



wwPDB EM Validation Summary Report ⓘ

Feb 22, 2024 – 09:25 PM 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.; Beck-
mann, 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

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>.

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

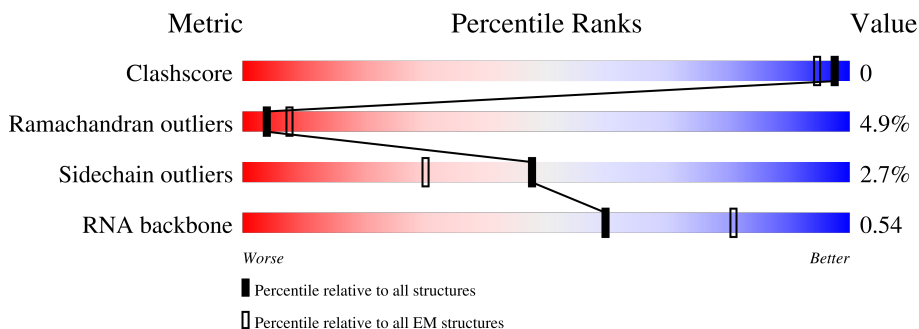
EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance i

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 ≥ 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	77% (Yellow), 20% (Orange), 3% (Red)
2	AX	11	27% (Red), 9% (Green), 45% (Yellow), 45% (Orange)
3	AV	77	75% (Yellow), 25% (Orange)
4	AZ	98	45% (Red), 76% (Green), 23% (Yellow)
5	A0	200	65% (Red), 96% (Green)
5	A1	200	41% (Red), 95% (Green)
6	AB	240	12% (Red), 94% (Green), 5% (Orange)

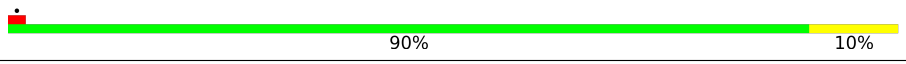
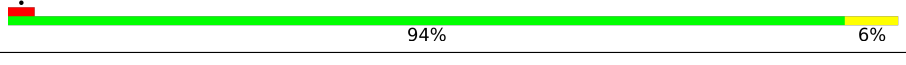
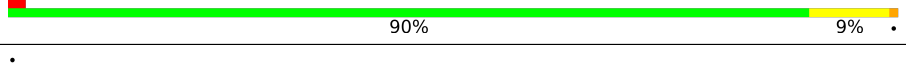
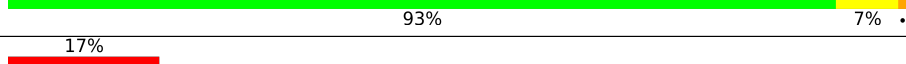

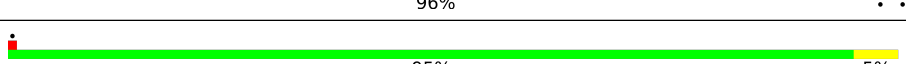
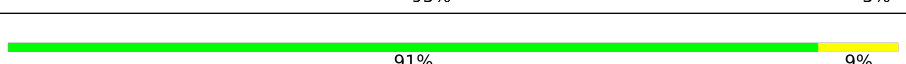
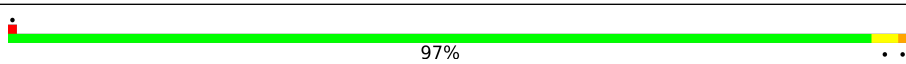
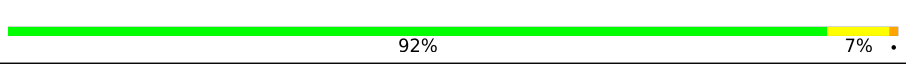
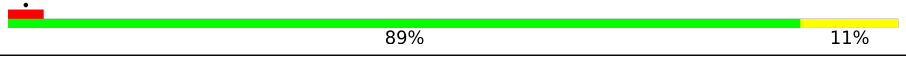
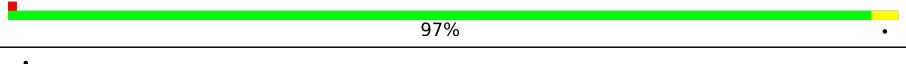
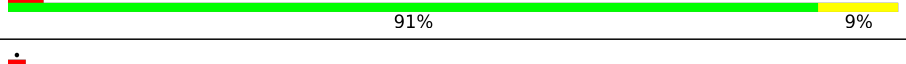
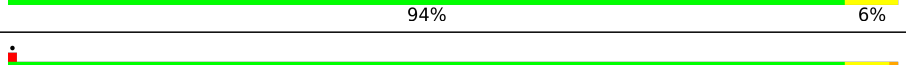
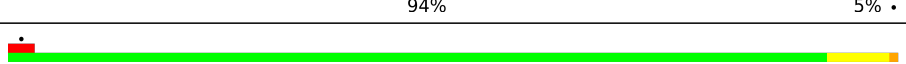
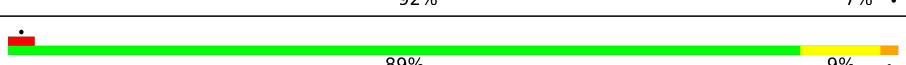
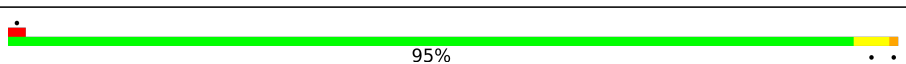
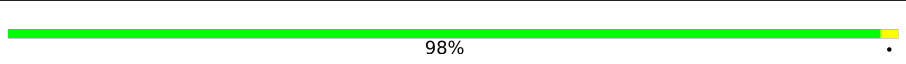
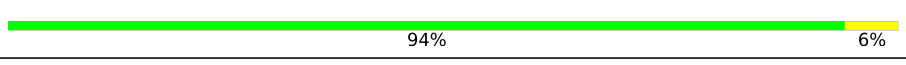
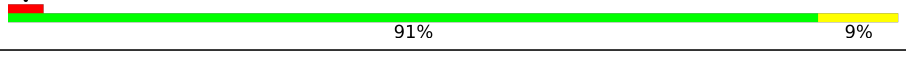
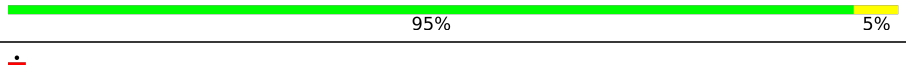
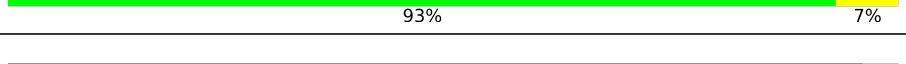
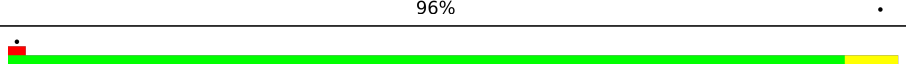
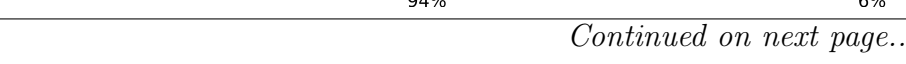


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Mol	Chain	Length	Quality of chain
7	AC	232	90% 9%
8	AD	205	91% 9%
9	AE	166	94% 5% 11%
10	AF	135	93% 7% 19%
11	AG	178	97%
12	AH	129	95% 5%
13	AI	129	90% 9%
14	AJ	103	88% 12%
15	AK	128	94% 6% 7%
16	AL	123	96%
17	AM	117	92% 7%
18	AN	100	88% 12%
19	AO	88	97%
20	AP	82	95%
21	AQ	83	87% 13%
22	AR	74	92% 8% 7%
23	AS	91	96%
24	AT	86	97%
25	AU	70	94% 6% 6%
26	B7	120	82% 18%
27	B8	2904	80% 18%
28	BA	435	80% 16% 40%
29	BB	116	89% 10% 34%
30	B5	234	95% 5% 24%
31	B6	272	93% 6%


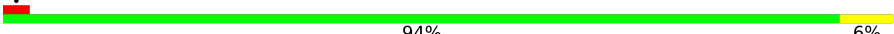

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Mol	Chain	Length	Quality of chain
32	BD	209	 90% 10%
33	BE	201	 94% 6%
34	BF	178	 90% 9%
35	BG	176	 93% 7%
36	BH	149	 17% 88% 11%
37	BI	141	 96%
38	BJ	142	 95% 5%
39	BK	123	 91% 9%
40	BL	144	 97%
41	BM	136	 92% 7%
42	BN	127	 89% 11%
43	BO	117	 97%
44	BP	114	 91% 9%
45	BQ	117	 94% 6%
46	BR	103	 94% 5%
47	BS	110	 92% 7%
48	BT	100	 89% 9%
49	BU	103	 95%
50	BV	94	 98%
51	BW	84	 94% 6%
52	BX	77	 91% 9%
53	BY	63	 95% 5%
54	BZ	58	 93% 7%
55	B0	56	 96%
56	B1	54	 94% 6%

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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 i

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
			Total	C	N	O	P		
1	AA	1542	33080	14754	6064	10720	1542	0	0

- Molecule 2 is a RNA chain called mRNA.

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

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

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

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

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

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
			Total	C	N	O	S		
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
			Total	C	N	O	S		
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
			Total	C	N	O	S		
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
			Total	C	N	O	S		
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
			Total	C	N	O	S		
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
			Total	C	N	O	S		
17	AM	117	910	564	183	160	3	0	0

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

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

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

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

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
			Total	C	N	O	S		
20	AP	82	649	406	128	114	1	0	0

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

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

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

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

- 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
			Total	C	N	O	S		
30	B5	234	1733	1081	315	330	7	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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		

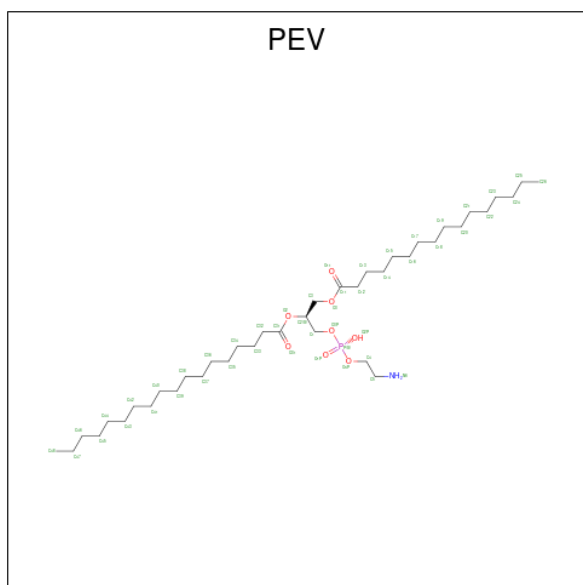
- Molecule 58 is a protein called 50S ribosomal protein L35.

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

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

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

- Molecule 60 is (1S)-2-[[[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (three-letter code: PEV) (formula: C₃₉H₇₈NO₈P).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
60	AZ	1	49	39	1	8	1	0
60	AZ	1	49	39	1	8	1	0
60	AZ	1	49	39	1	8	1	0
60	AZ	1	49	39	1	8	1	0
60	AZ	1	49	39	1	8	1	0
60	A0	1	49	39	1	8	1	0
60	A0	1	49	39	1	8	1	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
60	A0	1	49	39	1	8	1	0
60	A0	1	49	39	1	8	1	0
60	A0	1	49	39	1	8	1	0
60	A0	1	49	39	1	8	1	0
60	A0	1	49	39	1	8	1	0
60	A0	1	49	39	1	8	1	0
60	A0	1	49	39	1	8	1	0
60	A0	1	49	39	1	8	1	0
60	A0	1	49	39	1	8	1	0
60	A0	1	49	39	1	8	1	0
60	A0	1	49	39	1	8	1	0
60	A0	1	49	39	1	8	1	0
60	A0	1	49	39	1	8	1	0
60	A0	1	49	39	1	8	1	0
60	A0	1	49	39	1	8	1	0
60	A0	1	49	39	1	8	1	0
60	A0	1	49	39	1	8	1	0
60	A0	1	49	39	1	8	1	0
60	A0	1	49	39	1	8	1	0
60	A0	1	49	39	1	8	1	0
60	A1	1	49	39	1	8	1	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
60	A1	1	Total 49	C 39	N 1	O 8	P 1	0
60	A1	1	Total 49	C 39	N 1	O 8	P 1	0
60	A1	1	Total 49	C 39	N 1	O 8	P 1	0
60	A1	1	Total 49	C 39	N 1	O 8	P 1	0
60	A1	1	Total 49	C 39	N 1	O 8	P 1	0
60	A1	1	Total 49	C 39	N 1	O 8	P 1	0
60	A1	1	Total 49	C 39	N 1	O 8	P 1	0
60	A1	1	Total 49	C 39	N 1	O 8	P 1	0
60	A1	1	Total 49	C 39	N 1	O 8	P 1	0
60	A1	1	Total 49	C 39	N 1	O 8	P 1	0
60	A1	1	Total 49	C 39	N 1	O 8	P 1	0
60	A1	1	Total 49	C 39	N 1	O 8	P 1	0
60	A1	1	Total 49	C 39	N 1	O 8	P 1	0
60	A1	1	Total 49	C 39	N 1	O 8	P 1	0
60	A1	1	Total 49	C 39	N 1	O 8	P 1	0
60	A1	1	Total 49	C 39	N 1	O 8	P 1	0
60	A1	1	Total 49	C 39	N 1	O 8	P 1	0
60	A1	1	Total 49	C 39	N 1	O 8	P 1	0
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60	A1	1	Total 49	C 39	N 1	O 8	P 1	0
60	A1	1	Total 49	C 39	N 1	O 8	P 1	0
60	A1	1	Total 49	C 39	N 1	O 8	P 1	0
60	A1	1	Total 49	C 39	N 1	O 8	P 1	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
60	A1	1	49	39	1	8	1	0
60	A1	1	49	39	1	8	1	0
60	A1	1	49	39	1	8	1	0
60	B8	1	49	39	1	8	1	0
60	B8	1	49	39	1	8	1	0
60	B8	1	49	39	1	8	1	0
60	B8	1	49	39	1	8	1	0
60	B8	1	49	39	1	8	1	0
60	B8	1	49	39	1	8	1	0
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60	BA	1	49	39	1	8	1	0
60	BA	1	49	39	1	8	1	0
60	BA	1	49	39	1	8	1	0
60	BA	1	49	39	1	8	1	0
60	BA	1	49	39	1	8	1	0
60	BA	1	49	39	1	8	1	0
60	BA	1	49	39	1	8	1	0
60	BA	1	49	39	1	8	1	0
60	BA	1	49	39	1	8	1	0
60	BA	1	49	39	1	8	1	0
60	BA	1	49	39	1	8	1	0
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60	BA	1	49	39	1	8	1	0

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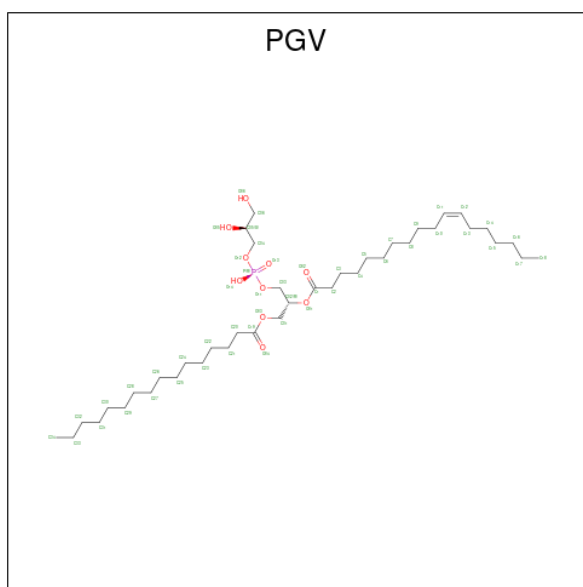
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
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60	BA	1	49	39	1	8	1	0
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60	BA	1	49	39	1	8	1	0
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60	BA	1	49	39	1	8	1	0
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60	BA	1	49	39	1	8	1	0
60	BA	1	49	39	1	8	1	0
60	BA	1	49	39	1	8	1	0
60	BB	1	49	39	1	8	1	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
60	BB	1	Total 49	C 39	N 1	O 8	P 1	0
60	BB	1	Total 49	C 39	N 1	O 8	P 1	0
60	BB	1	Total 49	C 39	N 1	O 8	P 1	0
60	BB	1	Total 49	C 39	N 1	O 8	P 1	0
60	BB	1	Total 49	C 39	N 1	O 8	P 1	0
60	BB	1	Total 49	C 39	N 1	O 8	P 1	0
60	BB	1	Total 49	C 39	N 1	O 8	P 1	0
60	BB	1	Total 49	C 39	N 1	O 8	P 1	0
60	BB	1	Total 49	C 39	N 1	O 8	P 1	0
60	BB	1	Total 49	C 39	N 1	O 8	P 1	0
60	BB	1	Total 49	C 39	N 1	O 8	P 1	0

- 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: C₄₀H₇₇O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
61	AZ	1	Total	C	O	P	0
			51	40	10	1	
61	AZ	1	Total	C	O	P	0
			51	40	10	1	
61	A0	1	Total	C	O	P	0
			51	40	10	1	
61	A0	1	Total	C	O	P	0
			51	40	10	1	
61	A0	1	Total	C	O	P	0
			51	40	10	1	
61	A0	1	Total	C	O	P	0
			51	40	10	1	
61	A0	1	Total	C	O	P	0
			51	40	10	1	
61	A0	1	Total	C	O	P	0
			51	40	10	1	
61	A0	1	Total	C	O	P	0
			51	40	10	1	
61	A0	1	Total	C	O	P	0
			51	40	10	1	
61	A0	1	Total	C	O	P	0
			51	40	10	1	
61	A1	1	Total	C	O	P	0
			51	40	10	1	
61	A1	1	Total	C	O	P	0
			51	40	10	1	
61	A1	1	Total	C	O	P	0
			51	40	10	1	
61	A1	1	Total	C	O	P	0
			51	40	10	1	
61	B8	1	Total	C	O	P	0
			51	40	10	1	
61	BA	1	Total	C	O	P	0
			51	40	10	1	
61	BA	1	Total	C	O	P	0
			51	40	10	1	
61	BA	1	Total	C	O	P	0
			51	40	10	1	
61	BA	1	Total	C	O	P	0
			51	40	10	1	
61	BA	1	Total	C	O	P	0
			51	40	10	1	

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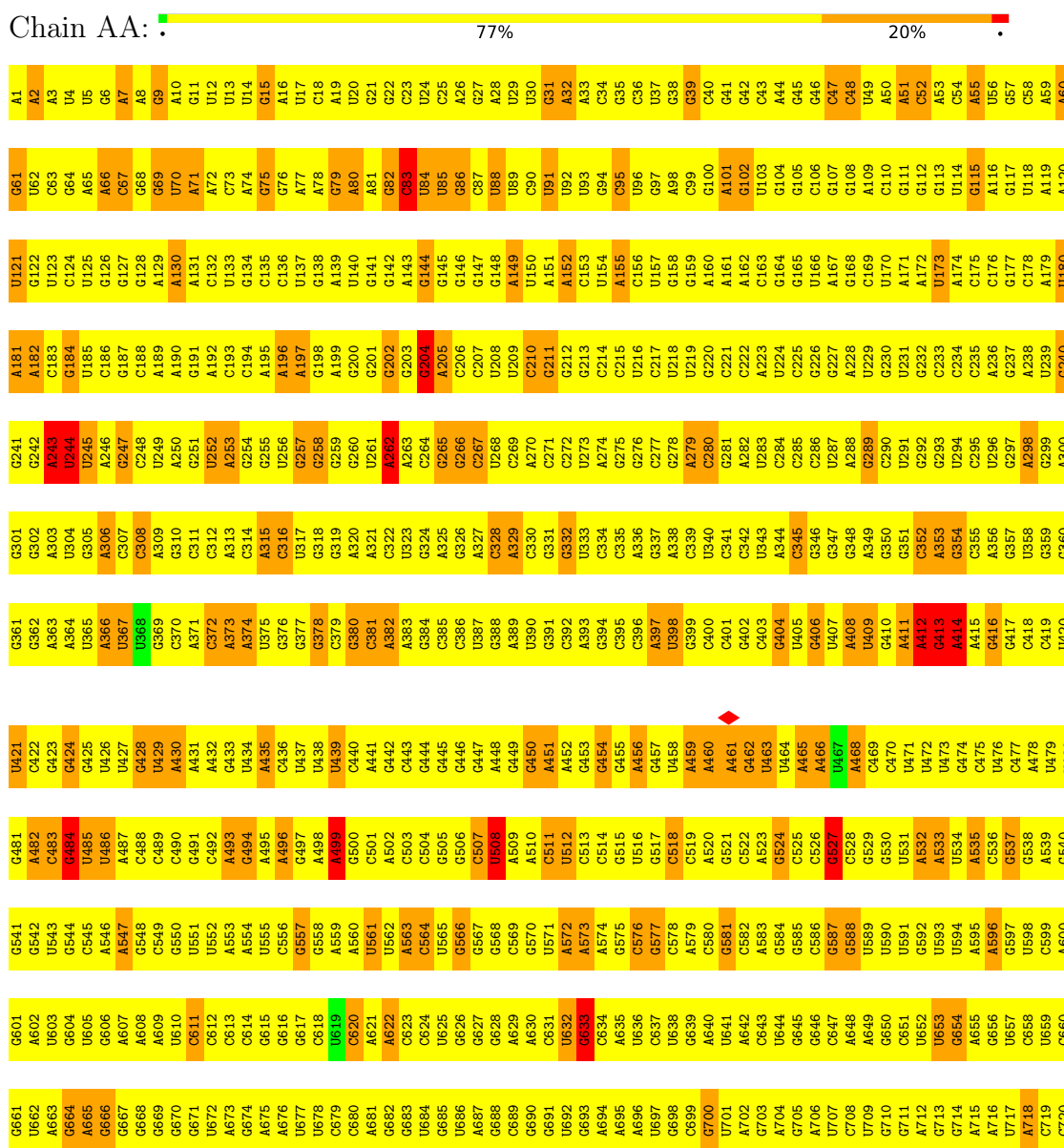
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
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61	BA	1	51	40	10	1	0
61	BA	1	51	40	10	1	0
61	BB	1	51	40	10	1	0
61	BB	1	51	40	10	1	0
61	BB	1	51	40	10	1	0
61	BB	1	51	40	10	1	0
61	BB	1	51	40	10	1	0
61	BB	1	51	40	10	1	0
61	BB	1	51	40	10	1	0
61	BB	1	51	40	10	1	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



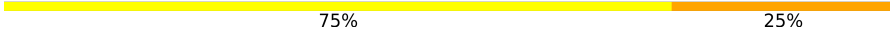
A1502	A1503	G1504	G1505	G1506	A1507	A1508	C1509	C1510	G1511	G1512	G1513	G1514	G1515	G1516	G1517	A1518	A1519	C1520	C1521	C1522	C1523	C1524	C1525	G1526	U1527	U1528	G1529	G1530	U1531	U1532	C1533	C1534	C1535	C1536	U1537	C1538	C1539	U1540	U1541	A1542																				
G1442	G1443	G1444	G1445	G1446	G1447	G1448	C1449	C1450	U1451	G1452	G1453	G1454	G1455	A1456	G1457	G1458	G1459	C1460	G1461	C1462	U1463	C1464	C1465	C1466	C1467	U1468	C1469	U1470	A1471	U1472	C1473	G1474	C1475	C1476	U1477	U1478	C1479	U1480	U1481	G1482	A1483	C1484	U1485	G1486	G1487	G1488	G1489	U1490	G1491	A1492	A1493	G1494	U1495	G1496	G1497	U1498	A1499	U1500	C1501	
C1322	G1323	C1324	C1325	G1326	G1327	C1328	A1329	U1330	G1331	A1332	G1333	G1334	U1335	C1336	G1337	A1338	G1339	C1340	G1401	C1402	C1403	C1404	G1405	C1406	C1407	A1408	C1409	U1410	C1411	C1412	C1413	U1414	C1415	G1416	U1417	A1418	G1419	U1420	G1421	G1422	C1423	U1424	U1425	G1426	C1427	A1428	A1429	U1430	A1431	A1432	A1433	A1434	U1435	U1436	G1437	C1438	G1439	U1440	A1441	
G1142	G1143	G1144	A1145	A1146	G1147	U1148	C1149	A1150	U1151	A1152	G1153	G1154	A1155	G1156	A1157	C1158	U1159	C1160	C1161	C1162	A1163	G1164	U1165	A1166	C1167	U1168	A1169	U1170	A1171	C1172	C1173	U1174	C1175	A1176	G1177	U1178	A1179	A1180	G1181	G1182	U1183	G1184	G1185	U1186	A1187	U1188	U1189	G1190	A1191	C1192	G1193	U1194	U1195	A1196	C1197	G1198	U1199	C1200	A1201	
U1202	C1203	A1204	U1205	G1206	G1207	C1208	C1209	C1210	U1211	A1212	A1213	C1214	G1215	A1216	C1217	A1218	G1219	A1220	G1221	G1222	C1223	U1224	A1225	C1226	A1227	C1228	A1229	C1230	U1231	U1232	U1233	C1234	U1235	A1236	C1237	U1238	A1239	U1240	G1241	G1242	C1243	G1244	C1245	A1246	U1247	U1248	C1249	G1310	A1251	G1312	G1313	A1254	U1315	A1256	C1317	A1318	A1319	C1320	U1321	
C1262	C1263	U1264	C1265	U1266	G1267	G1268	A1269	G1270	U1271	G1272	C1273	A1274	A1275	G1276	C1277	A1278	G1279	A1280	C1281	C1282	U1283	C1284	A1285	U1286	A1287	U1288	A1289	U1290	U1291	C1292	C1293	U1294	U1295	C1296	U1297	U1298	A1299	U1301	C1302	C1303	U1304	G1305	A1306	C1367	U1308	U1309	C1369	G1370	G1371	U1372	U1313	G1373	A1374	U1375	U1376	C1377	C1378	U1379	U1380	U1381
C1382	C1383	G1384	C1385	U1386	G1387	C1388	C1389	U1390	G1391	A1392	U1393	G1394	C1395	A1396	G1397	A1398	G1399	C1399	C1400	G1401	C1402	C1403	C1404	G1405	C1406	C1407	A1408	C1409	U1410	C1411	C1412	C1413	U1414	G1415	G1416	U1417	A1418	G1419	U1420	G1421	G1422	A1423	U1424	U1425	G1426	C1427	A1428	A1429	U1430	A1431	A1432	A1433	A1434	U1435	U1436	U1437	G1438	G1439	U1440	A1441
G1442	G1443	G1444	G1445	G1446	G1447	G1448	C1449	C1450	U1451	G1452	G1453	G1454	G1455	A1456	G1457	G1458	G1459	C1460	G1461	C1462	U1463	C1464	C1465	C1466	C1467	U1468	C1469	U1470	A1471	U1472	C1473	G1474	C1475	C1476	U1477	U1478	C1479	U1480	U1481	G1482	A1483	C1484	U1485	G1486	G1487	G1488	G1489	U1490	G1491	A1492	A1493	G1494	U1495	G1496	G1497	U1498	A1499	U1500	C1501	

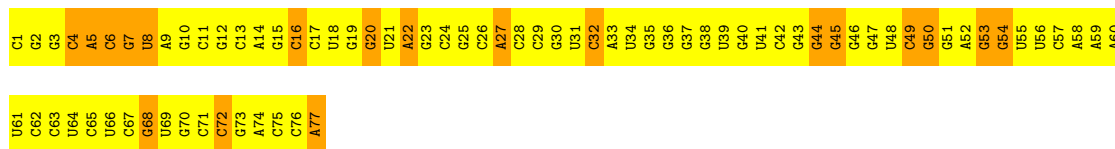
● Molecule 2: mRNA




U12	C13	G14	C15	C16	C17	C18	U19	G20	A21	A22
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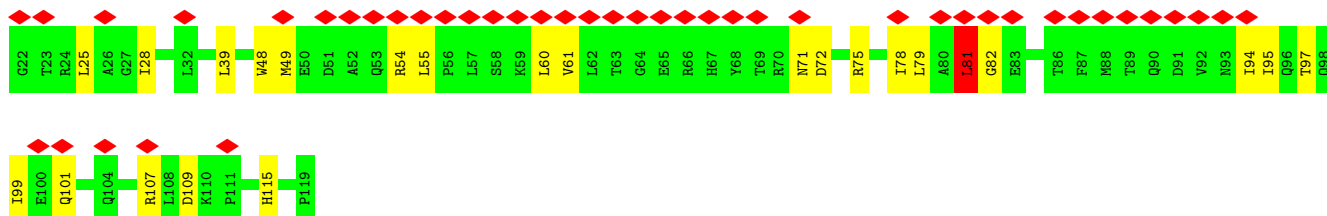
● Molecule 3: FtsQ nascent chain

Chain AV:  75% 25%



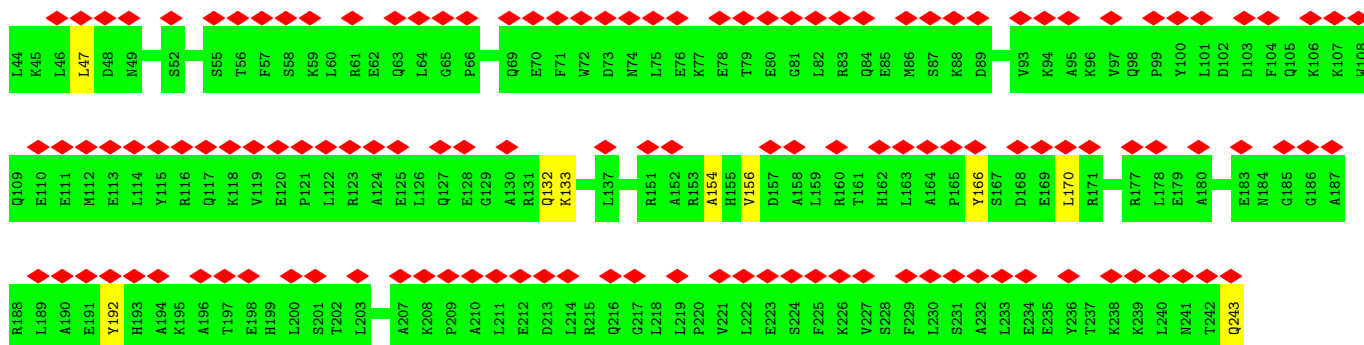
• Molecule 4: Cell division protein FtsQ

Chain AZ:  45% 76% 23%

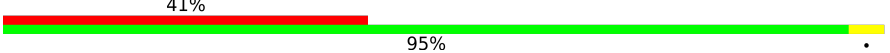


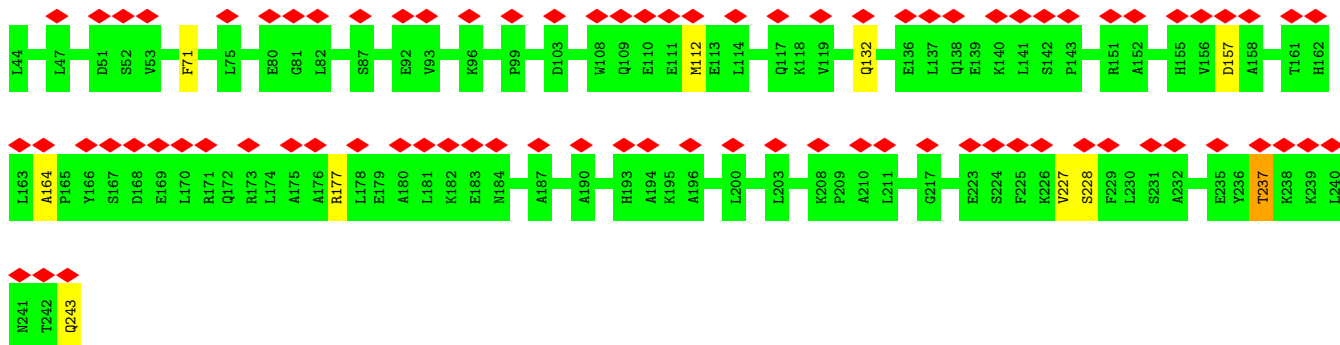
• Molecule 5: Apolipoprotein A-I

Chain A0:  65% 96%

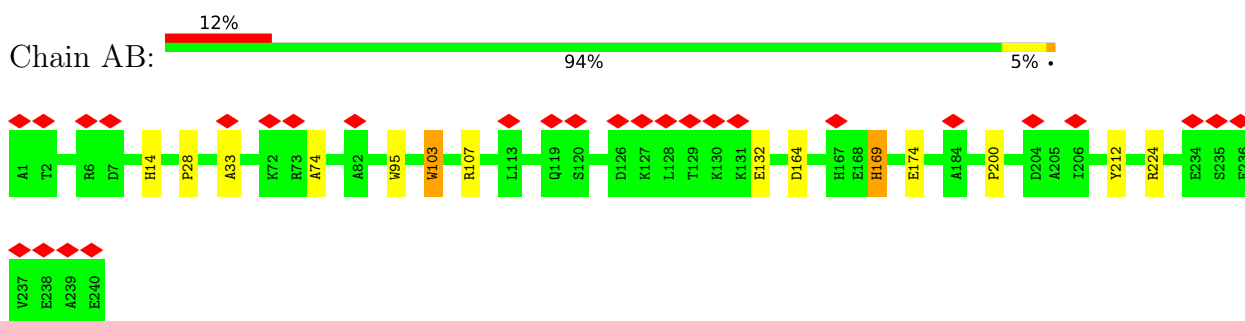


• Molecule 5: Apolipoprotein A-I

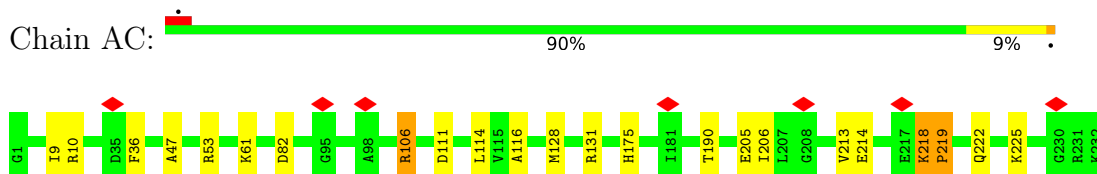
Chain A1:  41% 95%



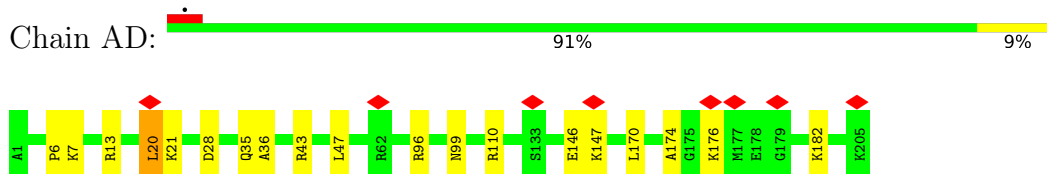
• Molecule 6: 30S ribosomal protein S2



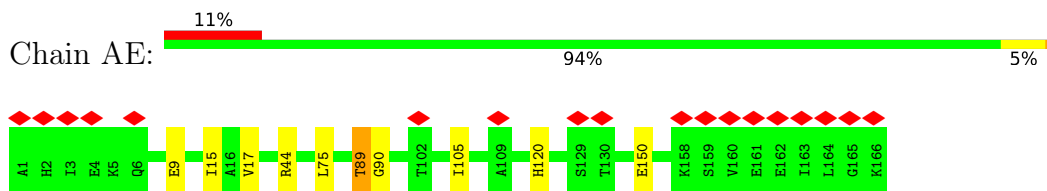
- Molecule 7: 30S ribosomal protein S3



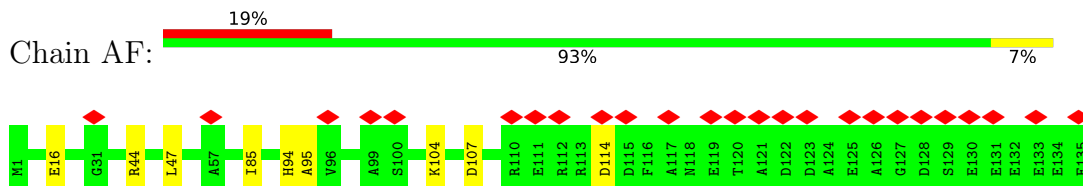
- Molecule 8: 30S ribosomal protein S4



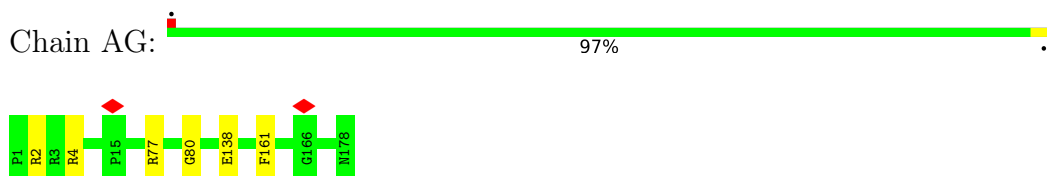
- Molecule 9: 30S ribosomal protein S5



- Molecule 10: 30S ribosomal protein S6

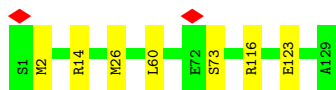


- Molecule 11: 30S ribosomal protein S7

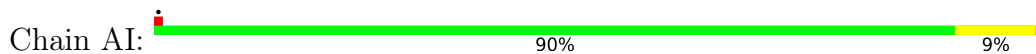


- Molecule 12: 30S ribosomal protein S8

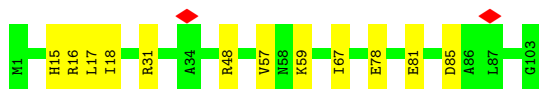
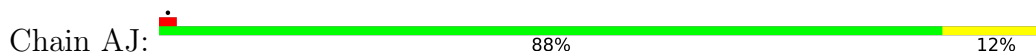




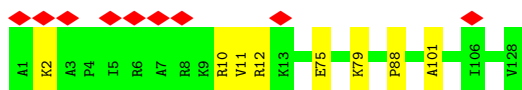
- Molecule 13: 30S ribosomal protein S9



- Molecule 14: 30S ribosomal protein S10



- Molecule 15: 30S ribosomal protein S11



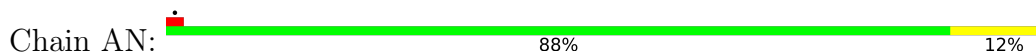
- Molecule 16: 30S ribosomal protein S12



- Molecule 17: 30S ribosomal protein S13



- Molecule 18: 30S ribosomal protein S14



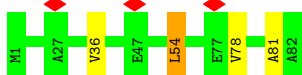
- Molecule 19: 30S ribosomal protein S15

Chain AO:  97%




- Molecule 20: 30S ribosomal protein S16

Chain AP:  95%



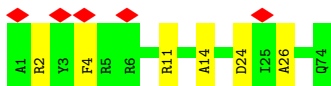
- Molecule 21: 30S ribosomal protein S17

Chain AQ:  87% 13%



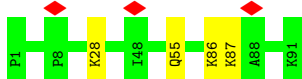
- Molecule 22: 30S ribosomal protein S18

Chain AR:  92% 8%



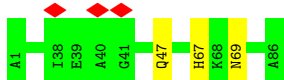
- Molecule 23: 30S ribosomal protein S19

Chain AS:  96%



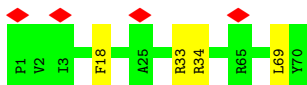
- Molecule 24: 30S ribosomal protein S20

Chain AT:  97%

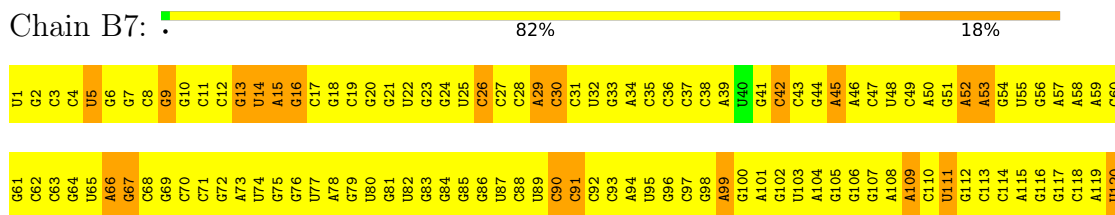


- Molecule 25: 30S ribosomal protein S21

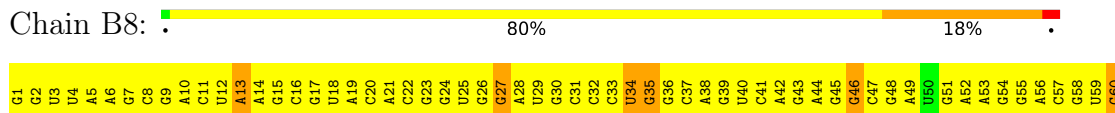
Chain AU:  94% 6%



● Molecule 26: 5S RIBOSOMAL RNA



● Molecule 27: 23S RIBOSOMAL RNA



C61	U62	A63	A64	U65	C66	G67	U68	C69	C70	A71	U72	A73	U74	G75	A76	C77	U78	A79	C79	U80	G81	A82	U83	A84	G85	U86	C87	U87	A88	C89	U90	A91	C91	U92	C93	A94	U95	A96	C97	C98	G99	A100	C101	C102	U103	A104	G105	C106	G107	U108	A109	C110	U111	A112	C113	U114	A115	U116	G117	A118	C119	U120
G121	G122	G123	G124	A125	A126	A127	C128	C129	C130	A131	G132	U133	G134	U135	A136	C137	U138	A139	U140	C141	G142	A143	C144	A145	C146	A147	U148	C149	A150	C151	U152	A153	G154	C155	A156	C157	U158	G159	A160	C161	A162	U163	C164	A165	C166	C167	A168	C169	U170	U171	A172	C173	U174	A175	U176	G177	A178	C179	U180			
A181	A182	C183	C184	G185	A186	G187	C188	A189	C190	A191	U192	C193	U194	A195	U196	A197	C198	A199	U200	C201	A202	U203	C204	A205	C206	U207	C208	A209	C210	U211	C212	A213	G214	A215	C216	U217	A218	C219	U220	A221	A222	C223	U224	C225	A226	C227	C228	C229	A230	U231	A232	C233	U234	A235	U236	C237	C238	A239	U240			
A241	G242	U243	A244	G245	C246	G247	C248	C249	G250	A251	C252	U253	G254	A255	U256	C257	U258	G259	C260	G261	A262	C263	A264	A265	C266	C267	C268	C269	A270	C311	A272	C313	C314	A315	C316	U317	C318	A319	U320	A321	C322	C323	A324	A325	C326	G327	C328	A329	U330	C331	U332	A333	C334	A335	C336	U337	C338	A339	U340			
G301	C302	G303	U304	U305	C306	G307	C308	A309	C310	A311	G312	C313	C314	G315	C316	U317	C318	G319	A320	U321	A322	C323	A324	A325	C326	G327	C328	A329	C330	C331	A332	C333	C334	A335	C336	U337	C338	U339	A340	C341	A342	C343	A344	A345	C346	A347	C348	U349	C350	U351	A352	C353	U354	A355	U356	C357	U358	A359	U360			
G361	A362	C363	C364	U365	C366	G367	A368	U369	C370	A371	G372	U373	A374	C375	G376	U377	C378	G379	A380	U381	A382	C383	A384	A385	C386	U387	C388	A389	U390	C391	A392	C393	C394	A395	U396	C397	U398	C399	A400	U401	A402	C403	U404	U405	C406	U407	C408	U409	C410	C411	A412	C413	U414	A415	C416	U417	A418	C419	U420			
C421	A422	A423	G424	C425	U426	U427	A428	A429	A430	U431	A432	C433	U434	C435	U436	A437	U438	A439	C440	U441	A442	A443	C444	A445	C446	A447	A448	A449	C450	U451	A452	C453	A454	A455	C456	A457	C458	U459	U460	A461	C462	U463	U464	A465	A466	C467	C468	U469	A470	U471	A472	C473	U474	A475	C476	A477	A478	U479	A480			
C481	A482	A483	C484	C485	U486	C487	G488	U489	C490	A491	U492	C493	G494	A495	U496	A497	C498	U499	A500	A501	A502	C503	A504	A505	C506	A507	A508	C509	U510	C511	A512	A513	A514	A515	C516	U517	C518	U519	U520	G521	U522	A523	C524	C525	U526	A527	C528	U529	A530	U531	C532	A533	U534	A535	C536	U537	C538	A539	U540			
A541	C542	G543	U544	U545	U546	A547	C548	U549	C550	C551	U552	C553	U554	C555	A556	U557	C558	U559	C560	A561	A562	C563	A564	C565	U566	U567	C568	U569	A570	C571	A572	C573	A574	U575	C576	U577	C578	U579	U580	C581	U582	A583	U584	C585	U586	C587	U588	C589	U590	C591	U592	A593	U594	A595	C596	U597	C598	A599	U600			
C601	A602	G603	C604	C605	U606	U607	C608	A609	U610	C611	U612	A613	A614	U615	A616	C617	U618	C619	G620	A621	U622	C623	A624	C625	U626	C627	U628	C629	A630	U631	A632	C633	A634	C635	U636	C637	U638	C639	A640	U641	C642	A643	A644	C645	U646	C647	C648	U649	C650	U651	A652	C653	U654	A655	C656	U657	U658	A659	U660			
A661	C662	G663	U664	C665	U666	U667	A668	C669	U670	A671	C672	C673	A674	A675	A676	C677	U678	C679	C680	U681	A682	C683	U684	A685	U686	C687	U688	A689	U690	C691	C692	A693	U694	C695	U696	C697	U698	C699	A700	U701	C702	U703	G704	A705	C706	U707	C708	U709	U710	C711	U712	C713	U714	A715	C716	U717	C718	U719	U720			
A721	C722	C723	U724	G725	A726	A727	C728	U729	A730	C731	C732	C733	A734	A735	C736	C737	U738	A739	C740	U741	A742	A743	U744	A745	U746	C747	U748	A749	U750	A751	C752	A753	U754	U755	A756	C757	C758	U759	A760	C761	U762	U763	A764	C765	U766	C767	U768	U769	U770	C771	U772	U773	C774	A775	C776	U777	C778	U779	U780			
A781	U782	C783	G784	C785	C786	C787	A788	U789	A790	C791	C792	A793	A794	C795	C796	G797	C798	C799	A800	C801	A802	U803	A804	C805	C806	U807	C808	C809	U810	U811	C812	U813	C814	C815	C816	C817	C818	A819	A820	A821	C822	C823	U824	A825	U826	U827	U828	A829	C830	C831	A833	C834	C835	C836	C837	C838	C839	U839	U840			

A1801	G1741	G1681	U1821	C1561	G1501	G1441	G1381	A1321	G1261	U1201	U1141	U1081	A1021	C961	C901	G841
A1802	U1742	G1682	G1622	U1562	A1502	U1442	G1382	A1322	A1262	G1202	A1142	U1082	G1022	G962	C902	U842
A1803	G1743	A1683	G1623	U1563	A1503	U1443	A1383	G1323	A1263	U1203	A1143	U1083	U1023	U963	C903	G843
A1804	U1744	G1684	U1624	U1564	A1504	U1444	A1384	G1324	A1264	A1204	A1144	A1084	G1024	G964	C904	A844
A1805	A1745	C1685	C1625	C1565	A1505	U1445	A1385	U1325	A1265	A1205	C1145	A1085	G1025	G965	C905	A845
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A1807	U1747	G1687	G1627	U1567	C1507	U1447	A1387	A1327	U1267	C1207	A1147	G1087	A1027	U967	C907	U847
A1808	U1748	U1688	G1628	U1568	A1508	U1448	A1388	A1328	A1268	C1208	A1148	A1088	A1028	C968	C908	C848
A1809	A1749	A1689	U1629	U1569	A1509	U1449	A1389	U1329	A1269	U1209	G1149	A1089	A1029	C969	C909	A849
A1810	A1750	A1690	A1630	A1570	A1510	A1450	A1390	U1330	C1270	C1210	A1150	A1090	C1030	G970	A910	U850
A1811	U1751	G1691	G1631	A1571	G1511	U1451	U1391	G1331	G1271	C1211	A1151	G1091	G1031	G971	A911	C851
A1812	U1752	U1692	A1632	A1572	C1512	U1452	A1392	A1332	A1272	G1212	C1152	C1092	A1032	A972	C912	U852
A1813	G1753	U1693	G1633	G1573	U1513	A1453	A1393	G1333	U1273	A1213	C1153	C1093	U1033	A973	C913	C853
A1814	A1754	G1694	A1634	C1574	U1514	U1454	U1394	G1334	A1274	A1214	G1154	U1094	G1034	G974	C914	C854
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A1817	A1757	G1697	U1637	U1577	G1517	U1457	U1397	G1337	G1277	U1217	G1157	U1097	G1037	G977	A917	G857
A1818	U1758	A1698	C1638	U1578	C1518	U1458	C1398	G1338	C1278	G1218	C1158	A1098	U1038	G978	A918	G858
A1819	A1759	G1699	C1639	U1579	G1519	U1459	C1399	U1339	G1279	U1219	U1159	A1099	A1039	A979	U919	G859
U1820	C1760	A1700	A1640	A1580	U1520	U1460	U1400	U1340	G1280	G1220	C1160	C1100	A1040	A980	A920	U860
A1821	C1761	A1701	A1641	U1581	G1521	U1461	G1401	U1341	G1281	G1221	C1161	U1101	G1041	A981	C921	A861
A1822	G1762	G1702	C1642	C1582	U1522	C1462	U1402	A1342	U1282	U1222	G1162	C1102	G1042	C982	C922	G862
A1823	G1763	G1703	C1643	U1583	U1523	C1463	A1403	G1343	G1283	G1223	G1163	A1103	C1043	A983	G923	A863
A1824	C1764	C1704	C1644	U1584	U1524	U1464	C1404	U1344	A1284	U1224	C1164	C1104	C1044	A984	G924	G864
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A1826	G1766	C1706	U1646	A1586	C1526	U1466	U1406	G1346	A1286	A1226	G1166	G1106	A1046	C986	G926	A866
A1827	U1767	G1707	U1647	U1587	U1527	U1467	G1407	A1347	A1287	G1227	C1167	U1107	G1047	C987	A927	C867
A1828	C1768	U1698	U1648	G1588	A1528	U1468	G1408	U1348	G1288	G1228	G1168	U1108	A1048	A988	A928	U868
A1829	U1769	U1699	U1649	U1589	G1529	A1469	U1409	C1349	C1289	C1229	C1169	C1109	C1049	C989	U929	G869
C1830	G1770	G1710	A1650	A1590	G1530	A1470	G1410	C1350	C1290	A1230	C1170	G1110	A1050	A990	G930	U870
A1831	C1771	A1711	G1651	A1591	C1531	G1471	U1411	C1351	C1291	U1231	G1171	A1111	C1051	C991	U931	U871
C1832	U1772	U1712	A1652	C1592	A1532	C1472	U1412	U1352	G1292	G1232	C1172	G1112	C1052	C992	U932	U872
A1833	G1773	A1713	G1653	U1593	C1533	G1473	U1413	A1353	C1293	C1233	U1173	G1113	C1053	C993	A933	C873
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A1835	U1775	G1715	A1655	A1595	A1535	G1475	U1415	G1355	C1295	G1235	U1175	G1115	A1055	C995	C935	G875
C1836	G1776	U1716	C1656	A1596	A1536	U1476	G1416	G1356	G1296	G1236	U1176	G1116	G1056	A996	A936	C876
C1837	U1777	A1717	U1657	U1597	G1537	U1477	C1417	C1357	C1297	G1237	U1177	C1117	A1057	G997	C937	A877
U1838	U1778	G1718	C1658	A1598	G1538	U1478	G1418	G1358	C1298	G1238	C1178	C1118	U1058	C998	G938	A878
A1839	U1779	U1699	G1659	U1599	U1539	U1479	A1419	A1359	G1299	G1239	U1179	U1119	G1059	U999	G939	G879
A1840	U1780	U1720	G1660	C1600	G1540	G1480	A1420	G1360	G1300	U1240	U1180	G1120	U1060	A1000	G940	G880
U1841	U1781	G1721	G1661	G1601	C1541	U1481	G1421	G1361	A1301	A1241	U1181	C1121	A1061	A1001	A941	G881
A1842	U1782	U1662	U1662	U1602	U1542	U1482	G1422	C1362	A1302	A1242	U1182	G1122	G1062	G1002	G942	G882
A1843	G1723	G1663	G1663	A1603	G1543	G1483	G1423	G1363	G1303	C1243	U1183	C1123	G1063	G1003	A943	G883
C1844	A1784	A1724	A1664	C1604	A1544	U1484	G1424	G1364	A1304	A1244	U1184	G1124	U1064	U1004	C944	U884
G1845	U1785	U1725	A1665	C1605	A1545	U1485	G1425	A1365	C1305	G1245	U1185	G1125	U1065	C1005	A945	C885
A1846	A1786	C1726	G1666	C1606	G1546	U1486	A1426	A1366	C1306	U1246	U1186	A1126	U1066	C1006	C946	A886
A1847	A1787	C1727	G1667	C1607	C1547	U1487	A1427	A1367	A1307	A1247	U1187	A1127	A1067	C1007	A947	U887
A1848	C1788	C1728	A1668	A1608	U1548	U1488	G1428	G1368	A1308	G1248	U1188	G1128	G1068	A1008	C948	C888
A1849	U1789	U1729	A1669	A1609	A1549	A1489	G1429	G1369	G1309	U1249	A1189	A1129	A1069	A1009	G949	C889
A1850	C1790	C1670	C1670	A1610	C1550	A1490	G1430	C1370	G1310	G1250	U1190	U1130	A1070	A1010	G950	C890
U1851	A1791	G1731	U1671	C1611	A1551	U1491	A1431	G1371	G1311	C1251	G1191	G1131	G1071	G1011	C951	G891
A1852	G1792	C1732	A1672	C1612	A1552	U1492	A1432	A1372	U1312	G1252	G1192	G1132	G1072	G1012	G952	A892
A1853	C1793	G1733	G1673	C1613	A1553	U1493	A1433	A1373	U1313	A1253	G1193	A1133	A1073	C1013	G953	C893
A1854	A1794	G1674	A1674	A1614	U1554	A1494	A1434	G1374	C1314	A1254	U1194	A1134	G1074	G1014	G954	U894
A1855	U1795	C1675	C1675	C1615	G1555	A1495	A1435	U1375	C1315	U1255	G1195	G1135	C1075	U1015	U955	U895
U1856	U1796	U1676	A1676	A1616	C1556	A1496	G1436	C1376	U1316	G1256	U1196	G1136	C1076	G1016	G956	A896
A1857	G1797	G1737	A1677	C1617	C1557	U1497	G1437	G1377	G1317	C1257	G1197	G1137	A1077	G1017	C957	C897
A1858	U1798	G1738	A1678	A1618	U1558	U1498	A1438	U1378	U1318	U1258	U1198	G1138	U1078	U1018	U958	C898
U1859	G1799	A1739	A1679	C1619	C1559	C1499	U1439	A1379	C1319	G1259	U1199	G1139	C1079	U1019	A959	A899
A1860	C1800	U1740	U1680	G1620	G1560	G1500	U1440	G1380	C1320	A1260	C1200	C1140	A1080	A1020	A960	A900

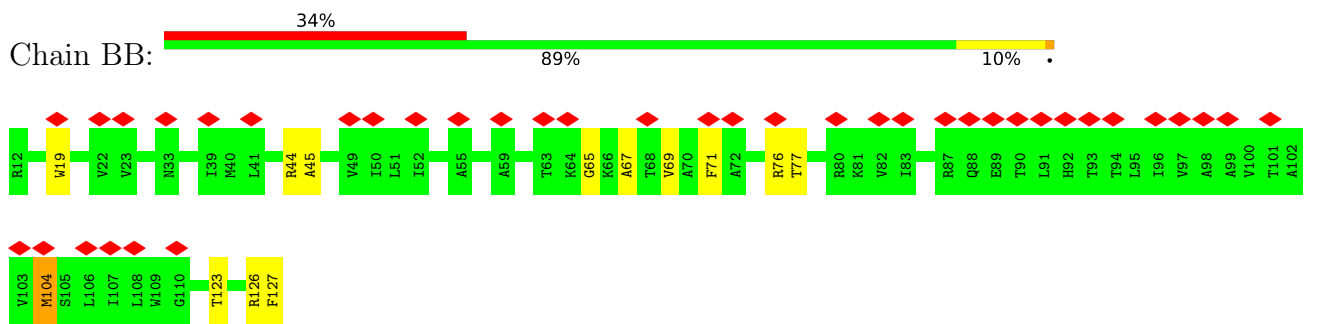
A8821	A2761	U2701	G2841	G5581	C2521	A2461	U2401	G2341	A2281	G2221	C2161	A2101	U2041	A1981	G1921	G1861
G2822	C2762	G2702	G2642	G2562	U2522	C2462	U2402	C2342	G2282	C2222	G2162	A2102	A2042	U1962	G1922	G1862
A2823	G2763	G2703	G2643	G2563	G2523	C2463	G2403	U2343	C2283	G2223	A2163	C2103	C2043	G1963	U1923	G1863
G2824	A2764	C2704	G2644	G2564	G2524	C2464	U2404	U2344	A2284	G2224	C2164	C2104	C2044	G1964	U1924	G1864
A2825	A2765	A2705	G2645	U2565	G2525	C2465	U2405	G2345	C2285	G2225	C2165	U2105	C2045	C1965	U1925	G1865
G2826	G2766	A2706	G2646	U2566	G2526	C2466	A2406	A2346	A2286	C2226	U2166	U2106	C2046	C1966	U1926	G1866
C2827	C2767	U2707	U2647	A2567	C2527	C2467	A2407	C2347	A2287	U2227	U2167	G2107	C2047	A1967	A1927	G1867
A2828	U2768	G2708	G2648	G2568	U2528	C2468	U2408	U2348	A2288	G2228	G2168	A2108	G2048	G1968	A1928	G1868
G2829	G2769	A2709	U2649	U2569	G2529	C2469	G2409	G2349	G2289	U2229	A2169	U2109	G2049	G1969	G1929	G1869
C2830	C2770	C2710	U2650	A2560	A2520	G2470	G2410	C2350	G2290	U2230	A2170	G2110	C2050	A1990	A1930	C1870
G2831	C2771	A2711	C2651	C2561	A2531	G2471	A2411	G2351	U2291	U2231	A2171	G2111	A2051	U1991	U1931	A1871
U2832	C2772	G2712	G2652	U2562	G2532	G2472	A2412	G2352	U2292	C2232	U2172	G2112	A2052	G1992	A1872	G1872
C2833	C2773	U2713	U2653	U2563	U2533	U2473	A2413	G2353	G2293	U2233	U2173	U2113	G2053	U1993	G1933	A1873
G2834	C2774	G2714	A2654	C2564	A2534	U2474	G2414	C2354	G2294	G2234	C2174	A2114	A2054	C1994	C1934	C1874
U2835	G2775	C2715	G2655	U2565	G2535	C2475	G2415	G2355	C2295	U2235	C2175	G2115	C2055	U1995	G1935	G1875
A2836	C2776	U2716	U2656	U2566	G2536	A2476	G2416	G2356	U2296	U2236	A2176	G2116	C2056	U1996	G1936	A1876
G2837	G2777	G2717	A2657	G2567	U2537	U2477	C2417	G2357	A2297	G2237	C2177	U2117	G2057	C1997	A1937	A1877
C2838	A2778	G2718	U2658	A2568	C2538	A2478	A2418	G2358	A2298	G2238	C2178	U2118	A2058	A1998	A1938	G1878
G2839	U2779	G2719	G2659	U2569	C2539	U2479	U2419	C2359	U2299	G2239	C2179	A2119	A2059	C1999	U1939	A1879
C2840	A2780	U2720	A2660	A2560	C2540	C2480	C2420	C2360	C2300	U2240	U2180	G2120	C2060	C2000	U1940	U1880
G2841	G2781	A2721	G2661	C2561	A2541	G2481	G2421	G2361	C2301	A2241	U2181	G2121	G2061	C2001	C1941	C1881
A2842	C2782	G2722	A2662	A2562	G2542	G2482	U2422	G2362	U2302	G2242	U2182	U2122	A2062	G2002	A1942	U1882
G2843	U2783	G2723	G2663	G2563	G2543	C2483	U2423	G2363	G2303	U2243	A2183	G2123	C2063	A2003	U1943	U1883
C2844	U2784	U2724	G2664	G2564	G2544	G2484	C2424	C2364	G2304	U2244	A2184	G2124	C2064	G2004	U1944	G1884
U2845	G2785	A2725	A2665	U2565	G2545	G2485	A2425	G2365	U2305	U2245	U2185	G2125	C2065	A2005	G1945	A1885
G2846	U2786	A2726	C2666	C2566	U2546	C2486	A2426	A2366	C2306	G2246	G2186	A2126	C2066	C2006	U1946	U1886
U2847	C2787	U2727	G2667	G2567	U2547	G2487	C2427	G2367	G2307	U2247	U2187	G2127	G2067	U2007	C1947	C1887
A2848	U2788	G2728	G2668	U2568	G2548	G2488	G2428	C2368	C2308	C2248	U2188	G2128	C2068	C2008	G1948	G1888
U2849	G2789	G2729	G2669	U2569	G2549	U2489	A2429	A2369	A2309	U2249	U2189	C2129	C2069	A1949	G1949	A1889
A2850	U2790	C2730	A2670	G2560	G2550	G2490	A2430	G2370	C2310	G2250	G2190	U2130	A2070	G2010	A1950	A1890
C2851	G2791	G2731	G2671	C2561	G2551	U2491	U2431	G2371	G2311	G2251	U2191	U2131	A2071	U2011	U1951	A1891
G2852	A2792	G2732	U2672	U2562	G2552	U2492	A2432	U2372	U2312	G2252	U2192	U2132	C2072	G2012	A1952	C1892
C2853	C2793	A2733	G2673	G2563	G2553	U2493	A2433	G2373	C2313	G2253	G2193	G2133	C2073	A2013	A1953	C1893
G2854	C2794	G2734	A2674	U2564	U2554	G2494	A2434	C2374	G2314	C2254	U2194	A2134	U2074	A2014	G1954	C1894
C2855	U2795	G2735	G2675	G2565	G2555	G2495	A2435	C2375	G2315	G2255	U2195	A2135	U2075	A2015	U1955	C1895
A2856	U2796	A2736	G2676	C2566	G2556	C2496	G2436	A2376	G2316	G2256	C2196	G2136	U2076	U2016	U1956	G1896
G2857	U2797	G2737	G2677	U2567	G2557	A2497	G2437	A2377	U2317	U2257	U2197	U2137	A2077	U2017	G1957	G1897
C2858	U2798	A2738	C2678	C2568	C2558	C2498	U2438	A2378	G2318	C2258	A2198	G2138	C2078	G2018	C1958	U1898
G2859	A2799	U2739	A2679	U2569	C2559	C2499	A2439	G2379	G2319	U2259	A2199	U2139	U2079	A2019	G1959	A1899
A2860	C2800	A2740	U2680	C2560	U2560	U2500	C2440	C2380	U2320	C2260	C2200	G2140	A2080	A2020	A1960	A1900
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G2862	G2802	G2742	A2682	U2562	U2562	G2502	C2442	G2382	A2322	U2262	U2202	A2142	A2082	U2022	C1962	A1902
C2863	G2803	U2743	C2683	G2563	G2563	A2503	C2443	G2383	G2323	C2263	U2203	C2143	A2083	C2023	U1963	G1903
G2864	U2804	G2744	U2684	U2564	A2564	U2504	G2444	U2384	U2324	C2264	G2204	G2144	C2084	G2024	G1964	G1904
C2865	C2805	C2745	G2685	G2565	A2565	G2505	G2445	C2385	G2325	U2265	A2205	C2145	U2085	C2025	C1965	C1905
U2866	C2806	U2746	U2686	A2566	U2566	U2506	G2446	C2386	C2326	A2266	C2206	C2146	U2086	U2026	A1966	G1906
A2867	U2807	G2747	G2687	G2567	G2567	C2507	G2447	U2387	A2327	A2267	C2207	A2147	U2087	G2027	C1967	G1907
G2868	G2808	A2748	U2688	U2568	U2568	A2508	A2448	A2388	A2328	A2268	G2208	G2148	A2088	U2028	C1968	C1908
C2869	U2809	U2749	U2689	G2569	G2569	G2509	U2449	A2389	U2329	G2269	U2209	G2149	A2089	G2029	A1969	C1909
G2870	A2810	A2750	U2690	U2560	G2570	C2510	A2450	U2390	G2330	A2270	U2210	C2150	A2090	A2030	A1970	G1910
C2871	G2811	G2751	C2691	U2561	U2571	U2511	A2451	G2391	C2331	G2271	A2211	G2151	C2091	A2031	U1971	U1911
A2872	G2812	C2752	A2692	A2562	A2572	C2512	A2452	C2392	C2332	U2272	U2212	G2152	C2092	G2032	G1972	A1912
G2873	A2813	U2753	G2693	C2563	C2573	A2513	A2453	A2393	A2333	A2273	U2213	C2153	G2093	A2033	G1973	A1913
C2874	A2814	U2754	U2694	G2564	G2574	U2514	G2454	C2394	U2334	A2274	C2214	A2154	A2094	U2034	C1974	A1914
G2875	C2815	G2755	U2695	A2565	C2575	A2515	G2455	C2395	A2335	G2275	G2215	U2155	A2095	G2035	U1975	U1915
U2876	G2816	U2756	U2696	U2566	G2576	C2516	A2456	G2396	A2336	G2276	G2216	U2156	A2096	C2036	G1976	A1916
C2877	U2817	A2757	G2697	A2567	A2577	C2517	U2457	G2397	G2337	G2277	G2217	G2157	A2097	A2037	A1977	U1917
A2878	U2818	U2758	U2698	G2568	G2578	A2518	G2458	U2398	C2338	A2278	U2218	A2158	U2098	G2038	A1978	A1918
G2879	G2819	U2759	G2699	U2569	C2579	A2519	A2459	G2399	C2339	G2279	U2219	G2159	U2099	U2039	A1979	A1919
C2880	A2820	C2760	U2700	U2640	U2580	C2520	U2460	G2400	A2340	G2240	U2180	G2120	C2060	C2000	G1980	C1920

U2881
A2882
U2883
U2884
G2885
A2886
A2887
C2888
C2889
U2890
G2891
G2892
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A2899
A2900
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C2902
U2903
U2904

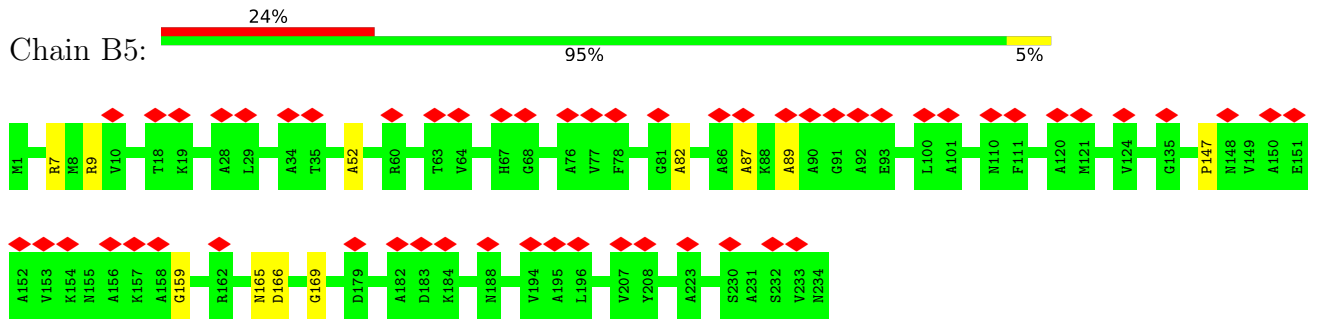
• Molecule 28: Preprotein translocase secY subunit



• Molecule 29: Preprotein translocase secE subunit

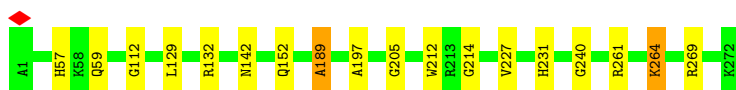


• Molecule 30: 50S ribosomal protein L1



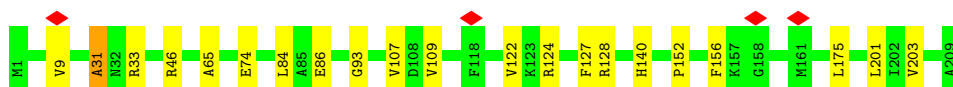
- Molecule 31: 50S ribosomal protein L2

Chain B6:  93% 6%



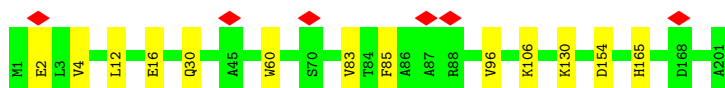
- Molecule 32: 50S ribosomal protein L3

Chain BD:  90% 10%



- Molecule 33: 50S ribosomal protein L4

Chain BE:  94% 6%



- Molecule 34: 50S ribosomal protein L5

Chain BF:  90% 9%




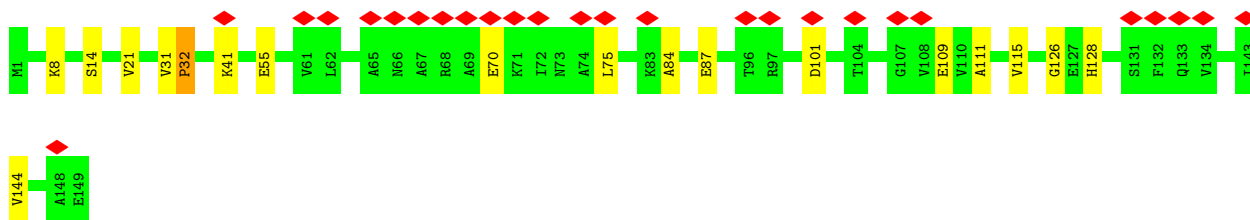
- Molecule 35: 50S ribosomal protein L6

Chain BG:  93% 7%



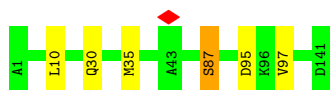
- Molecule 36: 50S ribosomal protein L9

Chain BH:  17% 88% 11%



- Molecule 37: 50S ribosomal protein L11

Chain BI:  96%



- Molecule 38: 50S ribosomal protein L13

Chain BJ:  95%



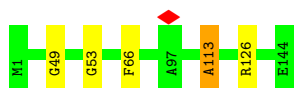
- Molecule 39: 50S ribosomal protein L14

Chain BK:  91%



- Molecule 40: 50S ribosomal protein L15

Chain BL:  97%



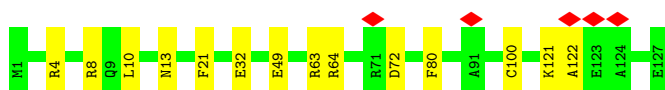
- Molecule 41: 50S ribosomal protein L16

Chain BM:  92%



- Molecule 42: 50S ribosomal protein L17

Chain BN:  89%




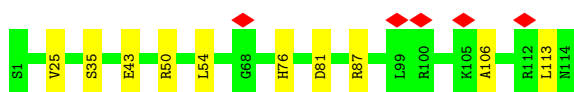
- Molecule 43: 50S ribosomal protein L18

Chain BO:  97%



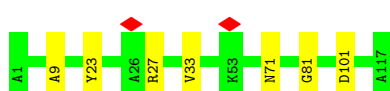
- Molecule 44: 50S ribosomal protein L19

Chain BP:  91% 9%



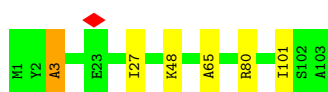
- Molecule 45: 50S ribosomal protein L20

Chain BQ:  94% 6%




- Molecule 46: 50S ribosomal protein L21

Chain BR:  94% 5%



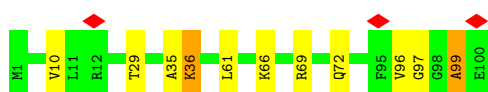
- Molecule 47: 50S ribosomal protein L22

Chain BS:  92% 7%



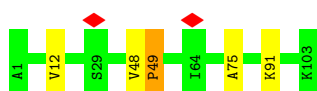
- Molecule 48: 50S ribosomal protein L23

Chain BT:  89% 9%



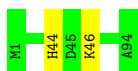
- Molecule 49: 50S ribosomal protein L24

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%



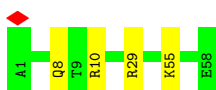
- Molecule 53: 50S ribosomal protein L29

Chain BY: 95% 5%



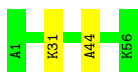
- Molecule 54: 50S ribosomal protein L30

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

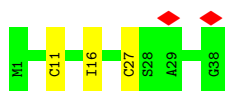
Chain B2: 87% 11%



- 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 (\AA)	396, 396, 396	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90, 90, 90	wwPDB
Pixel spacing (\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: PGV, PEV

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 [i](#)

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

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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 [i](#)

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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	309	-	48,48,48	0.79	1 (2%)	51,53,53	0.70	2 (3%)
60	PEV	BA	518	-	48,48,48	0.77	1 (2%)	51,53,53	0.67	2 (3%)
61	PGV	BA	516	-	50,50,50	1.06	2 (4%)	53,56,56	0.70	2 (3%)
60	PEV	A1	313	-	48,48,48	0.77	1 (2%)	51,53,53	0.73	2 (3%)
60	PEV	BB	216	-	48,48,48	0.78	1 (2%)	51,53,53	0.77	2 (3%)
60	PEV	A0	322	-	48,48,48	0.79	1 (2%)	51,53,53	0.74	2 (3%)
61	PGV	BA	515	-	50,50,50	1.05	2 (4%)	53,56,56	0.73	2 (3%)
60	PEV	BA	511	-	48,48,48	0.75	1 (2%)	51,53,53	0.70	2 (3%)
60	PEV	A0	303	-	48,48,48	0.80	1 (2%)	51,53,53	0.69	2 (3%)
60	PEV	A1	301	-	48,48,48	0.78	2 (4%)	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	BB	210	-	48,48,48	0.77	1 (2%)	51,53,53	0.72	2 (3%)
60	PEV	BA	520	-	48,48,48	0.78	1 (2%)	51,53,53	0.64	2 (3%)
60	PEV	BB	218	-	48,48,48	0.77	1 (2%)	51,53,53	0.70	2 (3%)
60	PEV	BA	503	-	48,48,48	0.79	1 (2%)	51,53,53	0.74	2 (3%)
61	PGV	BA	501	-	50,50,50	1.05	2 (4%)	53,56,56	0.81	2 (3%)
60	PEV	A0	321	-	48,48,48	0.79	1 (2%)	51,53,53	0.81	3 (5%)
60	PEV	A0	329	-	48,48,48	0.78	1 (2%)	51,53,53	0.72	2 (3%)
60	PEV	BA	533	-	48,48,48	2.69	1 (2%)	51,53,53	1.32	2 (3%)
60	PEV	BA	507	-	48,48,48	0.78	1 (2%)	51,53,53	0.69	2 (3%)
60	PEV	AZ	203	-	48,48,48	0.77	1 (2%)	51,53,53	0.63	2 (3%)
60	PEV	BA	502	-	48,48,48	0.77	1 (2%)	51,53,53	0.70	2 (3%)
60	PEV	A1	306	-	48,48,48	0.79	1 (2%)	51,53,53	0.63	2 (3%)
60	PEV	BB	214	-	48,48,48	0.78	1 (2%)	51,53,53	0.71	2 (3%)
61	PGV	AZ	207	-	50,50,50	1.05	2 (4%)	53,56,56	0.76	2 (3%)
60	PEV	AZ	206	-	48,48,48	0.78	1 (2%)	51,53,53	0.61	2 (3%)
60	PEV	BA	510	-	48,48,48	0.77	1 (2%)	51,53,53	0.69	2 (3%)
61	PGV	A0	304	-	50,50,50	1.06	2 (4%)	53,56,56	0.81	2 (3%)
60	PEV	BA	517	-	48,48,48	0.78	1 (2%)	51,53,53	0.69	2 (3%)
60	PEV	BA	531	-	48,48,48	0.77	1 (2%)	51,53,53	0.66	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
60	PEV	A0	330	-	48,48,48	0.78	1 (2%)	51,53,53	0.65	2 (3%)
60	PEV	BA	528	-	48,48,48	0.78	1 (2%)	51,53,53	0.73	2 (3%)
60	PEV	A0	316	-	48,48,48	0.80	1 (2%)	51,53,53	0.84	2 (3%)
60	PEV	A0	308	-	48,48,48	0.78	1 (2%)	51,53,53	0.75	2 (3%)
60	PEV	BA	524	-	48,48,48	0.80	1 (2%)	51,53,53	0.70	2 (3%)
60	PEV	BA	538	-	48,48,48	0.75	1 (2%)	51,53,53	0.65	2 (3%)
60	PEV	A1	326	-	48,48,48	0.76	1 (2%)	51,53,53	0.68	2 (3%)
61	PGV	BB	205	-	50,50,50	1.05	2 (4%)	53,56,56	0.80	2 (3%)
60	PEV	BB	202	-	48,48,48	0.78	1 (2%)	51,53,53	0.71	2 (3%)
60	PEV	BA	529	-	48,48,48	0.80	1 (2%)	51,53,53	0.70	2 (3%)
60	PEV	BA	523	-	48,48,48	0.78	1 (2%)	51,53,53	0.74	2 (3%)
60	PEV	AZ	202	-	48,48,48	0.77	1 (2%)	51,53,53	0.72	2 (3%)
60	PEV	A1	310	-	48,48,48	0.77	1 (2%)	51,53,53	0.72	2 (3%)
61	PGV	BB	203	-	50,50,50	1.06	2 (4%)	53,56,56	0.76	2 (3%)
60	PEV	A0	323	-	48,48,48	0.77	1 (2%)	51,53,53	0.71	2 (3%)
60	PEV	A0	326	-	48,48,48	0.76	1 (2%)	51,53,53	0.71	2 (3%)
60	PEV	BA	527	-	48,48,48	0.79	1 (2%)	51,53,53	0.76	2 (3%)
60	PEV	B8	3004	-	48,48,48	0.78	1 (2%)	51,53,53	0.70	2 (3%)
60	PEV	A0	320	-	48,48,48	0.80	1 (2%)	51,53,53	0.65	2 (3%)
61	PGV	A0	318	-	50,50,50	1.06	2 (4%)	53,56,56	0.74	2 (3%)
60	PEV	BA	530	-	48,48,48	0.77	1 (2%)	51,53,53	0.67	2 (3%)
61	PGV	A0	328	-	50,50,50	1.05	2 (4%)	53,56,56	0.76	2 (3%)
61	PGV	A1	318	-	50,50,50	1.06	2 (4%)	53,56,56	0.79	2 (3%)
60	PEV	A0	312	-	48,48,48	0.79	1 (2%)	51,53,53	0.61	2 (3%)
60	PEV	BA	504	-	48,48,48	0.79	1 (2%)	51,53,53	0.80	2 (3%)
60	PEV	BA	513	-	48,48,48	0.77	1 (2%)	51,53,53	0.68	2 (3%)
61	PGV	BA	512	-	50,50,50	1.04	2 (4%)	53,56,56	0.75	2 (3%)
61	PGV	BB	213	-	50,50,50	1.06	2 (4%)	53,56,56	0.81	2 (3%)
60	PEV	BA	535	-	48,48,48	0.78	1 (2%)	51,53,53	0.67	2 (3%)
61	PGV	BA	536	-	50,50,50	1.05	2 (4%)	53,56,56	0.73	2 (3%)
60	PEV	BA	539	-	48,48,48	0.78	1 (2%)	51,53,53	0.79	2 (3%)
60	PEV	A1	312	-	48,48,48	0.78	1 (2%)	51,53,53	0.68	2 (3%)
60	PEV	A1	314	-	48,48,48	0.78	1 (2%)	51,53,53	0.69	2 (3%)
61	PGV	BB	217	-	50,50,50	1.05	2 (4%)	53,56,56	0.76	2 (3%)
60	PEV	A1	327	-	48,48,48	0.76	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
60	PEV	A1	322	-	48,48,48	0.76	1 (2%)	51,53,53	0.69	2 (3%)
60	PEV	BA	509	-	48,48,48	0.79	1 (2%)	51,53,53	0.75	2 (3%)
60	PEV	BB	209	-	48,48,48	0.76	1 (2%)	51,53,53	0.69	2 (3%)
61	PGV	BB	208	-	50,50,50	1.06	2 (4%)	53,56,56	0.74	2 (3%)
61	PGV	A0	305	-	50,50,50	1.04	2 (4%)	53,56,56	0.73	2 (3%)
61	PGV	B8	3005	-	50,50,50	1.05	2 (4%)	53,56,56	0.72	2 (3%)
60	PEV	B8	3007	-	48,48,48	0.77	1 (2%)	51,53,53	0.64	2 (3%)
60	PEV	A0	313	-	48,48,48	0.80	1 (2%)	51,53,53	0.74	2 (3%)
60	PEV	A1	321	-	48,48,48	0.78	1 (2%)	51,53,53	0.67	2 (3%)
60	PEV	A0	302	-	48,48,48	0.77	1 (2%)	51,53,53	0.71	2 (3%)
60	PEV	A1	329	-	48,48,48	0.78	1 (2%)	51,53,53	0.72	2 (3%)
60	PEV	A1	305	-	48,48,48	0.78	1 (2%)	51,53,53	0.68	2 (3%)
60	PEV	A0	310	-	48,48,48	0.79	1 (2%)	51,53,53	0.82	2 (3%)
60	PEV	BB	206	-	48,48,48	0.78	1 (2%)	51,53,53	0.70	2 (3%)
60	PEV	B8	3003	-	48,48,48	0.79	1 (2%)	51,53,53	0.71	2 (3%)
60	PEV	A0	324	-	48,48,48	0.79	1 (2%)	51,53,53	0.71	2 (3%)
61	PGV	AZ	205	-	50,50,50	1.05	2 (4%)	53,56,56	0.76	2 (3%)
60	PEV	B8	3001	-	48,48,48	0.79	1 (2%)	51,53,53	0.71	2 (3%)
60	PEV	BB	212	-	48,48,48	0.78	1 (2%)	51,53,53	0.66	2 (3%)
60	PEV	BB	211	-	48,48,48	0.77	1 (2%)	51,53,53	0.73	2 (3%)
60	PEV	A1	324	-	48,48,48	0.78	1 (2%)	51,53,53	0.64	2 (3%)
60	PEV	A0	314	-	48,48,48	0.80	1 (2%)	51,53,53	0.69	2 (3%)
61	PGV	A0	317	-	50,50,50	1.05	2 (4%)	53,56,56	0.84	2 (3%)
61	PGV	A1	311	-	50,50,50	1.06	2 (4%)	53,56,56	0.80	2 (3%)
60	PEV	A1	325	-	48,48,48	0.78	1 (2%)	51,53,53	0.66	2 (3%)
60	PEV	BA	534	-	48,48,48	0.82	1 (2%)	51,53,53	0.75	2 (3%)
60	PEV	A1	323	-	48,48,48	0.76	1 (2%)	51,53,53	0.66	2 (3%)
61	PGV	A0	327	-	50,50,50	1.06	2 (4%)	53,56,56	0.71	2 (3%)
60	PEV	BB	215	-	48,48,48	0.76	1 (2%)	51,53,53	0.69	2 (3%)
60	PEV	A1	328	-	48,48,48	0.76	1 (2%)	51,53,53	0.68	2 (3%)
60	PEV	BA	514	-	48,48,48	0.80	1 (2%)	51,53,53	0.75	2 (3%)
60	PEV	BA	519	-	48,48,48	0.78	1 (2%)	51,53,53	0.74	2 (3%)
60	PEV	A0	307	-	48,48,48	0.77	1 (2%)	51,53,53	0.65	2 (3%)
60	PEV	A1	319	-	48,48,48	0.77	1 (2%)	51,53,53	0.65	1 (1%)
60	PEV	A0	315	-	48,48,48	0.76	1 (2%)	51,53,53	0.64	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
61	PGV	BA	540	-	50,50,50	1.04	2 (4%)	53,56,56	0.77	2 (3%)
61	PGV	A0	306	-	50,50,50	1.05	2 (4%)	53,56,56	0.75	2 (3%)
60	PEV	A0	311	-	48,48,48	0.78	1 (2%)	51,53,53	0.67	2 (3%)
60	PEV	A1	317	-	48,48,48	0.79	2 (4%)	51,53,53	0.69	2 (3%)
60	PEV	A1	320	-	48,48,48	0.79	1 (2%)	51,53,53	0.71	2 (3%)
60	PEV	A1	307	-	48,48,48	0.78	1 (2%)	51,53,53	0.70	2 (3%)
60	PEV	A1	304	-	48,48,48	0.77	1 (2%)	51,53,53	0.63	2 (3%)
60	PEV	BA	506	-	48,48,48	0.75	1 (2%)	51,53,53	0.70	2 (3%)
60	PEV	BA	526	-	48,48,48	0.77	1 (2%)	51,53,53	0.69	2 (3%)
60	PEV	BB	201	-	48,48,48	0.79	1 (2%)	51,53,53	0.70	2 (3%)
61	PGV	A0	325	-	50,50,50	1.05	2 (4%)	53,56,56	0.86	2 (3%)
61	PGV	BA	522	-	50,50,50	1.06	2 (4%)	53,56,56	0.71	2 (3%)
61	PGV	A1	315	-	50,50,50	1.07	2 (4%)	53,56,56	0.79	2 (3%)
60	PEV	AZ	204	-	48,48,48	0.78	1 (2%)	51,53,53	0.67	2 (3%)
60	PEV	A1	302	-	48,48,48	0.79	1 (2%)	51,53,53	0.71	2 (3%)
60	PEV	B8	3002	-	48,48,48	0.77	1 (2%)	51,53,53	0.66	2 (3%)
61	PGV	BB	204	-	50,50,50	1.06	2 (4%)	53,56,56	0.81	2 (3%)
60	PEV	A1	309	-	48,48,48	0.78	1 (2%)	51,53,53	0.74	2 (3%)
60	PEV	BA	508	-	48,48,48	0.78	1 (2%)	51,53,53	0.68	2 (3%)
60	PEV	AZ	201	-	48,48,48	0.75	1 (2%)	51,53,53	0.70	2 (3%)
60	PEV	BA	525	-	48,48,48	0.79	1 (2%)	51,53,53	0.74	2 (3%)
60	PEV	BA	521	-	48,48,48	0.78	1 (2%)	51,53,53	0.67	2 (3%)
61	PGV	A1	303	-	50,50,50	1.05	2 (4%)	53,56,56	0.75	2 (3%)
60	PEV	BA	532	-	48,48,48	0.76	1 (2%)	51,53,53	0.74	2 (3%)
60	PEV	A0	319	-	48,48,48	0.79	1 (2%)	51,53,53	0.75	2 (3%)
60	PEV	B8	3006	-	48,48,48	0.78	1 (2%)	51,53,53	0.67	2 (3%)
61	PGV	BB	207	-	50,50,50	1.06	2 (4%)	53,56,56	0.77	2 (3%)
60	PEV	A1	316	-	48,48,48	0.78	1 (2%)	51,53,53	0.74	2 (3%)
61	PGV	A0	332	-	50,50,50	1.06	2 (4%)	53,56,56	0.76	2 (3%)
61	PGV	A0	331	-	50,50,50	1.04	2 (4%)	53,56,56	0.77	2 (3%)
60	PEV	BA	537	-	48,48,48	0.80	2 (4%)	51,53,53	0.74	2 (3%)
60	PEV	A0	301	-	48,48,48	0.78	1 (2%)	51,53,53	0.68	2 (3%)
61	PGV	BA	505	-	50,50,50	1.05	2 (4%)	53,56,56	0.77	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	PGV	BA	516	-	2/2/5/7	7/55/55/55	-
60	PEV	A0	309	-	-	6/52/52/52	-
60	PEV	BA	518	-	-	9/52/52/52	-
60	PEV	A1	313	-	1/1/4/4	8/52/52/52	-
60	PEV	BB	216	-	-	5/52/52/52	-
60	PEV	A0	322	-	-	6/52/52/52	-
61	PGV	BA	515	-	2/2/5/7	6/55/55/55	-
60	PEV	BA	511	-	-	5/52/52/52	-
60	PEV	A0	303	-	-	7/52/52/52	-
60	PEV	A1	301	-	1/1/4/4	13/52/52/52	-
60	PEV	A1	308	-	-	12/52/52/52	-
60	PEV	BB	210	-	-	13/52/52/52	-
60	PEV	BA	520	-	-	5/52/52/52	-
60	PEV	BB	218	-	-	9/52/52/52	-
60	PEV	BA	503	-	-	11/52/52/52	-
61	PGV	BA	501	-	1/1/5/7	7/55/55/55	-
60	PEV	A0	321	-	-	11/52/52/52	-
60	PEV	A0	329	-	-	4/52/52/52	-
60	PEV	BA	533	-	-	10/52/52/52	-
60	PEV	BA	507	-	-	4/52/52/52	-
60	PEV	AZ	203	-	-	8/52/52/52	-
60	PEV	BA	502	-	1/1/4/4	8/52/52/52	-
60	PEV	A1	306	-	-	6/52/52/52	-
60	PEV	BB	214	-	-	8/52/52/52	-
61	PGV	AZ	207	-	2/2/5/7	8/55/55/55	-
60	PEV	AZ	206	-	-	4/52/52/52	-
60	PEV	BA	510	-	-	8/52/52/52	-
61	PGV	A0	304	-	2/2/5/7	5/55/55/55	-
60	PEV	BA	517	-	-	5/52/52/52	-
60	PEV	BA	531	-	-	3/52/52/52	-
60	PEV	A0	330	-	-	10/52/52/52	-
60	PEV	BA	528	-	-	9/52/52/52	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	PEV	A0	316	-	-	10/52/52/52	-
60	PEV	A0	308	-	1/1/4/4	5/52/52/52	-
60	PEV	BA	538	-	1/1/4/4	9/52/52/52	-
60	PEV	BA	524	-	-	12/52/52/52	-
61	PGV	BB	205	-	2/2/5/7	6/55/55/55	-
60	PEV	A1	326	-	-	4/52/52/52	-
60	PEV	BB	202	-	1/1/4/4	3/52/52/52	-
60	PEV	BA	529	-	-	4/52/52/52	-
60	PEV	BA	523	-	-	7/52/52/52	-
60	PEV	AZ	202	-	-	8/52/52/52	-
60	PEV	A1	310	-	-	8/52/52/52	-
61	PGV	BB	203	-	2/2/5/7	8/55/55/55	-
60	PEV	A0	323	-	1/1/4/4	7/52/52/52	-
60	PEV	A0	326	-	-	9/52/52/52	-
61	PGV	A0	318	-	2/2/5/7	9/55/55/55	-
60	PEV	B8	3004	-	-	9/52/52/52	-
60	PEV	A0	320	-	-	5/52/52/52	-
60	PEV	BA	527	-	-	8/52/52/52	-
60	PEV	BA	530	-	1/1/4/4	11/52/52/52	-
61	PGV	A0	328	-	2/2/5/7	10/55/55/55	-
61	PGV	A1	318	-	2/2/5/7	11/55/55/55	-
60	PEV	A0	312	-	-	7/52/52/52	-
61	PGV	BA	512	-	1/1/5/7	10/55/55/55	-
60	PEV	BA	504	-	-	5/52/52/52	-
60	PEV	BA	513	-	-	7/52/52/52	-
61	PGV	BB	213	-	1/1/5/7	9/55/55/55	-
60	PEV	BA	535	-	1/1/4/4	7/52/52/52	-
61	PGV	BA	536	-	2/2/5/7	7/55/55/55	-
60	PEV	BA	539	-	-	4/52/52/52	-
60	PEV	A1	312	-	-	5/52/52/52	-
60	PEV	A1	314	-	-	6/52/52/52	-
61	PGV	BB	217	-	2/2/5/7	7/55/55/55	-
60	PEV	A1	327	-	-	7/52/52/52	-
60	PEV	A1	322	-	-	4/52/52/52	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	PEV	BA	509	-	-	13/52/52/52	-
61	PGV	BB	208	-	2/2/5/7	8/55/55/55	-
60	PEV	BB	209	-	-	8/52/52/52	-
61	PGV	A0	305	-	1/1/5/7	10/55/55/55	-
61	PGV	B8	3005	-	2/2/5/7	8/55/55/55	-
60	PEV	B8	3007	-	-	3/52/52/52	-
60	PEV	A0	313	-	-	5/52/52/52	-
60	PEV	A1	321	-	-	7/52/52/52	-
60	PEV	A0	302	-	-	8/52/52/52	-
60	PEV	A1	329	-	-	5/52/52/52	-
60	PEV	A1	305	-	1/1/4/4	6/52/52/52	-
60	PEV	A0	310	-	-	5/52/52/52	-
60	PEV	BB	206	-	1/1/4/4	9/52/52/52	-
60	PEV	B8	3003	-	-	15/52/52/52	-
60	PEV	A0	324	-	-	7/52/52/52	-
61	PGV	AZ	205	-	2/2/5/7	15/55/55/55	-
60	PEV	B8	3001	-	1/1/4/4	3/52/52/52	-
60	PEV	BB	212	-	-	6/52/52/52	-
60	PEV	BB	211	-	-	8/52/52/52	-
60	PEV	A1	324	-	-	5/52/52/52	-
60	PEV	A0	314	-	1/1/4/4	8/52/52/52	-
61	PGV	A0	317	-	2/2/5/7	8/55/55/55	-
61	PGV	A1	311	-	2/2/5/7	8/55/55/55	-
60	PEV	A1	325	-	-	12/52/52/52	-
60	PEV	BA	534	-	-	5/52/52/52	-
60	PEV	A1	323	-	-	4/52/52/52	-
61	PGV	A0	327	-	2/2/5/7	6/55/55/55	-
60	PEV	BB	215	-	-	6/52/52/52	-
60	PEV	A1	328	-	-	12/52/52/52	-
60	PEV	BA	514	-	-	8/52/52/52	-
60	PEV	BA	519	-	-	11/52/52/52	-
60	PEV	A0	307	-	-	9/52/52/52	-
60	PEV	A1	319	-	-	4/52/52/52	-
61	PGV	BA	540	-	2/2/5/7	6/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	PEV	A0	315	-	-	9/52/52/52	-
61	PGV	A0	306	-	2/2/5/7	7/55/55/55	-
60	PEV	A0	311	-	-	7/52/52/52	-
60	PEV	A1	317	-	1/1/4/4	9/52/52/52	-
60	PEV	A1	320	-	-	9/52/52/52	-
60	PEV	A1	307	-	-	4/52/52/52	-
60	PEV	A1	304	-	-	5/52/52/52	-
60	PEV	BA	506	-	-	5/52/52/52	-
60	PEV	BA	526	-	1/1/4/4	5/52/52/52	-
60	PEV	BB	201	-	-	11/52/52/52	-
61	PGV	A0	325	-	2/2/5/7	8/55/55/55	-
61	PGV	BA	522	-	2/2/5/7	2/55/55/55	-
61	PGV	A1	315	-	2/2/5/7	13/55/55/55	-
60	PEV	AZ	204	-	1/1/4/4	8/52/52/52	-
60	PEV	A1	302	-	-	10/52/52/52	-
60	PEV	B8	3002	-	-	4/52/52/52	-
61	PGV	BB	204	-	2/2/5/7	10/55/55/55	-
60	PEV	A1	309	-	-	6/52/52/52	-
60	PEV	BA	508	-	1/1/4/4	5/52/52/52	-
60	PEV	AZ	201	-	-	5/52/52/52	-
60	PEV	BA	525	-	-	11/52/52/52	-
60	PEV	BA	521	-	-	8/52/52/52	-
61	PGV	A1	303	-	2/2/5/7	5/55/55/55	-
60	PEV	BA	532	-	-	12/52/52/52	-
60	PEV	A0	319	-	-	8/52/52/52	-
60	PEV	B8	3006	-	-	7/52/52/52	-
61	PGV	BB	207	-	2/2/5/7	4/55/55/55	-
60	PEV	A1	316	-	-	3/52/52/52	-
61	PGV	A0	332	-	2/2/5/7	7/55/55/55	-
61	PGV	A0	331	-	2/2/5/7	4/55/55/55	-
60	PEV	BA	537	-	1/1/4/4	9/52/52/52	-
60	PEV	A0	301	-	-	11/52/52/52	-
61	PGV	BA	505	-	2/2/5/7	7/55/55/55	-

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:

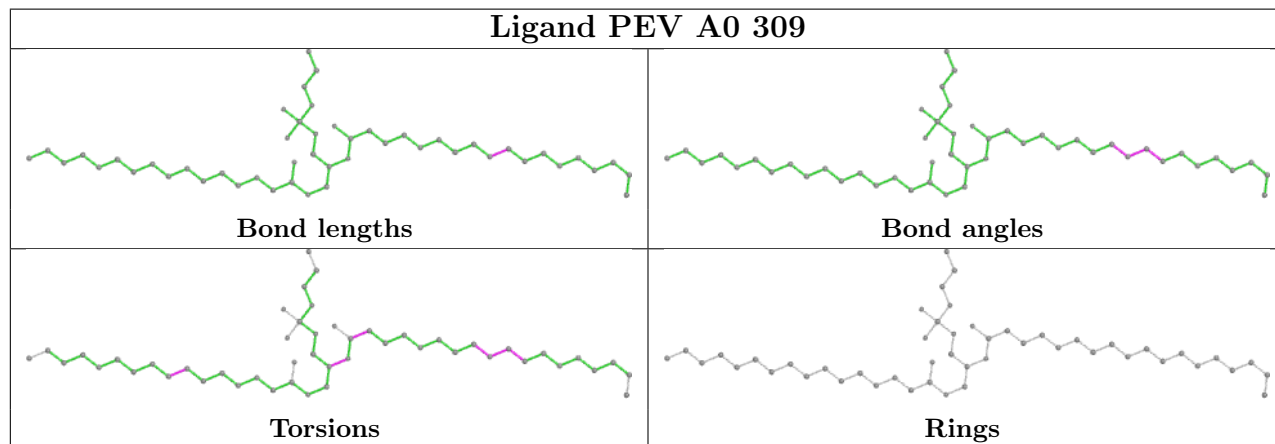
Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	A1	301	PEV	1	0
60	BA	520	PEV	1	0
60	BA	503	PEV	1	0
60	BA	533	PEV	29	0
60	BA	531	PEV	1	0

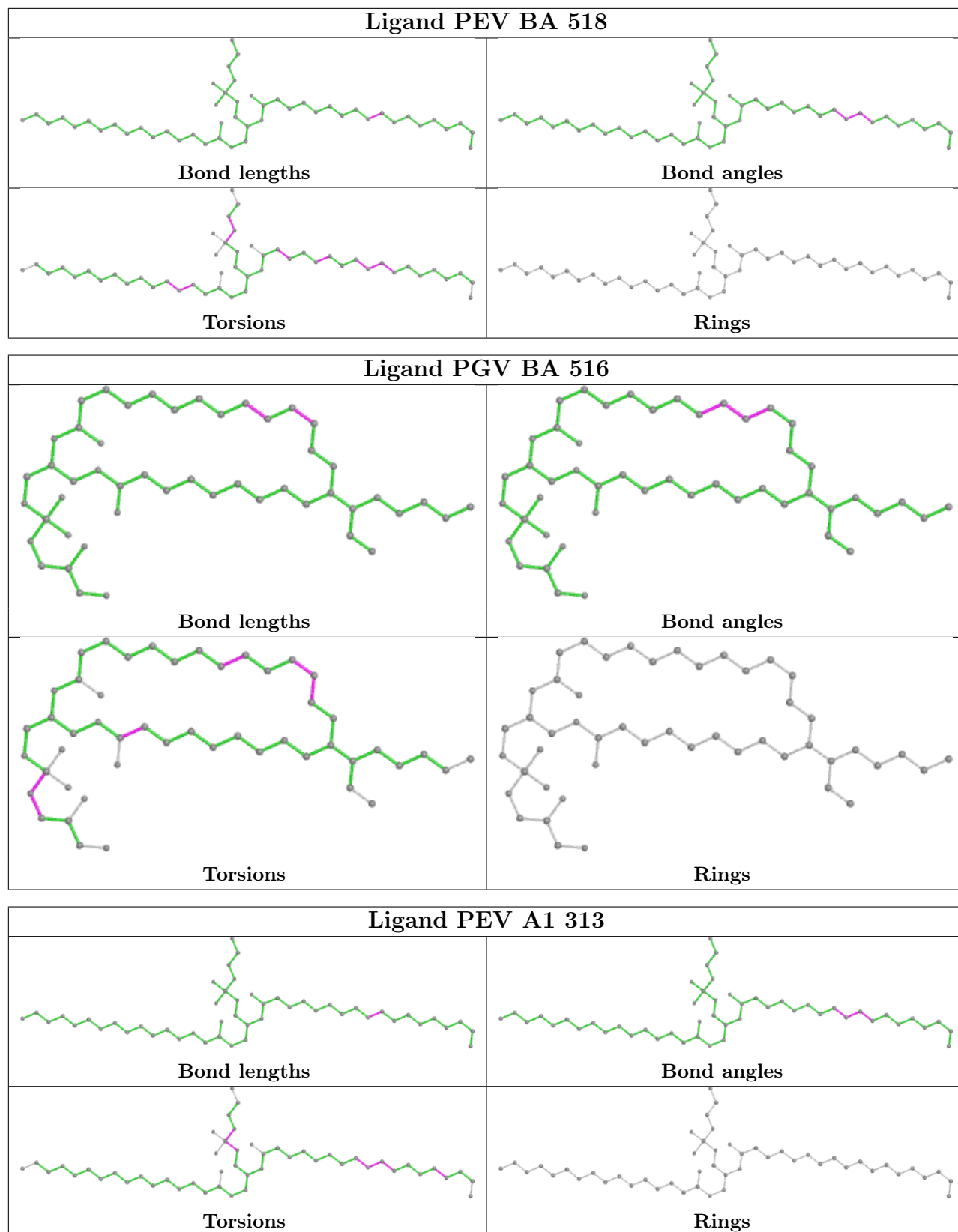
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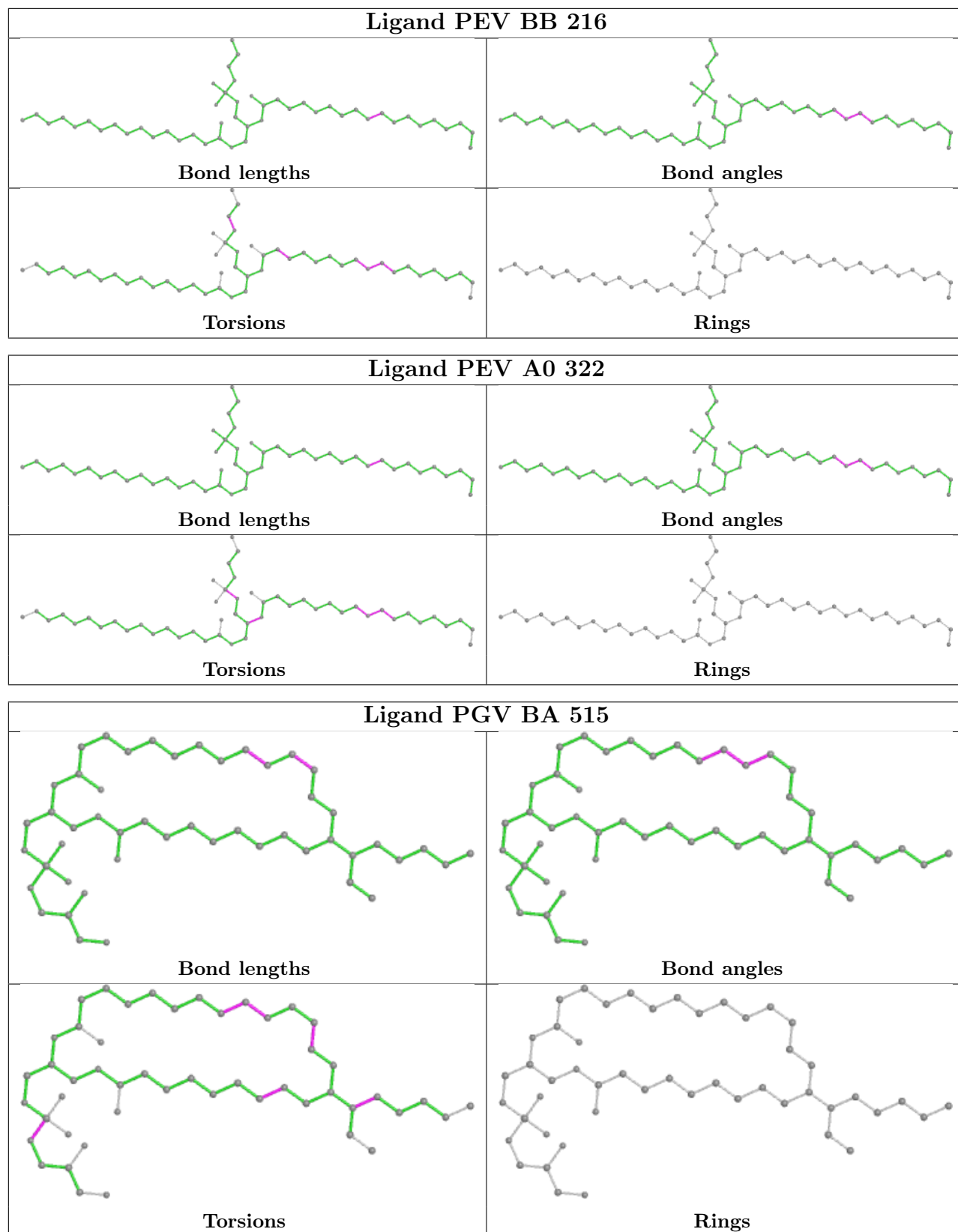
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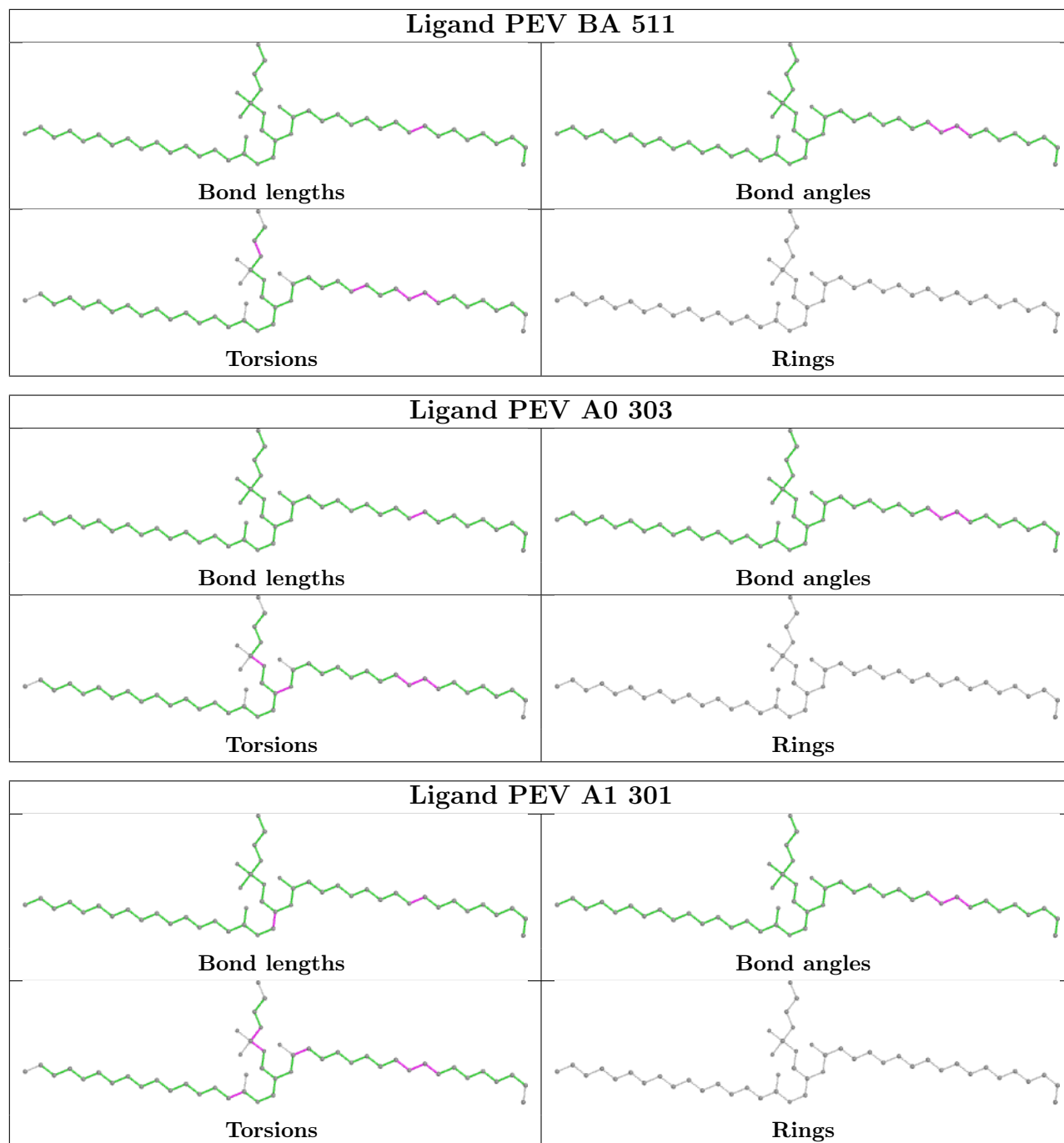
Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	BA	513	PEV	1	0
61	BA	512	PGV	1	0
60	B8	3001	PEV	1	0
60	A1	323	PEV	1	0
60	BA	514	PEV	1	0
60	A1	319	PEV	1	0
60	A0	315	PEV	1	0
60	BA	526	PEV	1	0
61	A1	315	PGV	1	0
60	A1	302	PEV	1	0
60	B8	3002	PEV	2	0
61	A1	303	PGV	1	0

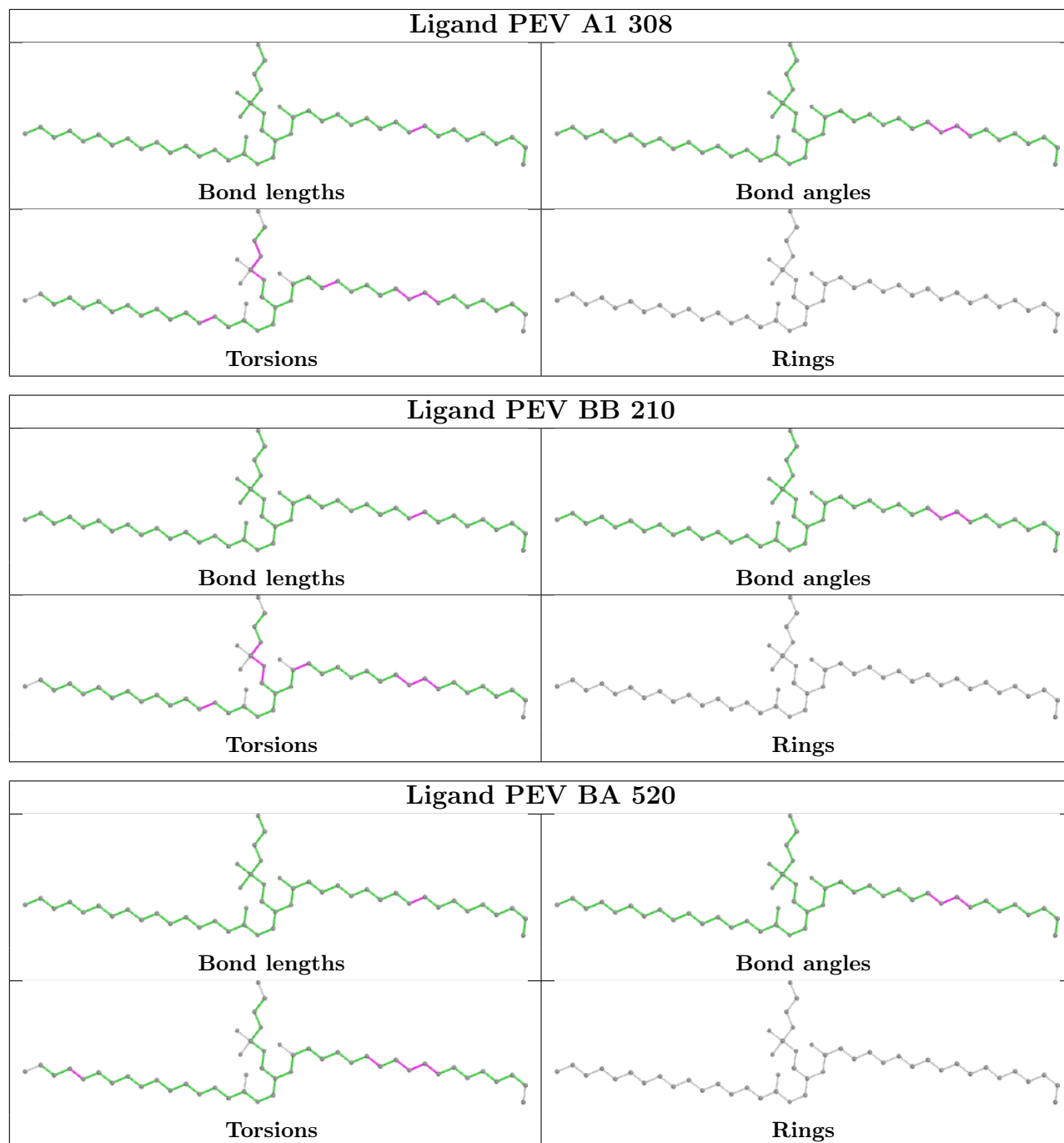
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

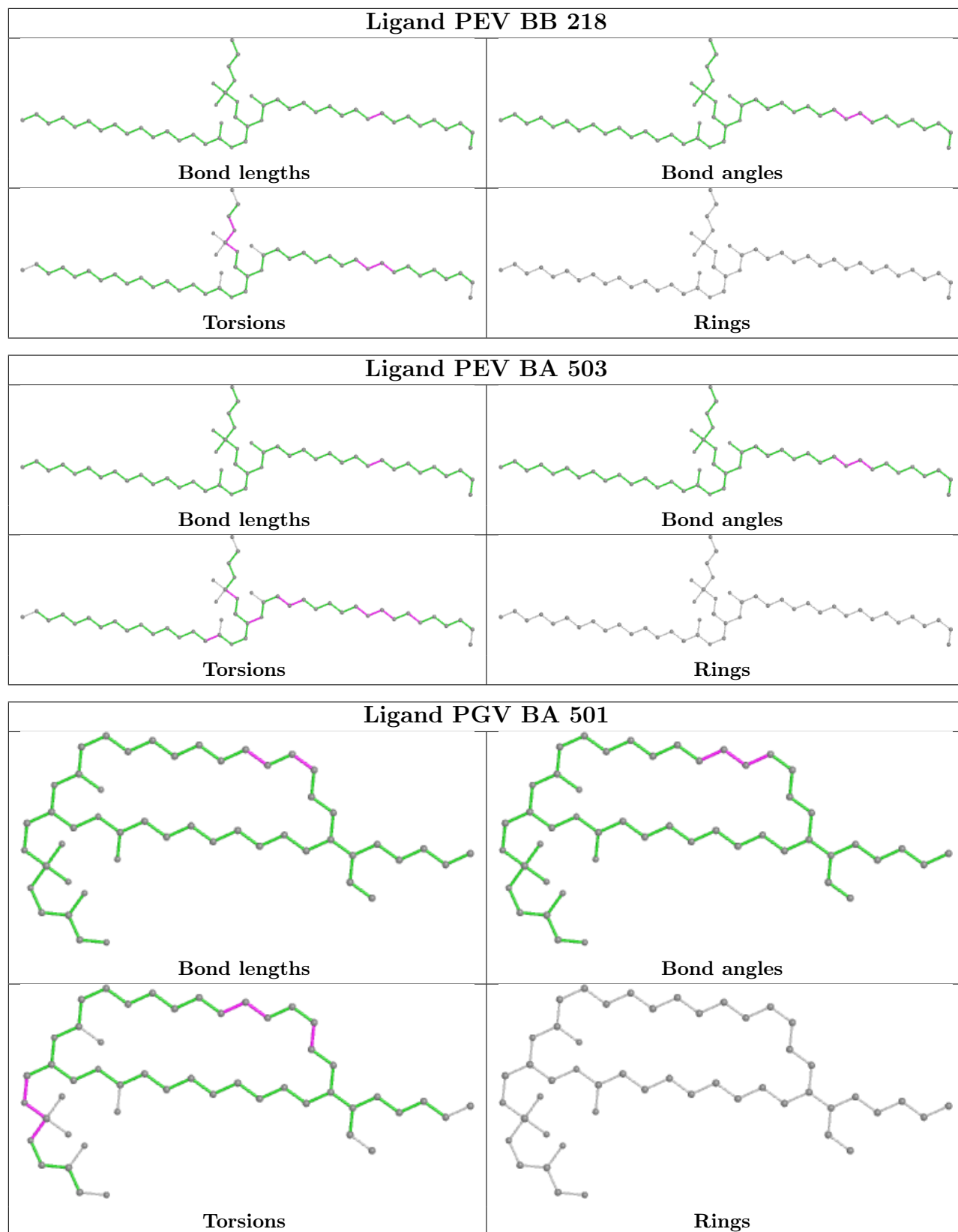


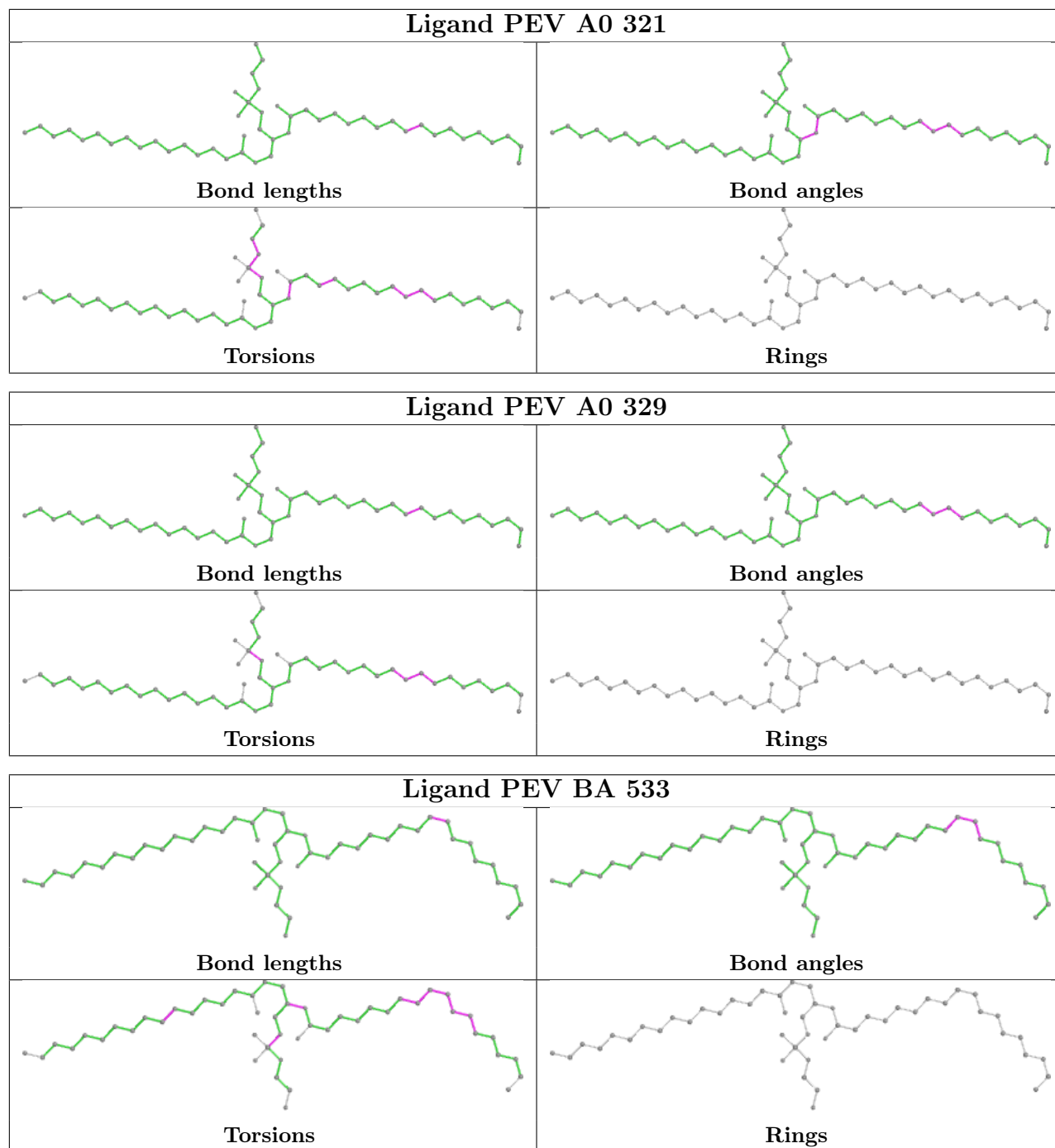


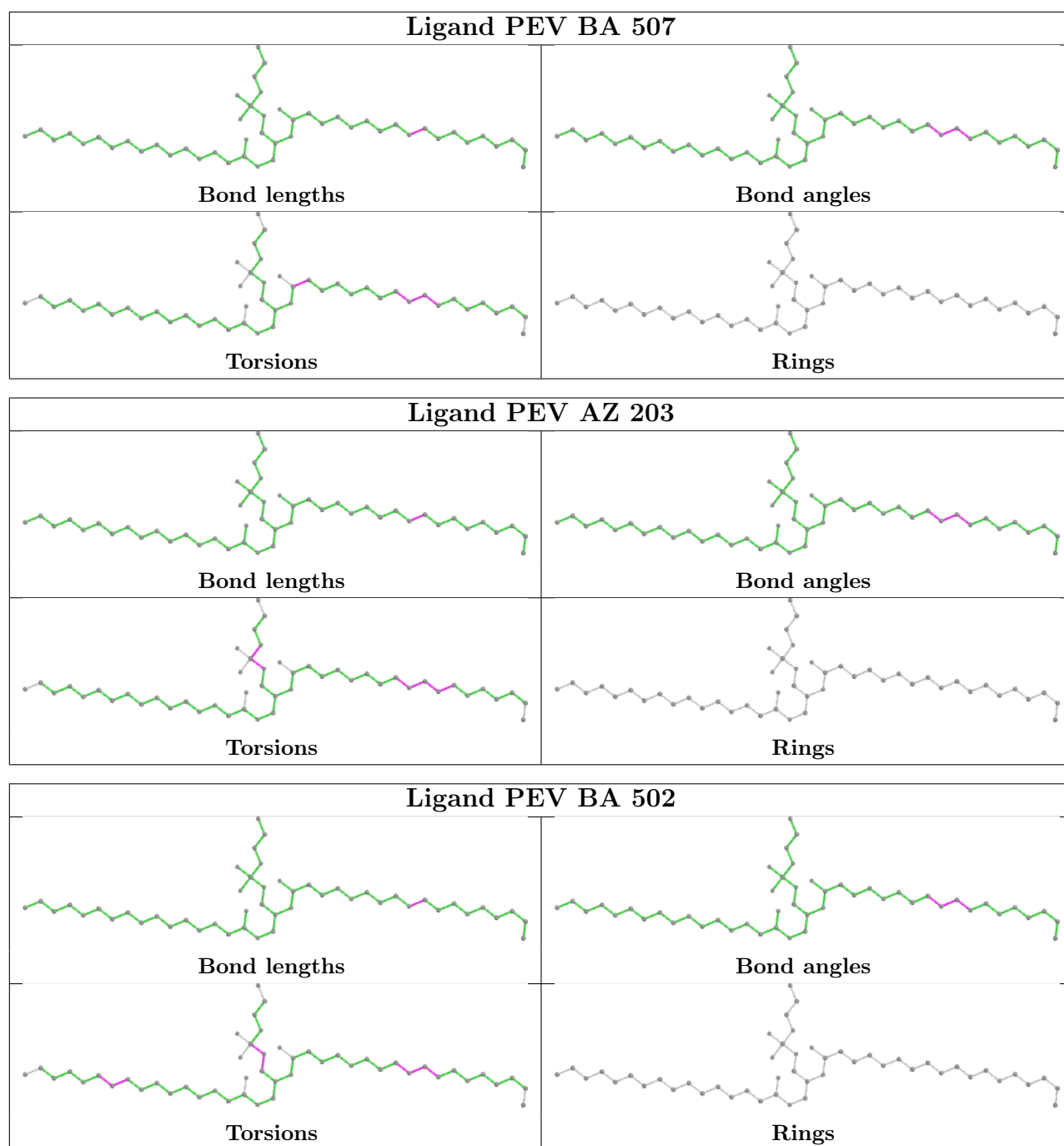


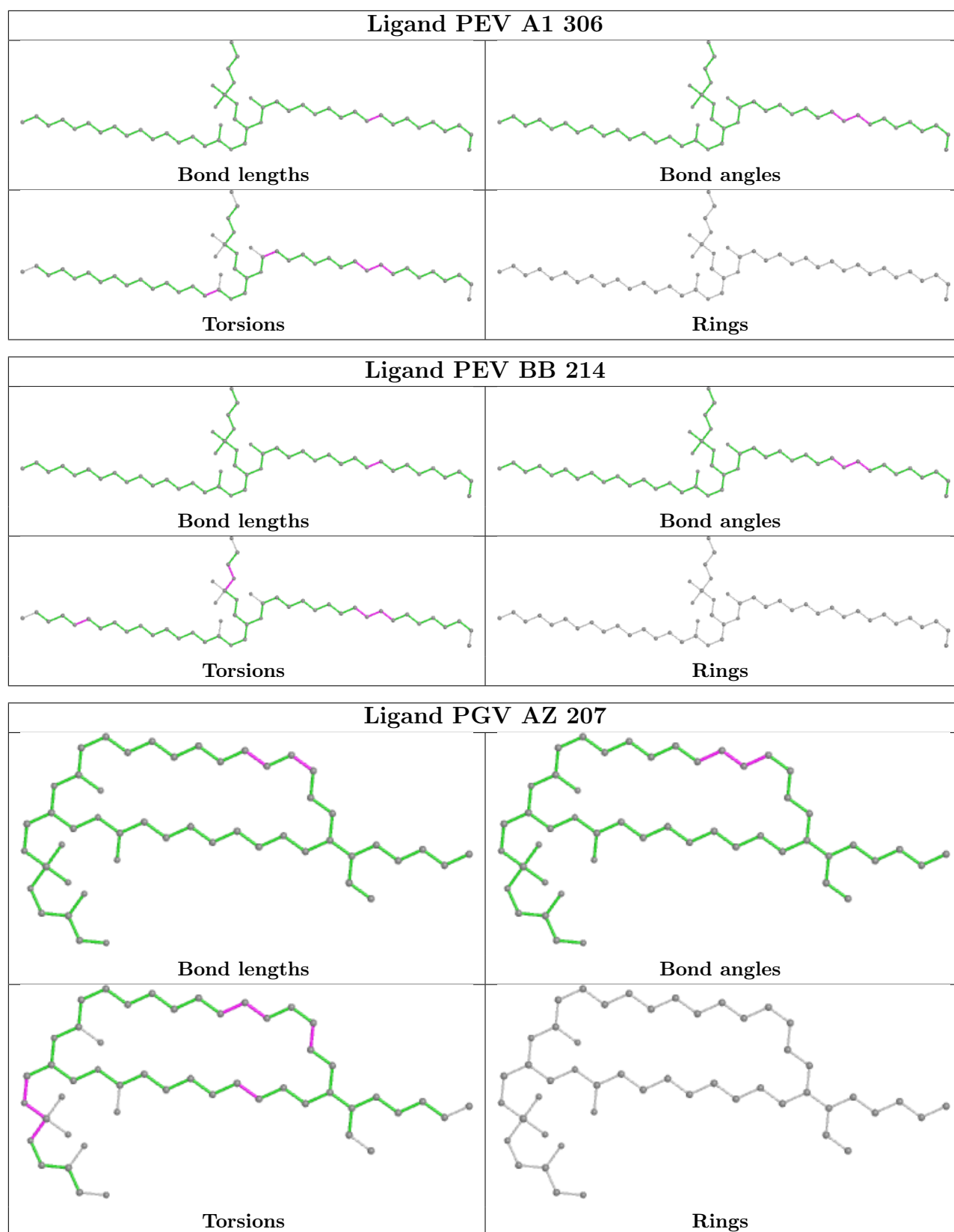


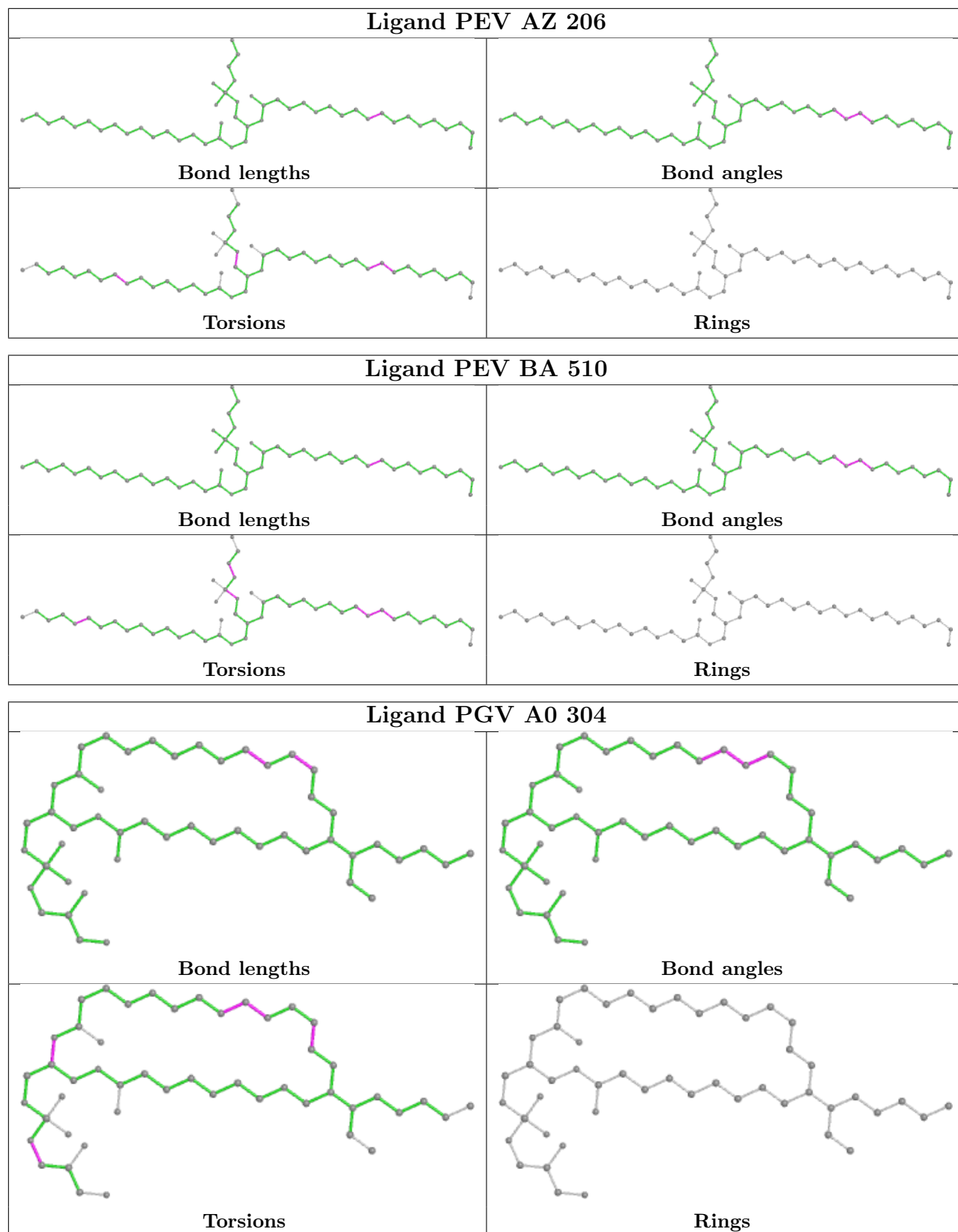


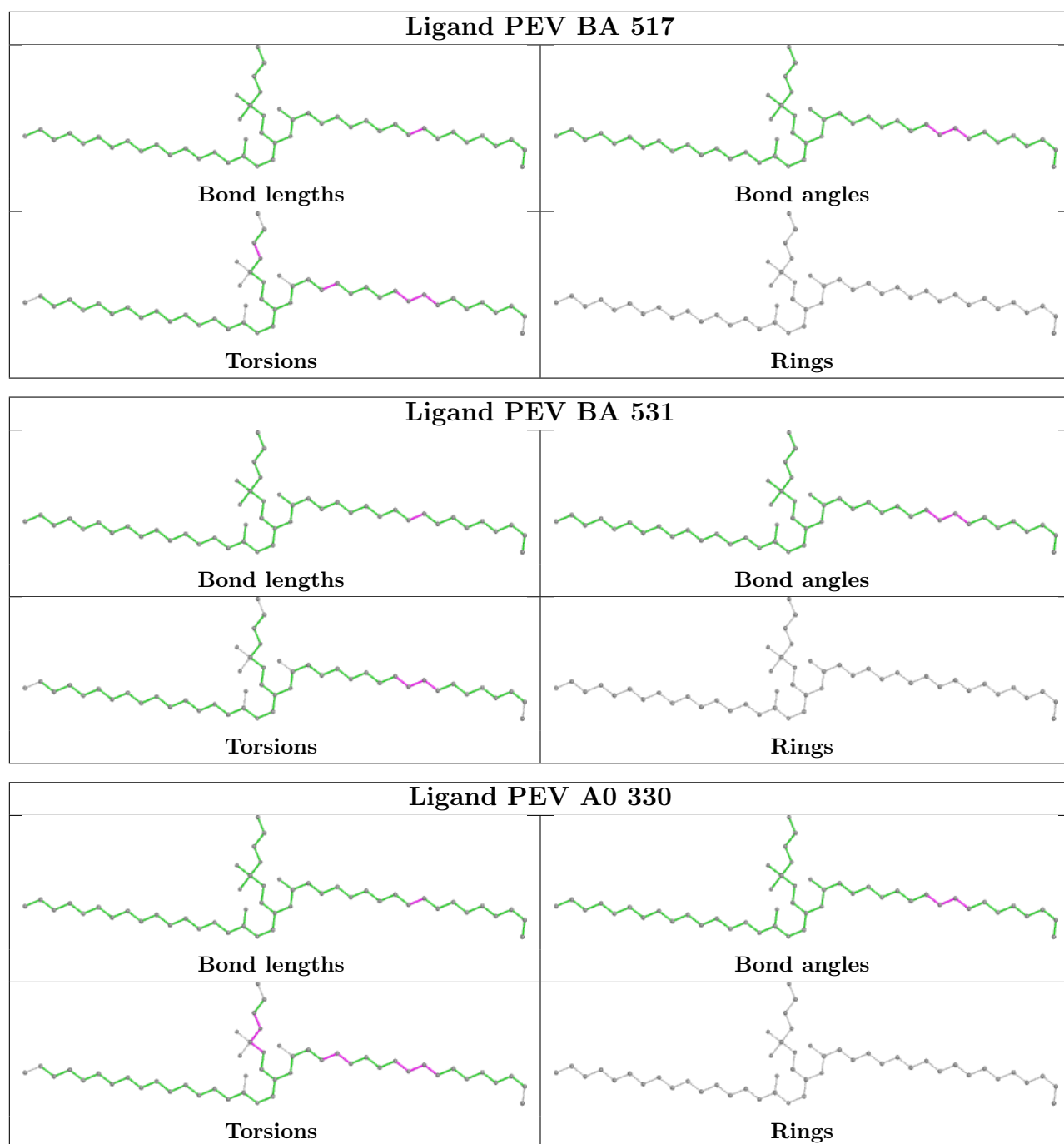


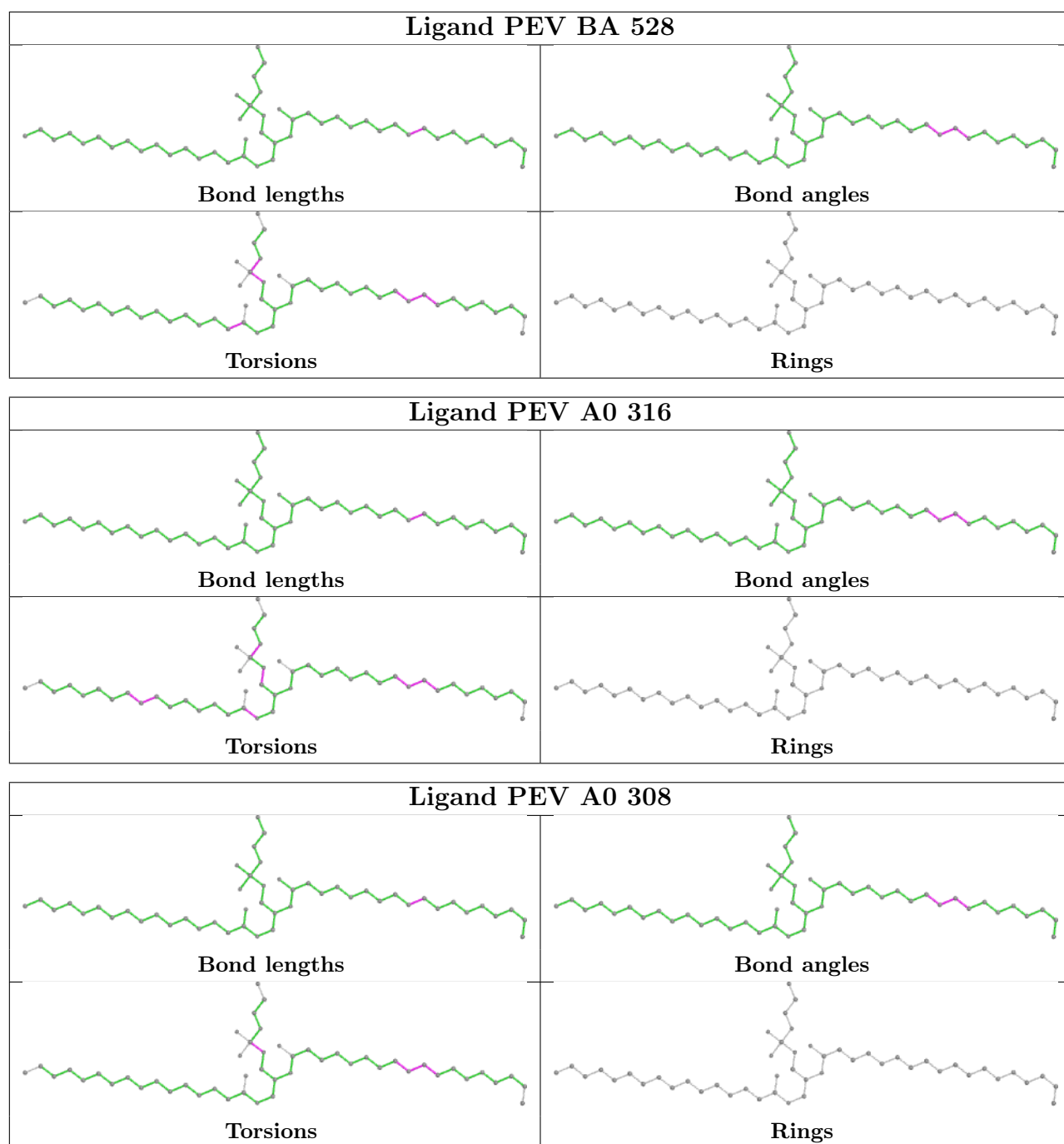


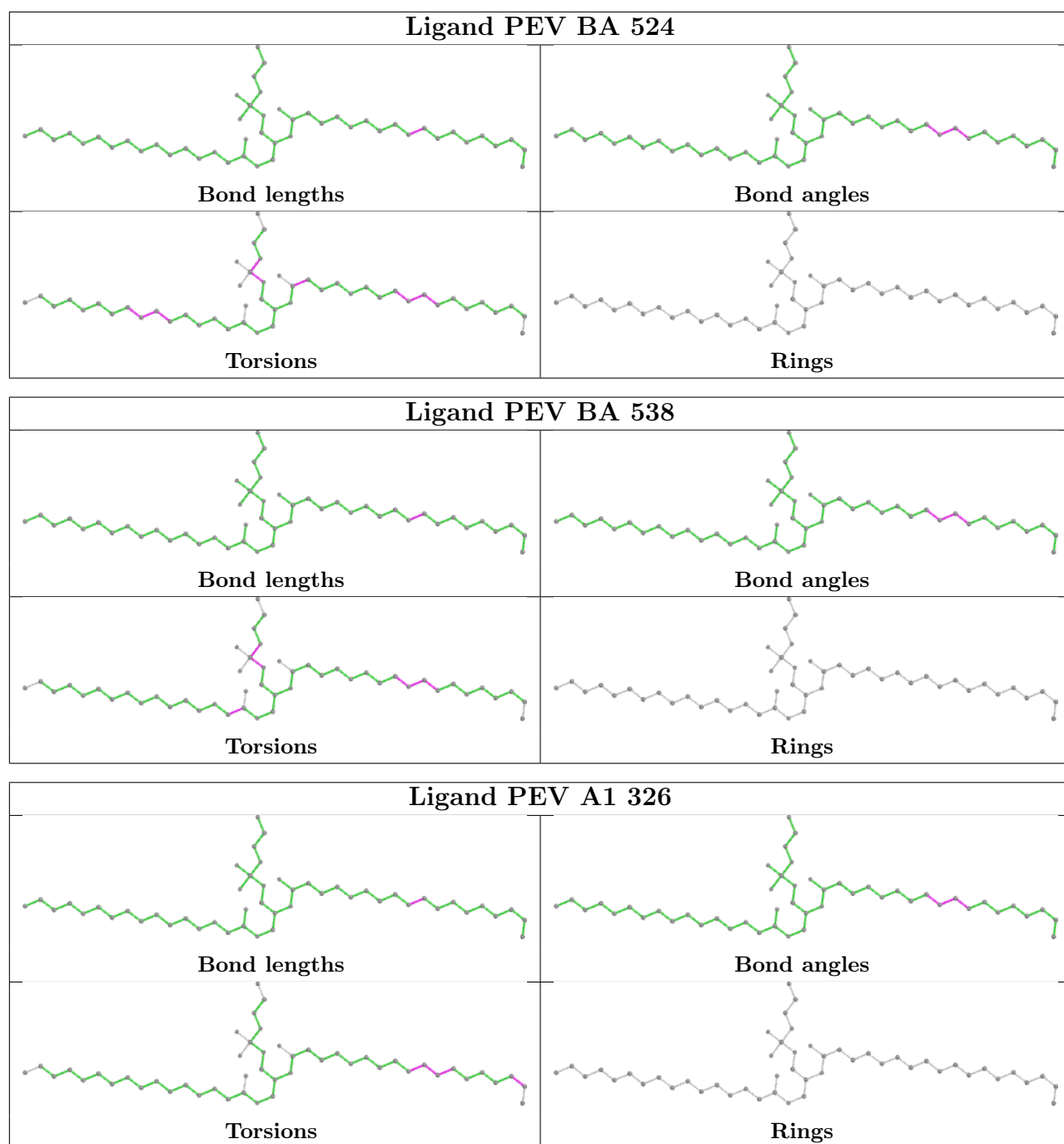


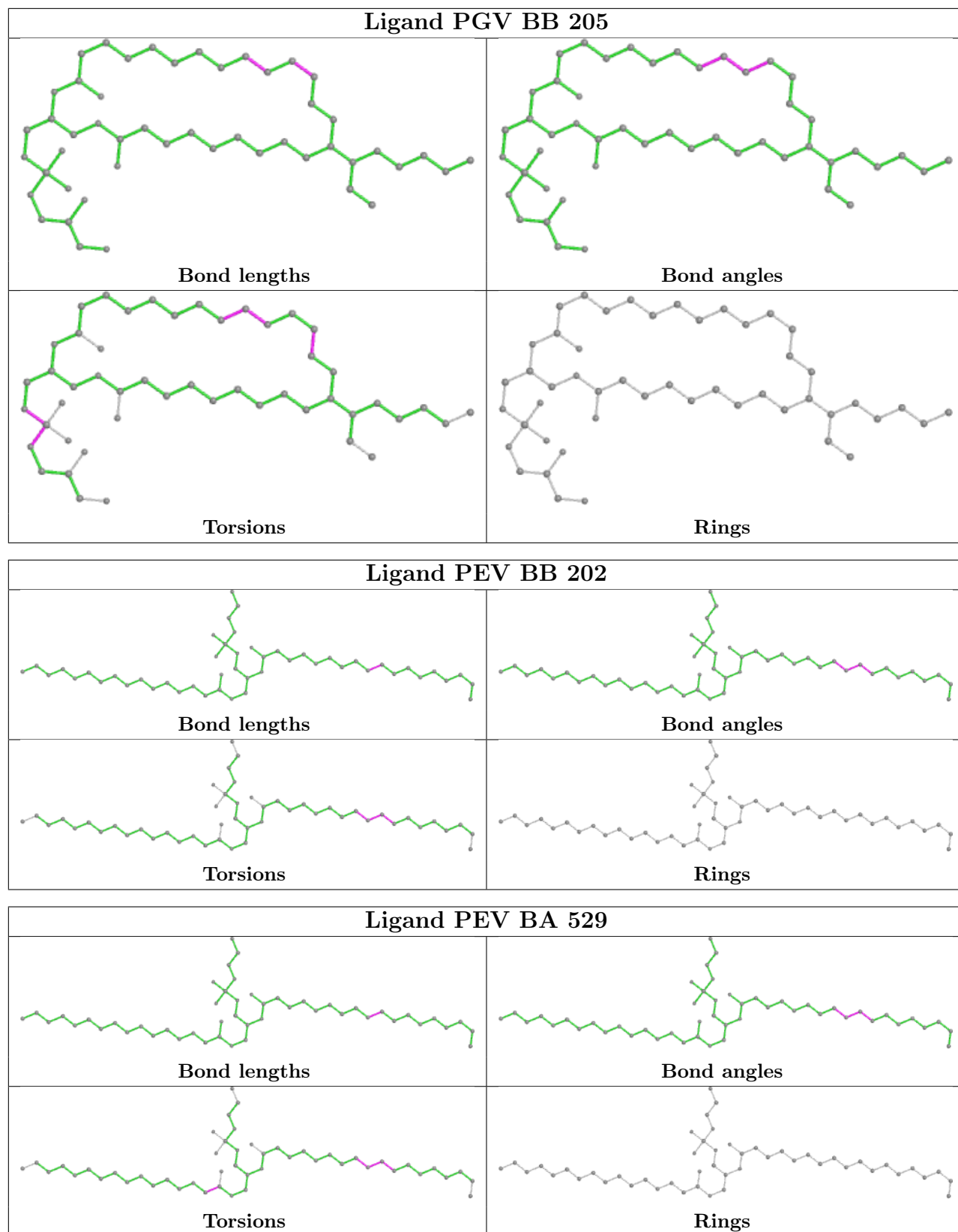


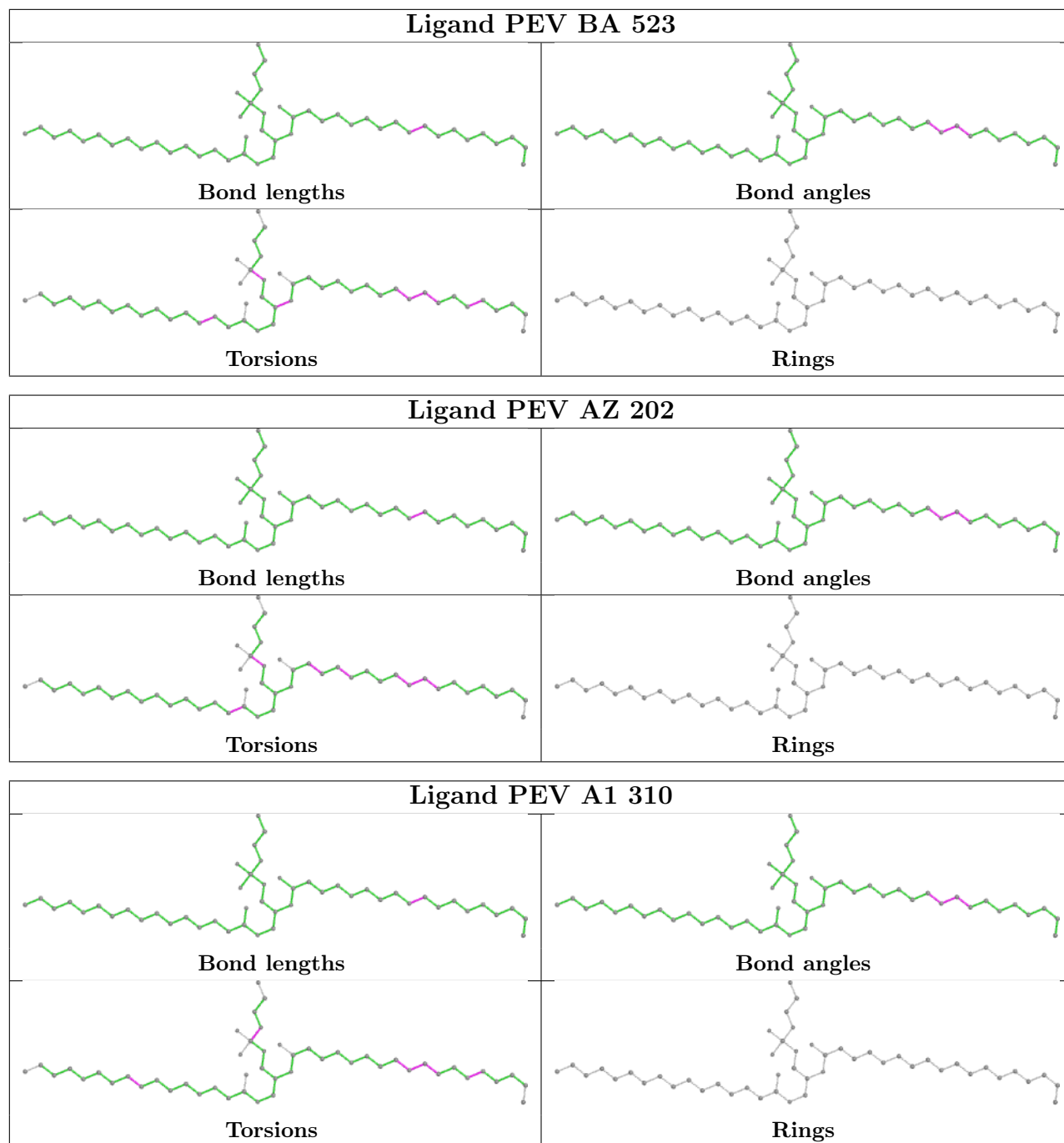


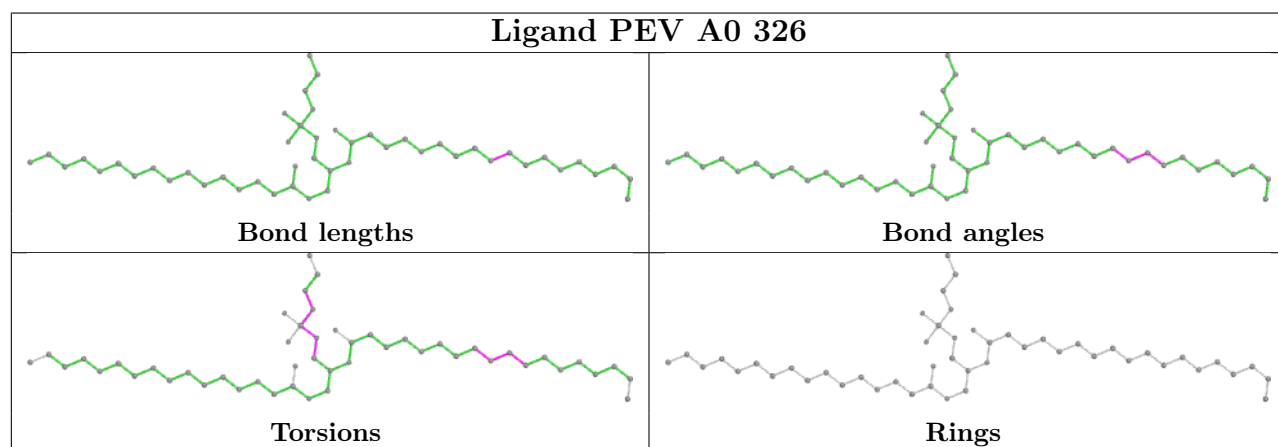
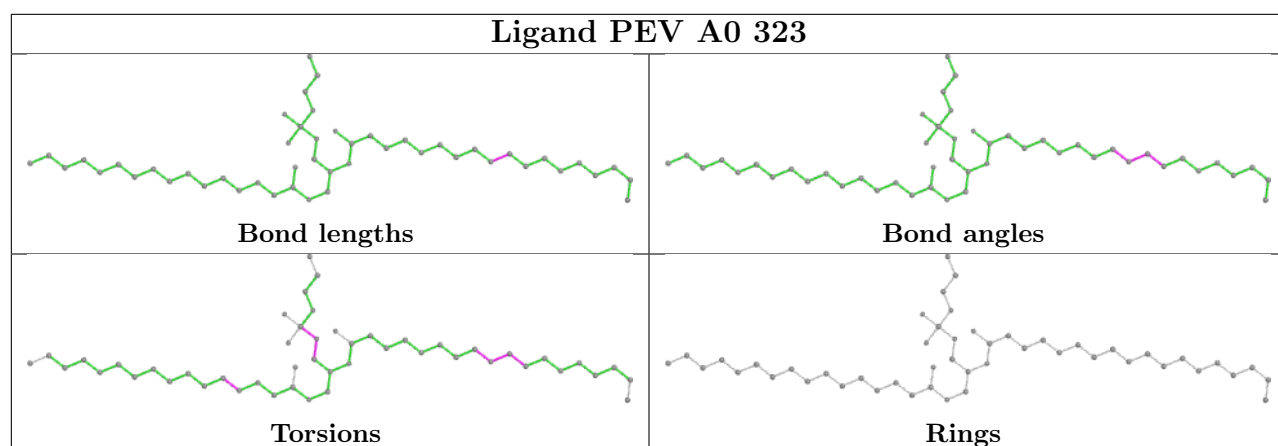
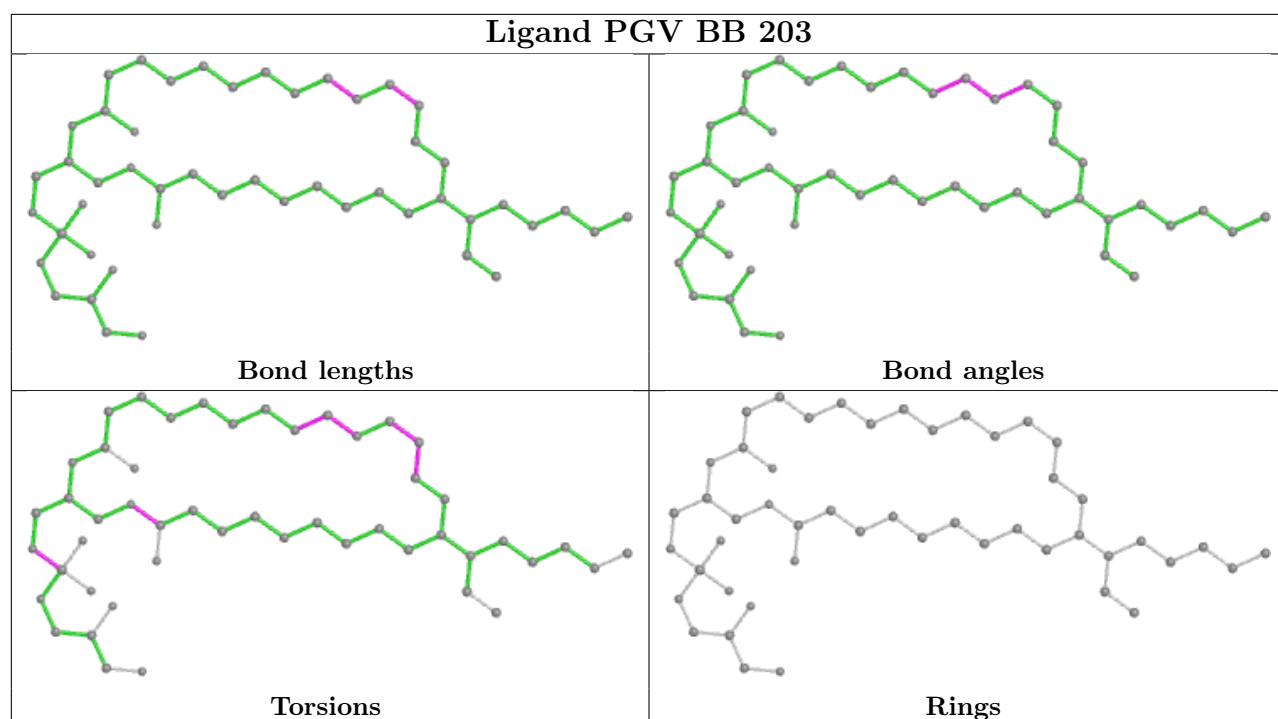


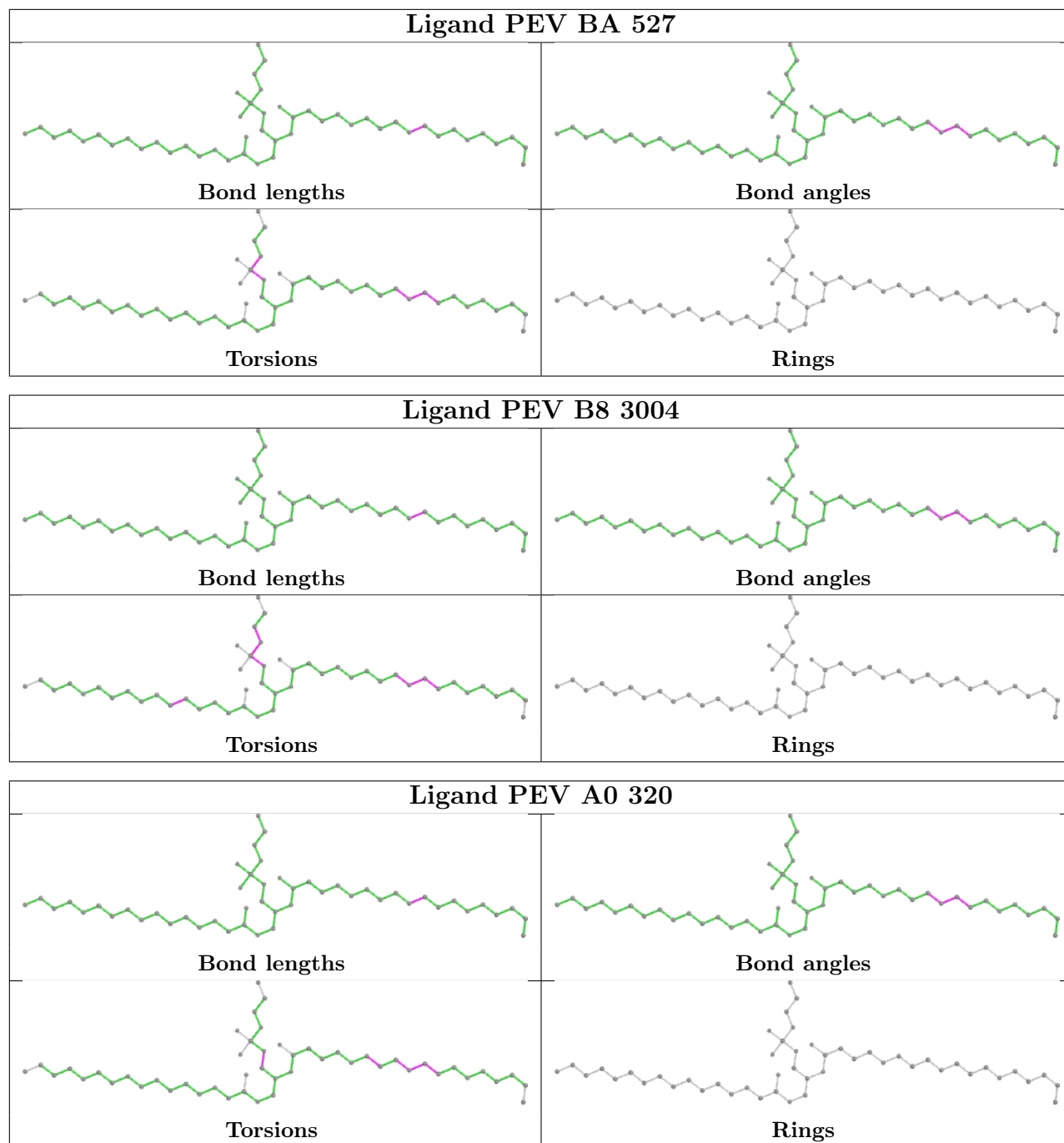


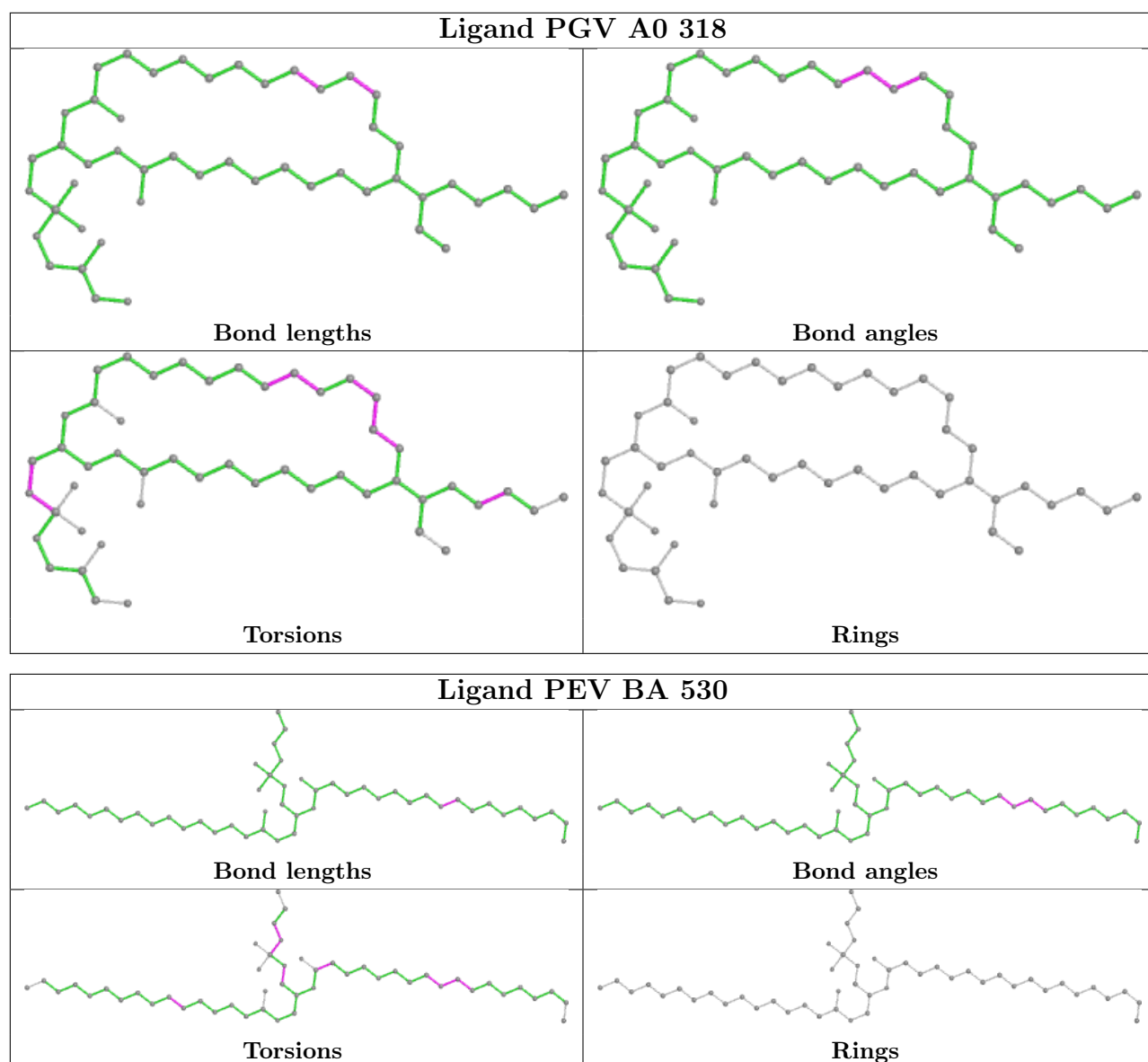


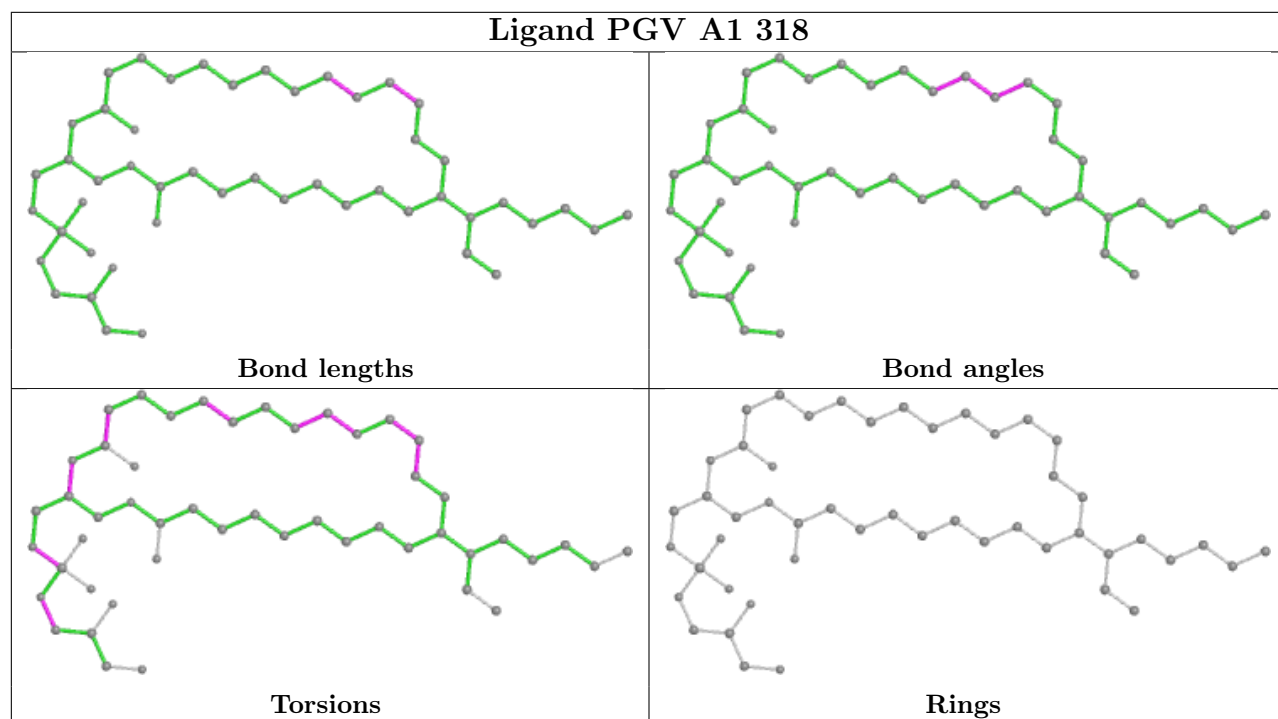
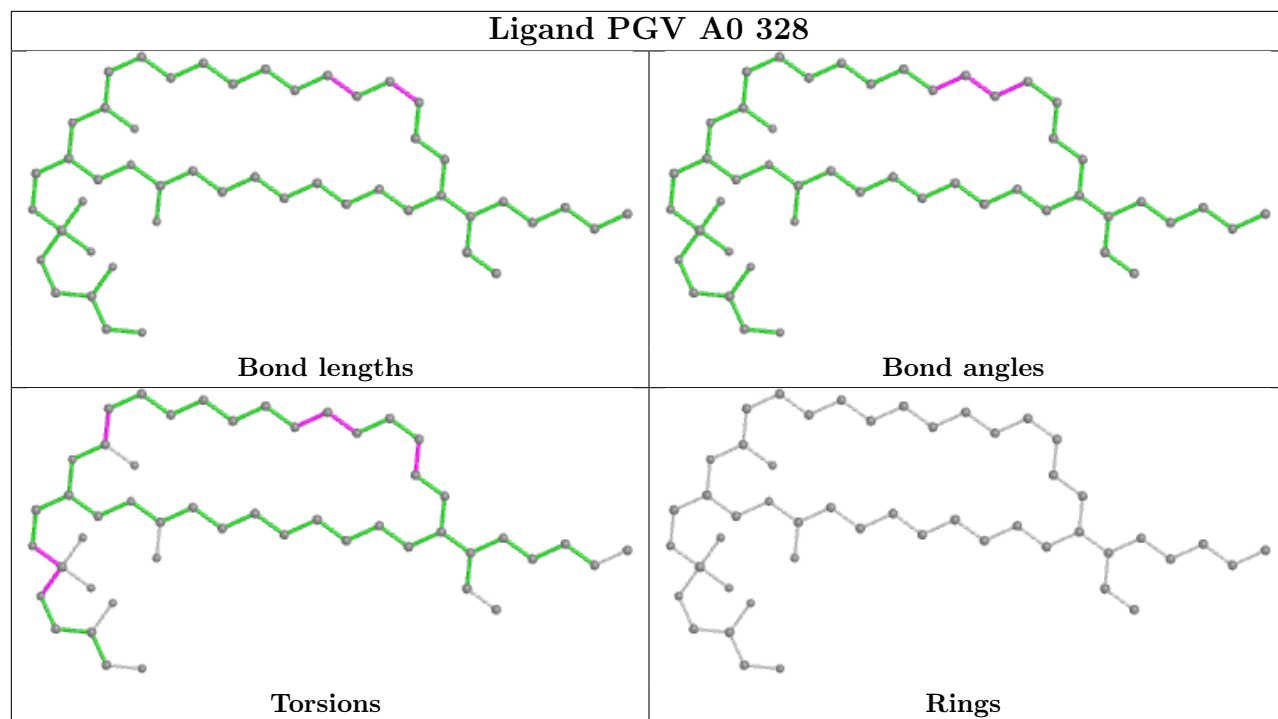


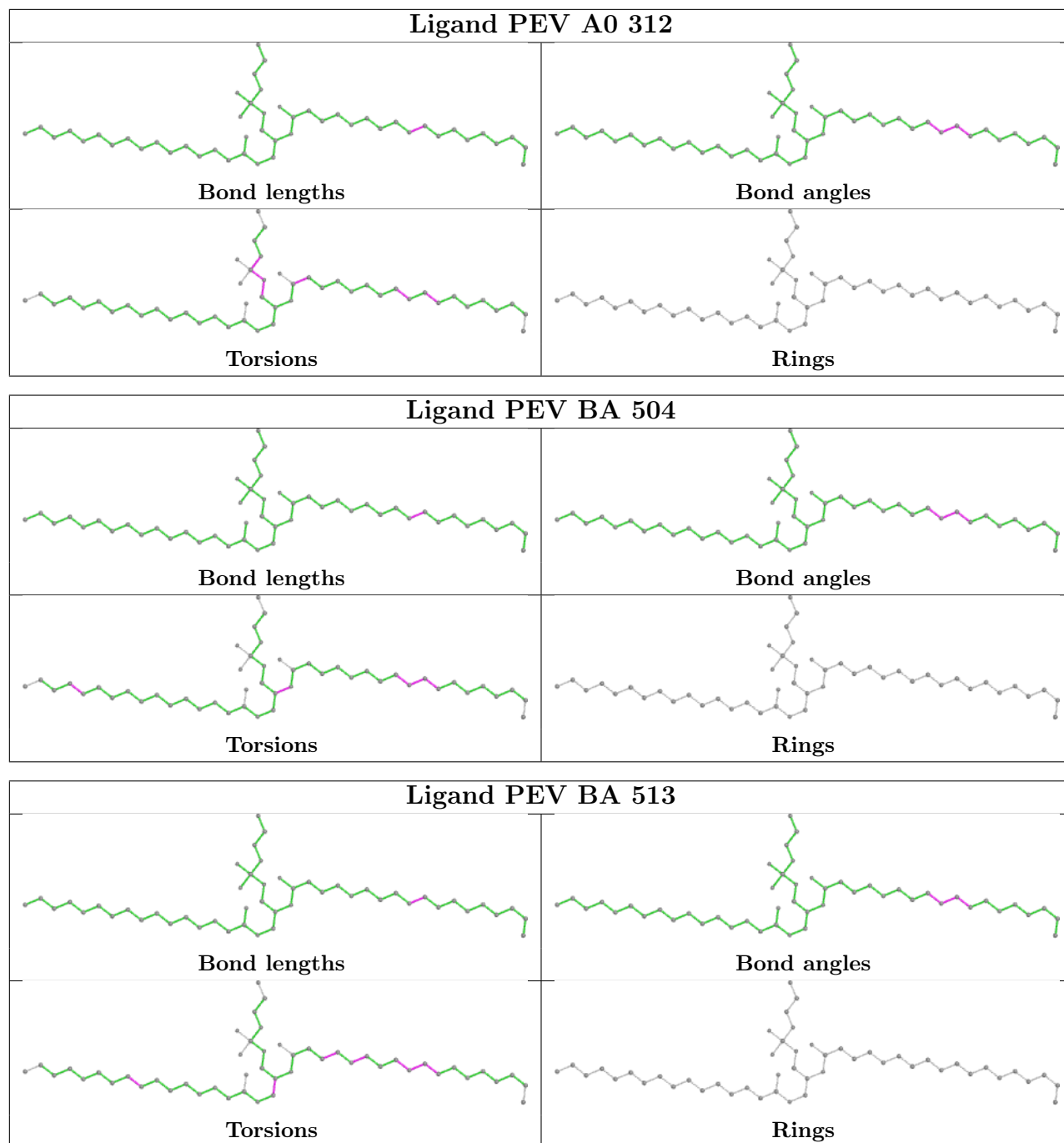


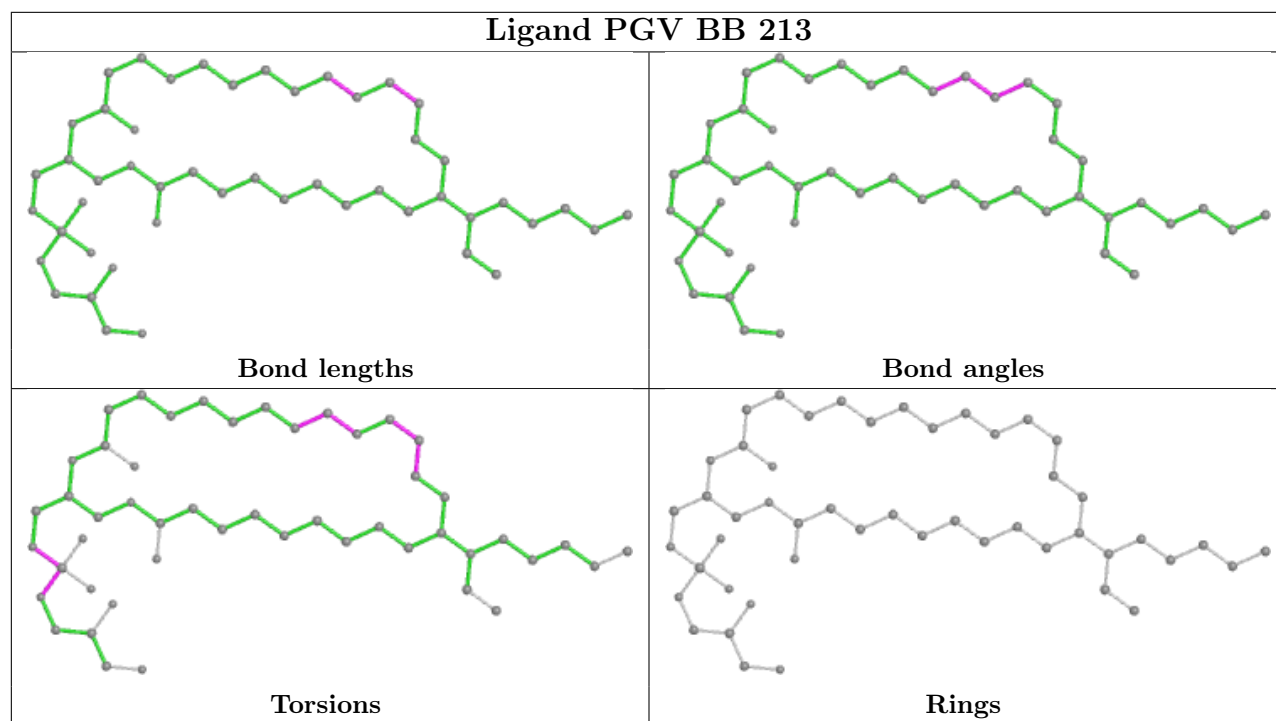
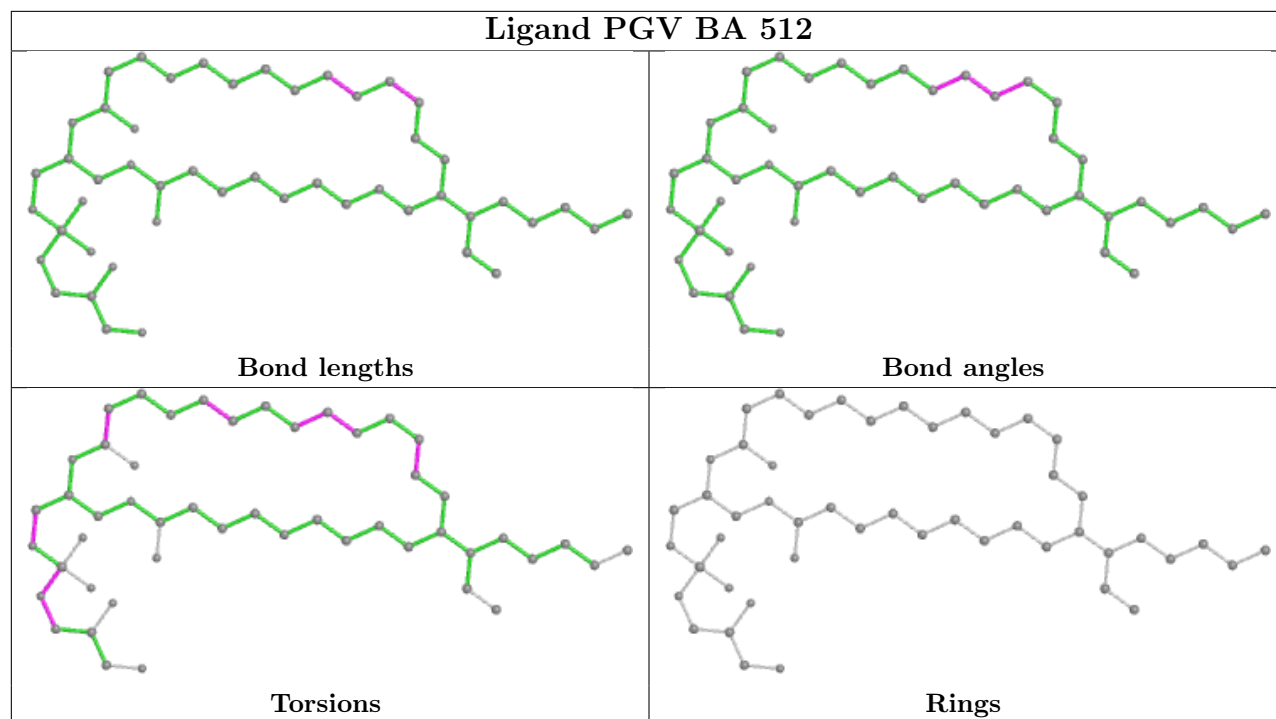


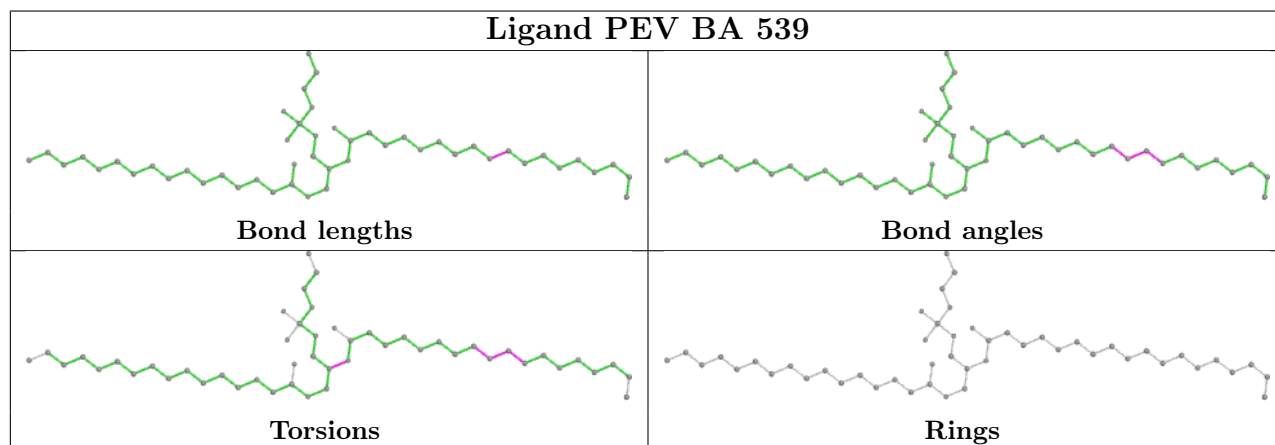
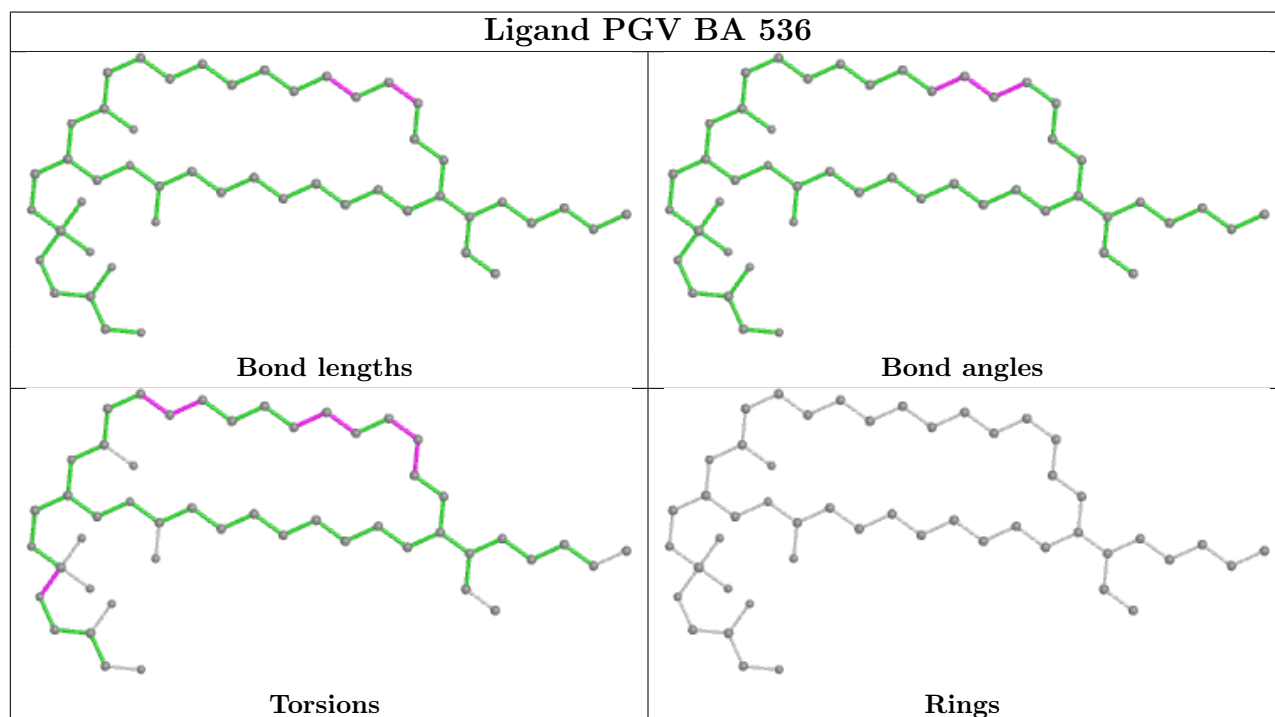
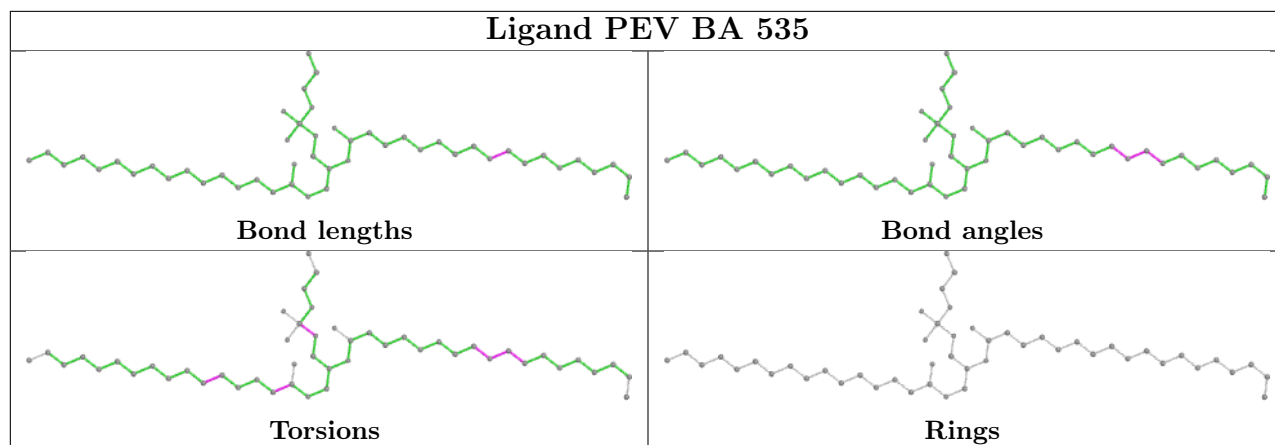


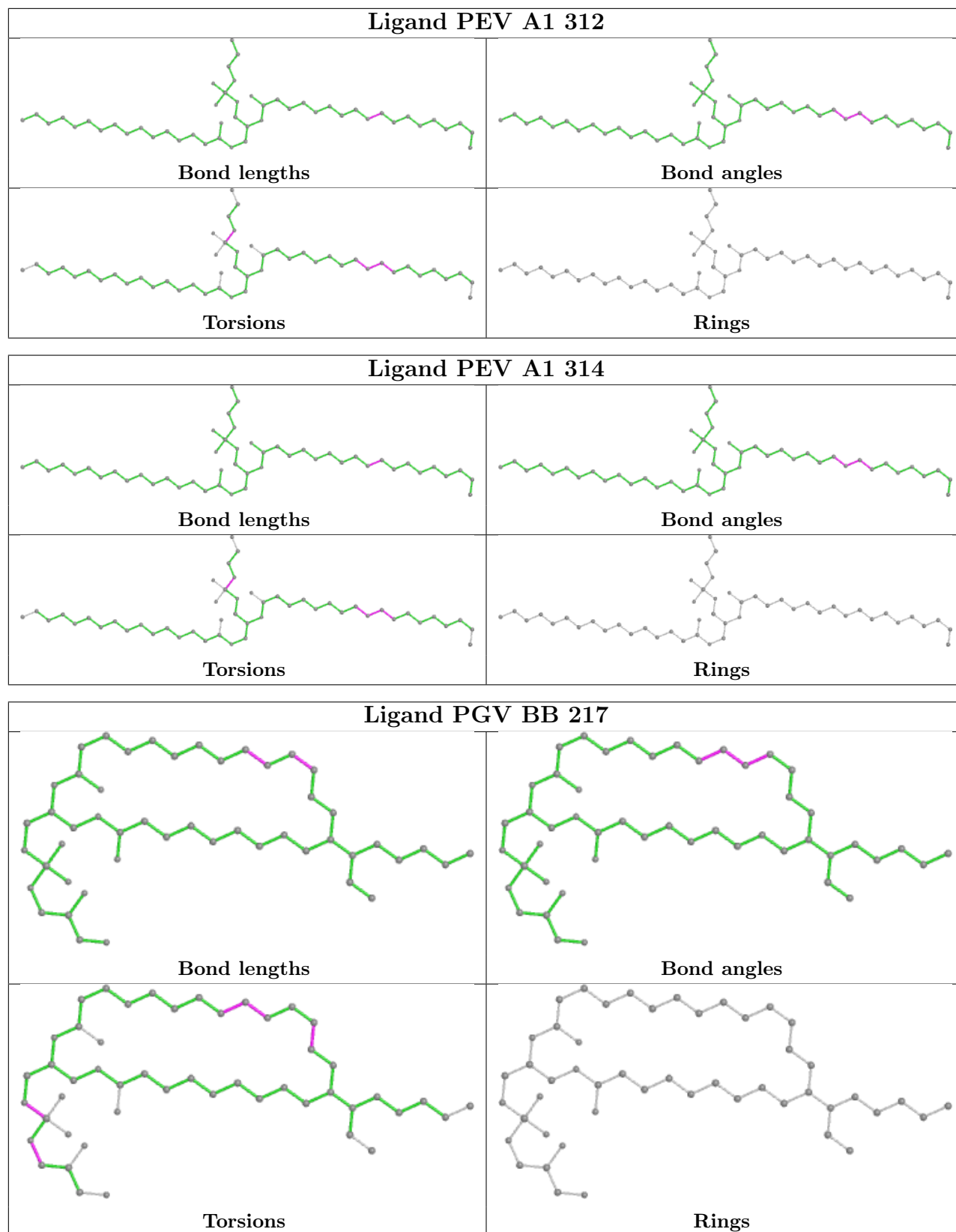


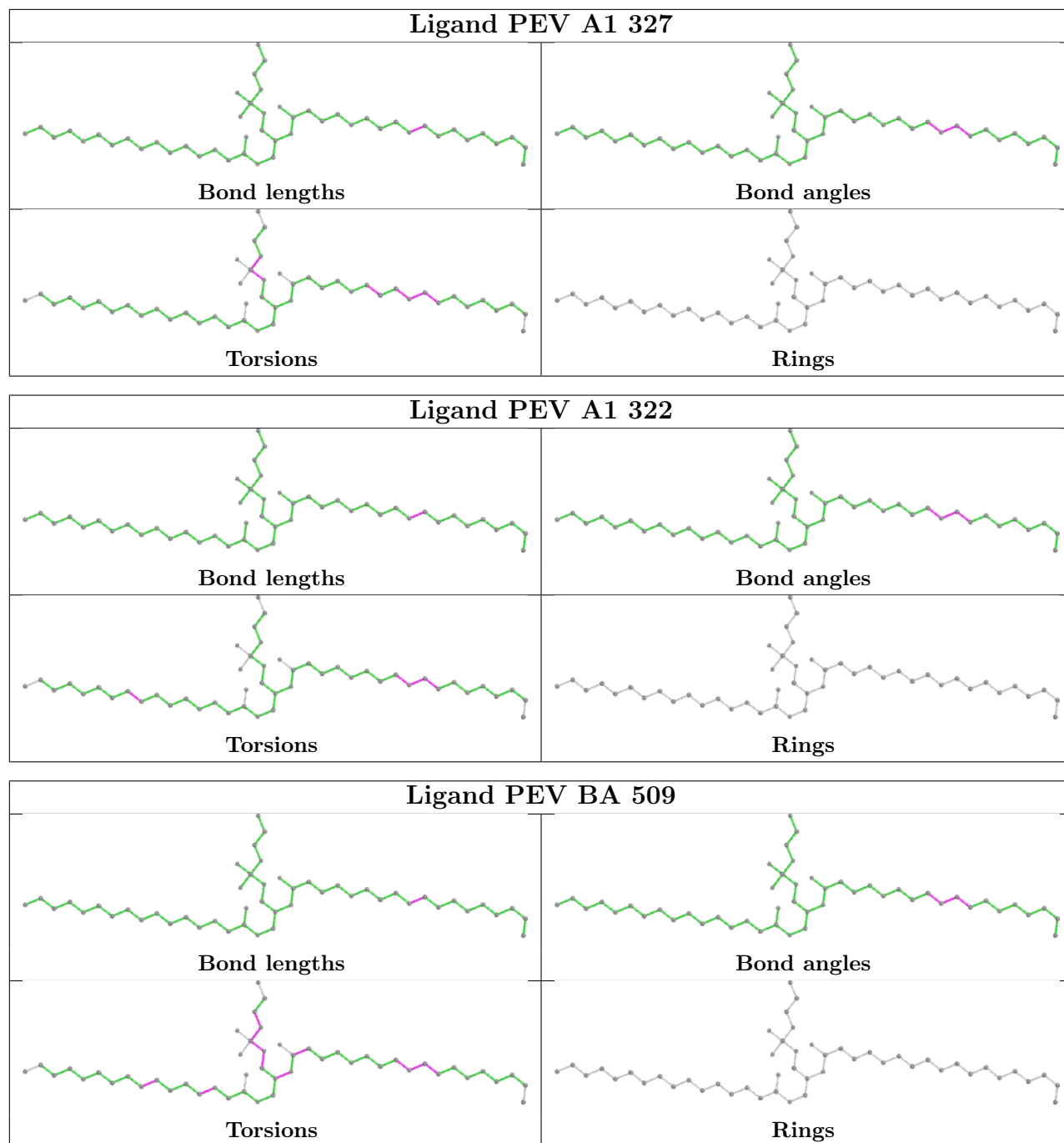


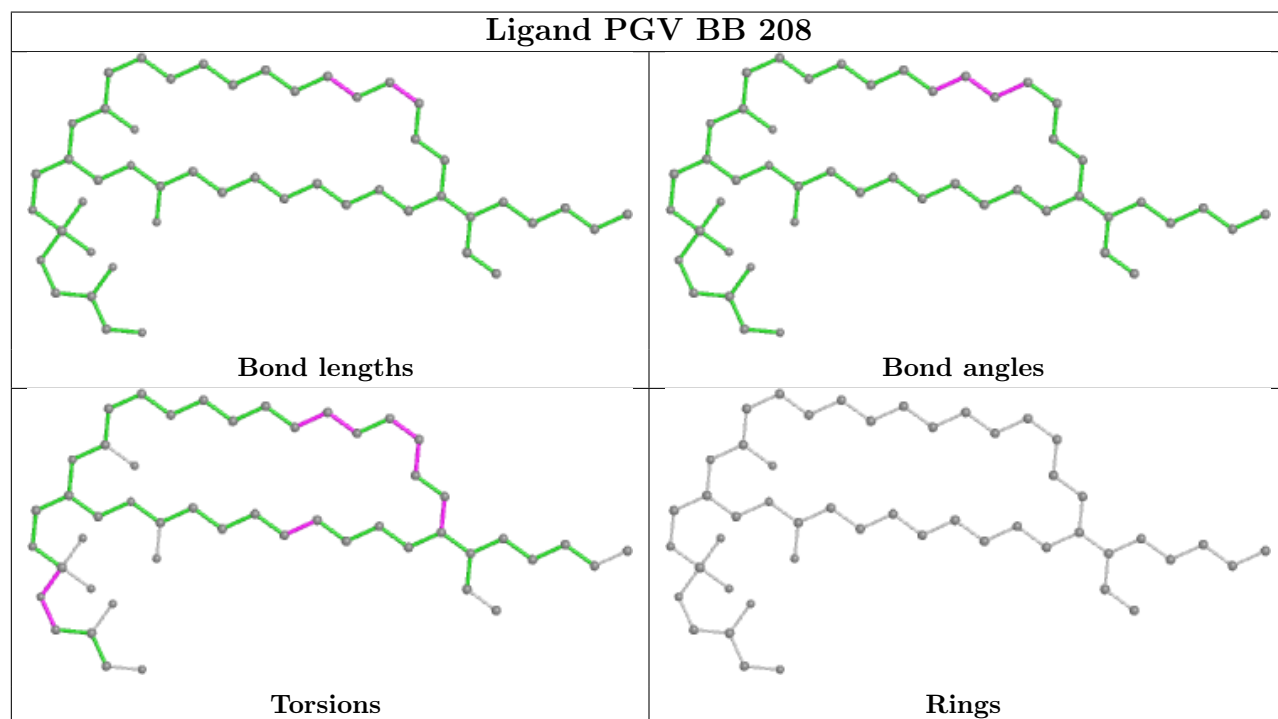
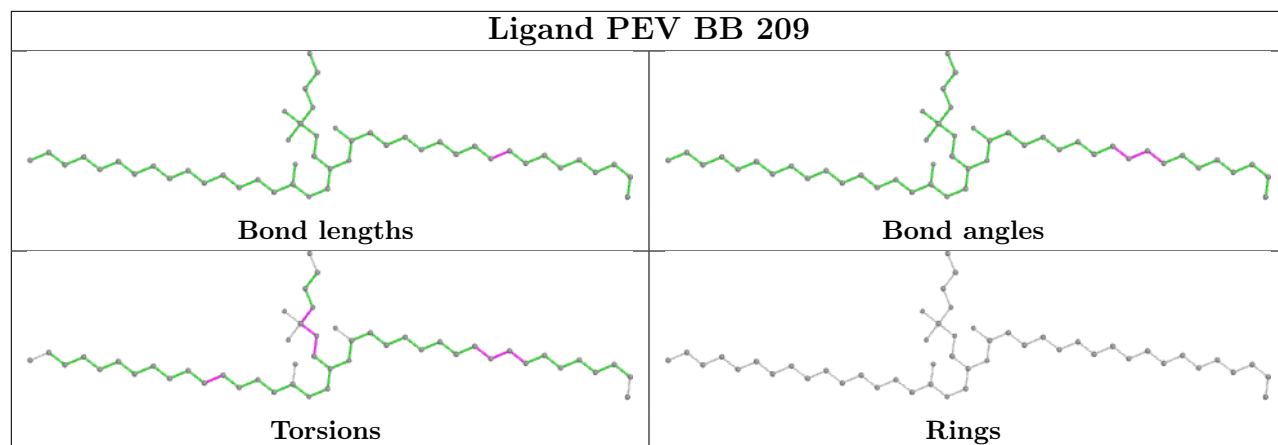


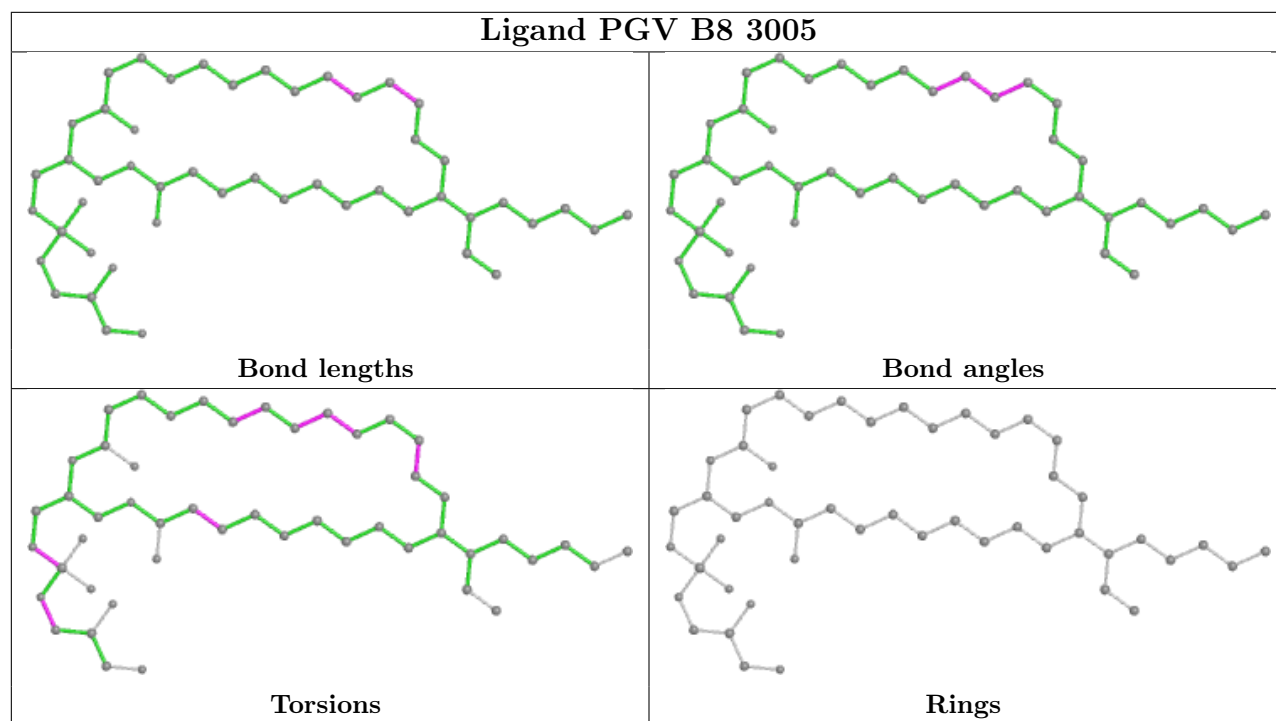
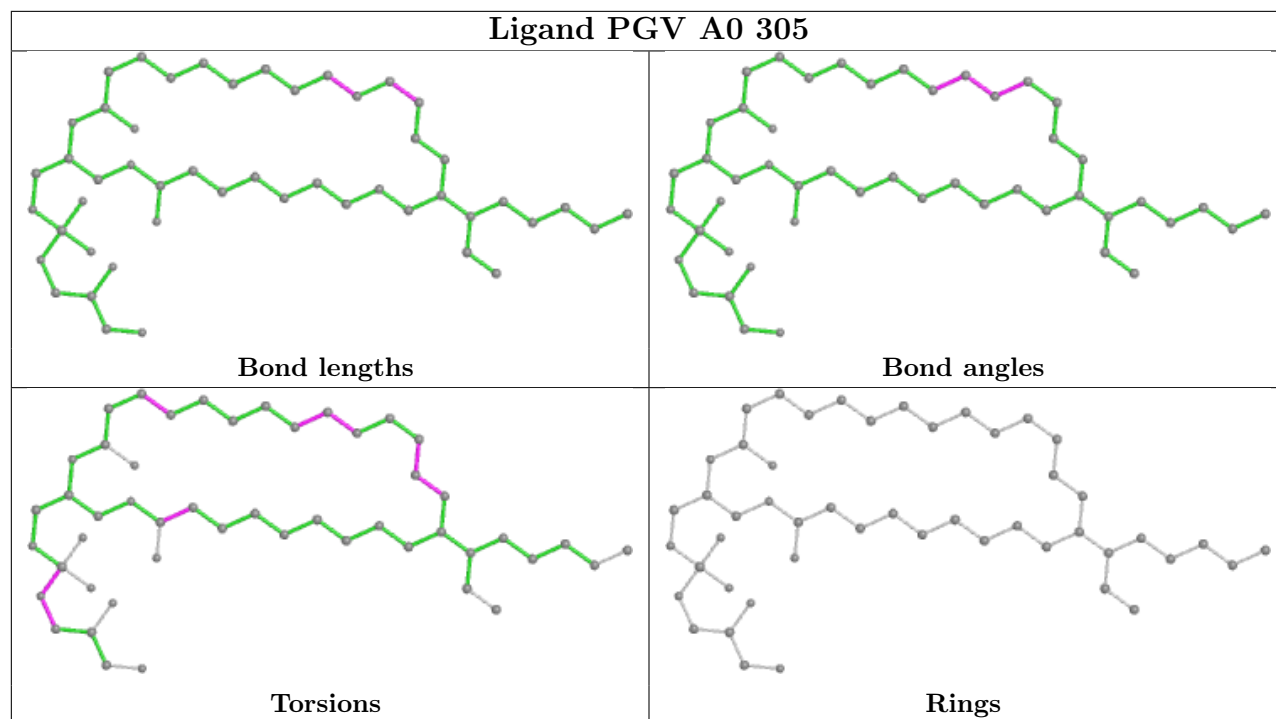


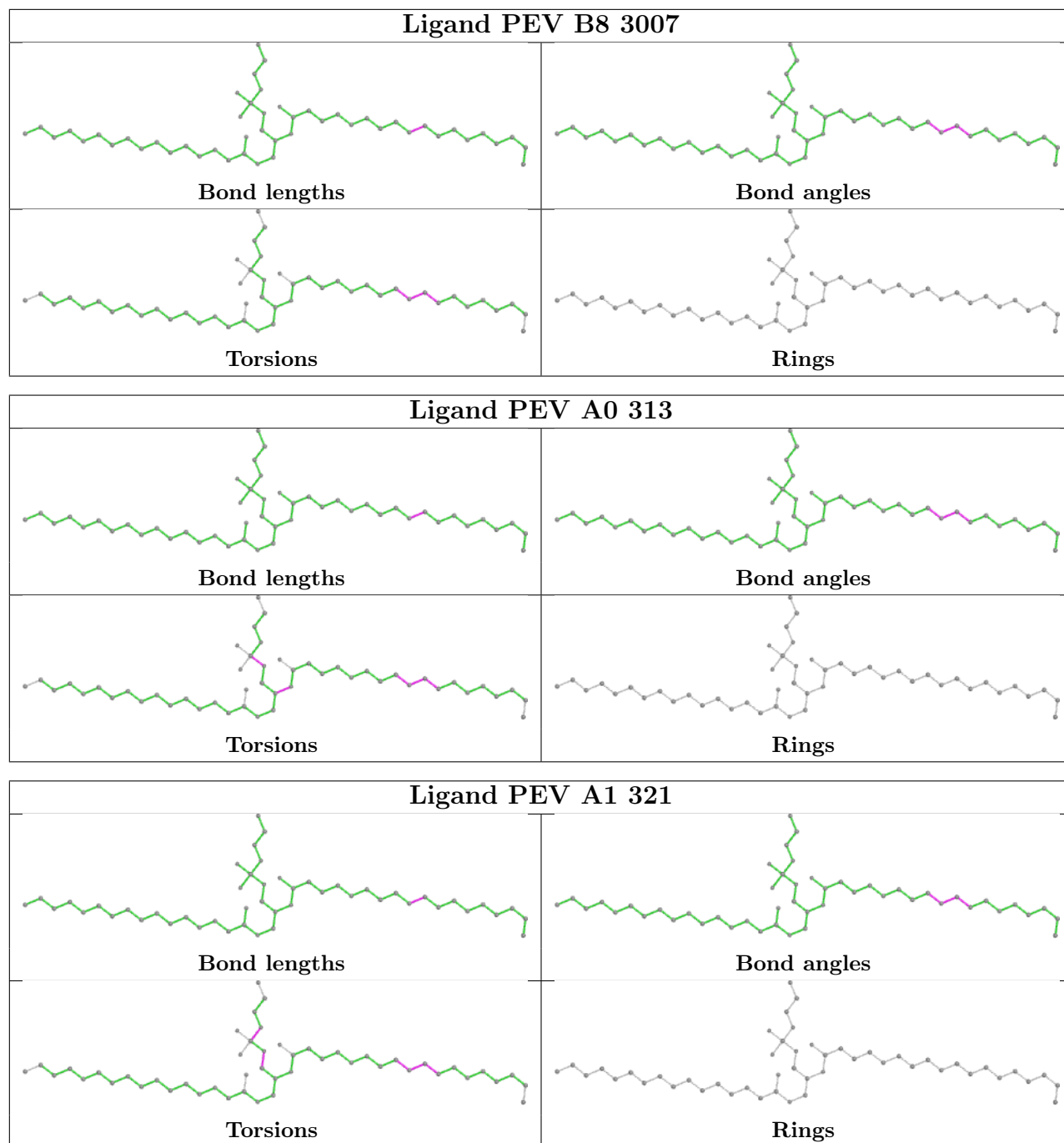


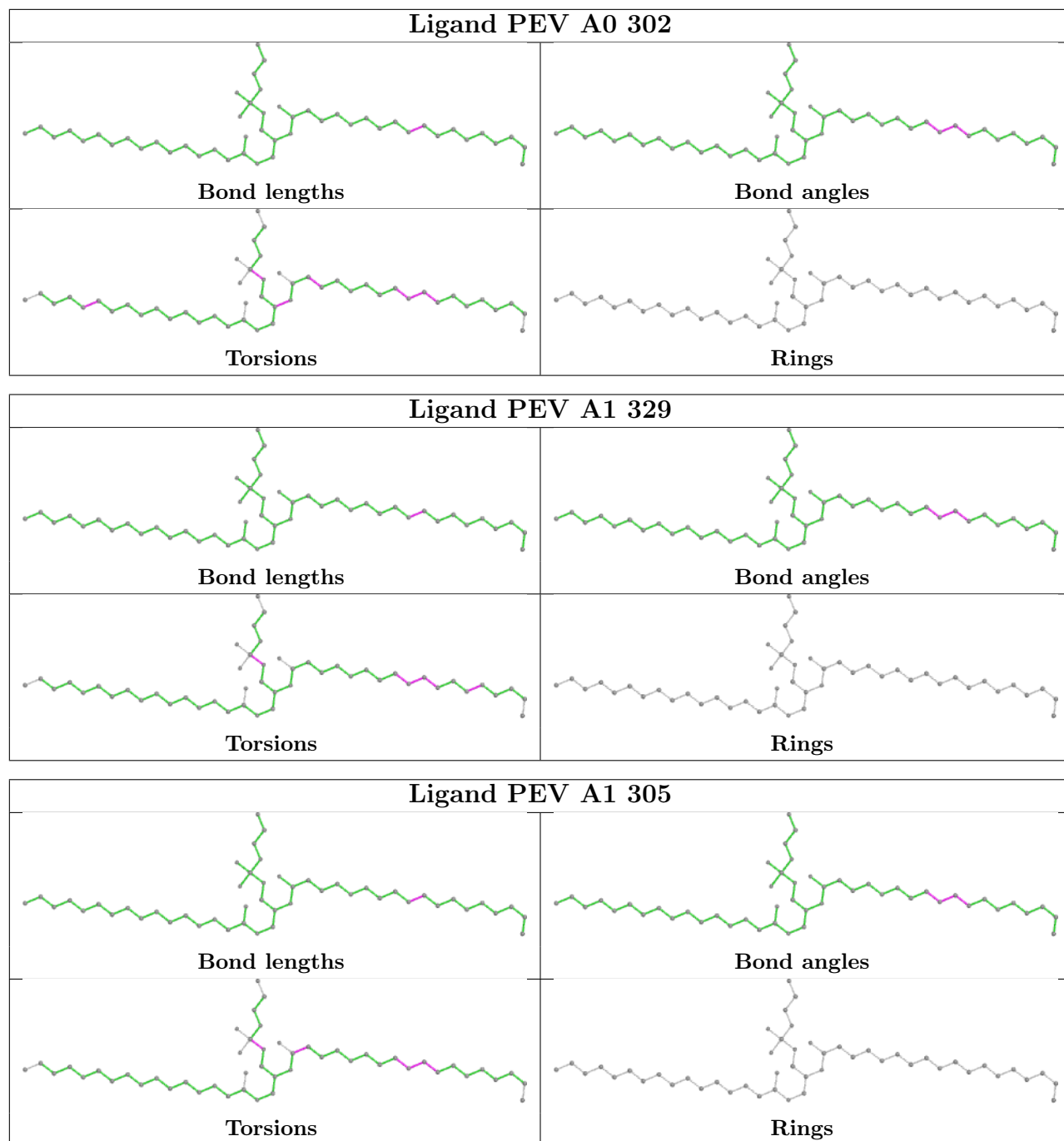


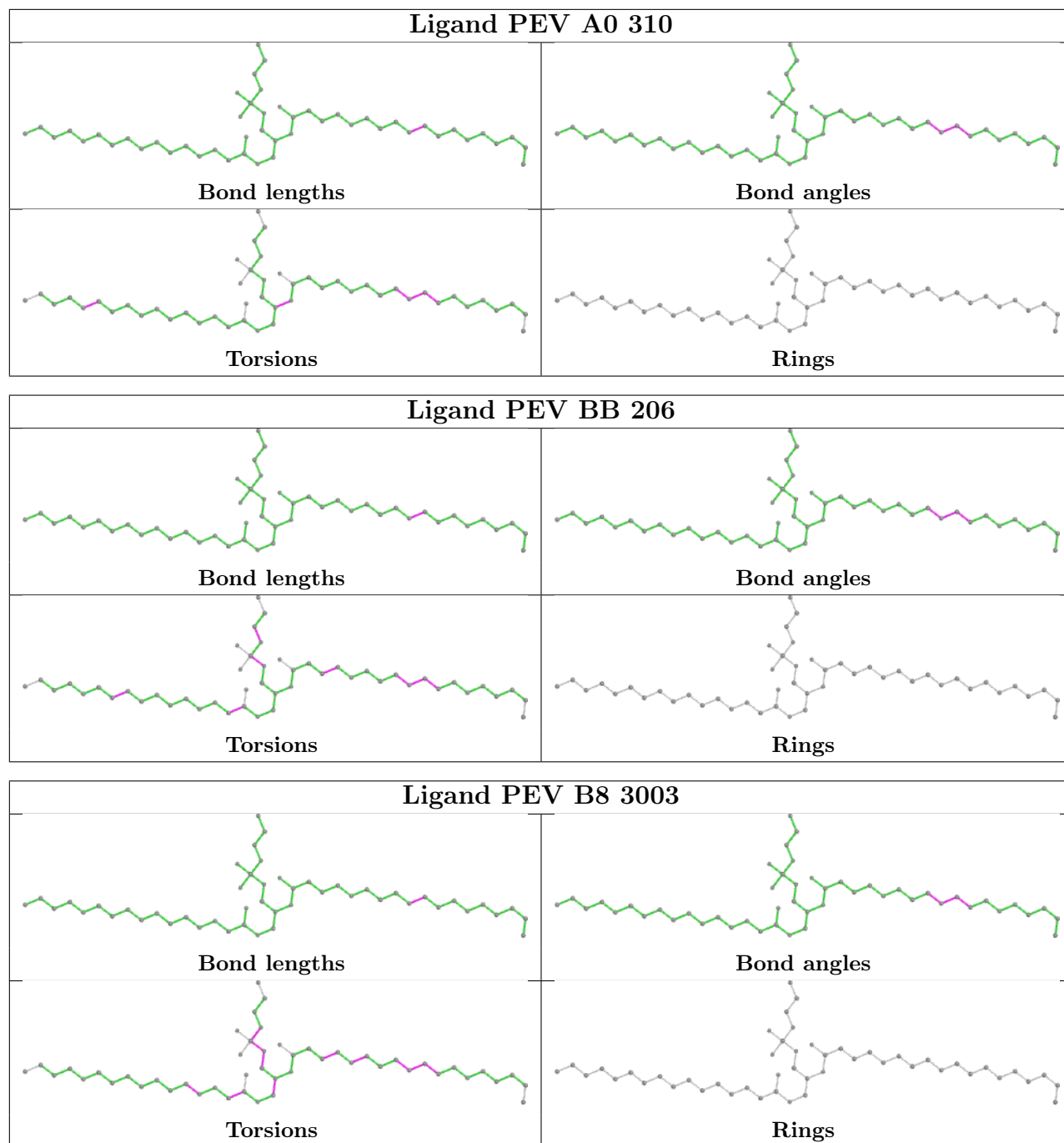


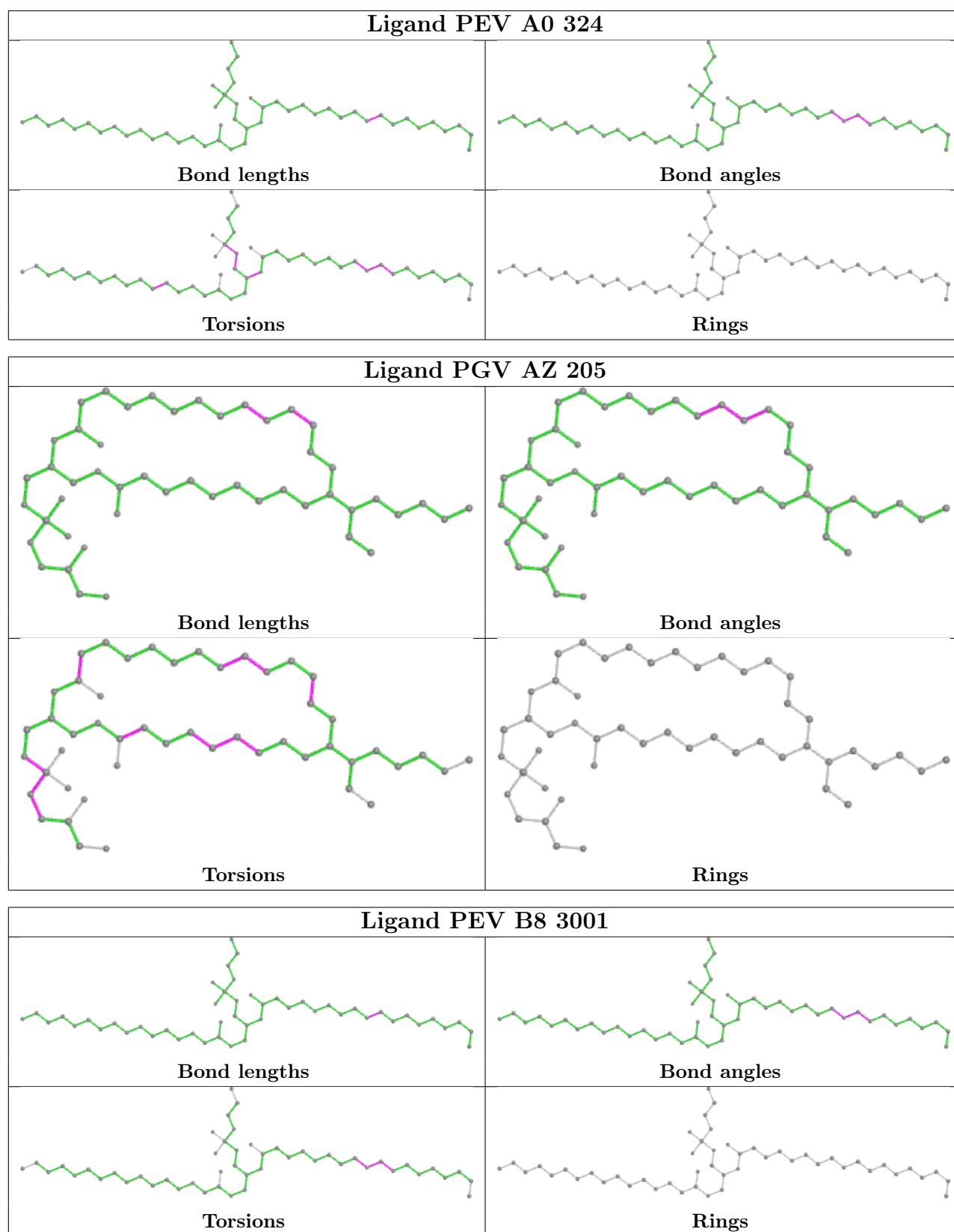


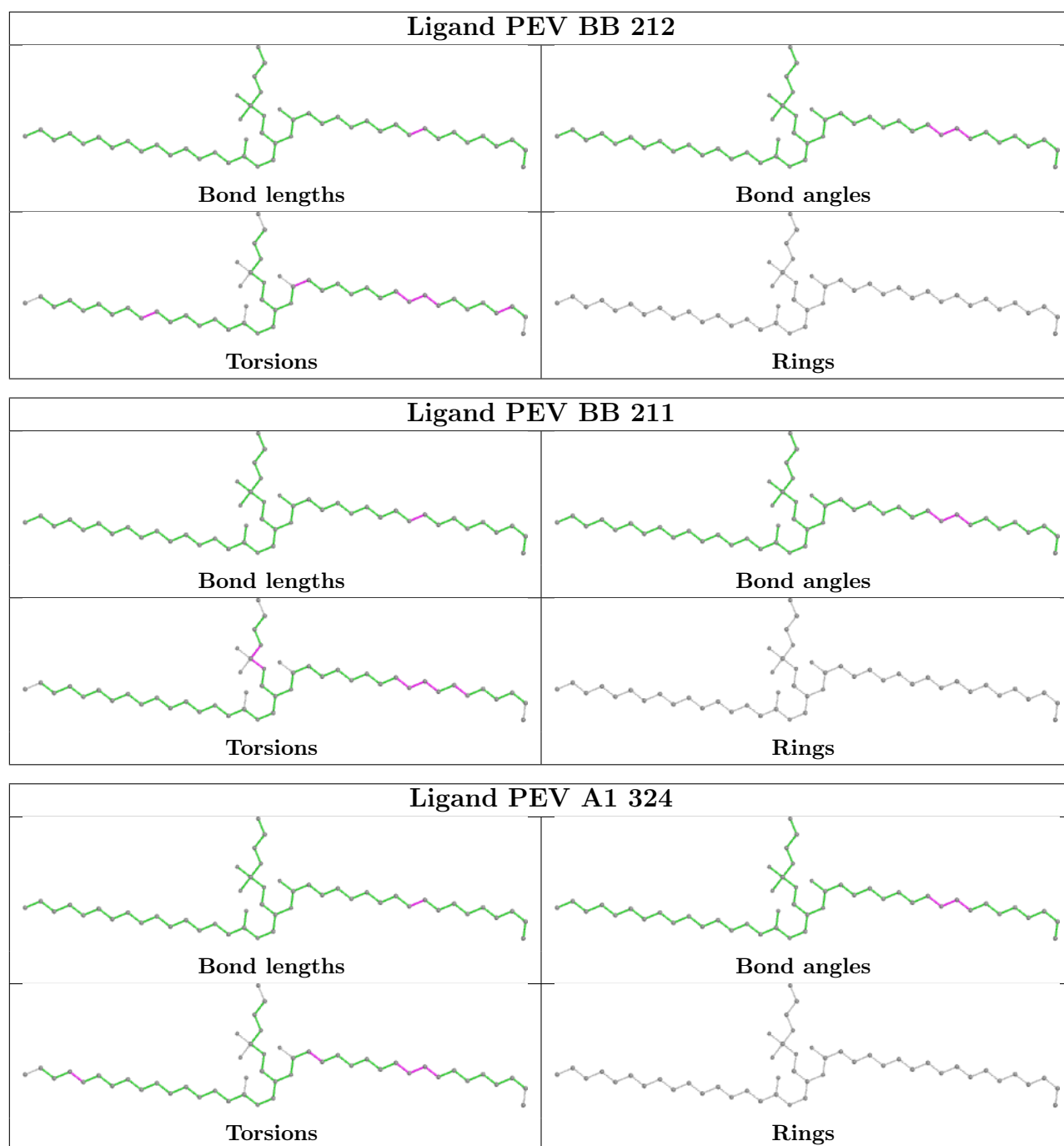


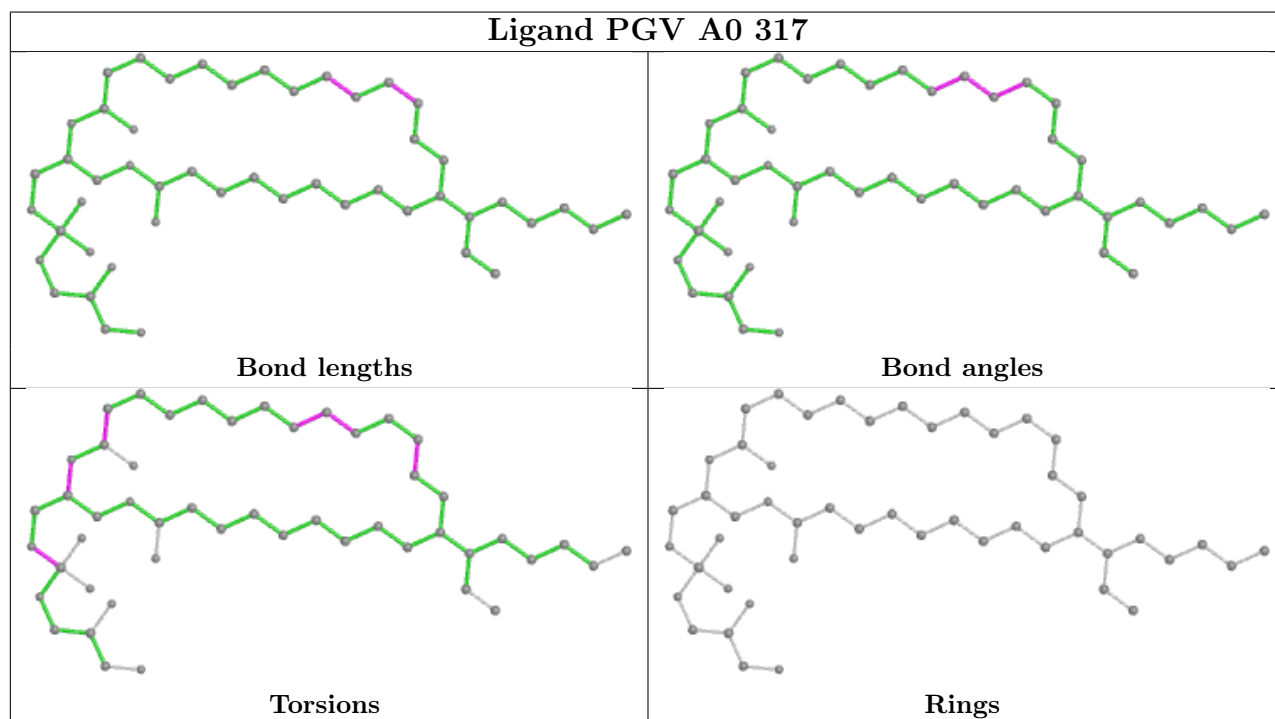
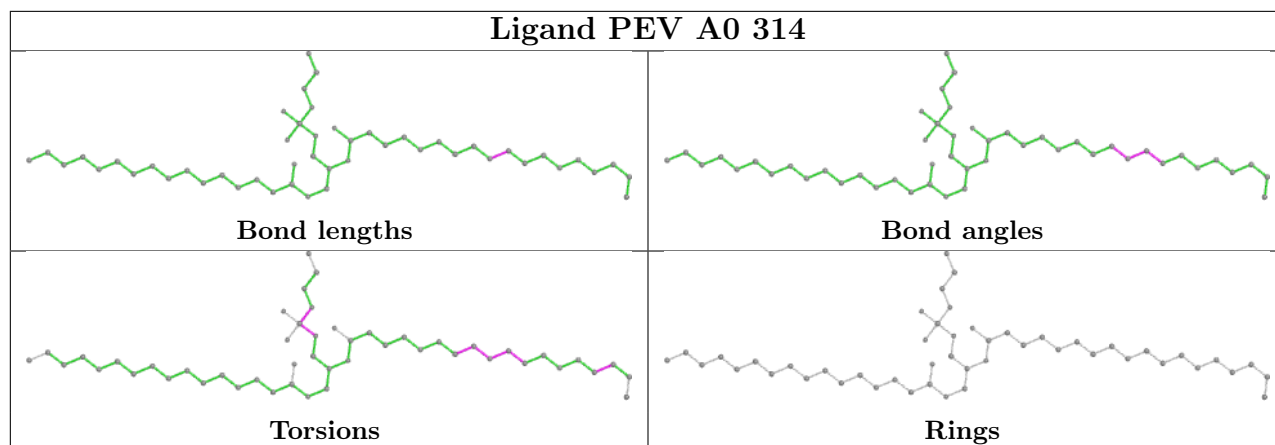


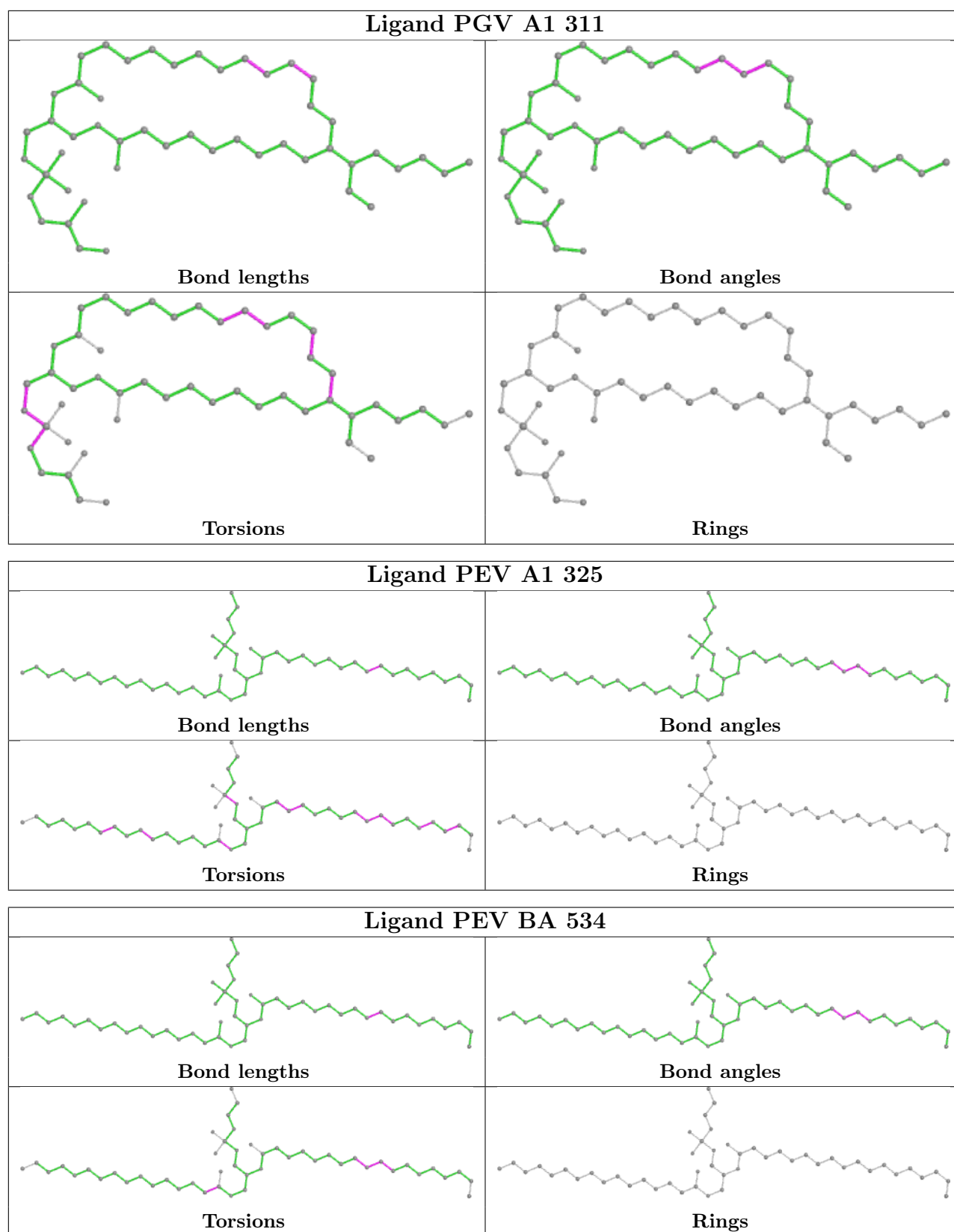


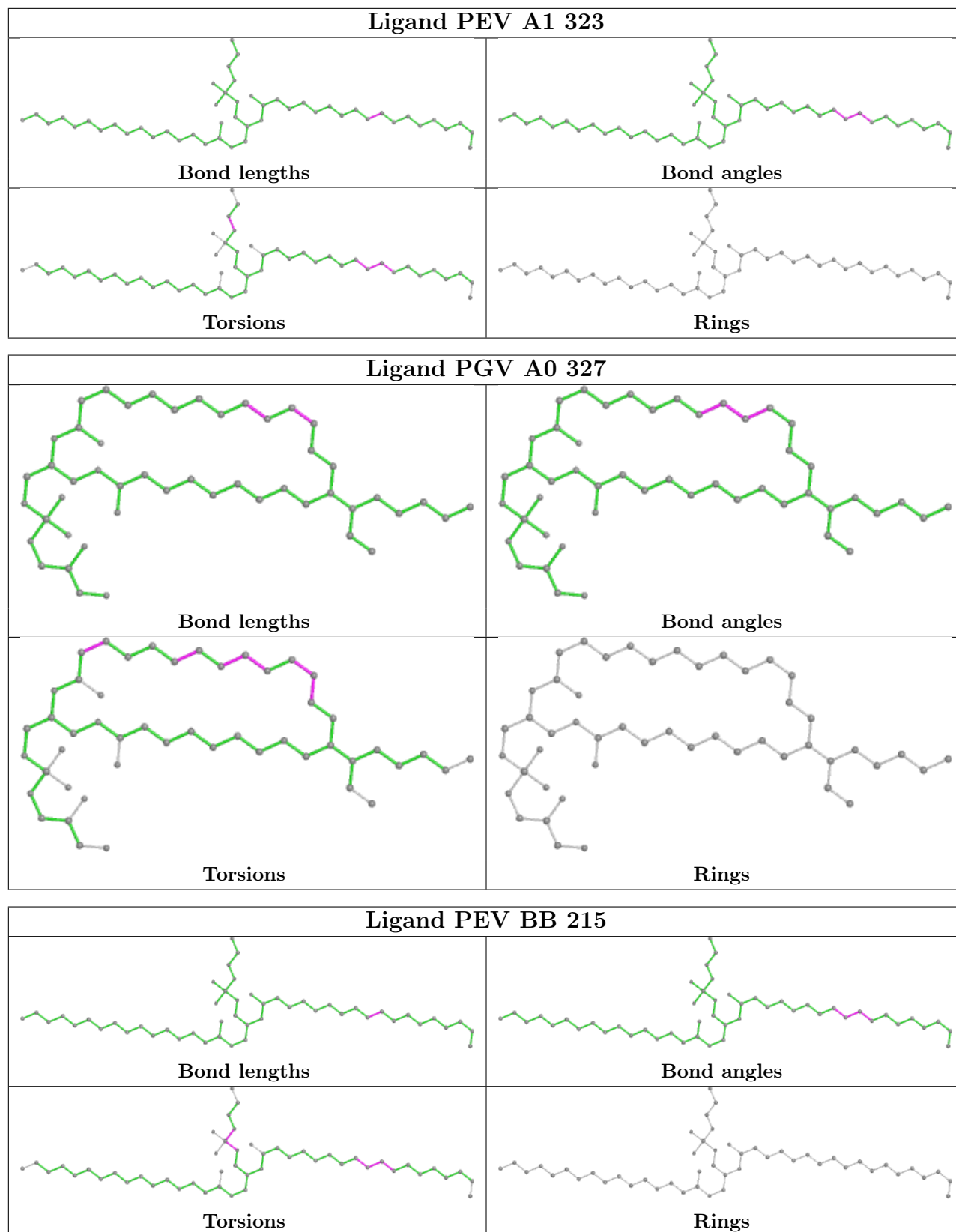


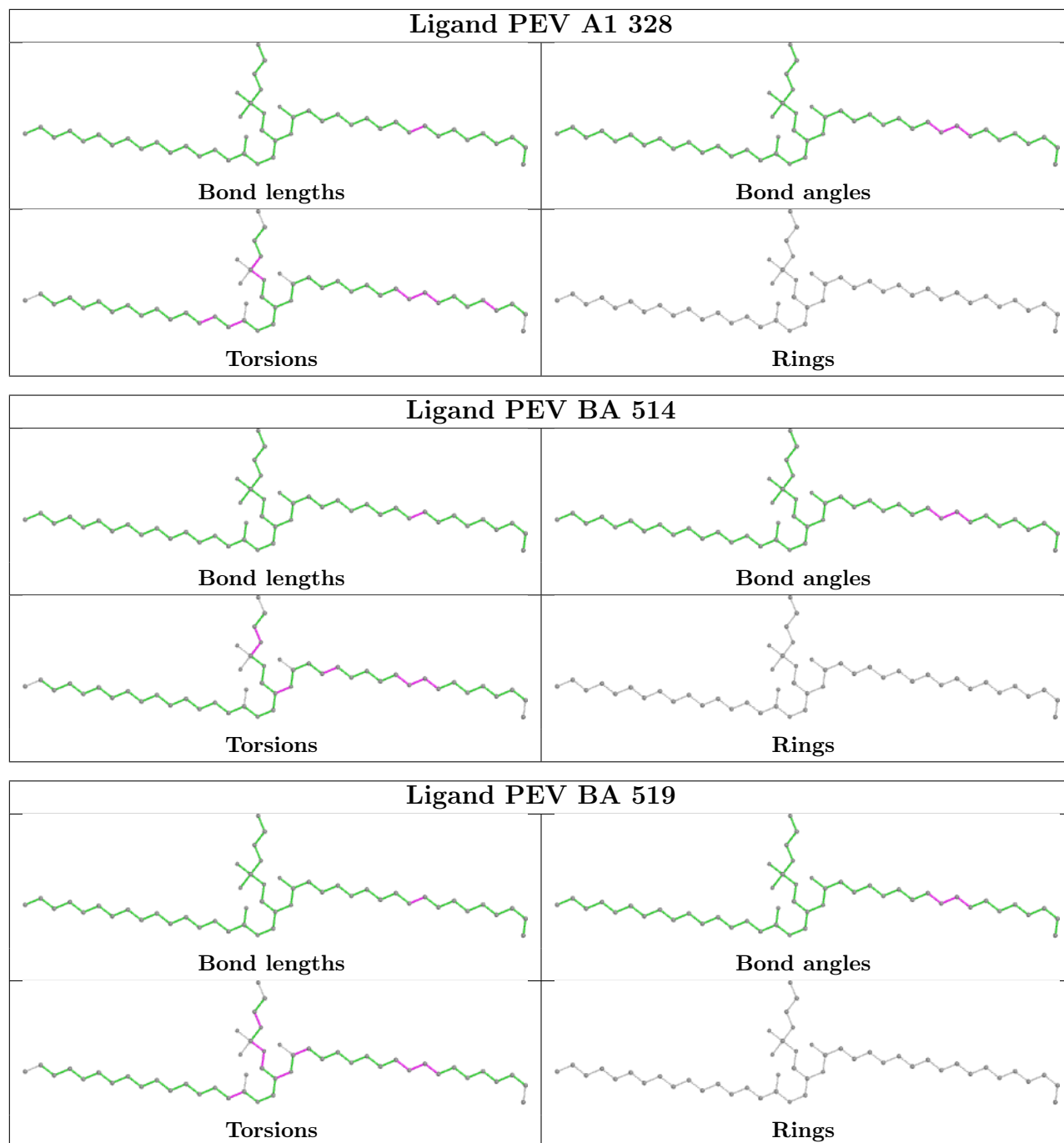


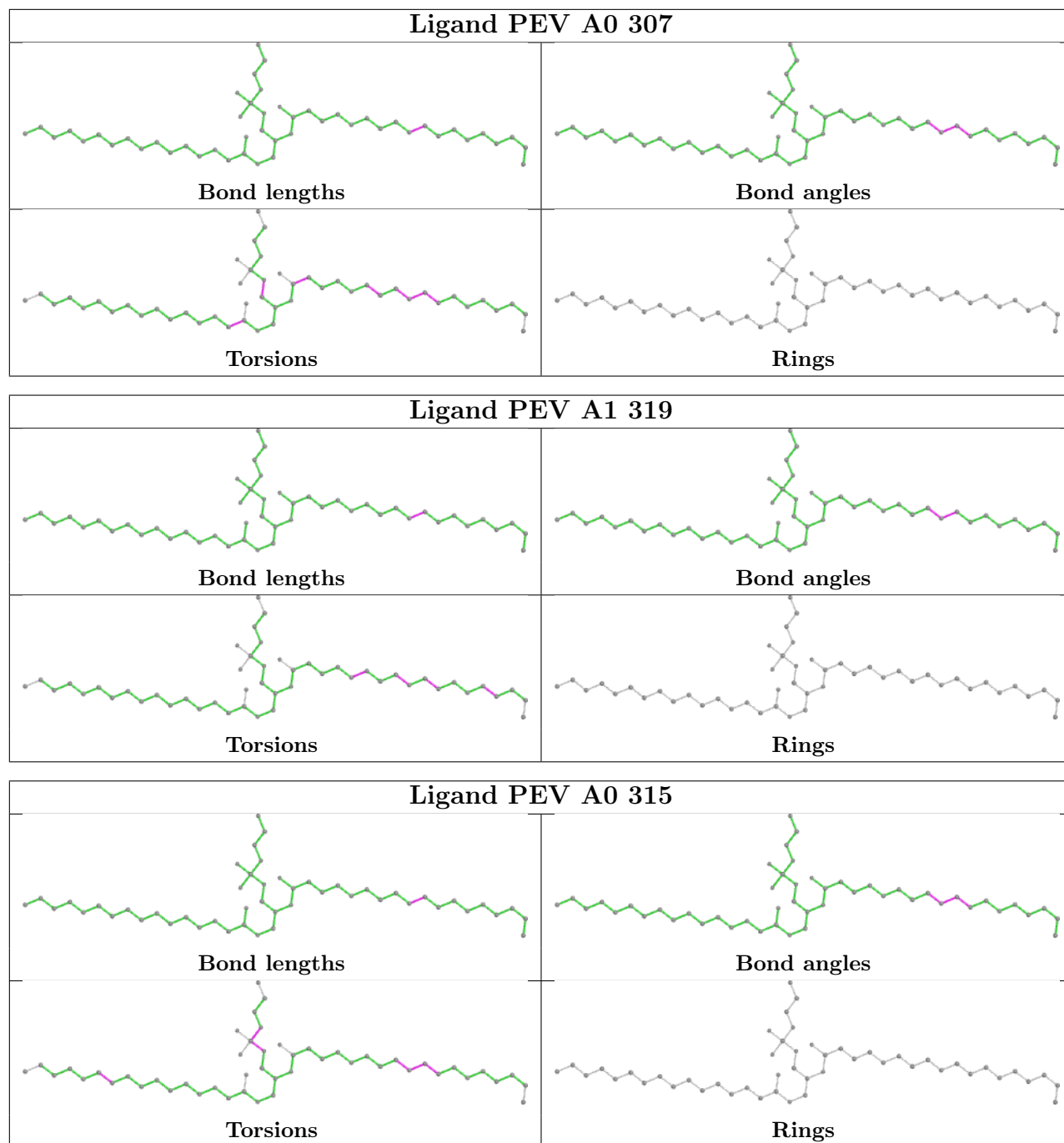


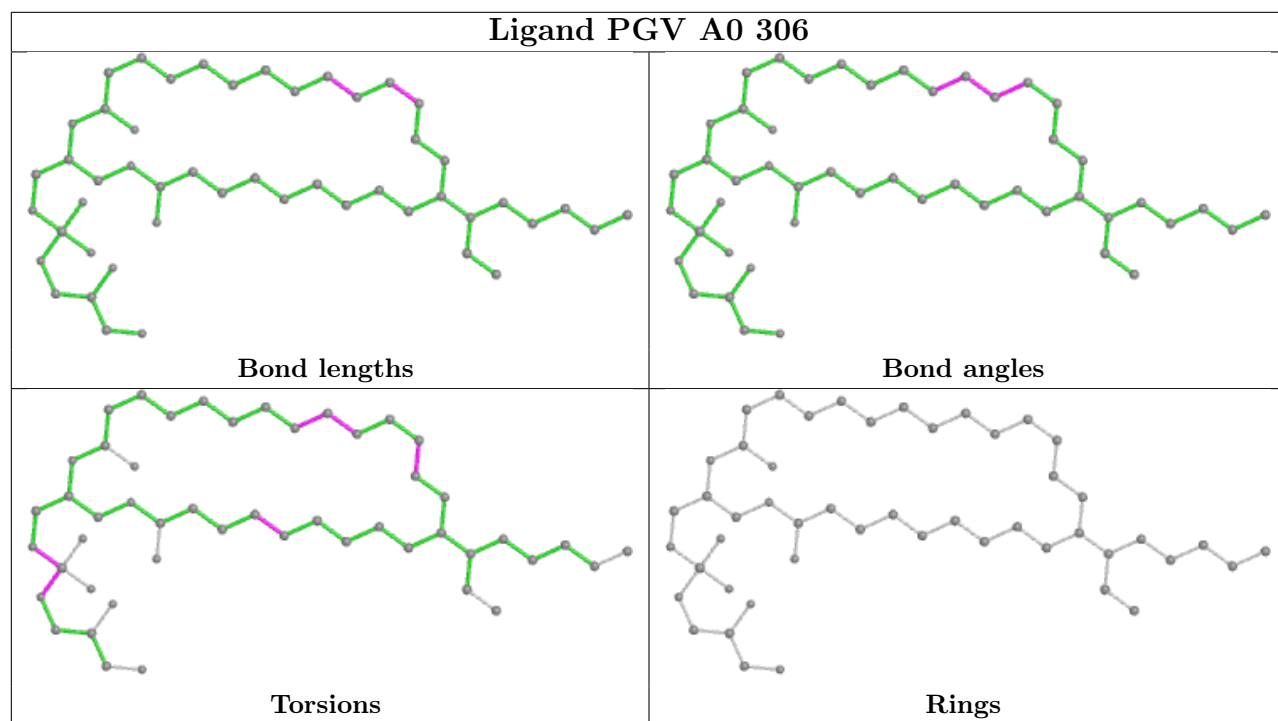
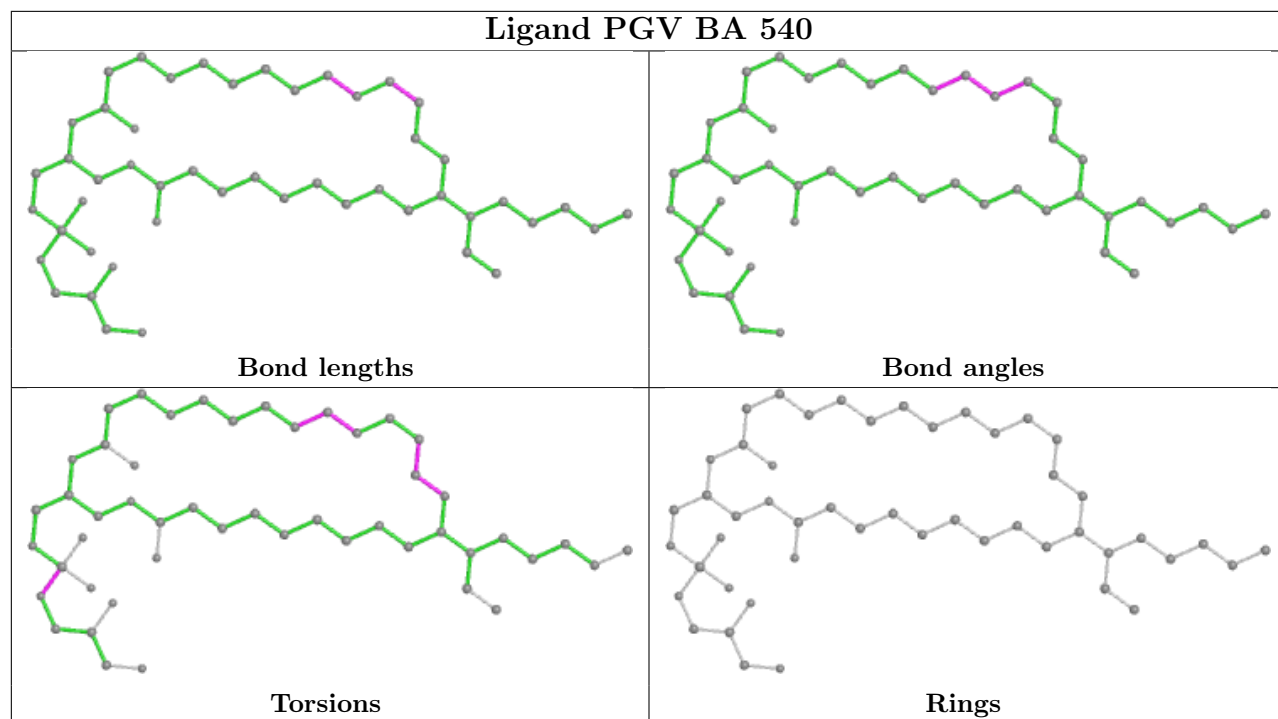


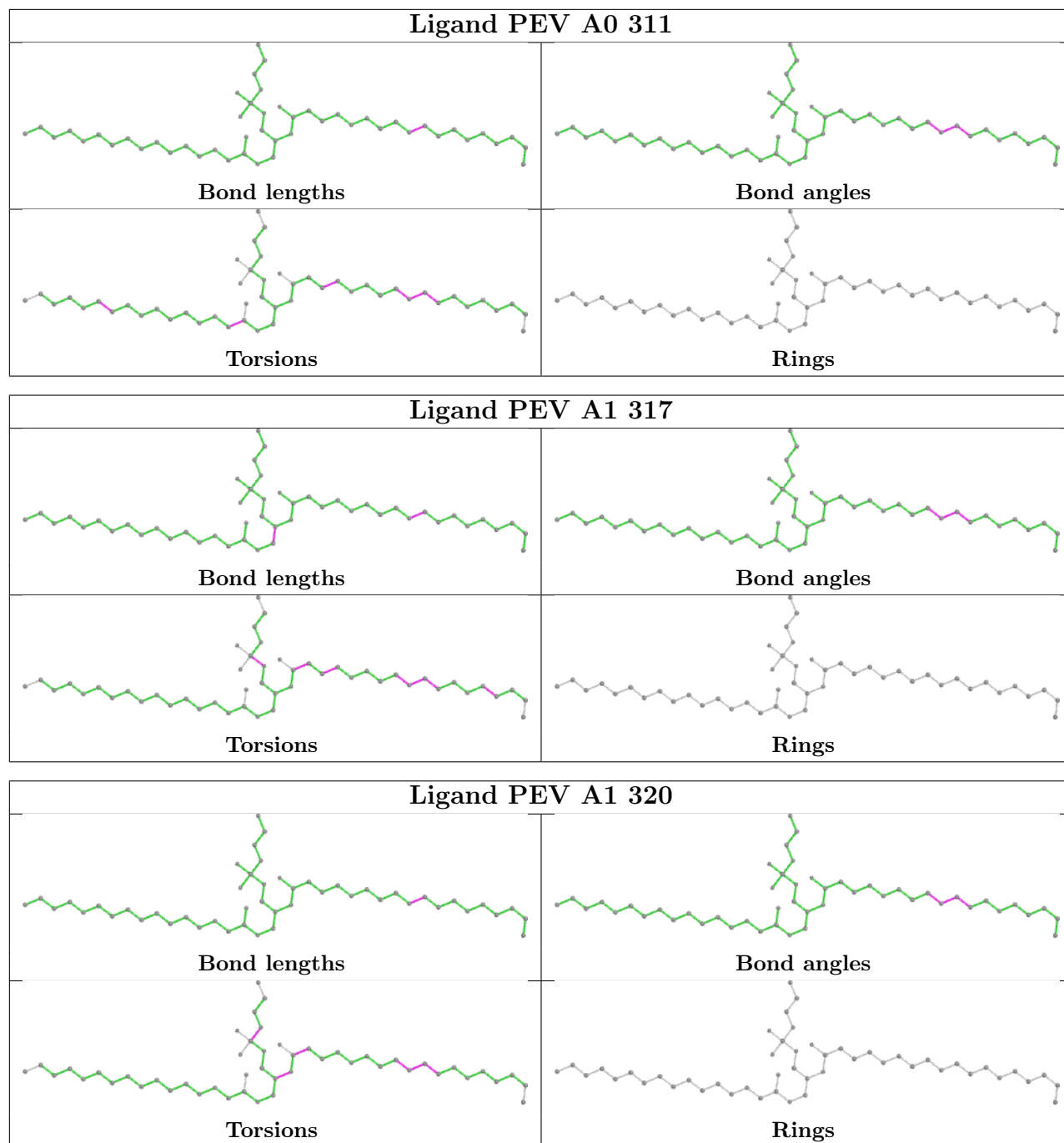


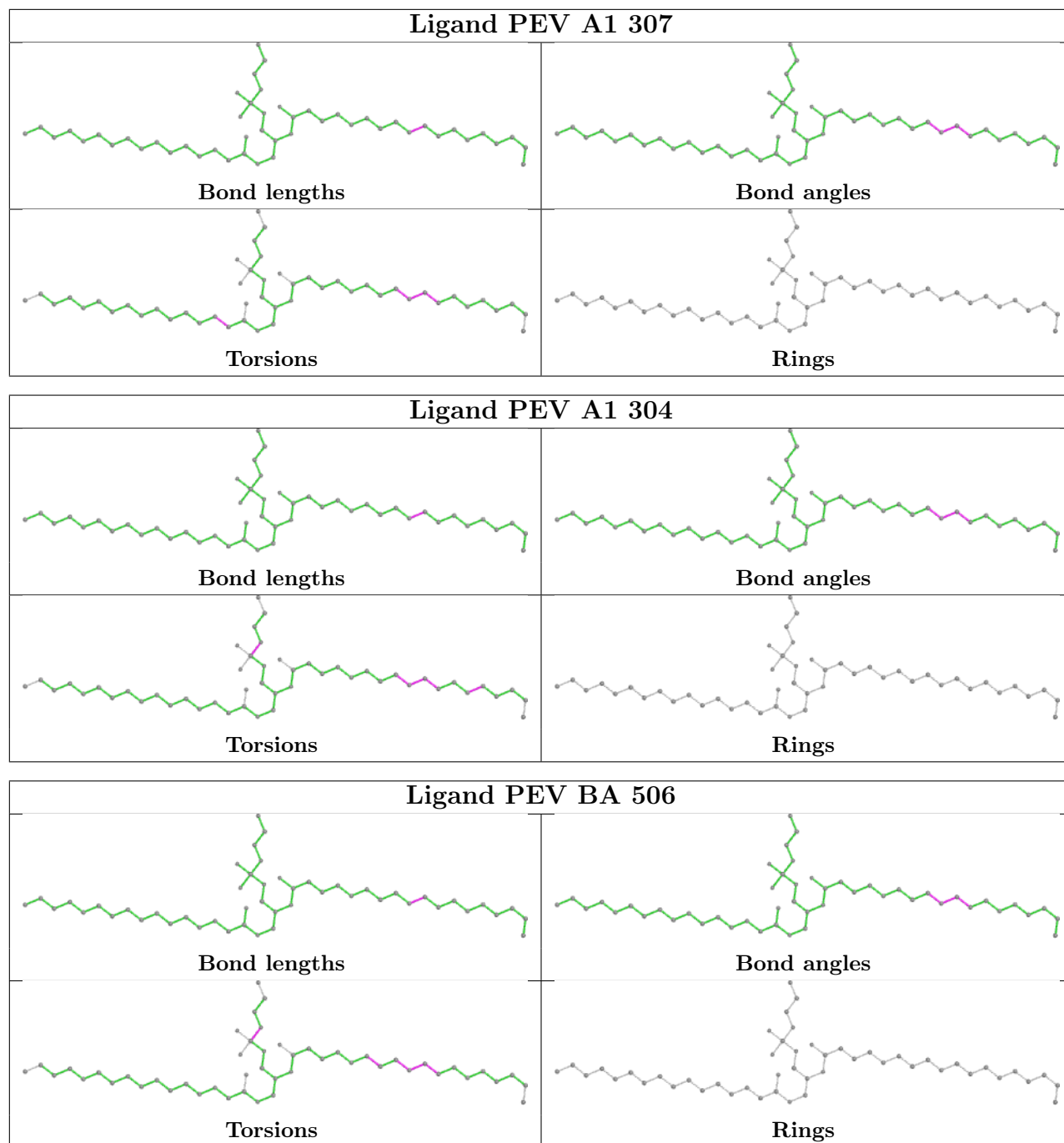


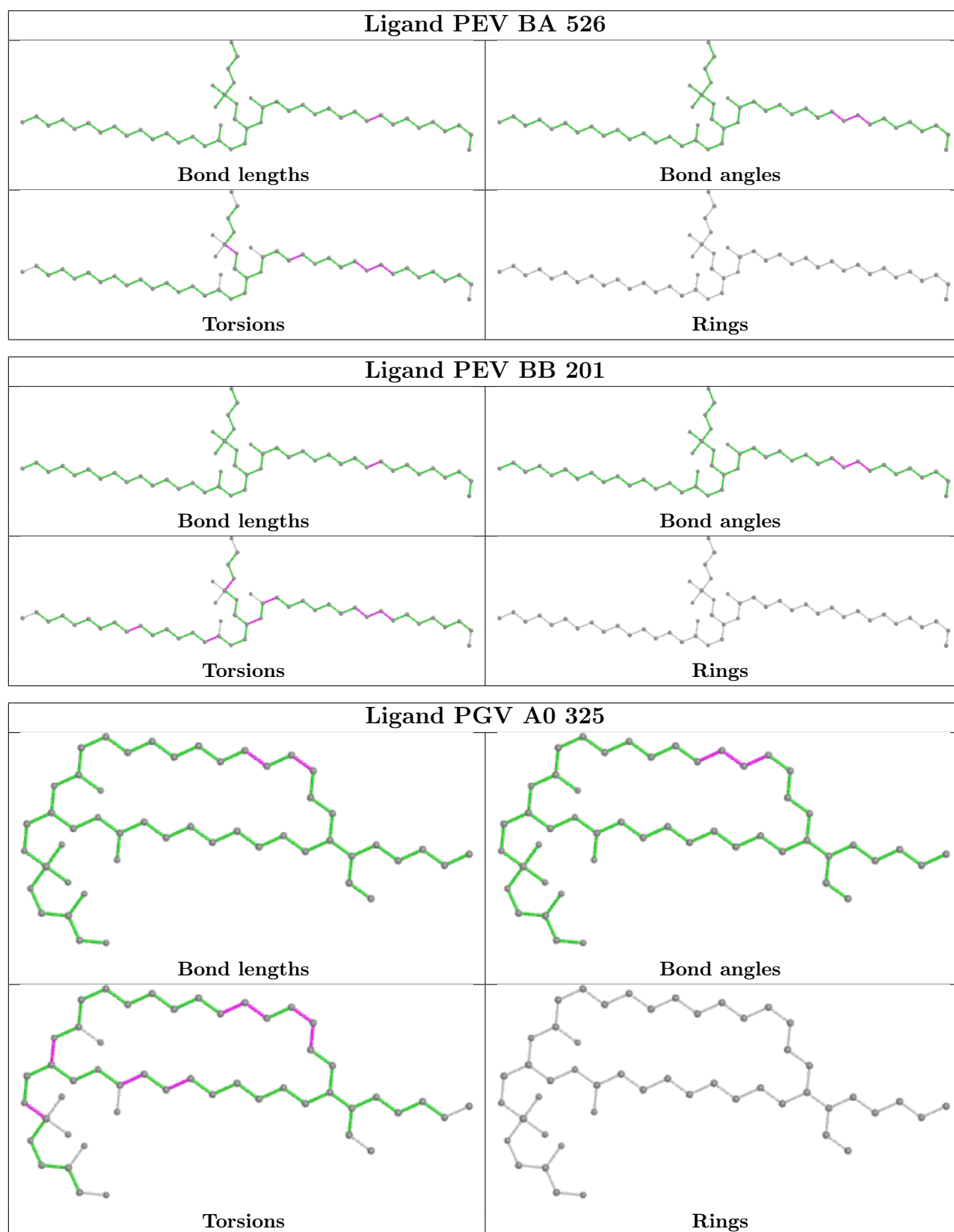


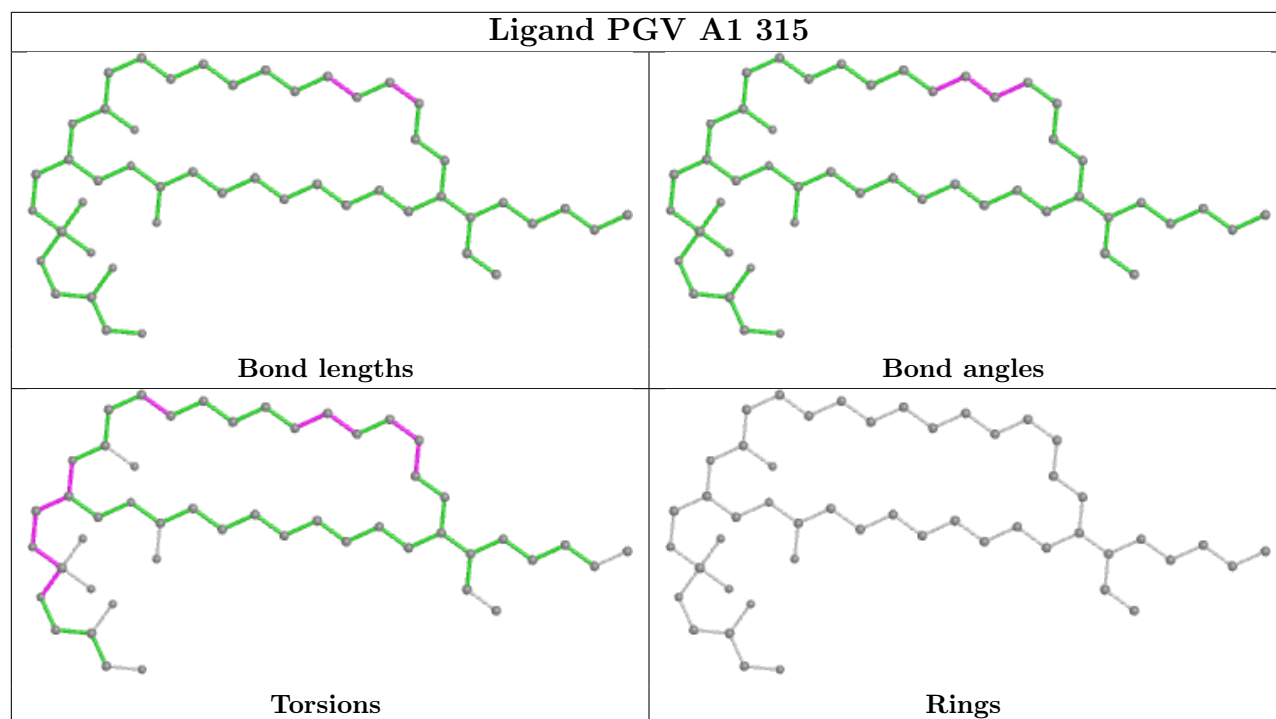
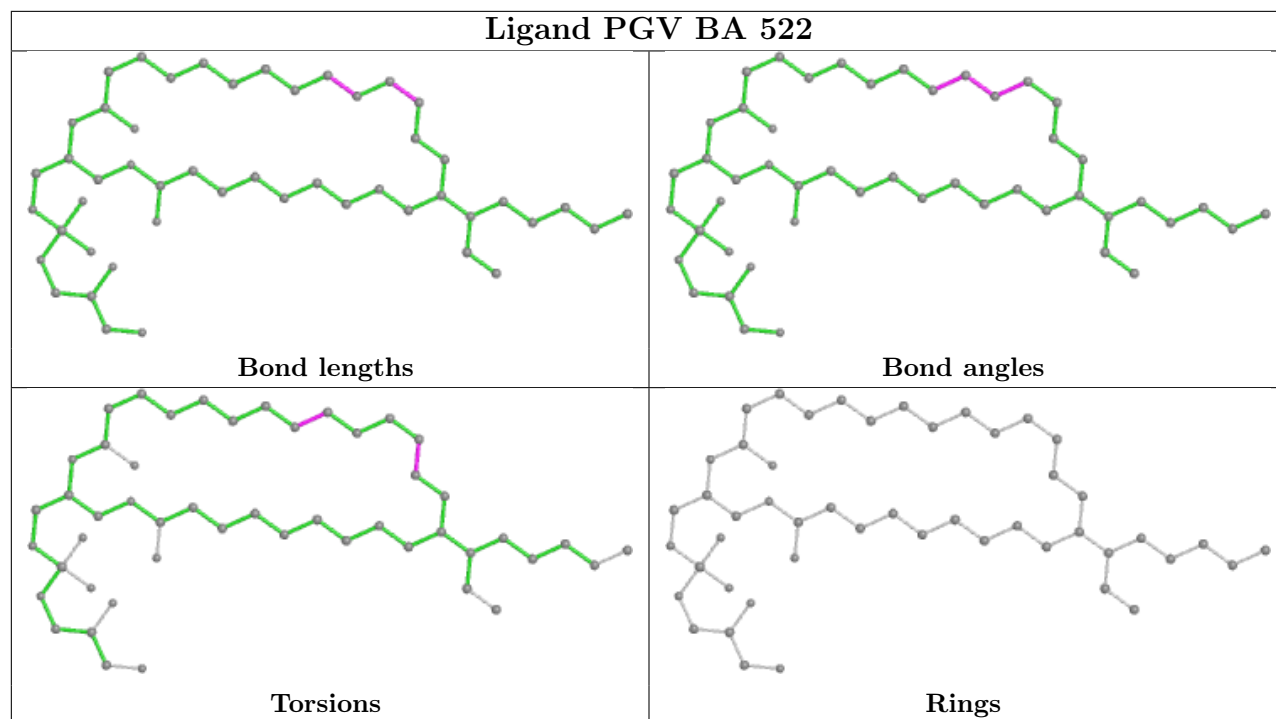


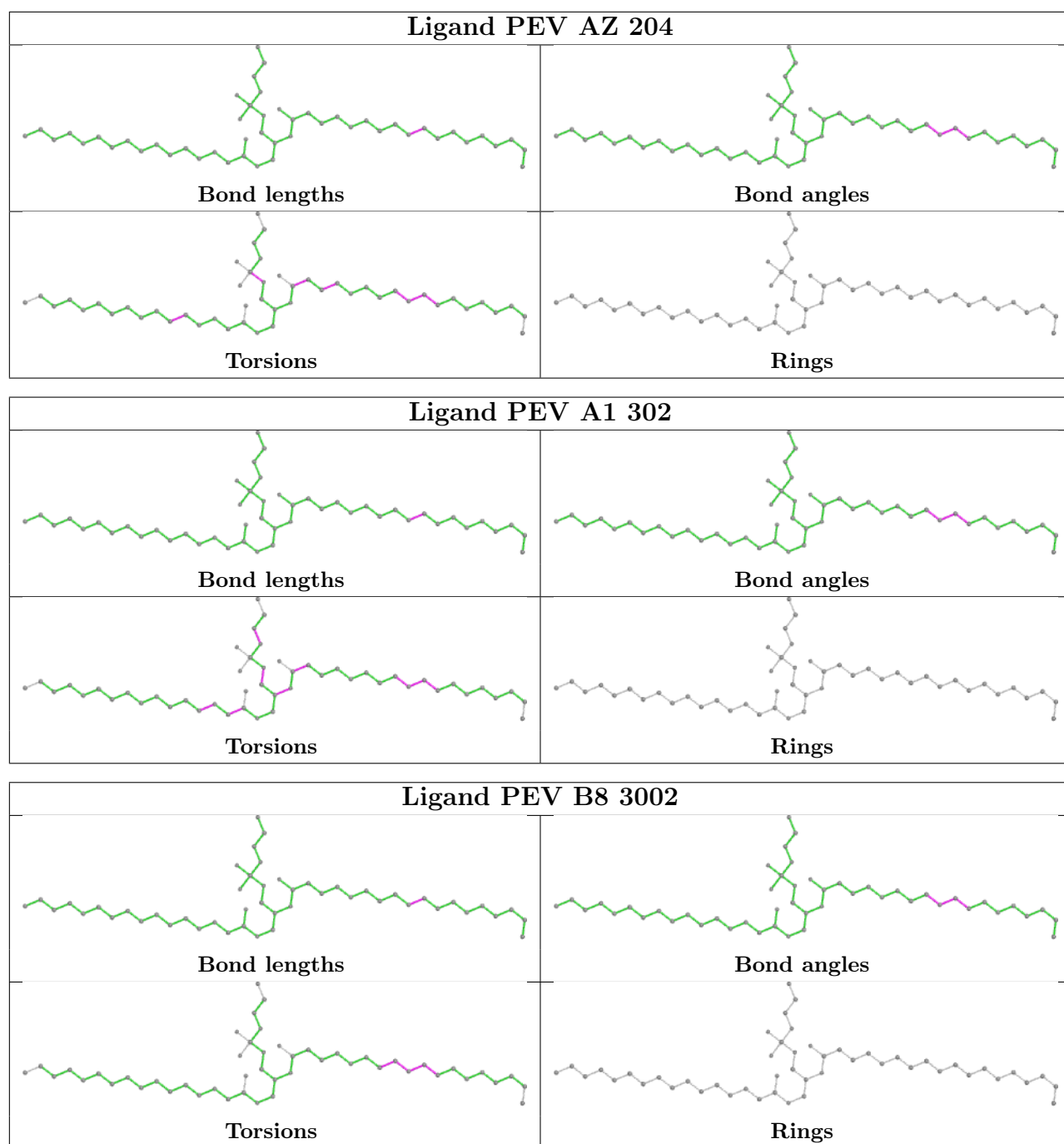


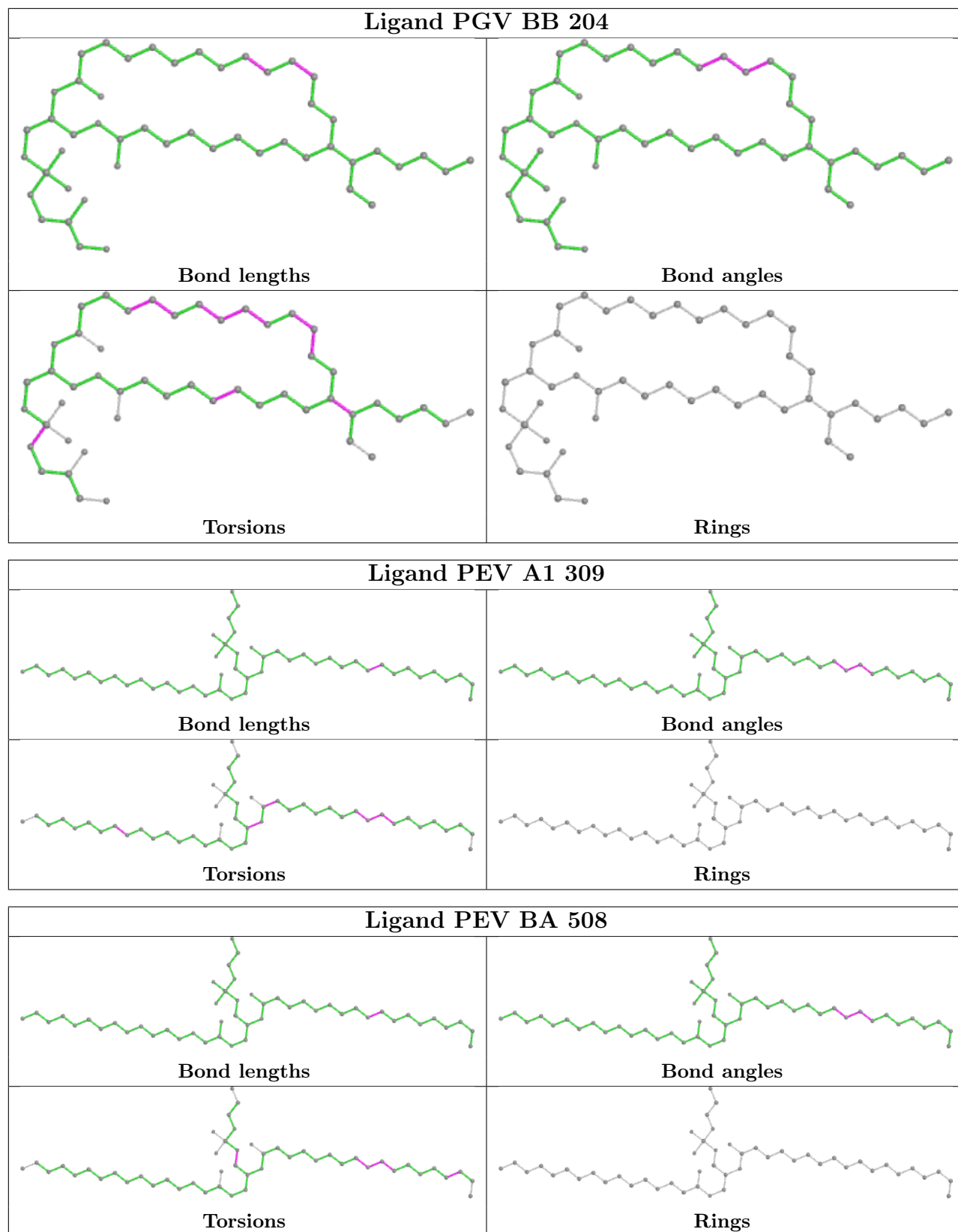


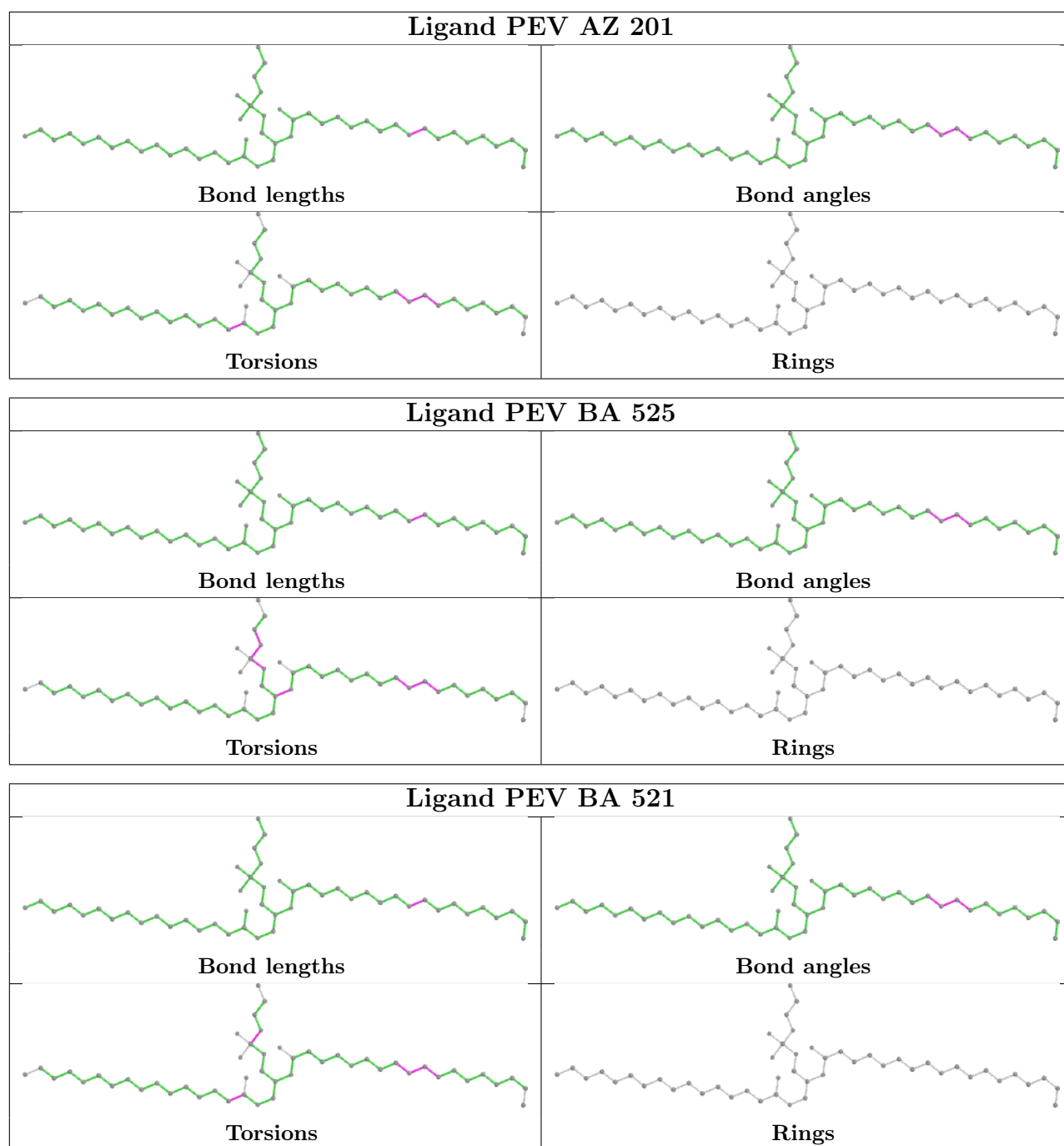


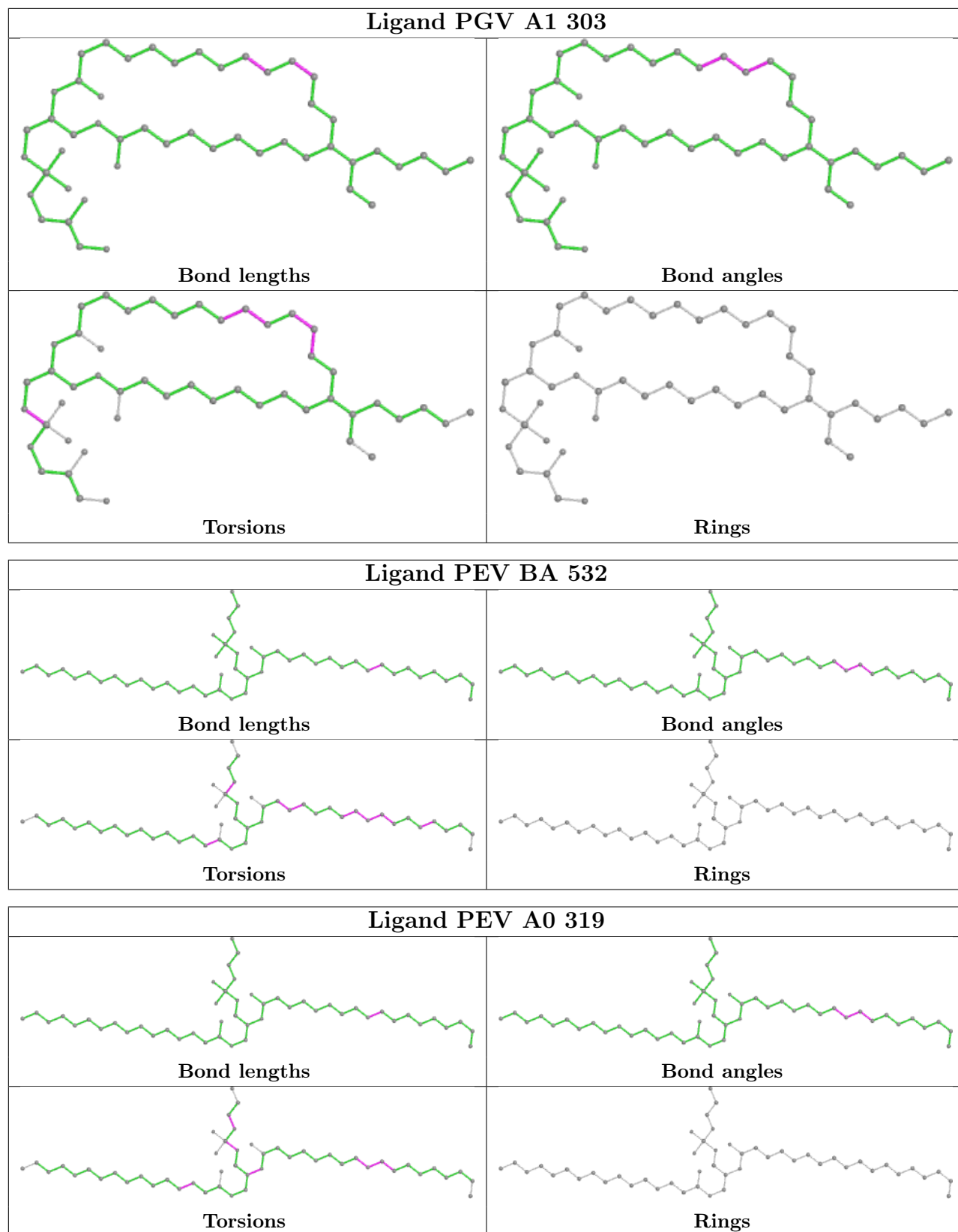


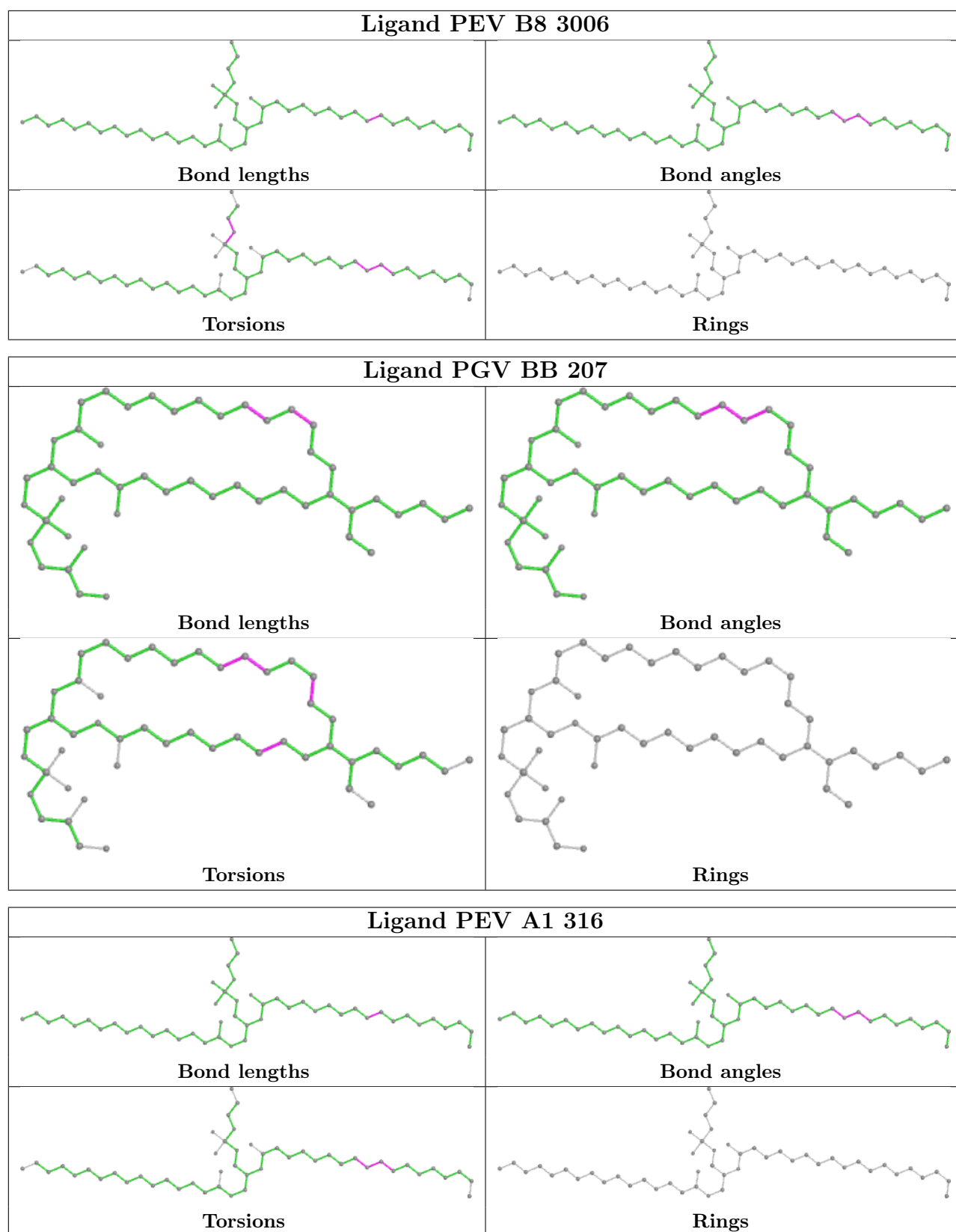


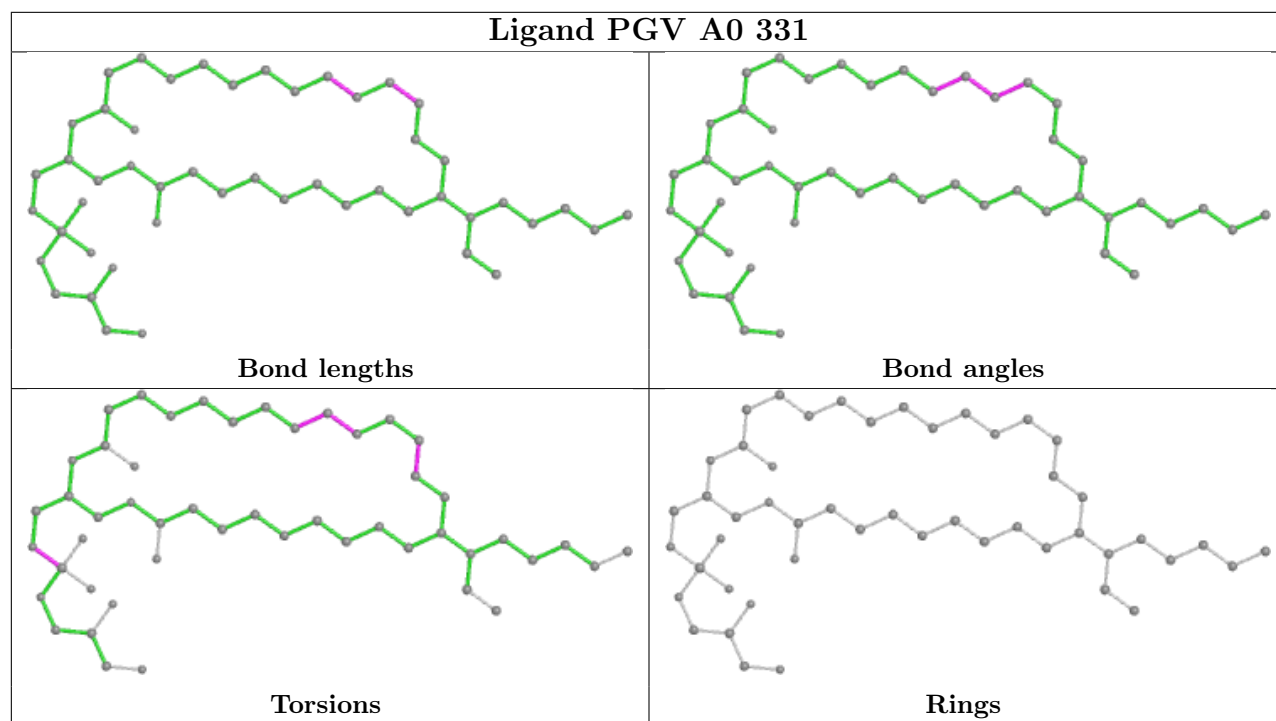
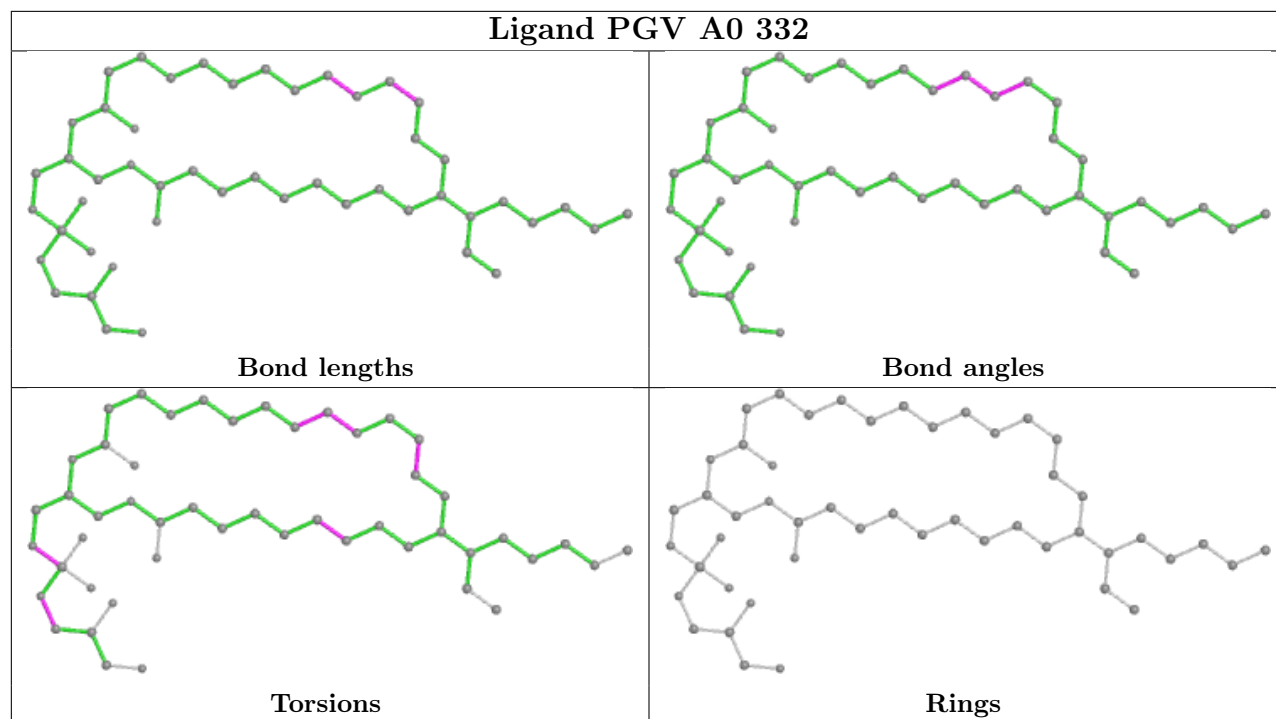


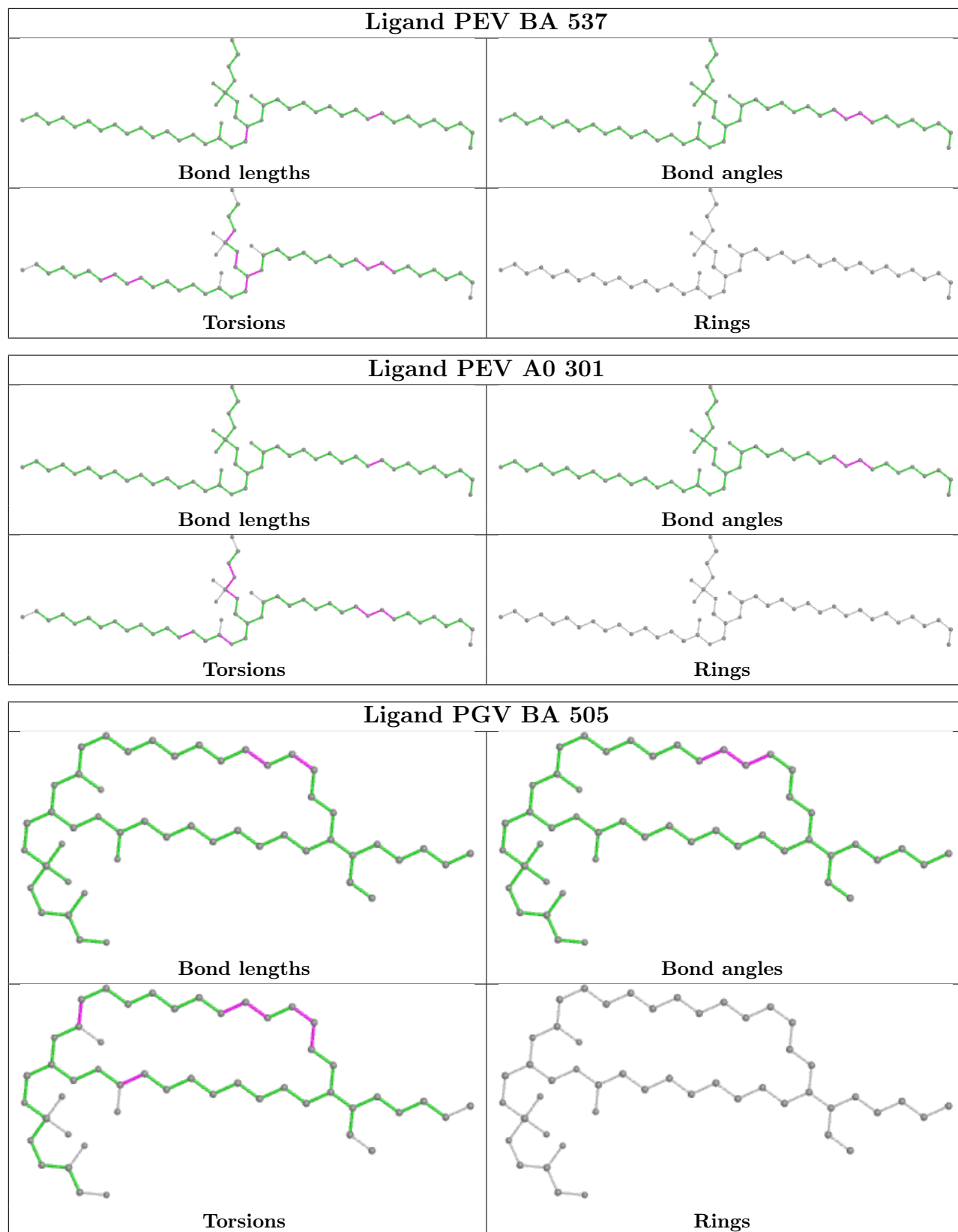












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

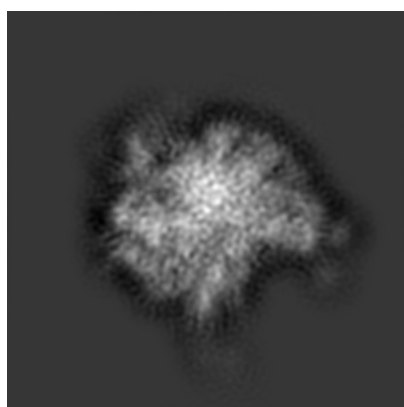
6 Map visualisation [i](#)

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.

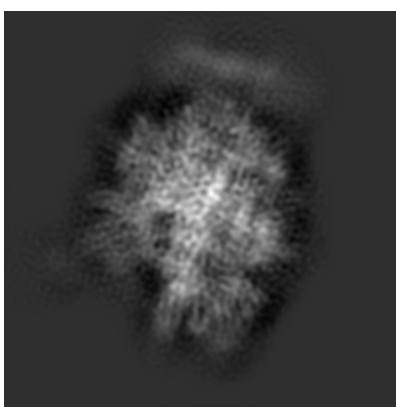
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

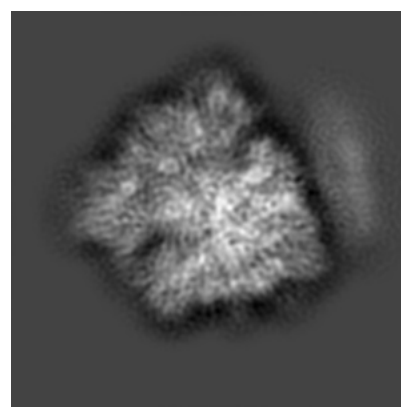
6.1.1 Primary map



X



Y

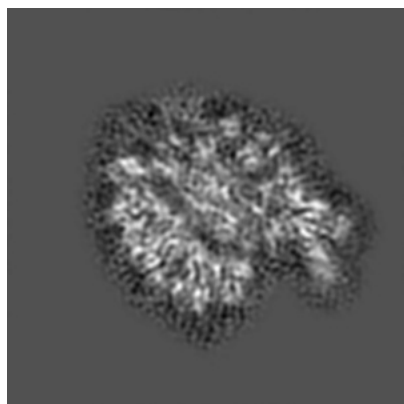


Z

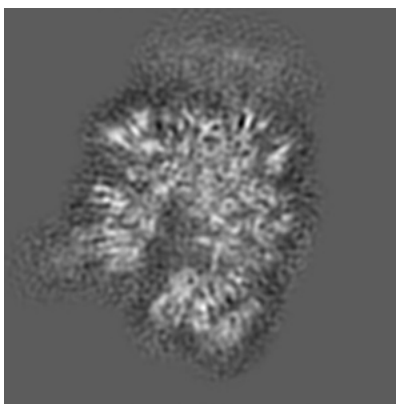
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

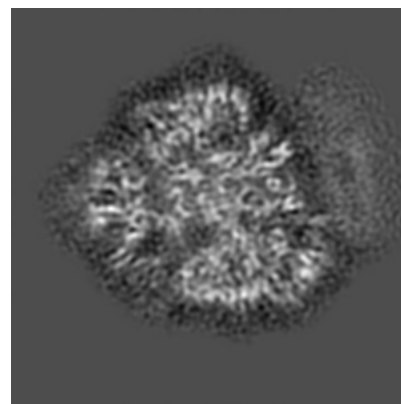
6.2.1 Primary map



X Index: 160



Y Index: 160

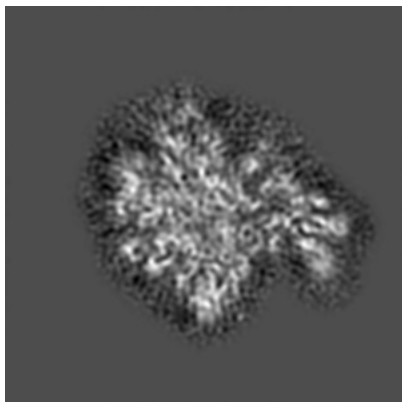


Z Index: 160

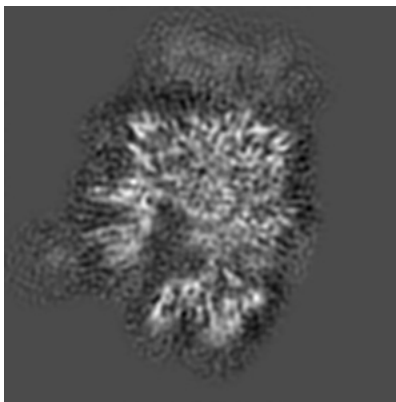
The images above show central slices of the map in three orthogonal directions.

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

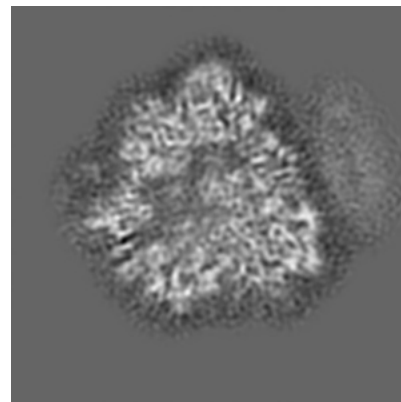
6.3.1 Primary map



X Index: 166



Y Index: 167



Z Index: 146

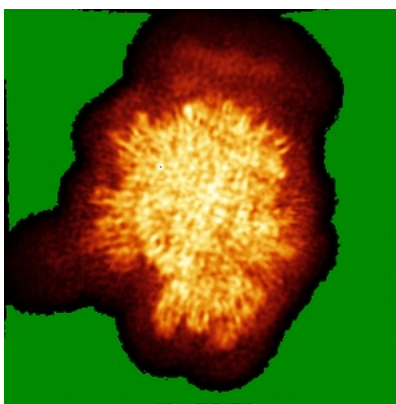
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [\(i\)](#)

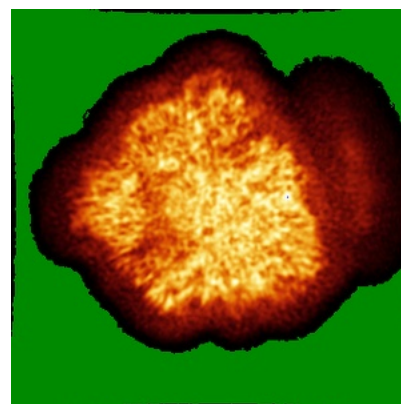
6.4.1 Primary map



X



Y

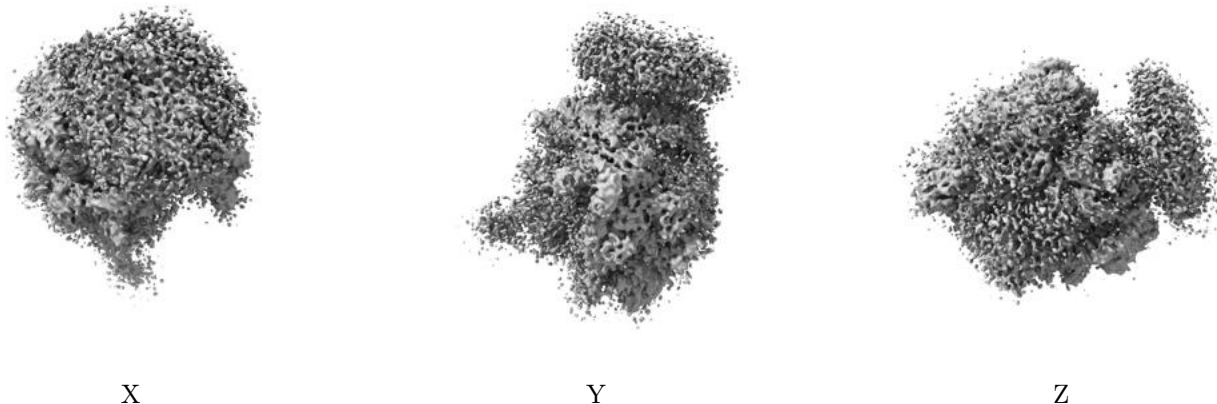


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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.

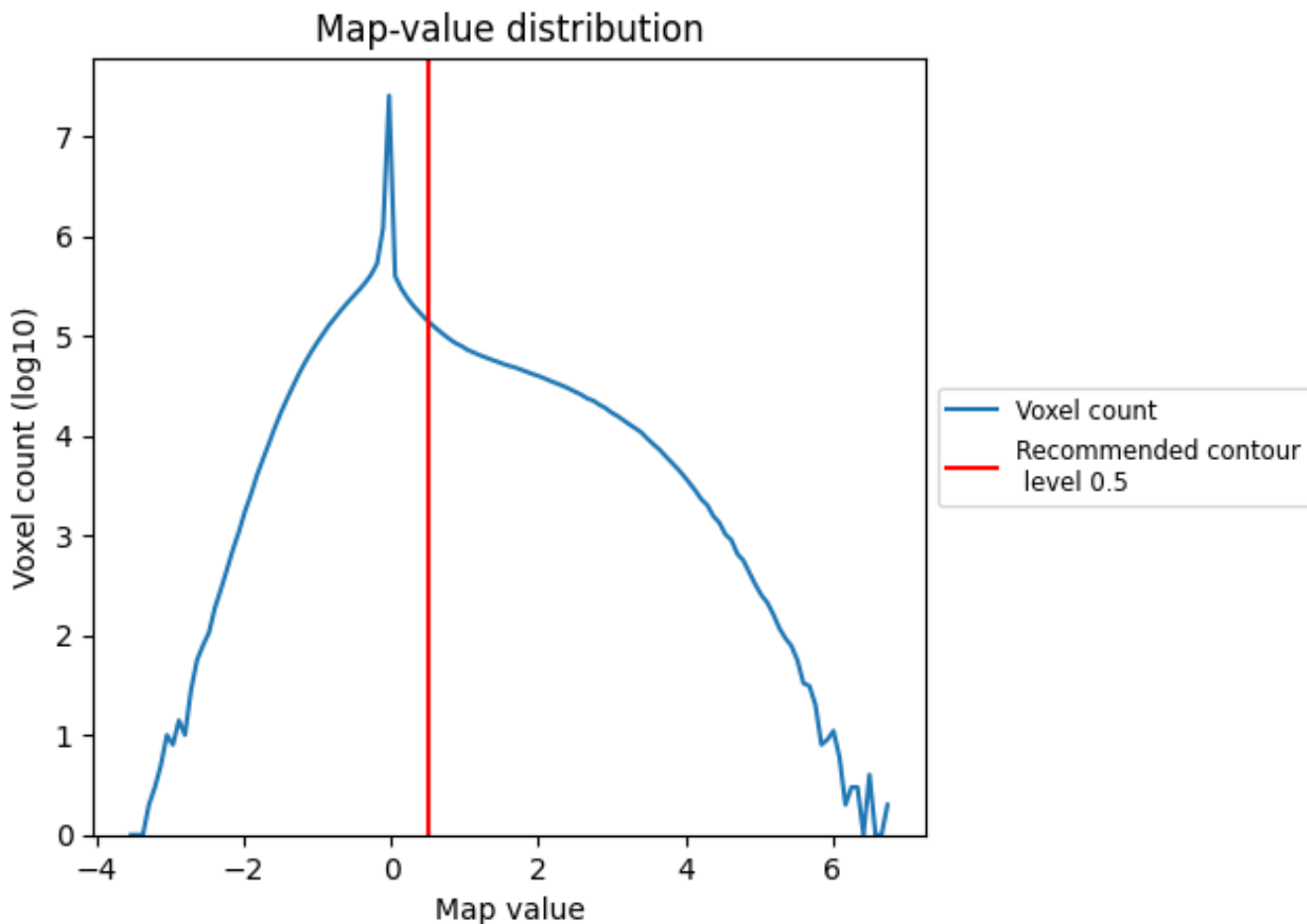
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

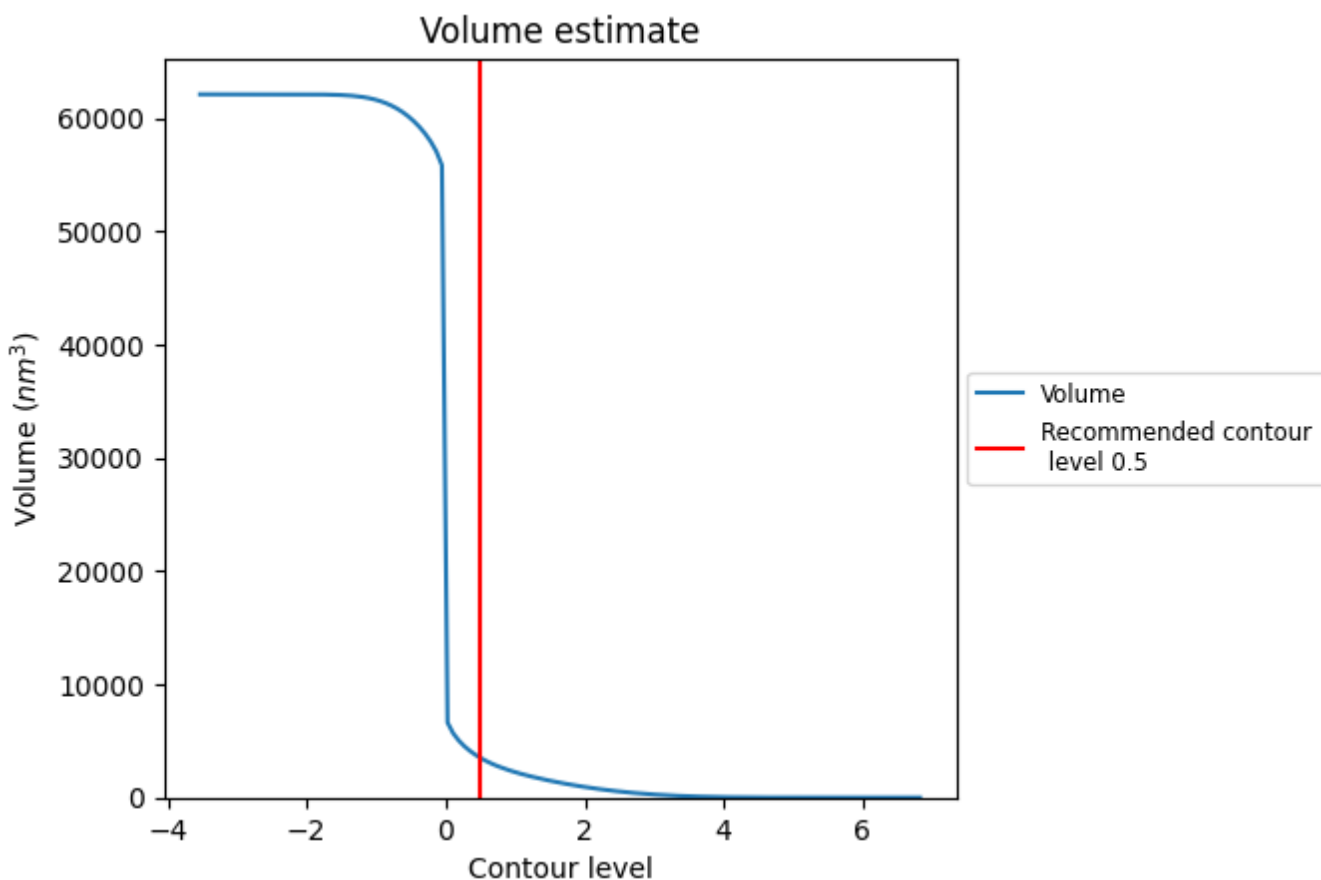
This section contains the results of statistical analysis of the map.

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.

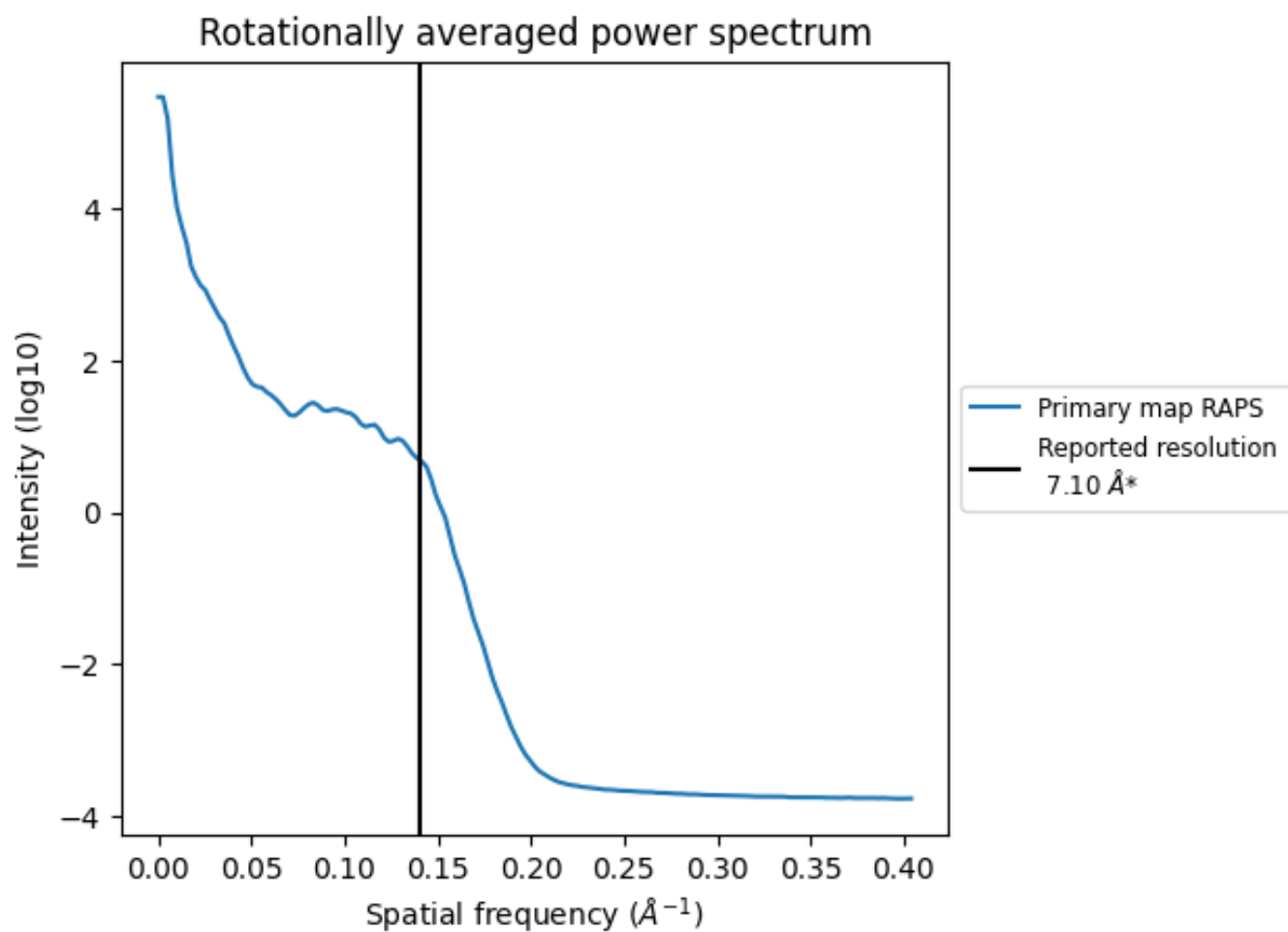
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3504 nm³; 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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.141 Å⁻¹

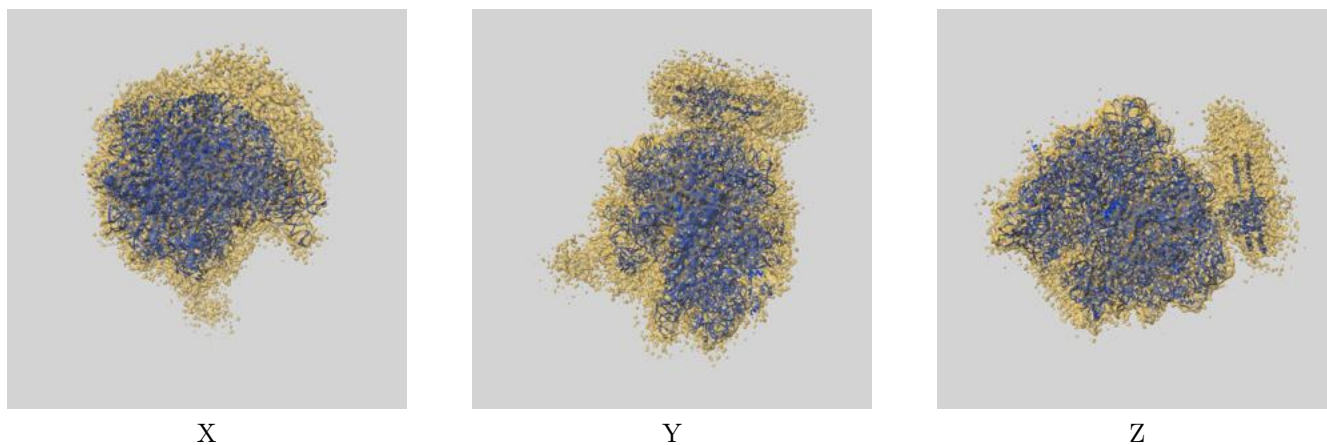
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

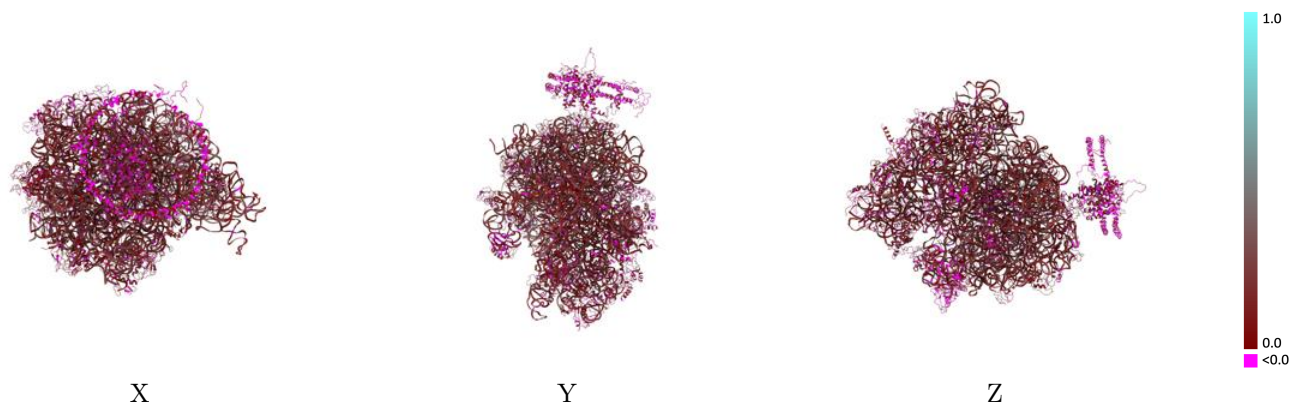
This section contains information regarding the fit between EMDB map EMD-1858 and PDB model 4V6M. Per-residue inclusion information can be found in section 3 on page 24.

9.1 Map-model overlay [i](#)



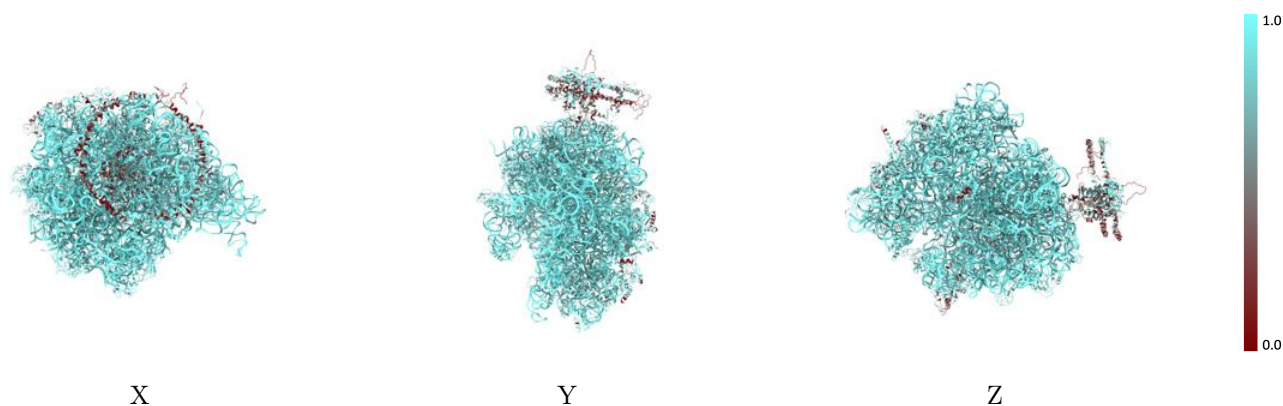
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



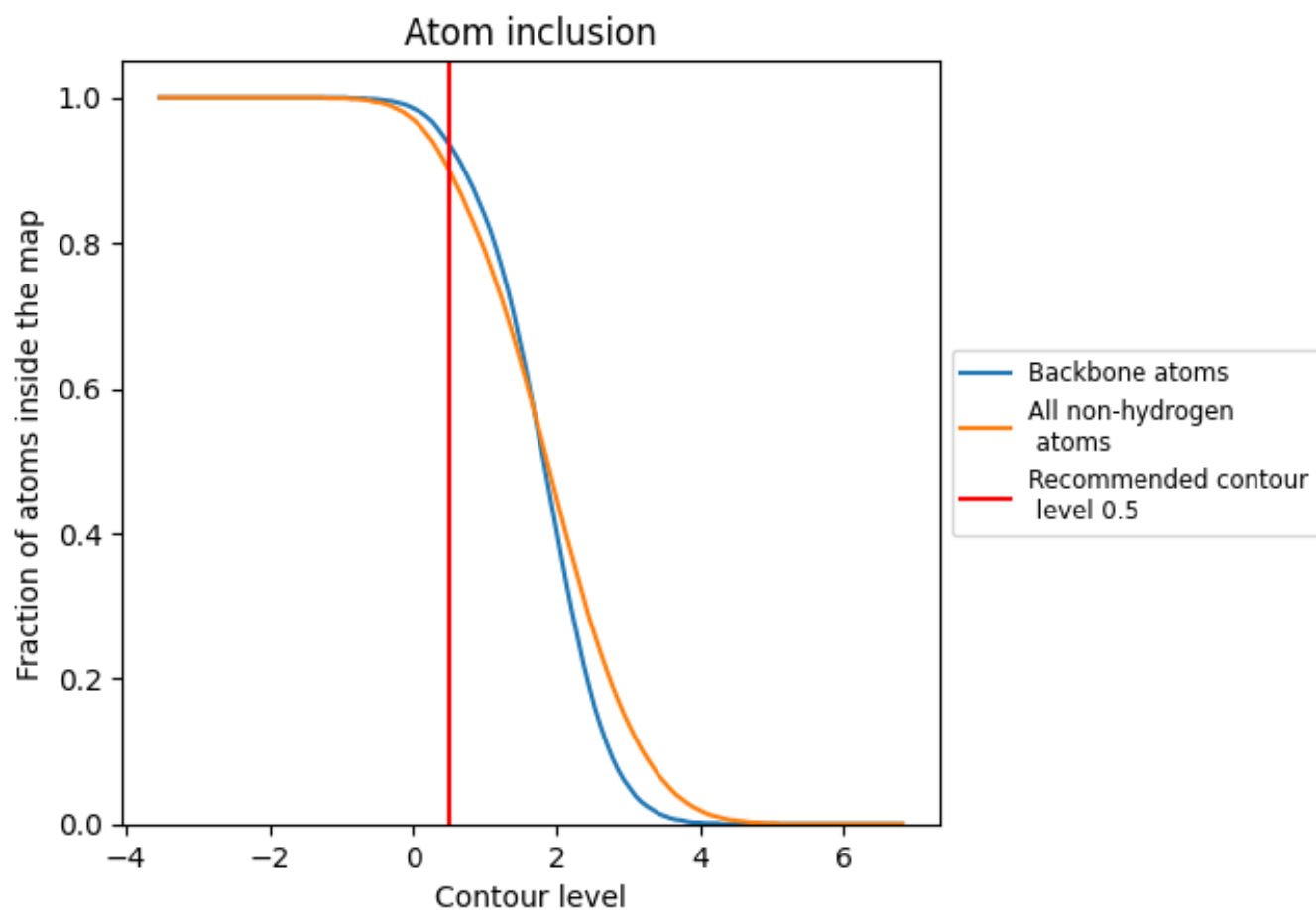
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.9010	 0.1450
A0	 0.3260	 0.0170
A1	 0.5620	 0.0090
AA	 0.9850	 0.1740
AB	 0.7510	 0.1210
AC	 0.8280	 0.1200
AD	 0.8390	 0.1240
AE	 0.7780	 0.1190
AF	 0.7180	 0.1060
AG	 0.9090	 0.1350
AH	 0.8540	 0.1350
AI	 0.8730	 0.0980
AJ	 0.8950	 0.0950
AK	 0.8480	 0.1140
AL	 0.9250	 0.1180
AM	 0.8860	 0.1220
AN	 0.8670	 0.1230
AO	 0.9170	 0.1390
AP	 0.8850	 0.1220
AQ	 0.8990	 0.1230
AR	 0.8000	 0.1240
AS	 0.8900	 0.1060
AT	 0.8290	 0.1370
AU	 0.8360	 0.1220
AV	 0.9590	 0.1410
AX	 0.7920	 0.1000
AZ	 0.5150	 0.0640
B0	 0.8550	 0.1190
B1	 0.9420	 0.1170
B2	 0.9270	 0.0860
B3	 0.8960	 0.1220
B4	 0.9140	 0.1000
B5	 0.6780	 0.0570
B6	 0.9290	 0.1300
B7	 0.9880	 0.1840



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Chain	Atom inclusion	Q-score
B8	 0.9840	 0.1750
BA	 0.4620	 0.0370
BB	 0.4380	 0.0650
BD	 0.8970	 0.1180
BE	 0.8830	 0.1230
BF	 0.8970	 0.1180
BG	 0.9330	 0.1550
BH	 0.7440	 0.1150
BI	 0.9710	 0.0670
BJ	 0.8960	 0.1410
BK	 0.8970	 0.1400
BL	 0.9100	 0.1230
BM	 0.9460	 0.1330
BN	 0.8440	 0.1070
BO	 0.8990	 0.1260
BP	 0.8680	 0.1360
BQ	 0.8390	 0.1050
BR	 0.8820	 0.1390
BS	 0.8110	 0.1050
BT	 0.7850	 0.1180
BU	 0.8800	 0.1290
BV	 0.9350	 0.1430
BW	 0.9010	 0.0760
BX	 0.8490	 0.1040
BY	 0.8550	 0.1100
BZ	 0.8790	 0.1540