



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 02:01 PM UTC

PDB ID : 2EIN / pdb\_00002ein  
Title : Zinc ion binding structure of bovine heart cytochrome C oxidase in the fully oxidized state  
Authors : Muramoto, K.; Hirata, K.; Shinzawa-Itoh, K.; Yoko-o, S.; Yamashita, E.; Aoyama, H.; Tsukihara, T.; Yoshikawa, S.  
Deposited on : 2007-03-13  
Resolution : 2.70 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 : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

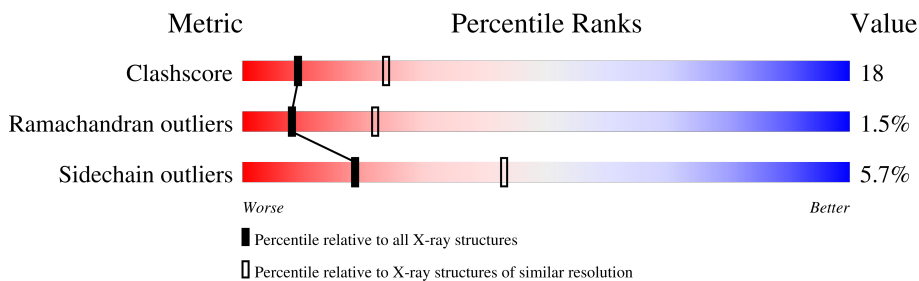
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	514	62% 35% .
1	N	514	60% 36% .
2	B	227	54% 37% 9%
2	O	227	47% 45% 8%
3	C	261	66% 30% ..
3	P	261	66% 32% ..
4	D	147	63% 33% ..
4	Q	147	64% 31% ...

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Mol	Chain	Length	Quality of chain	
5	E	109	68%	28%
5	R	109	66%	29%
6	F	98	69%	23%
6	S	98	58%	35%
7	G	85	59%	29%
7	T	85	61%	26%
8	H	85	55%	34%
8	U	85	62%	27%
9	I	73	73%	25%
9	V	73	70%	30%
10	J	59	75%	22%
10	W	59	75%	22%
11	K	56	64%	21%
11	X	56	57%	29%
12	L	47	64%	28%
12	Y	47	62%	30%
13	M	46	57%	24%
13	Z	46	39%	48%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	PSC	B	230	-	-	X	-
23	CHD	C	271	X	-	-	-
23	CHD	J	60	X	-	-	-
23	CHD	P	1271	X	-	-	-
23	CHD	W	1060	X	-	-	-
24	DMU	C	272	X	-	-	-
24	DMU	M	526	X	-	-	-

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<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
24	DMU	P	1272	X	-	-	-
24	DMU	Z	1526	X	-	-	-
26	CDL	G	269	-	-	X	-
26	CDL	T	1269	-	-	X	-

## 2 Entry composition [i](#)

There are 27 unique types of molecules in this entry. The entry contains 31815 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 polypeptide Va.

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

- Molecule 6 is a protein called Cytochrome c oxidase polypeptide Vb.

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

- Molecule 7 is a protein called Cytochrome c oxidase polypeptide VIa-heart.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
7	G	84	Total	C	N	O	P	S	0	0	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 VIb isoform 1.

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

- Molecule 9 is a protein called Cytochrome c oxidase polypeptide VIc.

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

- Molecule 10 is a protein called Cytochrome c oxidase polypeptide VIIa-heart.

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			
11	X	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			

- Molecule 12 is a protein called Cytochrome c oxidase polypeptide VIIc.

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

- Molecule 13 is a protein called Cytochrome c oxidase polypeptide VIII-heart.

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

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

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

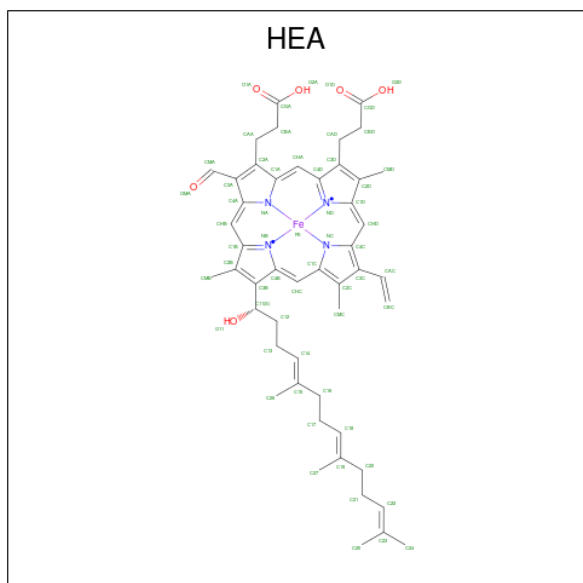
- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

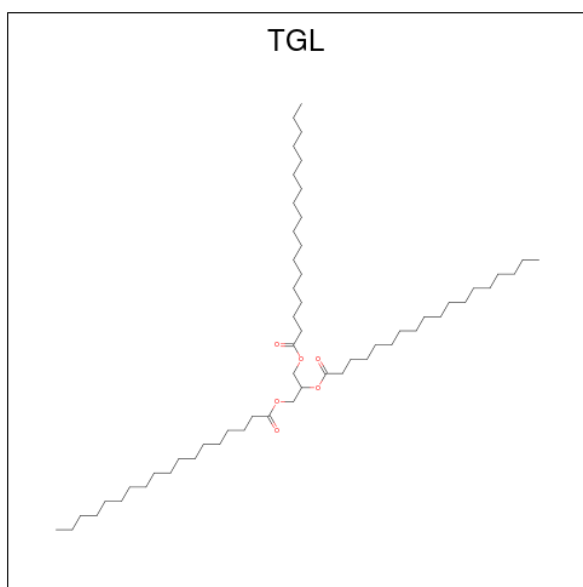
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	1	Total Na 1 1	0	0
16	N	1	Total Na 1 1	0	0

- Molecule 17 is HEME-A (CCD ID: HEA) (formula: C<sub>49</sub>H<sub>56</sub>FeN<sub>4</sub>O<sub>6</sub>).



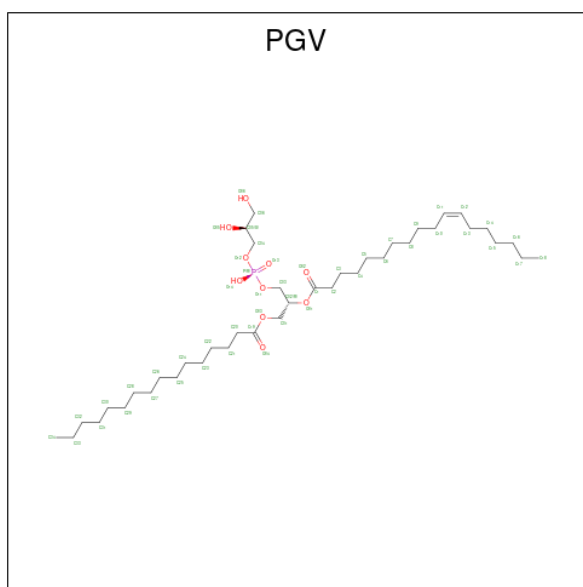
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total C Fe N O 60 49 1 4 6	0	0
17	A	1	Total C Fe N O 60 49 1 4 6	0	0
17	N	1	Total C Fe N O 60 49 1 4 6	0	0
17	N	1	Total C Fe N O 60 49 1 4 6	0	0

- Molecule 18 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: C<sub>57</sub>H<sub>110</sub>O<sub>6</sub>).



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

- Molecule 19 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C<sub>40</sub>H<sub>77</sub>O<sub>10</sub>P).



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

- Molecule 20 is ZINC ION (CCD ID: ZN) (formula: Zn).

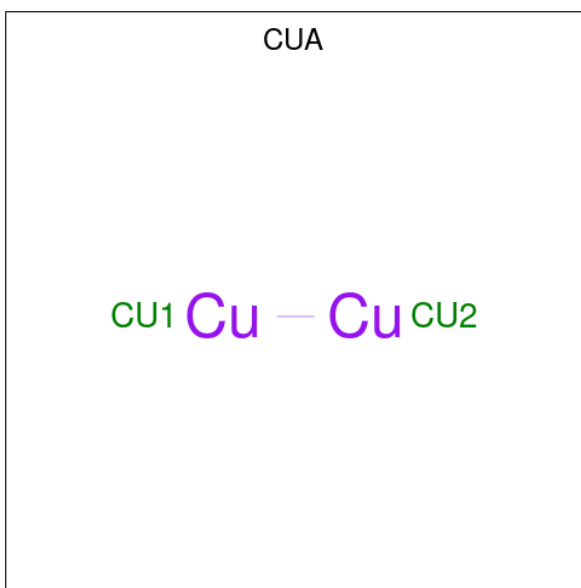
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	B	1	Total	Zn	0	0
			1	1		
20	C	1	Total	Zn	0	0
			1	1		
20	D	1	Total	Zn	0	0
			1	1		
20	F	2	Total	Zn	0	0
			2	2		

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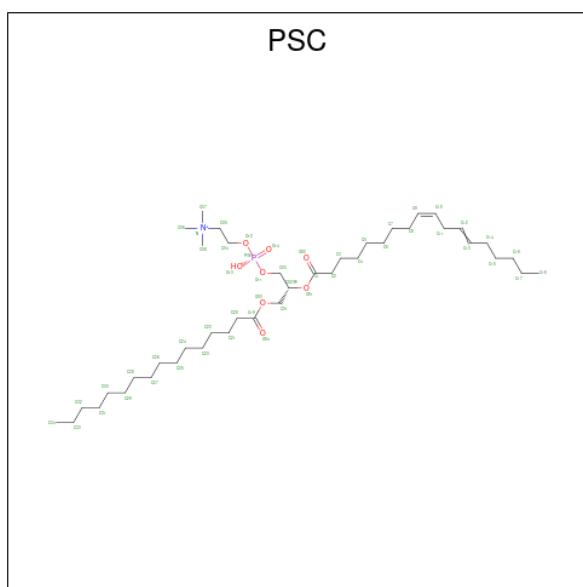
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	G	1	Total Zn 1 1	0	0
20	L	1	Total Zn 1 1	0	0
20	N	2	Total Zn 2 2	0	0
20	O	1	Total Zn 1 1	0	0
20	P	2	Total Zn 2 2	0	0
20	S	1	Total Zn 1 1	0	0
20	T	1	Total Zn 1 1	0	0

- Molecule 21 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu<sub>2</sub>).



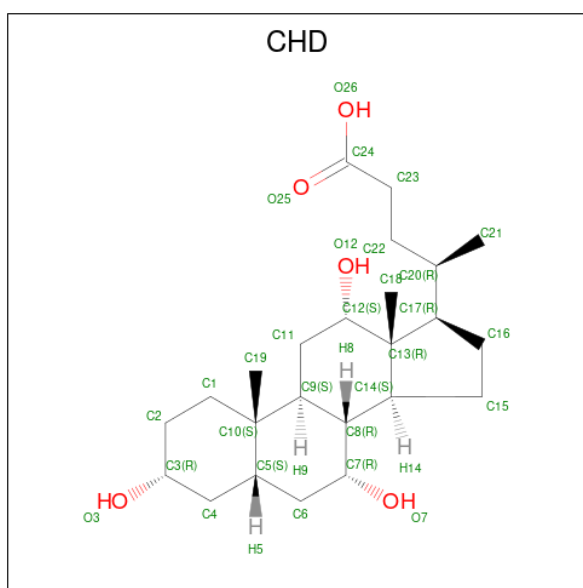
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	B	1	Total Cu 2 2	0	0
21	O	1	Total Cu 2 2	0	0

- Molecule 22 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (CCD ID: PSC) (formula: C<sub>42</sub>H<sub>81</sub>NO<sub>8</sub>P).



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

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



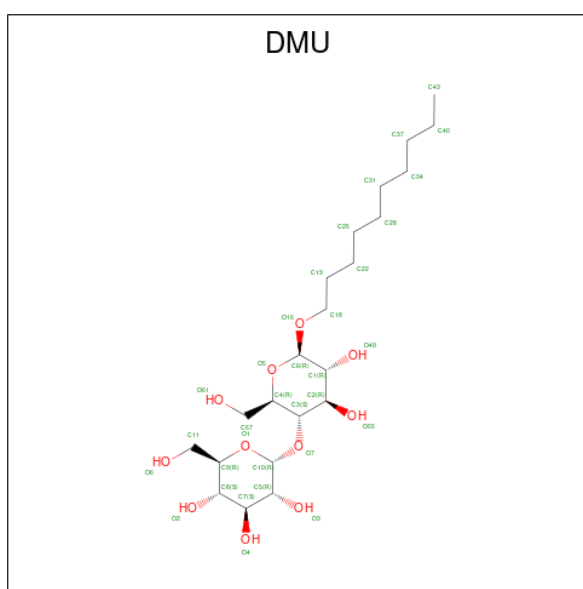
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	B	1	Total	C	O	0	0
			29	24	5		
23	C	1	Total	C	O	0	0
			29	24	5		

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

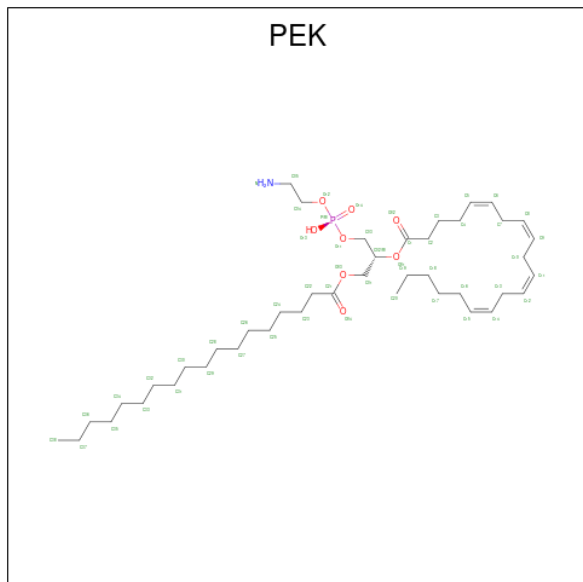
- Molecule 24 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula:  $C_{22}H_{42}O_{11}$ ).



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

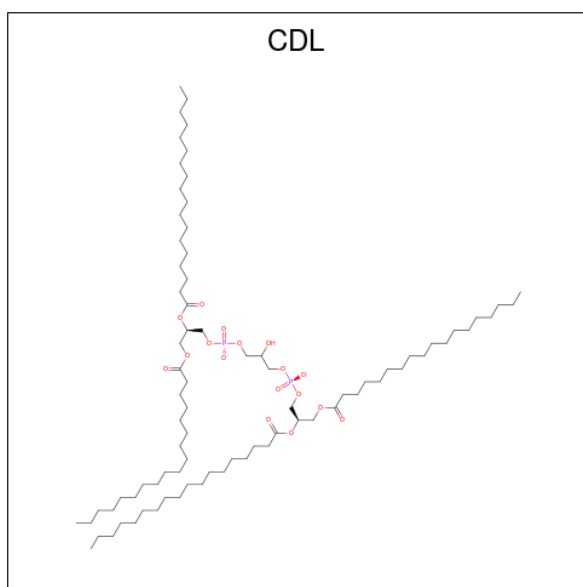
- Molecule 25 is (1S)-2-[[[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY]-1-[(ST

EAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE  
(CCD ID: PEK) (formula: C<sub>43</sub>H<sub>78</sub>NO<sub>8</sub>P).



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

- Molecule 26 is CARDIOLIPIN (CCD ID: CDL) (formula: C<sub>81</sub>H<sub>156</sub>O<sub>17</sub>P<sub>2</sub>).



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

- Molecule 27 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
27	A	160	160	160	0	0
27	B	86	86	86	0	0
27	C	73	73	73	0	0
27	D	38	38	38	0	0
27	E	23	23	23	0	0
27	F	37	37	37	0	0
27	G	29	29	29	0	0
27	H	31	31	31	0	0

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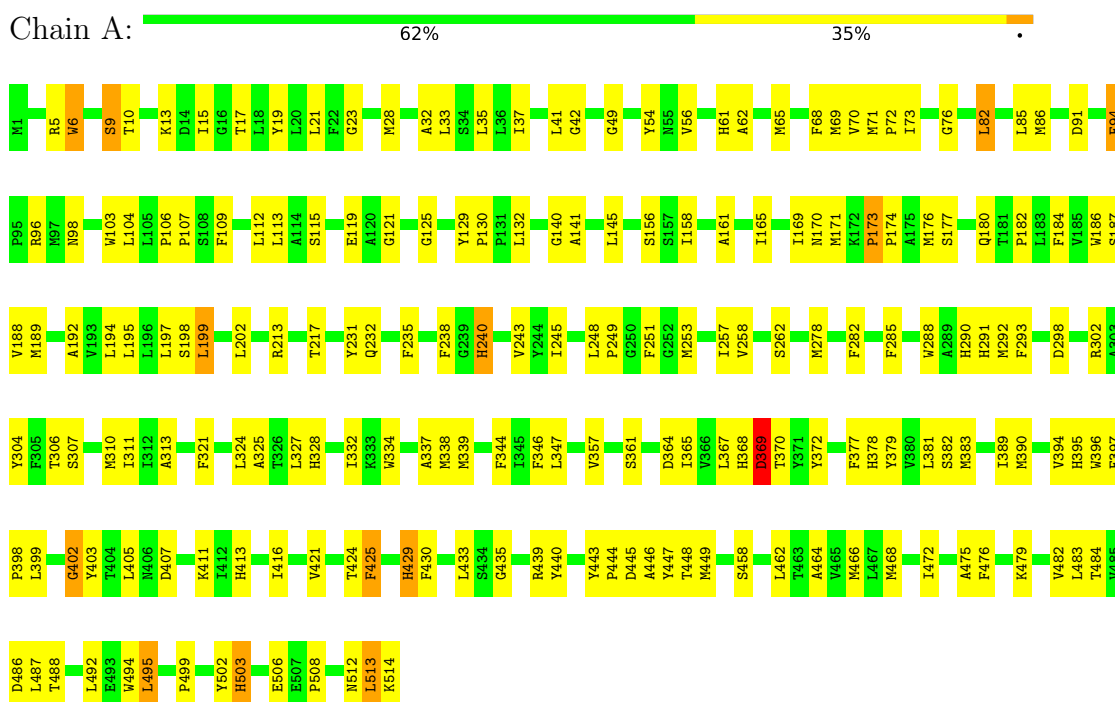
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	I	18	Total O 18 18	0	0
27	J	9	Total O 9 9	0	0
27	K	20	Total O 20 20	0	0
27	L	12	Total O 12 12	0	0
27	M	11	Total O 11 11	0	0
27	N	161	Total O 161 161	0	0
27	O	77	Total O 77 77	0	0
27	P	72	Total O 72 72	0	0
27	Q	42	Total O 42 42	0	0
27	R	22	Total O 22 22	0	0
27	S	39	Total O 39 39	0	0
27	T	26	Total O 26 26	0	0
27	U	28	Total O 28 28	0	0
27	V	17	Total O 17 17	0	0
27	W	13	Total O 13 13	0	0
27	X	13	Total O 13 13	0	0
27	Y	11	Total O 11 11	0	0
27	Z	5	Total O 5 5	0	0

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

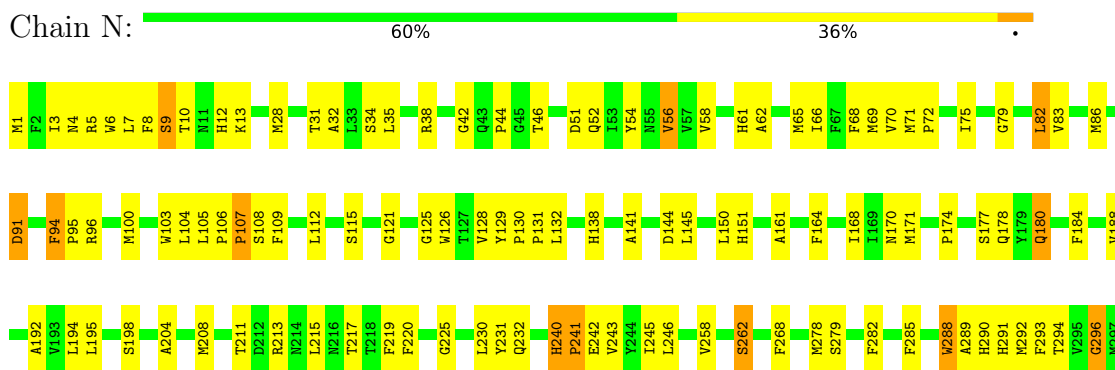
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

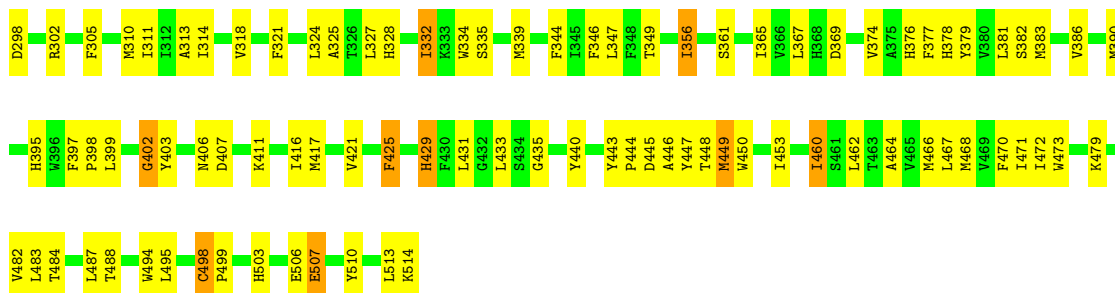
Note EDS was not executed.

- Molecule 1: Cytochrome c oxidase subunit 1



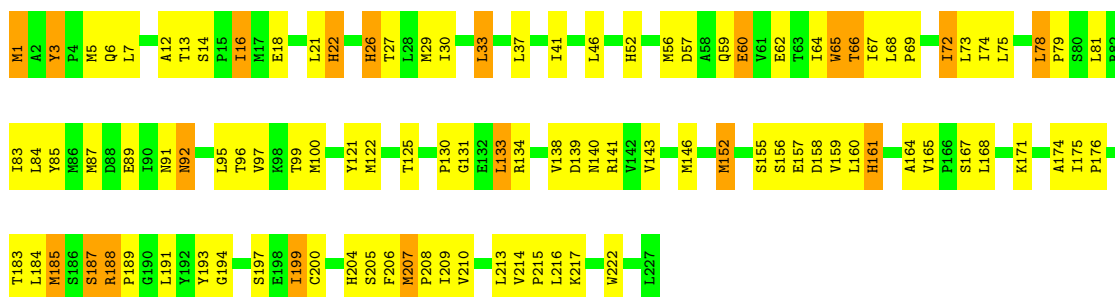
- Molecule 1: Cytochrome c oxidase subunit 1





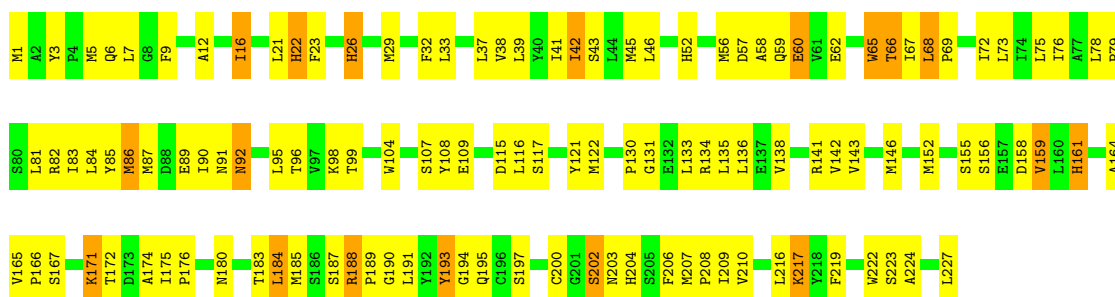
- Molecule 2: Cytochrome c oxidase subunit 2

Chain B: 54% 37% 9%



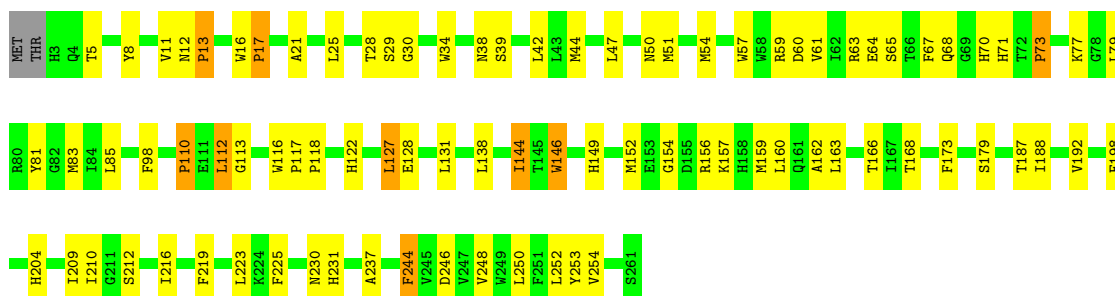
- Molecule 2: Cytochrome c oxidase subunit 2

Chain O: 47% 45% 8%



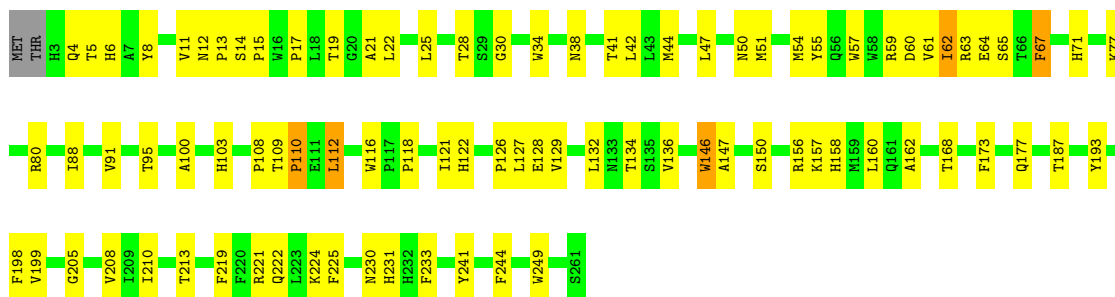
- Molecule 3: Cytochrome c oxidase subunit 3

Chain C: 66% 30% 4%



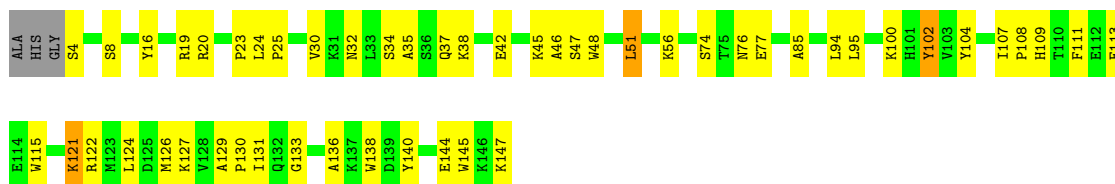
- Molecule 3: Cytochrome c oxidase subunit 3

Chain P:  66% 32% ..



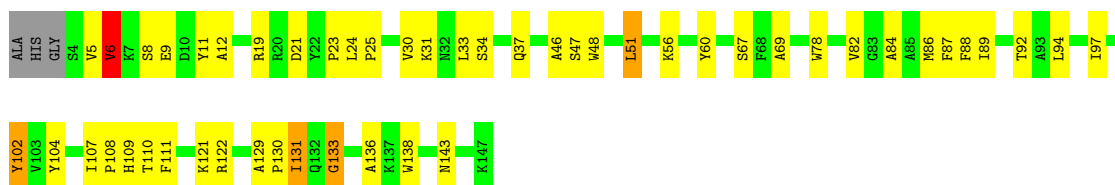
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain D:  63% 33% ..



- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain Q:  64% 31% ..



- Molecule 5: Cytochrome c oxidase polypeptide Va

Chain E:  68% 28% ..



- Molecule 5: Cytochrome c oxidase polypeptide Va

Chain R:  66% 29% ..



- Molecule 6: Cytochrome c oxidase polypeptide Vb

Chain F:  69% 23% 7%



- Molecule 6: Cytochrome c oxidase polypeptide Vb

Chain S:  58% 35% 5%



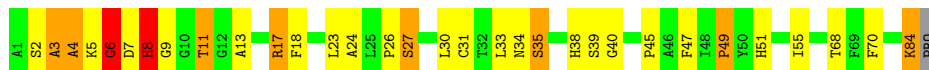
- Molecule 7: Cytochrome c oxidase polypeptide VIa-heart

Chain G:  59% 29% 9% ..



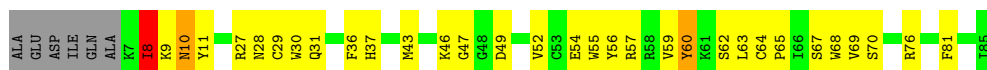
- Molecule 7: Cytochrome c oxidase polypeptide VIa-heart

Chain T:  61% 26% 9% ..



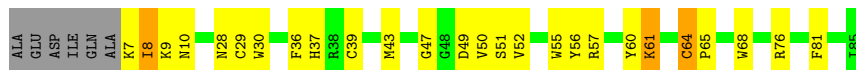
- Molecule 8: Cytochrome c oxidase subunit VIb isoform 1

Chain H:  55% 34% .. 7%



- Molecule 8: Cytochrome c oxidase subunit VIb isoform 1

Chain U:  62% 27% 7%

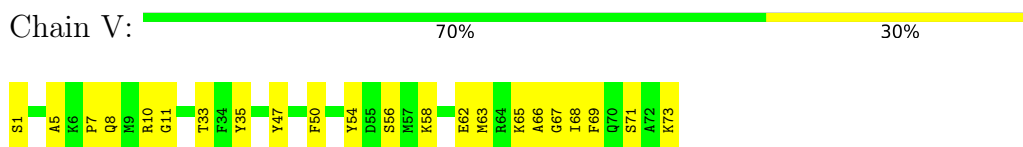


- Molecule 9: Cytochrome c oxidase polypeptide VIc

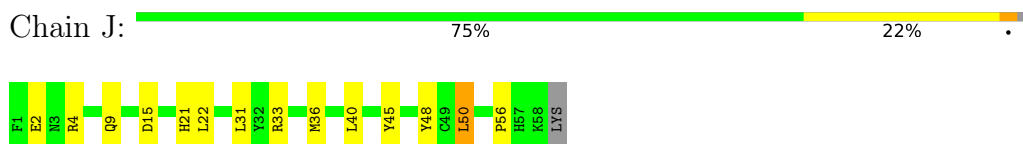
Chain I:  73% 25%



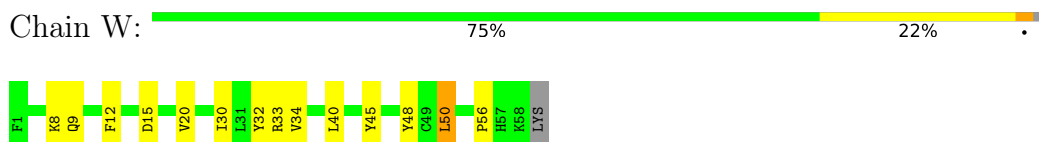
- Molecule 9: Cytochrome c oxidase polypeptide VIc



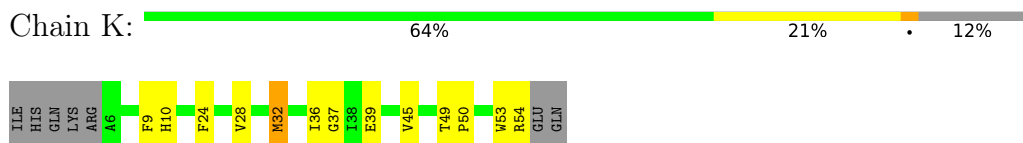
- Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart



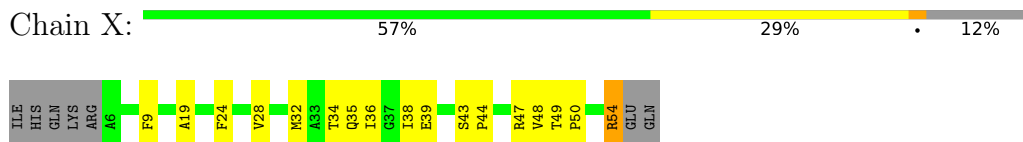
- Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart



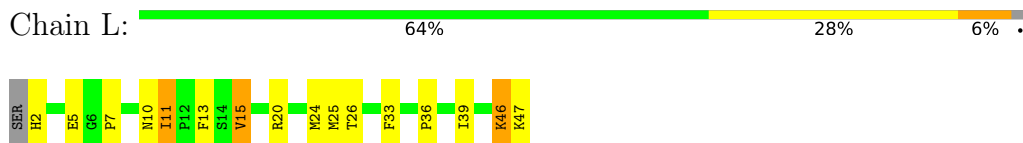
- Molecule 11: Cytochrome c oxidase polypeptide VIIb



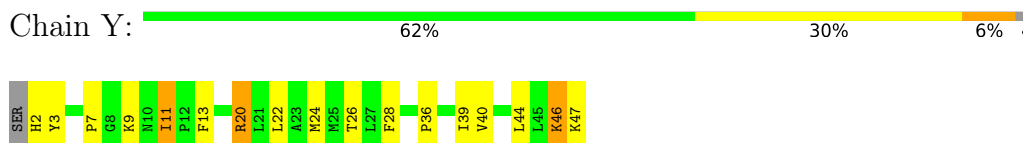
- Molecule 11: Cytochrome c oxidase polypeptide VIIb



- Molecule 12: Cytochrome c oxidase polypeptide VIIc

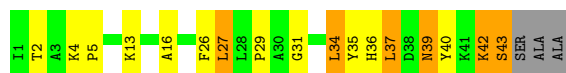


- Molecule 12: Cytochrome c oxidase polypeptide VIIc



- Molecule 13: Cytochrome c oxidase polypeptide VIII-heart

Chain M:  57% 24% 13% 7%



- Molecule 13: Cytochrome c oxidase polypeptide VIII-heart

Chain Z:  39% 48% 7% 7%



## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	187.81Å 203.58Å 177.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-2.70)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.208 , 0.258	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	31815	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: NA, ZN, PSC, PGV, DMU, TGL, TPO, SAC, FME, CDL, CU, MG, CUA, HEA, PEK, CHD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.86	1/4156 (0.0%)	1.19	35/5678 (0.6%)
1	N	0.72	1/4156 (0.0%)	1.14	32/5678 (0.6%)
2	B	0.88	2/1860 (0.1%)	1.26	16/2534 (0.6%)
2	O	0.86	2/1860 (0.1%)	1.21	16/2534 (0.6%)
3	C	0.83	0/2197	1.02	9/3005 (0.3%)
3	P	0.72	0/2197	1.07	11/3005 (0.4%)
4	D	0.72	0/1229	1.07	7/1658 (0.4%)
4	Q	0.73	2/1229 (0.2%)	1.04	4/1658 (0.2%)
5	E	0.74	0/871	1.08	4/1182 (0.3%)
5	R	0.67	0/871	1.07	3/1182 (0.3%)
6	F	0.79	0/765	1.27	6/1038 (0.6%)
6	S	0.82	0/765	1.25	8/1038 (0.8%)
7	G	0.83	0/690	1.15	3/937 (0.3%)
7	T	0.90	1/690 (0.1%)	1.12	3/937 (0.3%)
8	H	0.75	1/682 (0.1%)	1.15	6/921 (0.7%)
8	U	0.70	0/682	1.11	4/921 (0.4%)
9	I	0.70	0/605	0.99	1/802 (0.1%)
9	V	0.65	0/605	0.95	2/802 (0.2%)
10	J	0.69	0/471	1.02	0/636
10	W	0.64	0/471	1.07	0/636
11	K	0.75	0/398	1.23	3/546 (0.5%)
11	X	0.64	0/398	1.25	5/546 (0.9%)
12	L	0.98	2/393 (0.5%)	1.18	5/526 (1.0%)
12	Y	0.83	1/393 (0.3%)	1.16	4/526 (0.8%)
13	M	0.86	0/345	1.13	1/470 (0.2%)
13	Z	0.74	1/345 (0.3%)	1.17	1/470 (0.2%)
All	All	0.78	14/29324 (0.0%)	1.14	189/39866 (0.5%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	N	0	1
2	B	0	1
2	O	0	1
All	All	0	6

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	26	HIS	CD2-NE2	12.73	1.51	1.37
2	O	26	HIS	CD2-NE2	11.10	1.50	1.37
1	N	83	VAL	CA-CB	7.19	1.57	1.54
2	O	22	HIS	ND1-CE1	6.43	1.39	1.32
12	Y	2	HIS	CD2-NE2	6.41	1.45	1.37

The worst 5 of 189 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	82	LEU	N-CA-C	10.76	123.09	111.36
1	N	82	LEU	N-CA-C	10.32	122.60	111.36
5	E	81	ILE	N-CA-C	8.75	118.65	110.42
13	Z	27	LEU	N-CA-C	8.71	121.73	111.71
1	A	262	SER	N-CA-C	-8.70	102.45	113.23

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	A	372	TYR	Sidechain
1	A	502	TYR	Sidechain
2	B	85	TYR	Sidechain
1	N	240	HIS	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4027	0	4001	175	0
1	N	4027	0	4001	177	0
2	B	1824	0	1833	95	0
2	O	1824	0	1833	105	0
3	C	2110	0	2027	84	0
3	P	2110	0	2027	85	0
4	D	1195	0	1183	42	0
4	Q	1195	0	1183	39	0
5	E	852	0	845	16	0
5	R	852	0	845	22	0
6	F	748	0	728	18	0
6	S	748	0	728	26	0
7	G	675	0	644	38	0
7	T	675	0	644	46	0
8	H	662	0	623	21	0
8	U	662	0	623	17	0
9	I	601	0	613	15	0
9	V	601	0	613	20	0
10	J	460	0	459	10	0
10	W	460	0	459	11	0
11	K	384	0	366	12	0
11	X	384	0	366	14	0
12	L	380	0	380	17	0
12	Y	380	0	380	17	0
13	M	335	0	352	19	0
13	Z	335	0	352	13	0
14	A	1	0	0	0	0
14	N	1	0	0	0	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	120	0	108	17	0
17	N	120	0	108	18	0
18	A	126	0	220	12	0
18	L	63	0	110	20	0
18	N	63	0	110	9	0
18	O	63	0	110	8	0
18	Y	63	0	110	16	0
19	A	102	0	152	9	0
19	C	102	0	152	7	0
19	N	102	0	152	10	0
19	P	102	0	152	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	B	1	0	0	0	0
20	C	1	0	0	0	0
20	D	1	0	0	0	0
20	F	2	0	0	0	0
20	G	1	0	0	0	0
20	L	1	0	0	0	0
20	N	2	0	0	0	0
20	O	1	0	0	0	0
20	P	2	0	0	0	0
20	S	1	0	0	0	0
20	T	1	0	0	0	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	52	0	80	21	0
22	O	52	0	80	20	0
23	B	29	0	39	5	0
23	C	58	0	78	5	0
23	G	29	0	39	1	0
23	J	29	0	39	4	0
23	P	58	0	78	6	0
23	W	29	0	39	3	0
24	C	33	0	36	3	0
24	M	33	0	38	2	0
24	P	33	0	38	4	0
24	Z	33	0	38	1	0
25	C	106	0	154	20	0
25	G	53	0	77	10	0
25	P	53	0	77	10	0
25	T	106	0	154	23	0
26	C	100	0	156	17	0
26	G	100	0	156	23	0
26	P	100	0	156	17	0
26	T	100	0	156	32	0
27	A	160	0	0	8	0
27	B	86	0	0	3	0
27	C	73	0	0	5	0
27	D	38	0	0	3	0
27	E	23	0	0	2	0
27	F	37	0	0	1	0
27	G	29	0	0	5	0
27	H	31	0	0	2	0
27	I	18	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	J	9	0	0	0	0
27	K	20	0	0	0	0
27	L	12	0	0	0	0
27	M	11	0	0	1	0
27	N	161	0	0	9	0
27	O	77	0	0	5	0
27	P	72	0	0	7	0
27	Q	42	0	0	2	0
27	R	22	0	0	1	0
27	S	39	0	0	1	0
27	T	26	0	0	3	0
27	U	28	0	0	1	0
27	V	17	0	0	3	0
27	W	13	0	0	1	0
27	X	13	0	0	1	0
27	Y	11	0	0	2	0
27	Z	5	0	0	1	0
All	All	31815	0	31300	1133	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 18.

The worst 5 of 1133 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)
3:C:63:ARG:HE	26:C:270:CDL:HA22	1.12	1.11
25:C:264:PEK:H161	25:C:264:PEK:H102	1.38	1.04
7:T:31:CYS:SG	26:T:1269:CDL:H532	1.98	1.04
4:Q:34:SER:H	4:Q:37:GLN:HE21	1.08	1.01
22:O:1230:PSC:H142	22:O:1230:PSC:H343	1.45	0.99

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%)	466 (91%)	42 (8%)	4 (1%)	16	37
1	N	512/514 (100%)	469 (92%)	40 (8%)	3 (1%)	21	44
2	B	225/227 (99%)	202 (90%)	20 (9%)	3 (1%)	9	25
2	O	225/227 (99%)	198 (88%)	21 (9%)	6 (3%)	4	10
3	C	257/261 (98%)	247 (96%)	9 (4%)	1 (0%)	30	54
3	P	257/261 (98%)	246 (96%)	10 (4%)	1 (0%)	30	54
4	D	142/147 (97%)	135 (95%)	7 (5%)	0	100	100
4	Q	142/147 (97%)	134 (94%)	8 (6%)	0	100	100
5	E	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
5	R	103/109 (94%)	101 (98%)	2 (2%)	0	100	100
6	F	96/98 (98%)	80 (83%)	12 (12%)	4 (4%)	2	4
6	S	96/98 (98%)	83 (86%)	9 (9%)	4 (4%)	2	4
7	G	81/85 (95%)	60 (74%)	13 (16%)	8 (10%)	0	0
7	T	81/85 (95%)	61 (75%)	12 (15%)	8 (10%)	0	0
8	H	77/85 (91%)	66 (86%)	8 (10%)	3 (4%)	2	5
8	U	77/85 (91%)	66 (86%)	8 (10%)	3 (4%)	2	5
9	I	71/73 (97%)	67 (94%)	4 (6%)	0	100	100
9	V	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
10	J	56/59 (95%)	53 (95%)	2 (4%)	1 (2%)	6	18
10	W	56/59 (95%)	53 (95%)	2 (4%)	1 (2%)	6	18
11	K	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
11	X	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
12	L	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
12	Y	44/47 (94%)	42 (96%)	1 (2%)	1 (2%)	5	13
13	M	41/46 (89%)	36 (88%)	5 (12%)	0	100	100
13	Z	41/46 (89%)	36 (88%)	5 (12%)	0	100	100
All	All	3504/3614 (97%)	3204 (91%)	249 (7%)	51 (2%)	8	22

5 of 51 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	60	GLU
6	F	93	PRO
6	F	94	HIS
7	G	4	ALA
7	G	7	ASP

### 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	136/426 (32%)	132 (97%)	4 (3%)	37 67
1	N	426/426 (100%)	413 (97%)	13 (3%)	35 65
2	B	210/210 (100%)	192 (91%)	18 (9%)	10 25
2	O	210/210 (100%)	186 (89%)	24 (11%)	5 14
3	C	224/226 (99%)	211 (94%)	13 (6%)	18 42
3	P	224/226 (99%)	219 (98%)	5 (2%)	45 74
4	D	128/129 (99%)	122 (95%)	6 (5%)	23 51
4	Q	128/129 (99%)	120 (94%)	8 (6%)	16 39
5	E	92/95 (97%)	89 (97%)	3 (3%)	33 63
5	R	92/95 (97%)	89 (97%)	3 (3%)	33 63
6	F	81/81 (100%)	78 (96%)	3 (4%)	30 59
6	S	81/81 (100%)	75 (93%)	6 (7%)	13 32
7	G	67/68 (98%)	62 (92%)	5 (8%)	12 31
7	T	67/68 (98%)	61 (91%)	6 (9%)	9 23
8	H	71/75 (95%)	67 (94%)	4 (6%)	19 44
8	U	71/75 (95%)	68 (96%)	3 (4%)	26 55
9	I	57/57 (100%)	51 (90%)	6 (10%)	6 17
9	V	57/57 (100%)	55 (96%)	2 (4%)	32 61
10	J	49/50 (98%)	48 (98%)	1 (2%)	48 76
10	W	49/50 (98%)	48 (98%)	1 (2%)	48 76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	39/46 (85%)	37 (95%)	2 (5%)	21	48
11	X	39/46 (85%)	37 (95%)	2 (5%)	21	48
12	L	39/40 (98%)	37 (95%)	2 (5%)	21	48
12	Y	39/40 (98%)	37 (95%)	2 (5%)	21	48
13	M	37/38 (97%)	30 (81%)	7 (19%)	1	4
13	Z	37/38 (97%)	29 (78%)	8 (22%)	1	3
All	All	2750/3082 (89%)	2593 (94%)	157 (6%)	18	43

5 of 157 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	P	230	ASN
9	V	33	THR
4	Q	51	LEU
6	S	68	THR
13	Z	12	PRO

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

Mol	Chain	Res	Type
1	N	178	GLN
3	P	50	ASN
10	W	29	ASN
1	N	180	GLN
1	N	491	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	FME	N	1	1	8,9,10	0.97	0	8,9,11	0.81	0
2	FME	O	1	2	8,9,10	0.64	0	8,9,11	1.45	2 (25%)
7	TPO	G	11	7	8,10,11	1.93	4 (50%)	10,14,16	1.08	1 (10%)
1	FME	A	1	1	8,9,10	0.75	0	8,9,11	1.01	0
7	TPO	T	11	7	8,10,11	1.97	4 (50%)	10,14,16	1.12	1 (10%)
2	FME	B	1	2	8,9,10	0.71	0	8,9,11	1.50	2 (25%)
9	SAC	V	1	9	7,8,9	3.02	2 (28%)	7,9,11	1.93	3 (42%)
9	SAC	I	1	9	7,8,9	2.76	2 (28%)	7,9,11	1.62	2 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	N	1	1	-	5/7/9/11	-
2	FME	O	1	2	-	1/7/9/11	-
7	TPO	G	11	7	-	4/9/11/13	-
1	FME	A	1	1	-	4/7/9/11	-
7	TPO	T	11	7	-	4/9/11/13	-
2	FME	B	1	2	-	2/7/9/11	-
9	SAC	V	1	9	-	3/7/8/10	-
9	SAC	I	1	9	-	3/7/8/10	-

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	1	SAC	OAC-C1A	5.48	1.35	1.23
9	V	1	SAC	OAC-C1A	5.43	1.35	1.23
9	V	1	SAC	CA-N	5.27	1.54	1.46
9	I	1	SAC	CA-N	4.35	1.52	1.46
7	G	11	TPO	CB-CA	3.25	1.60	1.53

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CA-N-CN	-3.26	117.80	122.82
9	V	1	SAC	C2A-C1A-N	3.06	121.19	116.12
2	O	1	FME	C-CA-N	2.98	115.25	109.50
9	I	1	SAC	C2A-C1A-N	2.57	120.39	116.12
9	V	1	SAC	OAC-C1A-C2A	-2.55	117.52	122.05

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O1-CN-N-CA
2	B	1	FME	O1-CN-N-CA
7	G	11	TPO	N-CA-CB-CG2
7	G	11	TPO	N-CA-CB-OG1
7	G	11	TPO	C-CA-CB-CG2

There are no ring outliers.

4 monomers are involved in 6 short contacts:

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 64 ligands modelled in this entry, 20 are monoatomic - leaving 44 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CHD	B	1086	-	32,32,32	0.95	0	51,51,51	2.45	20 (39%)
18	TGL	O	1521	-	62,62,62	1.06	5 (8%)	65,65,65	1.54	10 (15%)
26	CDL	P	1270	-	99,99,99	1.32	13 (13%)	105,111,111	1.07	8 (7%)
17	HEA	A	515	1	67,67,67	1.42	10 (14%)	81,103,103	1.45	12 (14%)
22	PSC	B	230	-	51,51,51	1.60	10 (19%)	57,59,59	1.11	4 (7%)
23	CHD	P	1271	-	32,32,32	1.33	5 (15%)	51,51,51	3.79	26 (50%)
24	DMU	P	1272	-	34,34,34	2.81	14 (41%)	45,45,45	3.78	20 (44%)
18	TGL	Y	1522	-	62,62,62	1.43	5 (8%)	65,65,65	1.69	10 (15%)
24	DMU	C	272	-	34,34,34	2.75	14 (41%)	45,45,45	3.99	18 (40%)
17	HEA	N	515	1	67,67,67	1.56	11 (16%)	81,103,103	1.62	18 (22%)
18	TGL	N	1523	-	62,62,62	1.18	5 (8%)	65,65,65	1.44	9 (13%)
21	CUA	B	228	2	0,1,1	-	-	-	-	-
19	PGV	N	1266	-	50,50,50	1.25	6 (12%)	53,56,56	0.92	1 (1%)
23	CHD	J	60	-	32,32,32	1.56	3 (9%)	51,51,51	3.70	25 (49%)
18	TGL	L	522	-	62,62,62	1.39	5 (8%)	65,65,65	1.75	13 (20%)
23	CHD	C	525	-	32,32,32	1.32	2 (6%)	51,51,51	2.13	15 (29%)
23	CHD	C	271	-	32,32,32	1.30	4 (12%)	51,51,51	3.73	25 (49%)
19	PGV	N	1524	-	50,50,50	1.55	8 (16%)	53,56,56	1.07	5 (9%)
17	HEA	A	516	1	67,67,67	1.58	12 (17%)	81,103,103	1.73	21 (25%)
22	PSC	O	1230	-	51,51,51	1.65	10 (19%)	57,59,59	1.08	5 (8%)
19	PGV	A	524	-	50,50,50	1.55	8 (16%)	53,56,56	1.12	5 (9%)
23	CHD	G	86	-	32,32,32	1.22	3 (9%)	51,51,51	2.58	21 (41%)
23	CHD	W	1060	-	32,32,32	1.83	5 (15%)	51,51,51	3.62	25 (49%)
24	DMU	M	526	-	34,34,34	3.37	9 (26%)	45,45,45	3.56	21 (46%)
19	PGV	C	267	-	50,50,50	1.06	2 (4%)	53,56,56	1.08	6 (11%)
18	TGL	A	521	-	62,62,62	1.01	3 (4%)	65,65,65	1.52	11 (16%)
24	DMU	Z	1526	-	34,34,34	3.37	8 (23%)	45,45,45	3.47	21 (46%)
18	TGL	A	523	-	62,62,62	1.17	5 (8%)	65,65,65	1.42	10 (15%)
25	PEK	G	1263	-	52,52,52	2.36	15 (28%)	55,57,57	1.39	7 (12%)
26	CDL	C	270	-	99,99,99	1.26	13 (13%)	105,111,111	1.04	7 (6%)
19	PGV	P	1268	-	50,50,50	1.65	9 (18%)	53,56,56	0.89	2 (3%)
26	CDL	T	1269	-	99,99,99	1.48	15 (15%)	105,111,111	1.05	9 (8%)
25	PEK	T	1264	-	52,52,52	2.18	14 (26%)	55,57,57	1.54	10 (18%)
19	PGV	C	268	-	50,50,50	1.64	8 (16%)	53,56,56	0.93	2 (3%)
23	CHD	P	1525	-	32,32,32	1.53	5 (15%)	51,51,51	2.07	14 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
21	CUA	O	228	2	0,1,1	-	-	-	-	-
25	PEK	P	1265	-	52,52,52	1.87	12 (23%)	55,57,57	1.09	5 (9%)
19	PGV	P	1267	-	50,50,50	1.12	4 (8%)	53,56,56	0.88	2 (3%)
25	PEK	C	265	-	52,52,52	1.93	12 (23%)	55,57,57	1.12	5 (9%)
25	PEK	T	263	-	52,52,52	2.38	14 (26%)	55,57,57	1.39	8 (14%)
26	CDL	G	269	-	99,99,99	1.57	16 (16%)	105,111,111	1.04	7 (6%)
19	PGV	A	525	-	50,50,50	1.13	5 (10%)	53,56,56	0.99	2 (3%)
25	PEK	C	264	-	52,52,52	2.09	12 (23%)	55,57,57	1.55	11 (20%)
17	HEA	N	516	1	67,67,67	1.50	6 (8%)	81,103,103	1.92	25 (30%)

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
23	CHD	B	1086	-	-	2/9/74/74	0/4/4/4
18	TGL	O	1521	-	-	16/65/65/65	-
26	CDL	P	1270	-	-	71/110/110/110	-
17	HEA	A	515	1	-	11/36/76/76	-
22	PSC	B	230	-	-	34/55/55/55	-
23	CHD	P	1271	-	5/5/12/12	8/9/74/74	0/4/4/4
24	DMU	P	1272	-	6/6/10/10	11/19/59/59	0/2/2/2
18	TGL	Y	1522	-	-	17/65/65/65	-
24	DMU	C	272	-	6/6/10/10	10/19/59/59	0/2/2/2
17	HEA	N	515	1	-	11/36/76/76	-
18	TGL	N	1523	-	-	17/65/65/65	-
19	PGV	N	1266	-	-	11/55/55/55	-
23	CHD	J	60	-	5/5/12/12	8/9/74/74	0/4/4/4
18	TGL	L	522	-	-	15/65/65/65	-
23	CHD	C	525	-	-	2/9/74/74	0/4/4/4
23	CHD	C	271	-	5/5/12/12	8/9/74/74	0/4/4/4
19	PGV	N	1524	-	-	33/55/55/55	-
17	HEA	A	516	1	-	9/36/76/76	-
22	PSC	O	1230	-	-	34/55/55/55	-
19	PGV	A	524	-	-	33/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CHD	W	1060	-	5/5/12/12	8/9/74/74	0/4/4/4
23	CHD	G	86	-	-	2/9/74/74	0/4/4/4
24	DMU	M	526	-	5/5/10/10	9/19/59/59	0/2/2/2
19	PGV	C	267	-	-	18/55/55/55	-
18	TGL	A	521	-	-	14/65/65/65	-
24	DMU	Z	1526	-	5/5/10/10	9/19/59/59	0/2/2/2
18	TGL	A	523	-	-	17/65/65/65	-
25	PEK	G	1263	-	-	29/56/56/56	-
26	CDL	C	270	-	-	69/110/110/110	-
19	PGV	P	1268	-	-	35/55/55/55	-
26	CDL	T	1269	-	-	66/110/110/110	-
25	PEK	T	1264	-	-	22/56/56/56	-
19	PGV	C	268	-	-	34/55/55/55	-
23	CHD	P	1525	-	-	2/9/74/74	0/4/4/4
25	PEK	P	1265	-	-	17/56/56/56	-
19	PGV	P	1267	-	-	18/55/55/55	-
25	PEK	C	265	-	-	19/56/56/56	-
25	PEK	T	263	-	-	29/56/56/56	-
26	CDL	G	269	-	-	65/110/110/110	-
19	PGV	A	525	-	-	11/55/55/55	-
25	PEK	C	264	-	-	22/56/56/56	-
17	HEA	N	516	1	-	9/36/76/76	-

The worst 5 of 345 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Z	1526	DMU	O16-C6	-8.64	1.25	1.40
24	M	526	DMU	O16-C6	-8.38	1.26	1.40
24	M	526	DMU	O7-C3	-7.89	1.23	1.43
24	Z	1526	DMU	O7-C3	-7.62	1.24	1.43
17	N	516	HEA	FE-ND	-7.61	1.71	1.94

The worst 5 of 501 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	P	1272	DMU	O16-C6-C1	11.48	125.71	108.27
23	P	1271	CHD	C10-C9-C8	11.40	124.55	111.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	271	CHD	C10-C9-C8	11.28	124.42	111.84
23	J	60	CHD	C13-C17-C20	9.89	131.46	119.48
24	C	272	DMU	O16-C6-C1	9.56	122.80	108.27

5 of 42 chirality outliers are listed below:

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

5 of 885 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	A	515	HEA	C2A-C3A-CMA-OMA
17	A	515	HEA	C4A-C3A-CMA-OMA
17	N	515	HEA	C2A-C3A-CMA-OMA
17	N	515	HEA	C4A-C3A-CMA-OMA
18	A	521	TGL	CB2-CB1-OG2-CG2

There are no ring outliers.

42 monomers are involved in 347 short contacts:

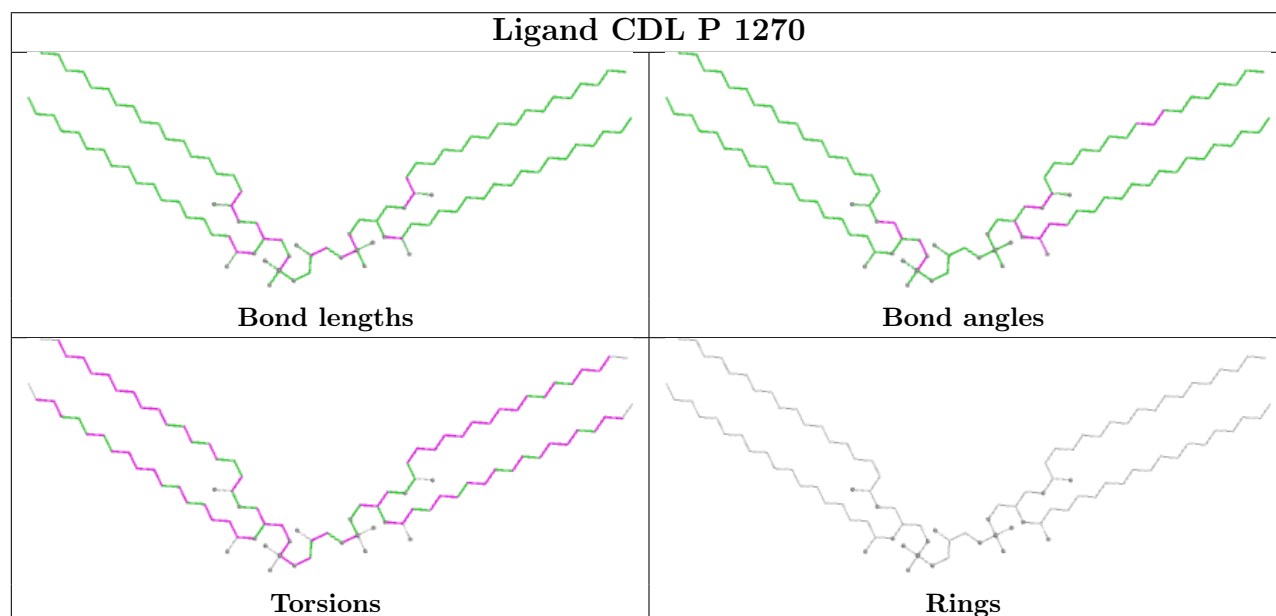
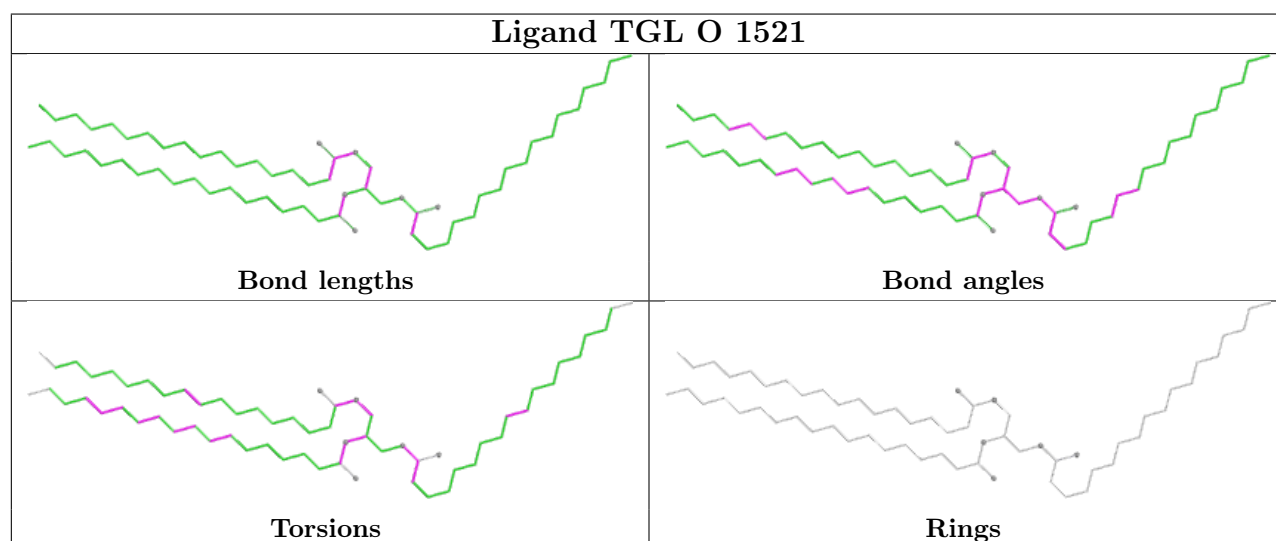
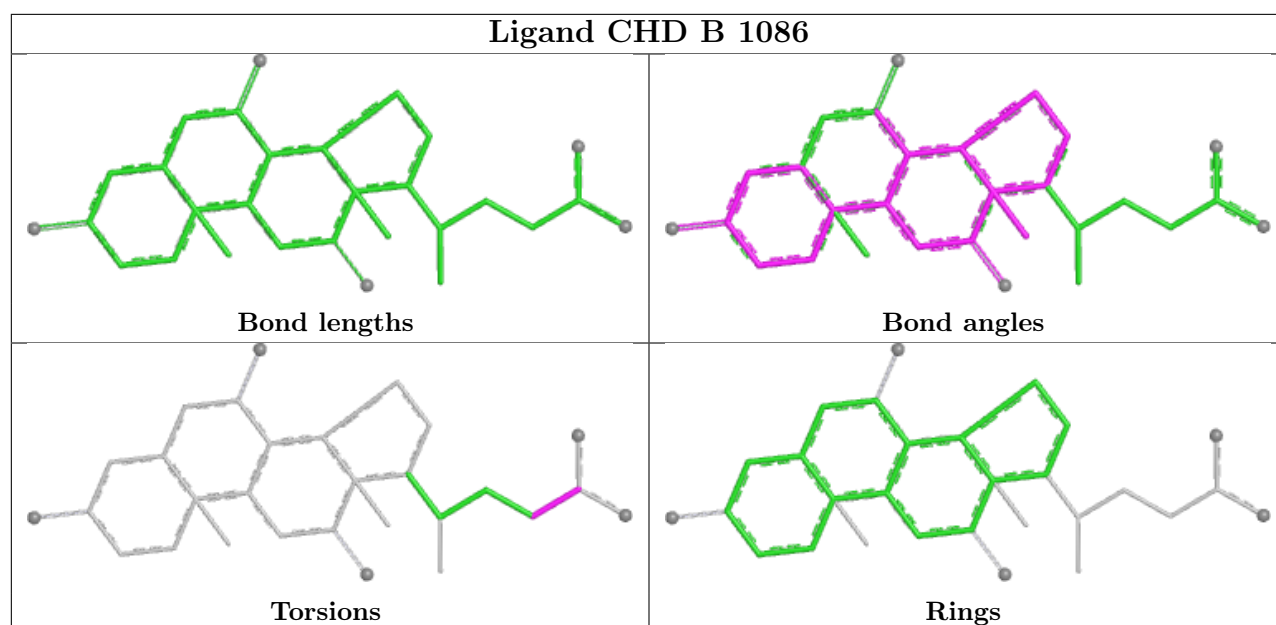
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	1086	CHD	5	0
18	O	1521	TGL	8	0
26	P	1270	CDL	17	0
17	A	515	HEA	15	0
22	B	230	PSC	21	0
23	P	1271	CHD	5	0
24	P	1272	DMU	4	0
18	Y	1522	TGL	16	0
24	C	272	DMU	3	0
17	N	515	HEA	12	0
18	N	1523	TGL	9	0
19	N	1266	PGV	3	0
23	J	60	CHD	4	0
18	L	522	TGL	20	0
23	C	525	CHD	1	0
23	C	271	CHD	4	0

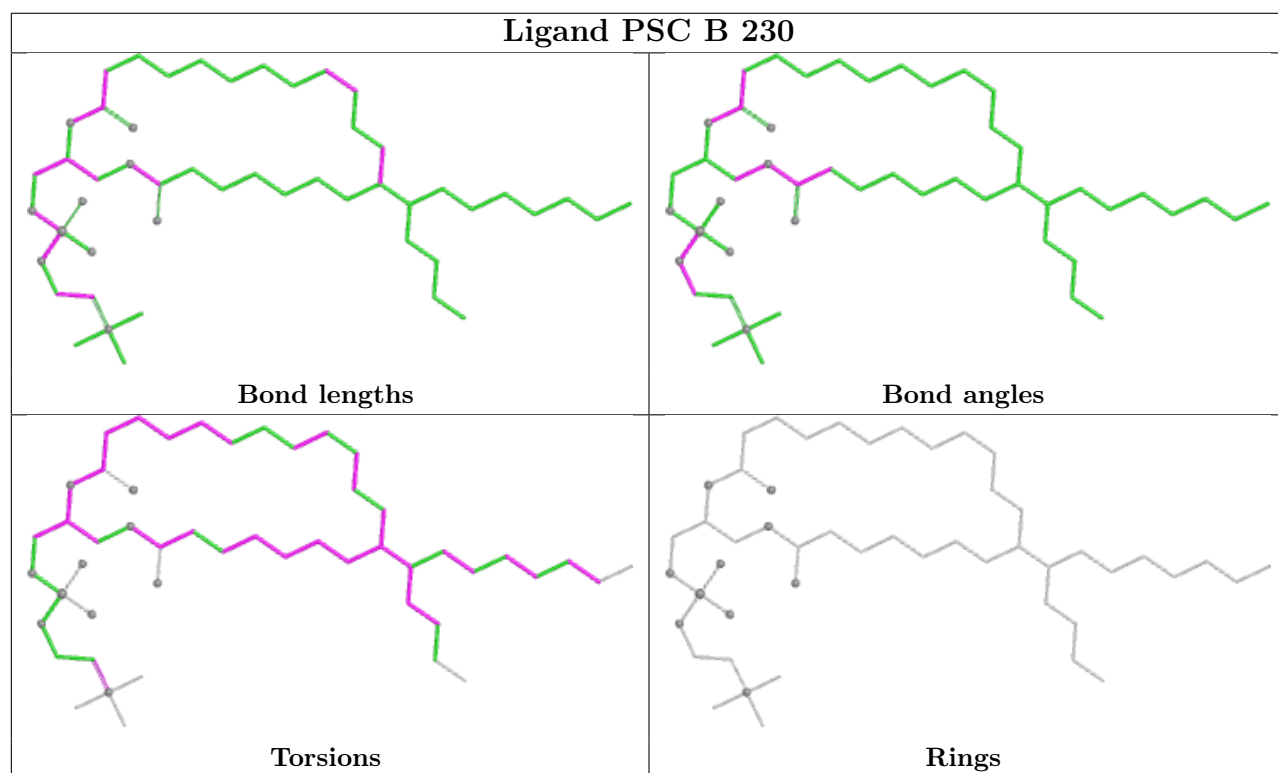
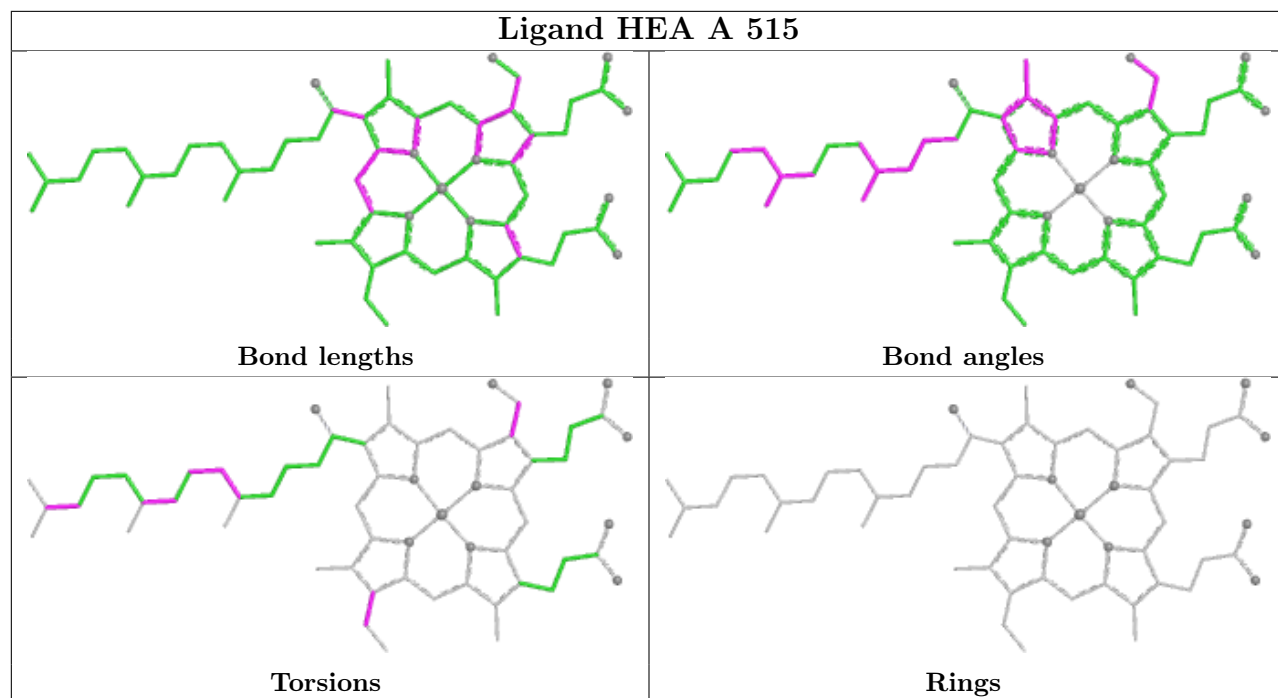
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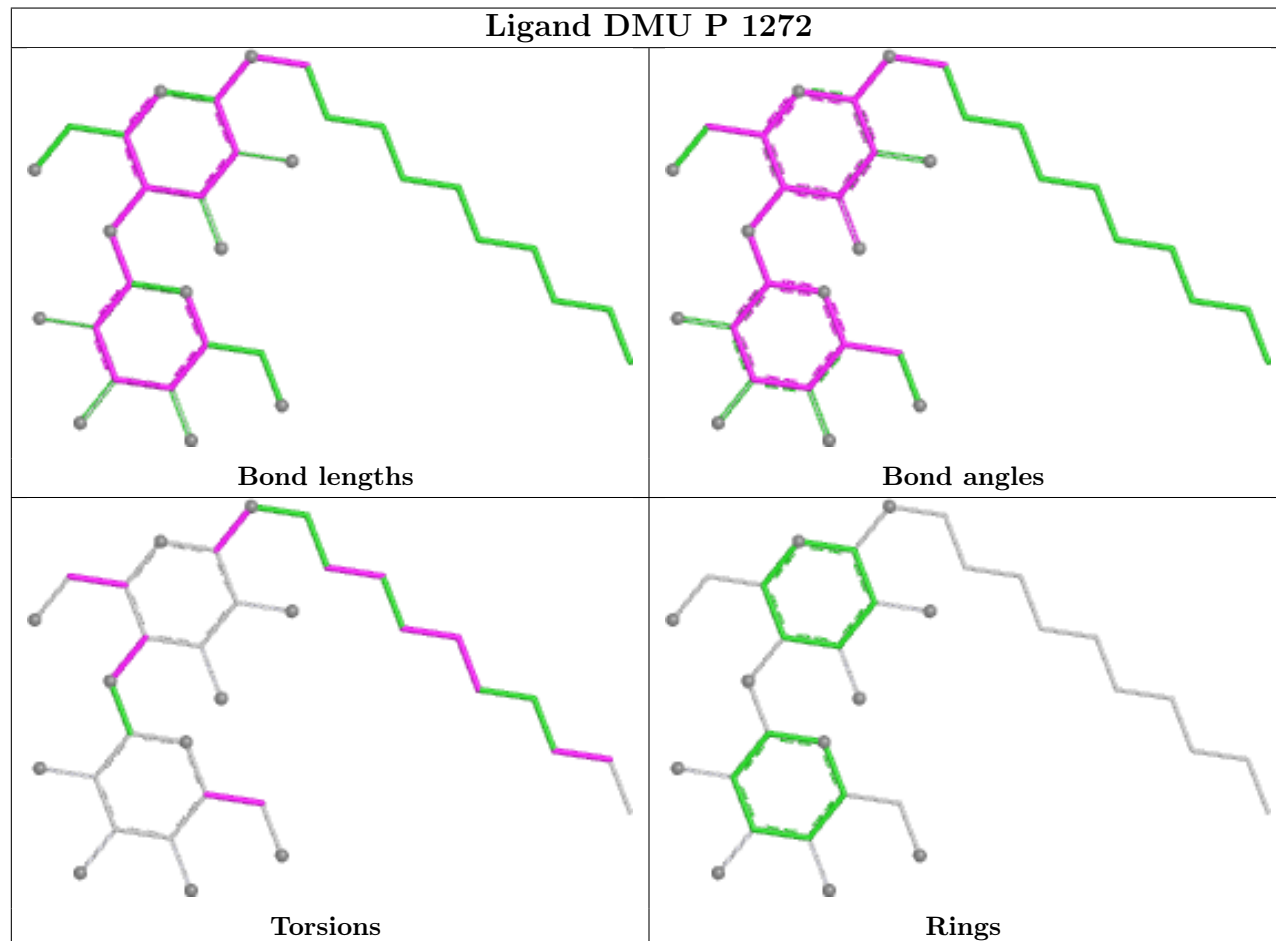
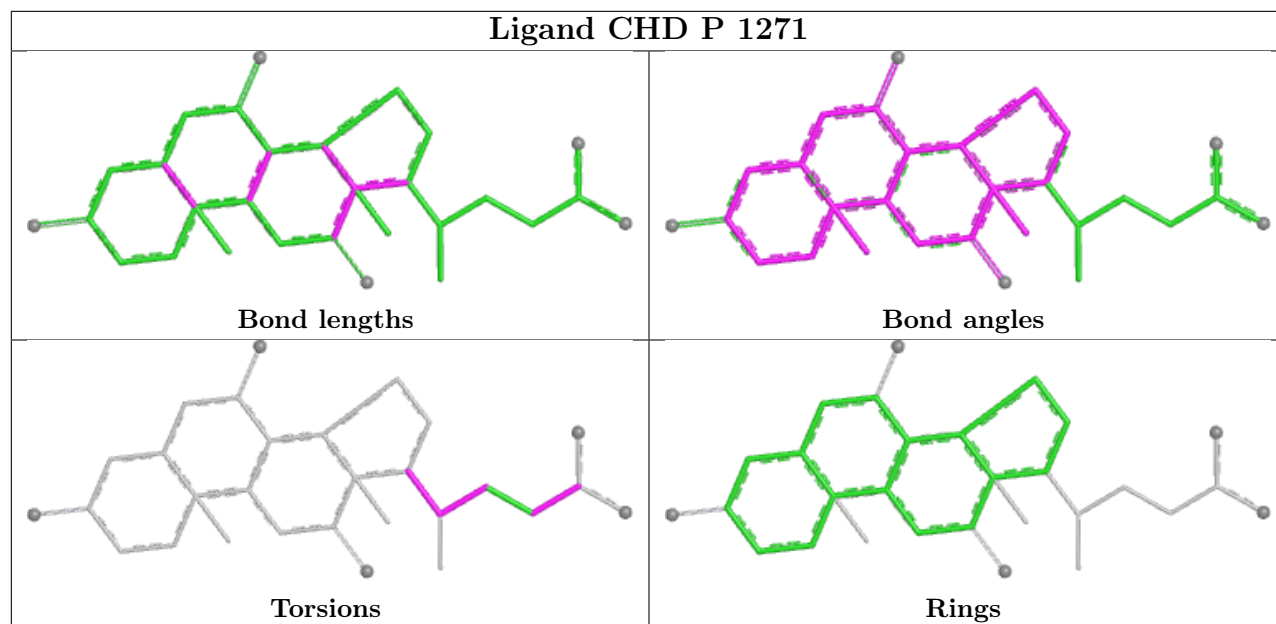
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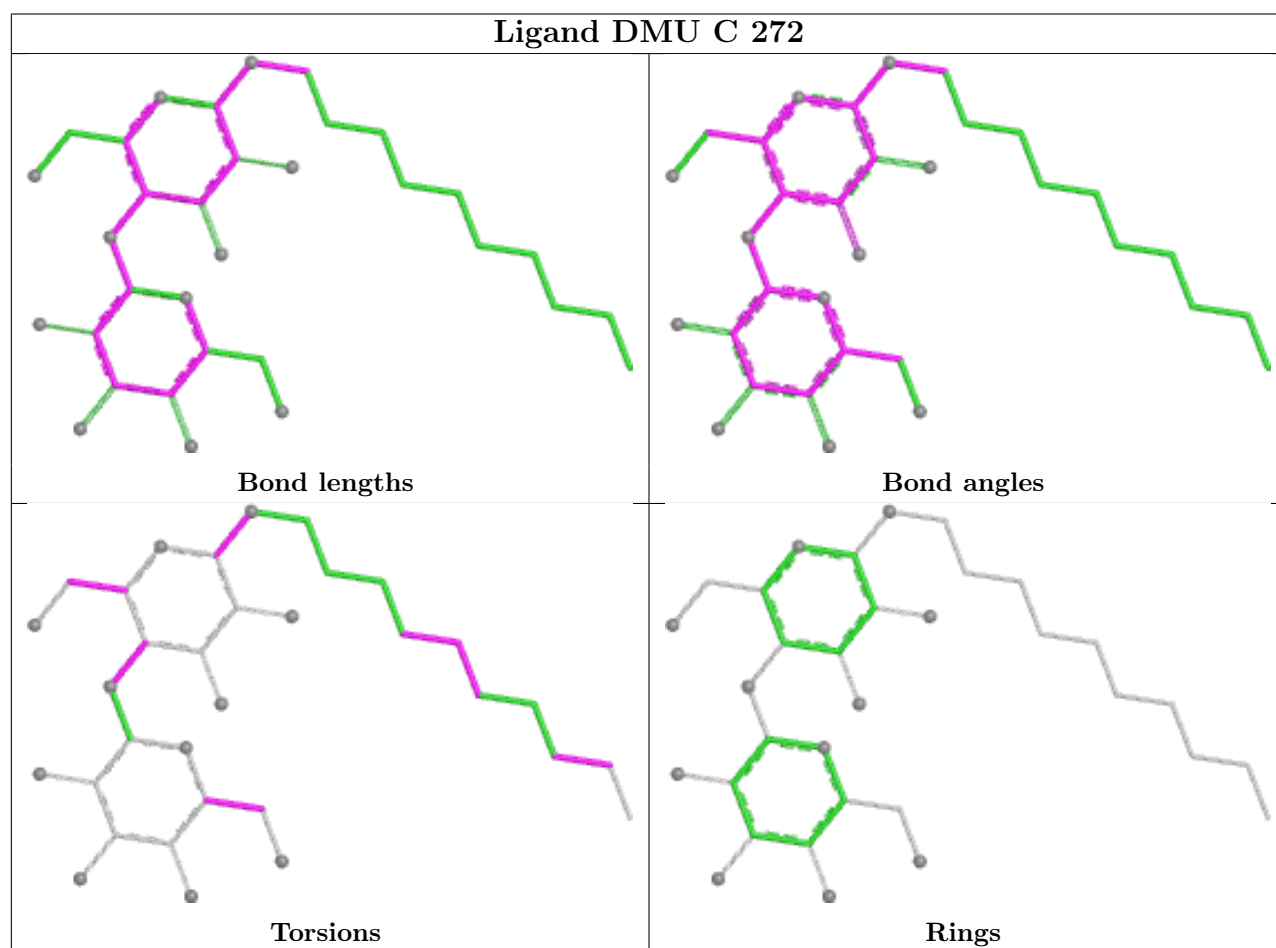
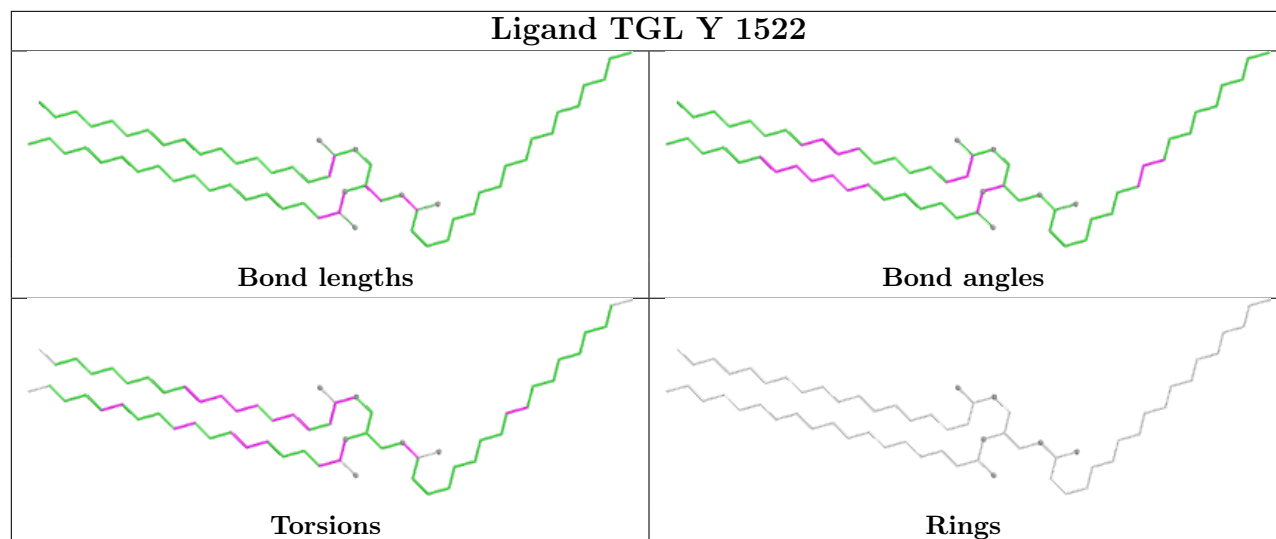
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	N	1524	PGV	7	0
17	A	516	HEA	2	0
22	O	1230	PSC	20	0
19	A	524	PGV	5	0
23	G	86	CHD	1	0
23	W	1060	CHD	3	0
24	M	526	DMU	2	0
19	C	267	PGV	6	0
18	A	521	TGL	8	0
24	Z	1526	DMU	1	0
18	A	523	TGL	4	0
25	G	1263	PEK	10	0
26	C	270	CDL	17	0
19	P	1268	PGV	2	0
26	T	1269	CDL	32	0
25	T	1264	PEK	12	0
19	C	268	PGV	1	0
23	P	1525	CHD	1	0
25	P	1265	PEK	10	0
19	P	1267	PGV	10	0
25	C	265	PEK	11	0
25	T	263	PEK	11	0
26	G	269	CDL	23	0
19	A	525	PGV	4	0
25	C	264	PEK	9	0
17	N	516	HEA	6	0

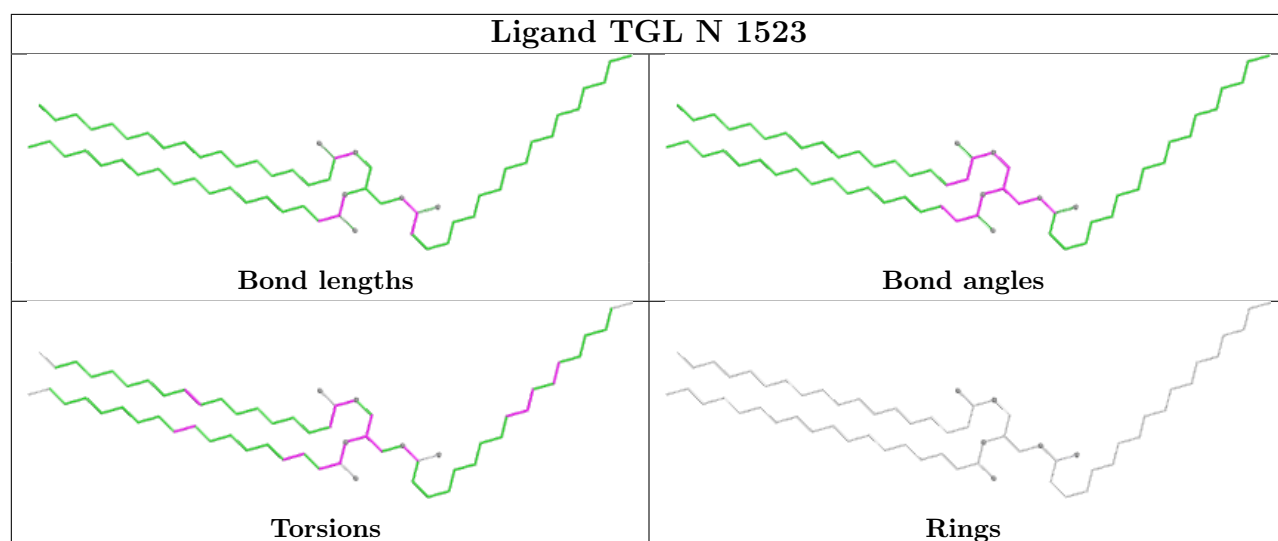
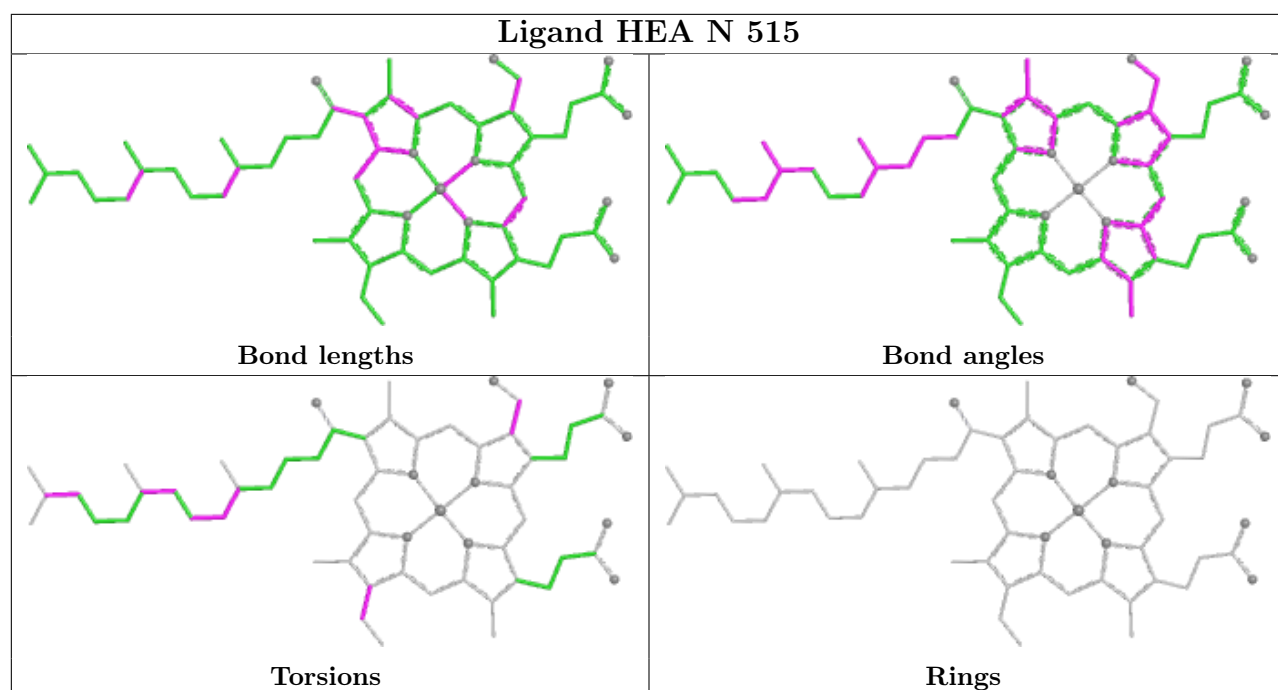
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

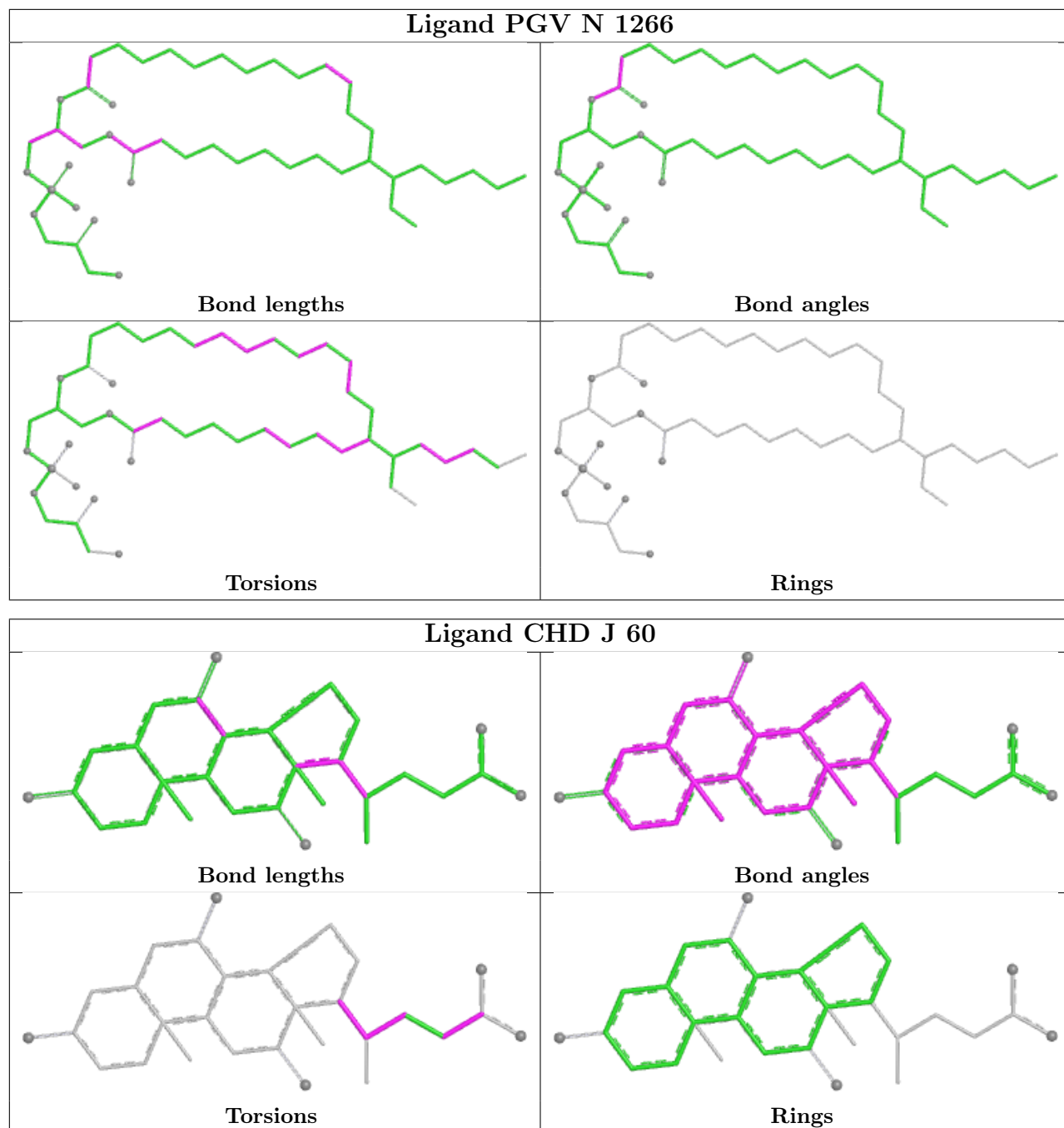


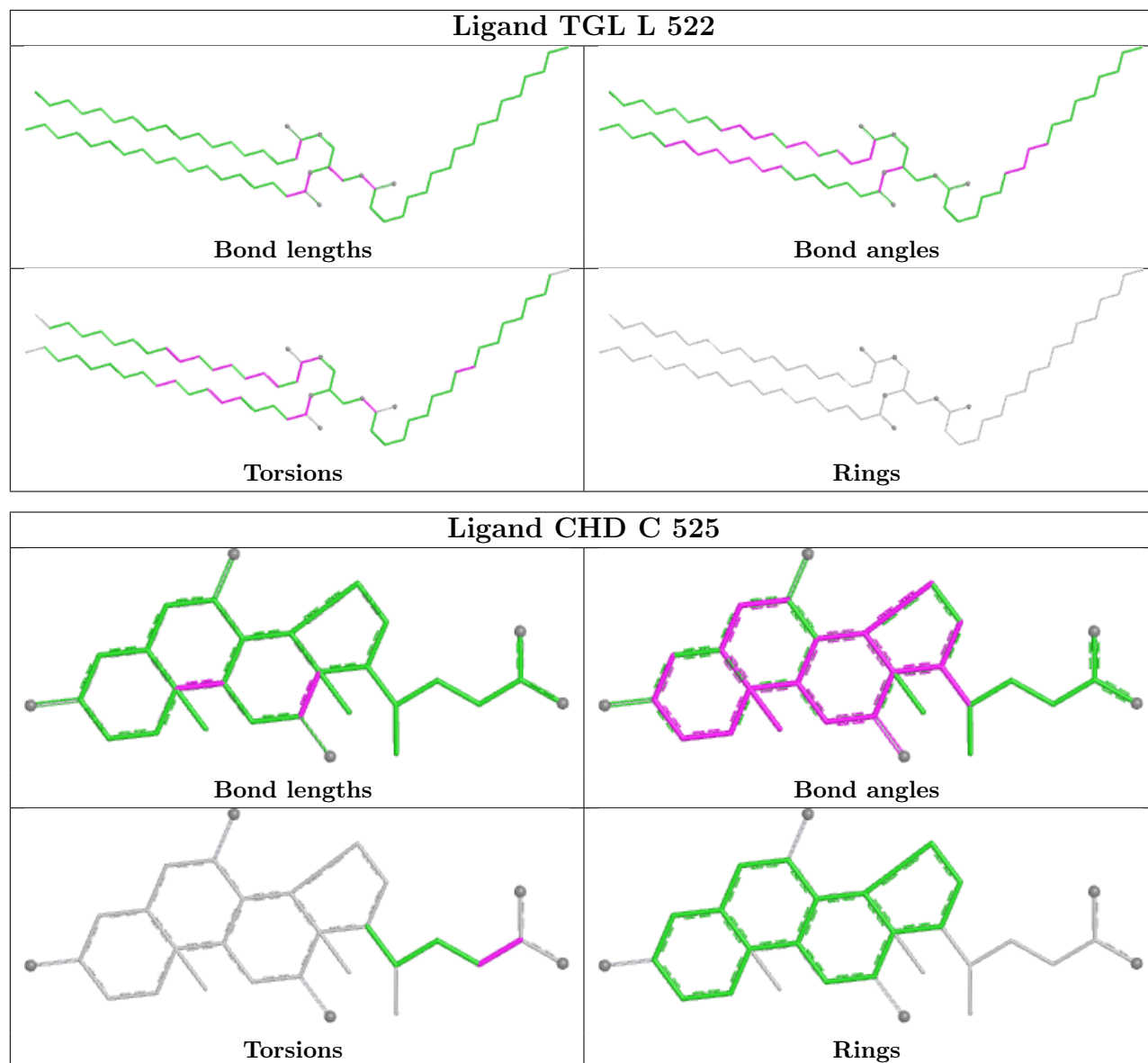


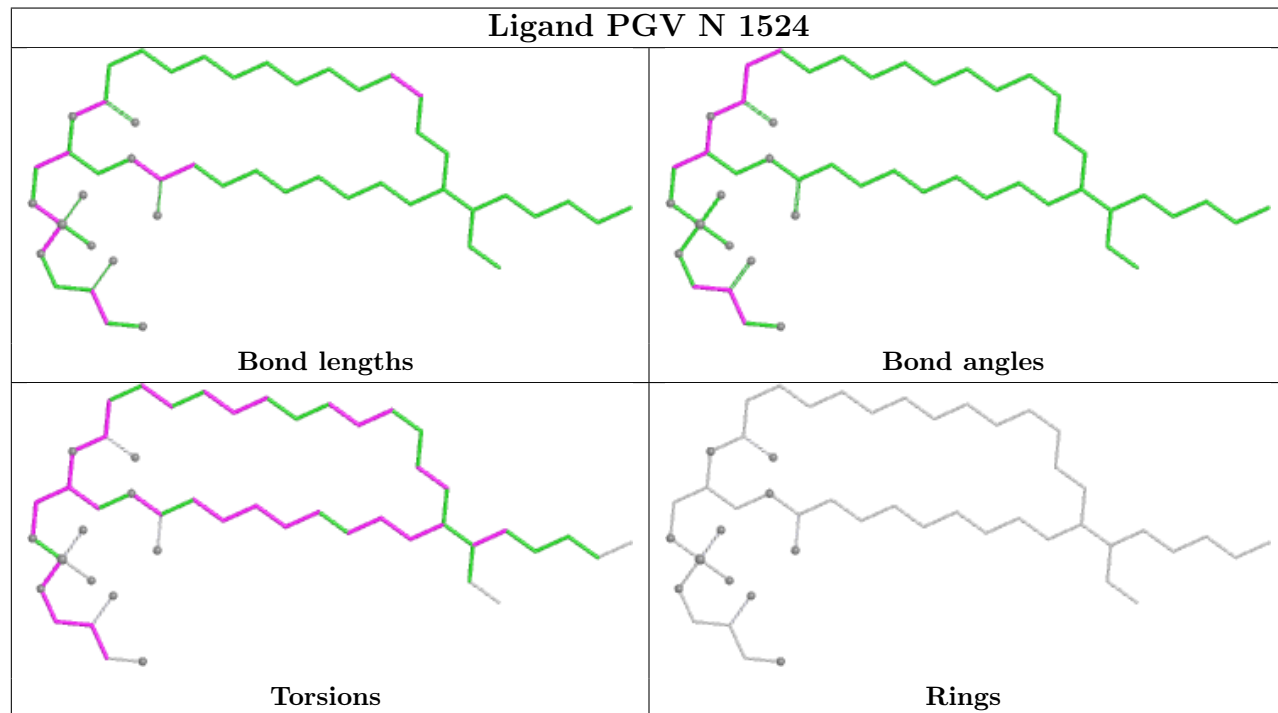
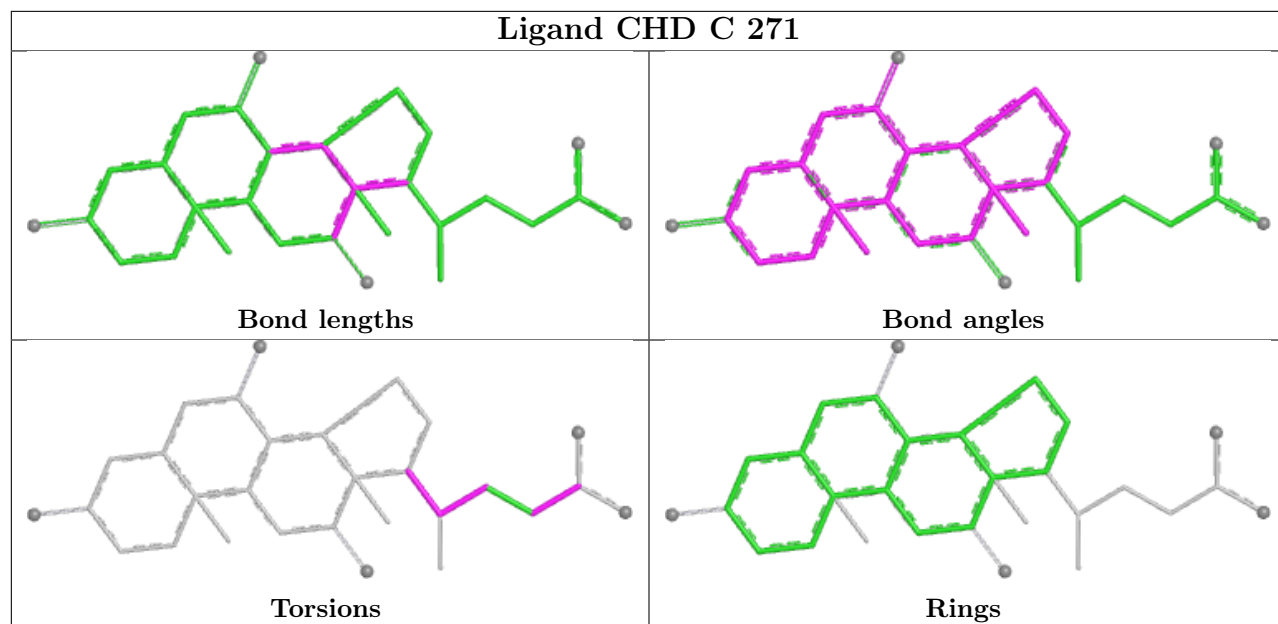


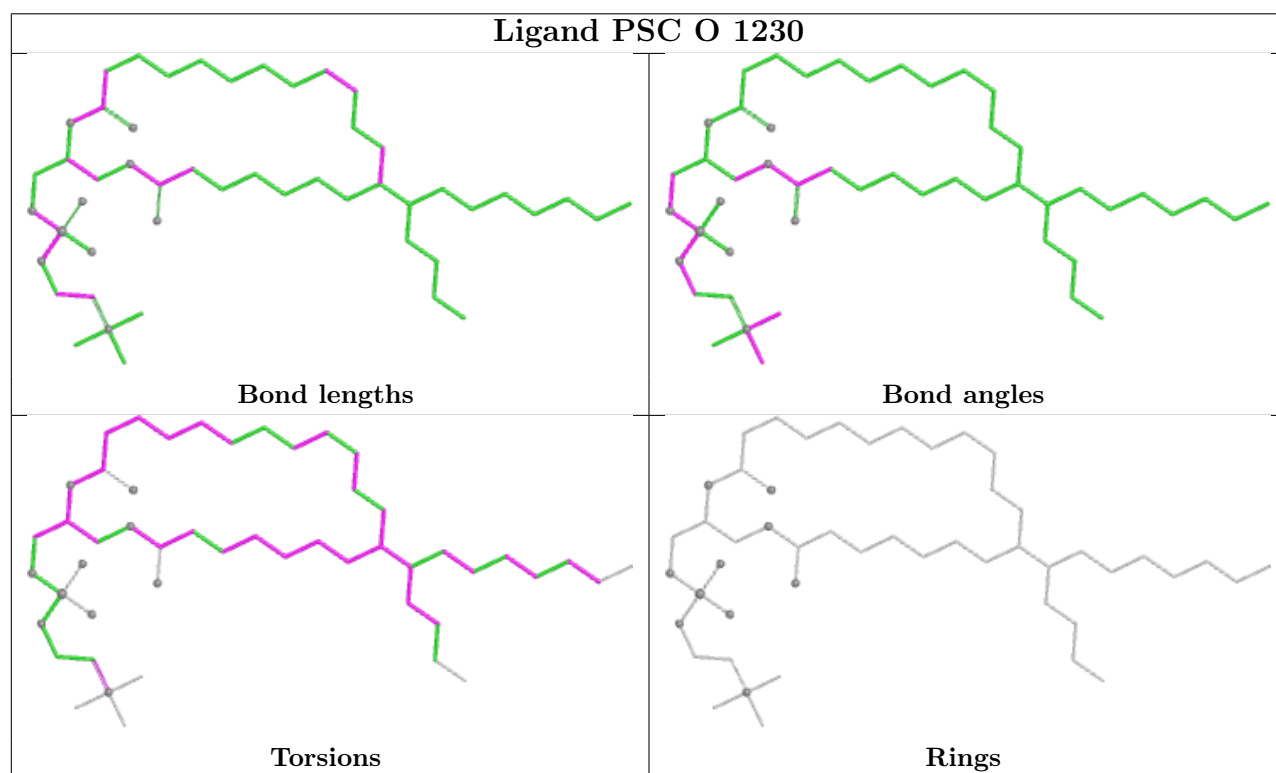
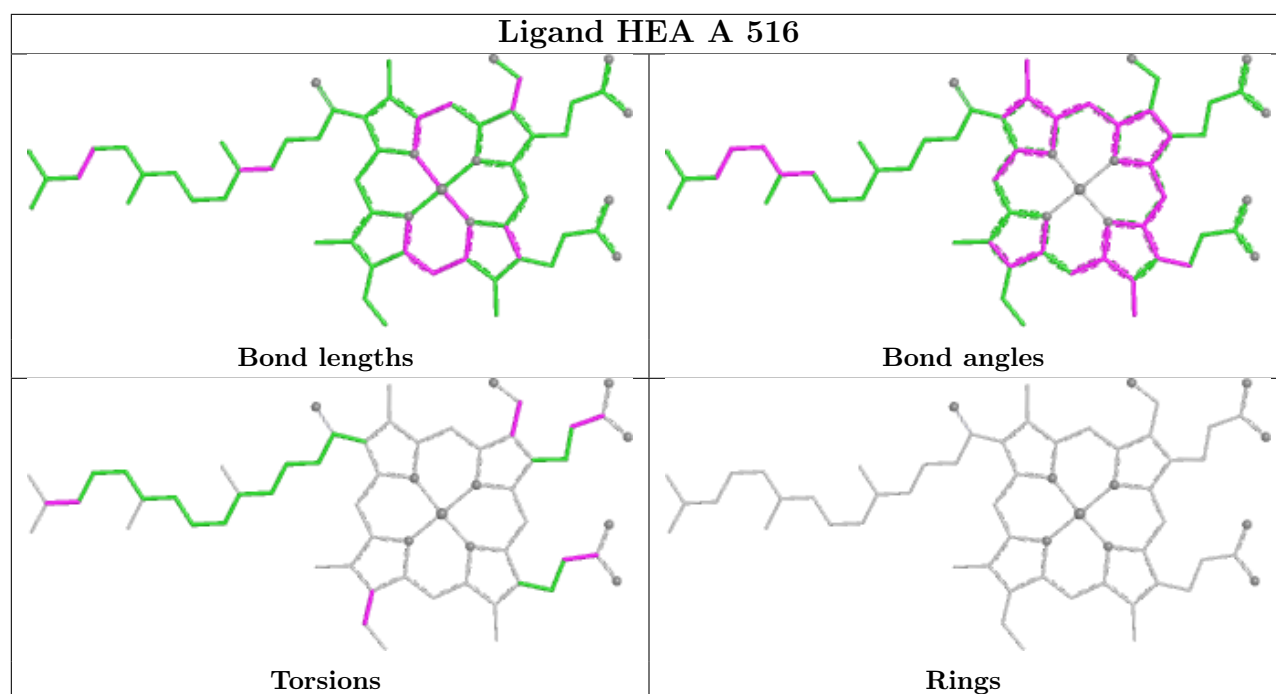


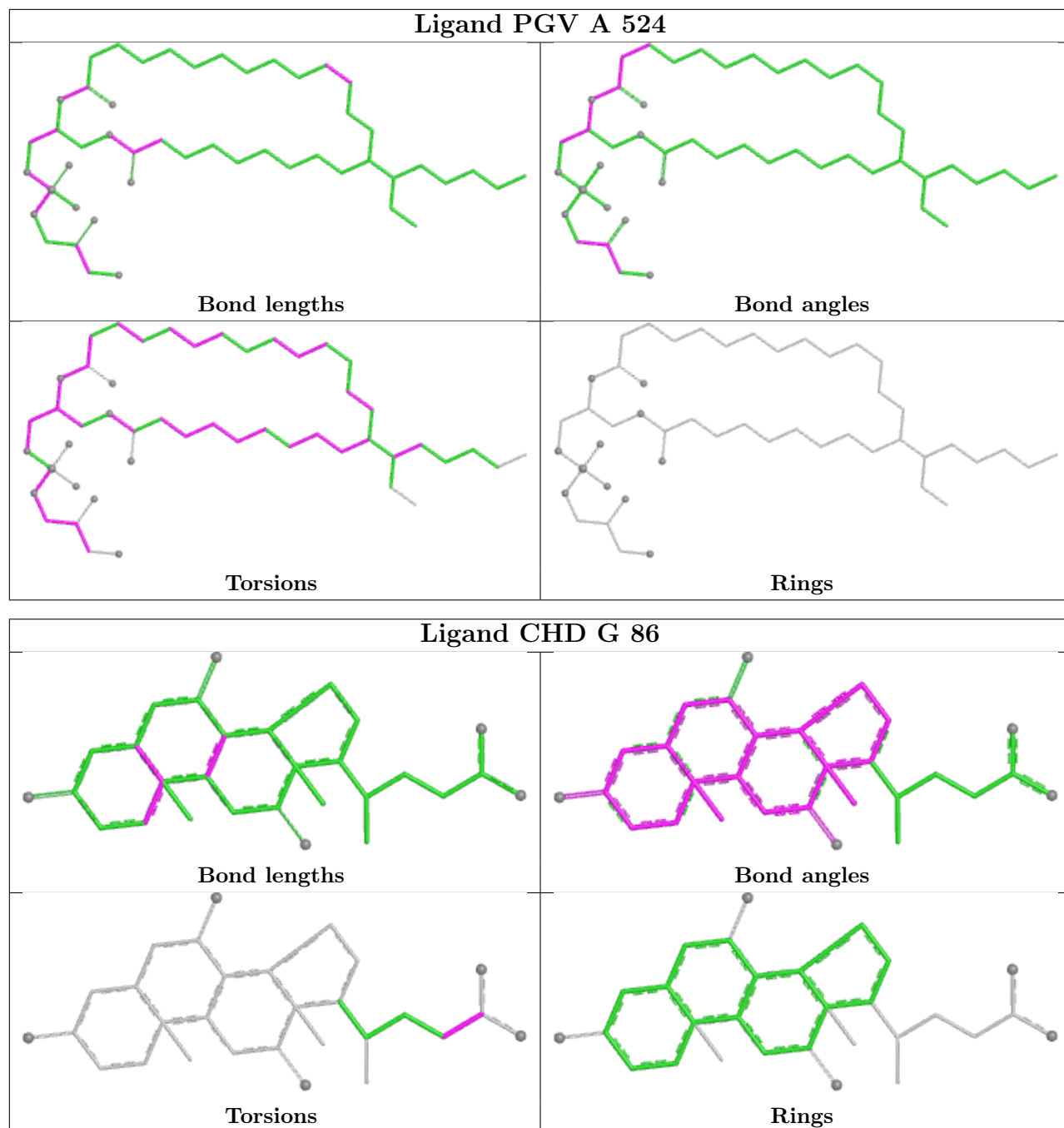


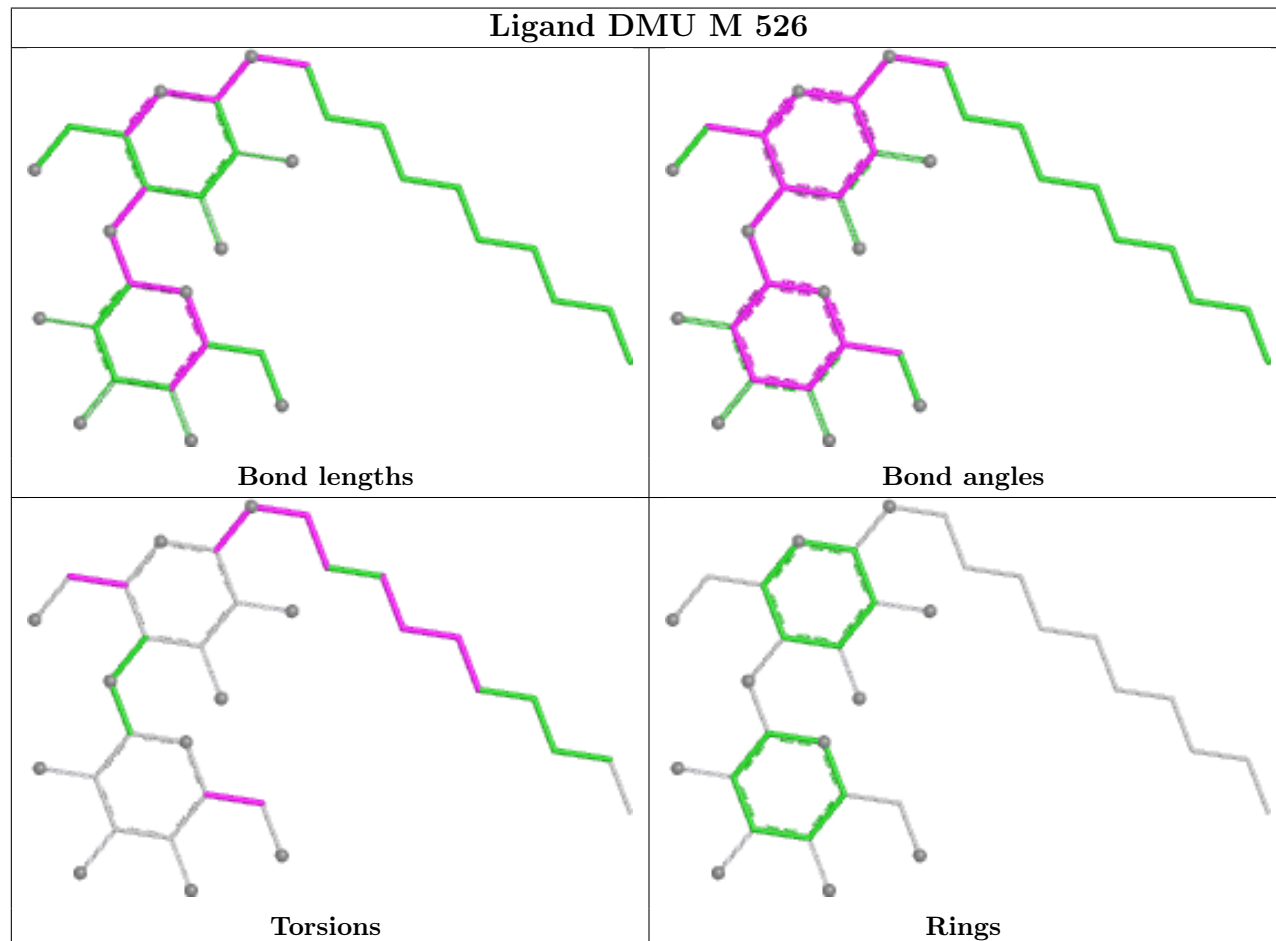
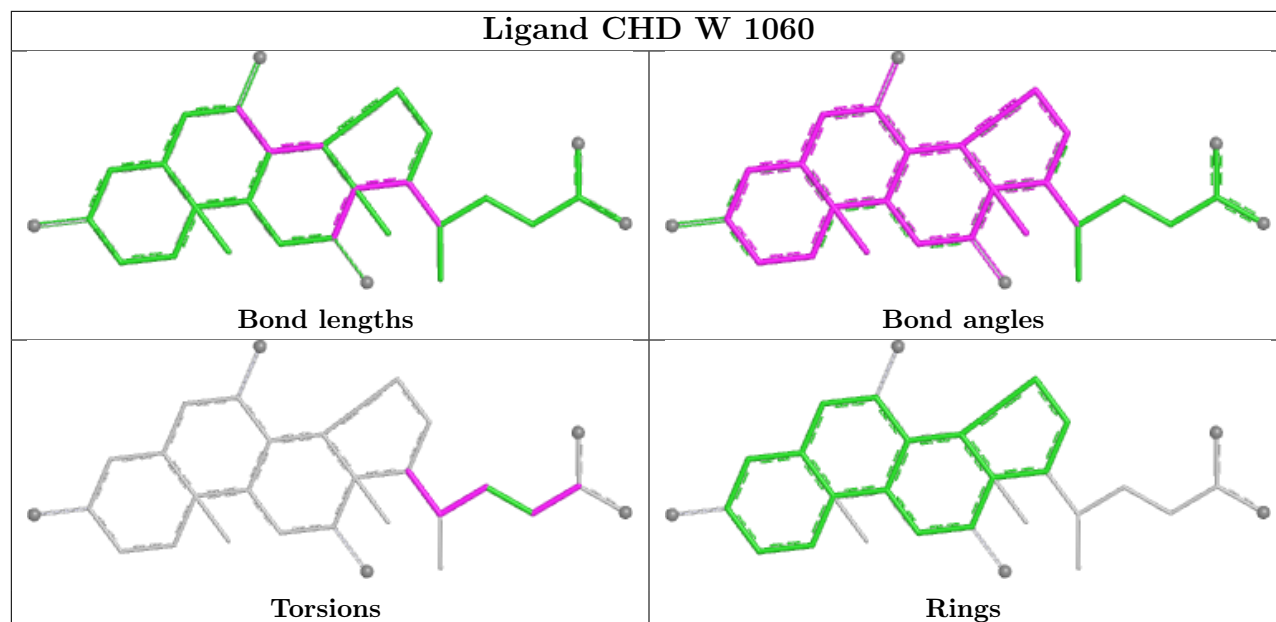


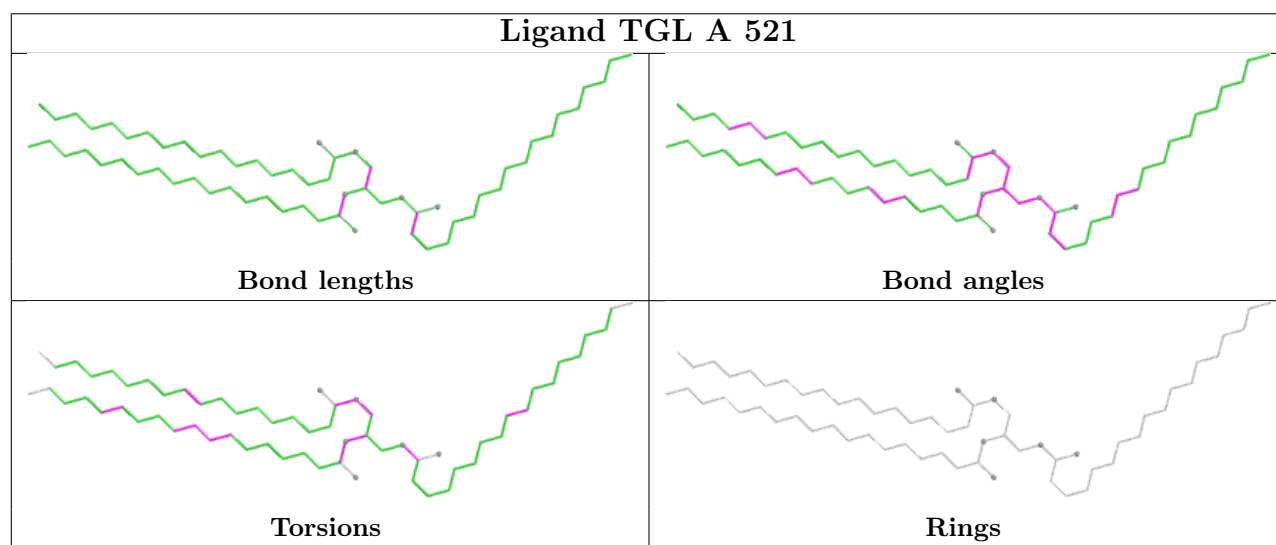
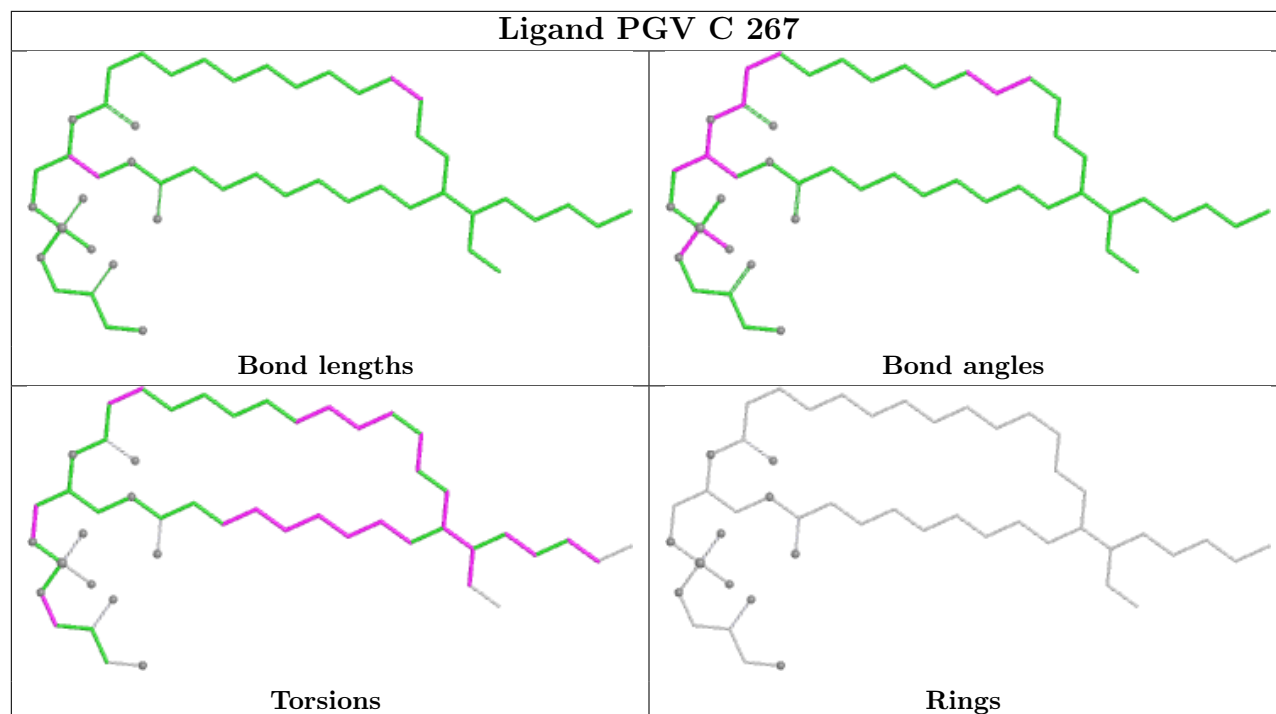


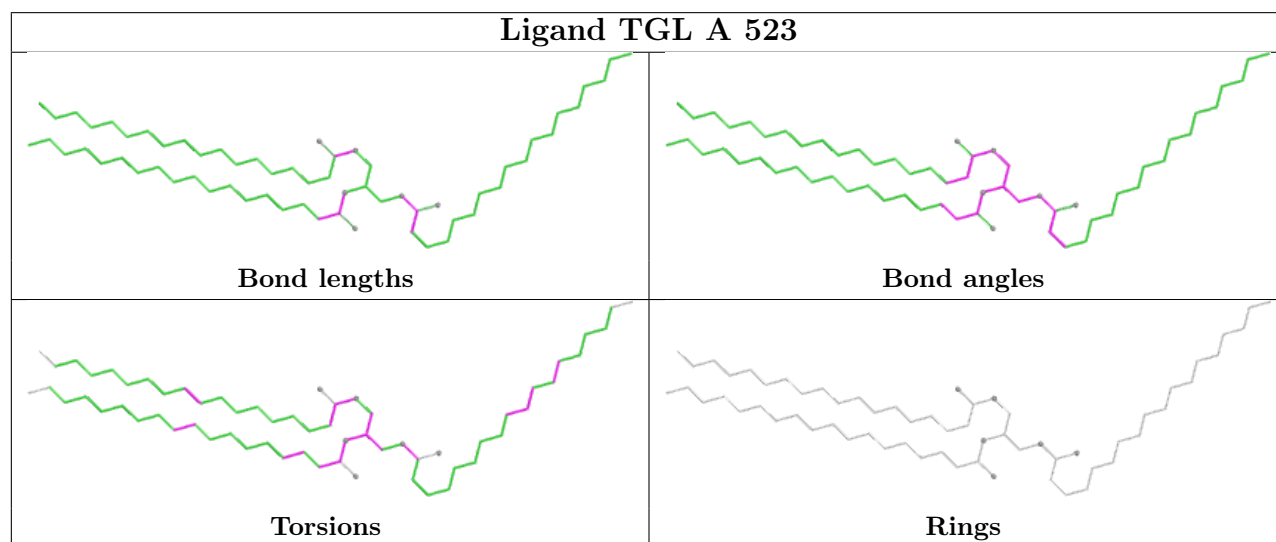
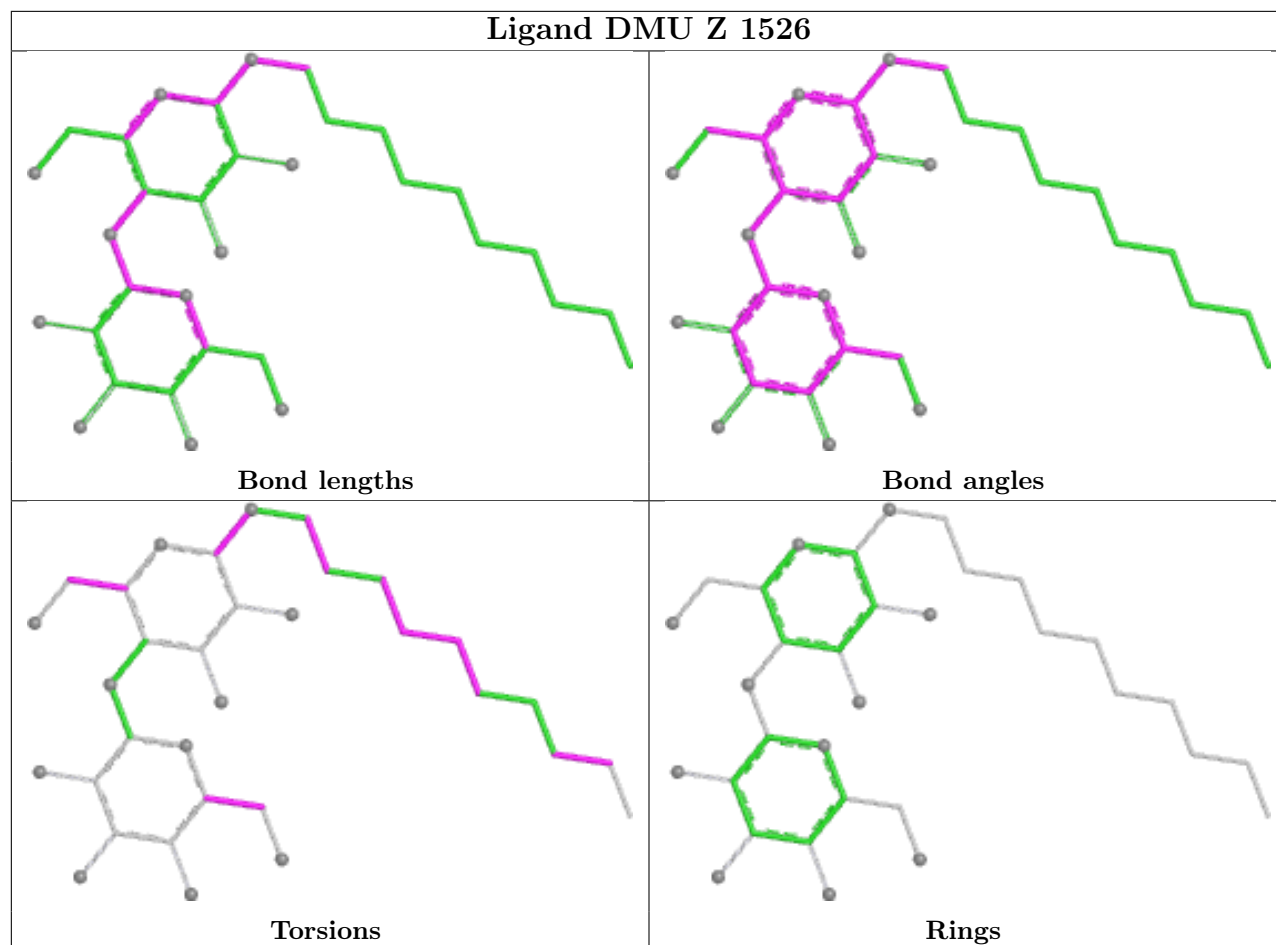


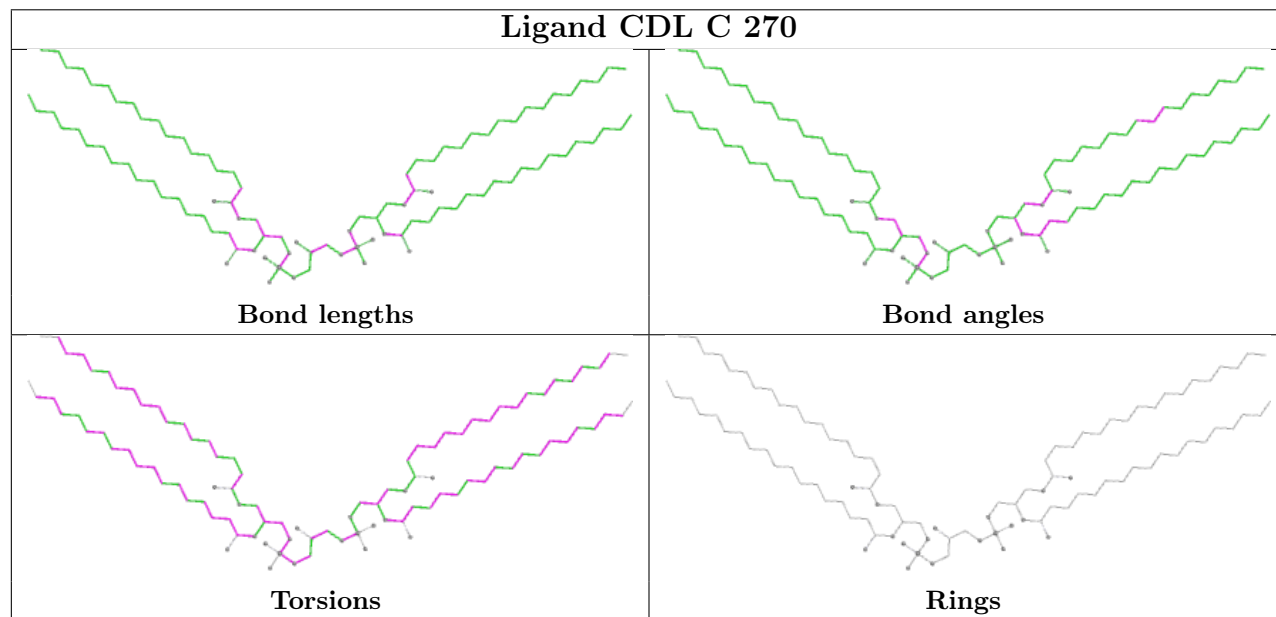
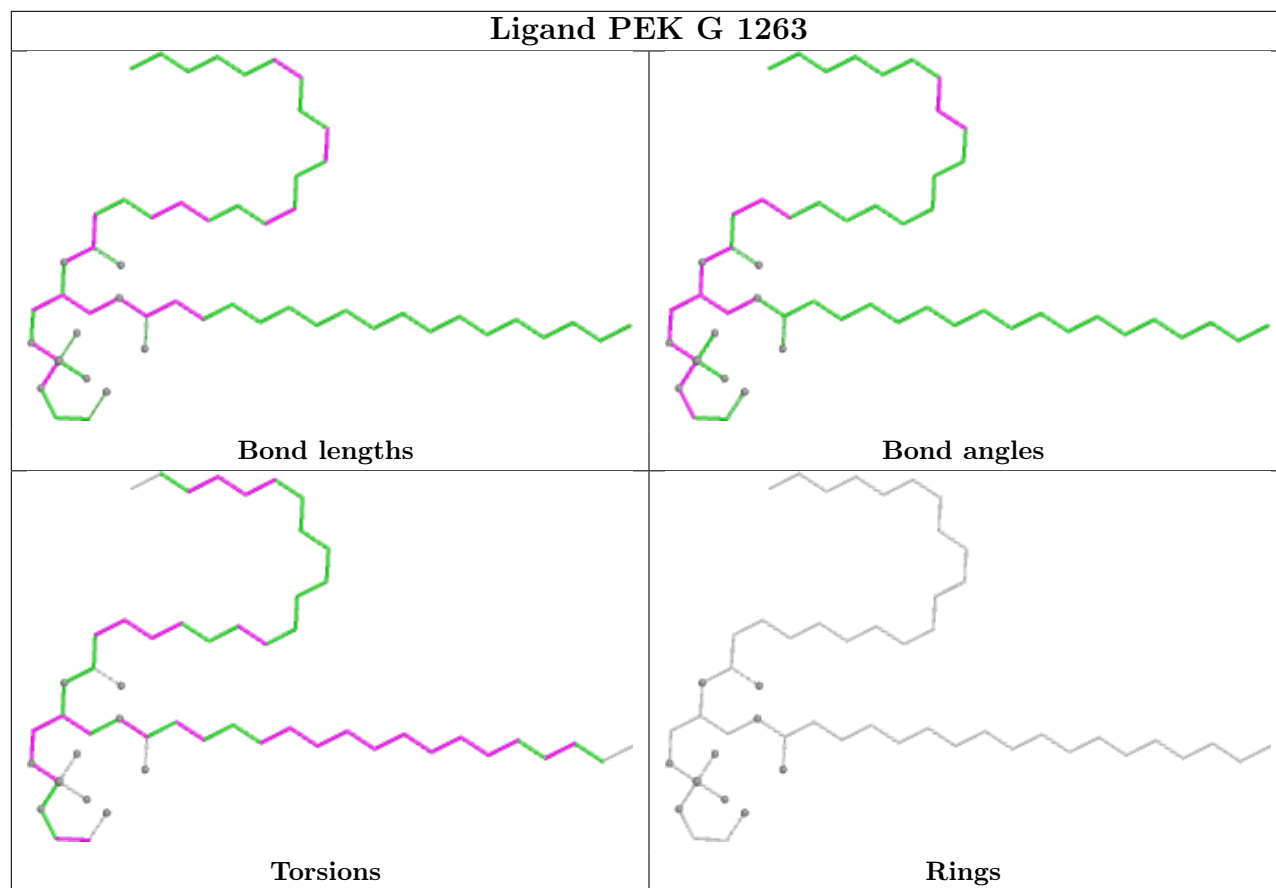


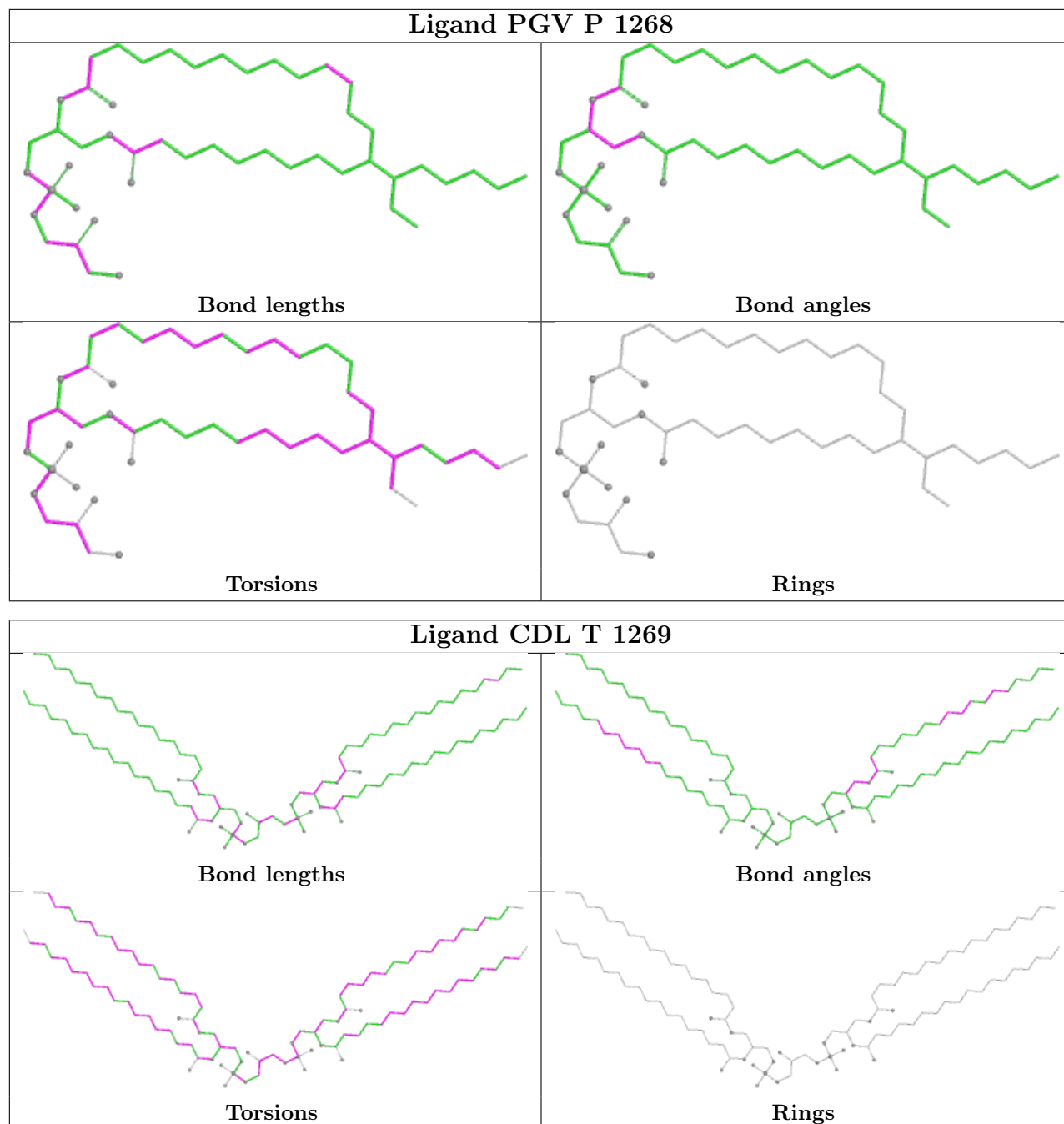


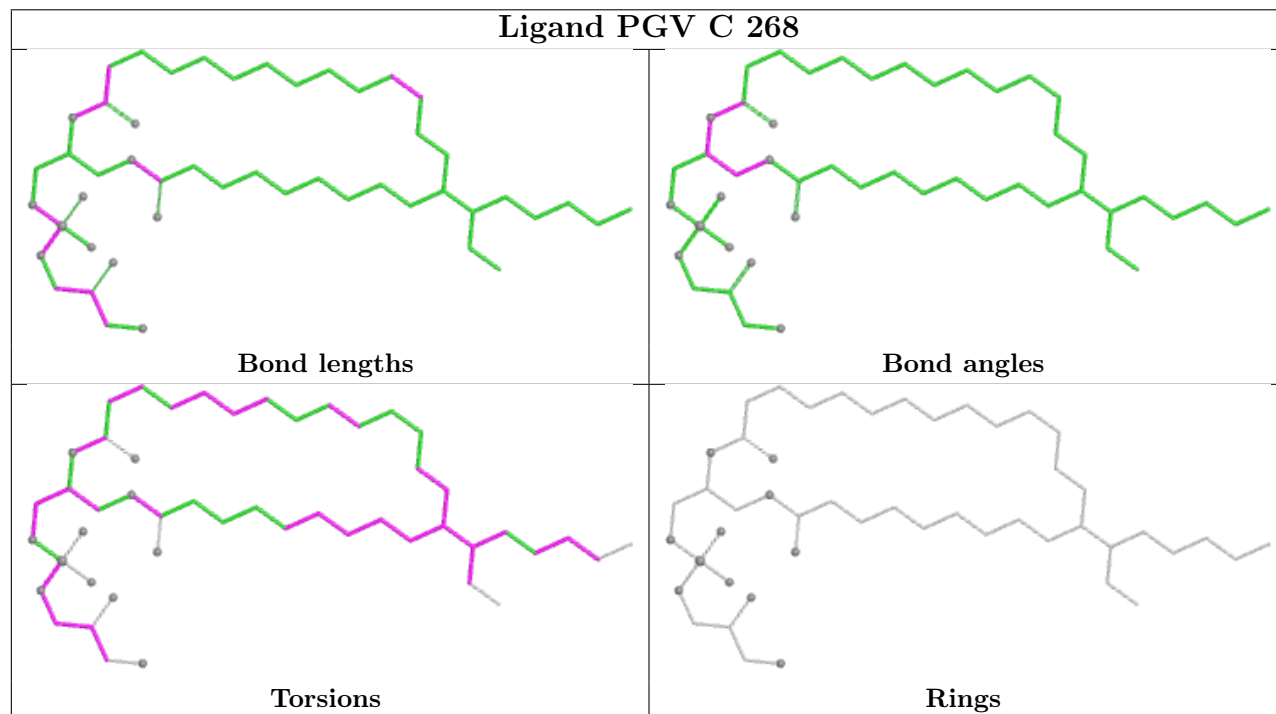
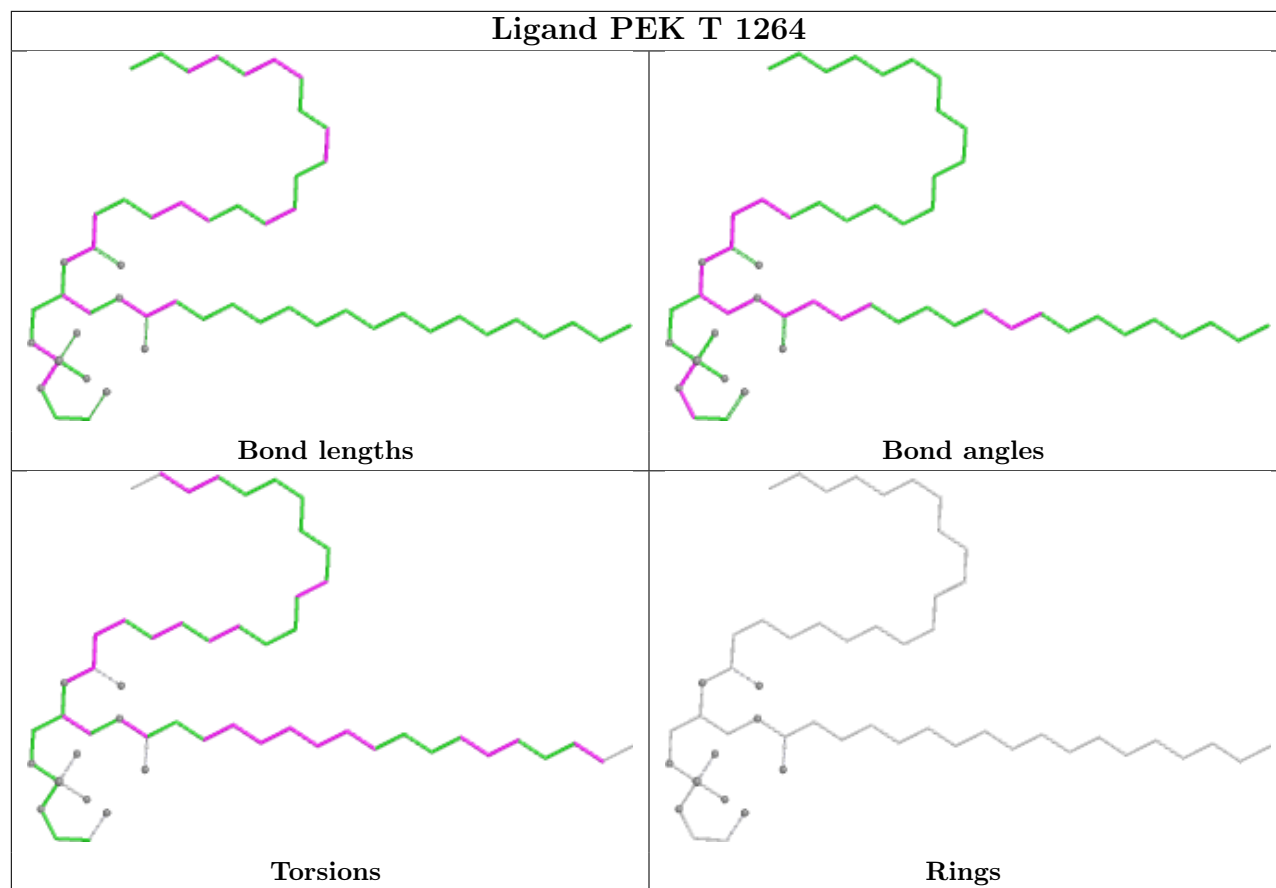


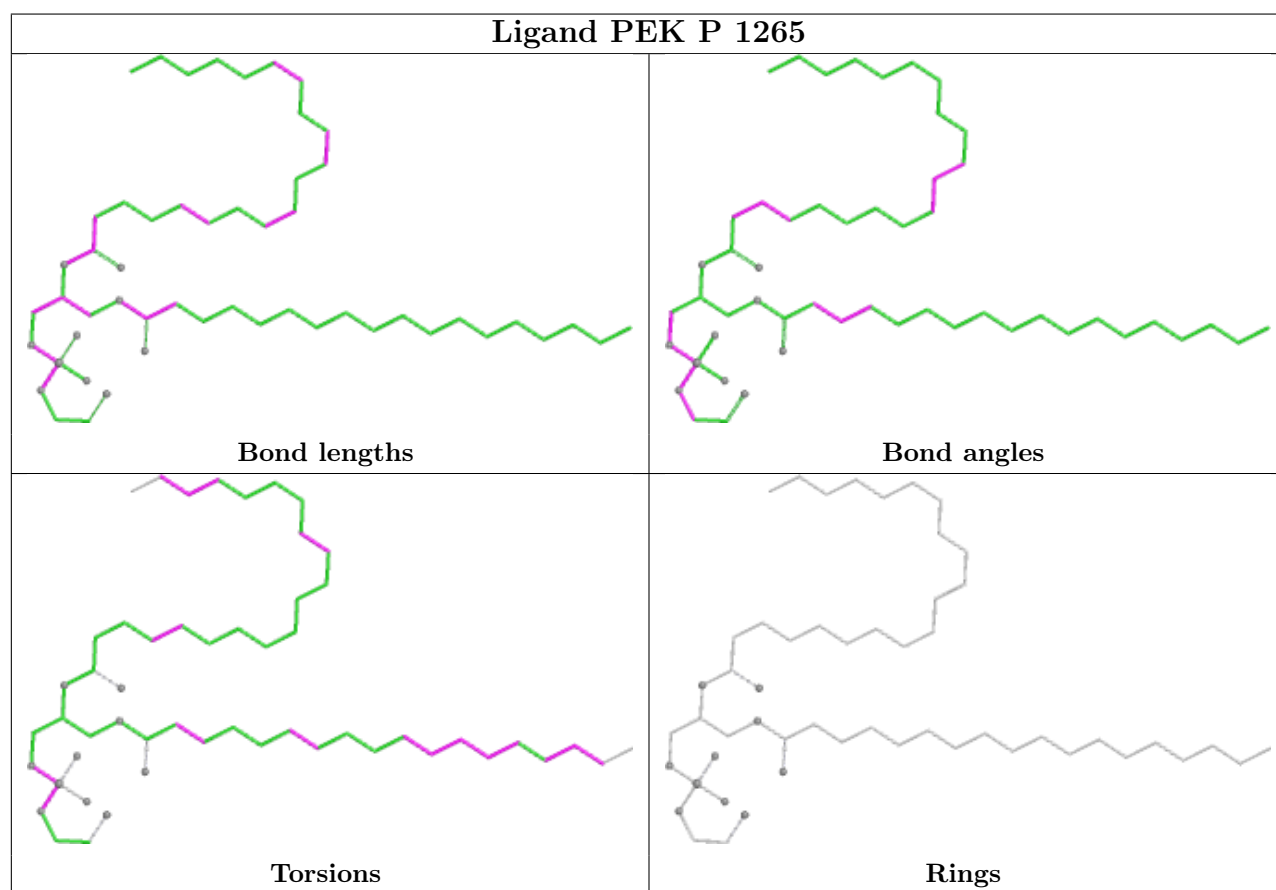
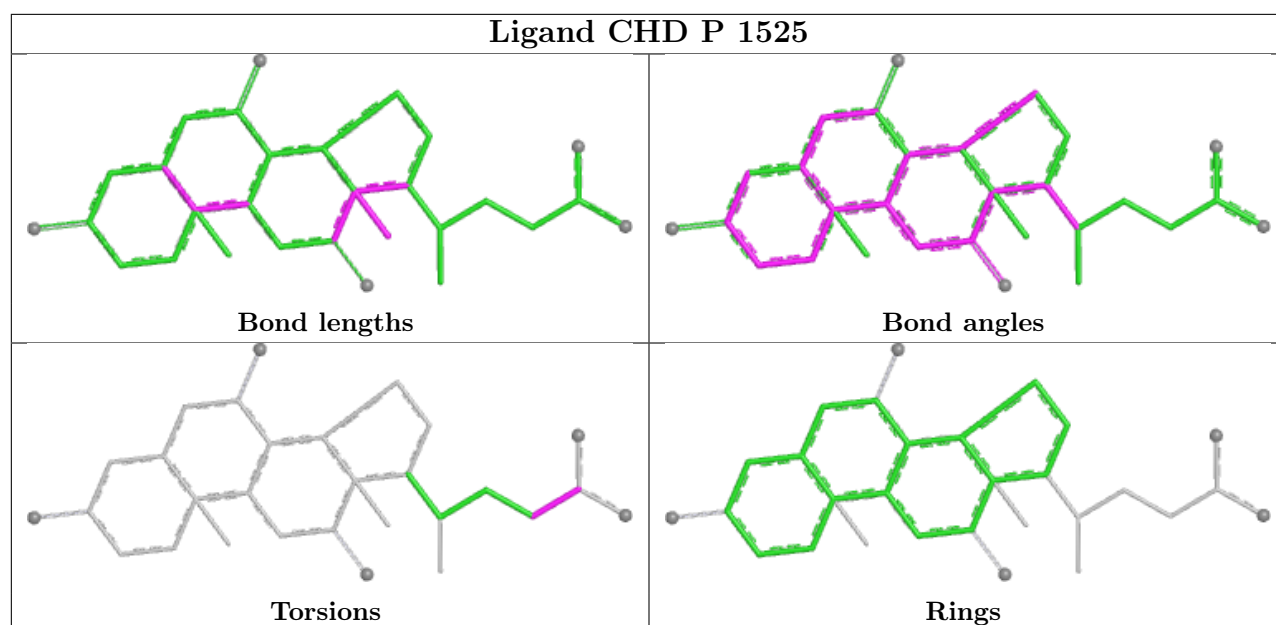


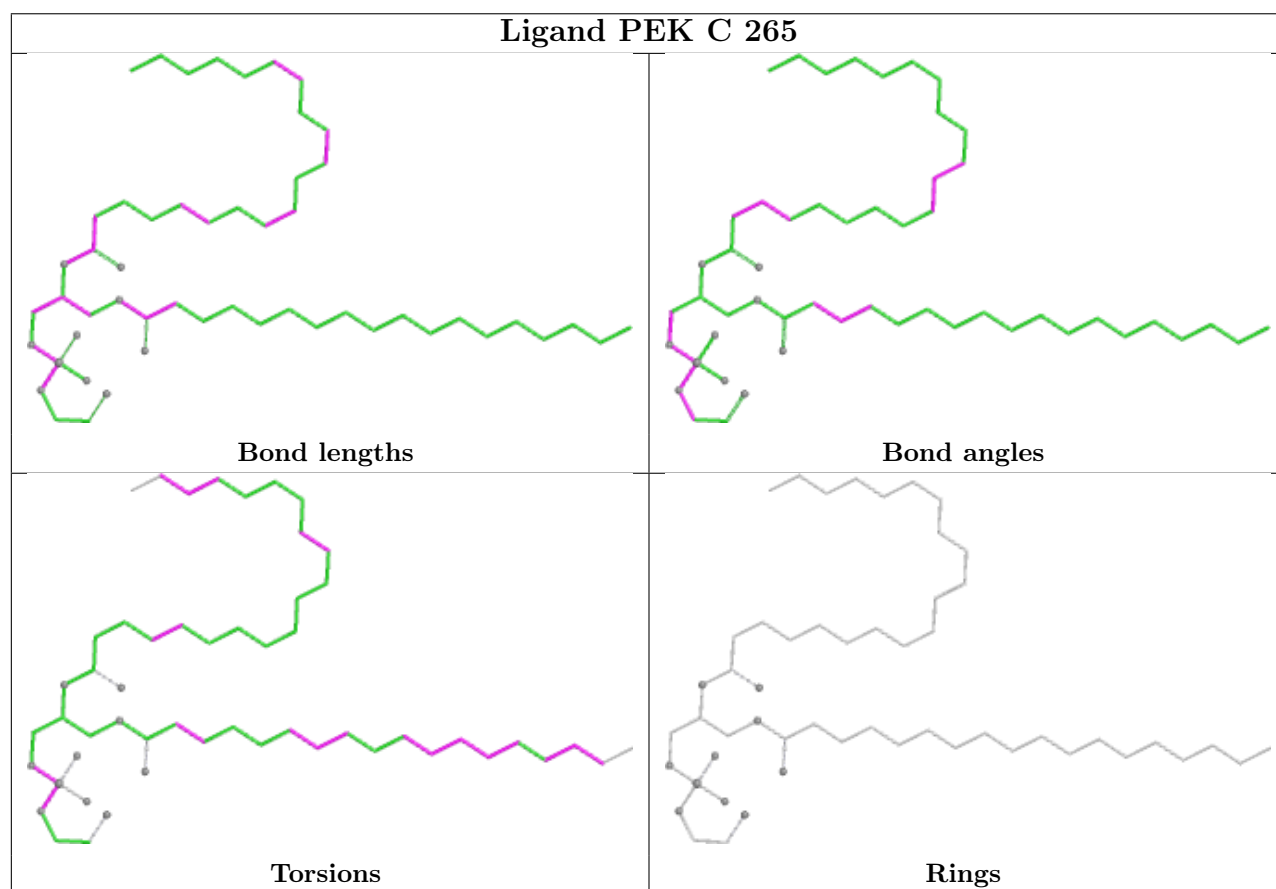
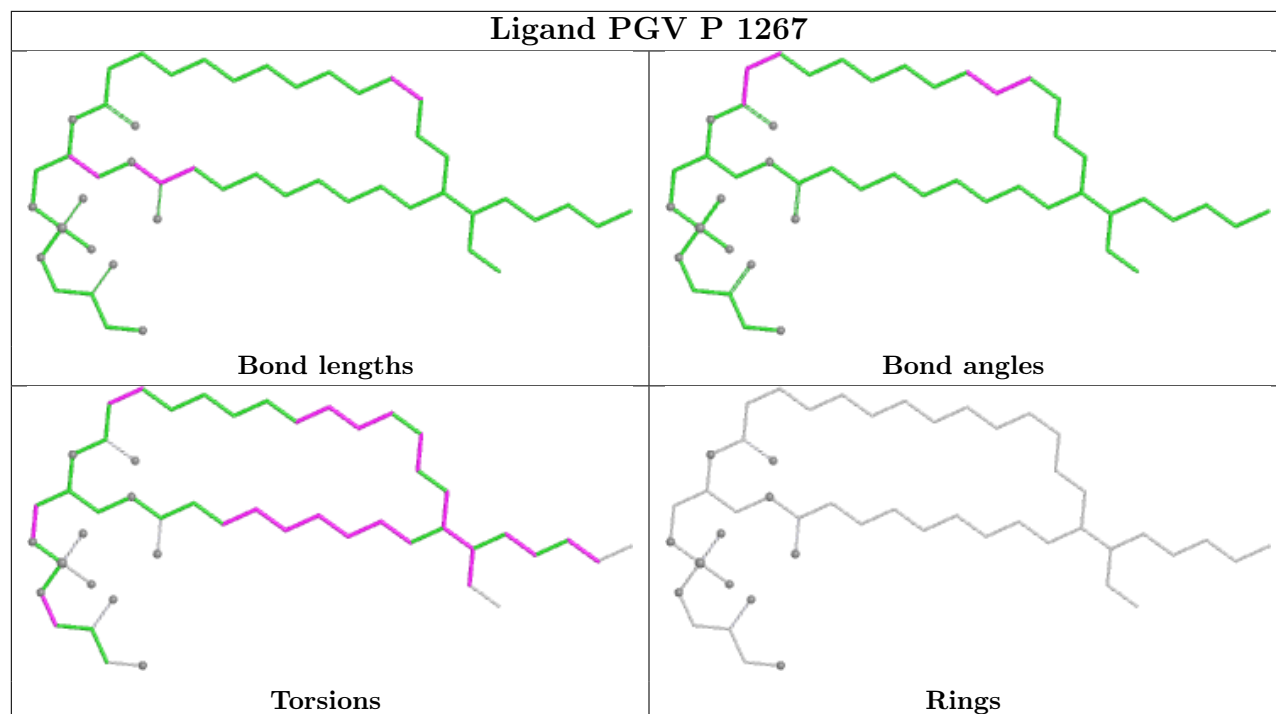


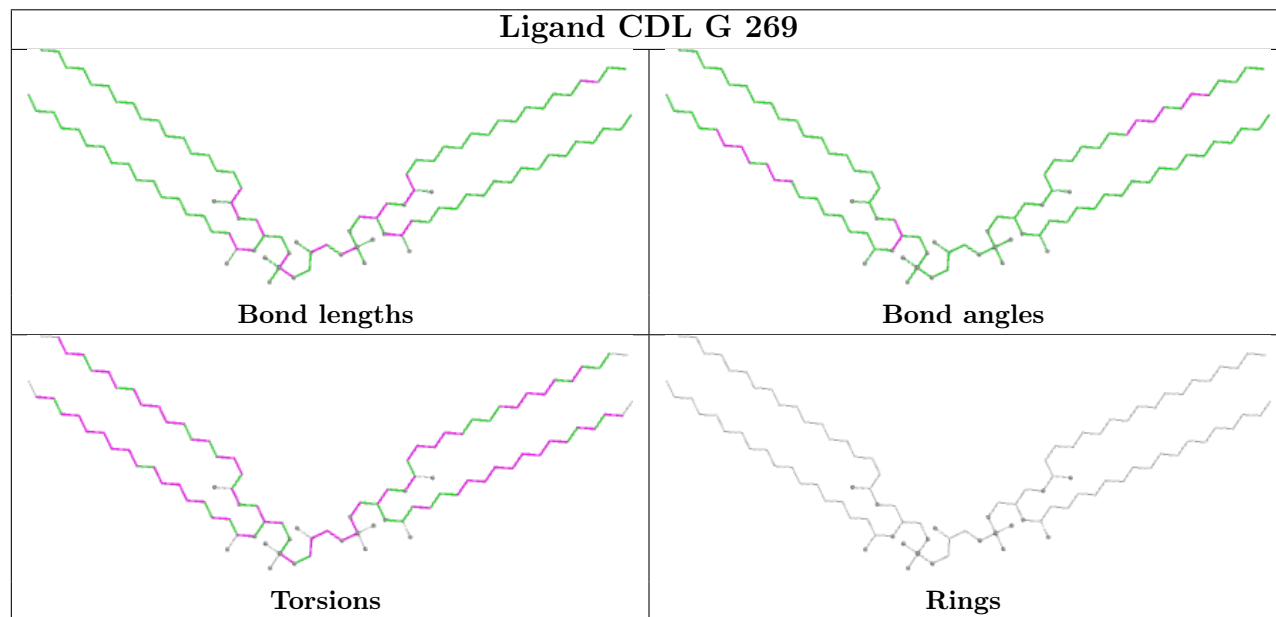
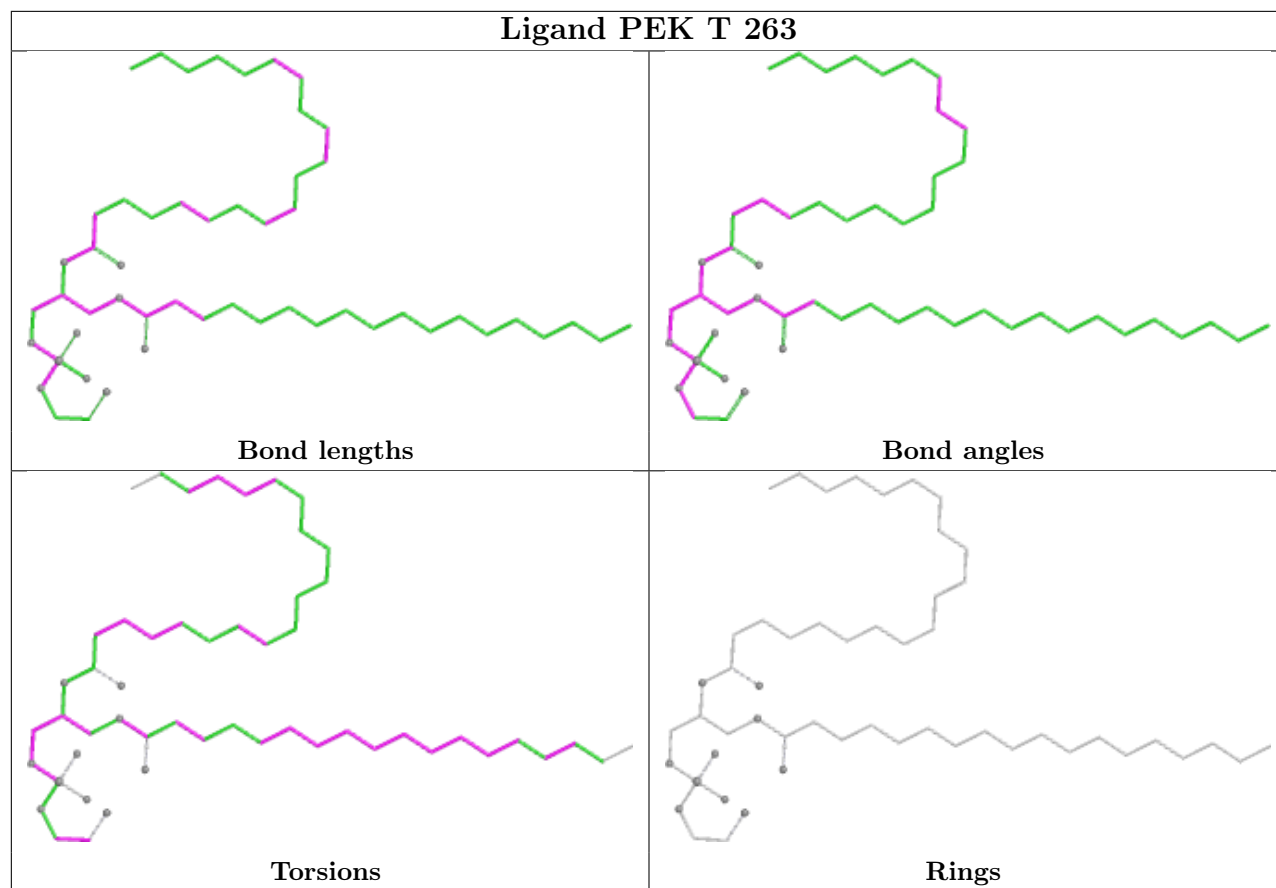


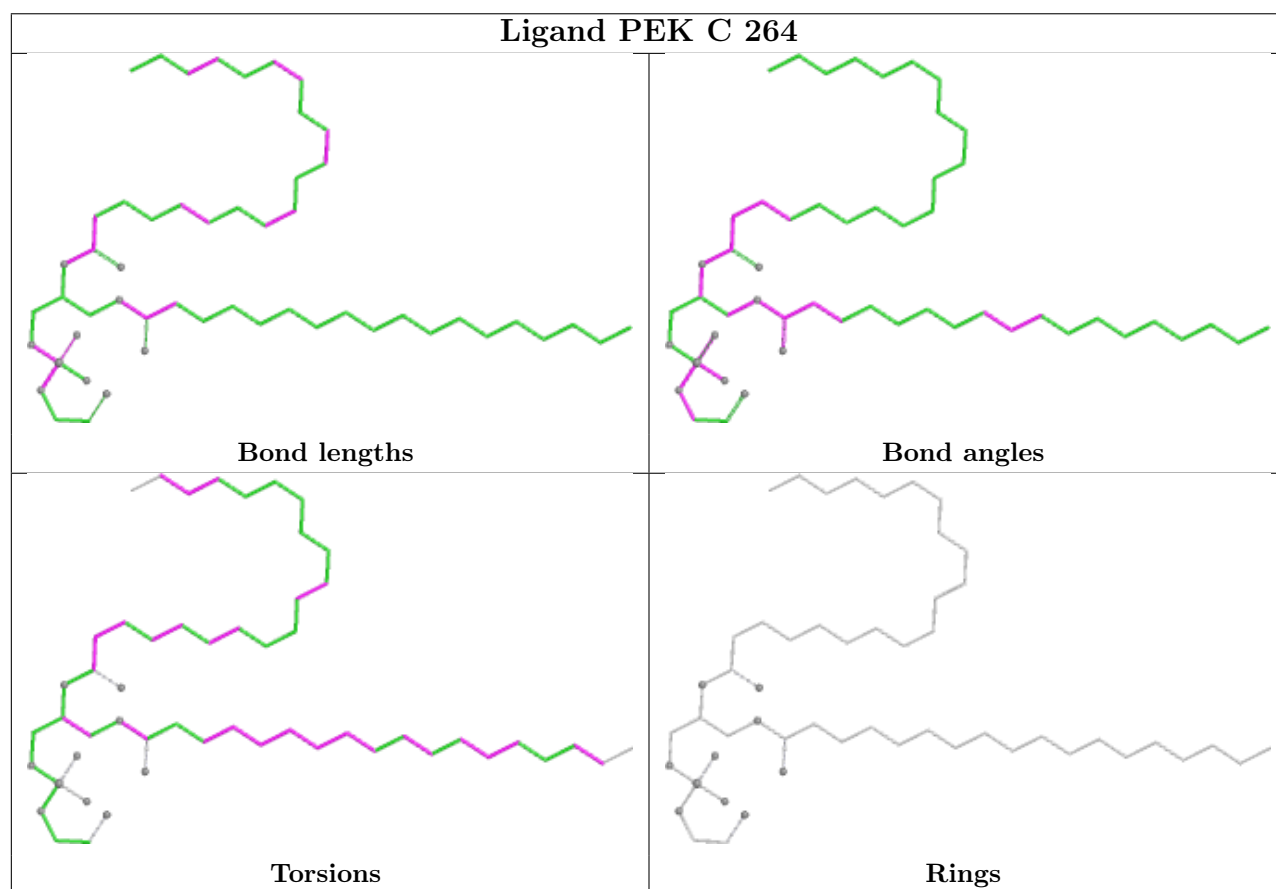
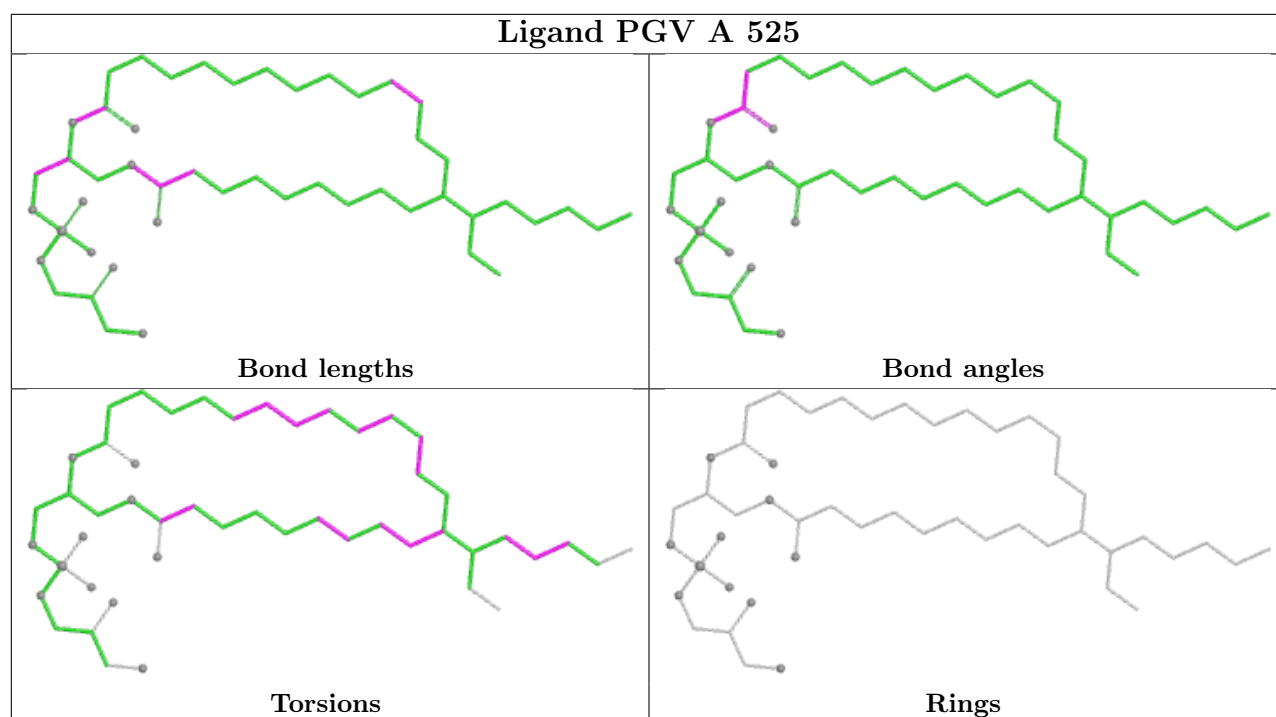


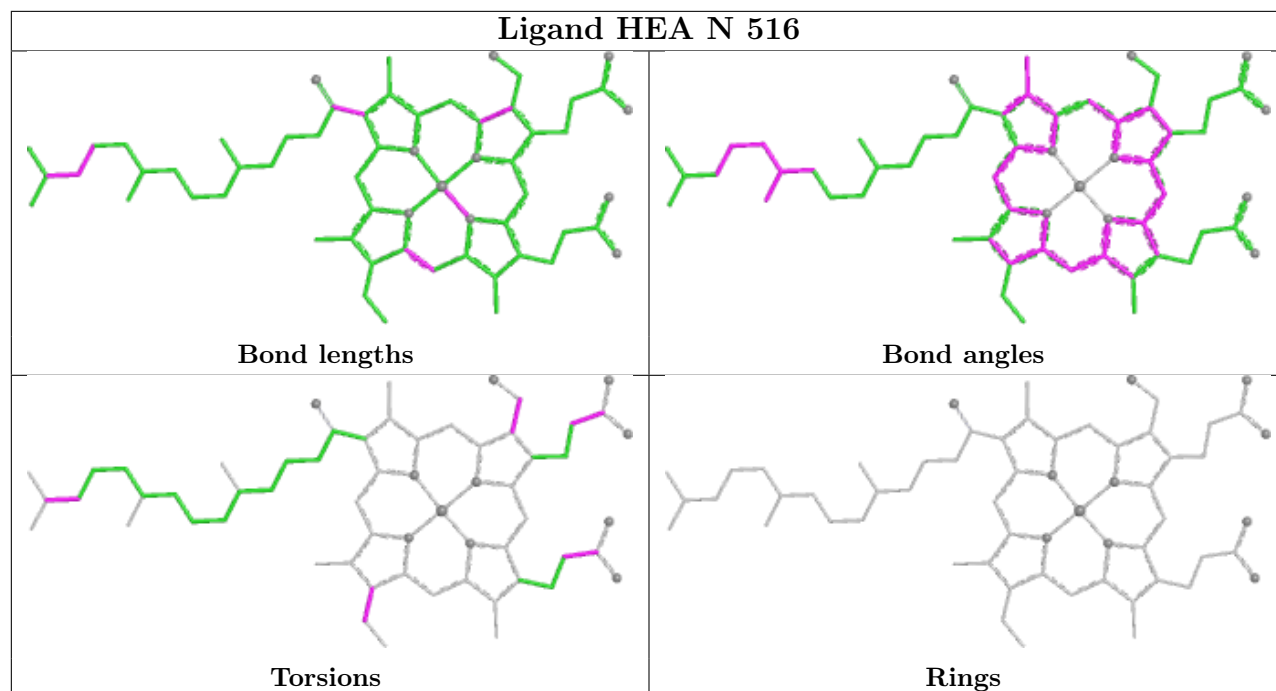












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

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

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.