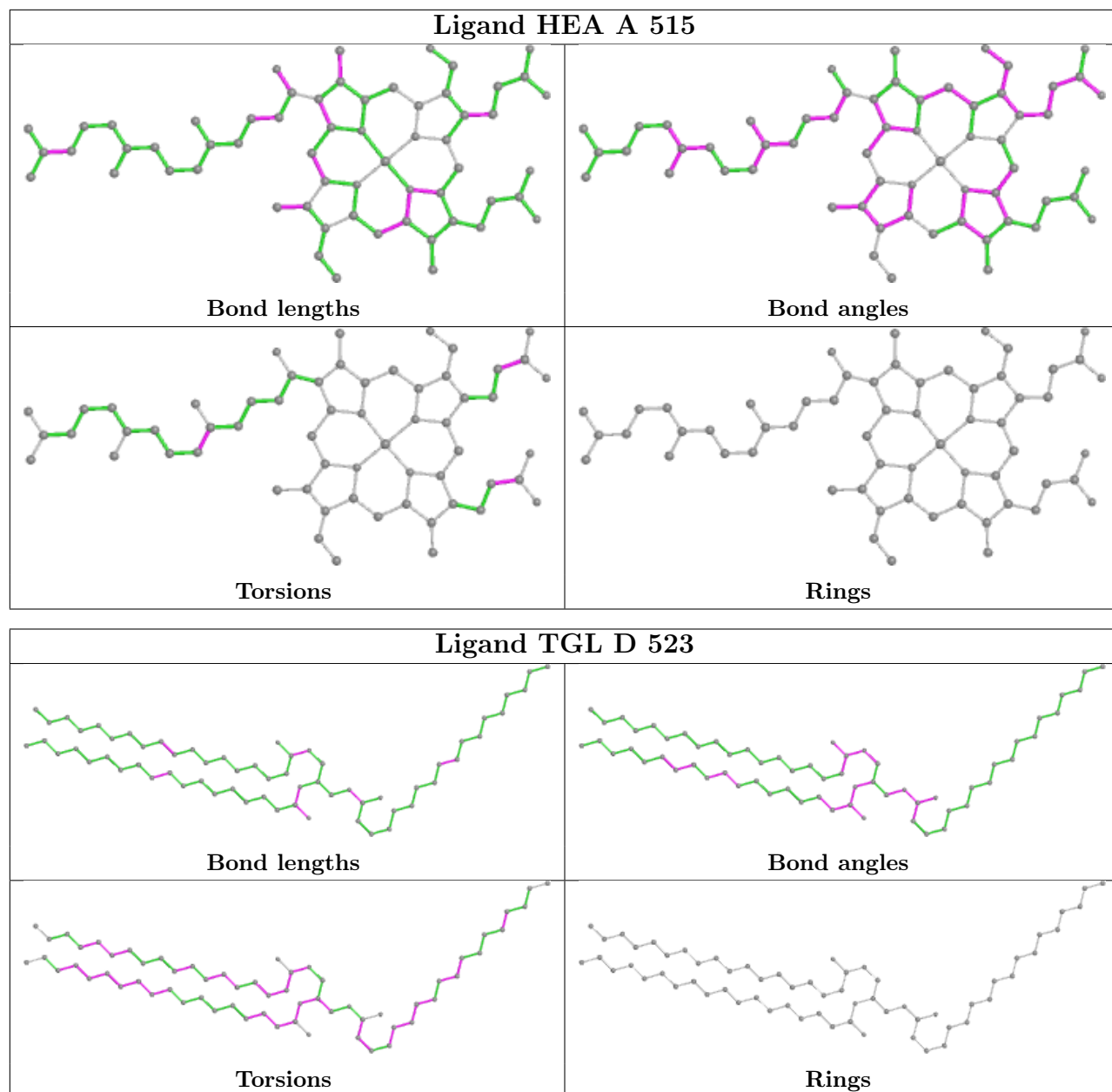


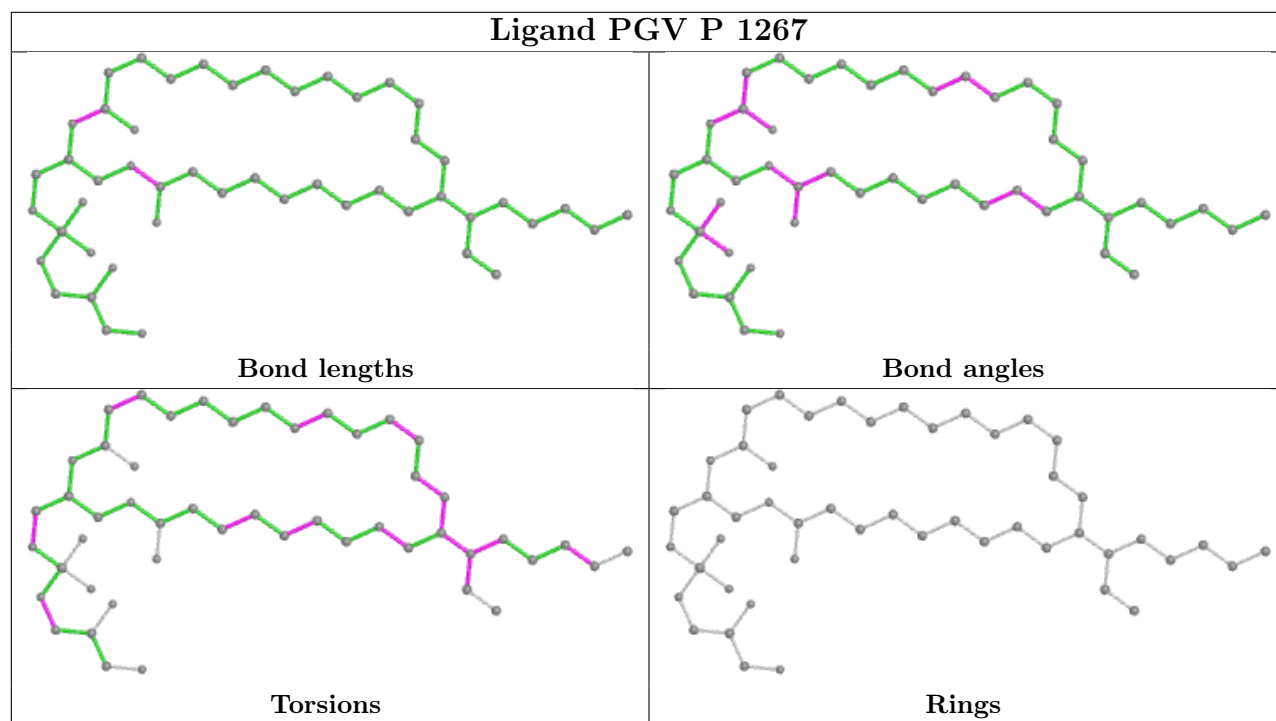
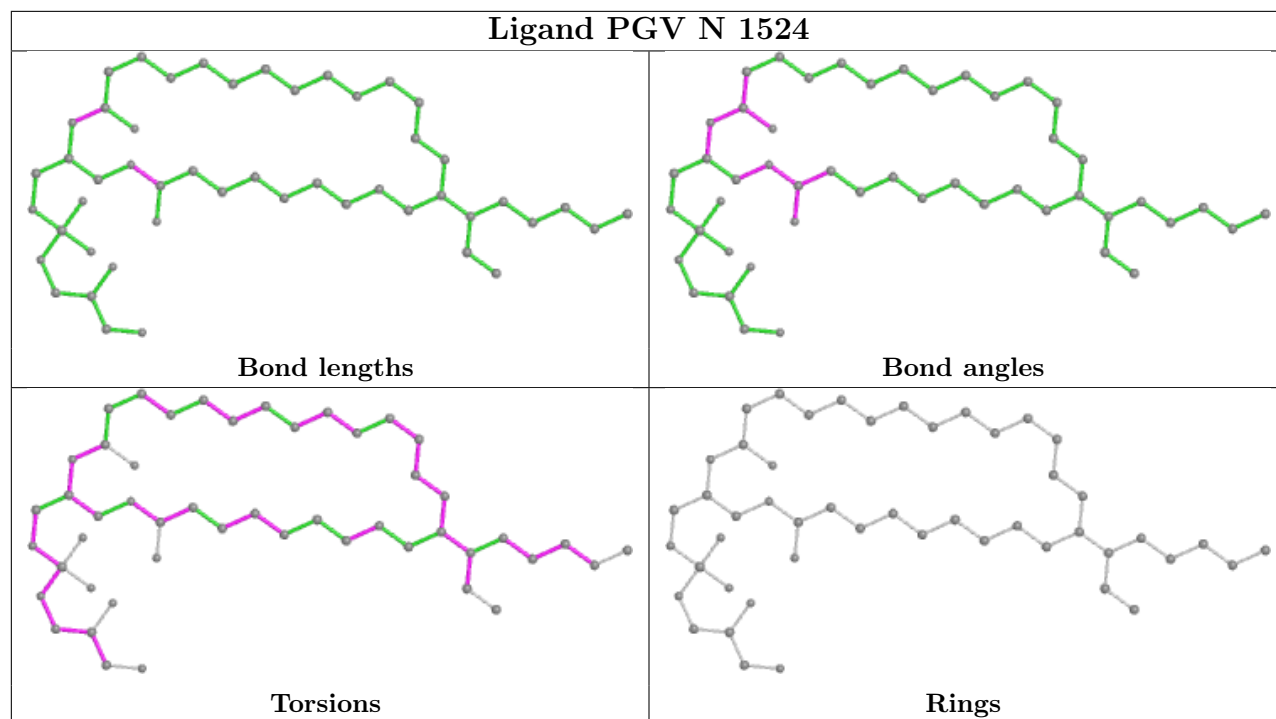


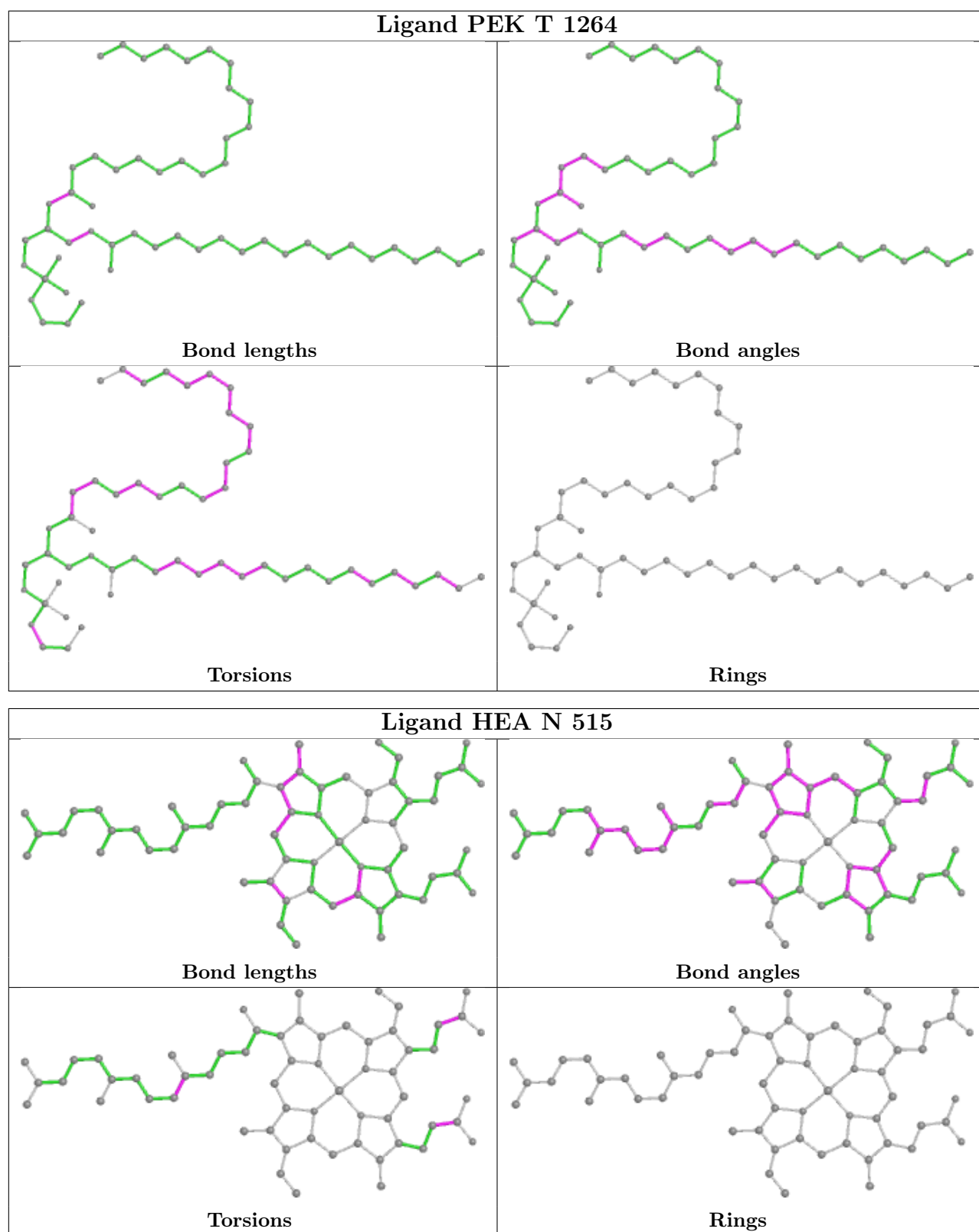




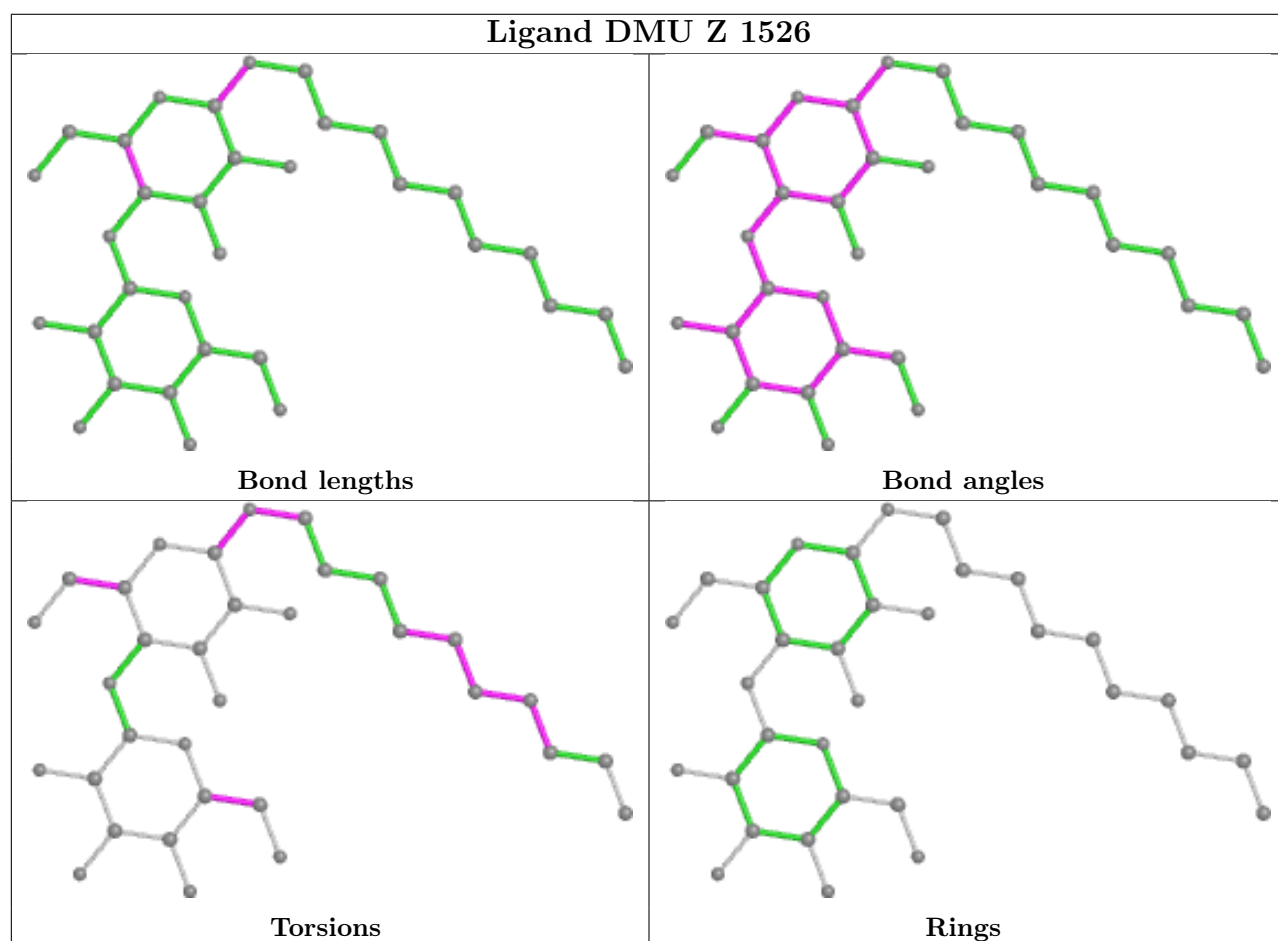
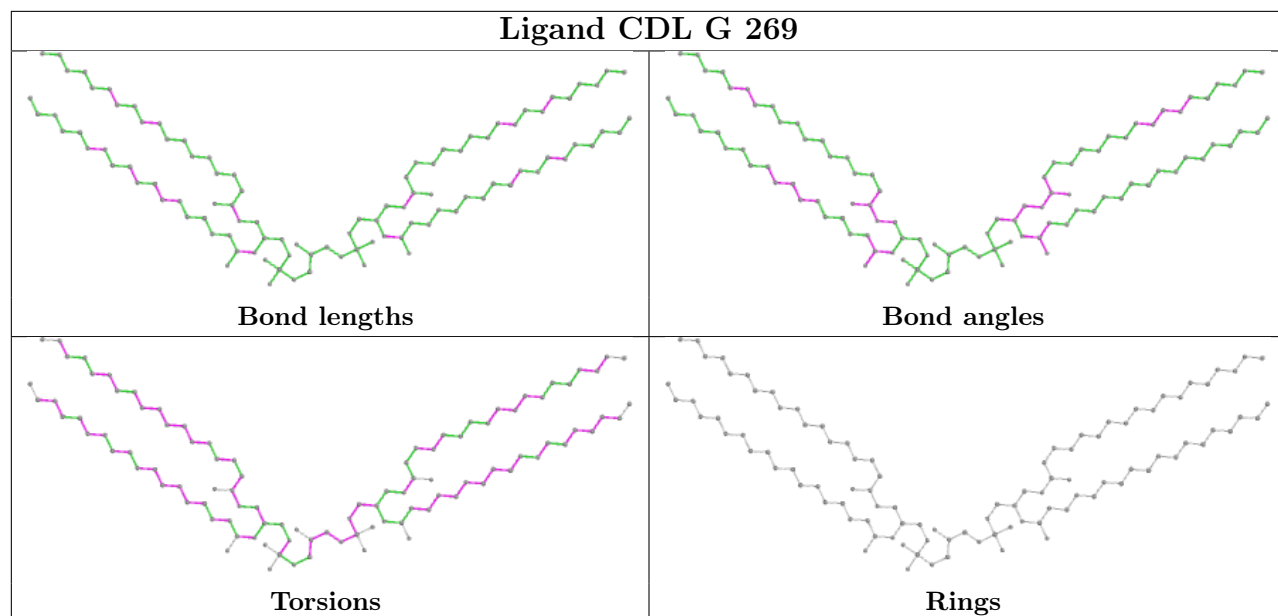


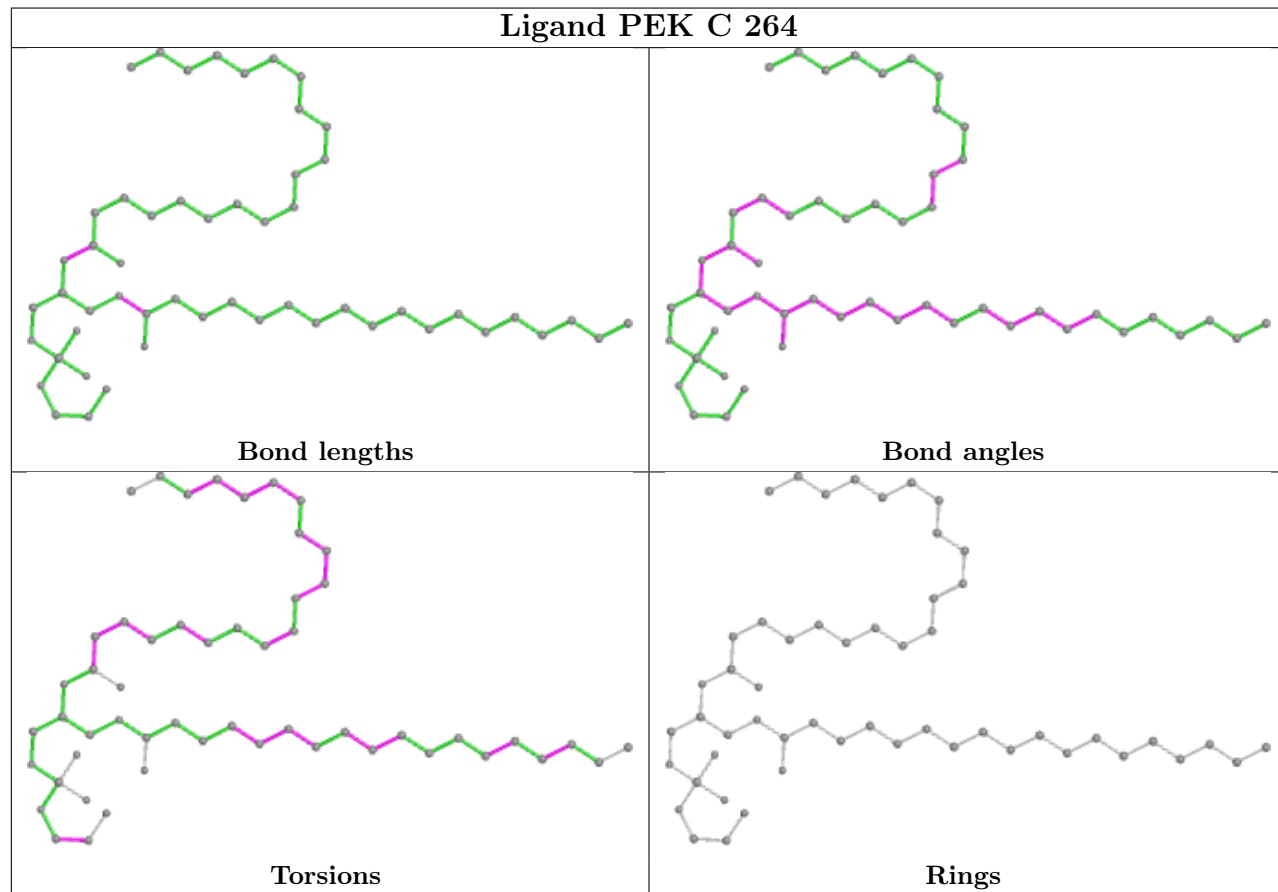
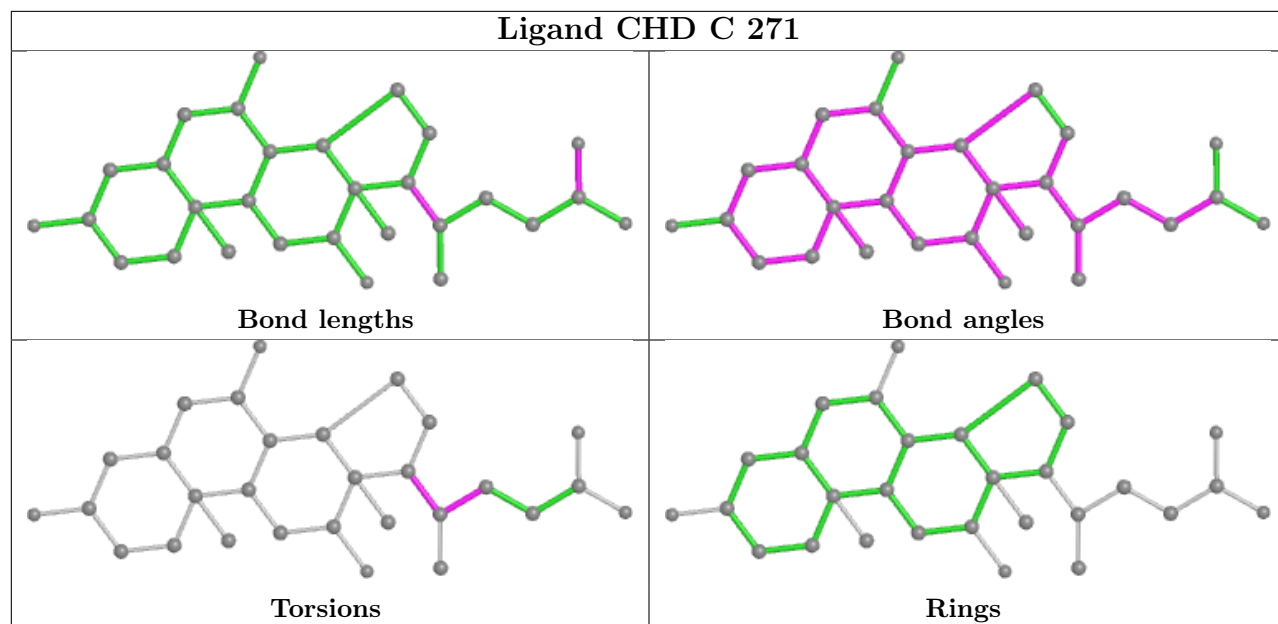


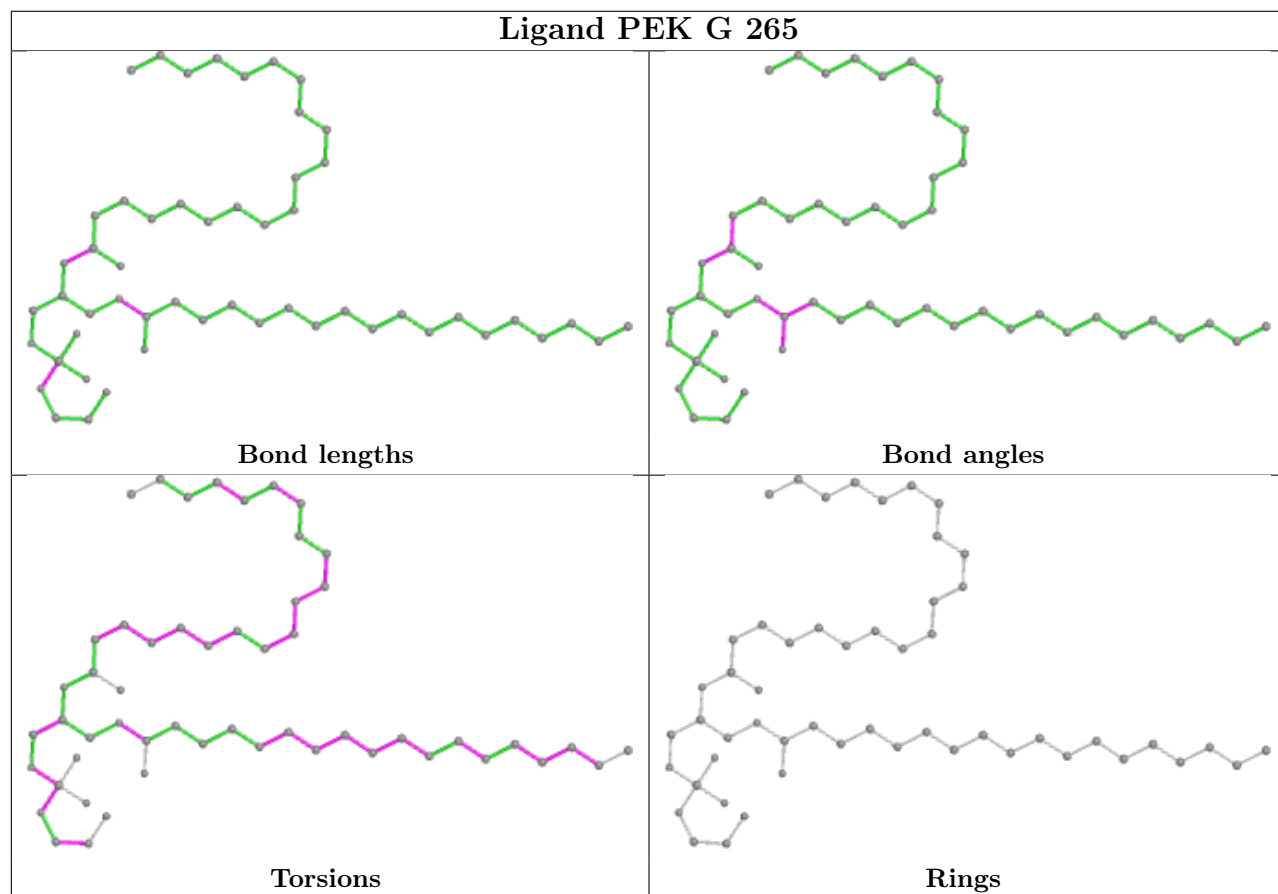
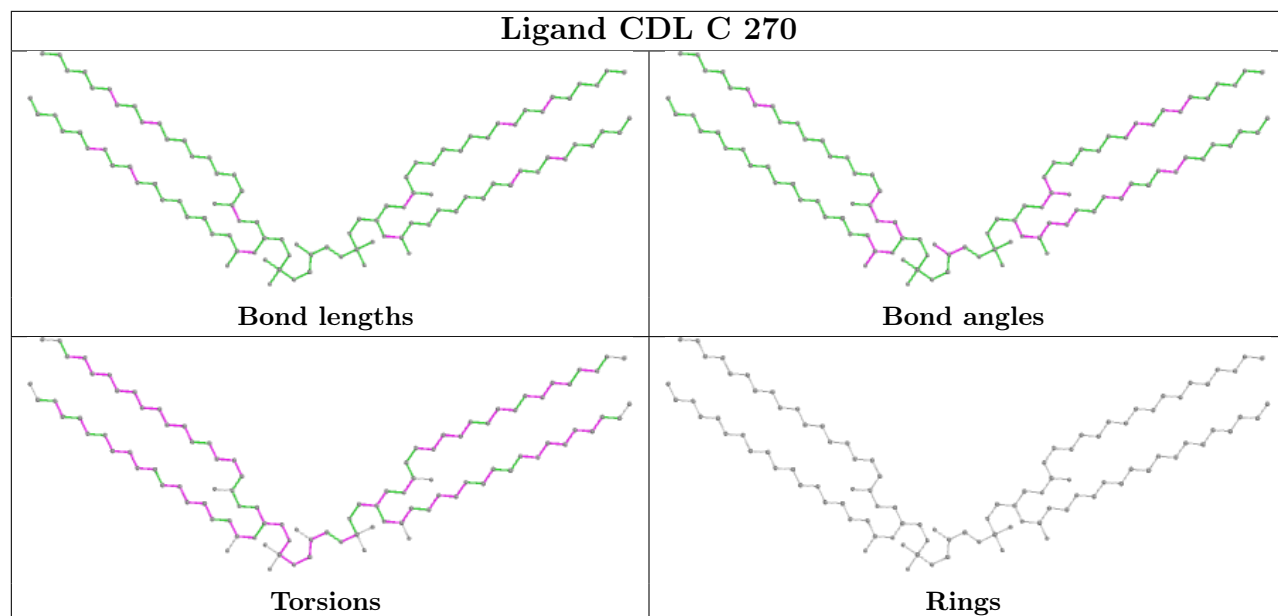


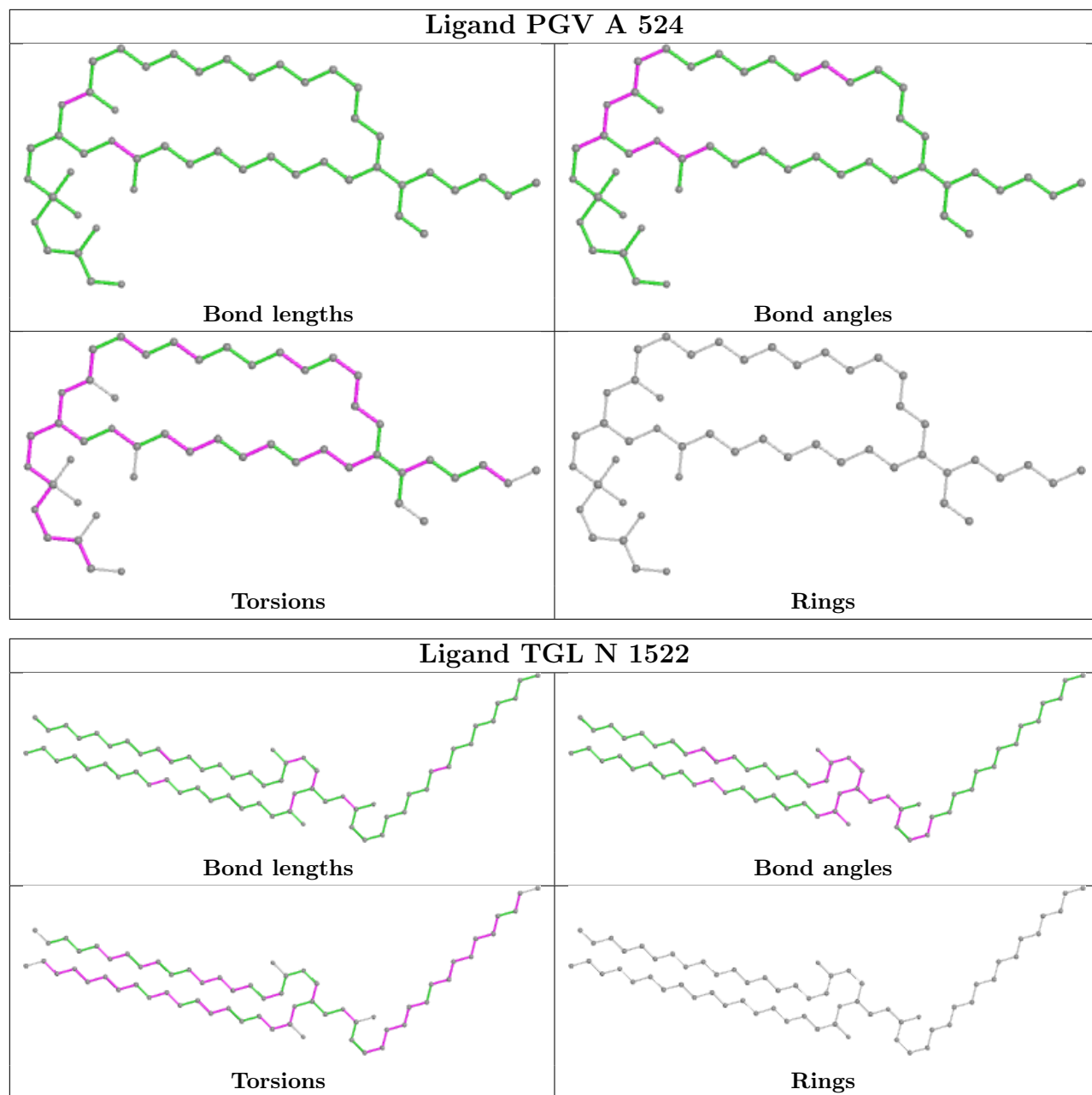


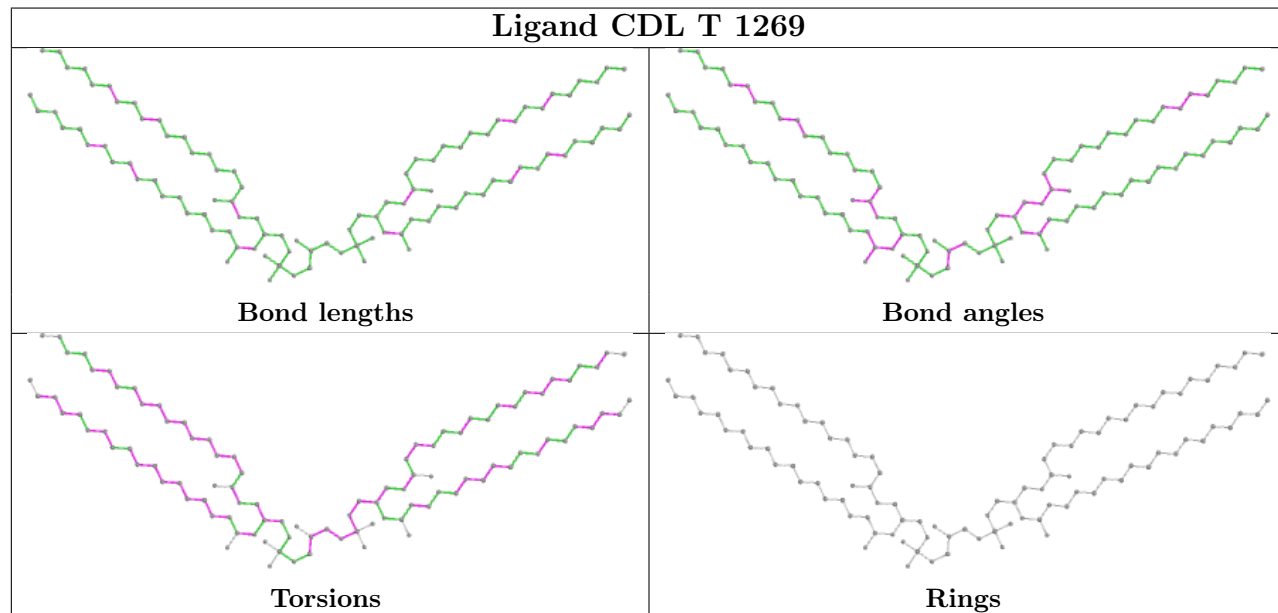
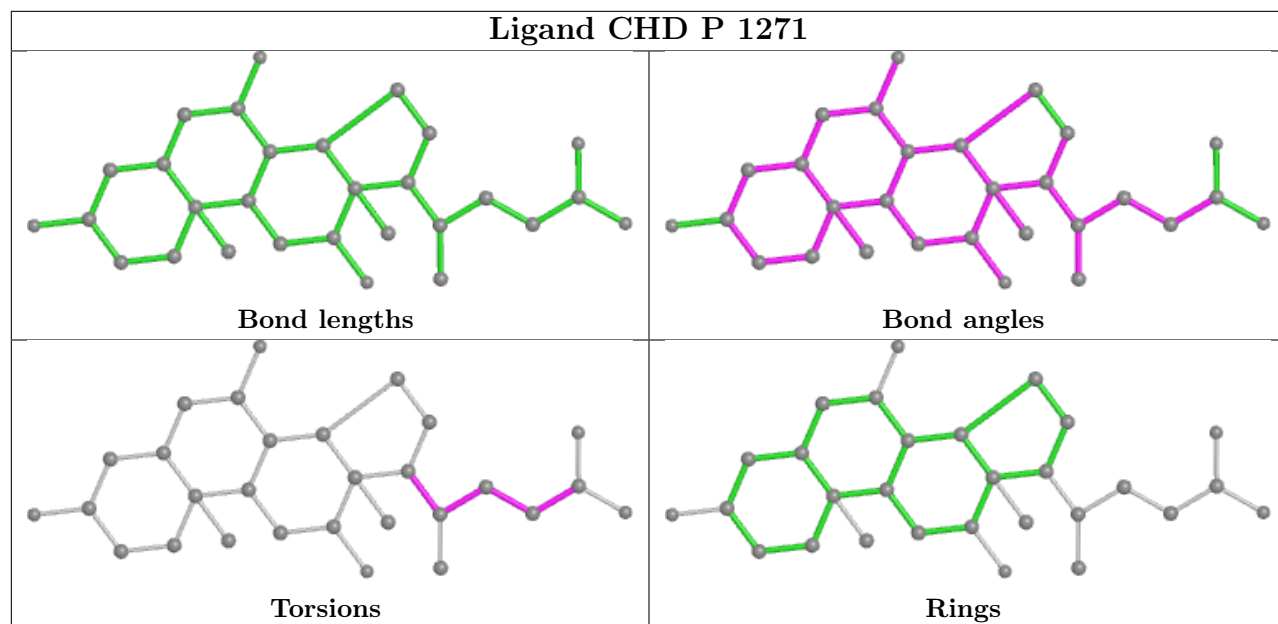


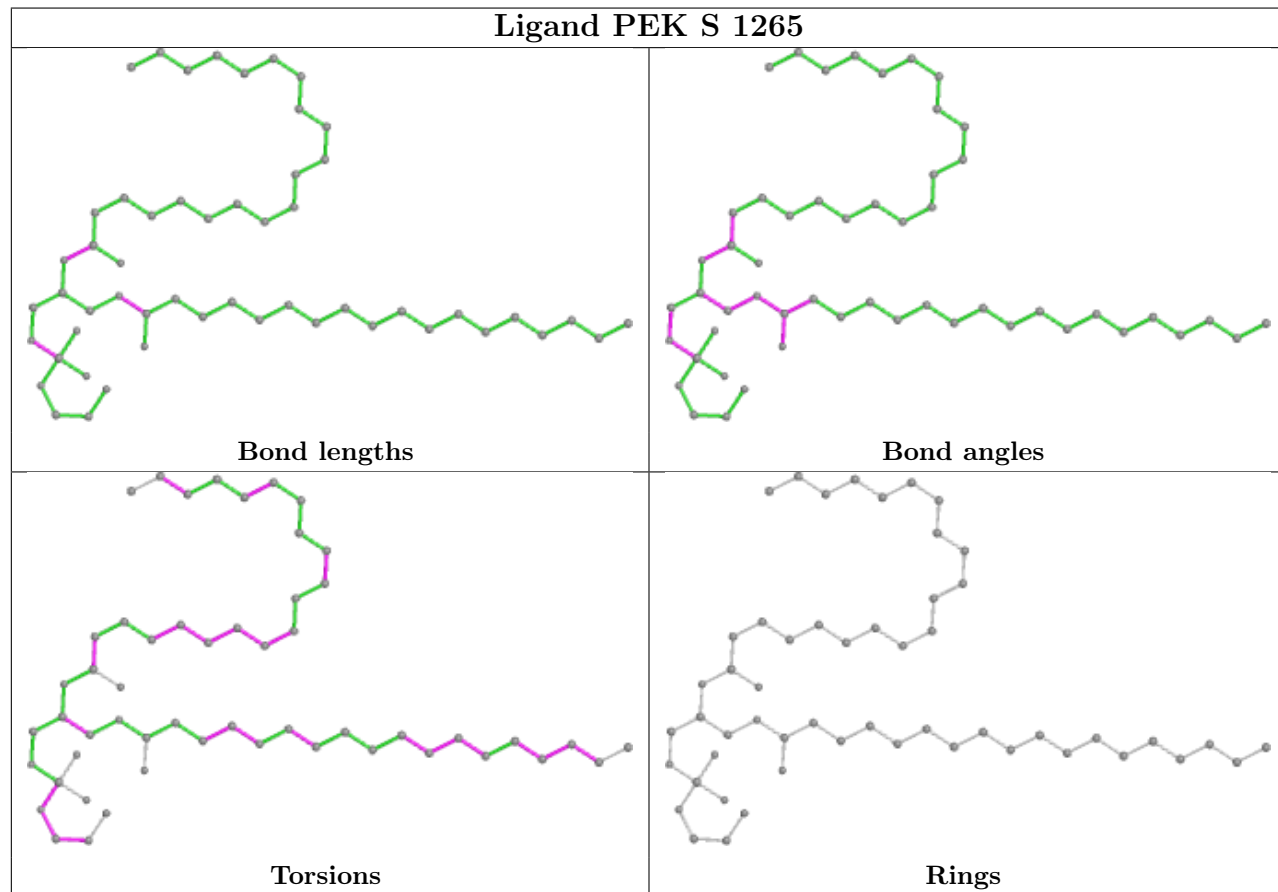
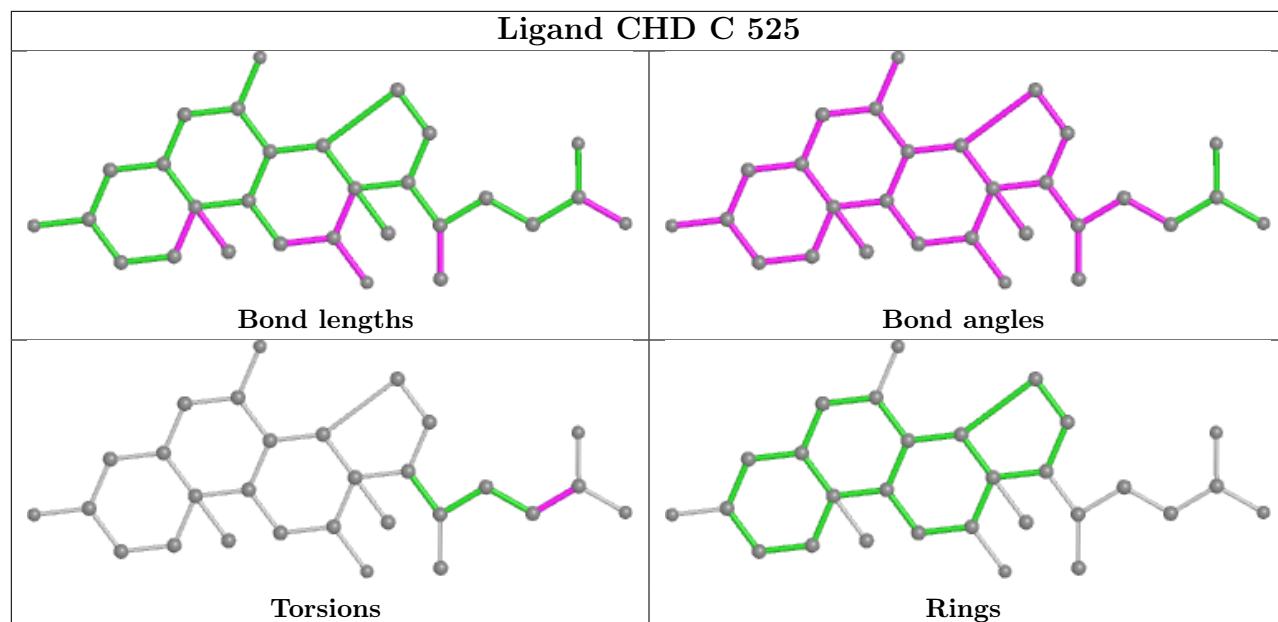


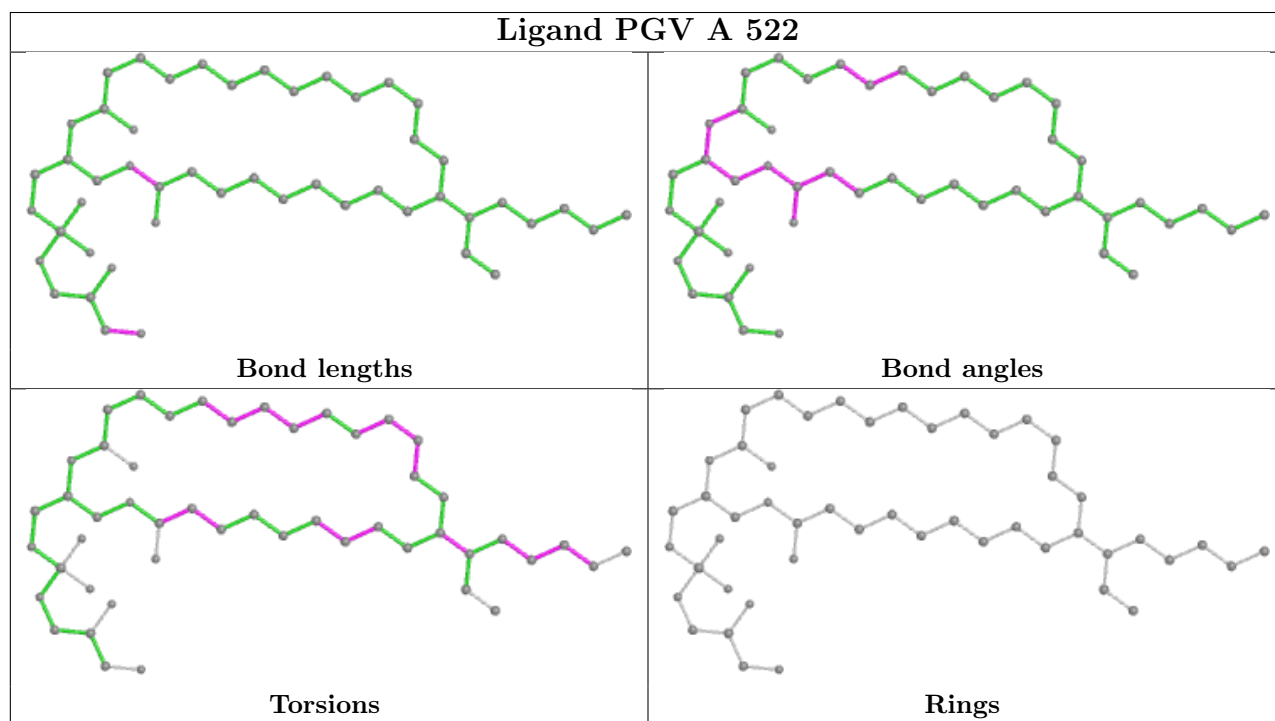
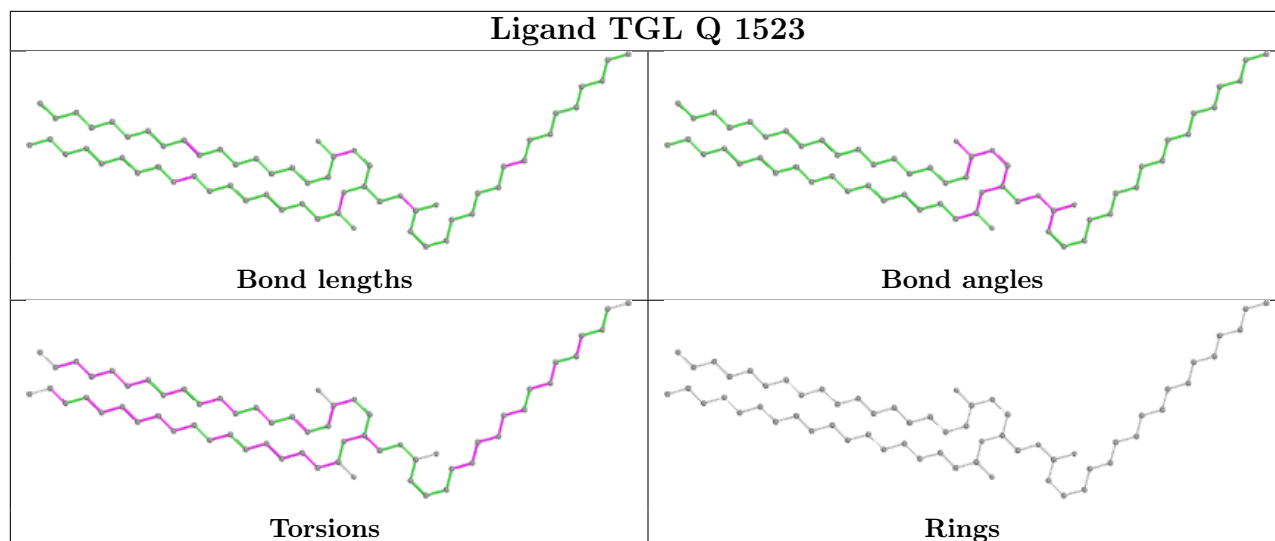


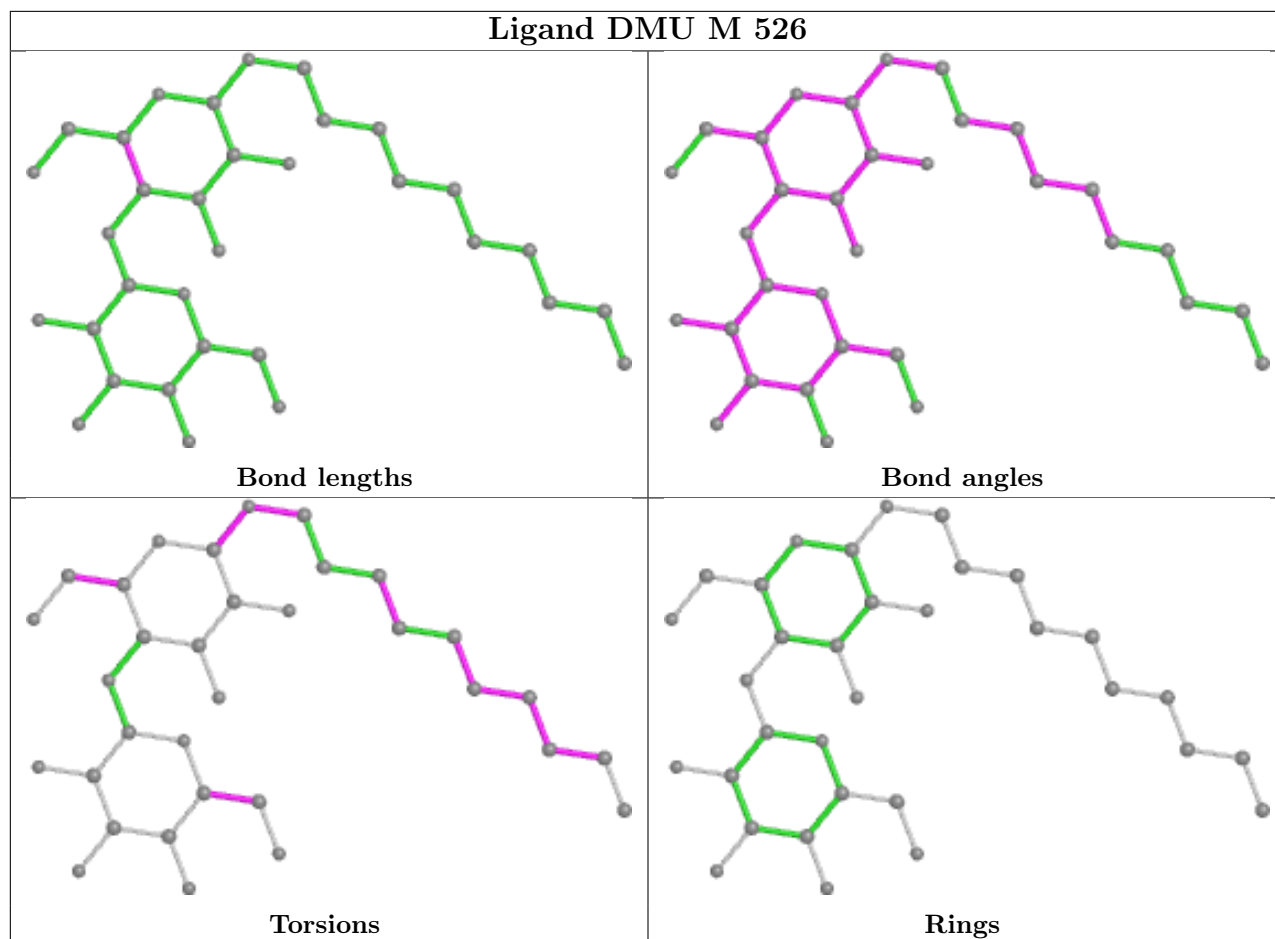




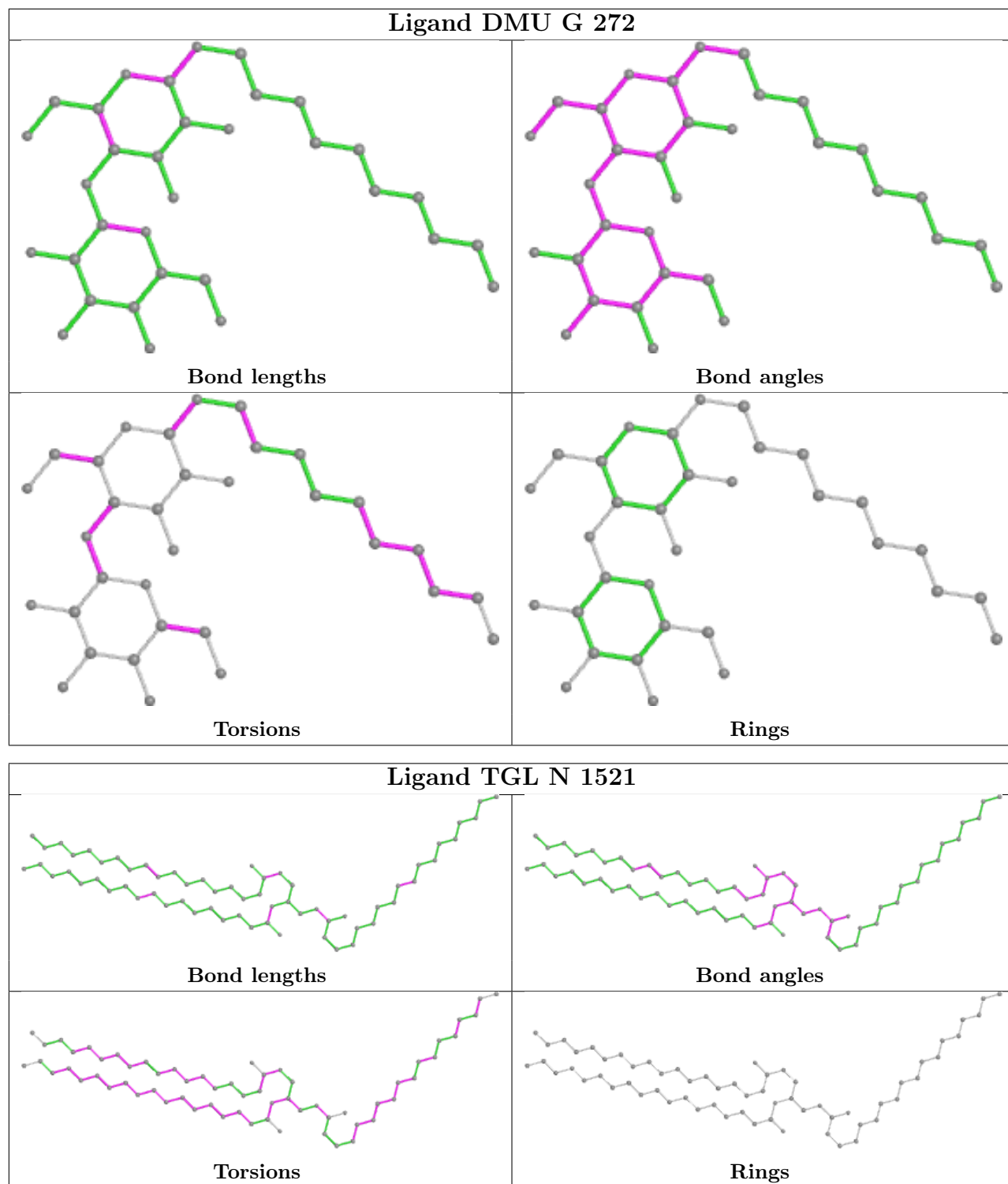


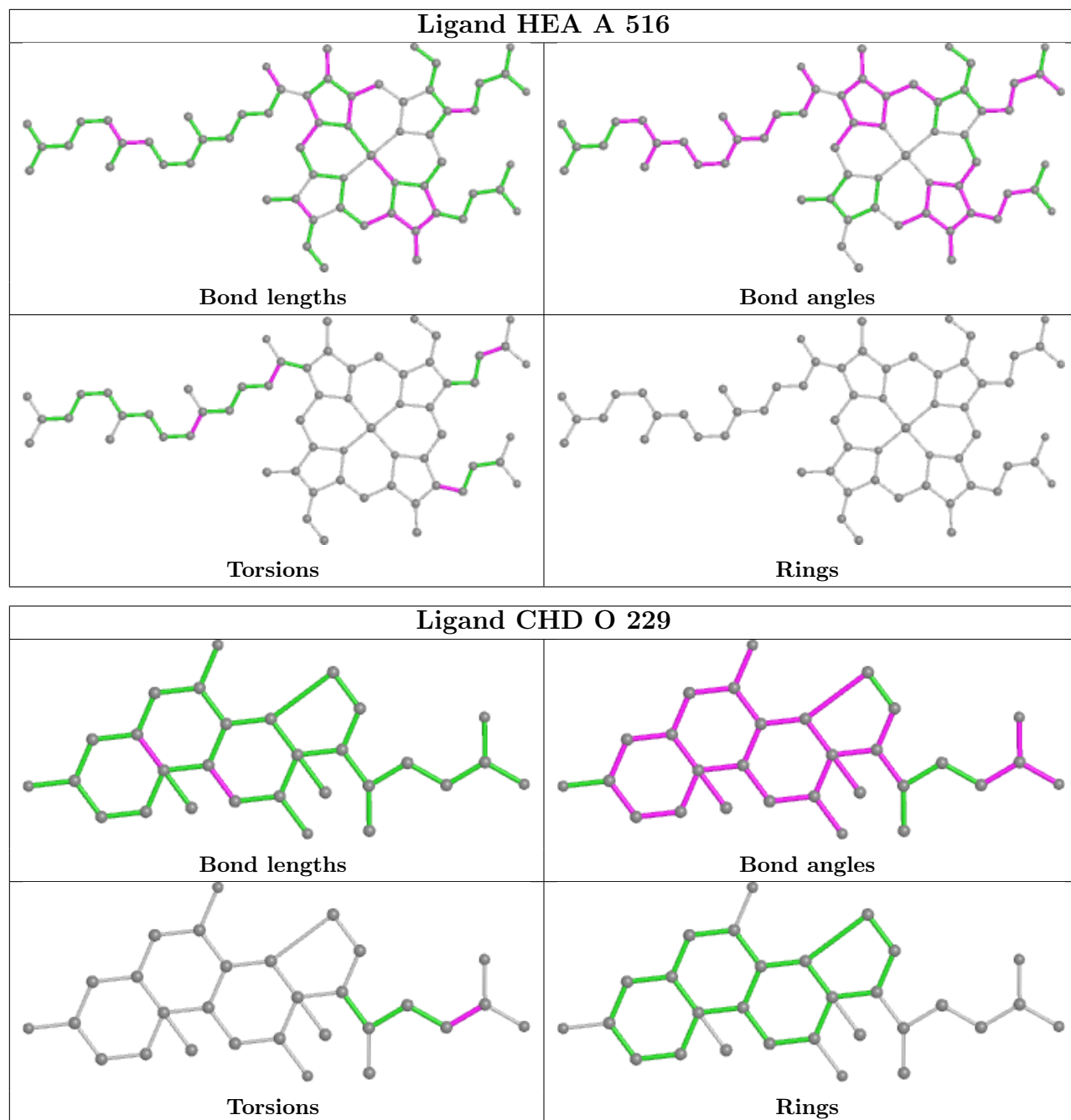


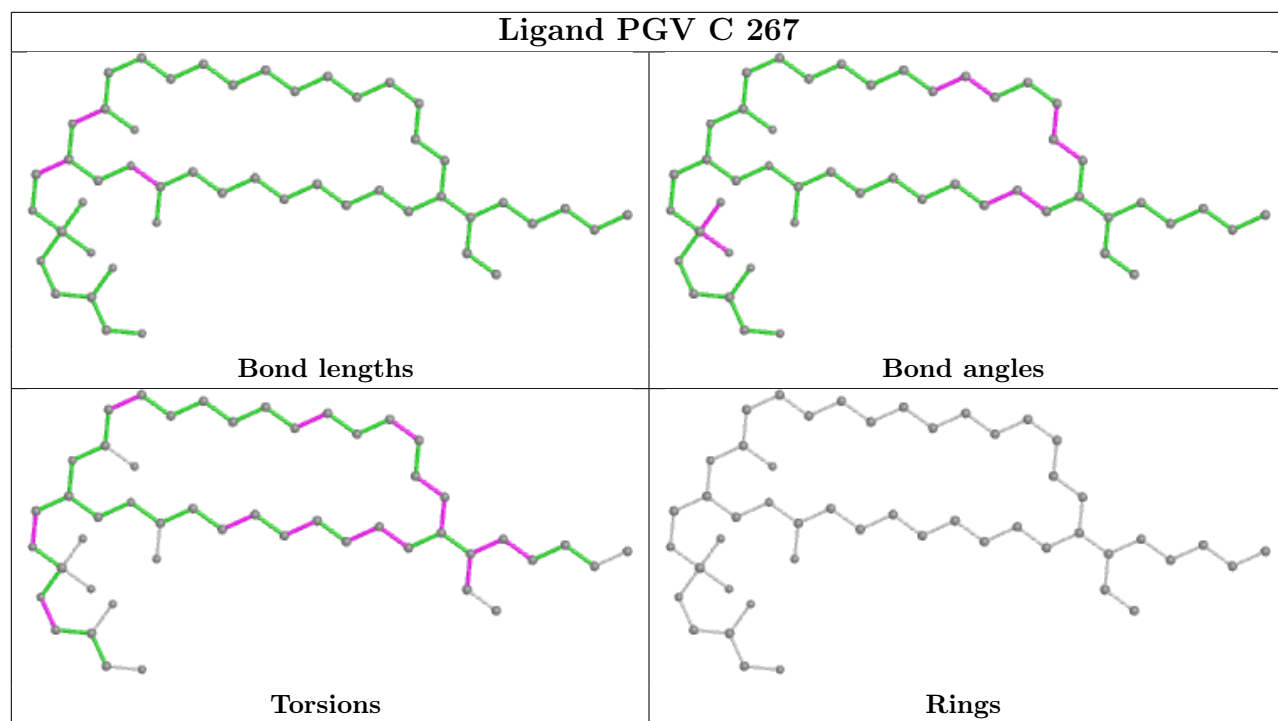
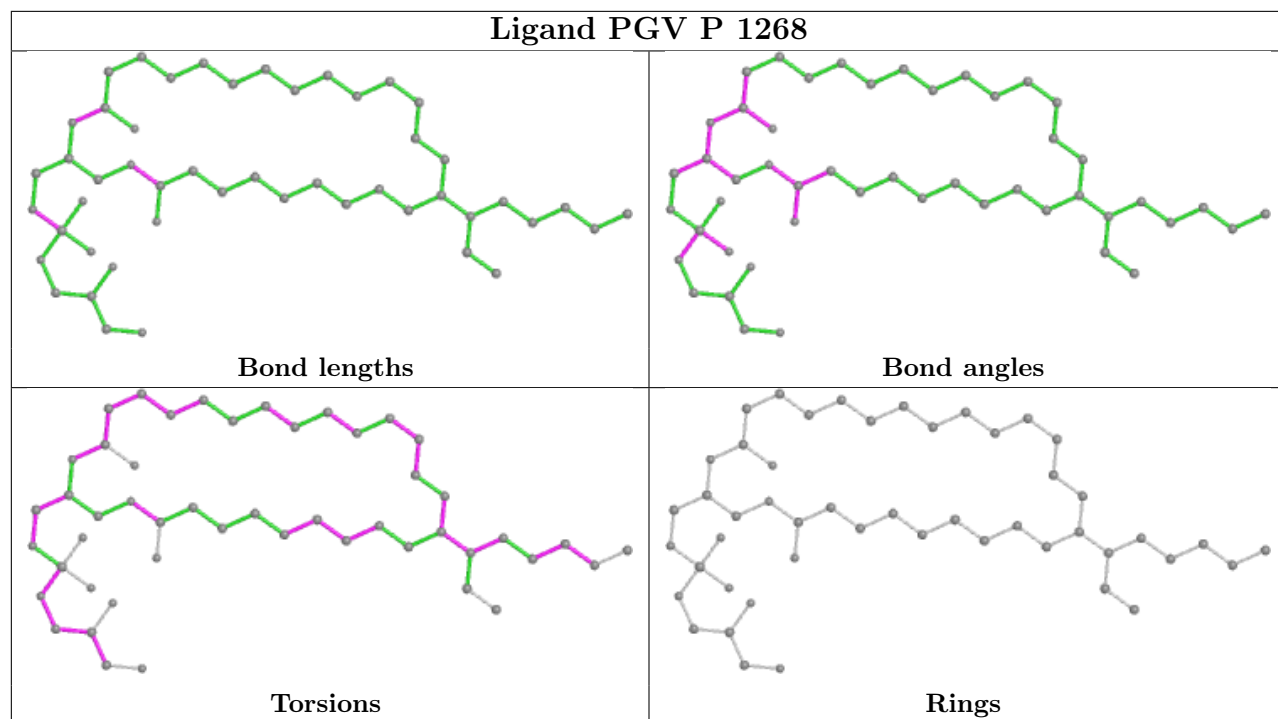


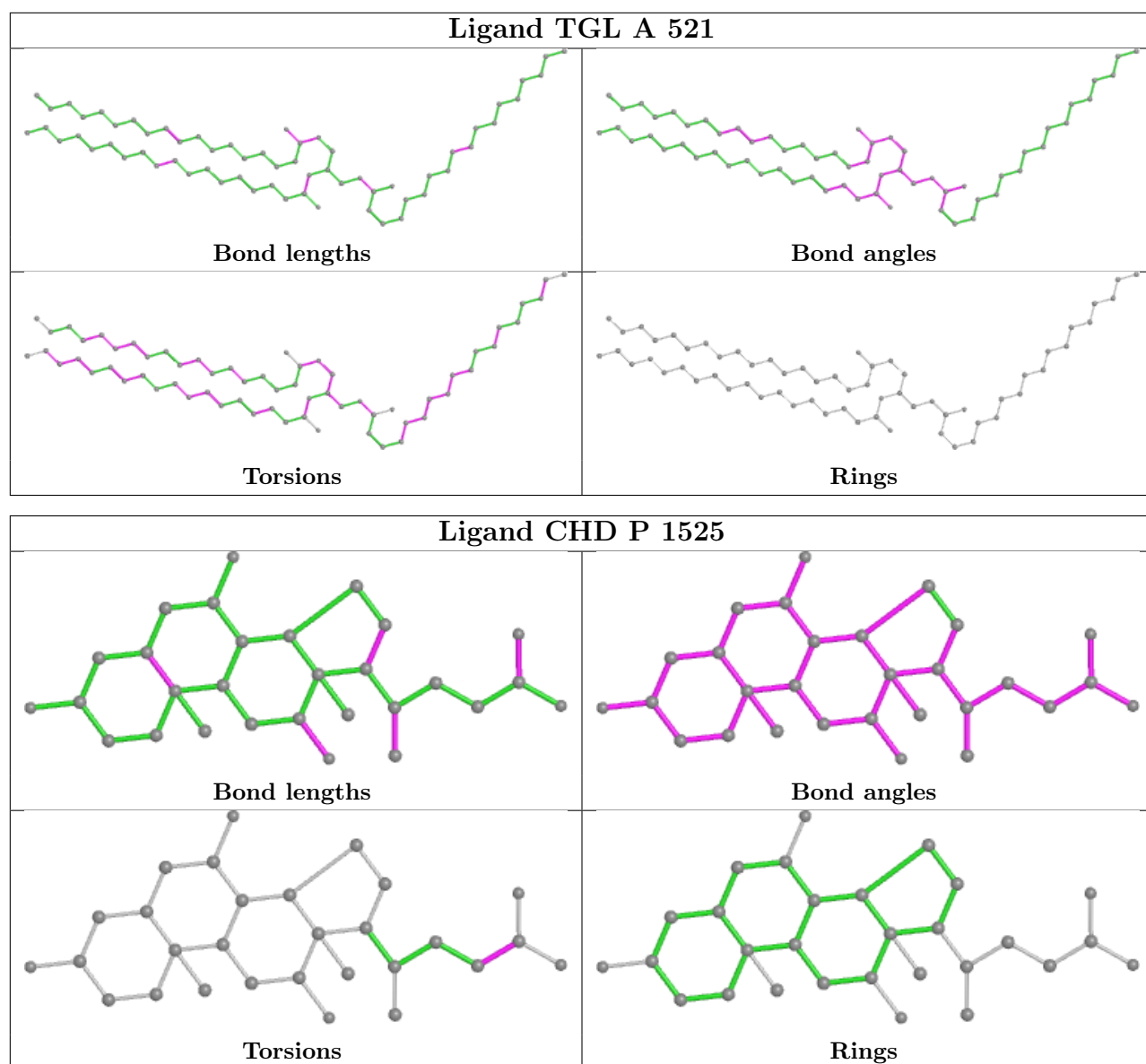












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data i

### 6.1 Protein, DNA and RNA chains i

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	513/514 (99%)	0.50	48 (9%) 8 9	23, 29, 40, 63	0
1	N	513/514 (99%)	0.29	29 (5%) 23 25	30, 36, 47, 68	0
2	B	226/227 (99%)	-0.33	3 (1%) 77 79	24, 35, 59, 78	0
2	O	226/227 (99%)	-0.07	5 (2%) 62 66	33, 45, 70, 88	0
3	C	259/261 (99%)	-0.43	1 (0%) 92 93	26, 32, 43, 62	0
3	P	259/261 (99%)	-0.44	3 (1%) 79 81	29, 36, 47, 67	0
4	D	144/147 (97%)	-0.44	1 (0%) 87 89	30, 37, 56, 70	0
4	Q	144/147 (97%)	1.22	28 (19%) 1 0	39, 52, 76, 118	0
5	E	105/109 (96%)	-0.03	2 (1%) 66 71	31, 38, 63, 99	0
5	R	105/109 (96%)	0.22	5 (4%) 30 33	36, 43, 68, 103	0
6	F	98/98 (100%)	0.34	8 (8%) 11 12	29, 39, 80, 127	0
6	S	98/98 (100%)	0.50	11 (11%) 5 5	34, 43, 86, 123	0
7	G	83/85 (97%)	0.70	15 (18%) 1 1	29, 39, 110, 113	0
7	T	83/85 (97%)	0.67	18 (21%) 0 0	29, 42, 102, 110	0
8	H	79/85 (92%)	0.32	12 (15%) 2 1	30, 41, 90, 112	0
8	U	79/85 (92%)	0.87	16 (20%) 1 0	37, 48, 94, 113	0
9	I	72/73 (98%)	0.21	6 (8%) 11 11	34, 46, 80, 83	0
9	V	72/73 (98%)	0.77	11 (15%) 2 1	39, 55, 82, 85	0
10	J	58/59 (98%)	0.21	8 (13%) 2 2	31, 41, 65, 96	0
10	W	58/59 (98%)	0.53	11 (18%) 1 0	34, 45, 69, 107	0
11	K	49/56 (87%)	-0.38	0 100 100	33, 41, 52, 62	0
11	X	49/56 (87%)	1.13	12 (24%) 0 0	44, 51, 64, 76	0
12	L	46/47 (97%)	-0.44	1 (2%) 62 66	29, 34, 50, 79	0
12	Y	46/47 (97%)	0.04	3 (6%) 18 20	34, 45, 61, 81	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	43/46 (93%)	-0.22	3 (6%) 16 18	30, 34, 71, 101	0
13	Z	43/46 (93%)	0.45	7 (16%) 1 1	41, 46, 90, 112	0
All	All	3550/3614 (98%)	0.18	267 (7%) 14 15	23, 38, 69, 127	0

The worst 5 of 267 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	6	VAL	30.7
6	S	97	ALA	13.6
4	Q	5	VAL	13.4
4	Q	4	SER	12.7
6	F	96	LEU	10.9

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
9	SAC	V	1	9/10	0.14	0.56	88,90,92,93	0
7	TPO	G	11	11/12	0.45	0.32	74,82,105,105	0
7	TPO	T	11	11/12	0.54	0.26	75,82,101,102	0
9	SAC	I	1	9/10	0.80	0.28	77,82,84,85	0
1	FME	N	1	10/11	0.87	0.23	50,54,74,77	0
1	FME	A	1	10/11	0.92	0.14	46,51,63,76	0
2	FME	O	1	10/11	0.95	0.14	41,42,49,55	0
2	FME	B	1	10/11	0.96	0.13	31,33,40,56	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
24	PEK	T	263	53/53	0.54	0.38	54,103,127,128	0
28	DMU	G	272	33/33	0.54	0.31	85,116,119,121	0
19	TGL	N	1522	63/63	0.55	0.33	54,76,92,95	0
24	PEK	G	265	53/53	0.55	0.27	51,91,109,114	0
28	DMU	P	1272	33/33	0.56	0.35	104,118,124,125	0
24	PEK	S	1265	53/53	0.59	0.30	50,87,111,114	0
23	UNX	C	262	1/1	0.64	0.58	49,49,49,49	0
25	CDL	G	269	100/100	0.64	0.34	72,99,122,124	0
25	CDL	T	1269	100/100	0.65	0.32	66,96,122,126	0
24	PEK	G	1263	53/53	0.66	0.37	59,107,131,132	0
26	PSC	R	1229	52/52	0.67	0.32	53,109,133,136	0
22	CHD	W	1059	29/29	0.67	0.47	107,115,119,120	0
20	PGV	P	1268	51/51	0.67	0.31	64,100,119,121	0
20	PGV	N	1524	51/51	0.68	0.33	54,81,117,119	0
25	CDL	P	1270	100/100	0.68	0.37	46,100,119,122	0
19	TGL	L	522	63/63	0.69	0.27	43,68,84,87	0
20	PGV	C	268	51/51	0.69	0.29	60,91,117,117	0
22	CHD	J	60	29/29	0.72	0.28	105,109,113,114	0
19	TGL	Q	1523	63/63	0.72	0.22	67,83,98,100	0
26	PSC	E	229	52/52	0.72	0.33	53,106,131,133	0
25	CDL	C	270	100/100	0.75	0.31	49,96,120,122	0
20	PGV	A	524	51/51	0.75	0.28	45,75,117,118	0
19	TGL	N	1521	63/63	0.76	0.23	71,92,105,109	0
19	TGL	D	523	63/63	0.77	0.22	48,70,93,94	0
28	DMU	Z	1526	33/33	0.78	0.26	44,59,75,75	0
23	UNX	P	262	1/1	0.80	0.60	49,49,49,49	0
19	TGL	A	521	63/63	0.81	0.21	49,82,106,110	0
22	CHD	C	271	29/29	0.85	0.31	72,84,87,90	0
15	CYN	N	520	2/2	0.88	0.15	42,42,42,43	0
28	DMU	M	526	33/33	0.89	0.16	36,51,69,71	0
22	CHD	P	1271	29/29	0.91	0.22	68,86,90,91	0
17	MG	N	518	1/1	0.92	0.12	33,33,33,33	0
18	NA	N	519	1/1	0.92	0.06	40,40,40,40	0
22	CHD	P	1525	29/29	0.94	0.11	28,38,43,51	0
24	PEK	T	1264	53/53	0.94	0.15	30,54,83,85	0
22	CHD	O	229	29/29	0.95	0.08	27,34,42,45	0
22	CHD	B	1085	29/29	0.95	0.09	29,34,40,50	0
24	PEK	C	264	53/53	0.95	0.13	27,50,76,79	0
14	HEA	N	516	60/60	0.96	0.19	32,40,54,57	0
20	PGV	C	267	51/51	0.96	0.13	23,36,72,75	0
22	CHD	C	525	29/29	0.96	0.11	25,35,39,46	0
14	HEA	A	516	60/60	0.97	0.17	23,35,51,52	0

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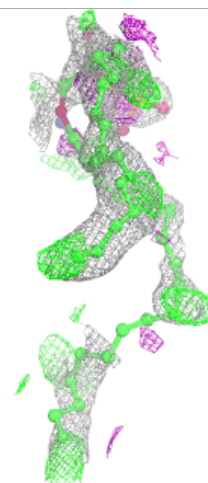
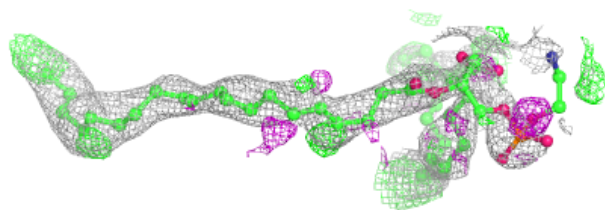
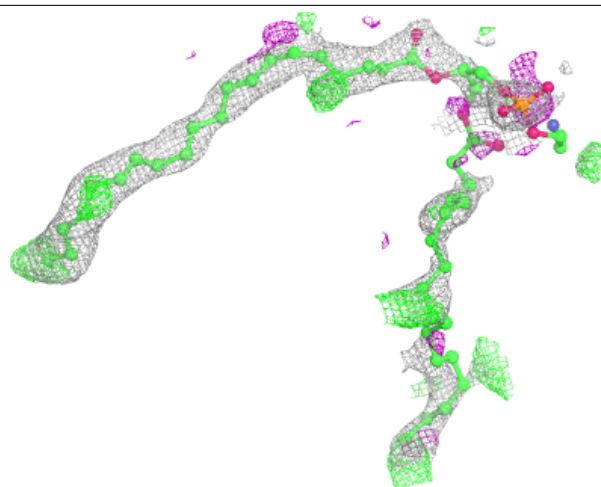
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
20	PGV	N	1266	51/51	0.97	0.15	28,43,70,75	0
20	PGV	P	1267	51/51	0.97	0.13	29,40,77,85	0
20	PGV	A	522	51/51	0.97	0.17	25,36,68,72	0
18	NA	A	519	1/1	0.97	0.09	30,30,30,30	0
14	HEA	N	515	60/60	0.97	0.20	30,36,50,52	0
14	HEA	A	515	60/60	0.98	0.20	18,27,40,45	0
21	CUA	O	228	2/2	0.98	0.09	36,36,36,37	0
17	MG	A	518	1/1	0.98	0.17	25,25,25,25	0
15	CYN	A	520	2/2	0.98	0.13	31,31,31,31	0
21	CUA	B	228	2/2	0.99	0.14	28,28,28,28	0
16	CU	N	517	1/1	0.99	0.16	37,37,37,37	0
27	ZN	F	99	1/1	0.99	0.07	35,35,35,35	0
27	ZN	S	99	1/1	0.99	0.07	38,38,38,38	0
16	CU	A	517	1/1	1.00	0.17	31,31,31,31	0

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



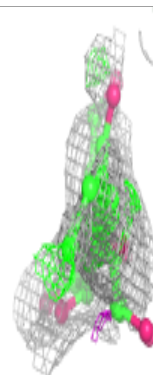
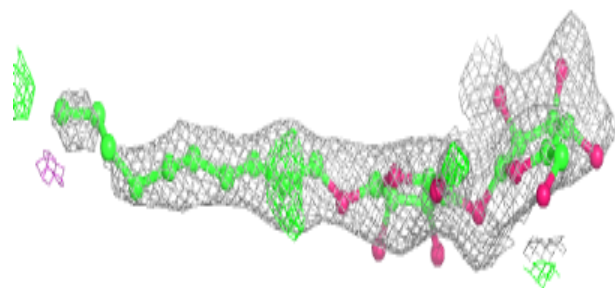
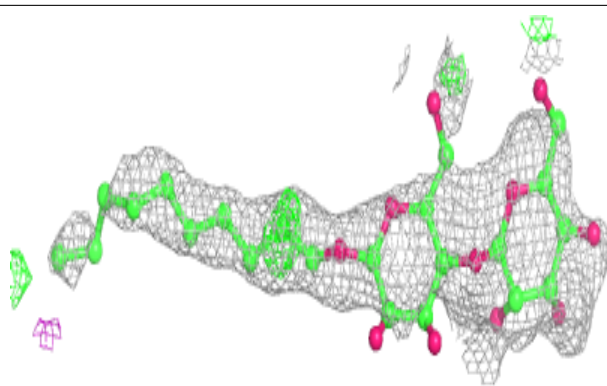
**Electron density around PEK T 263:**

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

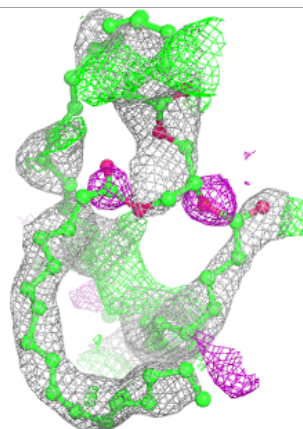
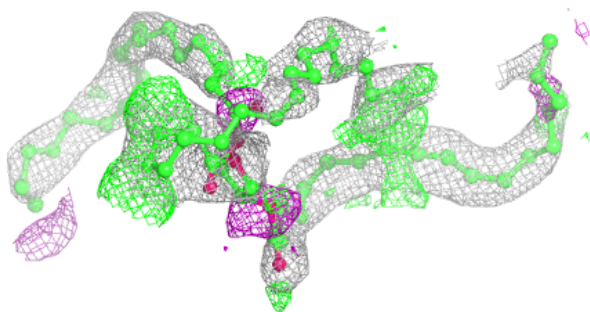
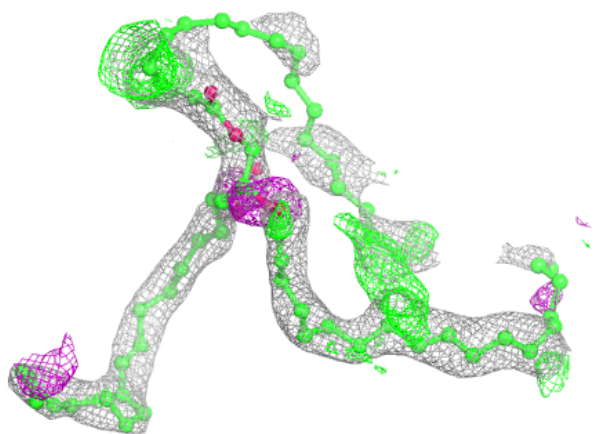


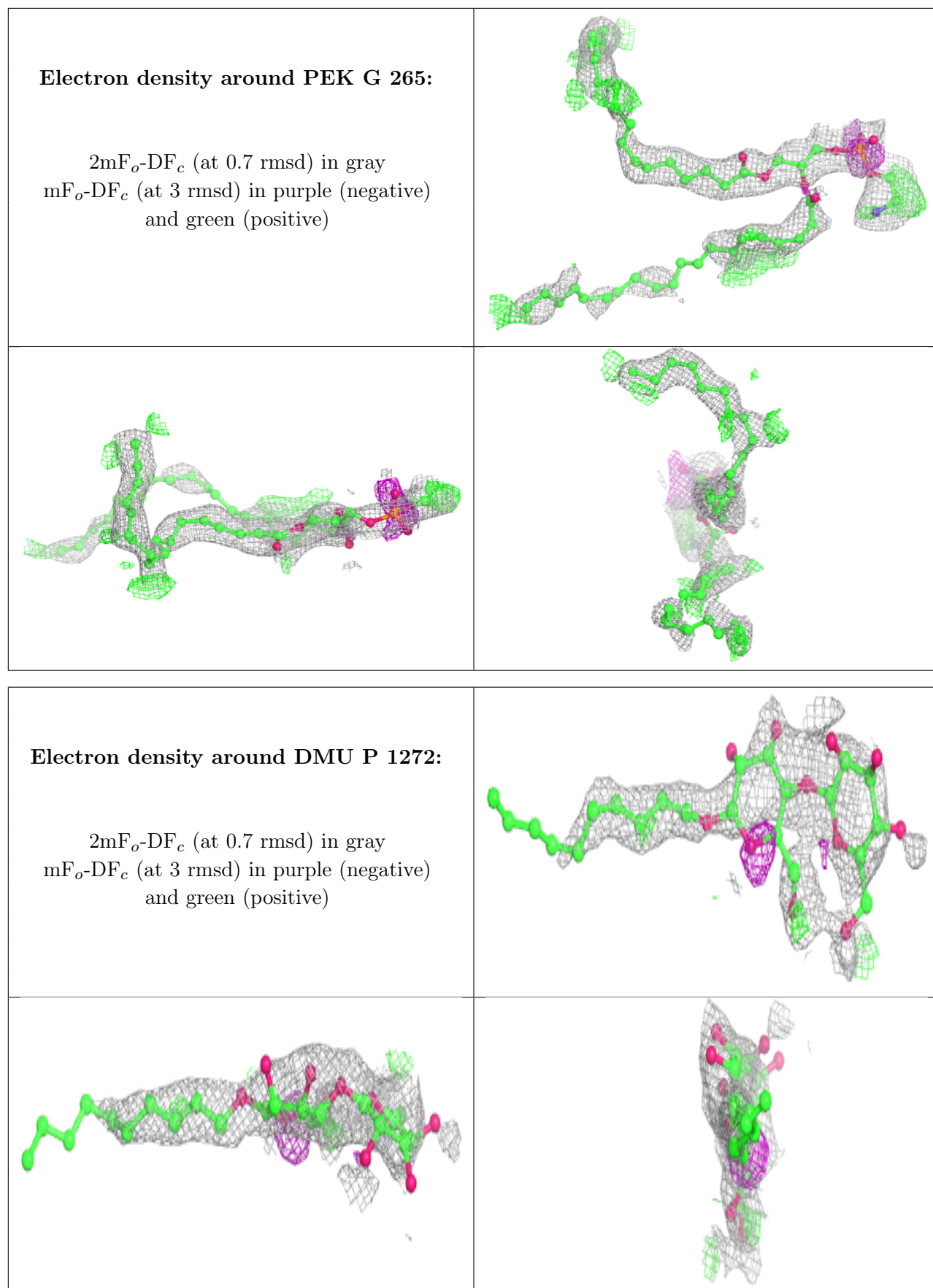
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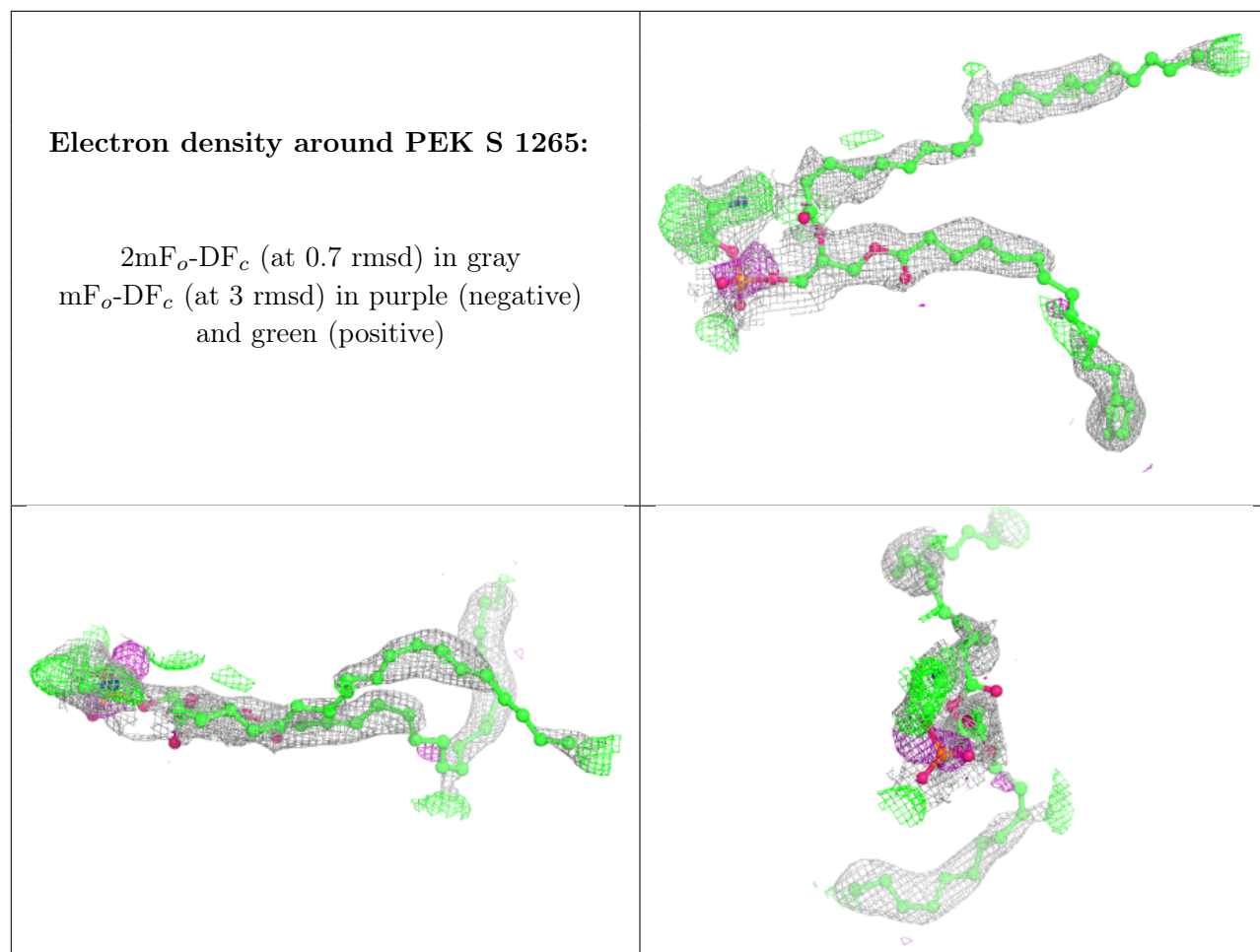
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

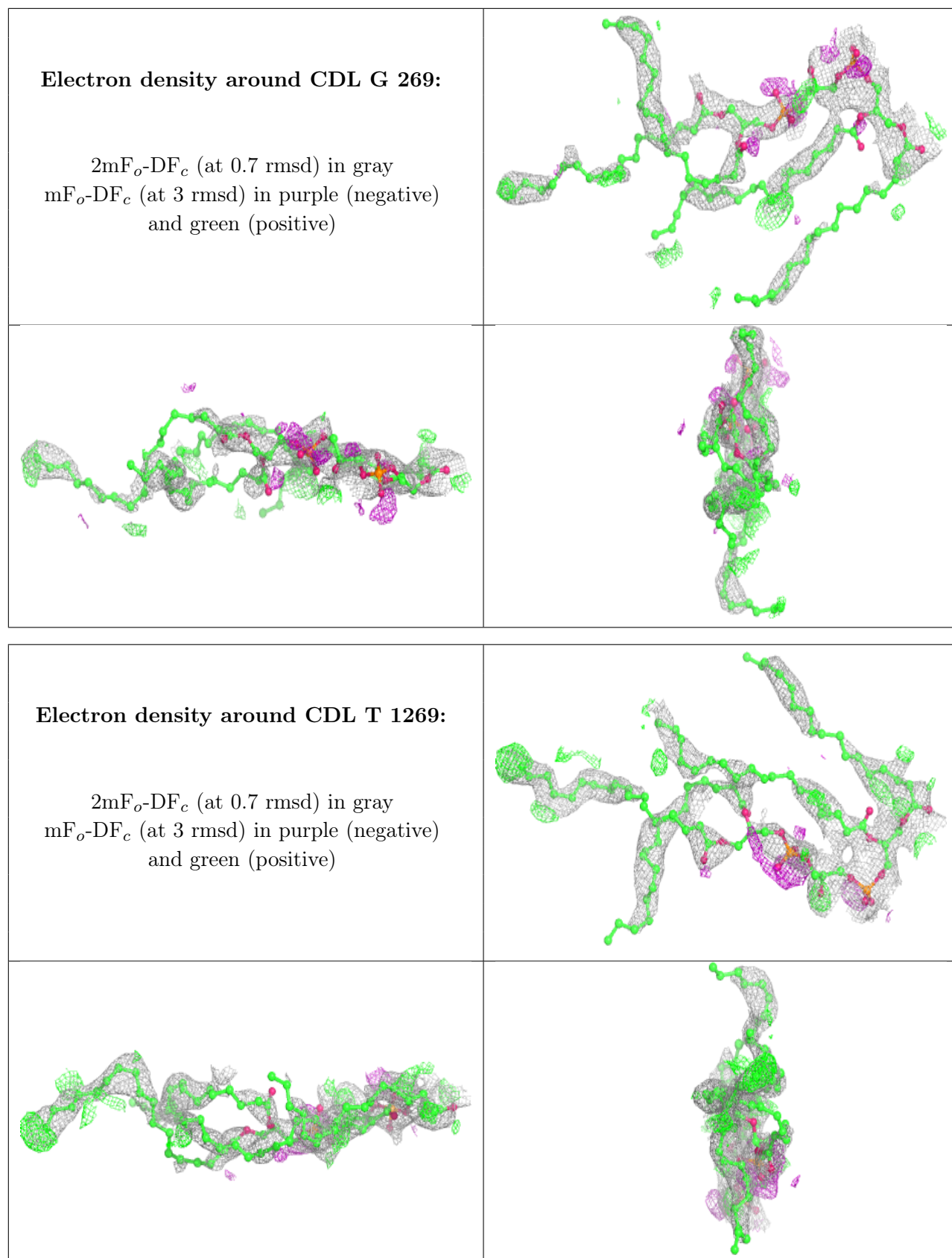
**Electron density around TGL N 1522:**

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



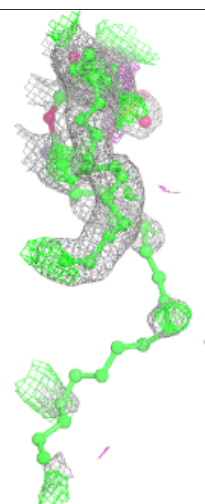
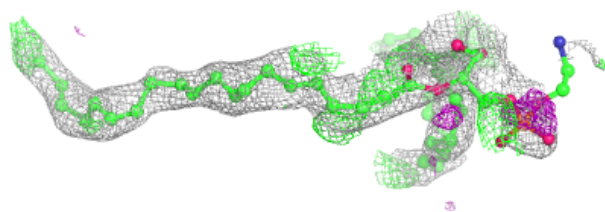
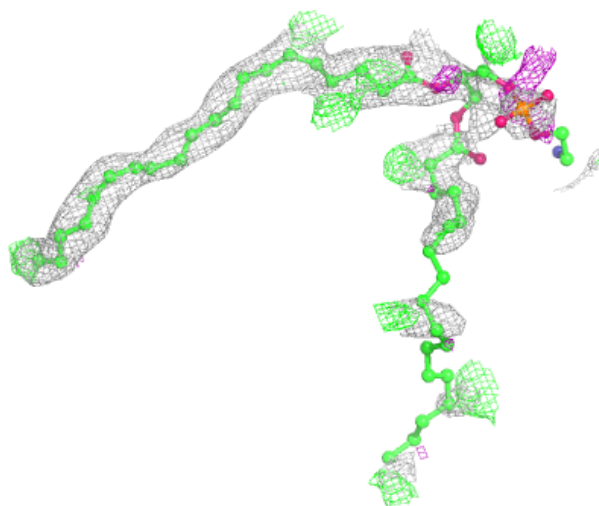






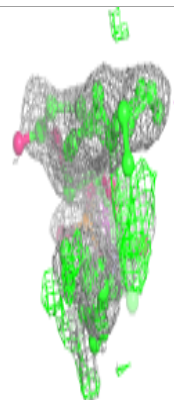
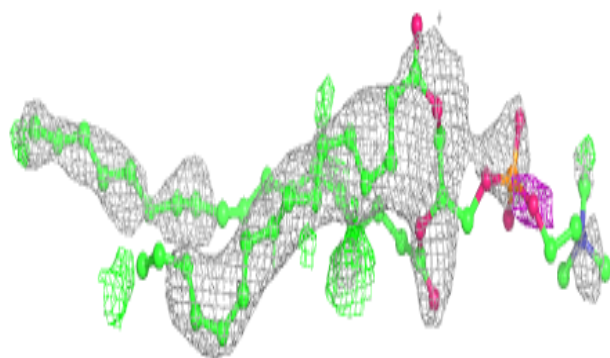
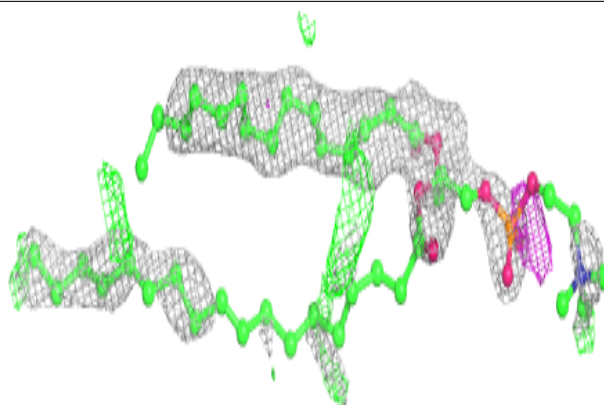
**Electron density around PEK G 1263:**

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and green (positive)

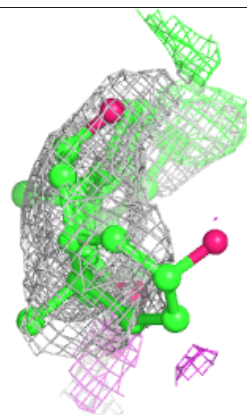
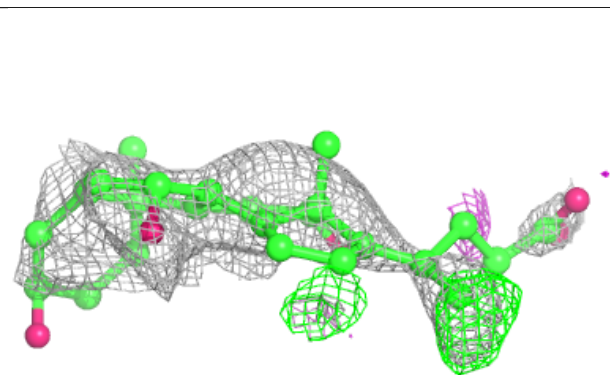
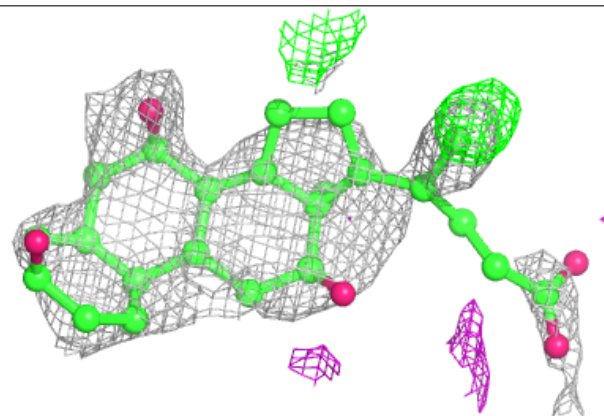


**Electron density around PSC R 1229:**

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

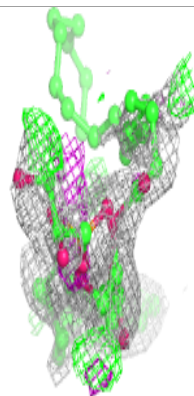
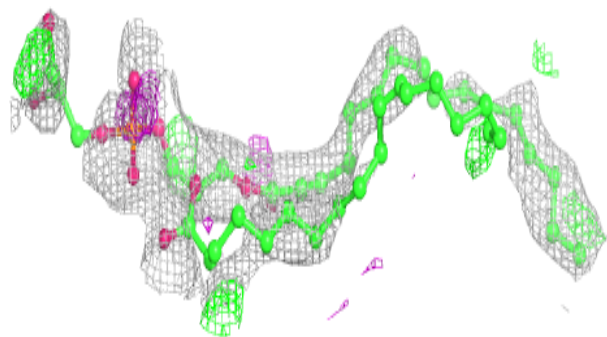
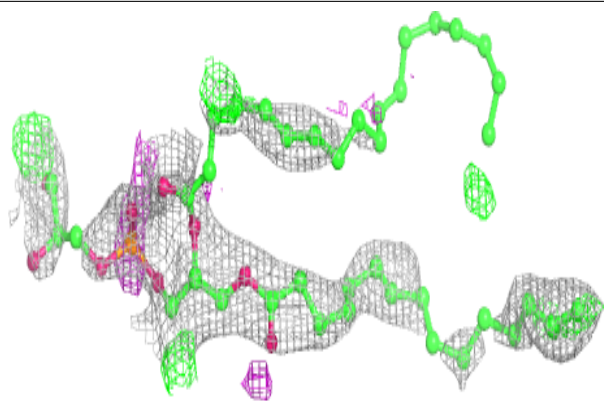
**Electron density around CHD W 1059:**

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

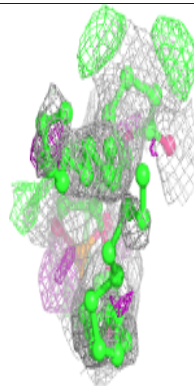
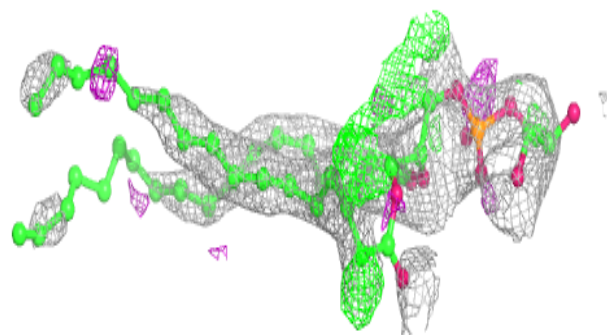
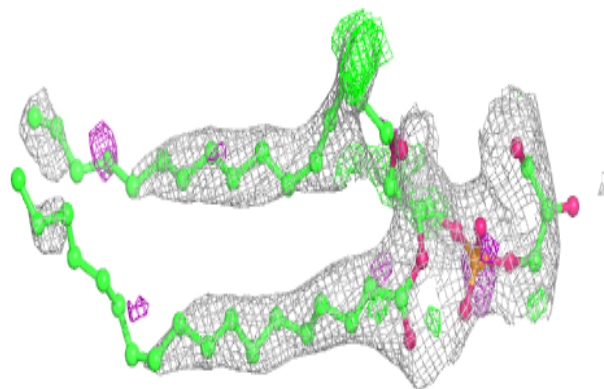


**Electron density around PGV P 1268:**

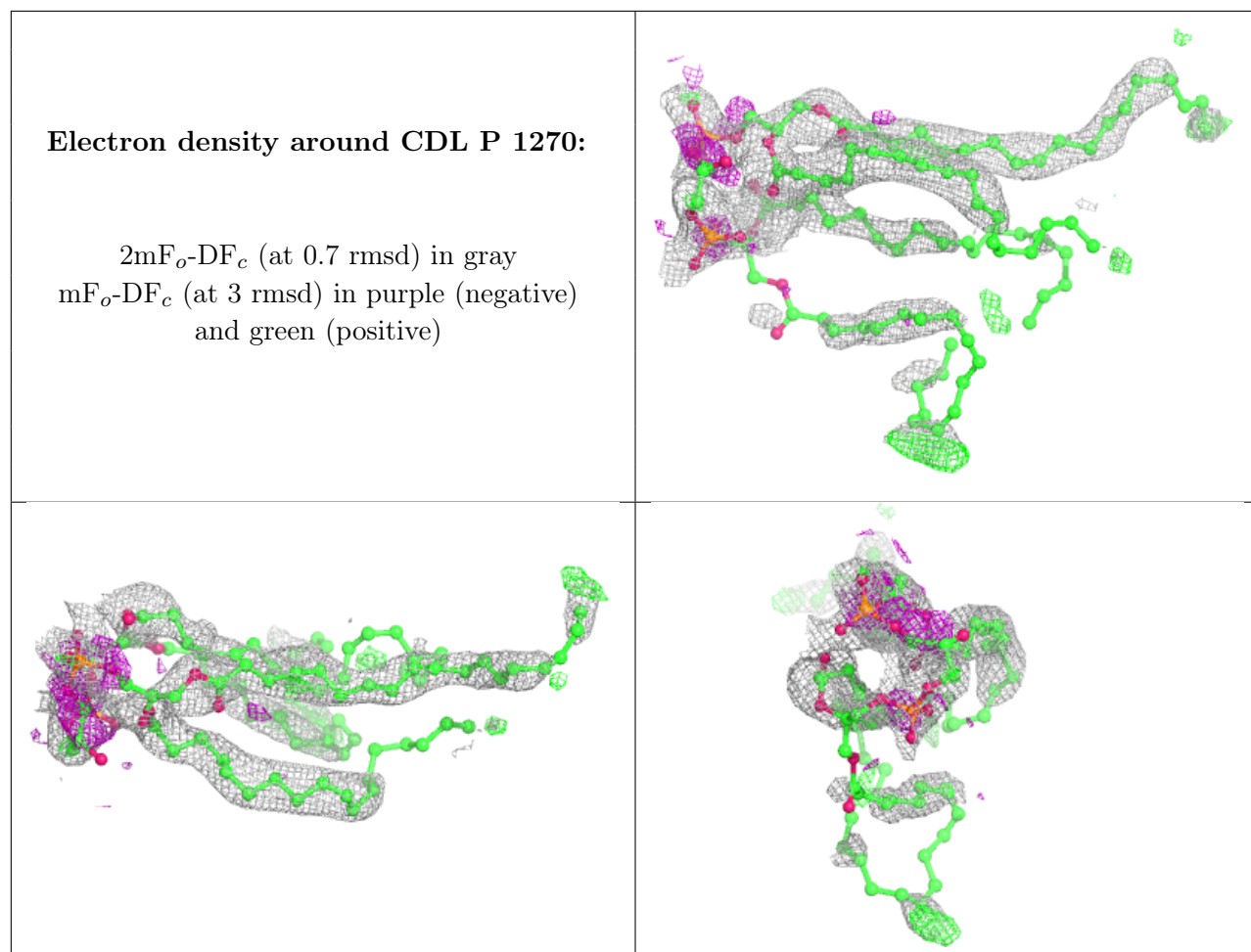
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around 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)

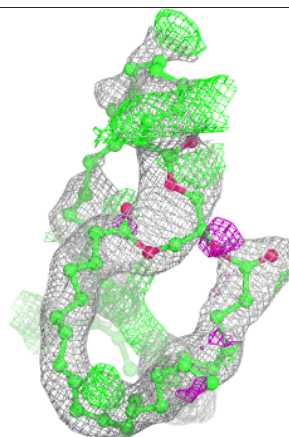
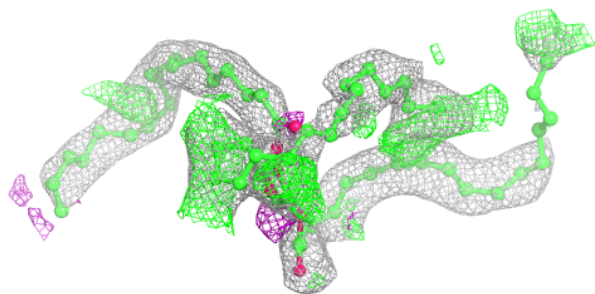
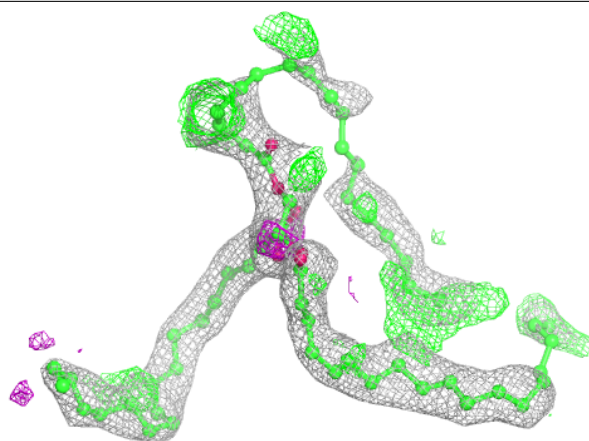




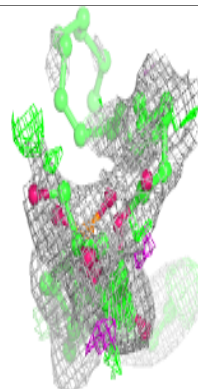
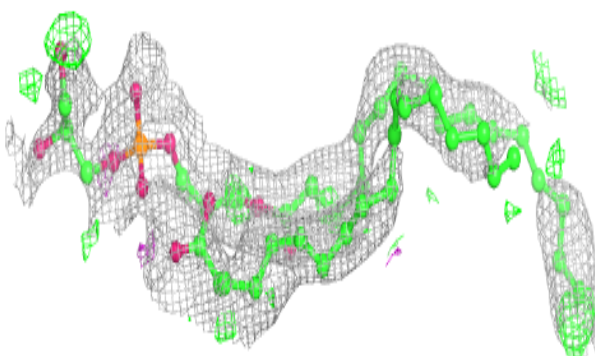
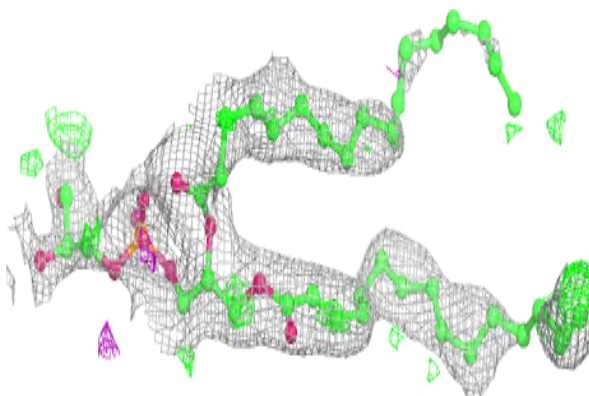


**Electron density around TGL L 522:**

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

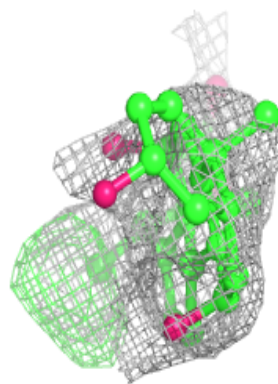
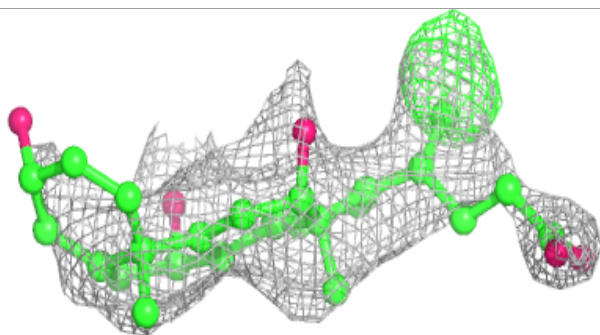
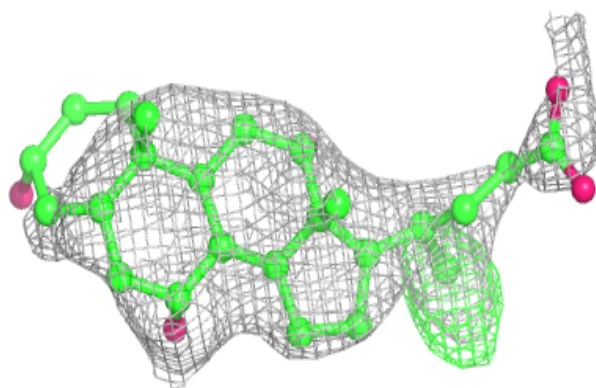
**Electron density around PGV C 268:**

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

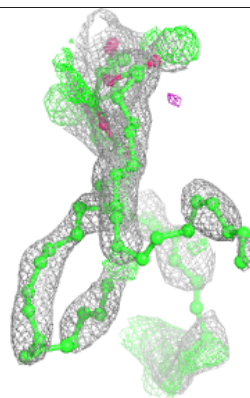
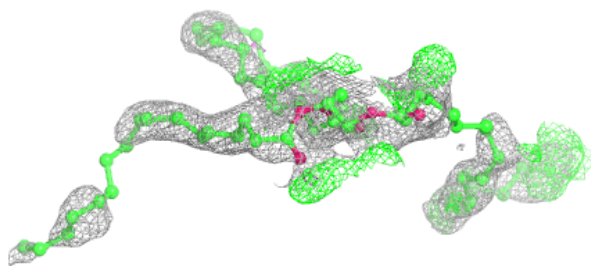
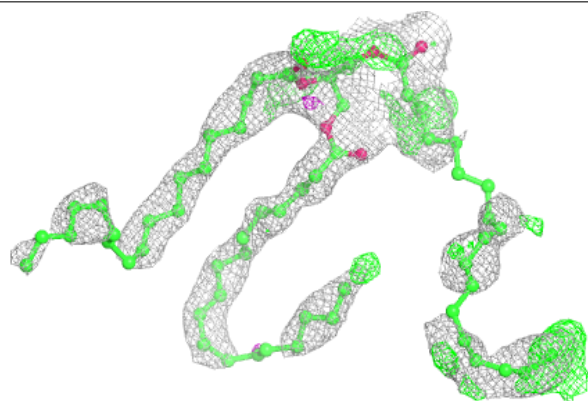


**Electron density around CHD J 60:**

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

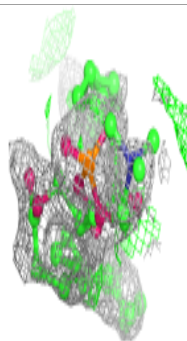
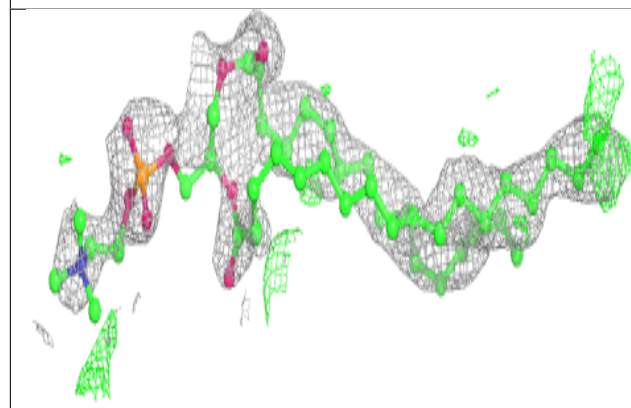
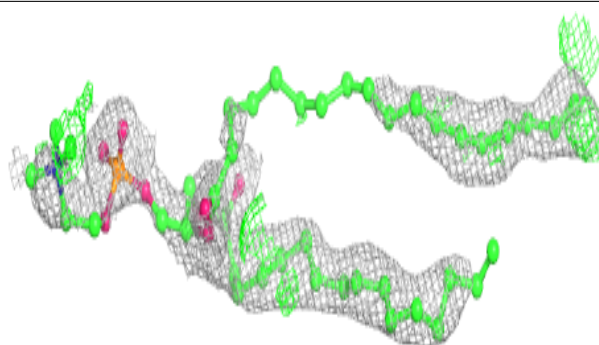
**Electron density around TGL Q 1523:**

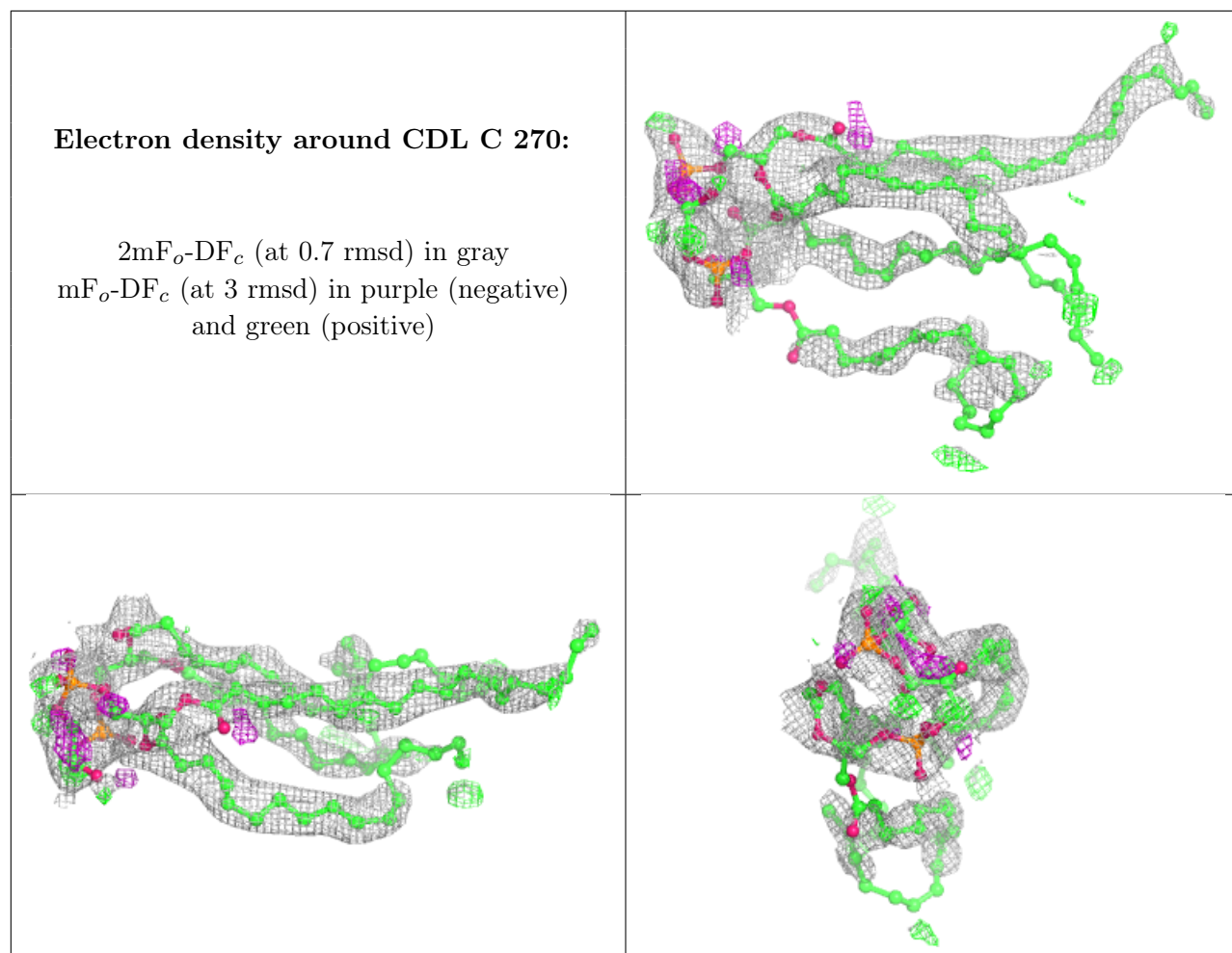
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around PSC E 229:**

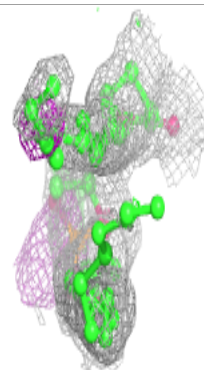
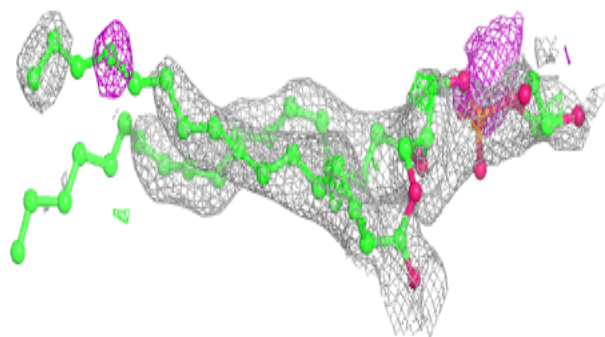
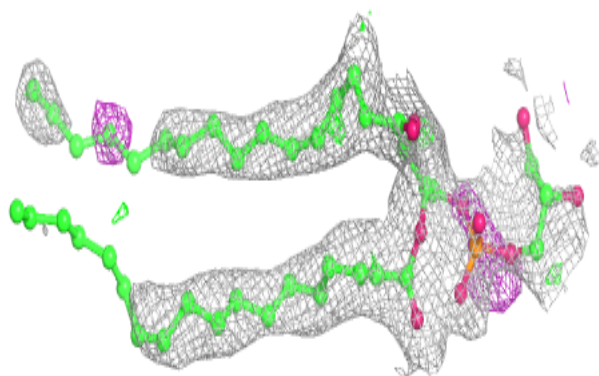
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



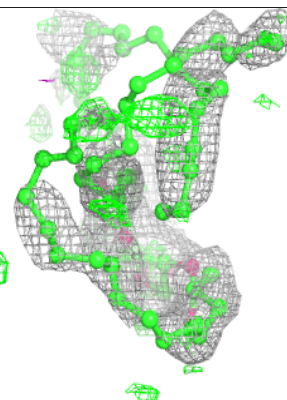
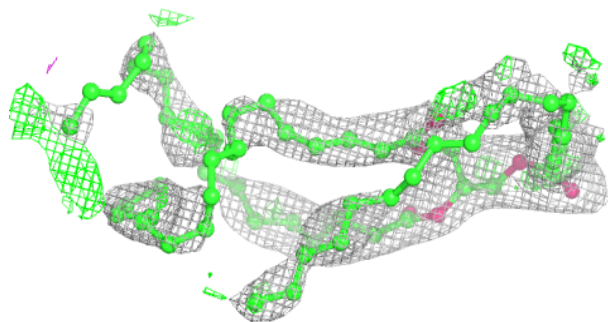
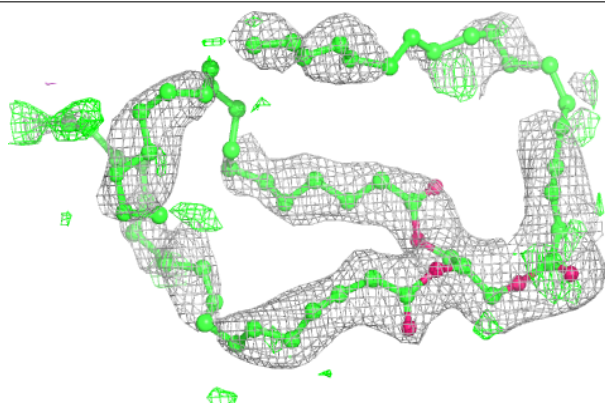


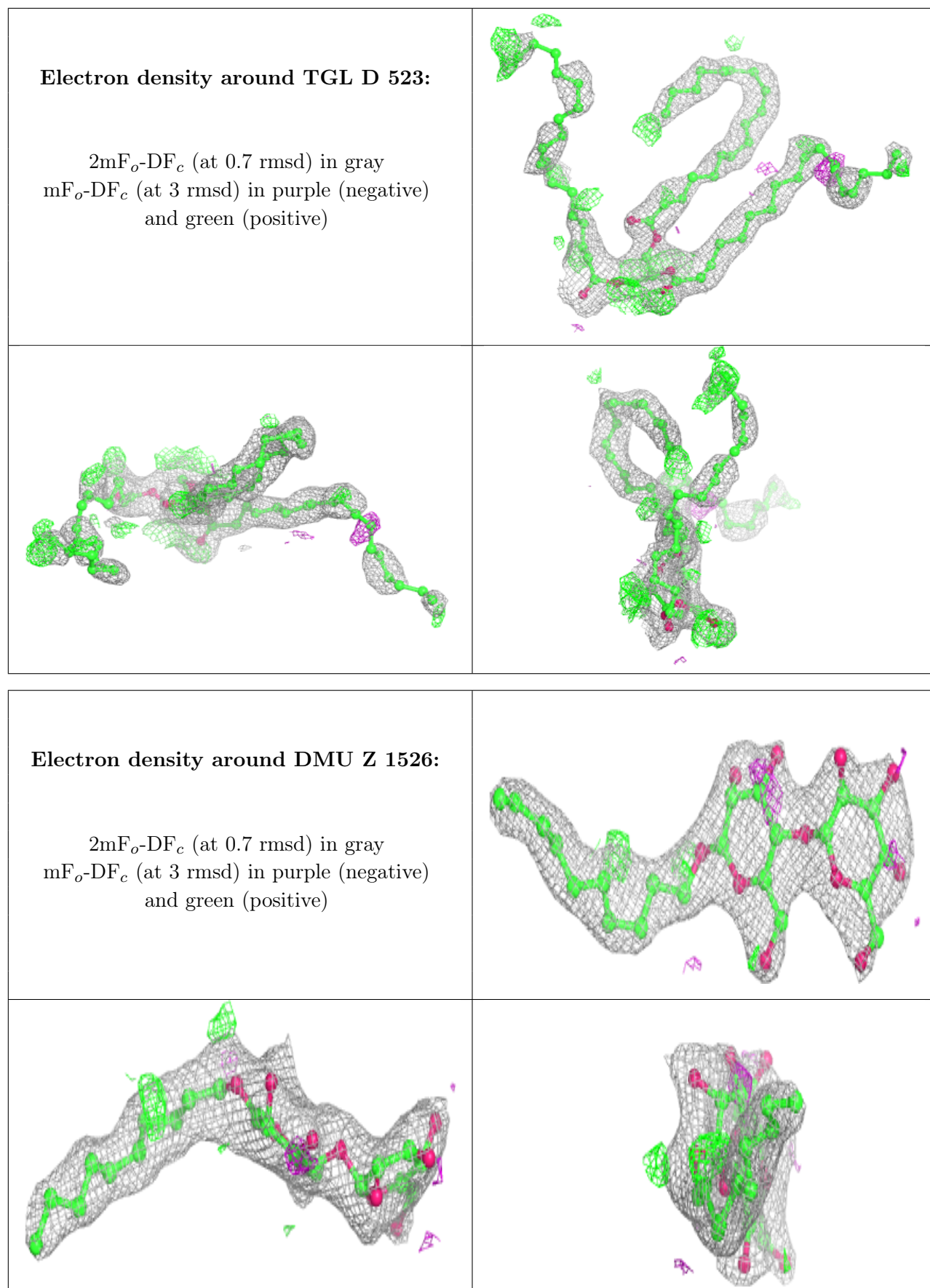
**Electron density around PGV A 524:**

$2mF_o-DF_c$  (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:**

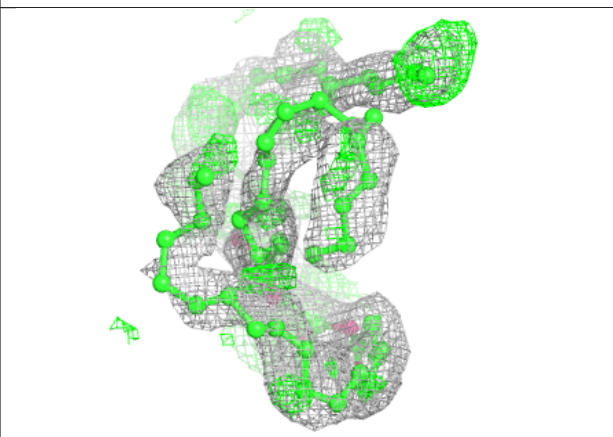
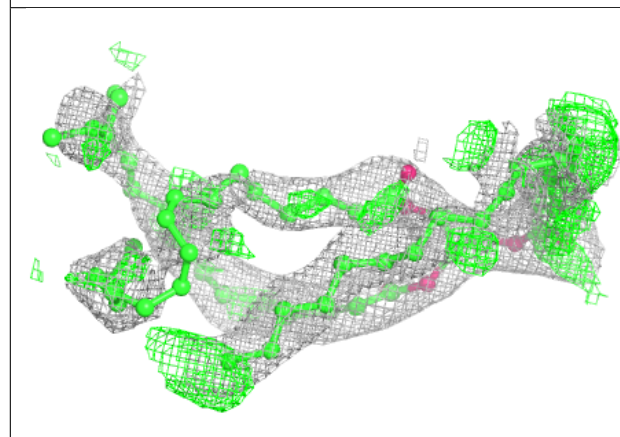
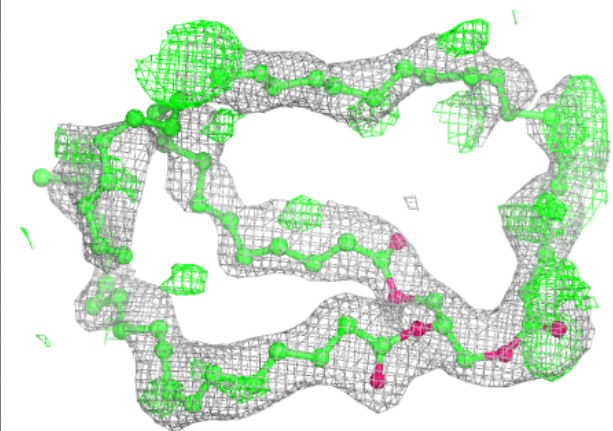
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



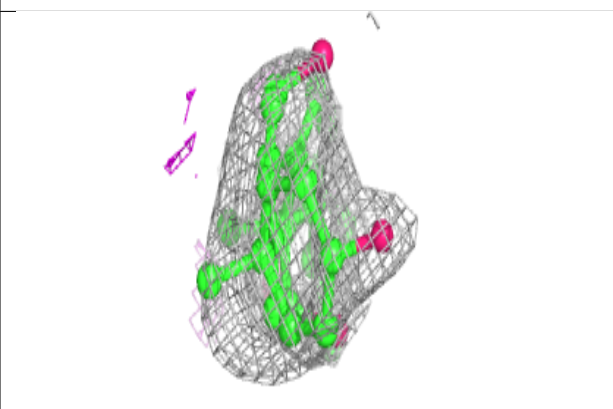
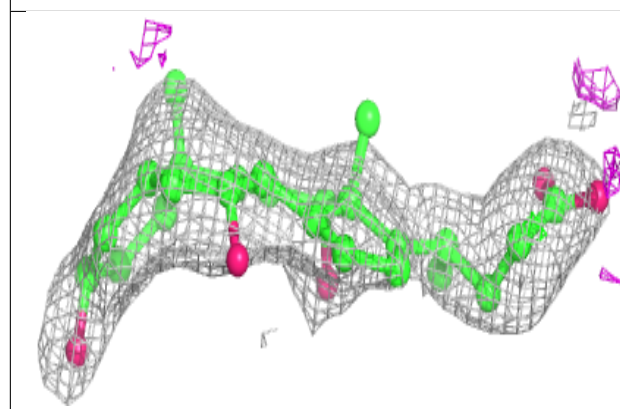
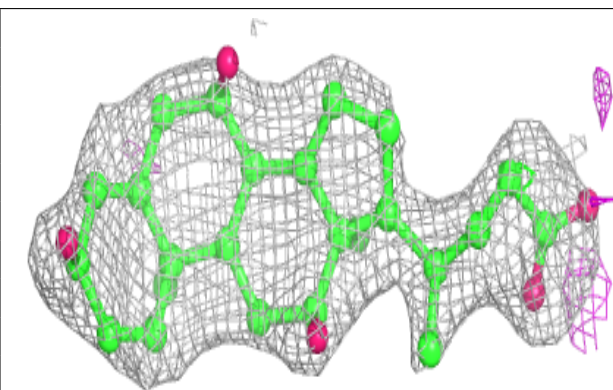


**Electron density around TGL A 521:**

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

**Electron density around CHD C 271:**

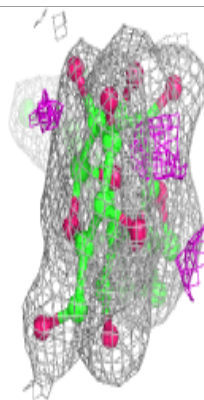
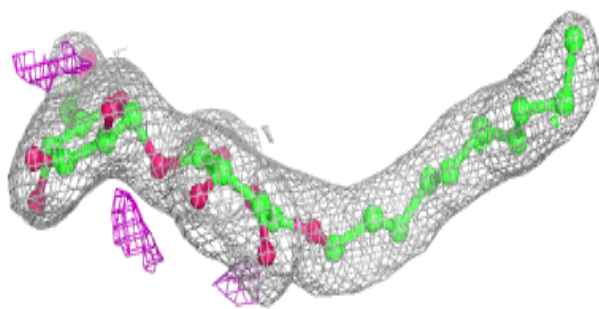
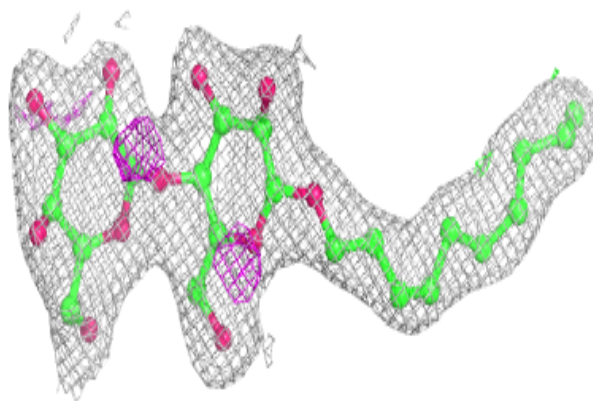
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



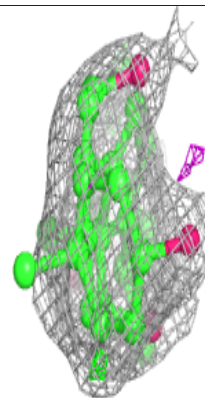
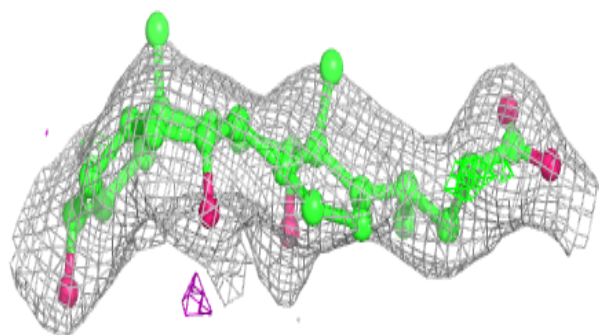
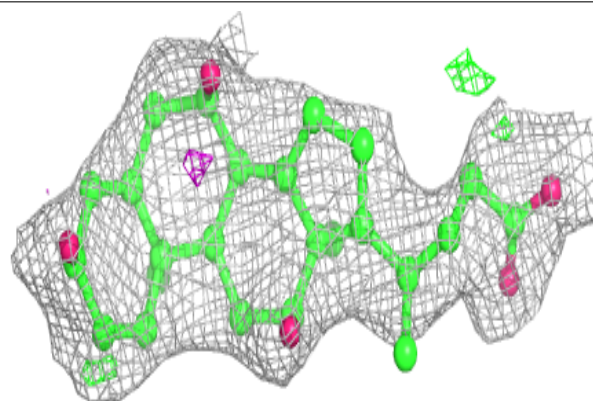


**Electron density around DMU M 526:**

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

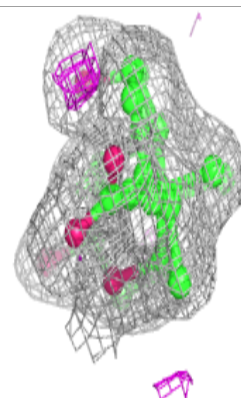
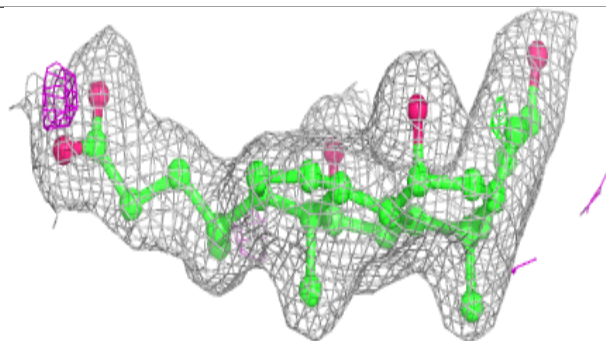
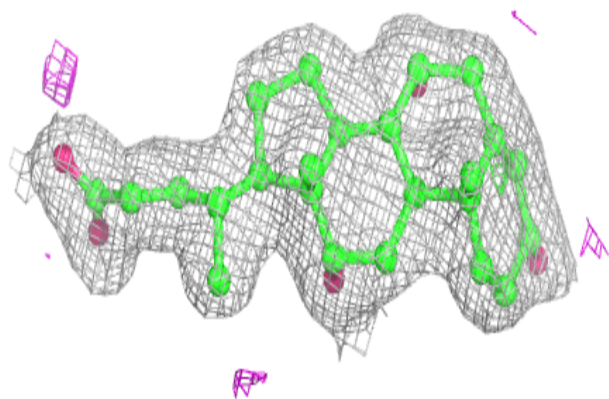
**Electron density around CHD P 1271:**

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

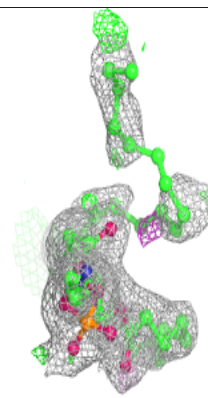
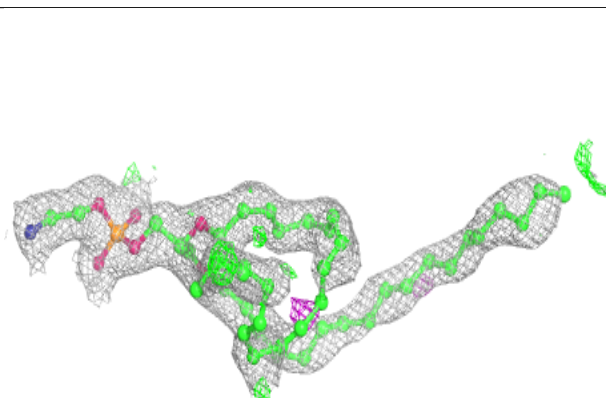
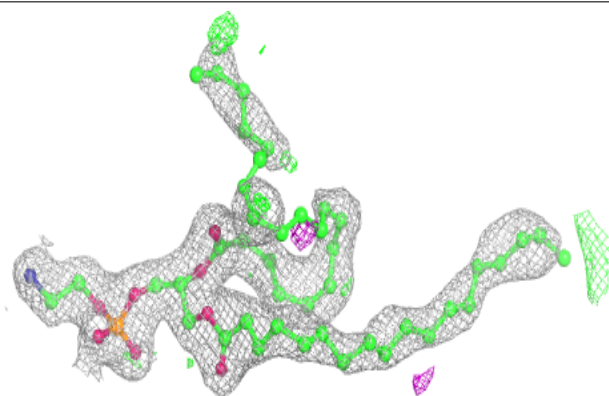


**Electron density around CHD P 1525:**

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

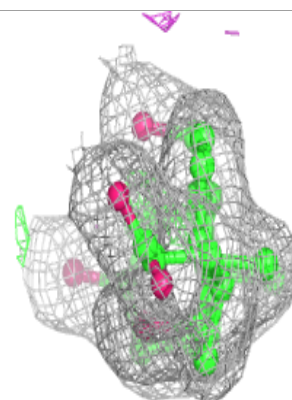
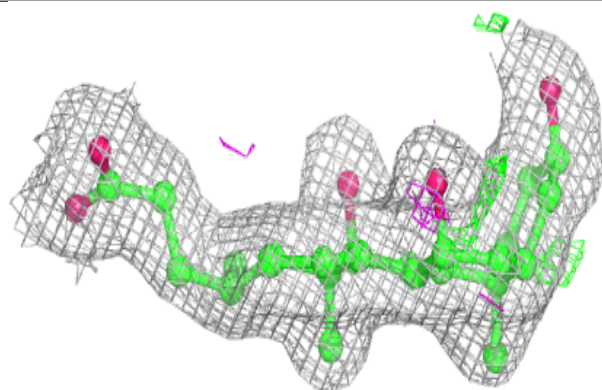
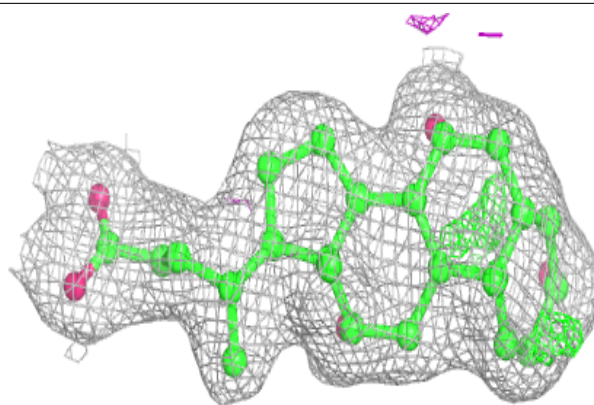
**Electron density around PEK T 1264:**

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

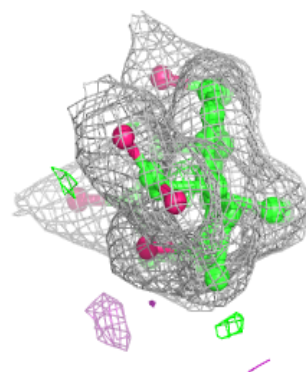
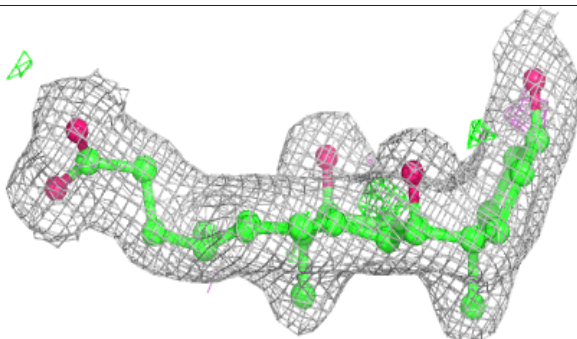
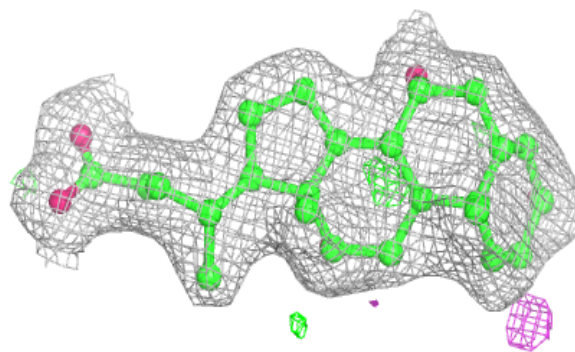


**Electron density around CHD O 229:**

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

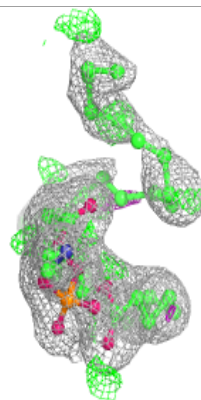
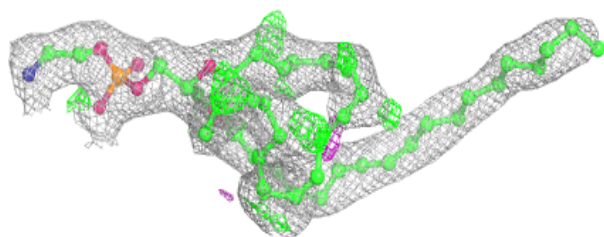
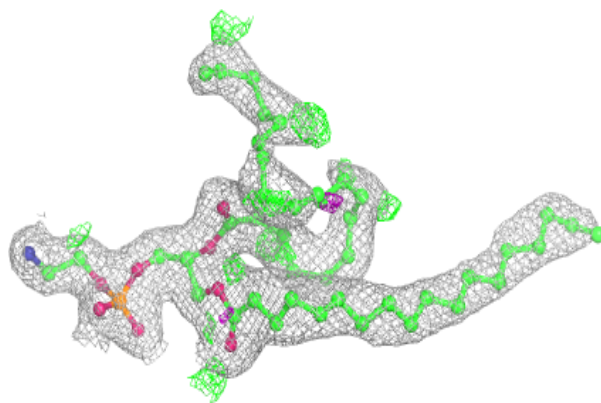
**Electron density around CHD B 1085:**

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

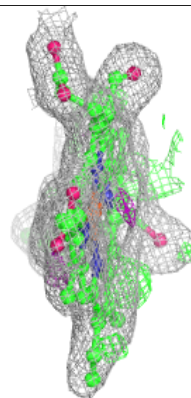
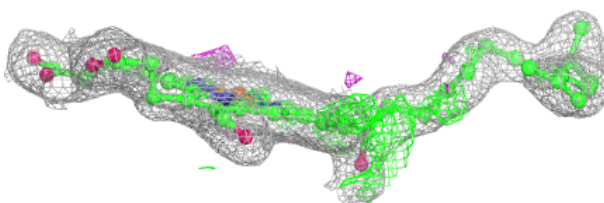
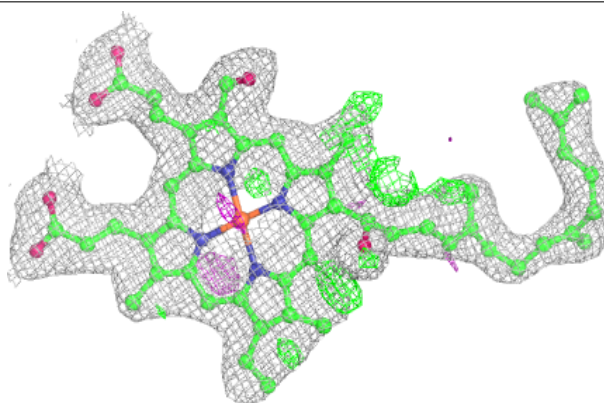


**Electron density around PEK C 264:**

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

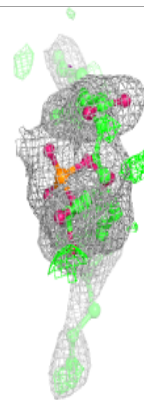
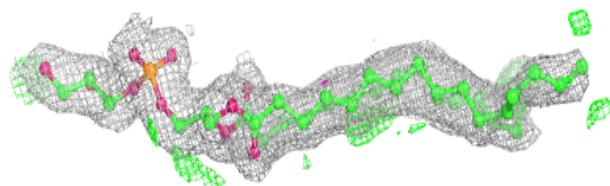
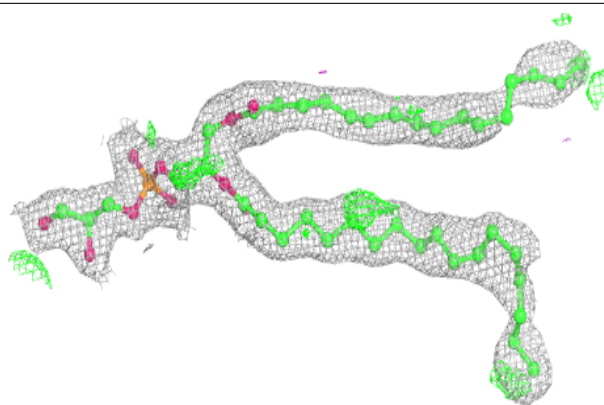
**Electron density around HEA N 516:**

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

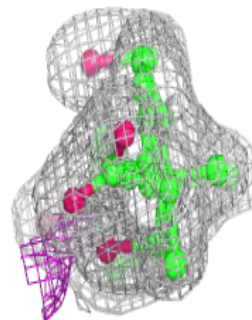
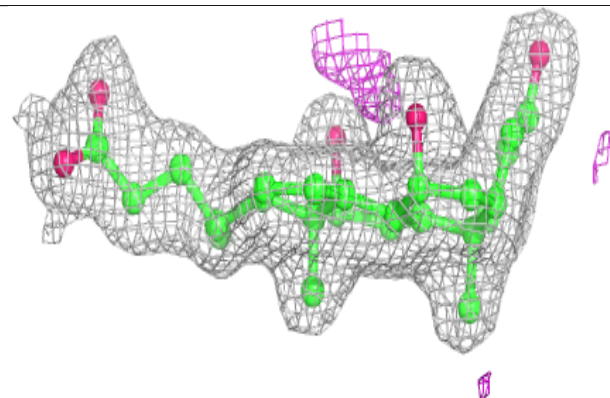
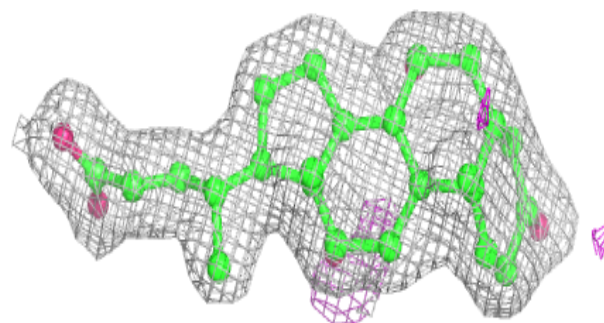


**Electron density around PGV C 267:**

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

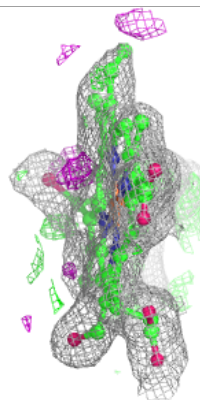
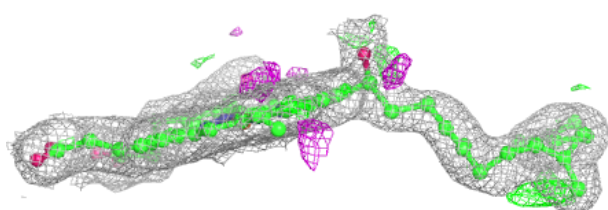
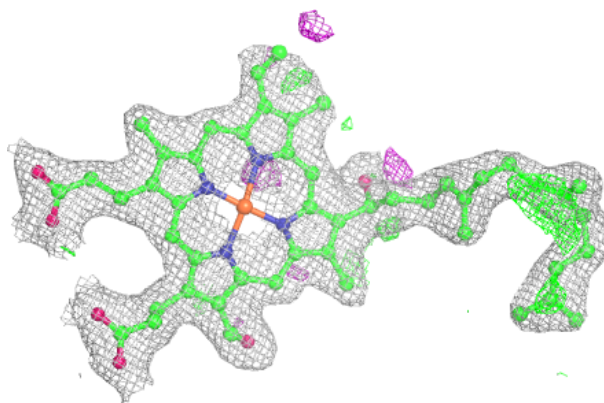
**Electron density around CHD C 525:**

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

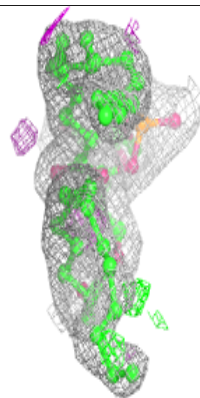
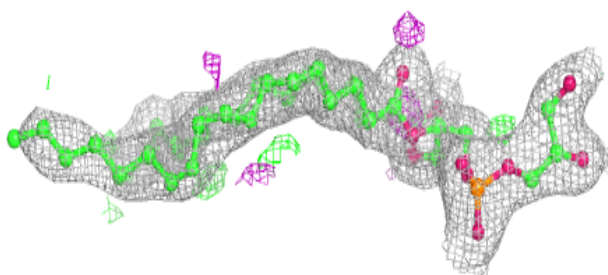
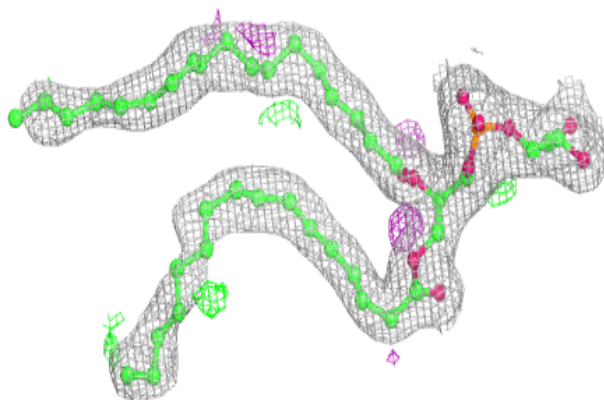


**Electron density around HEA A 516:**

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

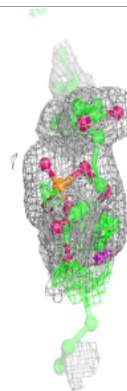
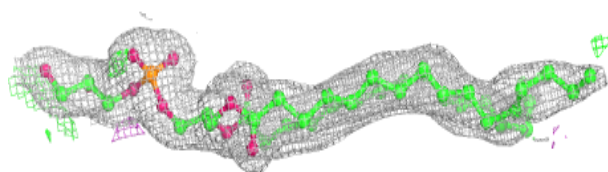
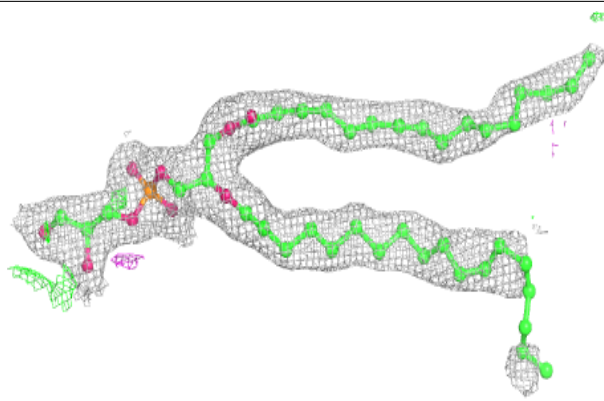
**Electron density around PGV N 1266:**

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

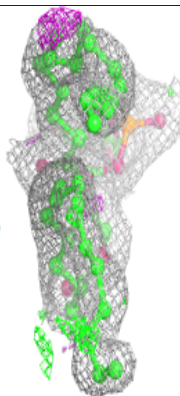
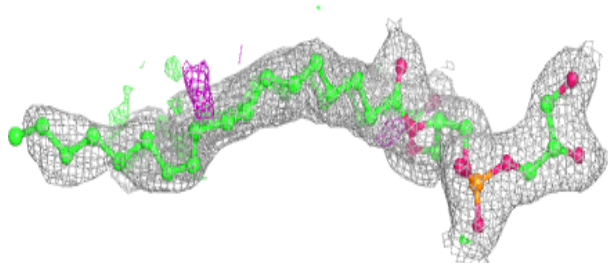
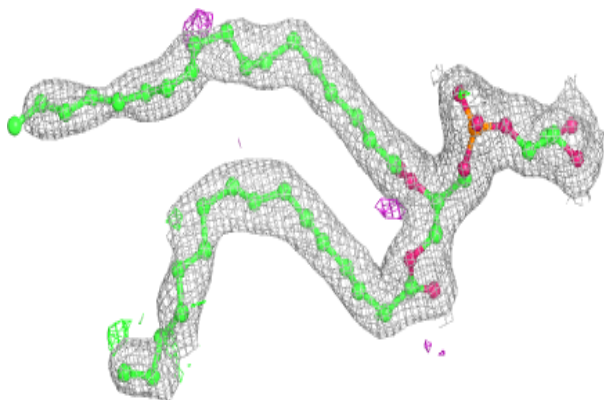


**Electron density around PGV P 1267:**

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

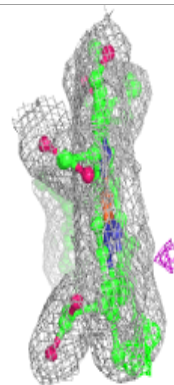
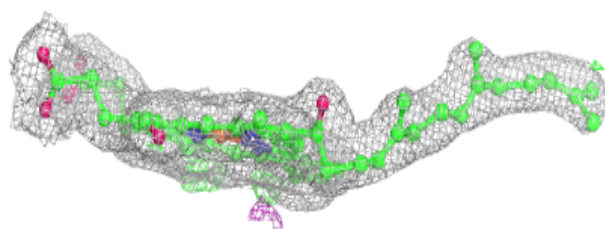
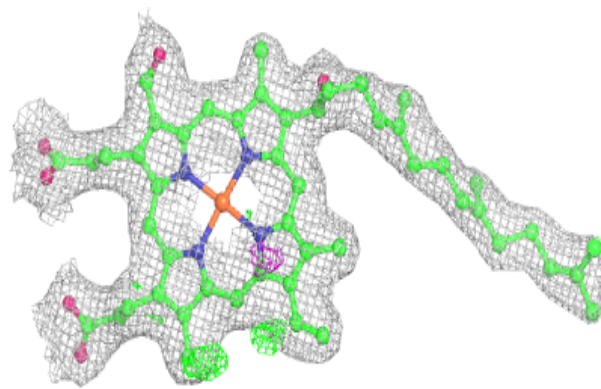
**Electron density around PGV A 522:**

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

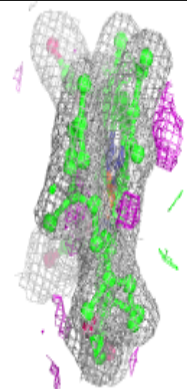
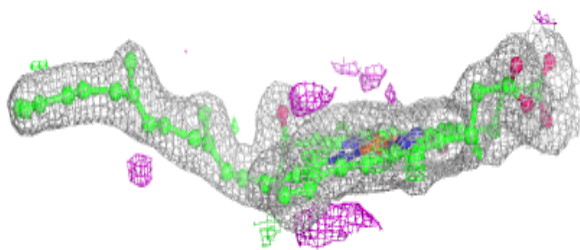
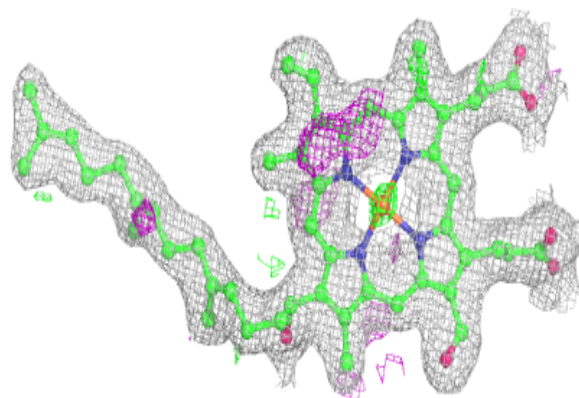


**Electron density around HEA N 515:**

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

**Electron density around HEA A 515:**

$2mF_o-DF_c$  (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.