



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 4, 2026 – 06:33 PM EDT

PDB ID : 1V54 / pdb_00001v54
Title : Bovine heart cytochrome c oxidase at the fully oxidized state
Authors : Tsukihara, T.; Shimokata, K.; Katayama, Y.; Shimada, H.; Muramoto, K.; Aoyama, H.; Mochizuki, M.; Shinzawa-Itoh, K.; Yamashita, E.; Yao, M.; Ishimura, Y.; Yoshikawa, S.
Deposited on : 2003-11-21
Resolution : 1.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
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)	:	2.50

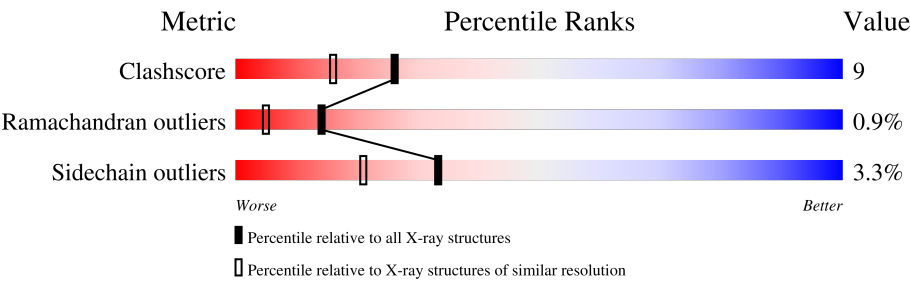
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	514	81% 17% .
1	N	514	79% 19% .
2	B	227	78% 17% .
2	O	227	70% 26% ..
3	C	261	87% 12% .
3	P	261	85% 14% .
4	D	147	87% 11% .
4	Q	147	74% 23% ..

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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
18	TGL	L	3522	-	-	X	-
21	CHD	C	3271	X	-	-	-
21	CHD	J	3060	X	-	-	-
21	CHD	P	4271	X	-	-	-
21	CHD	W	4060	X	-	-	-
25	PSC	O	4230	-	-	X	-
27	DMU	M	3526	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	DMU	Z	4526	X	-	-	-

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 32636 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 polypeptide I.

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 polypeptide II.

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 polypeptide III.

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 IV 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 polypeptide VIb.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

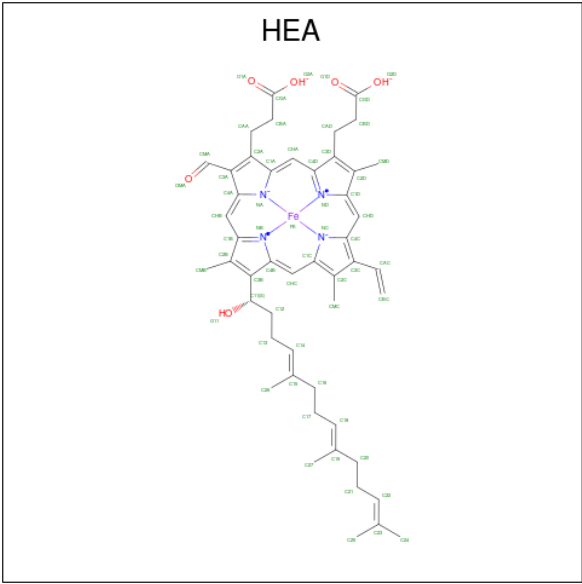
- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

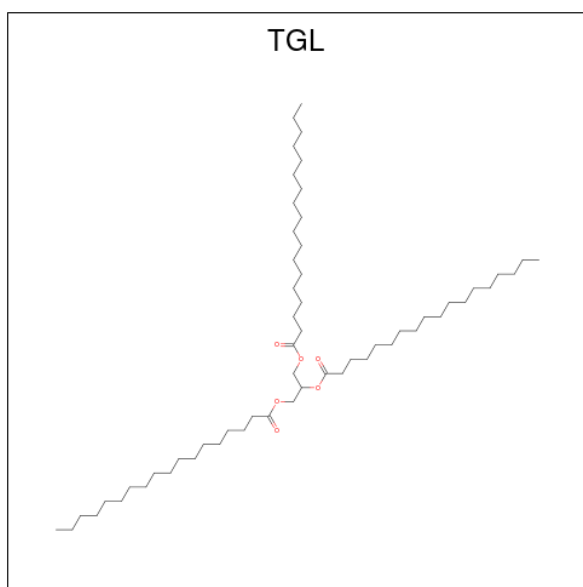
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Na	0	0
			1	1		
16	N	1	Total	Na	0	0
			1	1		

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



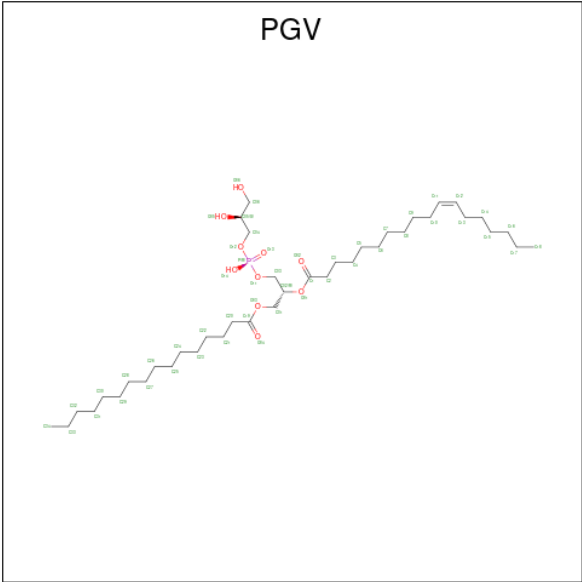
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
17	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
17	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
17	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

- Molecule 18 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: C₅₇H₁₁₀O₆).



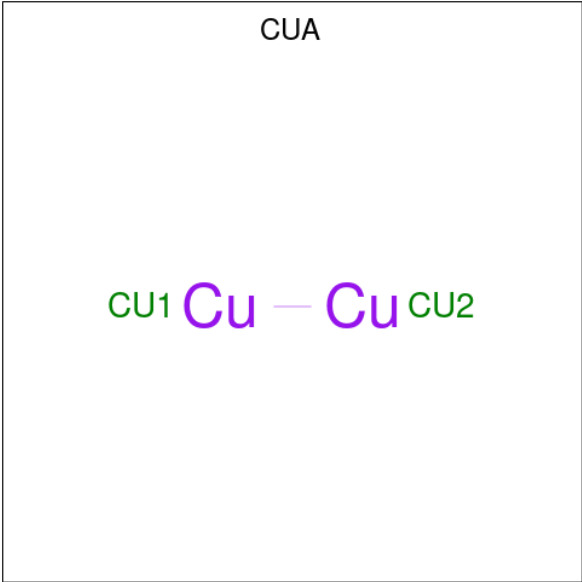
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	A	1	Total	C	O	0	0
			63	57	6		
18	D	1	Total	C	O	0	0
			63	57	6		
18	L	1	Total	C	O	0	0
			63	57	6		
18	N	1	Total	C	O	0	0
			63	57	6		
18	N	1	Total	C	O	0	0
			63	57	6		
18	Q	1	Total	C	O	0	0
			63	57	6		

- Molecule 19 is (1R)-2-{{[[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P).



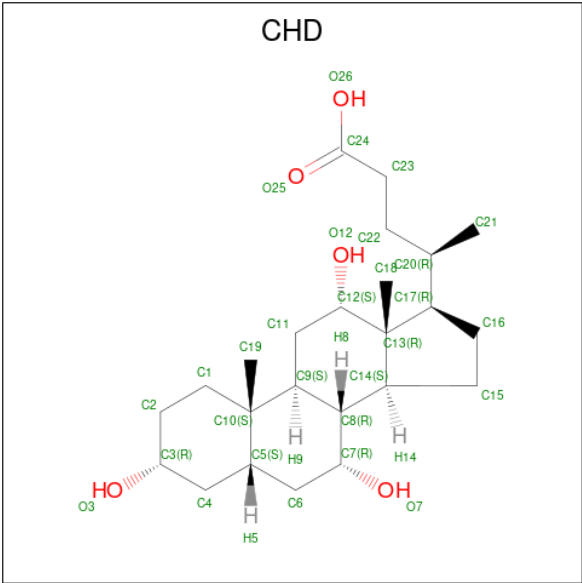
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	P	1	Total	C	O	P	0	0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

- Molecule 20 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



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

- Molecule 21 is CHOLIC ACID (CCD ID: CHD) (formula: C₂₄H₄₀O₅).



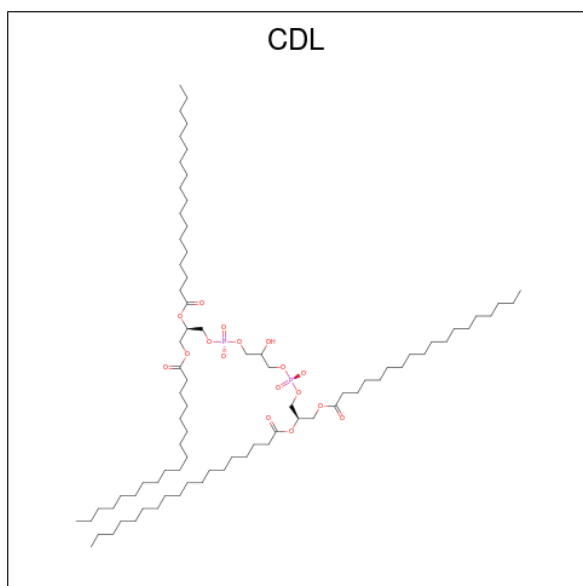
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	B	1	Total	C	O	0	0
			29	24	5		
21	C	1	Total	C	O	0	0
			29	24	5		

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

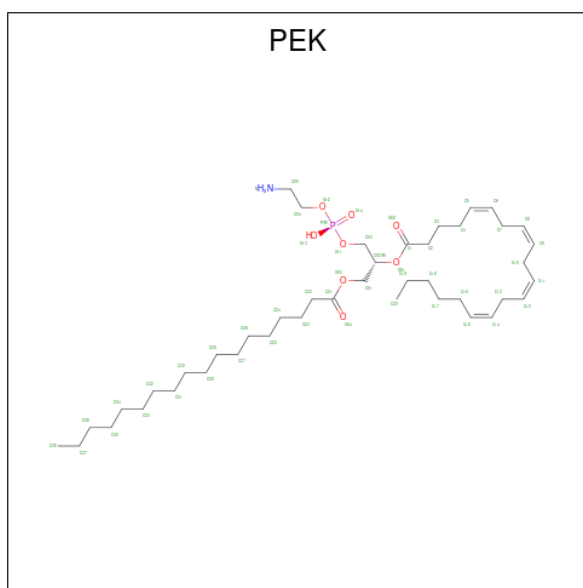
- Molecule 22 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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

- Molecule 23 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE

(CCD ID: PEK) (formula: C₄₃H₇₈NO₈P).

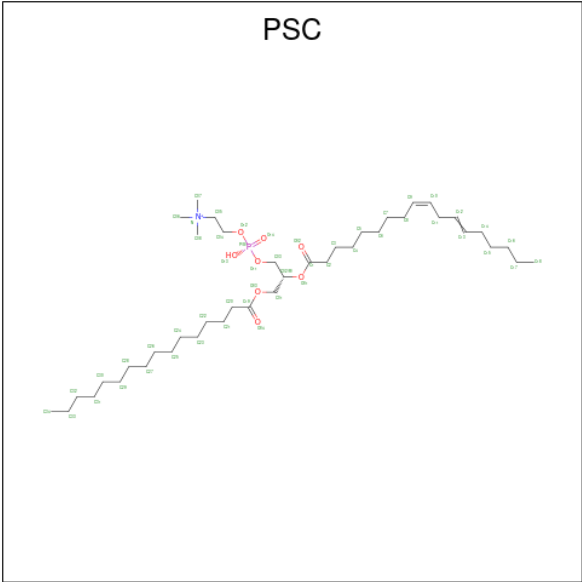


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

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

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

- Molecule 25 is (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: C₄₂H₈₁NO₈P).

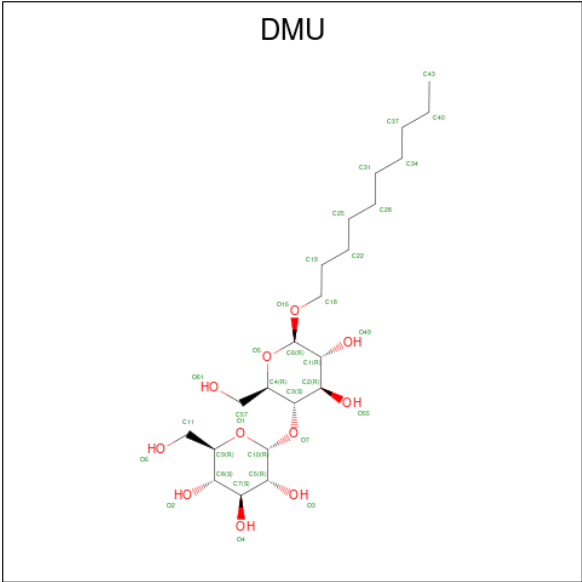


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	E	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
25	O	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 26 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 27 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: C₂₂H₄₂O₁₁).



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

- Molecule 28 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	227	Total	O	0	0
			227	227		
28	B	180	Total	O	0	0
			180	180		
28	C	116	Total	O	0	0
			116	116		
28	D	109	Total	O	0	0
			109	109		
28	E	68	Total	O	0	0
			68	68		
28	F	80	Total	O	0	0
			80	80		
28	G	59	Total	O	0	0
			59	59		
28	H	71	Total	O	0	0
			71	71		
28	I	61	Total	O	0	0
			61	61		
28	J	21	Total	O	0	0
			21	21		

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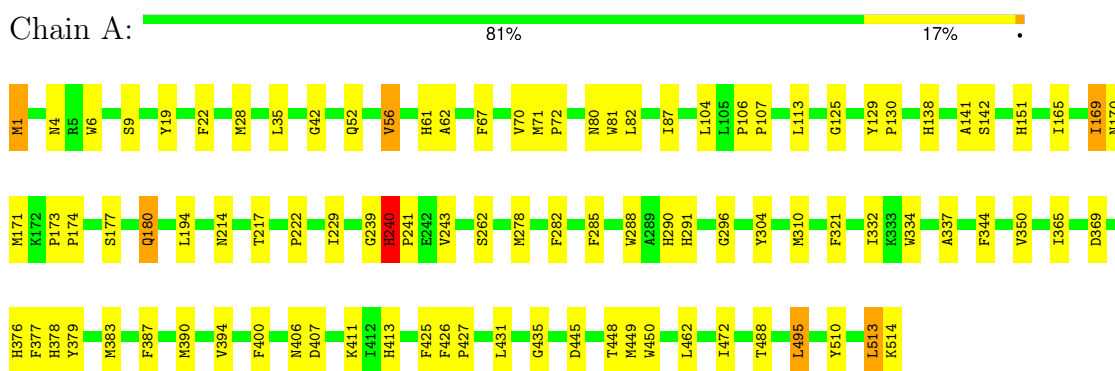
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	K	37	Total 37	O 37	0	0
28	L	23	Total 23	O 23	0	0
28	M	32	Total 32	O 32	0	0
28	N	217	Total 217	O 217	0	0
28	O	146	Total 146	O 146	0	0
28	P	120	Total 120	O 120	0	0
28	Q	73	Total 73	O 73	0	0
28	R	32	Total 32	O 32	0	0
28	S	54	Total 54	O 54	0	0
28	T	58	Total 58	O 58	0	0
28	U	65	Total 65	O 65	0	0
28	V	36	Total 36	O 36	0	0
28	W	13	Total 13	O 13	0	0
28	X	29	Total 29	O 29	0	0
28	Y	25	Total 25	O 25	0	0
28	Z	18	Total 18	O 18	0	0

3 Residue-property plots

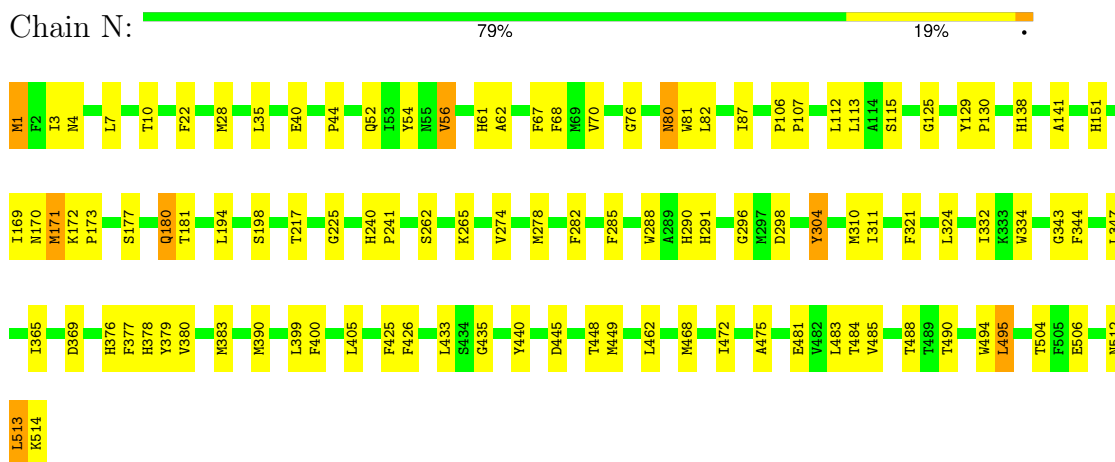
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

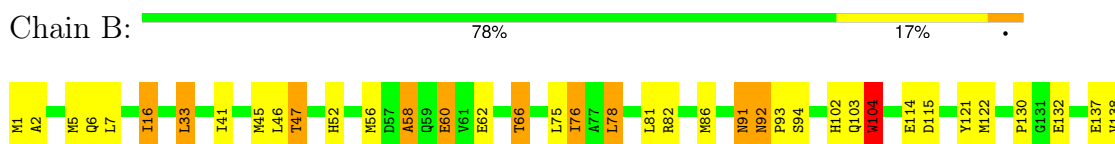
- Molecule 1: Cytochrome c oxidase polypeptide I



- Molecule 1: Cytochrome c oxidase polypeptide I



- Molecule 2: Cytochrome c oxidase polypeptide II





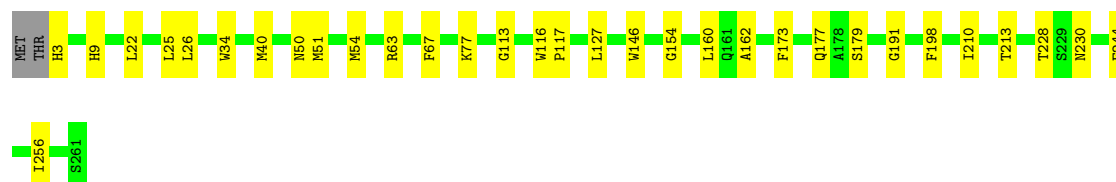
• Molecule 2: Cytochrome c oxidase polypeptide II

Chain O: 70% 26% ..



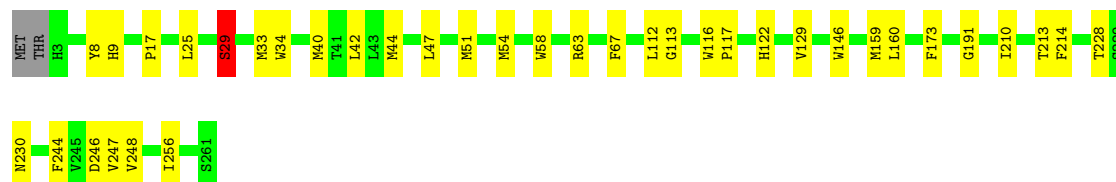
• Molecule 3: Cytochrome c oxidase polypeptide III

Chain C: 87% 12% ..



• Molecule 3: Cytochrome c oxidase polypeptide III

Chain P: 85% 14% ..



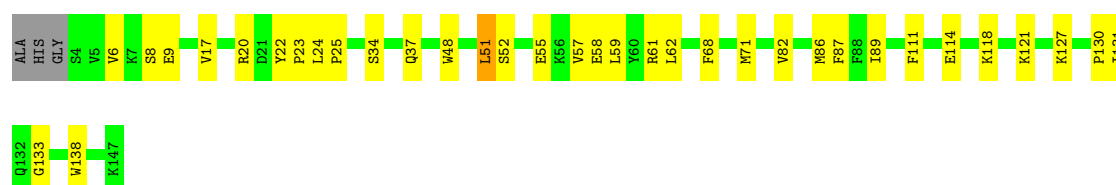
• Molecule 4: Cytochrome c oxidase subunit IV isoform 1

Chain D: 87% 11% ..



• Molecule 4: Cytochrome c oxidase subunit IV isoform 1

Chain Q: 74% 23% ..



- Molecule 5: Cytochrome c oxidase polypeptide Va

Chain E:  85% 11% .



- Molecule 5: Cytochrome c oxidase polypeptide Va

Chain R:  74% 21% . .



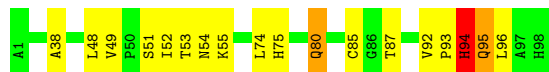
- Molecule 6: Cytochrome c oxidase polypeptide Vb

Chain F:  74% 21% . .



- Molecule 6: Cytochrome c oxidase polypeptide Vb

Chain S:  82% 15% . .



- Molecule 7: Cytochrome c oxidase polypeptide VIa-heart

Chain G:  69% 20% 9% .



- Molecule 7: Cytochrome c oxidase polypeptide VIa-heart

Chain T:  73% 19% 7% .



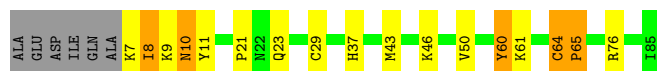
- Molecule 8: Cytochrome c oxidase polypeptide VIIb

Chain H:  76% 14% . 7%



- Molecule 8: Cytochrome c oxidase polypeptide VIIb

Chain U:  73% 14% 6% 7%



- Molecule 9: Cytochrome c oxidase polypeptide VIc

Chain I:  79% 19% .



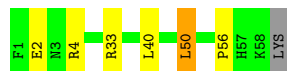
- Molecule 9: Cytochrome c oxidase polypeptide VIc

Chain V:  79% 21%

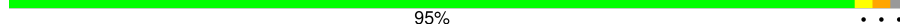


- Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart

Chain J:  88% 8% . .



- Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart

Chain W:  95% . . .



- Molecule 11: Cytochrome c oxidase polypeptide VIIb

Chain K:  79% 9% 12%



- Molecule 11: Cytochrome c oxidase polypeptide VIIb

Chain X:  75% 11% . 12%



- Molecule 12: Cytochrome c oxidase polypeptide VIIc

Chain L:  83% 9% 6% •



- Molecule 12: Cytochrome c oxidase polypeptide VIIc

Chain Y:  79% 17% ••



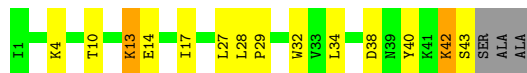
- Molecule 13: Cytochrome c oxidase polypeptide VIII-heart

Chain M:  74% 17% • 7%



- Molecule 13: Cytochrome c oxidase polypeptide VIII-heart

Chain Z:  63% 26% • 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, α , β , γ	182.59Å 205.14Å 178.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.80	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-1.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.202 , 0.227	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	32636	wwPDB-VP
Average B, all atoms (Å ²)	36.0	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: MG, TGL, SAC, HEA, PSC, UNX, ZN, CDL, NA, PEK, FME, CHD, TPO, CUA, DMU, CU, PGV

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	0.67	4/4156 (0.1%)	1.07	30/5678 (0.5%)
1	N	0.64	1/4156 (0.0%)	1.05	26/5678 (0.5%)
2	B	0.59	0/1860	1.06	8/2534 (0.3%)
2	O	0.62	0/1860	1.09	9/2534 (0.4%)
3	C	0.58	0/2197	0.90	5/3005 (0.2%)
3	P	0.56	0/2197	0.94	8/3005 (0.3%)
4	D	0.56	0/1229	1.00	1/1658 (0.1%)
4	Q	0.59	0/1229	1.00	4/1658 (0.2%)
5	E	0.58	0/871	0.96	1/1182 (0.1%)
5	R	0.57	0/871	1.06	4/1182 (0.3%)
6	F	0.62	0/765	1.18	8/1038 (0.8%)
6	S	0.66	0/765	1.15	5/1038 (0.5%)
7	G	0.60	0/690	1.00	1/937 (0.1%)
7	T	0.65	1/690 (0.1%)	1.03	1/937 (0.1%)
8	H	0.58	0/682	1.02	5/921 (0.5%)
8	U	0.57	0/682	1.03	3/921 (0.3%)
9	I	0.57	0/605	0.89	1/802 (0.1%)
9	V	0.56	0/605	0.86	1/802 (0.1%)
10	J	0.54	0/471	0.93	0/636
10	W	0.52	0/471	0.98	0/636
11	K	0.60	0/398	1.13	3/546 (0.5%)
11	X	0.58	0/398	1.06	1/546 (0.2%)
12	L	0.53	0/393	0.90	3/526 (0.6%)
12	Y	0.54	0/393	0.94	2/526 (0.4%)
13	M	0.56	0/345	0.95	1/470 (0.2%)
13	Z	0.51	0/345	0.98	1/470 (0.2%)
All	All	0.60	6/29324 (0.0%)	1.02	132/39866 (0.3%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	N	0	2
8	U	0	1
All	All	0	5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	61	HIS	CD2-NE2	5.92	1.44	1.37
7	T	5	LYS	CA-C	5.55	1.56	1.53
1	A	376	HIS	ND1-CE1	5.33	1.37	1.32
1	A	80	ASN	CG-OD1	5.29	1.33	1.23
1	A	130	PRO	CA-C	5.16	1.56	1.52

The worst 5 of 132 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	133	GLY	N-CA-C	12.65	127.17	112.50
4	Q	133	GLY	N-CA-C	12.22	126.67	112.50
6	F	93	PRO	N-CA-C	10.89	126.90	111.33
1	A	61	HIS	CB-CG-CD2	-9.24	119.19	131.20
1	A	125	GLY	N-CA-C	-9.20	101.35	112.48

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	19	TYR	Sidechain
1	A	240	HIS	Sidechain
1	N	240	HIS	Sidechain
1	N	304	TYR	Sidechain
8	U	11	TYR	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	69	0
1	N	4027	0	4001	75	0
2	B	1824	0	1833	37	0
2	O	1824	0	1833	53	0
3	C	2110	0	2027	22	0
3	P	2110	0	2027	28	0
4	D	1195	0	1183	15	0
4	Q	1195	0	1183	26	0
5	E	852	0	845	6	0
5	R	852	0	845	12	0
6	F	748	0	728	16	0
6	S	748	0	728	12	0
7	G	675	0	644	26	0
7	T	675	0	644	21	0
8	H	662	0	623	7	0
8	U	662	0	623	11	0
9	I	601	0	613	9	0
9	V	601	0	613	11	0
10	J	460	0	459	5	0
10	W	460	0	459	2	0
11	K	384	0	366	2	0
11	X	384	0	366	8	0
12	L	380	0	380	15	0
12	Y	380	0	380	11	0
13	M	335	0	352	5	0
13	Z	335	0	352	6	0
14	A	1	0	0	0	0
14	N	1	0	0	0	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	120	0	108	3	0
17	N	120	0	108	3	0
18	A	63	0	110	11	0
18	D	63	0	110	15	0
18	L	63	0	110	25	0
18	N	126	0	220	39	0
18	Q	63	0	110	15	0
19	A	102	0	152	7	0
19	C	102	0	152	8	0
19	N	102	0	152	5	0
19	P	102	0	152	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	B	2	0	0	0	0
20	O	2	0	0	0	0
21	B	29	0	39	1	0
21	C	58	0	78	3	0
21	J	29	0	39	2	0
21	O	29	0	39	1	0
21	P	58	0	78	2	0
21	W	29	0	39	2	0
22	C	100	0	156	14	0
22	G	100	0	156	14	0
22	P	100	0	156	19	0
22	T	100	0	156	15	0
23	C	106	0	154	7	0
23	G	53	0	77	10	0
23	P	106	0	154	6	0
23	T	53	0	77	9	0
24	C	1	0	0	0	0
24	P	1	0	0	0	0
25	E	52	0	80	13	0
25	O	52	0	80	21	0
26	F	1	0	0	0	0
26	S	1	0	0	0	0
27	M	33	0	36	0	0
27	Z	33	0	36	0	0
28	A	227	0	0	2	0
28	B	180	0	0	8	0
28	C	116	0	0	1	0
28	D	109	0	0	3	0
28	E	68	0	0	2	0
28	F	80	0	0	2	0
28	G	59	0	0	4	0
28	H	71	0	0	1	0
28	I	61	0	0	2	0
28	J	21	0	0	0	0
28	K	37	0	0	0	0
28	L	23	0	0	1	0
28	M	32	0	0	0	0
28	N	217	0	0	5	0
28	O	146	0	0	1	0
28	P	120	0	0	1	0
28	Q	73	0	0	5	0
28	R	32	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	S	54	0	0	3	0
28	T	58	0	0	2	0
28	U	65	0	0	1	0
28	V	36	0	0	2	0
28	W	13	0	0	0	0
28	X	29	0	0	1	0
28	Y	25	0	0	1	0
28	Z	18	0	0	0	0
All	All	32636	0	31222	580	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 580 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:84:LYS:H	7:G:84:LYS:HD2	1.14	1.08
22:C:3270:CDL:H662	19:C:3267:PGV:H182	1.41	1.03
3:P:63:ARG:HE	22:P:4270:CDL:HA22	1.24	1.03
7:T:84:LYS:HD2	7:T:84:LYS:H	1.23	1.02
3:C:63:ARG:HE	22:C:3270:CDL:HA22	1.23	1.01

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	512/514 (100%)	496 (97%)	16 (3%)	0	100	100
1	N	512/514 (100%)	500 (98%)	12 (2%)	0	100	100
2	B	225/227 (99%)	208 (92%)	14 (6%)	3 (1%)	9	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	O	225/227 (99%)	206 (92%)	16 (7%)	3 (1%)	9	3
3	C	257/261 (98%)	252 (98%)	5 (2%)	0	100	100
3	P	257/261 (98%)	252 (98%)	5 (2%)	0	100	100
4	D	142/147 (97%)	138 (97%)	4 (3%)	0	100	100
4	Q	142/147 (97%)	138 (97%)	4 (3%)	0	100	100
5	E	103/109 (94%)	103 (100%)	0	0	100	100
5	R	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
6	F	96/98 (98%)	89 (93%)	4 (4%)	3 (3%)	3	0
6	S	96/98 (98%)	89 (93%)	4 (4%)	3 (3%)	3	0
7	G	81/85 (95%)	68 (84%)	6 (7%)	7 (9%)	0	0
7	T	81/85 (95%)	65 (80%)	9 (11%)	7 (9%)	0	0
8	H	77/85 (91%)	70 (91%)	5 (6%)	2 (3%)	4	0
8	U	77/85 (91%)	70 (91%)	5 (6%)	2 (3%)	4	0
9	I	71/73 (97%)	67 (94%)	4 (6%)	0	100	100
9	V	71/73 (97%)	67 (94%)	4 (6%)	0	100	100
10	J	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
10	W	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
11	K	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
11	X	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
12	L	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
12	Y	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
13	M	41/46 (89%)	41 (100%)	0	0	100	100
13	Z	41/46 (89%)	41 (100%)	0	0	100	100
All	All	3504/3614 (97%)	3350 (96%)	124 (4%)	30 (1%)	14	5

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	95	GLN
7	G	4	ALA
7	G	7	ASP
7	G	8	HIS
7	G	39	SER

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%)	421 (99%)	5 (1%)	63	57
1	N	426/426 (100%)	416 (98%)	10 (2%)	44	33
2	B	210/210 (100%)	200 (95%)	10 (5%)	23	11
2	O	210/210 (100%)	198 (94%)	12 (6%)	18	8
3	C	224/226 (99%)	220 (98%)	4 (2%)	51	43
3	P	224/226 (99%)	219 (98%)	5 (2%)	45	34
4	D	128/129 (99%)	126 (98%)	2 (2%)	55	47
4	Q	128/129 (99%)	124 (97%)	4 (3%)	35	23
5	E	92/95 (97%)	90 (98%)	2 (2%)	45	34
5	R	92/95 (97%)	89 (97%)	3 (3%)	33	21
6	F	81/81 (100%)	78 (96%)	3 (4%)	30	18
6	S	81/81 (100%)	77 (95%)	4 (5%)	22	10
7	G	67/68 (98%)	63 (94%)	4 (6%)	17	7
7	T	67/68 (98%)	64 (96%)	3 (4%)	24	12
8	H	71/75 (95%)	68 (96%)	3 (4%)	26	14
8	U	71/75 (95%)	67 (94%)	4 (6%)	19	8
9	I	57/57 (100%)	53 (93%)	4 (7%)	14	4
9	V	57/57 (100%)	53 (93%)	4 (7%)	14	4
10	J	49/50 (98%)	48 (98%)	1 (2%)	48	38
10	W	49/50 (98%)	48 (98%)	1 (2%)	48	38
11	K	39/46 (85%)	39 (100%)	0	100	100
11	X	39/46 (85%)	38 (97%)	1 (3%)	40	28
12	L	39/40 (98%)	38 (97%)	1 (3%)	40	28
12	Y	39/40 (98%)	38 (97%)	1 (3%)	40	28
13	M	37/38 (97%)	32 (86%)	5 (14%)	4	1
13	Z	37/38 (97%)	33 (89%)	4 (11%)	6	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	3040/3082 (99%)	2940 (97%)	100 (3%)	33	21

5 of 100 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	O	66	THR
4	Q	8	SER
13	Z	42	LYS
2	O	75	LEU
2	O	217	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
1	N	170	ASN
3	P	3	HIS
10	W	57	HIS
1	N	178	GLN
1	N	503	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	$\# Z > 2$
7	TPO	T	11	7	8,10,11	1.37	1 (12%)	10,14,16	1.16	1 (10%)
9	SAC	I	1	9	7,8,9	2.55	2 (28%)	7,9,11	1.72	2 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	FME	A	1	1	8,9,10	0.66	0	8,9,11	1.08	1 (12%)
9	SAC	V	1	9	7,8,9	2.64	2 (28%)	7,9,11	2.00	3 (42%)
2	FME	O	1	2	8,9,10	0.67	0	8,9,11	1.73	2 (25%)
7	TPO	G	11	7	8,10,11	1.43	2 (25%)	10,14,16	1.15	1 (10%)
2	FME	B	1	2	8,9,10	0.77	0	8,9,11	2.30	2 (25%)
1	FME	N	1	1	8,9,10	0.79	0	8,9,11	1.82	2 (25%)

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

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

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	V	1	SAC	OAC-C1A	5.27	1.35	1.23
9	I	1	SAC	OAC-C1A	5.19	1.34	1.23
9	V	1	SAC	CA-N	4.15	1.52	1.46
9	I	1	SAC	CA-N	4.05	1.52	1.46
7	T	11	TPO	CB-CA	2.80	1.59	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CA-N-CN	-4.79	115.46	122.82
1	N	1	FME	CA-N-CN	-4.24	116.30	122.82
2	B	1	FME	C-CA-N	4.11	117.43	109.50
2	O	1	FME	C-CA-N	3.57	116.38	109.50
9	I	1	SAC	C-CA-N	-3.18	103.36	109.50

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

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

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	T	11	TPO	1	0
1	A	1	FME	5	0
2	O	1	FME	3	0
7	G	11	TPO	1	0
1	N	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 52 ligands modelled in this entry, 8 are monoatomic and 2 are unknown - leaving 42 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$
21	CHD	J	3060	-	32,32,32	0.93	1 (3%)	51,51,51	3.24	25 (49%)
18	TGL	D	3523	-	62,62,62	1.17	3 (4%)	65,65,65	1.13	7 (10%)
17	HEA	A	516	1	67,67,67	1.15	4 (5%)	81,103,103	1.03	3 (3%)
18	TGL	N	4521	-	62,62,62	1.02	4 (6%)	65,65,65	1.11	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CUA	B	228	2	0,1,1	-	-	-		
21	CHD	P	4271	-	32,32,32	0.83	0	51,51,51	3.54	22 (43%)
25	PSC	E	3230	-	51,51,51	1.25	3 (5%)	57,59,59	1.02	4 (7%)
19	PGV	P	4268	-	50,50,50	1.12	3 (6%)	53,56,56	0.67	0
21	CHD	C	3271	-	32,32,32	0.86	2 (6%)	51,51,51	3.61	22 (43%)
22	CDL	T	4269	-	99,99,99	0.95	4 (4%)	105,111,111	0.96	9 (8%)
19	PGV	C	3267	-	50,50,50	0.83	1 (2%)	53,56,56	0.94	4 (7%)
22	CDL	C	3270	-	99,99,99	0.80	3 (3%)	105,111,111	0.91	5 (4%)
19	PGV	A	3524	-	50,50,50	1.13	7 (14%)	53,56,56	1.26	8 (15%)
20	CUA	O	228	2	0,1,1	-	-	-		
18	TGL	A	3521	-	62,62,62	1.00	4 (6%)	65,65,65	1.14	6 (9%)
18	TGL	N	4522	-	62,62,62	1.43	6 (9%)	65,65,65	1.14	6 (9%)
23	PEK	T	3263	-	52,52,52	1.70	11 (21%)	55,57,57	1.00	3 (5%)
19	PGV	A	3266	-	50,50,50	0.91	1 (2%)	53,56,56	0.78	2 (3%)
21	CHD	B	4085	-	32,32,32	0.81	0	51,51,51	1.87	13 (25%)
21	CHD	C	3525	-	32,32,32	0.87	1 (3%)	51,51,51	1.60	12 (23%)
18	TGL	Q	4523	-	62,62,62	1.16	3 (4%)	65,65,65	1.06	4 (6%)
23	PEK	P	4265	-	52,52,52	1.71	12 (23%)	55,57,57	0.98	5 (9%)
17	HEA	A	515	1	67,67,67	0.99	2 (2%)	81,103,103	1.18	6 (7%)
21	CHD	O	3085	-	32,32,32	0.84	0	51,51,51	1.89	18 (35%)
19	PGV	P	4267	-	50,50,50	1.01	2 (4%)	53,56,56	1.06	3 (5%)
25	PSC	O	4230	-	51,51,51	1.21	3 (5%)	57,59,59	1.03	4 (7%)
23	PEK	C	3265	-	52,52,52	1.67	11 (21%)	55,57,57	1.00	4 (7%)
22	CDL	P	4270	-	99,99,99	0.83	4 (4%)	105,111,111	0.89	5 (4%)
23	PEK	C	3264	-	52,52,52	1.52	5 (9%)	55,57,57	1.29	7 (12%)
21	CHD	W	4060	-	32,32,32	1.01	2 (6%)	51,51,51	3.20	26 (50%)
27	DMU	Z	4526	-	34,34,34	3.24	8 (23%)	45,45,45	4.32	19 (42%)
23	PEK	G	4263	-	52,52,52	1.70	9 (17%)	55,57,57	1.01	3 (5%)
17	HEA	N	515	1	67,67,67	1.00	2 (2%)	81,103,103	1.17	8 (9%)
21	CHD	P	4525	-	32,32,32	0.92	2 (6%)	51,51,51	1.65	9 (17%)
19	PGV	N	4266	-	50,50,50	1.04	3 (6%)	53,56,56	1.00	3 (5%)
23	PEK	P	4264	-	52,52,52	1.51	5 (9%)	55,57,57	1.35	10 (18%)
27	DMU	M	3526	-	34,34,34	3.26	8 (23%)	45,45,45	4.36	19 (42%)
19	PGV	N	4524	-	50,50,50	1.13	3 (6%)	53,56,56	1.20	8 (15%)
17	HEA	N	516	1	67,67,67	1.14	6 (8%)	81,103,103	1.10	2 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CDL	G	3269	-	99,99,99	0.99	5 (5%)	105,111,111	0.94	7 (6%)
19	PGV	C	3268	-	50,50,50	1.12	3 (6%)	53,56,56	0.66	0
18	TGL	L	3522	-	62,62,62	1.40	6 (9%)	65,65,65	1.23	6 (9%)

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
21	CHD	J	3060	-	5/5/12/12	8/9/74/74	0/4/4/4
18	TGL	D	3523	-	-	29/65/65/65	-
17	HEA	A	516	1	-	7/36/76/76	-
21	CHD	P	4271	-	5/5/12/12	8/9/74/74	0/4/4/4
18	TGL	N	4521	-	-	32/65/65/65	-
25	PSC	E	3230	-	-	35/55/55/55	-
19	PGV	P	4268	-	-	33/55/55/55	-
21	CHD	C	3271	-	5/5/12/12	8/9/74/74	0/4/4/4
22	CDL	T	4269	-	-	67/110/110/110	-
19	PGV	C	3267	-	-	18/55/55/55	-
22	CDL	C	3270	-	-	71/110/110/110	-
19	PGV	A	3524	-	-	29/55/55/55	-
18	TGL	A	3521	-	-	31/65/65/65	-
18	TGL	N	4522	-	-	35/65/65/65	-
23	PEK	T	3263	-	-	23/56/56/56	-
19	PGV	A	3266	-	-	12/55/55/55	-
21	CHD	B	4085	-	-	2/9/74/74	0/4/4/4
21	CHD	C	3525	-	-	2/9/74/74	0/4/4/4
18	TGL	Q	4523	-	-	27/65/65/65	-
23	PEK	P	4265	-	-	24/56/56/56	-
17	HEA	A	515	1	-	6/36/76/76	-
21	CHD	O	3085	-	-	2/9/74/74	0/4/4/4
19	PGV	P	4267	-	-	15/55/55/55	-
25	PSC	O	4230	-	-	38/55/55/55	-
23	PEK	C	3265	-	-	24/56/56/56	-
22	CDL	P	4270	-	-	72/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	PEK	C	3264	-	-	16/56/56/56	-
21	CHD	W	4060	-	5/5/12/12	8/9/74/74	0/4/4/4
27	DMU	Z	4526	-	5/5/10/10	6/19/59/59	0/2/2/2
23	PEK	G	4263	-	-	22/56/56/56	-
17	HEA	N	515	1	-	7/36/76/76	-
21	CHD	P	4525	-	-	2/9/74/74	0/4/4/4
19	PGV	N	4266	-	-	15/55/55/55	-
23	PEK	P	4264	-	-	17/56/56/56	-
27	DMU	M	3526	-	5/5/10/10	6/19/59/59	0/2/2/2
19	PGV	N	4524	-	-	29/55/55/55	-
17	HEA	N	516	1	-	7/36/76/76	-
22	CDL	G	3269	-	-	68/110/110/110	-
19	PGV	C	3268	-	-	33/55/55/55	-
18	TGL	L	3522	-	-	33/65/65/65	-

The worst 5 of 162 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	M	3526	DMU	O7-C3	-8.46	1.22	1.43
27	Z	4526	DMU	O7-C3	-8.26	1.22	1.43
27	Z	4526	DMU	O16-C6	-7.80	1.27	1.40
27	M	3526	DMU	O16-C6	-7.35	1.28	1.40
27	M	3526	DMU	O1-C9	-7.05	1.27	1.44

The worst 5 of 333 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	C	3271	CHD	C17-C13-C14	10.50	110.64	100.11
27	M	3526	DMU	C10-C5-C7	10.43	131.95	110.01
27	Z	4526	DMU	C10-C5-C7	10.33	131.73	110.01
21	C	3271	CHD	C17-C13-C12	-10.12	108.56	117.67
21	P	4271	CHD	C17-C13-C14	10.08	110.22	100.11

5 of 30 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	C	3271	CHD	C12
21	C	3271	CHD	C3
21	C	3271	CHD	C8

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Mol	Chain	Res	Type	Atom
21	C	3271	CHD	C14
21	C	3271	CHD	C9

5 of 927 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	3521	TGL	CB2-CB1-OG2-CG2
18	A	3521	TGL	OB1-CB1-OG2-CG2
18	A	3521	TGL	OG1-CG1-CG2-OG2
18	D	3523	TGL	CB2-CB1-OG2-CG2
18	D	3523	TGL	OB1-CB1-OG2-CG2

There are no ring outliers.

32 monomers are involved in 270 short contacts:

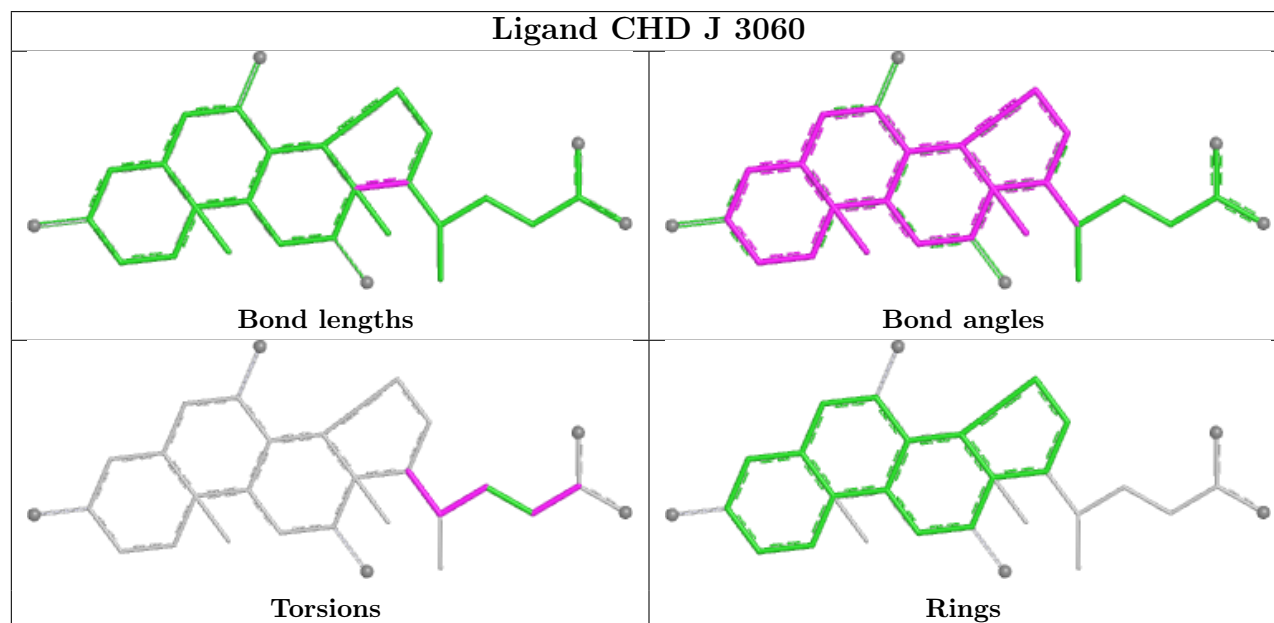
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	J	3060	CHD	2	0
18	D	3523	TGL	15	0
17	A	516	HEA	1	0
18	N	4521	TGL	19	0
21	P	4271	CHD	2	0
25	E	3230	PSC	13	0
21	C	3271	CHD	3	0
22	T	4269	CDL	15	0
19	C	3267	PGV	7	0
22	C	3270	CDL	14	0
19	A	3524	PGV	7	0
18	A	3521	TGL	11	0
18	N	4522	TGL	20	0
23	T	3263	PEK	9	0
21	B	4085	CHD	1	0
18	Q	4523	TGL	15	0
23	P	4265	PEK	2	0
17	A	515	HEA	2	0
21	O	3085	CHD	1	0
19	P	4267	PGV	9	0
25	O	4230	PSC	21	0
23	C	3265	PEK	3	0
22	P	4270	CDL	19	0
23	C	3264	PEK	4	0
21	W	4060	CHD	2	0
23	G	4263	PEK	10	0

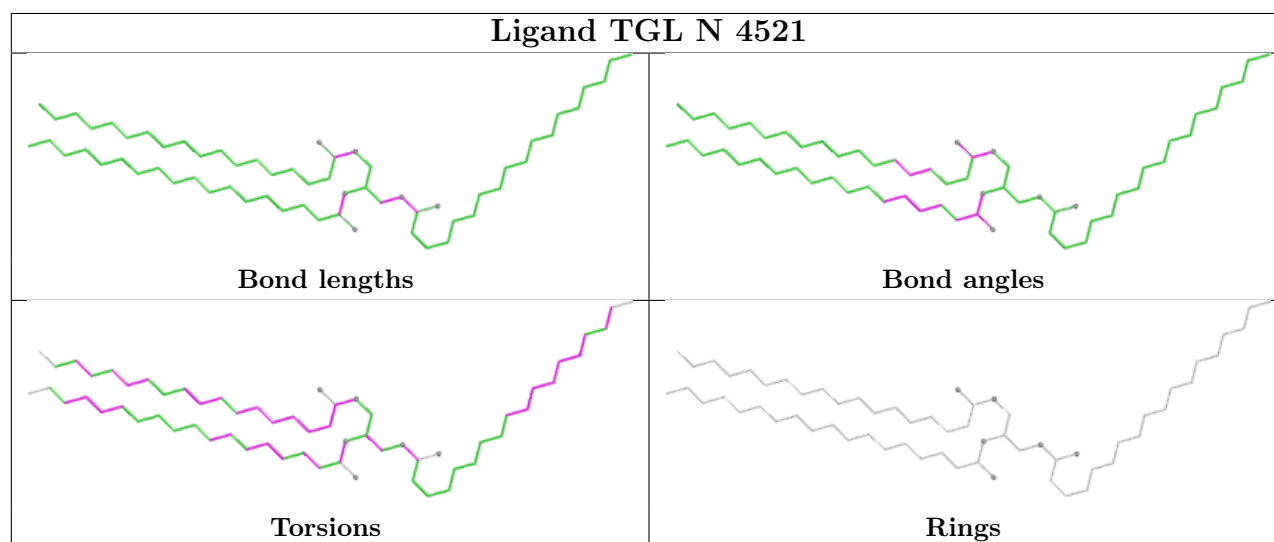
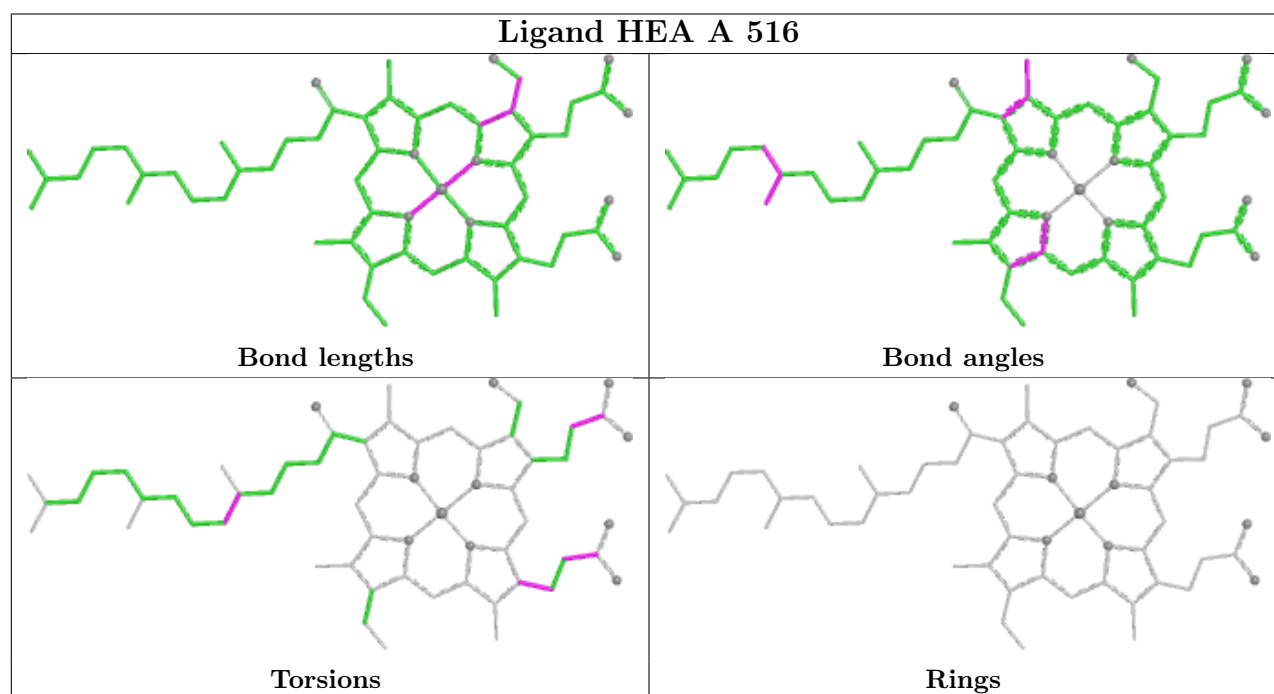
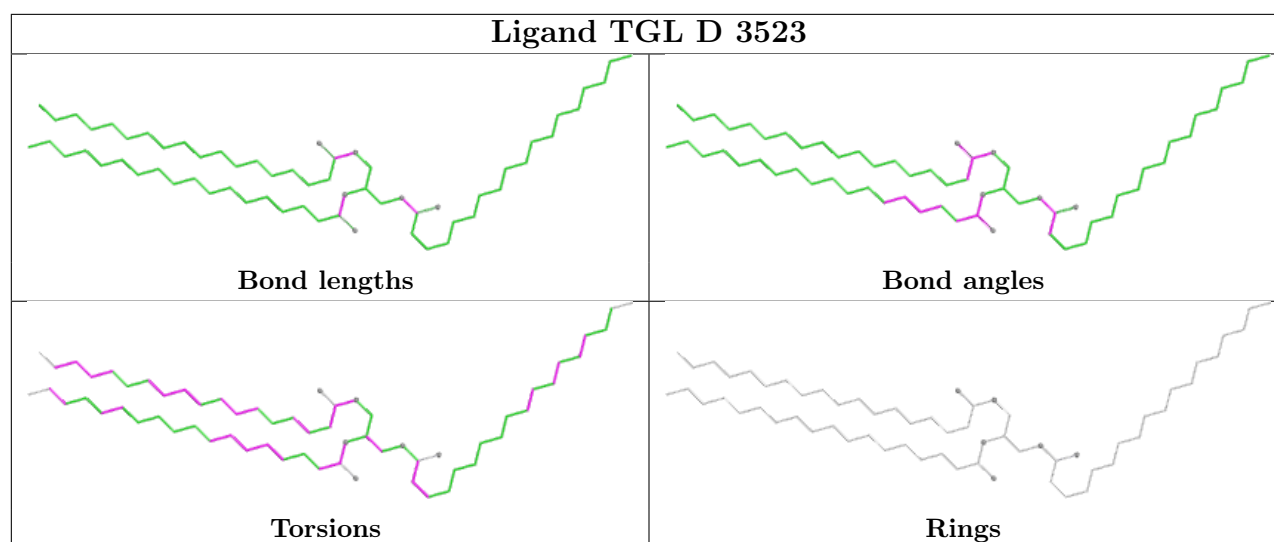
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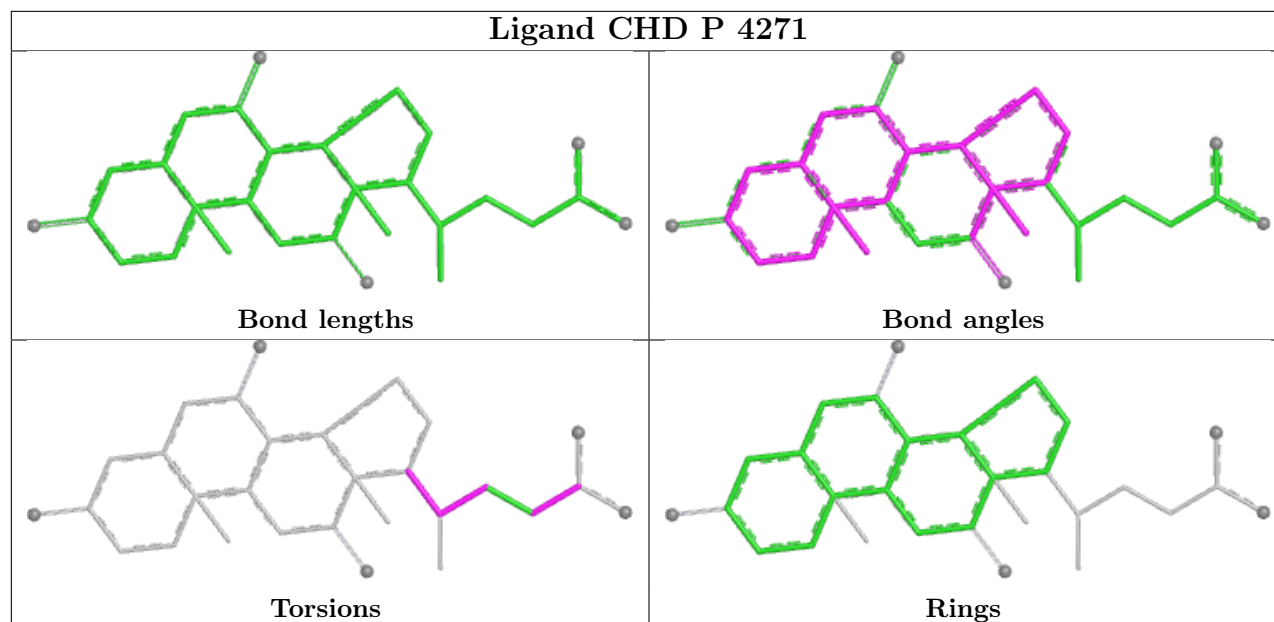
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	N	515	HEA	3	0
23	P	4264	PEK	4	0
19	N	4524	PGV	5	0
22	G	3269	CDL	14	0
19	C	3268	PGV	1	0
18	L	3522	TGL	25	0

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

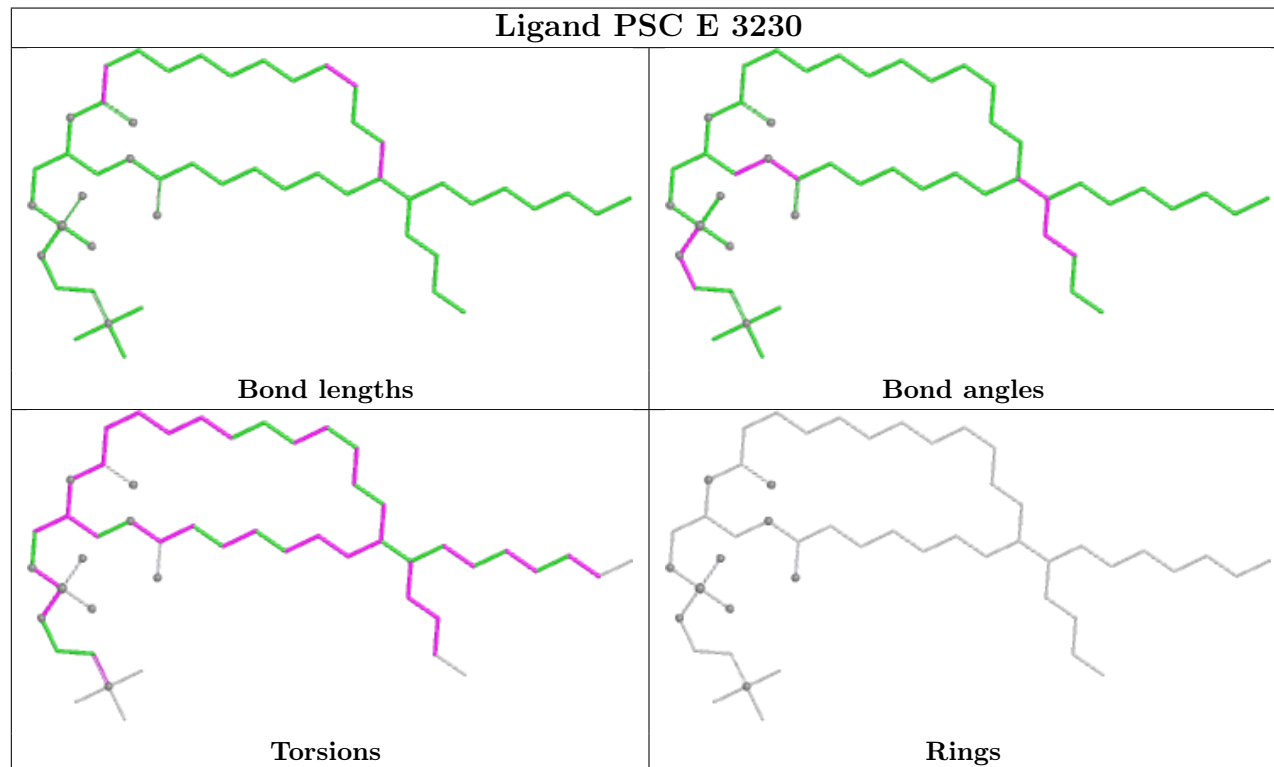


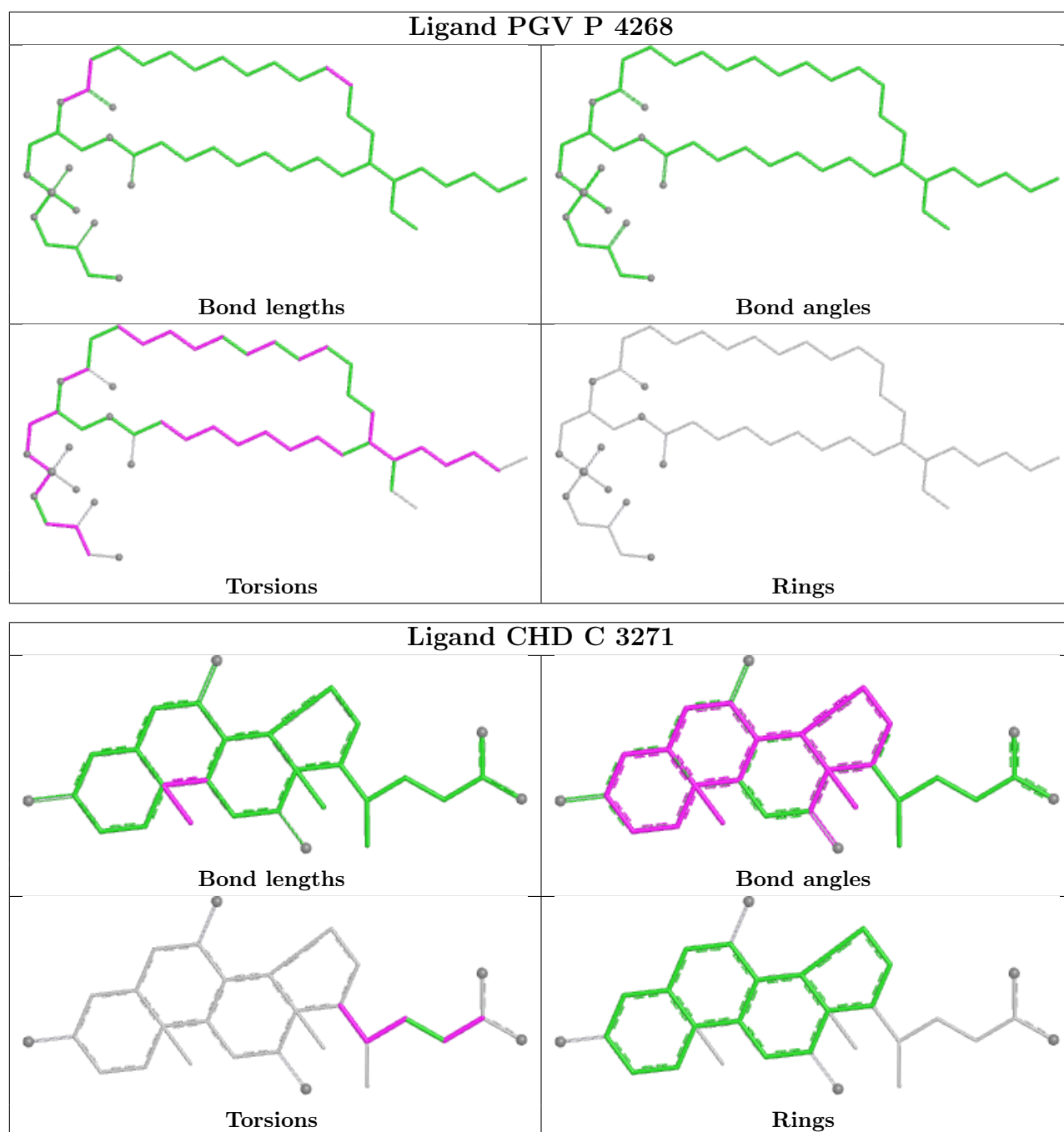


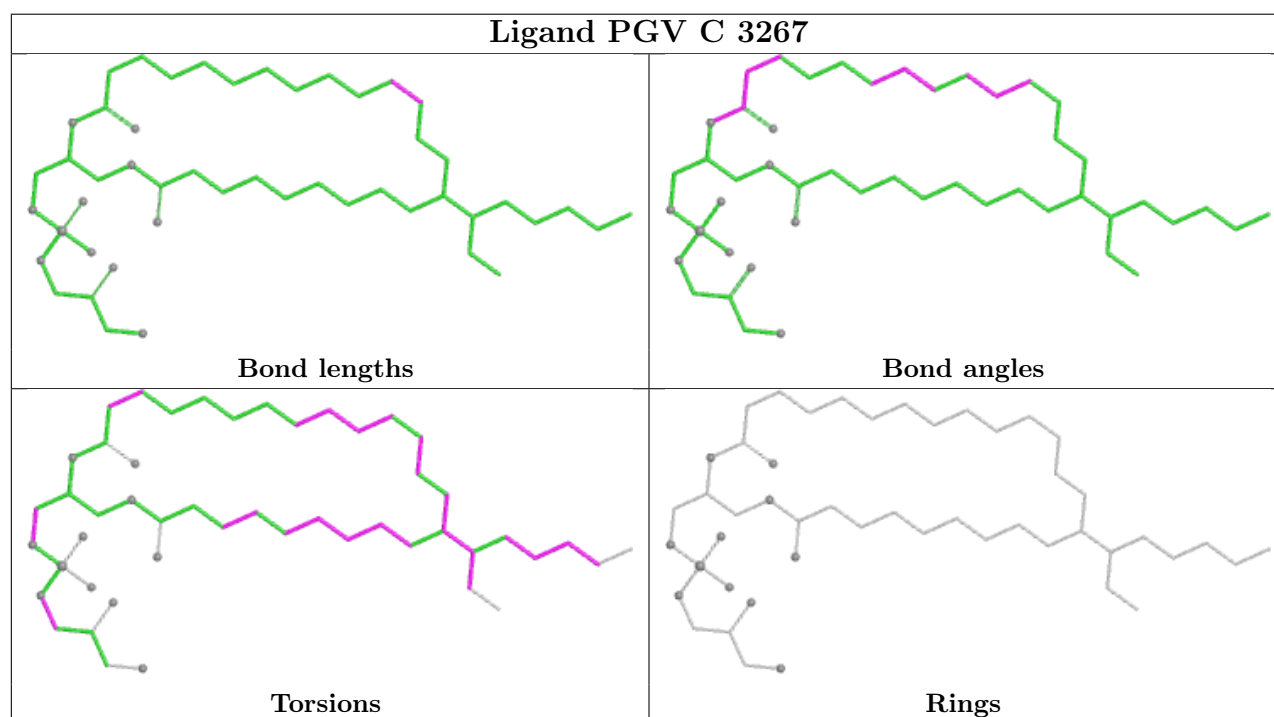
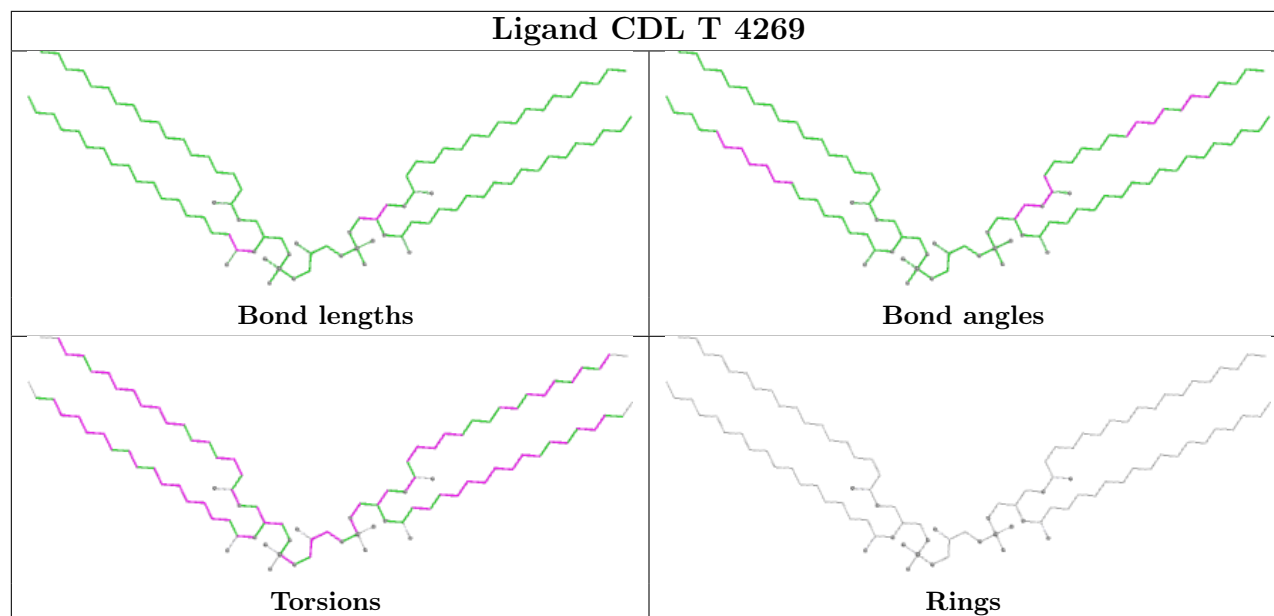
Ligand CHD P 4271

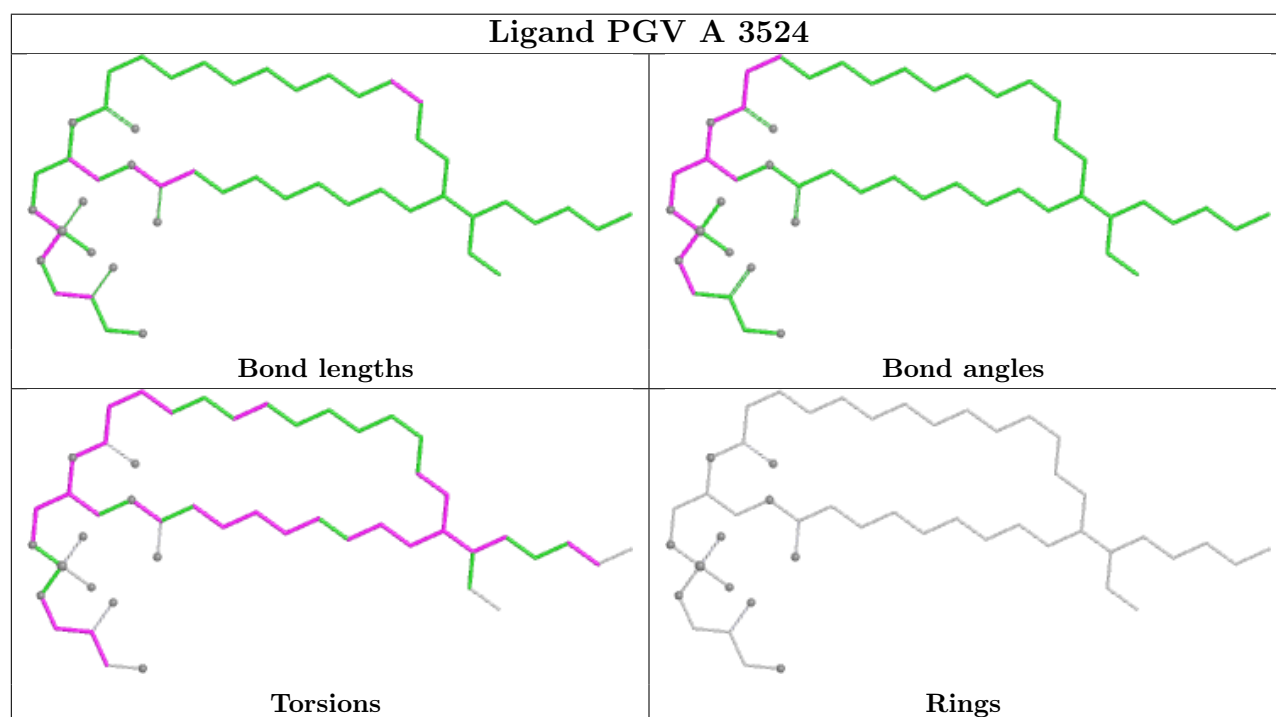
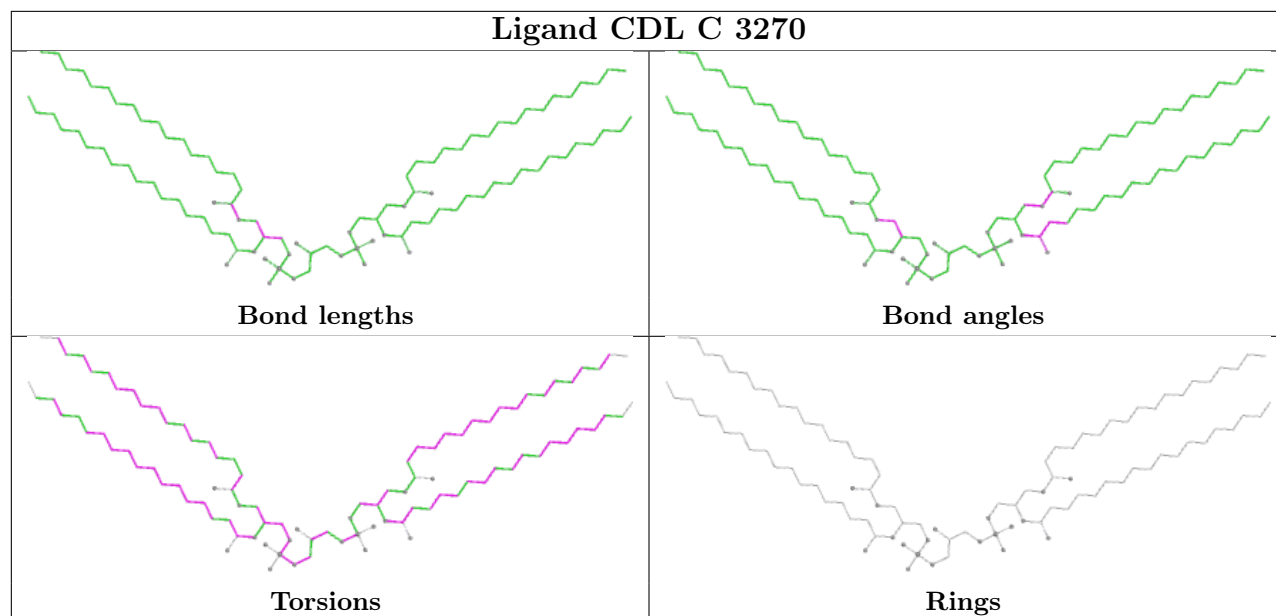


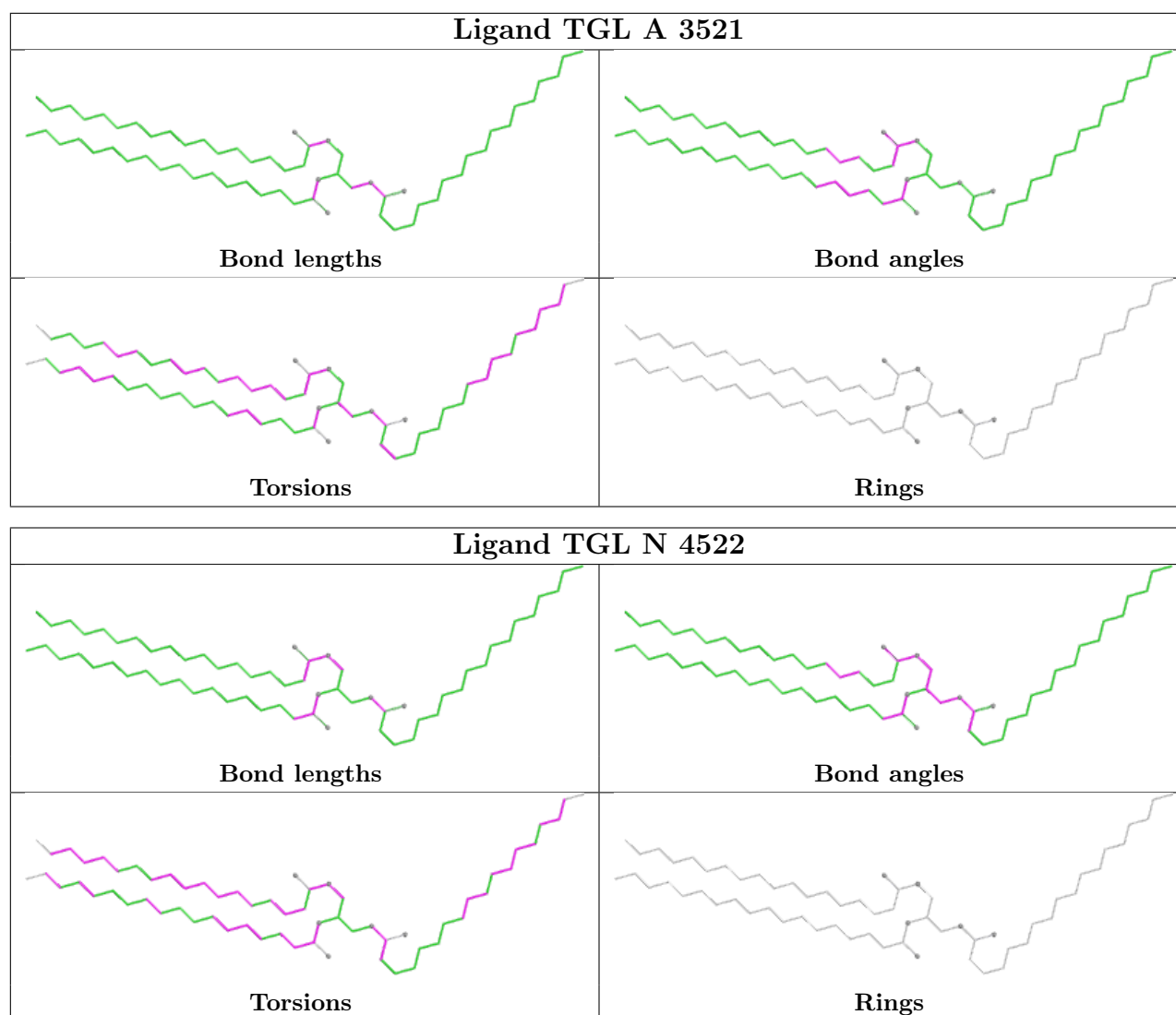
Ligand PSC E 3230

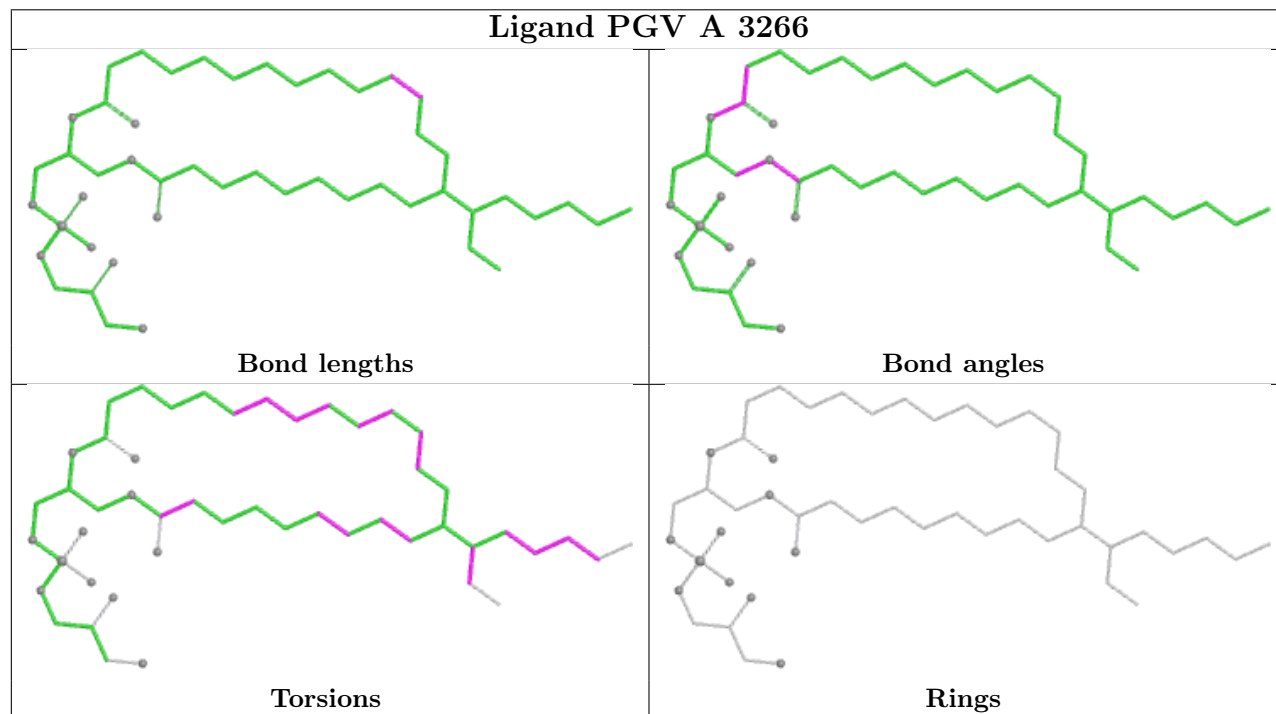
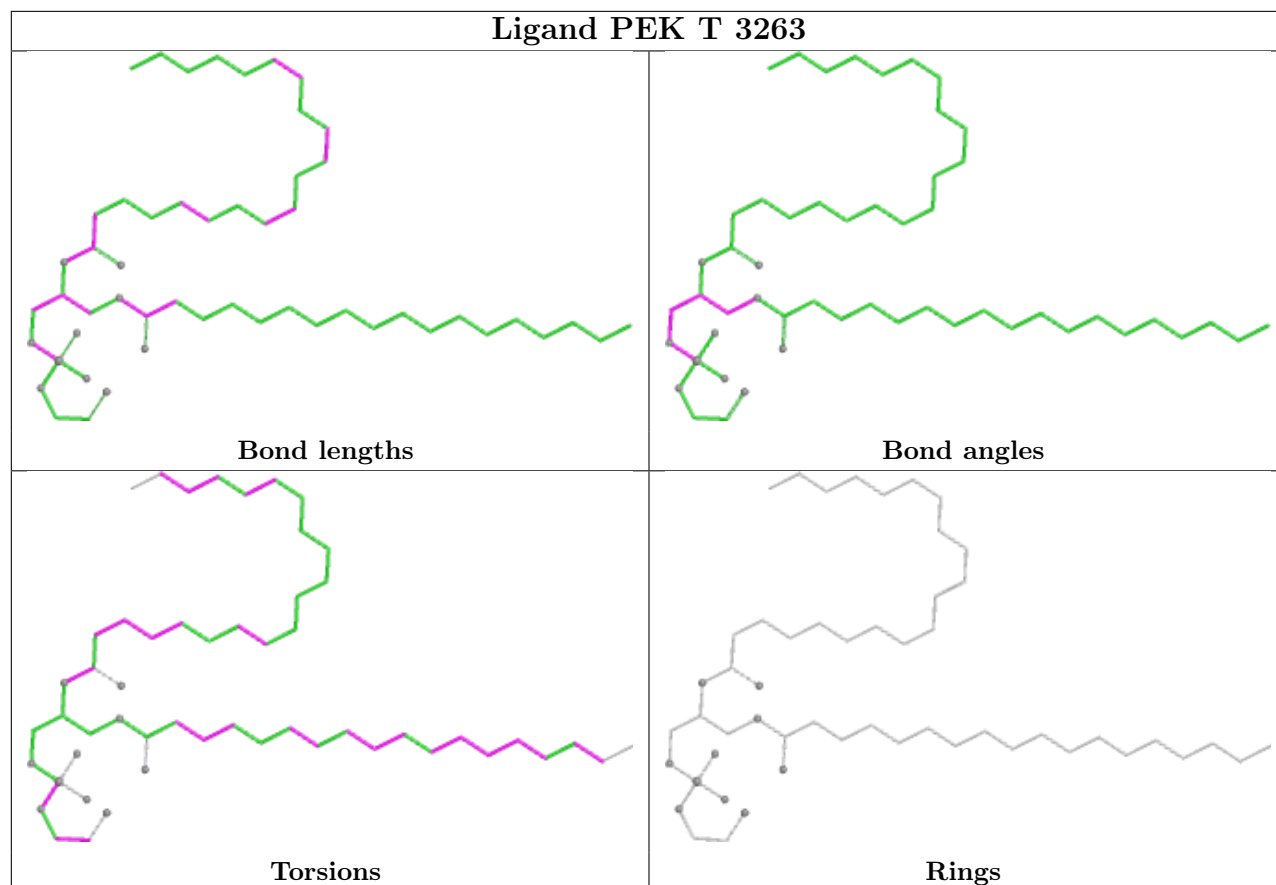




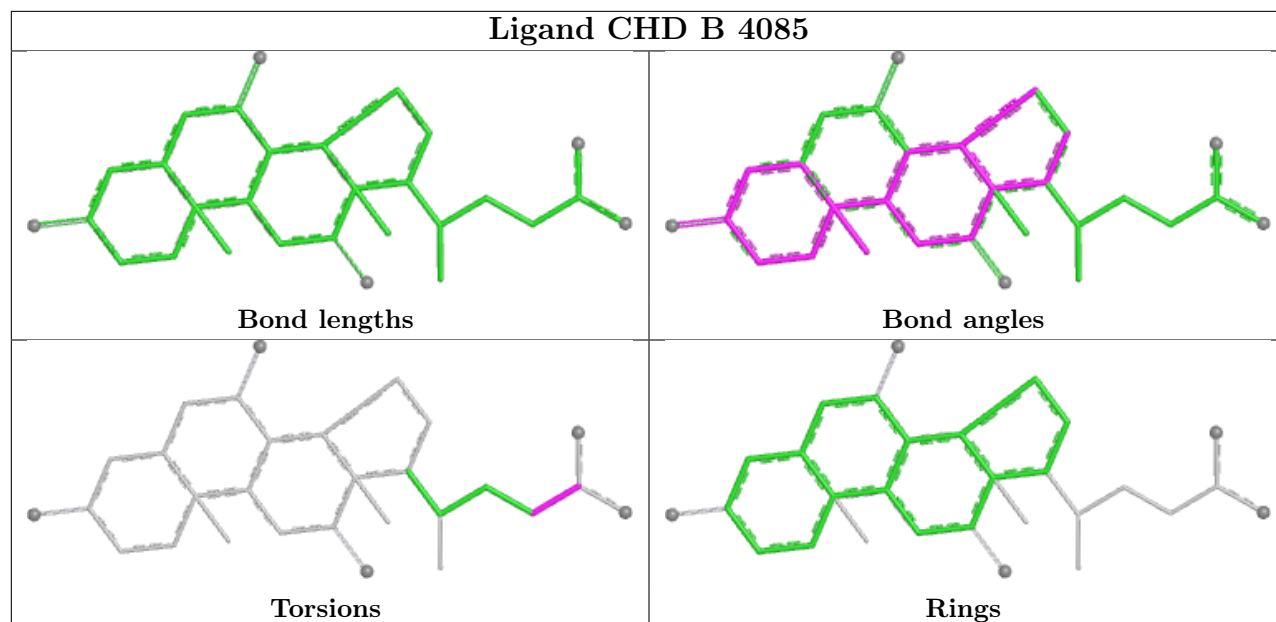




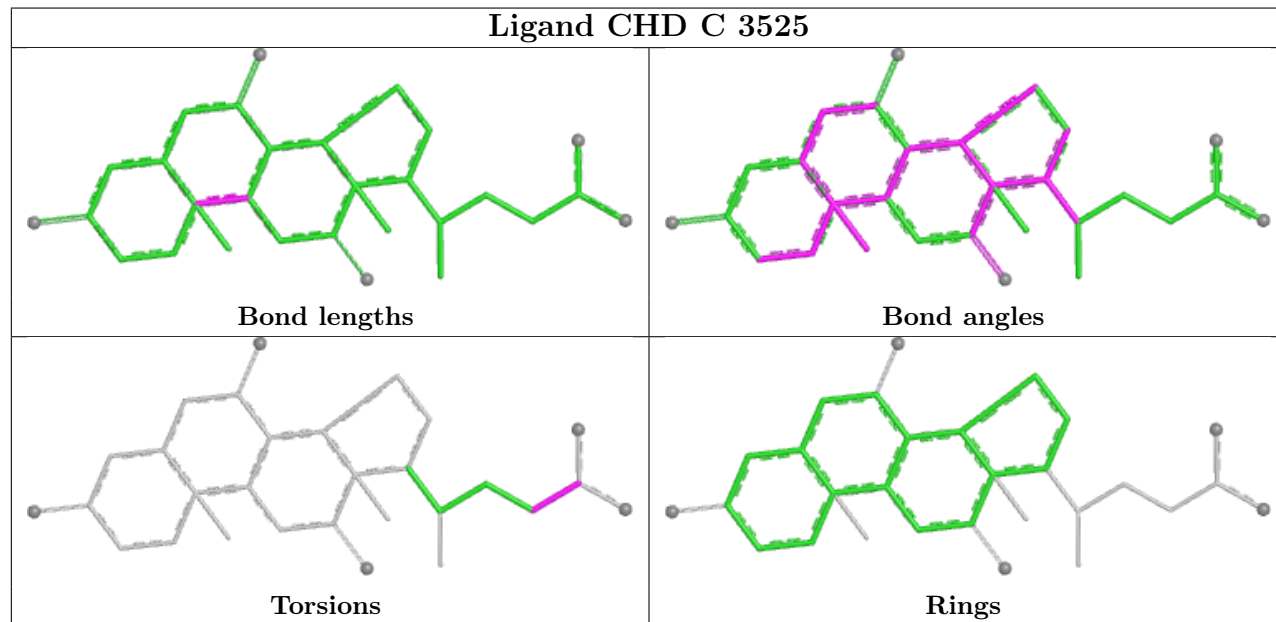


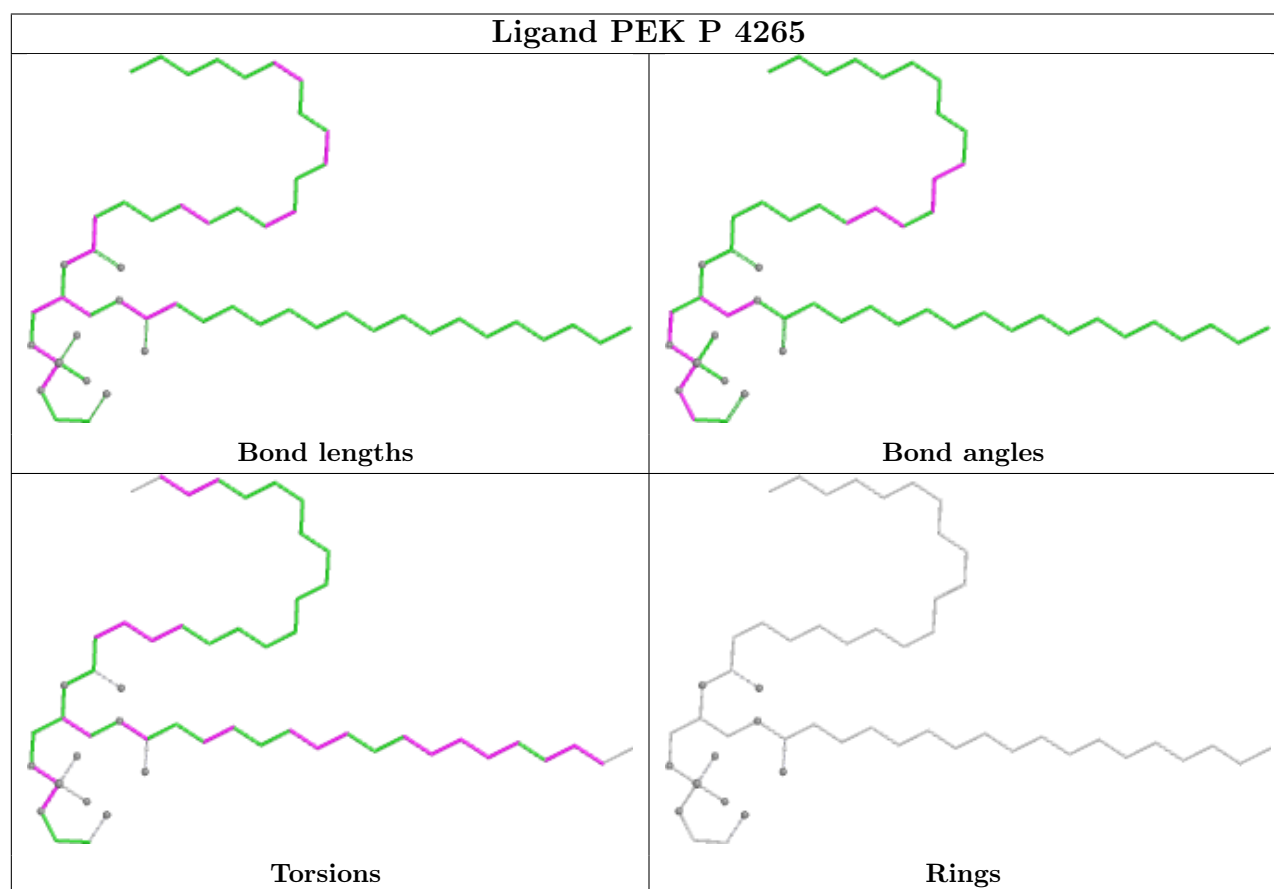
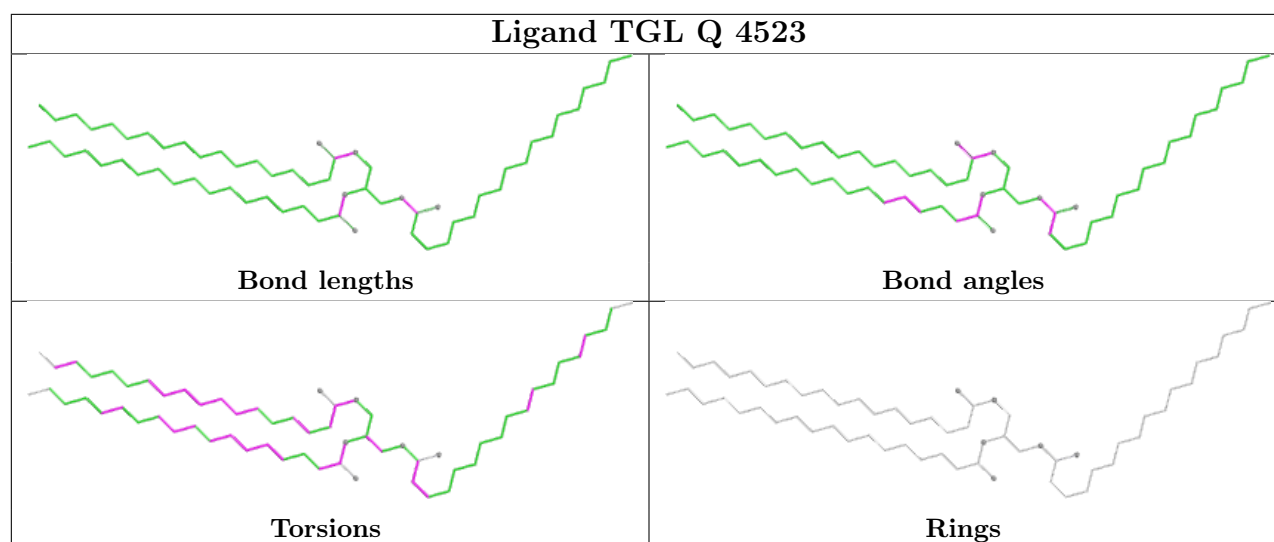


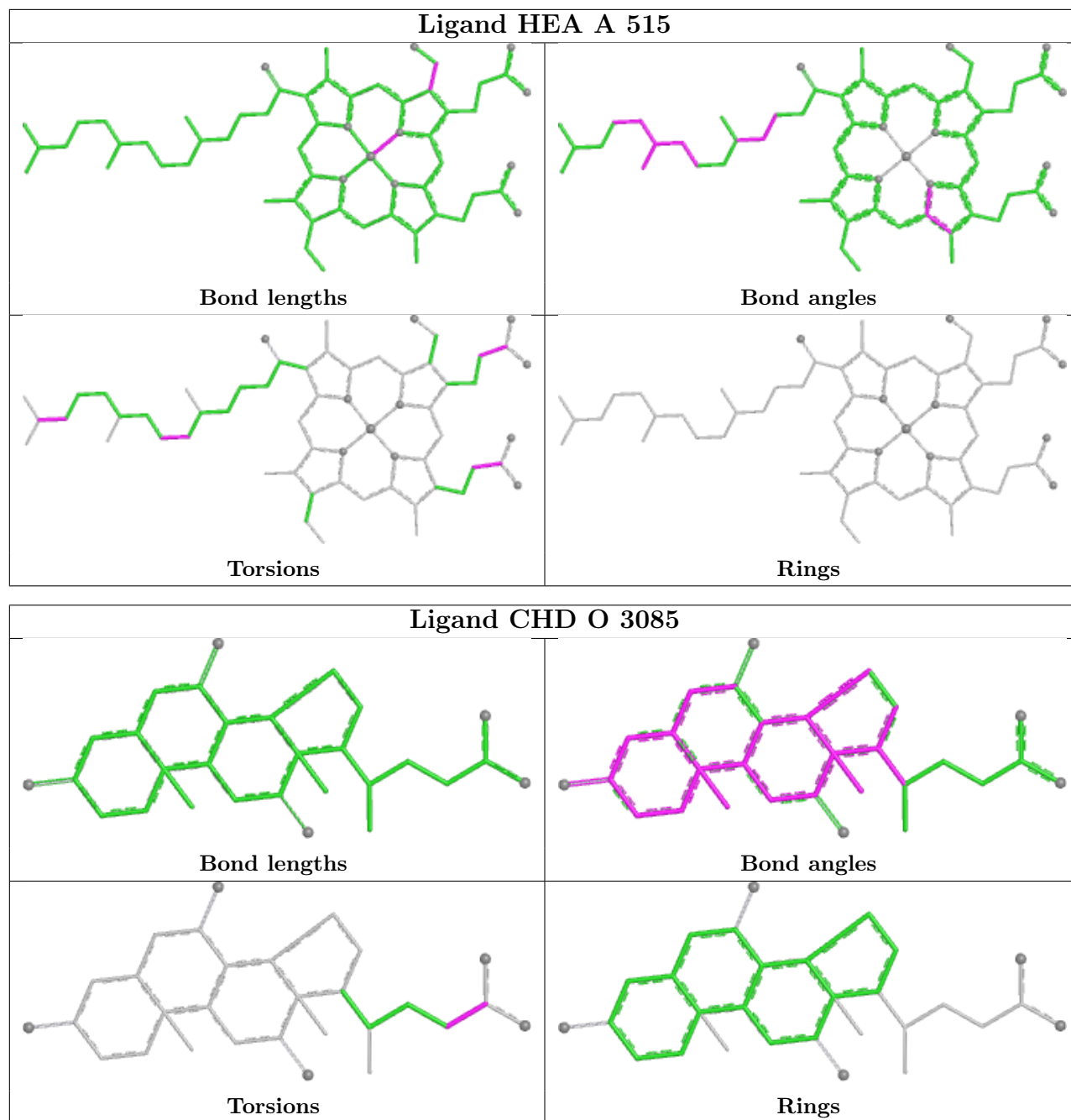
Ligand CHD B 4085

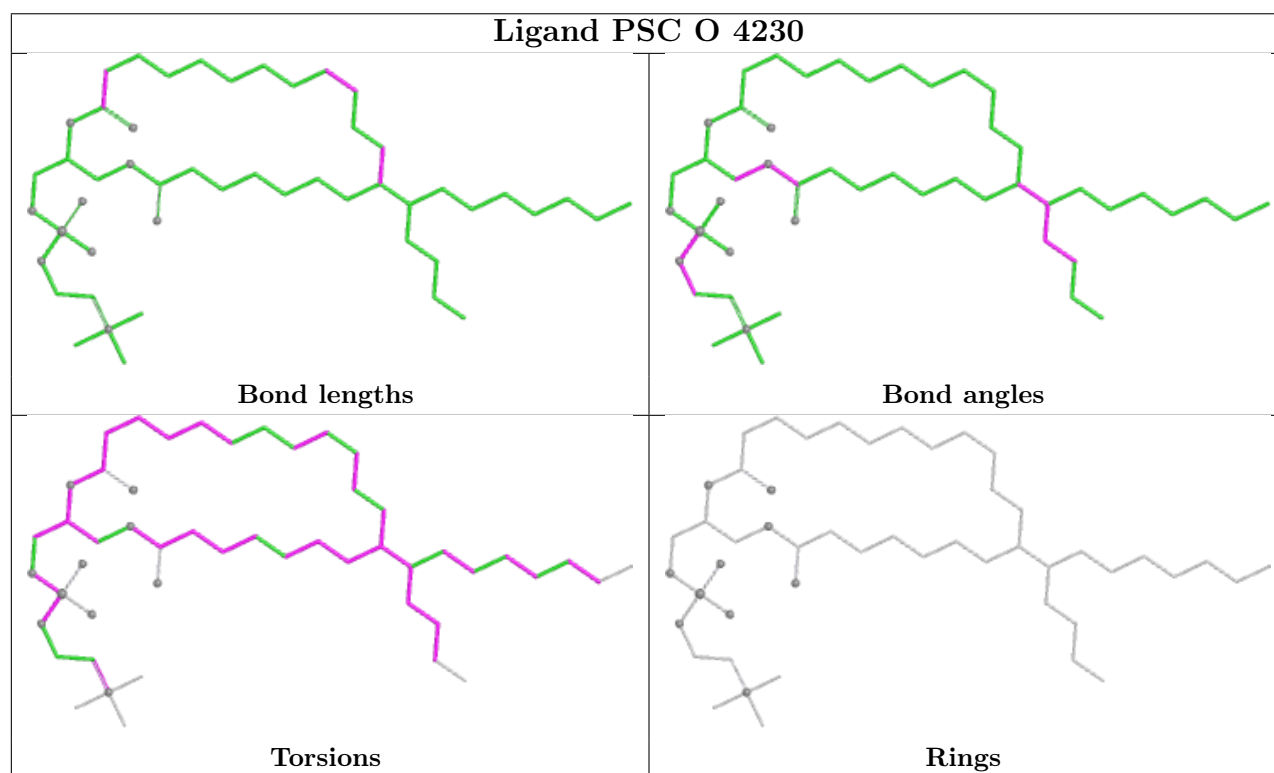
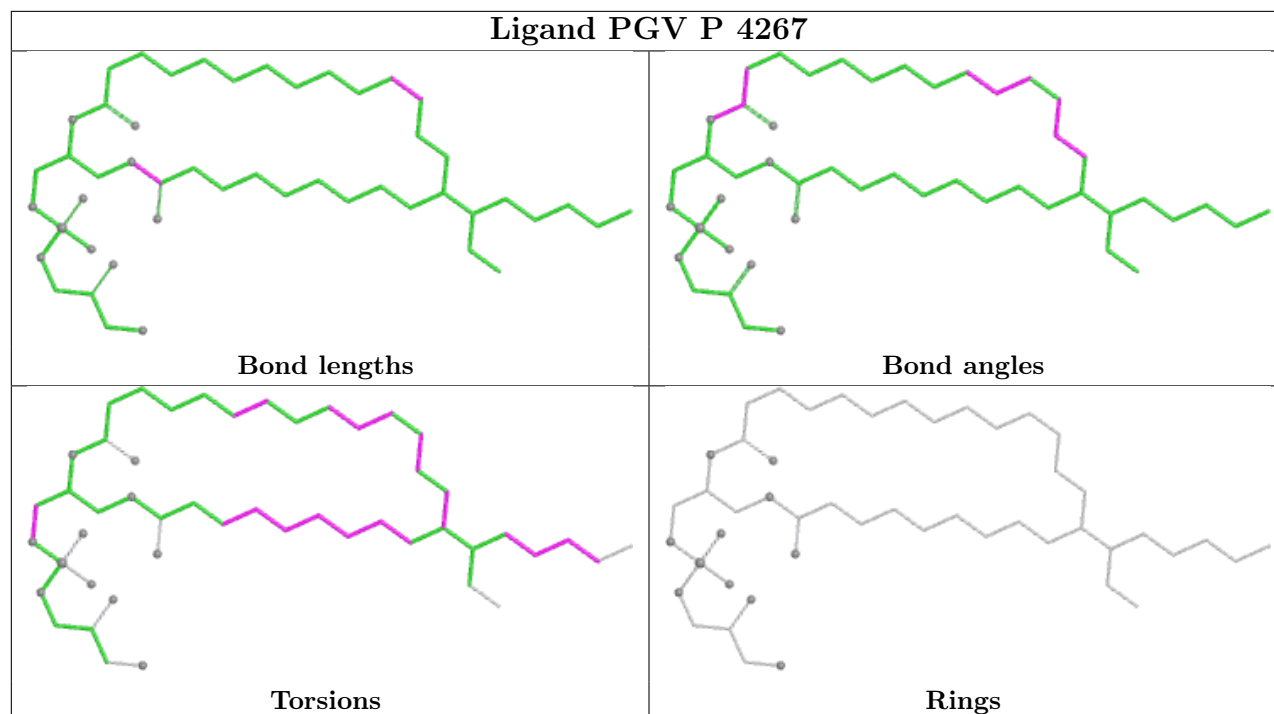


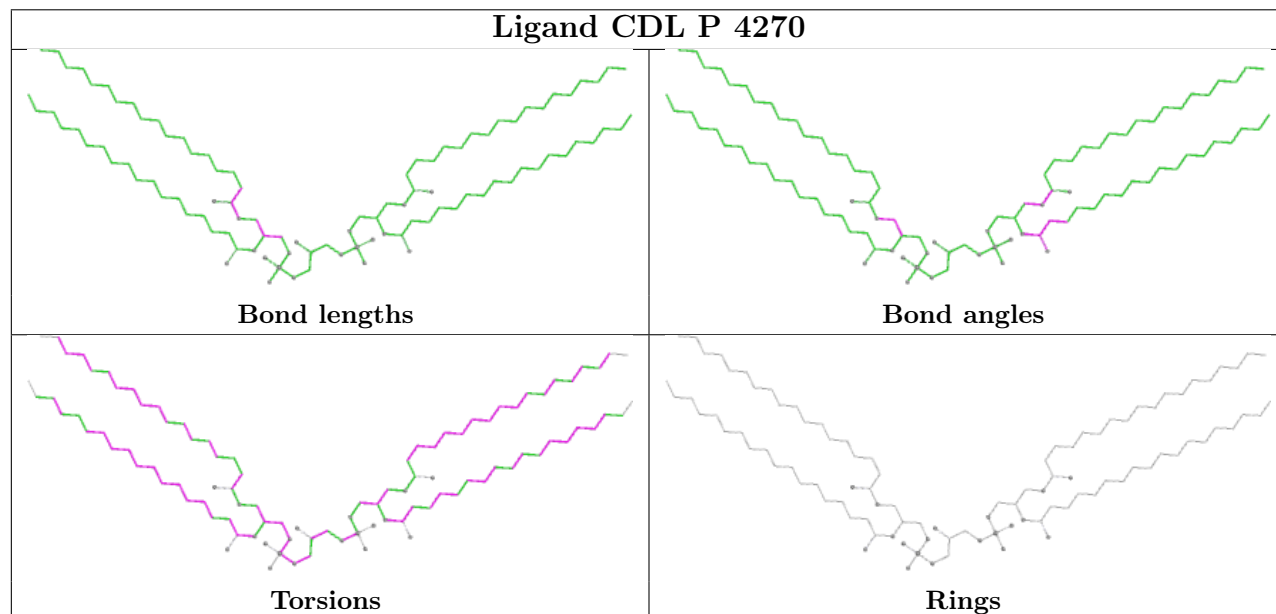
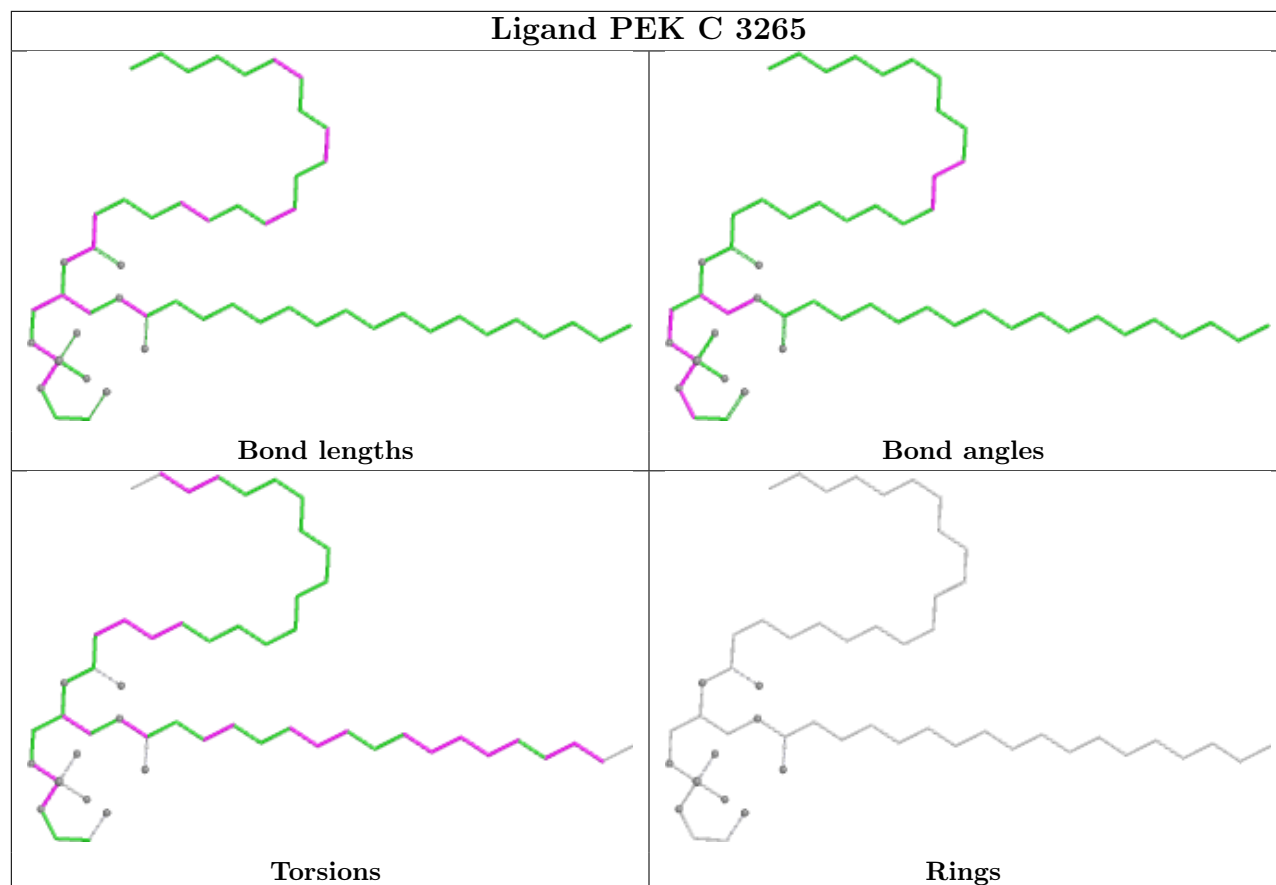
Ligand CHD C 3525

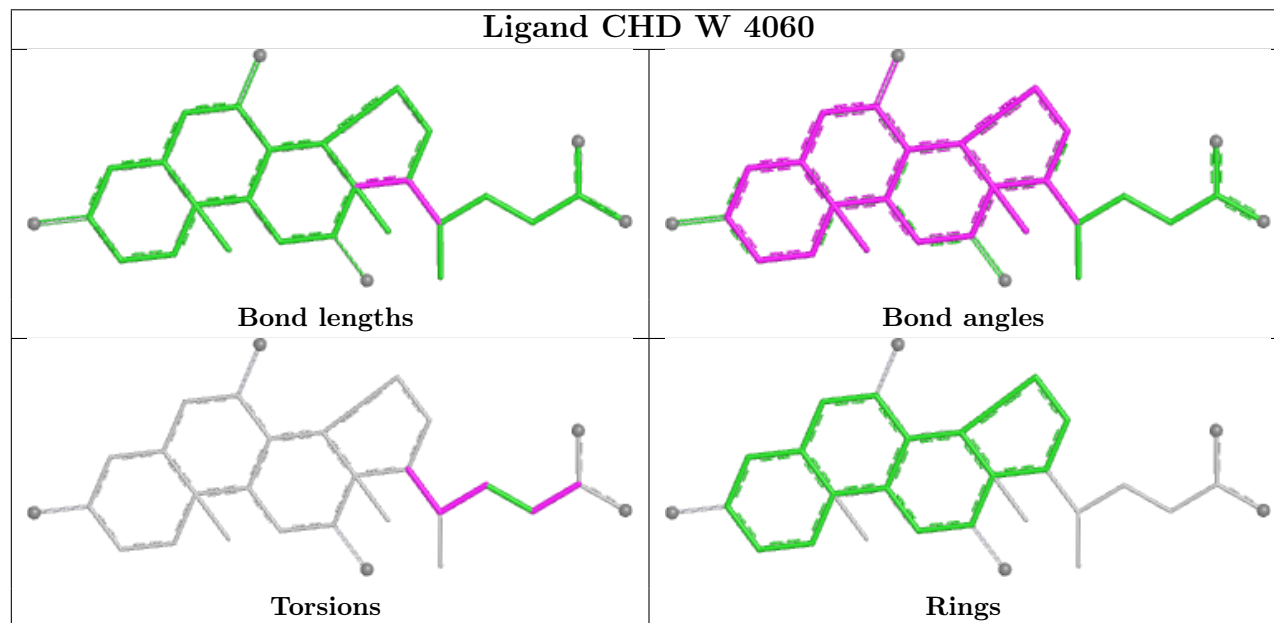
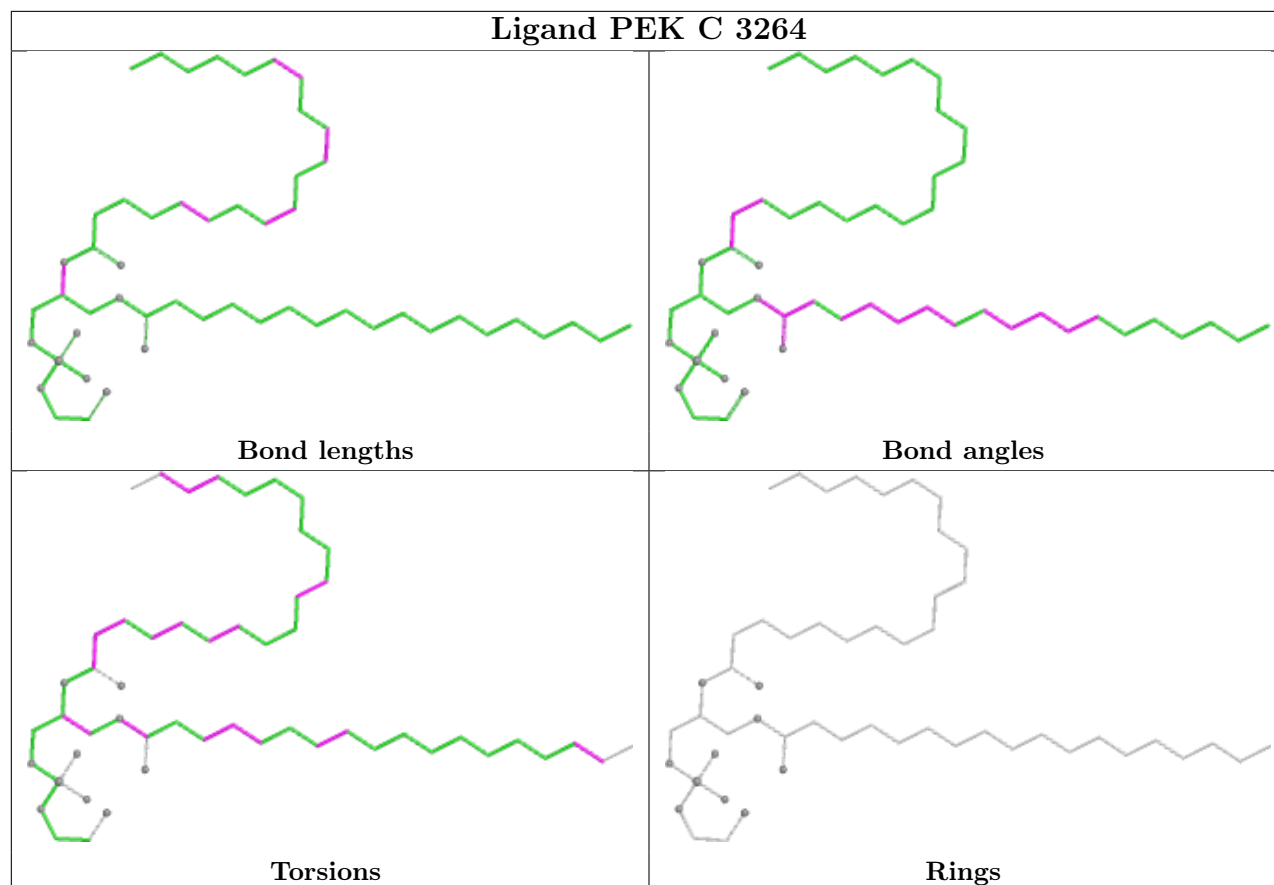


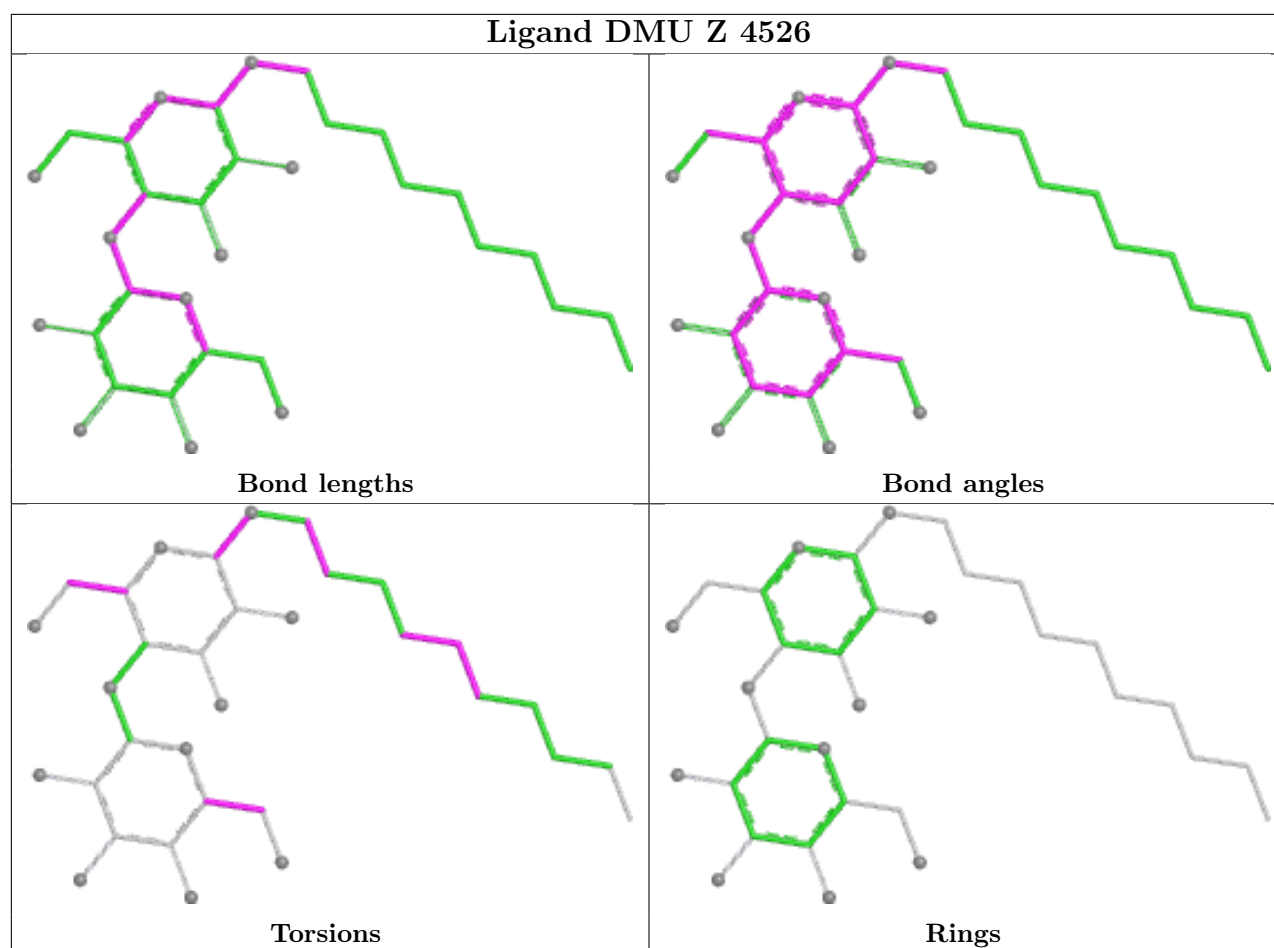


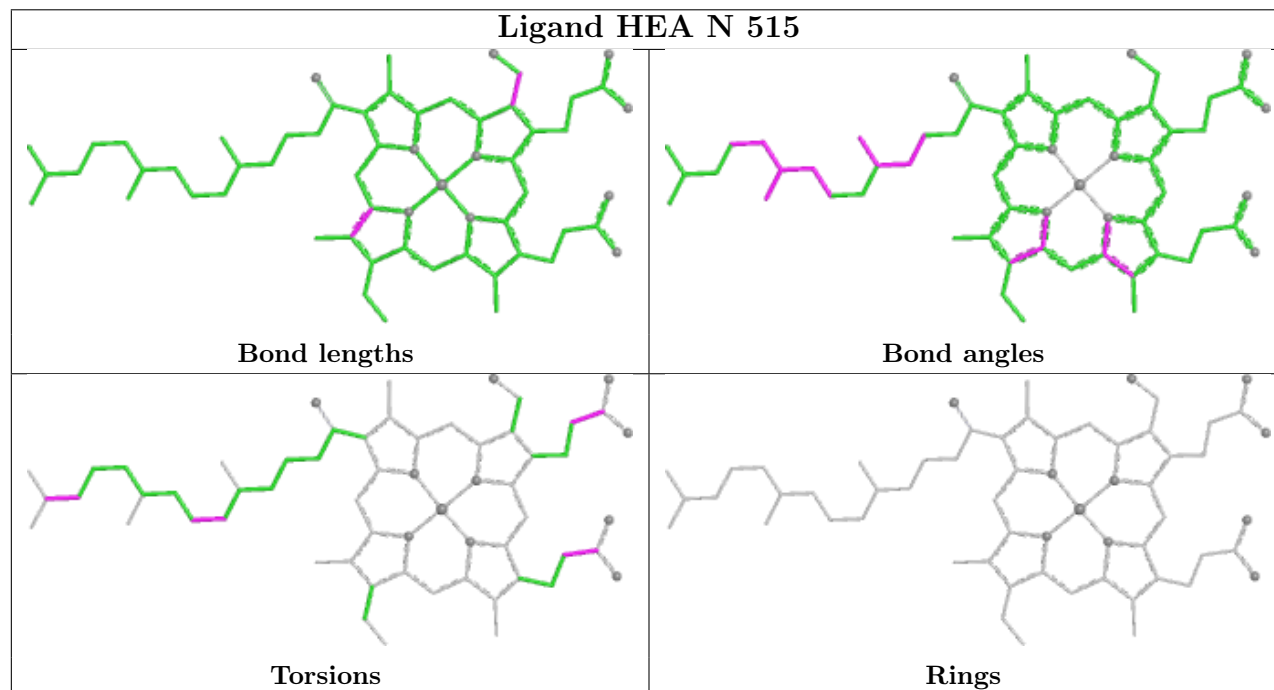
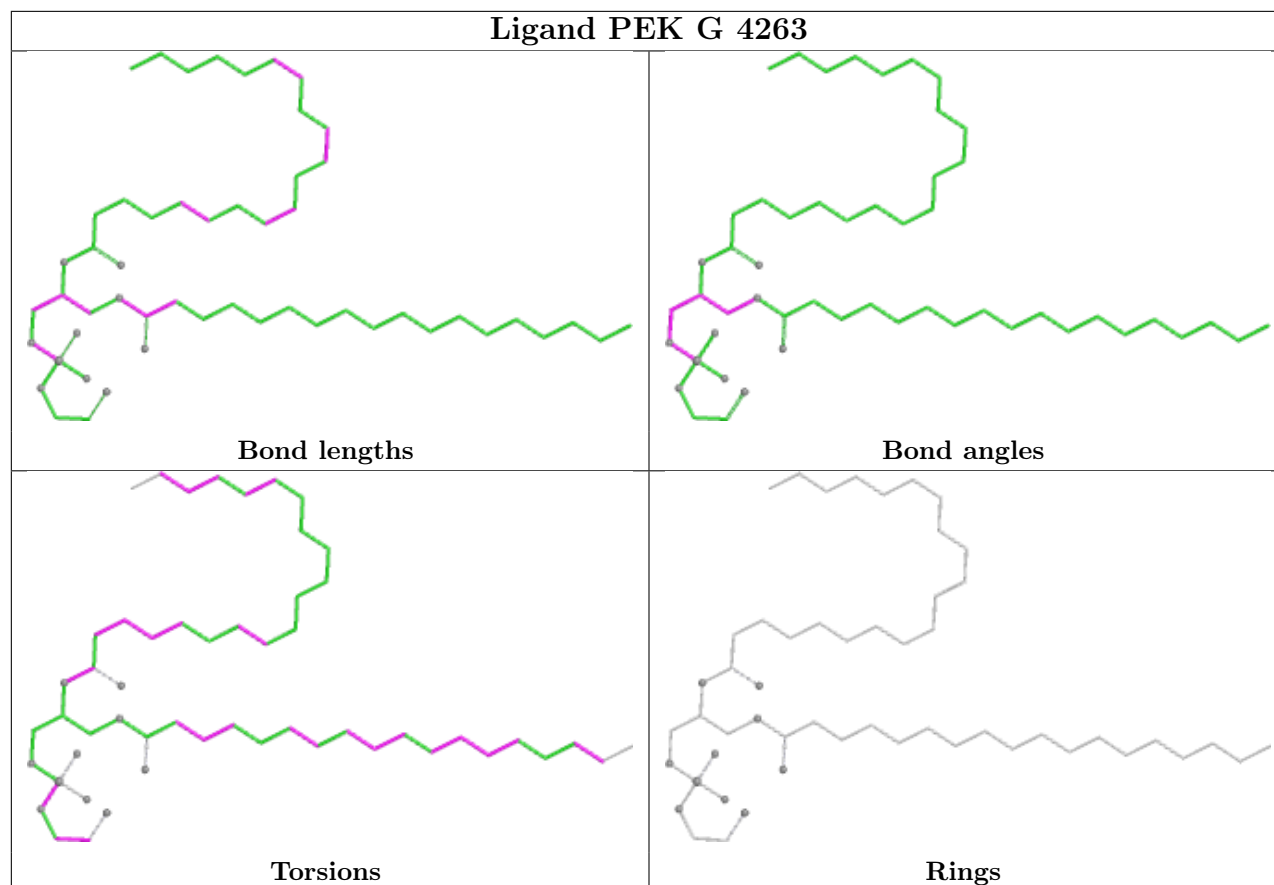


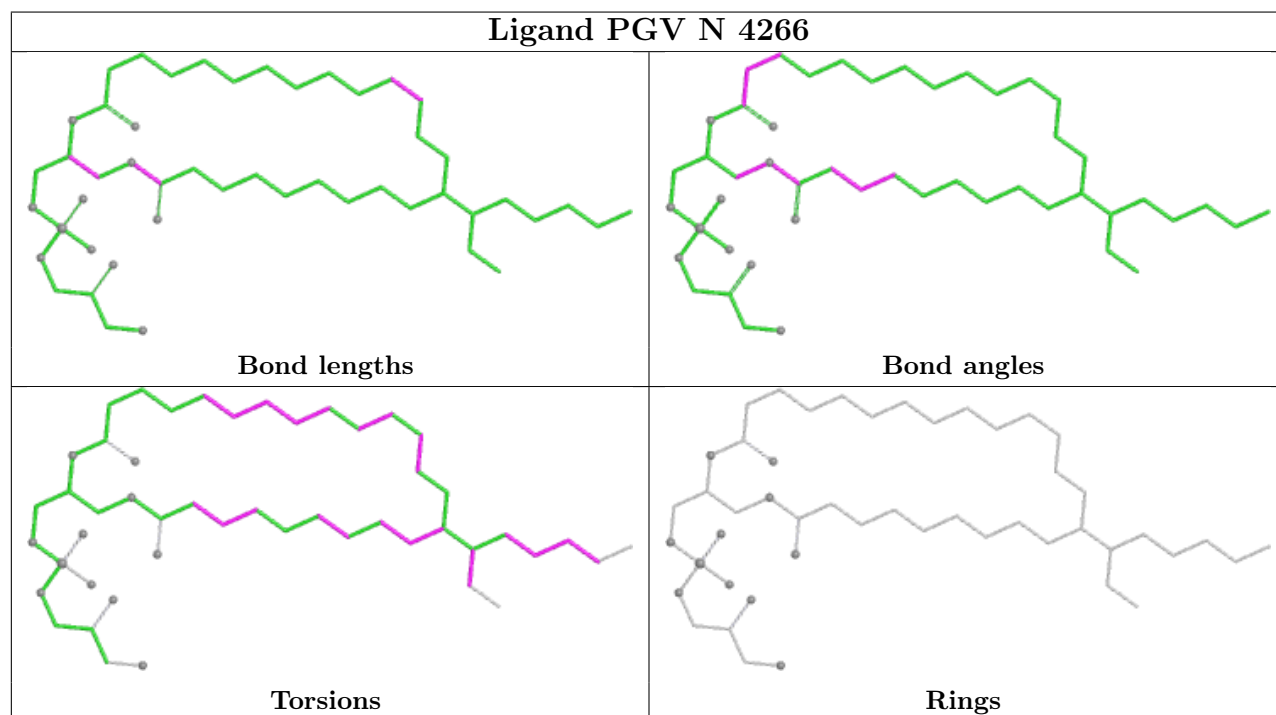
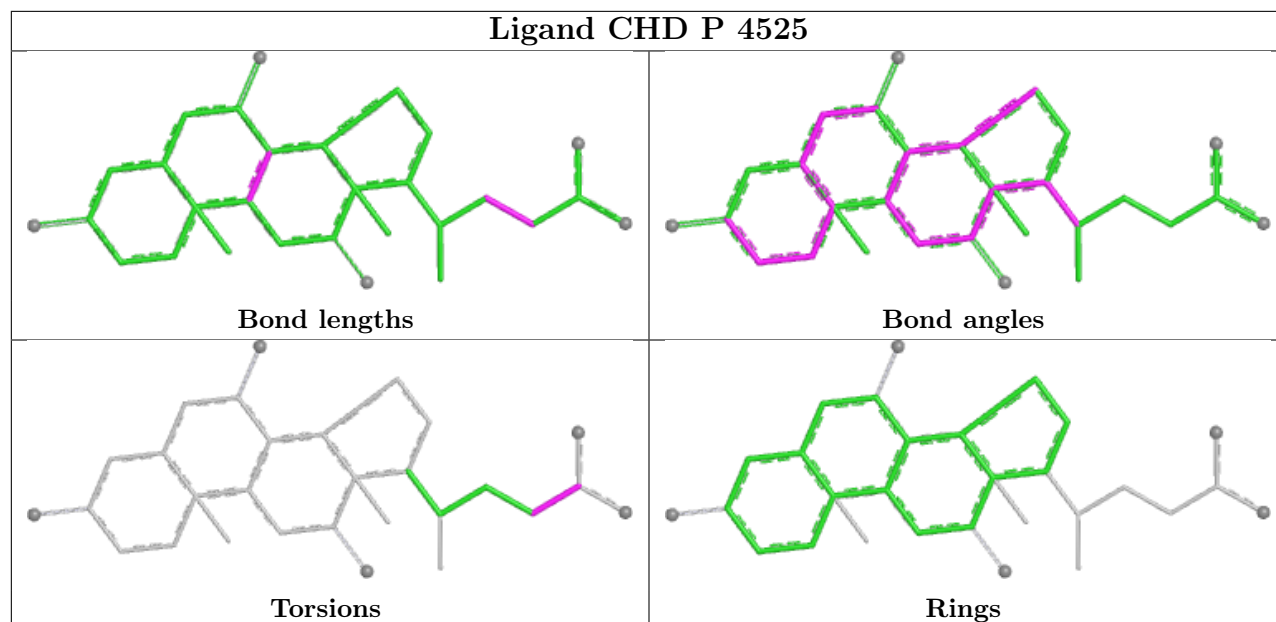


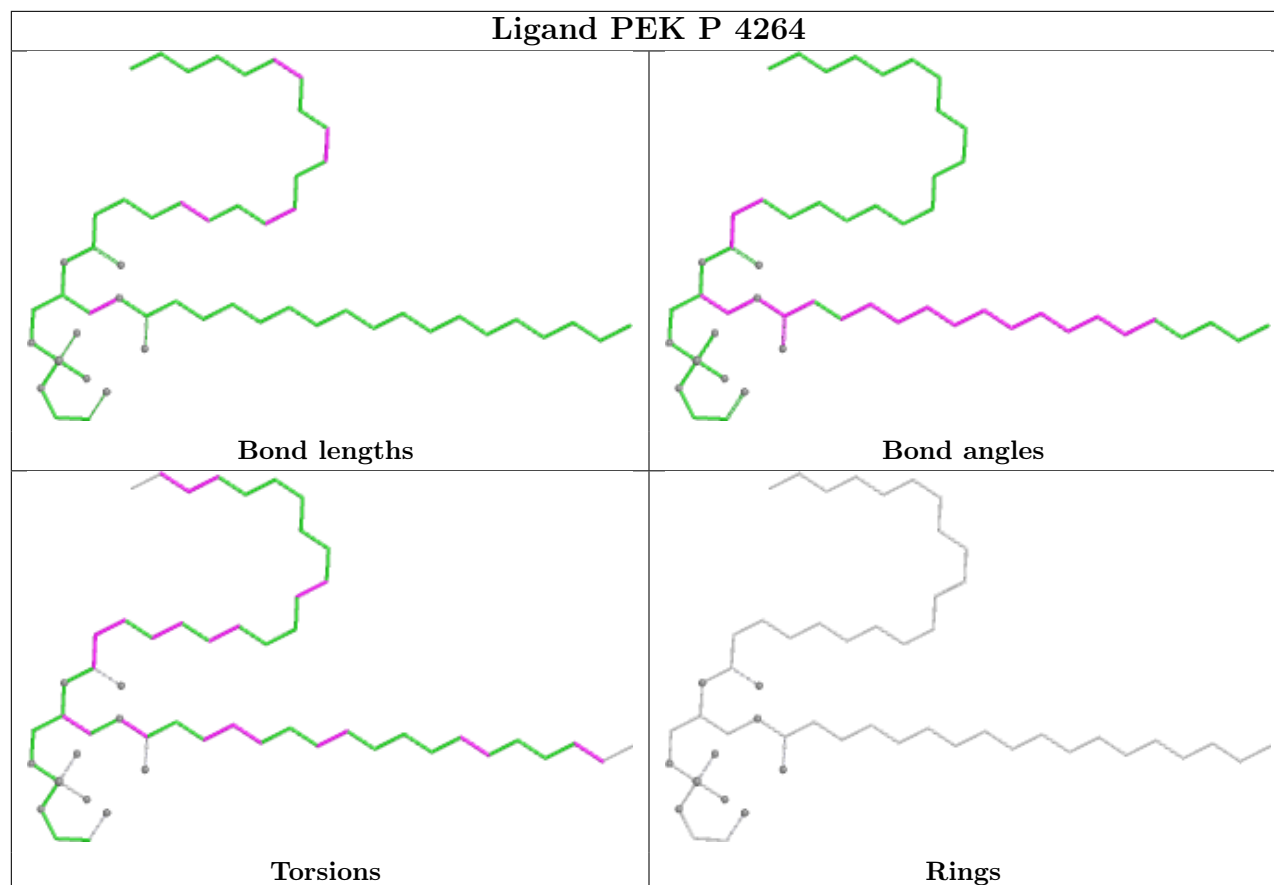




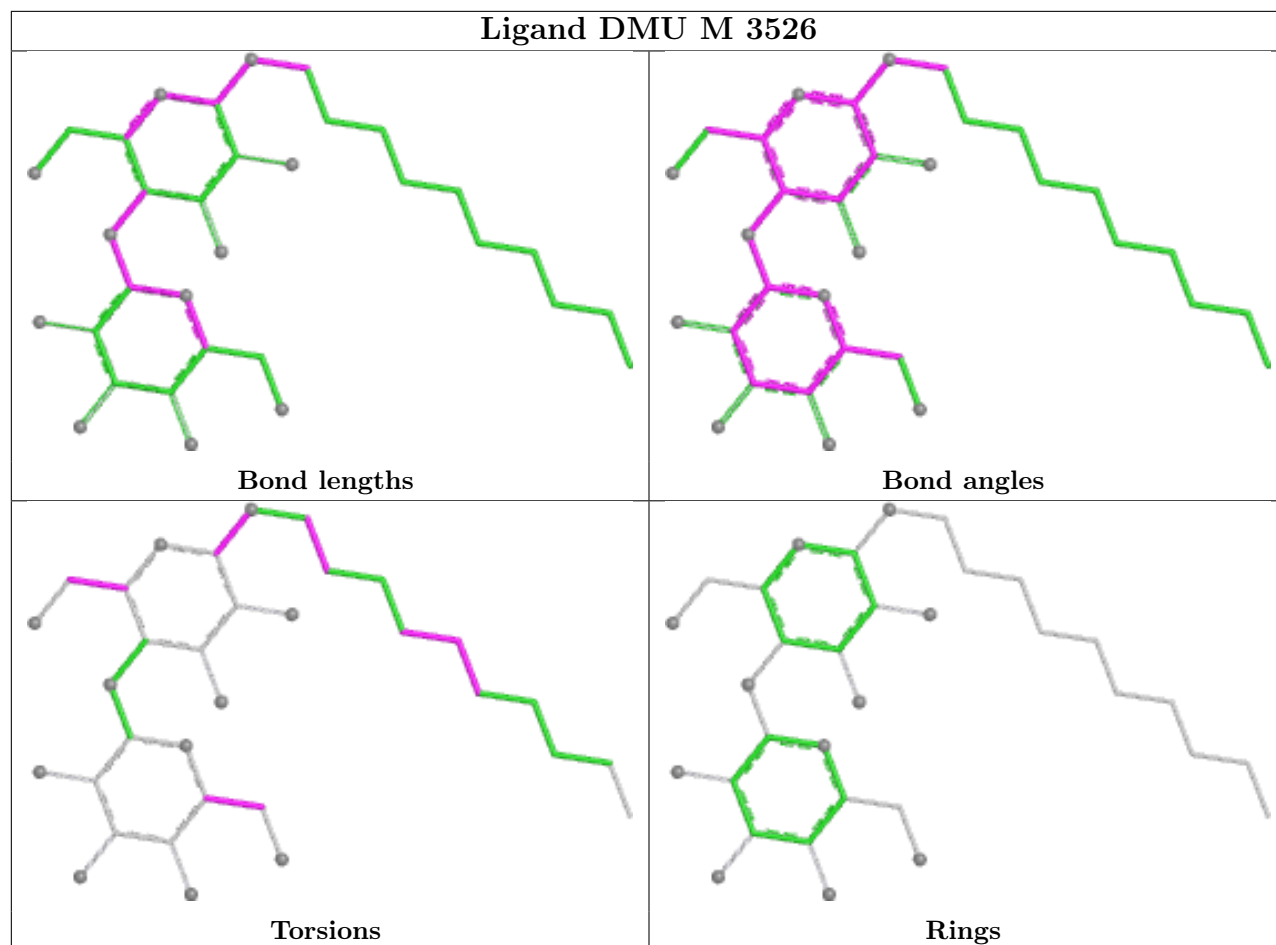




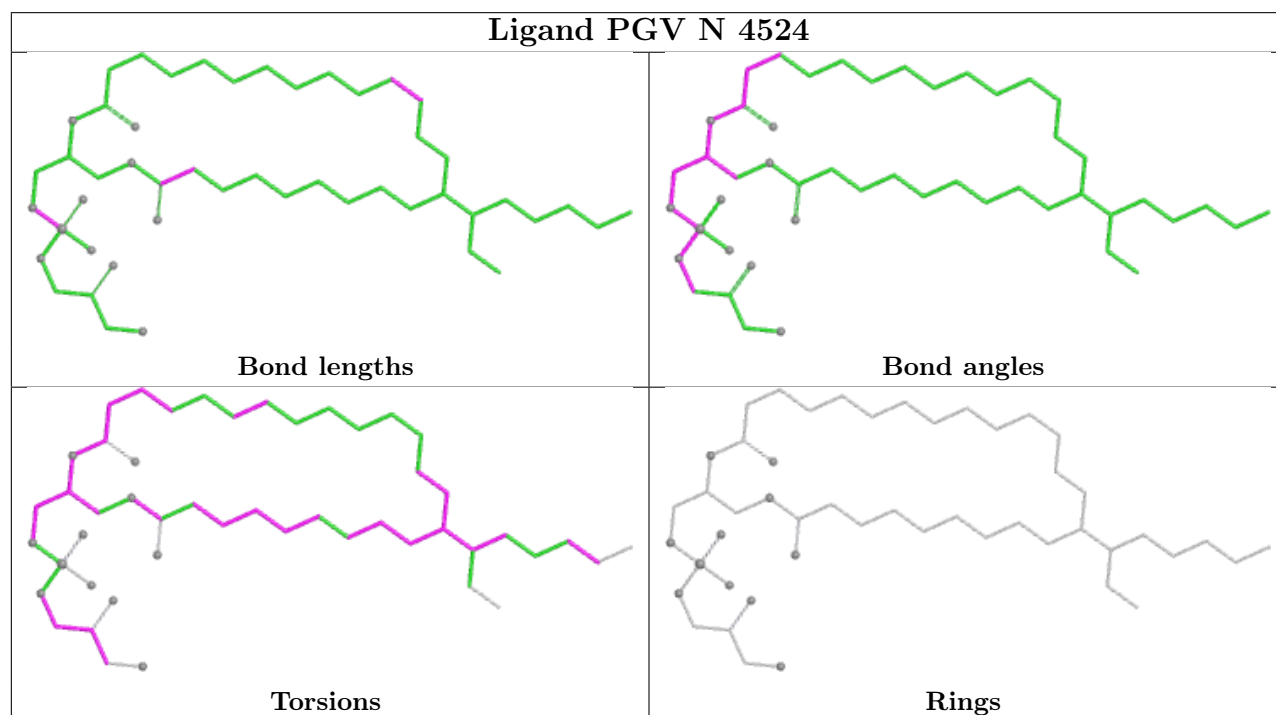


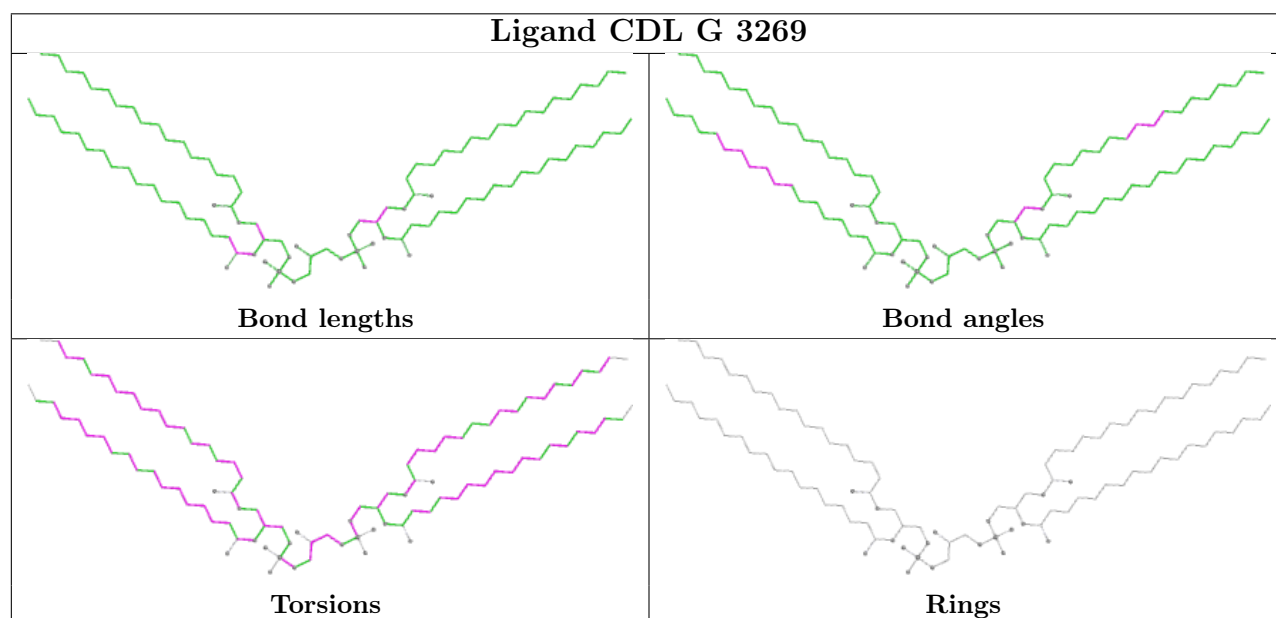
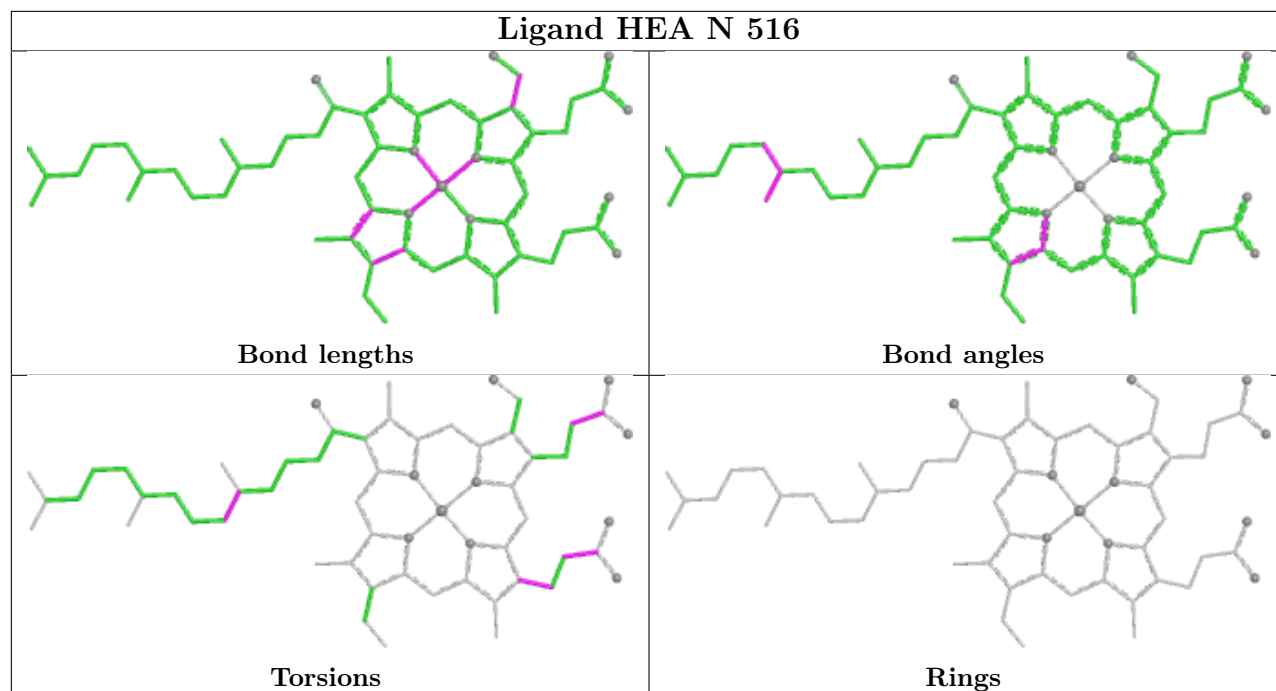


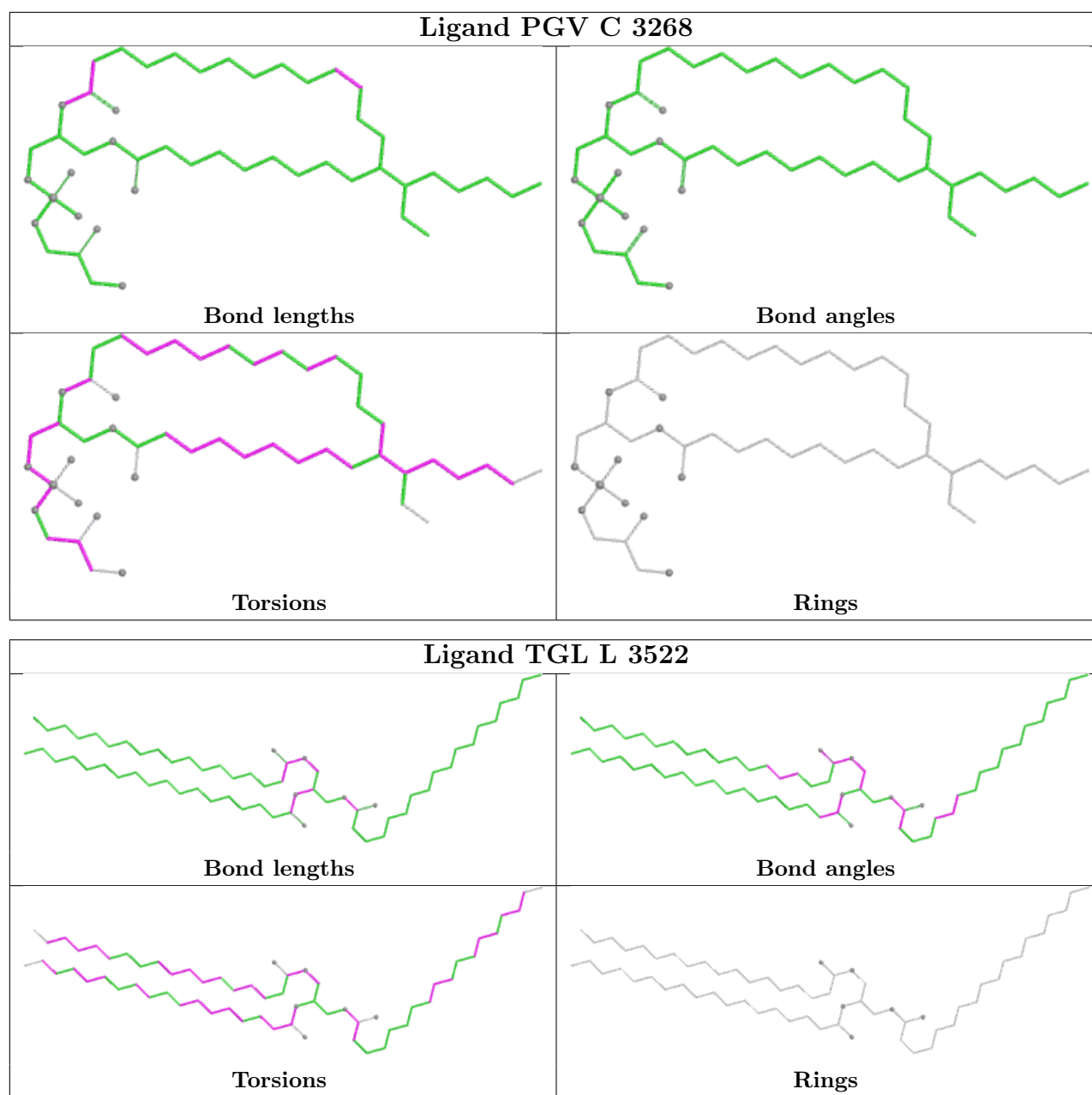
Ligand DMU M 3526



Ligand PGV N 4524







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.