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.; Beckmann, R.
Deposited on	:	2011-02-08
Resolution	:	7.10 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

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

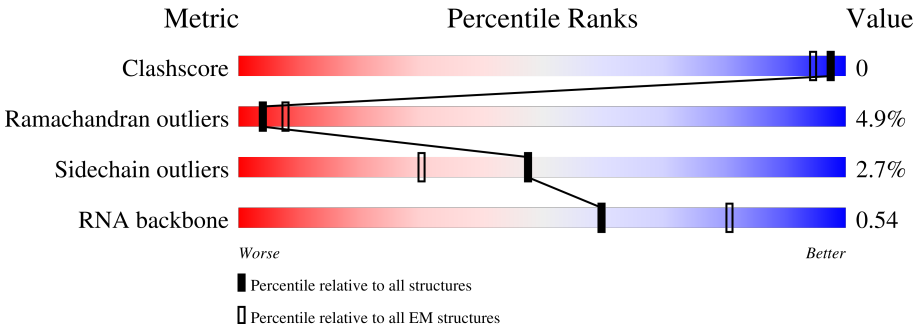
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance

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 <=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% 20%
2	AX	11	27% 9% 45% 45%
3	AV	77	75% 25%
4	AZ	98	45% 76% 23%
5	A0	200	65% 96%
5	A1	200	41% 95%
6	AB	240	12% 94% 5%

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Mol	Chain	Length	Quality of chain
7	AC	232	90% 9%
8	AD	205	91% 9%
9	AE	166	11% 94% 5%
10	AF	135	19% 93% 7%
11	AG	178	97%
12	AH	129	95% 5%
13	AI	129	90% 9%
14	AJ	103	88% 12%
15	AK	128	7% 94% 6%
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	7% 92% 8%
23	AS	91	96%
24	AT	86	97%
25	AU	70	6% 94% 6%
26	B7	120	82% 18%
27	B8	2904	80% 18%
28	BA	435	40% 80% 16%
29	BB	116	34% 89% 10%
30	B5	234	24% 95% 5%
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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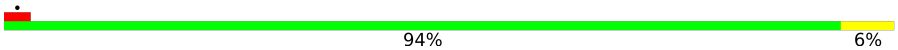
Mol	Chain	Length	Quality of chain
57	B2	46	
58	B3	64	
59	B4	38	

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

- Molecule 2 is a RNA chain called mRNA.

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

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

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

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

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

There are 16 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

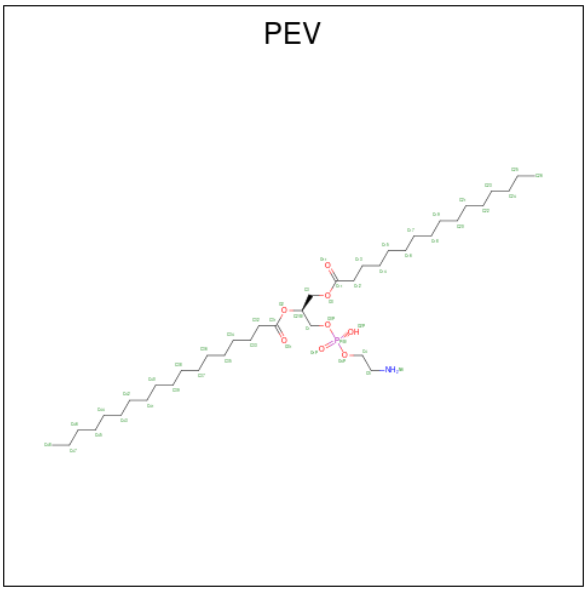
- Molecule 58 is a protein called 50S ribosomal protein L35.

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

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

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

- Molecule 60 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (three-letter code: PEV) (formula: $C_{39}H_{78}NO_8P$).



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

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

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

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

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

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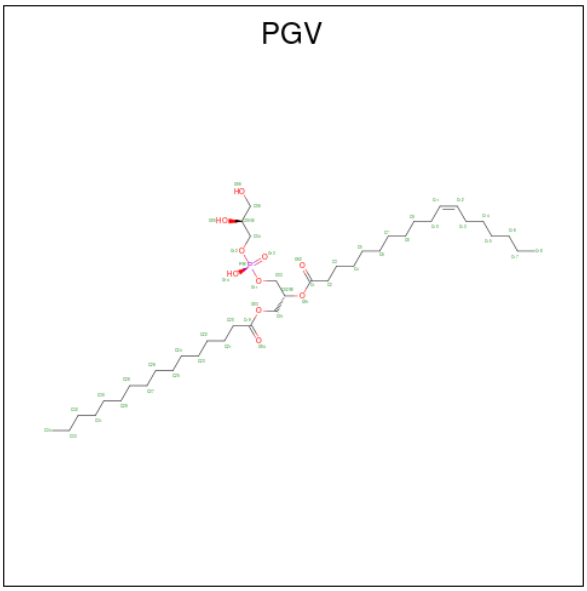
Mol	Chain	Residues	Atoms					AltConf
60	BB	1	Total	C	N	O	P	0
			49	39	1	8	1	
60	BB	1	Total	C	N	O	P	0
			49	39	1	8	1	
60	BB	1	Total	C	N	O	P	0
			49	39	1	8	1	
60	BB	1	Total	C	N	O	P	0
			49	39	1	8	1	
60	BB	1	Total	C	N	O	P	0
			49	39	1	8	1	
60	BB	1	Total	C	N	O	P	0
			49	39	1	8	1	
60	BB	1	Total	C	N	O	P	0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

- Molecule 61 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: $C_{40}H_{77}O_{10}P$).



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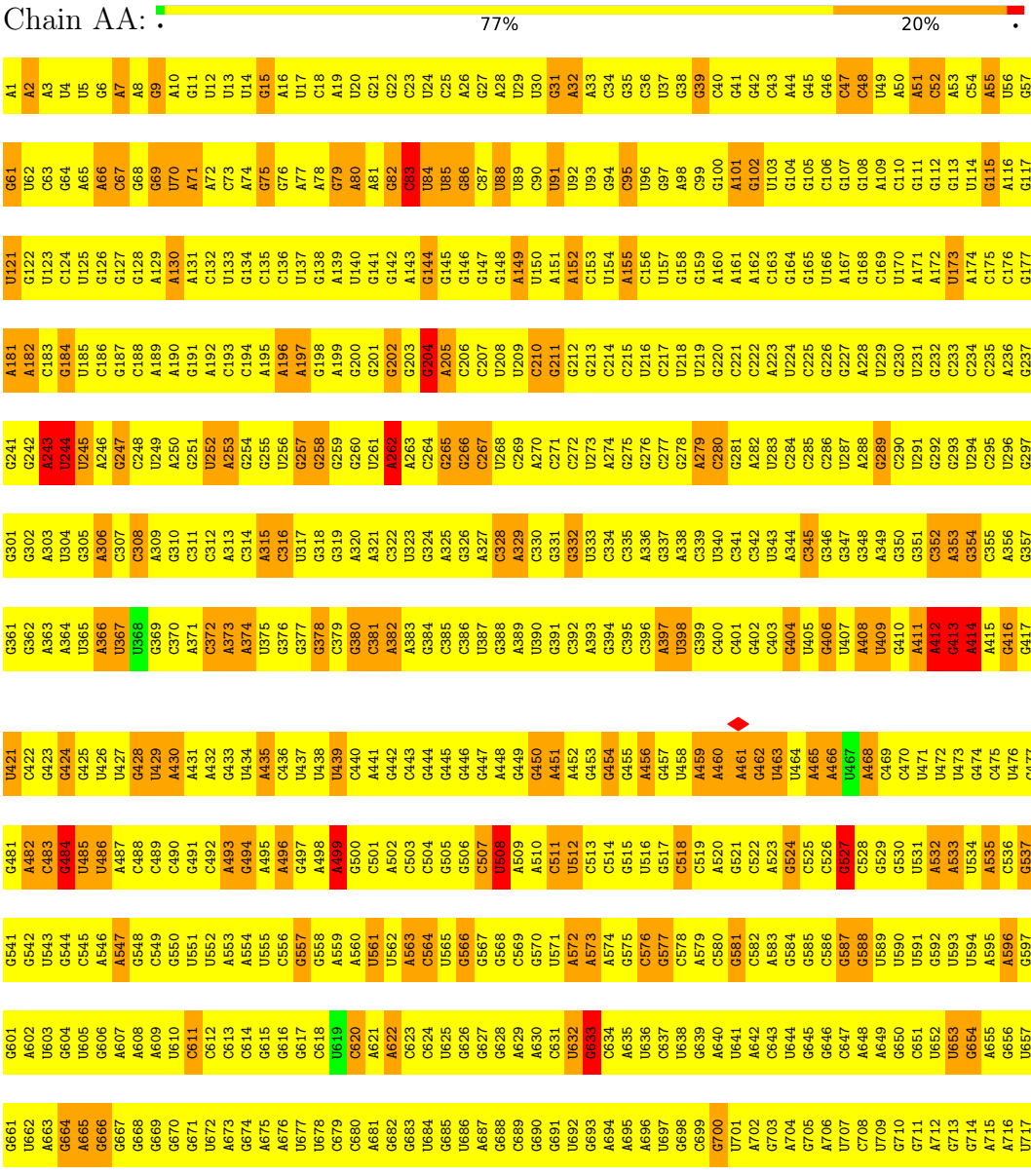
Mol	Chain	Residues	Atoms				AltConf
61	BA	1	Total	C	O	P	0
			51	40	10	1	
61	BA	1	Total	C	O	P	0
			51	40	10	1	
61	BA	1	Total	C	O	P	0
			51	40	10	1	
61	BB	1	Total	C	O	P	0
			51	40	10	1	
61	BB	1	Total	C	O	P	0
			51	40	10	1	
61	BB	1	Total	C	O	P	0
			51	40	10	1	
61	BB	1	Total	C	O	P	0
			51	40	10	1	
61	BB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

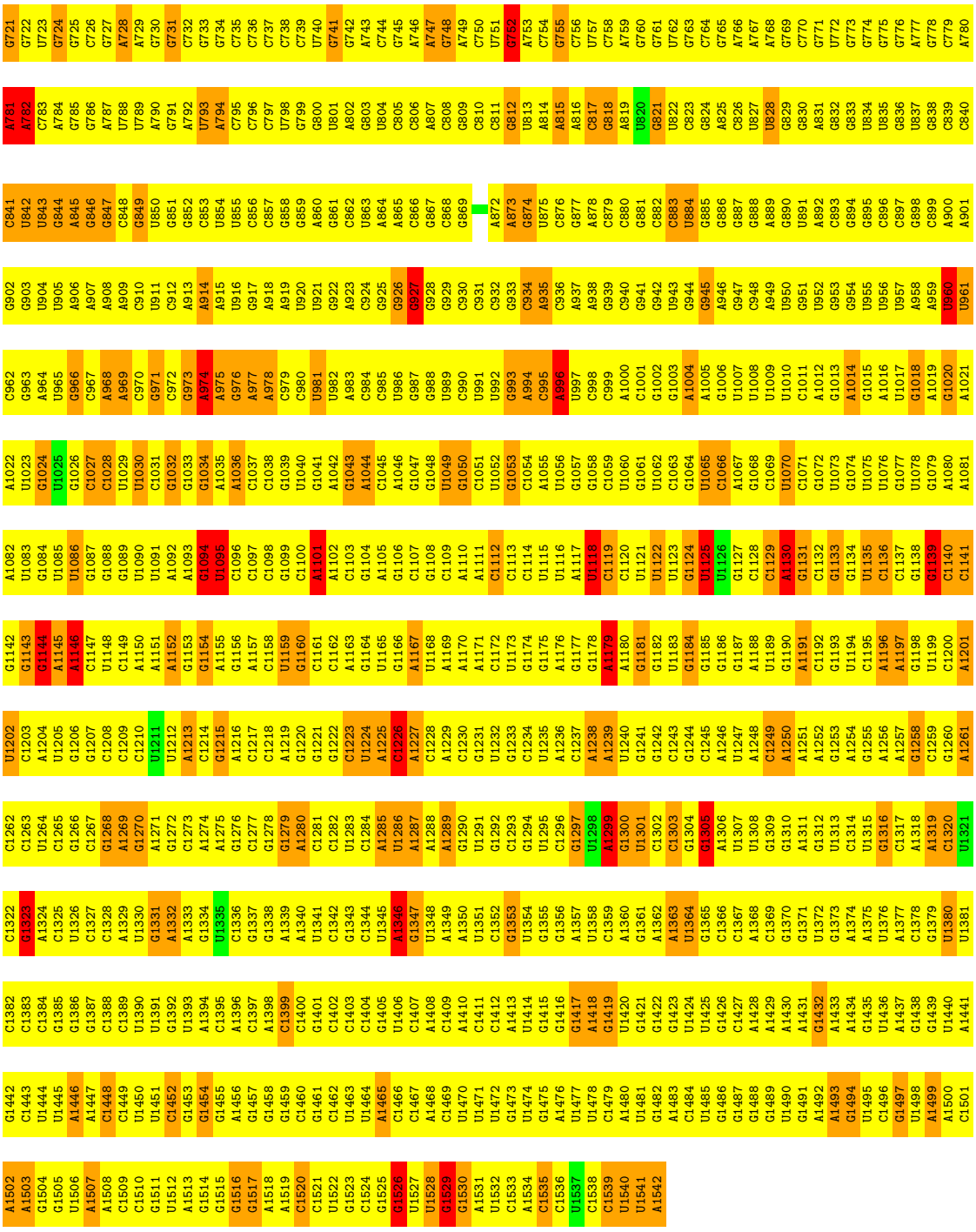
3 Residue-property plots (i)

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

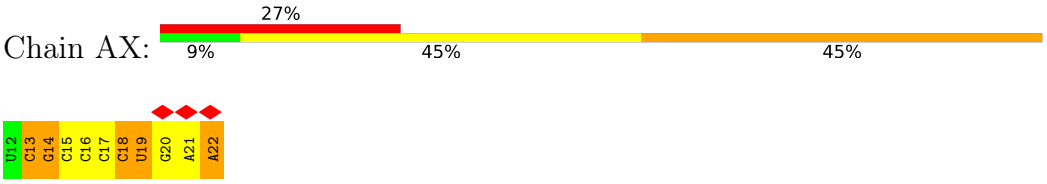
- Molecule 1: 16S RIBOSOMAL RNA

Chain AA:



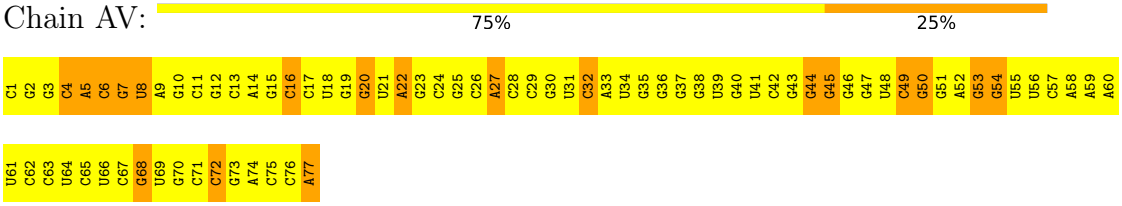


• Molecule 2: mRNA



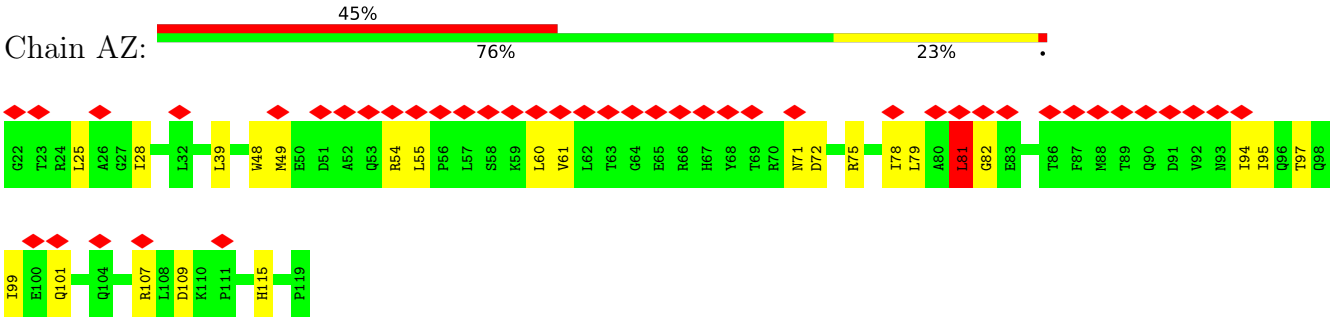
• Molecule 3: FtsQ nascent chain

Chain AV:



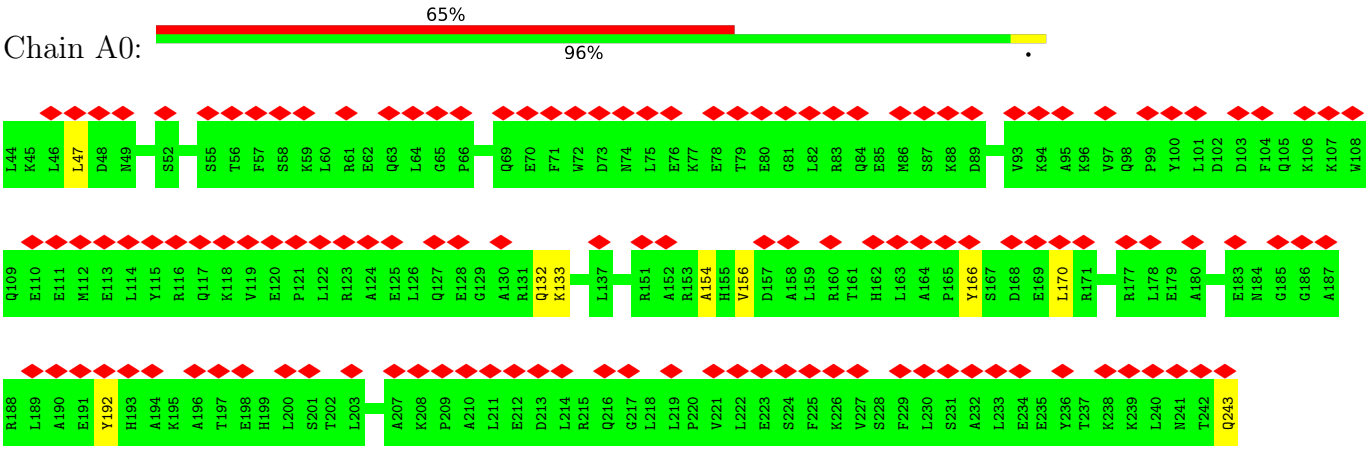
• Molecule 4: Cell division protein FtsQ

Chain AZ:



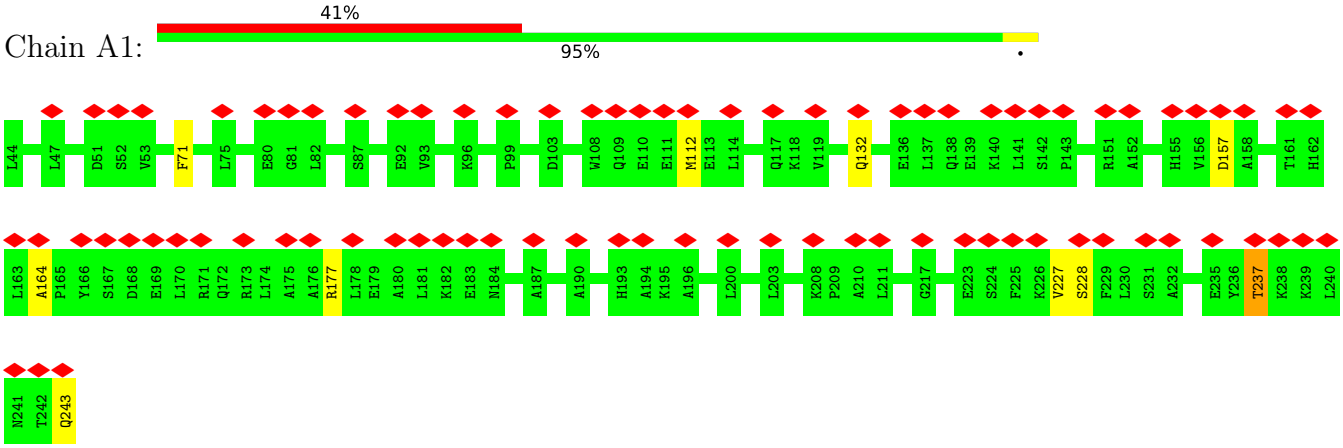
• Molecule 5: Apolipoprotein A-I

Chain A0:



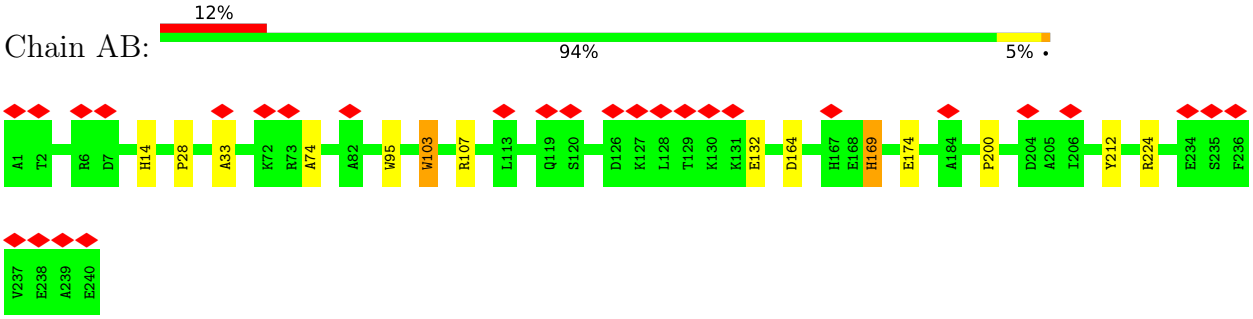
• Molecule 5: Apolipoprotein A-I

Chain A1:



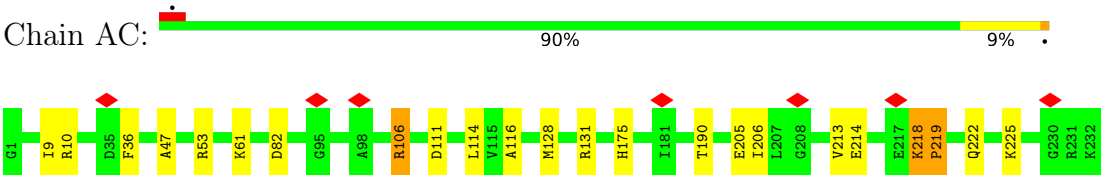
• Molecule 6: 30S ribosomal protein S2

Chain AB:



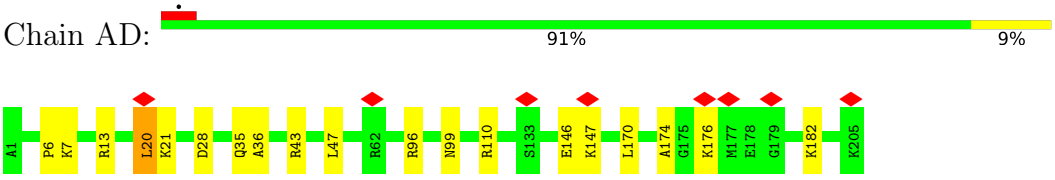
• Molecule 7: 30S ribosomal protein S3

Chain AC:



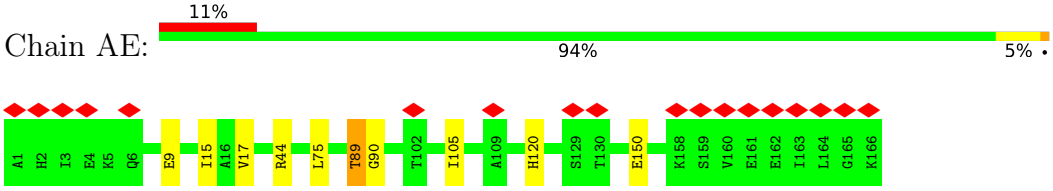
• Molecule 8: 30S ribosomal protein S4

Chain AD:



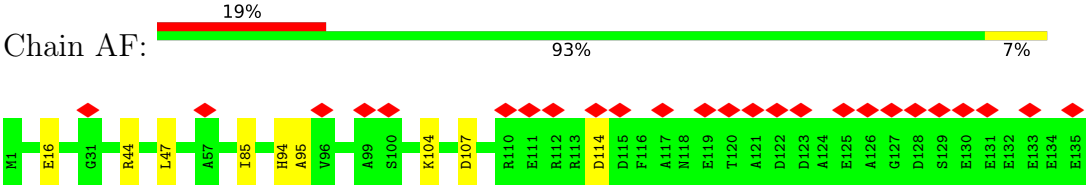
• Molecule 9: 30S ribosomal protein S5

Chain AE:



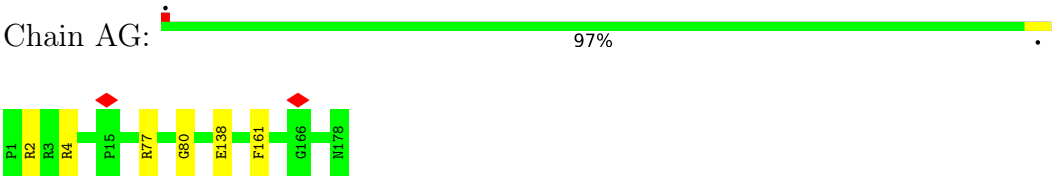
• Molecule 10: 30S ribosomal protein S6

Chain AF:



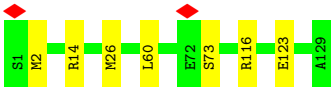
• Molecule 11: 30S ribosomal protein S7

Chain AG:



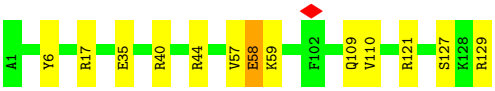
• Molecule 12: 30S ribosomal protein S8

Chain AH:



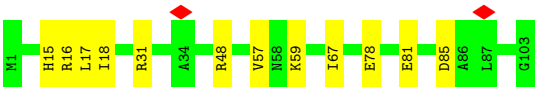
• Molecule 13: 30S ribosomal protein S9

Chain AI:



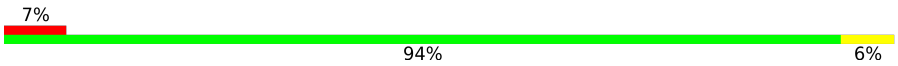
• Molecule 14: 30S ribosomal protein S10

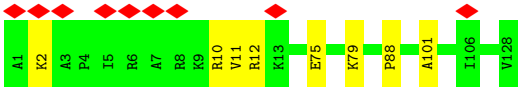
Chain AJ:



• Molecule 15: 30S ribosomal protein S11

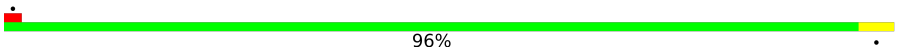
Chain AK:

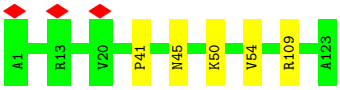




• Molecule 16: 30S ribosomal protein S12

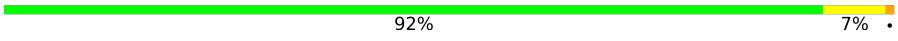
Chain AL:





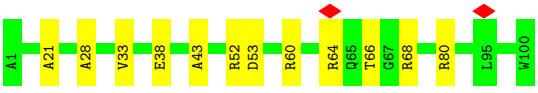
• Molecule 17: 30S ribosomal protein S13

Chain AM:



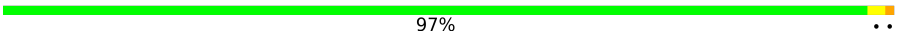
• Molecule 18: 30S ribosomal protein S14

Chain AN:



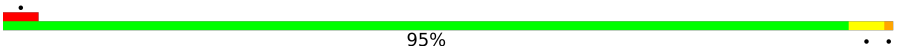
• Molecule 19: 30S ribosomal protein S15

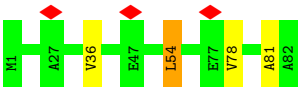
Chain AO:



• Molecule 20: 30S ribosomal protein S16

Chain AP:



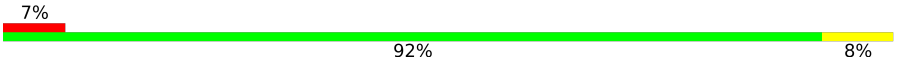


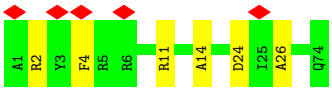
• Molecule 21: 30S ribosomal protein S17

Chain AQ:

• Molecule 22: 30S ribosomal protein S18

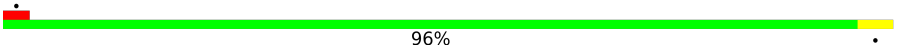
Chain AR:

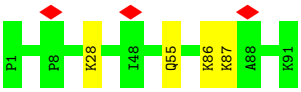




• Molecule 23: 30S ribosomal protein S19

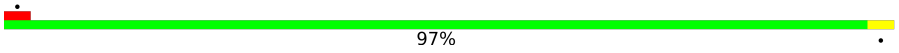
Chain AS:

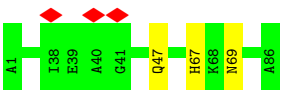




• Molecule 24: 30S ribosomal protein S20

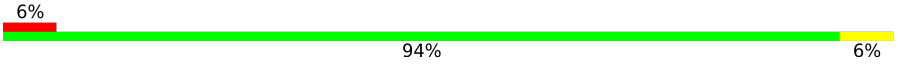
Chain AT:

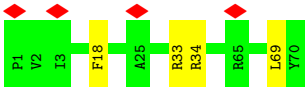




• Molecule 25: 30S ribosomal protein S21

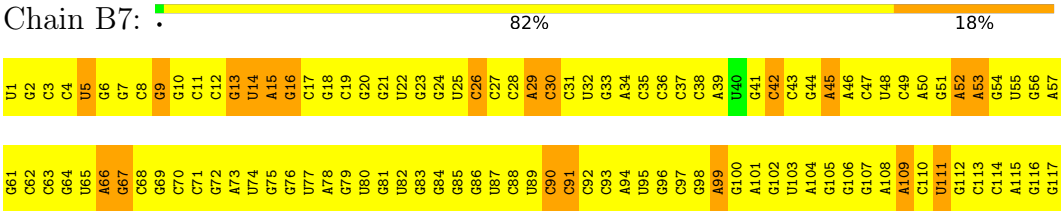
Chain AU:





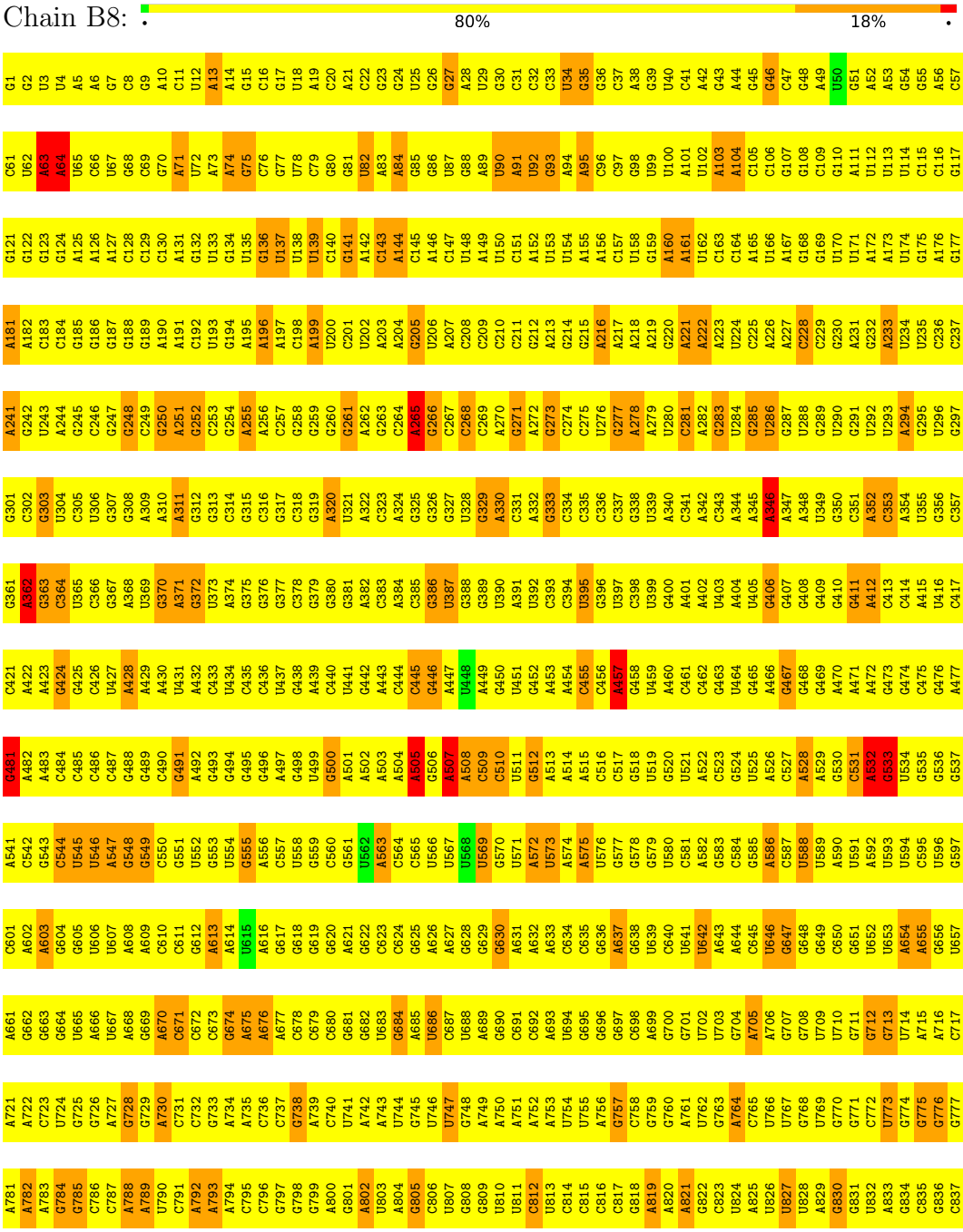
• Molecule 26: 5S RIBOSOMAL RNA

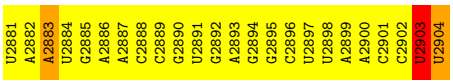
Chain B7:



• Molecule 27: 23S RIBOSOMAL RNA

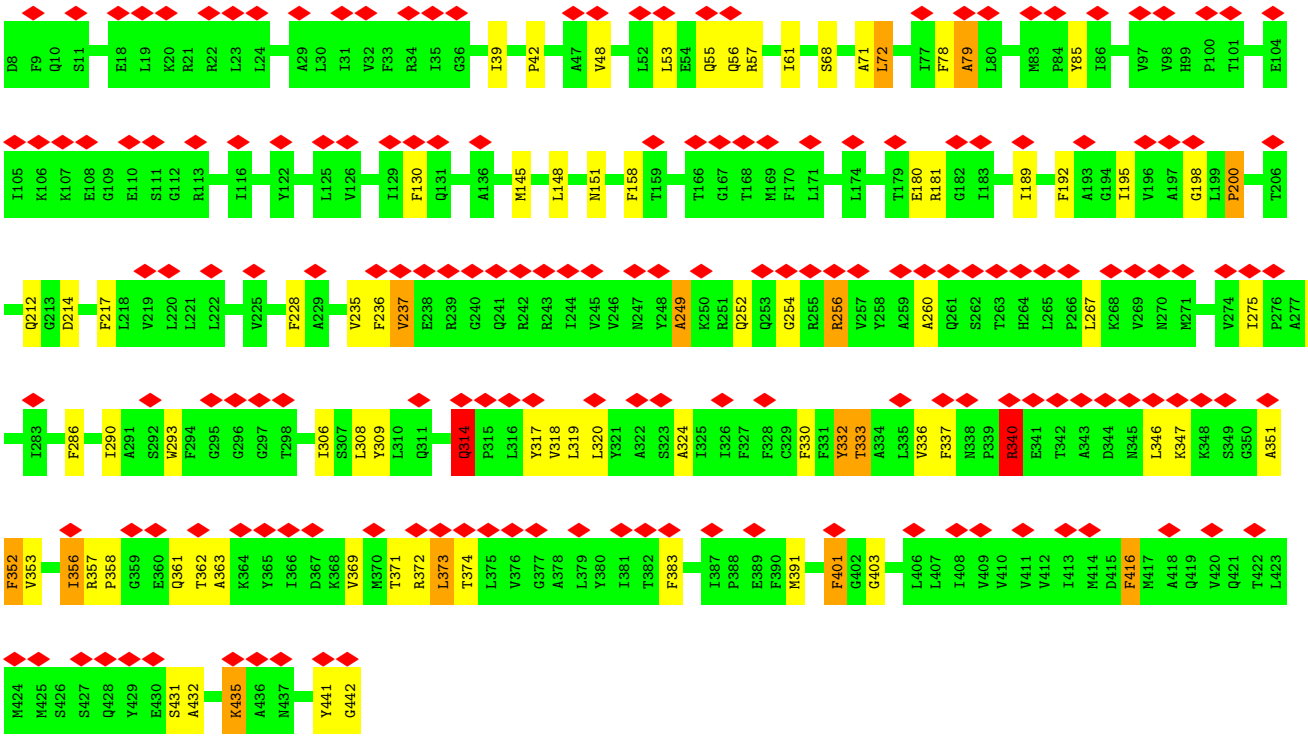
Chain B8:





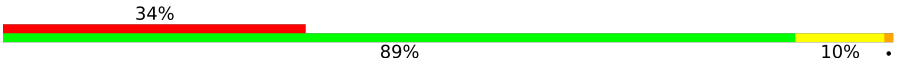
• Molecule 28: Preprotein translocase secY subunit

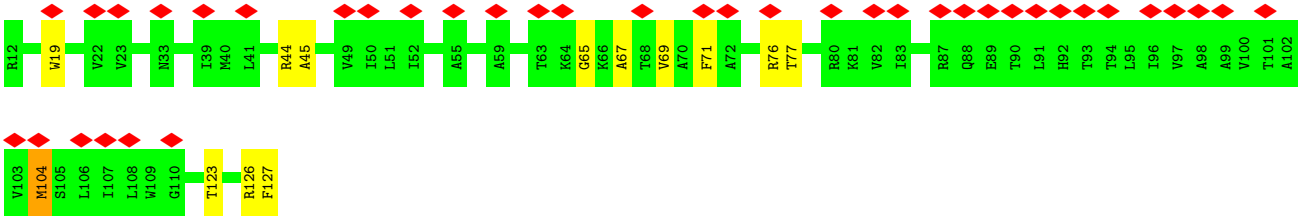
Chain BA:



• Molecule 29: Preprotein translocase secE subunit

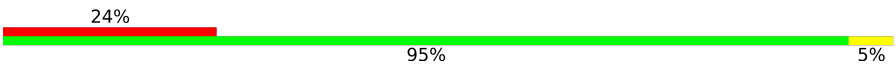
Chain BB:

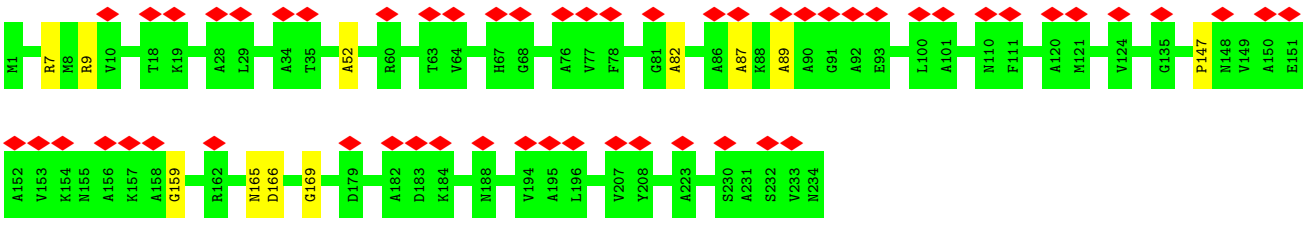




• Molecule 30: 50S ribosomal protein L1

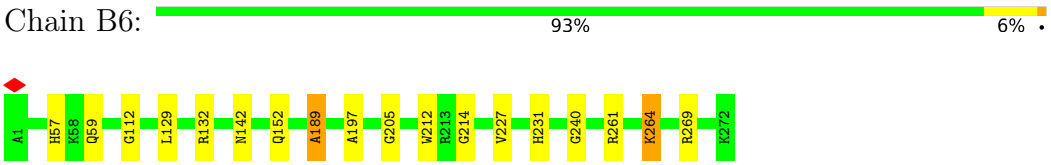
Chain B5:





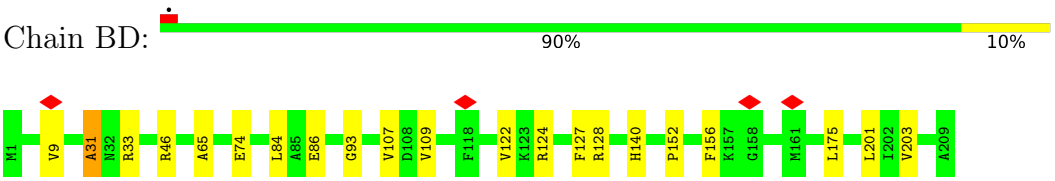
• Molecule 31: 50S ribosomal protein L2

Chain B6:



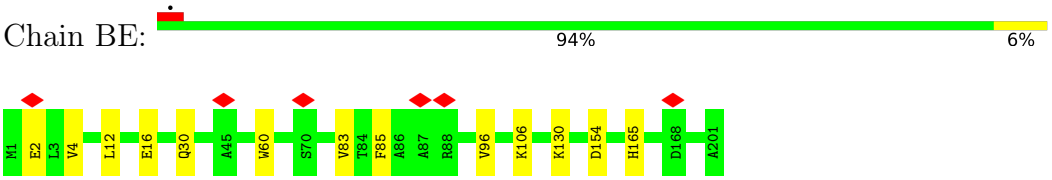
• Molecule 32: 50S ribosomal protein L3

Chain BD:



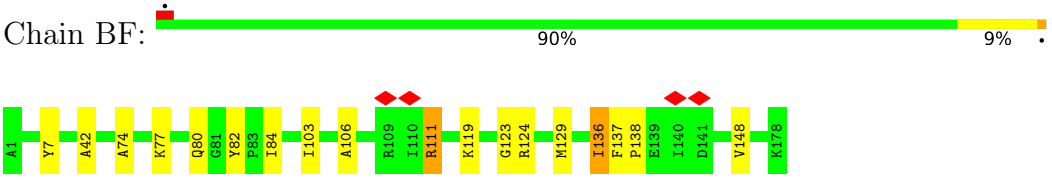
• Molecule 33: 50S ribosomal protein L4

Chain BE:



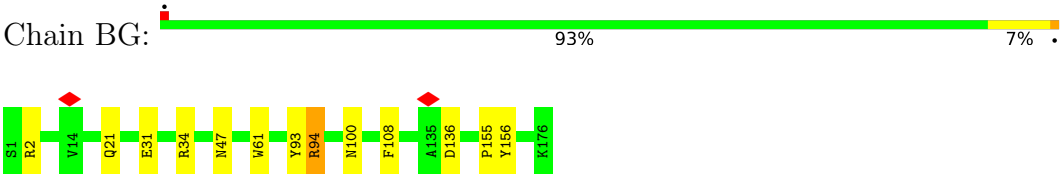
• Molecule 34: 50S ribosomal protein L5

Chain BF:



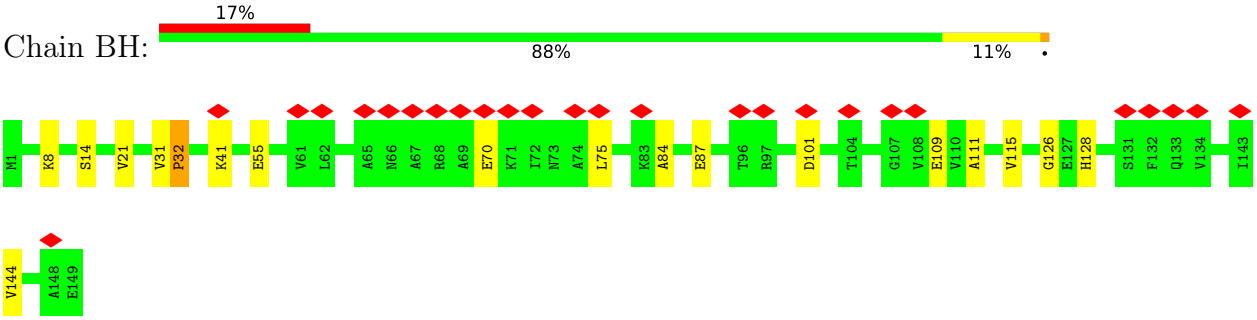
• Molecule 35: 50S ribosomal protein L6

Chain BG:



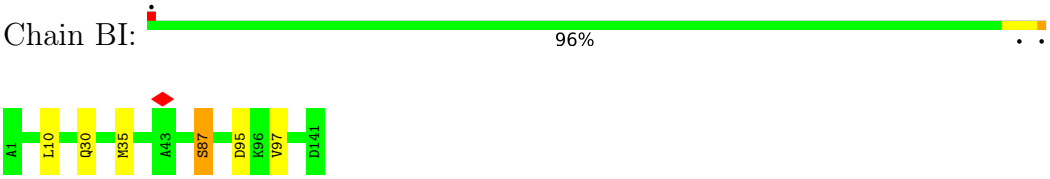
• Molecule 36: 50S ribosomal protein L9

Chain BH:



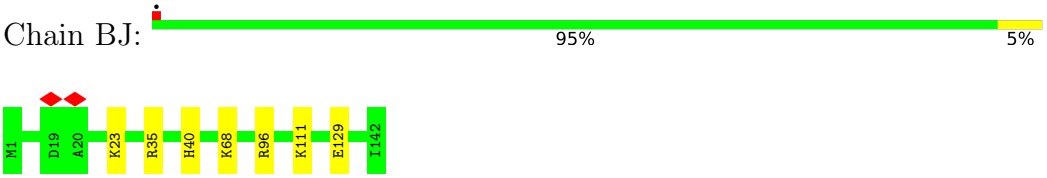
• Molecule 37: 50S ribosomal protein L11

Chain BI:



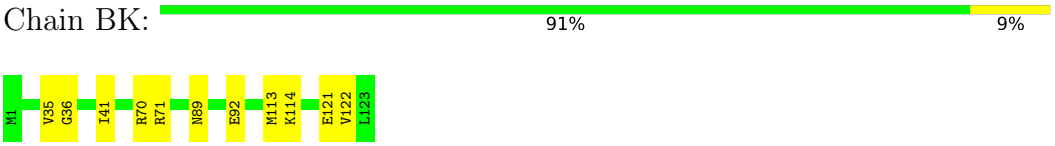
• Molecule 38: 50S ribosomal protein L13

Chain BJ:



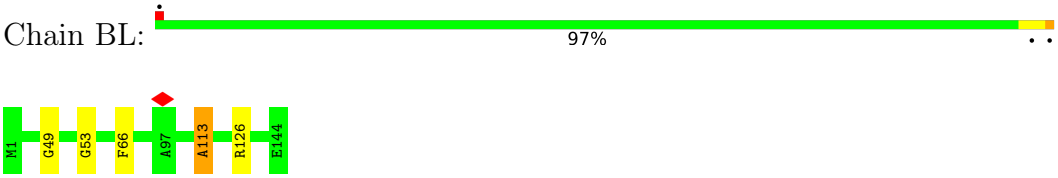
• Molecule 39: 50S ribosomal protein L14

Chain BK:



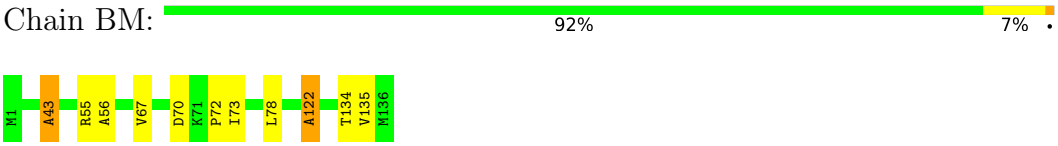
• Molecule 40: 50S ribosomal protein L15

Chain BL:



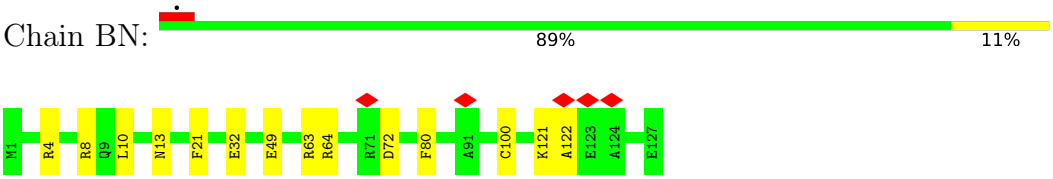
• Molecule 41: 50S ribosomal protein L16

Chain BM:



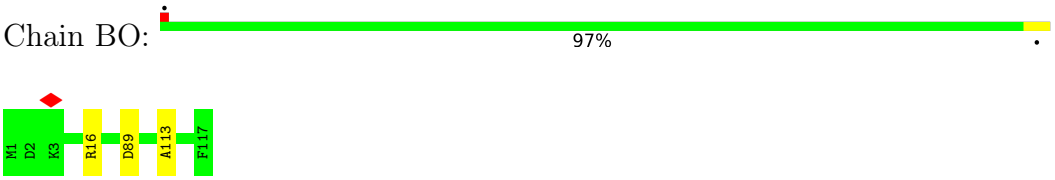
• Molecule 42: 50S ribosomal protein L17

Chain BN:



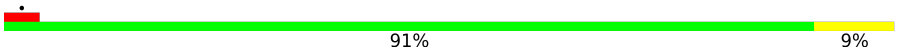
• Molecule 43: 50S ribosomal protein L18

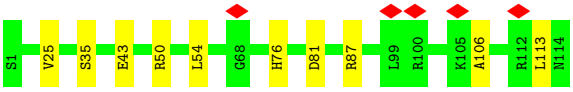
Chain BO:



• Molecule 44: 50S ribosomal protein L19

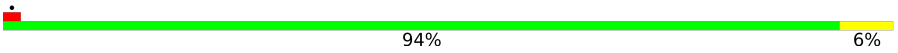
Chain BP:

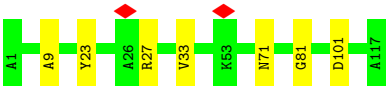




• Molecule 45: 50S ribosomal protein L20

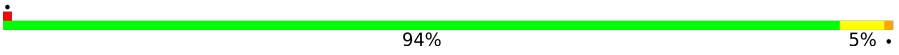
Chain BQ:





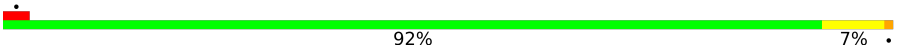
• Molecule 46: 50S ribosomal protein L21

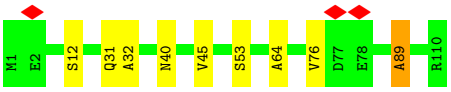
Chain BR:



• Molecule 47: 50S ribosomal protein L22

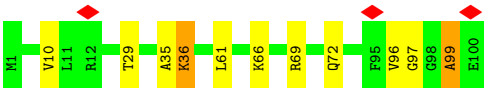
Chain BS:





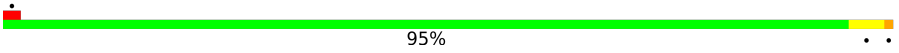
• Molecule 48: 50S ribosomal protein L23

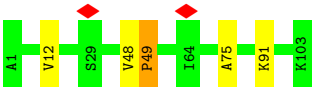
Chain BT:



• Molecule 49: 50S ribosomal protein L24

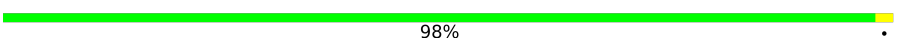
Chain BU:

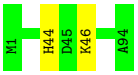




• Molecule 50: 50S ribosomal protein L25

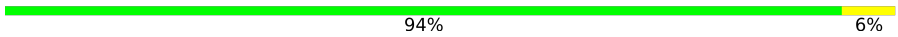
Chain BV:

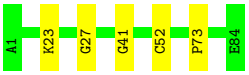




• Molecule 51: 50S ribosomal protein L27

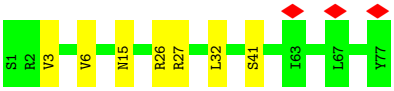
Chain BW:





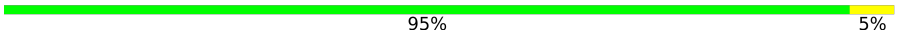
• Molecule 52: 50S ribosomal protein L28

Chain BX:



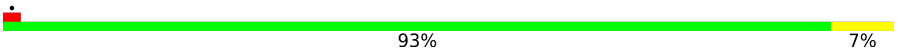
• Molecule 53: 50S ribosomal protein L29

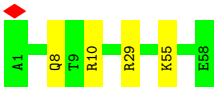
Chain BY:



• Molecule 54: 50S ribosomal protein L30

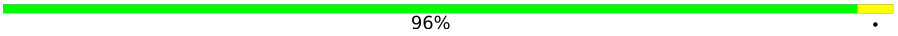
Chain BZ:

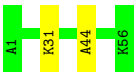




• Molecule 55: 50S ribosomal protein L32

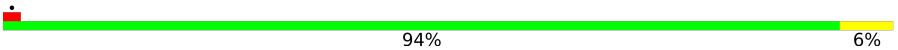
Chain B0:





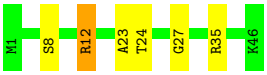
• Molecule 56: 50S ribosomal protein L33

Chain B1:



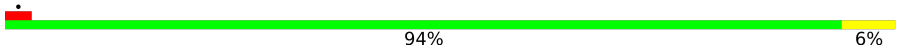
• Molecule 57: 50S ribosomal protein L34

Chain B2:



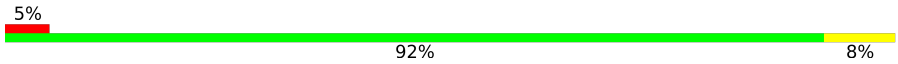
• Molecule 58: 50S ribosomal protein L35

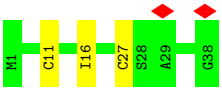
Chain B3:



• Molecule 59: 50S ribosomal protein L36

Chain B4:





4 Experimental information (i)

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 ($e^-/Å^2$)	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 (Å)	396, 396, 396	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90, 90, 90	wwPDB
Pixel spacing (Å)	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(^{o})	Ideal(^{o})
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

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

5 of 753 RNA backbone outliers are listed below:

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

5 of 73 RNA pucker outliers are listed below:

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

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

133 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
60	PEV	A0	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. '-' 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(^{o})	Ideal(^{o})
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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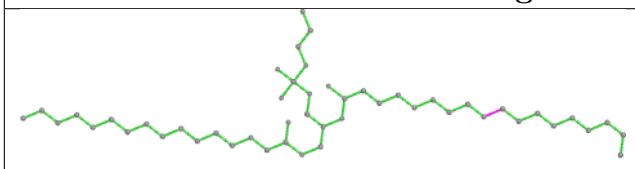
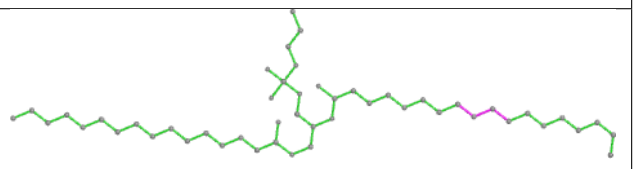
Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	BA	513	PEV	1	0
61	BA	512	PGV	1	0
60	B8	3001	PEV	1	0
60	A1	323	PEV	1	0
60	BA	514	PEV	1	0
60	A1	319	PEV	1	0
60	A0	315	PEV	1	0
60	BA	526	PEV	1	0
61	A1	315	PGV	1	0
60	A1	302	PEV	1	0
60	B8	3002	PEV	2	0
61	A1	303	PGV	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

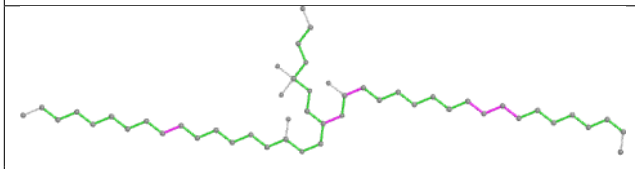
Ligand PEV A0 309



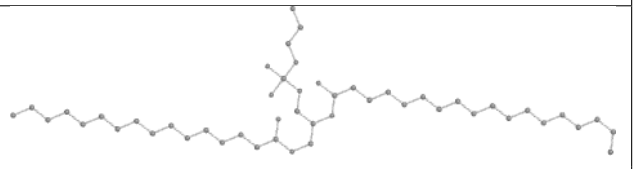
Bond lengths



Bond angles

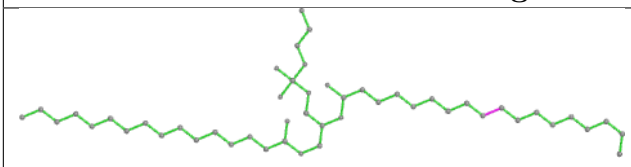


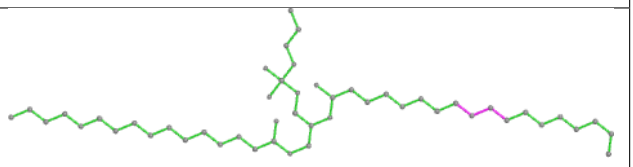
Torsions

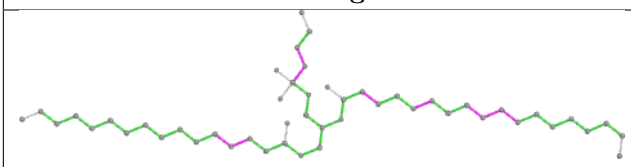


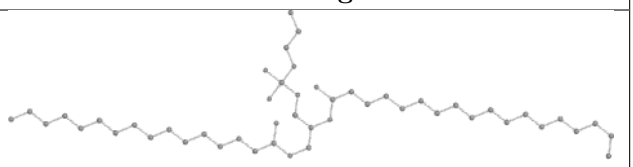
Rings

Ligand PEV BA 518

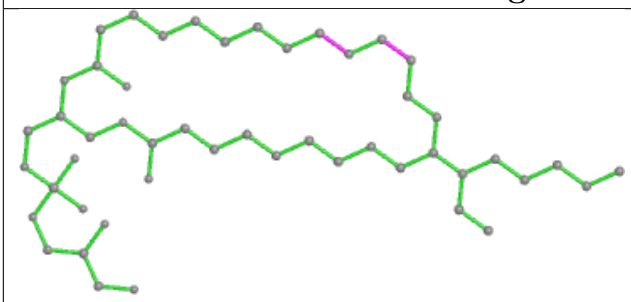

Bond lengths

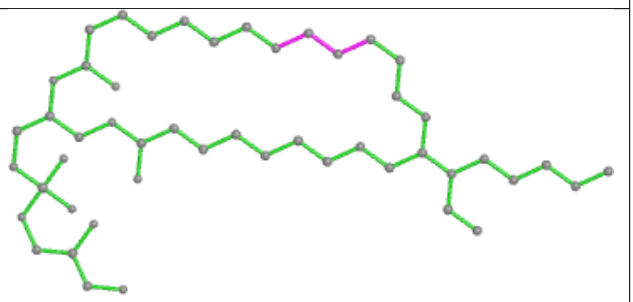

Bond angles

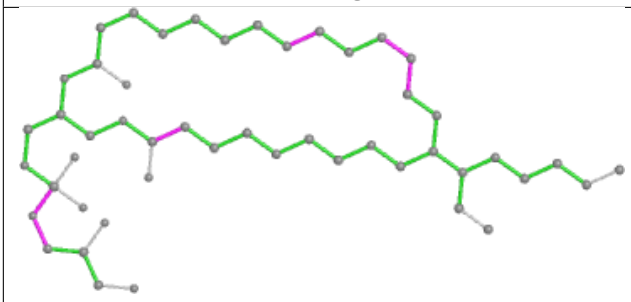

Torsions

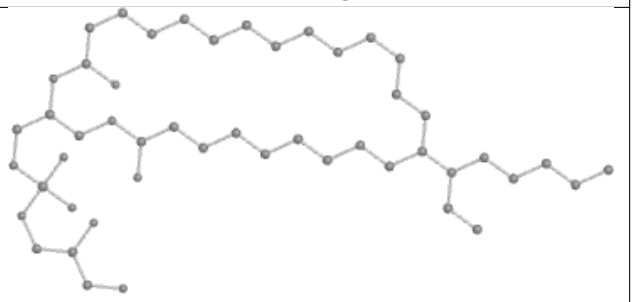

Rings

Ligand PGV BA 516

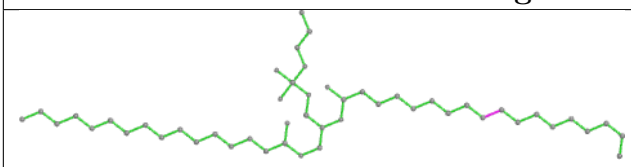

Bond lengths

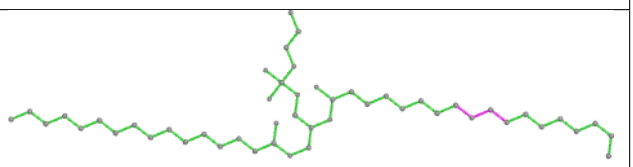

Bond angles

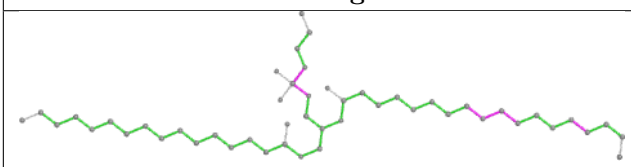

Torsions

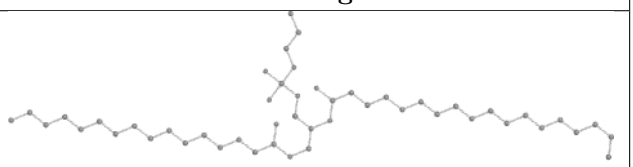

Rings

Ligand PEV A1 313

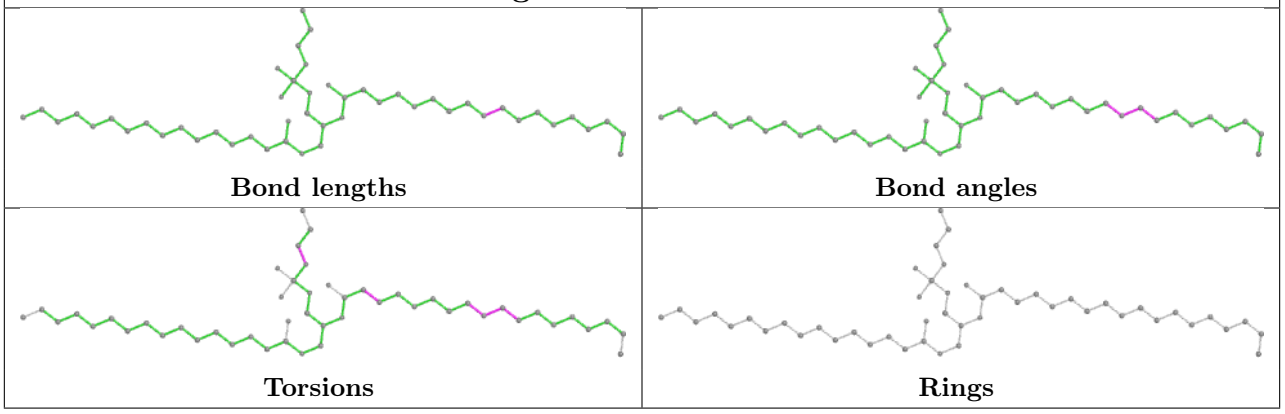

Bond lengths


Bond angles

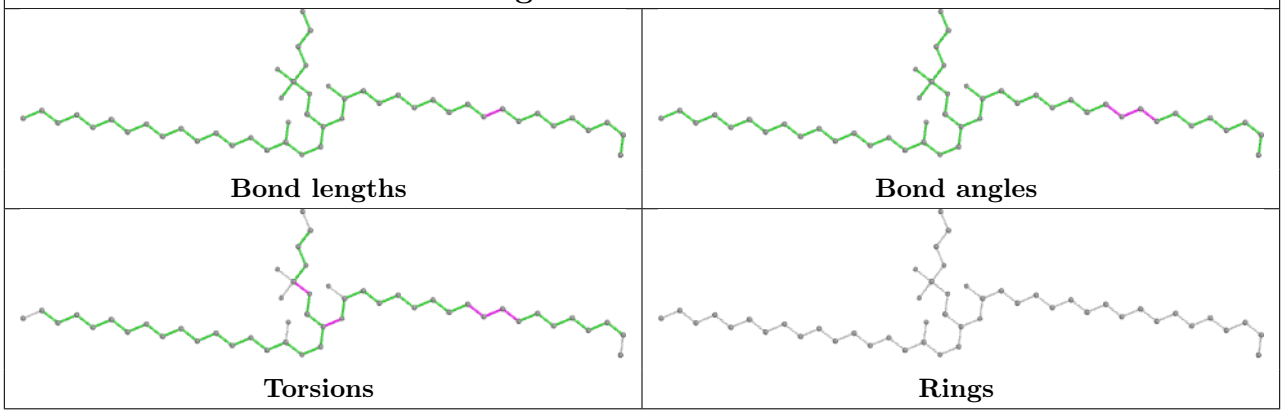

Torsions


Rings

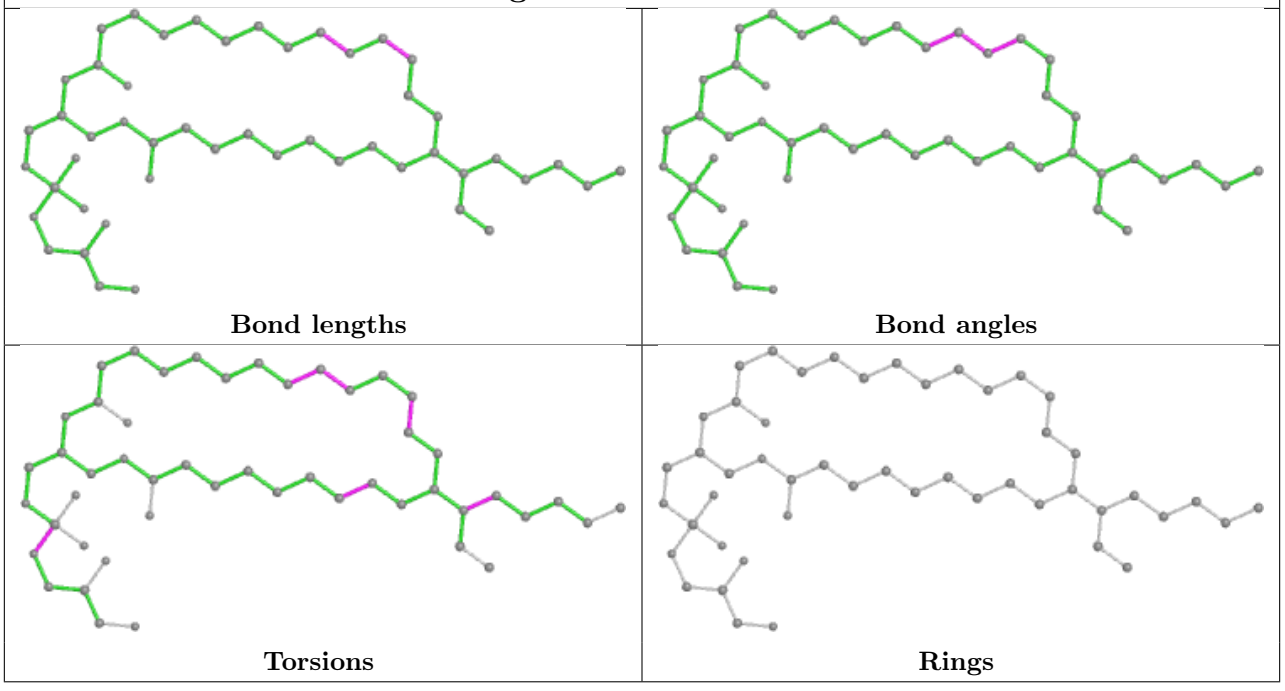
Ligand PEV BB 216



Ligand PEV A0 322



Ligand PGV BA 515



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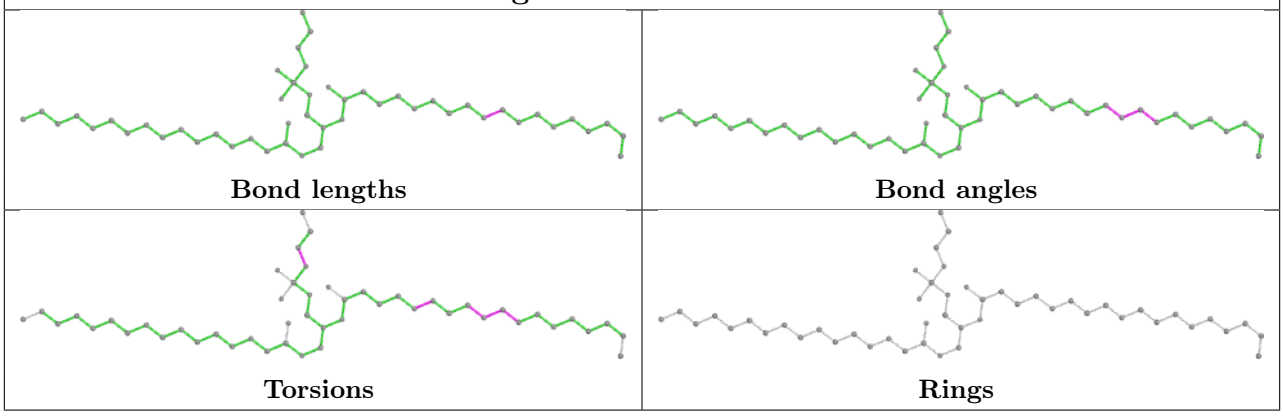

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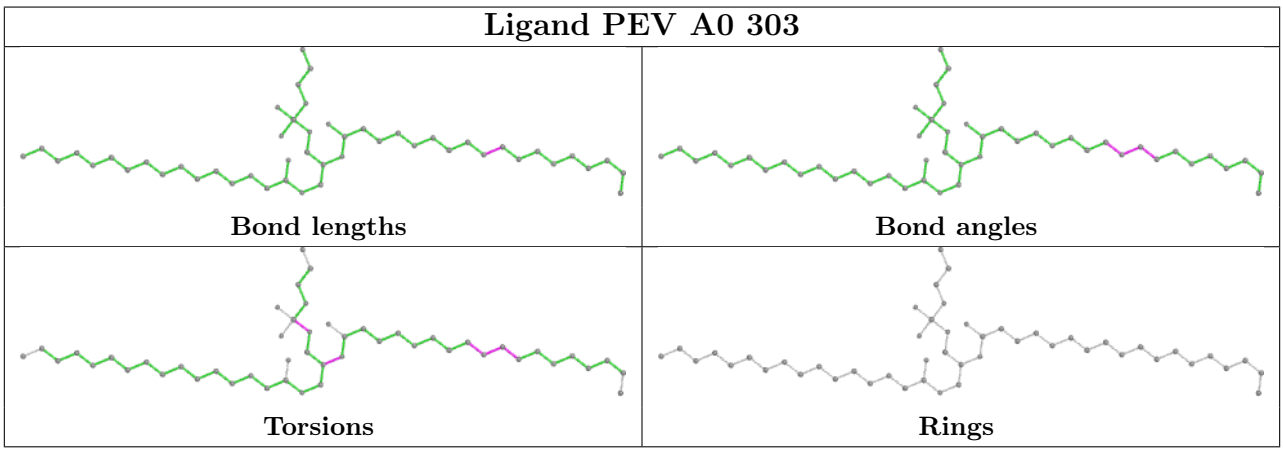

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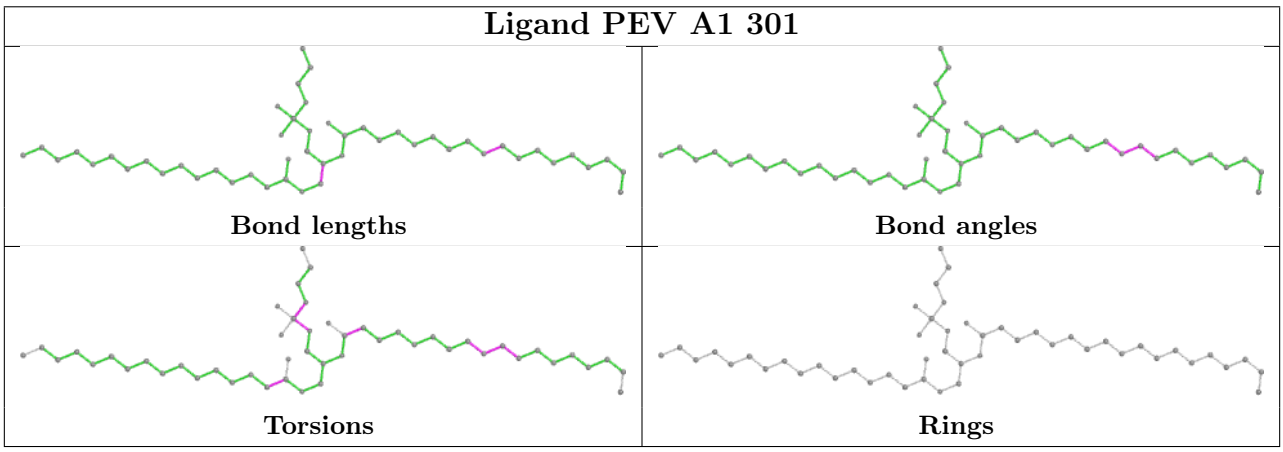

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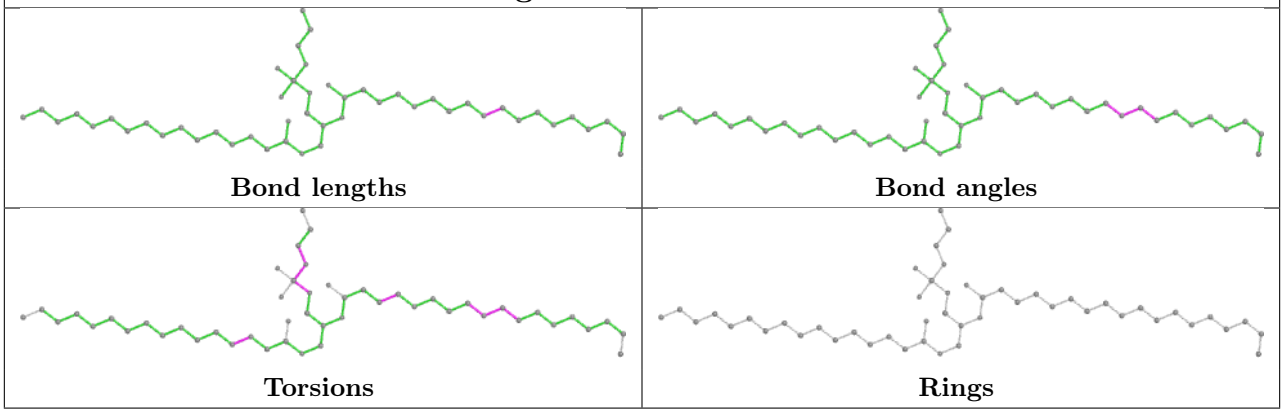

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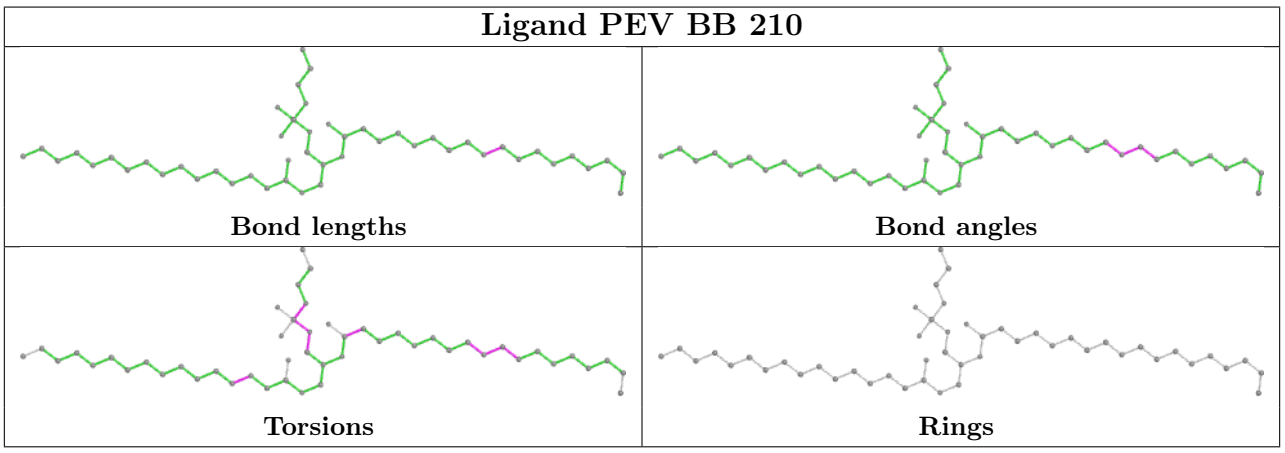

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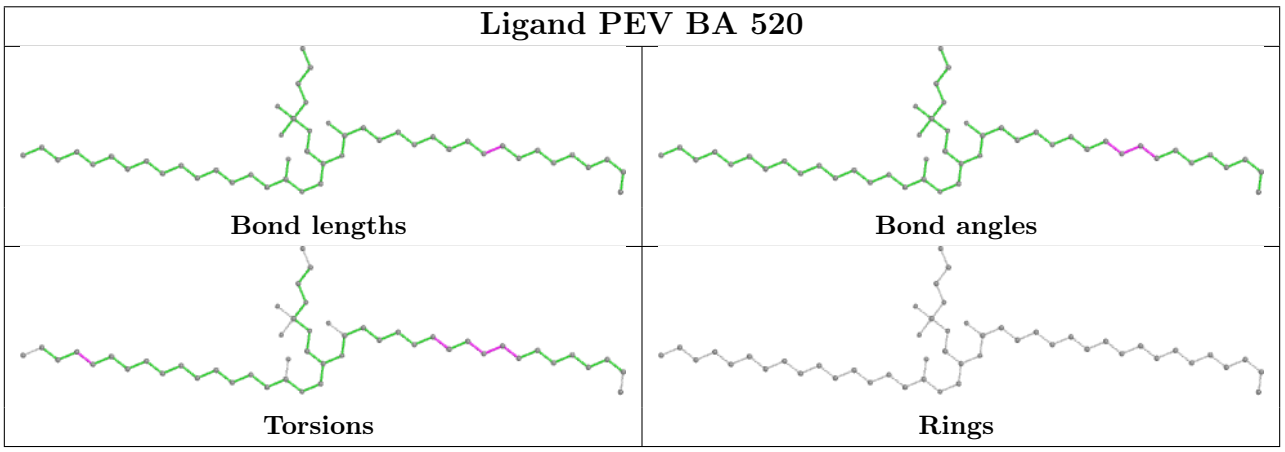

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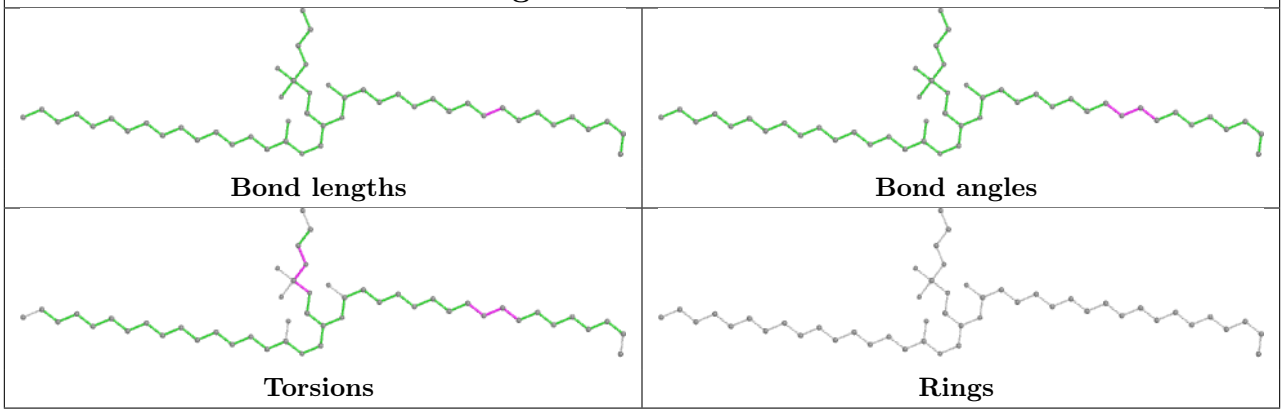

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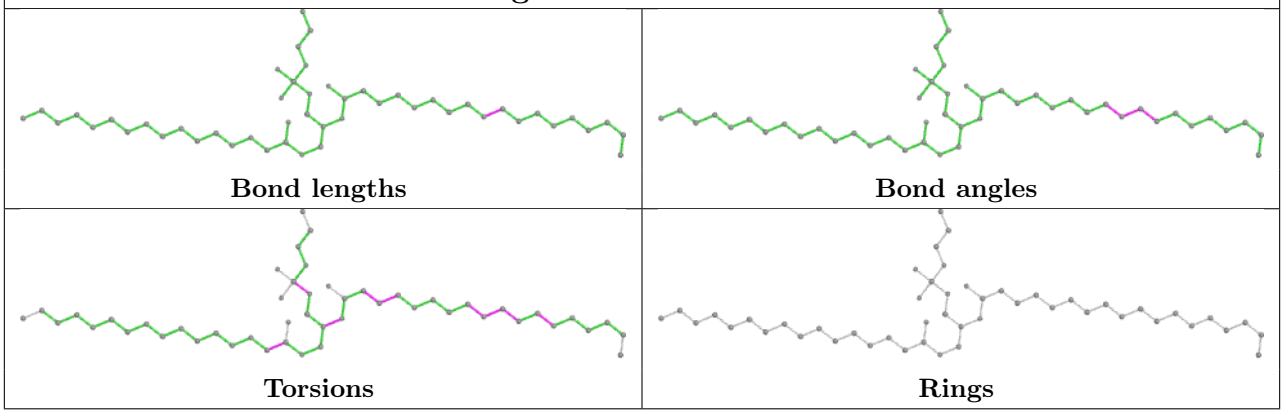
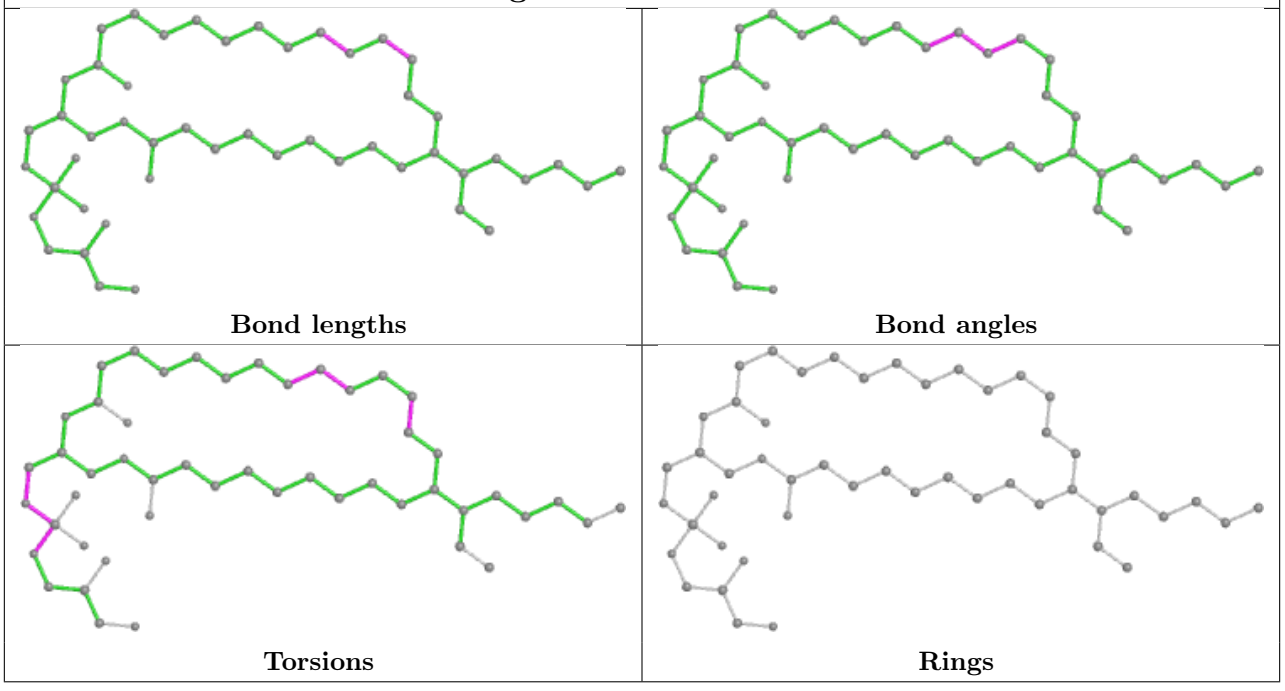
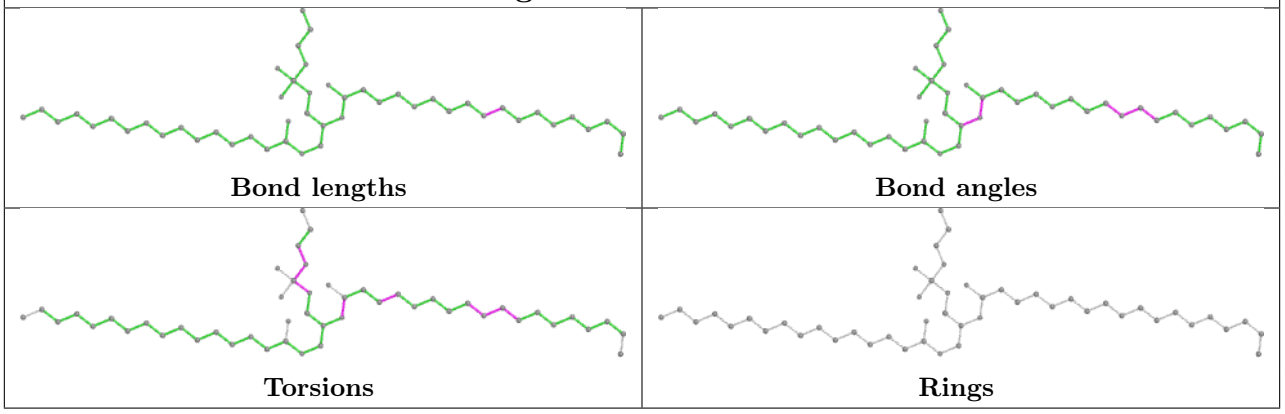


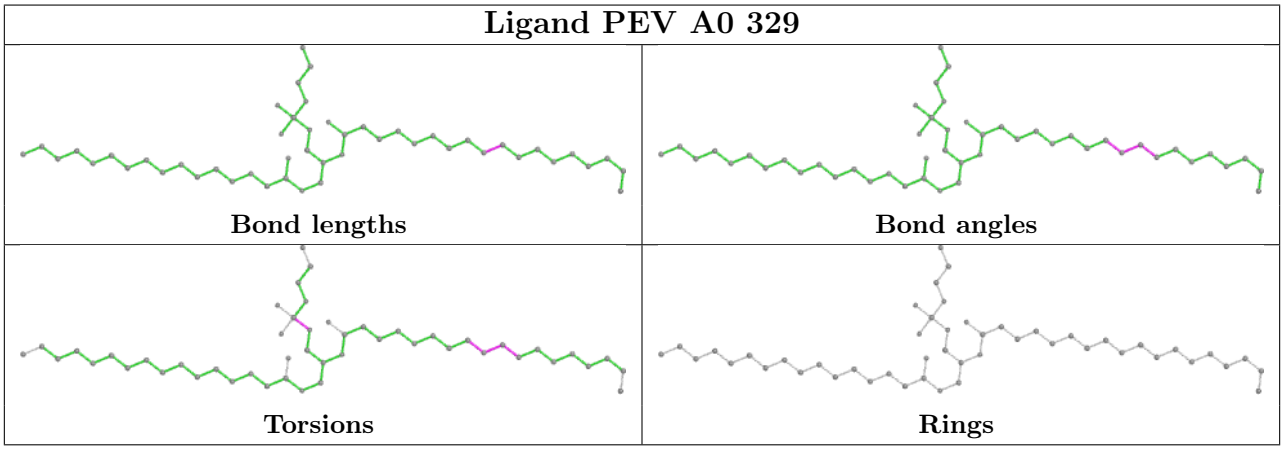
Ligand PGV BA 501



Ligand PEV A0 321



Ligand PEV A0 329



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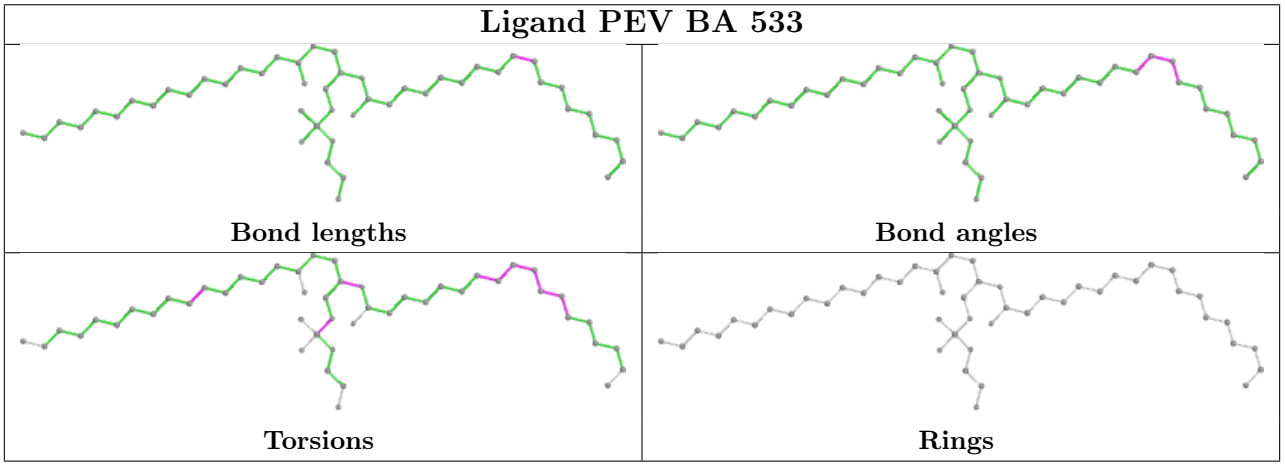

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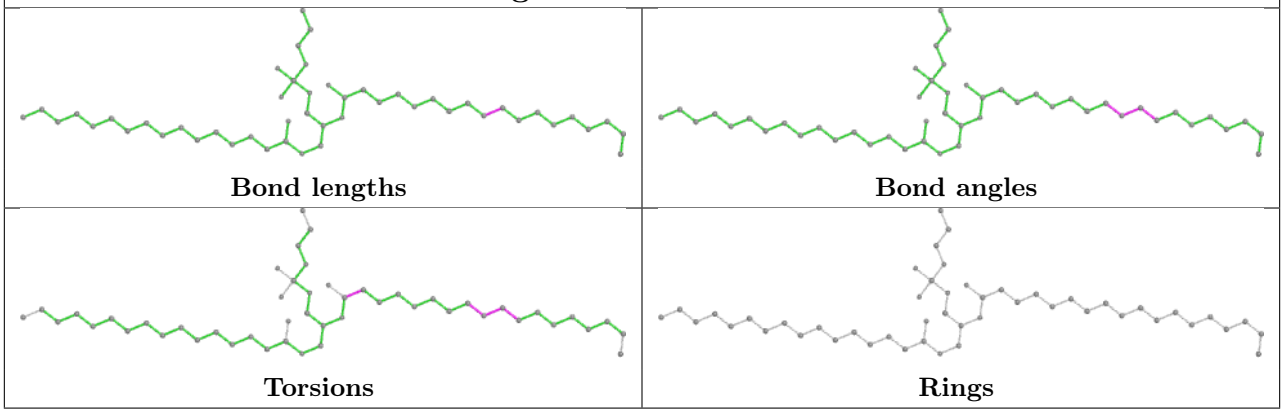

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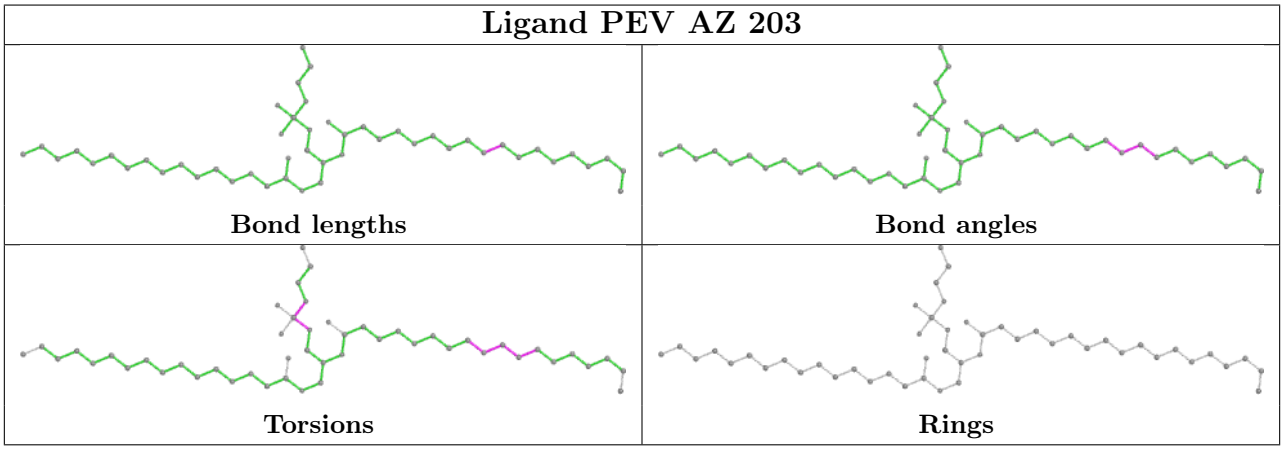

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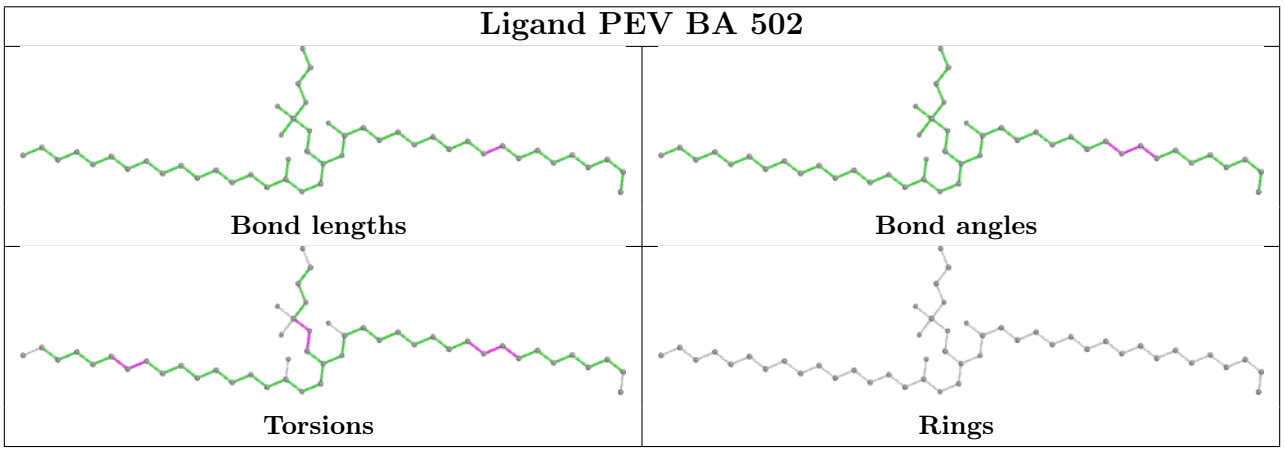
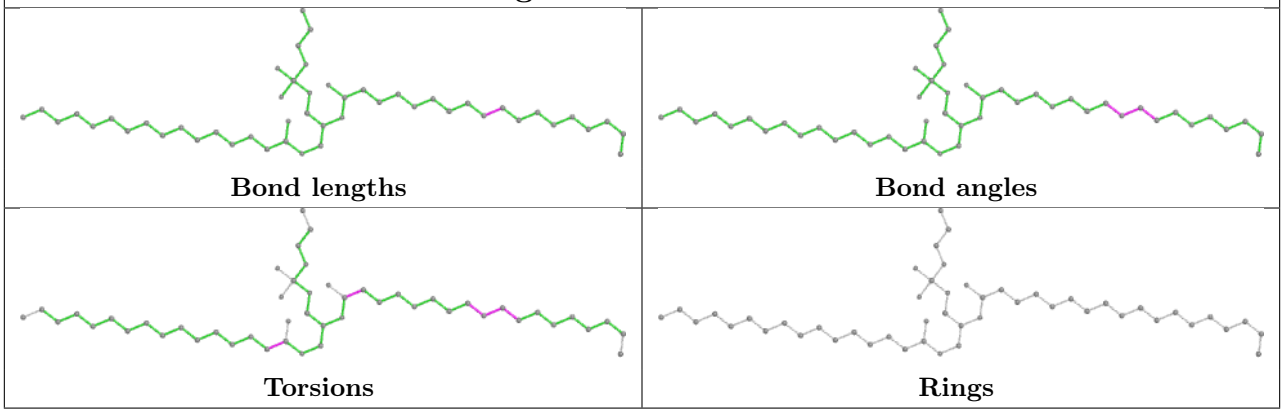


Ligand PEV A1 306



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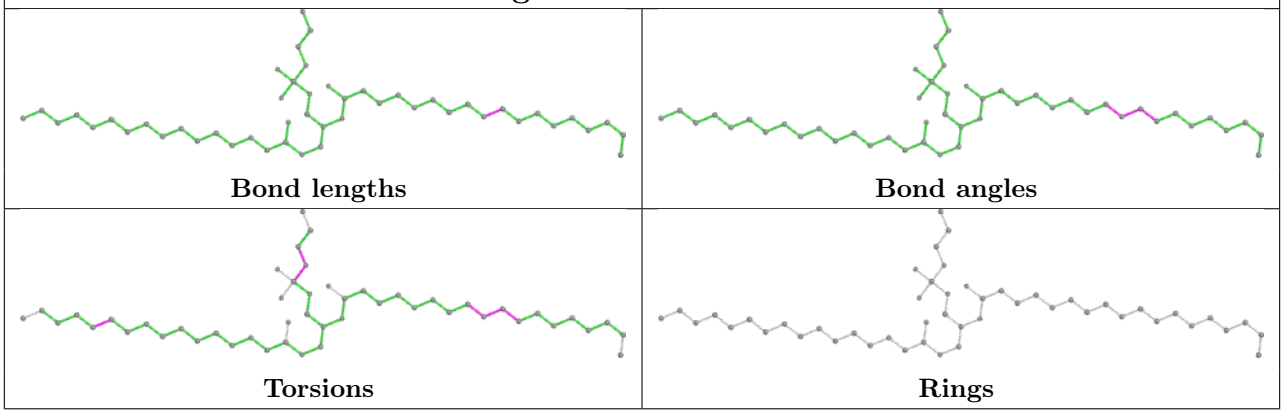

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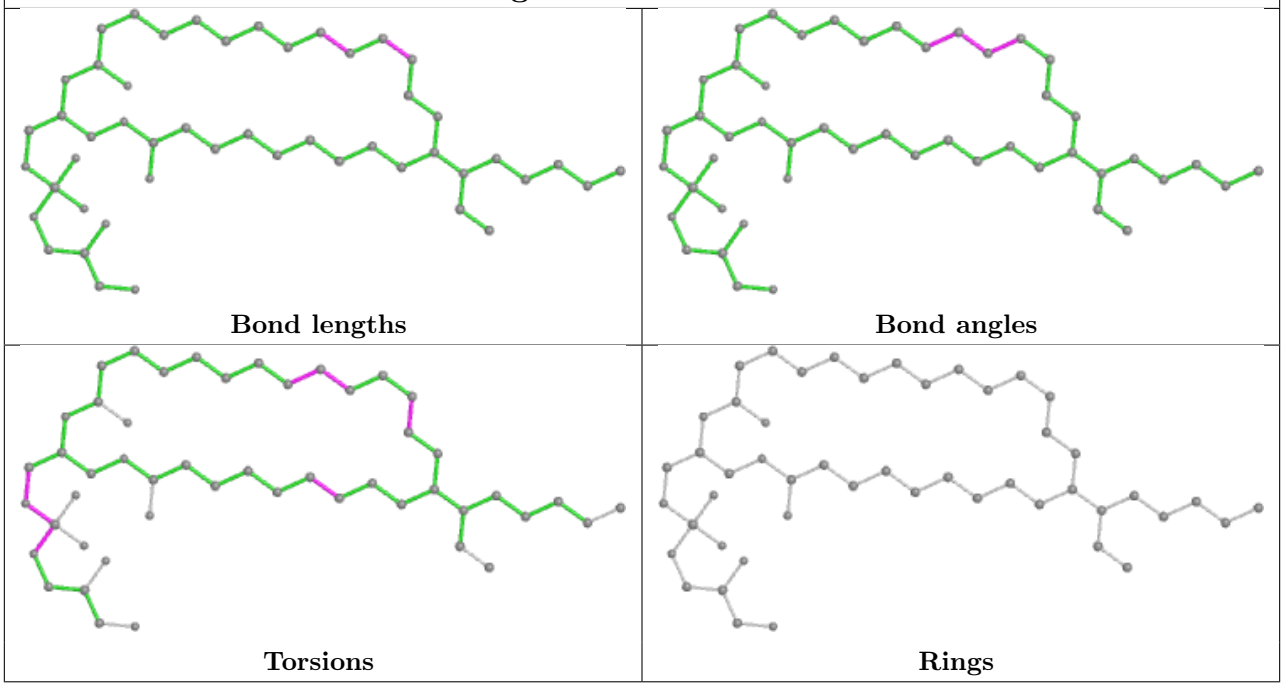

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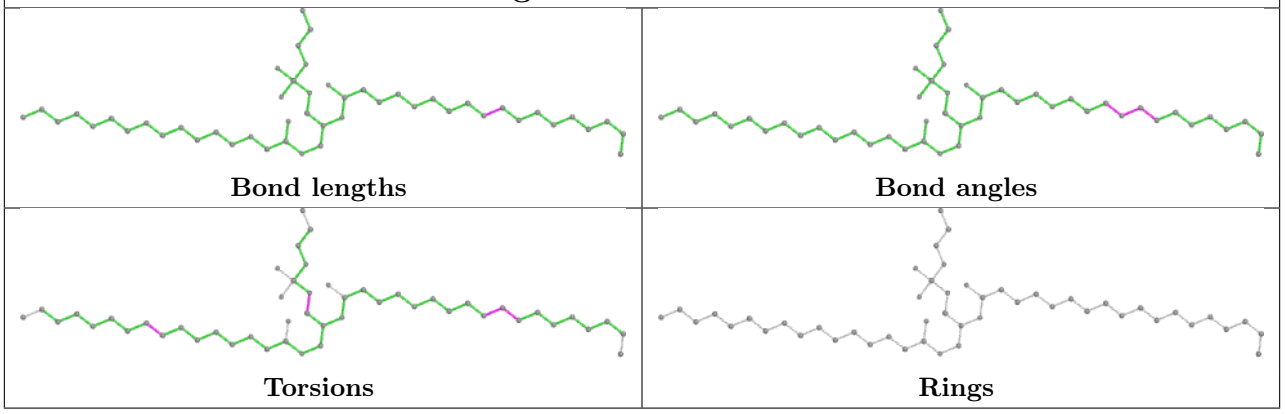

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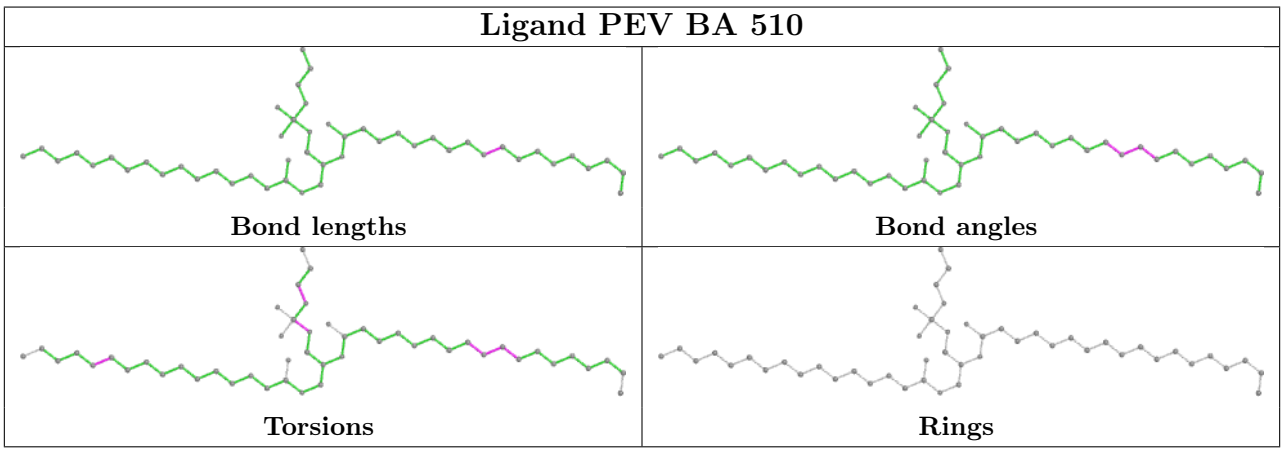
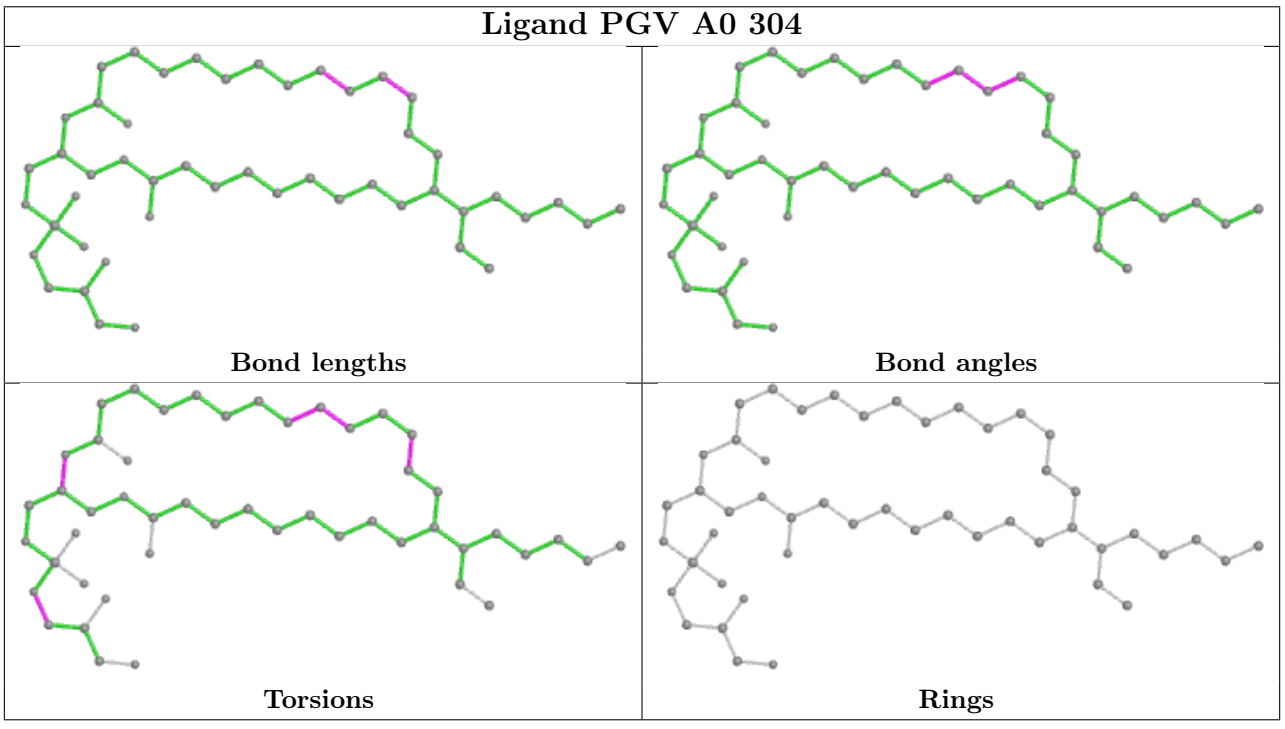


Ligand PGV A0 304



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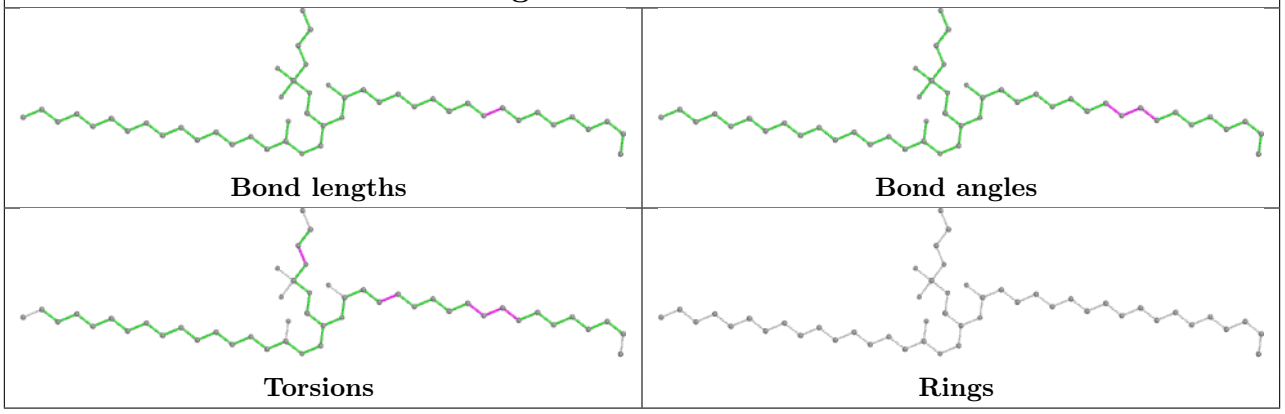
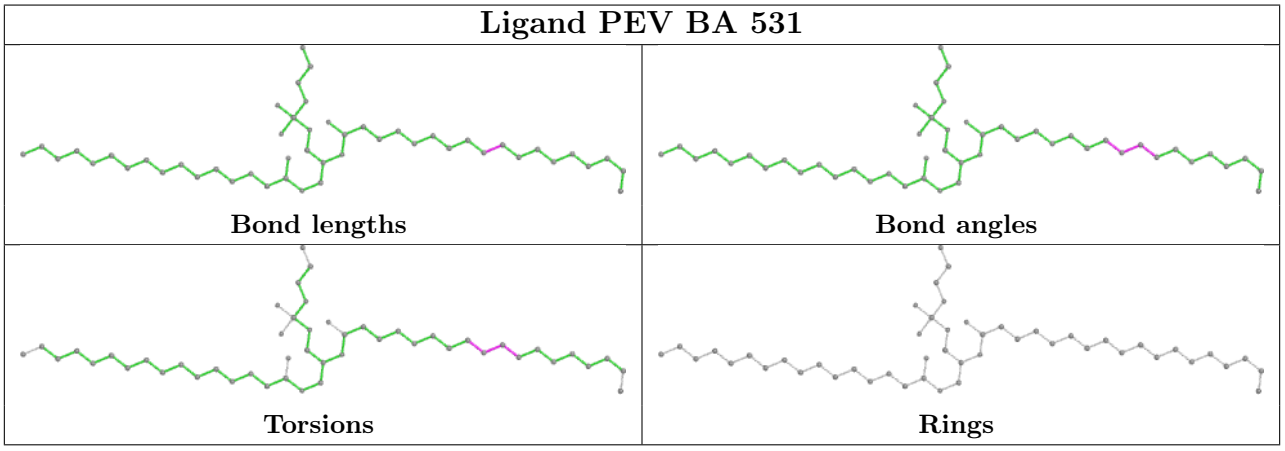
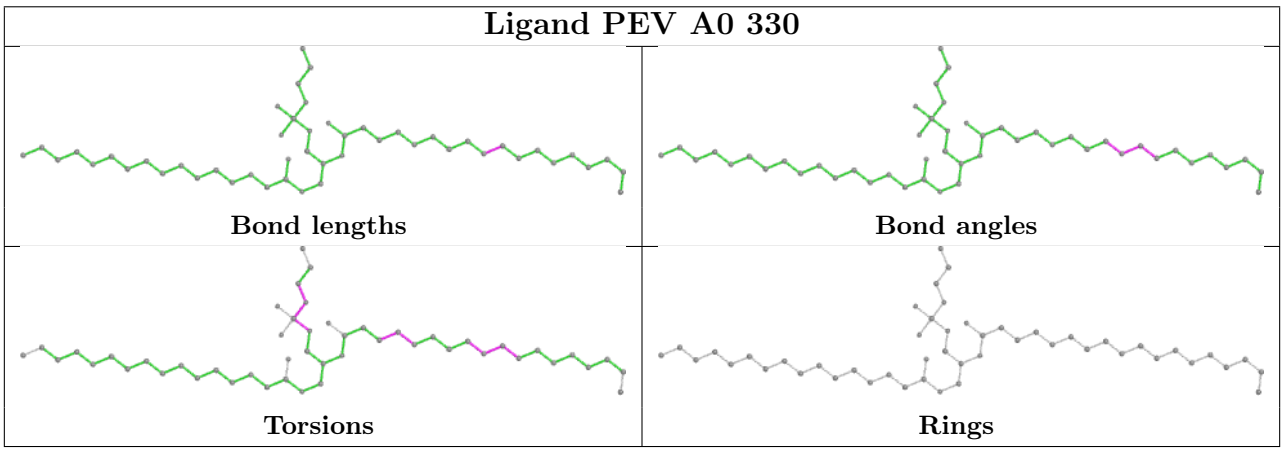


Ligand PEV BA 531



Ligand PEV A0 330



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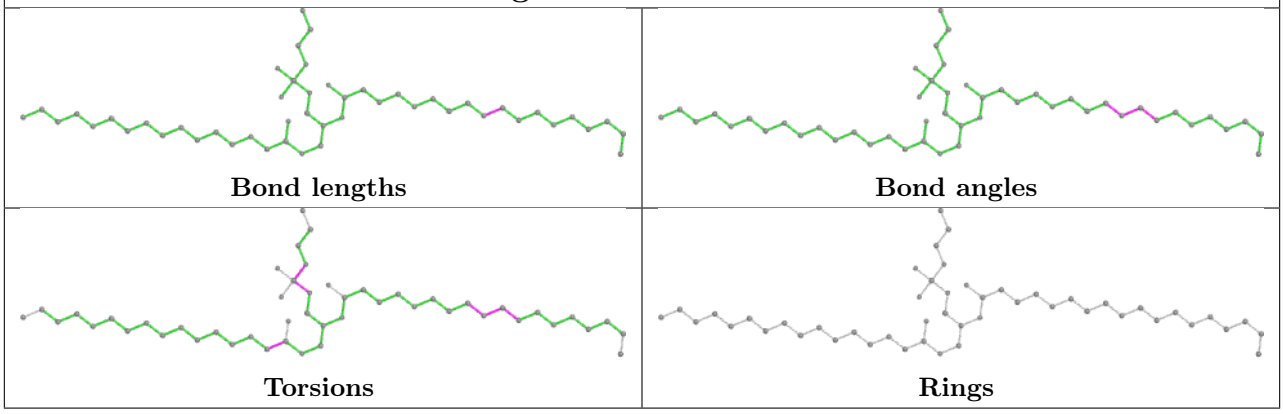
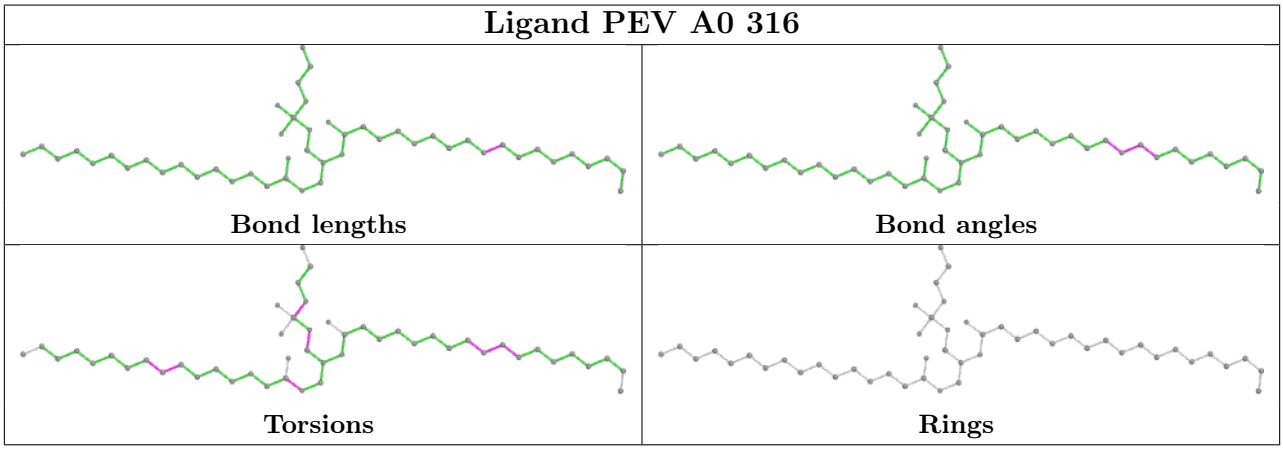


Ligand PEV A0 316



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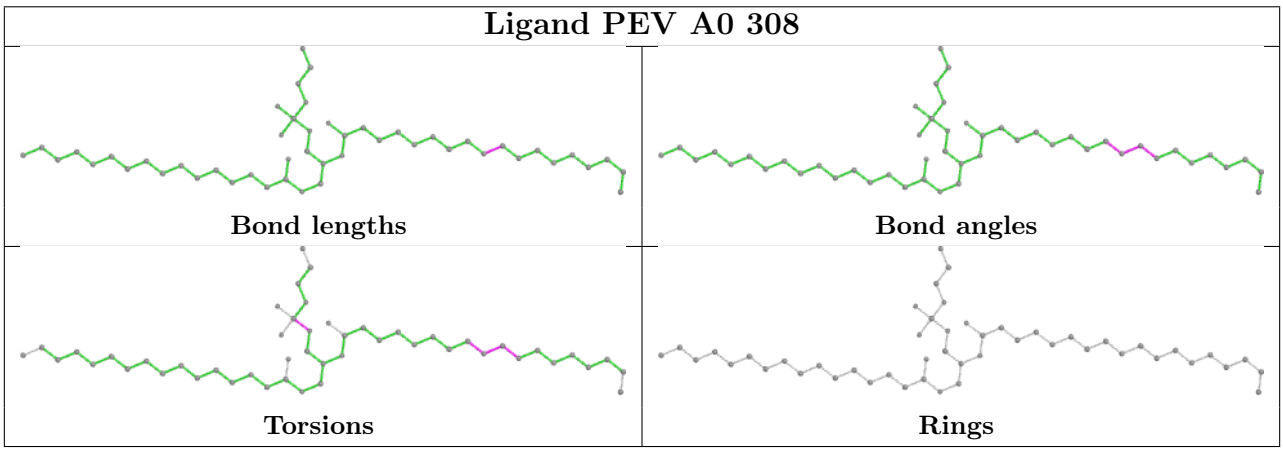

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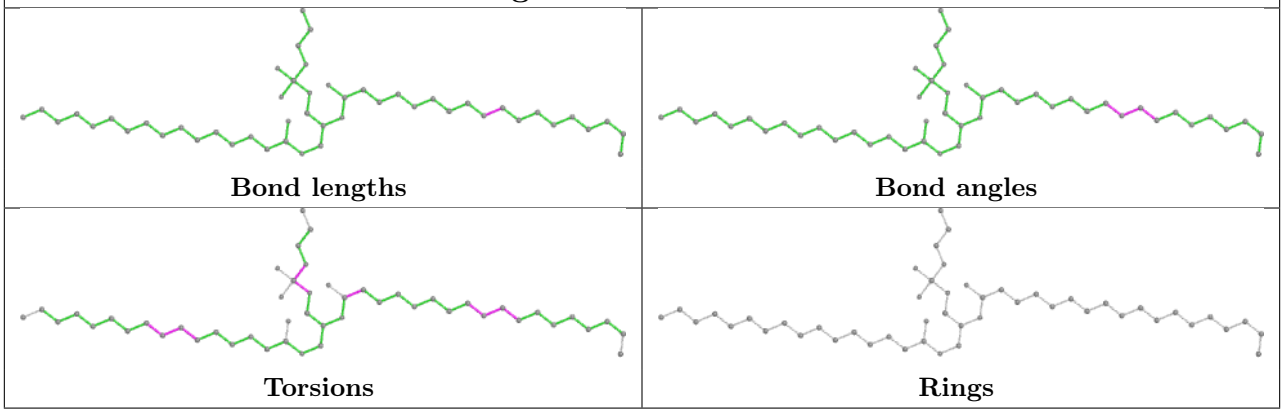
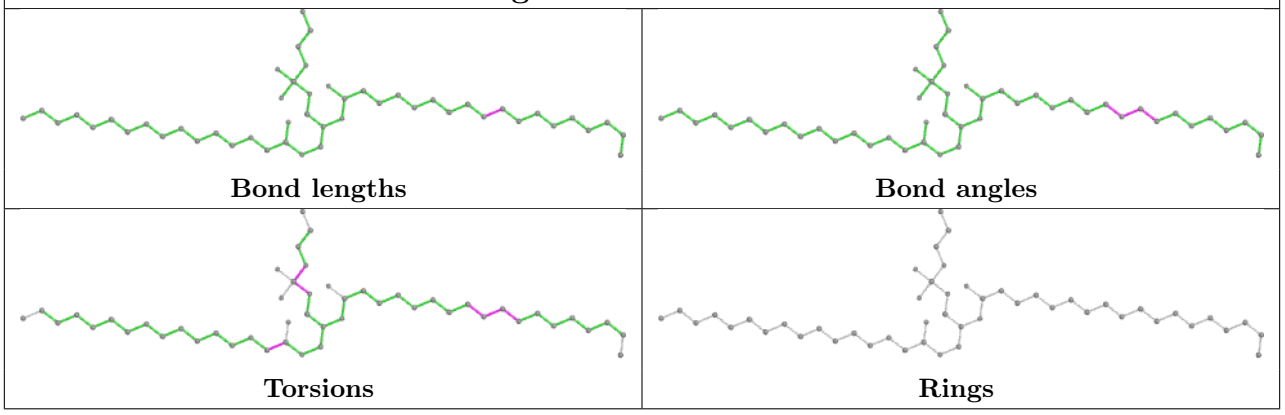
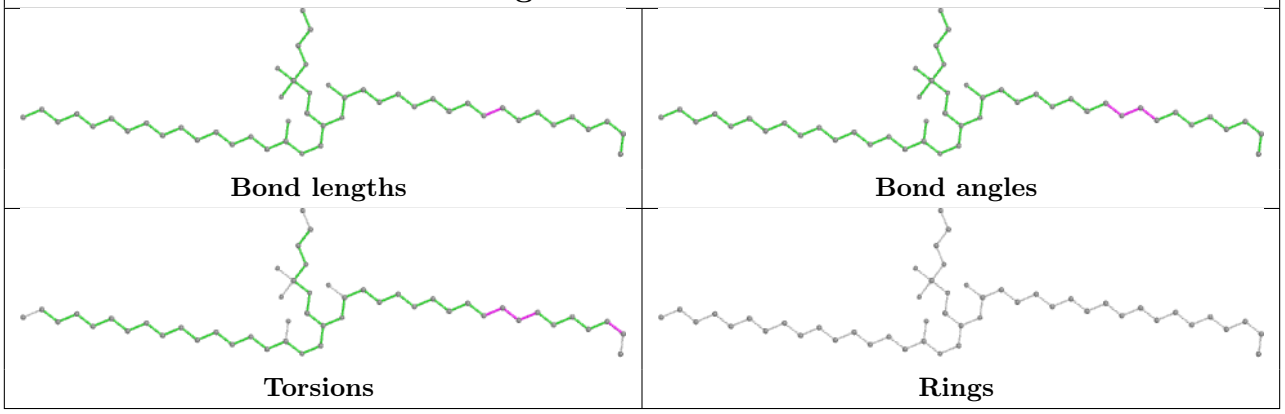


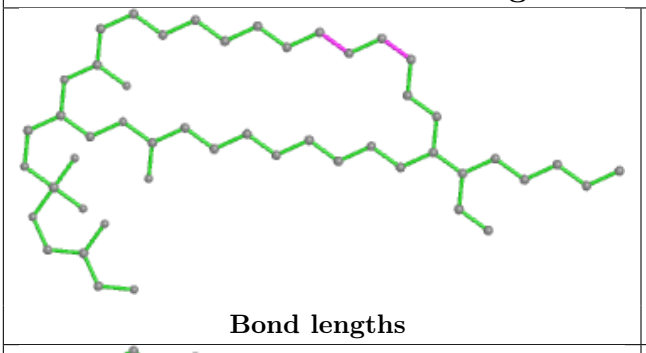
Ligand PEV BA 538



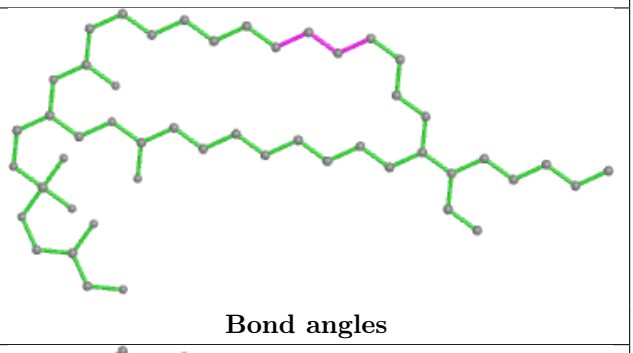
Ligand PEV A1 326



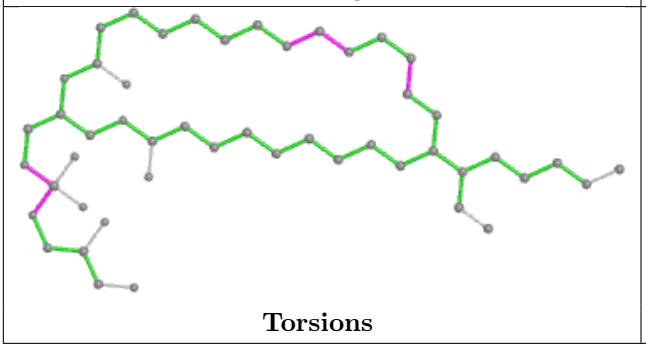
Ligand PGV BB 205



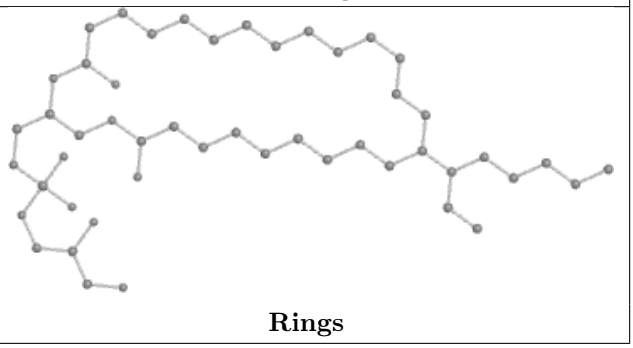
Bond lengths



Bond angles

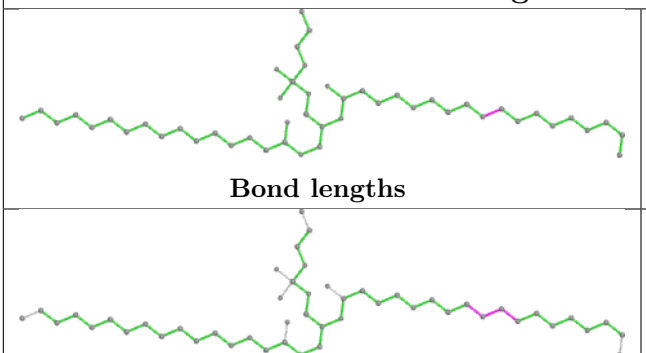


Torsions



Rings

Ligand PEV BB 202



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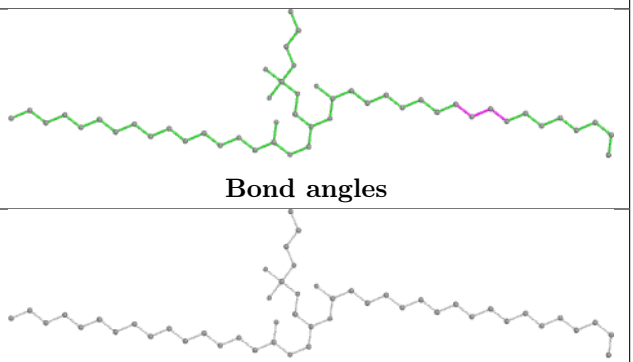
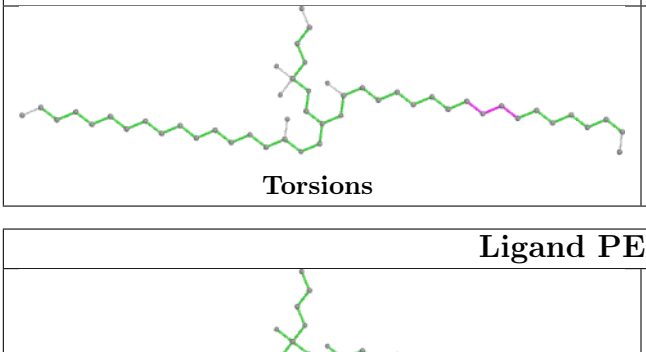
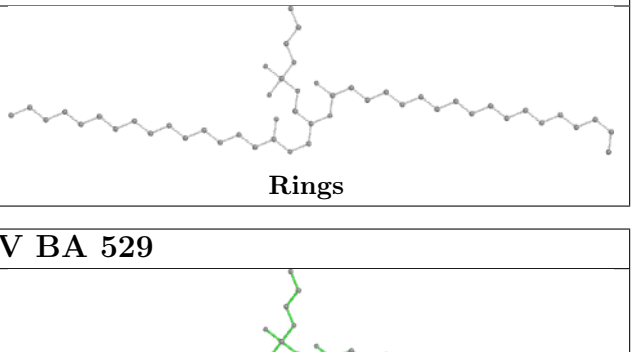


Bond angles

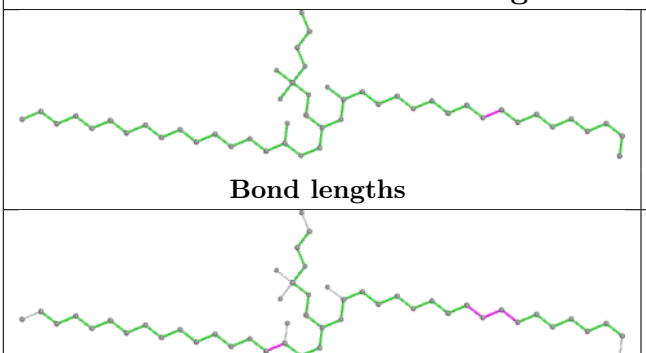


Torsions

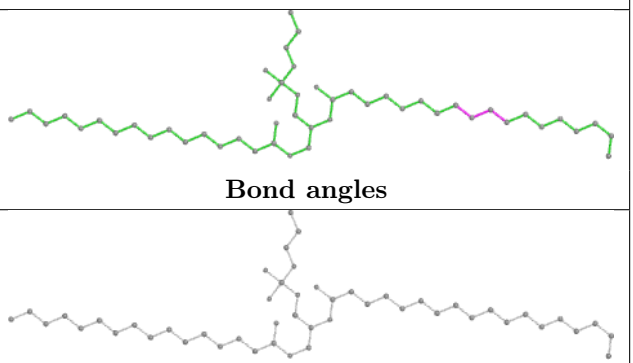


Rings

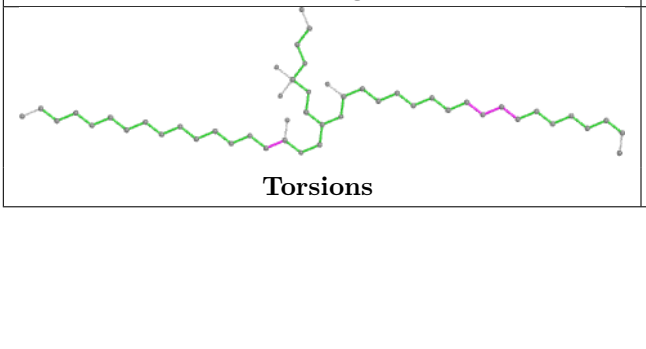
Ligand PEV BA 529



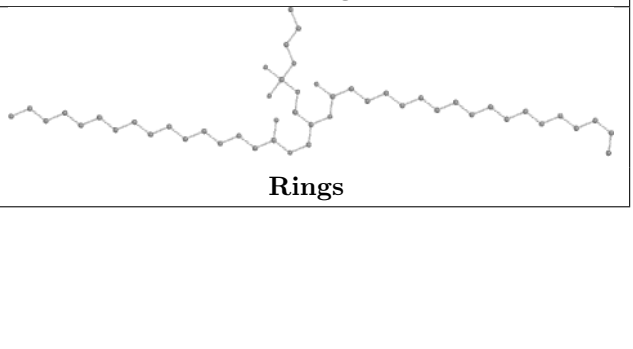
Bond lengths



Bond angles

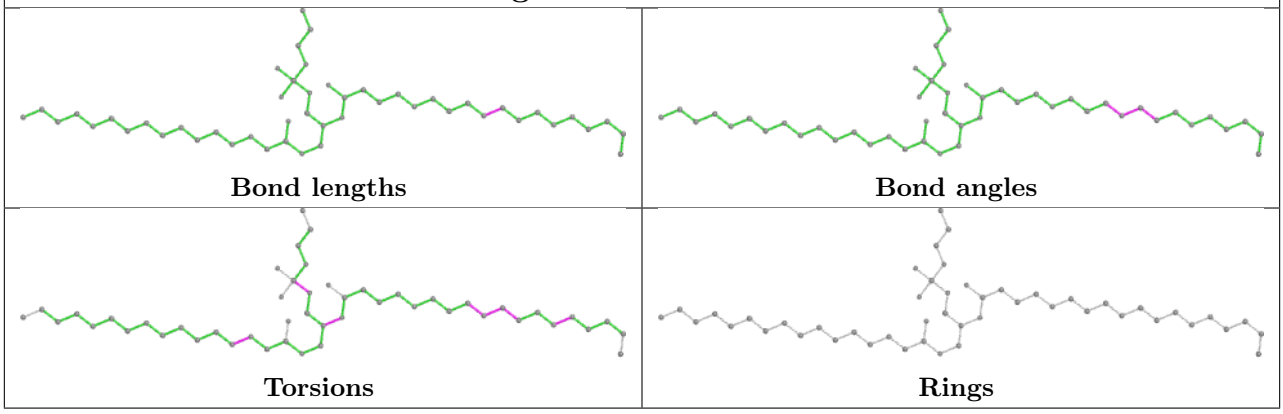


Torsions

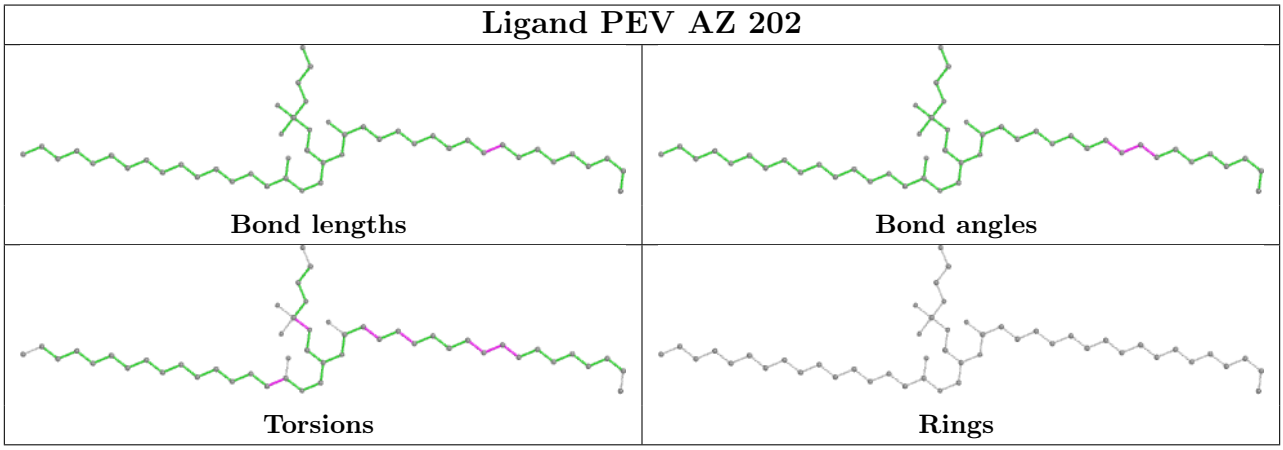


Rings

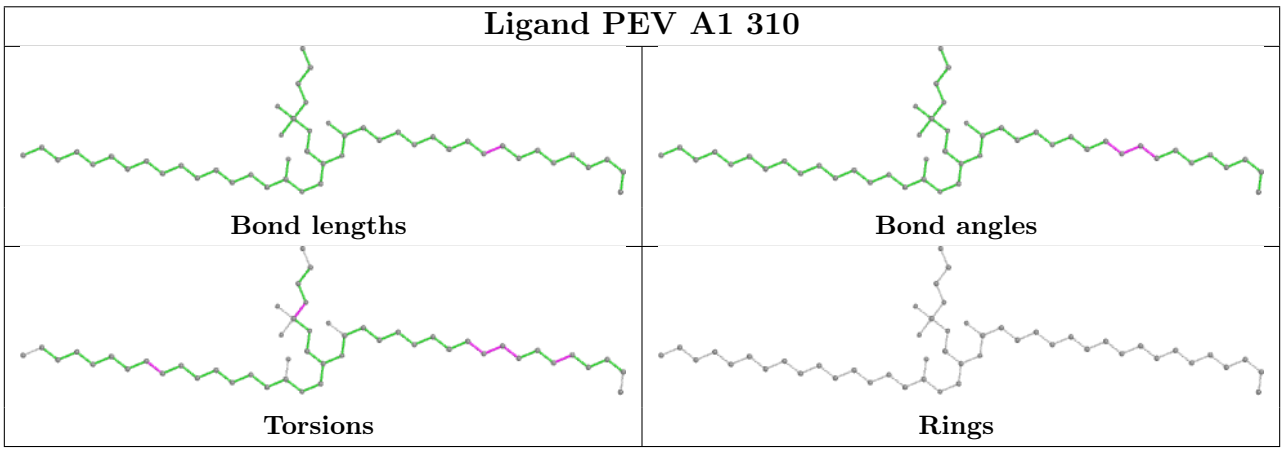
Ligand PEV BA 523



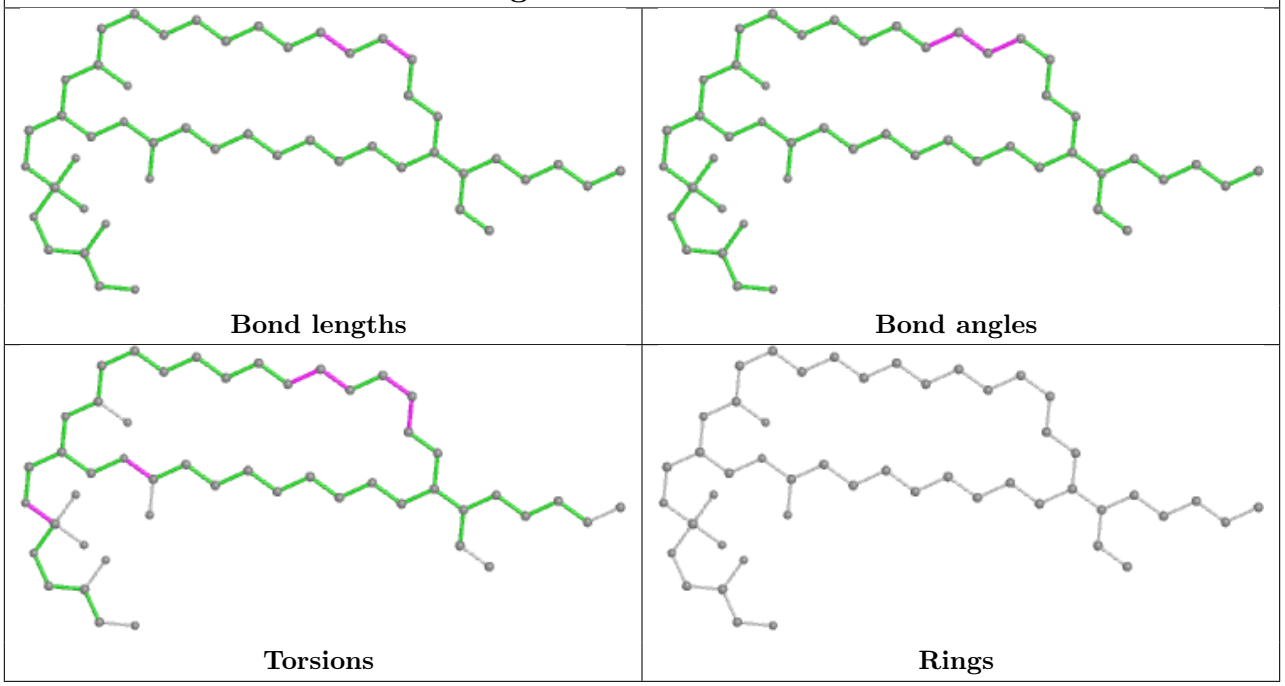
Ligand PEV AZ 202



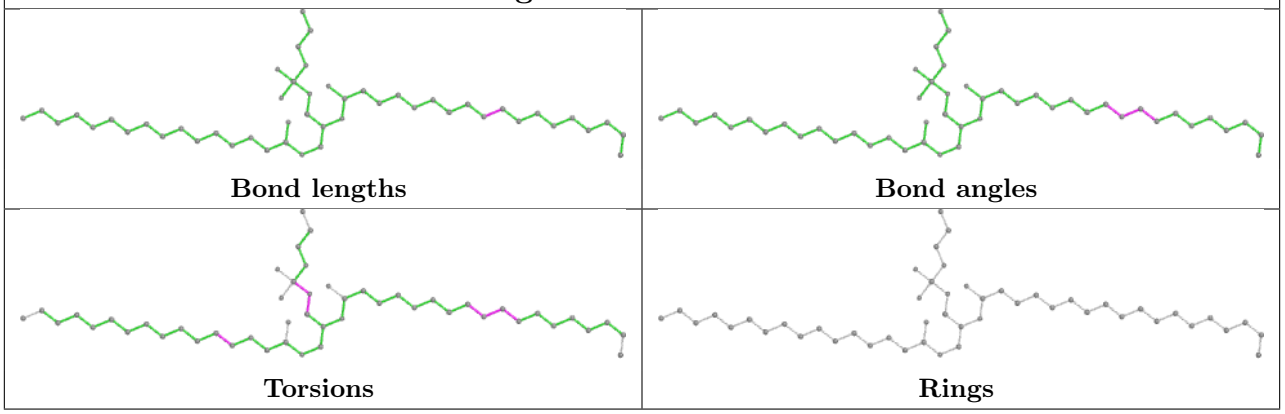
Ligand PEV A1 310



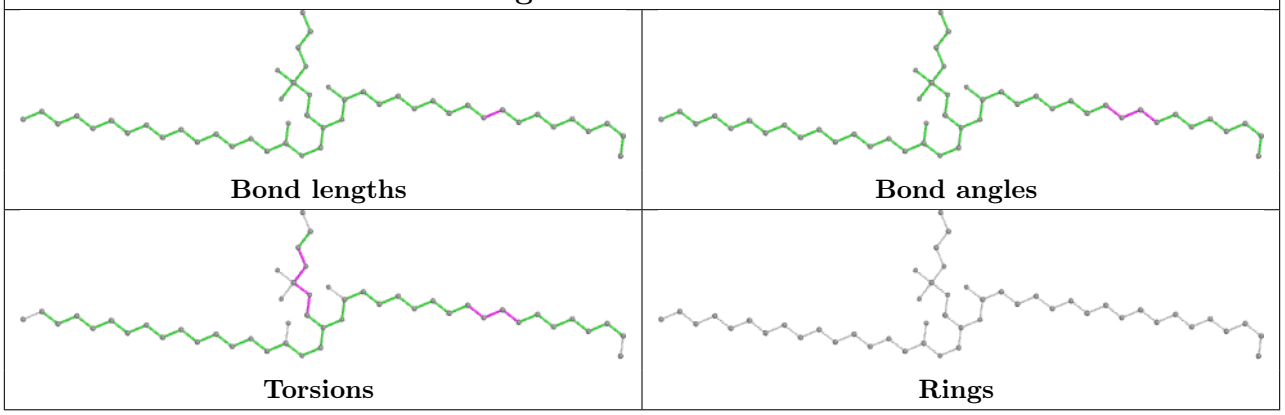
Ligand PGV BB 203



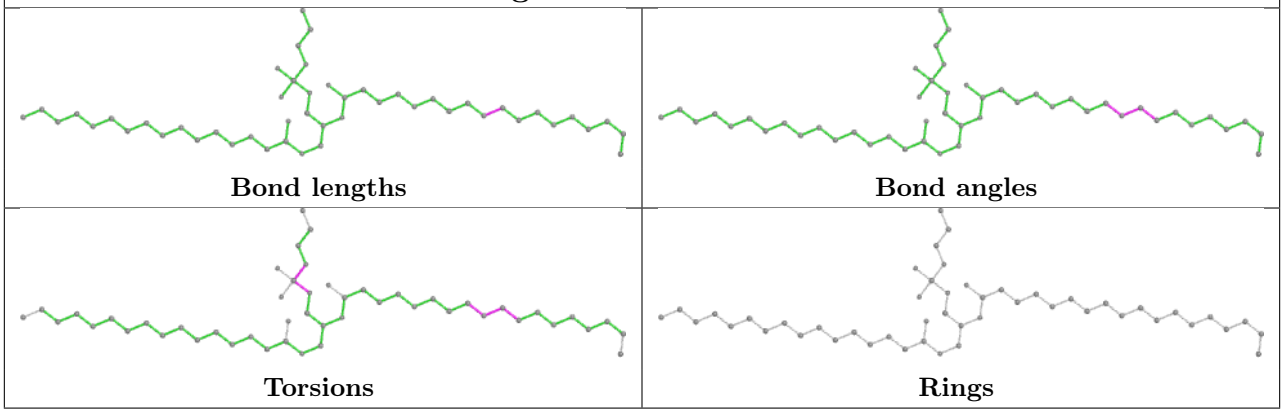
Ligand PEV A0 323



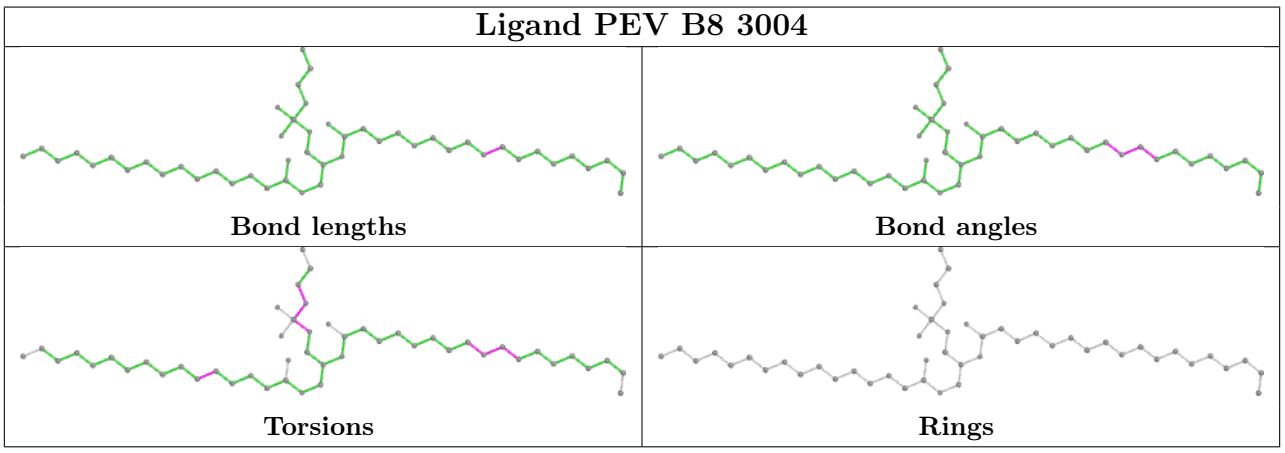
Ligand PEV A0 326



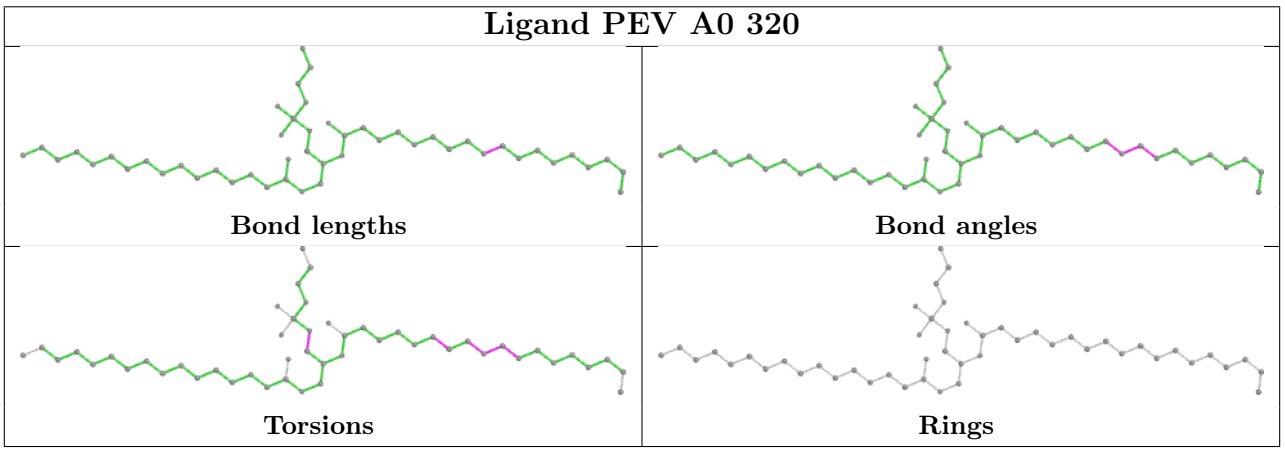
Ligand PEV BA 527



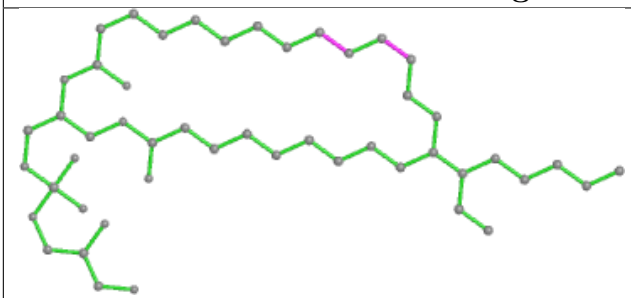
Ligand PEV B8 3004



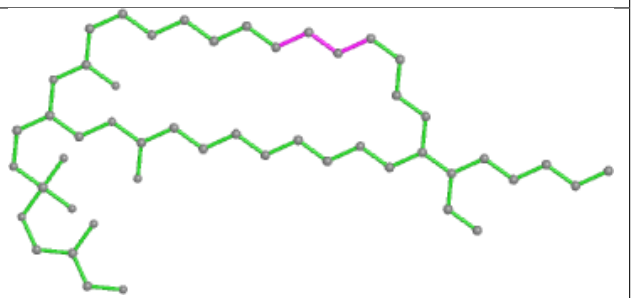
Ligand PEV A0 320



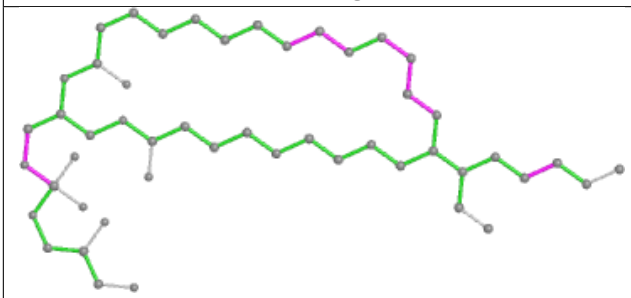
Ligand PGV A0 318



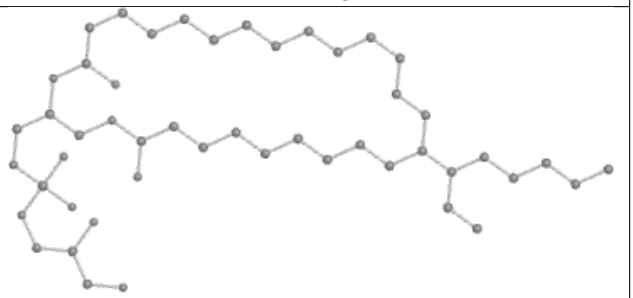
Bond lengths



Bond angles

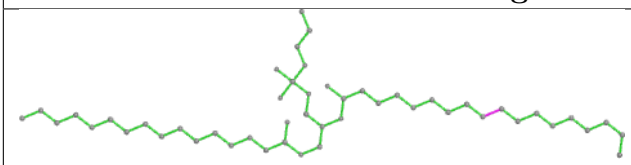


Torsions

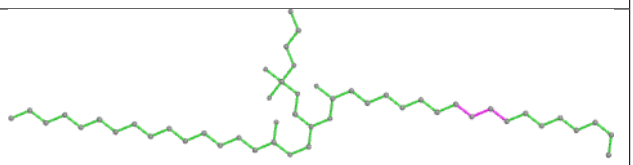


Rings

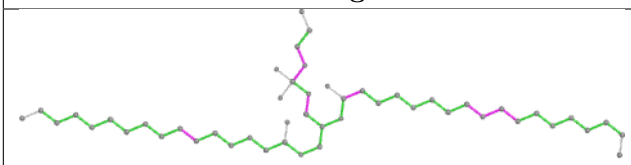
Ligand PEV BA 530



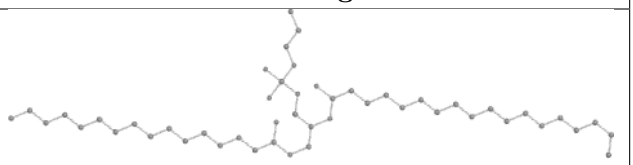
Bond lengths



Bond angles

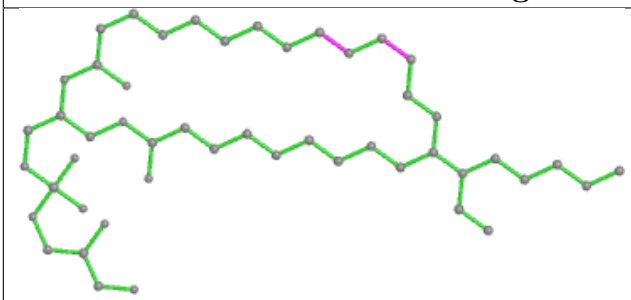


Torsions

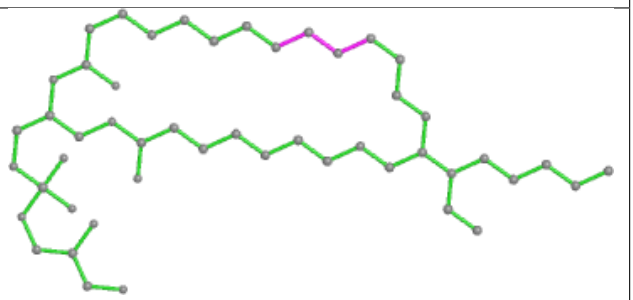


Rings

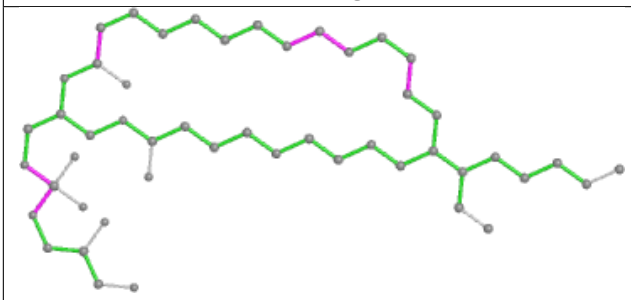
Ligand PGV A0 328



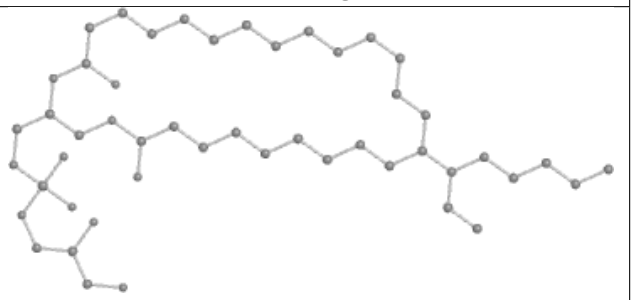
Bond lengths



Bond angles

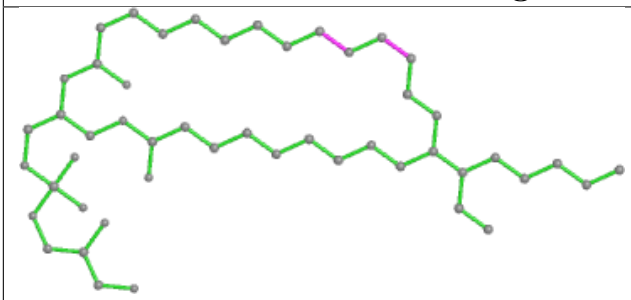


Torsions

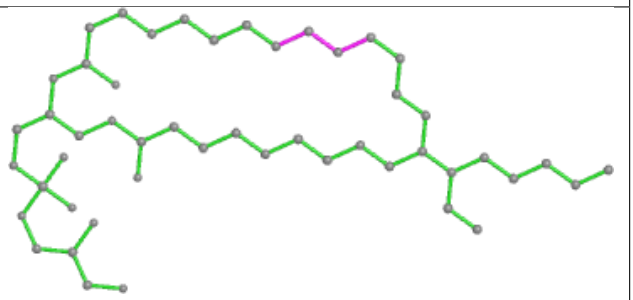


Rings

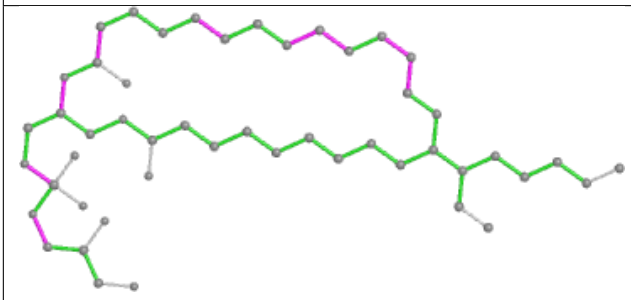
Ligand PGV A1 318



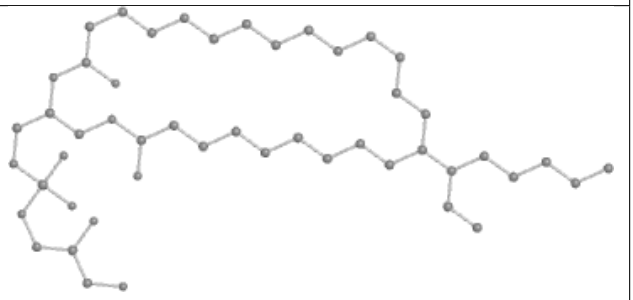
Bond lengths



Bond angles

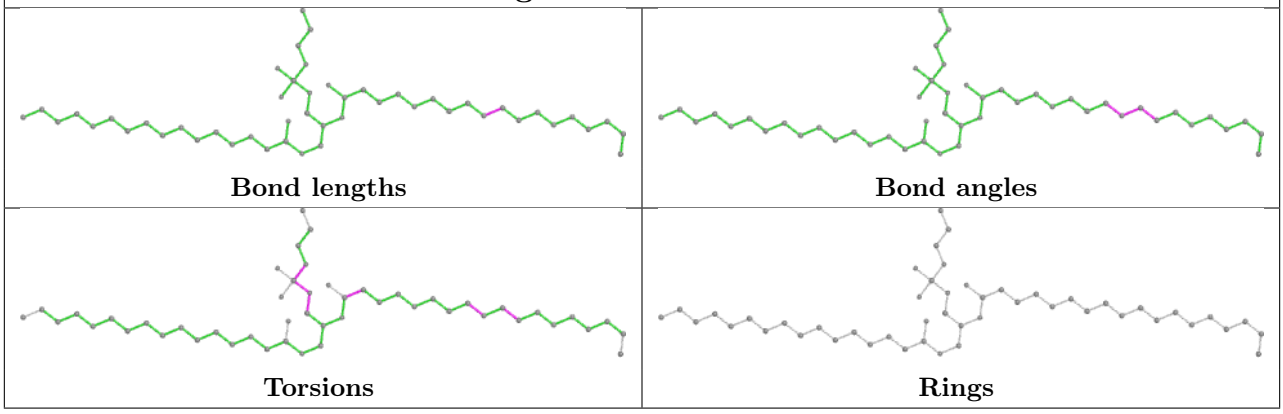


Torsions

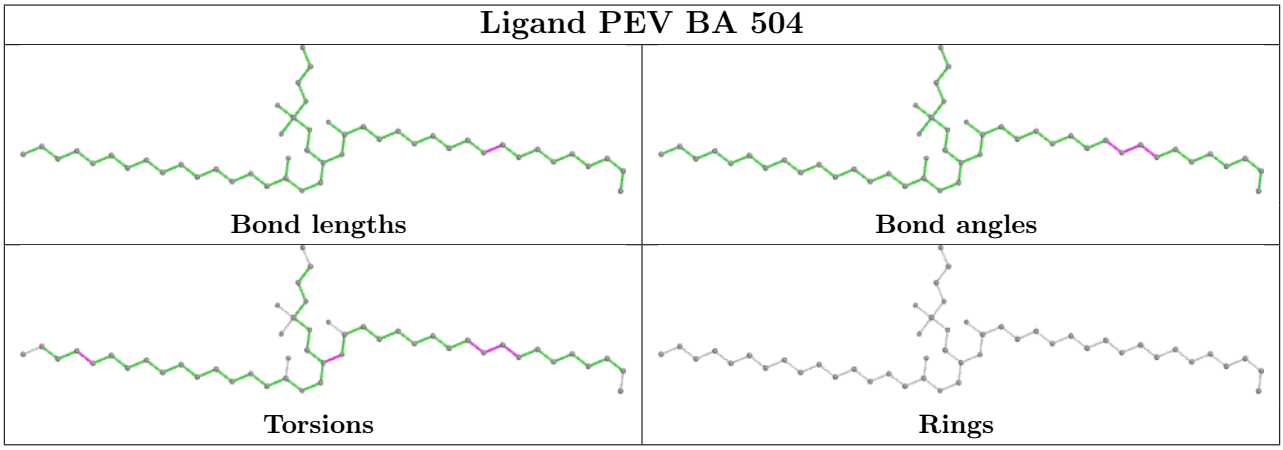


Rings

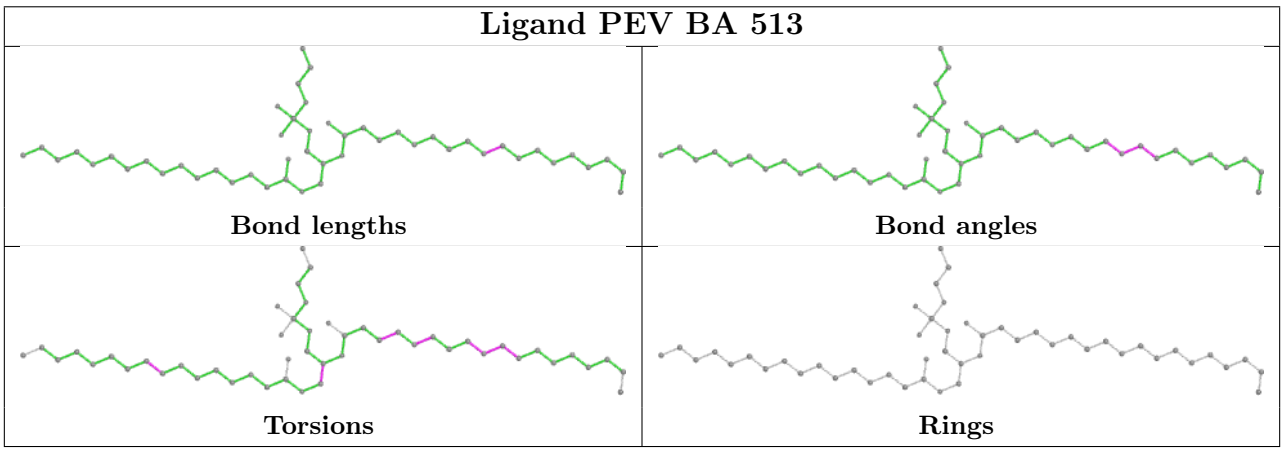
Ligand PEV A0 312



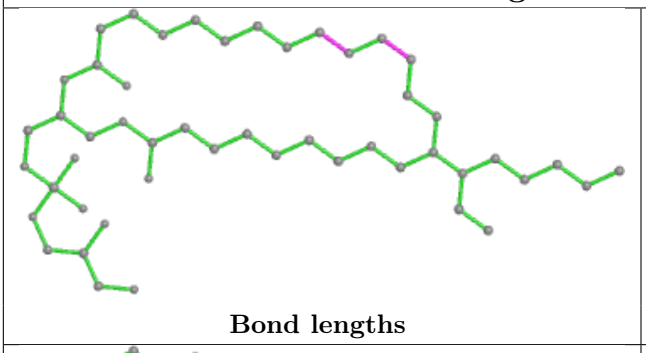
Ligand PEV BA 504



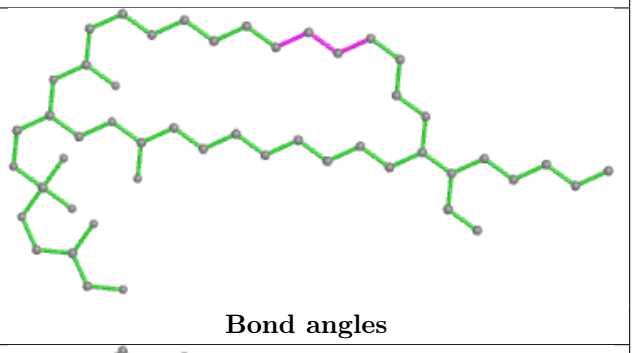
Ligand PEV BA 513



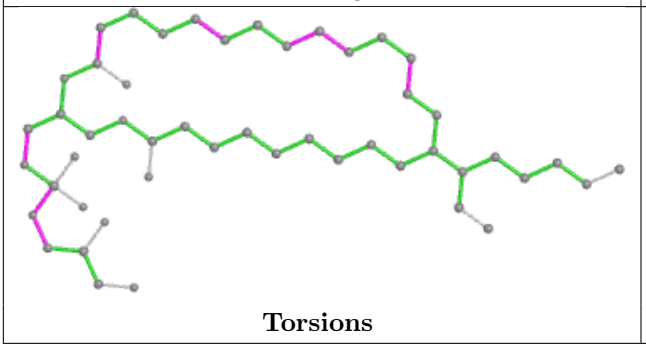
Ligand PGV BA 512



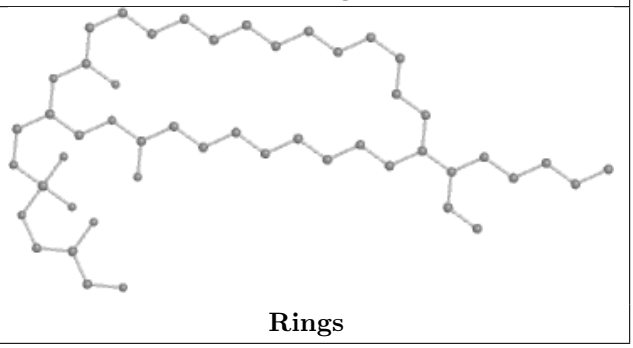
Bond lengths



Bond angles

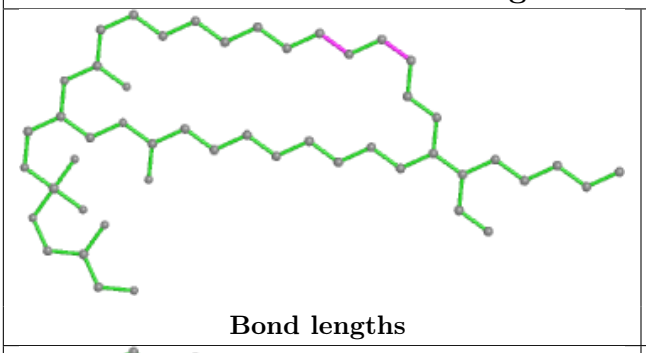


Torsions

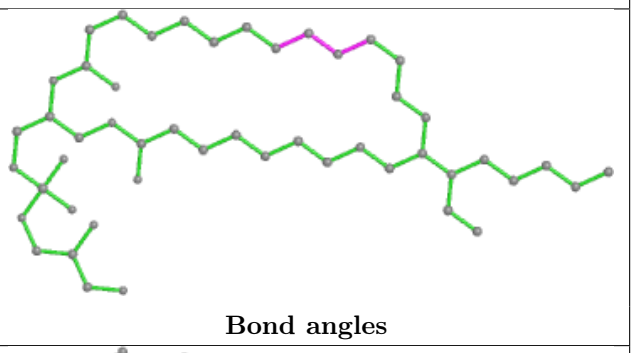


Rings

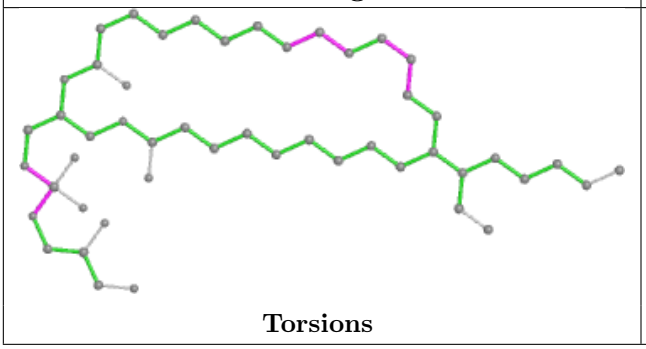
Ligand PGV BB 213



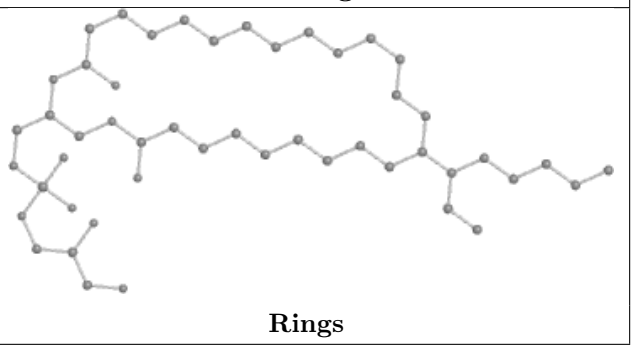
Bond lengths



Bond angles

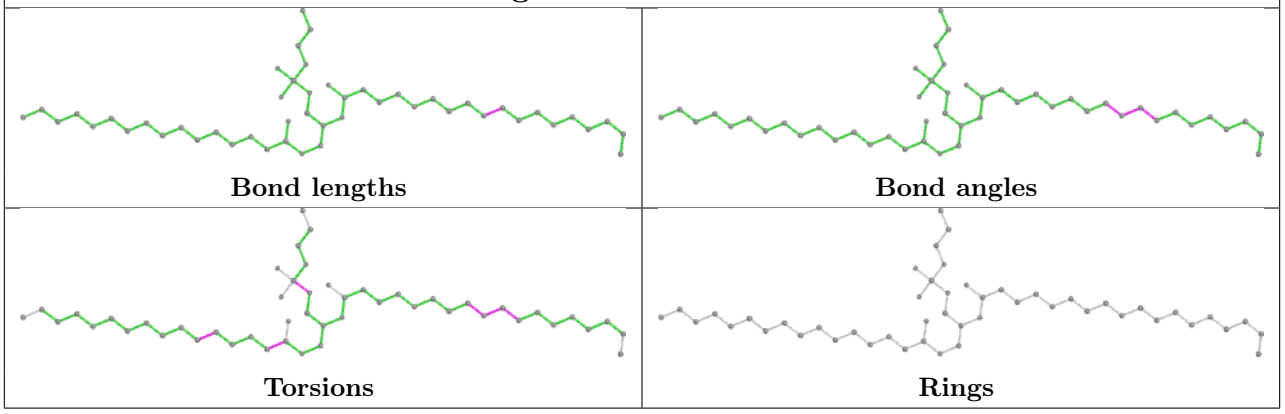


Torsions

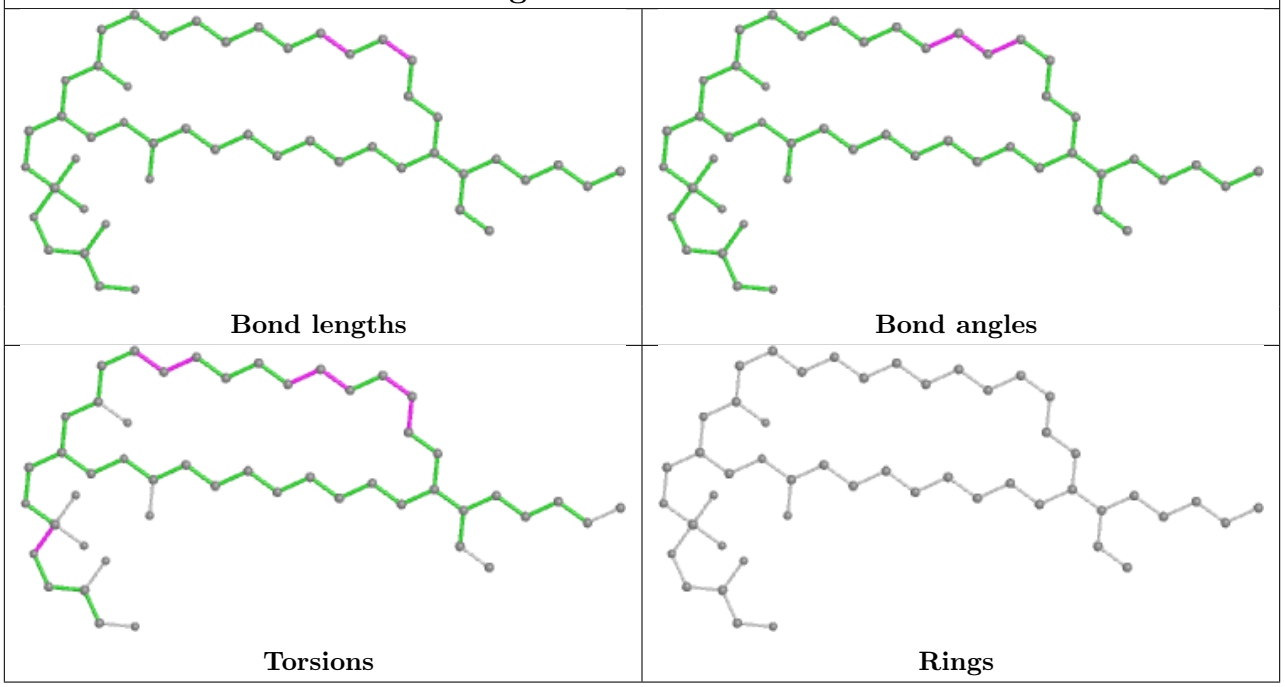


Rings

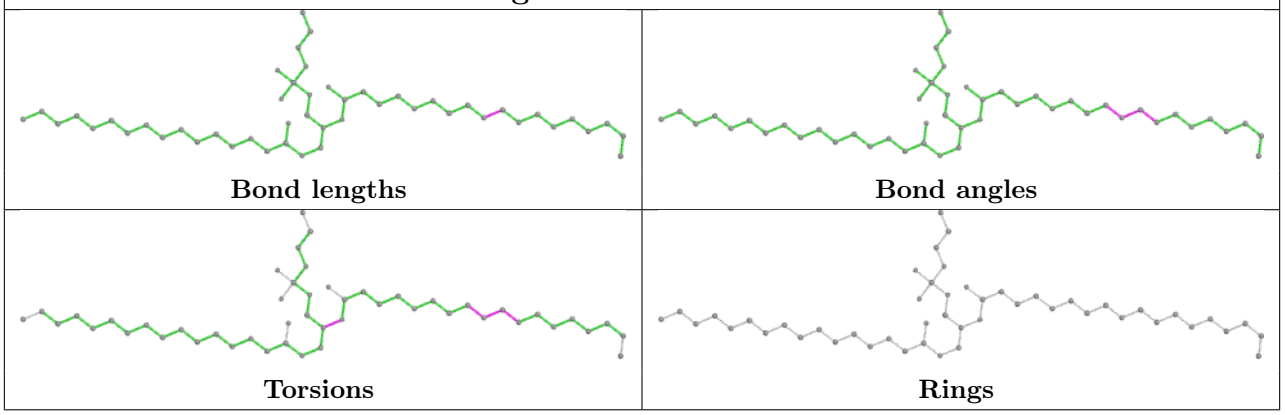
Ligand PEV BA 535



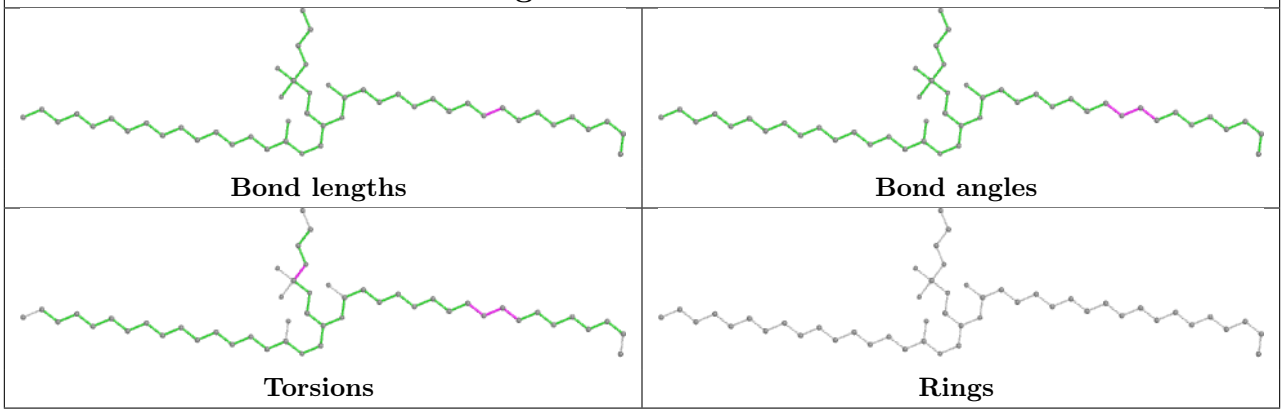
Ligand PGV BA 536



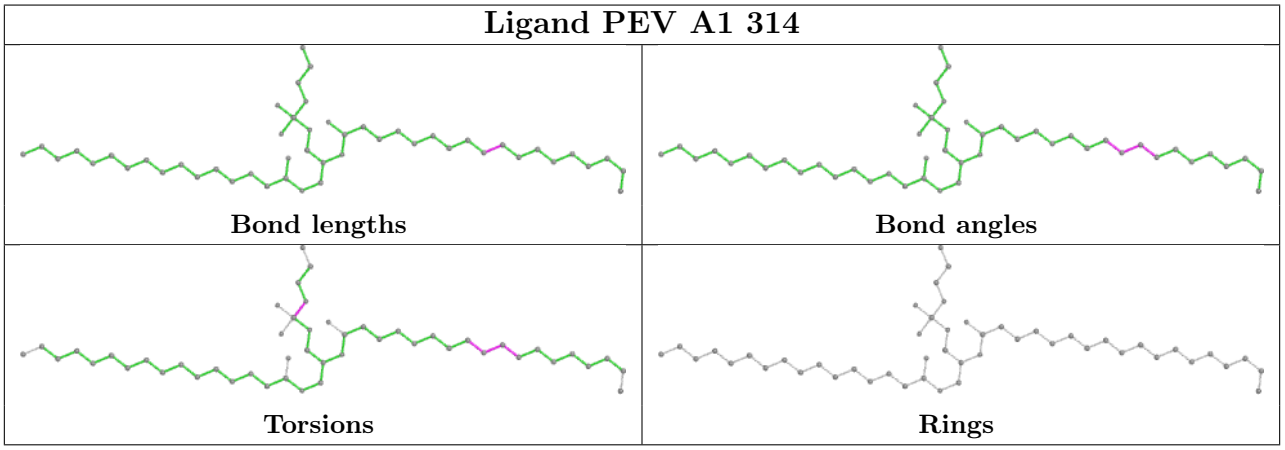
Ligand PEV BA 539



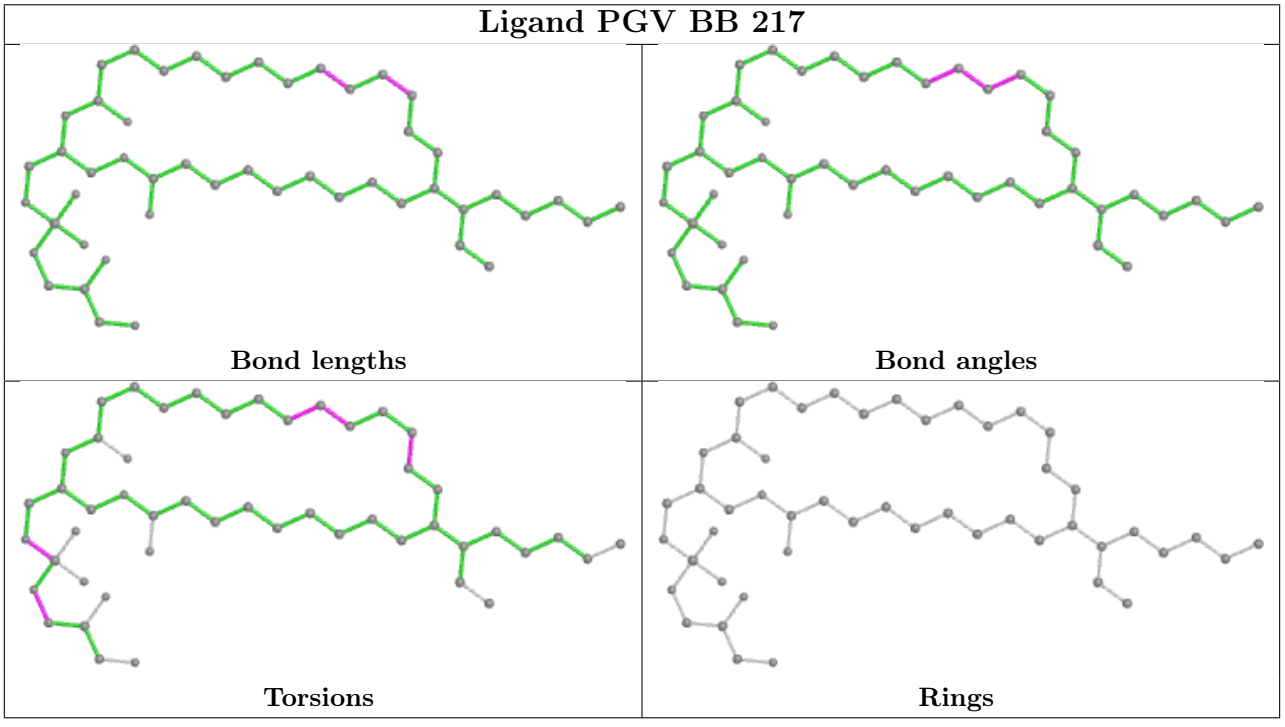
Ligand PEV A1 312



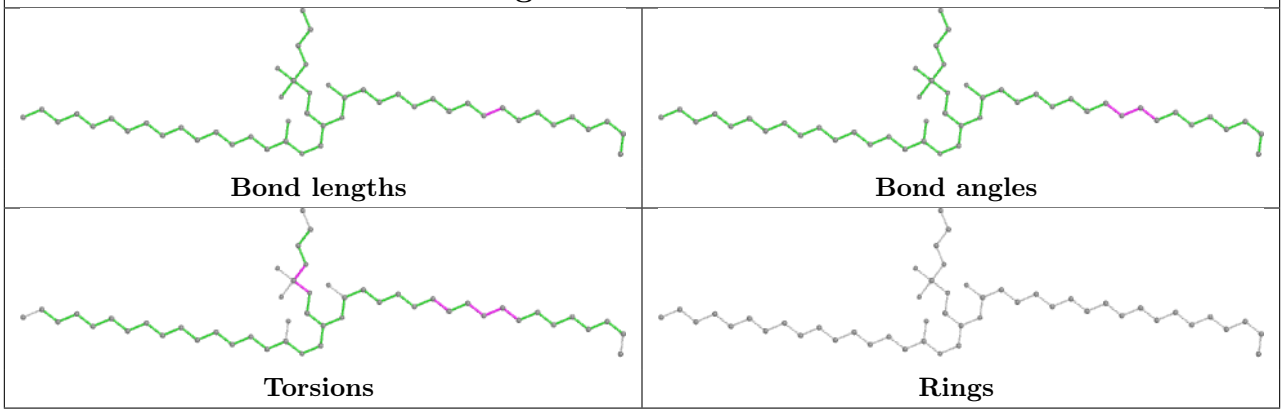
Ligand PEV A1 314



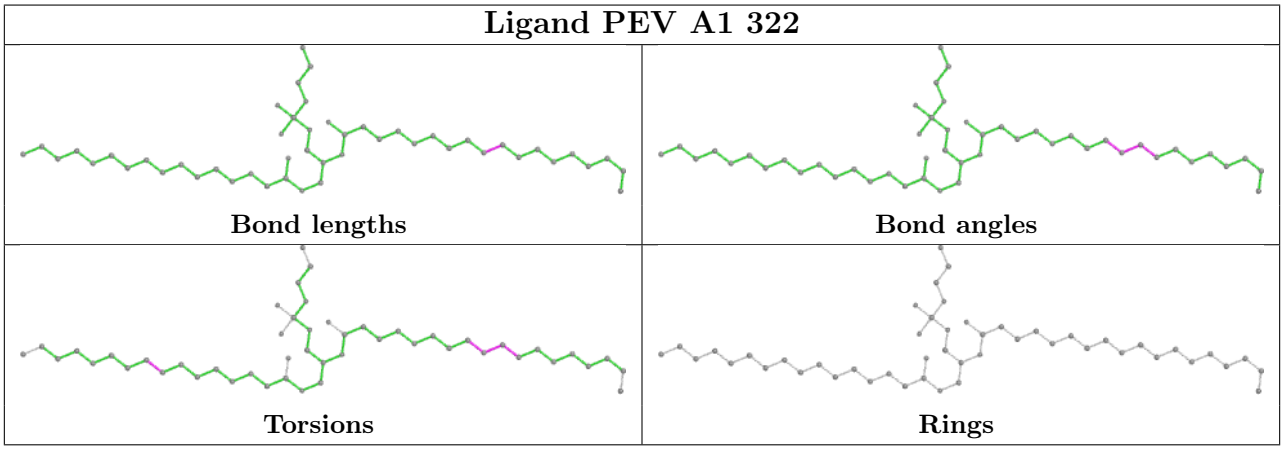
Ligand PGV BB 217



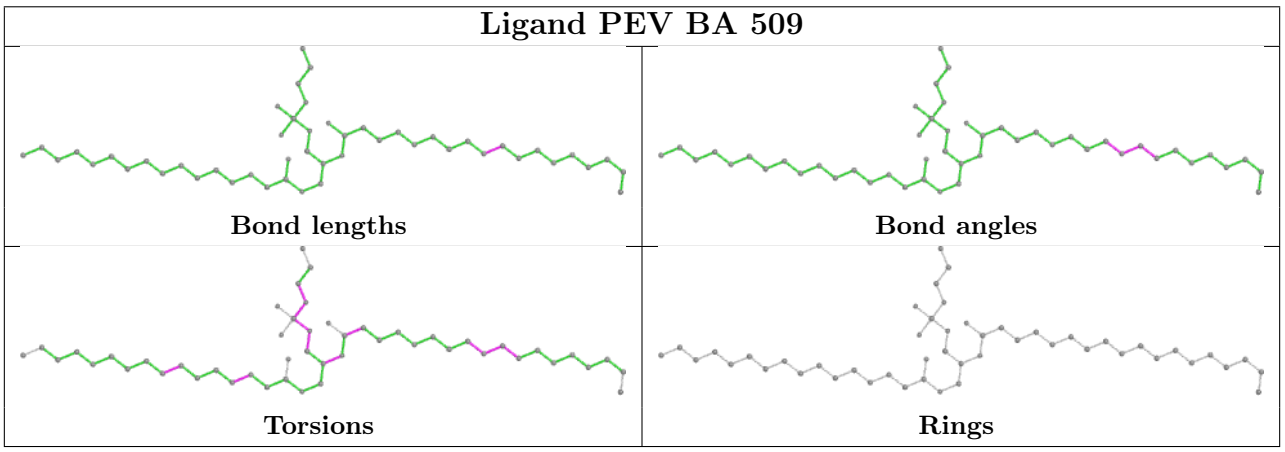
Ligand PEV A1 327



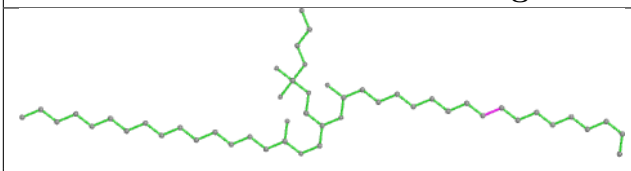
Ligand PEV A1 322



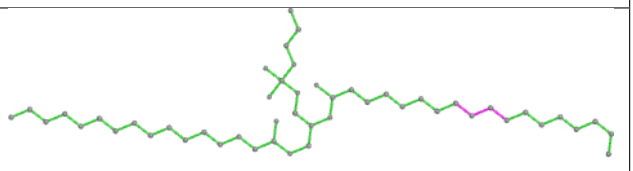
Ligand PEV BA 509



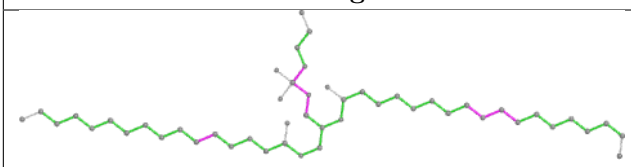
Ligand PEV BB 209



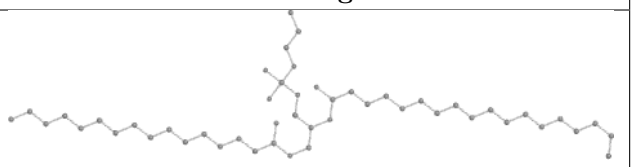
Bond lengths



Bond angles

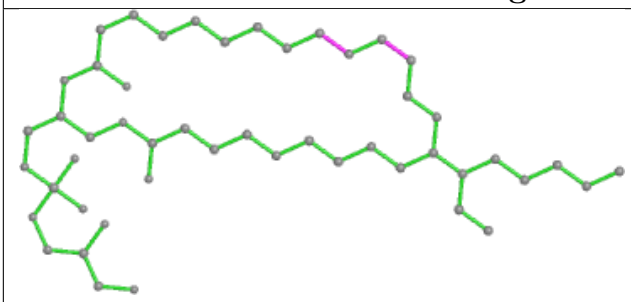


Torsions

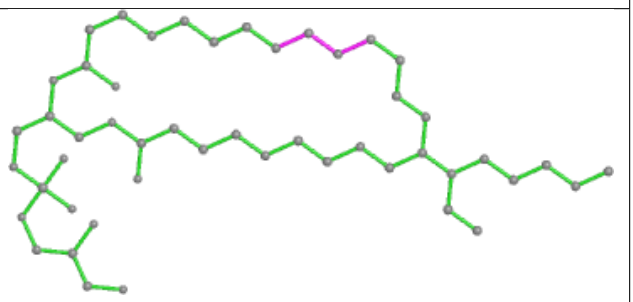


Rings

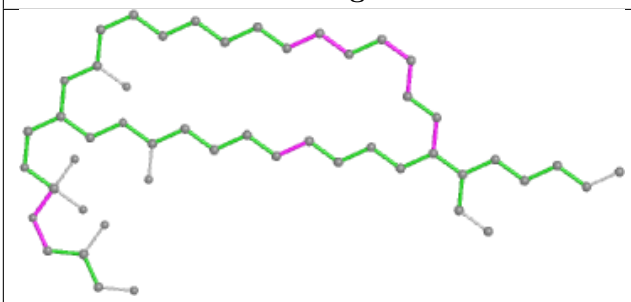
Ligand PGV BB 208



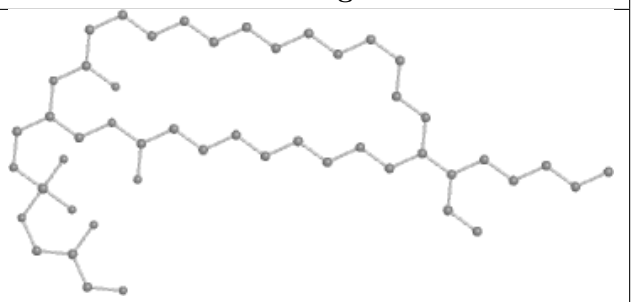
Bond lengths



Bond angles

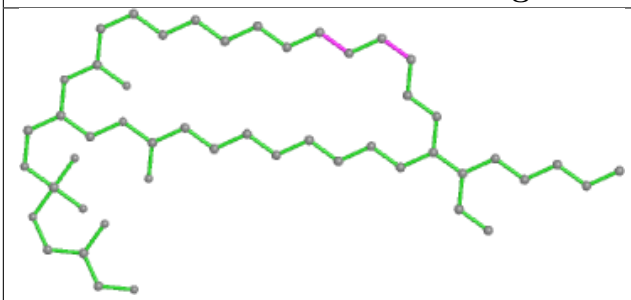


Torsions

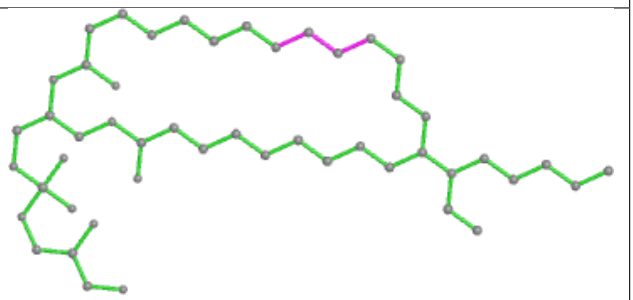


Rings

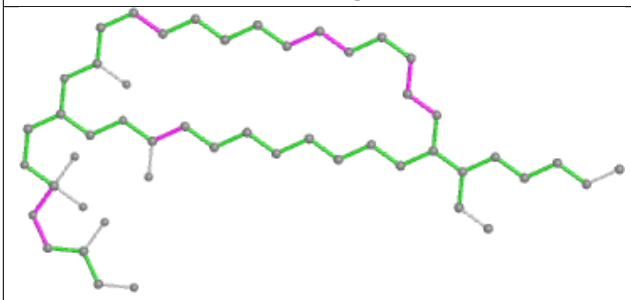
Ligand PGV A0 305



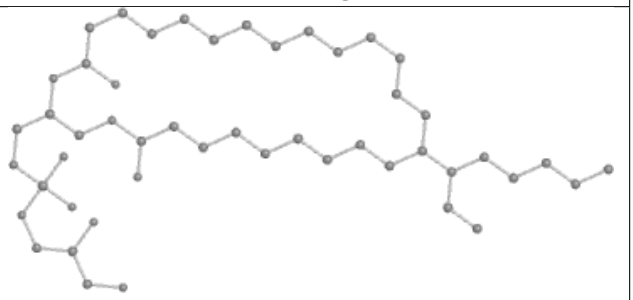
Bond lengths



Bond angles

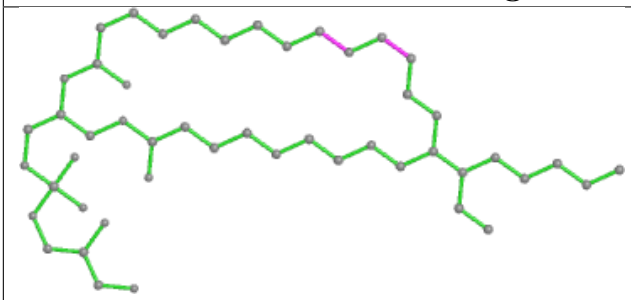


Torsions

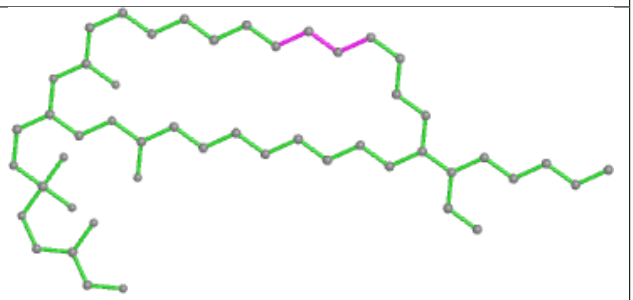


Rings

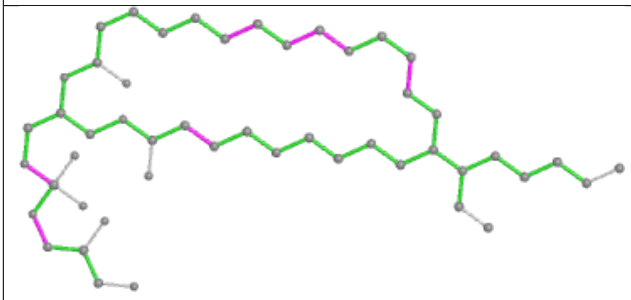
Ligand PGV B8 3005



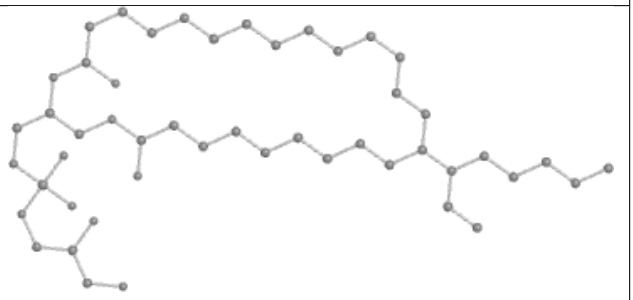
Bond lengths



Bond angles

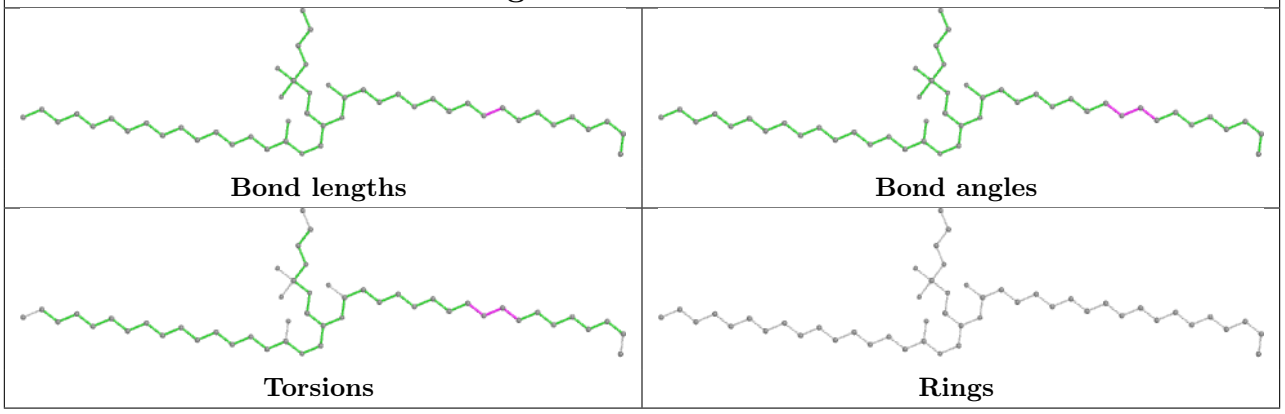


Torsions

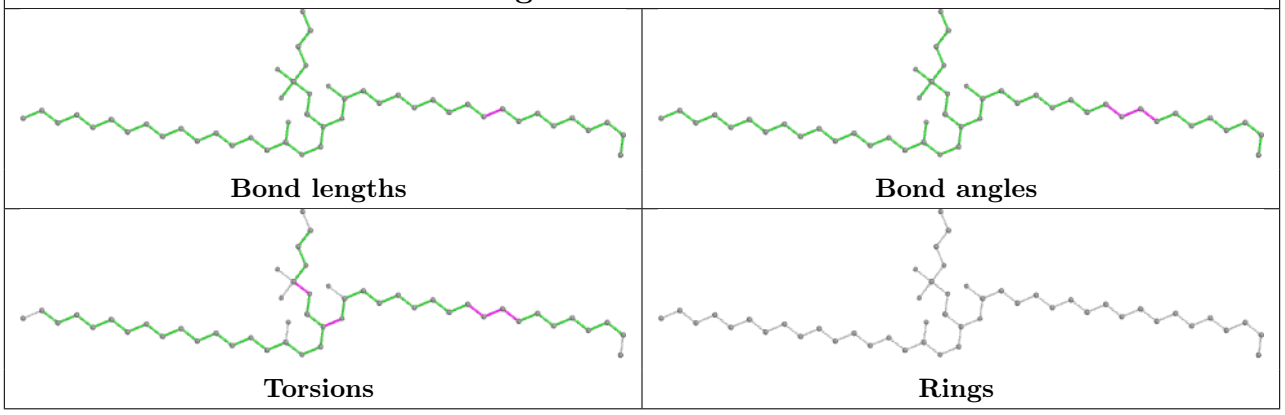


Rings

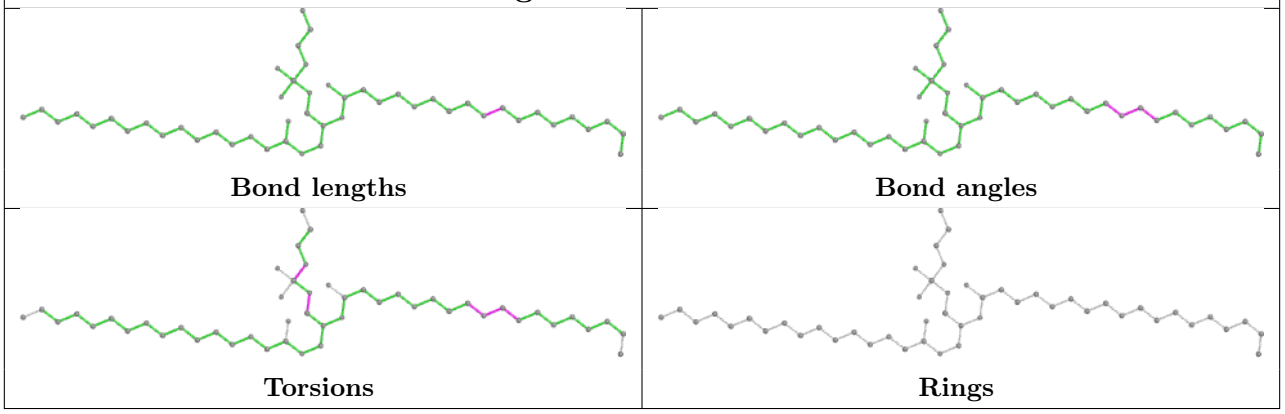
Ligand PEV B8 3007



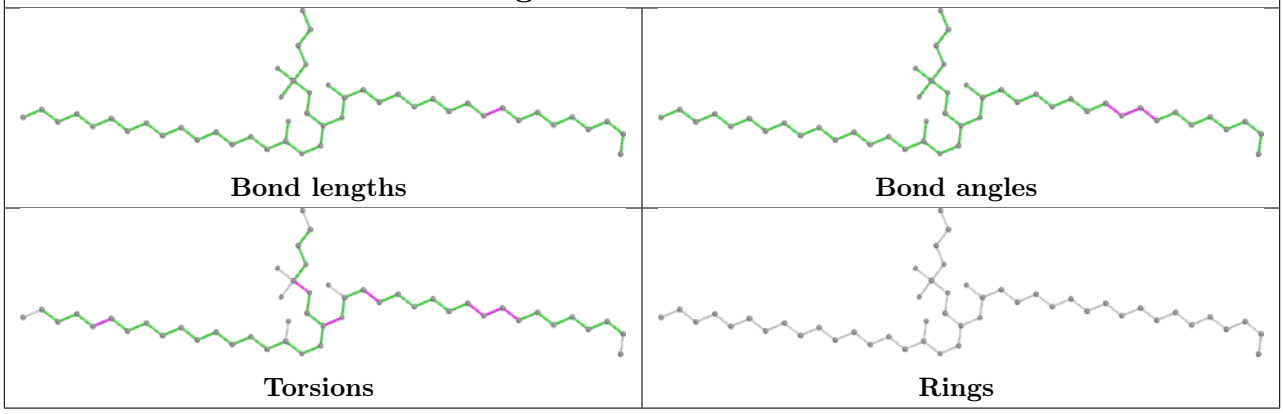
Ligand PEV A0 313



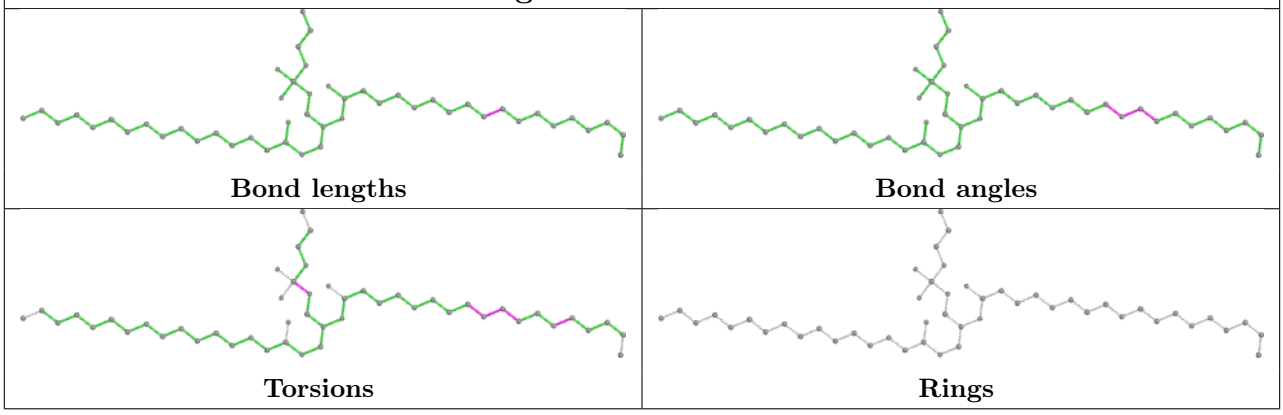
Ligand PEV A1 321



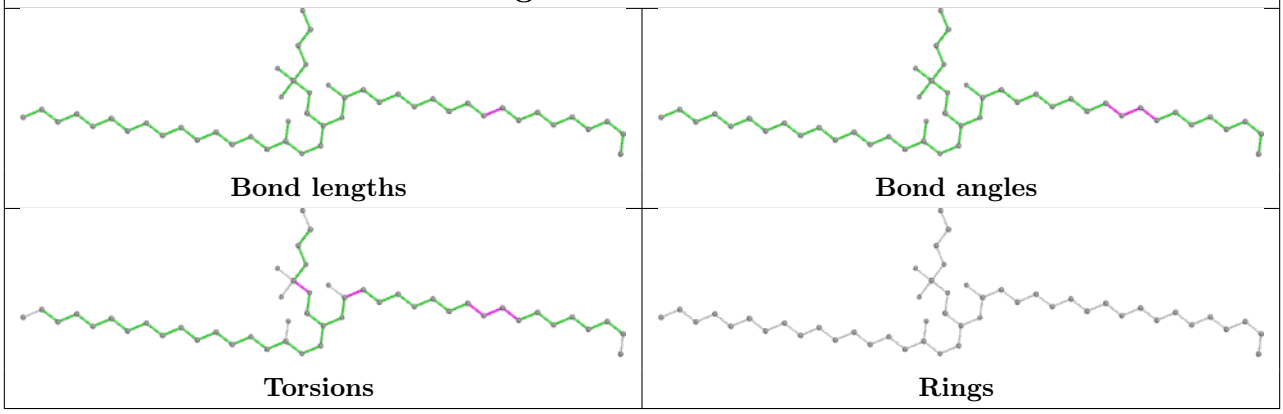
Ligand PEV A0 302



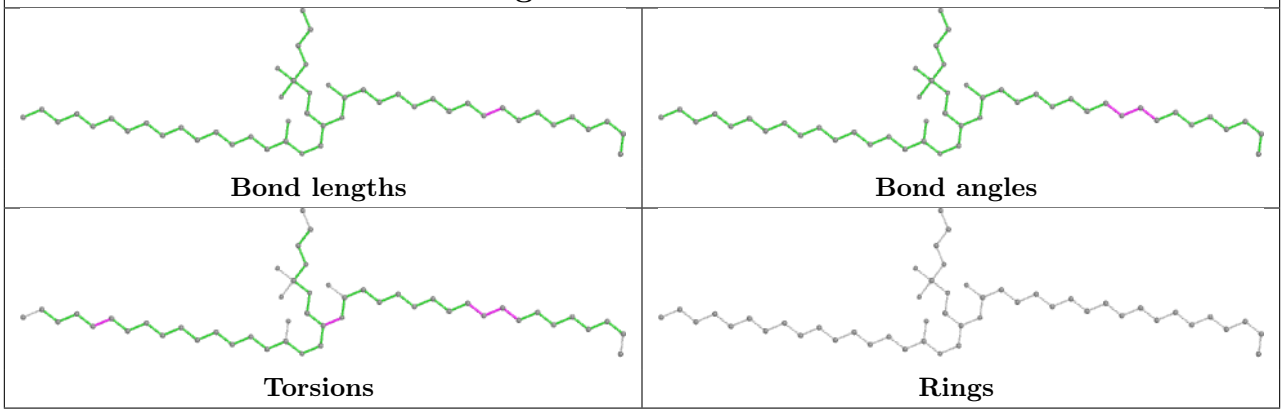
Ligand PEV A1 329



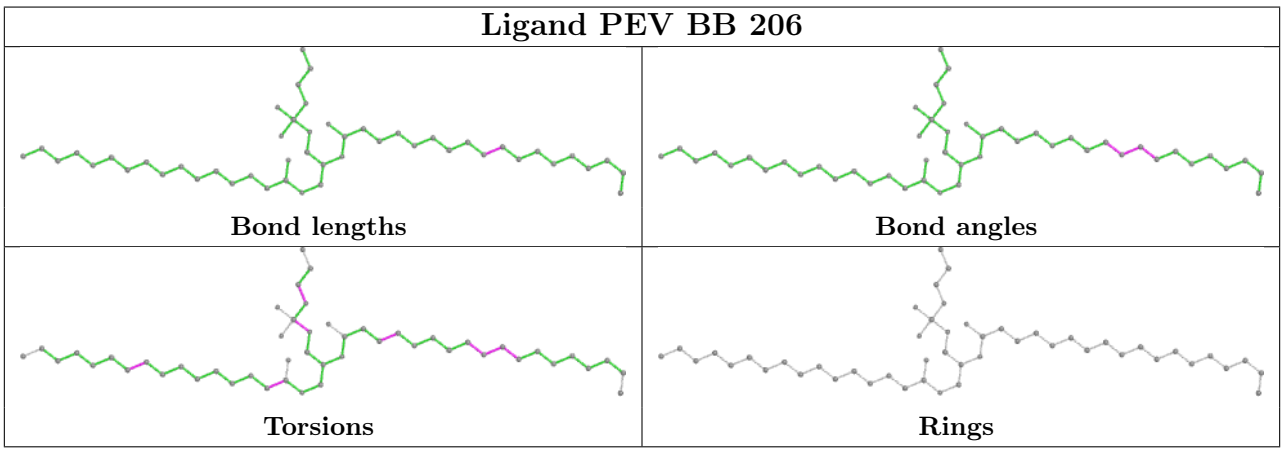
Ligand PEV A1 305



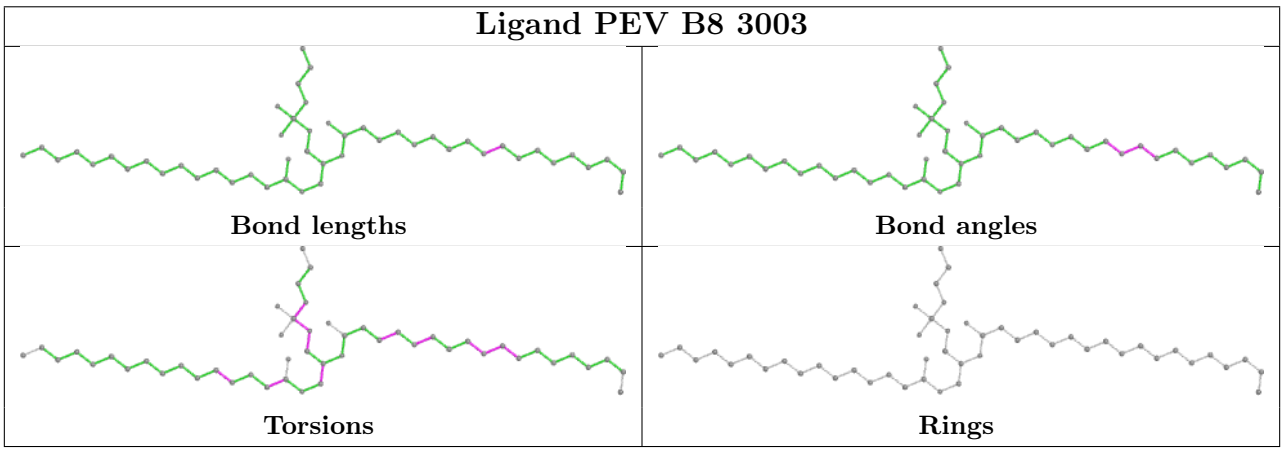
Ligand PEV A0 310



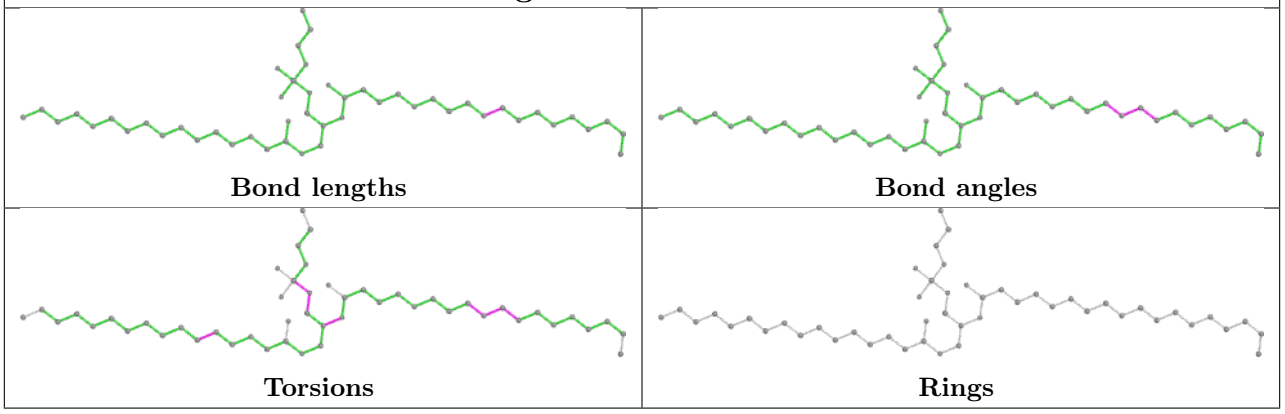
Ligand PEV BB 206



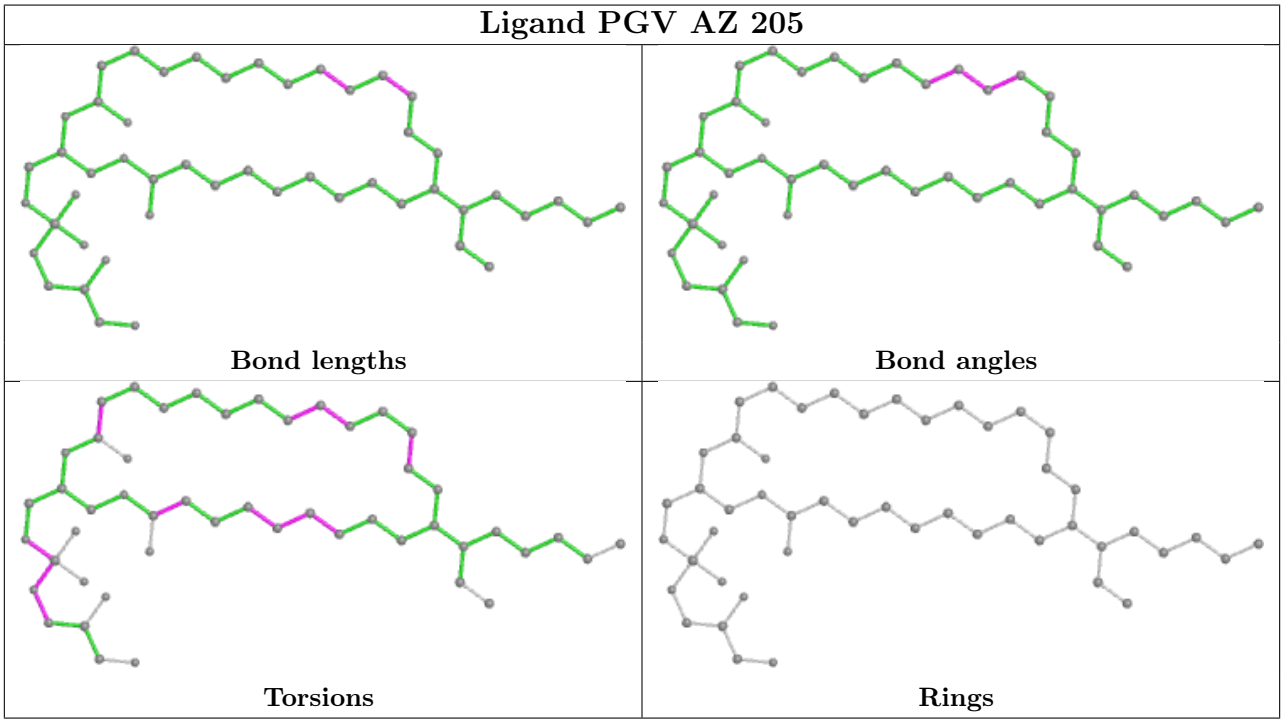
Ligand PEV B8 3003



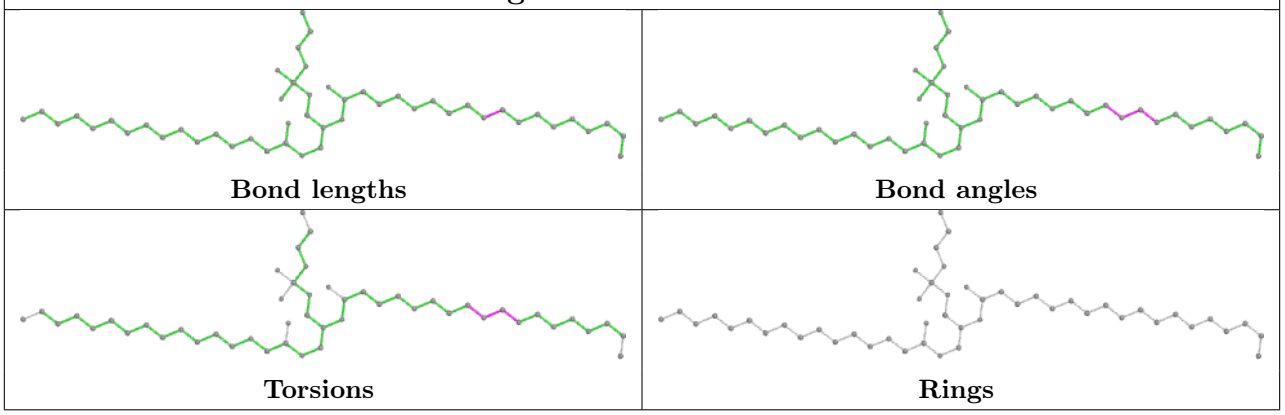
Ligand PEV A0 324



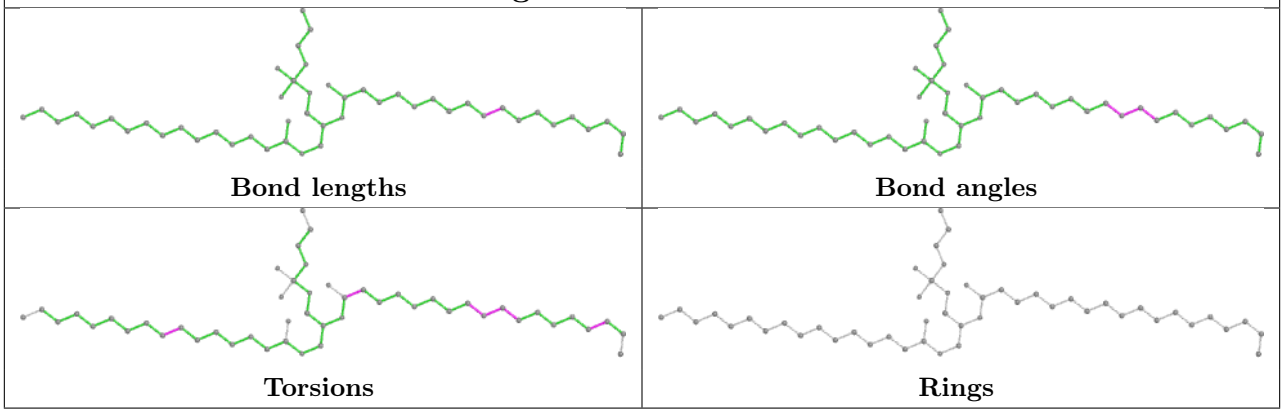
Ligand PGV AZ 205



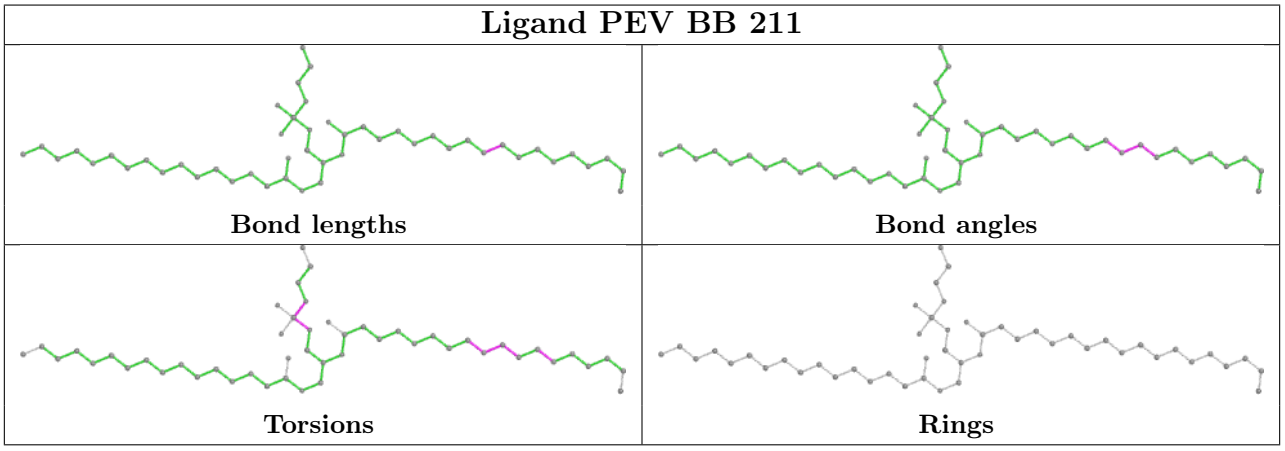
Ligand PEV B8 3001



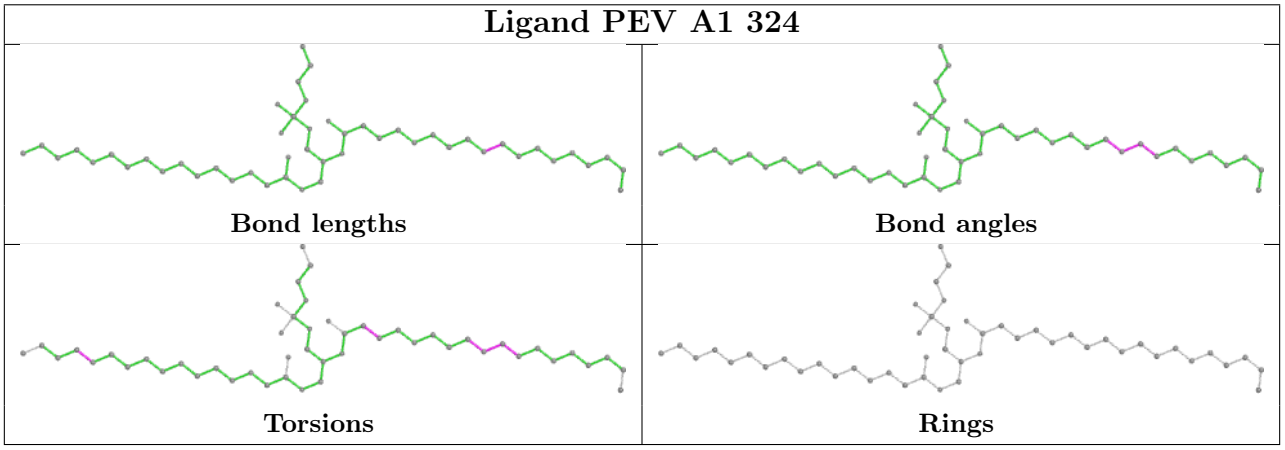
Ligand PEV BB 212



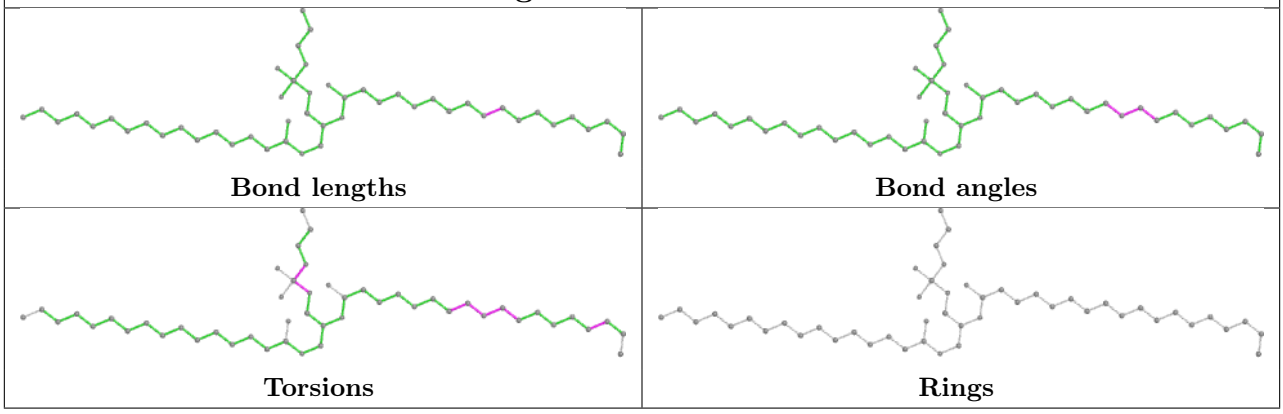
Ligand PEV BB 211



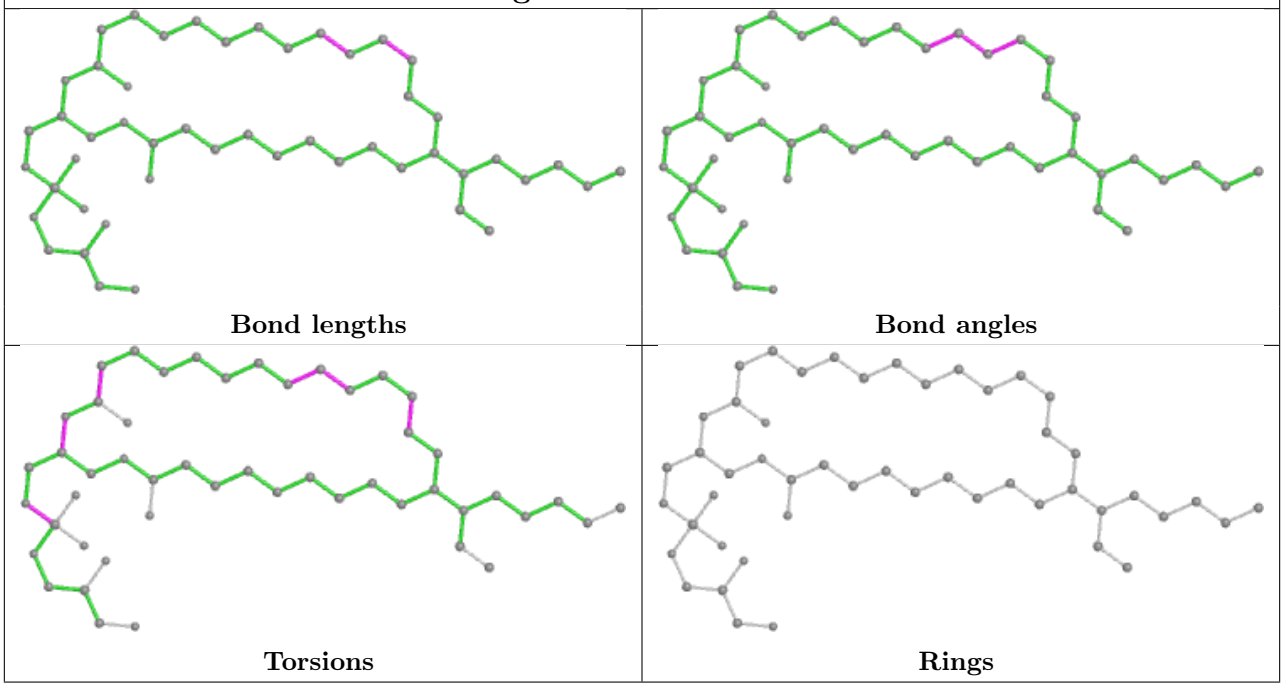
Ligand PEV A1 324



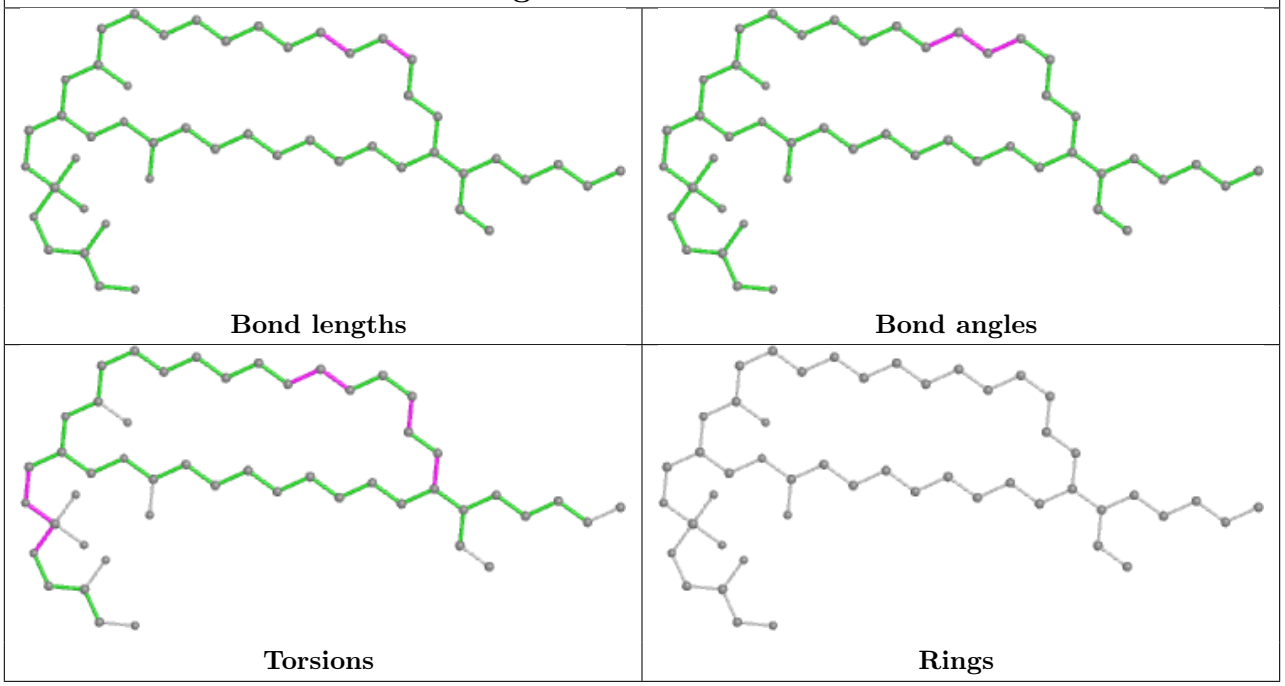
Ligand PEV A0 314



Ligand PGV A0 317



Ligand PGV A1 311



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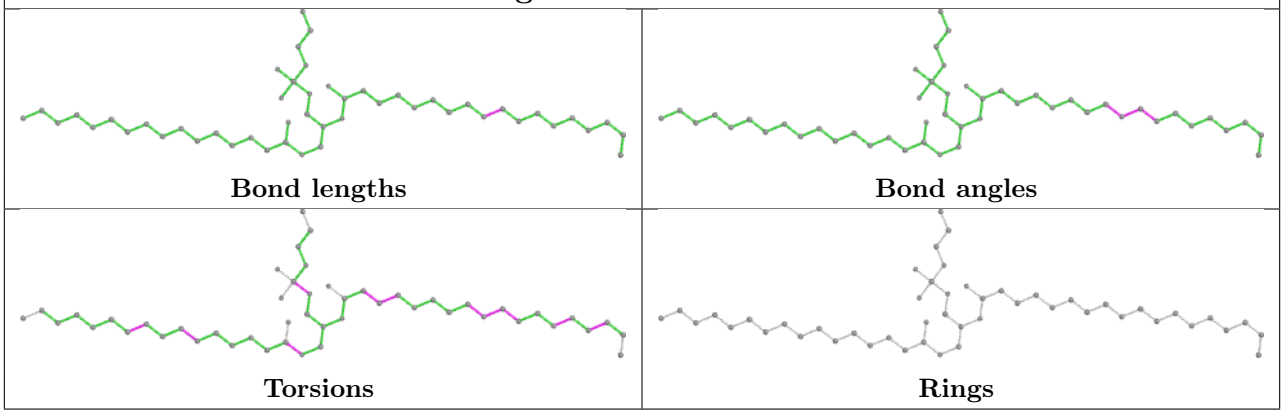

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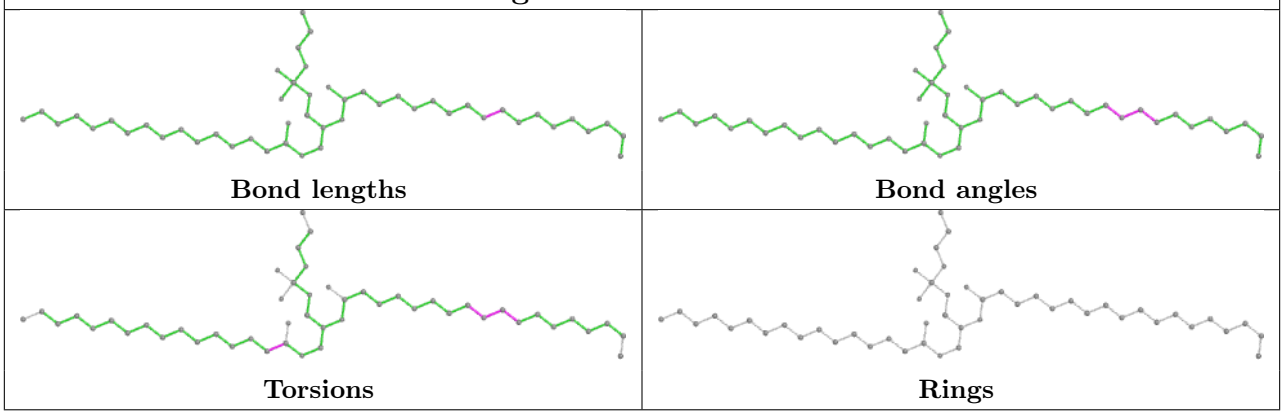

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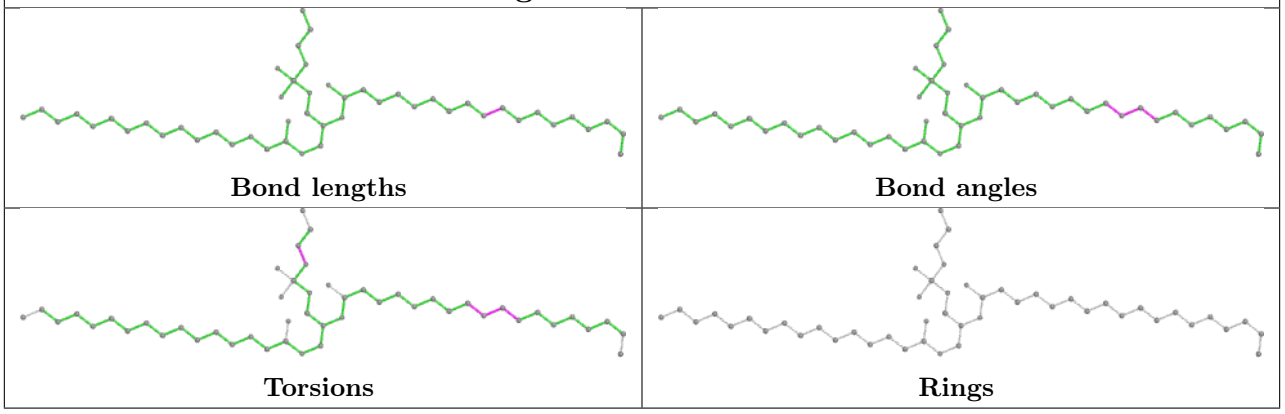
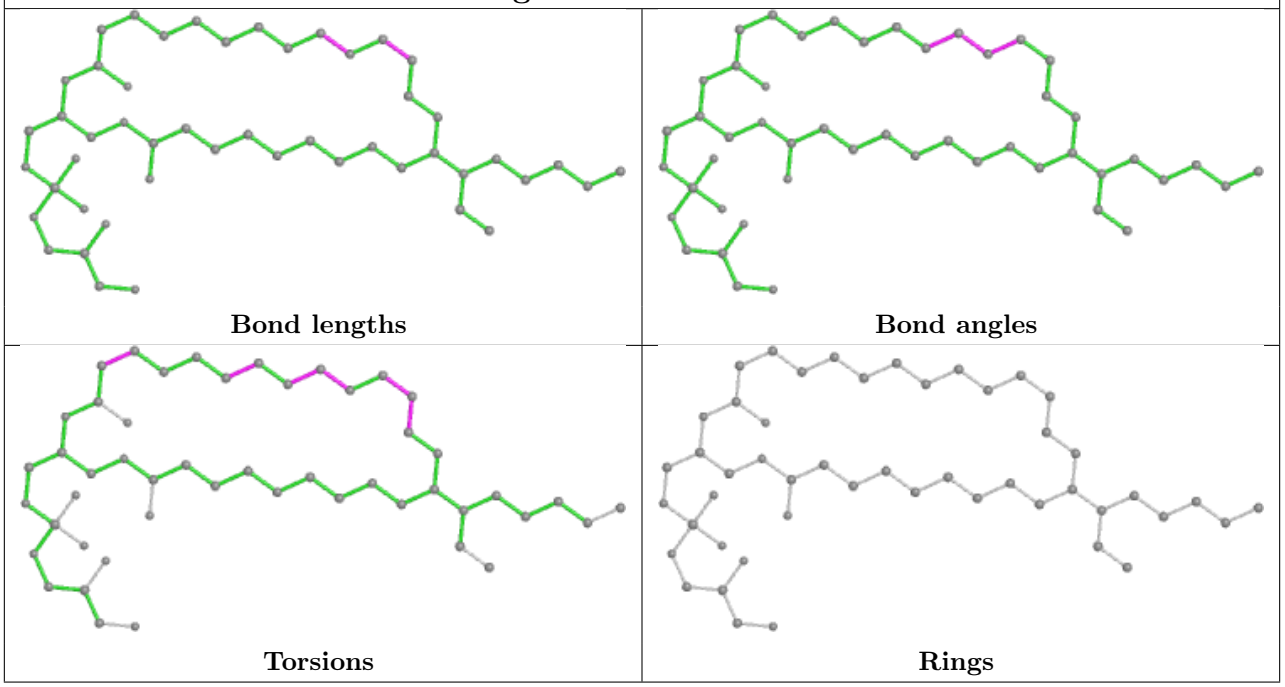
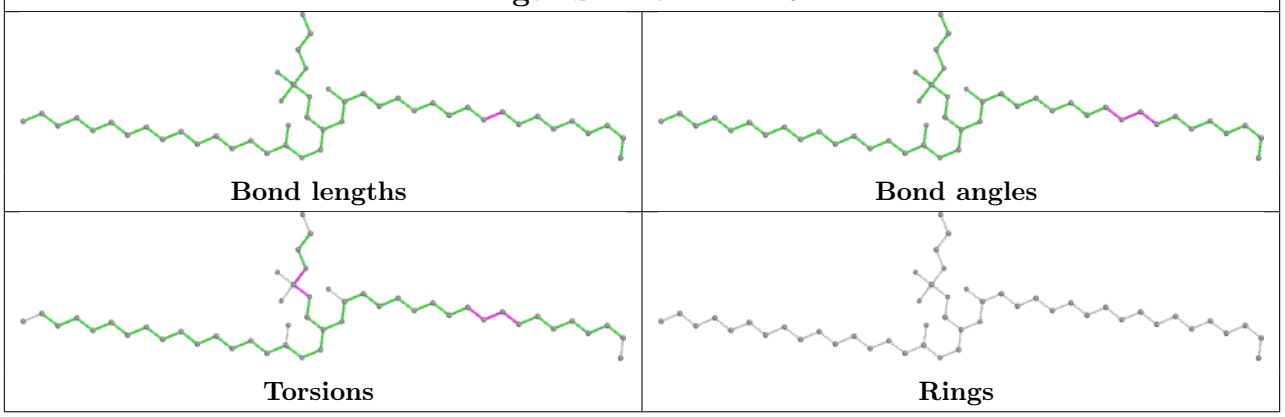


Ligand PGV A0 327



Ligand PEV BB 215



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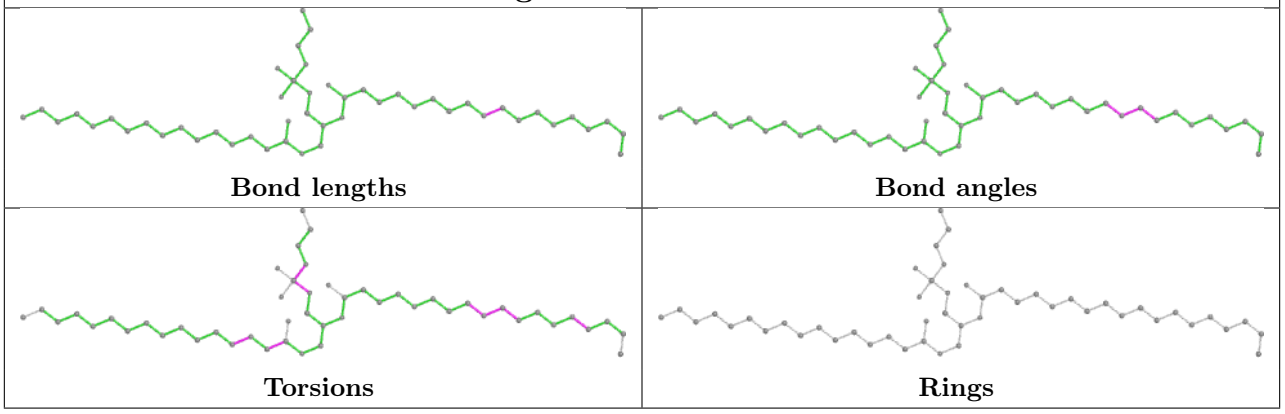

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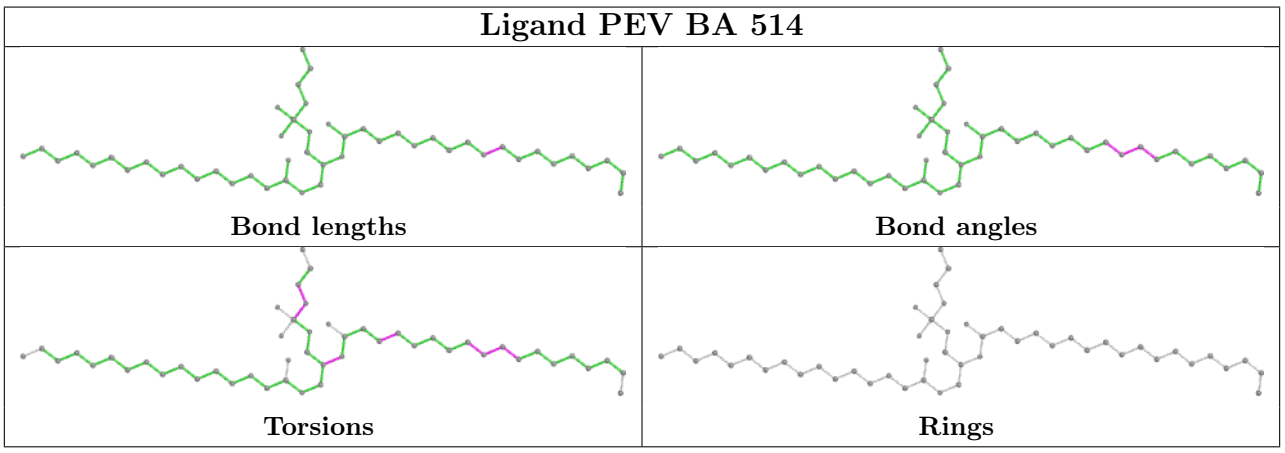

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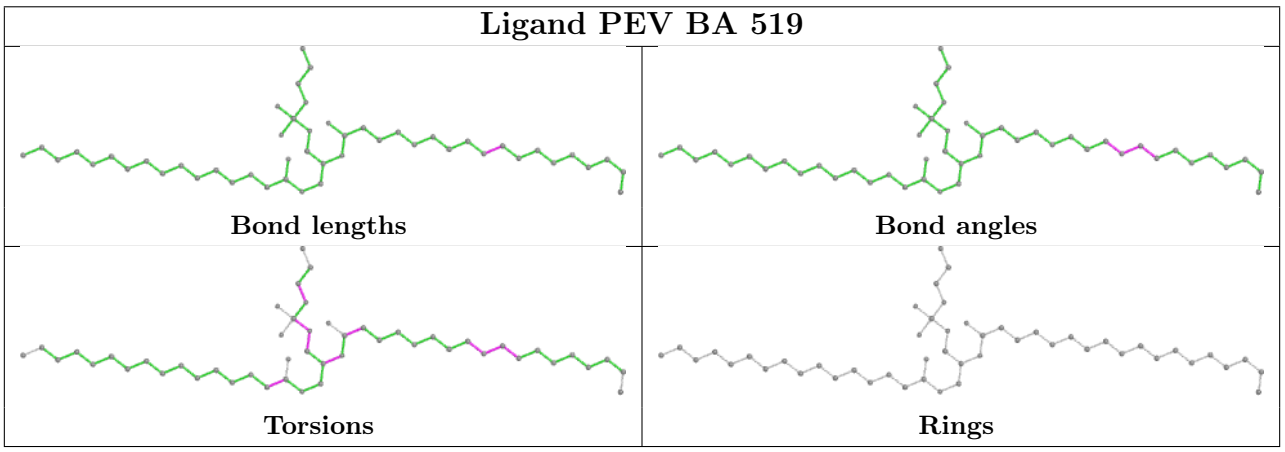
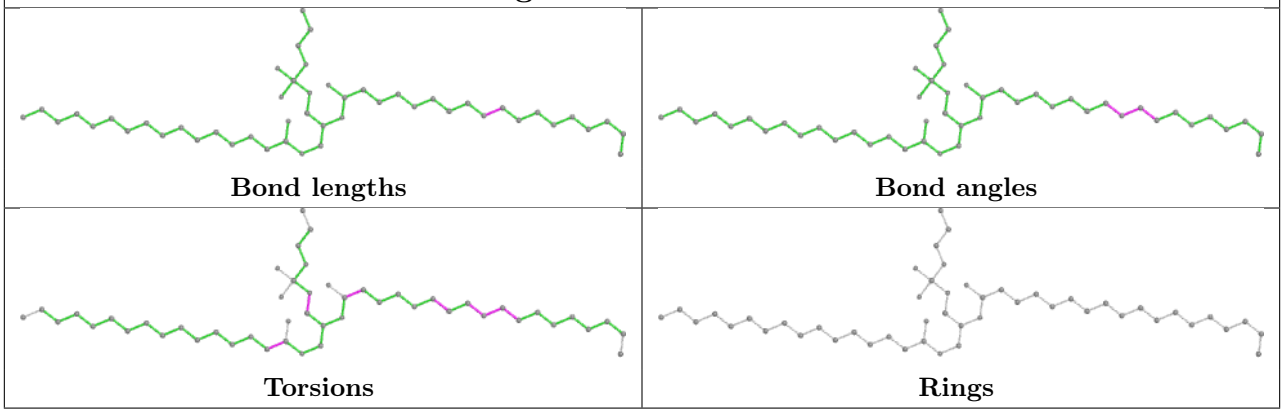
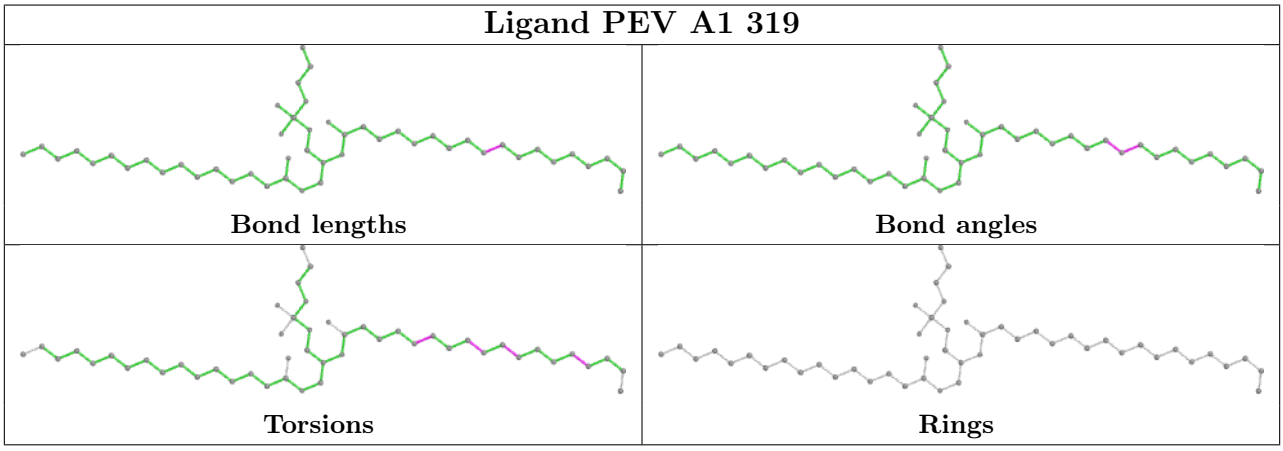


Ligand PEV A0 307



Ligand PEV A1 319



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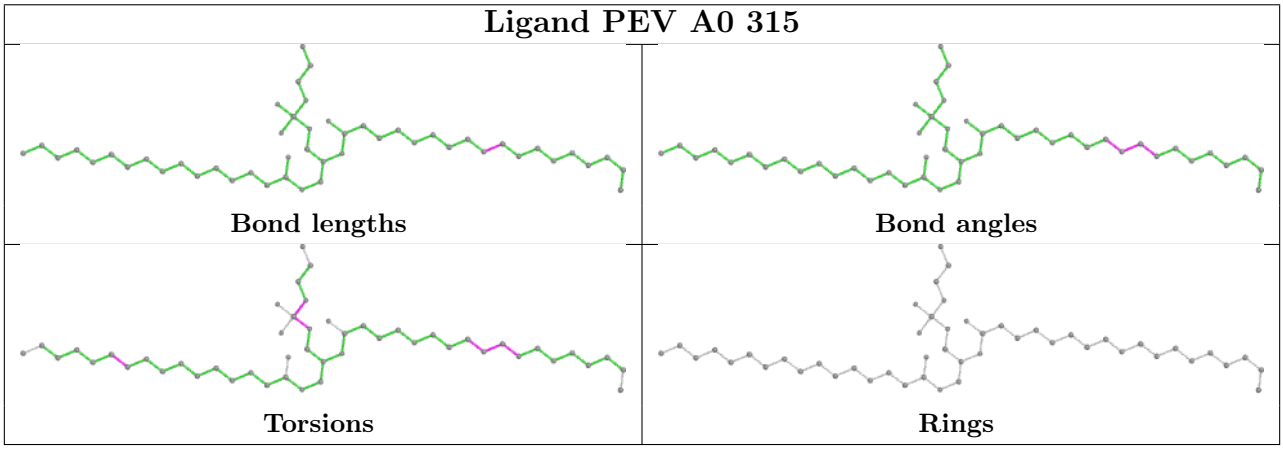

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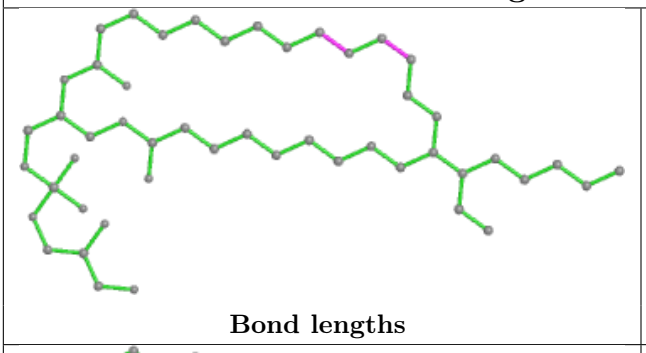
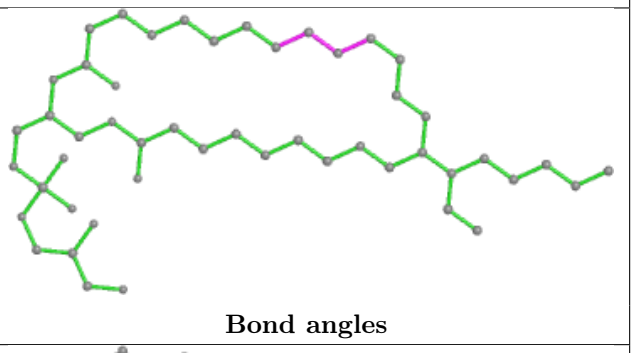
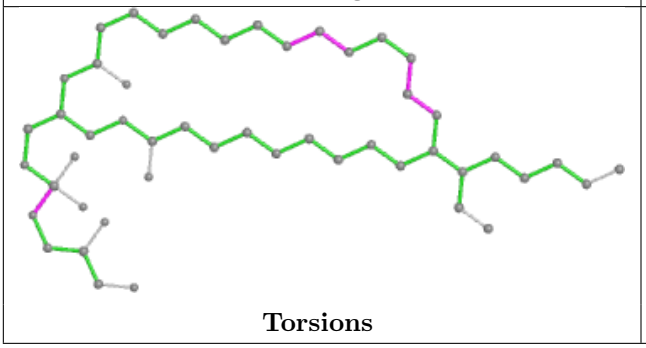


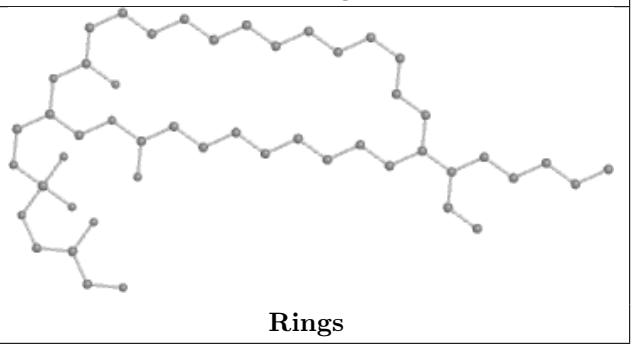
Bond lengths



Bond angles

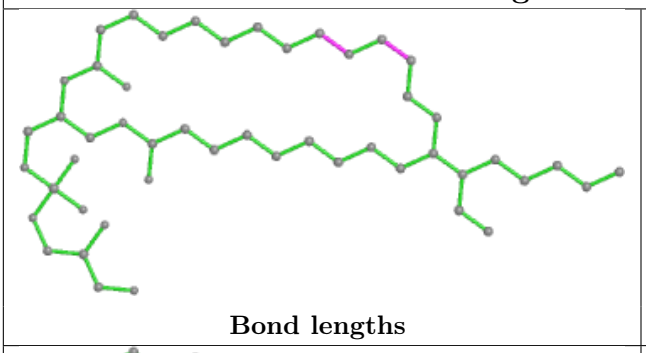


Torsions

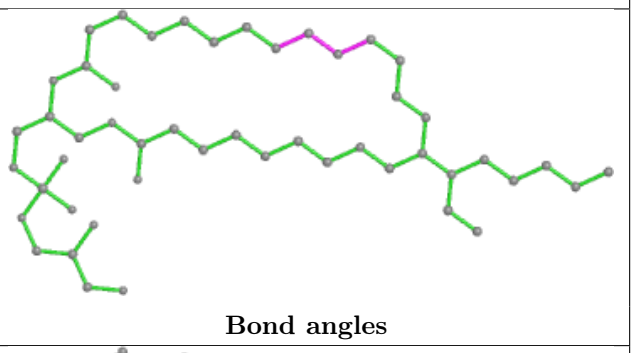


Rings

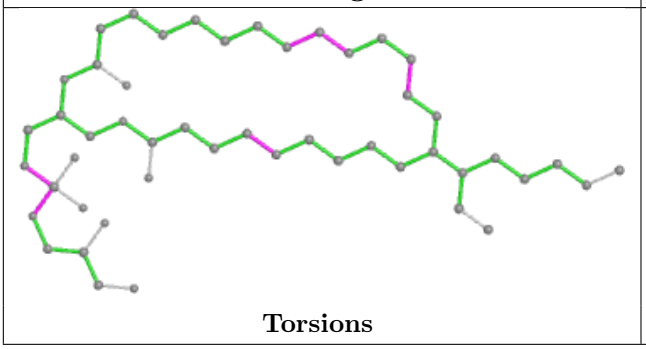
Ligand PGV A0 306



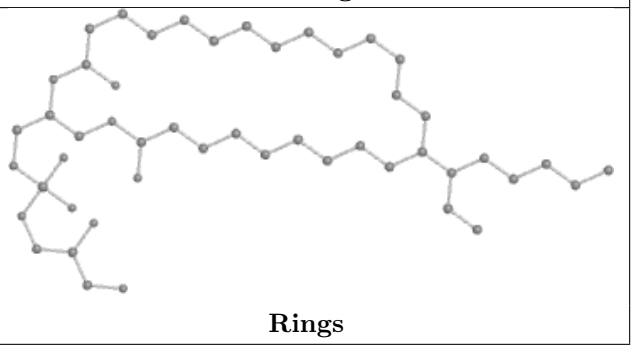
Bond lengths



Bond angles

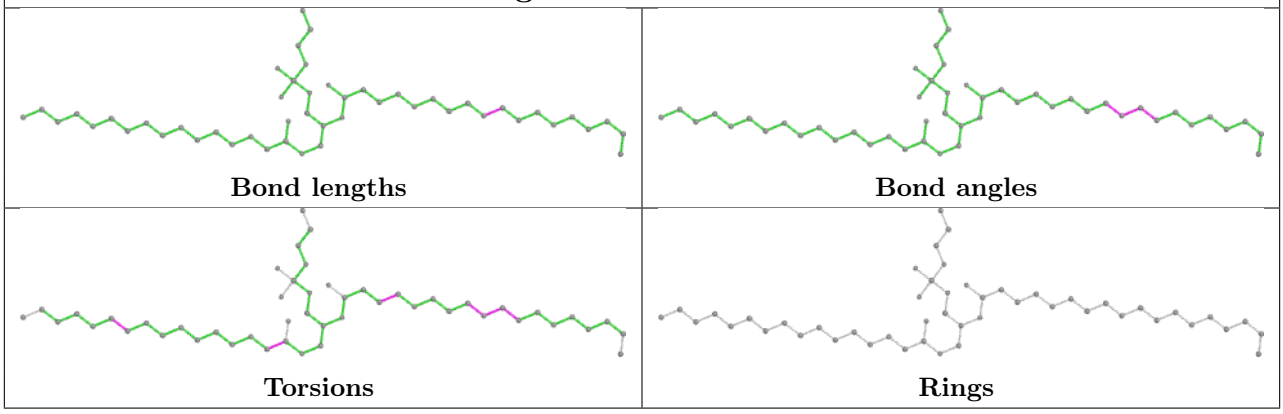


Torsions

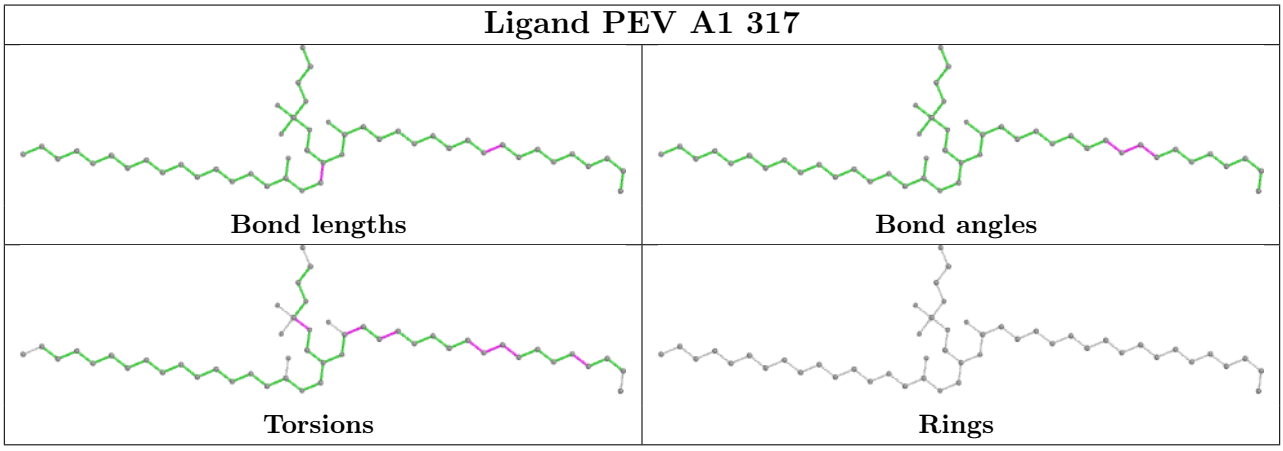


Rings

Ligand PEV A0 311



Ligand PEV A1 317



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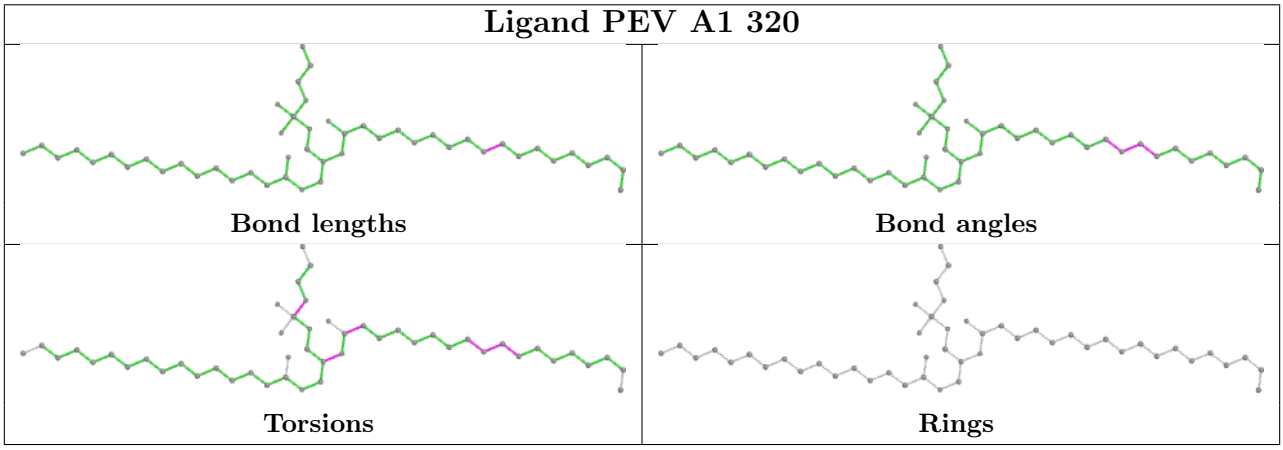
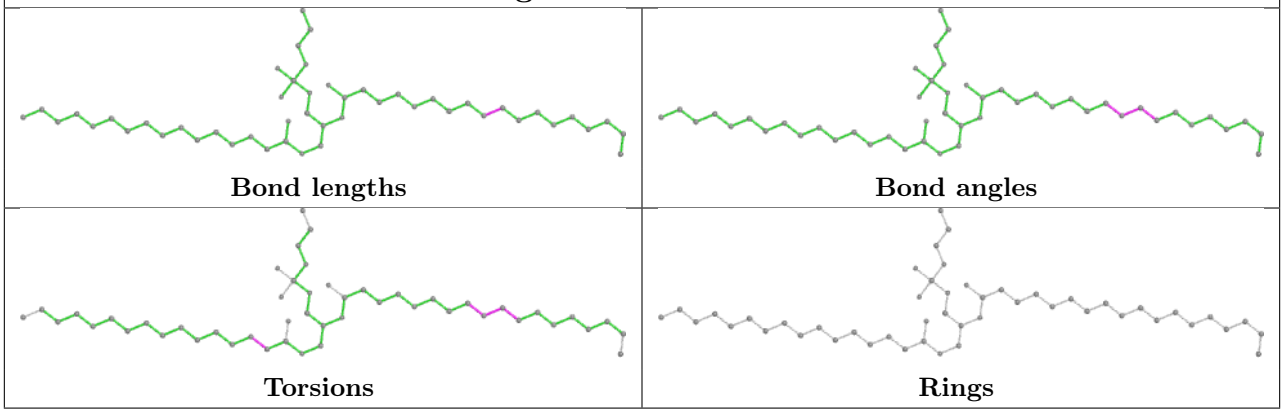
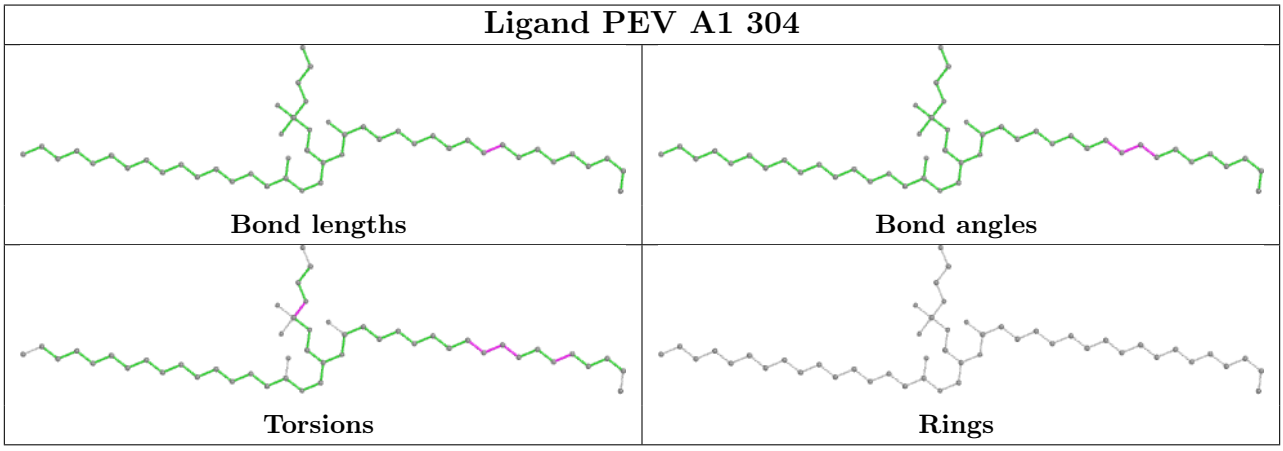


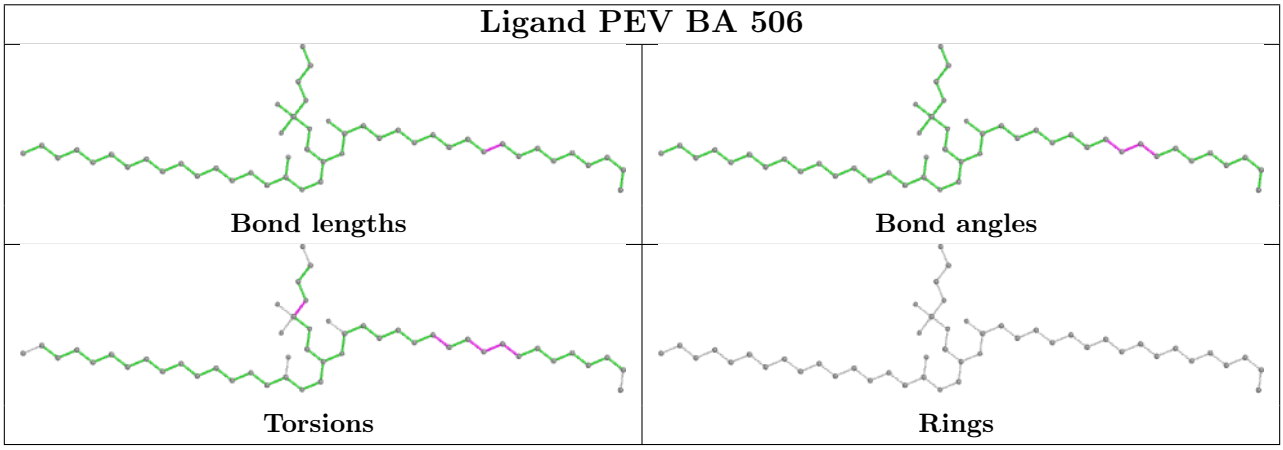
Ligand PEV A1 307



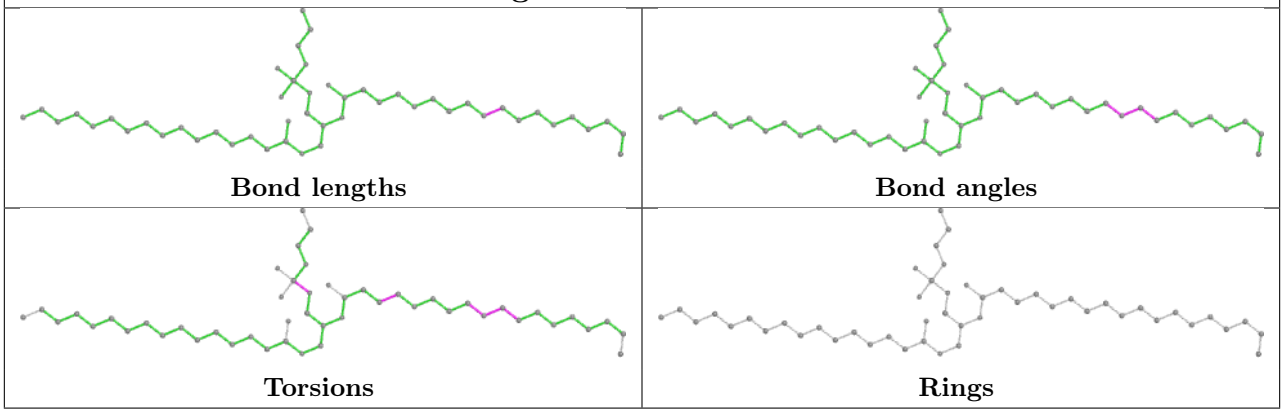
Ligand PEV A1 304



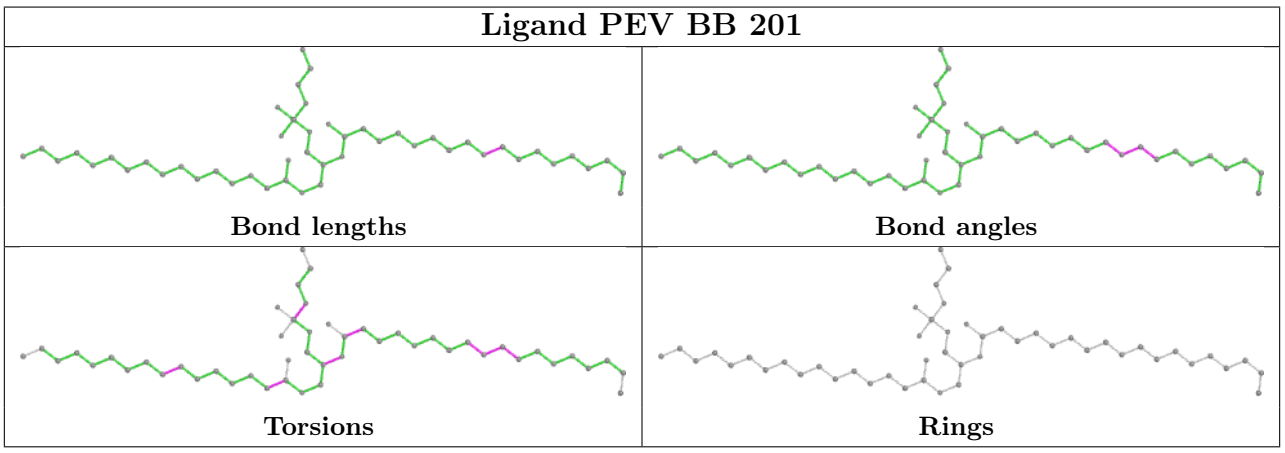
Ligand PEV BA 506



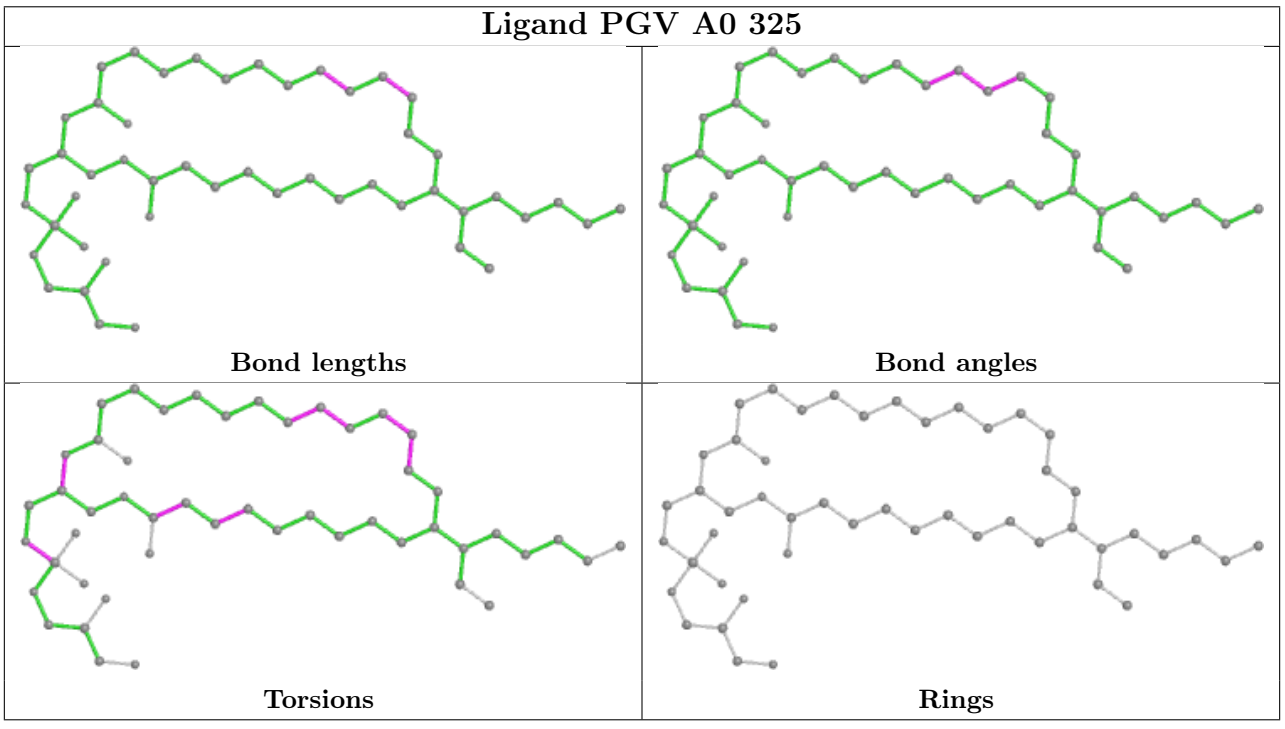
Ligand PEV BA 526



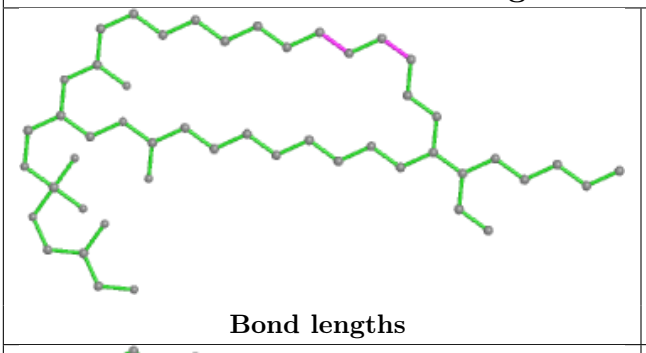
Ligand PEV BB 201



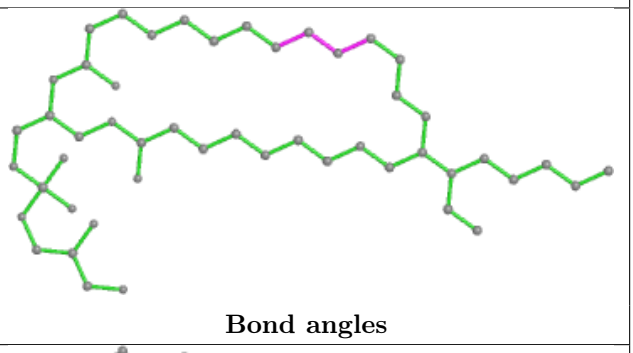
Ligand PGV A0 325



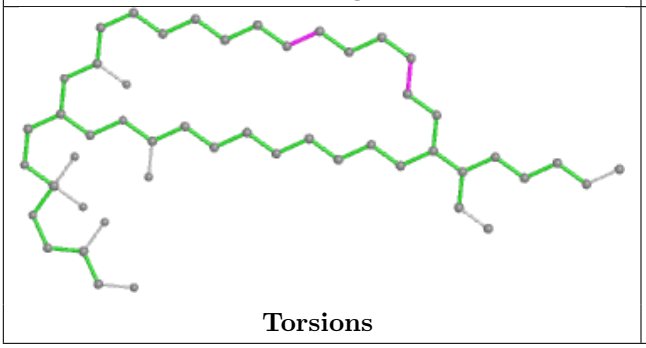
Ligand PGV BA 522



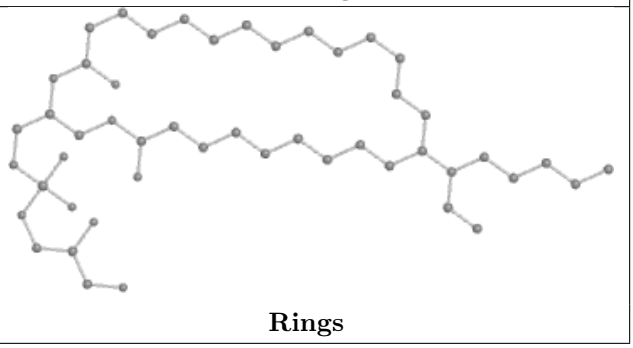
Bond lengths



Bond angles

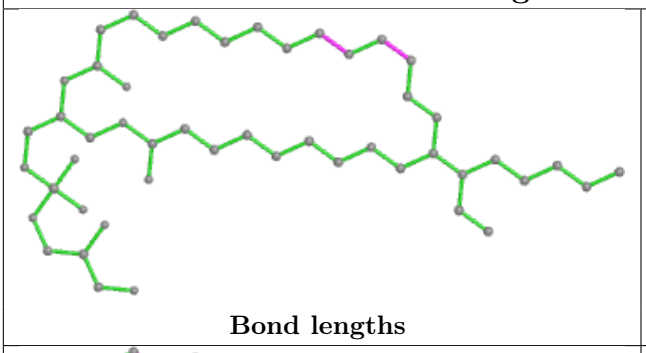


Torsions

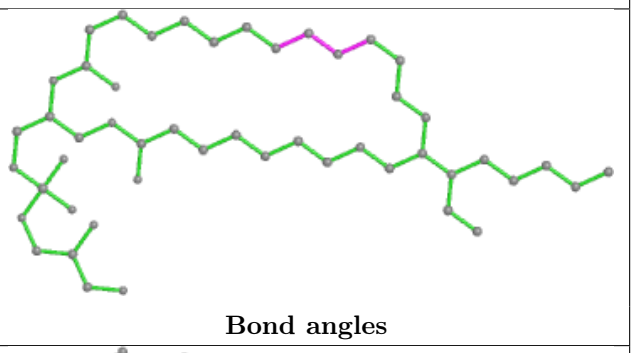


Rings

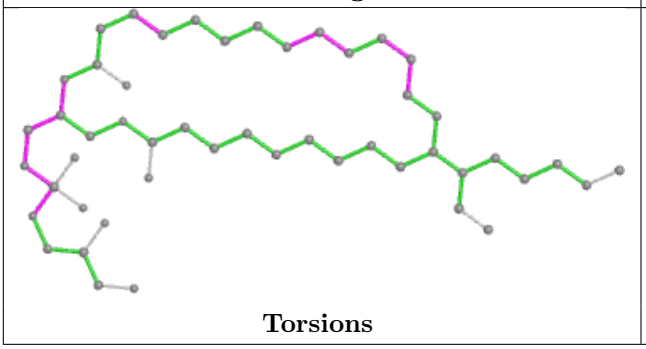
Ligand PGV A1 315



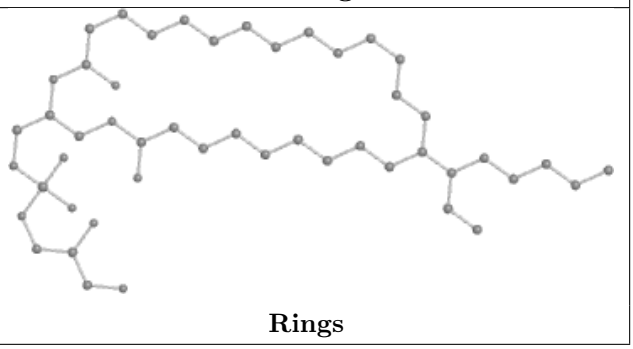
Bond lengths



Bond angles

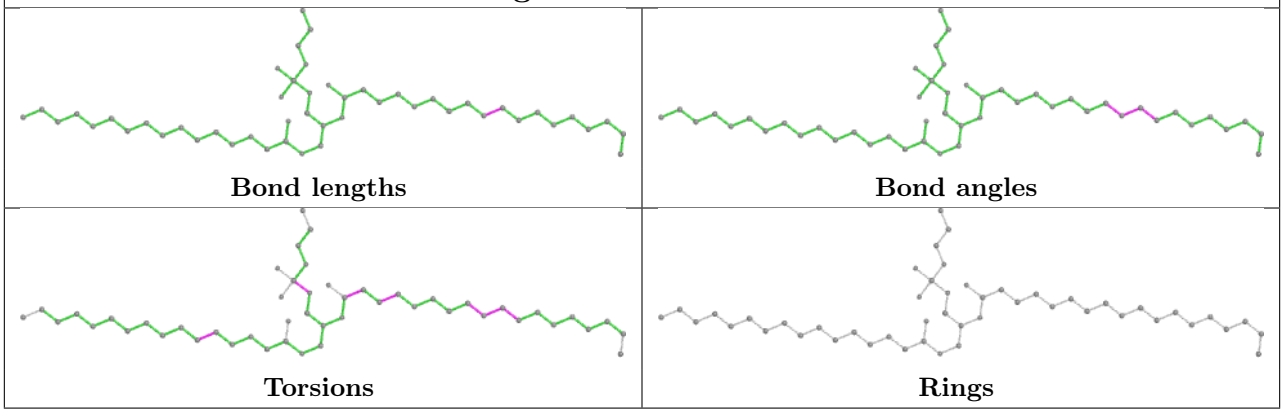


Torsions

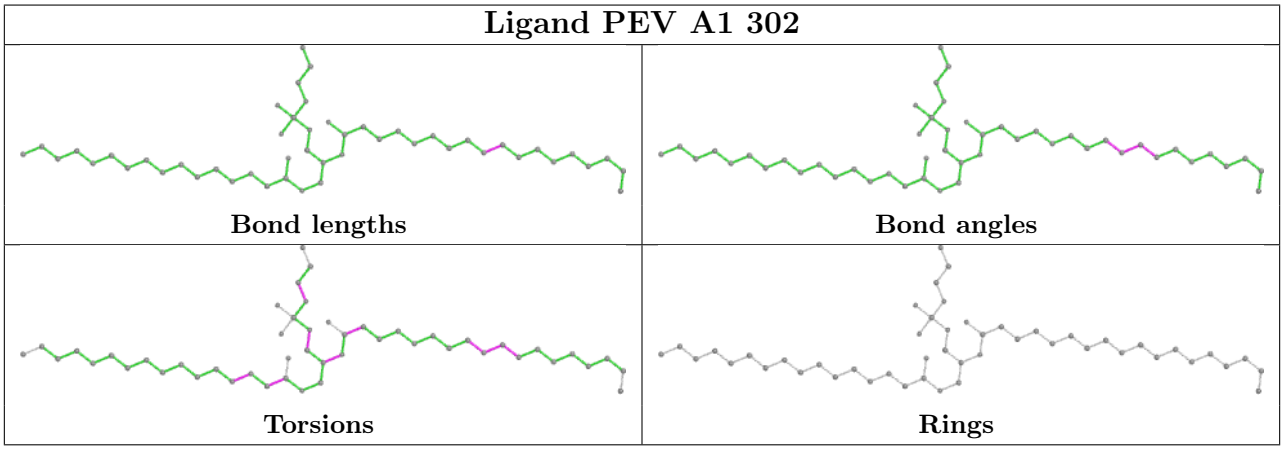


Rings

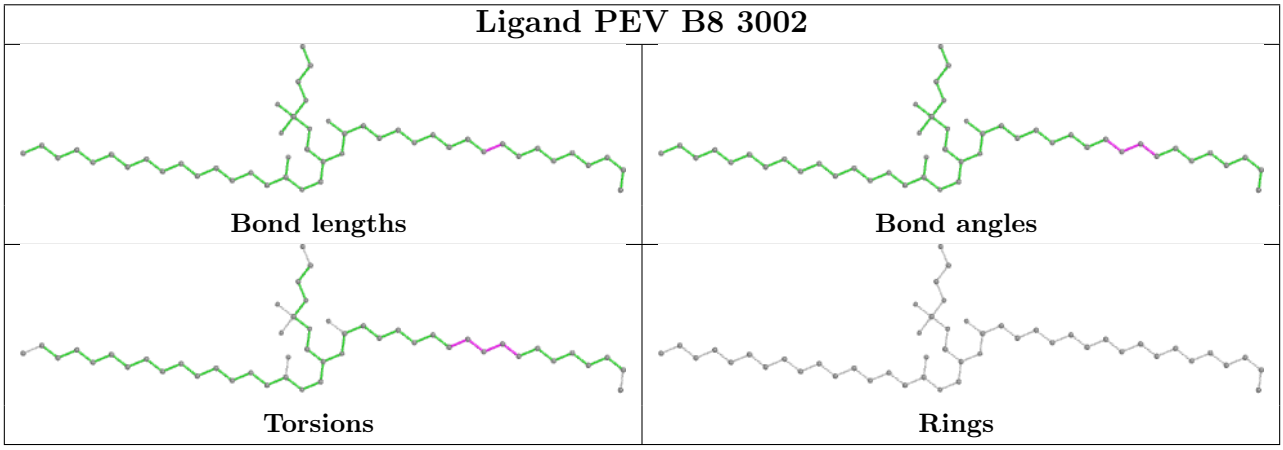
Ligand PEV AZ 204



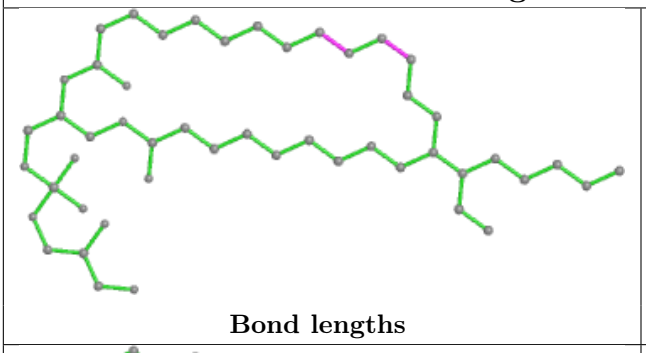
Ligand PEV A1 302



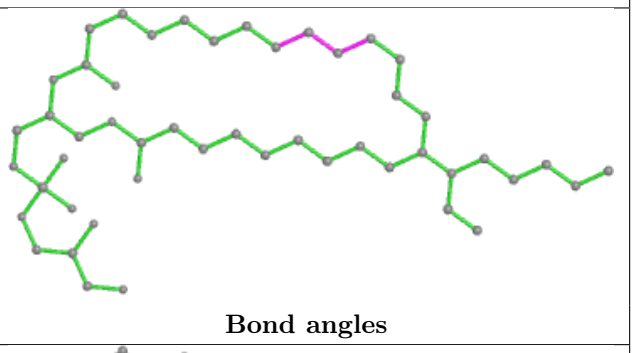
Ligand PEV B8 3002



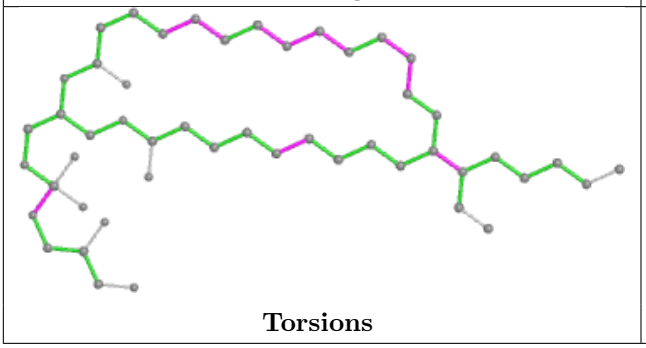
Ligand PGV BB 204



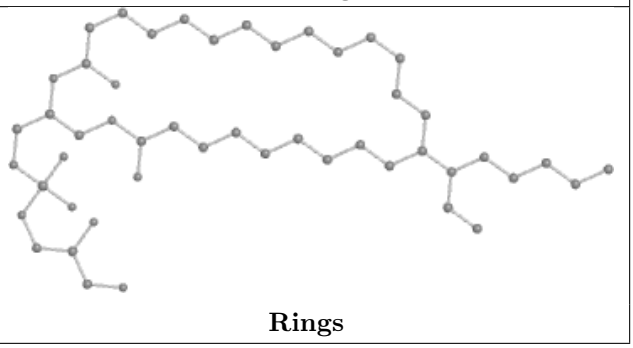
Bond lengths



Bond angles

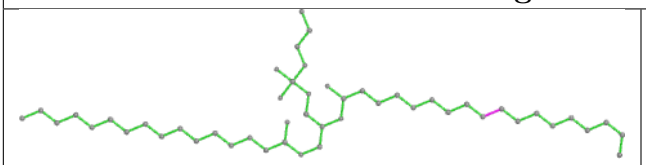


Torsions

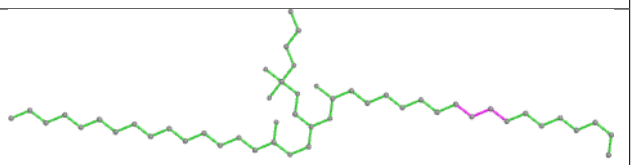


Rings

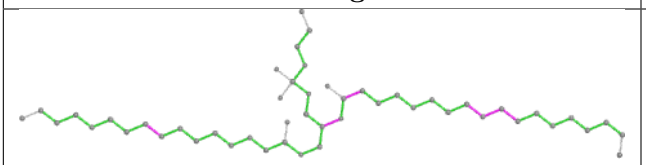
Ligand PEV A1 309



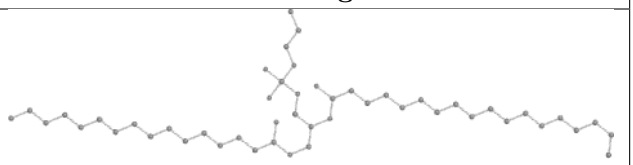
Bond lengths



Bond angles

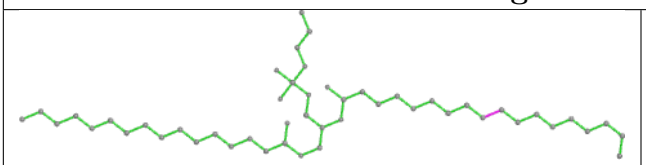


Torsions

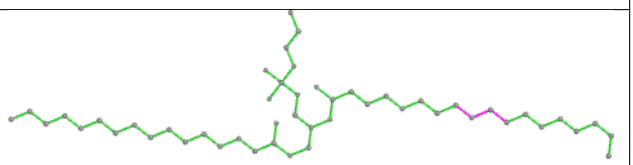


Rings

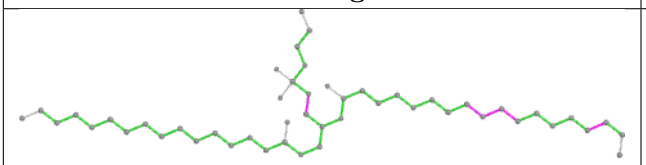
Ligand PEV BA 508



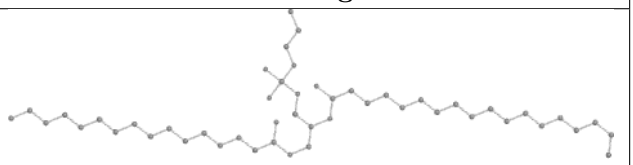
Bond lengths



Bond angles

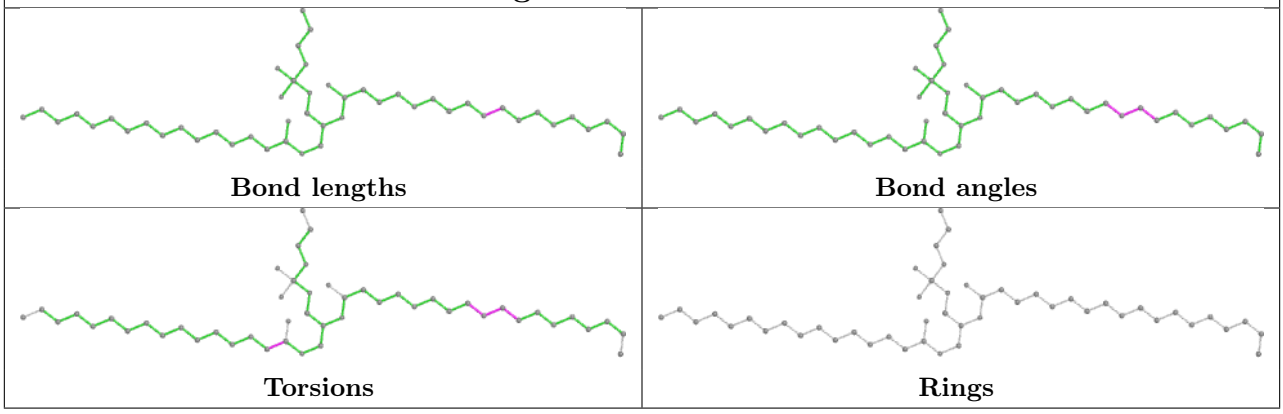


Torsions

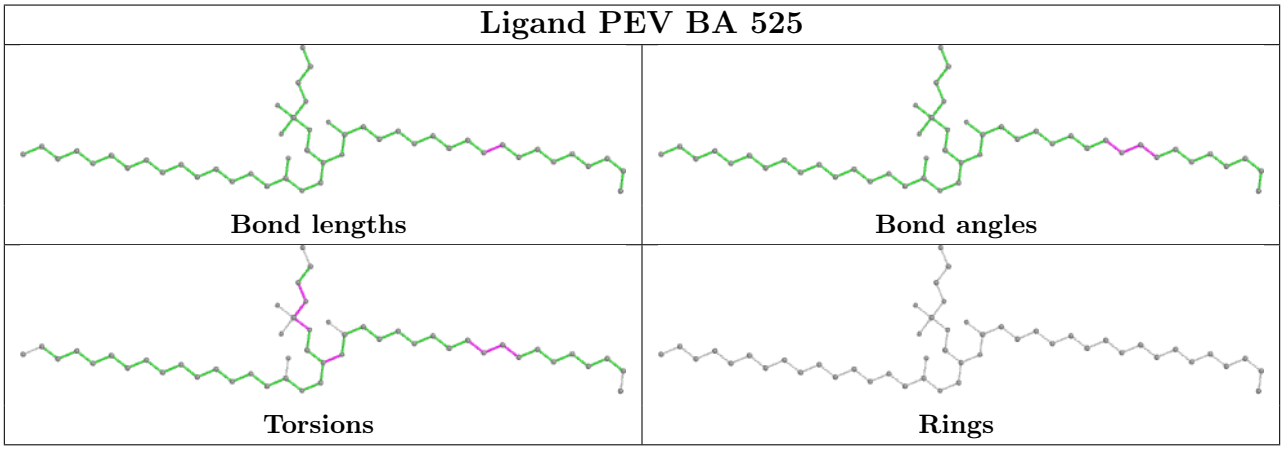


Rings

Ligand PEV AZ 201



Ligand PEV BA 525



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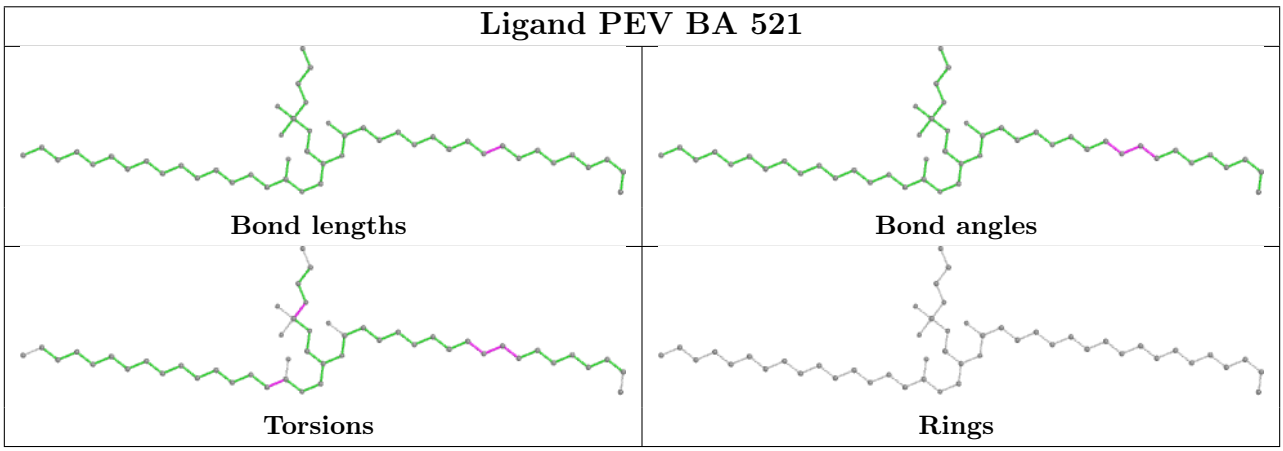
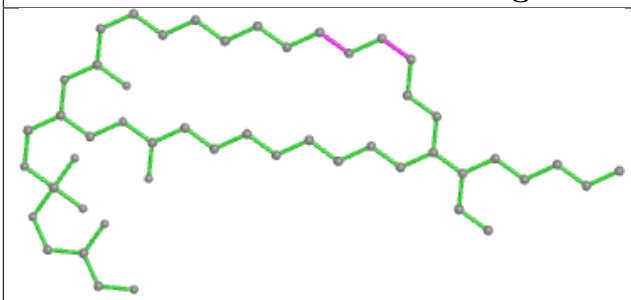
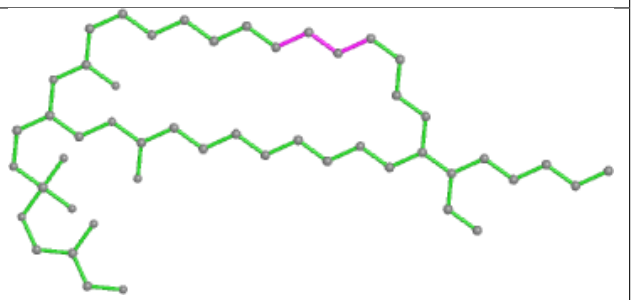


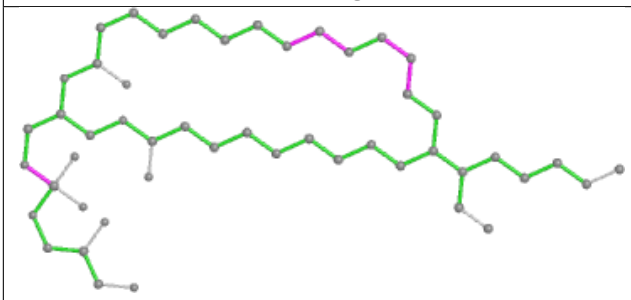
Ligand PGV A1 303



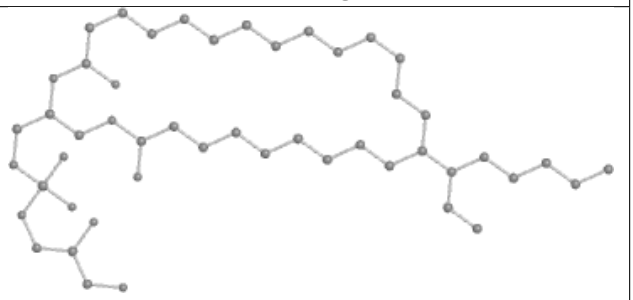
Bond lengths



Bond angles

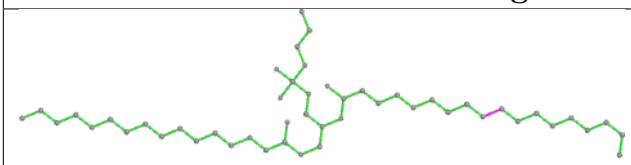


Torsions

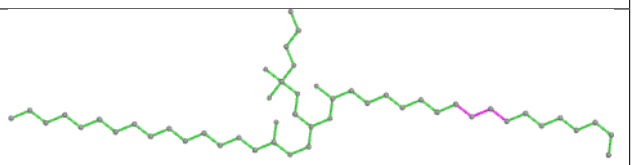


Rings

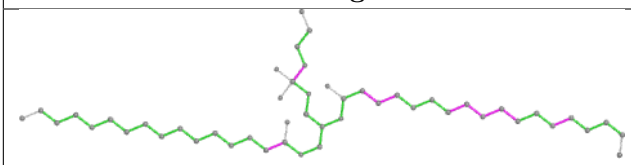
Ligand PEV BA 532



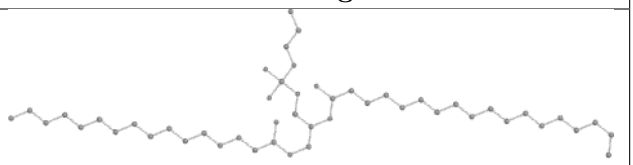
Bond lengths



Bond angles

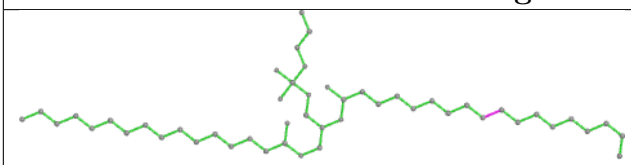


Torsions

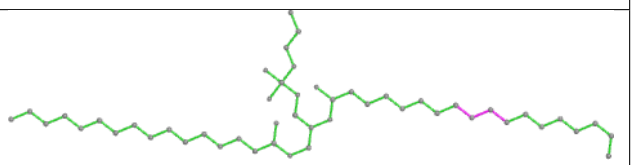


Rings

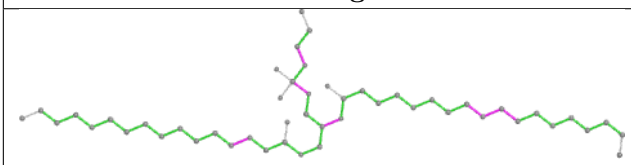
Ligand PEV A0 319



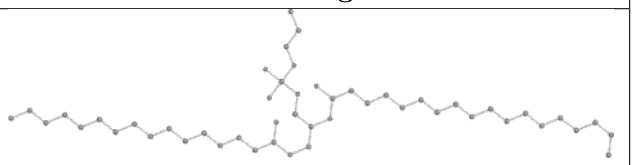
Bond lengths



Bond angles

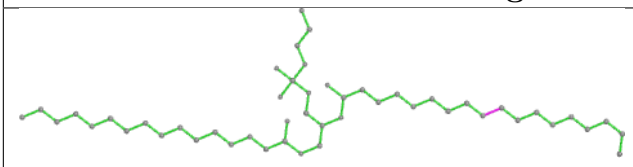


Torsions



Rings

Ligand PEV B8 3006



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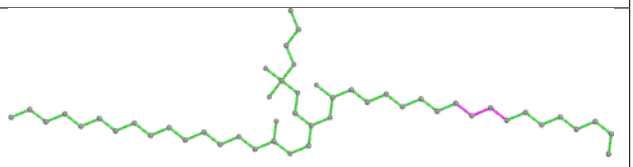
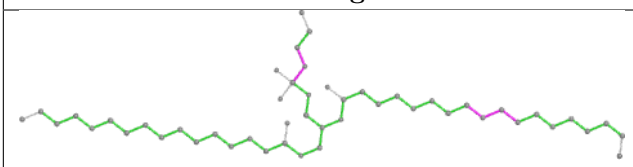
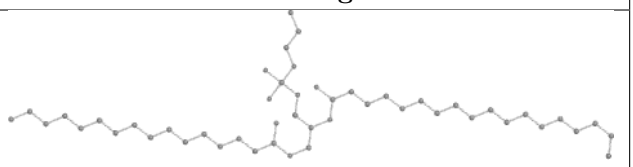


Bond angles

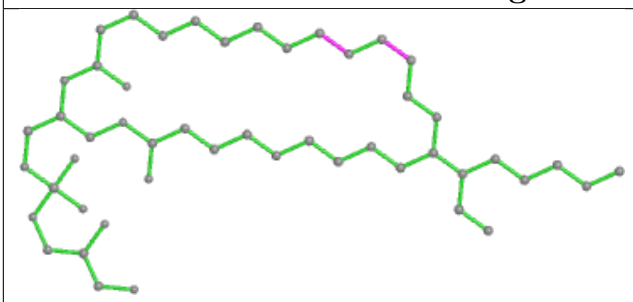


Torsions

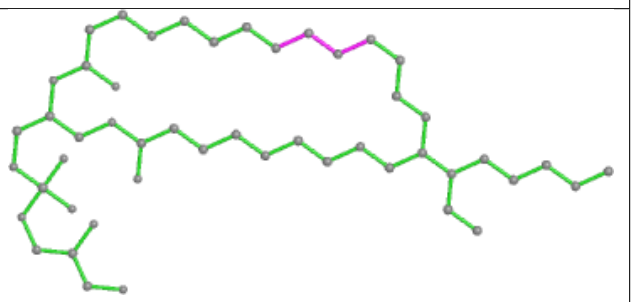


Rings

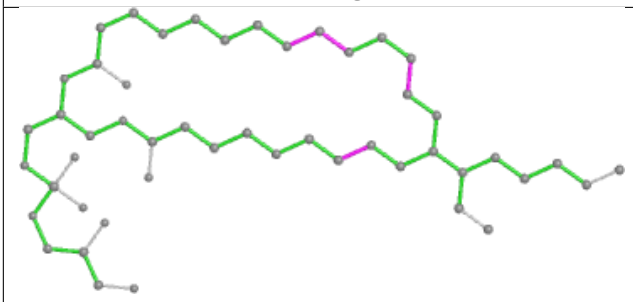
Ligand PGV BB 207



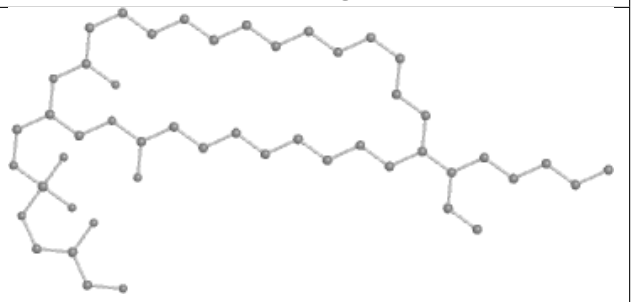
Bond lengths



Bond angles

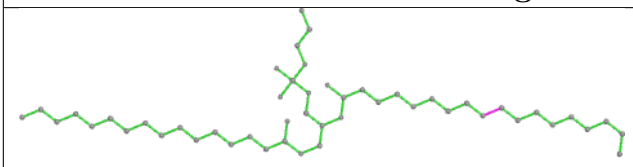


Torsions

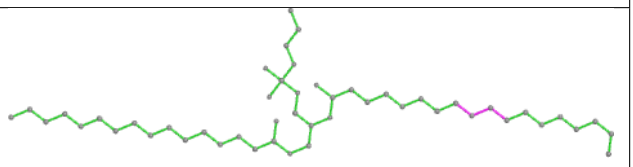


Rings

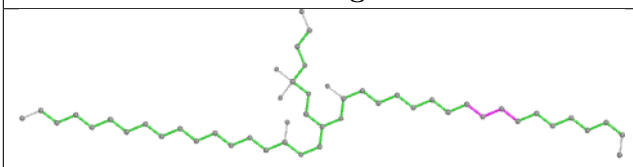
Ligand PEV A1 316



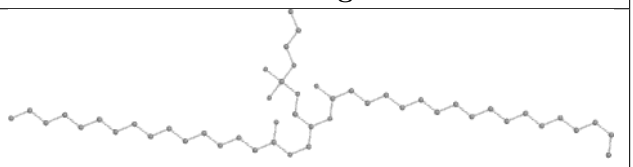
Bond lengths



Bond angles

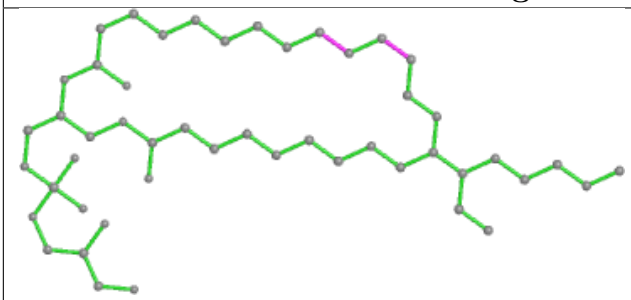


Torsions

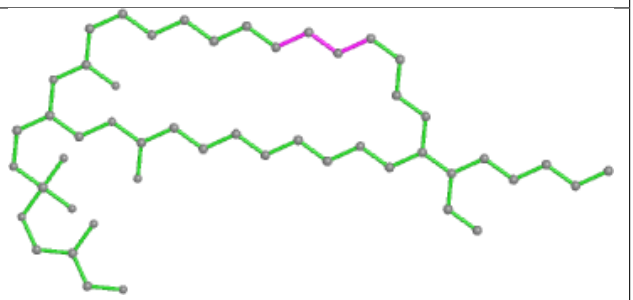


Rings

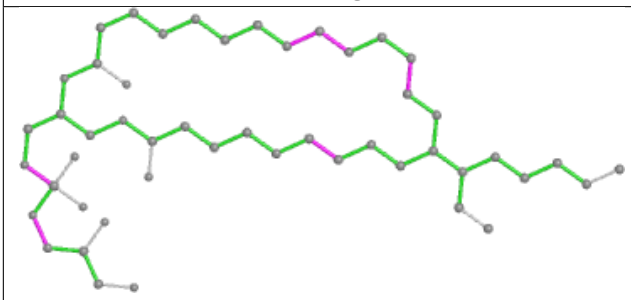
Ligand PGV A0 332



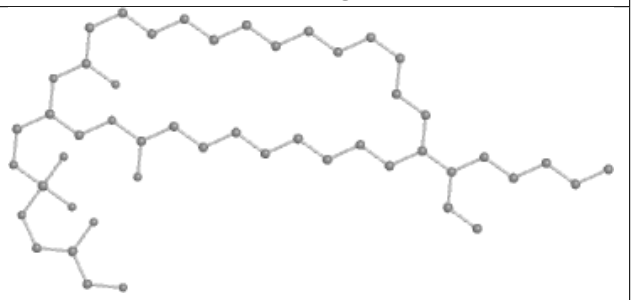
Bond lengths



Bond angles

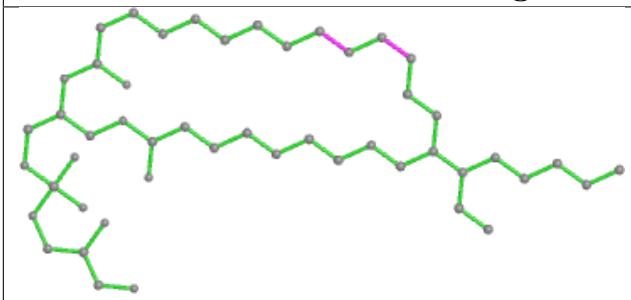


Torsions

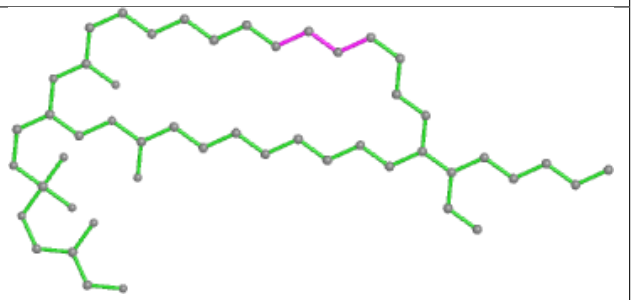


Rings

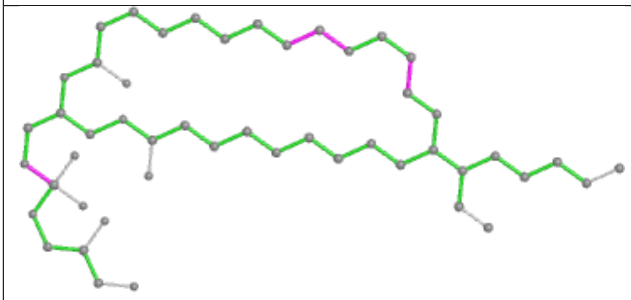
Ligand PGV A0 331



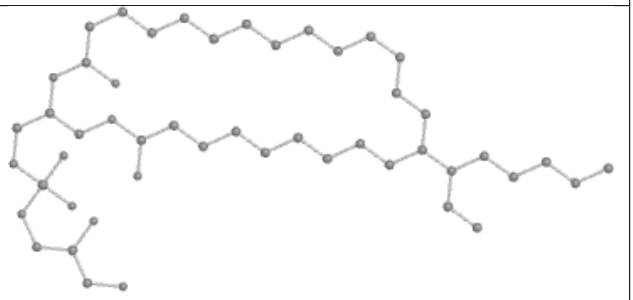
Bond lengths



Bond angles

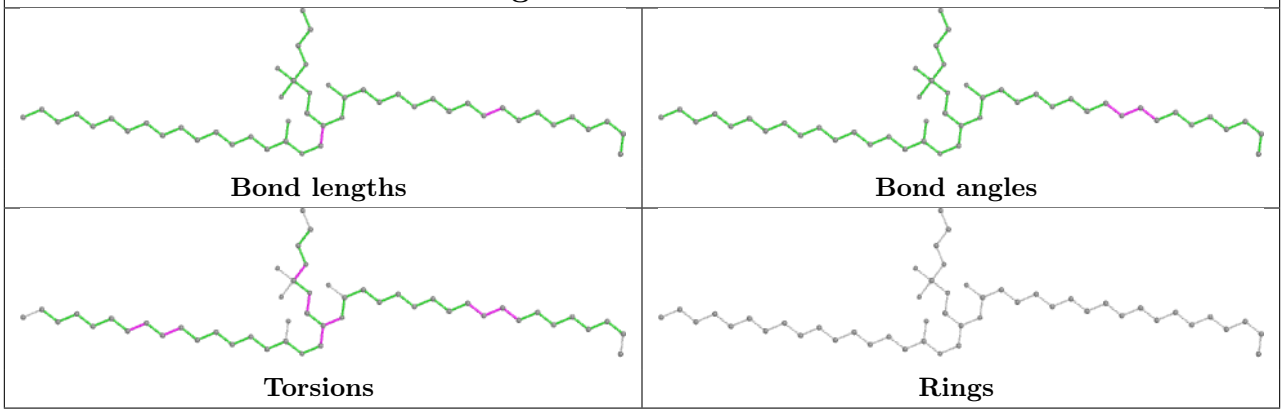


Torsions

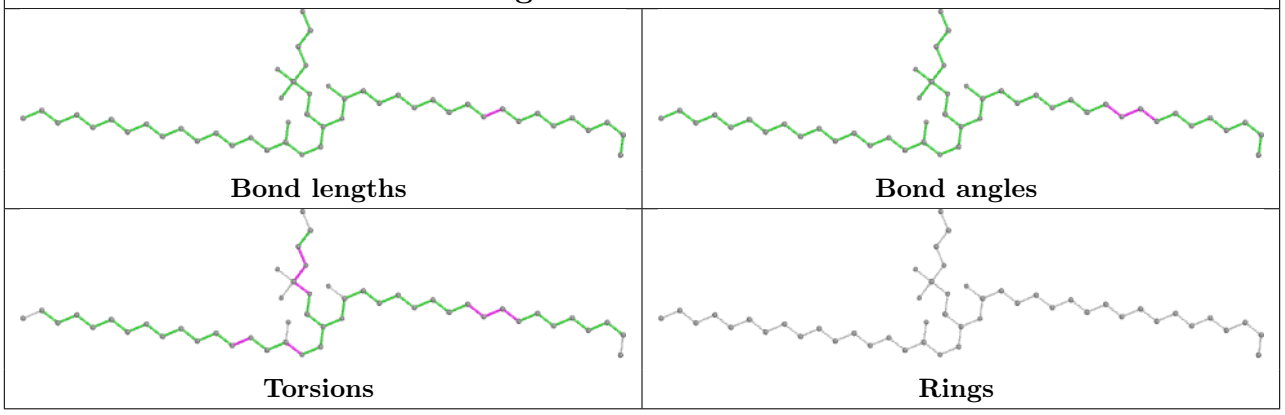


Rings

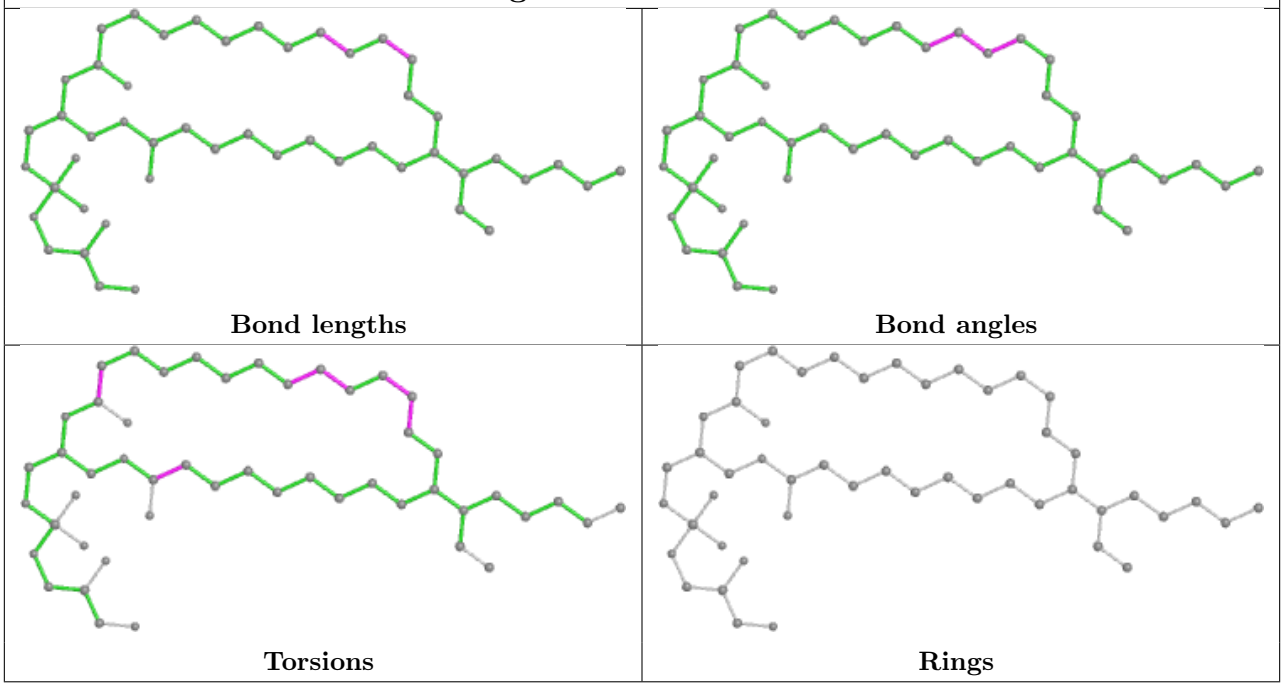
Ligand PEV BA 537



Ligand PEV A0 301



Ligand PGV BA 505



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.

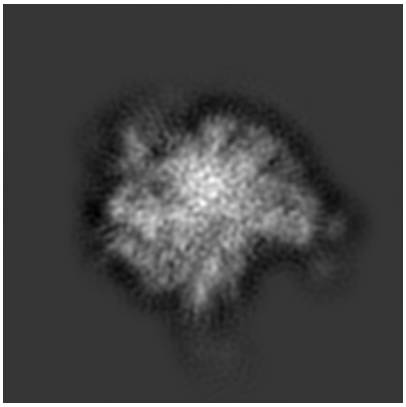
6 Map visualisation

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.

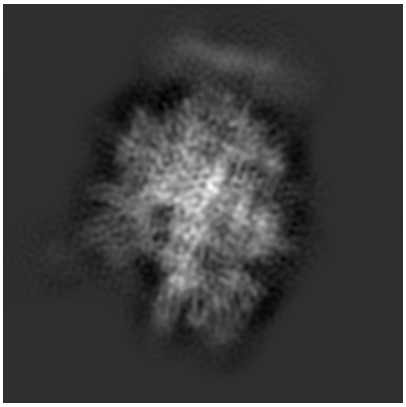
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

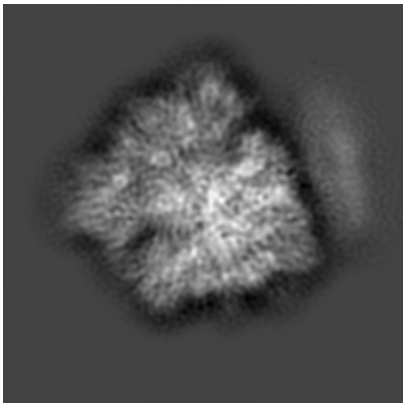
6.1.1 Primary map



X



Y

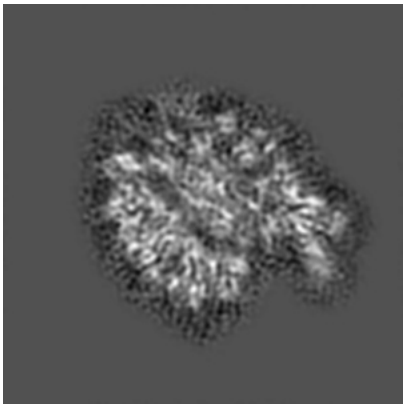


Z

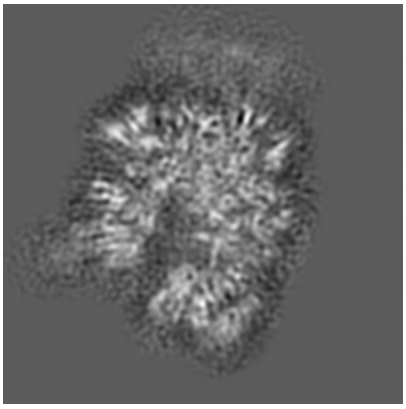
The images above show the map projected in three orthogonal directions.

6.2 Central slices

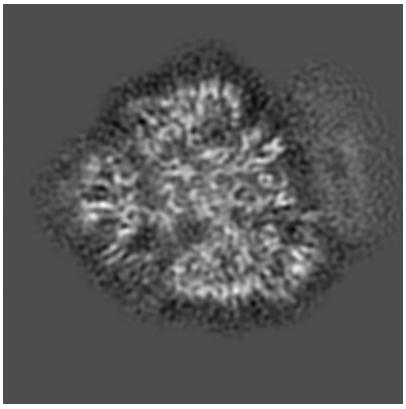
6.2.1 Primary map



X Index: 160



Y Index: 160

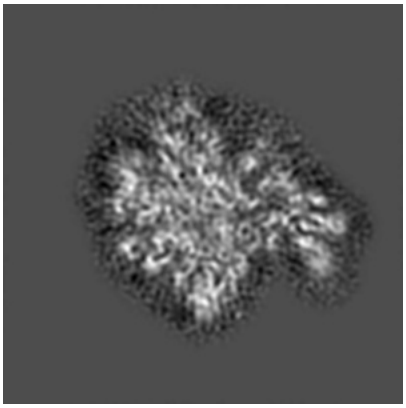


Z Index: 160

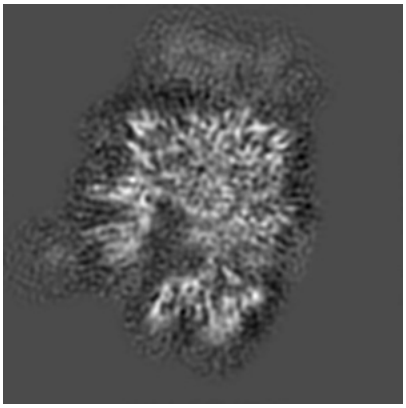
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

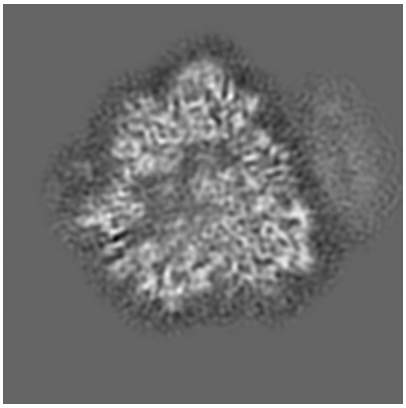
6.3.1 Primary map



X Index: 166



Y Index: 167



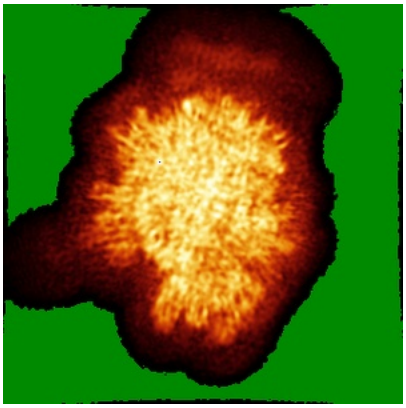
Z Index: 146

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

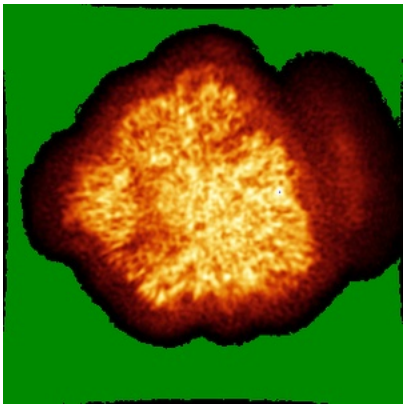
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map

X



Y

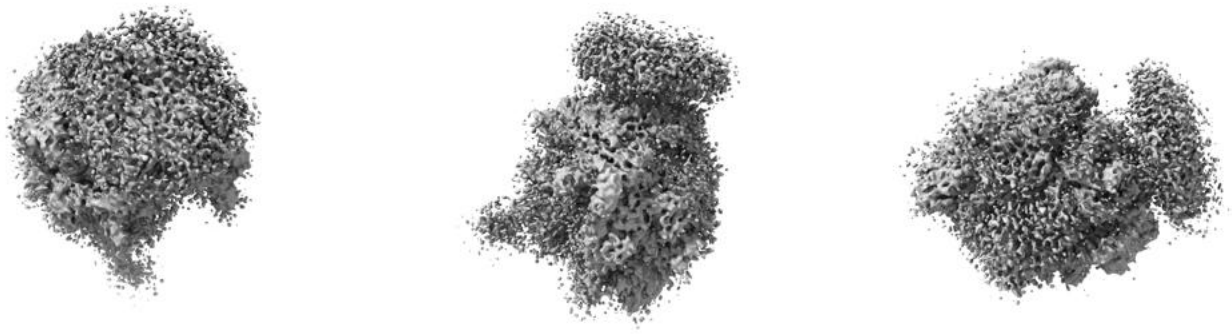


Z

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



X Y Z

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

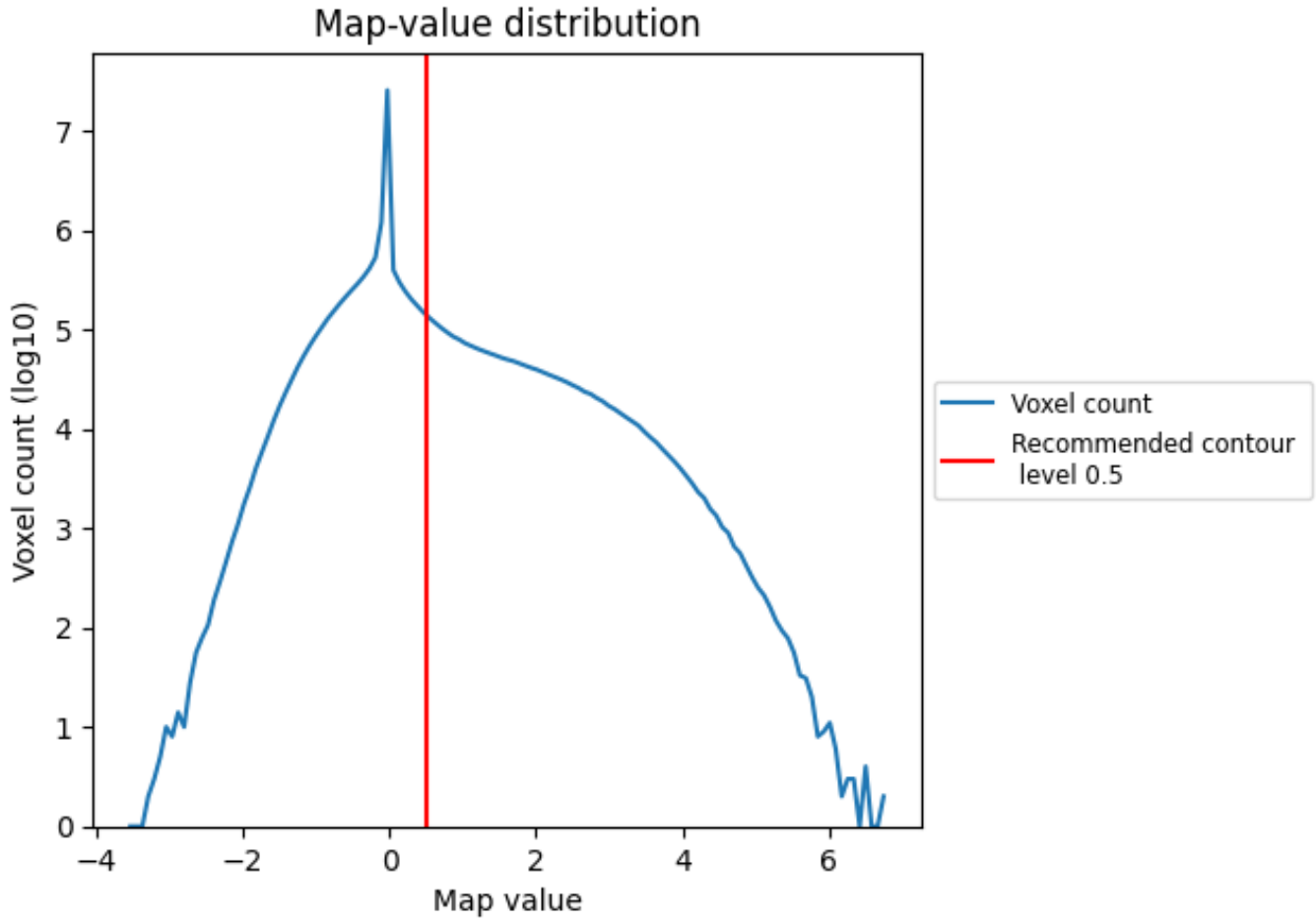
6.6 Mask visualisation (i)

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

7 Map analysis

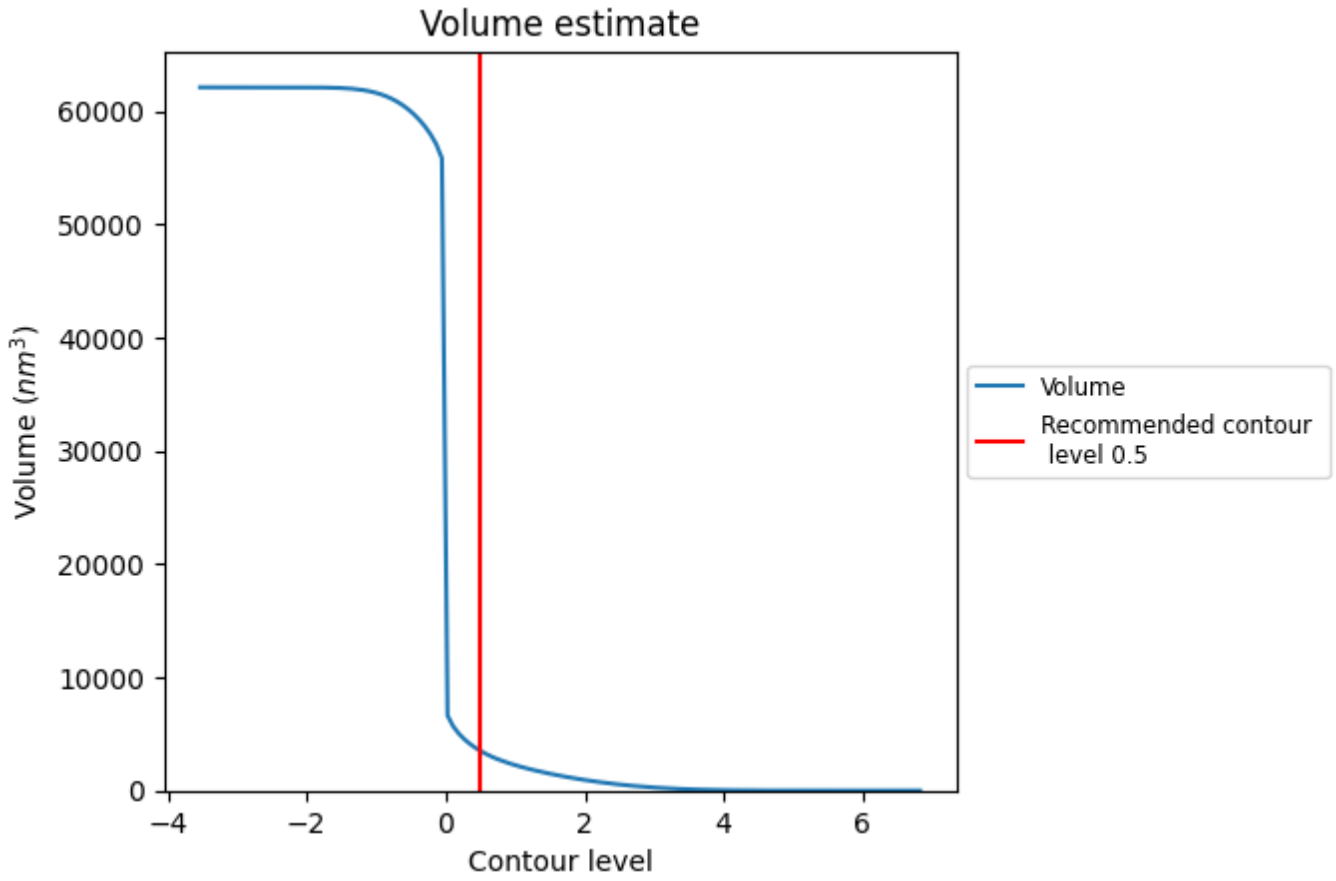
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

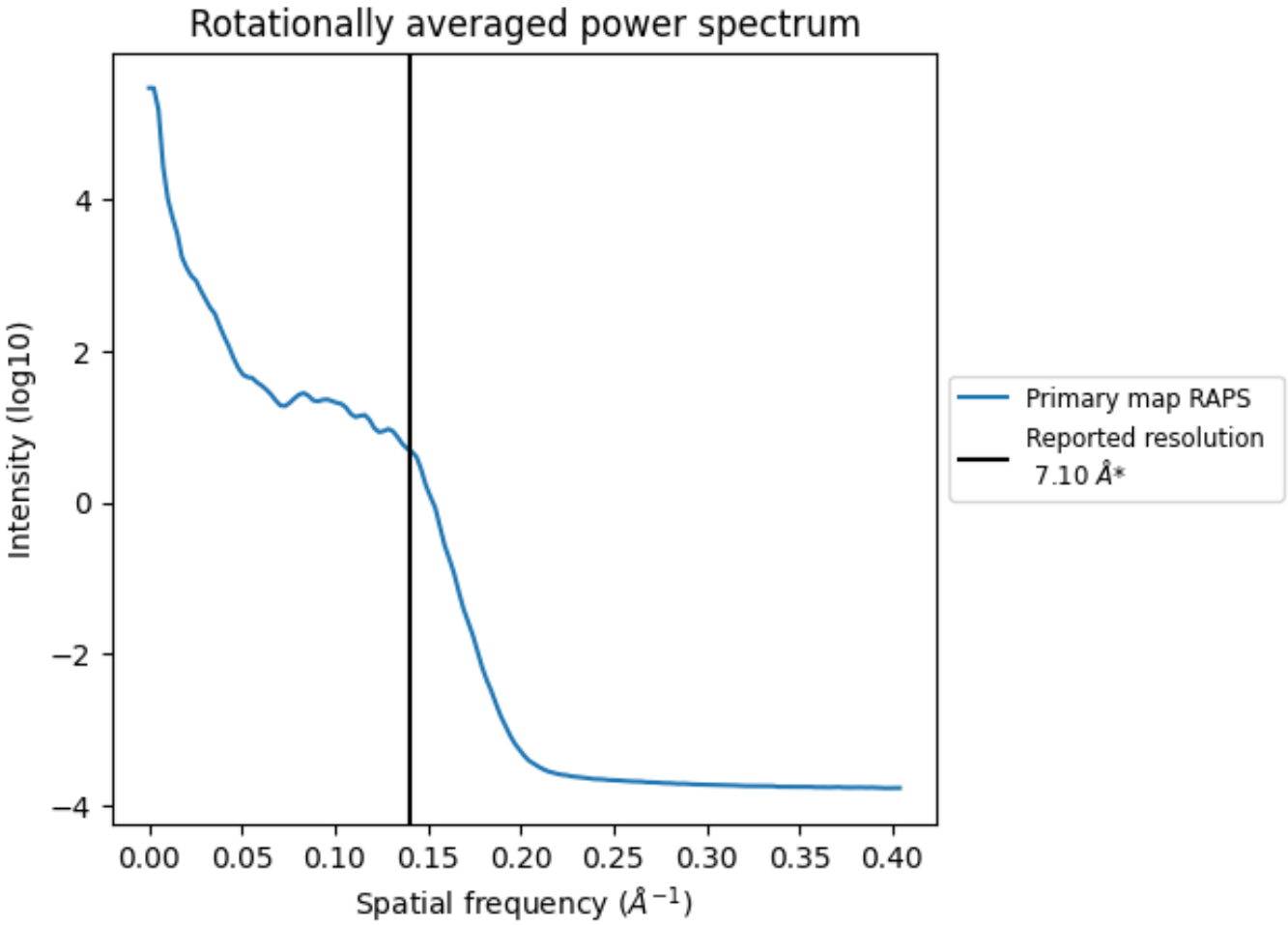
7.2 Volume estimate (i)



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

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.141 Å^{-1}

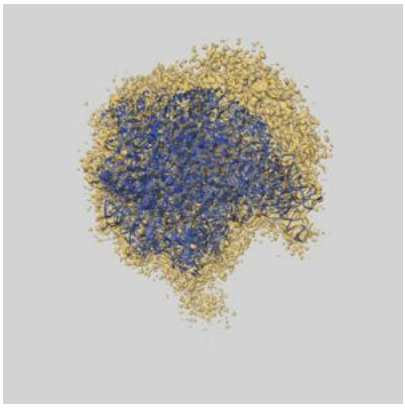
8 Fourier-Shell correlation

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

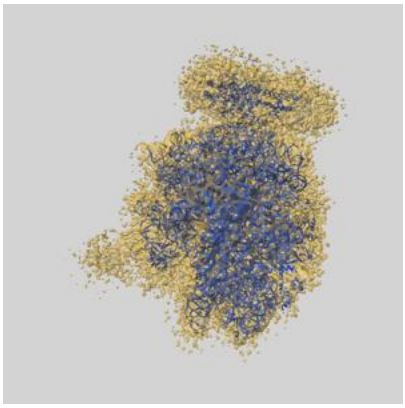
9 Map-model fit

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.

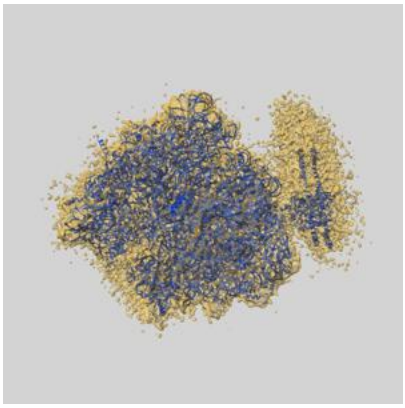
9.1 Map-model overlay



X



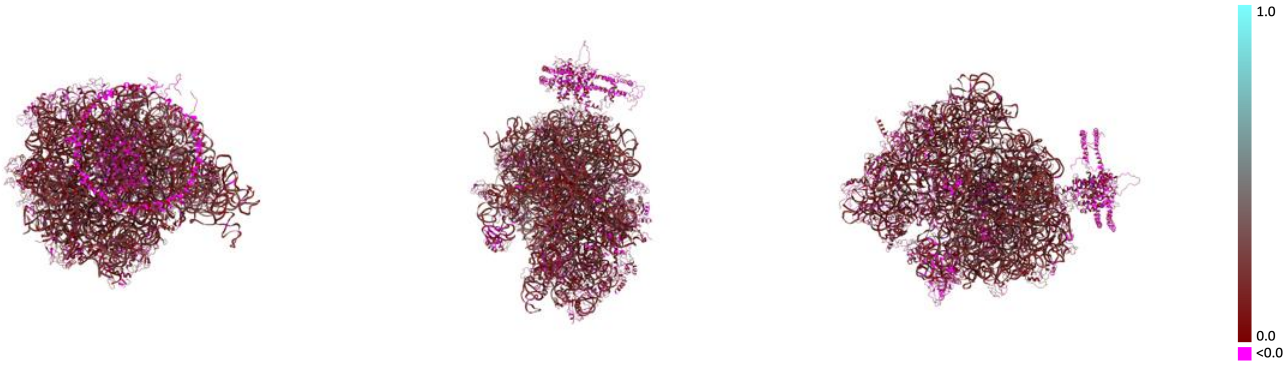
Y



Z

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.

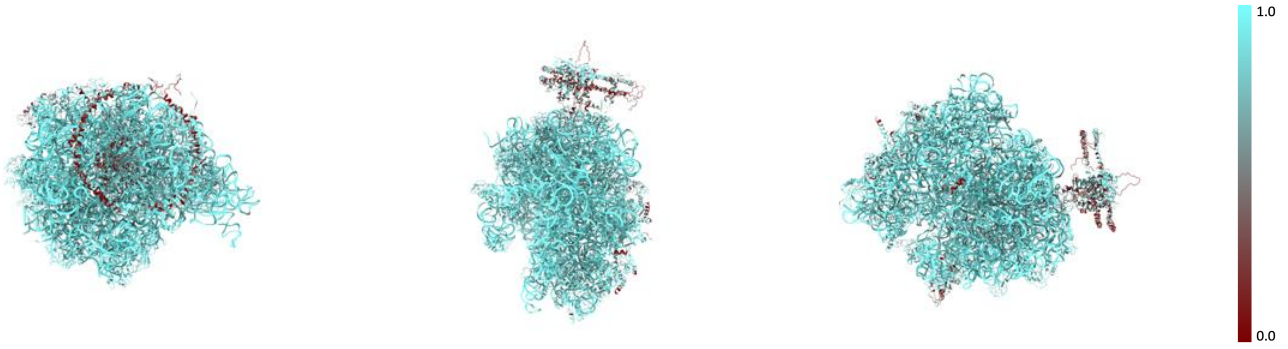
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according 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.

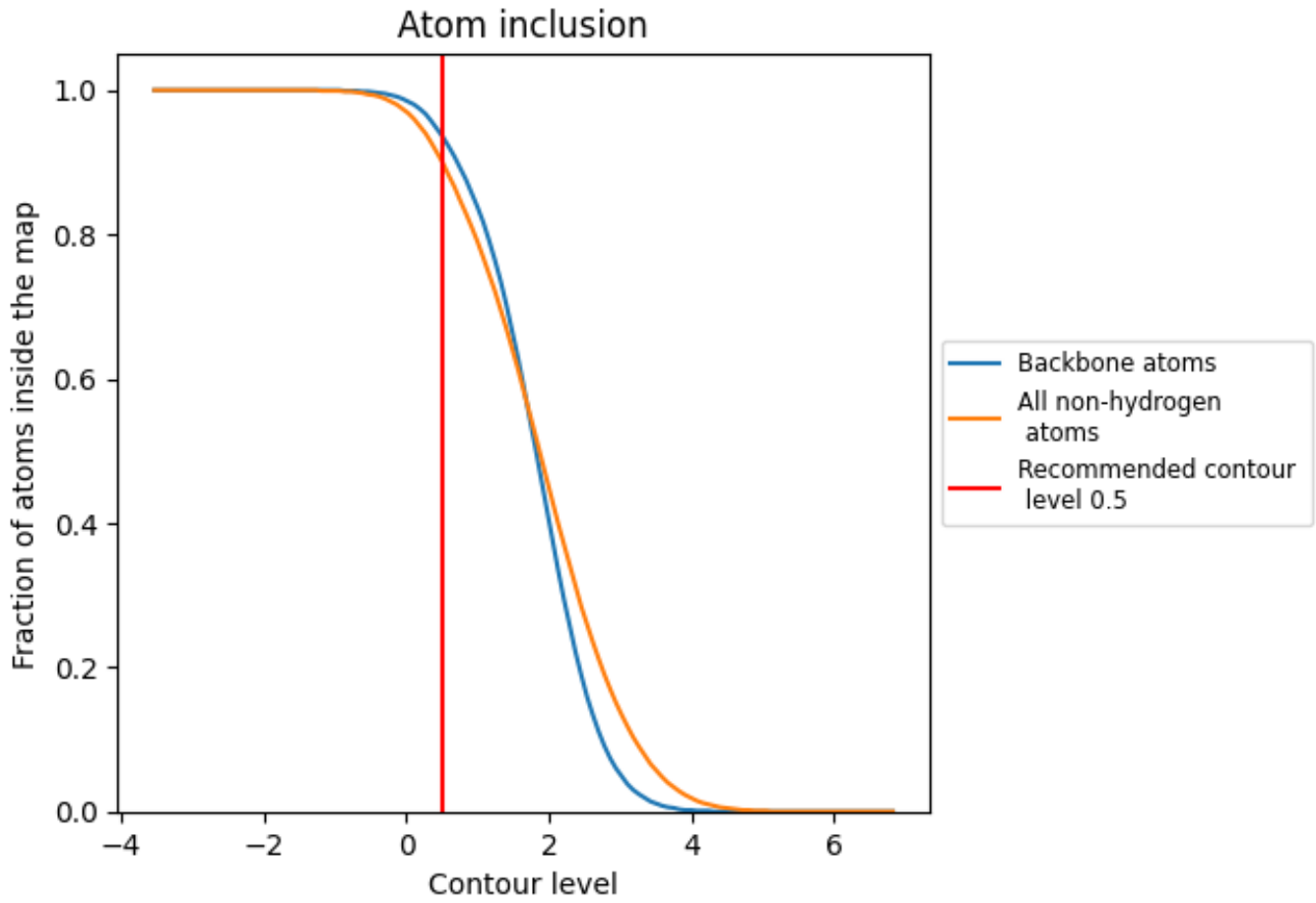
9.3 Atom inclusion mapped to coordinate model



X Y Z

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

Continued on next page...

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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