



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 24, 2020 – 05:49 pm BST

PDB ID : 2EIN  
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.

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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)	:	<b>NOT EXECUTED</b>
EDS	:	<b>NOT EXECUTED</b>
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

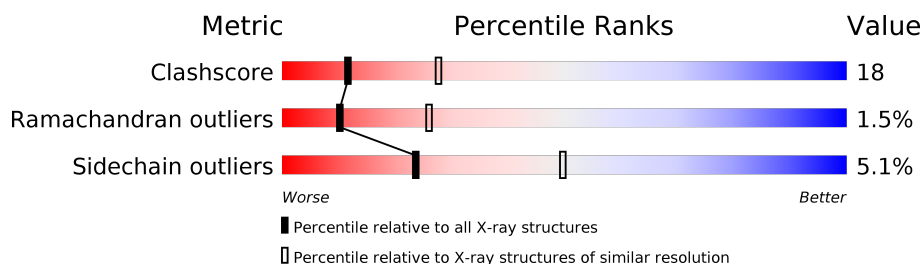
# 1 Overall quality at a glance

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	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)


















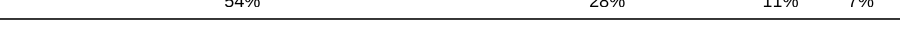
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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	68% 31% .
1	N	514	66% 33% .
2	B	227	56% 39% .
2	O	227	51% 45% .
3	C	261	70% 28% ..
3	P	261	67% 32% .
4	D	147	69% 27% ..
4	Q	147	68% 29% ..

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	HEA	A	515	X	-	-	-
17	HEA	A	516	X	-	-	-
17	HEA	N	515	X	-	-	-
17	HEA	N	516	X	-	-	-
22	PSC	B	230	-	-	X	-
23	CHD	C	271	X	-	-	-
23	CHD	J	60	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CHD	P	1271	X	-	-	-
23	CHD	W	1060	X	-	-	-
24	DMU	C	272	X	-	-	-
24	DMU	M	526	X	-	-	-
24	DMU	P	1272	X	-	-	-
24	DMU	Z	1526	X	-	-	-
26	CDL	G	269	-	-	X	-
26	CDL	T	1269	-	-	X	-
9	SAC	V	1	-	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
1	A	514	Total	C	N	O	S	0	0	0
			4027	2691	623	678	35			
1	N	514	Total	C	N	O	S	0	0	0
			4027	2691	623	678	35			

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

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

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

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

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

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

- Molecule 5 is a protein called Cytochrome c oxidase polypeptide Va.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 14 is COPPER (II) ION (three-letter code: 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		

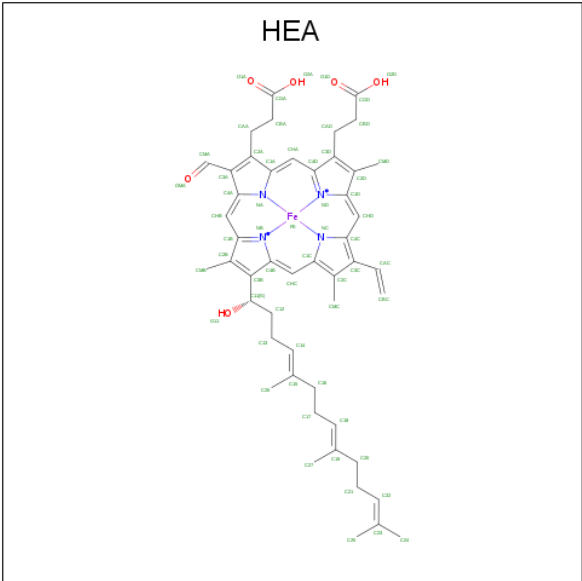
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

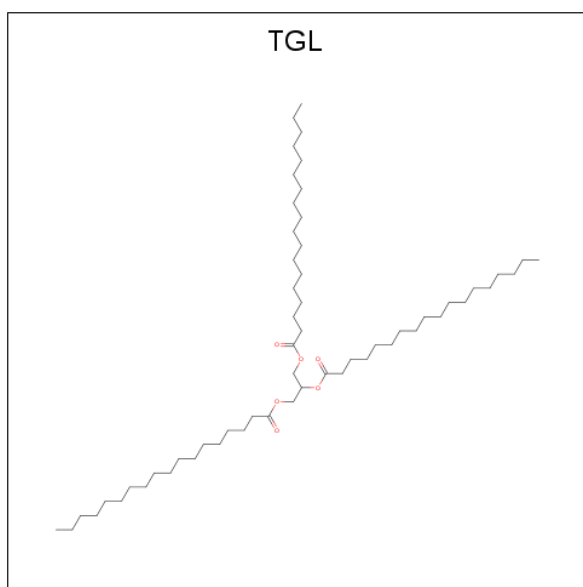
- Molecule 17 is HEME-A (three-letter code: HEA) (formula: C<sub>49</sub>H<sub>56</sub>FeN<sub>4</sub>O<sub>6</sub>).



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

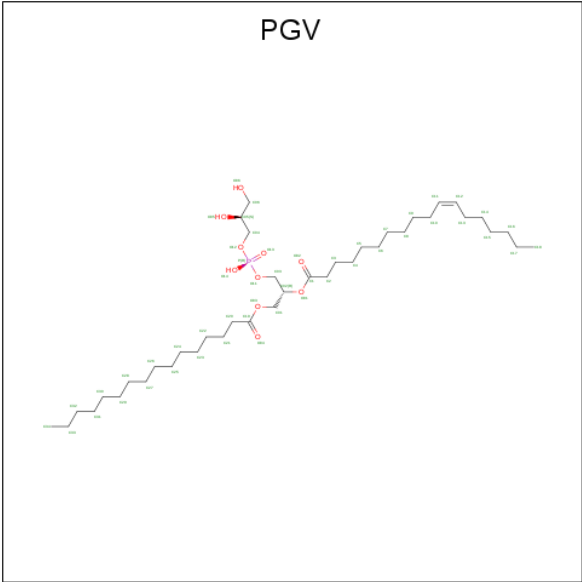
- Molecule 18 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C<sub>57</sub>H<sub>110</sub>O<sub>6</sub>).





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

- Molecule 19 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
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 (three-letter code: ZN) (formula: Zn).

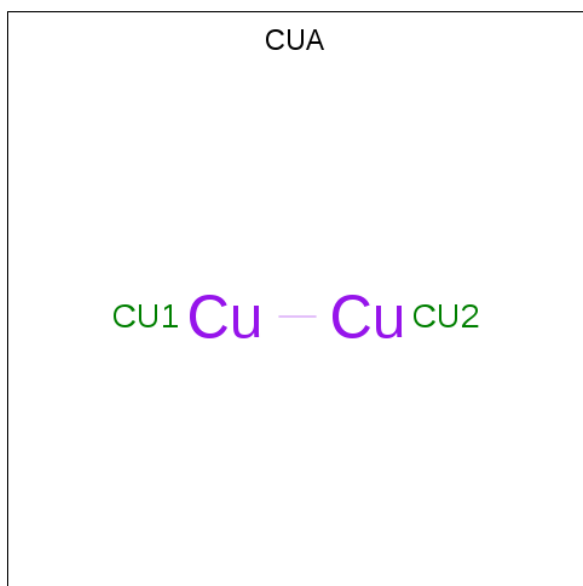
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	P	2	Total	Zn	0	0
			2	2		
20	G	1	Total	Zn	0	0
			1	1		
20	D	1	Total	Zn	0	0
			1	1		
20	B	1	Total	Zn	0	0
			1	1		

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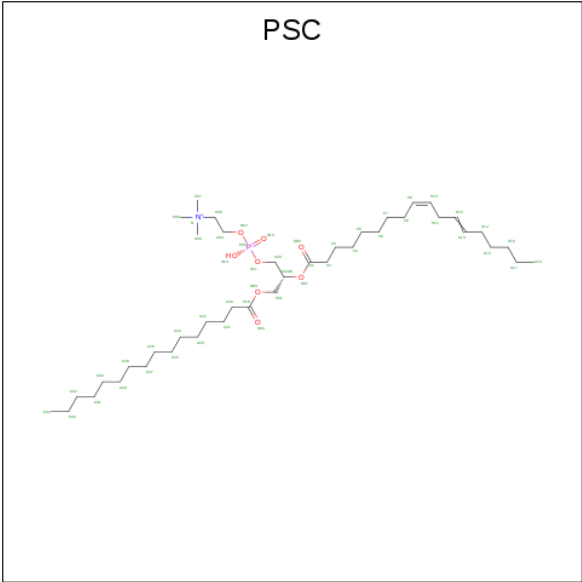
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	C	1	Total 1	Zn 1	0	0
20	T	1	Total 1	Zn 1	0	0
20	N	2	Total 2	Zn 2	0	0
20	O	1	Total 1	Zn 1	0	0
20	L	1	Total 1	Zn 1	0	0
20	S	1	Total 1	Zn 1	0	0
20	F	2	Total 2	Zn 2	0	0

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



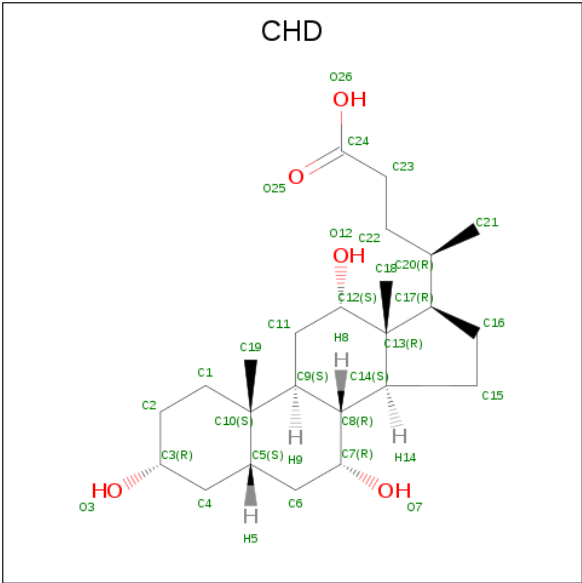
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	B	1	Total 2	Cu 2	0	0
21	O	1	Total 2	Cu 2	0	0

- 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 (three-letter code: 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 (three-letter code: CHD) (formula: C<sub>24</sub>H<sub>40</sub>O<sub>5</sub>).



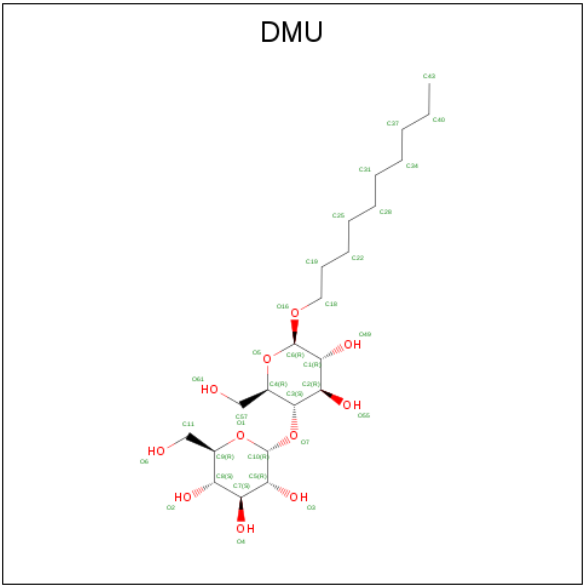
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	B	1	Total	C	O	0	0
			29	24	5		
23	C	1	Total	C	O	0	0
			29	24	5		

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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		

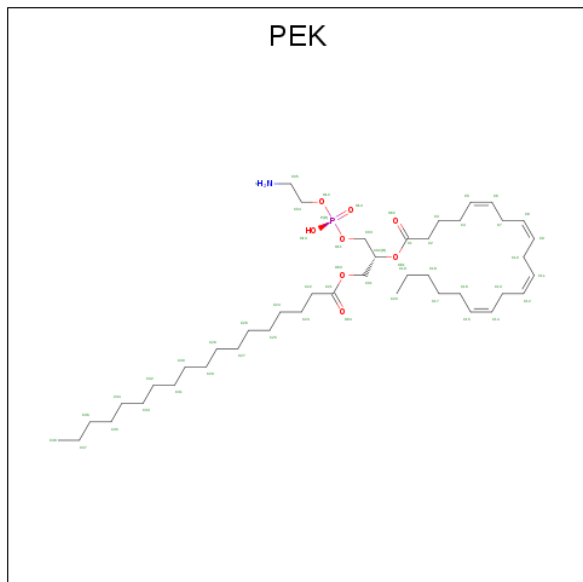
- Molecule 24 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: C<sub>22</sub>H<sub>42</sub>O<sub>11</sub>).



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		

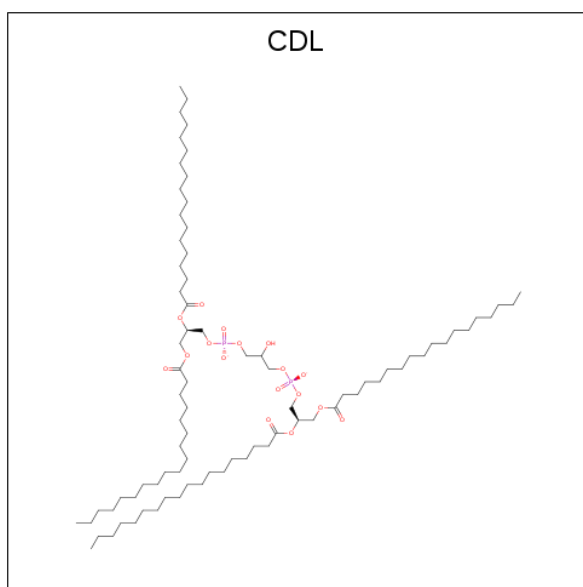
- Molecule 25 is (1S)-2-[[[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(ST

EAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE  
(three-letter code: PEK) (formula:  $C_{43}H_{78}NO_8P$ ).



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

- Molecule 26 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



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

- Molecule 27 is water.

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

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

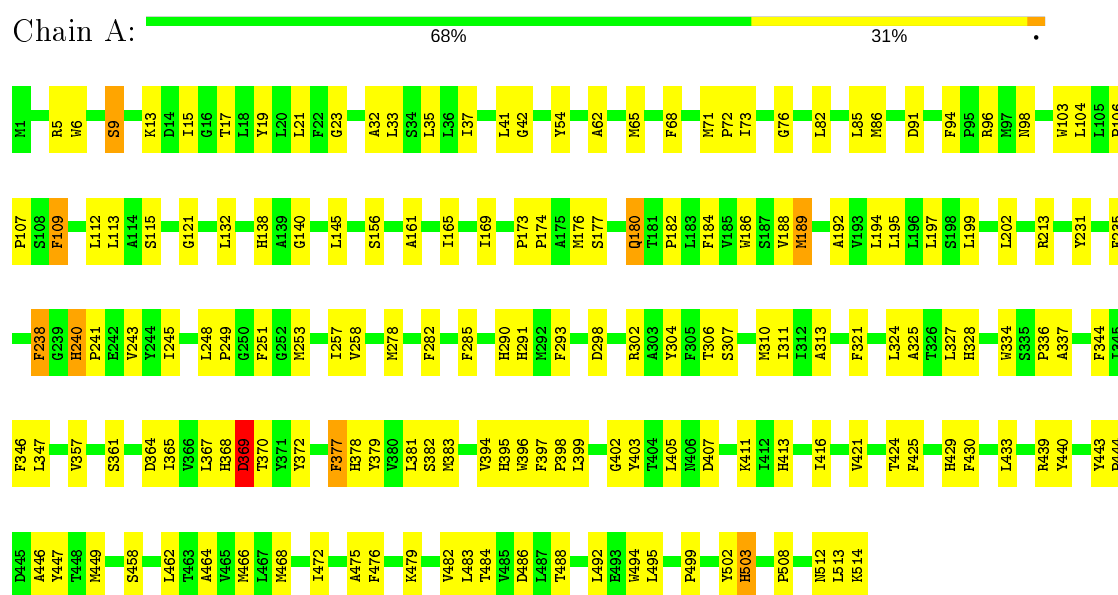


### 3 Residue-property plots [i](#)

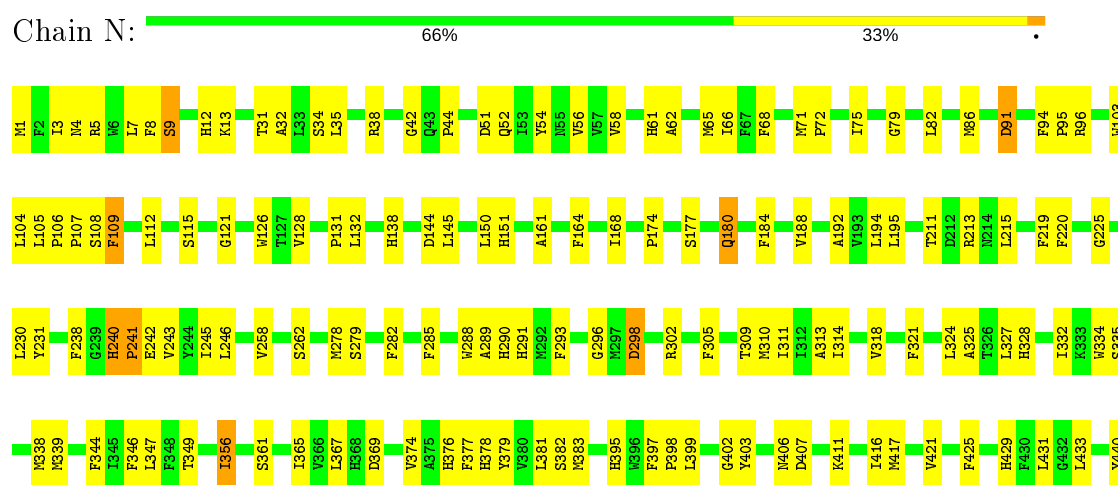
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

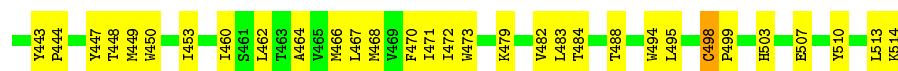
Note EDS was not executed.

- Molecule 1: Cytochrome c oxidase subunit 1

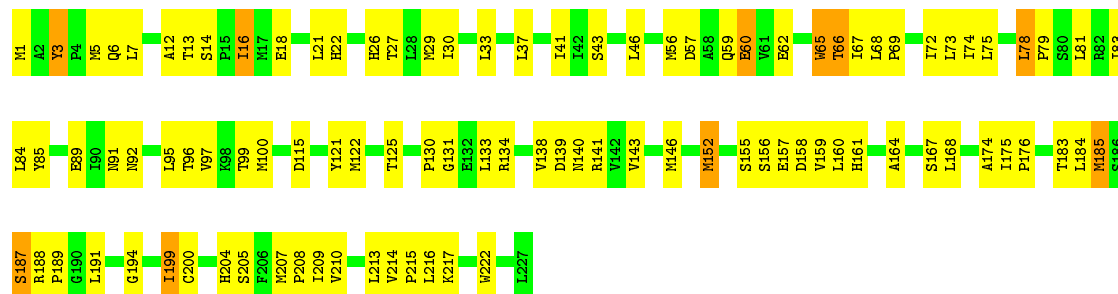


- Molecule 1: Cytochrome c oxidase subunit 1

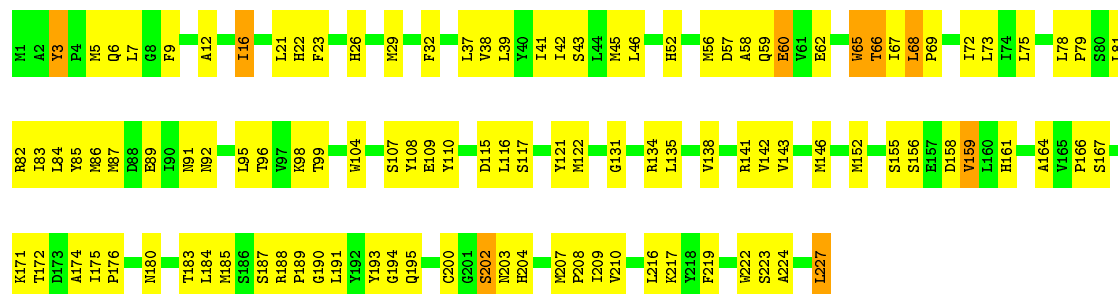




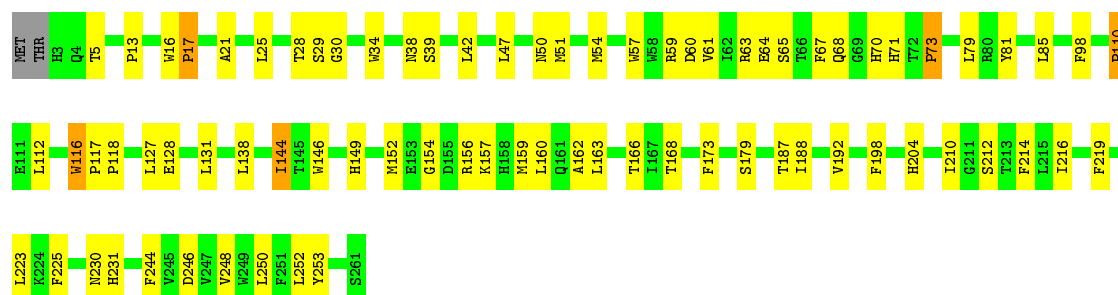
• Molecule 2: Cytochrome c oxidase subunit 2



• Molecule 2: Cytochrome c oxidase subunit 2



• Molecule 3: Cytochrome c oxidase subunit 3



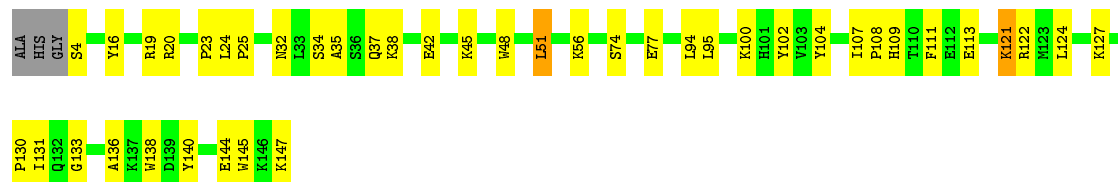
• Molecule 3: Cytochrome c oxidase subunit 3





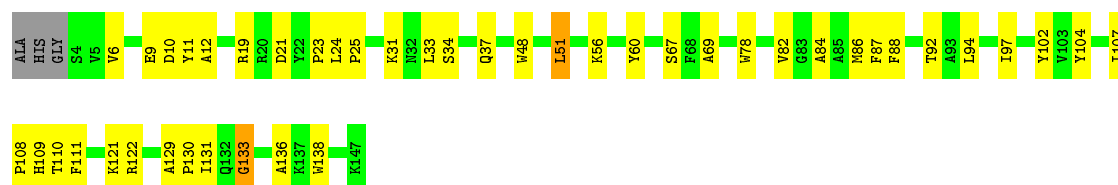
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain D: 69% 27% ..



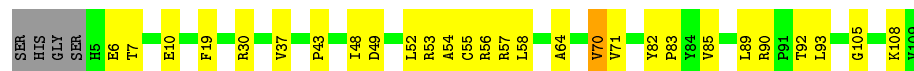
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain Q: 68% 29% ..



- Molecule 5: Cytochrome c oxidase polypeptide Va

Chain E: 71% 25% . .



- Molecule 5: Cytochrome c oxidase polypeptide Va

Chain R: 68% 27% . .



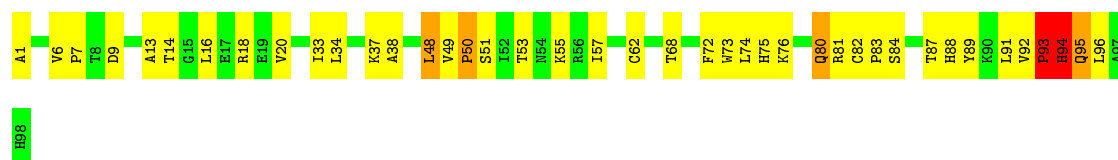
- Molecule 6: Cytochrome c oxidase polypeptide Vb

Chain F: 68% 28% .



- Molecule 6: Cytochrome c oxidase polypeptide Vb

Chain S: 



- Molecule 7: Cytochrome c oxidase polypeptide VIa-heart

Chain G: 



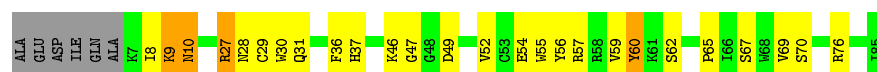
- Molecule 7: Cytochrome c oxidase polypeptide VIa-heart

Chain T: 



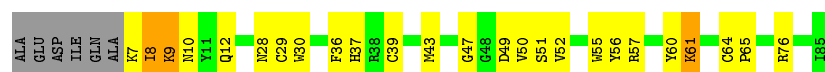
- Molecule 8: Cytochrome c oxidase subunit VIb isoform 1

Chain H: 



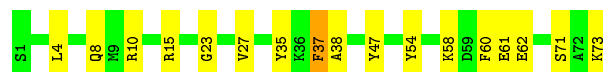
- Molecule 8: Cytochrome c oxidase subunit VIb isoform 1

Chain U: 



- Molecule 9: Cytochrome c oxidase polypeptide VIc

Chain I: 



- Molecule 9: Cytochrome c oxidase polypeptide VIc

Chain V: 



- Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart

Chain J:  73% 24% ..



- Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart

Chain W:  75% 22% ..



- Molecule 11: Cytochrome c oxidase polypeptide VIIb

Chain K:  70% 16% • 13%



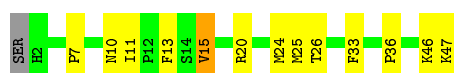
- Molecule 11: Cytochrome c oxidase polypeptide VIIb

Chain X:  66% 20% • 13%



- Molecule 12: Cytochrome c oxidase polypeptide VIIc

Chain L:  70% 26% ..



- Molecule 12: Cytochrome c oxidase polypeptide VIIc

Chain Y:  66% 30% ..



- Molecule 13: Cytochrome c oxidase polypeptide VIII-heart

Chain M:  54% 28% 11% 7%



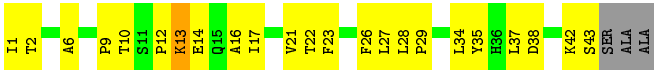
- Molecule 13: Cytochrome c oxidase polypeptide VIII-heart

Chain Z: 

43%

48%

• 7%



## 4 Data and refinement statistics

Xtriage (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.	Xtriage
Total number of atoms	31815	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.69	0/4156	0.79	0/5678
1	N	0.58	0/4156	0.73	0/5678
2	B	0.68	0/1860	0.87	0/2534
2	O	0.66	0/1860	0.84	1/2534 (0.0%)
3	C	0.69	1/2197 (0.0%)	0.69	0/3005
3	P	0.62	0/2197	0.69	0/3005
4	D	0.63	0/1229	0.74	1/1658 (0.1%)
4	Q	0.66	0/1229	0.71	1/1658 (0.1%)
5	E	0.62	0/871	0.71	0/1182
5	R	0.52	0/871	0.68	0/1182
6	F	0.70	0/765	0.94	3/1038 (0.3%)
6	S	0.67	0/765	0.89	3/1038 (0.3%)
7	G	0.67	1/690 (0.1%)	0.80	1/937 (0.1%)
7	T	0.71	0/690	0.78	1/937 (0.1%)
8	H	0.65	0/682	0.72	0/921
8	U	0.62	0/682	0.74	0/921
9	I	0.69	0/605	0.69	0/802
9	V	0.63	0/605	0.64	0/802
10	J	0.60	0/471	0.71	0/636
10	W	0.62	0/471	0.74	0/636
11	K	0.63	0/398	0.75	0/546
11	X	0.61	0/398	0.76	0/546
12	L	0.80	0/393	0.72	0/526
12	Y	0.64	0/393	0.68	0/526
13	M	0.64	0/345	0.76	0/470
13	Z	0.60	0/345	0.76	0/470
All	All	0.65	2/29324 (0.0%)	0.76	11/39866 (0.0%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	116	TRP	CB-CG	5.36	1.59	1.50
7	G	36	TRP	CB-CG	5.02	1.59	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	S	94	HIS	N-CA-C	6.42	128.32	111.00
6	S	9	ASP	CB-CG-OD2	6.35	124.02	118.30
6	F	94	HIS	N-CA-C	6.19	127.72	111.00
6	F	9	ASP	CB-CG-OD2	6.15	123.84	118.30
7	G	6	GLY	N-CA-C	5.79	127.59	113.10

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	162	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	4027	0	4001	165	0
2	B	1824	0	1833	91	0
2	O	1824	0	1833	101	0
3	C	2110	0	2027	79	0
3	P	2110	0	2027	83	0
4	D	1195	0	1183	38	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	643	38	0
7	T	675	0	643	46	0
8	H	662	0	623	18	0
8	U	662	0	623	15	0
9	I	601	0	613	15	0
9	V	601	0	613	20	0
10	J	460	0	459	11	0
10	W	460	0	459	11	0
11	K	384	0	366	11	0
11	X	384	0	366	13	0
12	L	380	0	380	17	0
12	Y	380	0	380	17	0
13	M	335	0	352	17	0
13	Z	335	0	352	12	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	15	0
17	N	120	0	108	18	0
18	A	126	0	220	11	0
18	L	63	0	110	20	0
18	N	63	0	110	8	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	9	0
19	P	102	0	152	11	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	1	0
24	P	33	0	38	4	0
24	Z	33	0	38	0	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	31298	1087	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 1087 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%)	19	43
1	N	512/514 (100%)	469 (92%)	40 (8%)	3 (1%)	25	50
2	B	225/227 (99%)	202 (90%)	20 (9%)	3 (1%)	12	30
2	O	225/227 (99%)	198 (88%)	21 (9%)	6 (3%)	5	12
3	C	257/261 (98%)	247 (96%)	9 (4%)	1 (0%)	34	60
3	P	257/261 (98%)	246 (96%)	10 (4%)	1 (0%)	34	60
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%)	3	5
6	S	96/98 (98%)	83 (86%)	9 (9%)	4 (4%)	3	5
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%)	3	6
8	U	77/85 (91%)	66 (86%)	8 (10%)	3 (4%)	3	6
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%)	8	21
10	W	56/59 (95%)	53 (95%)	2 (4%)	1 (2%)	8	21
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%)	6	16
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%)	10	26

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 ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	426/426 (100%)	415 (97%)	11 (3%)	46	75
1	N	426/426 (100%)	412 (97%)	14 (3%)	38	67
2	B	210/210 (100%)	192 (91%)	18 (9%)	10	24
2	O	210/210 (100%)	190 (90%)	20 (10%)	8	20
3	C	224/226 (99%)	213 (95%)	11 (5%)	25	52
3	P	224/226 (99%)	220 (98%)	4 (2%)	59	83
4	D	128/129 (99%)	123 (96%)	5 (4%)	32	61
4	Q	128/129 (99%)	123 (96%)	5 (4%)	32	61
5	E	92/95 (97%)	89 (97%)	3 (3%)	38	67
5	R	92/95 (97%)	88 (96%)	4 (4%)	29	57
6	F	81/81 (100%)	80 (99%)	1 (1%)	71	88
6	S	81/81 (100%)	74 (91%)	7 (9%)	10	24
7	G	67/68 (98%)	61 (91%)	6 (9%)	9	22
7	T	67/68 (98%)	61 (91%)	6 (9%)	9	22
8	H	71/75 (95%)	66 (93%)	5 (7%)	15	35
8	U	71/75 (95%)	66 (93%)	5 (7%)	15	35
9	I	57/57 (100%)	53 (93%)	4 (7%)	15	35
9	V	57/57 (100%)	55 (96%)	2 (4%)	36	65
10	J	49/50 (98%)	48 (98%)	1 (2%)	55	81
10	W	49/50 (98%)	48 (98%)	1 (2%)	55	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	39/46 (85%)	37 (95%)	2 (5%)	24	50
11	X	39/46 (85%)	37 (95%)	2 (5%)	24	50
12	L	39/40 (98%)	37 (95%)	2 (5%)	24	50
12	Y	39/40 (98%)	37 (95%)	2 (5%)	24	50
13	M	37/38 (97%)	29 (78%)	8 (22%)	1	3
13	Z	37/38 (97%)	30 (81%)	7 (19%)	1	4
All	All	3040/3082 (99%)	2884 (95%)	156 (5%)	24	50

5 of 156 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	M	13	LYS
1	N	369	ASP
10	W	50	LEU
13	M	37	LEU
1	N	138	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
11	K	35	GLN
1	N	180	GLN
10	W	9	GLN
11	K	41	ASN
1	N	151	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	FME	O	1	2	8,9,10	0.62	0	7,9,11	1.55	2 (28%)
7	TPO	G	11	7	8,10,11	1.86	3 (37%)	10,14,16	0.99	0
2	FME	B	1	2	8,9,10	0.74	0	7,9,11	1.61	2 (28%)
9	SAC	V	1	9	7,8,9	3.11	2 (28%)	8,9,11	3.11	5 (62%)
1	FME	N	1	1	8,9,10	0.98	0	7,9,11	0.86	0
7	TPO	T	11	7	8,10,11	1.91	4 (50%)	10,14,16	1.03	1 (10%)
9	SAC	I	1	9	7,8,9	2.82	2 (28%)	8,9,11	2.91	4 (50%)
1	FME	A	1	1	8,9,10	0.73	0	7,9,11	1.09	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FME	O	1	2	-	1/7/9/11	-
7	TPO	G	11	7	-	4/9/11/13	-
2	FME	B	1	2	-	2/7/9/11	-
9	SAC	V	1	9	-	3/7/8/10	-
1	FME	N	1	1	-	5/7/9/11	-
7	TPO	T	11	7	-	6/9/11/13	-
9	SAC	I	1	9	-	3/7/8/10	-
1	FME	A	1	1	-	4/7/9/11	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	V	1	SAC	CA-N	5.58	1.54	1.46
9	I	1	SAC	OAC-C1A	5.42	1.35	1.23
9	V	1	SAC	OAC-C1A	5.38	1.35	1.23
9	I	1	SAC	CA-N	4.64	1.52	1.46
7	G	11	TPO	CB-CA	3.06	1.60	1.53

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



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	V	1	SAC	CA-N-C1A	-6.67	110.85	123.15
9	I	1	SAC	CA-N-C1A	-6.55	111.06	123.15
2	B	1	FME	CA-N-CN	-3.26	117.80	122.82
2	O	1	FME	C-CA-N	3.06	115.25	109.73
9	V	1	SAC	C2A-C1A-N	3.01	121.19	116.10

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	O	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
2	B	1	FME	O1-CN-N-CA

There are no ring outliers.

4 monomers are involved in 6 short contacts:

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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
18	TGL	N	1523	-	62,62,62	1.14	5 (8%)	65,65,65	1.43	9 (13%)
23	CHD	C	525	-	29,32,32	1.27	2 (6%)	48,51,51	2.19	15 (31%)
23	CHD	P	1271	-	29,32,32	1.33	6 (20%)	48,51,51	3.92	25 (52%)
26	CDL	P	1270	-	99,99,99	1.28	13 (13%)	105,111,111	1.05	8 (7%)
18	TGL	L	522	-	62,62,62	1.35	5 (8%)	65,65,65	1.74	13 (20%)
25	PEK	T	263	-	52,52,52	2.35	14 (26%)	55,57,57	1.38	8 (14%)
26	CDL	T	1269	-	99,99,99	1.44	15 (15%)	105,111,111	1.03	9 (8%)
25	PEK	P	1265	-	52,52,52	1.84	12 (23%)	55,57,57	1.09	5 (9%)
19	PGV	C	268	-	50,50,50	1.60	8 (16%)	53,56,56	0.91	2 (3%)
22	PSC	B	230	-	51,51,51	1.57	10 (19%)	57,59,59	1.09	3 (5%)
23	CHD	J	60	-	29,32,32	1.53	3 (10%)	48,51,51	3.83	25 (52%)
19	PGV	P	1267	-	50,50,50	1.10	4 (8%)	53,56,56	0.87	2 (3%)
25	PEK	C	264	-	52,52,52	2.05	12 (23%)	55,57,57	1.57	11 (20%)
25	PEK	G	1263	-	52,52,52	2.33	15 (28%)	55,57,57	1.38	7 (12%)
21	CUA	O	228	2	0,1,1	0.00	-	-		
19	PGV	C	267	-	50,50,50	1.03	2 (4%)	53,56,56	1.07	6 (11%)
19	PGV	N	1266	-	50,50,50	1.23	6 (12%)	53,56,56	0.91	1 (1%)
22	PSC	O	1230	-	51,51,51	1.62	11 (21%)	57,59,59	1.06	4 (7%)
17	HEA	A	515	1	44,67,67	1.76	7 (15%)	37,103,103	1.66	9 (24%)
23	CHD	G	86	-	29,32,32	1.18	3 (10%)	48,51,51	2.66	21 (43%)
18	TGL	Y	1522	-	62,62,62	1.40	5 (8%)	65,65,65	1.68	10 (15%)
17	HEA	N	516	1	44,67,67	1.65	8 (18%)	37,103,103	1.49	5 (13%)
23	CHD	B	1086	-	29,32,32	0.88	0	48,51,51	2.51	20 (41%)
21	CUA	B	228	2	0,1,1	0.00	-	-		
18	TGL	O	1521	-	62,62,62	1.03	5 (8%)	65,65,65	1.52	10 (15%)
24	DMU	P	1272	-	34,34,34	2.82	14 (41%)	45,45,45	3.72	19 (42%)
23	CHD	W	1060	-	29,32,32	1.82	5 (17%)	48,51,51	3.75	25 (52%)
17	HEA	A	516	1	44,67,67	1.52	8 (18%)	37,103,103	1.44	5 (13%)
24	DMU	Z	1526	-	34,34,34	3.34	9 (26%)	45,45,45	3.43	21 (46%)
23	CHD	C	271	-	29,32,32	1.28	4 (13%)	48,51,51	3.86	25 (52%)
18	TGL	A	521	-	62,62,62	0.97	3 (4%)	65,65,65	1.49	12 (18%)
25	PEK	C	265	-	52,52,52	1.89	12 (23%)	55,57,57	1.12	5 (9%)
24	DMU	C	272	-	34,34,34	2.76	14 (41%)	45,45,45	3.92	18 (40%)
19	PGV	P	1268	-	50,50,50	1.61	9 (18%)	53,56,56	0.88	2 (3%)
17	HEA	N	515	1	44,67,67	2.26	10 (22%)	37,103,103	1.69	10 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	PEK	T	1264	-	52,52,52	2.14	13 (25%)	55,57,57	1.55	10 (18%)
18	TGL	A	523	-	62,62,62	1.13	5 (8%)	65,65,65	1.41	11 (16%)
19	PGV	A	524	-	50,50,50	1.52	8 (16%)	53,56,56	1.10	5 (9%)
23	CHD	P	1525	-	29,32,32	1.49	5 (17%)	48,51,51	2.13	14 (29%)
26	CDL	C	270	-	99,99,99	1.22	13 (13%)	105,111,111	1.02	7 (6%)
19	PGV	A	525	-	50,50,50	1.12	5 (10%)	53,56,56	0.98	2 (3%)
19	PGV	N	1524	-	50,50,50	1.52	8 (16%)	53,56,56	1.06	5 (9%)
24	DMU	M	526	-	34,34,34	3.35	10 (29%)	45,45,45	3.52	21 (46%)
26	CDL	G	269	-	99,99,99	1.53	16 (16%)	105,111,111	1.02	7 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	TGL	N	1523	-	-	17/65/65/65	-
23	CHD	C	525	-	-	0/7/74/74	0/4/4/4
23	CHD	P	1271	-	5/5/12/12	6/7/74/74	0/4/4/4
26	CDL	P	1270	-	-	73/110/110/110	-
18	TGL	L	522	-	-	15/65/65/65	-
25	PEK	T	263	-	-	29/56/56/56	-
26	CDL	T	1269	-	-	66/110/110/110	-
25	PEK	P	1265	-	-	18/56/56/56	-
19	PGV	C	268	-	-	34/55/55/55	-
19	PGV	C	267	-	-	19/55/55/55	-
22	PSC	B	230	-	-	34/55/55/55	-
23	CHD	J	60	-	5/5/12/12	6/7/74/74	0/4/4/4
19	PGV	P	1267	-	-	19/55/55/55	-
25	PEK	C	264	-	-	21/56/56/56	-
25	PEK	G	1263	-	-	29/56/56/56	-
24	DMU	Z	1526	-	5/5/10/10	10/19/59/59	0/2/2/2
19	PGV	N	1266	-	-	12/55/55/55	-
22	PSC	O	1230	-	-	34/55/55/55	-
17	HEA	A	515	1	3/3/7/16	7/24/76/76	-
23	CHD	G	86	-	-	0/7/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	TGL	Y	1522	-	-	17/65/65/65	-
17	HEA	N	516	1	3/3/7/16	2/24/76/76	-
23	CHD	B	1086	-	-	0/7/74/74	0/4/4/4
18	TGL	O	1521	-	-	16/65/65/65	-
24	DMU	P	1272	-	6/6/10/10	11/19/59/59	0/2/2/2
23	CHD	W	1060	-	5/5/12/12	6/7/74/74	0/4/4/4
17	HEA	A	516	1	3/3/7/16	2/24/76/76	-
25	PEK	T	1264	-	-	22/56/56/56	-
18	TGL	A	521	-	-	14/65/65/65	-
25	PEK	C	265	-	-	20/56/56/56	-
24	DMU	C	272	-	6/6/10/10	10/19/59/59	0/2/2/2
19	PGV	P	1268	-	-	35/55/55/55	-
17	HEA	N	515	1	3/3/7/16	7/24/76/76	-
23	CHD	C	271	-	5/5/12/12	6/7/74/74	0/4/4/4
18	TGL	A	523	-	-	17/65/65/65	-
19	PGV	A	524	-	-	34/55/55/55	-
23	CHD	P	1525	-	-	0/7/74/74	0/4/4/4
26	CDL	C	270	-	-	70/110/110/110	-
19	PGV	A	525	-	-	11/55/55/55	-
19	PGV	N	1524	-	-	34/55/55/55	-
24	DMU	M	526	-	5/5/10/10	9/19/59/59	0/2/2/2
26	CDL	G	269	-	-	66/110/110/110	-

The worst 5 of 342 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	N	515	HEA	C3B-C11	-11.25	1.44	1.52
24	Z	1526	DMU	O16-C6	-8.39	1.25	1.40
24	M	526	DMU	O16-C6	-8.14	1.26	1.40
17	A	515	HEA	C3B-C11	-7.88	1.46	1.52
24	M	526	DMU	O7-C3	-7.73	1.23	1.43

The worst 5 of 452 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	P	1271	CHD	C10-C9-C8	11.85	124.55	111.82
23	C	271	CHD	C10-C9-C8	11.73	124.42	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	P	1272	DMU	O16-C6-C1	11.15	125.71	108.30
23	J	60	CHD	C13-C17-C20	10.03	131.46	119.50
23	C	271	CHD	C17-C13-C14	9.48	109.65	100.09

5 of 54 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	P	1271	CHD	C12
23	P	1271	CHD	C8
23	P	1271	CHD	C3
23	P	1271	CHD	C9
23	P	1271	CHD	C14

5 of 858 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	P	1270	CDL	CA2-OA2-PA1-OA3
26	P	1270	CDL	CA2-OA2-PA1-OA4
26	P	1270	CDL	CA4-CA3-OA5-PA1
26	P	1270	CDL	C11-CA5-OA6-CA4
26	P	1270	CDL	CB2-OB2-PB2-OB3

There are no ring outliers.

41 monomers are involved in 339 short contacts:

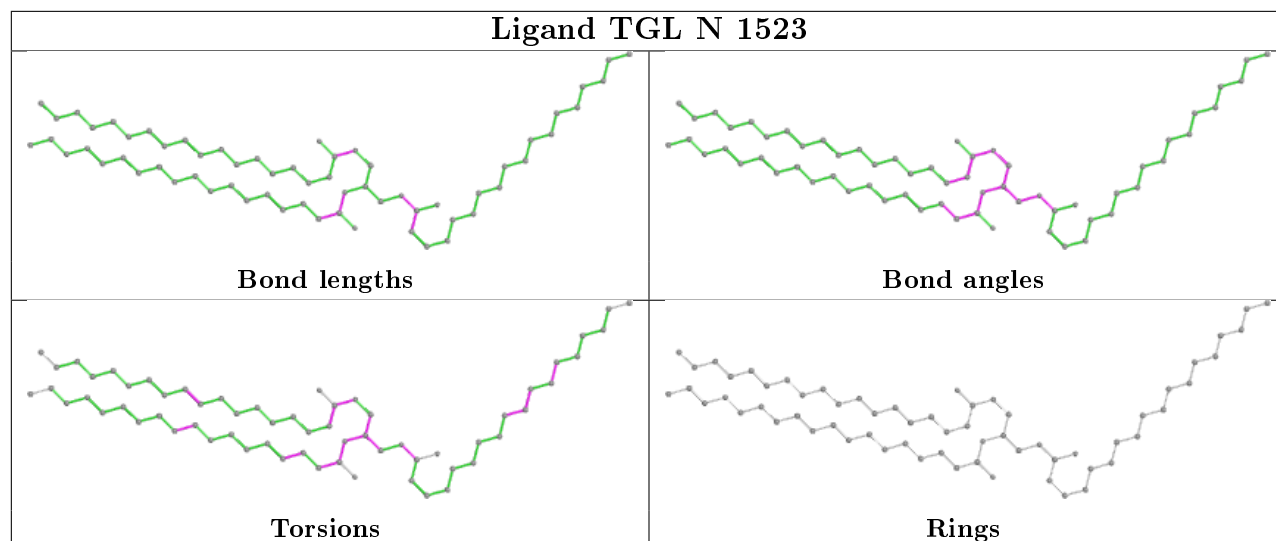
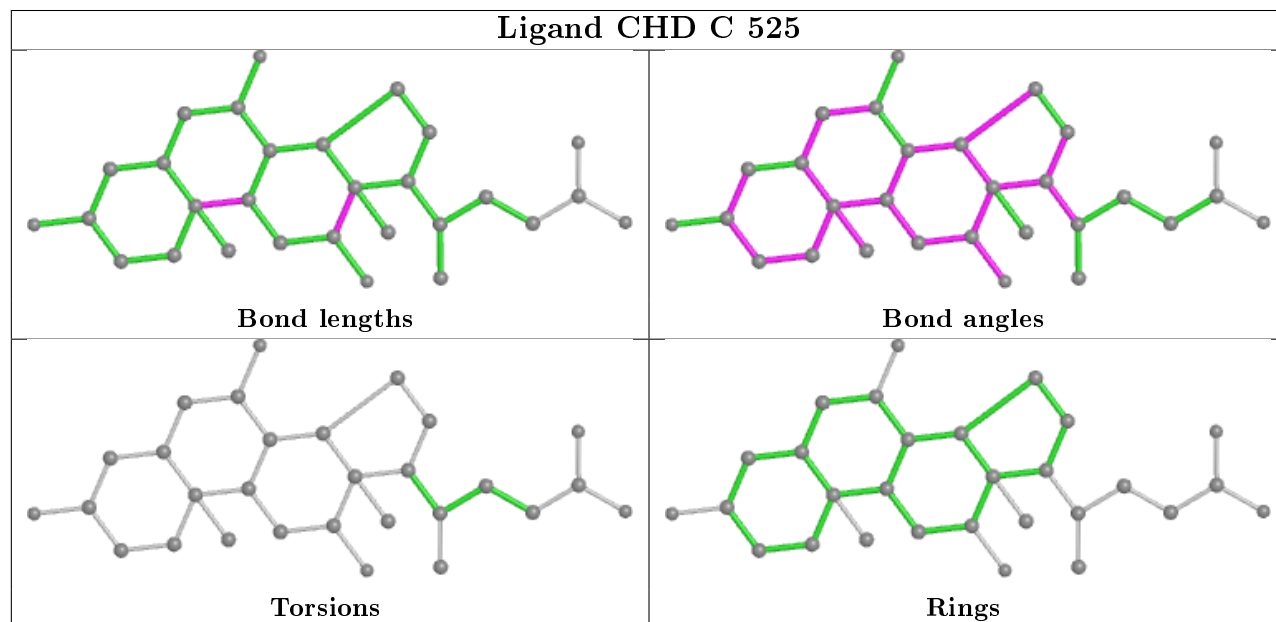
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	N	1523	TGL	8	0
23	C	525	CHD	1	0
23	P	1271	CHD	5	0
26	P	1270	CDL	17	0
18	L	522	TGL	20	0
25	T	263	PEK	11	0
26	T	1269	CDL	32	0
25	P	1265	PEK	10	0
19	C	268	PGV	1	0
22	B	230	PSC	21	0
23	J	60	CHD	4	0
19	P	1267	PGV	9	0
25	C	264	PEK	9	0
25	G	1263	PEK	10	0
19	C	267	PGV	6	0
19	N	1266	PGV	2	0

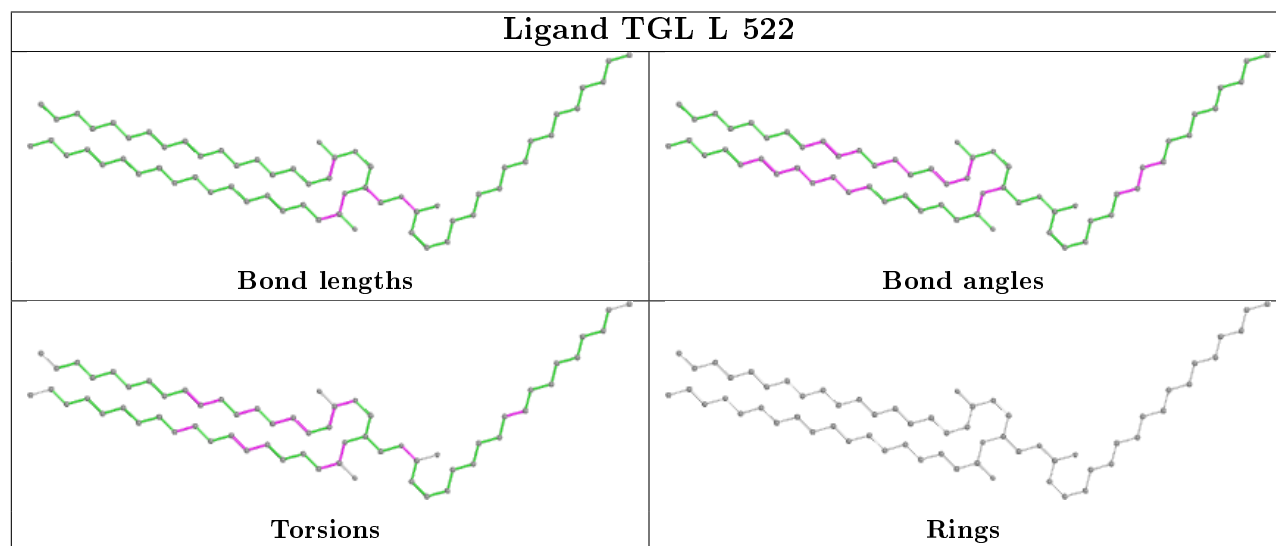
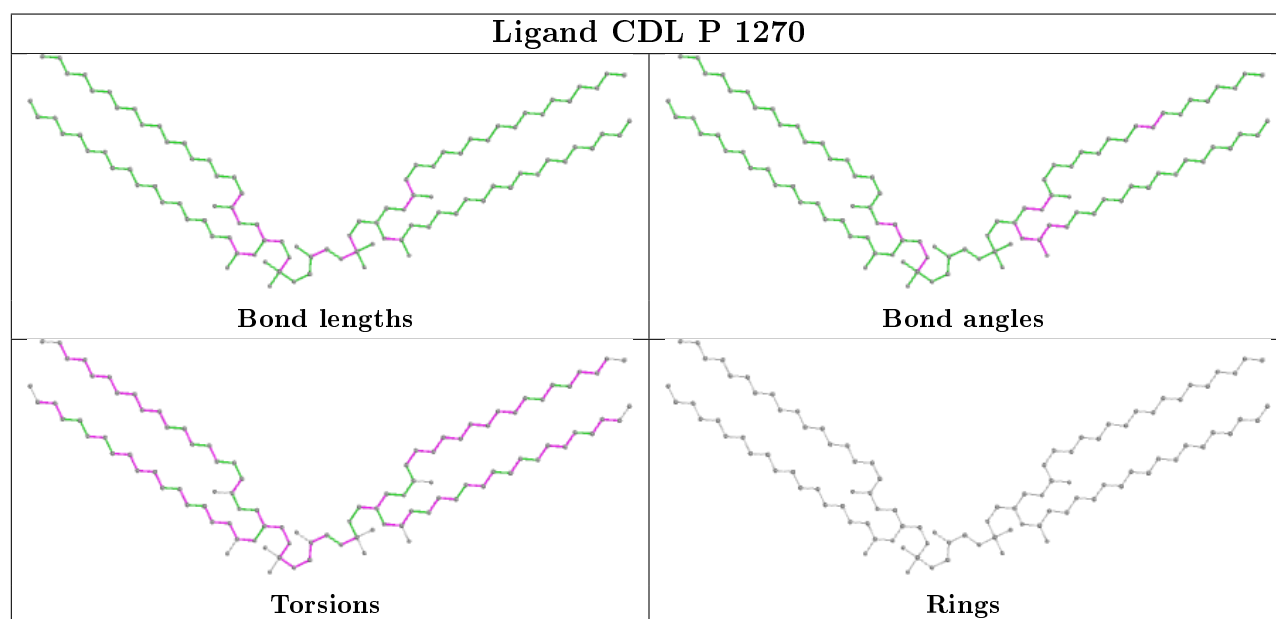
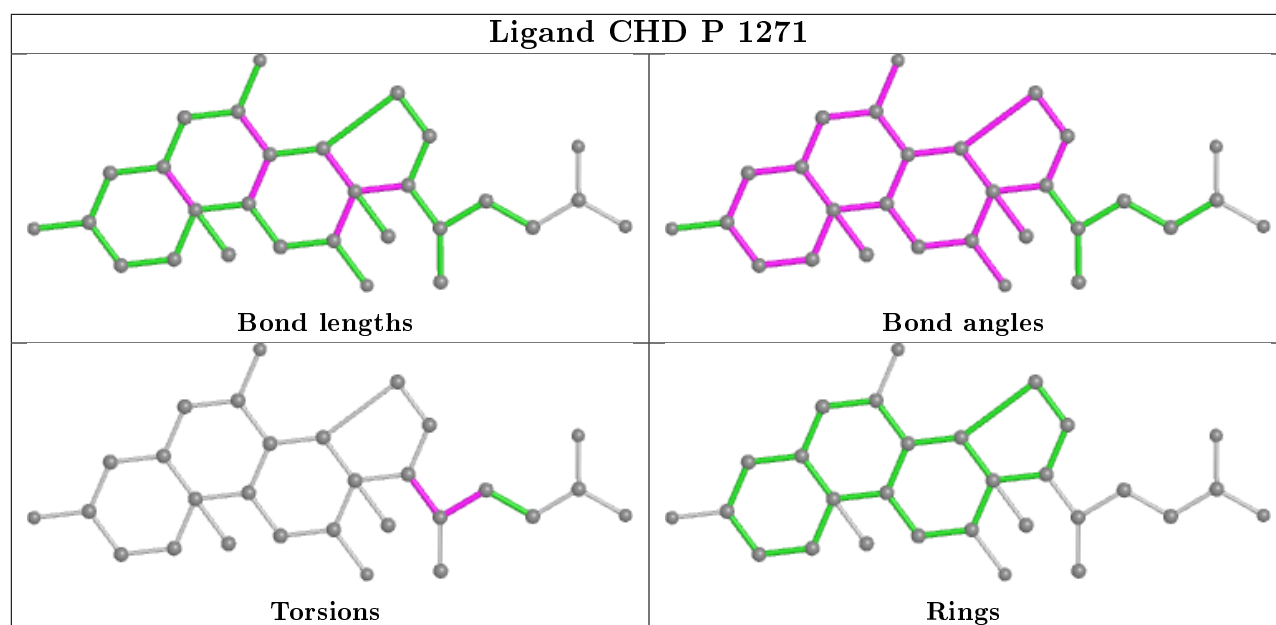
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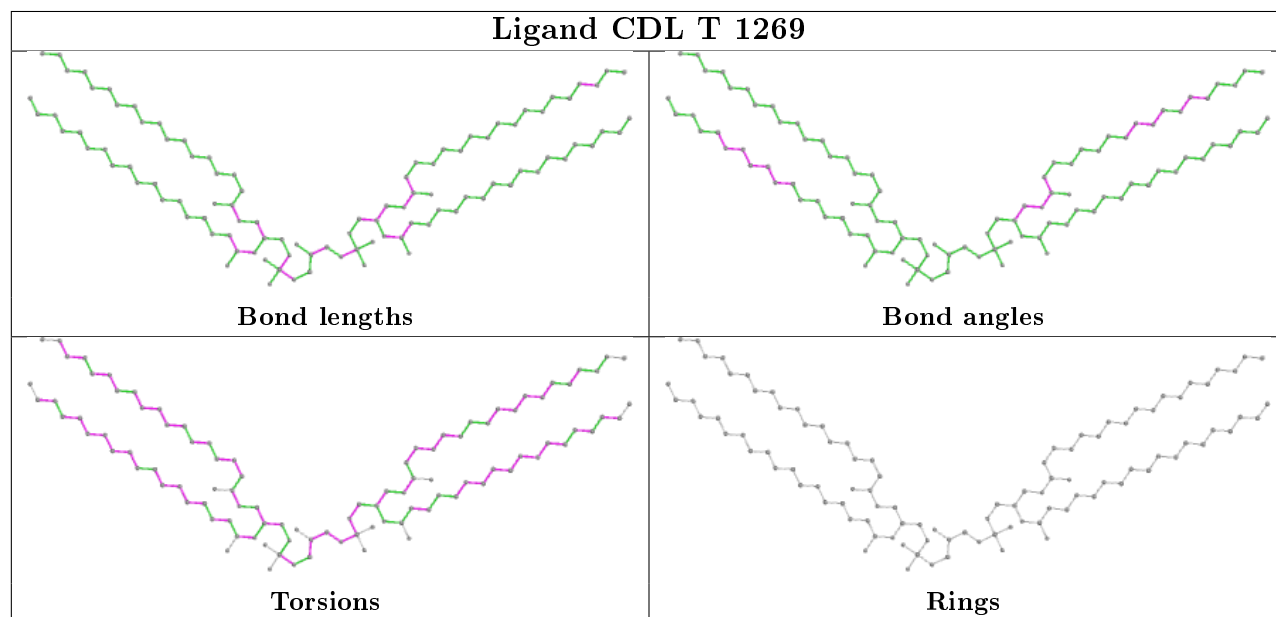
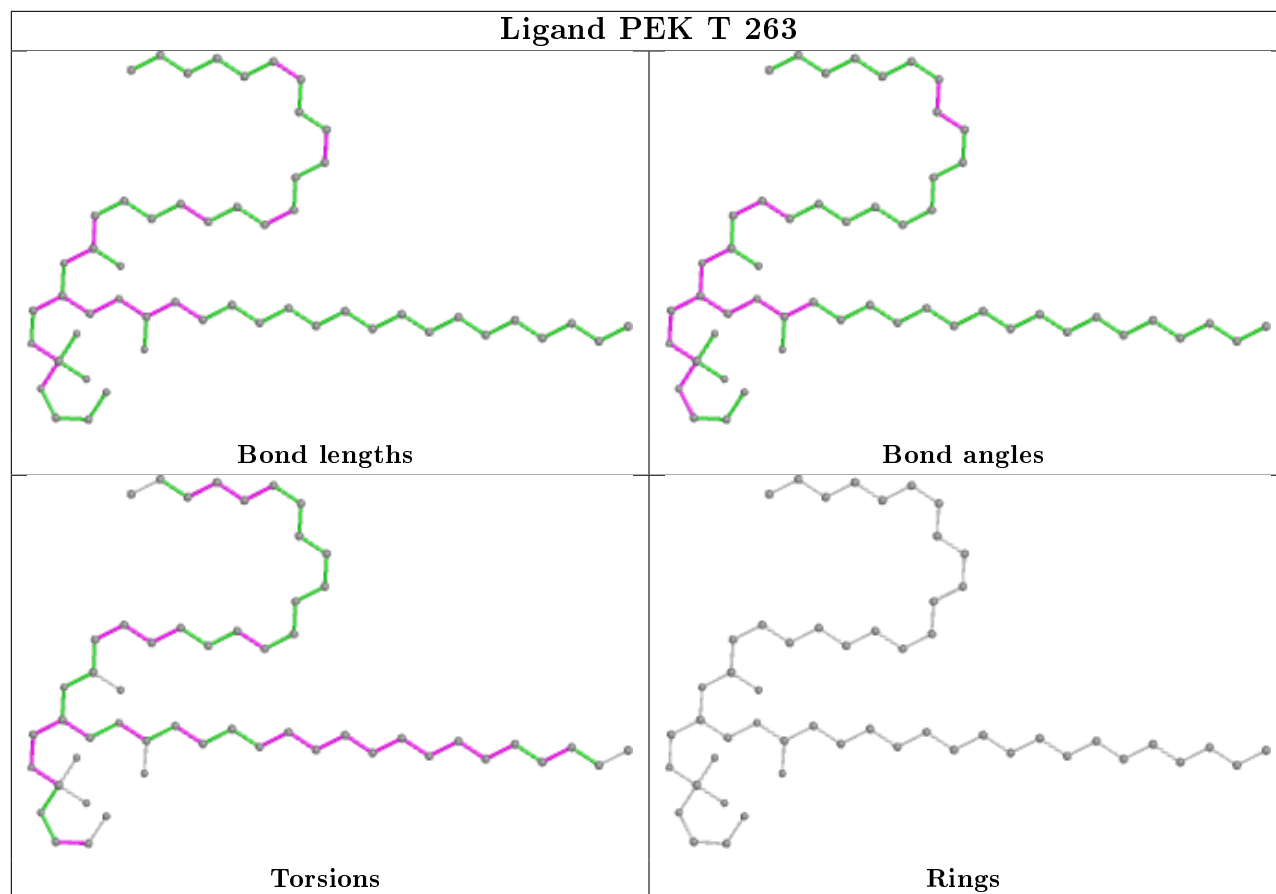
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	O	1230	PSC	20	0
17	A	515	HEA	12	0
23	G	86	CHD	1	0
18	Y	1522	TGL	16	0
17	N	516	HEA	9	0
23	B	1086	CHD	5	0
18	O	1521	TGL	8	0
24	P	1272	DMU	4	0
23	W	1060	CHD	3	0
17	A	516	HEA	3	0
23	C	271	CHD	4	0
18	A	521	TGL	8	0
25	C	265	PEK	11	0
24	C	272	DMU	3	0
19	P	1268	PGV	2	0
17	N	515	HEA	9	0
25	T	1264	PEK	12	0
18	A	523	TGL	3	0
19	A	524	PGV	5	0
23	P	1525	CHD	1	0
26	C	270	CDL	17	0
19	A	525	PGV	4	0
19	N	1524	PGV	7	0
24	M	526	DMU	1	0
26	G	269	CDL	23	0

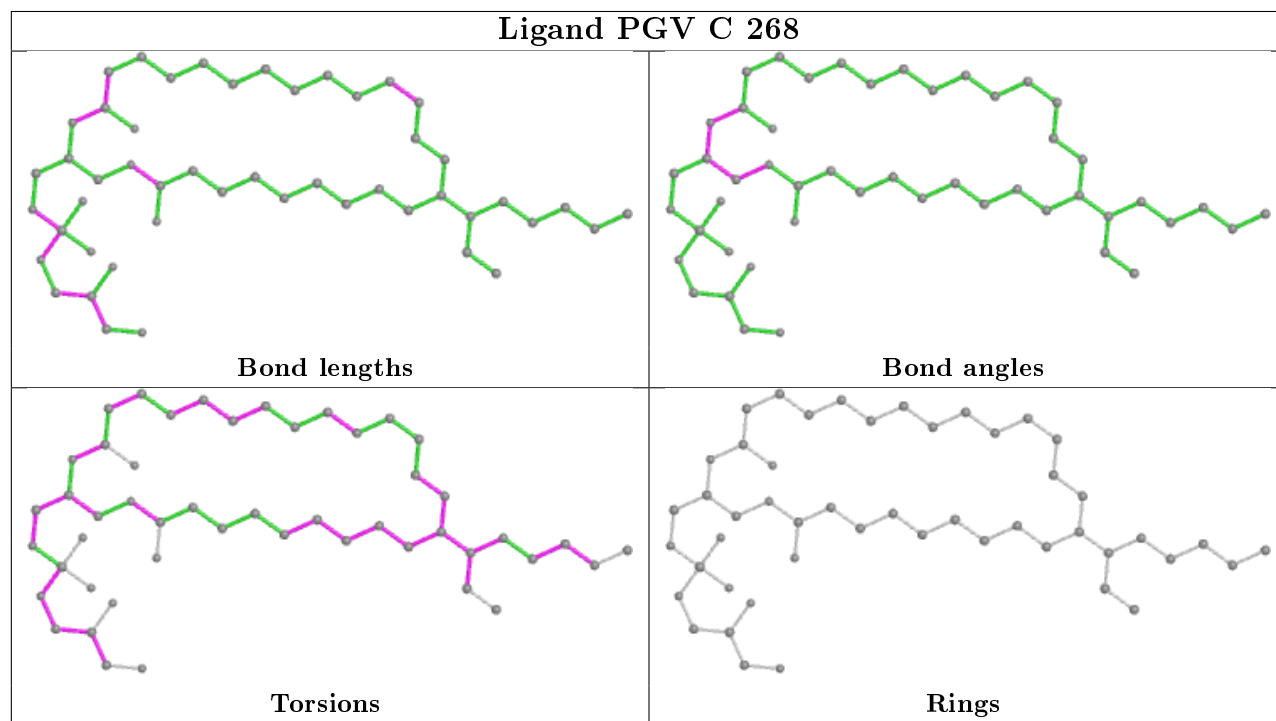
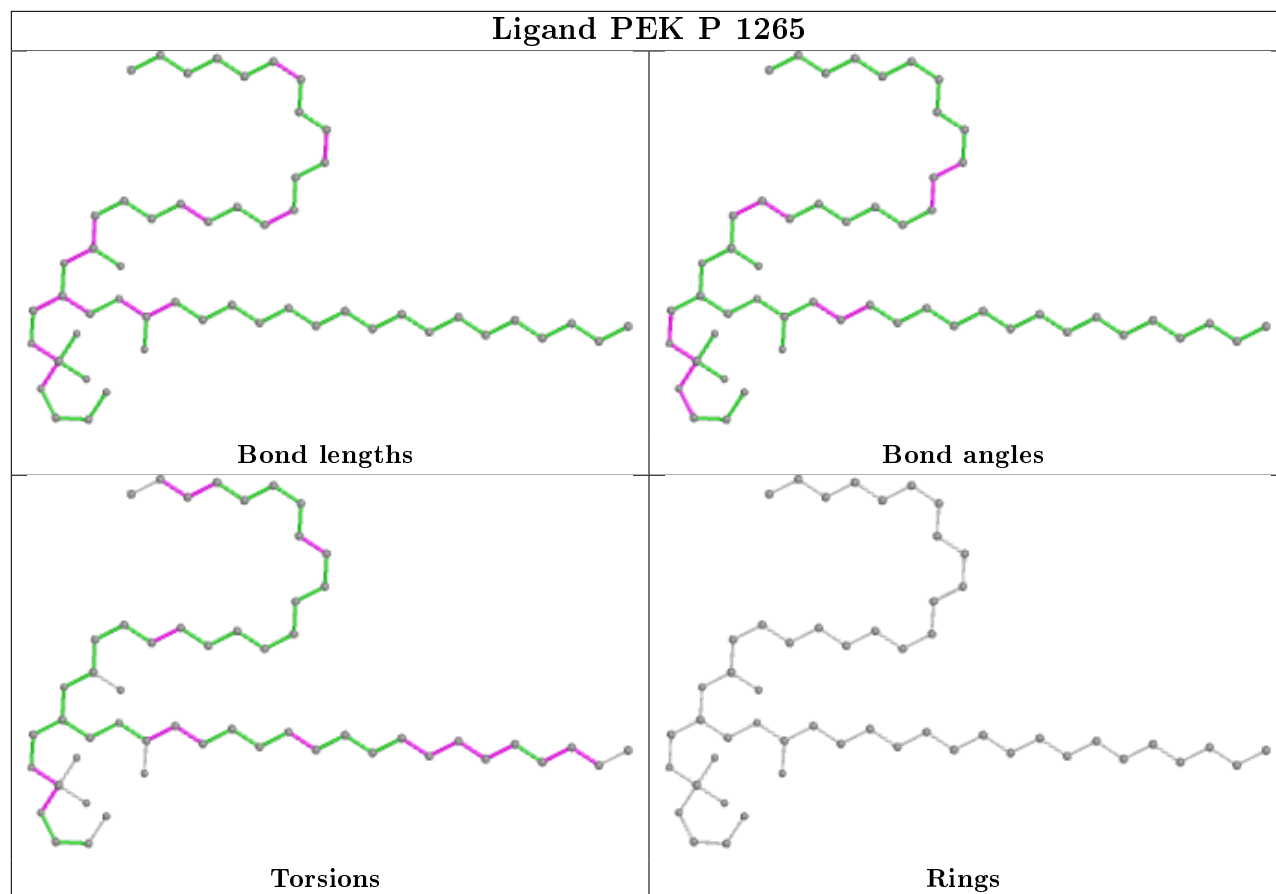
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

**Ligand TGL N 1523****Ligand CHD C 525**

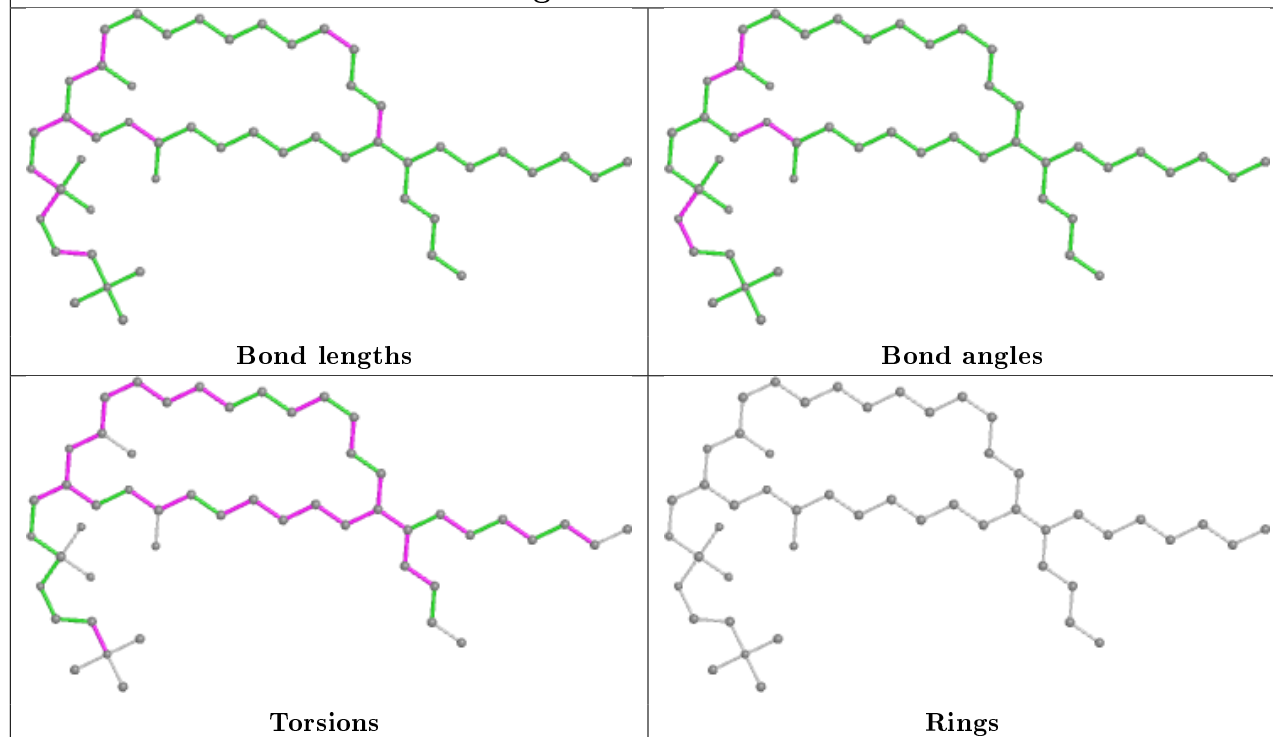




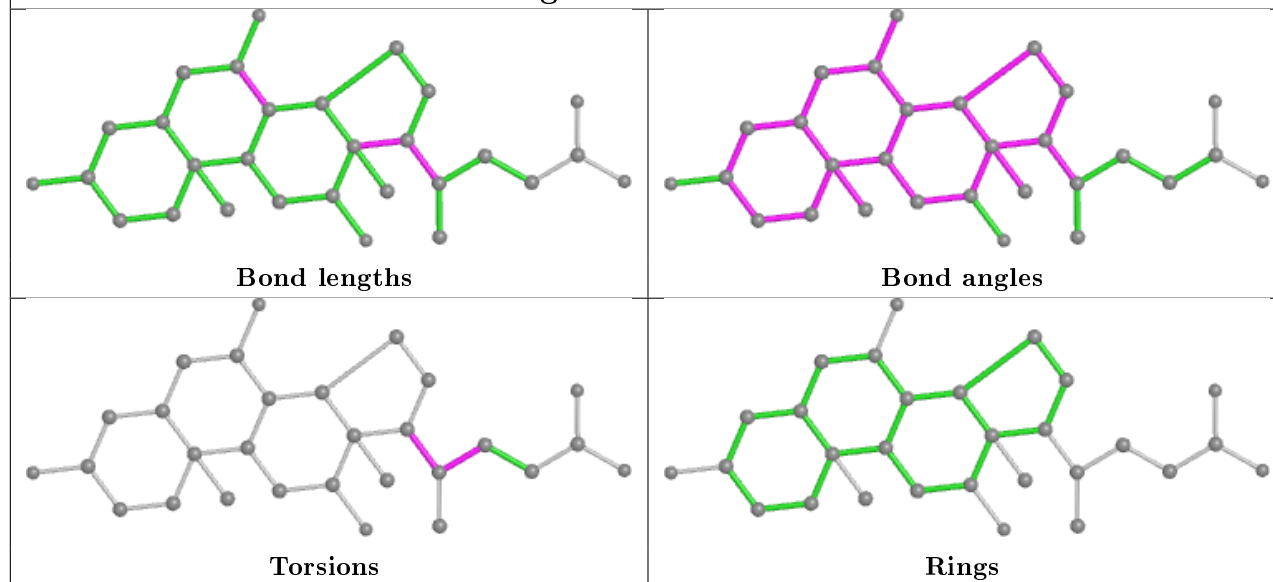


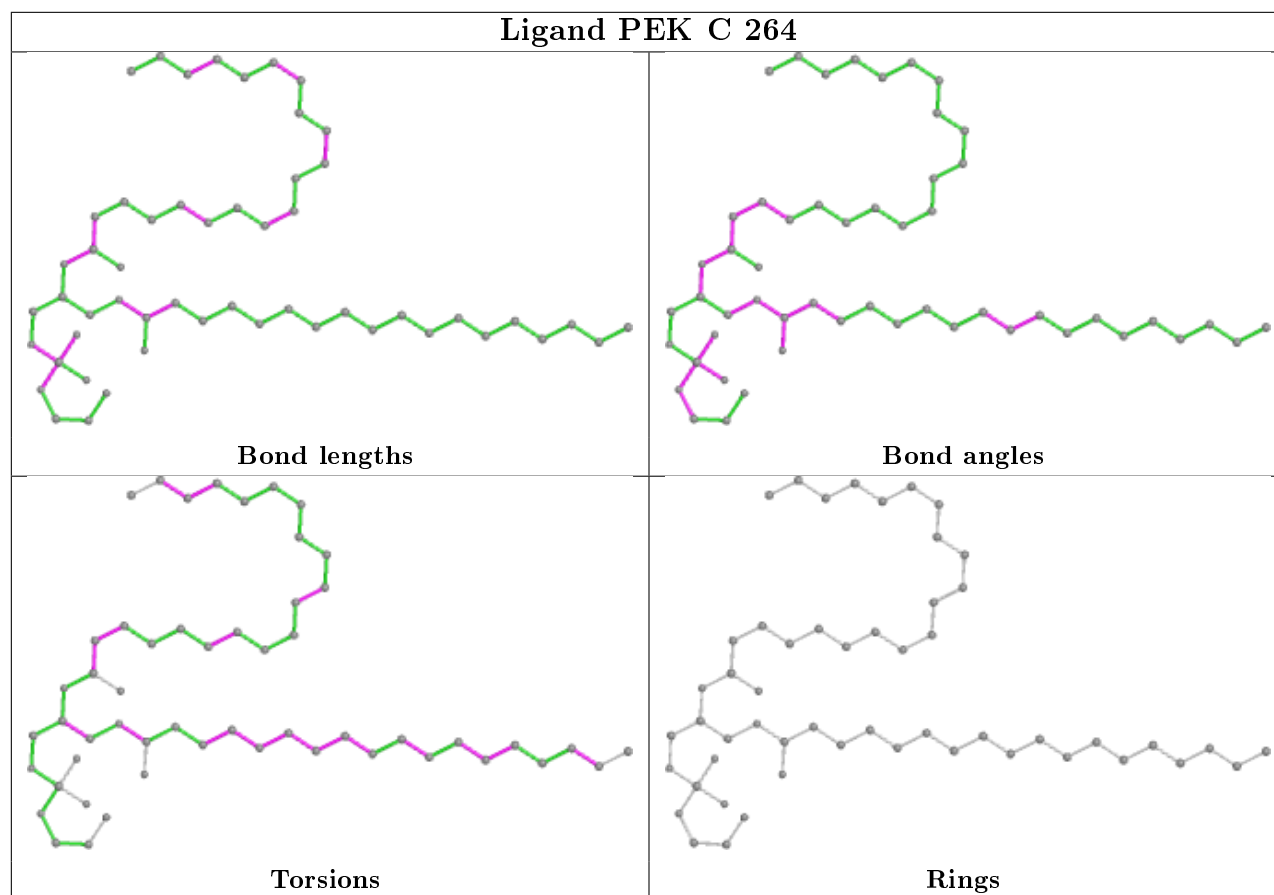
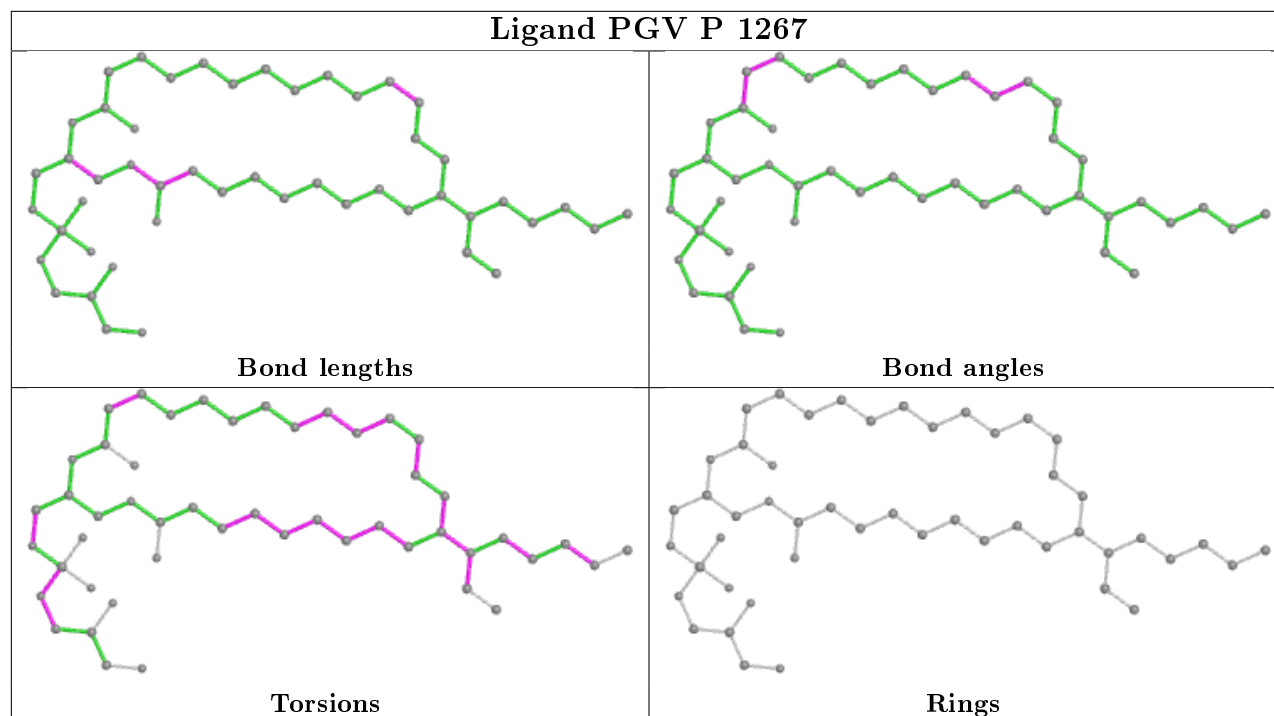


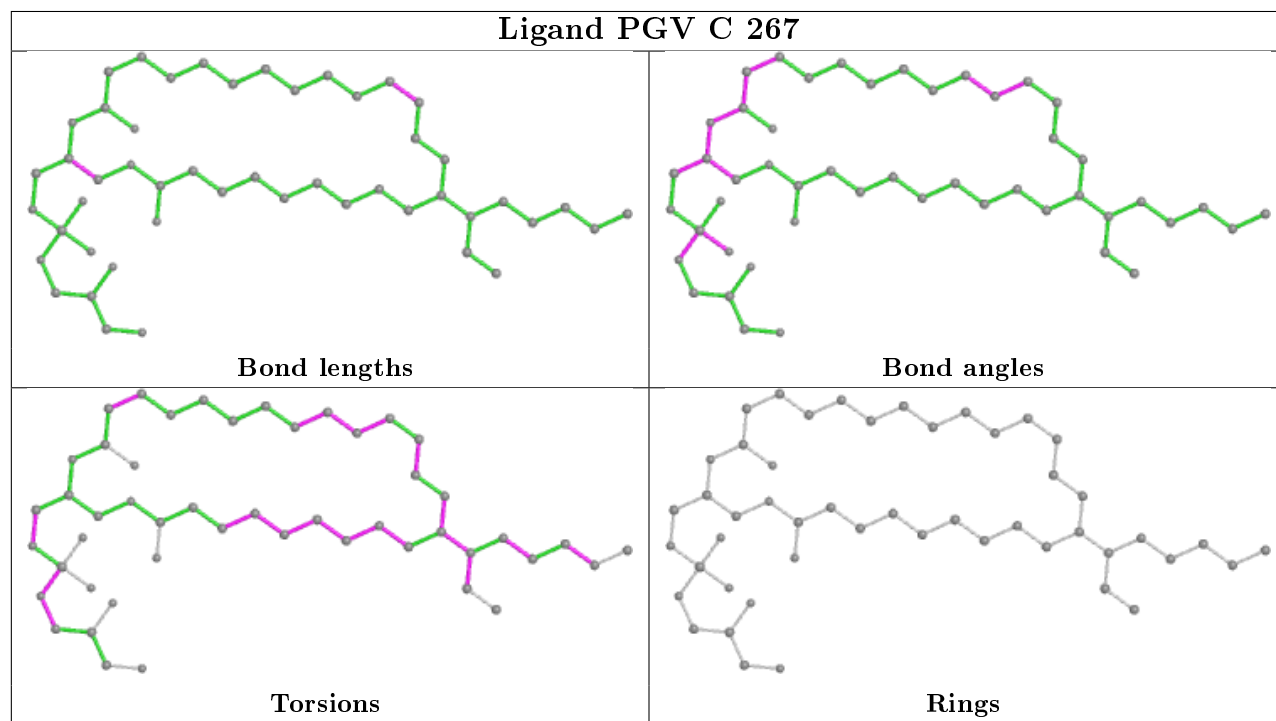
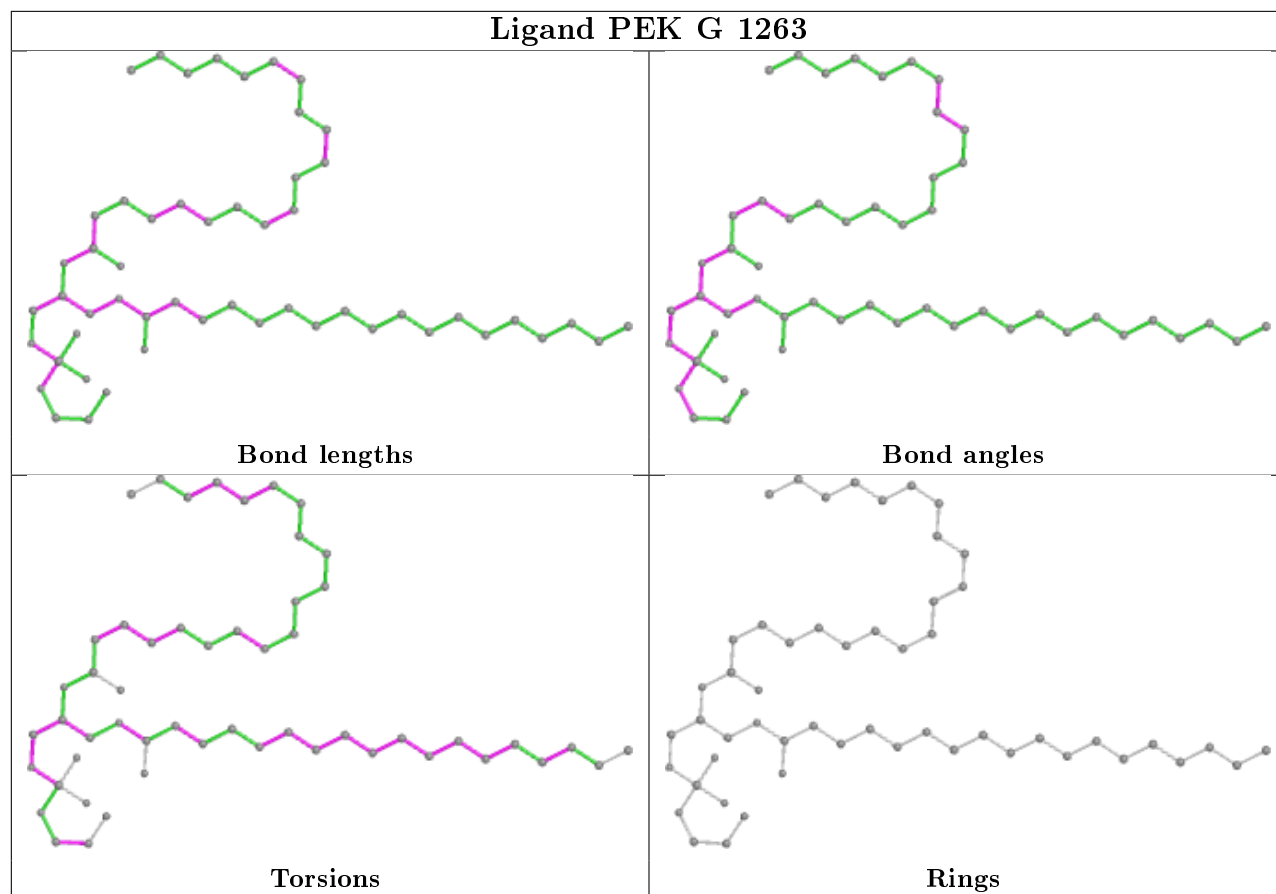
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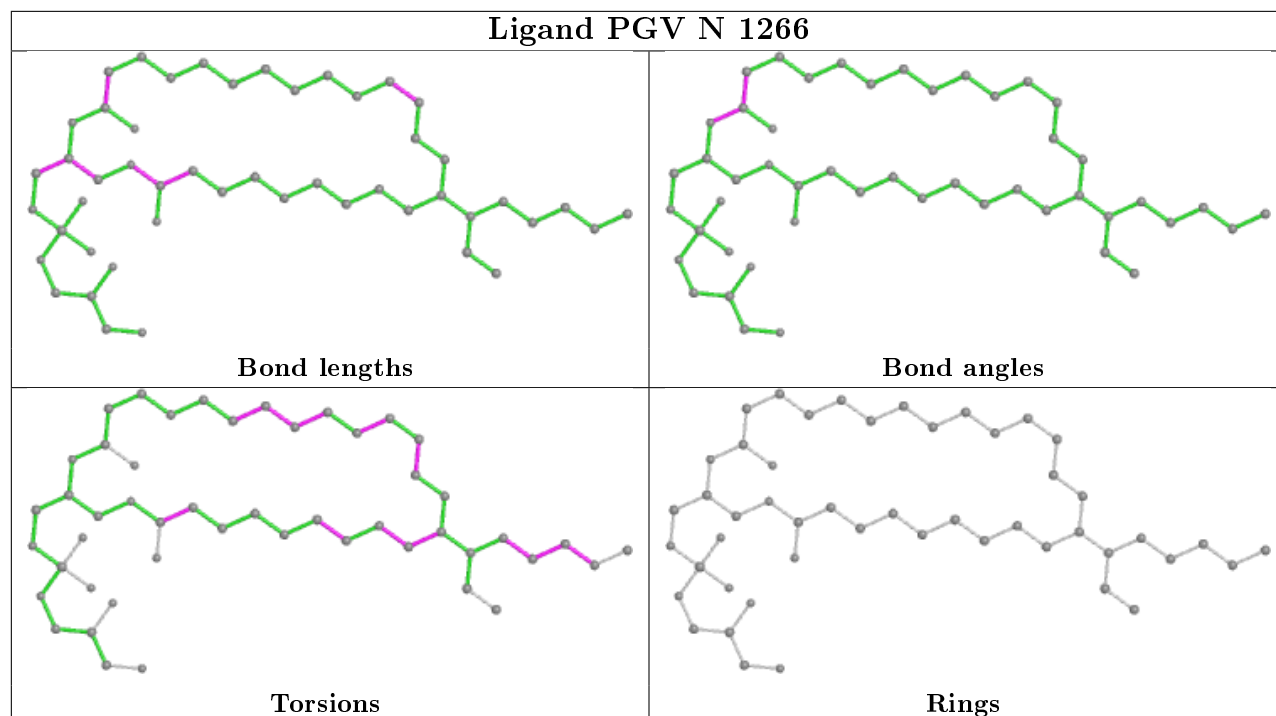
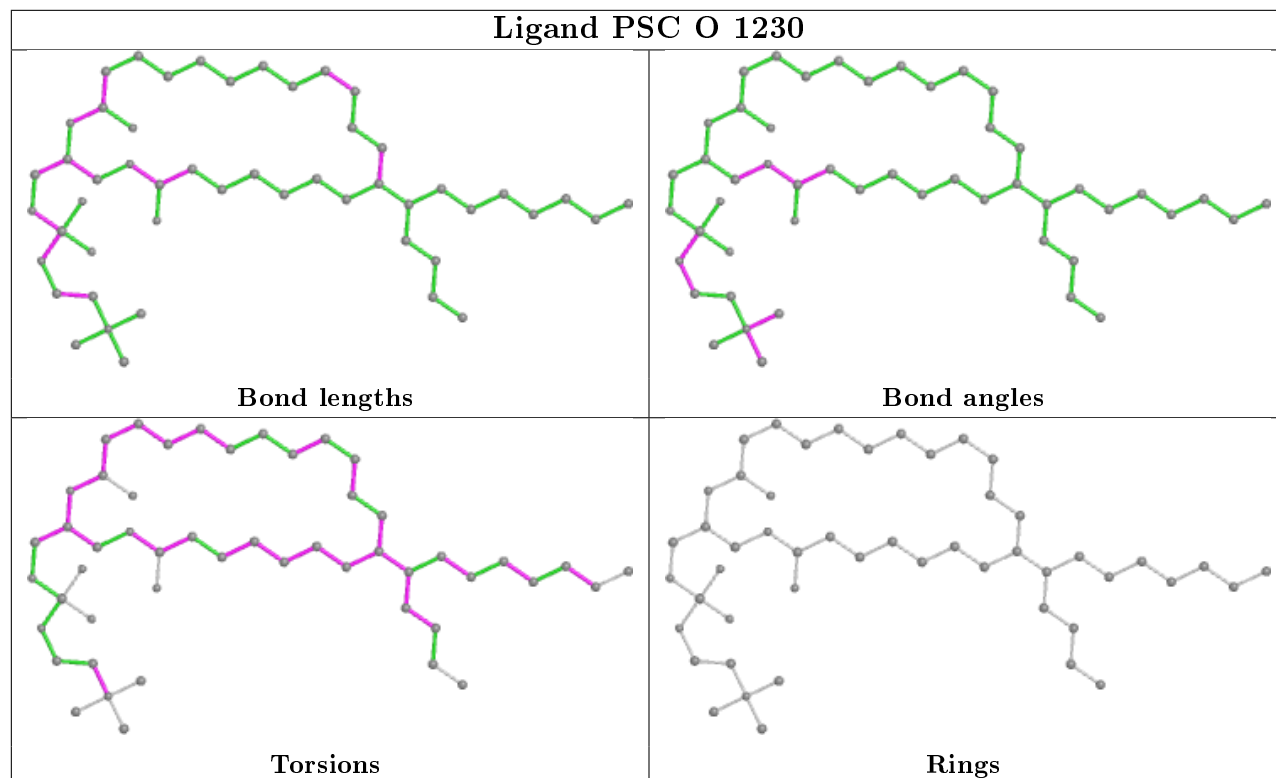


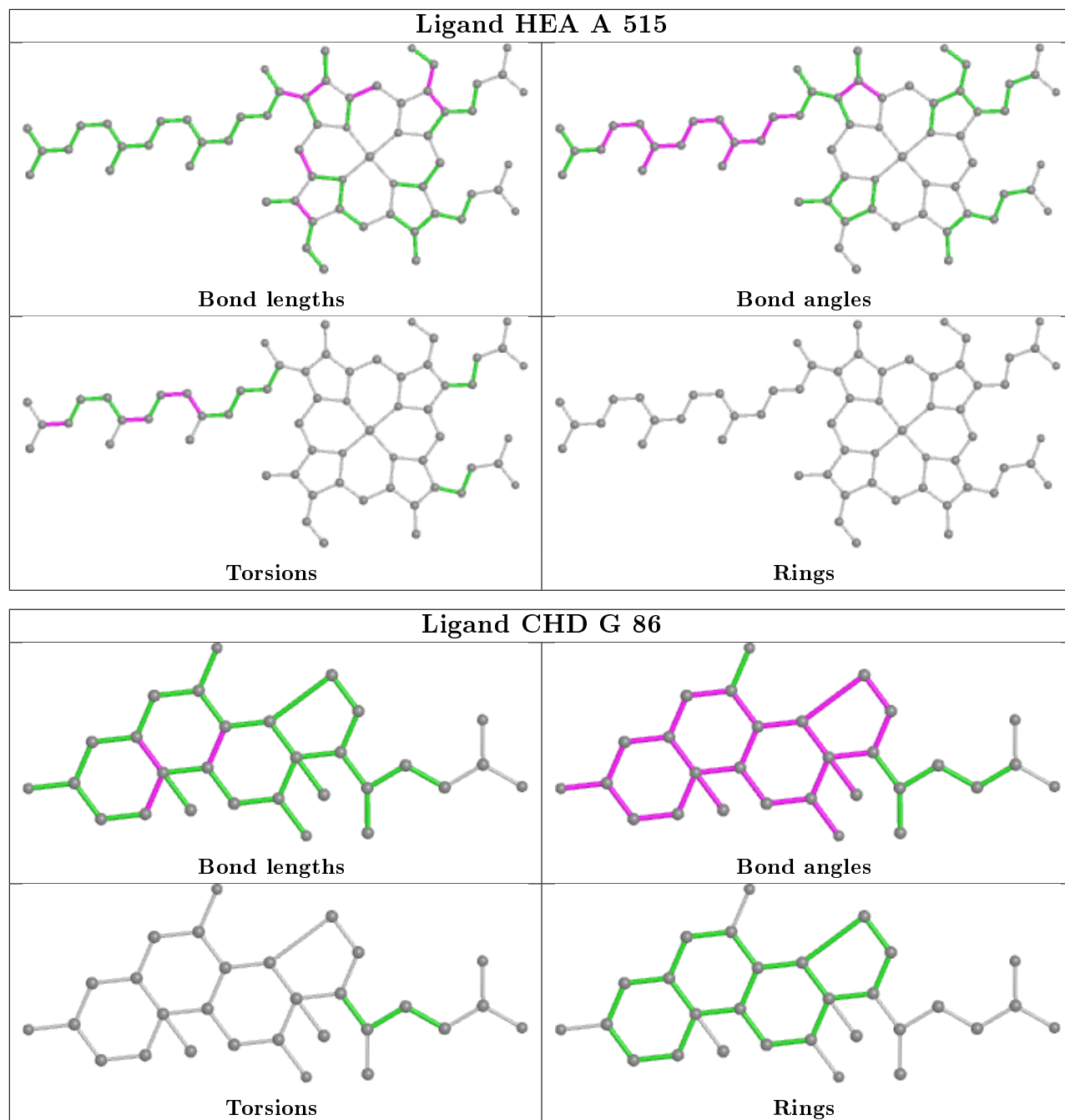
## Ligand CHD J 60

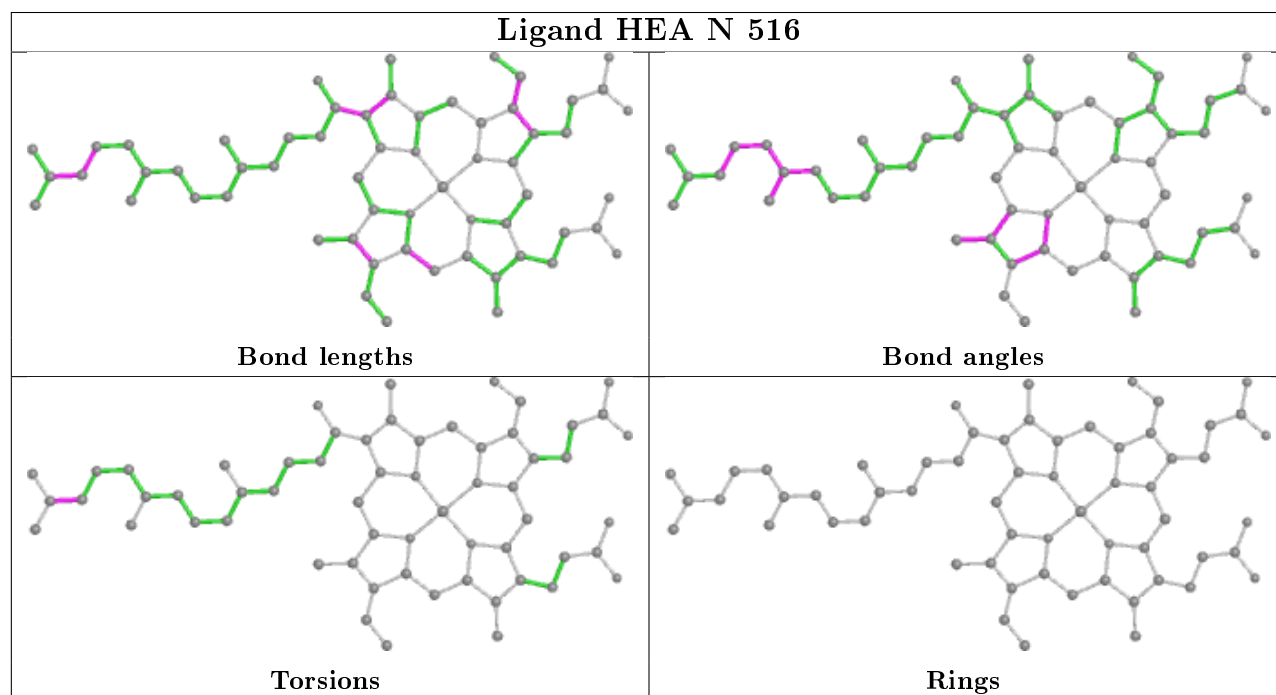
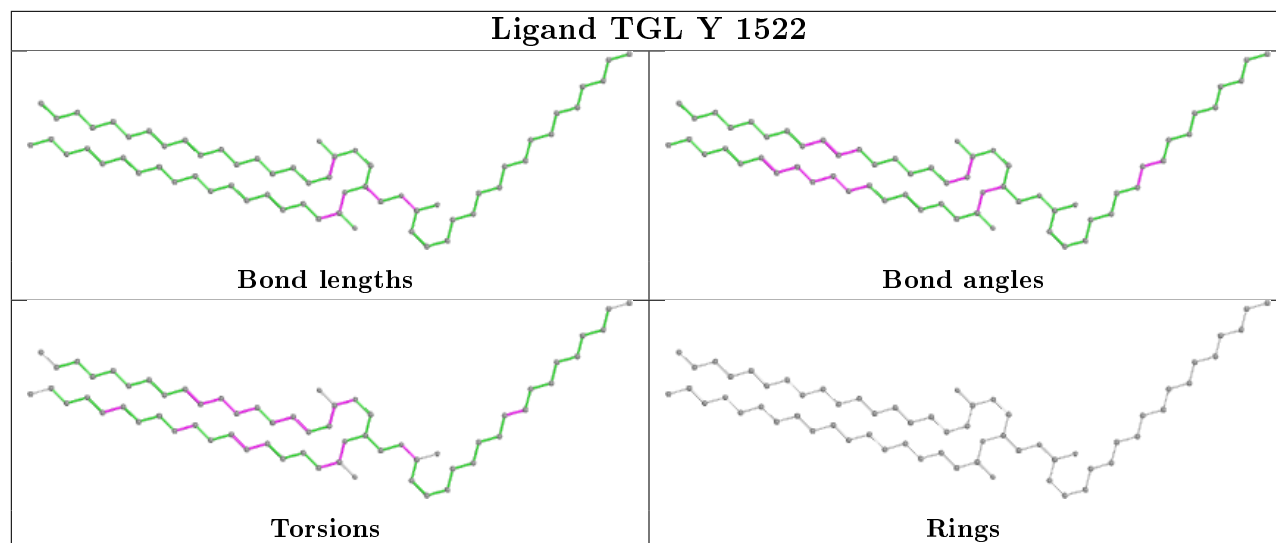




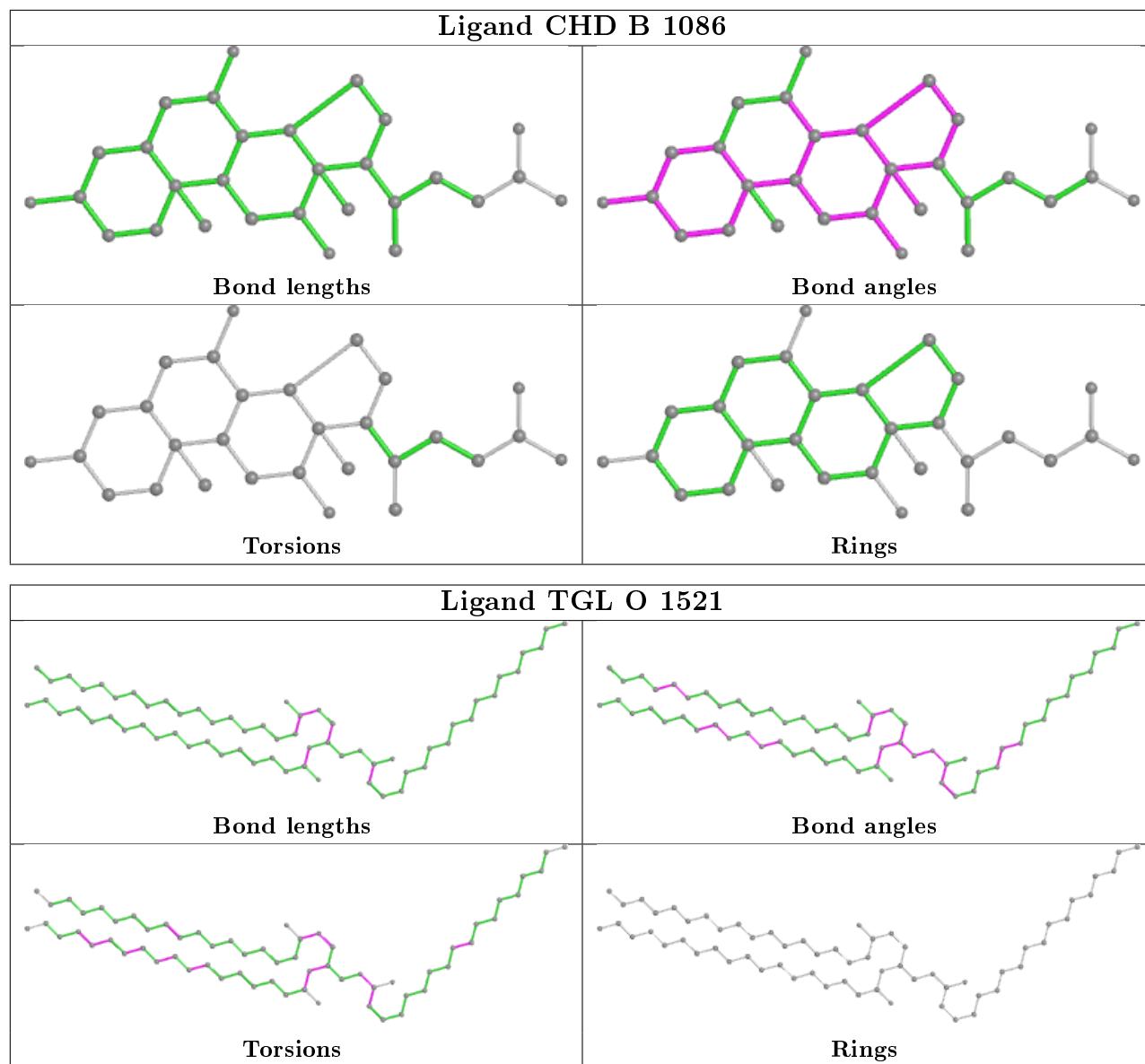


**Ligand PGV N 1266****Ligand PSC O 1230**

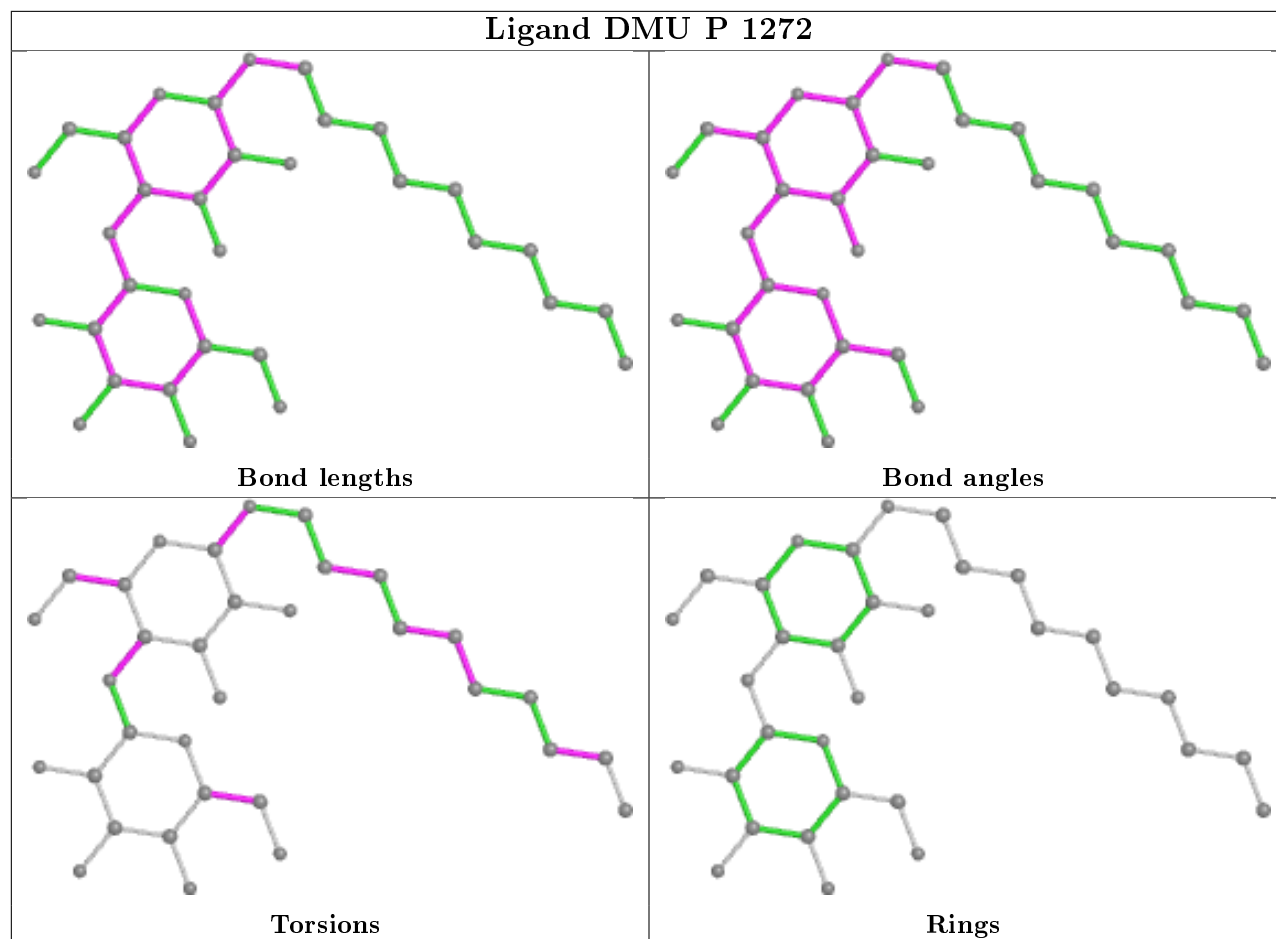




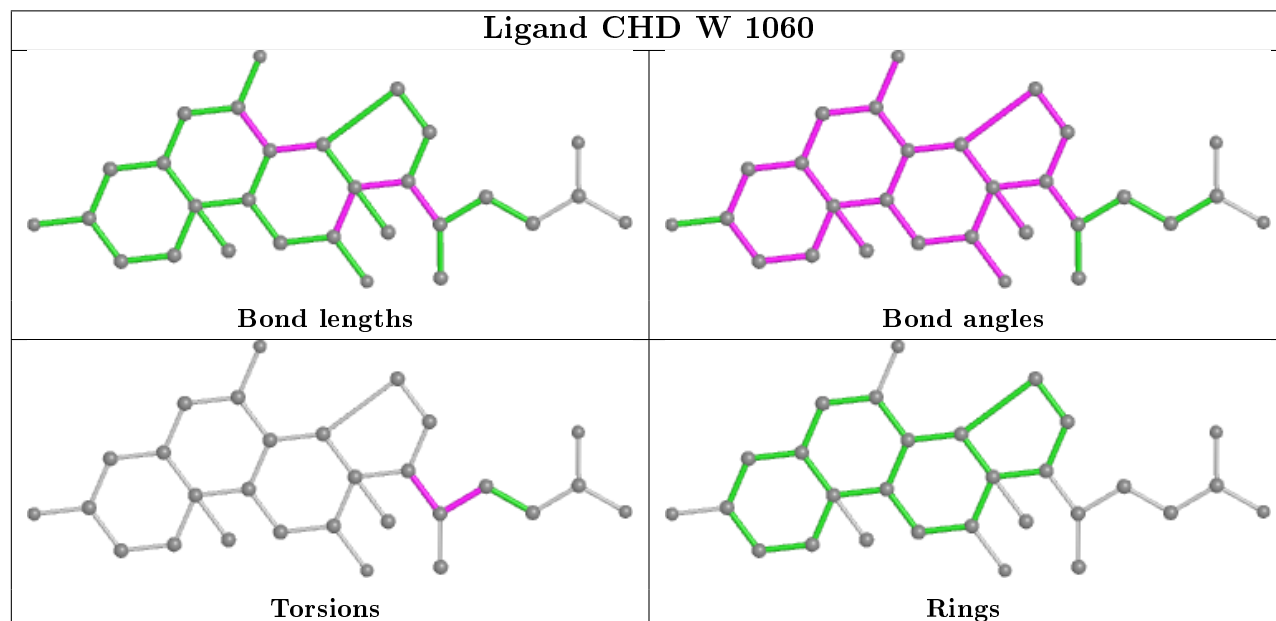


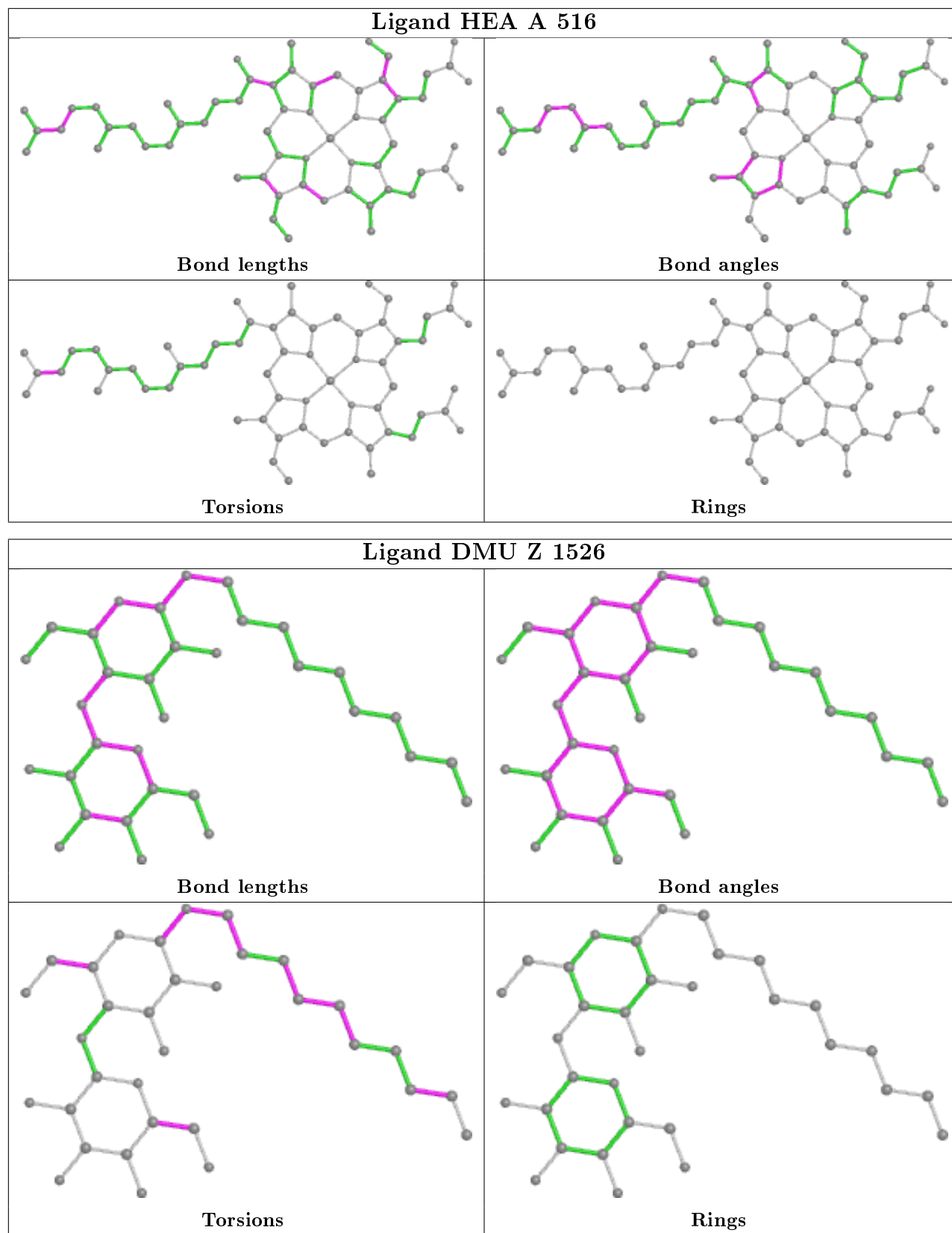


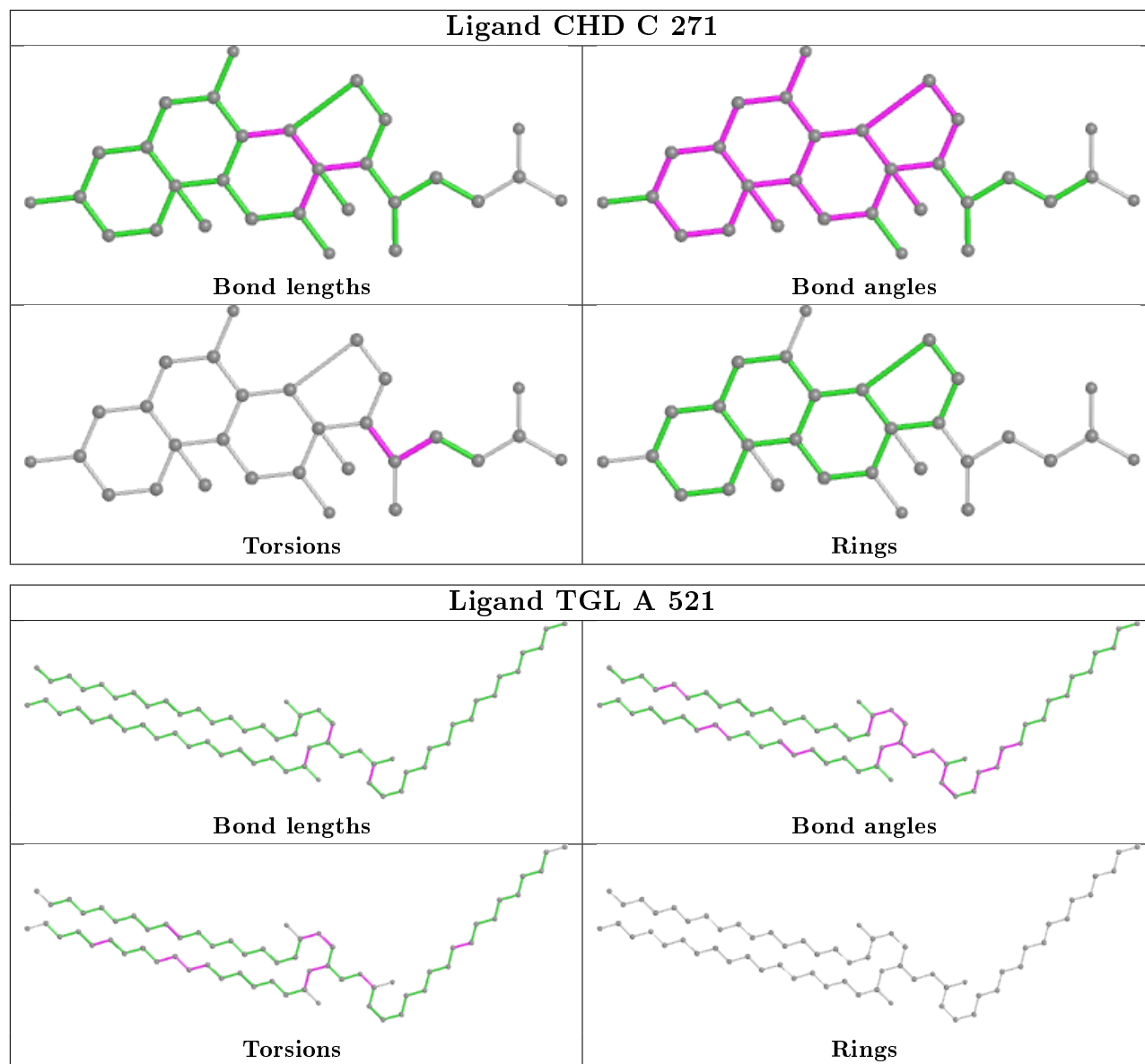
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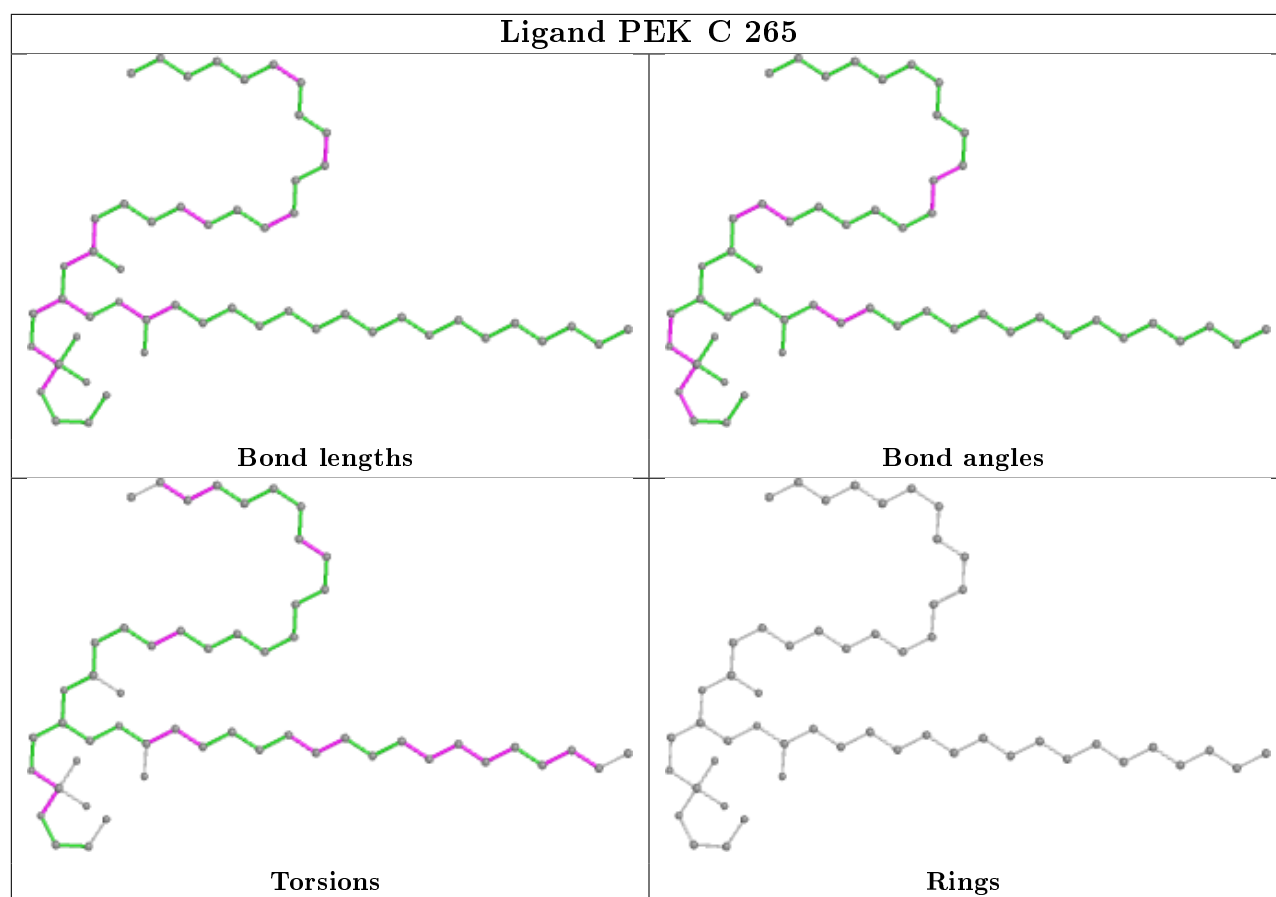


## Ligand CHD W 1060

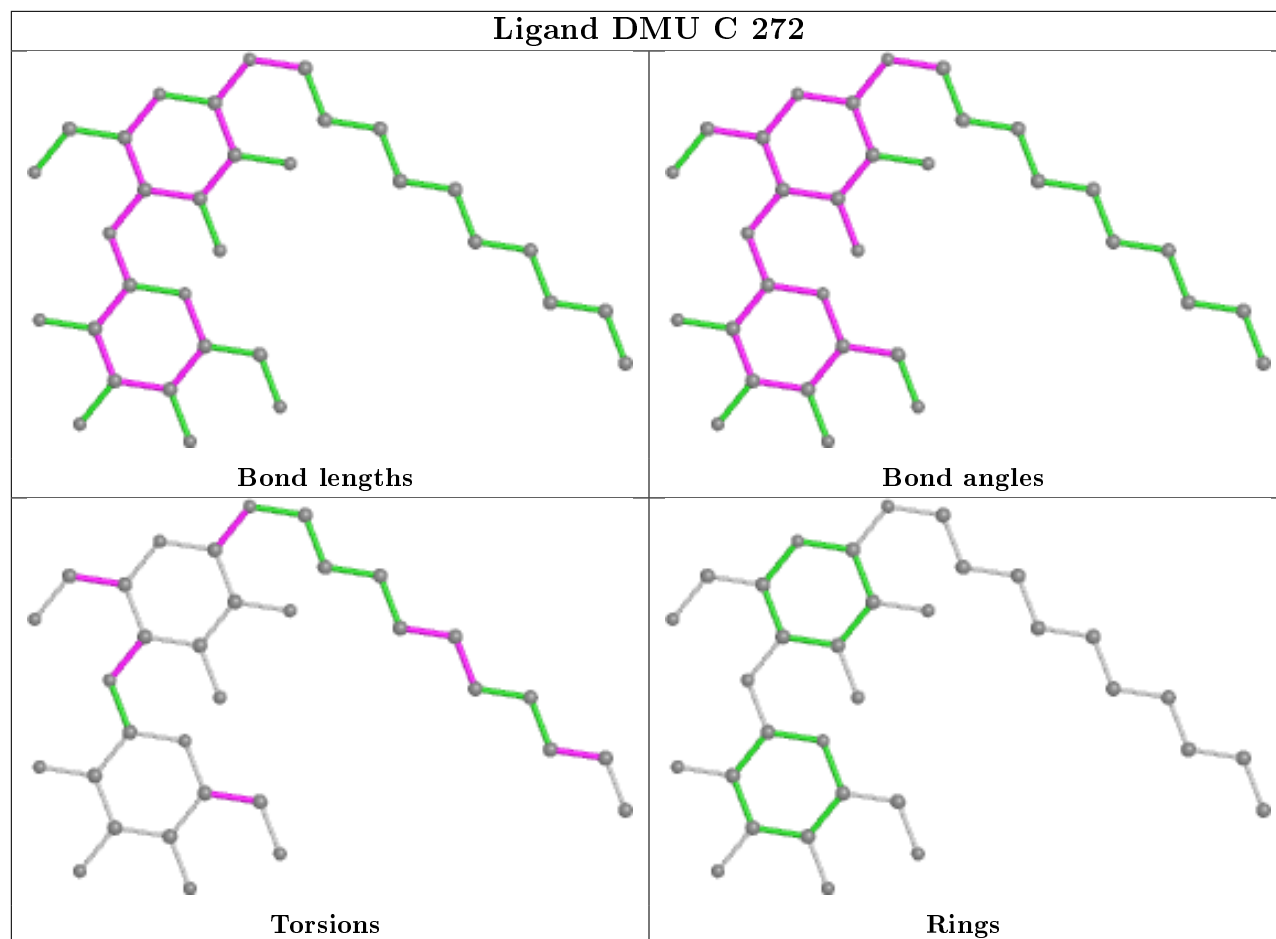




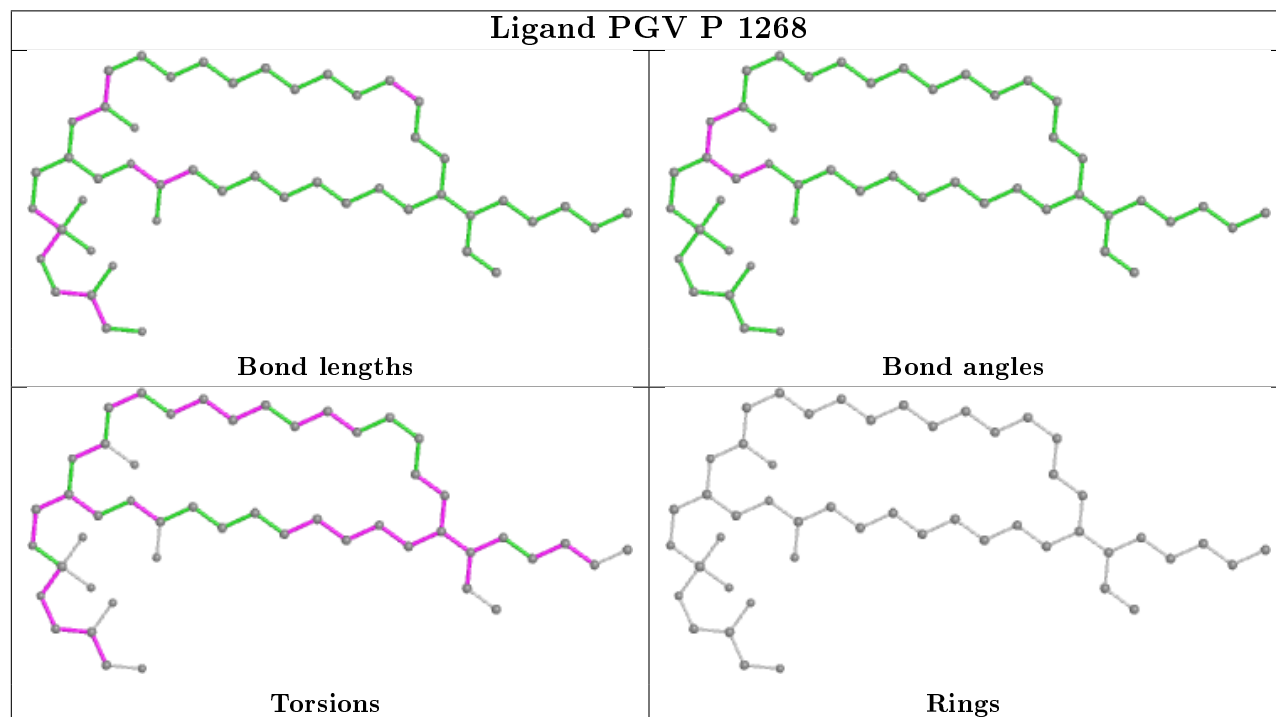


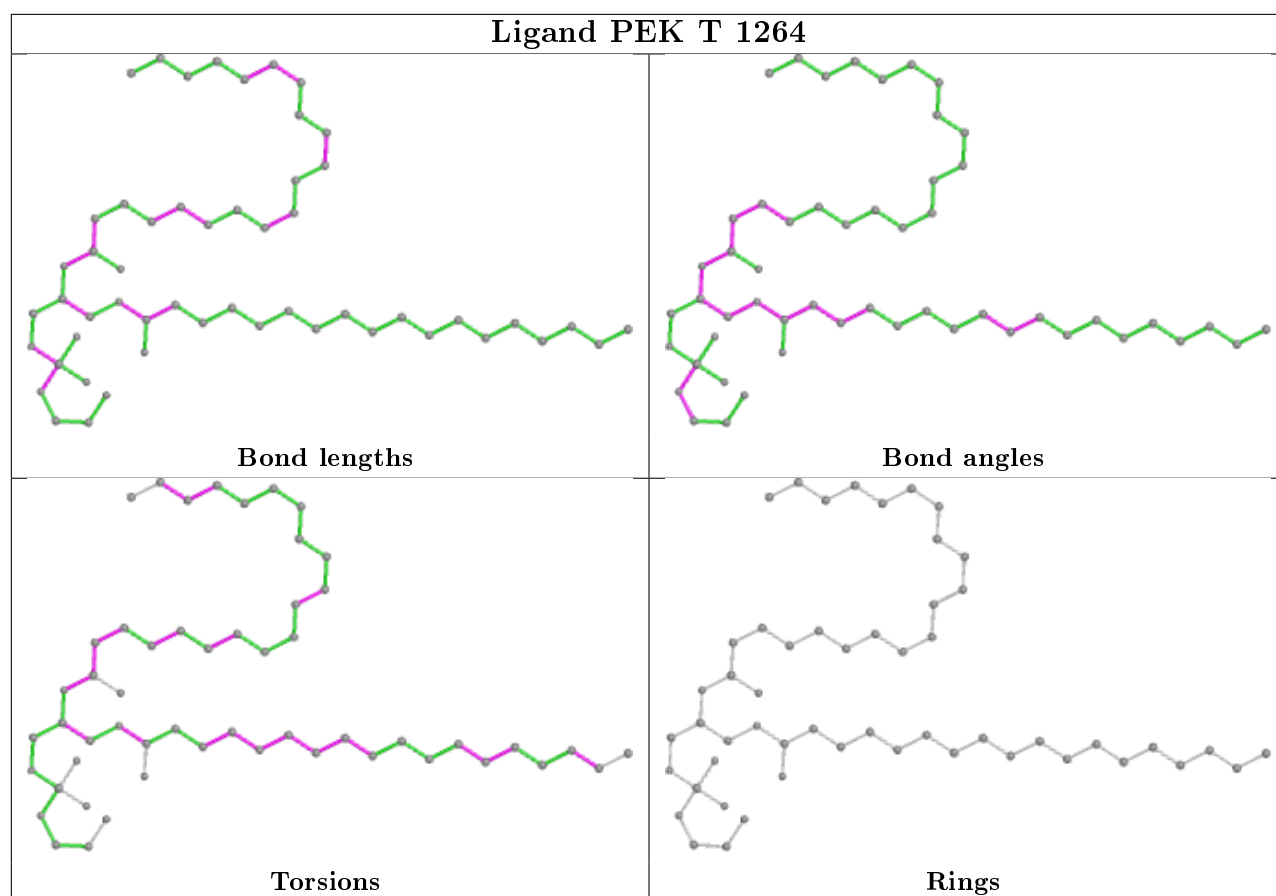
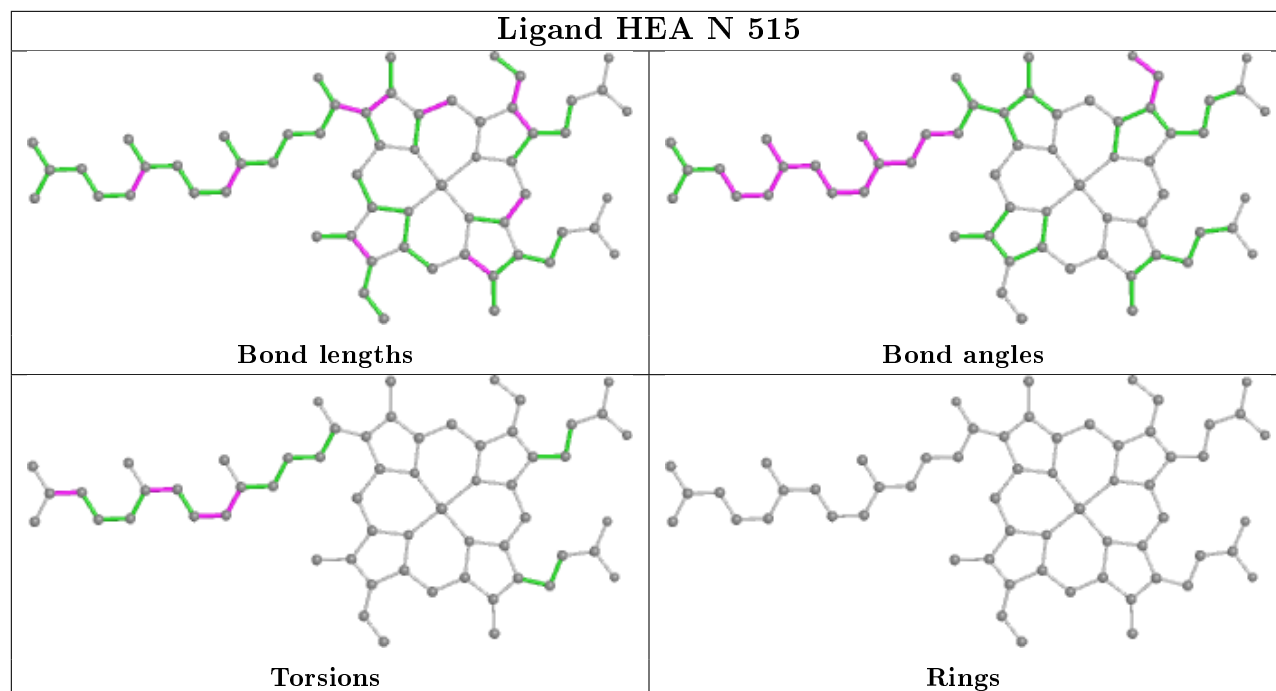


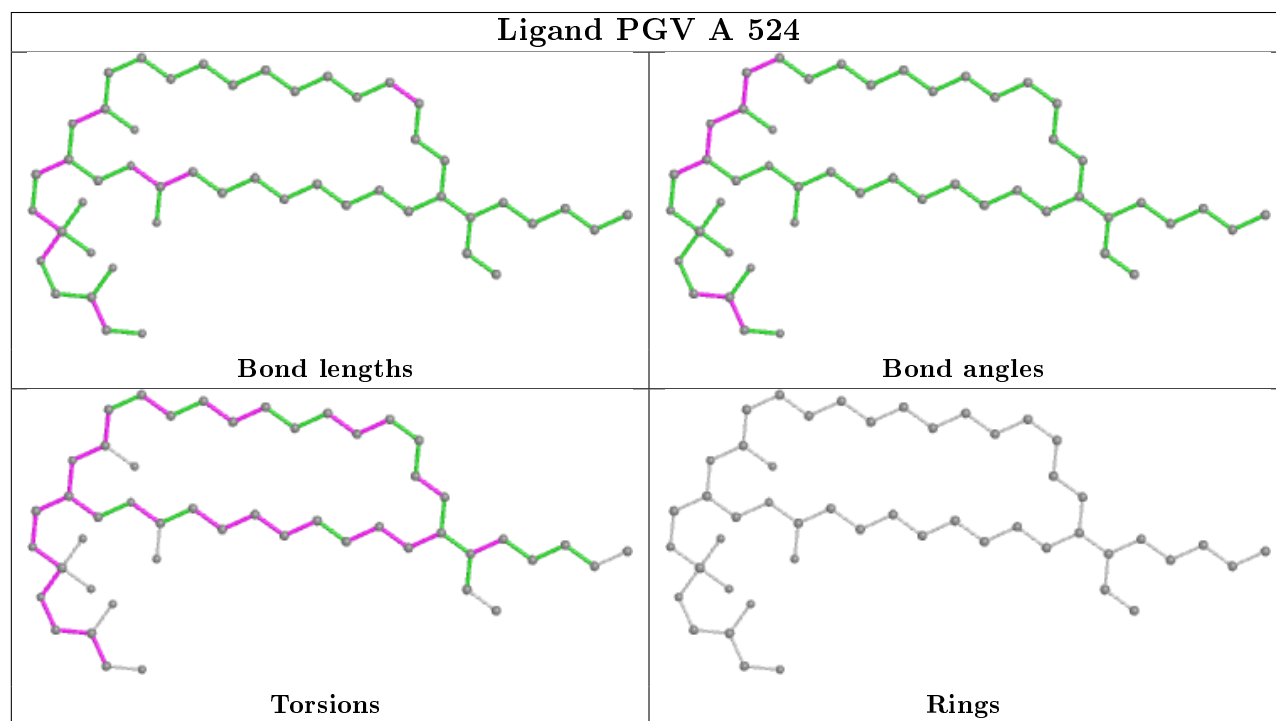
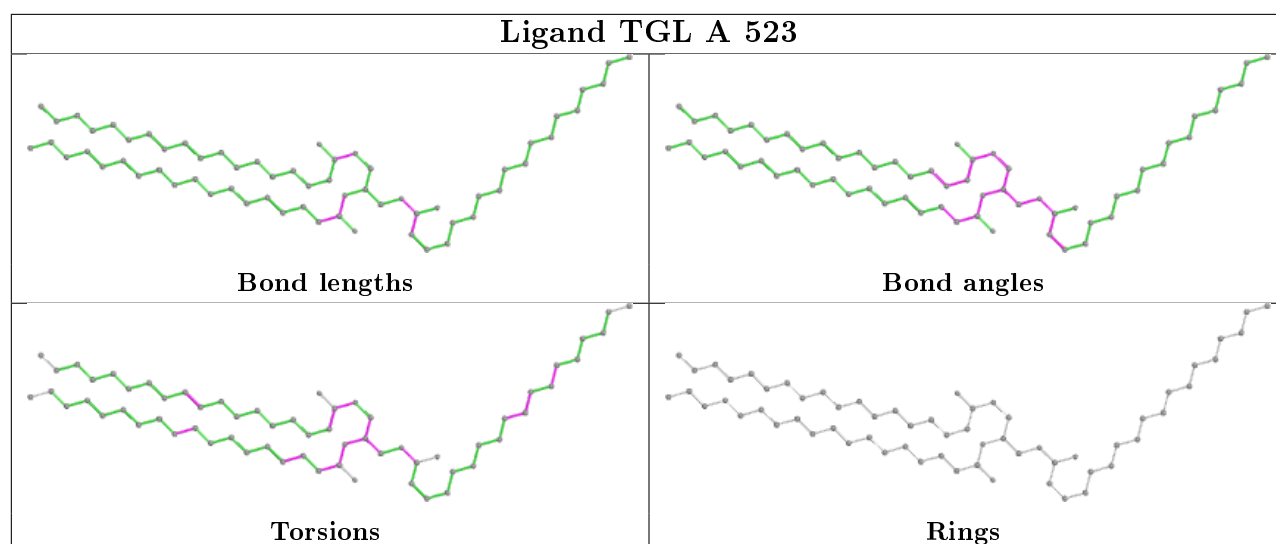
## Ligand DMU C 272



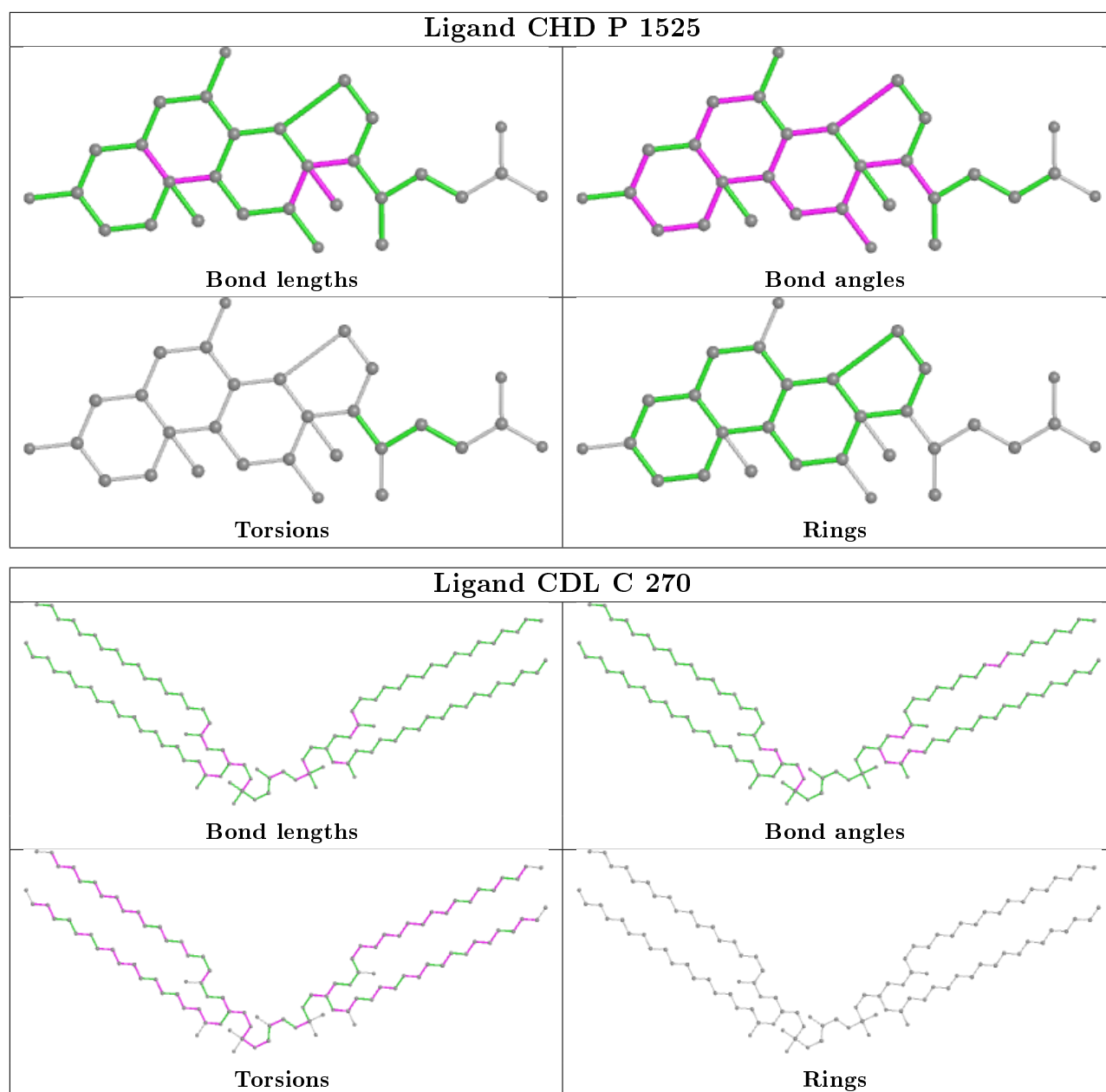
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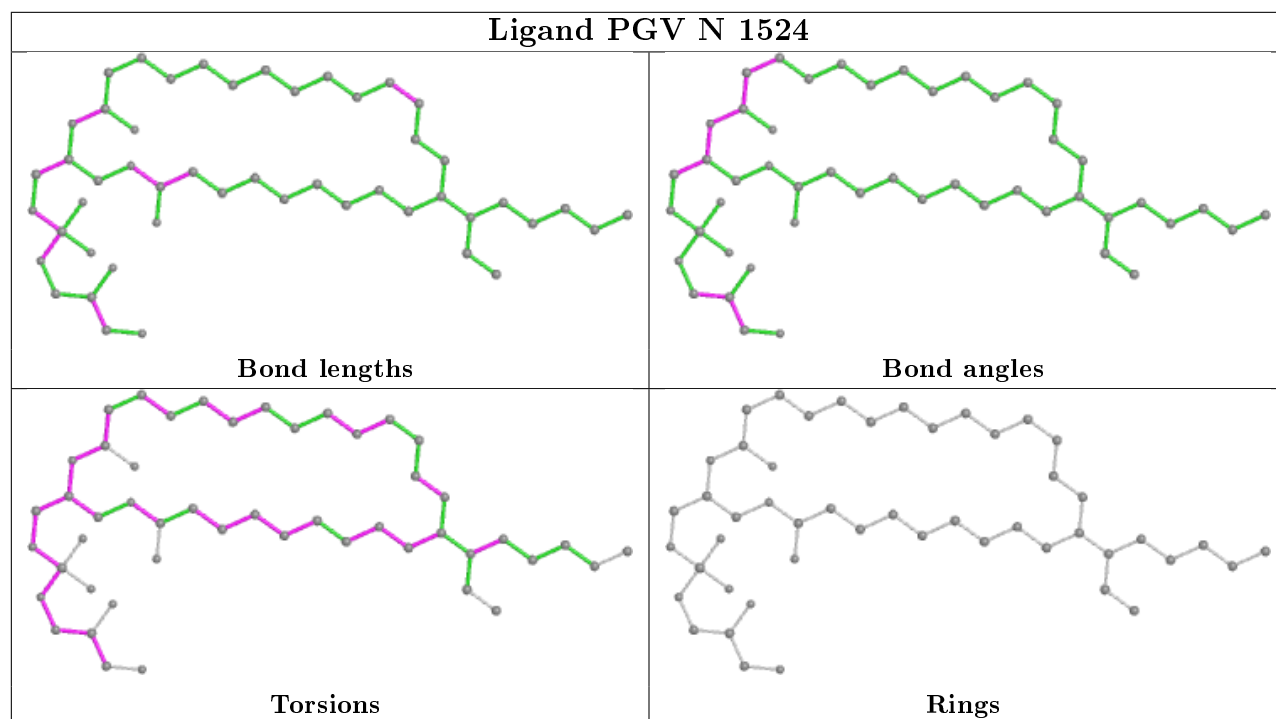
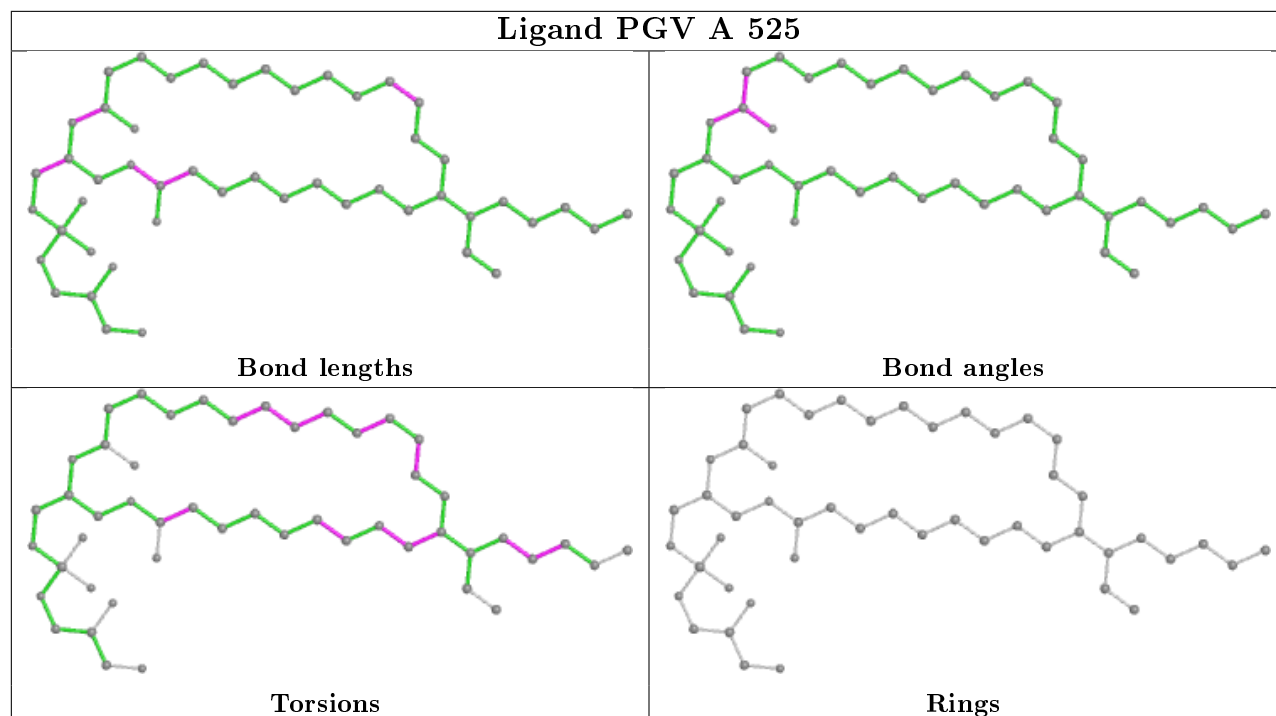


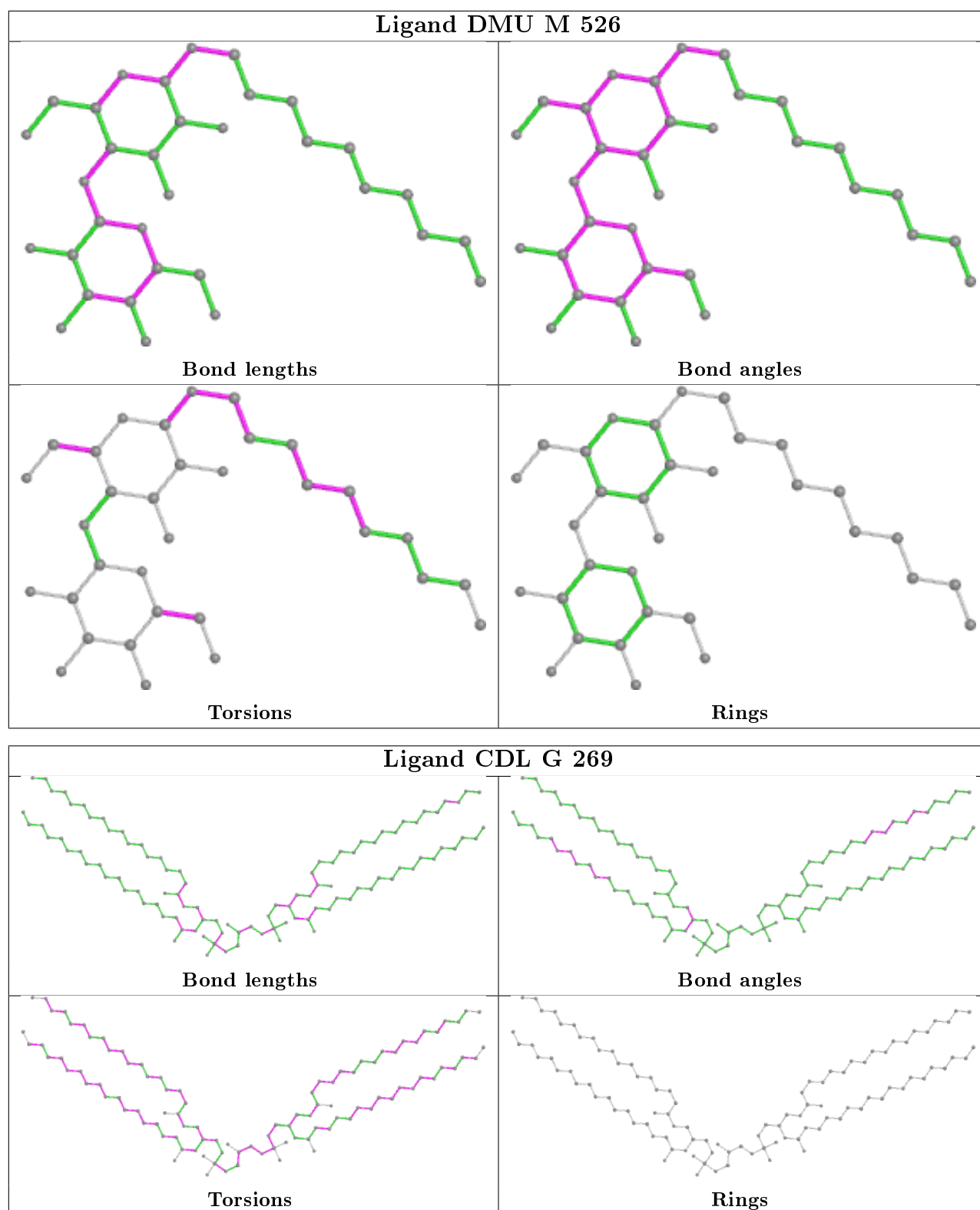












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.