



## wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 11:21 AM EST

PDB ID : 4V6M  
EMDB ID : EMD-1858  
Title : Structure of the ribosome-SecYE complex in the membrane environment  
Authors : Frauenfeld, J.; Gumbart, J.; van der Sluis, E.O.; Funes, S.; Gartmann, M.; Beatrix, B.; Mielke, T.; Berninghausen, O.; Becker, T.; Schulten, K.; Beckmann, R.  
Deposited on : 2011-02-08  
Resolution : 7.10 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

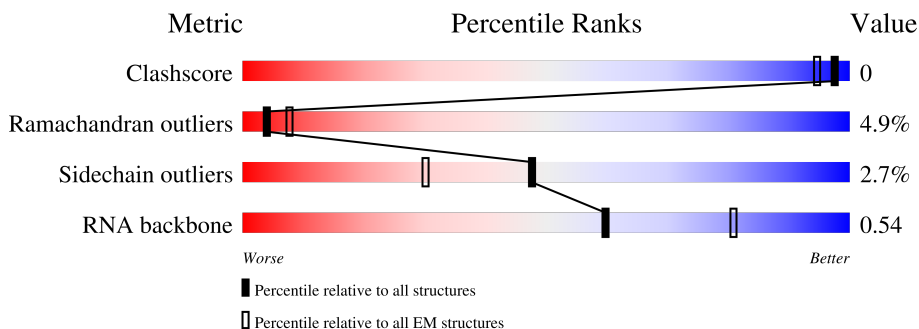
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 7.10 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.



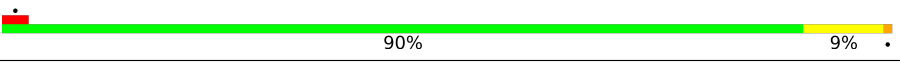
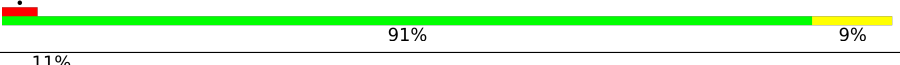
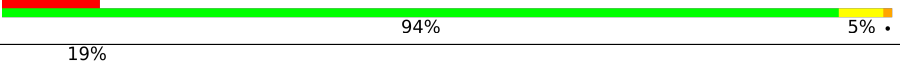
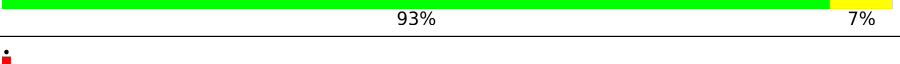
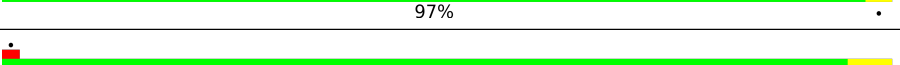
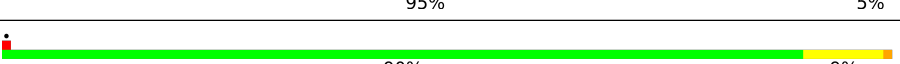
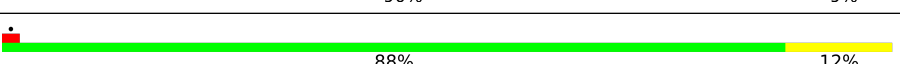
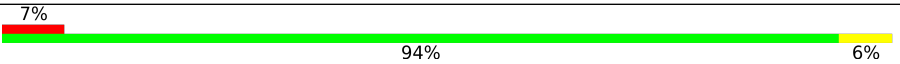
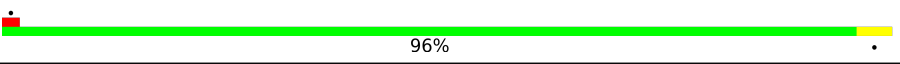
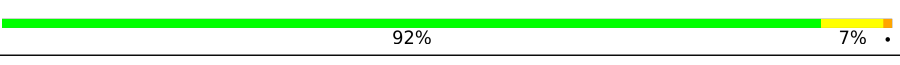
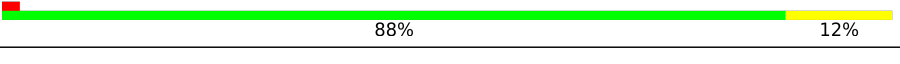
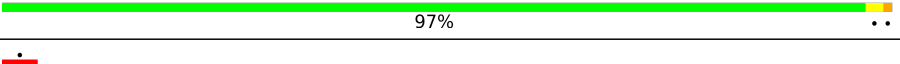
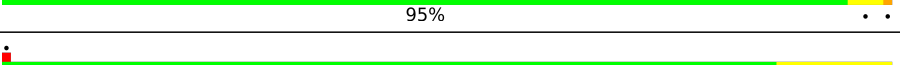
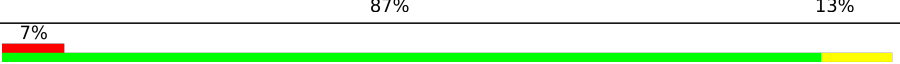
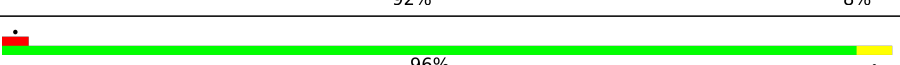
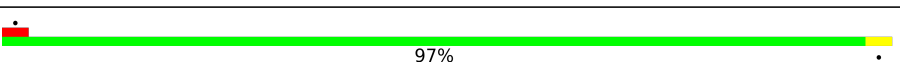
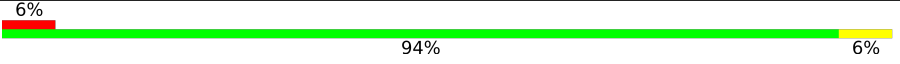
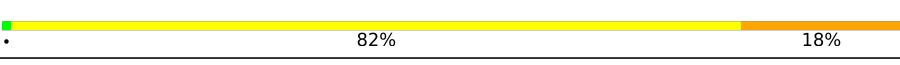
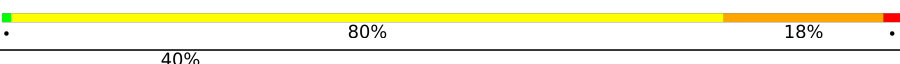

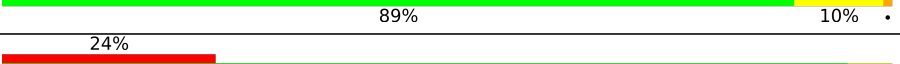
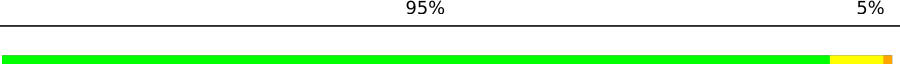
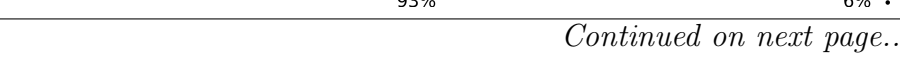


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	1542	
2	AX	11	
3	AV	77	
4	AZ	98	
5	A0	200	
5	A1	200	
6	AB	240	


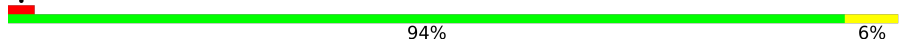
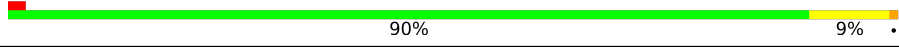
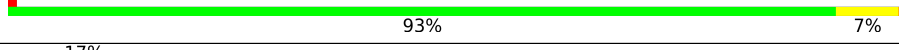

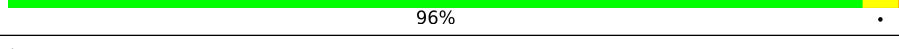
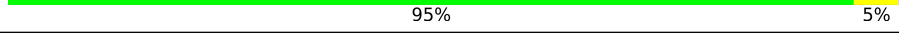
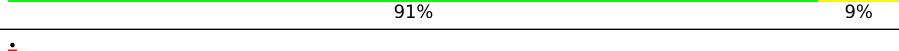
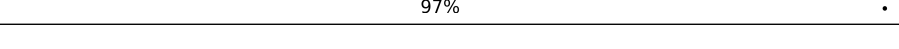
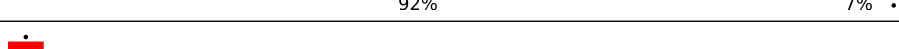
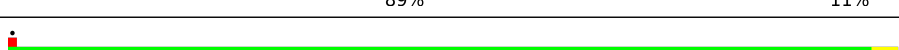
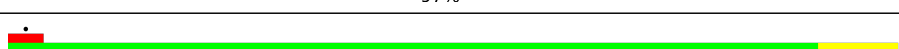
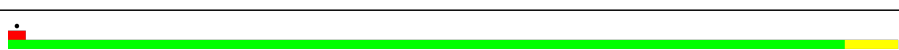
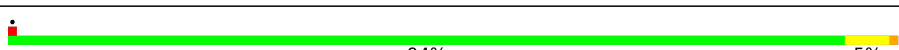
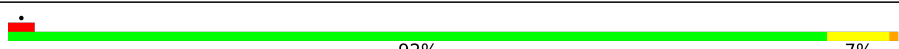

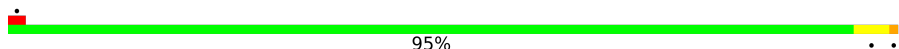
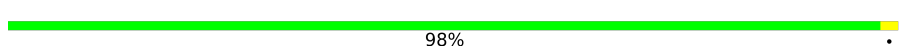
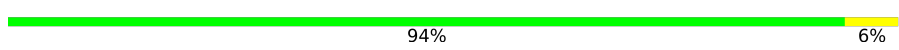

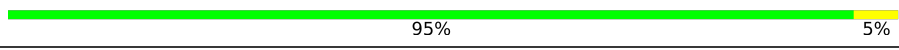
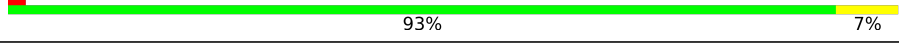
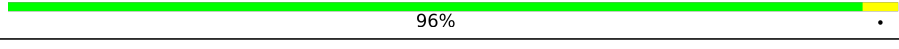
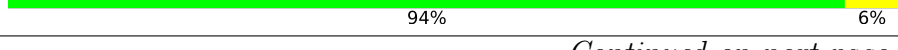

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Mol	Chain	Length	Quality of chain
7	AC	232	
8	AD	205	
9	AE	166	
10	AF	135	
11	AG	178	
12	AH	129	
13	AI	129	
14	AJ	103	
15	AK	128	
16	AL	123	
17	AM	117	
18	AN	100	
19	AO	88	
20	AP	82	
21	AQ	83	
22	AR	74	
23	AS	91	
24	AT	86	
25	AU	70	
26	B7	120	
27	B8	2904	
28	BA	435	
29	BB	116	
30	B5	234	
31	B6	272	


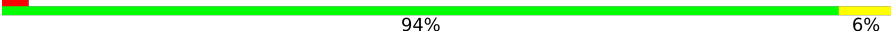

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Mol	Chain	Length	Quality of chain
32	BD	209	
33	BE	201	
34	BF	178	
35	BG	176	
36	BH	149	
37	BI	141	
38	BJ	142	
39	BK	123	
40	BL	144	
41	BM	136	
42	BN	127	
43	BO	117	
44	BP	114	
45	BQ	117	
46	BR	103	
47	BS	110	
48	BT	100	
49	BU	103	
50	BV	94	
51	BW	84	
52	BX	77	
53	BY	63	
54	BZ	58	
55	B0	56	
56	B1	54	

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Mol	Chain	Length	Quality of chain
57	B2	46	
58	B3	64	
59	B4	38	

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
60	PEV	A0	308	X	-	-	-
60	PEV	A0	314	X	-	-	-
60	PEV	A0	323	X	-	-	-
60	PEV	A1	301	X	-	-	-
60	PEV	A1	305	X	-	-	-
60	PEV	A1	313	X	-	-	-
60	PEV	A1	317	X	-	-	-
60	PEV	AZ	204	X	-	-	-
60	PEV	B8	3001	X	-	-	-
60	PEV	BA	502	X	-	-	-
60	PEV	BA	508	X	-	-	-
60	PEV	BA	526	X	-	-	-
60	PEV	BA	530	X	-	-	-
60	PEV	BA	533	-	-	X	-
60	PEV	BA	535	X	-	-	-
60	PEV	BA	537	X	-	-	-
60	PEV	BA	538	X	-	-	-
60	PEV	BB	202	X	-	-	-
60	PEV	BB	206	X	-	-	-
61	PGV	A0	304	X	-	-	-
61	PGV	A0	305	X	-	-	-
61	PGV	A0	306	X	-	-	-
61	PGV	A0	317	X	-	-	-
61	PGV	A0	318	X	-	-	-
61	PGV	A0	325	X	-	-	-
61	PGV	A0	327	X	-	-	-
61	PGV	A0	328	X	-	-	-
61	PGV	A0	331	X	-	-	-
61	PGV	A0	332	X	-	-	-
61	PGV	A1	303	X	-	-	-
61	PGV	A1	311	X	-	-	-
61	PGV	A1	315	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
61	PGV	A1	318	X	-	-	-
61	PGV	AZ	205	X	-	-	-
61	PGV	AZ	207	X	-	-	-
61	PGV	B8	3005	X	-	-	-
61	PGV	BA	501	X	-	-	-
61	PGV	BA	505	X	-	-	-
61	PGV	BA	512	X	-	-	-
61	PGV	BA	515	X	-	-	-
61	PGV	BA	516	X	-	-	-
61	PGV	BA	522	X	-	-	-
61	PGV	BA	536	X	-	-	-
61	PGV	BA	540	X	-	-	-
61	PGV	BB	203	X	-	-	-
61	PGV	BB	204	X	-	-	-
61	PGV	BB	205	X	-	-	-
61	PGV	BB	207	X	-	-	-
61	PGV	BB	208	X	-	-	-
61	PGV	BB	213	X	-	-	-
61	PGV	BB	217	X	-	-	-

## 2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 163040 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 RNA chain called 16S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	1542	Total	C	N	O	P	0	0
			33080	14754	6064	10720	1542		

- Molecule 2 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AX	11	Total	C	N	O	P	0	0
			231	103	39	78	11		

- Molecule 3 is a RNA chain called FtsQ nascent chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AV	77	Total	C	N	O	P	0	0
			1649	733	297	542	77		

- Molecule 4 is a protein called Cell division protein FtsQ.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AZ	98	Total	C	N	O	S	0	0
			779	496	142	138	3		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AZ	104	GLN	-	expression tag	UNP Q8X9Y5
AZ	105	HIS	-	expression tag	UNP Q8X9Y5
AZ	106	ALA	-	expression tag	UNP Q8X9Y5
AZ	107	ARG	-	expression tag	UNP Q8X9Y5
AZ	108	LEU	-	expression tag	UNP Q8X9Y5
AZ	109	ASP	-	expression tag	UNP Q8X9Y5
AZ	110	LYS	-	expression tag	UNP Q8X9Y5
AZ	111	PRO	-	expression tag	UNP Q8X9Y5
AZ	112	GLY	-	expression tag	UNP Q8X9Y5

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Chain	Residue	Modelled	Actual	Comment	Reference
AZ	113	ALA	-	expression tag	UNP Q8X9Y5
AZ	114	ARG	-	expression tag	UNP Q8X9Y5
AZ	115	HIS	-	expression tag	UNP Q8X9Y5
AZ	116	PRO	-	expression tag	UNP Q8X9Y5
AZ	117	CYS	-	expression tag	UNP Q8X9Y5
AZ	118	TRP	-	expression tag	UNP Q8X9Y5
AZ	119	PRO	-	expression tag	UNP Q8X9Y5

- Molecule 5 is a protein called Apolipoprotein A-I.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A0	200	Total	C	N	O	S	0	0
			1640	1028	290	319	3		
5	A1	200	Total	C	N	O	S	0	0
			1640	1028	290	319	3		

- Molecule 6 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AB	240	Total	C	N	O	S	0	0
			1872	1180	332	352	8		

- Molecule 7 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AC	232	Total	C	N	O	S	0	0
			1822	1149	346	323	4		

- Molecule 8 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AD	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 9 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AE	166	Total	C	N	O	S	0	0
			1225	761	232	226	6		

- Molecule 10 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AF	135	Total	C	N	O	S	0	0
			1101	677	198	219	7		

- Molecule 11 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AG	178	Total	C	N	O	S	0	0
			1400	874	269	253	4		

- Molecule 12 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AH	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 13 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AI	129	Total	C	N	O	S	0	0
			1036	642	208	183	3		

- Molecule 14 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AJ	103	Total	C	N	O	S	0	0
			825	514	158	151	2		

- Molecule 15 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AK	128	Total	C	N	O	S	0	0
			965	595	196	171	3		

- Molecule 16 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AL	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 17 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AM	117	Total	C	N	O	S	0	0
			910	564	183	160	3		

- Molecule 18 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AN	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 19 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AO	88	Total	C	N	O	S	0	0
			716	440	146	129	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AO	79	ARG	GLN	conflict	UNP P0ADZ4

- Molecule 20 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AP	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 21 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AQ	83	Total	C	N	O	S	0	0
			672	425	124	120	3		

- Molecule 22 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AR	74	Total	C	N	O	S	0	0
			626	395	123	107	1		

- Molecule 23 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AS	91	Total	C	N	O	S	0	0
			727	464	139	122	2		

- Molecule 24 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AT	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 25 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AU	70	Total	C	N	O	S	0	0
			590	366	125	98	1		

- Molecule 26 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	B7	120	Total	C	N	O	P	0	0
			2570	1144	468	838	120		

- Molecule 27 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	B8	2904	Total	C	N	O	P	0	0
			62341	27810	11469	20158	2904		

- Molecule 28 is a protein called Preprotein translocase secY subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BA	435	Total	C	N	O	S	0	0
			3362	2221	553	571	17		

- Molecule 29 is a protein called Preprotein translocase secE subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BB	116	Total	C	N	O	S	0	0
			889	587	154	145	3		

- Molecule 30 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	B5	234	Total	C	N	O	S	0	0
			1733	1081	315	330	7		

- Molecule 31 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	B6	272	Total	C	N	O	S	0	0
			2092	1294	425	366	7		

- Molecule 32 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	BD	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 33 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BE	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 34 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BF	178	Total	C	N	O	S	0	0
			1420	905	251	258	6		

- Molecule 35 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BG	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 36 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BH	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 37 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BI	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 38 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BJ	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 39 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BK	123	Total	C	N	O	S	0	0
			947	593	181	167	6		

- Molecule 40 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BL	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 41 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BM	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 42 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BN	127	Total	C	N	O	S	0	0
			1008	621	204	178	5		

- Molecule 43 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BO	117	Total	C	N	O	S	0	0
			900	557	179	163	1		

- Molecule 44 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BP	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 45 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BQ	117	Total	C	N	O		0	0
			947	604	192	151			

- Molecule 46 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BR	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 47 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BS	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 48 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BT	100	Total	C	N	O	S	0	0
			787	496	146	143	2		

- Molecule 49 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BU	103	Total	C	N	O		0	0
			789	498	148	143			

- Molecule 50 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BV	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 51 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	BW	84	Total	C	N	O	S	0	0
			634	391	129	113	1		

- Molecule 52 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	BX	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 53 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	BY	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 54 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	BZ	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 55 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	B0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 56 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
56	B1	54	Total	C	N	O	0	0
			441	284	81	76		

- Molecule 57 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	B2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

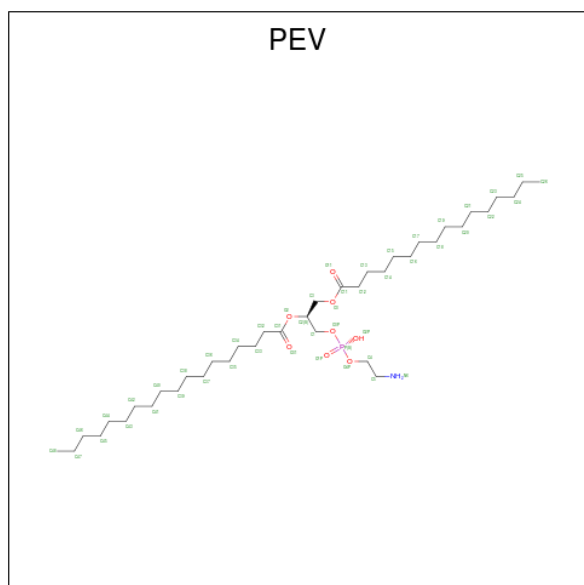
- Molecule 58 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	B3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 59 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	B4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 60 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (three-letter code: PEV) (formula: C<sub>39</sub>H<sub>78</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					AltConf
60	AZ	1	Total	C	N	O	P	0
			245	195	5	40	5	
60	AZ	1	Total	C	N	O	P	0
			245	195	5	40	5	
60	AZ	1	Total	C	N	O	P	0
			245	195	5	40	5	
60	AZ	1	Total	C	N	O	P	0
			245	195	5	40	5	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	

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Mol	Chain	Residues	Atoms					AltConf
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A1	1	Total	C	N	O	P	0
			1225	975	25	200	25	

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Mol	Chain	Residues	Atoms					AltConf
60	A1	1	Total	C	N	O	P	0
			1225	975	25	200	25	
60	A1	1	Total	C	N	O	P	0
			1225	975	25	200	25	
60	A1	1	Total	C	N	O	P	0
			1225	975	25	200	25	
60	B8	1	Total	C	N	O	P	0
			294	234	6	48	6	
60	B8	1	Total	C	N	O	P	0
			294	234	6	48	6	
60	B8	1	Total	C	N	O	P	0
			294	234	6	48	6	
60	B8	1	Total	C	N	O	P	0
			294	234	6	48	6	
60	B8	1	Total	C	N	O	P	0
			294	234	6	48	6	
60	B8	1	Total	C	N	O	P	0
			294	234	6	48	6	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	

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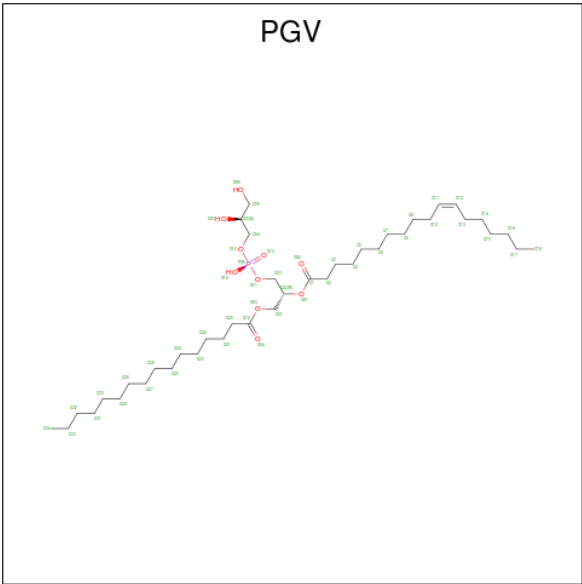
Mol	Chain	Residues	Atoms					AltConf
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BB	1	Total	C	N	O	P	0
			539	429	11	88	11	

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Mol	Chain	Residues	Atoms					AltConf
60	BB	1	Total	C	N	O	P	0
			539	429	11	88	11	
60	BB	1	Total	C	N	O	P	0
			539	429	11	88	11	
60	BB	1	Total	C	N	O	P	0
			539	429	11	88	11	
60	BB	1	Total	C	N	O	P	0
			539	429	11	88	11	
60	BB	1	Total	C	N	O	P	0
			539	429	11	88	11	
60	BB	1	Total	C	N	O	P	0
			539	429	11	88	11	
60	BB	1	Total	C	N	O	P	0
			539	429	11	88	11	
60	BB	1	Total	C	N	O	P	0
			539	429	11	88	11	

- Molecule 61 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				AltConf
61	AZ	1	Total	C	O	P	0
			102	80	20	2	
61	AZ	1	Total	C	O	P	0
			102	80	20	2	
61	A0	1	Total	C	O	P	0
			510	400	100	10	
61	A0	1	Total	C	O	P	0
			510	400	100	10	
61	A0	1	Total	C	O	P	0
			510	400	100	10	
61	A0	1	Total	C	O	P	0
			510	400	100	10	
61	A0	1	Total	C	O	P	0
			510	400	100	10	
61	A0	1	Total	C	O	P	0
			510	400	100	10	
61	A0	1	Total	C	O	P	0
			510	400	100	10	
61	A0	1	Total	C	O	P	0
			510	400	100	10	
61	A0	1	Total	C	O	P	0
			510	400	100	10	
61	A1	1	Total	C	O	P	0
			204	160	40	4	
61	A1	1	Total	C	O	P	0
			204	160	40	4	
61	A1	1	Total	C	O	P	0
			204	160	40	4	
61	A1	1	Total	C	O	P	0
			204	160	40	4	
61	B8	1	Total	C	O	P	0
			51	40	10	1	
61	BA	1	Total	C	O	P	0
			408	320	80	8	
61	BA	1	Total	C	O	P	0
			408	320	80	8	
61	BA	1	Total	C	O	P	0
			408	320	80	8	
61	BA	1	Total	C	O	P	0
			408	320	80	8	
61	BA	1	Total	C	O	P	0
			408	320	80	8	

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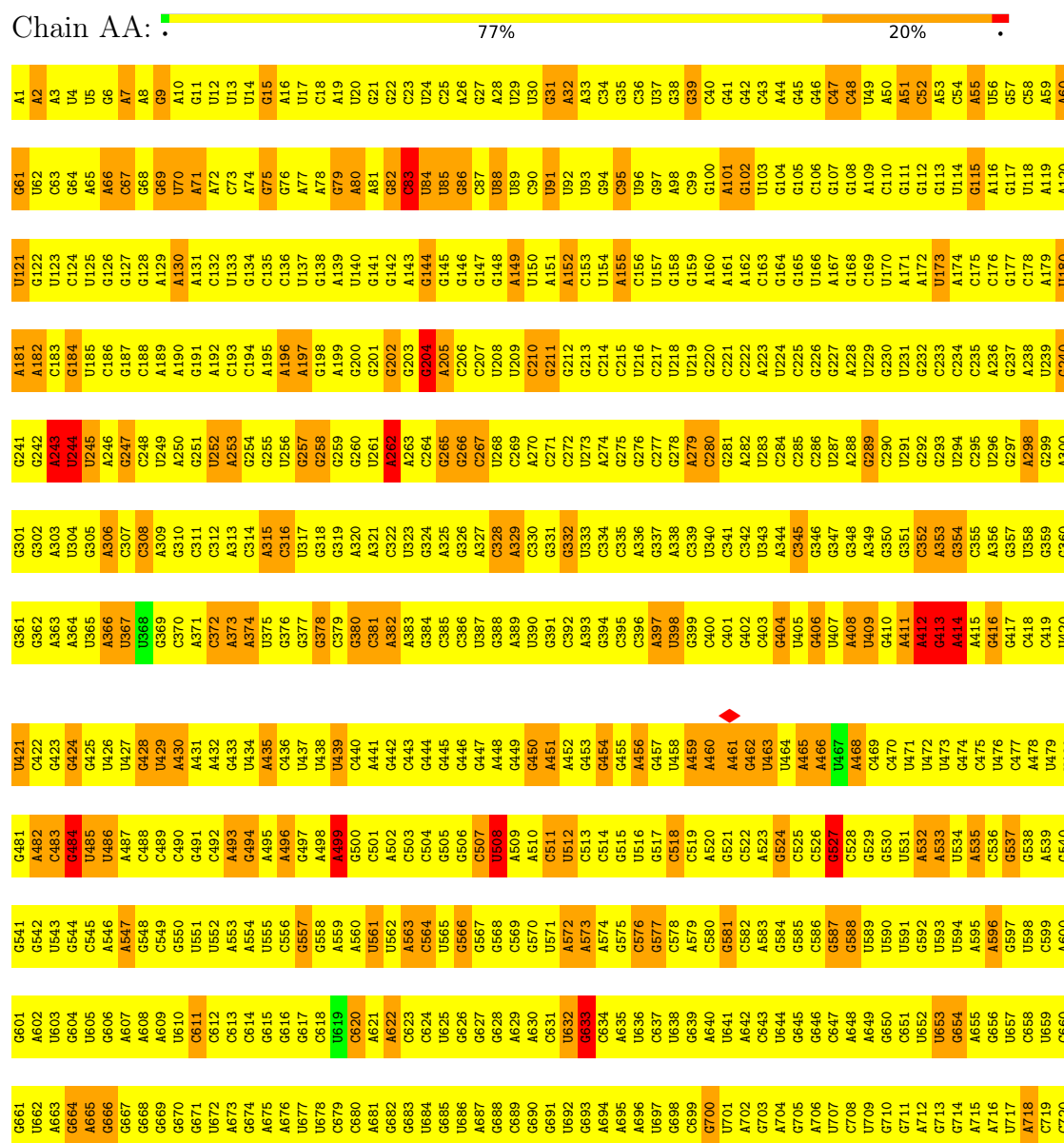
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Mol	Chain	Residues	Atoms				AltConf
61	BA	1	Total 408	C 320	O 80	P 8	0
61	BA	1	Total 408	C 320	O 80	P 8	0
61	BA	1	Total 408	C 320	O 80	P 8	0
61	BB	1	Total 357	C 280	O 70	P 7	0
61	BB	1	Total 357	C 280	O 70	P 7	0
61	BB	1	Total 357	C 280	O 70	P 7	0
61	BB	1	Total 357	C 280	O 70	P 7	0
61	BB	1	Total 357	C 280	O 70	P 7	0
61	BB	1	Total 357	C 280	O 70	P 7	0
61	BB	1	Total 357	C 280	O 70	P 7	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 and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: 16S RIBOSOMAL RNA



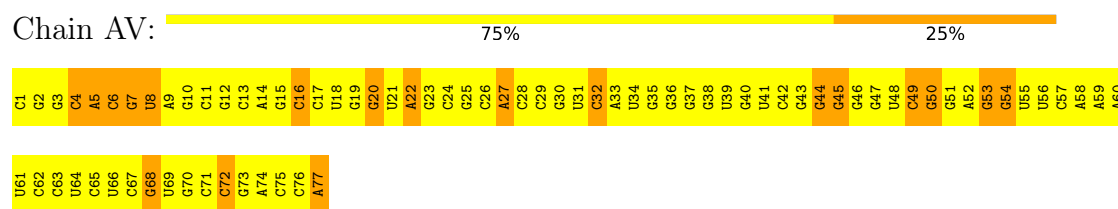
A1502	G1442	C1382	G1322	C1262	U1202	G1142	A1082	A1022	C962	G902	C841	A781	G721
A1503	C1443	C1383	G1323	C1263	C1203	G1143	U1083	U1023	G963	G903	U842	A782	G722
G1504	U1444	A1384	A1324	U1264	A1204	G1144	G1084	G1024	A964	U904	U843	A783	U723
G1505	U1445	G1385	C1325	C1265	U1205	G1145	U1085	U1025	U965	U905	G844	A784	G724
U1506	A1446	G1386	U1326	C1266	G1206	A1146	U1086	G1026	G966	A906	A845	G785	G725
A1507	A1447	G1387	C1327	C1267	G1207	G1147	G1087	G1027	C967	A907	G846	G786	G726
A1508	C1448	C1388	C1328	G1268	C1208	U1148	G1088	C1028	A968	A908	G847	A787	G727
C1509	U1449	A1389	A1329	G1269	C1209	C1149	G1089	U1029	A969	A909	C848	A788	A728
C1510	U1450	U1390	U1330	G1270	C1210	A1150	U1090	U1030	C970	C910	C849	U789	A729
G1511	U1451	U1391	G1331	A1271	U1211	A1151	U1091	C1031	G971	U911	U850	A790	G730
U1512	A1452	G1392	A1332	G1272	U1212	A1152	A1092	G1032	C972	C912	G851	G791	G731
A1513	G1453	U1393	C1333	C1273	A1213	G1153	G1093	G1033	G973	A913	G852	A792	G732
G1514	A1454	A1394	G1334	A1274	C1214	G1154	G1094	G1034	A974	A914	C853	U793	G733
G1515	G1455	C1395	U1385	A1275	G1215	A1155	U1095	A1035	A975	A915	U854	A794	G734
G1516	A1456	A1396	C1386	G1276	A1216	G1156	C1096	A1036	G976	U916	U855	C795	C735
G1517	A1457	G1397	G1337	C1277	C1217	A1157	C1097	C1037	A977	G917	C856	C796	C736
A1518	G1458	A1398	G1338	G1278	C1218	U1158	C1098	C1038	A978	A918	C857	C797	C737
A1519	G1459	C1399	A1339	G1279	A1219	U1159	G1099	G1039	C979	A919	G858	U798	C738
C1520	C1460	A1400	A1340	C1280	G1220	G1160	C1100	U1040	U980	U920	G859	C799	C739
C1521	G1461	G1401	U1341	C1281	G1221	C1161	A1101	G1041	U981	U921	A860	U740	U740
U1522	C1462	C1402	C1342	C1282	G1222	C1162	A1102	A1042	U982	G922	G861	G741	G741
G1523	U1463	G1403	G1343	U1283	C1223	A1163	C1103	G1043	A983	A923	C862	A802	G742
C1524	C1464	C1404	G1344	C1284	U1224	G1164	G1104	A1044	C984	C924	U863	G803	A743
G1525	A1465	G1405	U1345	A1285	C1225	U1165	A1105	C1045	C985	G925	A864	U804	C744
G1526	C1466	U1406	A1346	U1286	G1226	U1166	G1106	A1046	U986	G926	A865	C805	G745
U1527	C1467	C1407	G1347	A1287	A1227	A1167	C1107	G1047	G987	C927	C866	C806	A746
U1528	A1468	A1408	U1348	A1288	C1228	U1168	G1108	G1048	G988	G928	G867	A807	A747
G1529	C1469	A1409	A1349	A1289	C1229	U1169	G1109	U1049	U989	G929	C868	C808	G748
G1530	U1470	A1410	A1350	G1290	C1230	A1170	A1110	G1050	C990	C930	G869	C809	A749
A1531	U1471	C1411	U1351	U1291	G1231	A1171	A1111	C1051	U991	C931	C810	C810	C750
U1532	U1472	C1412	C1352	G1292	U1232	C1172	C1112	U1052	U992	C932	C811	C811	U751
C1533	G1473	A1413	G1353	C1293	G1233	U1173	C1113	G1053	G993	C933	A872	G812	G752
U1534	U1474	U1414	U1354	G1294	C1234	G1174	C1114	C1054	A994	C934	G873	U813	A753
C1535	G1475	G1415	G1355	U1295	U1235	G1175	U1115	U1055	A995	A935	U875	A814	G754
C1536	A1476	G1416	G1356	C1296	A1236	A1176	U1116	U1056	A996	C936	C876	A815	G755
U1537	G1477	G1417	A1357	G1297	C1237	G1177	A1117	G1057	U997	A937	G877	A816	C756
G1538	U1478	A1418	U1358	U1298	A1238	G1178	U1118	G1058	C998	A938	A878	C817	U757
C1539	C1479	G1419	C1359	A1299	A1239	A1179	C1119	C1059	C999	C939	C879	G818	C758
U1540	A1480	U1420	A1360	G1300	U1240	A1180	C1120	U1060	A1000	C940	C880	A819	A759
U1541	U1481	G1421	G1361	U1301	G1241	G1181	U1121	G1061	C1001	G941	G881	U820	G760
A1542	G1482	G1422	A1362	C1302	G1242	G1182	U1122	U1062	G1002	G942	C882	G821	G761
	A1483	G1423	A1363	C1303	C1243	U1183	U1123	C1063	G1003	U943	C883	U822	U762
	C1484	U1424	U1364	G1304	G1244	G1184	U1124	G1064	A1004	G944	U884	G823	G763
	U1485	U1425	G1365	G1305	C1245	G1185	U1125	U1065	A1005	G945	G885	G824	C764
	G1486	G1426	C1366	A1306	A1246	G1186	U1126	C1066	G1006	A946	G886	A825	G765
	G1487	C1427	C1367	U1307	U1247	G1187	G1127	U1067	U1007	G947	G887	C826	A766
	G1488	A1428	A1368	U1308	A1248	G1188	C1128	G1068	U1008	C948	G888	U827	A767
	G1489	A1429	C1369	G1309	C1249	U1189	C1129	C1069	U1009	A949	A889	U828	A768
	U1490	A1430	G1370	G1310	A1250	G1190	A1130	U1070	U1010	U950	G890	G829	G769
	G1491	A1431	G1371	A1311	A1251	A1191	G1131	C1071	C1011	G951	U891	G830	C770
	A1492	G1432	U1372	G1312	A1252	C1192	C1132	G1072	A1012	U952	A892	A831	G771
	A1493	A1433	G1373	U1313	G1253	G1193	G1133	U1073	G1013	G953	C893	G832	U772
	G1494	A1434	A1374	C1314	A1254	U1194	G1134	G1074	A1014	G954	G894	G833	G773
	U1495	G1435	A1375	U1315	G1255	U1195	U1135	U1075	G1015	U955	G895	U834	G774
	G1496	A1436	U1376	G1316	A1256	A1196	U1136	U1076	A1016	U956	C896	U835	G775
	G1497	A1437	C1377	C1317	A1257	A1197	G1137	G1077	U1017	A957	C897	G836	G776
	U1498	G1438	C1378	A1318	G1258	G1198	G1138	U1078	G1018	A958	G898	U837	A777
	A1499	G1439	G1379	A1319	C1259	U1199	G1139	G1079	A1019	A959	C899	G838	G778
	U1500	U1440	C1380	C1320	G1260	C1200	G1140	U1080	A1020	U960	A900	C839	C779
	C1501	A1441	U1381	U1321	A1261	A1201	C1141	A1081	A1021	U961	A901	C840	A780

● Molecule 2: mRNA



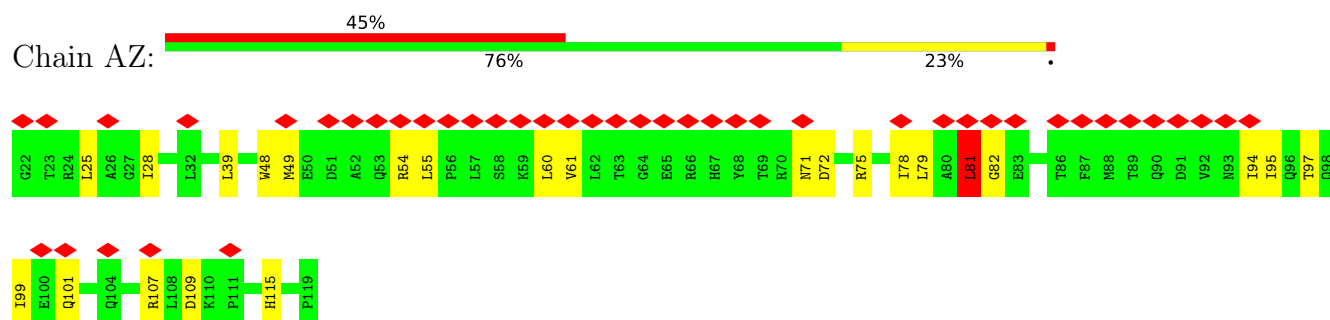
● Molecule 3: FtsQ nascent chain

Chain AV:

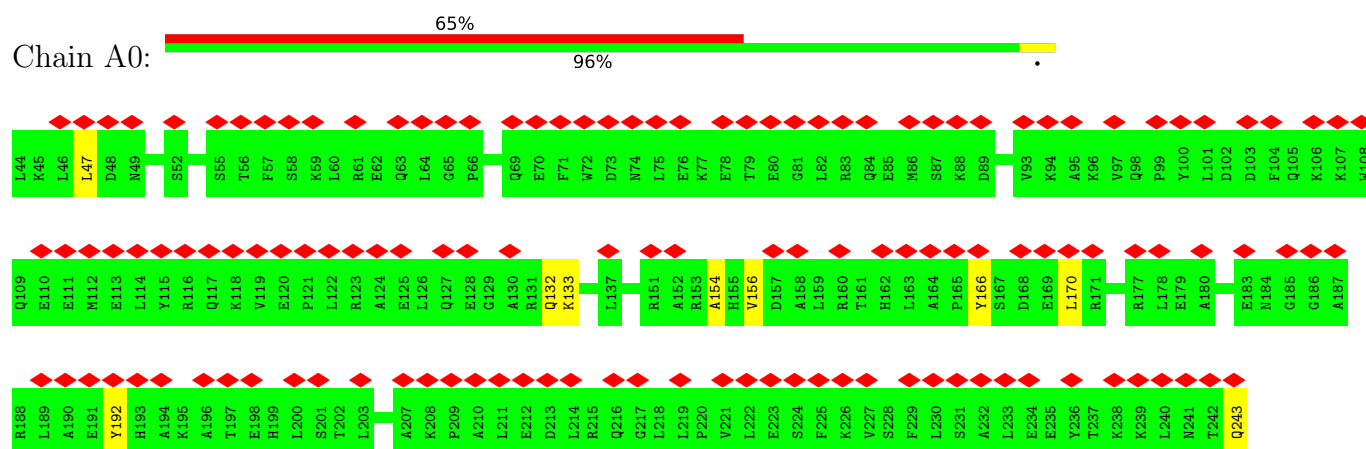


- Molecule 4: Cell division protein FtsQ

Chain AZ:

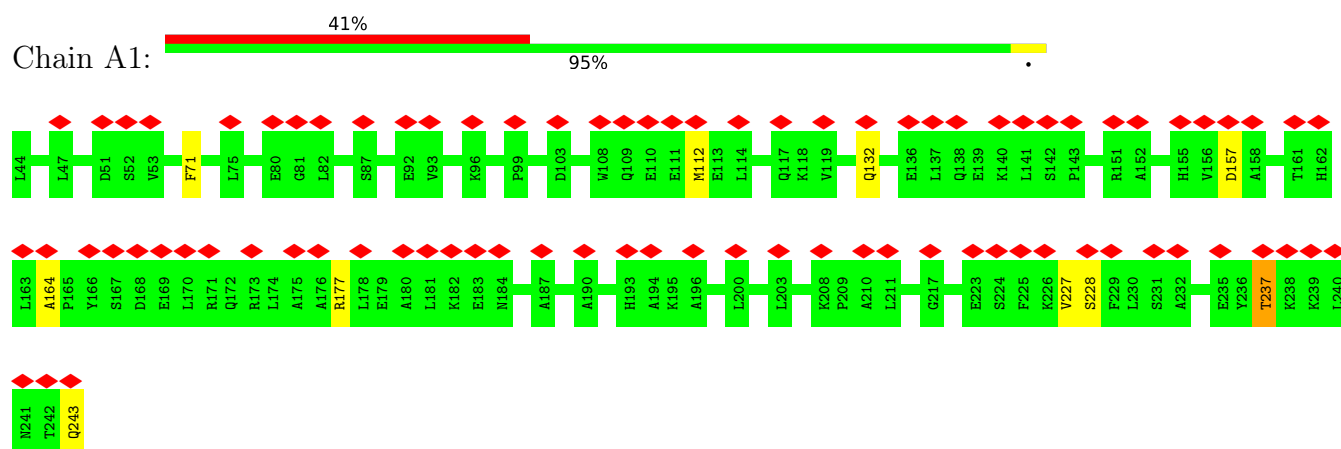


- Molecule 5: Apolipoprotein A-I

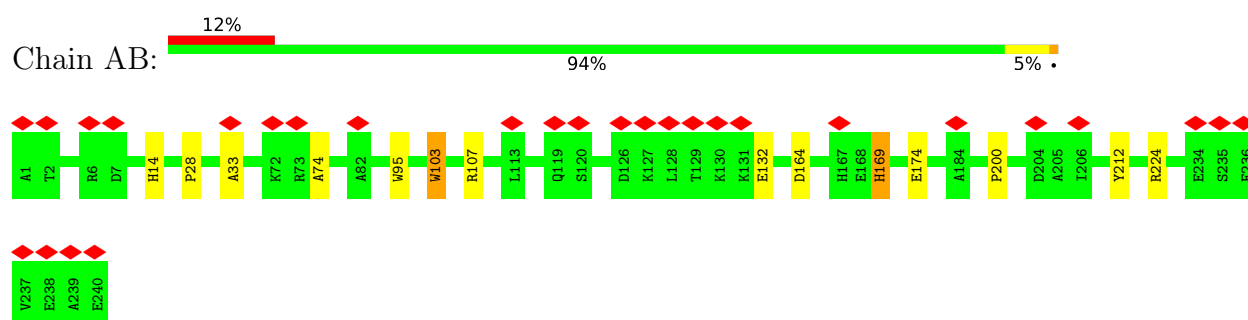


- Molecule 5: Apolipoprotein A-I

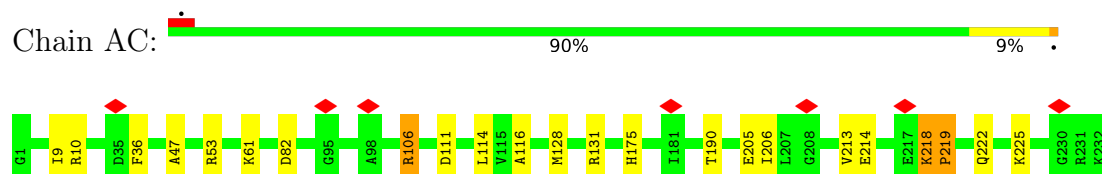
Chain A1:



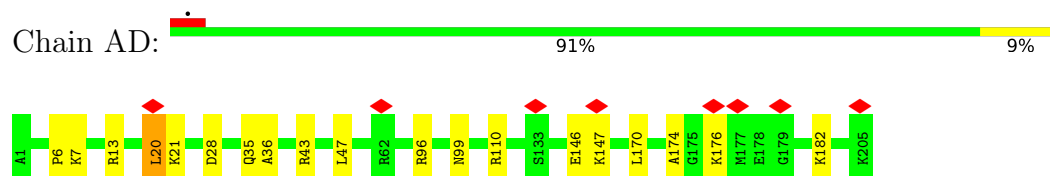
- Molecule 6: 30S ribosomal protein S2



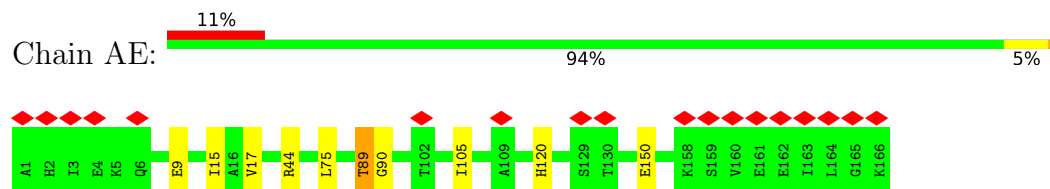
- Molecule 7: 30S ribosomal protein S3



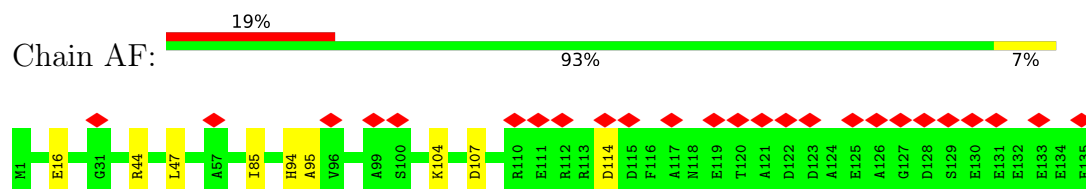
- Molecule 8: 30S ribosomal protein S4



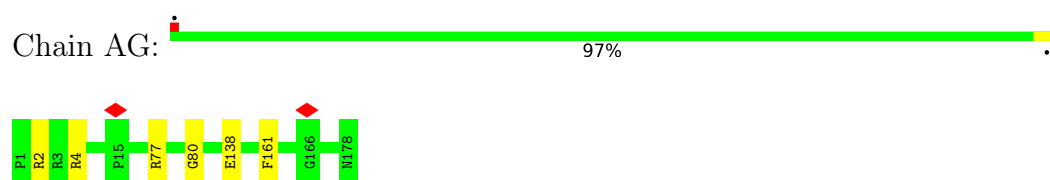
- Molecule 9: 30S ribosomal protein S5



- Molecule 10: 30S ribosomal protein S6

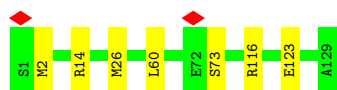


- Molecule 11: 30S ribosomal protein S7

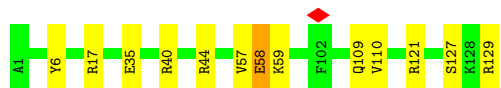


- Molecule 12: 30S ribosomal protein S8





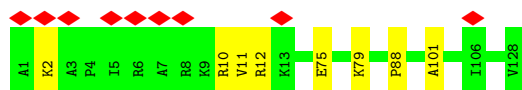
- Molecule 13: 30S ribosomal protein S9



- Molecule 14: 30S ribosomal protein S10



- Molecule 15: 30S ribosomal protein S11



- Molecule 16: 30S ribosomal protein S12



- Molecule 17: 30S ribosomal protein S13



- Molecule 18: 30S ribosomal protein S14



- Molecule 19: 30S ribosomal protein S15

Chain AO:  97% ..



- Molecule 20: 30S ribosomal protein S16

Chain AP:  95% ..



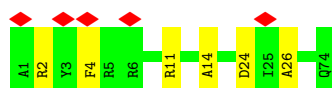
- Molecule 21: 30S ribosomal protein S17

Chain AQ:  87% 13%



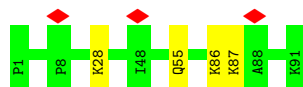
- Molecule 22: 30S ribosomal protein S18

Chain AR:  7% 92% 8%



- Molecule 23: 30S ribosomal protein S19

Chain AS:  96% .



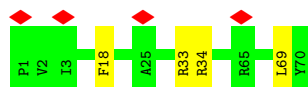
- Molecule 24: 30S ribosomal protein S20

Chain AT:  97% .




- Molecule 25: 30S ribosomal protein S21

Chain AU:  6% 94% 6%

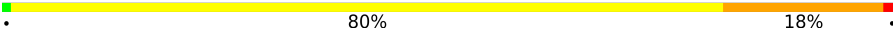


## ● Molecule 26: 5S RIBOSOMAL RNA

Chain B7:  82% 18%

U1	G2	C3	C4	U5	G6	G7	C8	G9	G10	C11	C12	G13	U14	A15	G16	C17	U18	C19	G20	G21	U22	G23	G24	G25	C26	C27	C28	C29	C30	C31	U32	C33	A34	C35	C36	C37	C38	A39	U40	G41	C42	C43	A44	A45	A46	C47	U48	A49	C50	U51	G52	C53	G54	U55	A56	G57	A58	A59	C60
G61	C62	C63	G64	U65	A66	G67	C68	G69	C70	C71	G72	A73	U74	G75	C76	U77	A78	G79	U80	G81	U82	G83	G84	G85	C86	U87	C88	U89	C90	C91	C92	C93	A94	U95	C96	C97	C98	A99	G100	A101	C102	U103	A104	G105	C106	G107	U108	A109	C110	U111	G112	C113	C114	A115	G116	G117	C118	A119	U120

## ● Molecule 27: 23S RIBOSOMAL RNA

Chain B8:  80% 18%

A781	A721	A661	C601	A541	G481	C421	G361	G301	A241	A181	G121	C61	G1
A782	A722	A662	A602	C542	A482	A422	A362	C302	G242	A182	G122	U62	G2
A783	C723	G663	A603	C543	A483	A423	G363	C303	U243	C183	G123	A63	U3
C784	A724	G664	G604	C544	C484	C424	C364	U304	A244	C184	G124	A64	U4
G785	C725	U665	G605	U545	C485	C425	U365	C305	G245	C185	A125	U65	A5
C786	C726	A666	U606	U546	C486	C426	C366	U306	C246	G186	A126	C66	A6
C787	A727	U667	U607	A547	C487	U427	G367	G307	G247	G187	A127	U67	G7
A788	C728	A668	A608	G548	C488	A428	A368	G308	G248	G188	C128	C68	C8
A789	C729	C669	A609	G549	C489	A429	U369	A309	C249	G189	C129	C69	G9
C790	A730	C670	C610	C550	C490	A430	G370	A310	G250	A190	C130	C70	A10
C791	C731	C671	C611	C551	G491	U431	A371	A311	A251	A191	A131	A71	C11
A792	C732	C672	G612	U552	A492	A432	C372	G312	G252	C192	G132	U72	U12
C793	C733	C673	A613	G553	C493	C433	U373	G313	C253	U193	U133	A73	A13
A794	A734	A674	A614	G554	C494	U434	A374	C314	G254	G194	G134	A74	A14
C795	A735	A675	U615	G555	C495	C435	G375	G315	A255	A195	U135	G75	G15
C796	C736	A676	A616	A556	C496	C436	G376	C316	C256	A196	G136	C76	C16
C797	C737	A677	G617	C557	A497	U437	G377	G317	C257	A197	U137	C77	G17
C798	C738	C678	G618	U558	C498	C438	C378	C318	G258	C198	U138	U78	U18
C799	A739	C679	G619	G559	U499	A439	G379	G319	G259	A199	U139	C79	A19
A800	C740	C680	G620	C560	C440	C440	G380	A320	G260	U200	C140	C80	C20
C801	U741	A681	U621	U561	A501	U441	G381	U321	G261	C201	G141	C81	C21
A802	A742	G682	G622	U562	A502	C442	A382	A322	A262	U202	A142	U82	C22
U803	C743	A683	C623	A563	A503	A443	C383	C323	G263	C203	C143	A83	C23
A804	A744	G684	C624	C564	A504	C444	A384	A324	C264	A204	A144	A84	C24
G805	C745	A685	G625	C565	A505	C445	C385	G325	A265	G205	C145	C85	U25
C806	U746	A686	A626	U566	G506	U446	G386	G326	C266	U206	A146	C86	G26
U807	U747	C687	U627	U567	A507	A447	U387	G327	C267	A207	C147	U87	G27
C808	C748	U688	G628	U568	A508	U448	G388	U328	C268	C208	U148	C88	A28
A809	A749	C689	G629	U569	C509	A449	G389	G329	C269	C209	A149	A89	U29
U810	C750	C690	G630	C570	C510	C450	U390	A330	A270	C210	U150	U90	C30
U811	A751	C691	A631	U571	U511	U451	A391	C331	G271	C211	C151	A91	C31
C812	C752	C692	A632	A572	C512	C452	U392	A332	A272	G212	A152	U92	C32
U813	A753	A693	A633	U573	A513	A453	C393	G333	G273	C213	U153	G93	C33
C814	C754	C694	C634	A574	A514	A454	C394	C334	C274	G214	U154	A94	U34
U815	C755	G695	C635	A575	A515	C455	U395	C335	C275	G215	A155	A95	G35
C816	A756	G696	C636	U576	C516	C456	C396	C336	U276	A216	A156	C96	G36
C817	C757	G697	A637	C577	C517	A457	U397	C337	G277	A217	C157	C97	C37
A818	C758	C698	G638	C578	C518	C458	C398	U338	A278	C218	U158	C98	A38
C819	A759	A699	U639	G579	U519	U459	U399	U339	A279	A219	G159	U99	G39
C820	C760	G700	C640	G620	C620	A460	C400	A340	U280	G220	A160	U100	U40
A821	A761	C701	U641	C581	U521	C461	A401	C341	C281	A221	A161	A101	C41
C822	C762	U702	U642	A582	A522	C462	A402	A342	A282	A222	U162	U102	A42
C823	C763	C703	A643	C583	C523	U463	U403	C343	G283	C223	C163	A103	G43
U824	A764	A704	A644	C584	C524	U464	A404	A344	U284	U224	C164	A104	A44
C825	C765	A705	A645	G585	U525	C465	U405	A345	G285	C225	A165	C105	G45
A826	U766	U706	U646	A586	A526	A466	A406	A346	U286	A226	U166	C106	G46
U827	C767	C707	G647	C587	C527	C467	G407	A347	G287	A227	A167	G107	C47
C828	U768	C708	G648	U588	A528	C468	C408	A348	U288	C228	G168	C108	A48
C829	A769	C709	U649	U589	A529	C469	C409	U349	G289	C229	G169	C109	A49
G830	C770	C650	A650	G590	C630	A470	G410	C350	U290	G230	U170	U110	G50
C831	C771	G711	C511	C531	A531	A471	C411	C351	G291	A231	U171	A111	G51
U832	C772	G712	U652	A592	A532	A472	A412	A352	U292	G232	A172	U112	A52
C833	C773	G713	C513	U593	G533	C473	C413	C353	U293	A233	A173	U113	A53
A834	C774	U714	A654	U594	U534	C474	C414	A354	A294	U234	U174	U114	G54
C835	C775	A715	A655	C595	G535	C475	C415	U355	G295	U235	G175	C115	G55
C836	C776	U716	G656	U596	C636	A476	U416	C356	U296	C236	G176	A116	A56
C837	C777	U717	U657	G597	G537	A477	C417	C357	G297	C237	G177	A117	C57
C838	C778	A718	U658	U598	A538	A478	C418	U358	G298	C238	G178	A118	G58
U839	U779	C719	G659	A599	C639	A479	U419	G359	A299	C239	C179	U119	U59
C840	C780	U720	C660	C500	A540	A480	C420	U360	A300	C240	G180	C60	G60

A1801	G1741	G1681	U1821	C1561	G1501	G1441	G1381	A1321	G1261	U1201	U1141	U1081	A1021	C961	C801	G841
A1802	U1742	G1682	G1622	U1562	A1502	U1442	G1382	A1322	A1262	G1202	A1142	U1082	G1022	G962	C902	U842
A1803	G1743	U1683	G1623	U1563	A1503	U1443	A1383	C1323	U1263	U1203	A1143	U1083	U1023	U963	C903	G843
A1804	U1744	G1684	G1624	U1564	A1504	U1444	A1384	A1324	A1264	A1204	A1144	A1084	G1024	G964	G904	A844
A1805	A1745	C1685	G1625	C1565	A1505	U1445	A1385	U1325	A1265	A1205	C1145	A1085	G1025	C965	A905	A845
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A1810	A1750	A1690	A1630	A1570	G1510	U1450	U1390	C1330	G1270	C1210	A1150	G1090	C1030	U970	A910	U850
A1811	U1751	G1691	G1631	A1571	G1511	U1451	U1391	G1331	G1271	C1211	A1151	G1091	C1031	G971	A911	C851
U1812	C1752	U1692	A1632	A1572	C1512	U1452	A1392	G1332	A1272	G1212	C1152	G1092	A972	C972	C912	U852
G1813	G1633	G1573	G1633	G1573	U1513	U1453	A1393	G1333	U1273	A1213	C1153	G1093	U1033	A973	U913	C853
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C1816	G1756	G1696	U1636	U1576	G1516	U1456	U1396	A1336	A1276	G1216	A1156	A1096	U1036	G976	G916	G856
G1817	A1757	G1697	A1637	C1577	G1517	U1457	U1397	G1337	G1277	U1217	C1157	U1097	G1037	G977	A917	G857
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A1819	A1759	G1699	C1639	U1579	G1519	U1459	C1399	G1339	G1279	U1219	U1159	A1099	A1039	A979	U919	G859
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C1822	A1762	G1702	C1642	C1582	A1522	U1462	U1402	A1342	U1282	U1222	C1162	C1102	G1042	C982	C922	G862
G1823	G1703	G1703	G1643	A1583	C1523	U1463	A1403	A1343	G1283	G1223	G1163	A1103	C1043	G983	G923	A863
A1824	C1764	U1704	A1644	U1584	G1524	U1464	C1404	U1344	A1284	U1224	C1164	C1104	C1044	A984	G924	G864
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C1832	A1772	C1592	A1652	C1592	A1532	U1472	U1412	U1352	C1292	G1232	C1172	G1112	C1052	C992	U932	U872
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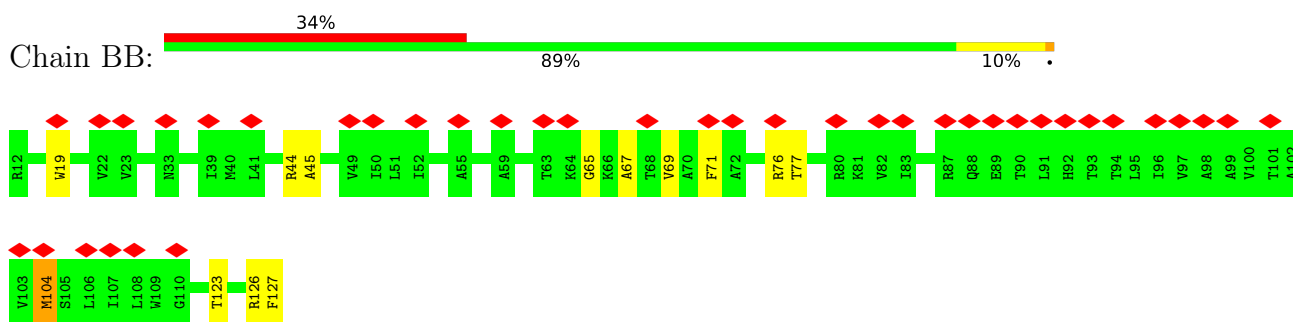
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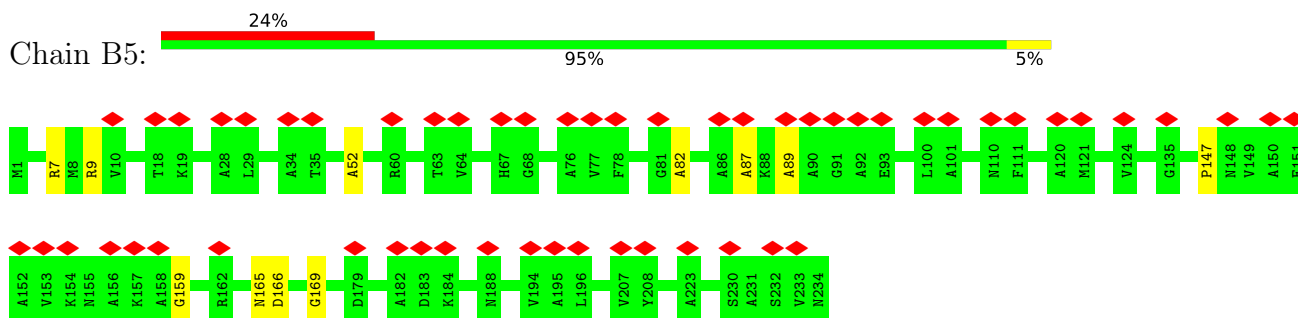
• Molecule 28: Preprotein translocase secY subunit



• Molecule 29: Preprotein translocase secE subunit

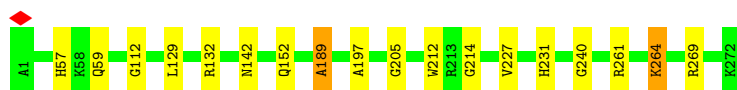


• Molecule 30: 50S ribosomal protein L1



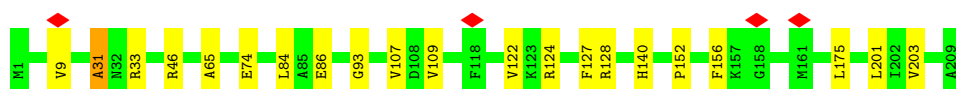
- Molecule 31: 50S ribosomal protein L2

Chain B6:  93% 6% .



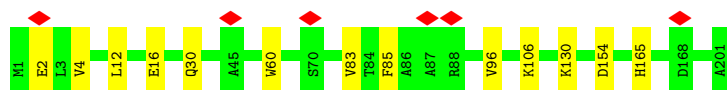
- Molecule 32: 50S ribosomal protein L3

Chain BD:  90% 10% .



- Molecule 33: 50S ribosomal protein L4

Chain BE:  94% 6% .



- Molecule 34: 50S ribosomal protein L5

Chain BF:  90% 9% .




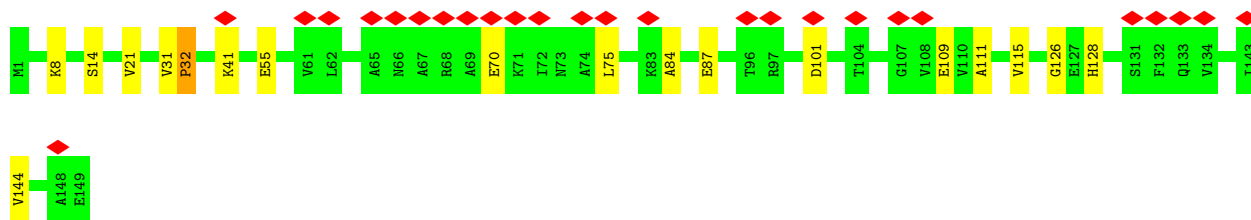
- Molecule 35: 50S ribosomal protein L6

Chain BG:  93% 7% .



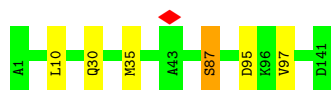
- Molecule 36: 50S ribosomal protein L9

Chain BH:  17% 88% 11% .



- Molecule 37: 50S ribosomal protein L11

Chain BI:  96% . .



- Molecule 38: 50S ribosomal protein L13

Chain BJ:  95% 5%



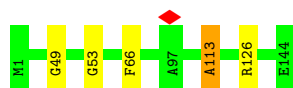
- Molecule 39: 50S ribosomal protein L14

Chain BK:  91% 9%



- Molecule 40: 50S ribosomal protein L15

Chain BL:  97% . .




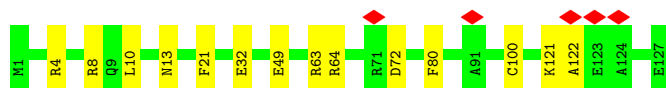
- Molecule 41: 50S ribosomal protein L16

Chain BM:  92% 7% .



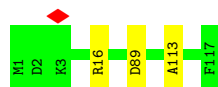
- Molecule 42: 50S ribosomal protein L17

Chain BN:  89% 11%



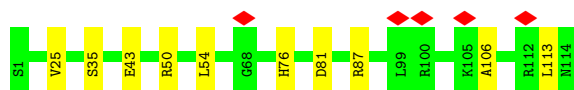
- Molecule 43: 50S ribosomal protein L18

Chain BO:  97% .



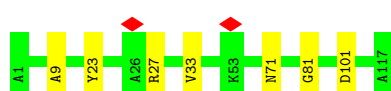
- Molecule 44: 50S ribosomal protein L19

Chain BP:  91% 9%



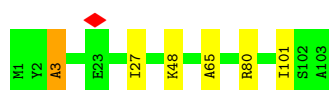
- Molecule 45: 50S ribosomal protein L20

Chain BQ:  94% 6%



- Molecule 46: 50S ribosomal protein L21

Chain BR:  94% 5%



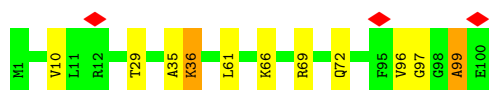
- Molecule 47: 50S ribosomal protein L22

Chain BS:  92% 7%



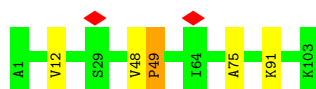
- Molecule 48: 50S ribosomal protein L23

Chain BT:  89% 9%



- Molecule 49: 50S ribosomal protein L24

Chain BU:  95%



- Molecule 50: 50S ribosomal protein L25

Chain BV:  98%



- Molecule 51: 50S ribosomal protein L27

Chain BW: 94% 6%



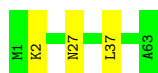
- Molecule 52: 50S ribosomal protein L28

Chain BX: 91% 9%



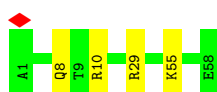
- Molecule 53: 50S ribosomal protein L29

Chain BY: 95% 5%



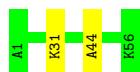
- Molecule 54: 50S ribosomal protein L30

Chain BZ: 93% 7%



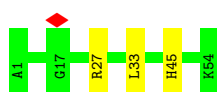
- Molecule 55: 50S ribosomal protein L32

Chain B0: 96%



- Molecule 56: 50S ribosomal protein L33

Chain B1: 94% 6%



- Molecule 57: 50S ribosomal protein L34

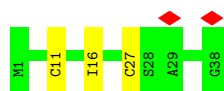
Chain B2: 87% 11%



- Molecule 58: 50S ribosomal protein L35



- Molecule 59: 50S ribosomal protein L36



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	85664	Depositor
Resolution determination method	Not provided	
CTF correction method	DEFOCUS GROUP VOLUMES	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	22	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	38000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	6.823	Depositor
Minimum map value	-3.534	Depositor
Average map value	0.051	Depositor
Map value standard deviation	0.456	Depositor
Recommended contour level	0.5	Depositor
Map size ( $\text{\AA}$ )	396, 396, 396	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90, 90, 90	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.2375, 1.2375, 1.2375	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PEV, 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	AA	1.60	46/37039 (0.1%)	2.50	4339/57778 (7.5%)
2	AX	1.56	0/256	2.32	28/394 (7.1%)
3	AV	1.61	1/1842 (0.1%)	2.43	211/2870 (7.4%)
4	AZ	0.98	0/795	1.16	0/1082
5	A0	0.96	1/1667 (0.1%)	0.95	3/2240 (0.1%)
5	A1	0.97	1/1667 (0.1%)	0.95	0/2240
6	AB	0.92	0/1904	0.98	1/2565 (0.0%)
7	AC	1.00	0/1852	1.06	1/2490 (0.0%)
8	AD	1.04	0/1665	0.99	0/2227
9	AE	0.97	0/1239	1.03	0/1664
10	AF	0.99	0/1121	1.06	0/1509
11	AG	1.03	0/1422	1.01	2/1908 (0.1%)
12	AH	0.96	0/989	1.01	0/1326
13	AI	1.12	0/1048	1.01	0/1394
14	AJ	1.03	0/835	1.03	0/1127
15	AK	1.05	0/982	1.05	0/1323
16	AL	1.07	0/969	1.01	0/1300
17	AM	1.05	0/919	0.99	1/1226 (0.1%)
18	AN	1.07	0/817	1.05	1/1088 (0.1%)
19	AO	1.06	0/724	0.92	0/966
20	AP	1.07	0/659	1.03	0/884
21	AQ	0.99	0/681	1.05	0/913
22	AR	1.14	0/637	1.05	2/851 (0.2%)
23	AS	0.96	0/744	0.96	0/995
24	AT	0.96	0/676	0.94	0/895
25	AU	1.18	0/598	0.99	0/792
26	B7	1.59	2/2873 (0.1%)	2.49	325/4478 (7.3%)
27	B8	1.60	100/69822 (0.1%)	2.50	8171/108926 (7.5%)
28	BA	1.68	7/3439 (0.2%)	1.14	15/4662 (0.3%)
29	BB	0.98	1/902 (0.1%)	1.05	1/1228 (0.1%)
30	B5	0.92	0/1748	0.97	0/2355
31	B6	1.04	0/2131	1.03	1/2863 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	BD	0.97	0/1586	1.08	4/2134 (0.2%)
33	BE	0.95	0/1571	1.01	2/2113 (0.1%)
34	BF	1.01	0/1444	1.06	1/1937 (0.1%)
35	BG	0.96	0/1343	1.06	4/1816 (0.2%)
36	BH	0.93	0/1122	1.05	0/1515
37	BI	0.86	0/1046	1.00	1/1410 (0.1%)
38	BJ	0.97	0/1152	1.01	0/1551
39	BK	1.03	0/956	1.03	0/1279
40	BL	1.04	0/1062	0.98	1/1413 (0.1%)
41	BM	1.03	0/1093	1.06	2/1460 (0.1%)
42	BN	1.10	0/1021	1.03	1/1364 (0.1%)
43	BO	1.07	0/910	0.98	0/1219
44	BP	1.06	0/929	1.03	0/1242
45	BQ	1.09	0/960	1.00	2/1278 (0.2%)
46	BR	1.01	0/829	1.07	1/1107 (0.1%)
47	BS	0.99	0/864	1.04	1/1156 (0.1%)
48	BT	0.98	0/794	1.09	1/1060 (0.1%)
49	BU	0.96	0/797	1.04	0/1062
50	BV	0.96	0/766	1.02	0/1025
51	BW	1.04	0/642	1.05	0/848
52	BX	1.09	0/635	1.04	0/848
53	BY	1.00	0/510	0.90	0/677
54	BZ	0.99	0/453	0.99	0/605
55	B0	1.05	0/450	0.97	0/599
56	B1	0.93	0/448	1.01	0/594
57	B2	1.25	0/380	1.06	0/498
58	B3	0.98	0/513	0.98	0/676
59	B4	1.20	2/303 (0.7%)	1.03	0/397
All	All	1.44	161/169241 (0.1%)	2.16	13123/251442 (5.2%)

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	AA	0	72
3	AV	0	2
5	A1	0	1
7	AC	0	1
12	AH	0	1
13	AI	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
26	B7	0	2
27	B8	0	100
28	BA	0	5
34	BF	0	1
36	BH	0	1
49	BU	0	1
57	B2	0	1
All	All	0	189

The worst 5 of 161 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	BA	416	PHE	CG-CD2	41.52	2.01	1.38
28	BA	416	PHE	CG-CD1	39.62	1.98	1.38
28	BA	416	PHE	CE2-CZ	30.78	1.95	1.37
28	BA	416	PHE	CE1-CZ	30.54	1.95	1.37
28	BA	416	PHE	CD2-CE2	27.89	1.95	1.39

The worst 5 of 13123 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	85	U	P-O3'-C3'	19.51	143.11	119.70
27	B8	670	A	P-O3'-C3'	17.35	140.52	119.70
27	B8	2076	U	P-O3'-C3'	15.69	138.53	119.70
27	B8	6	A	N1-C6-N6	14.72	127.43	118.60
1	AA	1252	A	N1-C6-N6	14.43	127.26	118.60

There are no chirality outliers.

5 of 189 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	102	G	Sidechain
1	AA	115	G	Sidechain
1	AA	13	U	Sidechain
1	AA	69	G	Sidechain
1	AA	95	C	Sidechain

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

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	33080	0	16649	21	0
2	AX	231	0	120	0	0
3	AV	1649	0	834	1	0
4	AZ	779	0	798	4	0
5	A0	1640	0	1641	0	0
5	A1	1640	0	1641	0	0
6	AB	1872	0	1885	3	0
7	AC	1822	0	1913	2	0
8	AD	1643	0	1710	1	0
9	AE	1225	0	1273	1	0
10	AF	1101	0	1050	1	0
11	AG	1400	0	1449	0	0
12	AH	979	0	1034	1	0
13	AI	1036	0	1084	0	0
14	AJ	825	0	865	2	0
15	AK	965	0	997	0	0
16	AL	955	0	1019	2	0
17	AM	910	0	981	0	0
18	AN	805	0	847	1	0
19	AO	716	0	742	0	0
20	AP	649	0	666	2	0
21	AQ	672	0	716	1	0
22	AR	626	0	651	0	0
23	AS	727	0	769	0	0
24	AT	670	0	722	2	0
25	AU	590	0	631	1	0
26	B7	2570	0	1301	0	0
27	B8	62341	0	31354	41	0
28	BA	3362	0	3511	38	0
29	BB	889	0	982	1	0
30	B5	1733	0	1824	1	0
31	B6	2092	0	2170	2	0
32	BD	1565	0	1616	1	0
33	BE	1552	0	1619	1	0
34	BF	1420	0	1460	1	0
35	BG	1323	0	1374	0	0
36	BH	1111	0	1148	2	0
37	BI	1032	0	1088	0	0
38	BJ	1129	0	1162	0	0
39	BK	947	0	1023	0	0
40	BL	1053	0	1129	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	BM	1074	0	1157	1	0
42	BN	1008	0	1045	1	0
43	BO	900	0	935	0	0
44	BP	917	0	965	0	0
45	BQ	947	0	1022	0	0
46	BR	816	0	839	1	0
47	BS	857	0	922	0	0
48	BT	787	0	846	0	0
49	BU	789	0	847	0	0
50	BV	753	0	780	0	0
51	BW	634	0	656	0	0
52	BX	625	0	655	0	0
53	BY	509	0	543	0	0
54	BZ	449	0	491	0	0
55	B0	444	0	461	0	0
56	B1	441	0	485	2	0
57	B2	377	0	418	1	0
58	B3	504	0	574	1	0
59	B4	302	0	343	0	0
60	A0	1078	0	1694	1	0
60	A1	1225	0	1925	4	0
60	AZ	245	0	385	0	0
60	B8	294	0	462	2	0
60	BA	1568	0	2464	34	0
60	BB	539	0	847	0	0
61	A0	510	0	760	0	0
61	A1	204	0	304	2	0
61	AZ	102	0	152	0	0
61	B8	51	0	76	0	0
61	BA	408	0	608	1	0
61	BB	357	0	532	0	0
All	All	163040	0	119641	141	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 0.

The worst 5 of 141 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)
28:BA:416:PHE:CD1	28:BA:416:PHE:CE1	1.92	1.58
28:BA:416:PHE:CD2	28:BA:416:PHE:CE2	1.95	1.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:BA:416:PHE:CE2	28:BA:416:PHE:CZ	1.95	1.53
28:BA:416:PHE:CE1	28:BA:416:PHE:CZ	1.95	1.51
28:BA:416:PHE:CD1	28:BA:416:PHE:CG	1.98	1.49

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 PDB entries followed by that with respect to all EM entries.

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	
4	AZ	96/98 (98%)	74 (77%)	13 (14%)	9 (9%)	0	10
5	A0	198/200 (99%)	174 (88%)	20 (10%)	4 (2%)	7	38
5	A1	198/200 (99%)	169 (85%)	23 (12%)	6 (3%)	4	28
6	AB	238/240 (99%)	190 (80%)	42 (18%)	6 (2%)	5	32
7	AC	230/232 (99%)	184 (80%)	31 (14%)	15 (6%)	1	16
8	AD	203/205 (99%)	163 (80%)	28 (14%)	12 (6%)	1	17
9	AE	164/166 (99%)	137 (84%)	21 (13%)	6 (4%)	3	24
10	AF	133/135 (98%)	109 (82%)	22 (16%)	2 (2%)	10	46
11	AG	176/178 (99%)	142 (81%)	29 (16%)	5 (3%)	5	30
12	AH	127/129 (98%)	102 (80%)	23 (18%)	2 (2%)	9	44
13	AI	127/129 (98%)	108 (85%)	11 (9%)	8 (6%)	1	17
14	AJ	101/103 (98%)	85 (84%)	9 (9%)	7 (7%)	1	15
15	AK	126/128 (98%)	106 (84%)	15 (12%)	5 (4%)	3	23
16	AL	121/123 (98%)	108 (89%)	12 (10%)	1 (1%)	19	60
17	AM	115/117 (98%)	96 (84%)	13 (11%)	6 (5%)	2	19
18	AN	98/100 (98%)	81 (83%)	9 (9%)	8 (8%)	1	12
19	AO	86/88 (98%)	79 (92%)	5 (6%)	2 (2%)	6	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	AP	80/82 (98%)	73 (91%)	5 (6%)	2 (2%)	5	32
21	AQ	81/83 (98%)	67 (83%)	8 (10%)	6 (7%)	1	13
22	AR	72/74 (97%)	59 (82%)	9 (12%)	4 (6%)	2	18
23	AS	89/91 (98%)	73 (82%)	12 (14%)	4 (4%)	2	22
24	AT	84/86 (98%)	76 (90%)	7 (8%)	1 (1%)	13	50
25	AU	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
28	BA	433/435 (100%)	313 (72%)	66 (15%)	54 (12%)	0	5
29	BB	114/116 (98%)	96 (84%)	12 (10%)	6 (5%)	2	19
30	B5	232/234 (99%)	211 (91%)	15 (6%)	6 (3%)	5	31
31	B6	270/272 (99%)	227 (84%)	31 (12%)	12 (4%)	2	22
32	BD	207/209 (99%)	172 (83%)	24 (12%)	11 (5%)	2	19
33	BE	199/201 (99%)	169 (85%)	20 (10%)	10 (5%)	2	20
34	BF	176/178 (99%)	137 (78%)	27 (15%)	12 (7%)	1	15
35	BG	174/176 (99%)	137 (79%)	28 (16%)	9 (5%)	2	19
36	BH	147/149 (99%)	108 (74%)	31 (21%)	8 (5%)	2	19
37	BI	139/141 (99%)	125 (90%)	11 (8%)	3 (2%)	6	35
38	BJ	140/142 (99%)	117 (84%)	19 (14%)	4 (3%)	4	29
39	BK	121/123 (98%)	99 (82%)	16 (13%)	6 (5%)	2	20
40	BL	142/144 (99%)	129 (91%)	10 (7%)	3 (2%)	7	36
41	BM	134/136 (98%)	107 (80%)	17 (13%)	10 (8%)	1	13
42	BN	125/127 (98%)	104 (83%)	12 (10%)	9 (7%)	1	14
43	BO	115/117 (98%)	97 (84%)	15 (13%)	3 (3%)	5	31
44	BP	112/114 (98%)	94 (84%)	11 (10%)	7 (6%)	1	17
45	BQ	115/117 (98%)	94 (82%)	15 (13%)	6 (5%)	2	19
46	BR	101/103 (98%)	83 (82%)	13 (13%)	5 (5%)	2	20
47	BS	108/110 (98%)	81 (75%)	18 (17%)	9 (8%)	1	12
48	BT	98/100 (98%)	71 (72%)	20 (20%)	7 (7%)	1	14
49	BU	101/103 (98%)	84 (83%)	14 (14%)	3 (3%)	4	28
50	BV	92/94 (98%)	82 (89%)	9 (10%)	1 (1%)	14	52
51	BW	82/84 (98%)	59 (72%)	19 (23%)	4 (5%)	2	20
52	BX	75/77 (97%)	57 (76%)	12 (16%)	6 (8%)	1	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	BY	61/63 (97%)	48 (79%)	11 (18%)	2 (3%)	4	26
54	BZ	56/58 (97%)	49 (88%)	4 (7%)	3 (5%)	2	19
55	B0	54/56 (96%)	47 (87%)	6 (11%)	1 (2%)	8	38
56	B1	52/54 (96%)	46 (88%)	5 (10%)	1 (2%)	8	38
57	B2	44/46 (96%)	31 (70%)	10 (23%)	3 (7%)	1	15
58	B3	62/64 (97%)	52 (84%)	9 (14%)	1 (2%)	9	44
59	B4	36/38 (95%)	32 (89%)	3 (8%)	1 (3%)	5	30
All	All	7128/7238 (98%)	5877 (82%)	904 (13%)	347 (5%)	4	20

5 of 347 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	AZ	48	TRP
4	AZ	61	VAL
4	AZ	81	LEU
5	A1	177	ARG
7	AC	206	ILE

### 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 PDB entries followed by that with respect to all EM entries.

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	
4	AZ	85/85 (100%)	72 (85%)	13 (15%)	2	14
5	A0	176/176 (100%)	174 (99%)	2 (1%)	73	84
5	A1	176/176 (100%)	173 (98%)	3 (2%)	60	78
6	AB	198/198 (100%)	194 (98%)	4 (2%)	55	74
7	AC	189/189 (100%)	183 (97%)	6 (3%)	39	61
8	AD	172/172 (100%)	166 (96%)	6 (4%)	36	59
9	AE	125/125 (100%)	122 (98%)	3 (2%)	49	69
10	AF	116/116 (100%)	111 (96%)	5 (4%)	29	53
11	AG	146/146 (100%)	146 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	AH	104/104 (100%)	101 (97%)	3 (3%)	42	64
13	AI	106/106 (100%)	101 (95%)	5 (5%)	26	51
14	AJ	90/90 (100%)	88 (98%)	2 (2%)	52	71
15	AK	98/98 (100%)	95 (97%)	3 (3%)	40	62
16	AL	103/103 (100%)	102 (99%)	1 (1%)	76	86
17	AM	95/95 (100%)	92 (97%)	3 (3%)	39	61
18	AN	83/83 (100%)	81 (98%)	2 (2%)	49	69
19	AO	76/76 (100%)	74 (97%)	2 (3%)	46	66
20	AP	65/65 (100%)	65 (100%)	0	100	100
21	AQ	77/77 (100%)	74 (96%)	3 (4%)	32	56
22	AR	64/64 (100%)	63 (98%)	1 (2%)	62	79
23	AS	78/78 (100%)	78 (100%)	0	100	100
24	AT	65/65 (100%)	65 (100%)	0	100	100
25	AU	60/60 (100%)	58 (97%)	2 (3%)	38	61
28	BA	353/353 (100%)	326 (92%)	27 (8%)	13	37
29	BB	92/92 (100%)	88 (96%)	4 (4%)	29	53
30	B5	181/181 (100%)	178 (98%)	3 (2%)	60	78
31	B6	217/217 (100%)	212 (98%)	5 (2%)	50	70
32	BD	164/164 (100%)	158 (96%)	6 (4%)	34	58
33	BE	165/165 (100%)	164 (99%)	1 (1%)	86	92
34	BF	149/149 (100%)	145 (97%)	4 (3%)	44	65
35	BG	137/137 (100%)	134 (98%)	3 (2%)	52	71
36	BH	114/114 (100%)	108 (95%)	6 (5%)	22	47
37	BI	109/109 (100%)	106 (97%)	3 (3%)	43	65
38	BJ	116/116 (100%)	113 (97%)	3 (3%)	46	66
39	BK	104/104 (100%)	99 (95%)	5 (5%)	25	50
40	BL	103/103 (100%)	102 (99%)	1 (1%)	76	86
41	BM	109/109 (100%)	109 (100%)	0	100	100
42	BN	103/103 (100%)	100 (97%)	3 (3%)	42	64
43	BO	87/87 (100%)	87 (100%)	0	100	100
44	BP	99/99 (100%)	96 (97%)	3 (3%)	41	63

*Continued on next page...*

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	BQ	89/89 (100%)	89 (100%)	0	100	100
46	BR	84/84 (100%)	84 (100%)	0	100	100
47	BS	93/93 (100%)	93 (100%)	0	100	100
48	BT	84/84 (100%)	79 (94%)	5 (6%)	19	44
49	BU	84/84 (100%)	82 (98%)	2 (2%)	49	69
50	BV	78/78 (100%)	77 (99%)	1 (1%)	69	81
51	BW	62/62 (100%)	61 (98%)	1 (2%)	62	79
52	BX	67/67 (100%)	66 (98%)	1 (2%)	65	80
53	BY	55/55 (100%)	54 (98%)	1 (2%)	59	77
54	BZ	48/48 (100%)	47 (98%)	1 (2%)	53	72
55	B0	47/47 (100%)	46 (98%)	1 (2%)	53	72
56	B1	48/48 (100%)	47 (98%)	1 (2%)	53	72
57	B2	38/38 (100%)	37 (97%)	1 (3%)	46	66
58	B3	51/51 (100%)	50 (98%)	1 (2%)	55	74
59	B4	34/34 (100%)	34 (100%)	0	100	100
All	All	5911/5911 (100%)	5749 (97%)	162 (3%)	48	65

5 of 162 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
34	BF	80	GLN
44	BP	43	GLU
35	BG	34	ARG
37	BI	95	ASP
48	BT	96	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
36	BH	20	ASN
42	BN	16	HIS
36	BH	128	HIS
38	BJ	132	HIS
45	BQ	13	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1541/1542 (99%)	273 (17%)	23 (1%)
2	AX	10/11 (90%)	5 (50%)	0
26	B7	119/120 (99%)	19 (15%)	2 (1%)
27	B8	2903/2904 (99%)	442 (15%)	47 (1%)
3	AV	76/77 (98%)	14 (18%)	1 (1%)
All	All	4649/4654 (99%)	753 (16%)	73 (1%)

5 of 753 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	2	A
1	AA	5	U
1	AA	7	A
1	AA	9	G
1	AA	15	G

5 of 73 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
27	B8	2159	G
27	B8	2797	U
27	B8	2172	U
27	B8	2425	A
26	B7	14	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

133 ligands 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
60	PEV	A0	316	-	48,48,48	0.80	1 (2%)	51,53,53	0.84	2 (3%)
60	PEV	A0	322	-	48,48,48	0.79	1 (2%)	51,53,53	0.74	2 (3%)
60	PEV	AZ	201	-	48,48,48	0.75	1 (2%)	51,53,53	0.70	2 (3%)
60	PEV	A0	329	-	48,48,48	0.78	1 (2%)	51,53,53	0.72	2 (3%)
61	PGV	BA	515	-	50,50,50	1.05	2 (4%)	53,56,56	0.73	2 (3%)
61	PGV	A0	331	-	50,50,50	1.04	2 (4%)	53,56,56	0.77	2 (3%)
60	PEV	A1	304	-	48,48,48	0.77	1 (2%)	51,53,53	0.63	2 (3%)
60	PEV	BA	530	-	48,48,48	0.77	1 (2%)	51,53,53	0.67	2 (3%)
60	PEV	A1	321	-	48,48,48	0.78	1 (2%)	51,53,53	0.67	2 (3%)
60	PEV	A0	311	-	48,48,48	0.78	1 (2%)	51,53,53	0.67	2 (3%)
61	PGV	A0	305	-	50,50,50	1.04	2 (4%)	53,56,56	0.73	2 (3%)
60	PEV	BB	211	-	48,48,48	0.77	1 (2%)	51,53,53	0.73	2 (3%)
60	PEV	BA	520	-	48,48,48	0.78	1 (2%)	51,53,53	0.64	2 (3%)
60	PEV	BB	214	-	48,48,48	0.78	1 (2%)	51,53,53	0.71	2 (3%)
60	PEV	BB	210	-	48,48,48	0.77	1 (2%)	51,53,53	0.72	2 (3%)
60	PEV	A0	309	-	48,48,48	0.79	1 (2%)	51,53,53	0.70	2 (3%)
60	PEV	BA	506	-	48,48,48	0.75	1 (2%)	51,53,53	0.70	2 (3%)
60	PEV	A1	323	-	48,48,48	0.76	1 (2%)	51,53,53	0.66	2 (3%)
61	PGV	BB	207	-	50,50,50	1.06	2 (4%)	53,56,56	0.77	2 (3%)
60	PEV	A1	302	-	48,48,48	0.79	1 (2%)	51,53,53	0.71	2 (3%)
60	PEV	A1	301	-	48,48,48	0.78	2 (4%)	51,53,53	0.71	2 (3%)
60	PEV	A1	328	-	48,48,48	0.76	1 (2%)	51,53,53	0.68	2 (3%)
60	PEV	A1	319	-	48,48,48	0.77	1 (2%)	51,53,53	0.65	1 (1%)
60	PEV	B8	3004	-	48,48,48	0.78	1 (2%)	51,53,53	0.70	2 (3%)
60	PEV	BB	218	-	48,48,48	0.77	1 (2%)	51,53,53	0.70	2 (3%)
60	PEV	B8	3006	-	48,48,48	0.78	1 (2%)	51,53,53	0.67	2 (3%)
60	PEV	A0	313	-	48,48,48	0.80	1 (2%)	51,53,53	0.74	2 (3%)
60	PEV	BB	215	-	48,48,48	0.76	1 (2%)	51,53,53	0.69	2 (3%)
60	PEV	A1	313	-	48,48,48	0.77	1 (2%)	51,53,53	0.73	2 (3%)
60	PEV	BA	526	-	48,48,48	0.77	1 (2%)	51,53,53	0.69	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
61	PGV	A0	328	-	50,50,50	1.05	2 (4%)	53,56,56	0.76	2 (3%)
60	PEV	BA	539	-	48,48,48	0.78	1 (2%)	51,53,53	0.79	2 (3%)
60	PEV	A0	330	-	48,48,48	0.78	1 (2%)	51,53,53	0.65	2 (3%)
60	PEV	AZ	203	-	48,48,48	0.77	1 (2%)	51,53,53	0.63	2 (3%)
60	PEV	BB	216	-	48,48,48	0.78	1 (2%)	51,53,53	0.77	2 (3%)
60	PEV	BB	201	-	48,48,48	0.79	1 (2%)	51,53,53	0.70	2 (3%)
60	PEV	BA	529	-	48,48,48	0.80	1 (2%)	51,53,53	0.70	2 (3%)
61	PGV	A1	311	-	50,50,50	1.06	2 (4%)	53,56,56	0.80	2 (3%)
60	PEV	B8	3003	-	48,48,48	0.79	1 (2%)	51,53,53	0.71	2 (3%)
60	PEV	BA	504	-	48,48,48	0.79	1 (2%)	51,53,53	0.80	2 (3%)
61	PGV	BA	501	-	50,50,50	1.05	2 (4%)	53,56,56	0.81	2 (3%)
61	PGV	BA	512	-	50,50,50	1.04	2 (4%)	53,56,56	0.75	2 (3%)
61	PGV	A0	332	-	50,50,50	1.06	2 (4%)	53,56,56	0.76	2 (3%)
61	PGV	BA	505	-	50,50,50	1.05	2 (4%)	53,56,56	0.77	2 (3%)
60	PEV	BB	202	-	48,48,48	0.78	1 (2%)	51,53,53	0.71	2 (3%)
60	PEV	A1	308	-	48,48,48	0.79	1 (2%)	51,53,53	0.65	2 (3%)
60	PEV	A1	314	-	48,48,48	0.78	1 (2%)	51,53,53	0.69	2 (3%)
60	PEV	A1	309	-	48,48,48	0.78	1 (2%)	51,53,53	0.74	2 (3%)
60	PEV	A1	329	-	48,48,48	0.78	1 (2%)	51,53,53	0.72	2 (3%)
60	PEV	AZ	202	-	48,48,48	0.77	1 (2%)	51,53,53	0.72	2 (3%)
60	PEV	BA	535	-	48,48,48	0.78	1 (2%)	51,53,53	0.67	2 (3%)
60	PEV	B8	3007	-	48,48,48	0.77	1 (2%)	51,53,53	0.64	2 (3%)
60	PEV	A1	310	-	48,48,48	0.77	1 (2%)	51,53,53	0.72	2 (3%)
60	PEV	A1	316	-	48,48,48	0.78	1 (2%)	51,53,53	0.74	2 (3%)
60	PEV	A0	321	-	48,48,48	0.79	1 (2%)	51,53,53	0.81	3 (5%)
60	PEV	A0	315	-	48,48,48	0.76	1 (2%)	51,53,53	0.64	2 (3%)
61	PGV	BB	205	-	50,50,50	1.05	2 (4%)	53,56,56	0.80	2 (3%)
60	PEV	B8	3001	-	48,48,48	0.79	1 (2%)	51,53,53	0.71	2 (3%)
60	PEV	A1	320	-	48,48,48	0.79	1 (2%)	51,53,53	0.71	2 (3%)
61	PGV	A0	306	-	50,50,50	1.05	2 (4%)	53,56,56	0.75	2 (3%)
61	PGV	A0	304	-	50,50,50	1.06	2 (4%)	53,56,56	0.81	2 (3%)
60	PEV	BA	502	-	48,48,48	0.77	1 (2%)	51,53,53	0.70	2 (3%)
60	PEV	BA	537	-	48,48,48	0.80	2 (4%)	51,53,53	0.74	2 (3%)
60	PEV	BB	206	-	48,48,48	0.78	1 (2%)	51,53,53	0.70	2 (3%)
61	PGV	A1	303	-	50,50,50	1.05	2 (4%)	53,56,56	0.75	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
60	PEV	A1	327	-	48,48,48	0.76	1 (2%)	51,53,53	0.69	2 (3%)
60	PEV	AZ	204	-	48,48,48	0.78	1 (2%)	51,53,53	0.67	2 (3%)
60	PEV	A1	322	-	48,48,48	0.76	1 (2%)	51,53,53	0.69	2 (3%)
60	PEV	BA	528	-	48,48,48	0.78	1 (2%)	51,53,53	0.73	2 (3%)
61	PGV	BA	536	-	50,50,50	1.05	2 (4%)	53,56,56	0.73	2 (3%)
61	PGV	BB	213	-	50,50,50	1.06	2 (4%)	53,56,56	0.81	2 (3%)
60	PEV	BA	532	-	48,48,48	0.76	1 (2%)	51,53,53	0.74	2 (3%)
60	PEV	A1	317	-	48,48,48	0.79	2 (4%)	51,53,53	0.69	2 (3%)
61	PGV	BB	203	-	50,50,50	1.06	2 (4%)	53,56,56	0.76	2 (3%)
60	PEV	BA	525	-	48,48,48	0.79	1 (2%)	51,53,53	0.74	2 (3%)
61	PGV	BB	208	-	50,50,50	1.06	2 (4%)	53,56,56	0.74	2 (3%)
60	PEV	A1	324	-	48,48,48	0.78	1 (2%)	51,53,53	0.64	2 (3%)
60	PEV	BA	521	-	48,48,48	0.78	1 (2%)	51,53,53	0.67	2 (3%)
61	PGV	A0	327	-	50,50,50	1.06	2 (4%)	53,56,56	0.71	2 (3%)
60	PEV	BA	524	-	48,48,48	0.80	1 (2%)	51,53,53	0.70	2 (3%)
60	PEV	A1	325	-	48,48,48	0.78	1 (2%)	51,53,53	0.66	2 (3%)
60	PEV	BA	531	-	48,48,48	0.77	1 (2%)	51,53,53	0.66	2 (3%)
60	PEV	BA	507	-	48,48,48	0.78	1 (2%)	51,53,53	0.69	2 (3%)
61	PGV	BA	516	-	50,50,50	1.06	2 (4%)	53,56,56	0.70	2 (3%)
61	PGV	BA	522	-	50,50,50	1.06	2 (4%)	53,56,56	0.71	2 (3%)
61	PGV	AZ	207	-	50,50,50	1.05	2 (4%)	53,56,56	0.76	2 (3%)
61	PGV	B8	3005	-	50,50,50	1.05	2 (4%)	53,56,56	0.72	2 (3%)
60	PEV	A0	320	-	48,48,48	0.80	1 (2%)	51,53,53	0.65	2 (3%)
61	PGV	A0	325	-	50,50,50	1.05	2 (4%)	53,56,56	0.86	2 (3%)
60	PEV	BA	533	-	48,48,48	2.69	1 (2%)	51,53,53	1.32	2 (3%)
61	PGV	BA	540	-	50,50,50	1.04	2 (4%)	53,56,56	0.77	2 (3%)
61	PGV	A0	318	-	50,50,50	1.06	2 (4%)	53,56,56	0.74	2 (3%)
60	PEV	BA	514	-	48,48,48	0.80	1 (2%)	51,53,53	0.75	2 (3%)
60	PEV	A0	307	-	48,48,48	0.77	1 (2%)	51,53,53	0.65	2 (3%)
60	PEV	B8	3002	-	48,48,48	0.77	1 (2%)	51,53,53	0.66	2 (3%)
60	PEV	BA	503	-	48,48,48	0.79	1 (2%)	51,53,53	0.74	2 (3%)
61	PGV	A1	315	-	50,50,50	1.07	2 (4%)	53,56,56	0.79	2 (3%)
60	PEV	BA	518	-	48,48,48	0.77	1 (2%)	51,53,53	0.67	2 (3%)
60	PEV	A0	310	-	48,48,48	0.79	1 (2%)	51,53,53	0.82	2 (3%)
60	PEV	BA	519	-	48,48,48	0.78	1 (2%)	51,53,53	0.74	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
61	PGV	BB	204	-	50,50,50	1.06	2 (4%)	53,56,56	0.81	2 (3%)
60	PEV	A0	303	-	48,48,48	0.80	1 (2%)	51,53,53	0.69	2 (3%)
60	PEV	A0	319	-	48,48,48	0.79	1 (2%)	51,53,53	0.75	2 (3%)
60	PEV	BA	538	-	48,48,48	0.75	1 (2%)	51,53,53	0.65	2 (3%)
60	PEV	BA	517	-	48,48,48	0.78	1 (2%)	51,53,53	0.69	2 (3%)
60	PEV	BB	212	-	48,48,48	0.78	1 (2%)	51,53,53	0.66	2 (3%)
60	PEV	A0	314	-	48,48,48	0.80	1 (2%)	51,53,53	0.69	2 (3%)
60	PEV	A0	326	-	48,48,48	0.76	1 (2%)	51,53,53	0.71	2 (3%)
60	PEV	BA	509	-	48,48,48	0.79	1 (2%)	51,53,53	0.75	2 (3%)
60	PEV	AZ	206	-	48,48,48	0.78	1 (2%)	51,53,53	0.61	2 (3%)
60	PEV	A0	324	-	48,48,48	0.79	1 (2%)	51,53,53	0.71	2 (3%)
60	PEV	A0	302	-	48,48,48	0.77	1 (2%)	51,53,53	0.71	2 (3%)
60	PEV	BA	513	-	48,48,48	0.77	1 (2%)	51,53,53	0.68	2 (3%)
60	PEV	BA	510	-	48,48,48	0.77	1 (2%)	51,53,53	0.69	2 (3%)
60	PEV	BA	534	-	48,48,48	0.82	1 (2%)	51,53,53	0.75	2 (3%)
60	PEV	BA	527	-	48,48,48	0.79	1 (2%)	51,53,53	0.76	2 (3%)
60	PEV	A0	323	-	48,48,48	0.77	1 (2%)	51,53,53	0.71	2 (3%)
60	PEV	A1	306	-	48,48,48	0.79	1 (2%)	51,53,53	0.63	2 (3%)
60	PEV	A0	301	-	48,48,48	0.78	1 (2%)	51,53,53	0.68	2 (3%)
60	PEV	A1	305	-	48,48,48	0.78	1 (2%)	51,53,53	0.68	2 (3%)
60	PEV	A0	308	-	48,48,48	0.78	1 (2%)	51,53,53	0.75	2 (3%)
61	PGV	BB	217	-	50,50,50	1.05	2 (4%)	53,56,56	0.76	2 (3%)
60	PEV	A1	326	-	48,48,48	0.76	1 (2%)	51,53,53	0.68	2 (3%)
60	PEV	A0	312	-	48,48,48	0.79	1 (2%)	51,53,53	0.61	2 (3%)
60	PEV	BA	508	-	48,48,48	0.78	1 (2%)	51,53,53	0.68	2 (3%)
60	PEV	BB	209	-	48,48,48	0.76	1 (2%)	51,53,53	0.69	2 (3%)
60	PEV	BA	511	-	48,48,48	0.75	1 (2%)	51,53,53	0.70	2 (3%)
61	PGV	A0	317	-	50,50,50	1.05	2 (4%)	53,56,56	0.84	2 (3%)
61	PGV	A1	318	-	50,50,50	1.06	2 (4%)	53,56,56	0.79	2 (3%)
60	PEV	BA	523	-	48,48,48	0.78	1 (2%)	51,53,53	0.74	2 (3%)
60	PEV	A1	312	-	48,48,48	0.78	1 (2%)	51,53,53	0.68	2 (3%)
61	PGV	AZ	205	-	50,50,50	1.05	2 (4%)	53,56,56	0.76	2 (3%)
60	PEV	A1	307	-	48,48,48	0.78	1 (2%)	51,53,53	0.70	2 (3%)

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
60	PEV	A0	316	-	-	10/52/52/52	-
60	PEV	A0	322	-	-	6/52/52/52	-
60	PEV	AZ	201	-	-	5/52/52/52	-
61	PGV	BA	515	-	2/2/5/7	6/55/55/55	-
60	PEV	A0	329	-	-	4/52/52/52	-
61	PGV	A0	331	-	2/2/5/7	4/55/55/55	-
60	PEV	A1	304	-	-	5/52/52/52	-
60	PEV	BA	530	-	1/1/4/4	11/52/52/52	-
60	PEV	A1	321	-	-	7/52/52/52	-
60	PEV	A0	311	-	-	7/52/52/52	-
61	PGV	A0	305	-	1/1/5/7	10/55/55/55	-
60	PEV	BB	211	-	-	8/52/52/52	-
60	PEV	BA	520	-	-	5/52/52/52	-
60	PEV	BB	214	-	-	8/52/52/52	-
60	PEV	BB	210	-	-	13/52/52/52	-
60	PEV	A0	309	-	-	6/52/52/52	-
60	PEV	BA	506	-	-	5/52/52/52	-
60	PEV	A1	323	-	-	4/52/52/52	-
61	PGV	BB	207	-	2/2/5/7	4/55/55/55	-
60	PEV	A1	302	-	-	10/52/52/52	-
60	PEV	A1	301	-	1/1/4/4	13/52/52/52	-
60	PEV	A1	328	-	-	12/52/52/52	-
60	PEV	A1	319	-	-	4/52/52/52	-
60	PEV	B8	3004	-	-	9/52/52/52	-
60	PEV	BB	218	-	-	9/52/52/52	-
60	PEV	B8	3006	-	-	7/52/52/52	-
60	PEV	A0	313	-	-	5/52/52/52	-
60	PEV	BB	215	-	-	6/52/52/52	-
60	PEV	A1	313	-	1/1/4/4	8/52/52/52	-
60	PEV	BA	526	-	1/1/4/4	5/52/52/52	-
61	PGV	A0	328	-	2/2/5/7	10/55/55/55	-
60	PEV	BA	539	-	-	4/52/52/52	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	PEV	A0	330	-	-	10/52/52/52	-
60	PEV	AZ	203	-	-	8/52/52/52	-
60	PEV	BB	216	-	-	5/52/52/52	-
60	PEV	BB	201	-	-	11/52/52/52	-
60	PEV	BA	529	-	-	4/52/52/52	-
61	PGV	A1	311	-	2/2/5/7	8/55/55/55	-
60	PEV	B8	3003	-	-	15/52/52/52	-
60	PEV	BA	504	-	-	5/52/52/52	-
61	PGV	BA	501	-	1/1/5/7	7/55/55/55	-
61	PGV	BA	512	-	1/1/5/7	10/55/55/55	-
61	PGV	A0	332	-	2/2/5/7	7/55/55/55	-
61	PGV	BA	505	-	2/2/5/7	7/55/55/55	-
60	PEV	BB	202	-	1/1/4/4	3/52/52/52	-
60	PEV	A1	308	-	-	12/52/52/52	-
60	PEV	A1	314	-	-	6/52/52/52	-
60	PEV	A1	309	-	-	6/52/52/52	-
60	PEV	A1	329	-	-	5/52/52/52	-
60	PEV	AZ	202	-	-	8/52/52/52	-
60	PEV	BA	535	-	1/1/4/4	7/52/52/52	-
60	PEV	B8	3007	-	-	3/52/52/52	-
60	PEV	A1	310	-	-	8/52/52/52	-
60	PEV	A1	316	-	-	3/52/52/52	-
60	PEV	A0	321	-	-	11/52/52/52	-
60	PEV	A0	315	-	-	9/52/52/52	-
61	PGV	BB	205	-	2/2/5/7	6/55/55/55	-
60	PEV	B8	3001	-	1/1/4/4	3/52/52/52	-
60	PEV	A1	320	-	-	9/52/52/52	-
61	PGV	A0	306	-	2/2/5/7	7/55/55/55	-
61	PGV	A0	304	-	2/2/5/7	5/55/55/55	-
60	PEV	BA	502	-	1/1/4/4	8/52/52/52	-
60	PEV	BA	537	-	1/1/4/4	9/52/52/52	-
60	PEV	BB	206	-	1/1/4/4	9/52/52/52	-
61	PGV	A1	303	-	2/2/5/7	5/55/55/55	-
60	PEV	A1	327	-	-	7/52/52/52	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	PEV	AZ	204	-	1/1/4/4	8/52/52/52	-
61	PGV	BA	536	-	2/2/5/7	7/55/55/55	-
61	PGV	BB	213	-	1/1/5/7	9/55/55/55	-
60	PEV	A1	322	-	-	4/52/52/52	-
60	PEV	BA	528	-	-	9/52/52/52	-
60	PEV	BA	532	-	-	12/52/52/52	-
60	PEV	A1	317	-	1/1/4/4	9/52/52/52	-
61	PGV	BB	203	-	2/2/5/7	8/55/55/55	-
60	PEV	BA	525	-	-	11/52/52/52	-
61	PGV	BB	208	-	2/2/5/7	8/55/55/55	-
60	PEV	A1	324	-	-	5/52/52/52	-
61	PGV	A0	327	-	2/2/5/7	6/55/55/55	-
60	PEV	BA	521	-	-	8/52/52/52	-
60	PEV	BA	524	-	-	12/52/52/52	-
60	PEV	A1	325	-	-	12/52/52/52	-
60	PEV	BA	531	-	-	3/52/52/52	-
61	PGV	BA	516	-	2/2/5/7	7/55/55/55	-
60	PEV	BA	507	-	-	4/52/52/52	-
61	PGV	BA	522	-	2/2/5/7	2/55/55/55	-
61	PGV	AZ	207	-	2/2/5/7	8/55/55/55	-
61	PGV	B8	3005	-	2/2/5/7	8/55/55/55	-
60	PEV	A0	320	-	-	5/52/52/52	-
61	PGV	A0	325	-	2/2/5/7	8/55/55/55	-
61	PGV	BA	540	-	2/2/5/7	6/55/55/55	-
60	PEV	BA	533	-	-	10/52/52/52	-
61	PGV	A0	318	-	2/2/5/7	9/55/55/55	-
60	PEV	BA	514	-	-	8/52/52/52	-
60	PEV	A0	307	-	-	9/52/52/52	-
60	PEV	B8	3002	-	-	4/52/52/52	-
61	PGV	A1	315	-	2/2/5/7	13/55/55/55	-
60	PEV	BA	503	-	-	11/52/52/52	-
60	PEV	BA	518	-	-	9/52/52/52	-
60	PEV	A0	310	-	-	5/52/52/52	-
60	PEV	BA	519	-	-	11/52/52/52	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	PGV	BB	204	-	2/2/5/7	10/55/55/55	-
60	PEV	A0	303	-	-	7/52/52/52	-
60	PEV	BA	538	-	1/1/4/4	9/52/52/52	-
60	PEV	A0	319	-	-	8/52/52/52	-
60	PEV	BA	517	-	-	5/52/52/52	-
60	PEV	BB	212	-	-	6/52/52/52	-
60	PEV	A0	314	-	1/1/4/4	8/52/52/52	-
60	PEV	A0	326	-	-	9/52/52/52	-
60	PEV	BA	509	-	-	13/52/52/52	-
60	PEV	AZ	206	-	-	4/52/52/52	-
60	PEV	A0	324	-	-	7/52/52/52	-
60	PEV	A0	302	-	-	8/52/52/52	-
60	PEV	BA	513	-	-	7/52/52/52	-
60	PEV	BA	510	-	-	8/52/52/52	-
60	PEV	BA	534	-	-	5/52/52/52	-
60	PEV	BA	527	-	-	8/52/52/52	-
60	PEV	A0	323	-	1/1/4/4	7/52/52/52	-
60	PEV	A1	306	-	-	6/52/52/52	-
60	PEV	A0	301	-	-	11/52/52/52	-
60	PEV	A1	305	-	1/1/4/4	6/52/52/52	-
60	PEV	A0	308	-	1/1/4/4	5/52/52/52	-
61	PGV	BB	217	-	2/2/5/7	7/55/55/55	-
60	PEV	A1	326	-	-	4/52/52/52	-
60	PEV	A0	312	-	-	7/52/52/52	-
60	PEV	BA	508	-	1/1/4/4	5/52/52/52	-
61	PGV	A0	317	-	2/2/5/7	8/55/55/55	-
60	PEV	BA	511	-	-	5/52/52/52	-
60	PEV	BB	209	-	-	8/52/52/52	-
61	PGV	A1	318	-	2/2/5/7	11/55/55/55	-
60	PEV	BA	523	-	-	7/52/52/52	-
60	PEV	A1	312	-	-	5/52/52/52	-
61	PGV	AZ	205	-	2/2/5/7	15/55/55/55	-
60	PEV	A1	307	-	-	4/52/52/52	-

The worst 5 of 168 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	BA	533	PEV	C39-C40	17.92	2.52	1.51
61	BA	516	PGV	C9-C10	-4.44	1.34	1.52
61	BB	213	PGV	C9-C10	-4.42	1.34	1.52
61	BA	522	PGV	C9-C10	-4.38	1.34	1.52
61	A1	315	PGV	C9-C10	-4.38	1.34	1.52

The worst 5 of 266 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	BA	533	PEV	C39-C40-C41	6.06	145.17	114.42
60	BA	533	PEV	C38-C39-C40	5.54	142.55	114.42
60	A0	316	PEV	C38-C39-C40	3.57	132.56	114.42
61	A0	325	PGV	C8-C9-C10	3.34	128.33	113.79
61	BB	205	PGV	C8-C9-C10	3.26	127.98	113.79

5 of 78 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
60	AZ	204	PEV	C2
60	A0	308	PEV	C2
60	A0	314	PEV	C2
60	A0	323	PEV	C2
60	A1	301	PEV	C2

5 of 987 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	AZ	203	PEV	C4-O4P-P-O2P
60	A0	301	PEV	C4-O4P-P-O2P
60	A0	301	PEV	O11-C11-O3-C3
60	A0	301	PEV	C12-C11-O3-C3
60	A0	303	PEV	C1-O3P-P-O1P

There are no ring outliers.

17 monomers are involved in 41 short contacts:

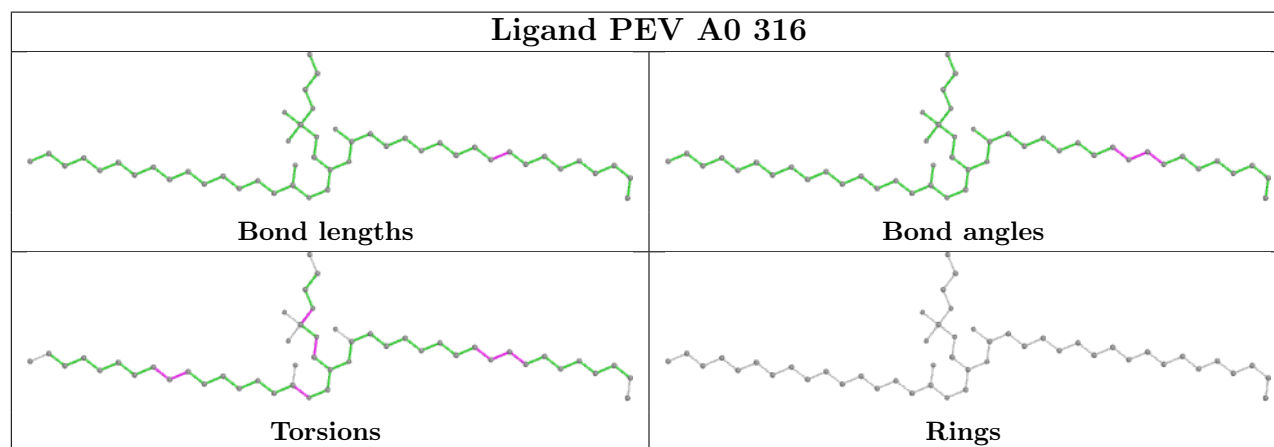
Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	BA	520	PEV	1	0
60	A1	323	PEV	1	0
60	A1	302	PEV	1	0
60	A1	301	PEV	1	0
60	A1	319	PEV	1	0

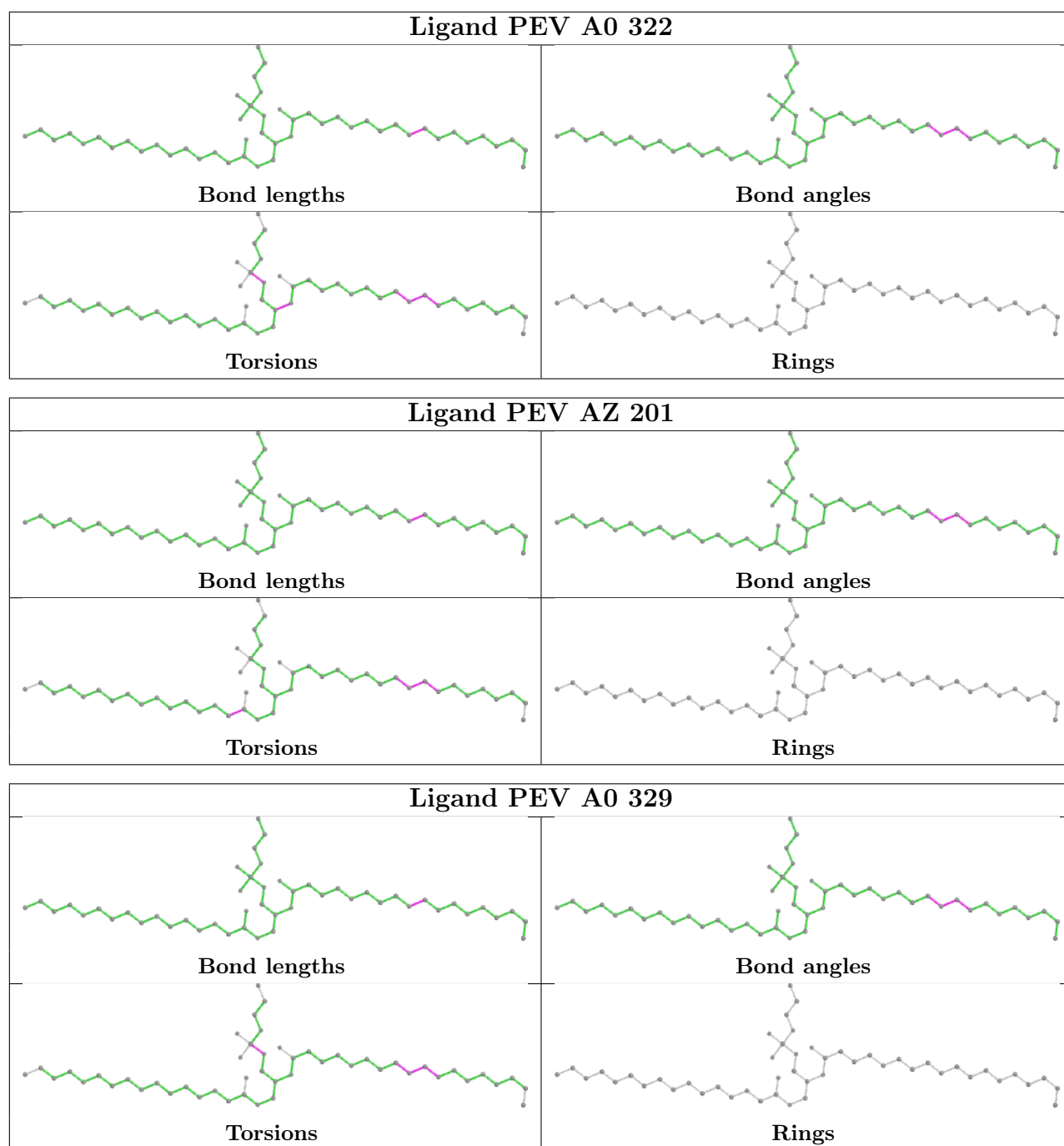
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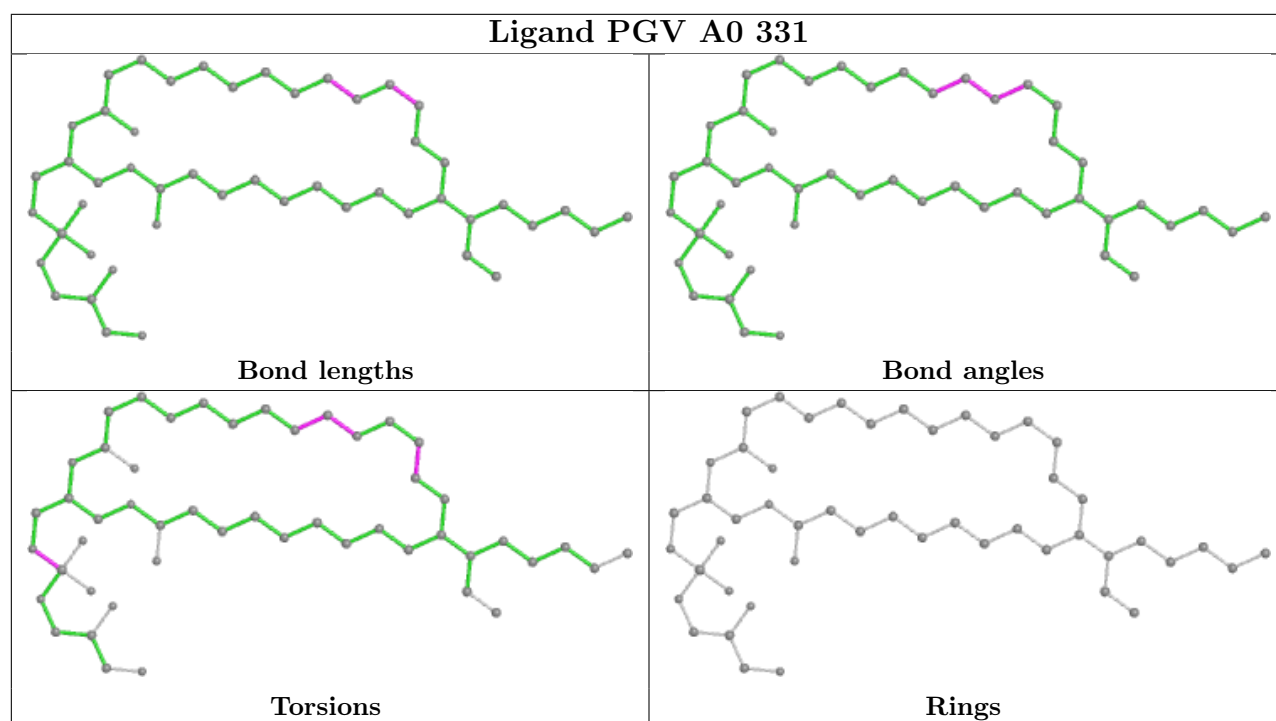
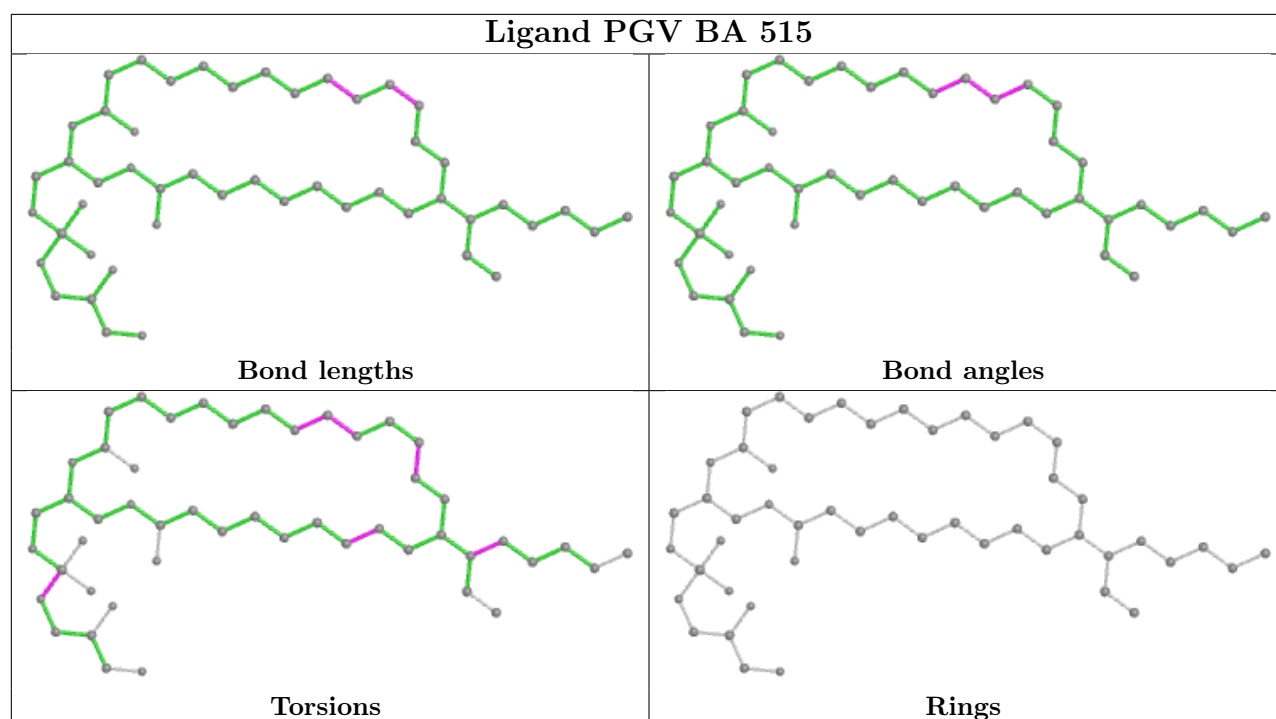
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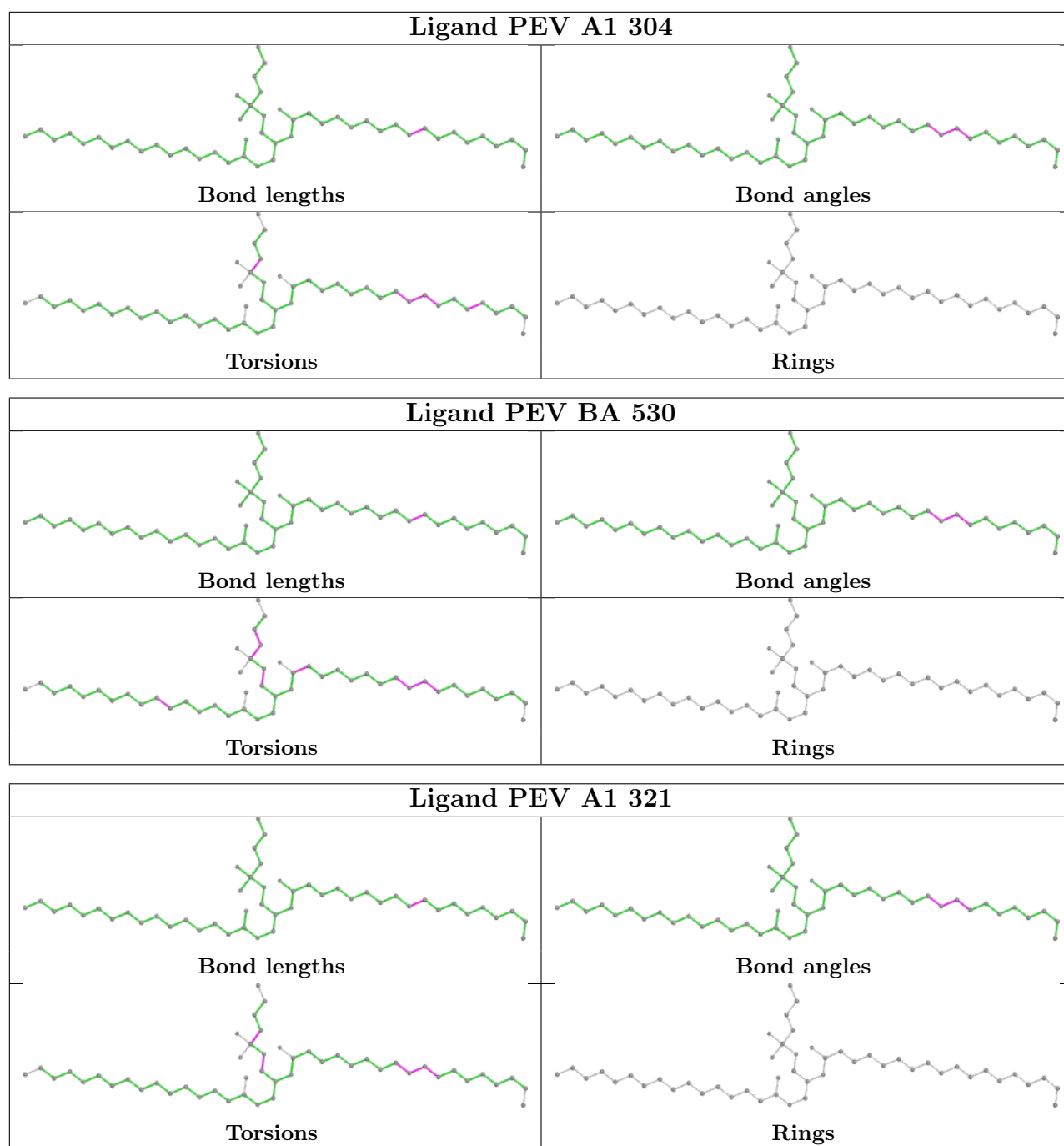
Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	BA	526	PEV	1	0
61	BA	512	PGV	1	0
60	A0	315	PEV	1	0
60	B8	3001	PEV	1	0
61	A1	303	PGV	1	0
60	BA	531	PEV	1	0
60	BA	533	PEV	29	0
60	BA	514	PEV	1	0
60	B8	3002	PEV	2	0
60	BA	503	PEV	1	0
61	A1	315	PGV	1	0
60	BA	513	PEV	1	0

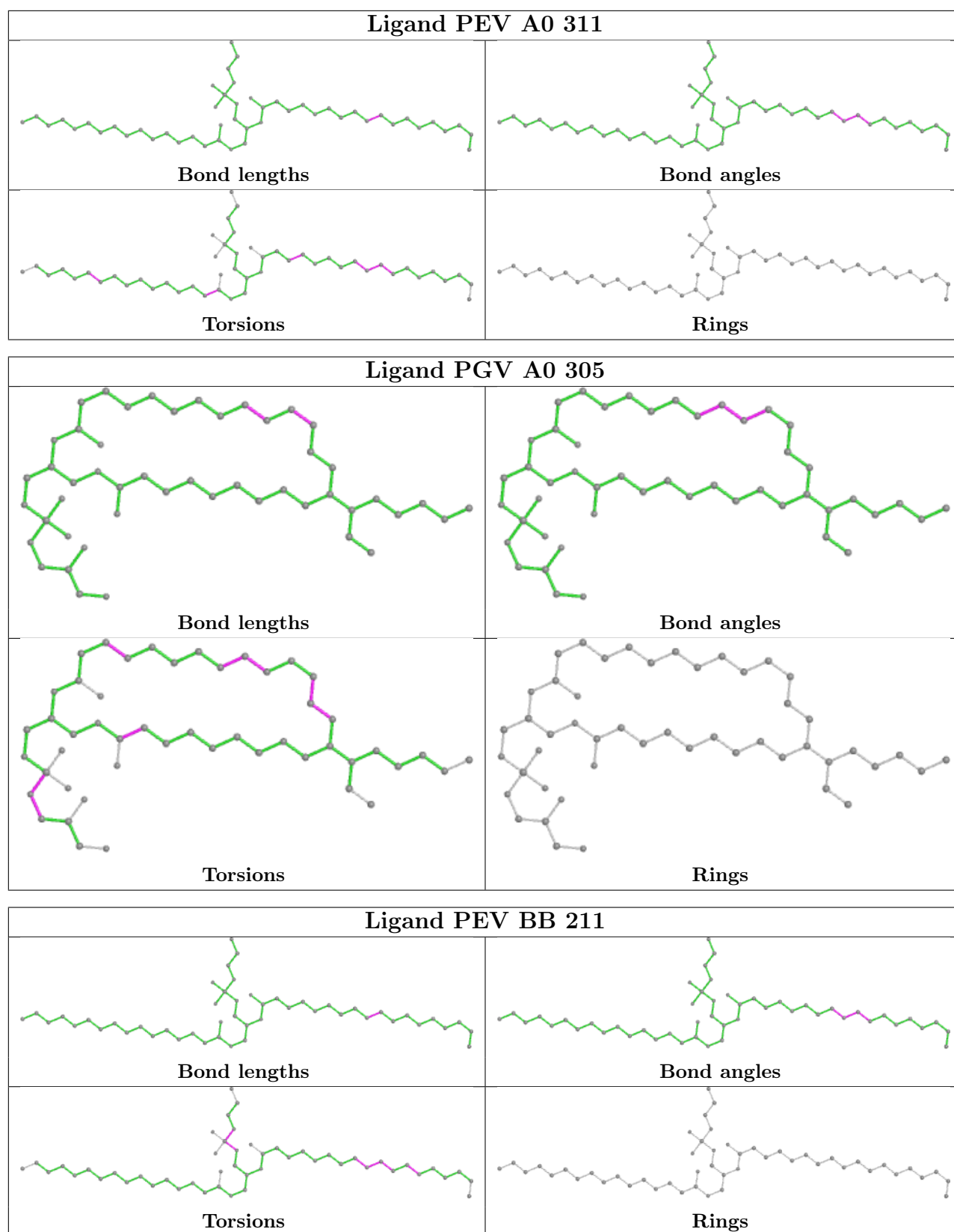
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

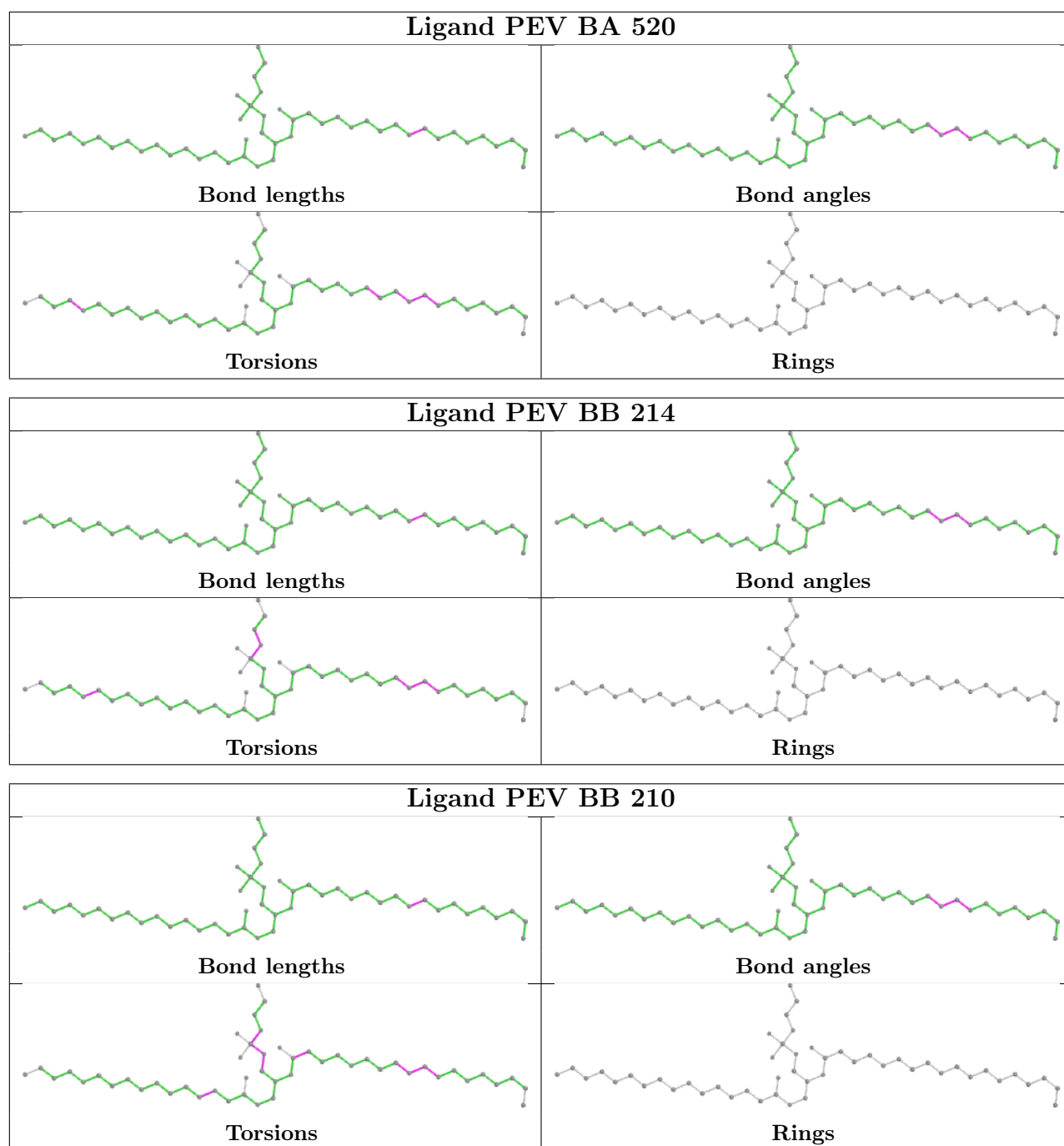


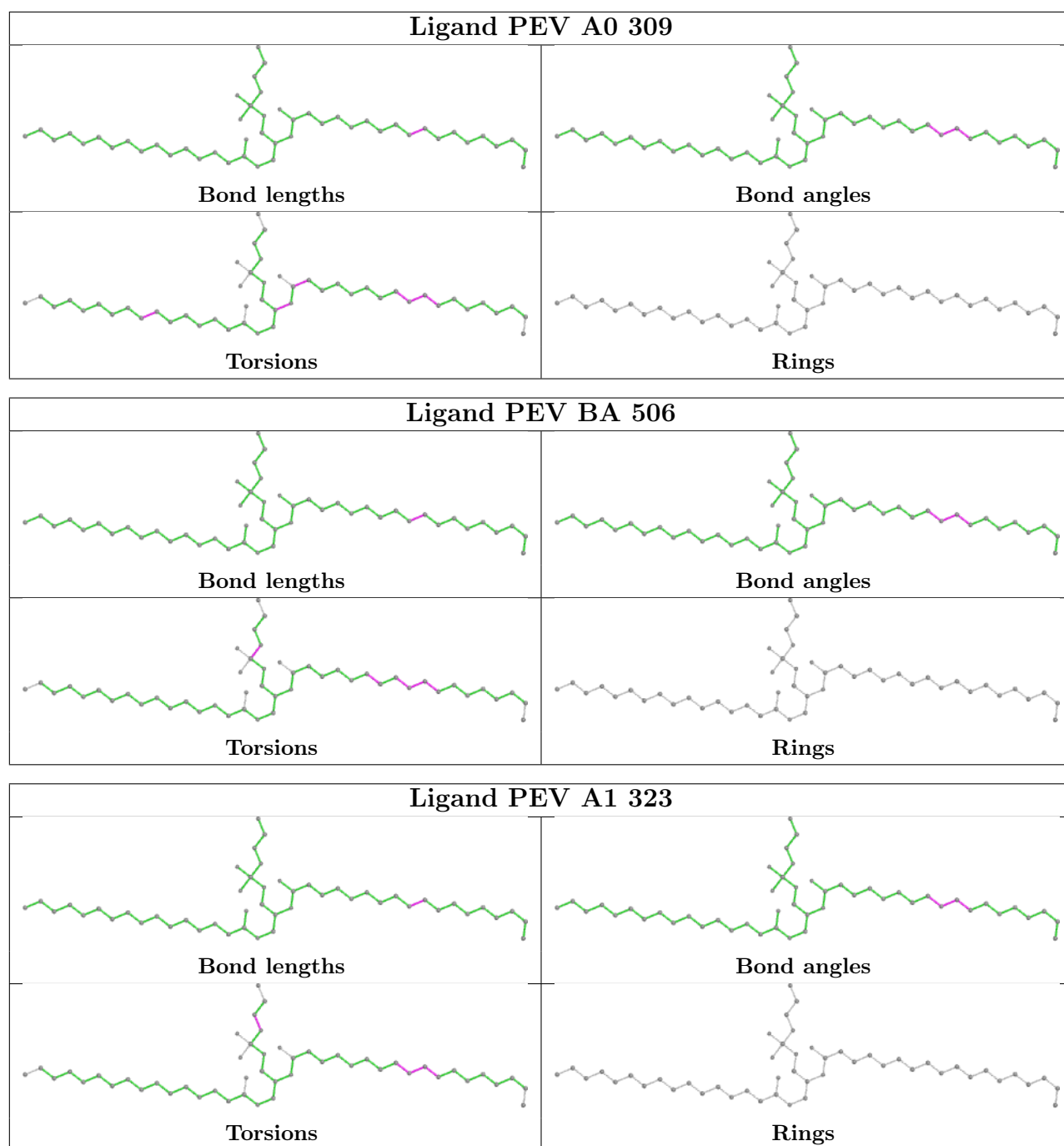


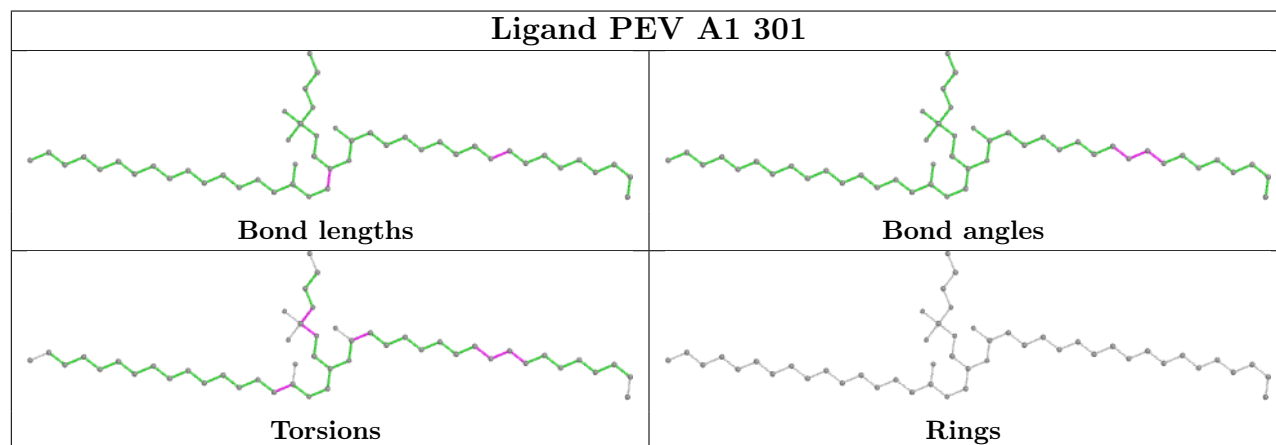
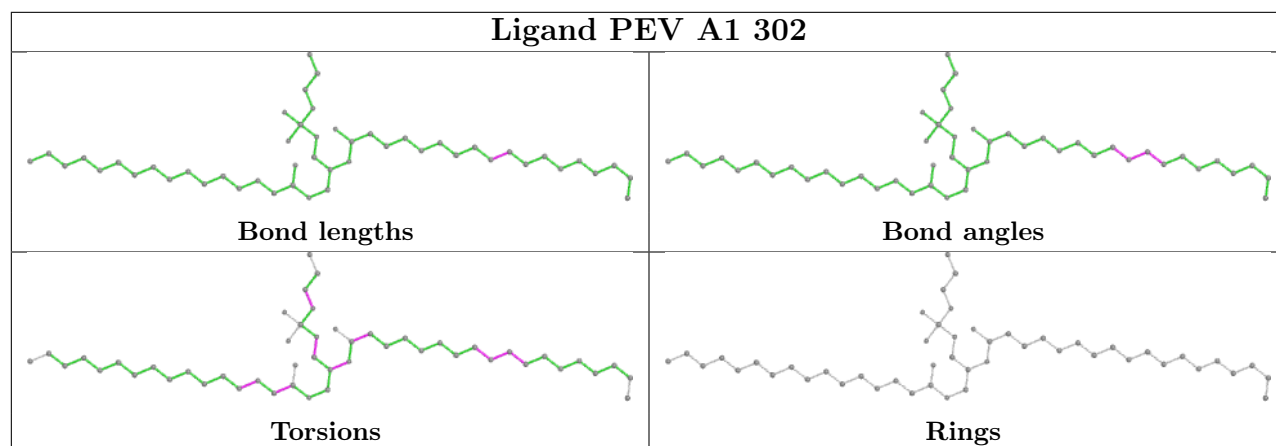
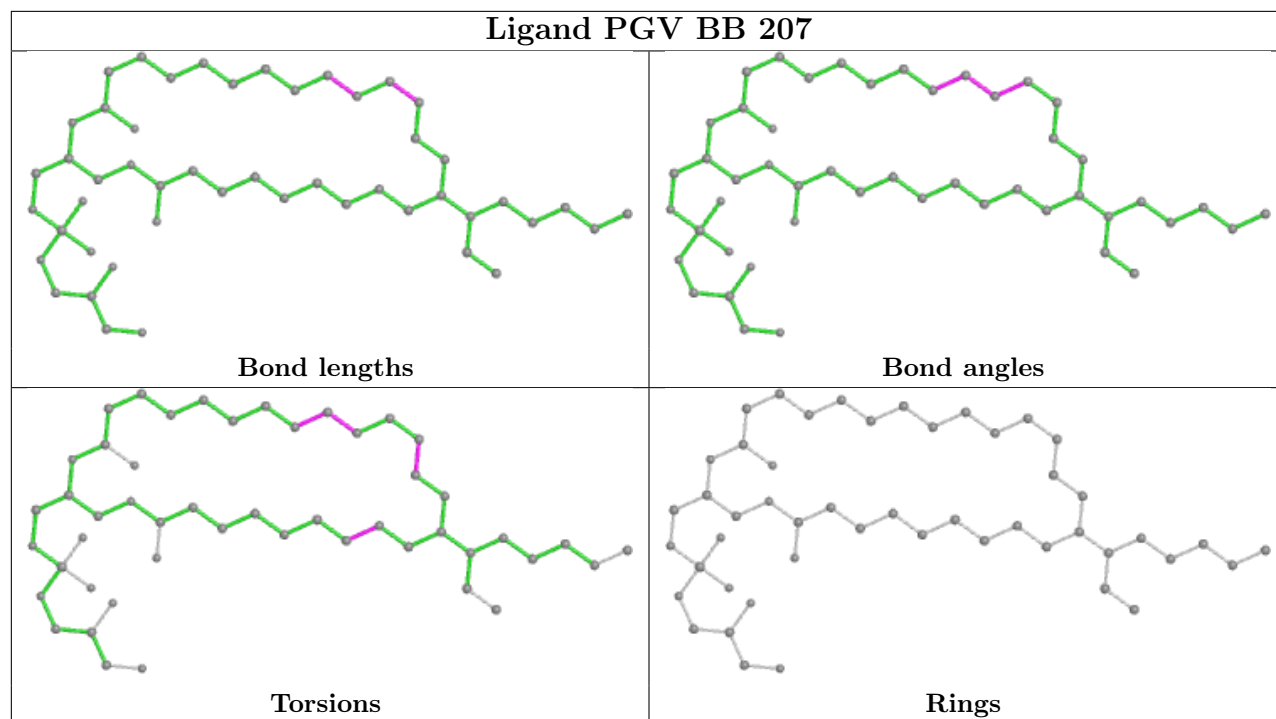


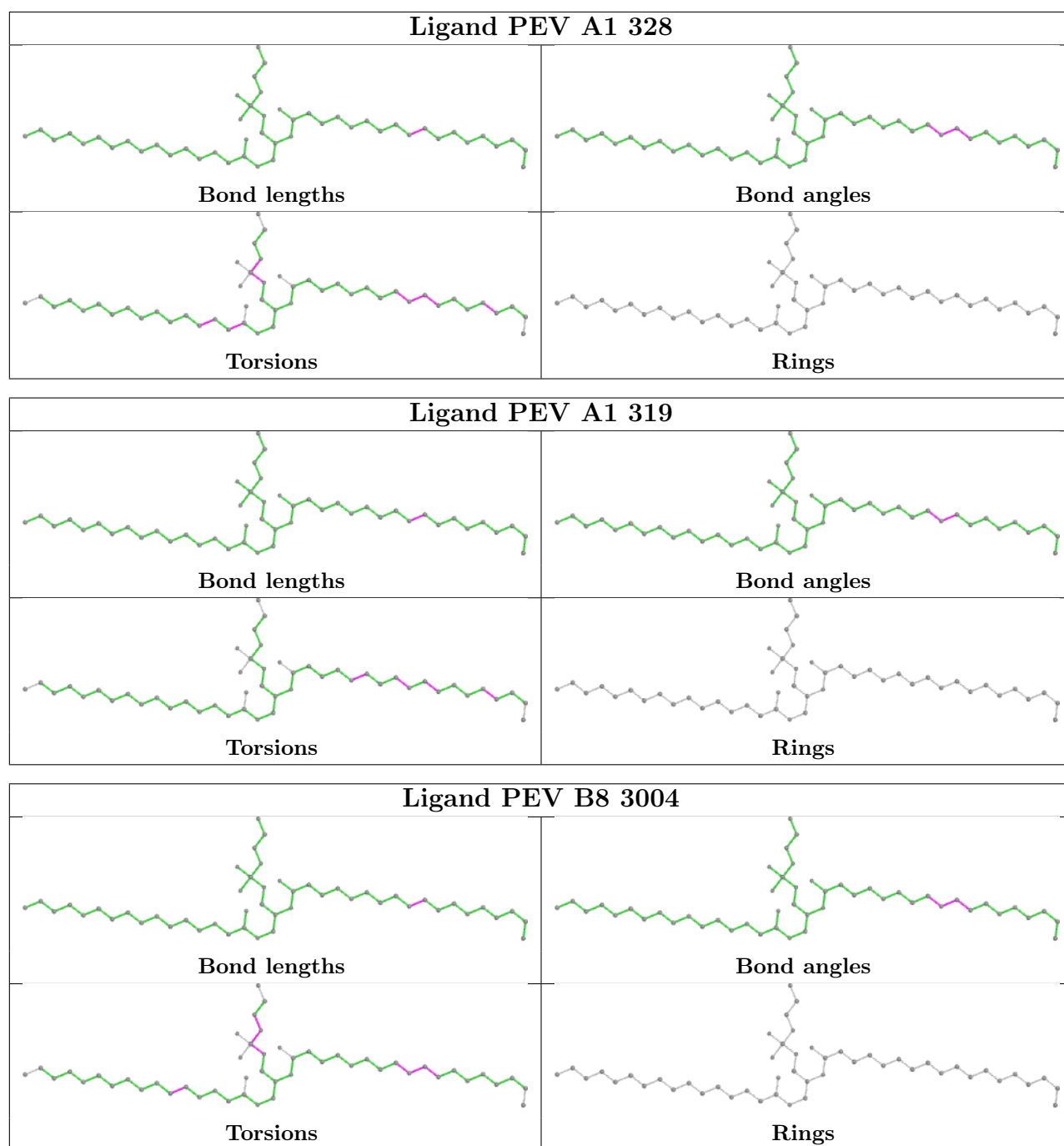


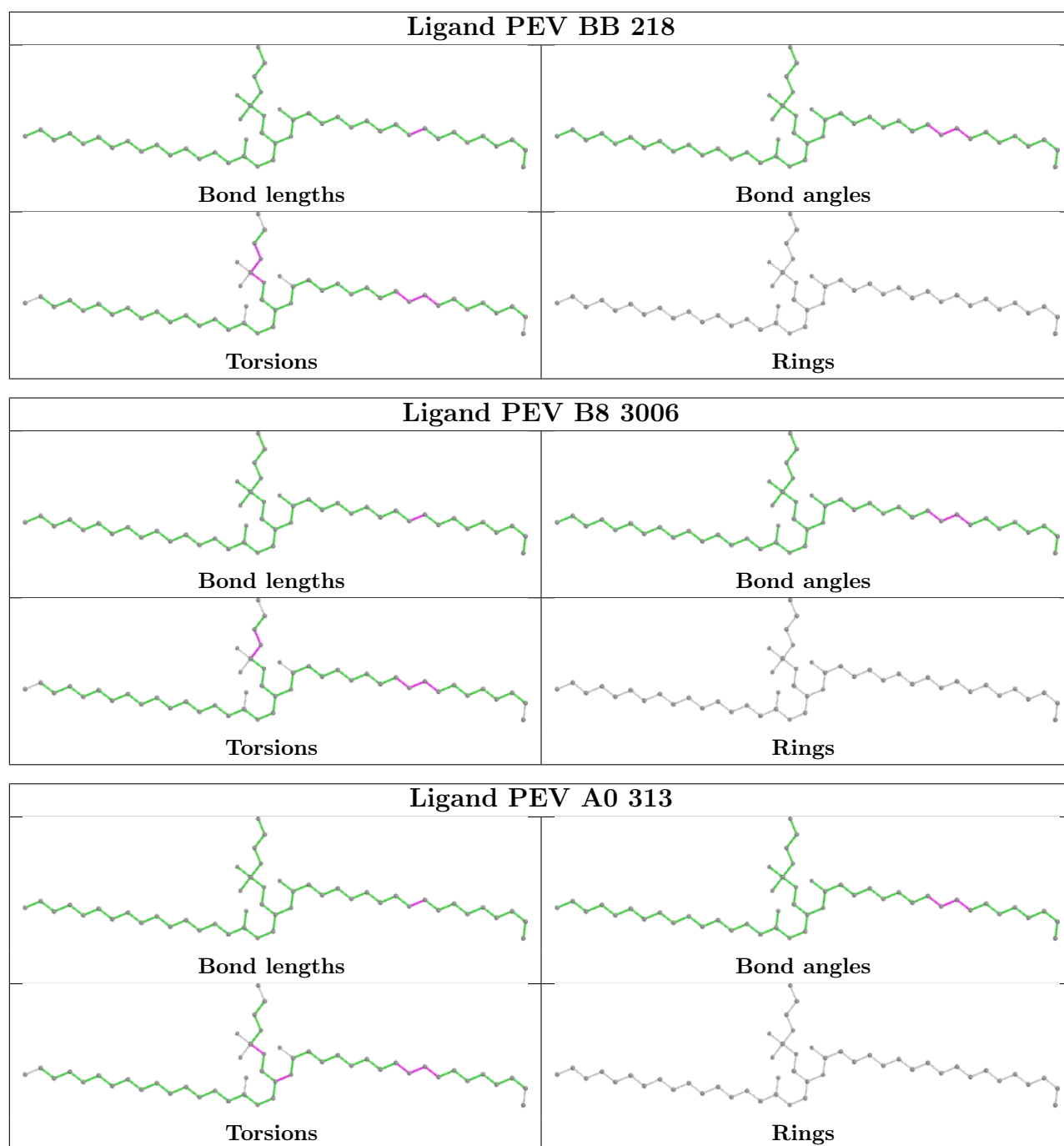


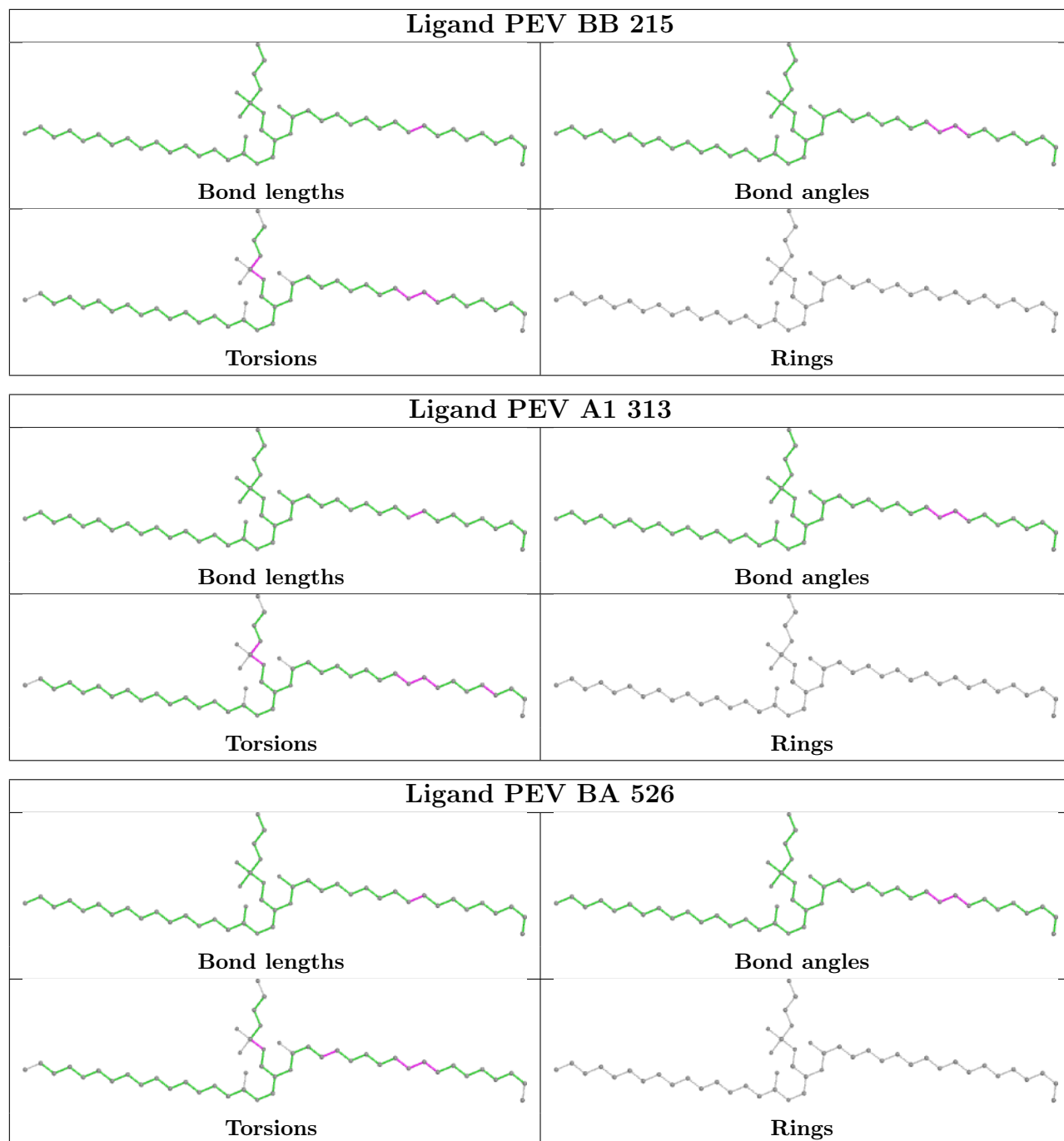


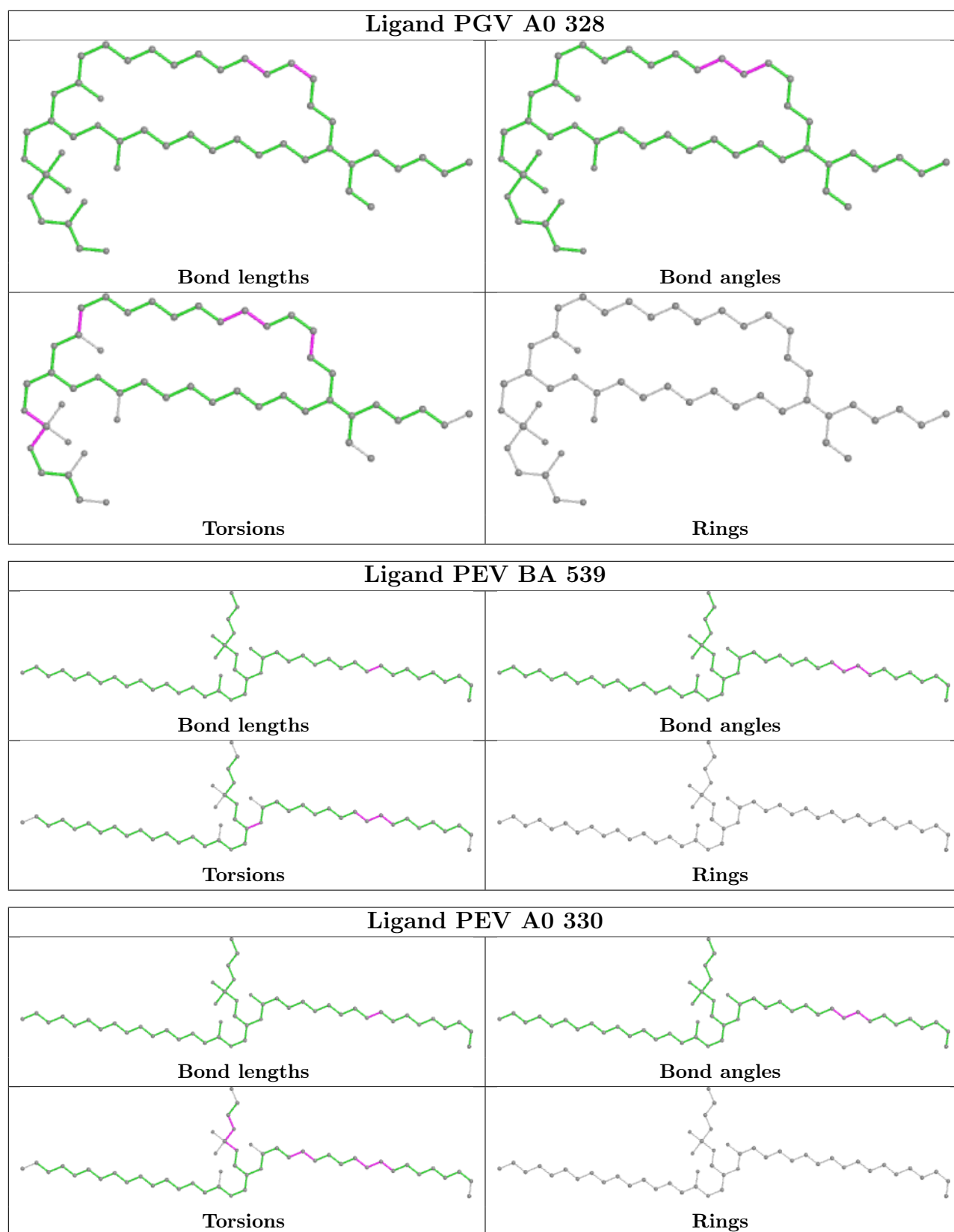


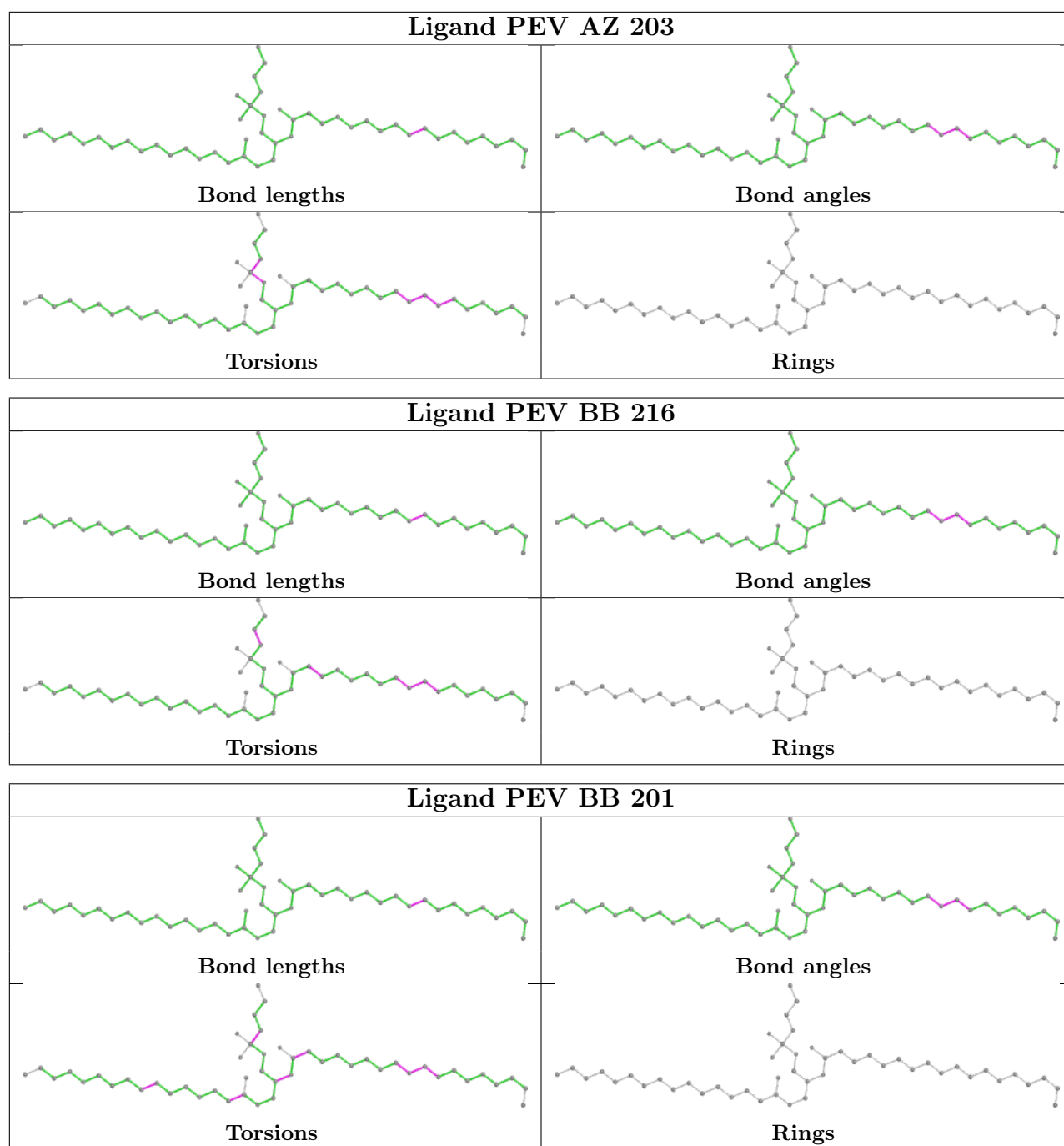


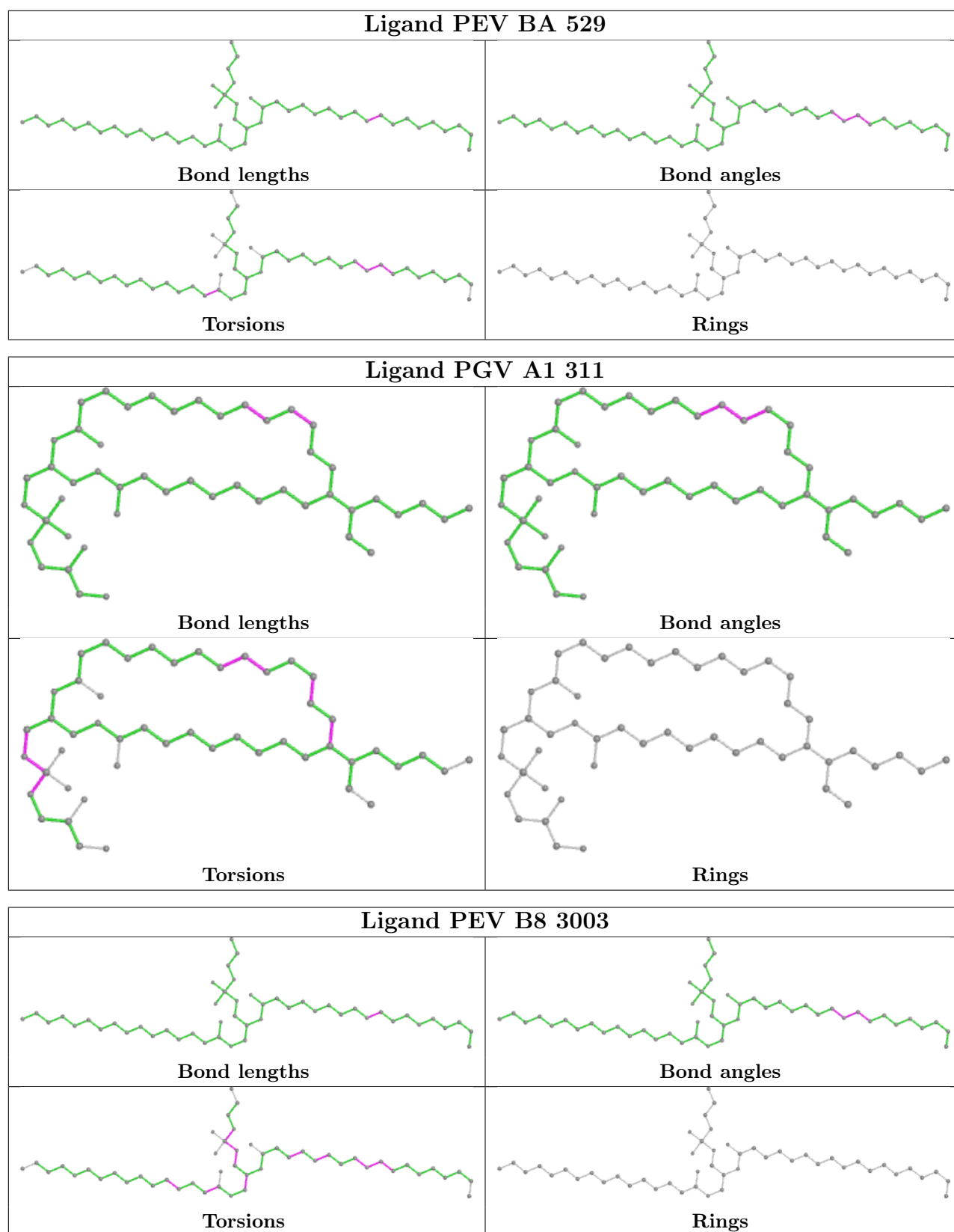


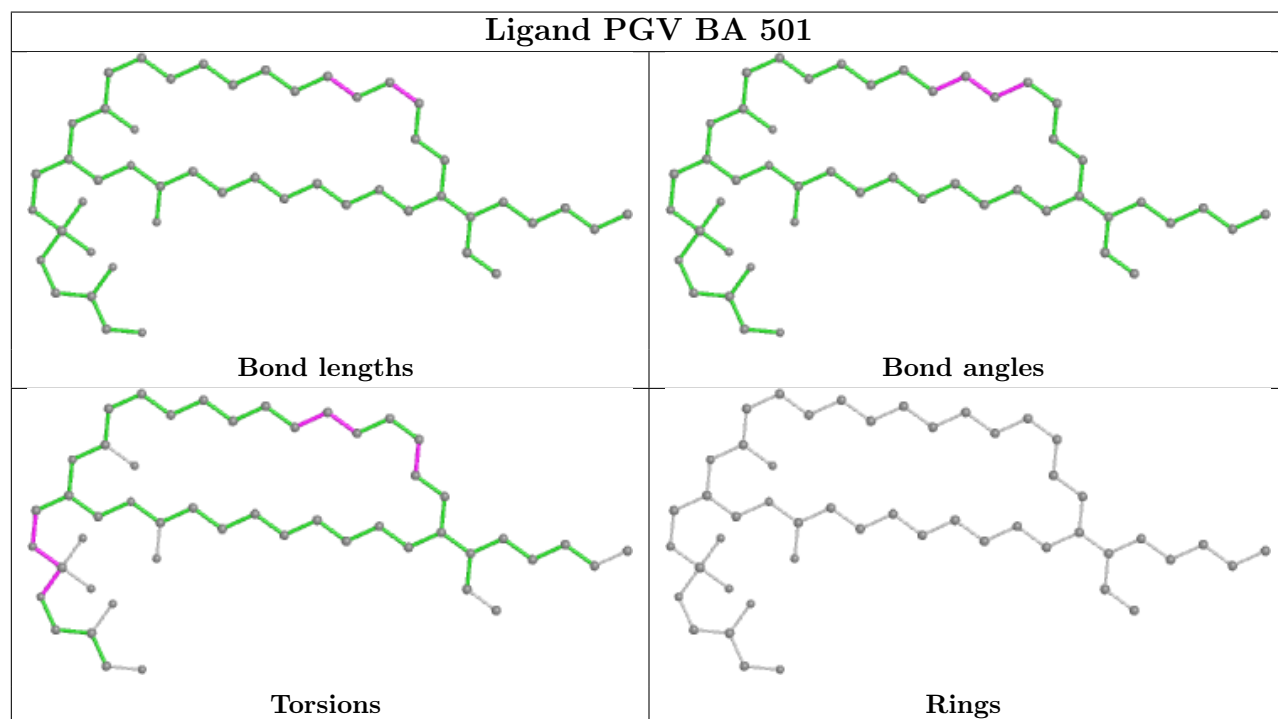
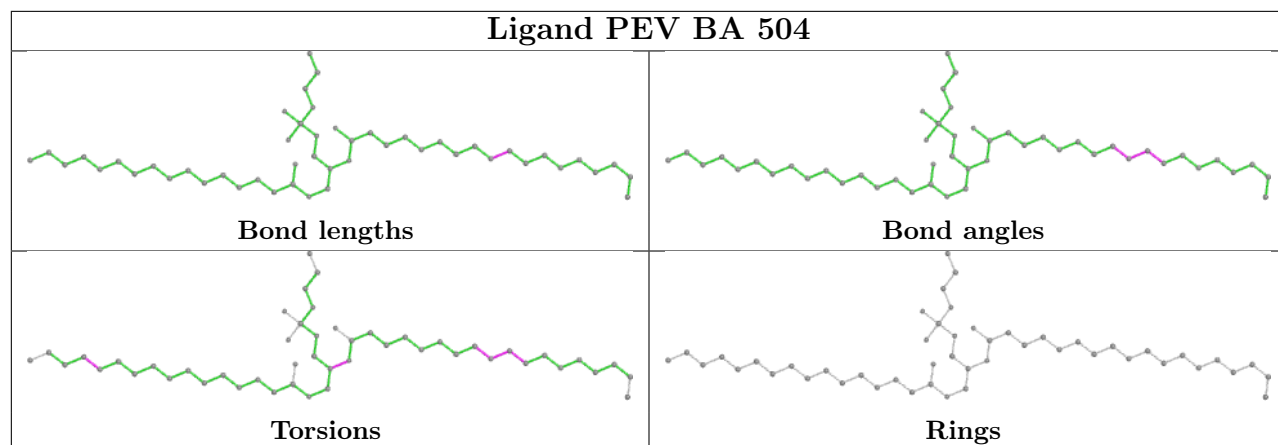




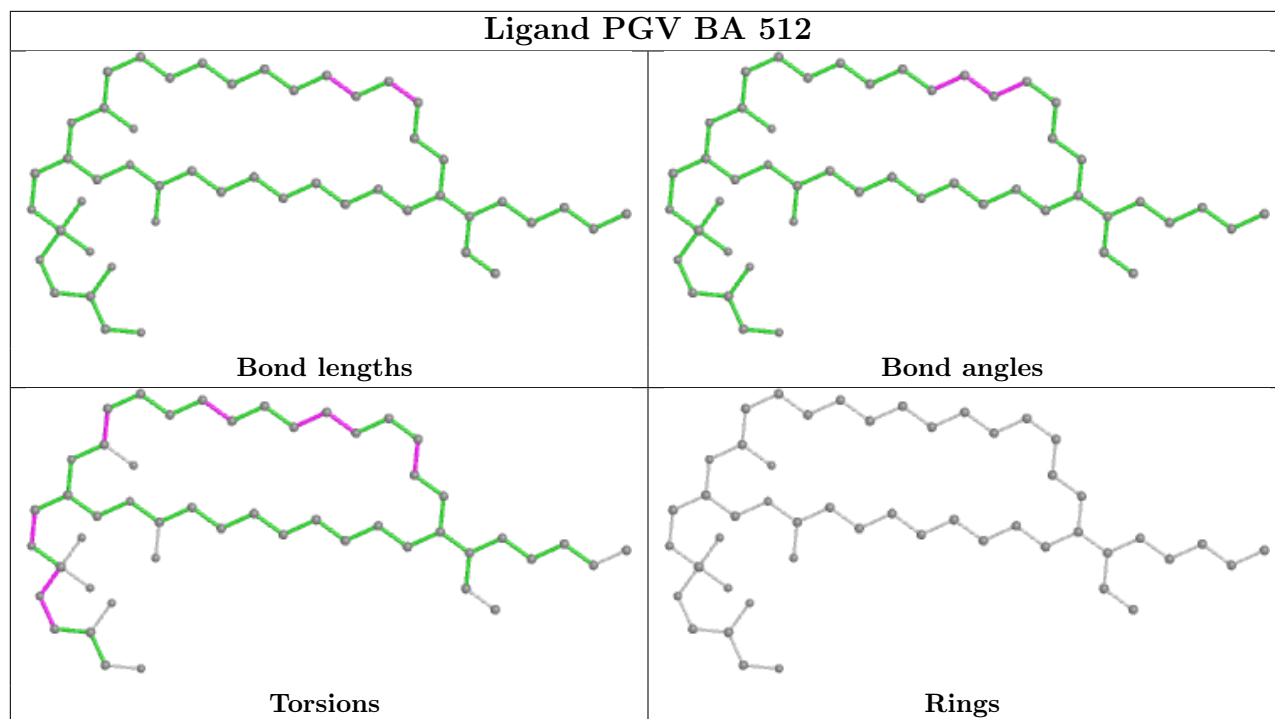




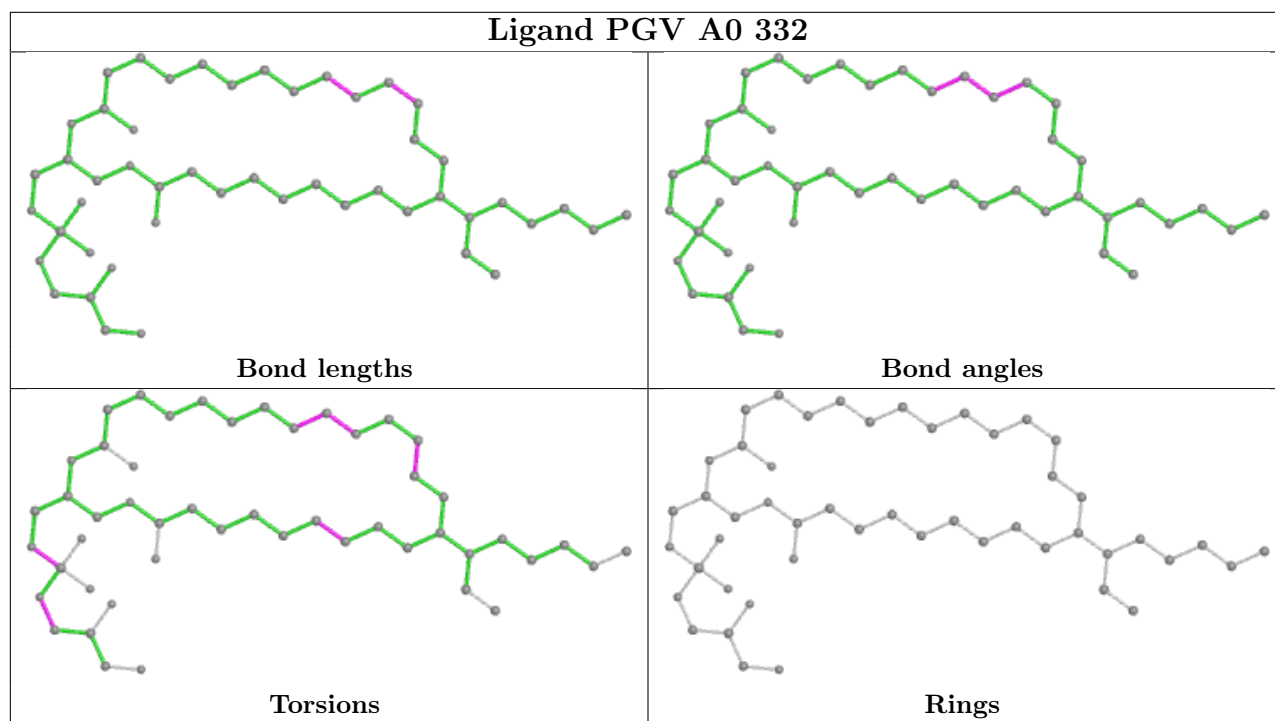


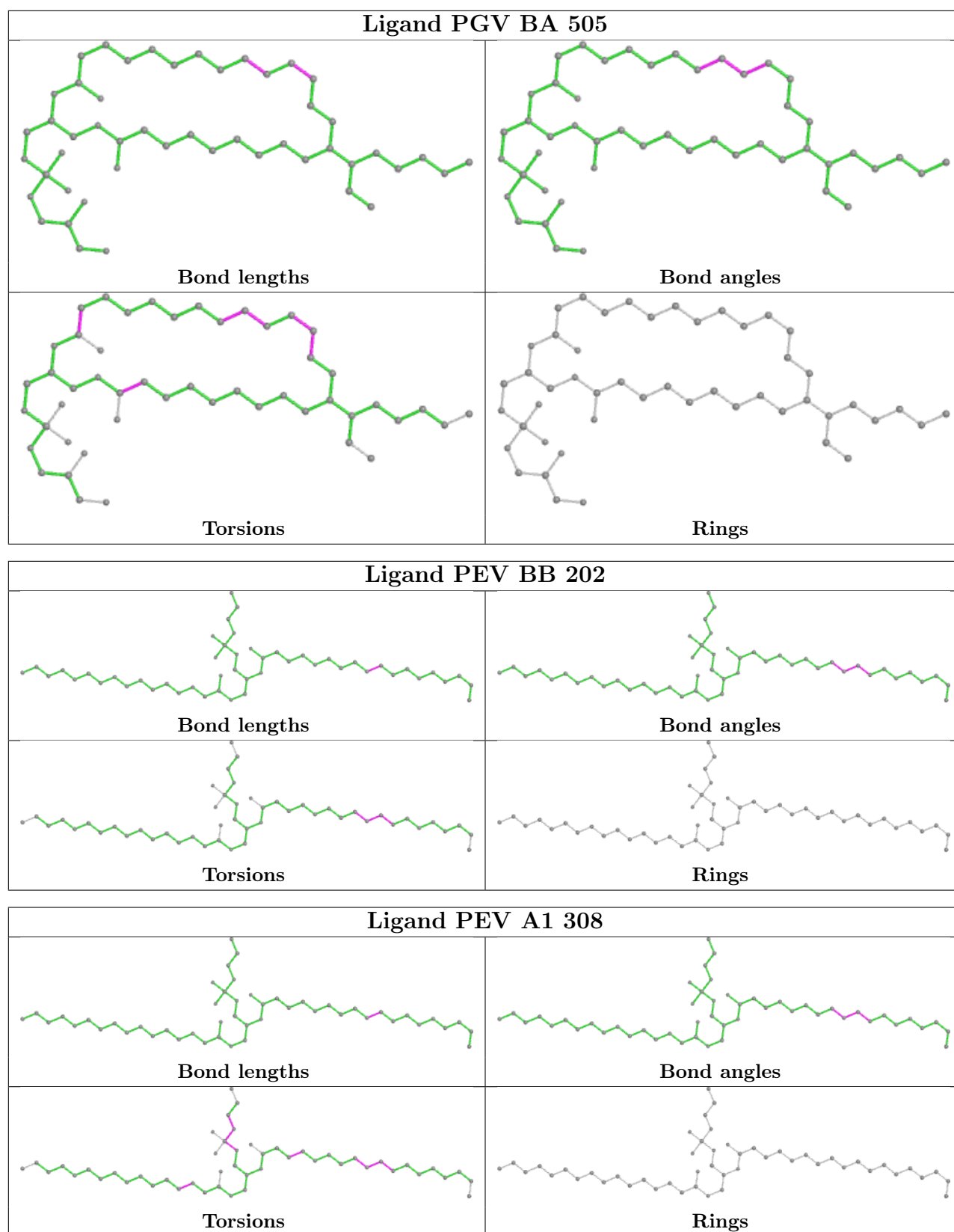


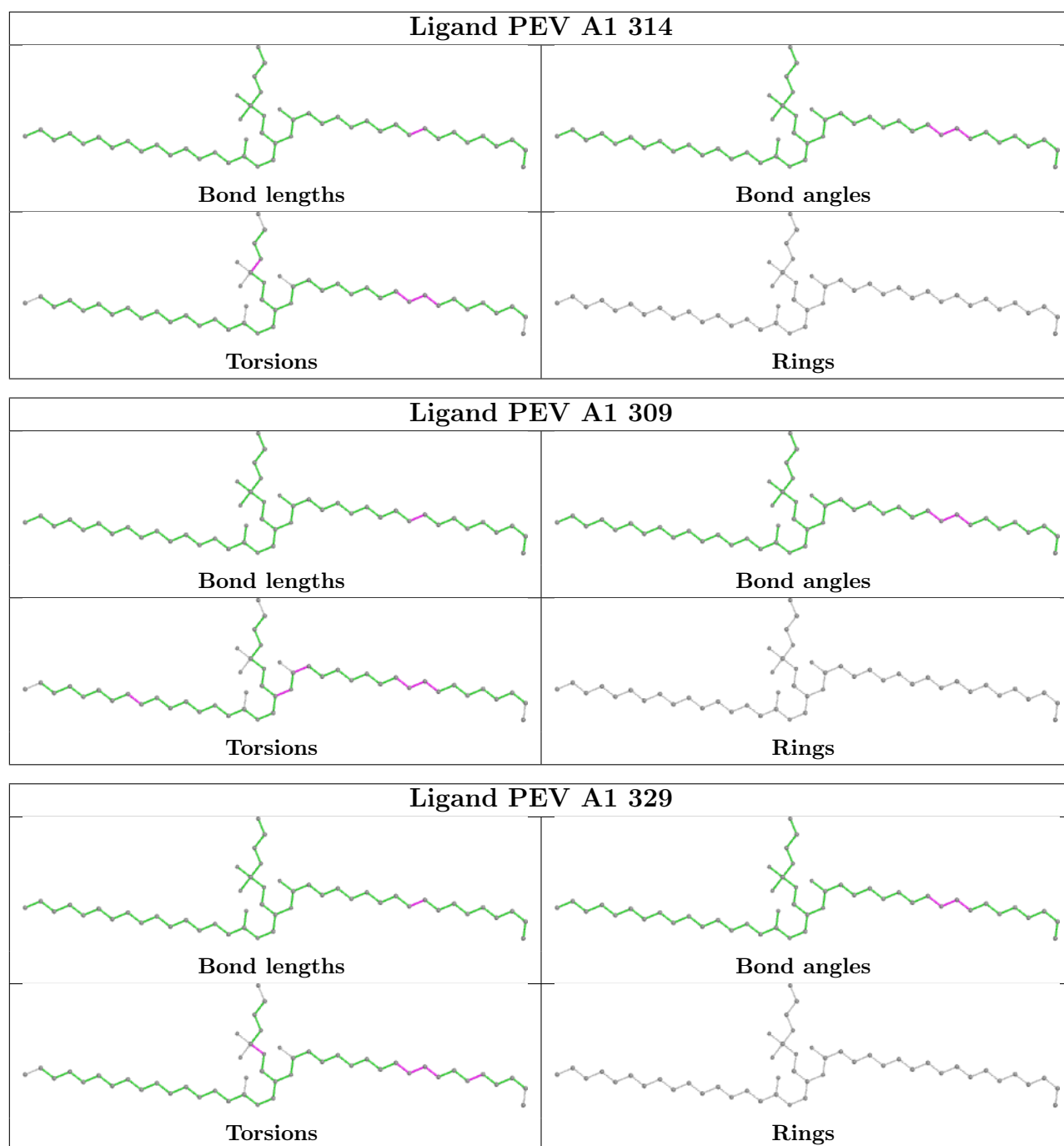
## Ligand PGV BA 512

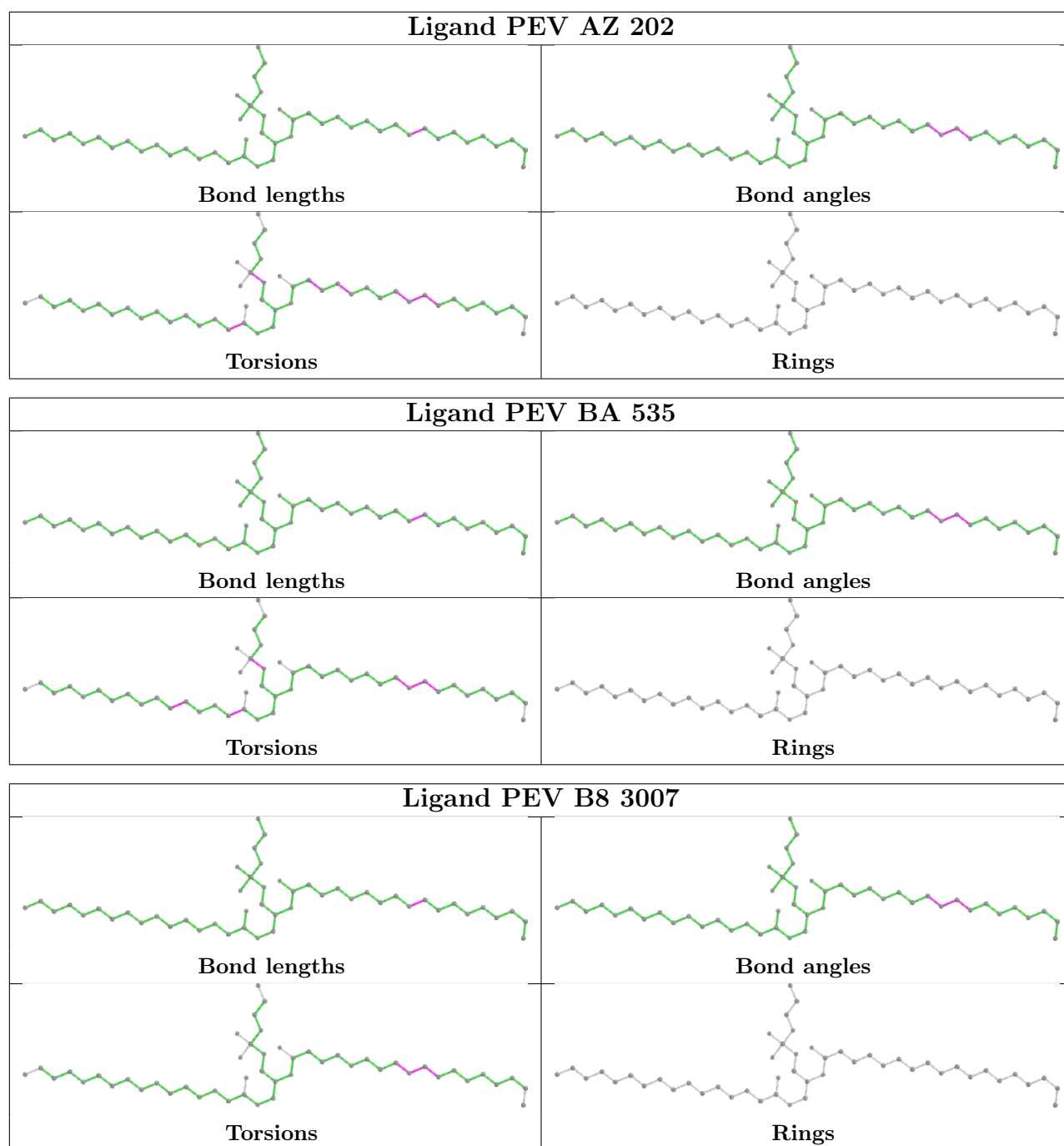


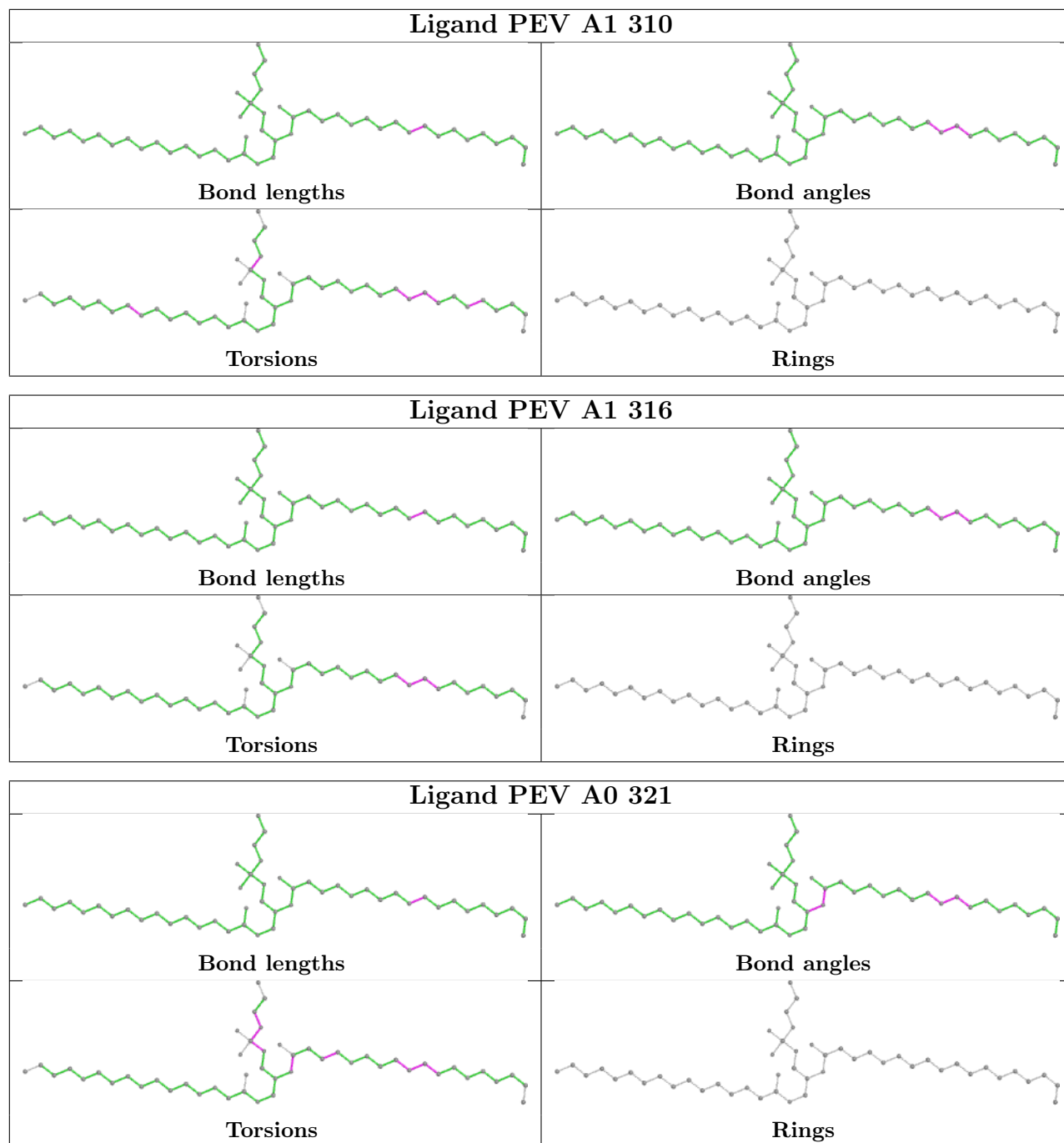
## Ligand PGV A0 332

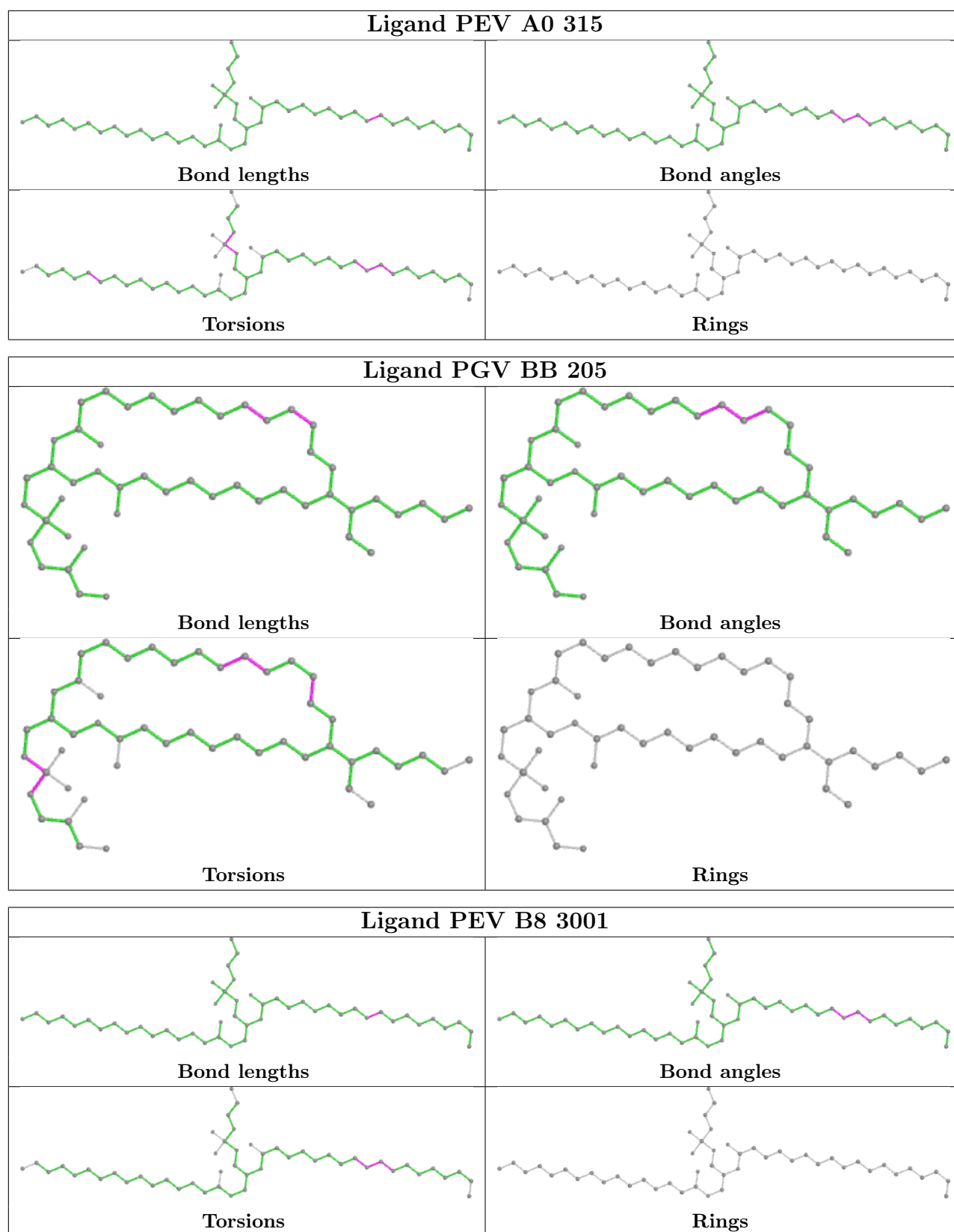


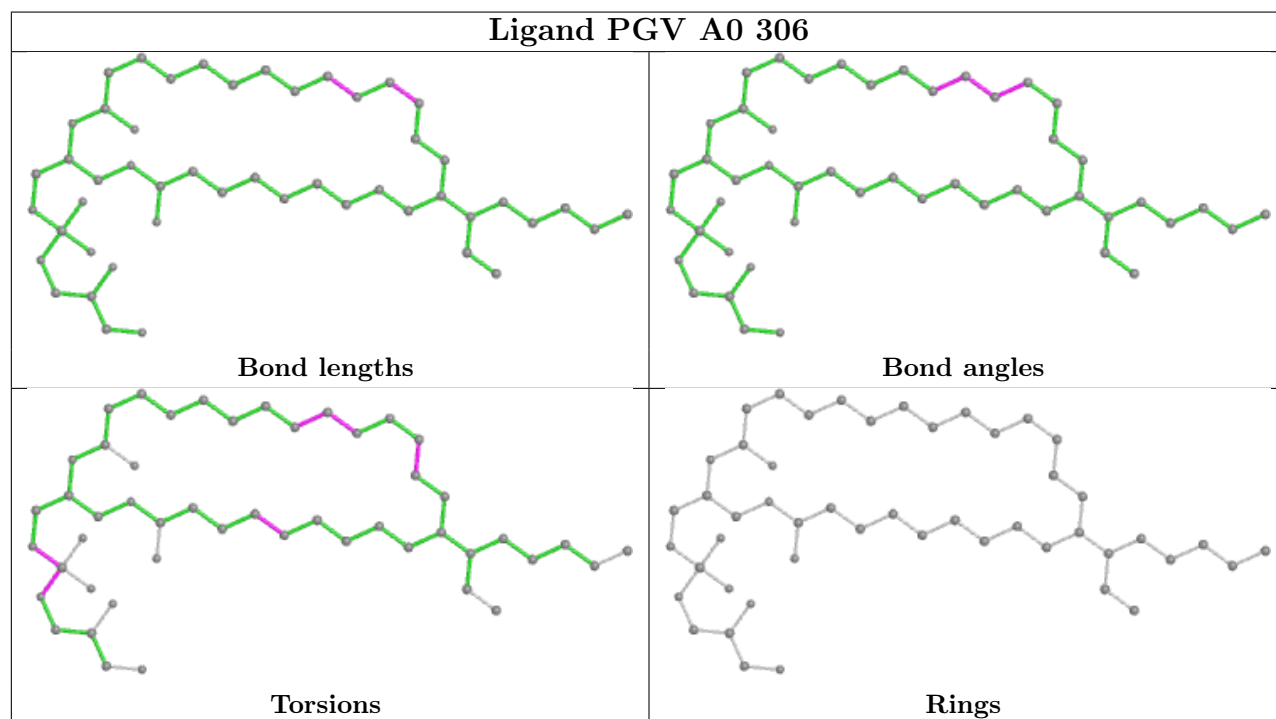
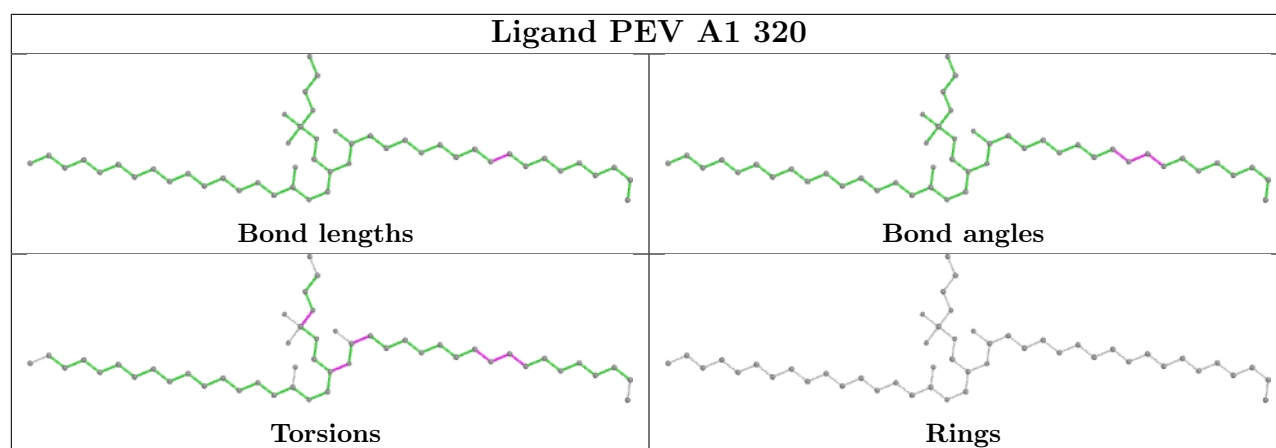


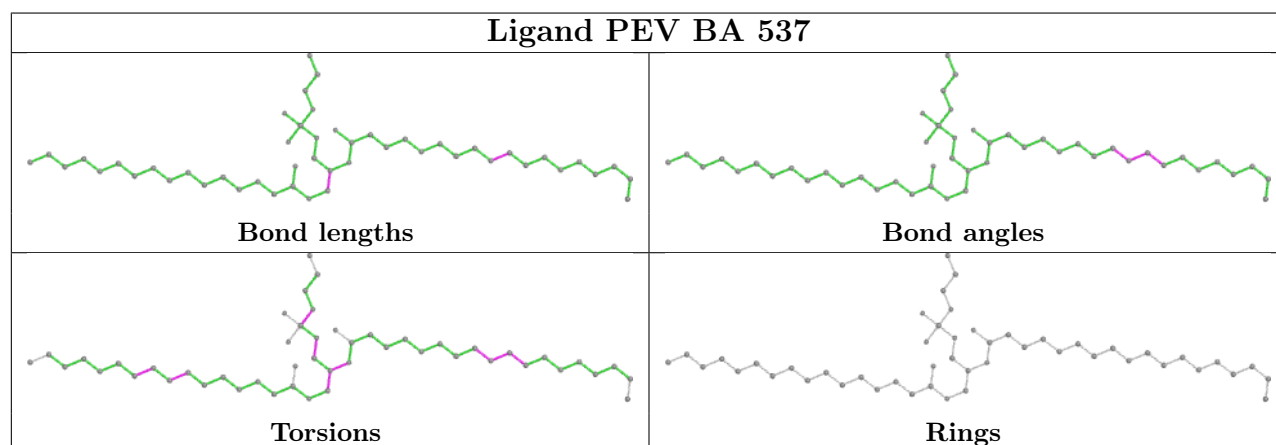
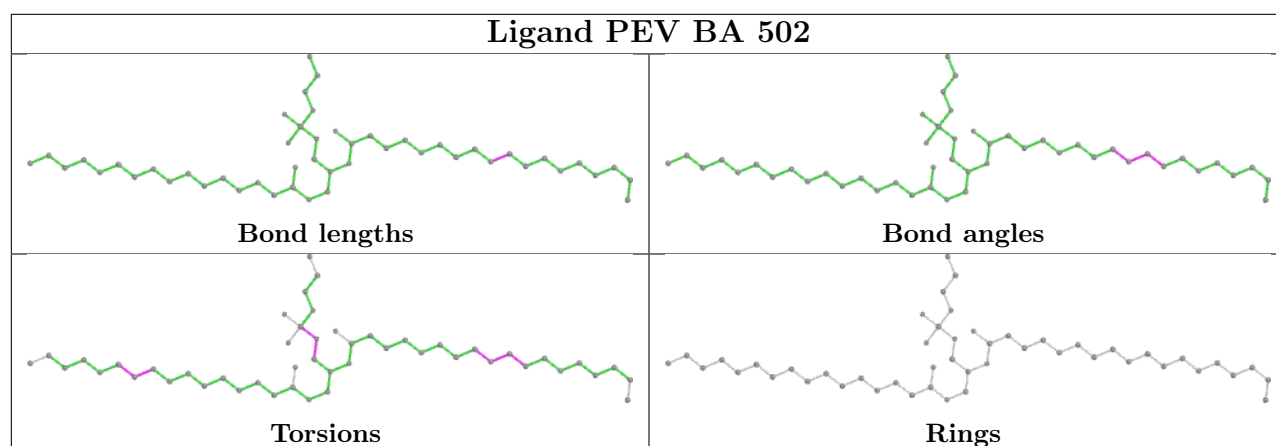
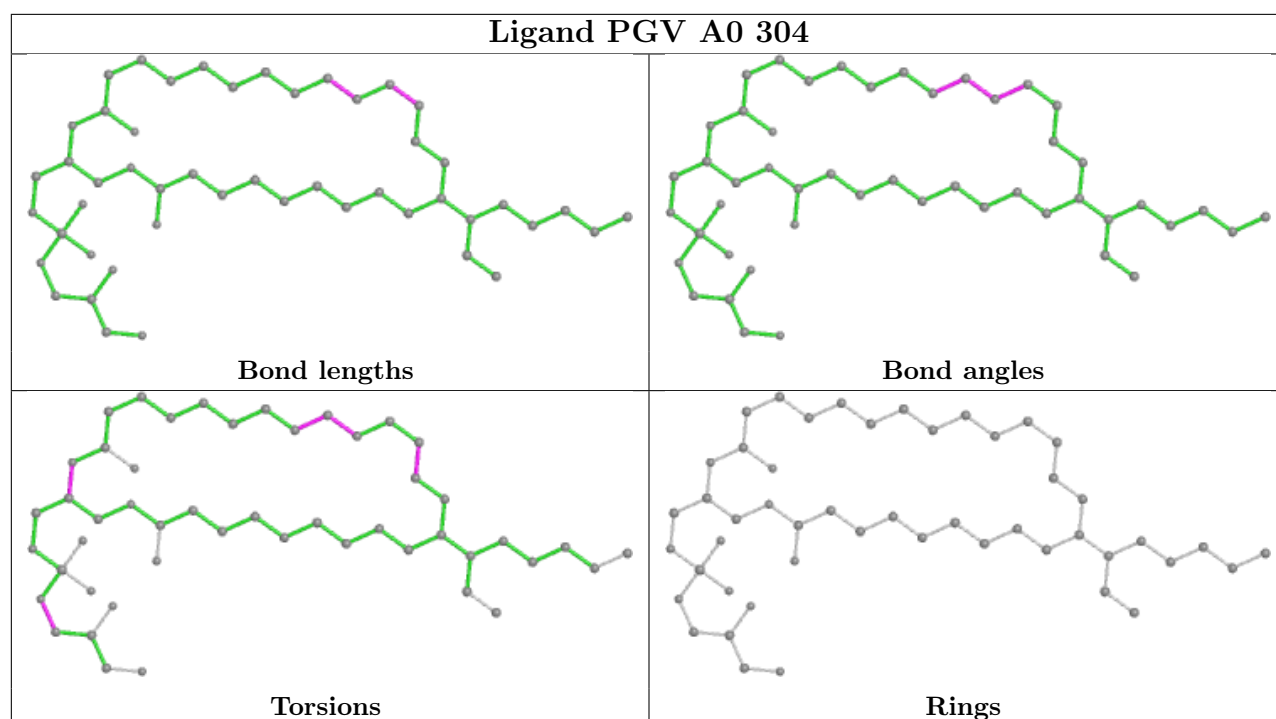


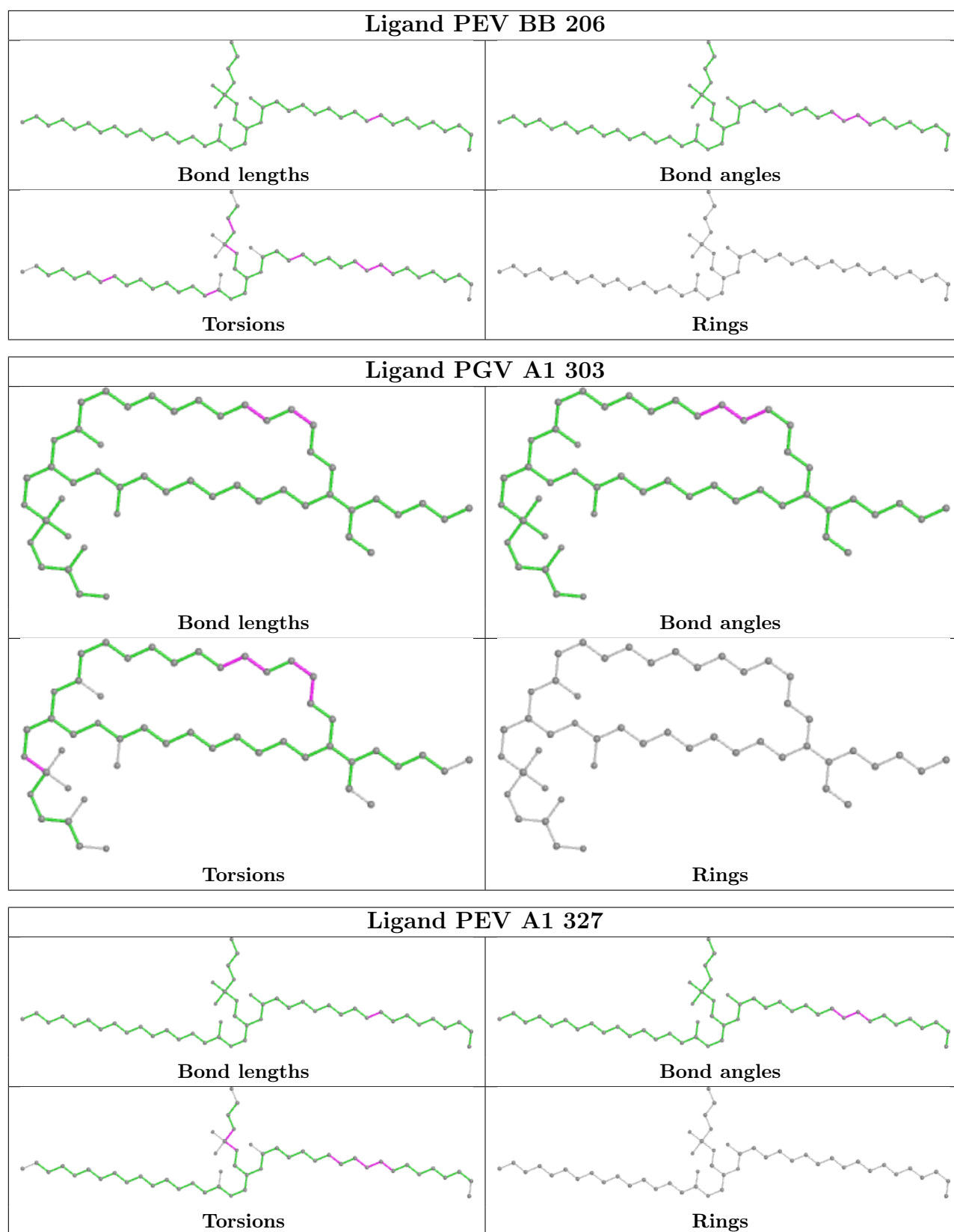


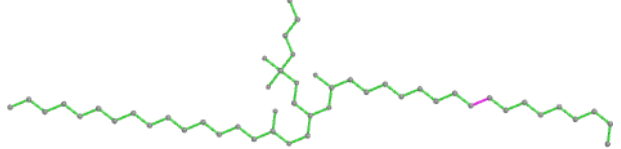
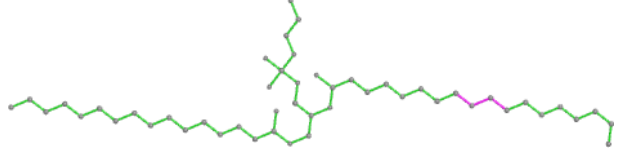
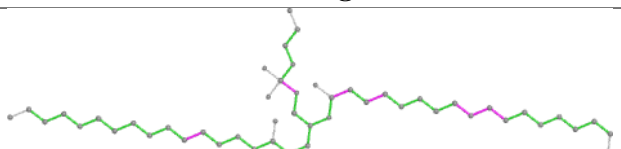
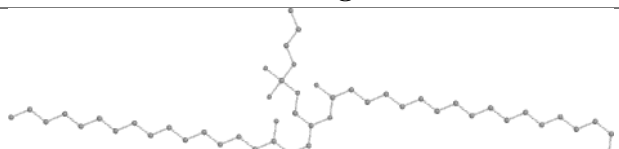
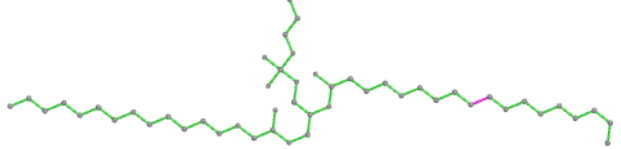
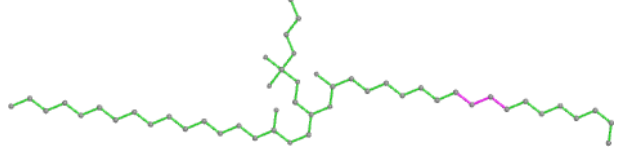
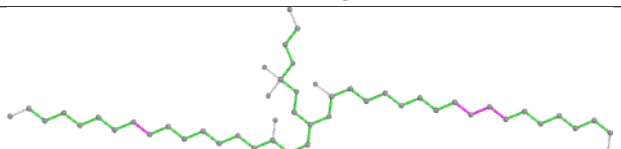
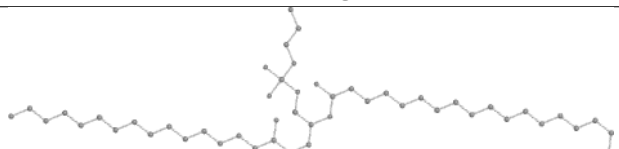
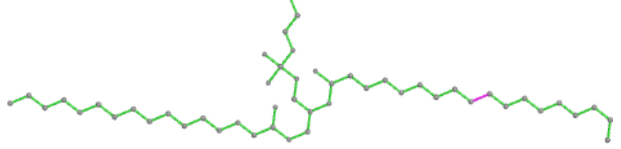
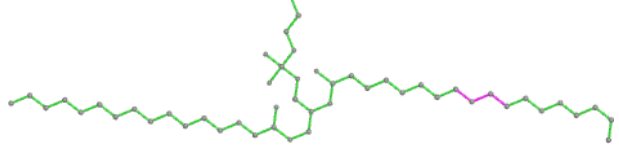
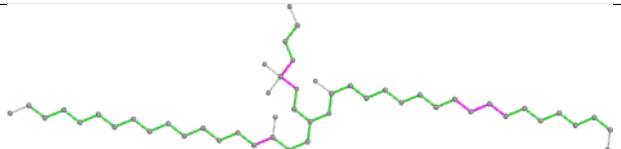
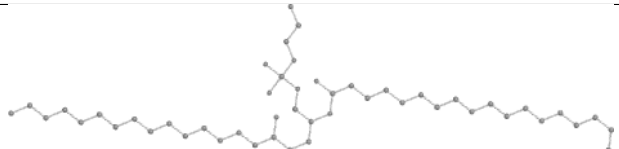




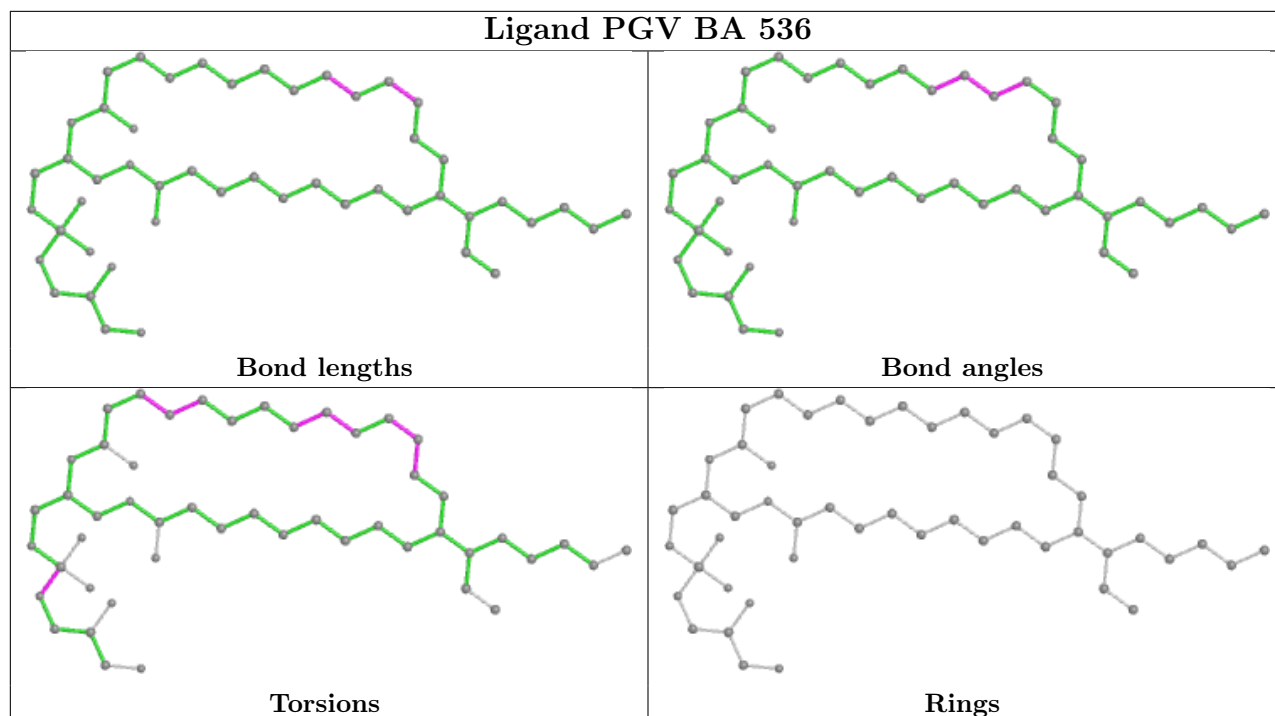




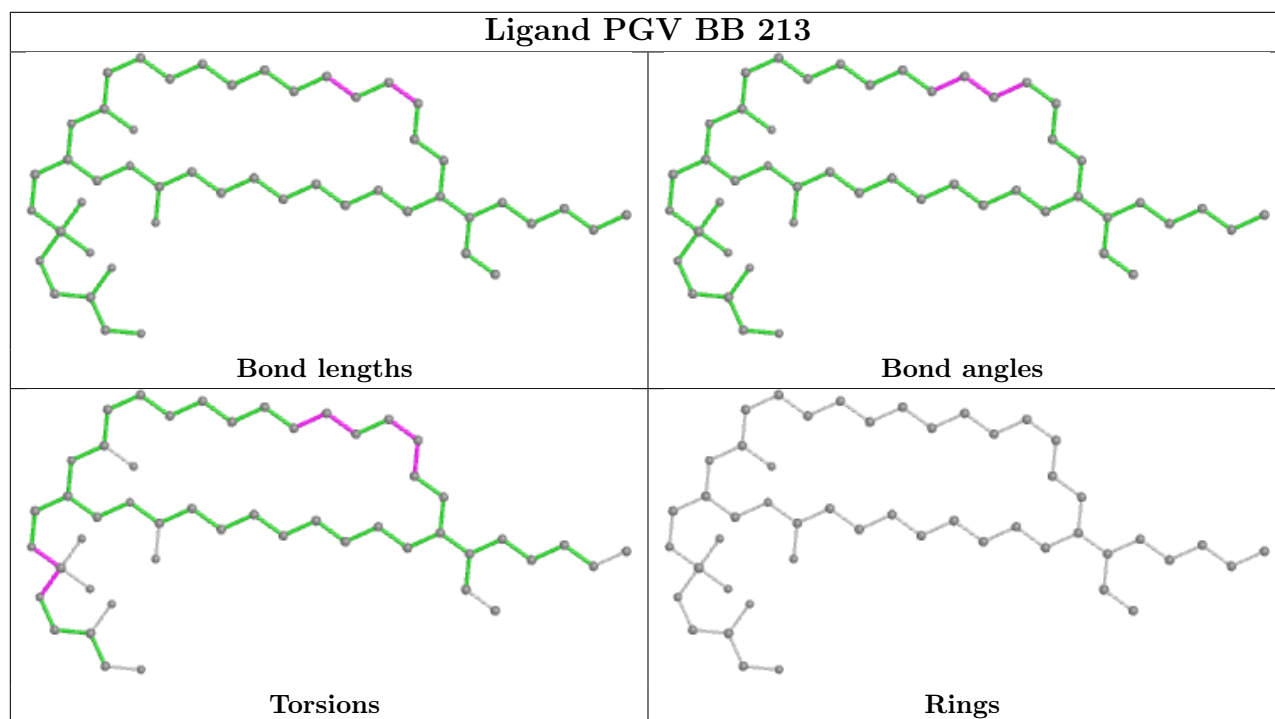


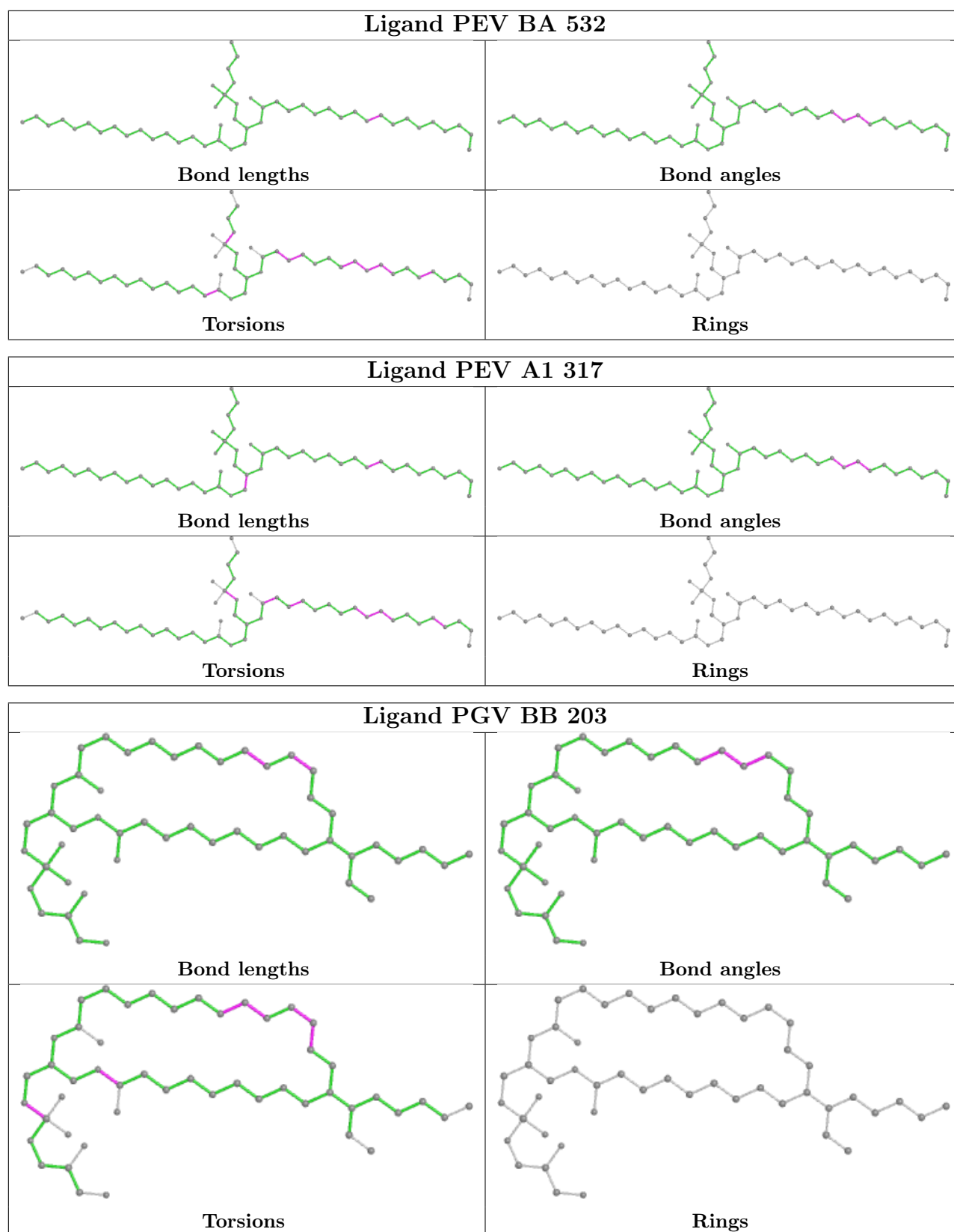
Ligand PEV AZ 204	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand PEV A1 322	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand PEV BA 528	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

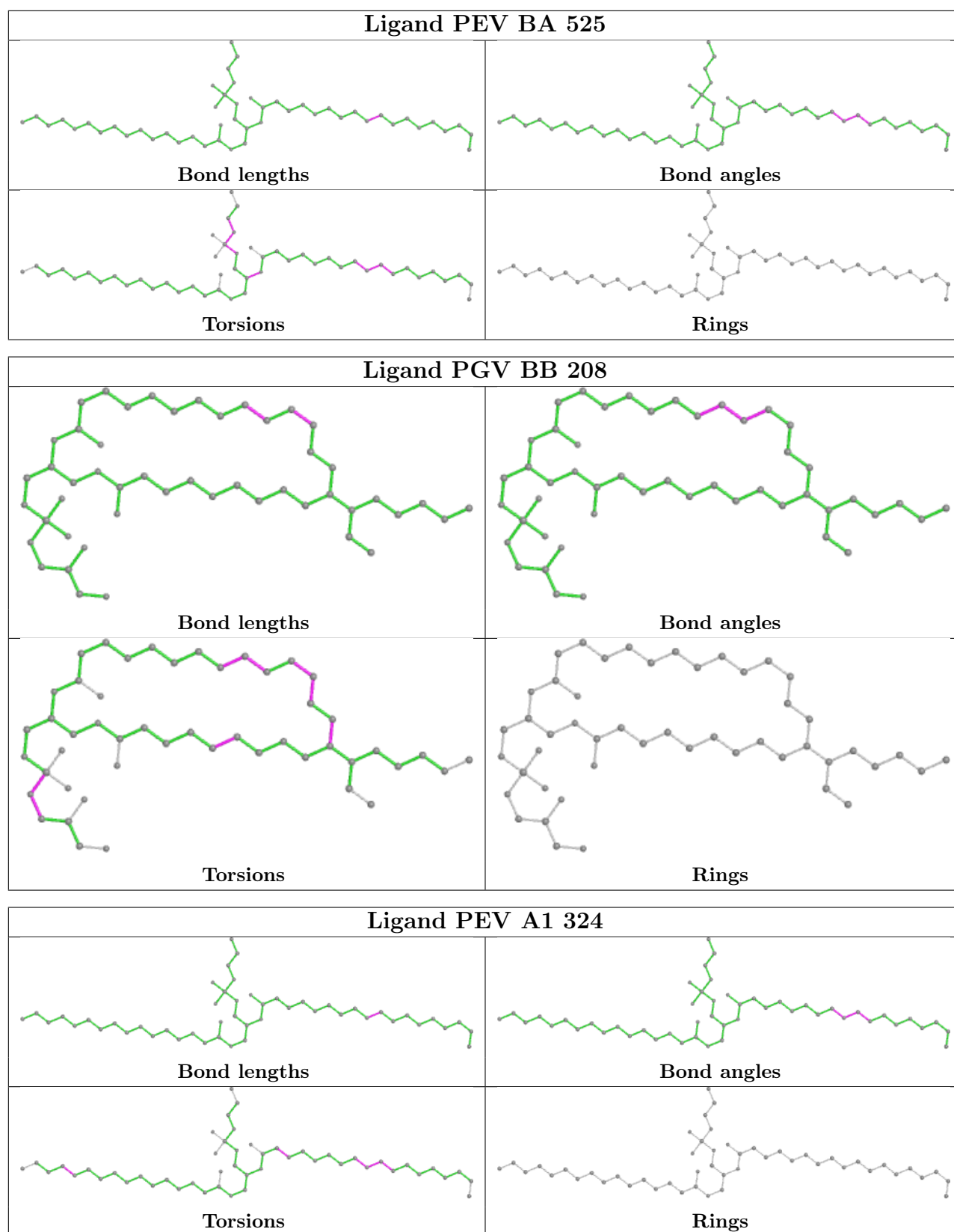
## Ligand PGV BA 536

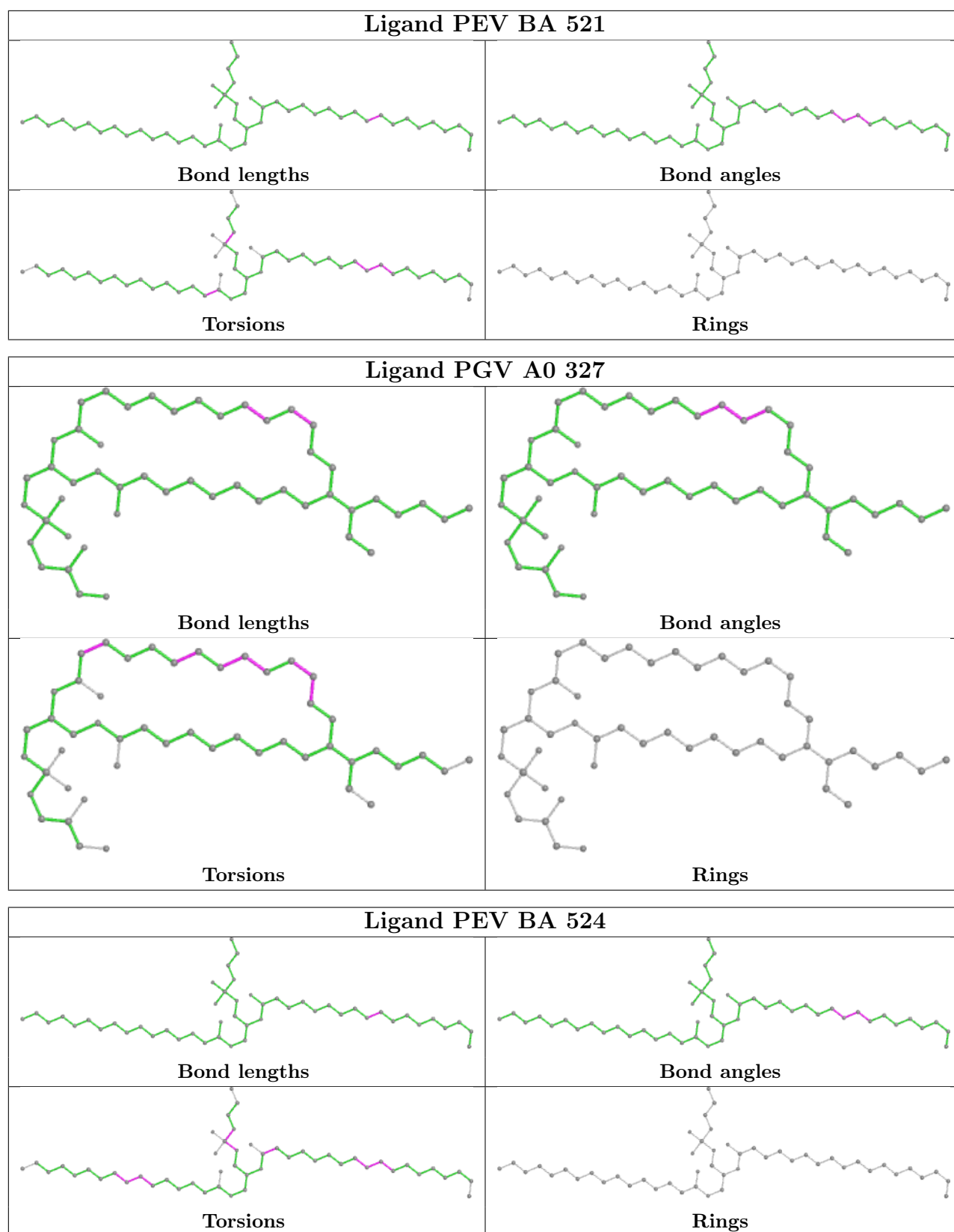


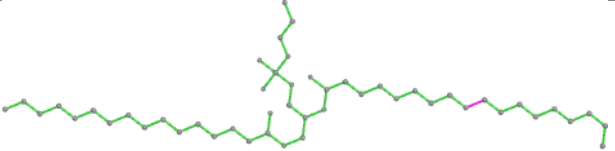
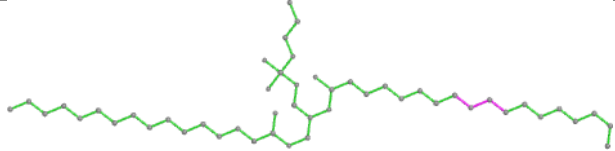
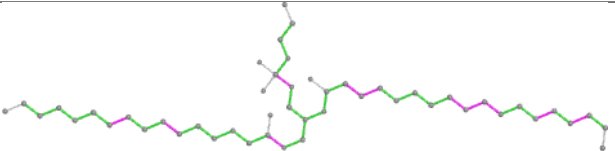
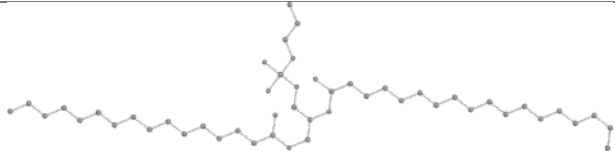
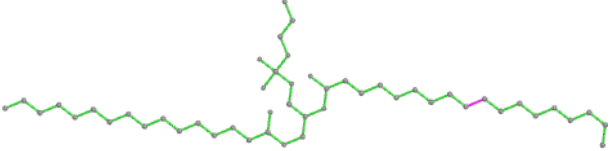
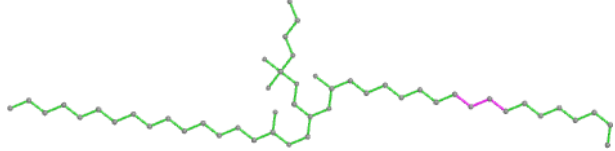
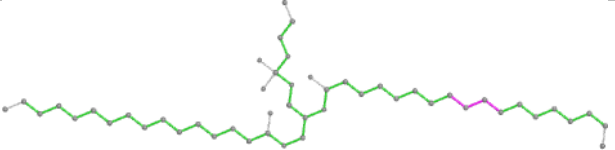
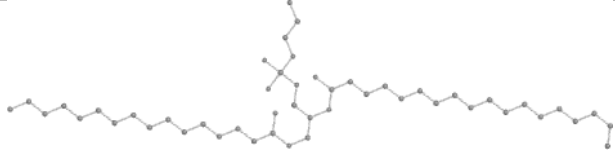
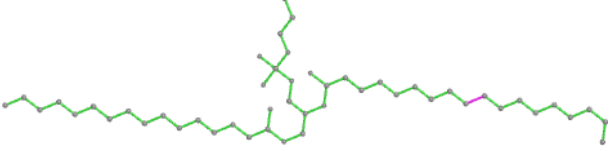
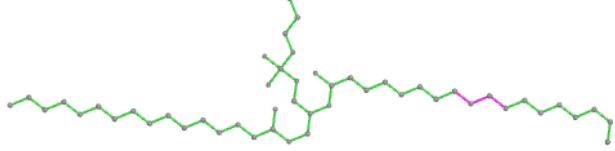
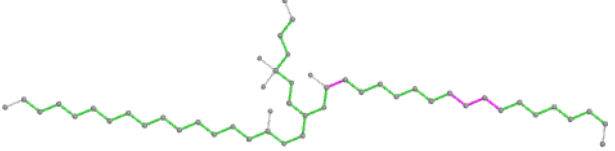
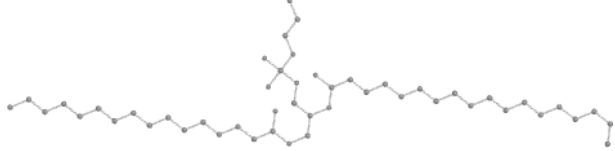
## Ligand PGV BB 213

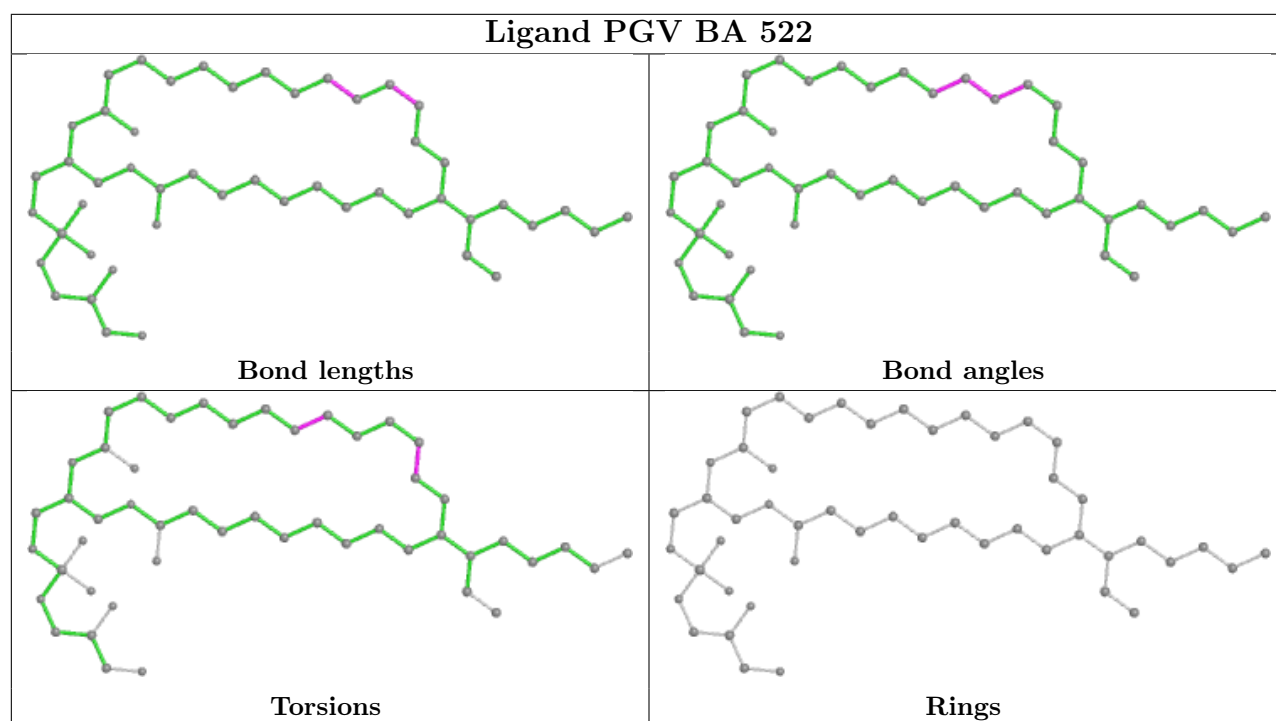
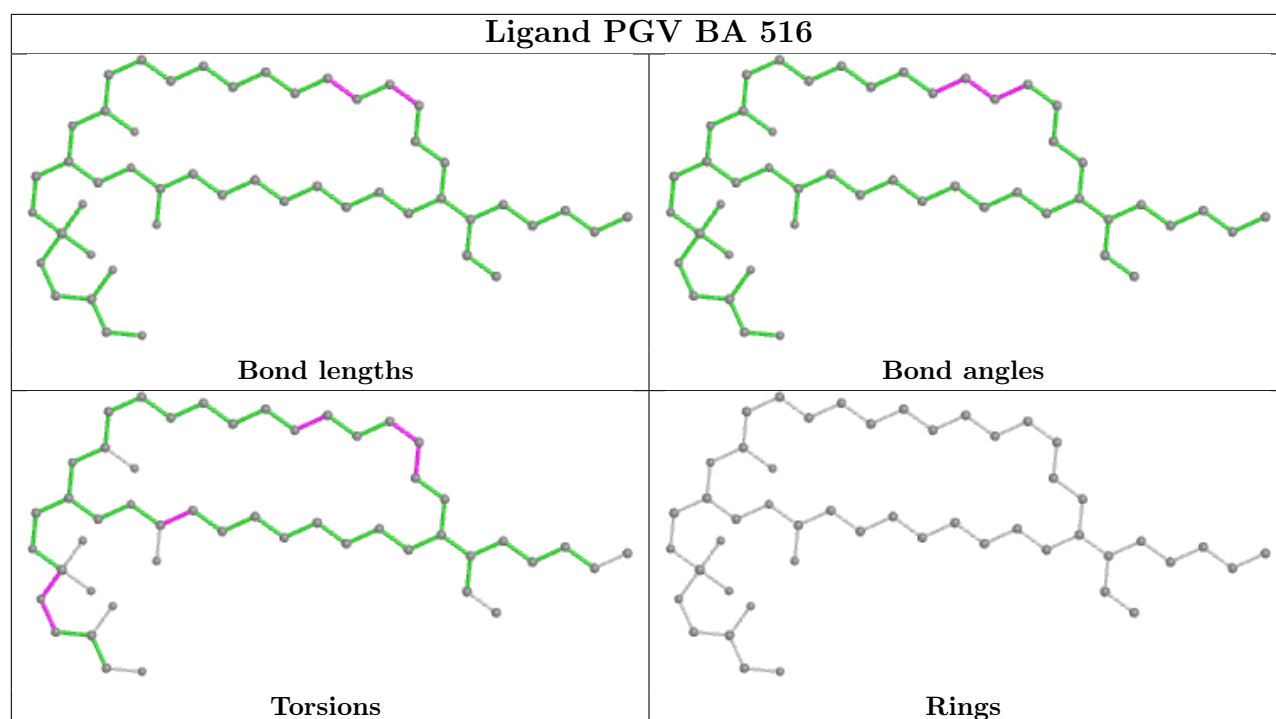


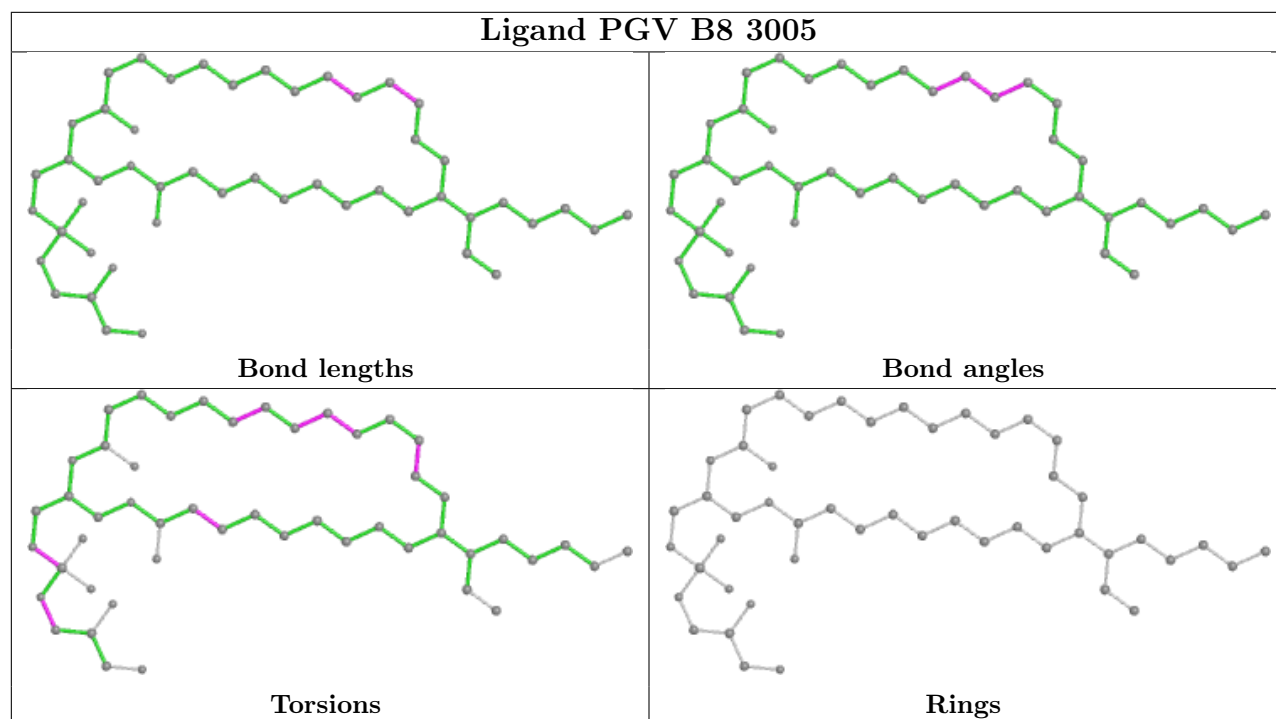
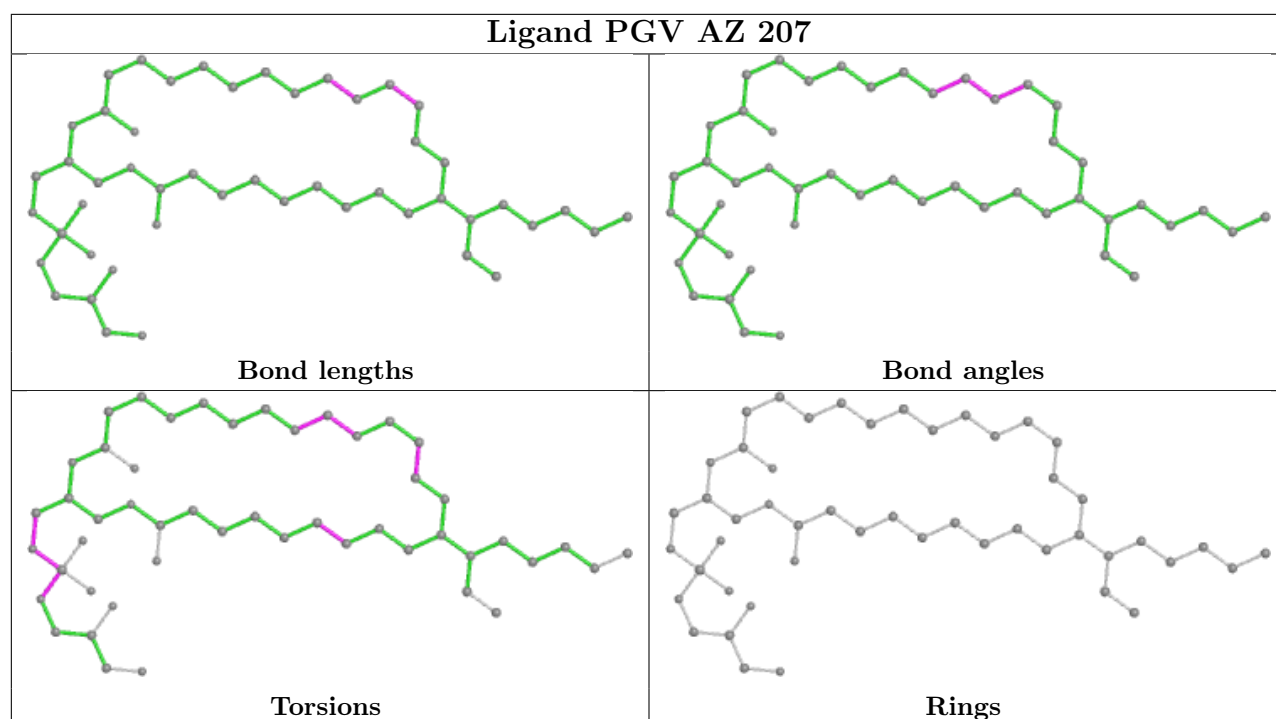


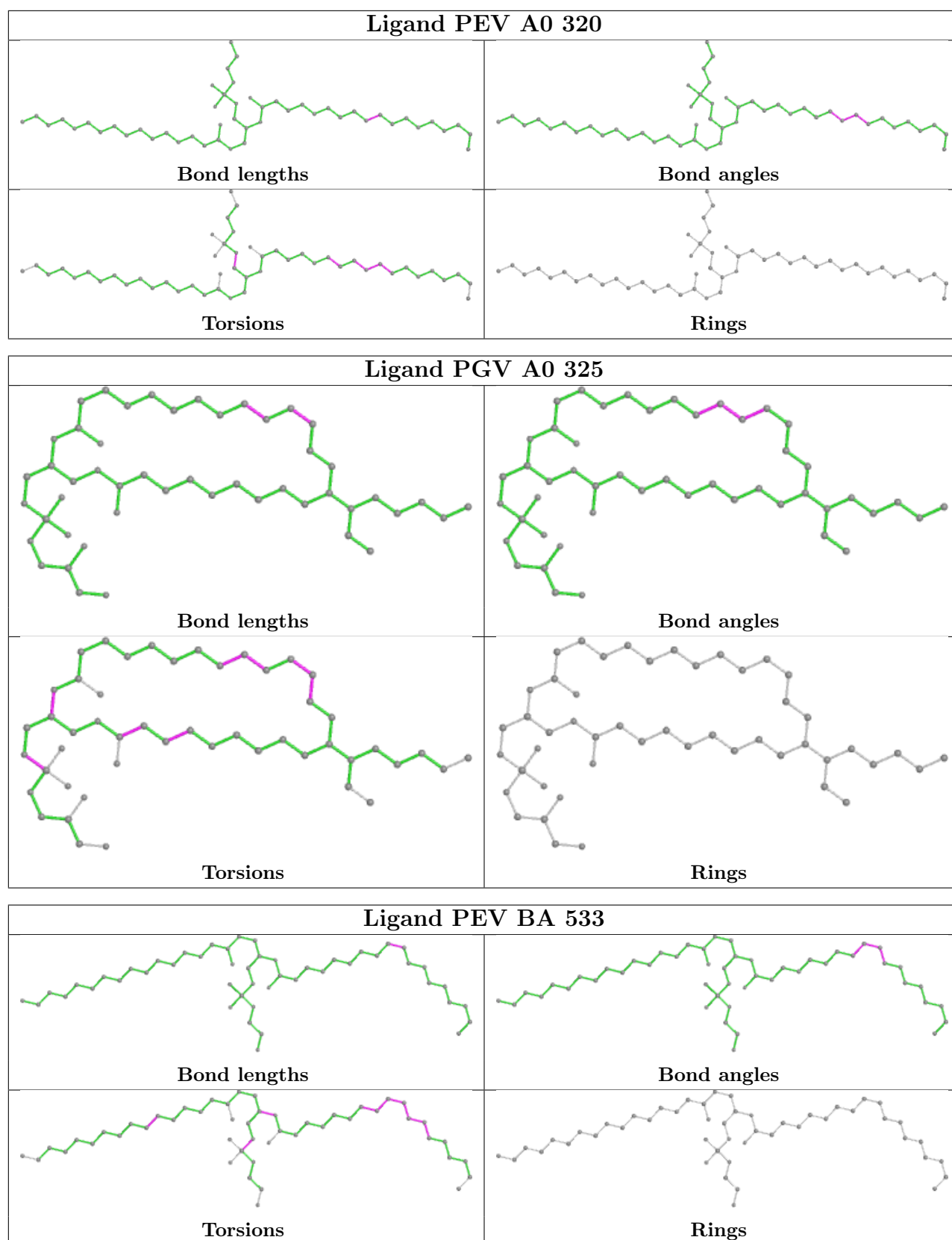


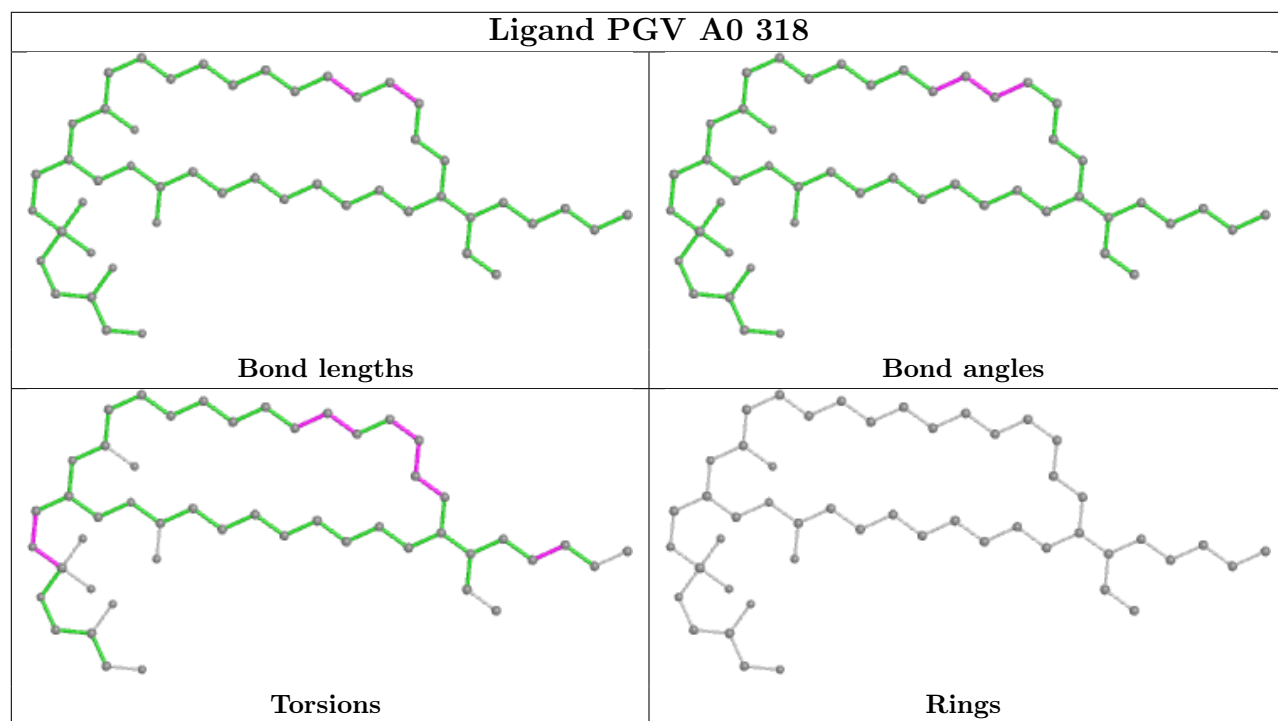
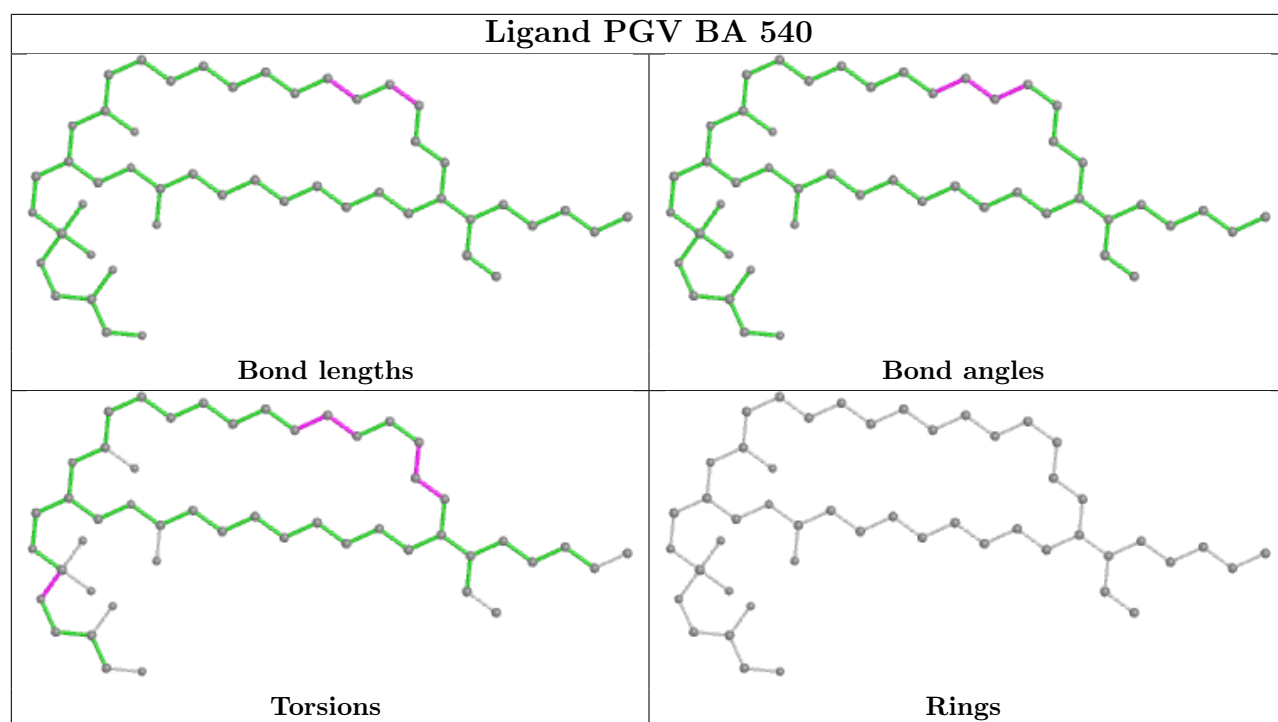


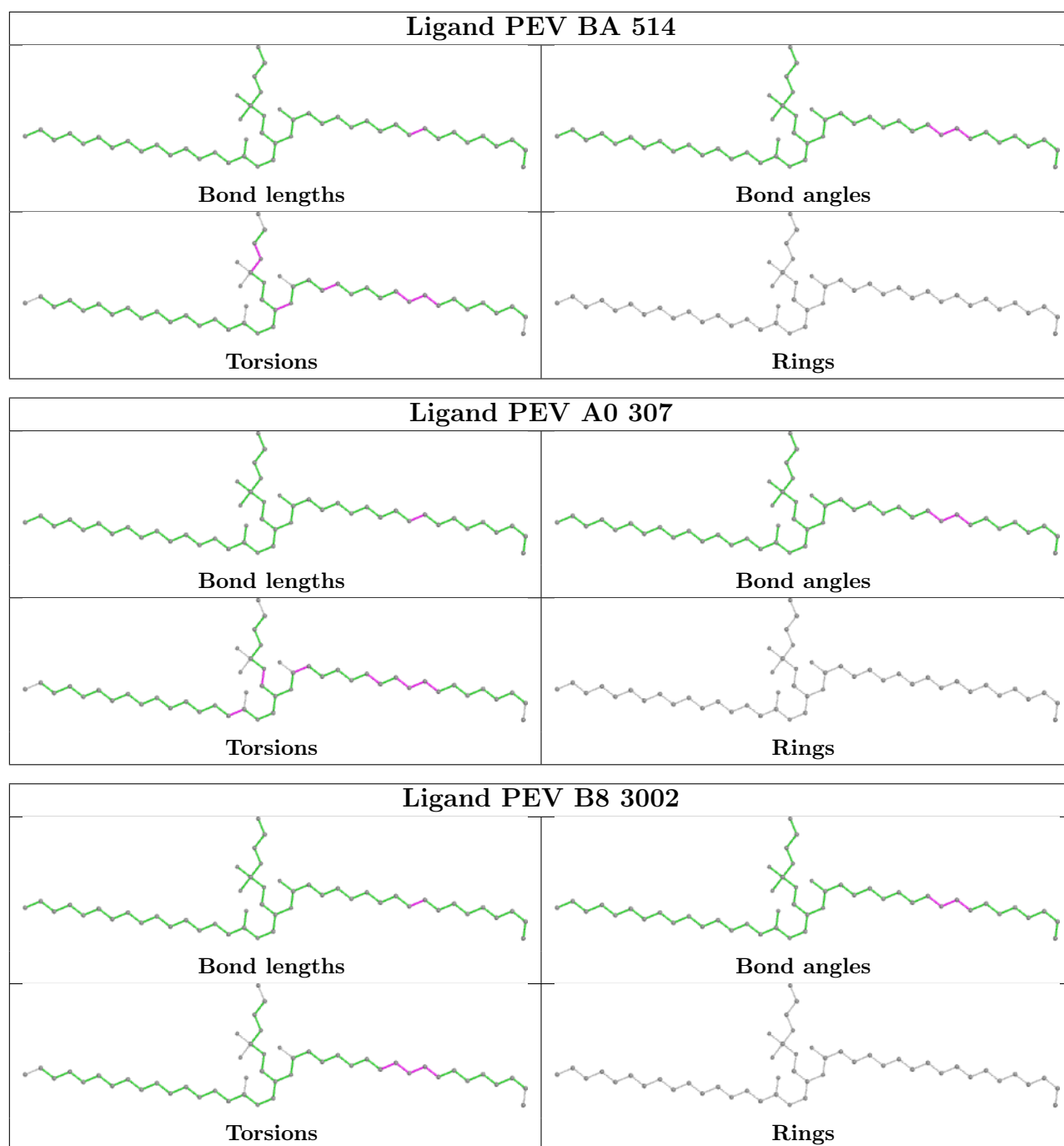
Ligand PEV A1 325	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand PEV BA 531	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand PEV BA 507	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

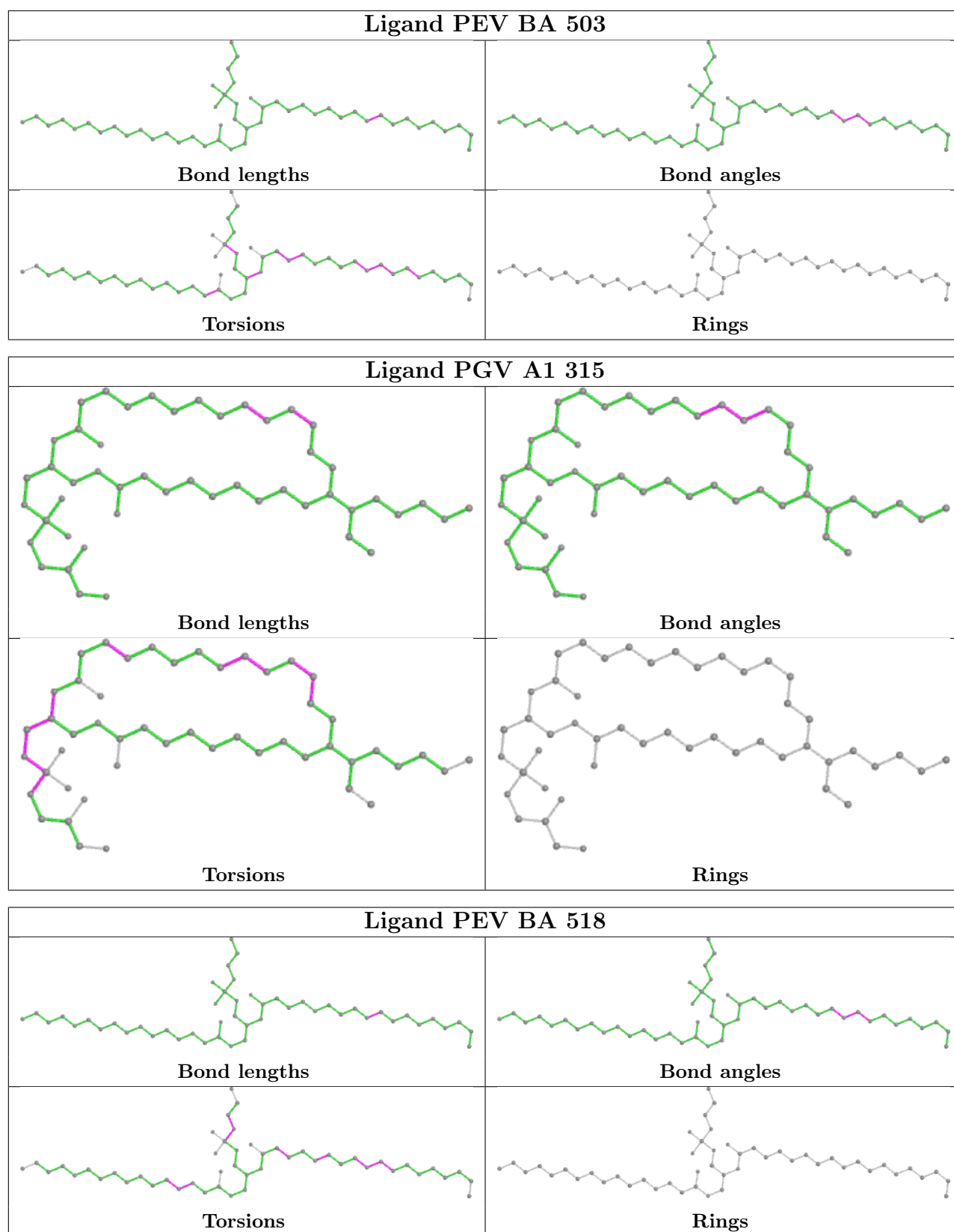


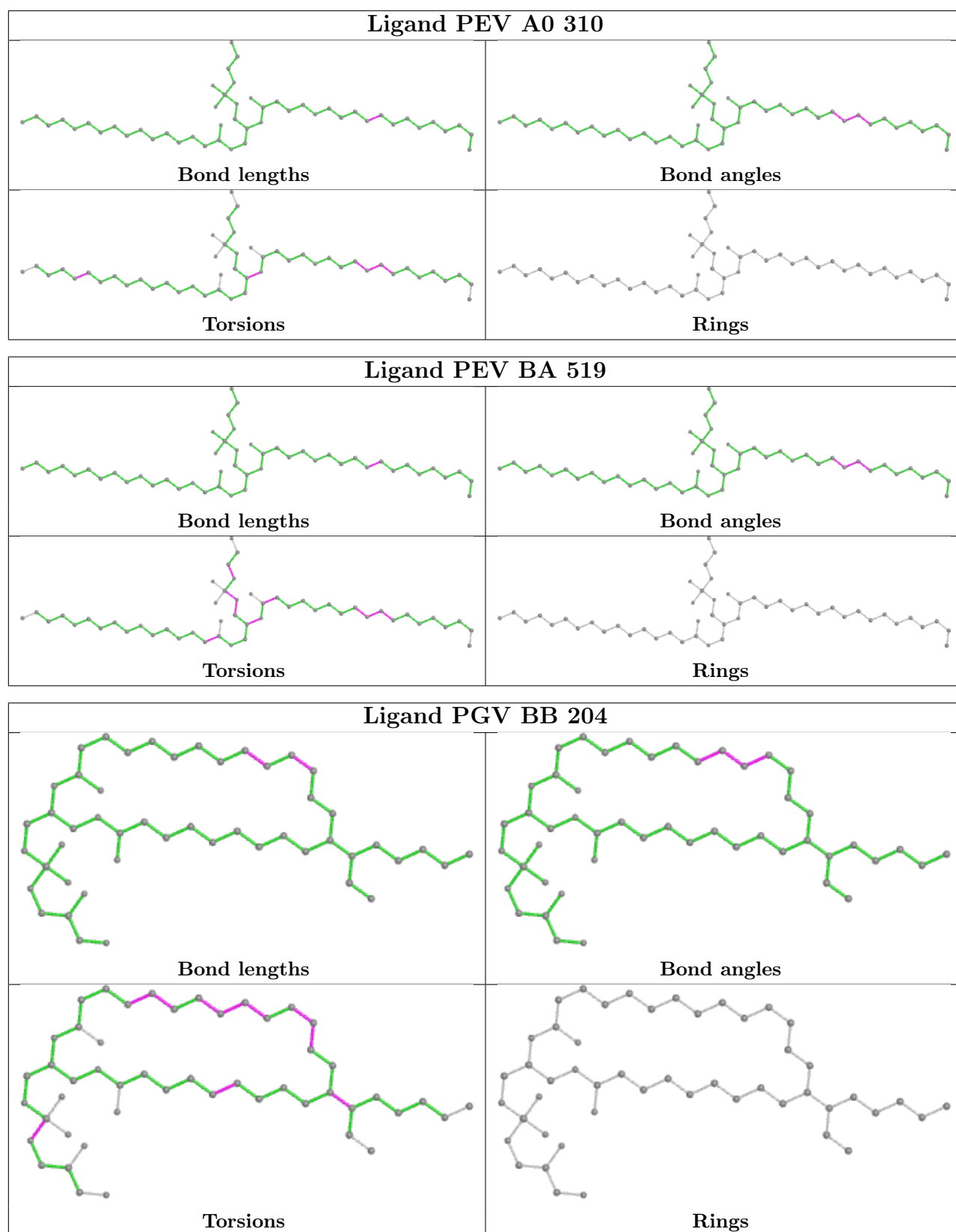


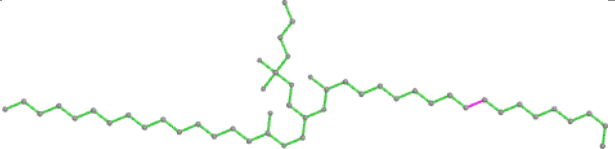
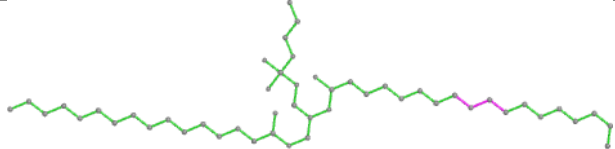
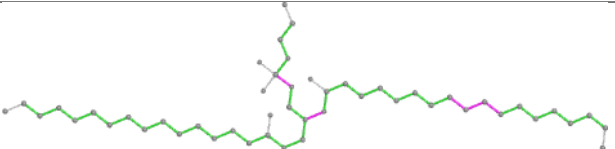
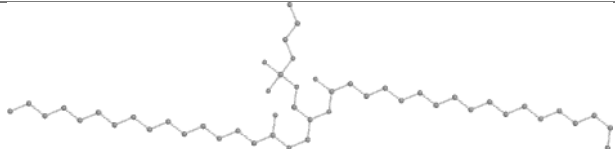
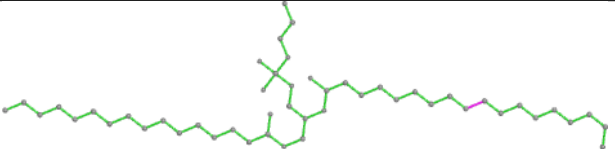
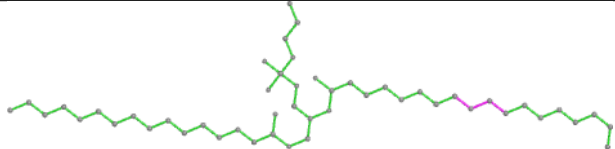
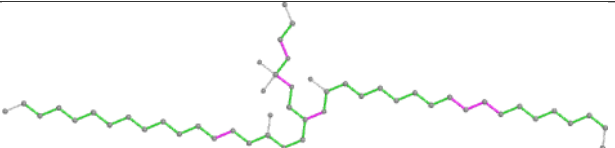
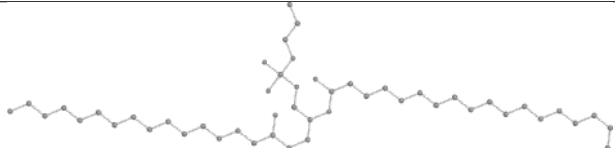
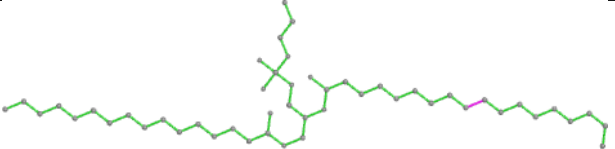
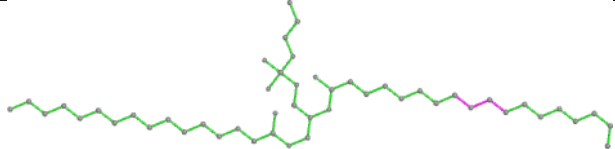
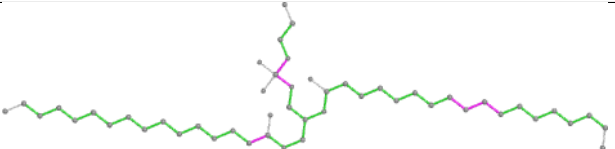
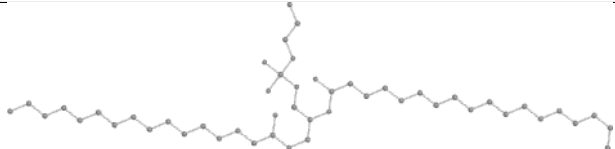


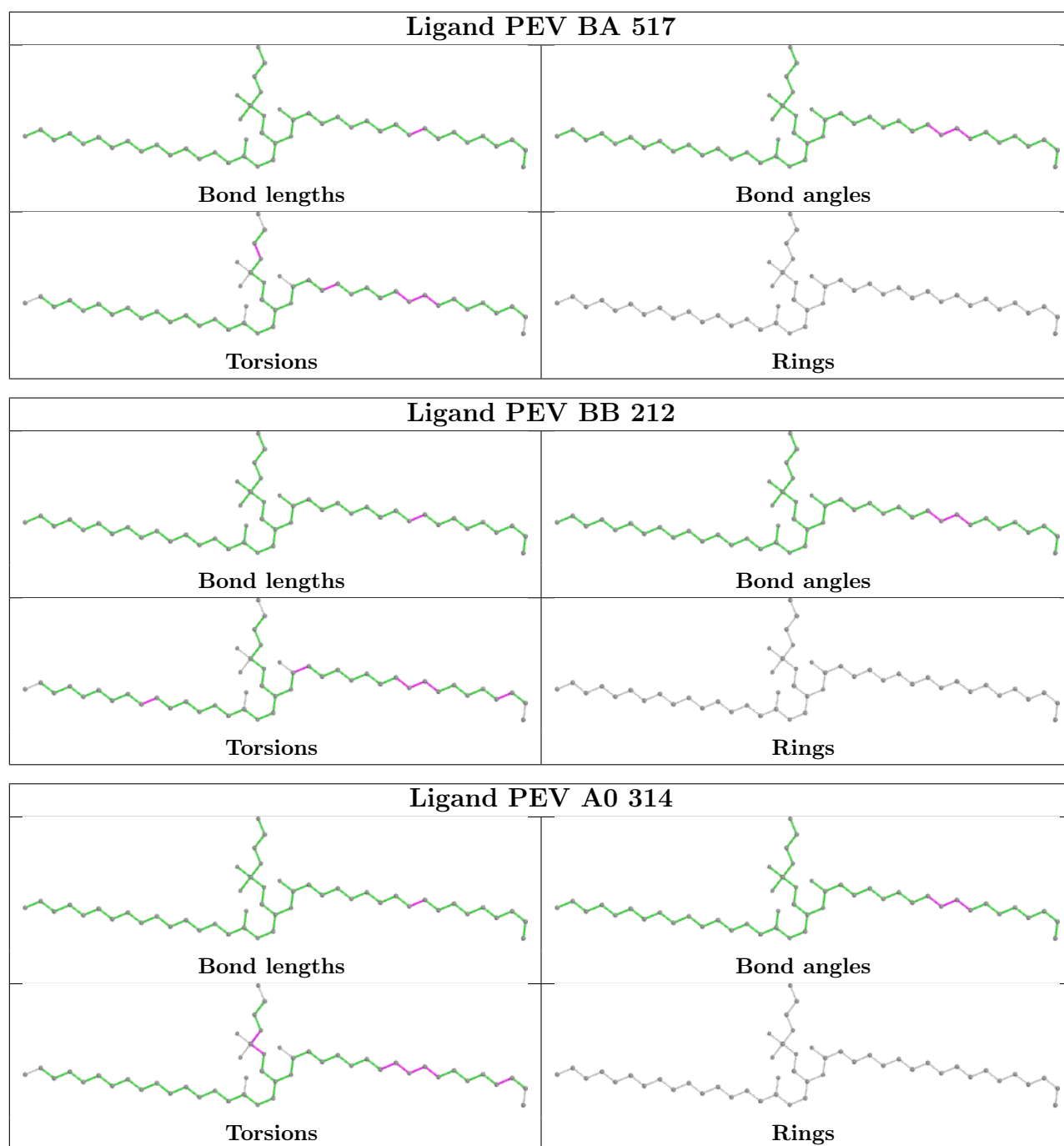


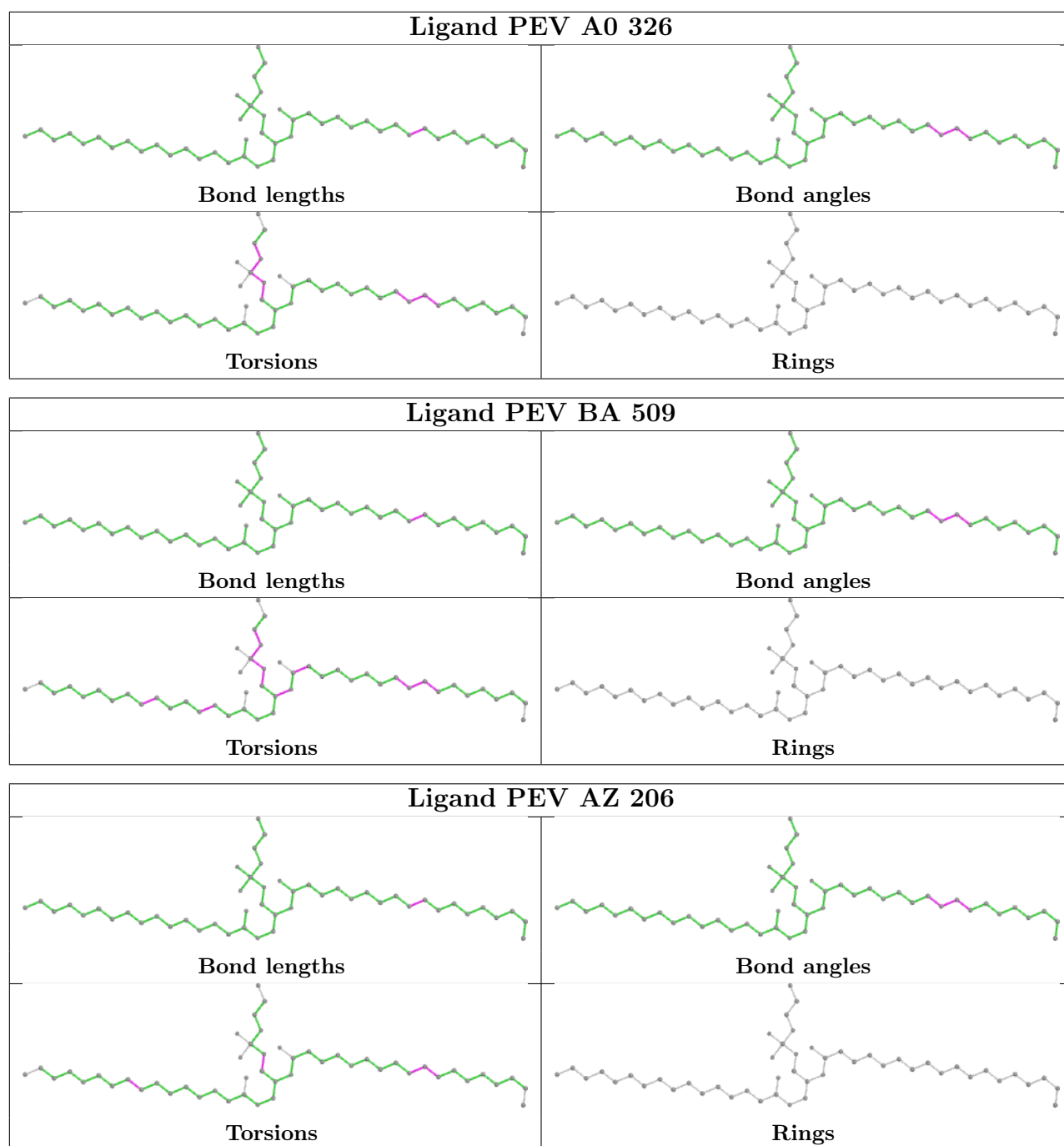


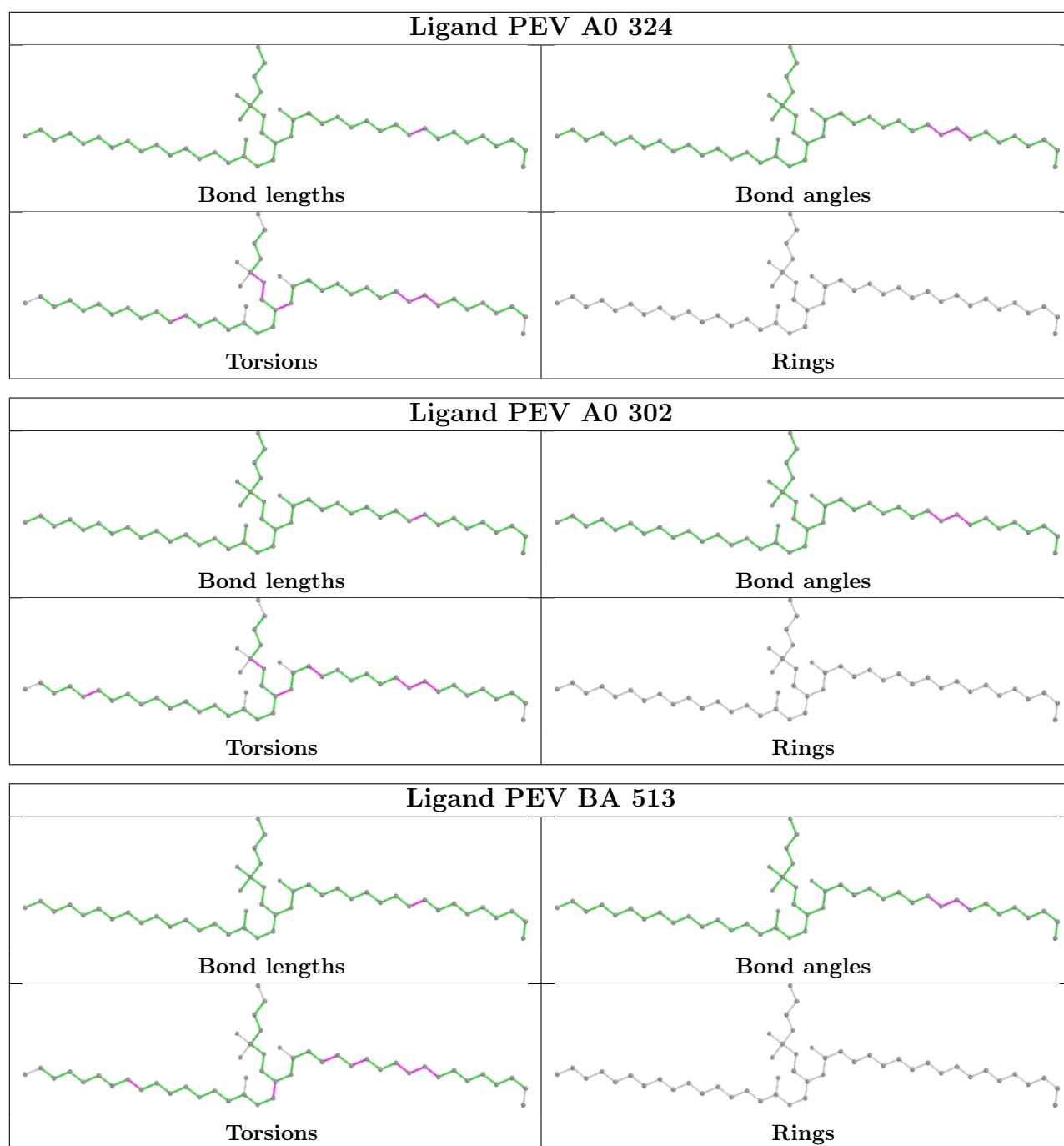


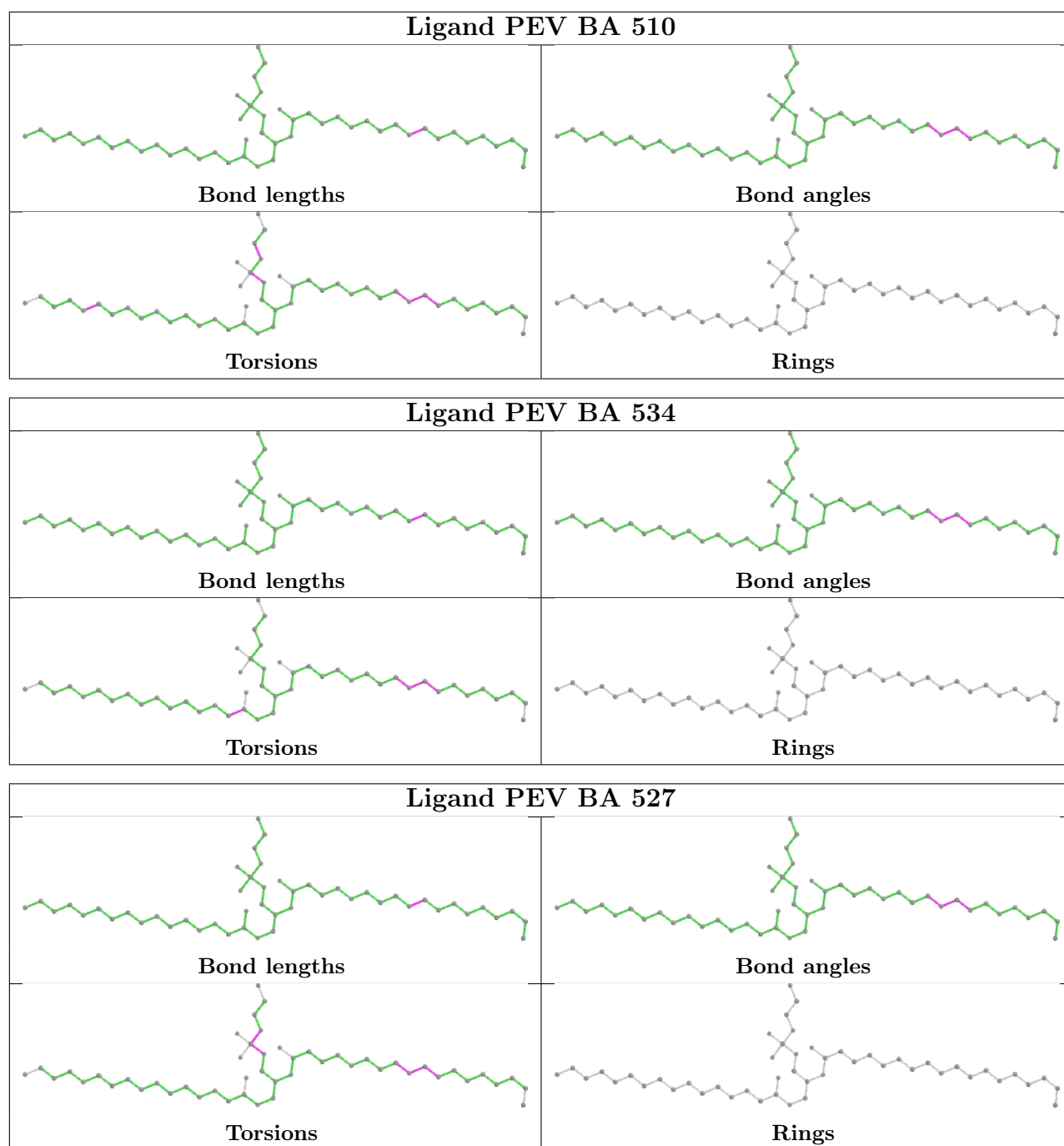


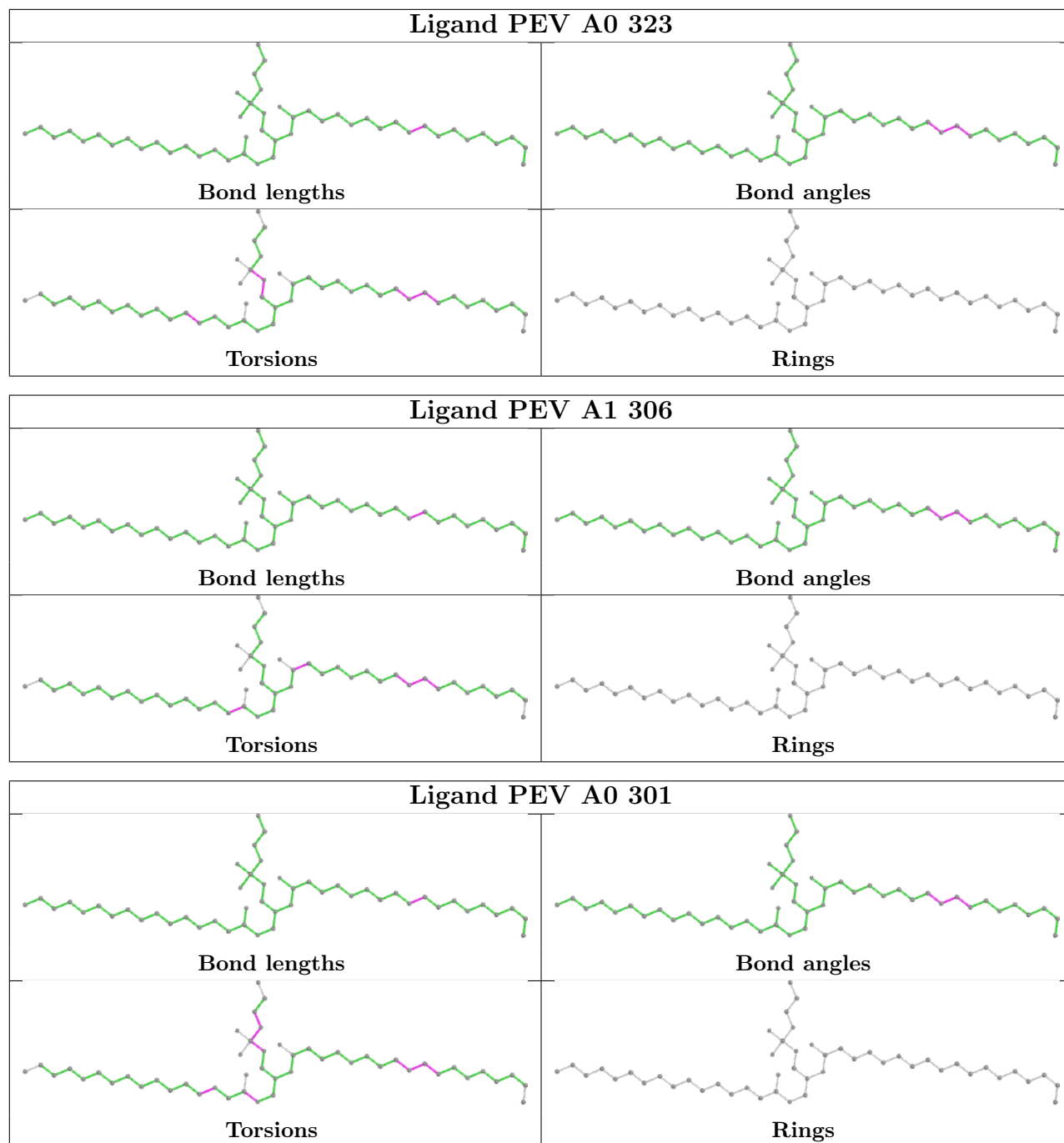
Ligand PEV A0 303	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand PEV A0 319	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand PEV BA 538	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

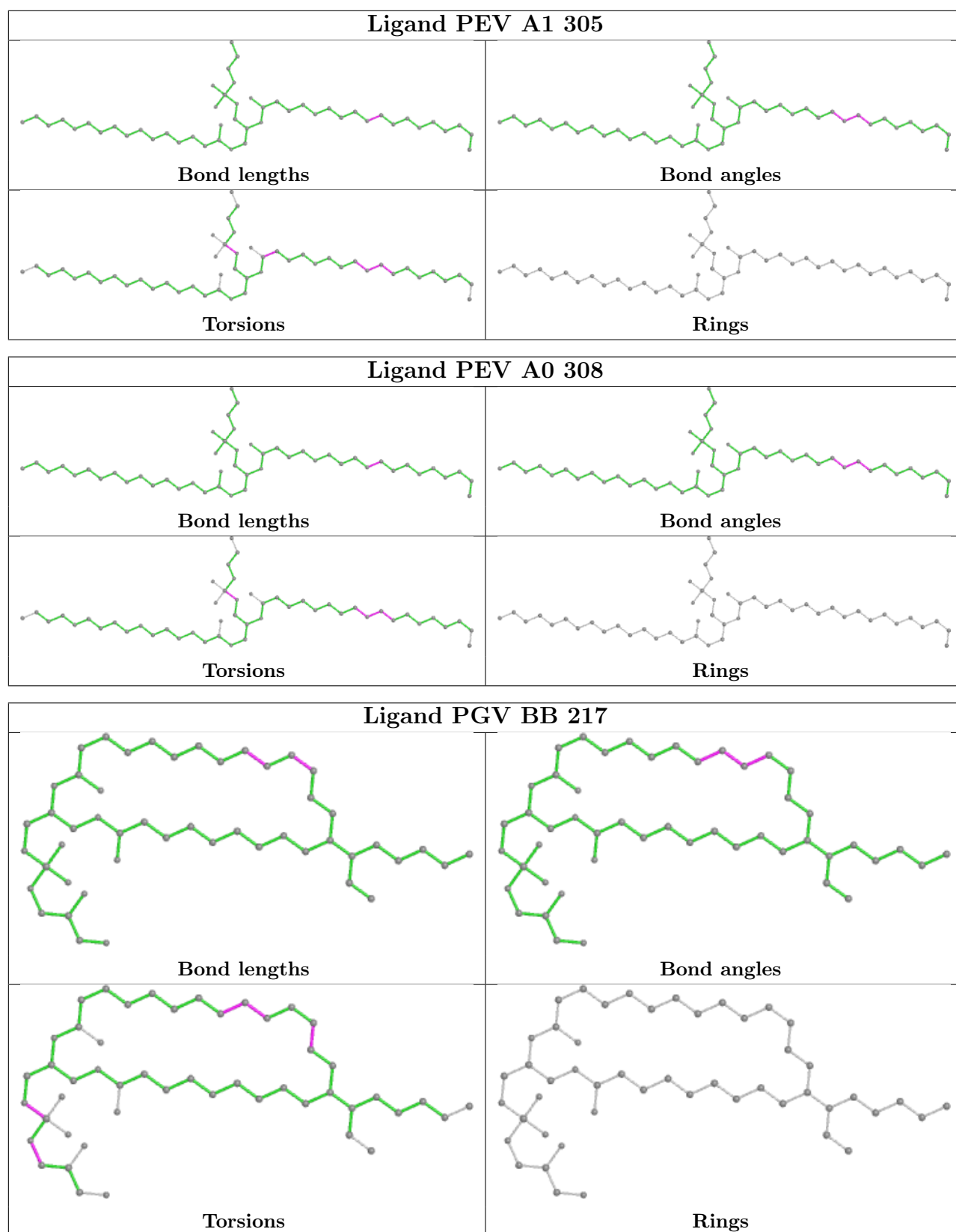


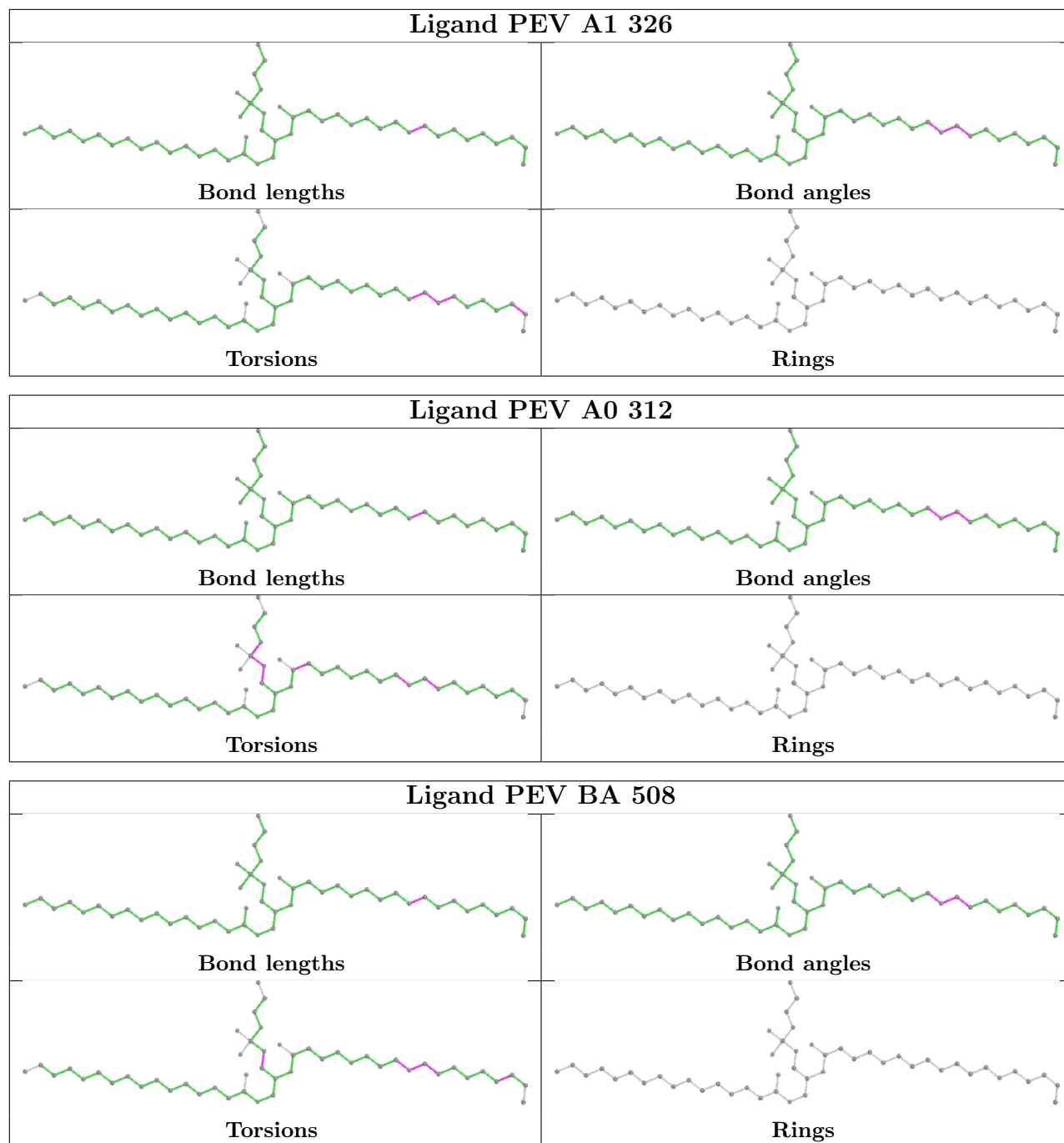


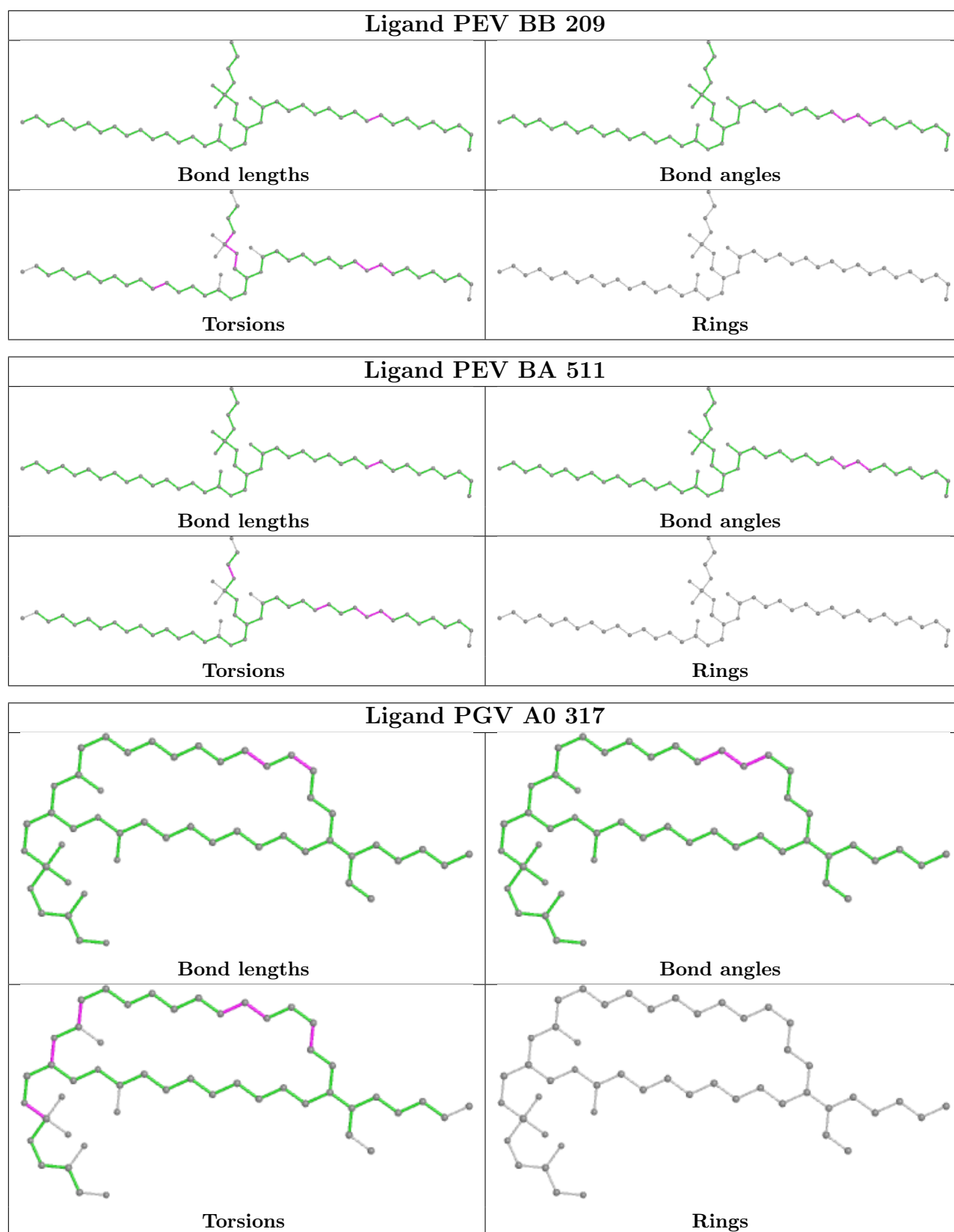


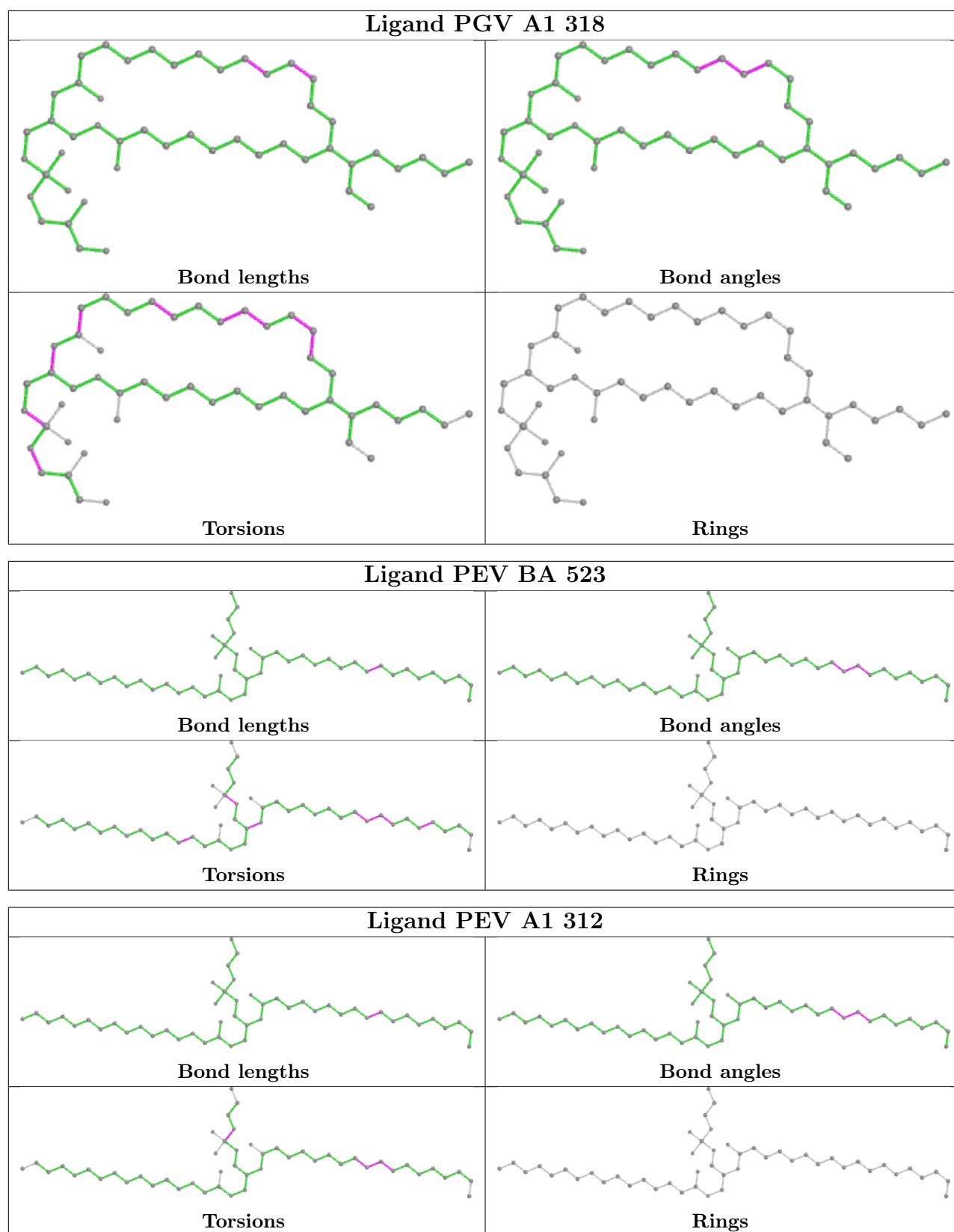


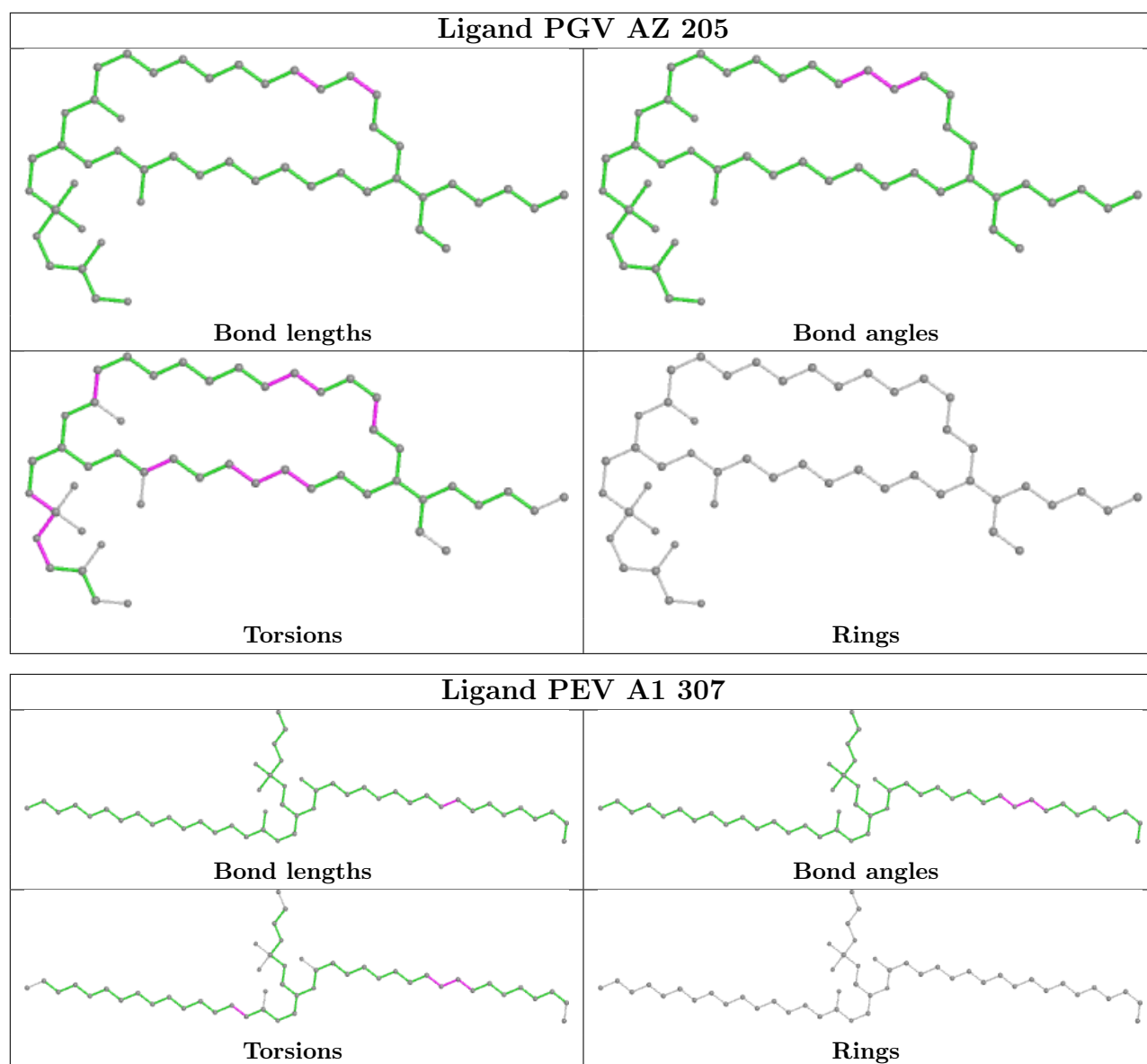












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

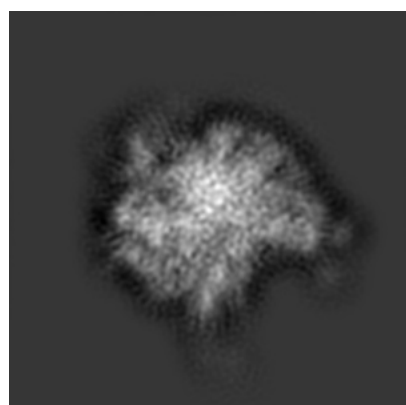
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1858. These allow visual inspection of the internal detail of the map and identification of artifacts.

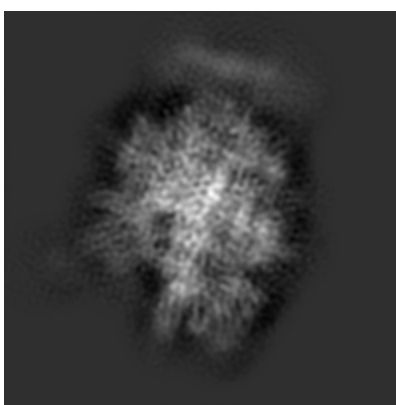
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

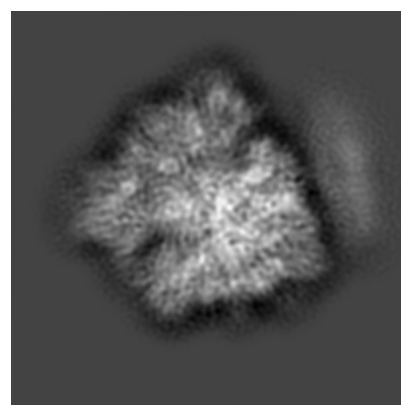
#### 6.1.1 Primary map



X



Y

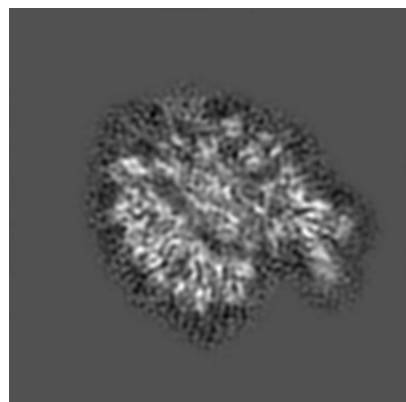


Z

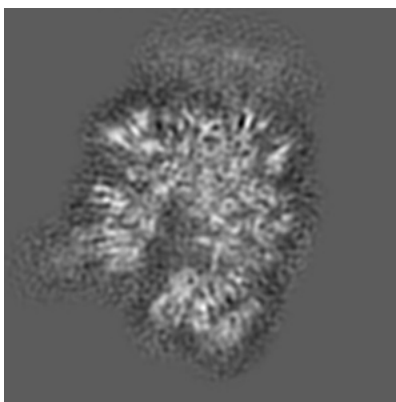
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

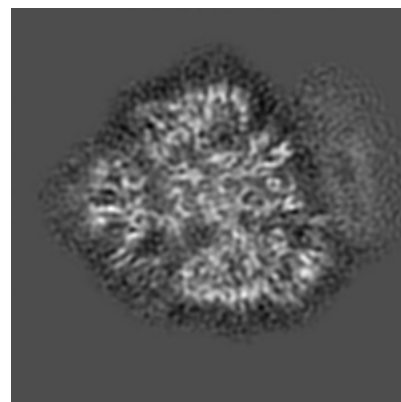
#### 6.2.1 Primary map



X Index: 160



Y Index: 160

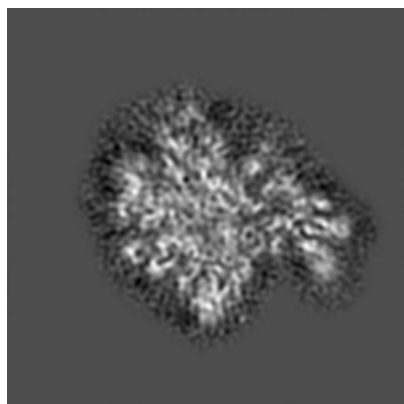


Z Index: 160

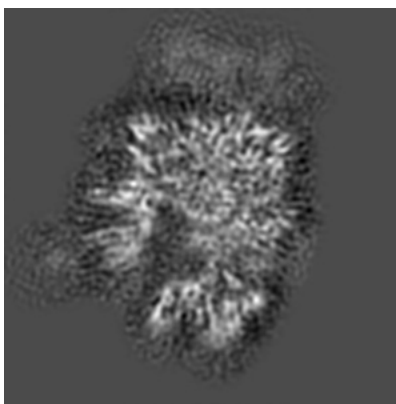
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

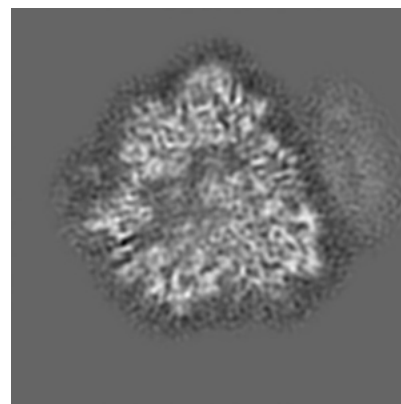
### 6.3.1 Primary map



X Index: 166



Y Index: 167

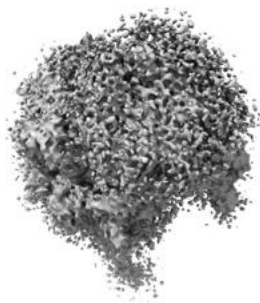


Z Index: 146

The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

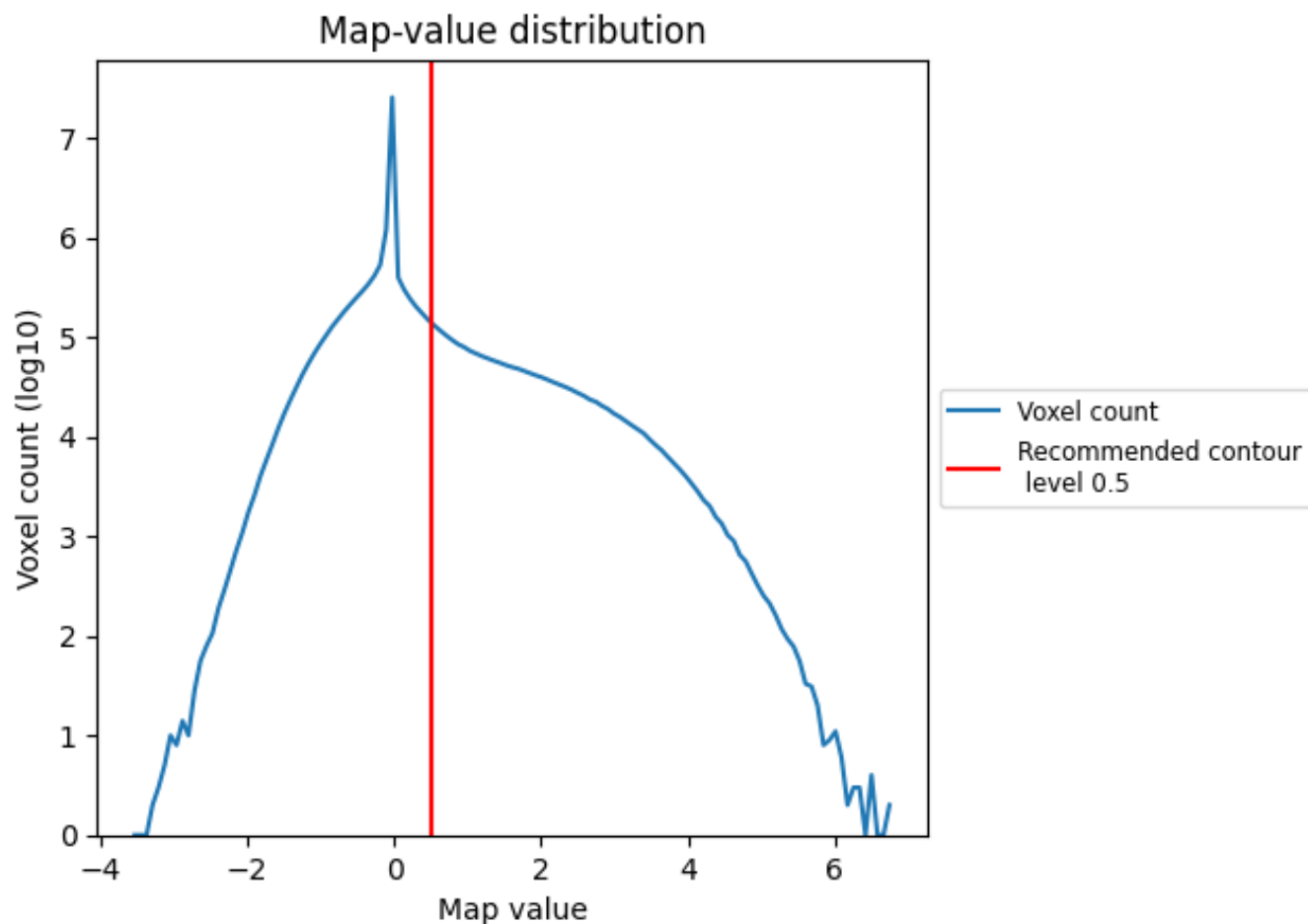
## 6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

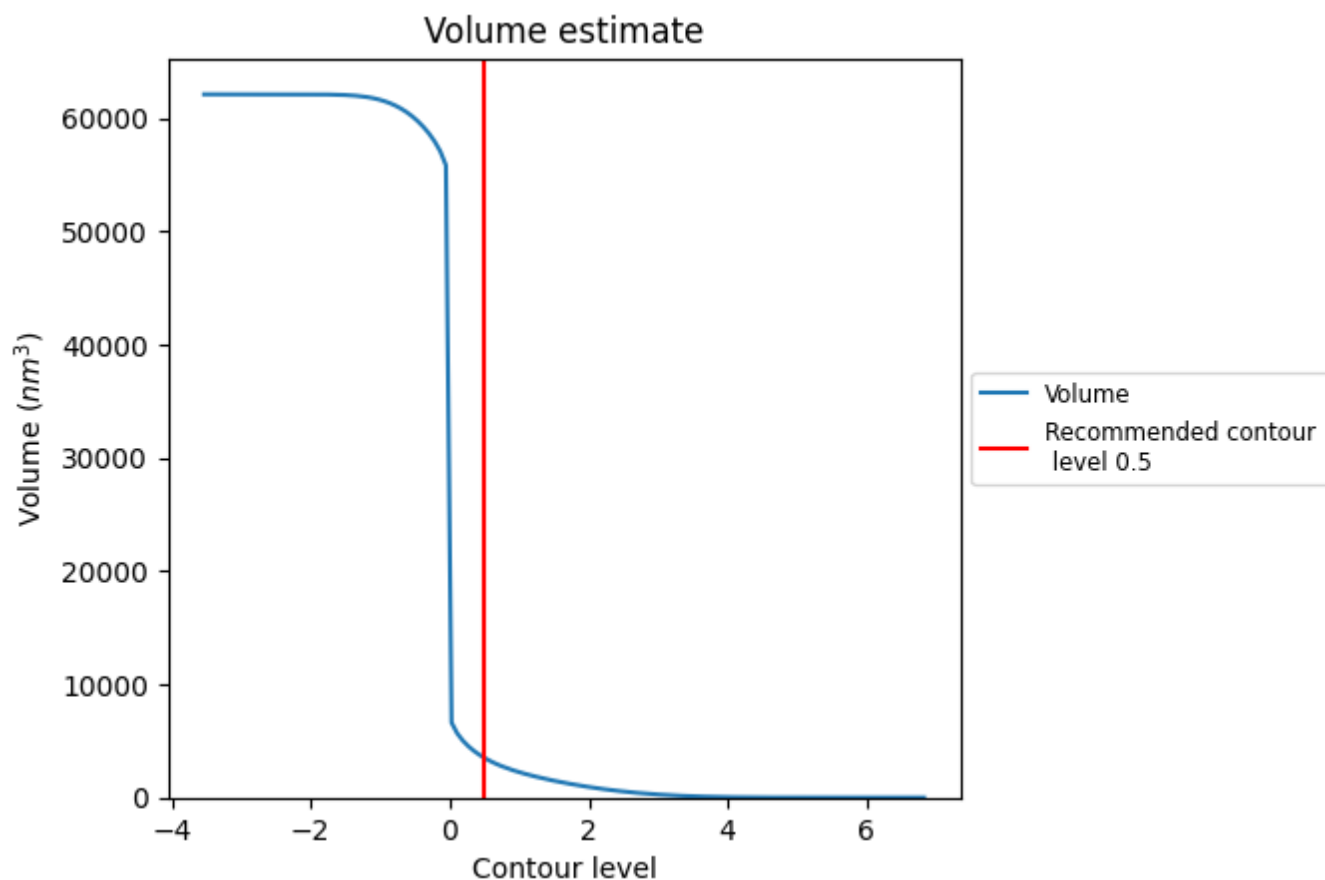
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

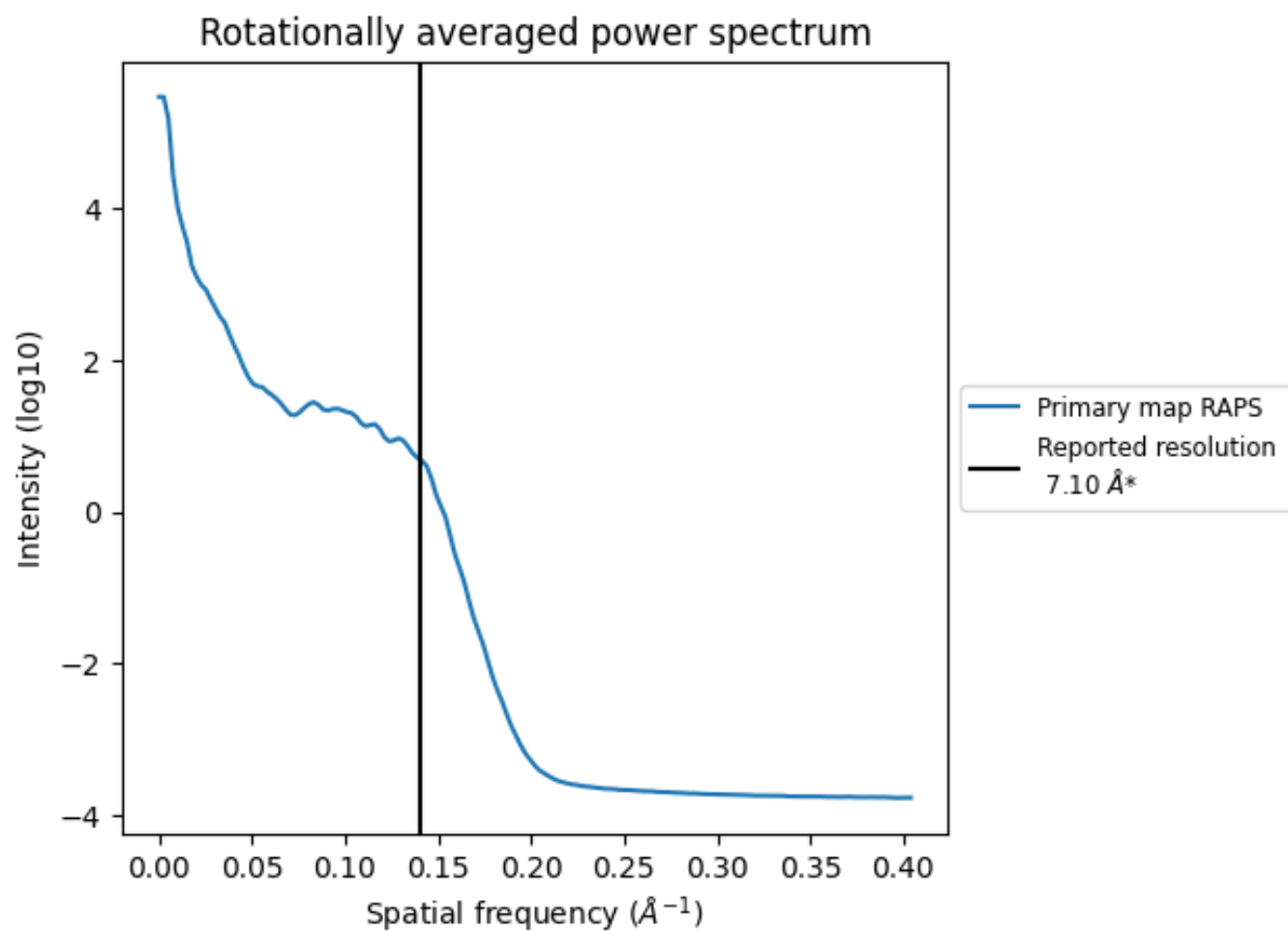
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3504  $\text{nm}^3$ ; this corresponds to an approximate mass of 3166 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.141 Å<sup>-1</sup>

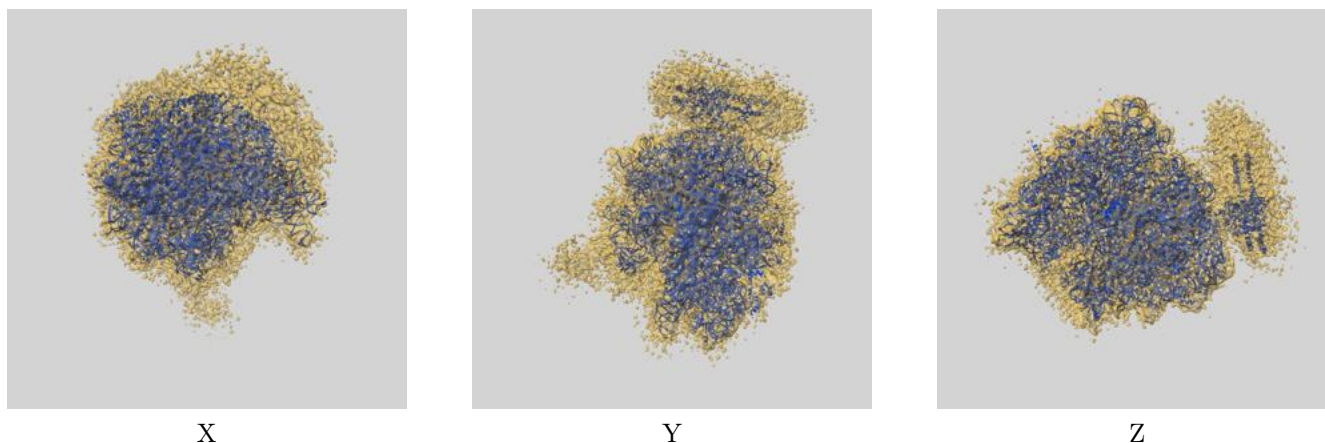
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

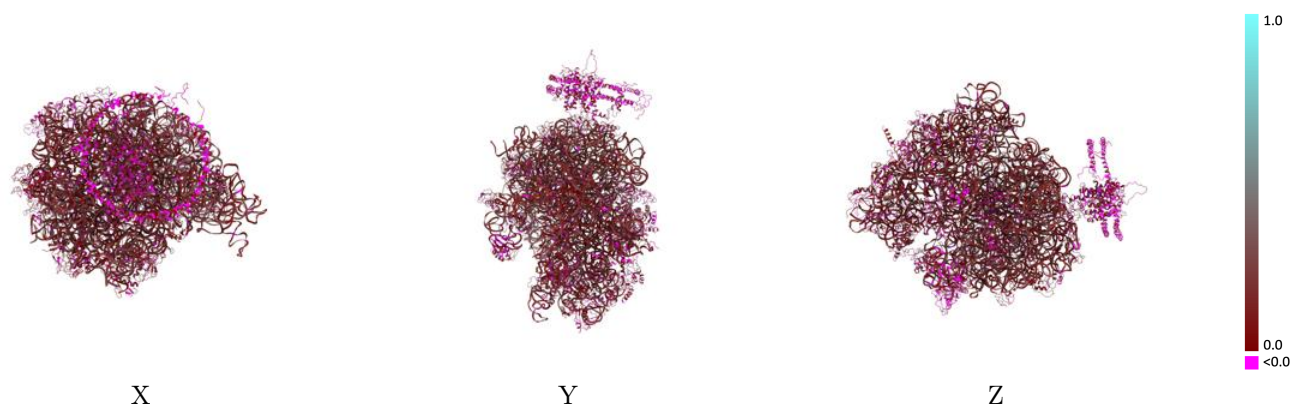
This section contains information regarding the fit between EMDB map EMD-1858 and PDB model 4V6M. Per-residue inclusion information can be found in section [3](#) on page [24](#).

### 9.1 Map-model overlay [i](#)



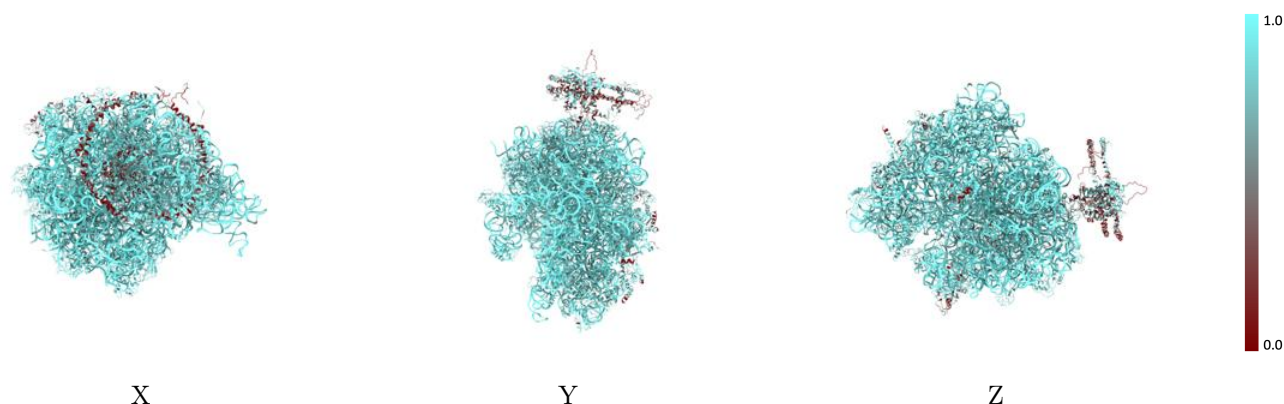
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



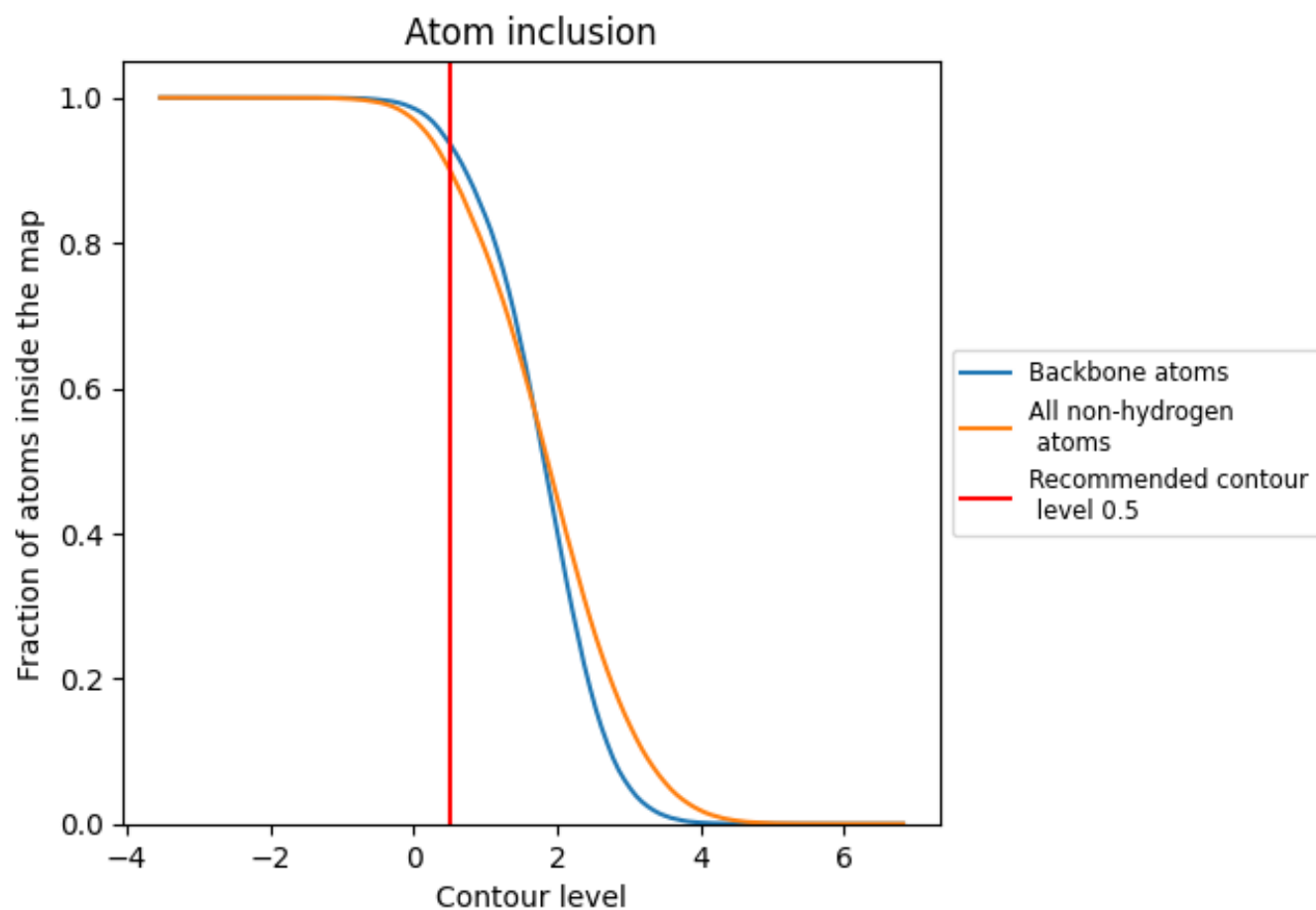
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ





















































The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9008	 0.1450
A0	 0.3258	 0.0170
A1	 0.5625	 0.0090
AA	 0.9846	 0.1740
AB	 0.7507	 0.1210
AC	 0.8279	 0.1200
AD	 0.8390	 0.1240
AE	 0.7781	 0.1190
AF	 0.7183	 0.1060
AG	 0.9093	 0.1350
AH	 0.8542	 0.1350
AI	 0.8731	 0.0980
AJ	 0.8950	 0.0950
AK	 0.8481	 0.1140
AL	 0.9251	 0.1180
AM	 0.8861	 0.1220
AN	 0.8669	 0.1230
AO	 0.9174	 0.1390
AP	 0.8852	 0.1220
AQ	 0.8994	 0.1230
AR	 0.8003	 0.1240
AS	 0.8903	 0.1060
AT	 0.8290	 0.1370
AU	 0.8357	 0.1220
AV	 0.9588	 0.1410
AX	 0.7922	 0.1000
AZ	 0.5154	 0.0640
B0	 0.8551	 0.1190
B1	 0.9423	 0.1170
B2	 0.9268	 0.0860
B3	 0.8961	 0.1220
B4	 0.9144	 0.1000
B5	 0.6780	 0.0570
B6	 0.9294	 0.1300
B7	 0.9883	 0.1840



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
B8	 0.9841	 0.1750
BA	 0.4615	 0.0370
BB	 0.4381	 0.0650
BD	 0.8973	 0.1180
BE	 0.8829	 0.1230
BF	 0.8966	 0.1180
BG	 0.9329	 0.1550
BH	 0.7436	 0.1150
BI	 0.9706	 0.0670
BJ	 0.8964	 0.1410
BK	 0.8970	 0.1400
BL	 0.9102	 0.1230
BM	 0.9463	 0.1330
BN	 0.8443	 0.1070
BO	 0.8990	 0.1260
BP	 0.8682	 0.1360
BQ	 0.8392	 0.1050
BR	 0.8821	 0.1390
BS	 0.8110	 0.1050
BT	 0.7847	 0.1180
BU	 0.8803	 0.1290
BV	 0.9350	 0.1430
BW	 0.9013	 0.0760
BX	 0.8486	 0.1040
BY	 0.8551	 0.1100
BZ	 0.8787	 0.1540