



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 11:26 AM UTC

PDB ID : 4V6M / pdb_00004v6m
EMDB ID : EMD-1858
Title : Structure of the ribosome-SecYE complex in the membrane environment
Authors : Frauenfeld, J.; Gumbart, J.; van der Sluis, E.O.; Funes, S.; Gartmann, M.;
Beatrix, B.; Mielke, T.; Berninghausen, O.; Becker, T.; Schulten, K.; Beck-
mann, R.
Deposited on : 2011-02-08
Resolution : 7.10 Å(reported)

This is a Full wwPDB EM Validation 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:

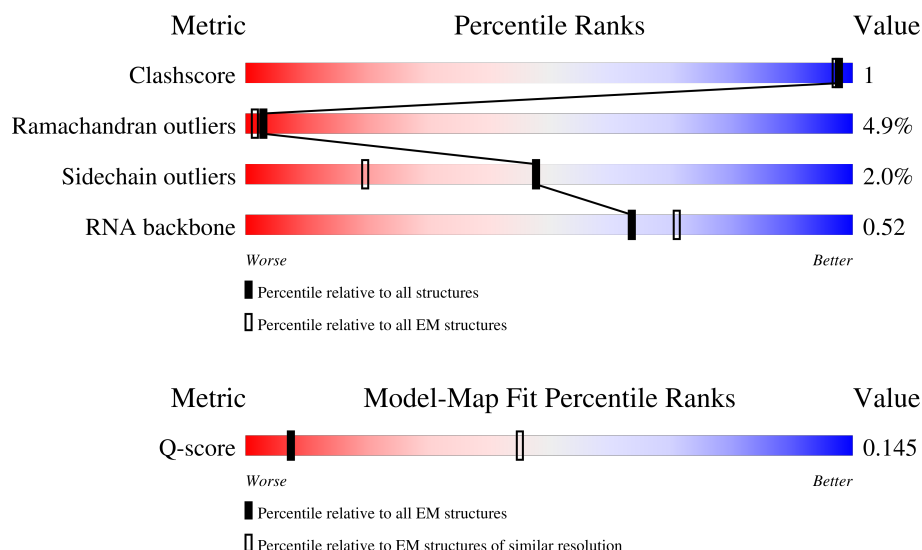
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

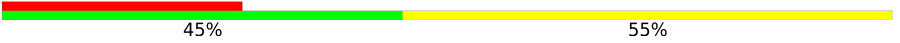
The reported resolution of this entry is 7.10 Å.

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	464 (6.60 - 7.60)

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

Mol	Chain	Length	Quality of chain
1	AA	1542	
2	AX	11	
3	AV	77	

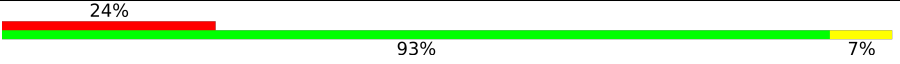
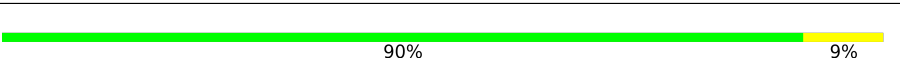
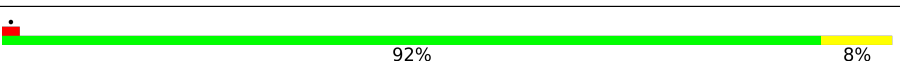
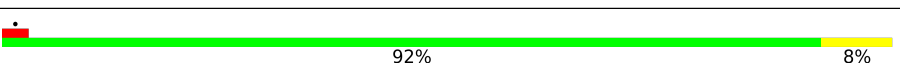
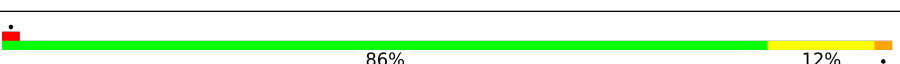
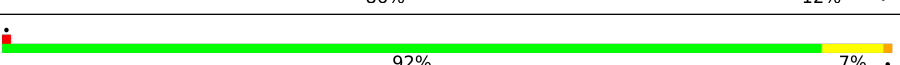
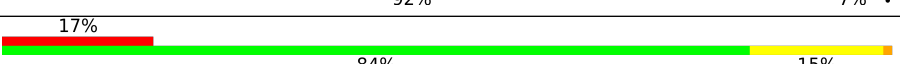
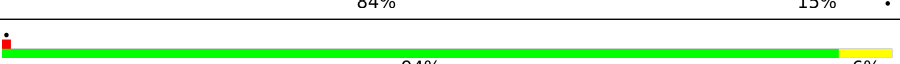
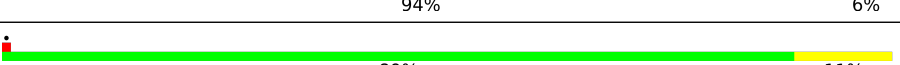
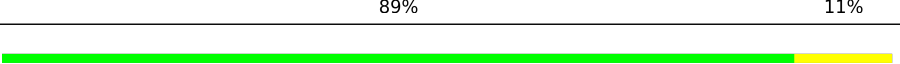
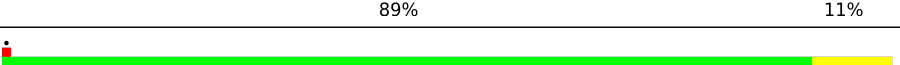
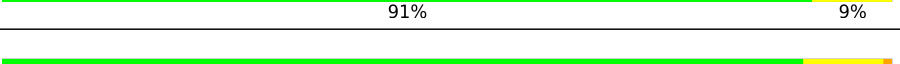
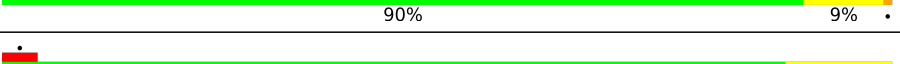
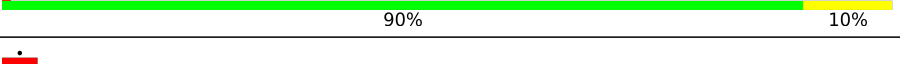
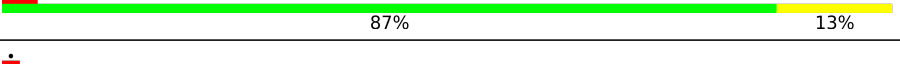
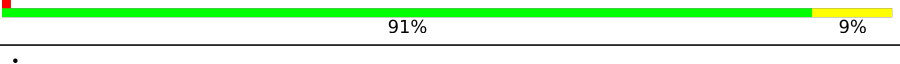
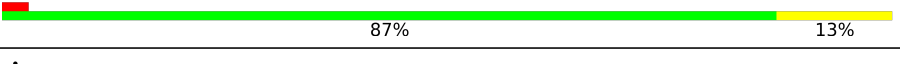
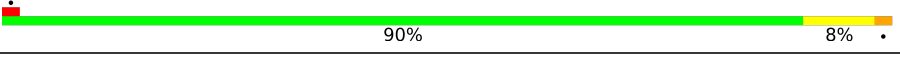
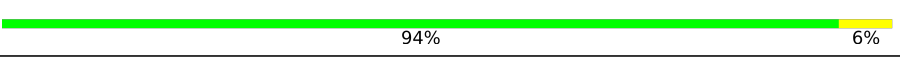
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Mol	Chain	Length	Quality of chain
4	AZ	98	
5	A0	200	
5	A1	200	
6	AB	240	
7	AC	232	
8	AD	205	
9	AE	166	
10	AF	135	
11	AG	178	
12	AH	129	
13	AI	129	
14	AJ	103	
15	AK	128	
16	AL	123	
17	AM	117	
18	AN	100	
19	AO	88	
20	AP	82	
21	AQ	83	
22	AR	74	
23	AS	91	
24	AT	86	
25	AU	70	
26	B7	120	
27	B8	2904	

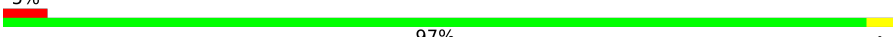
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Mol	Chain	Length	Quality of chain
28	BA	435	
29	BB	116	
30	B5	234	
31	B6	272	
32	BD	209	
33	BE	201	
34	BF	178	
35	BG	176	
36	BH	149	
37	BI	141	
38	BJ	142	
39	BK	123	
40	BL	144	
41	BM	136	
42	BN	127	
43	BO	117	
44	BP	114	
45	BQ	117	
46	BR	103	
47	BS	110	
48	BT	100	
49	BU	103	
50	BV	94	
51	BW	84	
52	BX	77	

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Mol	Chain	Length	Quality of chain
53	BY	63	
54	BZ	58	
55	B0	56	
56	B1	54	
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	-	-	-

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

2 Entry composition

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

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S RIBOSOMAL RNA.

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

- Molecule 2 is a RNA chain called mRNA.

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

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

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

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

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

There are 16 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

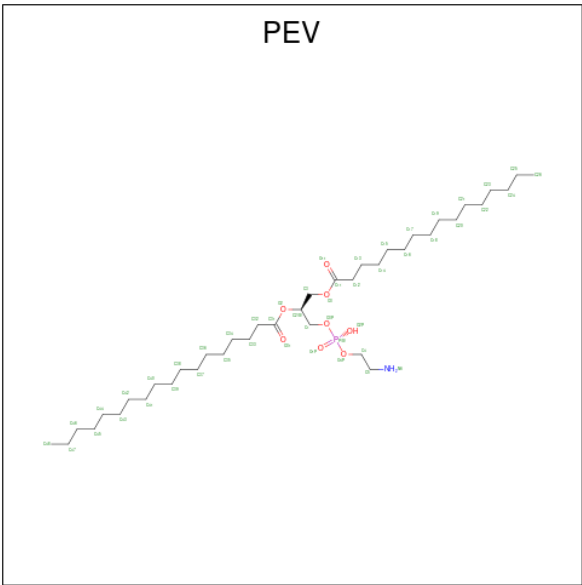
- Molecule 58 is a protein called 50S ribosomal protein L35.

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

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

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

- Molecule 60 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(PAL MITOYLOXY)METHYL]ETHYL STEARATE (CCD ID: PEV) (formula: C₃₉H₇₈NO₈P).



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

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

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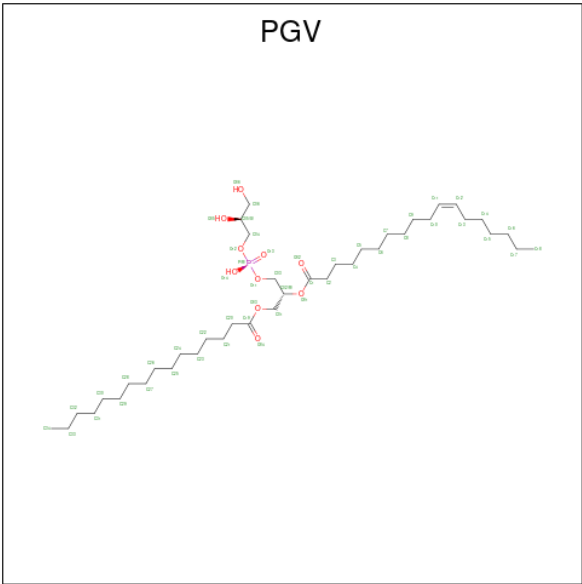
Mol	Chain	Residues	Atoms					AltConf
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60	BA	1	Total 49	C 39	N 1	O 8	P 1	0
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Mol	Chain	Residues	Atoms					AltConf
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60	BB	1	Total	C	N	O	P	0
			49	39	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 (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P).



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

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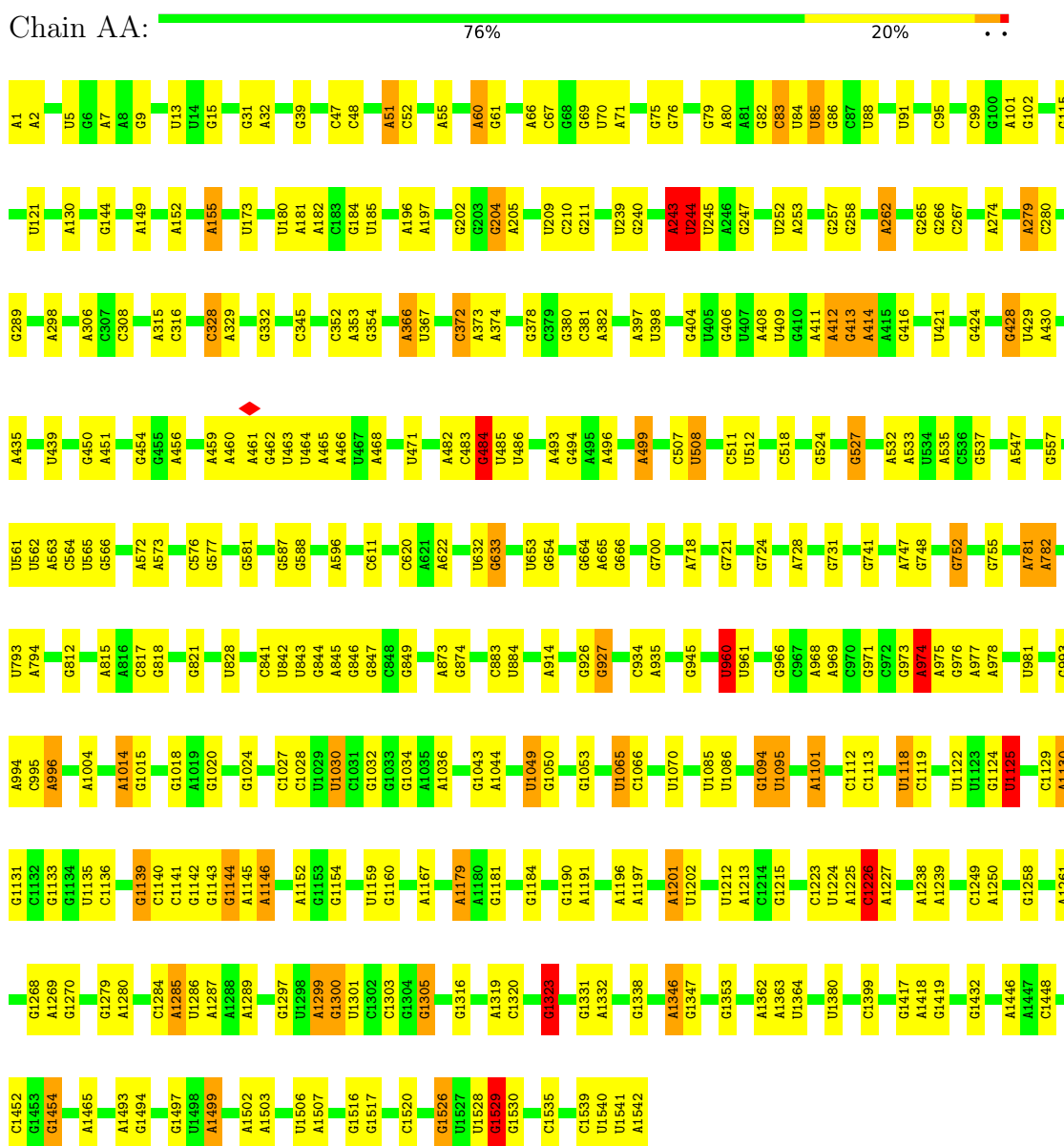
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Mol	Chain	Residues	Atoms				AltConf
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			51	40	10	1	
61	BA	1	Total	C	O	P	0
			51	40	10	1	
61	BA	1	Total	C	O	P	0
			51	40	10	1	
61	BB	1	Total	C	O	P	0
			51	40	10	1	
61	BB	1	Total	C	O	P	0
			51	40	10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

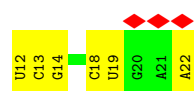
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

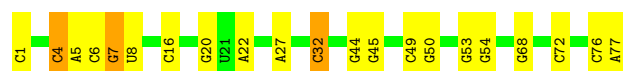
• Molecule 1: 16S RIBOSOMAL RNA



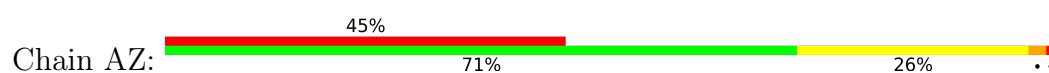
• Molecule 2: mRNA



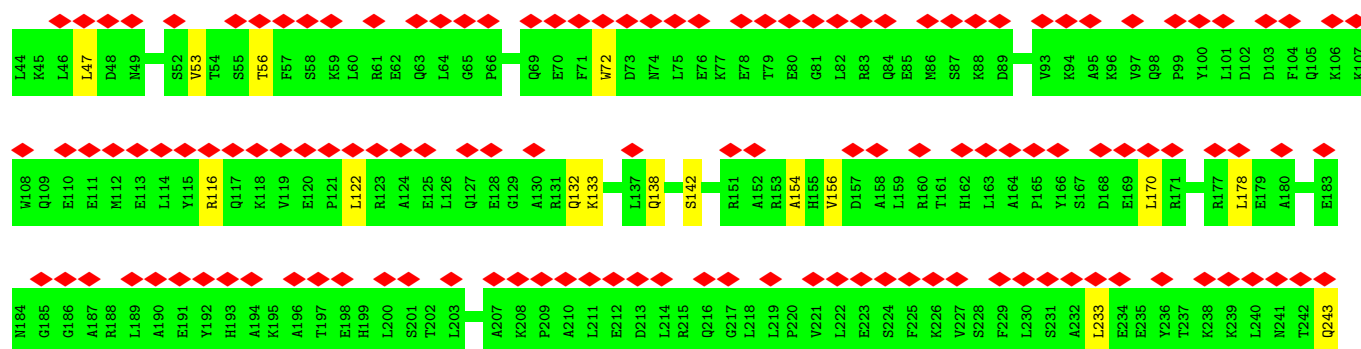
- Molecule 3: FtsQ nascent chain



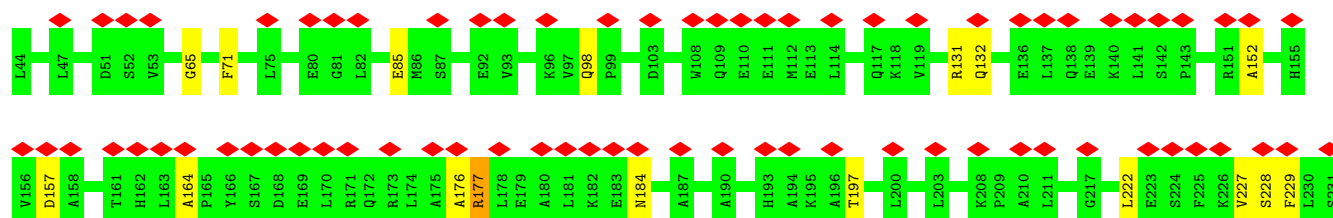
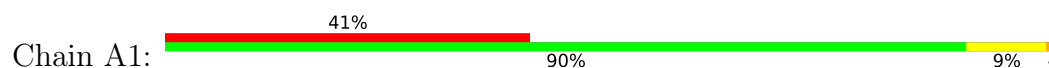
- Molecule 4: Cell division protein FtsQ

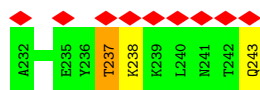


- Molecule 5: Apolipoprotein A-I

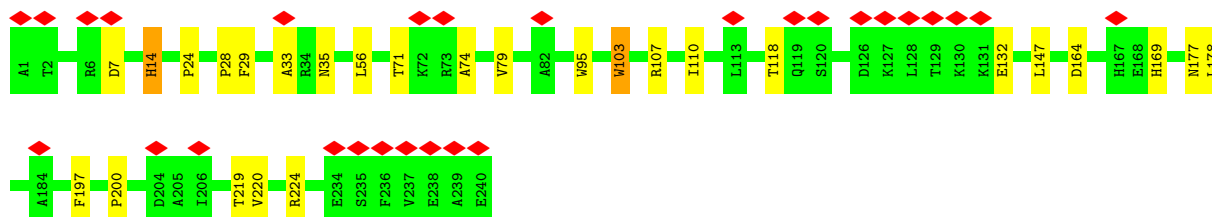
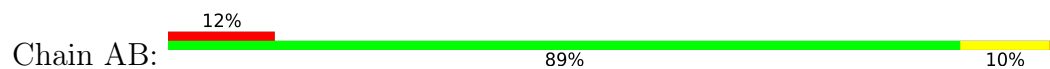


- Molecule 5: Apolipoprotein A-I

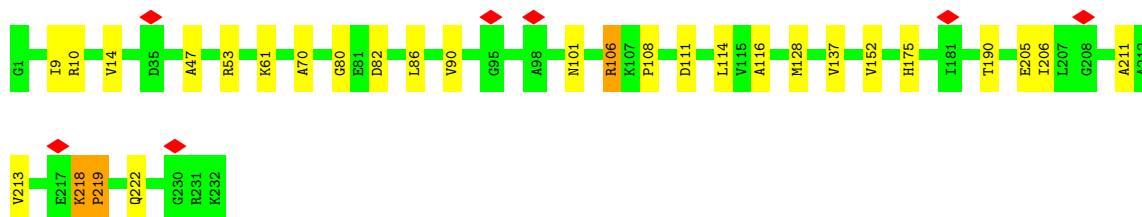
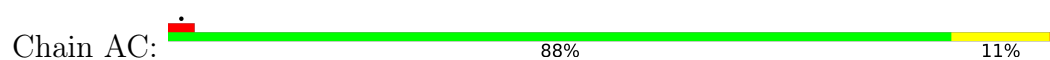




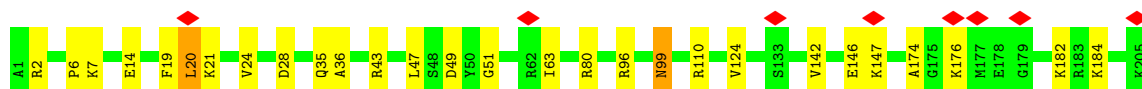
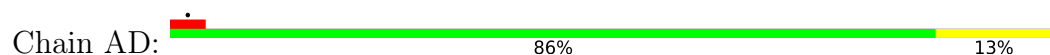
- Molecule 6: 30S ribosomal protein S2



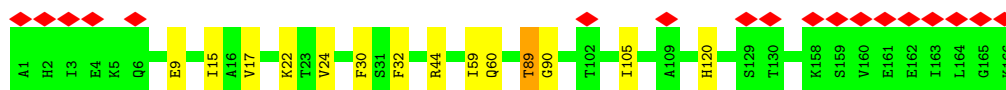
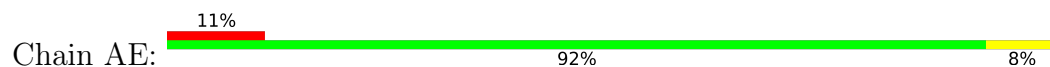
- Molecule 7: 30S ribosomal protein S3



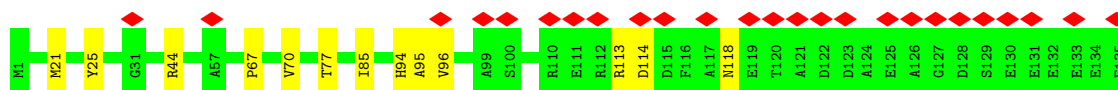
- Molecule 8: 30S ribosomal protein S4



- Molecule 9: 30S ribosomal protein S5

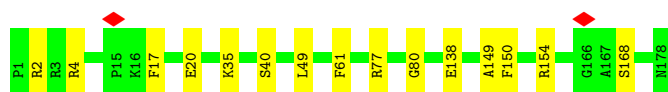


- Molecule 10: 30S ribosomal protein S6



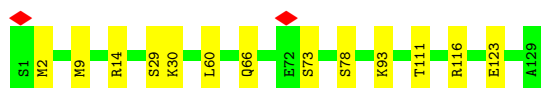
- Molecule 11: 30S ribosomal protein S7

Chain AG:  92% 8%



- Molecule 12: 30S ribosomal protein S8

Chain AH:  90% 10%



- Molecule 13: 30S ribosomal protein S9

Chain AI:  84% 16%



- Molecule 14: 30S ribosomal protein S10

Chain AJ:  87% 12%



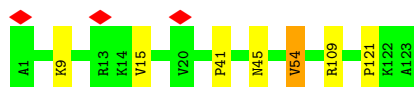
- Molecule 15: 30S ribosomal protein S11

Chain AK:  7% 88% 12%



- Molecule 16: 30S ribosomal protein S12

Chain AL:  94% 5%



- Molecule 17: 30S ribosomal protein S13

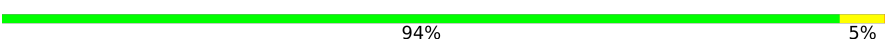
Chain AM:  90% 10%



• Molecule 18: 30S ribosomal protein S14

Chain AN:  85% 14%

• Molecule 19: 30S ribosomal protein S15

Chain AO:  94% 5%

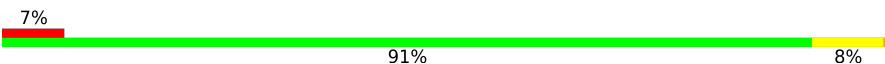
• Molecule 20: 30S ribosomal protein S16

Chain AP:  90% 9%

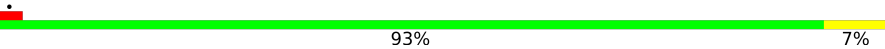
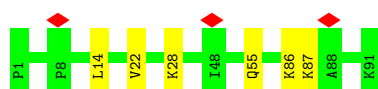
• Molecule 21: 30S ribosomal protein S17

Chain AQ:  83% 17%

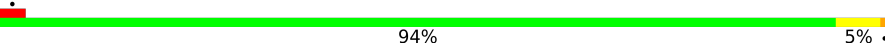
• Molecule 22: 30S ribosomal protein S18

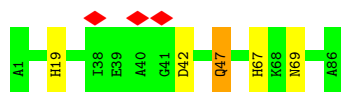
Chain AR:  7% 91% 8%

• Molecule 23: 30S ribosomal protein S19

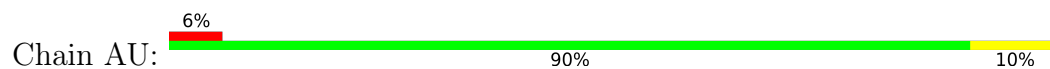
Chain AS:  93% 7%

• Molecule 24: 30S ribosomal protein S20

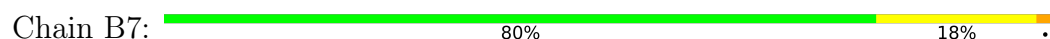
Chain AT:  94% 5%



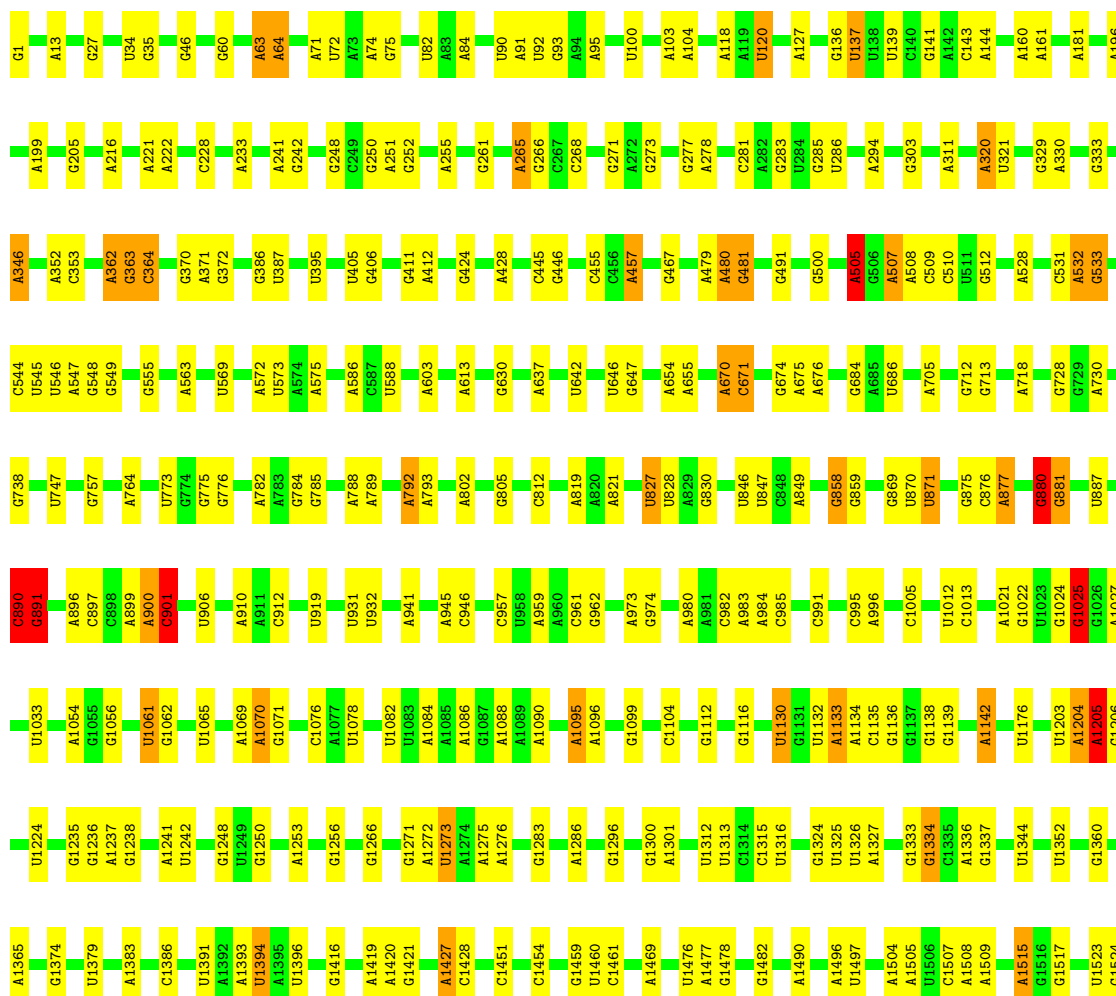
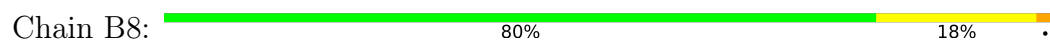
- Molecule 25: 30S ribosomal protein S21

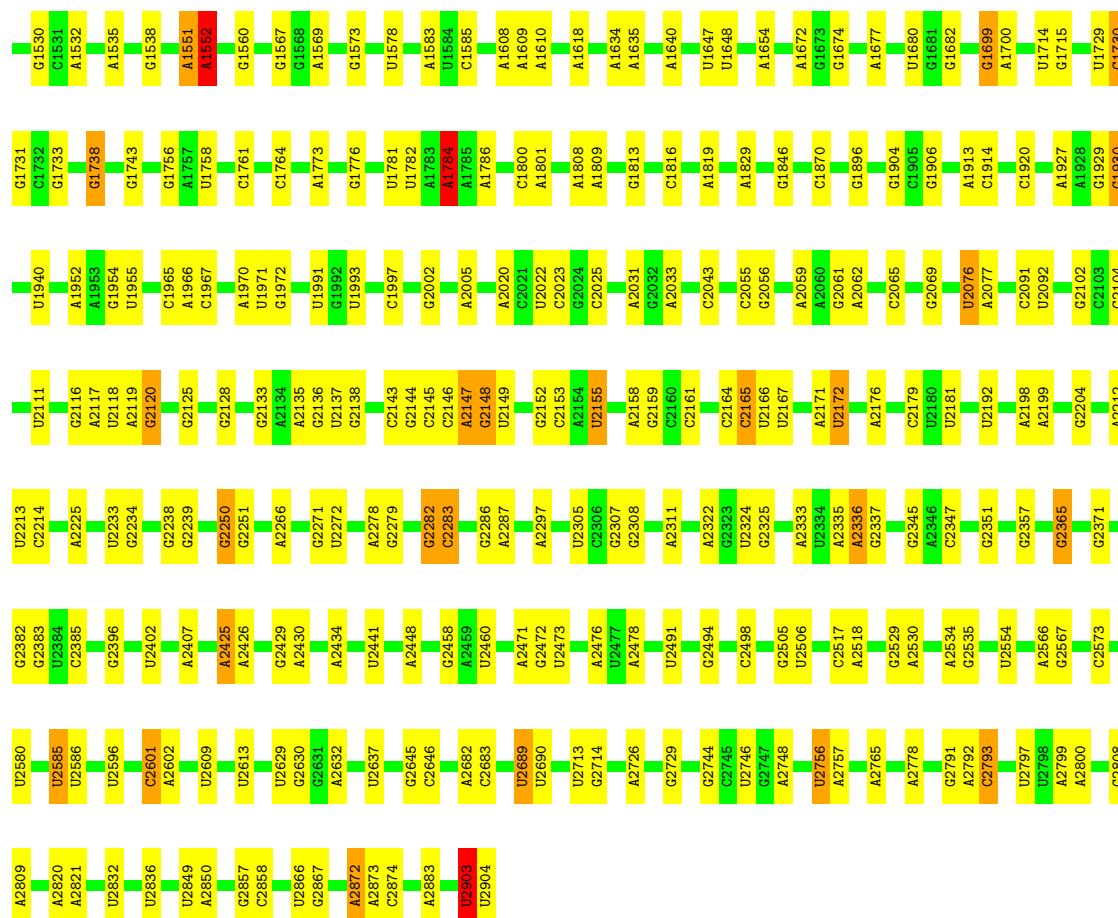


- Molecule 26: 5S RIBOSOMAL RNA

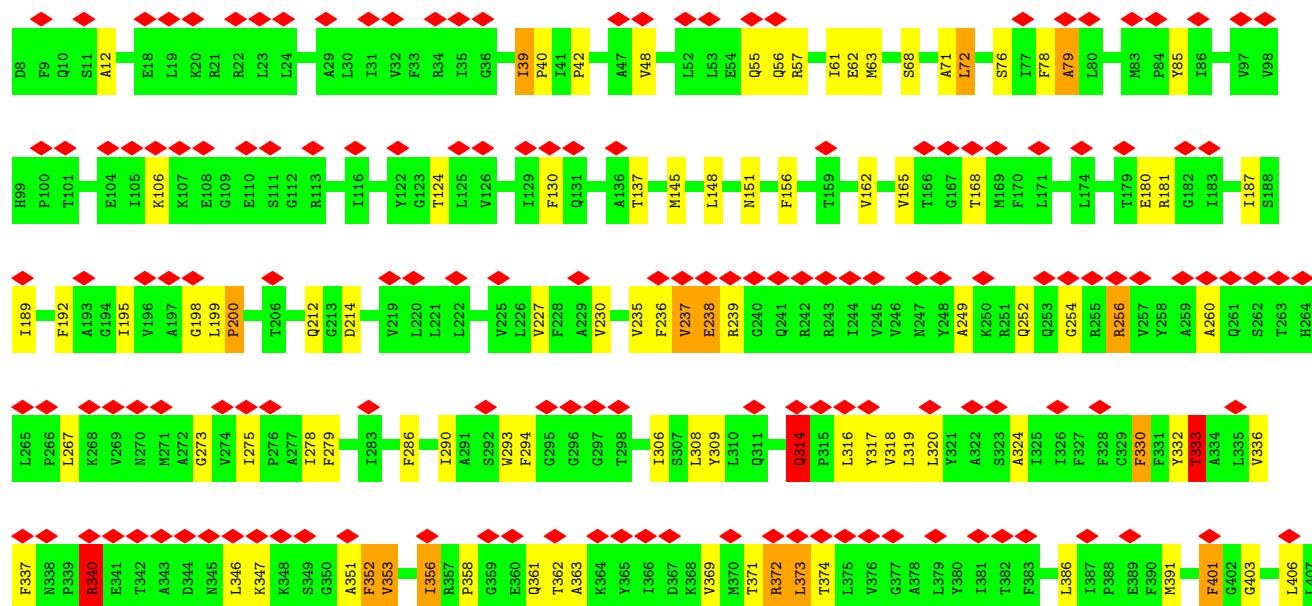
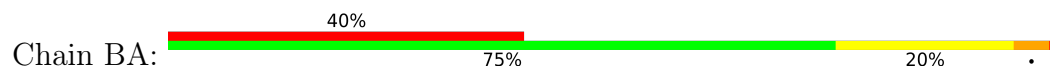


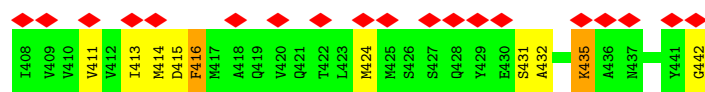
- Molecule 27: 23S RIBOSOMAL RNA



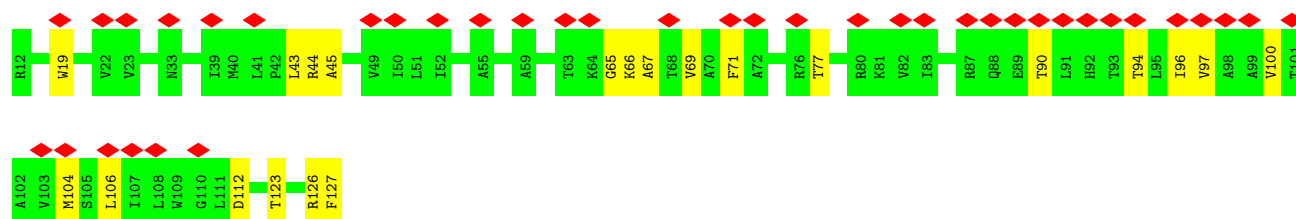
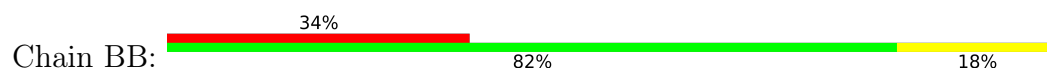


• Molecule 28: Preprotein translocase secY subunit

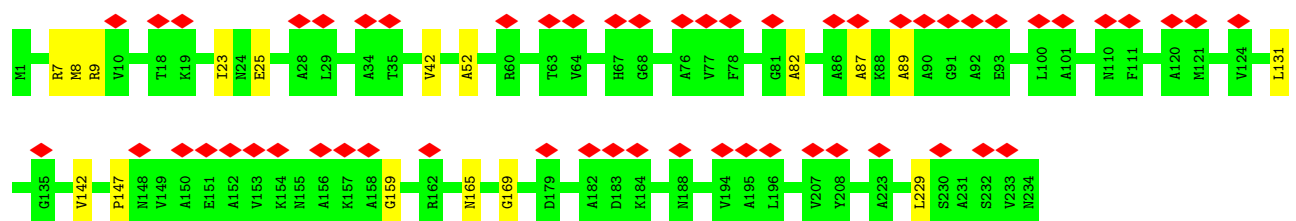




- Molecule 29: Preprotein translocase secE subunit



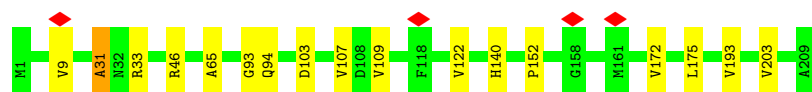
- Molecule 30: 50S ribosomal protein L1



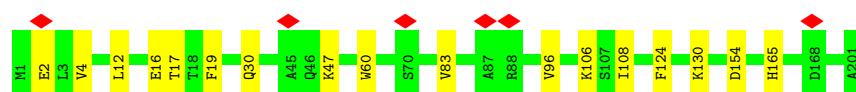
- Molecule 31: 50S ribosomal protein L2



- Molecule 32: 50S ribosomal protein L3



- Molecule 33: 50S ribosomal protein L4



- Molecule 34: 50S ribosomal protein L5

Chain BF:  86% 12%



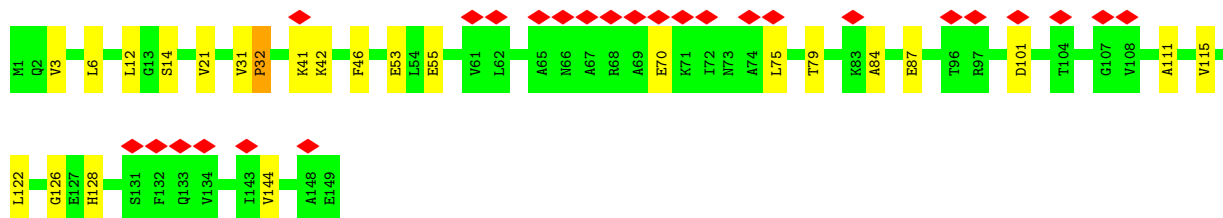
- Molecule 35: 50S ribosomal protein L6

Chain BG:  92% 7%



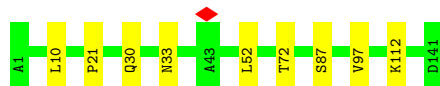
- Molecule 36: 50S ribosomal protein L9

Chain BH:  17% 84% 15%



- Molecule 37: 50S ribosomal protein L11

Chain BI:  94% 6%



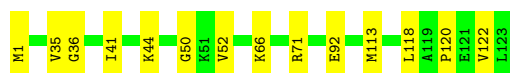
- Molecule 38: 50S ribosomal protein L13

Chain BJ:  89% 11%



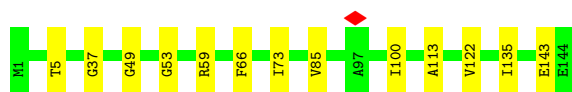
- Molecule 39: 50S ribosomal protein L14

Chain BK:  89% 11%



- Molecule 40: 50S ribosomal protein L15

Chain BL:  91% 9%



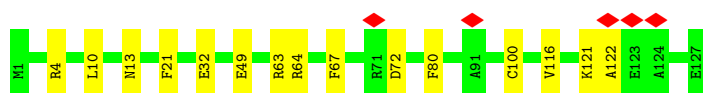
- Molecule 41: 50S ribosomal protein L16

Chain BM: 90% 9%



- Molecule 42: 50S ribosomal protein L17

Chain BN: 88% 12%



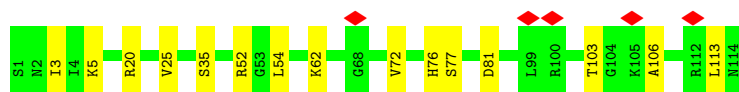
- Molecule 43: 50S ribosomal protein L18

Chain BO: 90% 10%



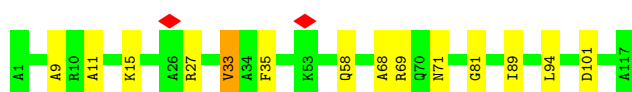
- Molecule 44: 50S ribosomal protein L19

Chain BP: 87% 13%



- Molecule 45: 50S ribosomal protein L20

Chain BQ: 88% 11%



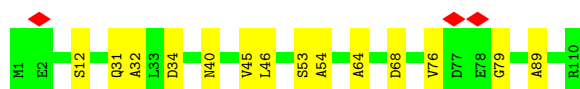
- Molecule 46: 50S ribosomal protein L21

Chain BR: 91% 9%



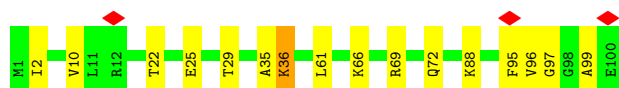
- Molecule 47: 50S ribosomal protein L22

Chain BS:  87% 13%



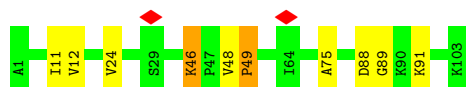
- Molecule 48: 50S ribosomal protein L23

Chain BT:  84% 15%

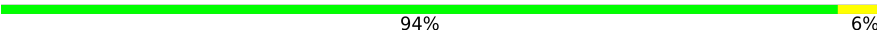


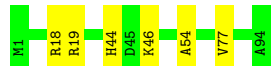
- Molecule 49: 50S ribosomal protein L24

Chain BU:  90% 8%



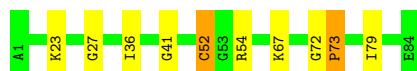
- Molecule 50: 50S ribosomal protein L25

Chain BV:  94% 6%



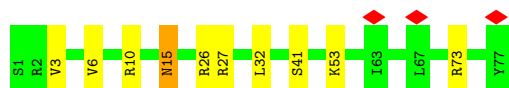
- Molecule 51: 50S ribosomal protein L27

Chain BW:  88% 10%



- Molecule 52: 50S ribosomal protein L28

Chain BX:  87% 12%



- Molecule 53: 50S ribosomal protein L29

Chain BY:  90% 10%



- Molecule 54: 50S ribosomal protein L30

Chain BZ:  88% 12%



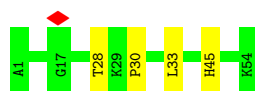
- Molecule 55: 50S ribosomal protein L32

Chain B0:  91% 9%



- Molecule 56: 50S ribosomal protein L33

Chain B1:  93% 7%



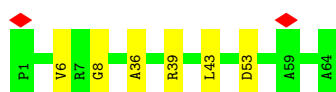
- Molecule 57: 50S ribosomal protein L34

Chain B2:  87% 11%

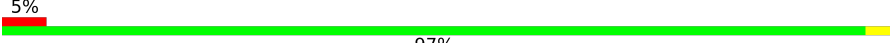


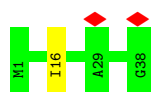
- Molecule 58: 50S ribosomal protein L35

Chain B3:  91% 9%



- Molecule 59: 50S ribosomal protein L36

Chain B4:  5% 97%



4 Experimental information

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PEV, PGV

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AA	0.90	1/37039 (0.0%)	1.11	46/57778 (0.1%)
2	AX	0.96	1/256 (0.4%)	1.09	0/394
3	AV	0.92	1/1842 (0.1%)	1.09	4/2870 (0.1%)
4	AZ	1.28	0/795	1.68	11/1082 (1.0%)
5	A0	1.19	1/1667 (0.1%)	1.58	13/2240 (0.6%)
5	A1	1.20	1/1667 (0.1%)	1.59	17/2240 (0.8%)
6	AB	1.20	0/1904	1.59	19/2565 (0.7%)
7	AC	1.28	0/1852	1.51	15/2490 (0.6%)
8	AD	1.28	0/1665	1.54	14/2227 (0.6%)
9	AE	1.26	0/1239	1.49	8/1664 (0.5%)
10	AF	1.29	0/1121	1.67	15/1509 (1.0%)
11	AG	1.29	1/1422 (0.1%)	1.61	8/1908 (0.4%)
12	AH	1.26	0/989	1.48	10/1326 (0.8%)
13	AI	1.36	0/1048	1.46	13/1394 (0.9%)
14	AJ	1.32	0/835	1.40	2/1127 (0.2%)
15	AK	1.33	0/982	1.55	13/1323 (1.0%)
16	AL	1.36	0/969	1.39	4/1300 (0.3%)
17	AM	1.31	0/919	1.62	7/1226 (0.6%)
18	AN	1.33	0/817	1.60	10/1088 (0.9%)
19	AO	1.33	0/724	1.75	6/966 (0.6%)
20	AP	1.34	0/659	1.48	7/884 (0.8%)
21	AQ	1.31	0/681	1.36	6/913 (0.7%)
22	AR	1.36	0/637	1.54	5/851 (0.6%)
23	AS	1.24	0/744	1.40	2/995 (0.2%)
24	AT	1.24	0/676	1.74	6/895 (0.7%)
25	AU	1.41	0/598	1.49	4/792 (0.5%)
26	B7	0.90	1/2873 (0.0%)	1.13	4/4478 (0.1%)
27	B8	0.89	1/69822 (0.0%)	1.10	49/108926 (0.0%)
28	BA	1.51	7/3439 (0.2%)	1.71	52/4662 (1.1%)
29	BB	1.22	1/902 (0.1%)	1.76	20/1228 (1.6%)
30	B5	1.20	0/1748	1.47	9/2355 (0.4%)
31	B6	1.33	0/2131	1.48	16/2863 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	BD	1.27	0/1586	1.45	6/2134 (0.3%)
33	BE	1.24	0/1571	1.53	4/2113 (0.2%)
34	BF	1.28	0/1444	1.53	12/1937 (0.6%)
35	BG	1.25	0/1343	1.44	5/1816 (0.3%)
36	BH	1.23	0/1122	1.54	10/1515 (0.7%)
37	BI	1.13	0/1046	1.62	8/1410 (0.6%)
38	BJ	1.25	0/1152	1.54	14/1551 (0.9%)
39	BK	1.31	0/956	1.46	8/1279 (0.6%)
40	BL	1.29	0/1062	1.45	10/1413 (0.7%)
41	BM	1.29	0/1093	1.45	3/1460 (0.2%)
42	BN	1.37	0/1021	1.48	3/1364 (0.2%)
43	BO	1.35	0/910	1.49	12/1219 (1.0%)
44	BP	1.34	0/929	1.50	10/1242 (0.8%)
45	BQ	1.33	0/960	1.66	13/1278 (1.0%)
46	BR	1.30	0/829	1.42	6/1107 (0.5%)
47	BS	1.32	0/864	1.56	8/1156 (0.7%)
48	BT	1.28	0/794	1.52	5/1060 (0.5%)
49	BU	1.26	0/797	1.44	7/1062 (0.7%)
50	BV	1.27	0/766	1.49	6/1025 (0.6%)
51	BW	1.34	0/642	1.50	7/848 (0.8%)
52	BX	1.36	0/635	1.52	6/848 (0.7%)
53	BY	1.27	0/510	1.61	6/677 (0.9%)
54	BZ	1.29	0/453	1.55	5/605 (0.8%)
55	B0	1.37	0/450	1.58	5/599 (0.8%)
56	B1	1.21	0/448	1.36	2/594 (0.3%)
57	B2	1.50	0/380	1.56	2/498 (0.4%)
58	B3	1.25	0/513	1.44	3/676 (0.4%)
59	B4	1.43	0/303	1.33	0/397
All	All	1.05	16/169241 (0.0%)	1.26	601/251442 (0.2%)

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

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	BA	416	PHE	CG-CD2	29.61	2.01	1.38
28	BA	416	PHE	CG-CD1	28.25	1.98	1.38
28	BA	416	PHE	CE2-CZ	19.06	1.95	1.38
28	BA	416	PHE	CE1-CZ	18.91	1.95	1.38
28	BA	416	PHE	CD2-CE2	18.79	1.95	1.38
28	BA	416	PHE	CD1-CE1	17.84	1.92	1.38
28	BA	442	GLY	C-OXT	6.87	1.37	1.23
5	A0	243	GLN	C-OXT	6.87	1.37	1.23
5	A1	243	GLN	C-OXT	6.85	1.37	1.23
29	BB	127	PHE	C-OXT	6.82	1.37	1.23
2	AX	12	U	OP3-P	5.90	1.60	1.48
3	AV	1	C	OP3-P	5.89	1.60	1.48
27	B8	1	G	OP3-P	5.83	1.60	1.48
26	B7	1	U	OP3-P	5.78	1.60	1.48
1	AA	1	A	OP3-P	5.45	1.59	1.48
11	AG	61	PHE	CA-C	-5.05	1.49	1.52

All (601) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	85	U	P-O3'-C3'	15.28	143.11	120.20
27	B8	670	A	P-O3'-C3'	13.55	140.52	120.20
27	B8	2076	U	P-O3'-C3'	12.22	138.53	120.20
1	AA	328	C	P-O3'-C3'	11.20	137.00	120.20
27	B8	890	C	P-O3'-C3'	11.03	136.75	120.20
1	AA	1014	A	P-O3'-C3'	10.79	136.38	120.20
27	B8	880	G	P-O3'-C3'	10.77	136.36	120.20
27	B8	1205	A	P-O3'-C3'	10.37	135.75	120.20
1	AA	1226	C	P-O3'-C3'	10.21	135.51	120.20
27	B8	1061	U	P-O3'-C3'	9.93	135.09	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2336	A	P-O3'-C3'	9.72	134.78	120.20
1	AA	1065	U	P-O3'-C3'	9.61	134.62	120.20
1	AA	960	U	P-O3'-C3'	9.59	134.59	120.20
41	BM	36	VAL	N-CA-C	-9.30	104.31	112.12
4	AZ	46	LEU	CA-C-N	9.16	130.29	120.03
4	AZ	46	LEU	C-N-CA	9.16	130.29	120.03
1	AA	484	G	P-O3'-C3'	9.03	133.74	120.20
1	AA	243	A	C2'-C3'-O3'	8.76	122.64	109.50
9	AE	59	ILE	N-CA-C	-8.76	104.76	112.12
27	B8	2425	A	P-O3'-C3'	8.74	133.31	120.20
1	AA	60	A	P-O3'-C3'	8.68	133.22	120.20
27	B8	1315	C	P-O3'-C3'	8.63	133.15	120.20
43	BO	74	VAL	N-CA-C	-8.48	104.48	112.96
27	B8	2282	G	C2'-C3'-O3'	8.45	122.18	109.50
15	AK	107	THR	N-CA-C	-8.42	105.02	114.62
6	AB	110	ILE	N-CA-C	-8.39	104.57	112.96
28	BA	415	ASP	CA-C-N	8.28	131.20	120.44
28	BA	415	ASP	C-N-CA	8.28	131.20	120.44
18	AN	53	ASP	CA-CB-CG	-8.24	104.36	112.60
1	AA	366	A	P-O3'-C3'	8.22	132.53	120.20
11	AG	168	SER	N-CA-C	-8.18	105.30	114.62
25	AU	12	ASP	N-CA-C	-8.03	103.31	113.43
1	AA	1201	A	P-O3'-C3'	7.81	131.92	120.20
1	AA	372	C	P-O3'-C3'	7.81	131.92	120.20
27	B8	2601	C	P-O3'-C3'	7.81	131.91	120.20
1	AA	1284	C	P-O3'-C3'	7.75	131.83	120.20
1	AA	279	A	P-O3'-C3'	7.72	131.78	120.20
27	B8	2147	A	P-O3'-C3'	7.63	131.65	120.20
40	BL	85	VAL	N-CA-C	-7.59	105.44	112.43
1	AA	960	U	C2'-C3'-O3'	7.59	120.88	109.50
43	BO	58	ILE	N-CA-C	-7.52	105.87	113.47
7	AC	137	VAL	N-CA-C	-7.46	105.50	112.96
29	BB	100	VAL	N-CA-C	-7.42	105.54	112.96
48	BT	22	THR	N-CA-C	-7.38	104.14	113.43
26	B7	66	A	P-O3'-C3'	7.38	131.26	120.20
45	BQ	35	PHE	N-CA-C	-7.26	103.42	112.72
48	BT	25	GLU	N-CA-C	-7.20	106.41	114.62
27	B8	792	A	P-O3'-C3'	7.20	130.99	120.20
28	BA	314	GLN	CA-C-O	-7.17	110.33	120.16
38	BJ	28	LEU	N-CA-C	-7.13	104.21	113.12
27	B8	827	U	P-O3'-C3'	7.12	130.88	120.20
40	BL	143	GLU	N-CA-C	-7.12	105.52	114.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	BJ	78	THR	N-CA-C	-7.08	105.83	114.75
48	BT	88	LYS	N-CA-C	-7.04	105.61	114.56
27	B8	1730	C	P-O3'-C3'	7.00	130.70	120.20
6	AB	29	PHE	N-CA-C	-6.97	106.67	114.62
4	AZ	28	ILE	N-CA-CB	6.96	120.01	110.54
44	BP	5	LYS	N-CA-C	-6.93	104.45	113.12
38	BJ	81	ILE	N-CA-C	-6.93	106.54	113.20
37	BI	21	PRO	N-CA-C	6.93	119.16	110.70
27	B8	1333	G	P-O3'-C3'	6.83	130.45	120.20
32	BD	94	GLN	N-CA-C	-6.80	106.18	114.75
16	AL	15	VAL	N-CA-C	-6.79	106.03	113.43
8	AD	14	GLU	N-CA-C	-6.77	105.58	114.31
27	B8	2282	G	P-O3'-C3'	6.76	130.33	120.20
39	BK	66	LYS	N-CA-C	-6.74	106.94	114.62
28	BA	137	THR	N-CA-C	-6.73	105.20	113.41
28	BA	40	PRO	CA-C-N	6.73	124.48	120.24
28	BA	40	PRO	C-N-CA	6.73	124.48	120.24
28	BA	401	PHE	N-CA-CB	6.72	121.84	110.49
9	AE	32	PHE	CA-CB-CG	-6.71	107.09	113.80
56	B1	28	THR	N-CA-C	-6.69	105.40	113.97
27	B8	670	A	C2'-C3'-O3'	6.61	119.41	109.50
34	BF	72	SER	N-CA-C	-6.61	103.96	113.21
27	B8	1551	A	P-O3'-C3'	6.57	130.05	120.20
26	B7	27	C	P-O5'-C5'	6.55	130.72	120.90
1	AA	85	U	C2'-C3'-O3'	6.54	119.31	109.50
36	BH	12	LEU	CA-C-N	6.53	126.19	119.92
36	BH	12	LEU	C-N-CA	6.53	126.19	119.92
3	AV	7	G	P-O3'-C3'	6.52	129.98	120.20
29	BB	43	LEU	N-CA-C	-6.47	105.54	113.50
28	BA	314	GLN	CB-CA-C	6.46	122.89	110.17
6	AB	147	LEU	CA-C-N	6.46	127.26	120.03
6	AB	147	LEU	C-N-CA	6.46	127.26	120.03
45	BQ	11	ALA	N-CA-C	-6.43	106.06	114.04
28	BA	279	PHE	N-CA-C	6.42	117.94	111.07
13	AI	103	VAL	N-CA-C	-6.39	106.76	112.90
6	AB	177	ASN	N-CA-C	-6.39	105.12	113.17
45	BQ	58	GLN	N-CA-C	-6.36	104.58	112.72
42	BN	116	VAL	N-CA-C	-6.35	106.55	112.83
1	AA	1049	U	P-O3'-C3'	6.34	129.72	120.20
44	BP	103	THR	CA-C-N	6.33	126.00	119.92
44	BP	103	THR	C-N-CA	6.33	126.00	119.92
1	AA	51	A	C2'-C3'-O3'	6.32	118.98	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	AZ	47	GLY	N-CA-C	6.30	120.52	112.83
13	AI	71	ILE	N-CA-C	-6.30	105.59	111.45
4	AZ	24	ARG	N-CA-C	-6.29	106.14	113.88
48	BT	2	ILE	N-CA-C	-6.29	106.67	112.96
44	BP	72	VAL	N-CA-C	-6.28	99.00	108.17
34	BF	155	ILE	N-CA-C	-6.26	106.70	112.96
48	BT	95	PHE	CA-CB-CG	-6.26	107.54	113.80
29	BB	90	THR	CA-C-N	6.25	128.66	120.28
29	BB	90	THR	C-N-CA	6.25	128.66	120.28
8	AD	124	VAL	N-CA-C	-6.24	99.06	108.17
8	AD	24	VAL	N-CA-C	-6.22	106.71	112.43
28	BA	200	PRO	N-CA-C	6.22	118.29	110.70
1	AA	279	A	C2'-C3'-O3'	6.21	118.82	109.50
1	AA	76	G	P-O5'-C5'	6.19	130.19	120.90
29	BB	112	ASP	N-CA-C	6.19	118.03	111.28
28	BA	340	ARG	N-CA-CB	6.19	120.94	110.49
6	AB	14	HIS	N-CA-C	-6.17	107.59	114.62
1	AA	51	A	P-O3'-C3'	6.15	129.43	120.20
52	BX	73	ARG	N-CA-C	-6.14	106.11	113.97
1	AA	1454	G	P-O5'-C5'	6.12	130.09	120.90
28	BA	124	THR	N-CA-C	-6.12	106.41	114.31
5	A1	229	PHE	N-CA-C	-6.12	105.72	113.43
38	BJ	131	ASN	N-CA-C	-6.12	104.65	113.21
28	BA	294	PHE	N-CA-C	-6.10	105.01	112.88
44	BP	52	ARG	N-CA-C	-6.09	107.08	114.75
1	AA	1300	G	P-O3'-C3'	6.07	129.30	120.20
15	AK	117	HIS	N-CA-C	-6.07	105.19	112.59
6	AB	178	LEU	N-CA-C	-6.03	107.16	114.75
27	B8	901	C	P-O5'-C5'	6.02	129.94	120.90
52	BX	53	LYS	CA-C-N	6.02	127.66	120.14
52	BX	53	LYS	C-N-CA	6.02	127.66	120.14
31	B6	66	PHE	N-CA-C	-6.02	107.17	114.75
1	AA	155	A	P-O5'-C5'	6.00	129.90	120.90
12	AH	66	GLN	N-CA-C	-5.99	104.83	113.21
18	AN	45	LEU	CA-C-N	5.99	128.22	120.44
18	AN	45	LEU	C-N-CA	5.99	128.22	120.44
28	BA	156	PHE	N-CA-C	-5.96	106.98	114.56
27	B8	2283	C	P-O5'-C5'	5.96	129.84	120.90
34	BF	137	PHE	CA-C-N	5.95	127.28	119.84
34	BF	137	PHE	C-N-CA	5.95	127.28	119.84
27	B8	1552	A	P-O5'-C5'	5.95	129.82	120.90
13	AI	3	ASN	N-CA-C	-5.94	104.89	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B7	117	G	P-O3'-C3'	5.94	129.11	120.20
36	BH	42	LYS	CA-C-N	5.93	129.04	120.38
36	BH	42	LYS	C-N-CA	5.93	129.04	120.38
13	AI	72	SER	CA-C-N	5.93	126.56	119.98
13	AI	72	SER	C-N-CA	5.93	126.56	119.98
50	BV	19	ARG	CA-C-N	5.93	128.15	120.44
50	BV	19	ARG	C-N-CA	5.93	128.15	120.44
44	BP	62	LYS	N-CA-C	-5.93	106.38	113.97
11	AG	40	SER	CA-C-N	5.92	128.24	120.60
11	AG	40	SER	C-N-CA	5.92	128.24	120.60
31	B6	220	ARG	CA-C-N	5.92	126.55	119.98
31	B6	220	ARG	C-N-CA	5.92	126.55	119.98
1	AA	428	G	P-O3'-C3'	5.91	129.07	120.20
28	BA	187	ILE	CA-C-N	5.91	128.79	120.28
28	BA	187	ILE	C-N-CA	5.91	128.79	120.28
45	BQ	89	ILE	N-CA-C	-5.91	107.23	112.90
1	AA	1190	G	P-O3'-C3'	5.90	129.04	120.20
6	AB	35	ASN	N-CA-C	-5.90	106.13	113.38
27	B8	2120	G	P-O3'-C3'	5.90	129.04	120.20
28	BA	76	SER	CA-C-N	5.89	128.39	120.50
28	BA	76	SER	C-N-CA	5.89	128.39	120.50
24	AT	47	GLN	CA-C-N	5.89	129.65	120.82
24	AT	47	GLN	C-N-CA	5.89	129.65	120.82
41	BM	8	LYS	N-CA-C	-5.88	107.34	114.75
30	B5	229	LEU	N-CA-C	-5.88	106.08	113.72
47	BS	46	LEU	N-CA-C	-5.88	106.65	113.88
49	BU	11	ILE	N-CA-C	-5.87	107.03	113.43
31	B6	267	VAL	N-CA-C	-5.87	106.09	111.67
23	AS	22	VAL	N-CA-C	-5.85	107.28	112.90
23	AS	14	LEU	N-CA-C	-5.85	106.68	113.88
4	AZ	37	THR	CA-C-N	5.85	127.93	120.56
4	AZ	37	THR	C-N-CA	5.85	127.93	120.56
1	AA	243	A	C4'-C3'-C2'	5.84	108.44	102.60
27	B8	2161	C	P-O3'-C3'	5.82	128.93	120.20
34	BF	76	PHE	N-CA-C	-5.81	106.05	114.12
33	BE	17	THR	N-CA-C	-5.80	106.54	113.97
28	BA	200	PRO	CA-C-O	-5.80	112.15	120.56
39	BK	120	PRO	N-CA-C	-5.79	108.03	114.92
47	BS	54	ALA	CA-C-N	5.79	127.86	120.56
47	BS	54	ALA	C-N-CA	5.79	127.86	120.56
27	B8	671	C	C5'-C4'-C3'	-5.79	107.32	116.00
46	BR	53	PHE	CA-CB-CG	-5.79	108.02	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	BQ	68	ALA	CA-C-N	5.78	128.34	120.54
45	BQ	68	ALA	C-N-CA	5.78	128.34	120.54
31	B6	242	HIS	CA-C-N	5.78	125.79	119.90
31	B6	242	HIS	C-N-CA	5.78	125.79	119.90
7	AC	80	GLY	CA-C-N	5.78	128.34	120.54
7	AC	80	GLY	C-N-CA	5.78	128.34	120.54
27	B8	363	G	P-O5'-C5'	5.78	129.56	120.90
6	AB	7	ASP	CA-C-N	5.77	128.01	120.28
6	AB	7	ASP	C-N-CA	5.77	128.01	120.28
28	BA	353	VAL	N-CA-CB	5.77	119.28	111.21
29	BB	104	MET	CA-C-N	5.76	128.00	120.28
29	BB	104	MET	C-N-CA	5.76	128.00	120.28
43	BO	78	VAL	N-CA-C	-5.76	107.37	112.90
27	B8	2165	C	P-O3'-C3'	5.75	128.83	120.20
53	BY	51	ALA	CA-C-N	5.75	129.45	120.82
53	BY	51	ALA	C-N-CA	5.75	129.45	120.82
6	AB	118	THR	N-CA-C	-5.75	106.61	113.97
40	BL	122	VAL	N-CA-C	-5.74	105.80	111.77
40	BL	73	ILE	N-CA-C	-5.74	107.53	113.10
51	BW	79	ILE	N-CA-C	-5.74	99.79	108.17
38	BJ	50	THR	CA-C-N	5.73	125.42	119.92
38	BJ	50	THR	C-N-CA	5.73	125.42	119.92
39	BK	52	VAL	N-CA-C	-5.72	107.69	113.47
6	AB	220	VAL	N-CA-C	-5.72	107.24	112.96
29	BB	66	LYS	CA-C-N	5.72	132.46	121.54
29	BB	66	LYS	C-N-CA	5.72	132.46	121.54
9	AE	60	GLN	CA-C-N	5.71	128.51	120.28
9	AE	60	GLN	C-N-CA	5.71	128.51	120.28
10	AF	25	TYR	CA-C-N	5.71	128.20	120.38
10	AF	25	TYR	C-N-CA	5.71	128.20	120.38
6	AB	24	PRO	N-CA-C	-5.70	108.13	114.92
8	AD	99	ASN	CA-CB-CG	-5.70	106.90	112.60
35	BG	66	THR	CA-C-N	5.70	128.19	120.38
35	BG	66	THR	C-N-CA	5.70	128.19	120.38
16	AL	121	PRO	N-CA-C	-5.69	108.15	114.92
36	BH	122	LEU	N-CA-C	-5.69	106.50	113.50
6	AB	71	THR	N-CA-C	-5.69	105.74	114.16
22	AR	66	LEU	N-CA-C	-5.68	106.90	113.88
38	BJ	27	ARG	N-CA-C	-5.68	105.29	114.09
18	AN	73	LEU	CA-C-N	5.67	128.20	120.54
18	AN	73	LEU	C-N-CA	5.67	128.20	120.54
1	AA	484	G	C2'-C3'-O3'	5.67	118.00	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	AN	6	LYS	CA-C-N	5.65	128.17	120.54
18	AN	6	LYS	C-N-CA	5.65	128.17	120.54
27	B8	127	A	C5'-C4'-C3'	-5.65	107.52	116.00
27	B8	137	U	P-O5'-C5'	5.64	129.36	120.90
34	BF	5	ASP	CA-C-N	5.64	128.11	120.38
34	BF	5	ASP	C-N-CA	5.64	128.11	120.38
28	BA	435	LYS	N-CA-CB	5.64	120.02	110.49
34	BF	140	ILE	N-CA-C	-5.64	106.81	112.17
53	BY	12	GLU	CA-C-N	5.63	127.83	120.28
53	BY	12	GLU	C-N-CA	5.63	127.83	120.28
14	AJ	95	GLY	N-CA-C	-5.63	106.78	116.01
37	BI	52	LEU	CA-C-N	5.62	125.63	119.90
37	BI	52	LEU	C-N-CA	5.62	125.63	119.90
27	B8	891	G	C1'-O4'-C4'	-5.62	104.28	109.90
28	BA	330	PHE	CA-C-N	5.61	128.59	120.79
28	BA	330	PHE	C-N-CA	5.61	128.59	120.79
21	AQ	33	TYR	N-CA-C	-5.61	106.26	114.39
29	BB	112	ASP	CA-C-N	5.61	127.20	120.13
29	BB	112	ASP	C-N-CA	5.61	127.20	120.13
57	B2	24	THR	CA-C-N	5.61	128.06	120.38
57	B2	24	THR	C-N-CA	5.61	128.06	120.38
58	B3	43	LEU	N-CA-C	-5.60	106.58	113.41
15	AK	45	THR	CA-C-N	5.59	127.78	120.28
15	AK	45	THR	C-N-CA	5.59	127.78	120.28
55	B0	6	LYS	CA-C-N	5.59	125.59	119.89
55	B0	6	LYS	C-N-CA	5.59	125.59	119.89
38	BJ	31	GLU	N-CA-C	-5.59	107.01	113.88
27	B8	2872	A	C2'-C3'-O3'	5.57	117.85	109.50
1	AA	1142	G	P-O3'-C3'	5.56	128.54	120.20
39	BK	50	GLY	N-CA-C	-5.56	107.57	115.30
45	BQ	15	LYS	CA-C-N	5.56	127.56	120.56
45	BQ	15	LYS	C-N-CA	5.56	127.56	120.56
5	A1	65	GLY	CA-C-N	5.56	126.78	119.84
5	A1	65	GLY	C-N-CA	5.56	126.78	119.84
18	AN	79	SER	CA-C-N	5.55	132.15	121.54
18	AN	79	SER	C-N-CA	5.55	132.15	121.54
28	BA	162	VAL	N-CA-CB	5.55	117.04	110.55
27	B8	2585	U	P-O3'-C3'	5.54	128.51	120.20
11	AG	20	GLU	N-CA-C	-5.54	106.52	113.72
3	AV	76	C	P-O5'-C5'	5.54	129.21	120.90
43	BO	83	LEU	N-CA-C	-5.54	106.88	113.97
5	A0	178	LEU	N-CA-C	-5.53	108.32	114.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	AK	51	PHE	CA-CB-CG	-5.53	108.27	113.80
28	BA	273	GLY	CA-C-N	5.52	128.03	120.35
28	BA	273	GLY	C-N-CA	5.52	128.03	120.35
42	BN	67	PHE	N-CA-C	-5.52	106.21	113.17
5	A1	98	GLN	CA-C-N	5.52	124.98	119.24
5	A1	98	GLN	C-N-CA	5.52	124.98	119.24
11	AG	154	ARG	N-CA-C	5.52	117.30	111.28
6	AB	197	PHE	CA-CB-CG	-5.52	108.28	113.80
1	AA	1201	A	C2'-C3'-O3'	5.51	117.77	109.50
4	AZ	78	ILE	N-CA-C	-5.51	101.07	108.35
7	AC	86	LEU	CA-C-N	5.51	127.94	120.38
7	AC	86	LEU	C-N-CA	5.51	127.94	120.38
1	AA	372	C	C2'-C3'-O3'	5.51	117.77	109.50
38	BJ	35	ARG	CA-C-N	5.51	127.93	120.38
38	BJ	35	ARG	C-N-CA	5.51	127.93	120.38
27	B8	320	A	P-O3'-C3'	5.50	128.46	120.20
1	AA	562	U	P-O3'-C3'	5.50	128.46	120.20
33	BE	124	PHE	N-CA-C	-5.50	105.51	113.21
44	BP	20	ARG	N-CA-C	-5.50	100.60	109.40
49	BU	46	LYS	CA-C-N	5.48	125.49	119.90
49	BU	46	LYS	C-N-CA	5.48	125.49	119.90
49	BU	88	ASP	N-CA-C	-5.48	106.48	112.72
7	AC	152	VAL	N-CA-C	-5.47	101.12	108.35
37	BI	21	PRO	CA-C-O	-5.47	112.62	120.56
49	BU	89	GLY	N-CA-C	-5.47	107.80	114.92
30	B5	25	GLU	CA-C-N	5.47	127.93	120.54
30	B5	25	GLU	C-N-CA	5.47	127.93	120.54
29	BB	97	VAL	CA-C-N	5.47	127.61	120.28
29	BB	97	VAL	C-N-CA	5.47	127.61	120.28
34	BF	171	ALA	N-CA-C	-5.47	106.61	113.28
13	AI	61	ASP	N-CA-C	-5.47	99.40	108.75
31	B6	6	LYS	CA-C-N	5.46	125.47	119.90
31	B6	6	LYS	C-N-CA	5.46	125.47	119.90
27	B8	2903	U	O4'-C1'-N1	5.46	116.69	108.50
54	BZ	57	GLU	N-CA-C	-5.45	107.88	114.75
28	BA	414	MET	CA-C-N	5.45	127.59	120.28
28	BA	414	MET	C-N-CA	5.45	127.59	120.28
1	AA	1113	C	P-O5'-C5'	5.45	129.08	120.90
27	B8	1496	A	O3'-P-O5'	-5.45	95.83	104.00
43	BO	2	ASP	CA-C-N	5.44	127.83	120.38
43	BO	2	ASP	C-N-CA	5.44	127.83	120.38
1	AA	1049	U	C2'-C3'-O3'	5.43	117.65	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BZ	22	THR	CA-C-N	5.43	127.87	120.54
54	BZ	22	THR	C-N-CA	5.43	127.87	120.54
5	A0	142	SER	CA-C-N	5.43	125.77	119.47
5	A0	142	SER	C-N-CA	5.43	125.77	119.47
1	AA	1323	G	O3'-P-O5'	-5.43	95.86	104.00
15	AK	93	GLU	N-CA-C	-5.42	107.68	114.56
10	AF	70	VAL	N-CA-C	-5.40	107.17	111.81
24	AT	42	ASP	CA-C-N	5.39	127.77	120.38
24	AT	42	ASP	C-N-CA	5.39	127.77	120.38
31	B6	150	GLY	CA-C-N	5.39	125.22	120.10
31	B6	150	GLY	C-N-CA	5.39	125.22	120.10
44	BP	77	SER	CA-C-N	5.39	125.47	119.32
44	BP	77	SER	C-N-CA	5.39	125.47	119.32
8	AD	49	ASP	CA-C-N	5.39	127.50	120.28
8	AD	49	ASP	C-N-CA	5.39	127.50	120.28
1	AA	99	C	O4'-C1'-N1	5.39	116.58	108.50
52	BX	10	ARG	CA-C-N	5.38	125.39	119.90
52	BX	10	ARG	C-N-CA	5.38	125.39	119.90
35	BG	107	GLY	N-CA-C	-5.37	107.62	115.63
18	AN	29	ILE	N-CA-C	5.37	116.10	110.62
12	AH	111	THR	CA-C-N	5.37	127.47	120.28
12	AH	111	THR	C-N-CA	5.37	127.47	120.28
39	BK	118	LEU	N-CA-C	-5.36	106.23	114.16
10	AF	67	PRO	CA-C-N	5.36	127.72	120.38
10	AF	67	PRO	C-N-CA	5.36	127.72	120.38
28	BA	165	VAL	N-CA-CB	5.36	116.82	110.55
38	BJ	112	GLY	CA-C-N	5.36	125.00	119.05
38	BJ	112	GLY	C-N-CA	5.36	125.00	119.05
50	BV	54	ALA	CA-C-N	5.35	127.71	120.38
50	BV	54	ALA	C-N-CA	5.35	127.71	120.38
3	AV	4	C	C2'-C3'-O3'	5.35	117.53	109.50
45	BQ	69	ARG	CA-C-N	5.35	127.45	120.28
45	BQ	69	ARG	C-N-CA	5.35	127.45	120.28
12	AH	29	SER	CA-C-N	5.35	128.22	120.79
12	AH	29	SER	C-N-CA	5.35	128.22	120.79
22	AR	26	ALA	CA-C-N	5.35	127.70	120.38
22	AR	26	ALA	C-N-CA	5.35	127.70	120.38
28	BA	372	ARG	N-CA-CB	5.35	118.08	110.06
28	BA	106	LYS	N-CA-C	-5.34	105.41	112.94
5	A1	152	ALA	CA-C-N	5.34	127.43	120.28
5	A1	152	ALA	C-N-CA	5.34	127.43	120.28
5	A1	238	LYS	N-CA-C	5.34	117.79	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	BO	70	ALA	N-CA-C	-5.34	106.44	113.17
36	BH	6	LEU	N-CA-C	-5.34	104.40	112.99
22	AR	10	CYS	N-CA-C	-5.33	105.74	113.21
27	B8	2025	C	P-O5'-C5'	5.33	128.90	120.90
10	AF	77	THR	N-CA-CB	5.33	117.92	109.82
31	B6	225	ASN	CA-C-N	5.33	126.50	119.84
31	B6	225	ASN	C-N-CA	5.33	126.50	119.84
6	AB	56	LEU	N-CA-C	-5.32	105.49	112.41
12	AH	9	MET	CA-C-N	5.32	127.67	120.38
12	AH	9	MET	C-N-CA	5.32	127.67	120.38
10	AF	21	MET	CA-C-N	5.32	127.46	120.60
10	AF	21	MET	C-N-CA	5.32	127.46	120.60
33	BE	19	PHE	N-CA-C	-5.32	105.49	112.41
47	BS	34	ASP	CA-C-N	5.32	127.46	120.60
47	BS	34	ASP	C-N-CA	5.32	127.46	120.60
5	A0	53	VAL	N-CA-C	-5.32	107.59	111.90
52	BX	15	ASN	N-CA-CB	5.32	119.48	110.49
47	BS	68	ASP	N-CA-C	-5.32	104.22	111.56
55	B0	8	THR	CA-C-N	5.32	127.40	120.28
55	B0	8	THR	C-N-CA	5.32	127.40	120.28
39	BK	50	GLY	CA-C-N	5.31	128.25	120.71
39	BK	50	GLY	C-N-CA	5.31	128.25	120.71
1	AA	274	A	P-O3'-C3'	5.31	128.16	120.20
27	B8	1930	G	P-O3'-C3'	5.31	128.16	120.20
28	BA	39	ILE	N-CA-CB	5.31	118.64	111.21
37	BI	72	THR	CA-C-N	5.30	125.84	120.38
37	BI	72	THR	C-N-CA	5.30	125.84	120.38
28	BA	79	ALA	N-CA-CB	5.30	119.45	110.49
11	AG	150	PHE	CA-CB-CG	-5.30	108.50	113.80
26	B7	15	A	O4'-C1'-N9	5.30	116.15	108.20
44	BP	3	ILE	N-CA-C	-5.30	107.22	113.42
28	BA	168	THR	CA-C-N	5.29	127.37	120.28
28	BA	168	THR	C-N-CA	5.29	127.37	120.28
43	BO	111	ARG	N-CA-C	-5.29	106.88	113.38
21	AQ	27	PHE	CA-CB-CG	-5.29	108.51	113.80
7	AC	106	ARG	N-CA-CB	5.28	119.42	110.49
37	BI	33	ASN	CA-C-N	5.28	127.69	120.77
37	BI	33	ASN	C-N-CA	5.28	127.69	120.77
27	B8	1025	G	P-O5'-C5'	5.28	128.82	120.90
5	A0	72	TRP	CA-C-N	5.28	128.74	120.82
5	A0	72	TRP	C-N-CA	5.28	128.74	120.82
13	AI	36	GLN	N-CA-C	-5.28	107.50	114.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1125	U	C2'-C3'-O3'	5.27	117.41	109.50
6	AB	219	THR	N-CA-C	-5.27	108.11	114.75
28	BA	386	LEU	CA-C-N	5.27	124.55	120.33
28	BA	386	LEU	C-N-CA	5.27	124.55	120.33
7	AC	108	PRO	N-CA-C	-5.27	108.65	114.92
28	BA	227	VAL	CA-C-N	5.27	127.34	120.28
28	BA	227	VAL	C-N-CA	5.27	127.34	120.28
35	BG	59	ASP	N-CA-C	-5.27	104.51	112.99
29	BB	106	LEU	CA-C-N	5.26	127.19	120.56
29	BB	106	LEU	C-N-CA	5.26	127.19	120.56
15	AK	121	ARG	CA-C-N	5.26	123.50	119.66
15	AK	121	ARG	C-N-CA	5.26	123.50	119.66
12	AH	30	LYS	CA-C-N	5.26	127.32	120.28
12	AH	30	LYS	C-N-CA	5.26	127.32	120.28
21	AQ	66	LEU	N-CA-C	-5.26	108.13	114.75
36	BH	46	PHE	CA-C-N	5.26	128.10	120.79
36	BH	46	PHE	C-N-CA	5.26	128.10	120.79
1	AA	1285	A	C5'-C4'-C3'	-5.25	107.32	115.20
13	AI	82	ILE	N-CA-C	-5.25	105.67	113.39
28	BA	63	MET	CA-C-N	5.25	127.31	120.28
28	BA	63	MET	C-N-CA	5.25	127.31	120.28
22	AR	64	LEU	N-CA-C	-5.25	105.54	112.94
46	BR	37	GLU	CA-C-N	5.25	127.64	120.35
46	BR	37	GLU	C-N-CA	5.25	127.64	120.35
27	B8	1730	C	C2'-C3'-O3'	5.25	117.37	109.50
17	AM	98	GLY	CA-C-N	5.24	128.21	120.82
17	AM	98	GLY	C-N-CA	5.24	128.21	120.82
46	BR	53	PHE	CA-C-N	5.24	127.64	120.35
46	BR	53	PHE	C-N-CA	5.24	127.64	120.35
30	B5	42	VAL	N-CA-C	-5.24	101.03	108.58
10	AF	113	ARG	N-CA-C	-5.24	105.18	112.30
17	AM	21	ILE	N-CA-C	-5.24	99.62	107.37
30	B5	142	VAL	N-CA-C	-5.24	107.87	112.90
27	B8	1344	U	P-O5'-C5'	5.24	128.76	120.90
4	AZ	41	SER	CA-C-N	5.24	125.75	119.94
4	AZ	41	SER	C-N-CA	5.24	125.75	119.94
8	AD	2	ARG	N-CA-C	-5.23	105.18	112.03
15	AK	68	ARG	CA-C-N	5.22	127.28	120.28
15	AK	68	ARG	C-N-CA	5.22	127.28	120.28
32	BD	193	VAL	CA-C-N	5.22	125.23	119.90
32	BD	193	VAL	C-N-CA	5.22	125.23	119.90
7	AC	211	ALA	N-CA-C	-5.22	106.59	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BF	101	ARG	N-CA-C	-5.22	106.43	114.16
42	BN	21	PHE	N-CA-C	-5.22	105.74	112.68
27	B8	2632	A	C5'-C4'-C3'	-5.22	108.17	116.00
27	B8	1076	C	O4'-C1'-N1	5.21	116.32	108.50
21	AQ	4	ILE	N-CA-C	-5.21	106.35	111.77
9	AE	30	PHE	CA-CB-CG	-5.21	108.59	113.80
20	AP	70	ARG	CA-C-N	5.21	127.31	120.60
20	AP	70	ARG	C-N-CA	5.21	127.31	120.60
7	AC	70	ALA	N-CA-C	-5.20	106.33	113.30
17	AM	101	THR	N-CA-C	-5.20	106.96	113.72
1	AA	1499	A	C5'-C4'-C3'	5.20	123.80	116.00
27	B8	1133	A	P-O3'-C3'	5.20	127.99	120.20
5	A0	122	LEU	N-CA-C	5.19	116.63	111.07
15	AK	96	ILE	CA-C-N	5.19	127.49	120.38
15	AK	96	ILE	C-N-CA	5.19	127.49	120.38
30	B5	23	ILE	N-CA-C	5.19	115.91	110.62
5	A1	85	GLU	N-CA-C	-5.18	106.64	113.12
17	AM	70	ARG	CA-C-N	5.18	129.43	121.19
17	AM	70	ARG	C-N-CA	5.18	129.43	121.19
5	A1	197	THR	CA-C-N	5.18	127.22	120.28
5	A1	197	THR	C-N-CA	5.18	127.22	120.28
1	AA	1338	G	O4'-C1'-N9	5.18	116.27	108.50
7	AC	14	VAL	N-CA-C	-5.18	107.36	113.42
58	B3	8	GLY	CA-C-N	5.18	127.22	120.28
58	B3	8	GLY	C-N-CA	5.18	127.22	120.28
5	A1	184	ASN	CA-C-N	5.18	125.69	119.94
5	A1	184	ASN	C-N-CA	5.18	125.69	119.94
10	AF	118	ASN	CA-C-N	5.18	127.22	120.28
10	AF	118	ASN	C-N-CA	5.18	127.22	120.28
39	BK	44	LYS	N-CA-C	-5.18	107.34	113.97
14	AJ	76	ILE	N-CA-C	-5.17	102.22	108.53
29	BB	94	THR	CA-C-N	5.17	127.16	120.44
29	BB	94	THR	C-N-CA	5.17	127.16	120.44
27	B8	364	C	C5'-C4'-C3'	-5.17	108.25	116.00
1	AA	1362	A	O3'-P-O5'	-5.17	96.25	104.00
32	BD	103	ASP	N-CA-C	-5.17	107.65	114.31
5	A1	176	ALA	CA-C-N	5.16	131.40	121.54
5	A1	176	ALA	C-N-CA	5.16	131.40	121.54
13	AI	48	ARG	CA-C-N	5.16	126.55	120.09
13	AI	48	ARG	C-N-CA	5.16	126.55	120.09
46	BR	47	VAL	N-CA-C	-5.16	100.21	107.75
1	AA	1030	U	O4'-C1'-N1	5.16	115.94	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	AG	149	ALA	N-CA-C	-5.16	105.00	113.50
40	BL	5	THR	N-CA-C	-5.16	108.01	114.56
4	AZ	81	LEU	N-CA-CB	5.15	119.20	110.49
50	BV	18	ARG	CA-C-N	5.15	127.18	120.28
50	BV	18	ARG	C-N-CA	5.15	127.18	120.28
11	AG	17	PHE	N-CA-C	-5.15	108.75	114.62
7	AC	101	ASN	CA-C-N	5.14	127.50	120.35
7	AC	101	ASN	C-N-CA	5.14	127.50	120.35
6	AB	79	VAL	CA-C-N	5.14	127.48	120.54
6	AB	79	VAL	C-N-CA	5.14	127.48	120.54
28	BA	413	ILE	CA-C-N	5.14	127.17	120.28
28	BA	413	ILE	C-N-CA	5.14	127.17	120.28
13	AI	75	ALA	CA-C-N	5.14	125.68	119.98
13	AI	75	ALA	C-N-CA	5.14	125.68	119.98
13	AI	86	LEU	N-CA-C	-5.14	107.68	114.31
28	BA	316	LEU	CA-C-N	5.14	127.67	120.28
28	BA	316	LEU	C-N-CA	5.14	127.67	120.28
5	A1	177	ARG	N-CA-CB	5.13	119.16	110.49
21	AQ	35	LYS	CA-C-N	5.13	128.49	120.75
21	AQ	35	LYS	C-N-CA	5.13	128.49	120.75
47	BS	79	GLY	CA-C-N	5.12	126.24	119.84
47	BS	79	GLY	C-N-CA	5.12	126.24	119.84
51	BW	72	GLY	CA-C-N	5.12	126.25	119.84
51	BW	72	GLY	C-N-CA	5.12	126.25	119.84
20	AP	53	ASP	CA-C-N	5.12	131.32	121.54
20	AP	53	ASP	C-N-CA	5.12	131.32	121.54
29	BB	66	LYS	N-CA-C	-5.12	104.75	112.99
36	BH	53	GLU	CA-C-N	5.12	127.90	120.79
36	BH	53	GLU	C-N-CA	5.12	127.90	120.79
51	BW	54	ARG	N-CA-C	-5.12	106.35	112.59
5	A0	116	ARG	CA-C-N	5.12	127.09	120.44
5	A0	116	ARG	C-N-CA	5.12	127.09	120.44
16	AL	9	LYS	CA-C-N	5.11	125.11	119.89
16	AL	9	LYS	C-N-CA	5.11	125.11	119.89
1	AA	471	U	P-O5'-C5'	5.11	128.56	120.90
30	B5	8	MET	CA-C-N	5.11	127.08	120.44
30	B5	8	MET	C-N-CA	5.11	127.08	120.44
20	AP	27	ALA	CA-C-N	5.11	127.12	120.28
20	AP	27	ALA	C-N-CA	5.11	127.12	120.28
20	AP	46	LYS	N-CA-C	-5.11	106.30	112.88
27	B8	1784	A	P-O3'-C3'	5.10	127.86	120.20
19	AO	73	ASP	CA-C-N	5.10	127.18	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	AO	73	ASP	C-N-CA	5.10	127.18	120.60
27	B8	1515	A	O4'-C1'-N9	5.10	116.16	108.50
31	B6	21	PRO	N-CA-C	-5.10	108.15	114.68
55	B0	50	GLY	N-CA-C	-5.10	108.03	115.63
15	AK	122	PRO	CA-C-O	-5.10	117.23	120.90
24	AT	19	HIS	CA-C-N	5.10	127.37	120.38
24	AT	19	HIS	C-N-CA	5.10	127.37	120.38
25	AU	60	ALA	CA-C-N	5.10	127.11	120.28
25	AU	60	ALA	C-N-CA	5.10	127.11	120.28
33	BE	108	ILE	N-CA-C	-5.09	106.18	111.58
27	B8	2336	A	C2'-C3'-O3'	5.09	117.14	109.50
32	BD	172	VAL	N-CA-C	-5.09	107.33	112.17
49	BU	24	VAL	CA-C-N	5.09	127.41	120.54
49	BU	24	VAL	C-N-CA	5.09	127.41	120.54
5	A1	222	LEU	N-CA-C	-5.09	105.91	112.68
12	AH	78	SER	N-CA-C	-5.09	105.55	112.26
40	BL	135	ILE	N-CA-C	-5.09	107.80	112.83
25	AU	48	LYS	N-CA-C	-5.08	107.11	113.72
28	BA	199	LEU	CA-C-O	-5.08	113.20	120.16
8	AD	63	ILE	N-CA-C	-5.08	106.98	113.22
19	AO	53	ARG	CA-C-N	5.08	125.57	119.94
19	AO	53	ARG	C-N-CA	5.08	125.57	119.94
56	B1	30	PRO	N-CA-C	-5.08	108.88	114.92
9	AE	24	VAL	CA-C-N	5.07	127.08	120.28
9	AE	24	VAL	C-N-CA	5.07	127.08	120.28
1	AA	464	U	C5'-C4'-C3'	-5.07	108.40	116.00
30	B5	131	LEU	N-CA-C	-5.07	106.51	113.30
3	AV	32	C	P-O5'-C5'	5.07	128.50	120.90
10	AF	113	ARG	CA-C-N	5.07	131.22	121.54
10	AF	113	ARG	C-N-CA	5.07	131.22	121.54
27	B8	1324	G	C5'-C4'-C3'	-5.06	107.61	115.20
10	AF	96	VAL	CA-C-N	5.06	127.06	120.28
10	AF	96	VAL	C-N-CA	5.06	127.06	120.28
28	BA	12	ALA	N-CA-C	-5.06	106.12	113.21
31	B6	103	ILE	N-CA-C	-5.06	100.61	108.81
28	BA	165	VAL	CA-C-N	5.06	127.06	120.28
28	BA	165	VAL	C-N-CA	5.06	127.06	120.28
34	BF	172	PHE	N-CA-C	-5.06	106.80	113.17
43	BO	7	ARG	CA-C-N	5.06	127.39	120.77
43	BO	7	ARG	C-N-CA	5.06	127.39	120.77
53	BY	4	LYS	CA-C-N	5.06	127.37	120.54
53	BY	4	LYS	C-N-CA	5.06	127.37	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	AD	51	GLY	CA-C-N	5.05	127.39	120.77
8	AD	51	GLY	C-N-CA	5.05	127.39	120.77
9	AE	22	LYS	N-CA-C	-5.05	101.51	109.50
19	AO	34	GLN	CA-C-N	5.05	126.93	120.56
19	AO	34	GLN	C-N-CA	5.05	126.93	120.56
7	AC	90	VAL	CA-C-N	5.05	127.30	120.38
7	AC	90	VAL	C-N-CA	5.05	127.30	120.38
40	BL	59	ARG	N-CA-C	-5.05	106.36	112.88
45	BQ	58	GLN	CA-C-N	5.05	127.36	120.54
45	BQ	58	GLN	C-N-CA	5.05	127.36	120.54
8	AD	19	PHE	CA-CB-CG	-5.05	108.75	113.80
41	BM	43	ALA	N-CA-CB	5.05	119.02	110.49
31	B6	208	GLY	CA-C-N	5.05	127.04	120.28
31	B6	208	GLY	C-N-CA	5.05	127.04	120.28
34	BF	175	PRO	N-CA-C	-5.05	107.63	114.80
8	AD	184	LYS	CA-C-N	5.04	126.14	119.84
8	AD	184	LYS	C-N-CA	5.04	126.14	119.84
1	AA	1529	G	C5'-C4'-O4'	5.04	117.35	109.80
35	BG	30	GLY	N-CA-C	-5.03	101.26	113.18
45	BQ	94	LEU	N-CA-C	-5.03	106.73	112.92
5	A0	56	THR	CA-C-N	5.03	127.02	120.28
5	A0	56	THR	C-N-CA	5.03	127.02	120.28
8	AD	80	ARG	N-CA-C	-5.02	107.19	113.72
32	BD	31	ALA	N-CA-CB	5.02	118.98	110.49
27	B8	242	G	C2'-C3'-O3'	5.02	117.03	109.50
28	BA	411	VAL	N-CA-C	5.02	115.24	110.42
43	BO	5	SER	CA-C-N	5.02	127.26	120.38
43	BO	5	SER	C-N-CA	5.02	127.26	120.38
40	BL	37	GLY	CA-C-N	5.02	127.50	120.28
40	BL	37	GLY	C-N-CA	5.02	127.50	120.28
28	BA	62	GLU	CA-C-N	5.02	127.00	120.28
28	BA	62	GLU	C-N-CA	5.02	127.00	120.28
38	BJ	89	PHE	CA-C-N	5.01	127.24	120.38
38	BJ	89	PHE	C-N-CA	5.01	127.24	120.38
40	BL	100	ILE	N-CA-C	-5.01	106.03	113.39
51	BW	73	PRO	CA-C-N	5.01	126.99	120.28
51	BW	73	PRO	C-N-CA	5.01	126.99	120.28
29	BB	96	ILE	CA-C-N	5.01	126.87	120.56
29	BB	96	ILE	C-N-CA	5.01	126.87	120.56
5	A0	138	GLN	CA-C-N	5.00	126.94	120.44
5	A0	138	GLN	C-N-CA	5.00	126.94	120.44
51	BW	52	CYS	N-CA-CB	5.00	118.95	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	AM	25	GLY	N-CA-C	-5.00	106.79	112.79
54	BZ	24	LEU	CA-C-N	5.00	126.43	120.13
54	BZ	24	LEU	C-N-CA	5.00	126.43	120.13

There are no chirality outliers.

All (189) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	A1	237	THR	Peptide
1	AA	102	G	Sidechain
1	AA	1024	G	Sidechain
1	AA	1027	C	Sidechain
1	AA	1044	A	Sidechain
1	AA	1094	G	Sidechain
1	AA	1095	U	Sidechain
1	AA	1101	A	Sidechain
1	AA	1125	U	Sidechain
1	AA	1129	C	Sidechain
1	AA	1131	G	Sidechain
1	AA	1139	G	Sidechain
1	AA	1144	G	Sidechain
1	AA	115	G	Sidechain
1	AA	1179	A	Sidechain
1	AA	1226	C	Sidechain
1	AA	1268	G	Sidechain
1	AA	1269	A	Sidechain
1	AA	1289	A	Sidechain
1	AA	1299	A	Sidechain
1	AA	13	U	Sidechain
1	AA	130	A	Sidechain
1	AA	1323	G	Sidechain
1	AA	1346	A	Sidechain
1	AA	1347	G	Sidechain
1	AA	1417	G	Sidechain
1	AA	1418	A	Sidechain
1	AA	1465	A	Sidechain
1	AA	1502	A	Sidechain
1	AA	1516	G	Sidechain
1	AA	152	A	Sidechain
1	AA	1526	G	Sidechain
1	AA	1529	G	Sidechain
1	AA	173	U	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	180	U	Sidechain
1	AA	181	A	Sidechain
1	AA	184	G	Sidechain
1	AA	185	U	Sidechain
1	AA	202	G	Sidechain
1	AA	204	G	Sidechain
1	AA	244	U	Sidechain
1	AA	262	A	Sidechain
1	AA	265	G	Sidechain
1	AA	298	A	Sidechain
1	AA	315	A	Sidechain
1	AA	353	A	Sidechain
1	AA	378	G	Sidechain
1	AA	380	G	Sidechain
1	AA	439	U	Sidechain
1	AA	450	G	Sidechain
1	AA	454	G	Sidechain
1	AA	496	A	Sidechain
1	AA	527	G	Sidechain
1	AA	557	G	Sidechain
1	AA	565	U	Sidechain
1	AA	566	G	Sidechain
1	AA	581	G	Sidechain
1	AA	587	G	Sidechain
1	AA	588	G	Sidechain
1	AA	620	C	Sidechain
1	AA	622	A	Sidechain
1	AA	69	G	Sidechain
1	AA	718	A	Sidechain
1	AA	728	A	Sidechain
1	AA	752	G	Sidechain
1	AA	874	G	Sidechain
1	AA	883	C	Sidechain
1	AA	884	U	Sidechain
1	AA	927	G	Sidechain
1	AA	95	C	Sidechain
1	AA	960	U	Sidechain
1	AA	974	A	Sidechain
1	AA	978	A	Sidechain
7	AC	218	LYS	Peptide
12	AH	14	ARG	Sidechain
13	AI	6	TYR	Sidechain

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Mol	Chain	Res	Type	Group
3	AV	53	G	Sidechain
3	AV	7	G	Sidechain
57	B2	12	ARG	Sidechain
26	B7	111	U	Sidechain
26	B7	5	U	Sidechain
27	B8	1025	G	Sidechain
27	B8	1027	A	Sidechain
27	B8	1070	A	Sidechain
27	B8	1084	A	Sidechain
27	B8	1095	A	Sidechain
27	B8	1099	G	Sidechain
27	B8	1130	U	Sidechain
27	B8	1138	G	Sidechain
27	B8	120	U	Sidechain
27	B8	1204	A	Sidechain
27	B8	1224	U	Sidechain
27	B8	1235	G	Sidechain
27	B8	1236	G	Sidechain
27	B8	1296	G	Sidechain
27	B8	1327	A	Sidechain
27	B8	1334	G	Sidechain
27	B8	1360	G	Sidechain
27	B8	1383	A	Sidechain
27	B8	1394	U	Sidechain
27	B8	1427	A	Sidechain
27	B8	1515	A	Sidechain
27	B8	1517	G	Sidechain
27	B8	1530	G	Sidechain
27	B8	1573	G	Sidechain
27	B8	161	A	Sidechain
27	B8	1672	A	Sidechain
27	B8	1680	U	Sidechain
27	B8	1682	G	Sidechain
27	B8	1699	G	Sidechain
27	B8	1738	G	Sidechain
27	B8	1743	G	Sidechain
27	B8	1784	A	Sidechain
27	B8	1813	G	Sidechain
27	B8	1846	G	Sidechain
27	B8	1904	G	Sidechain
27	B8	1920	C	Sidechain
27	B8	1927	A	Sidechain

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Mol	Chain	Res	Type	Group
27	B8	1952	A	Sidechain
27	B8	1954	G	Sidechain
27	B8	2005	A	Sidechain
27	B8	205	G	Sidechain
27	B8	2125	G	Sidechain
27	B8	2143	C	Sidechain
27	B8	2148	G	Sidechain
27	B8	2155	U	Sidechain
27	B8	2272	U	Sidechain
27	B8	2345	G	Sidechain
27	B8	2365	G	Sidechain
27	B8	2382	G	Sidechain
27	B8	2460	U	Sidechain
27	B8	2471	A	Sidechain
27	B8	250	G	Sidechain
27	B8	2517	C	Sidechain
27	B8	2580	U	Sidechain
27	B8	2596	U	Sidechain
27	B8	261	G	Sidechain
27	B8	2637	U	Sidechain
27	B8	265	A	Sidechain
27	B8	2689	U	Sidechain
27	B8	27	G	Sidechain
27	B8	2746	U	Sidechain
27	B8	2756	U	Sidechain
27	B8	2857	G	Sidechain
27	B8	2858	C	Sidechain
27	B8	2866	U	Sidechain
27	B8	2903	U	Sidechain
27	B8	303	G	Sidechain
27	B8	346	A	Sidechain
27	B8	362	A	Sidechain
27	B8	370	G	Sidechain
27	B8	395	U	Sidechain
27	B8	428	A	Sidechain
27	B8	445	C	Sidechain
27	B8	446	G	Sidechain
27	B8	457	A	Sidechain
27	B8	467	G	Sidechain
27	B8	480	A	Sidechain
27	B8	505	A	Sidechain
27	B8	507	A	Sidechain

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Mol	Chain	Res	Type	Group
27	B8	532	A	Sidechain
27	B8	569	U	Sidechain
27	B8	60	G	Sidechain
27	B8	630	G	Sidechain
27	B8	642	U	Sidechain
27	B8	674	G	Sidechain
27	B8	675	A	Sidechain
27	B8	676	A	Sidechain
27	B8	684	G	Sidechain
27	B8	705	A	Sidechain
27	B8	712	G	Sidechain
27	B8	72	U	Sidechain
27	B8	728	G	Sidechain
27	B8	738	G	Sidechain
27	B8	773	U	Sidechain
27	B8	821	A	Sidechain
27	B8	849	A	Sidechain
27	B8	858	G	Sidechain
27	B8	877	A	Sidechain
27	B8	899	A	Sidechain
27	B8	959	A	Sidechain
28	BA	181	ARG	Peptide
28	BA	198	GLY	Peptide
28	BA	293	TRP	Peptide
28	BA	314	GLN	Peptide
28	BA	72	LEU	Peptide
34	BF	137	PHE	Peptide
36	BH	31	VAL	Peptide
49	BU	48	VAL	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1	0
20	AP	649	0	666	2	0
21	AQ	672	0	716	2	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	40	0
28	BA	3362	0	3511	39	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	1	0
40	BL	1053	0	1129	1	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	144	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 1.

All (144) 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
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
28:BA:416:PHE:CD2	28:BA:416:PHE:CG	2.01	1.46
28:BA:416:PHE:CG	60:BA:533:PEV:H401	1.82	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:BA:416:PHE:CD2	60:BA:533:PEV:C39	2.32	1.12
28:BA:416:PHE:CE2	60:BA:533:PEV:C39	2.33	1.12
28:BA:416:PHE:CD1	60:BA:533:PEV:C39	2.33	1.12
28:BA:416:PHE:CD2	60:BA:533:PEV:H392	1.84	1.12
28:BA:416:PHE:CE2	60:BA:533:PEV:C40	2.33	1.12
28:BA:416:PHE:CG	60:BA:533:PEV:C40	2.33	1.12
28:BA:416:PHE:CD1	60:BA:533:PEV:C40	2.33	1.11
28:BA:416:PHE:CD2	60:BA:533:PEV:H402	1.85	1.11
28:BA:416:PHE:CE1	60:BA:533:PEV:C39	2.33	1.11
28:BA:416:PHE:CD2	60:BA:533:PEV:C40	2.32	1.11
28:BA:416:PHE:CZ	60:BA:533:PEV:C40	2.33	1.11
28:BA:416:PHE:CE1	60:BA:533:PEV:C40	2.34	1.11
28:BA:416:PHE:CZ	60:BA:533:PEV:C39	2.33	1.11
28:BA:416:PHE:CG	60:BA:533:PEV:C39	2.33	1.10
28:BA:416:PHE:CG	60:BA:533:PEV:H391	1.86	1.10
28:BA:416:PHE:CE2	60:BA:533:PEV:H402	1.91	1.04
28:BA:416:PHE:CD1	60:BA:533:PEV:H391	1.94	1.03
28:BA:416:PHE:CE2	60:BA:533:PEV:H392	1.96	1.01
28:BA:416:PHE:CD1	60:BA:533:PEV:H401	1.97	0.99
60:BA:533:PEV:C39	60:BA:533:PEV:C40	2.52	0.87
4:AZ:81:LEU:HD13	4:AZ:82:GLY:H	1.53	0.72
28:BA:324:ALA:HB2	60:BA:531:PEV:H402	1.73	0.70
28:BA:416:PHE:CZ	60:BA:533:PEV:C38	2.77	0.68
28:BA:416:PHE:CE1	60:BA:533:PEV:C38	2.79	0.65
28:BA:416:PHE:CZ	60:BA:533:PEV:H381	2.33	0.63
28:BA:416:PHE:CE1	60:BA:533:PEV:C41	2.82	0.62
28:BA:416:PHE:CZ	60:BA:533:PEV:C41	2.85	0.59
28:BA:416:PHE:CE1	60:BA:533:PEV:H381	2.39	0.57
27:B8:2091:C:H3'	27:B8:2092:U:H5''	1.87	0.56
27:B8:1021:A:H61	27:B8:1142:A:H61	1.53	0.56
3:AV:27:A:H61	3:AV:45:G:H1	1.52	0.55
27:B8:1024:G:H3'	27:B8:1025:G:H5''	1.88	0.55
1:AA:664:G:H22	1:AA:741:G:H1	1.54	0.55
27:B8:500:G:H21	27:B8:505:A:H62	1.55	0.55
27:B8:2792:A:H3'	27:B8:2793:C:H5''	1.90	0.53
27:B8:871:U:H3	27:B8:906:U:H3	1.56	0.53
27:B8:962:G:H21	27:B8:2250:G:H1	1.57	0.53
27:B8:870:U:H2'	27:B8:871:U:H5''	1.90	0.53
61:BA:512:PGV:H72	60:BA:513:PEV:H401	1.91	0.53
14:AJ:15:HIS:CD2	14:AJ:16:ARG:HE	2.29	0.51
1:AA:507:C:H3'	1:AA:508:U:H5''	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AZ:39:LEU:HD13	28:BA:286:PHE:HB3	1.93	0.50
60:B8:3001:PEV:H401	60:B8:3002:PEV:H401	1.92	0.50
21:AQ:18:LYS:H	21:AQ:50:ASN:HD21	1.59	0.50
1:AA:1239:A:H62	1:AA:1299:A:H62	1.60	0.50
25:AU:33:ARG:HE	25:AU:34:ARG:H	1.59	0.50
1:AA:1305:G:H21	1:AA:1332:A:H8	1.59	0.49
27:B8:1065:U:H3	27:B8:1069:A:H2'	1.76	0.49
36:BH:126:GLY:H	36:BH:128:HIS:CE1	2.30	0.49
1:AA:82:G:H3'	1:AA:83:C:H4'	1.95	0.49
27:B8:713:G:H21	27:B8:718:A:H2	1.60	0.49
1:AA:632:U:H3'	1:AA:633:G:H5'	1.95	0.49
28:BA:416:PHE:CZ	60:BA:533:PEV:H411	2.48	0.49
27:B8:870:U:C2'	27:B8:871:U:H5''	2.43	0.48
1:AA:243:A:H4'	1:AA:244:U:H5'	1.94	0.48
27:B8:1551:A:H3'	27:B8:1552:A:H5''	1.95	0.48
9:AE:89:THR:HG22	9:AE:90:GLY:H	1.77	0.48
20:AP:54:LEU:H	20:AP:54:LEU:HD12	1.78	0.48
60:BA:503:PEV:H442	60:BA:503:PEV:H401	1.95	0.48
1:AA:1122:U:H5''	7:AC:222:GLN:H	1.78	0.48
28:BA:416:PHE:CE1	60:BA:533:PEV:H411	2.48	0.48
12:AH:60:LEU:H	12:AH:60:LEU:HD23	1.79	0.48
20:AP:78:VAL:HG23	20:AP:81:ALA:H	1.79	0.48
60:A1:301:PEV:H392	61:A1:303:PGV:H02	1.96	0.47
24:AT:67:HIS:CD2	24:AT:69:ASN:H	2.32	0.47
27:B8:82:U:H3	27:B8:104:A:H61	1.63	0.47
30:B5:165:ASN:HD21	30:B5:169:GLY:H	1.63	0.47
1:AA:1223:C:H3'	1:AA:1224:U:C5'	2.45	0.47
58:B3:36:ALA:H	58:B3:39:ARG:HE	1.62	0.47
60:A0:315:PEV:H391	60:A1:302:PEV:H401	1.96	0.47
27:B8:957:C:H42	27:B8:2494:G:H21	1.61	0.47
27:B8:2091:C:H3'	27:B8:2092:U:C5'	2.46	0.46
36:BH:101:ASP:H	36:BH:111:ALA:HB3	1.80	0.46
4:AZ:25:LEU:CB	28:BA:333:THR:HG23	2.46	0.46
27:B8:2371:G:H21	56:B1:45:HIS:HE1	1.63	0.46
27:B8:63:A:H2'	27:B8:64:A:C8	2.51	0.46
60:A1:323:PEV:H142	60:A1:323:PEV:H392	1.97	0.46
27:B8:2171:A:H1'	27:B8:2172:U:C6	2.50	0.45
27:B8:480:A:H3'	27:B8:481:G:H5''	1.98	0.45
1:AA:262:A:H4'	24:AT:67:HIS:CD2	2.52	0.44
60:A1:319:PEV:H361	60:A1:319:PEV:H392	1.91	0.44
27:B8:2371:G:H21	56:B1:45:HIS:CE1	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:973:G:H3'	1:AA:974:A:H5''	1.99	0.44
6:AB:14:HIS:CE1	6:AB:200:PRO:HB3	2.53	0.44
27:B8:890:C:H3'	27:B8:891:G:H4'	2.00	0.44
27:B8:1203:U:H3'	27:B8:1204:A:H5''	1.99	0.44
10:AF:94:HIS:CG	10:AF:95:ALA:H	2.37	0.43
1:AA:404:G:H1	1:AA:499:A:H62	1.65	0.43
8:AD:96:ARG:HB2	8:AD:99:ASN:HD22	1.82	0.43
32:BD:33:ARG:HH11	32:BD:93:GLY:H	1.67	0.43
27:B8:1273:U:H3	27:B8:2002:G:H21	1.67	0.43
27:B8:2874:C:H4'	42:BN:4:ARG:HH21	1.84	0.43
39:BK:1:MET:HA	39:BK:1:MET:HE2	2.00	0.43
27:B8:532:A:H4'	27:B8:533:G:C8	2.54	0.43
57:B2:24:THR:HG23	57:B2:27:GLY:H	1.84	0.43
27:B8:572:A:H5''	46:BR:80:ARG:HH21	1.84	0.43
27:B8:1567:G:H5'	31:B6:57:HIS:CD2	2.54	0.43
6:AB:103:TRP:HE1	6:AB:107:ARG:HH21	1.66	0.42
27:B8:2682:A:C2	27:B8:2683:C:C5	3.06	0.42
27:B8:1205:A:C5	33:BE:165:HIS:HB3	2.54	0.42
27:B8:880:G:H2'	27:B8:881:G:C8	2.55	0.42
27:B8:877:A:C2	27:B8:901:C:C2	3.08	0.42
27:B8:1391:U:H2'	27:B8:1393:A:C2	2.53	0.42
29:BB:123:THR:HA	29:BB:126:ARG:HH12	1.84	0.42
21:AQ:17:GLU:H	21:AQ:17:GLU:CD	2.28	0.42
31:B6:264:LYS:H	31:B6:264:LYS:HD2	1.85	0.42
34:BF:106:ALA:HA	34:BF:111:ARG:HH11	1.85	0.42
1:AA:413:G:H4'	1:AA:414:A:H5''	2.02	0.42
6:AB:169:HIS:H	6:AB:169:HIS:CD2	2.37	0.42
27:B8:962:G:N2	27:B8:2250:G:H1	2.17	0.42
27:B8:2233:U:H2'	27:B8:2234:G:C8	2.55	0.42
1:AA:995:C:H2'	1:AA:996:A:H5''	2.02	0.42
1:AA:537:G:H5''	16:AL:109:ARG:HH12	1.85	0.41
1:AA:1130:A:H61	1:AA:1144:G:H1'	1.86	0.41
1:AA:1144:G:N2	1:AA:1146:A:H62	2.19	0.41
16:AL:41:PRO:HG2	16:AL:45:ASN:H	1.85	0.41
27:B8:900:A:H2'	27:B8:901:C:H5'	2.02	0.41
28:BA:238:GLU:CD	28:BA:239:ARG:H	2.28	0.41
27:B8:1082:U:N3	27:B8:1086:A:C2	2.88	0.41
1:AA:412:A:H3'	1:AA:413:G:C5'	2.51	0.41
60:BA:514:PEV:H362	60:BA:514:PEV:H391	1.94	0.41
27:B8:1283:G:H22	27:B8:1286:A:H5'	1.85	0.41
27:B8:251:A:H4'	40:BL:49:GLY:HA2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B8:2351:G:H2'	27:B8:2365:G:H22	1.84	0.41
4:AZ:25:LEU:HB3	28:BA:333:THR:HG23	2.03	0.41
61:A1:315:PGV:H132	61:A1:315:PGV:H102	1.98	0.41
1:AA:781:A:H2'	1:AA:782:A:H5'	2.02	0.41
19:AO:25:GLU:H	19:AO:25:GLU:CD	2.28	0.41
27:B8:2645:G:H3'	27:B8:2646:C:H5'	2.02	0.41
60:B8:3002:PEV:H362	60:B8:3002:PEV:H392	1.94	0.41
1:AA:1118:U:H1'	1:AA:1179:A:C4	2.55	0.41
7:AC:10:ARG:HH21	7:AC:175:HIS:HA	1.85	0.40
14:AJ:15:HIS:HA	14:AJ:18:ILE:HG22	2.01	0.40
60:BA:520:PEV:H402	60:BA:526:PEV:H441	2.04	0.40
1:AA:483:C:H2'	1:AA:484:G:C8	2.57	0.40
18:AN:60:ARG:HA	18:AN:60:ARG:HE	1.86	0.40
41:BM:78:LEU:H	41:BM:78:LEU:HD23	1.86	0.40

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	8
5	A0	198/200 (99%)	174 (88%)	20 (10%)	4 (2%)	6	31
5	A1	198/200 (99%)	169 (85%)	23 (12%)	6 (3%)	3	22
6	AB	238/240 (99%)	190 (80%)	42 (18%)	6 (2%)	4	26
7	AC	230/232 (99%)	184 (80%)	31 (14%)	15 (6%)	1	12
8	AD	203/205 (99%)	163 (80%)	28 (14%)	12 (6%)	1	13
9	AE	164/166 (99%)	137 (84%)	21 (13%)	6 (4%)	2	20
10	AF	133/135 (98%)	109 (82%)	22 (16%)	2 (2%)	8	40
11	AG	176/178 (99%)	142 (81%)	29 (16%)	5 (3%)	4	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	AH	127/129 (98%)	102 (80%)	23 (18%)	2 (2%)	7	38
13	AI	127/129 (98%)	108 (85%)	11 (9%)	8 (6%)	1	13
14	AJ	101/103 (98%)	85 (84%)	9 (9%)	7 (7%)	1	11
15	AK	126/128 (98%)	106 (84%)	15 (12%)	5 (4%)	2	18
16	AL	121/123 (98%)	108 (89%)	12 (10%)	1 (1%)	16	54
17	AM	115/117 (98%)	96 (84%)	13 (11%)	6 (5%)	1	15
18	AN	98/100 (98%)	81 (83%)	9 (9%)	8 (8%)	0	9
19	AO	86/88 (98%)	79 (92%)	5 (6%)	2 (2%)	5	28
20	AP	80/82 (98%)	73 (91%)	5 (6%)	2 (2%)	4	26
21	AQ	81/83 (98%)	67 (83%)	8 (10%)	6 (7%)	1	10
22	AR	72/74 (97%)	59 (82%)	9 (12%)	4 (6%)	1	14
23	AS	89/91 (98%)	73 (82%)	12 (14%)	4 (4%)	2	17
24	AT	84/86 (98%)	76 (90%)	7 (8%)	1 (1%)	10	44
25	AU	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
28	BA	433/435 (100%)	313 (72%)	66 (15%)	54 (12%)	0	4
29	BB	114/116 (98%)	96 (84%)	12 (10%)	6 (5%)	1	15
30	B5	232/234 (99%)	211 (91%)	15 (6%)	6 (3%)	4	25
31	B6	270/272 (99%)	227 (84%)	31 (12%)	12 (4%)	2	17
32	BD	207/209 (99%)	172 (83%)	24 (12%)	11 (5%)	1	15
33	BE	199/201 (99%)	169 (85%)	20 (10%)	10 (5%)	1	16
34	BF	176/178 (99%)	137 (78%)	27 (15%)	12 (7%)	1	11
35	BG	174/176 (99%)	137 (79%)	28 (16%)	9 (5%)	1	15
36	BH	147/149 (99%)	108 (74%)	31 (21%)	8 (5%)	1	15
37	BI	139/141 (99%)	125 (90%)	11 (8%)	3 (2%)	5	29
38	BJ	140/142 (99%)	117 (84%)	19 (14%)	4 (3%)	3	23
39	BK	121/123 (98%)	99 (82%)	16 (13%)	6 (5%)	1	16
40	BL	142/144 (99%)	129 (91%)	10 (7%)	3 (2%)	5	30
41	BM	134/136 (98%)	107 (80%)	17 (13%)	10 (8%)	1	10
42	BN	125/127 (98%)	104 (83%)	12 (10%)	9 (7%)	1	11
43	BO	115/117 (98%)	97 (84%)	15 (13%)	3 (3%)	4	25
44	BP	112/114 (98%)	94 (84%)	11 (10%)	7 (6%)	1	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	BQ	115/117 (98%)	94 (82%)	15 (13%)	6 (5%)	1	15
46	BR	101/103 (98%)	83 (82%)	13 (13%)	5 (5%)	1	16
47	BS	108/110 (98%)	81 (75%)	18 (17%)	9 (8%)	0	9
48	BT	98/100 (98%)	71 (72%)	20 (20%)	7 (7%)	1	11
49	BU	101/103 (98%)	84 (83%)	14 (14%)	3 (3%)	3	22
50	BV	92/94 (98%)	82 (89%)	9 (10%)	1 (1%)	11	46
51	BW	82/84 (98%)	59 (72%)	19 (23%)	4 (5%)	1	16
52	BX	75/77 (97%)	57 (76%)	12 (16%)	6 (8%)	1	9
53	BY	61/63 (97%)	48 (79%)	11 (18%)	2 (3%)	3	21
54	BZ	56/58 (97%)	49 (88%)	4 (7%)	3 (5%)	1	15
55	B0	54/56 (96%)	47 (87%)	6 (11%)	1 (2%)	6	32
56	B1	52/54 (96%)	46 (88%)	5 (10%)	1 (2%)	6	32
57	B2	44/46 (96%)	31 (70%)	10 (23%)	3 (7%)	1	11
58	B3	62/64 (97%)	52 (84%)	9 (14%)	1 (2%)	7	38
59	B4	36/38 (95%)	32 (89%)	3 (8%)	1 (3%)	4	24
All	All	7128/7238 (98%)	5877 (82%)	904 (13%)	347 (5%)	3	16

All (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
7	AC	219	PRO
9	AE	17	VAL
13	AI	127	SER
14	AJ	57	VAL
14	AJ	67	ILE
17	AM	3	ILE
18	AN	80	ARG
28	BA	48	VAL
28	BA	56	GLN
28	BA	68	SER
28	BA	72	LEU
28	BA	79	ALA

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Mol	Chain	Res	Type
28	BA	148	LEU
28	BA	200	PRO
28	BA	237	VAL
28	BA	249	ALA
28	BA	275	ILE
28	BA	314	GLN
28	BA	319	LEU
28	BA	332	TYR
28	BA	353	VAL
28	BA	358	PRO
28	BA	373	LEU
29	BB	67	ALA
31	B6	132	ARG
31	B6	197	ALA
31	B6	231	HIS
31	B6	261	ARG
33	BE	4	VAL
34	BF	82	TYR
34	BF	136	ILE
35	BG	2	ARG
35	BG	94	ARG
36	BH	32	PRO
36	BH	115	VAL
38	BJ	40	HIS
39	BK	71	ARG
41	BM	43	ALA
41	BM	56	ALA
41	BM	122	ALA
44	BP	25	VAL
45	BQ	71	ASN
46	BR	3	ALA
46	BR	48	LYS
46	BR	101	ILE
47	BS	76	VAL
48	BT	35	ALA
48	BT	36	LYS
48	BT	99	ALA
49	BU	49	PRO
4	AZ	49	MET
6	AB	95	TRP
6	AB	224	ARG
7	AC	190	THR

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Mol	Chain	Res	Type
8	AD	7	LYS
10	AF	85	ILE
11	AG	77	ARG
12	AH	73	SER
14	AJ	85	ASP
15	AK	11	VAL
16	AL	54	VAL
17	AM	29	SER
17	AM	87	GLY
18	AN	21	ALA
21	AQ	12	VAL
21	AQ	13	SER
21	AQ	81	ALA
22	AR	24	ASP
23	AS	28	LYS
28	BA	235	VAL
28	BA	256	ARG
28	BA	267	LEU
28	BA	308	LEU
28	BA	320	LEU
28	BA	333	THR
28	BA	340	ARG
28	BA	351	ALA
28	BA	362	THR
28	BA	363	ALA
28	BA	369	VAL
28	BA	371	THR
28	BA	401	PHE
28	BA	431	SER
29	BB	19	TRP
29	BB	71	PHE
31	B6	142	ASN
32	BD	31	ALA
32	BD	46	ARG
32	BD	107	VAL
33	BE	12	LEU
33	BE	30	GLN
34	BF	74	ALA
34	BF	84	ILE
34	BF	103	ILE
34	BF	138	PRO
37	BI	87	SER

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Mol	Chain	Res	Type
40	BL	113	ALA
41	BM	55	ARG
41	BM	72	PRO
41	BM	73	ILE
41	BM	135	VAL
42	BN	63	ARG
44	BP	106	ALA
45	BQ	101	ASP
46	BR	65	ALA
47	BS	12	SER
47	BS	53	SER
47	BS	89	ALA
48	BT	72	GLN
53	BY	2	LYS
53	BY	37	LEU
4	AZ	109	ASP
5	A0	170	LEU
5	A1	228	SER
7	AC	53	ARG
7	AC	106	ARG
7	AC	116	ALA
8	AD	6	PRO
8	AD	21	LYS
8	AD	146	GLU
8	AD	176	LYS
9	AE	120	HIS
11	AG	80	GLY
11	AG	138	GLU
12	AH	116	ARG
13	AI	35	GLU
13	AI	59	LYS
14	AJ	17	LEU
17	AM	105	ALA
19	AO	87	ARG
20	AP	54	LEU
23	AS	86	LYS
28	BA	57	ARG
28	BA	71	ALA
28	BA	78	PHE
28	BA	145	MET
28	BA	236	PHE
28	BA	254	GLY

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Mol	Chain	Res	Type
28	BA	260	ALA
28	BA	278	ILE
28	BA	356	ILE
28	BA	391	MET
28	BA	432	ALA
29	BB	45	ALA
29	BB	69	VAL
30	B5	87	ALA
30	B5	159	GLY
31	B6	112	GLY
31	B6	152	GLN
31	B6	189	ALA
31	B6	205	GLY
32	BD	65	ALA
32	BD	140	HIS
32	BD	175	LEU
33	BE	16	GLU
33	BE	130	LYS
33	BE	154	ASP
34	BF	42	ALA
34	BF	77	LYS
34	BF	123	GLY
34	BF	124	ARG
35	BG	21	GLN
36	BH	14	SER
36	BH	75	LEU
36	BH	84	ALA
38	BJ	111	LYS
39	BK	36	GLY
40	BL	53	GLY
42	BN	13	ASN
42	BN	122	ALA
43	BO	89	ASP
43	BO	113	ALA
44	BP	54	LEU
44	BP	113	LEU
48	BT	97	GLY
50	BV	44	HIS
51	BW	27	GLY
51	BW	41	GLY
51	BW	52	CYS
52	BX	27	ARG

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Mol	Chain	Res	Type
52	BX	32	LEU
54	BZ	8	GLN
54	BZ	10	ARG
57	B2	23	ALA
57	B2	35	ARG
4	AZ	55	LEU
4	AZ	101	GLN
5	A0	154	ALA
5	A1	71	PHE
5	A1	164	ALA
6	AB	74	ALA
7	AC	82	ASP
8	AD	20	LEU
8	AD	28	ASP
8	AD	35	GLN
8	AD	36	ALA
8	AD	174	ALA
9	AE	9	GLU
10	AF	114	ASP
13	AI	121	ARG
14	AJ	78	GLU
15	AK	2	LYS
17	AM	16	ILE
18	AN	38	GLU
18	AN	68	ARG
21	AQ	15	LYS
21	AQ	51	GLU
22	AR	2	ARG
22	AR	26	ALA
23	AS	55	GLN
23	AS	87	LYS
28	BA	39	ILE
28	BA	42	PRO
28	BA	151	ASN
28	BA	214	ASP
28	BA	346	LEU
28	BA	352	PHE
28	BA	435	LYS
30	B5	52	ALA
30	B5	82	ALA
30	B5	89	ALA
30	B5	147	PRO

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Mol	Chain	Res	Type
31	B6	214	GLY
31	B6	240	GLY
32	BD	122	VAL
32	BD	203	VAL
33	BE	106	LYS
35	BG	31	GLU
35	BG	47	ASN
37	BI	97	VAL
38	BJ	68	LYS
39	BK	113	MET
40	BL	66	PHE
41	BM	134	THR
42	BN	10	LEU
42	BN	32	GLU
42	BN	80	PHE
42	BN	121	LYS
43	BO	16	ARG
44	BP	35	SER
44	BP	81	ASP
45	BQ	9	ALA
46	BR	27	ILE
47	BS	31	GLN
47	BS	64	ALA
49	BU	12	VAL
49	BU	75	ALA
52	BX	15	ASN
54	BZ	29	ARG
57	B2	8	SER
4	AZ	72	ASP
4	AZ	94	ILE
5	A1	157	ASP
6	AB	28	PRO
6	AB	33	ALA
7	AC	9	ILE
7	AC	47	ALA
7	AC	61	LYS
7	AC	128	MET
7	AC	218	LYS
8	AD	47	LEU
8	AD	147	LYS
9	AE	44	ARG
11	AG	2	ARG

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Mol	Chain	Res	Type
11	AG	4	ARG
14	AJ	59	LYS
15	AK	101	ALA
17	AM	116	LYS
18	AN	28	ALA
18	AN	43	ALA
18	AN	66	THR
19	AO	73	ASP
24	AT	47	GLN
28	BA	61	ILE
28	BA	330	PHE
29	BB	65	GLY
32	BD	9	VAL
32	BD	109	VAL
33	BE	2	GLU
33	BE	83	VAL
33	BE	96	VAL
34	BF	148	VAL
35	BG	100	ASN
35	BG	136	ASP
35	BG	155	PRO
36	BH	55	GLU
36	BH	87	GLU
39	BK	92	GLU
39	BK	122	VAL
41	BM	67	VAL
42	BN	72	ASP
44	BP	76	HIS
45	BQ	27	ARG
45	BQ	81	GLY
47	BS	32	ALA
47	BS	40	ASN
48	BT	10	VAL
52	BX	41	SER
56	B1	33	LEU
5	A0	47	LEU
5	A0	156	VAL
6	AB	132	GLU
7	AC	111	ASP
7	AC	205	GLU
7	AC	213	VAL
13	AI	58	GLU

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Mol	Chain	Res	Type
13	AI	109	GLN
13	AI	110	VAL
14	AJ	48	ARG
15	AK	12	ARG
22	AR	14	ALA
28	BA	337	PHE
31	B6	59	GLN
34	BF	111	ARG
35	BG	156	TYR
36	BH	41	LYS
37	BI	30	GLN
41	BM	70	ASP
42	BN	100	CYS
48	BT	29	THR
52	BX	3	VAL
52	BX	6	VAL
55	B0	44	ALA
58	B3	53	ASP
5	A1	227	VAL
13	AI	57	VAL
18	AN	33	VAL
59	B4	16	ILE
9	AE	15	ILE
20	AP	36	VAL
39	BK	35	VAL
45	BQ	33	VAL
9	AE	105	ILE
15	AK	88	PRO
21	AQ	11	VAL
28	BA	306	ILE
28	BA	403	GLY
32	BD	152	PRO
38	BJ	96	ARG
28	BA	318	VAL
51	BW	73	PRO
47	BS	45	VAL

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%)	73 (86%)	12 (14%)	3	13
5	A0	176/176 (100%)	173 (98%)	3 (2%)	53	69
5	A1	176/176 (100%)	173 (98%)	3 (2%)	53	69
6	AB	198/198 (100%)	196 (99%)	2 (1%)	68	78
7	AC	189/189 (100%)	187 (99%)	2 (1%)	65	76
8	AD	172/172 (100%)	167 (97%)	5 (3%)	37	58
9	AE	125/125 (100%)	124 (99%)	1 (1%)	73	80
10	AF	116/116 (100%)	115 (99%)	1 (1%)	70	79
11	AG	146/146 (100%)	144 (99%)	2 (1%)	59	72
12	AH	104/104 (100%)	101 (97%)	3 (3%)	37	58
13	AI	106/106 (100%)	104 (98%)	2 (2%)	50	67
14	AJ	90/90 (100%)	88 (98%)	2 (2%)	45	64
15	AK	98/98 (100%)	96 (98%)	2 (2%)	48	66
16	AL	103/103 (100%)	102 (99%)	1 (1%)	68	78
17	AM	95/95 (100%)	94 (99%)	1 (1%)	65	76
18	AN	83/83 (100%)	82 (99%)	1 (1%)	63	75
19	AO	76/76 (100%)	76 (100%)	0	100	100
20	AP	65/65 (100%)	65 (100%)	0	100	100
21	AQ	77/77 (100%)	77 (100%)	0	100	100
22	AR	64/64 (100%)	64 (100%)	0	100	100
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%)	33	55
28	BA	353/353 (100%)	325 (92%)	28 (8%)	11	32
29	BB	92/92 (100%)	90 (98%)	2 (2%)	45	64
30	B5	181/181 (100%)	179 (99%)	2 (1%)	65	76
31	B6	217/217 (100%)	214 (99%)	3 (1%)	59	72
32	BD	164/164 (100%)	164 (100%)	0	100	100
33	BE	165/165 (100%)	163 (99%)	2 (1%)	63	75
34	BF	149/149 (100%)	146 (98%)	3 (2%)	48	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	BG	137/137 (100%)	135 (98%)	2 (2%)	57	72
36	BH	114/114 (100%)	108 (95%)	6 (5%)	20	41
37	BI	109/109 (100%)	107 (98%)	2 (2%)	51	68
38	BJ	116/116 (100%)	115 (99%)	1 (1%)	70	79
39	BK	104/104 (100%)	103 (99%)	1 (1%)	68	78
40	BL	103/103 (100%)	103 (100%)	0	100	100
41	BM	109/109 (100%)	109 (100%)	0	100	100
42	BN	103/103 (100%)	101 (98%)	2 (2%)	50	67
43	BO	87/87 (100%)	87 (100%)	0	100	100
44	BP	99/99 (100%)	99 (100%)	0	100	100
45	BQ	89/89 (100%)	88 (99%)	1 (1%)	65	76
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%)	17	39
49	BU	84/84 (100%)	81 (96%)	3 (4%)	31	52
50	BV	78/78 (100%)	76 (97%)	2 (3%)	40	62
51	BW	62/62 (100%)	59 (95%)	3 (5%)	23	44
52	BX	67/67 (100%)	66 (98%)	1 (2%)	57	72
53	BY	55/55 (100%)	54 (98%)	1 (2%)	51	68
54	BZ	48/48 (100%)	47 (98%)	1 (2%)	47	65
55	B0	47/47 (100%)	46 (98%)	1 (2%)	47	65
56	B1	48/48 (100%)	48 (100%)	0	100	100
57	B2	38/38 (100%)	38 (100%)	0	100	100
58	B3	51/51 (100%)	50 (98%)	1 (2%)	48	66
59	B4	34/34 (100%)	34 (100%)	0	100	100
All	All	5911/5911 (100%)	5793 (98%)	118 (2%)	48	66

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	AZ	28	ILE
4	AZ	29	LEU
4	AZ	44	VAL

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Mol	Chain	Res	Type
4	AZ	54	ARG
4	AZ	60	LEU
4	AZ	78	ILE
4	AZ	79	LEU
4	AZ	81	LEU
4	AZ	95	ILE
4	AZ	97	THR
4	AZ	99	ILE
4	AZ	115	HIS
5	A0	132	GLN
5	A0	133	LYS
5	A0	233	LEU
5	A1	131	ARG
5	A1	132	GLN
5	A1	237	THR
6	AB	103	TRP
6	AB	164	ASP
7	AC	114	LEU
7	AC	219	PRO
8	AD	20	LEU
8	AD	43	ARG
8	AD	110	ARG
8	AD	142	VAL
8	AD	182	LYS
9	AE	89	THR
10	AF	44	ARG
11	AG	35	LYS
11	AG	49	LEU
12	AH	2	MET
12	AH	93	LYS
12	AH	123	GLU
13	AI	17	ARG
13	AI	44	ARG
14	AJ	31	ARG
14	AJ	76	ILE
15	AK	10	ARG
15	AK	79	LYS
16	AL	54	VAL
17	AM	91	ARG
18	AN	53	ASP
25	AU	18	PHE
25	AU	69	LEU

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Mol	Chain	Res	Type
28	BA	55	GLN
28	BA	85	TYR
28	BA	130	PHE
28	BA	180	GLU
28	BA	189	ILE
28	BA	192	PHE
28	BA	195	ILE
28	BA	212	GLN
28	BA	230	VAL
28	BA	237	VAL
28	BA	238	GLU
28	BA	252	GLN
28	BA	256	ARG
28	BA	290	ILE
28	BA	309	TYR
28	BA	317	TYR
28	BA	333	THR
28	BA	336	VAL
28	BA	340	ARG
28	BA	347	LYS
28	BA	352	PHE
28	BA	356	ILE
28	BA	361	GLN
28	BA	372	ARG
28	BA	373	LEU
28	BA	374	THR
28	BA	406	LEU
28	BA	424	MET
29	BB	44	ARG
29	BB	77	THR
30	B5	7	ARG
30	B5	9	ARG
31	B6	129	LEU
31	B6	227	VAL
31	B6	264	LYS
33	BE	47	LYS
33	BE	60	TRP
34	BF	80	GLN
34	BF	119	LYS
34	BF	136	ILE
35	BG	34	ARG
35	BG	94	ARG

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Mol	Chain	Res	Type
36	BH	3	VAL
36	BH	21	VAL
36	BH	32	PRO
36	BH	70	GLU
36	BH	79	THR
36	BH	144	VAL
37	BI	10	LEU
37	BI	112	LYS
38	BJ	23	LYS
39	BK	41	ILE
42	BN	49	GLU
42	BN	64	ARG
45	BQ	33	VAL
48	BT	36	LYS
48	BT	61	LEU
48	BT	66	LYS
48	BT	69	ARG
48	BT	96	VAL
49	BU	46	LYS
49	BU	49	PRO
49	BU	91	LYS
50	BV	46	LYS
50	BV	77	VAL
51	BW	23	LYS
51	BW	36	ILE
51	BW	67	LYS
52	BX	26	ARG
53	BY	27	ASN
54	BZ	55	LYS
55	B0	31	LYS
58	B3	6	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (175) such sidechains are listed below:

Mol	Chain	Res	Type
4	AZ	76	GLN
4	AZ	101	GLN
4	AZ	104	GLN
5	A0	49	ASN
5	A0	109	GLN
5	A0	138	GLN
5	A0	162	HIS

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Mol	Chain	Res	Type
5	A0	184	ASN
5	A1	69	GLN
5	A1	109	GLN
5	A1	199	HIS
6	AB	14	HIS
6	AB	23	ASN
6	AB	41	ASN
6	AB	57	ASN
6	AB	88	GLN
6	AB	145	ASN
6	AB	169	HIS
6	AB	189	ASN
7	AC	24	ASN
7	AC	175	HIS
7	AC	189	HIS
7	AC	226	GLN
8	AD	39	GLN
8	AD	40	HIS
8	AD	73	ASN
8	AD	99	ASN
8	AD	135	GLN
9	AE	76	ASN
9	AE	81	GLN
9	AE	131	ASN
9	AE	134	ASN
9	AE	145	ASN
10	AF	17	GLN
10	AF	37	HIS
10	AF	46	GLN
10	AF	55	HIS
10	AF	94	HIS
10	AF	118	ASN
11	AG	8	GLN
11	AG	51	GLN
11	AG	67	ASN
11	AG	129	ASN
11	AG	141	HIS
11	AG	164	GLN
12	AH	17	GLN
12	AH	75	GLN
14	AJ	4	GLN
14	AJ	15	HIS

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Mol	Chain	Res	Type
15	AK	23	HIS
15	AK	27	ASN
15	AK	28	ASN
15	AK	39	ASN
15	AK	63	GLN
15	AK	100	ASN
15	AK	108	ASN
16	AL	4	ASN
16	AL	19	ASN
16	AL	71	HIS
16	AL	74	GLN
17	AM	7	ASN
19	AO	45	HIS
19	AO	49	HIS
19	AO	50	HIS
20	AP	9	HIS
20	AP	26	ASN
20	AP	40	ASN
20	AP	63	GLN
21	AQ	44	HIS
21	AQ	49	ASN
21	AQ	50	ASN
22	AR	53	GLN
22	AR	74	GLN
23	AS	13	HIS
23	AS	42	ASN
23	AS	51	HIS
23	AS	52	ASN
23	AS	56	HIS
24	AT	2	ASN
24	AT	19	HIS
24	AT	67	HIS
24	AT	83	ASN
28	BA	55	GLN
28	BA	56	GLN
28	BA	146	GLN
28	BA	151	ASN
28	BA	209	GLN
28	BA	252	GLN
28	BA	311	GLN
28	BA	361	GLN
29	BB	33	ASN

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Mol	Chain	Res	Type
30	B5	24	ASN
30	B5	47	ASN
30	B5	80	GLN
30	B5	168	ASN
31	B6	36	ASN
31	B6	57	HIS
31	B6	141	HIS
31	B6	152	GLN
31	B6	162	GLN
31	B6	229	HIS
31	B6	231	HIS
31	B6	238	ASN
31	B6	242	HIS
32	BD	36	GLN
32	BD	130	GLN
32	BD	134	HIS
32	BD	136	ASN
32	BD	140	HIS
32	BD	148	GLN
32	BD	173	GLN
32	BD	185	ASN
33	BE	29	HIS
33	BE	97	ASN
33	BE	195	GLN
34	BF	80	GLN
35	BG	21	GLN
35	BG	44	HIS
35	BG	100	ASN
35	BG	115	GLN
35	BG	142	GLN
36	BH	11	ASN
36	BH	43	ASN
36	BH	73	ASN
36	BH	128	HIS
36	BH	135	HIS
36	BH	145	ASN
37	BI	42	ASN
37	BI	104	GLN
38	BJ	40	HIS
38	BJ	77	HIS
38	BJ	80	HIS
38	BJ	86	GLN

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Mol	Chain	Res	Type
38	BJ	132	HIS
39	BK	3	GLN
39	BK	29	HIS
39	BK	93	GLN
40	BL	93	ASN
40	BL	99	ASN
40	BL	104	GLN
42	BN	3	HIS
42	BN	11	ASN
42	BN	16	HIS
43	BO	34	HIS
44	BP	14	GLN
44	BP	40	GLN
44	BP	55	HIS
44	BP	74	GLN
44	BP	76	HIS
45	BQ	13	HIS
45	BQ	55	GLN
45	BQ	70	GLN
45	BQ	71	ASN
45	BQ	80	ASN
46	BR	82	HIS
46	BR	87	GLN
47	BS	102	HIS
48	BT	28	ASN
49	BU	52	ASN
49	BU	65	GLN
49	BU	73	ASN
50	BV	12	GLN
50	BV	24	ASN
50	BV	49	ASN
50	BV	88	HIS
52	BX	35	HIS
53	BY	36	GLN
53	BY	39	GLN
53	BY	41	HIS
55	B0	4	GLN
55	B0	18	HIS
55	B0	41	HIS
56	B1	18	HIS
57	B2	16	HIS
58	B3	42	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%)	446 (15%)	47 (1%)
3	AV	76/77 (98%)	14 (18%)	1 (1%)
All	All	4649/4654 (99%)	757 (16%)	73 (1%)

All (757) 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
1	AA	31	G
1	AA	32	A
1	AA	39	G
1	AA	47	C
1	AA	48	C
1	AA	51	A
1	AA	52	C
1	AA	55	A
1	AA	61	G
1	AA	66	A
1	AA	67	C
1	AA	70	U
1	AA	71	A
1	AA	75	G
1	AA	79	G
1	AA	80	A
1	AA	83	C
1	AA	84	U
1	AA	85	U
1	AA	86	G
1	AA	88	U
1	AA	91	U
1	AA	101	A
1	AA	121	U
1	AA	144	G
1	AA	149	A

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Mol	Chain	Res	Type
1	AA	155	A
1	AA	182	A
1	AA	196	A
1	AA	197	A
1	AA	204	G
1	AA	205	A
1	AA	209	U
1	AA	210	C
1	AA	211	G
1	AA	239	U
1	AA	240	G
1	AA	243	A
1	AA	244	U
1	AA	245	U
1	AA	247	G
1	AA	252	U
1	AA	253	A
1	AA	257	G
1	AA	258	G
1	AA	266	G
1	AA	267	C
1	AA	280	C
1	AA	289	G
1	AA	306	A
1	AA	308	C
1	AA	316	C
1	AA	328	C
1	AA	329	A
1	AA	332	G
1	AA	345	C
1	AA	352	C
1	AA	354	G
1	AA	367	U
1	AA	373	A
1	AA	374	A
1	AA	381	C
1	AA	382	A
1	AA	397	A
1	AA	398	U
1	AA	406	G
1	AA	408	A
1	AA	409	U

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Mol	Chain	Res	Type
1	AA	411	A
1	AA	412	A
1	AA	413	G
1	AA	414	A
1	AA	416	G
1	AA	421	U
1	AA	424	G
1	AA	429	U
1	AA	430	A
1	AA	435	A
1	AA	451	A
1	AA	456	A
1	AA	459	A
1	AA	460	A
1	AA	461	A
1	AA	462	G
1	AA	463	U
1	AA	465	A
1	AA	466	A
1	AA	468	A
1	AA	482	A
1	AA	484	G
1	AA	485	U
1	AA	486	U
1	AA	493	A
1	AA	494	G
1	AA	499	A
1	AA	508	U
1	AA	511	C
1	AA	512	U
1	AA	518	C
1	AA	524	G
1	AA	527	G
1	AA	532	A
1	AA	533	A
1	AA	535	A
1	AA	547	A
1	AA	561	U
1	AA	563	A
1	AA	564	C
1	AA	572	A
1	AA	573	A

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Mol	Chain	Res	Type
1	AA	576	C
1	AA	577	G
1	AA	596	A
1	AA	611	C
1	AA	633	G
1	AA	653	U
1	AA	654	G
1	AA	665	A
1	AA	666	G
1	AA	721	G
1	AA	724	G
1	AA	731	G
1	AA	747	A
1	AA	748	G
1	AA	752	G
1	AA	755	G
1	AA	781	A
1	AA	782	A
1	AA	793	U
1	AA	794	A
1	AA	812	G
1	AA	815	A
1	AA	817	C
1	AA	818	G
1	AA	821	G
1	AA	828	U
1	AA	841	C
1	AA	842	U
1	AA	843	U
1	AA	844	G
1	AA	845	A
1	AA	846	G
1	AA	847	G
1	AA	849	G
1	AA	873	A
1	AA	914	A
1	AA	926	G
1	AA	927	G
1	AA	934	C
1	AA	935	A
1	AA	945	G
1	AA	960	U

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Mol	Chain	Res	Type
1	AA	961	U
1	AA	966	G
1	AA	968	A
1	AA	969	A
1	AA	971	G
1	AA	974	A
1	AA	975	A
1	AA	976	G
1	AA	977	A
1	AA	981	U
1	AA	993	G
1	AA	994	A
1	AA	996	A
1	AA	1004	A
1	AA	1014	A
1	AA	1015	G
1	AA	1018	G
1	AA	1020	G
1	AA	1028	C
1	AA	1030	U
1	AA	1032	G
1	AA	1034	G
1	AA	1036	A
1	AA	1043	G
1	AA	1050	G
1	AA	1053	G
1	AA	1065	U
1	AA	1066	C
1	AA	1070	U
1	AA	1085	U
1	AA	1086	U
1	AA	1094	G
1	AA	1095	U
1	AA	1101	A
1	AA	1112	C
1	AA	1118	U
1	AA	1119	C
1	AA	1124	G
1	AA	1125	U
1	AA	1130	A
1	AA	1133	G
1	AA	1135	U

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Mol	Chain	Res	Type
1	AA	1136	C
1	AA	1139	G
1	AA	1140	C
1	AA	1141	C
1	AA	1143	G
1	AA	1145	A
1	AA	1146	A
1	AA	1152	A
1	AA	1154	G
1	AA	1159	U
1	AA	1160	G
1	AA	1167	A
1	AA	1181	G
1	AA	1184	G
1	AA	1191	A
1	AA	1196	A
1	AA	1197	A
1	AA	1202	U
1	AA	1212	U
1	AA	1213	A
1	AA	1215	G
1	AA	1225	A
1	AA	1226	C
1	AA	1227	A
1	AA	1238	A
1	AA	1249	C
1	AA	1250	A
1	AA	1258	G
1	AA	1261	A
1	AA	1270	G
1	AA	1279	G
1	AA	1280	A
1	AA	1285	A
1	AA	1286	U
1	AA	1287	A
1	AA	1297	G
1	AA	1300	G
1	AA	1301	U
1	AA	1303	C
1	AA	1305	G
1	AA	1316	G
1	AA	1320	C

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Mol	Chain	Res	Type
1	AA	1323	G
1	AA	1331	G
1	AA	1346	A
1	AA	1353	G
1	AA	1363	A
1	AA	1364	U
1	AA	1380	U
1	AA	1399	C
1	AA	1419	G
1	AA	1432	G
1	AA	1446	A
1	AA	1448	C
1	AA	1452	C
1	AA	1454	G
1	AA	1493	A
1	AA	1494	G
1	AA	1497	G
1	AA	1499	A
1	AA	1503	A
1	AA	1506	U
1	AA	1507	A
1	AA	1517	G
1	AA	1520	C
1	AA	1526	G
1	AA	1528	U
1	AA	1529	G
1	AA	1530	G
1	AA	1535	C
1	AA	1539	C
1	AA	1540	U
1	AA	1541	U
1	AA	1542	A
2	AX	13	C
2	AX	14	G
2	AX	18	C
2	AX	19	U
2	AX	22	A
3	AV	4	C
3	AV	5	A
3	AV	6	C
3	AV	8	U
3	AV	20	G

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Mol	Chain	Res	Type
3	AV	22	A
3	AV	32	C
3	AV	44	G
3	AV	49	C
3	AV	50	G
3	AV	54	G
3	AV	68	G
3	AV	72	C
3	AV	77	A
26	B7	9	G
26	B7	13	G
26	B7	14	U
26	B7	15	A
26	B7	16	G
26	B7	26	C
26	B7	29	A
26	B7	30	C
26	B7	42	C
26	B7	45	A
26	B7	52	A
26	B7	53	A
26	B7	66	A
26	B7	67	G
26	B7	90	C
26	B7	91	C
26	B7	99	A
26	B7	109	A
26	B7	120	U
27	B8	13	A
27	B8	34	U
27	B8	35	G
27	B8	46	G
27	B8	63	A
27	B8	64	A
27	B8	71	A
27	B8	74	A
27	B8	75	G
27	B8	84	A
27	B8	90	U
27	B8	91	A
27	B8	92	U
27	B8	93	G

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Mol	Chain	Res	Type
27	B8	95	A
27	B8	100	U
27	B8	103	A
27	B8	118	A
27	B8	120	U
27	B8	136	G
27	B8	137	U
27	B8	139	U
27	B8	141	G
27	B8	143	C
27	B8	144	A
27	B8	160	A
27	B8	181	A
27	B8	196	A
27	B8	199	A
27	B8	216	A
27	B8	221	A
27	B8	222	A
27	B8	228	C
27	B8	233	A
27	B8	241	A
27	B8	248	G
27	B8	252	G
27	B8	255	A
27	B8	265	A
27	B8	266	G
27	B8	268	C
27	B8	271	G
27	B8	273	G
27	B8	277	G
27	B8	278	A
27	B8	281	C
27	B8	283	G
27	B8	285	G
27	B8	286	U
27	B8	294	A
27	B8	311	A
27	B8	321	U
27	B8	329	G
27	B8	330	A
27	B8	333	G
27	B8	346	A

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Mol	Chain	Res	Type
27	B8	352	A
27	B8	353	C
27	B8	362	A
27	B8	363	G
27	B8	364	C
27	B8	371	A
27	B8	372	G
27	B8	386	G
27	B8	387	U
27	B8	405	U
27	B8	406	G
27	B8	411	G
27	B8	412	A
27	B8	424	G
27	B8	455	C
27	B8	457	A
27	B8	479	A
27	B8	481	G
27	B8	491	G
27	B8	505	A
27	B8	508	A
27	B8	509	C
27	B8	510	C
27	B8	512	G
27	B8	528	A
27	B8	531	C
27	B8	533	G
27	B8	544	C
27	B8	545	U
27	B8	546	U
27	B8	547	A
27	B8	548	G
27	B8	549	G
27	B8	555	G
27	B8	563	A
27	B8	573	U
27	B8	575	A
27	B8	586	A
27	B8	588	U
27	B8	603	A
27	B8	613	A
27	B8	637	A

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Mol	Chain	Res	Type
27	B8	646	U
27	B8	647	G
27	B8	654	A
27	B8	655	A
27	B8	671	C
27	B8	686	U
27	B8	730	A
27	B8	747	U
27	B8	757	G
27	B8	764	A
27	B8	775	G
27	B8	776	G
27	B8	782	A
27	B8	784	G
27	B8	785	G
27	B8	788	A
27	B8	789	A
27	B8	792	A
27	B8	793	A
27	B8	802	A
27	B8	805	G
27	B8	812	C
27	B8	819	A
27	B8	827	U
27	B8	828	U
27	B8	830	G
27	B8	846	U
27	B8	847	U
27	B8	858	G
27	B8	859	G
27	B8	869	G
27	B8	871	U
27	B8	875	G
27	B8	876	C
27	B8	881	G
27	B8	887	U
27	B8	891	G
27	B8	896	A
27	B8	897	C
27	B8	900	A
27	B8	901	C
27	B8	910	A

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Mol	Chain	Res	Type
27	B8	912	C
27	B8	919	U
27	B8	931	U
27	B8	932	U
27	B8	941	A
27	B8	945	A
27	B8	946	C
27	B8	961	C
27	B8	973	A
27	B8	974	G
27	B8	980	A
27	B8	982	C
27	B8	983	A
27	B8	984	A
27	B8	985	C
27	B8	991	C
27	B8	995	C
27	B8	996	A
27	B8	1005	C
27	B8	1012	U
27	B8	1013	C
27	B8	1022	G
27	B8	1025	G
27	B8	1033	U
27	B8	1054	A
27	B8	1056	G
27	B8	1061	U
27	B8	1062	G
27	B8	1070	A
27	B8	1071	G
27	B8	1078	U
27	B8	1088	A
27	B8	1090	A
27	B8	1095	A
27	B8	1096	A
27	B8	1104	C
27	B8	1112	G
27	B8	1116	G
27	B8	1130	U
27	B8	1132	U
27	B8	1133	A
27	B8	1134	A

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Mol	Chain	Res	Type
27	B8	1135	C
27	B8	1136	G
27	B8	1139	G
27	B8	1142	A
27	B8	1176	U
27	B8	1206	G
27	B8	1237	A
27	B8	1238	G
27	B8	1241	A
27	B8	1242	U
27	B8	1248	G
27	B8	1250	G
27	B8	1253	A
27	B8	1256	G
27	B8	1266	G
27	B8	1271	G
27	B8	1272	A
27	B8	1273	U
27	B8	1275	A
27	B8	1276	A
27	B8	1300	G
27	B8	1301	A
27	B8	1312	U
27	B8	1313	U
27	B8	1316	U
27	B8	1325	U
27	B8	1326	U
27	B8	1334	G
27	B8	1336	A
27	B8	1337	G
27	B8	1352	U
27	B8	1365	A
27	B8	1374	G
27	B8	1379	U
27	B8	1386	C
27	B8	1394	U
27	B8	1396	U
27	B8	1416	G
27	B8	1419	A
27	B8	1420	A
27	B8	1421	G
27	B8	1427	A

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Mol	Chain	Res	Type
27	B8	1428	C
27	B8	1451	C
27	B8	1454	C
27	B8	1459	G
27	B8	1460	U
27	B8	1461	C
27	B8	1469	A
27	B8	1476	U
27	B8	1477	A
27	B8	1478	G
27	B8	1482	G
27	B8	1490	A
27	B8	1497	U
27	B8	1504	A
27	B8	1505	A
27	B8	1507	C
27	B8	1508	A
27	B8	1509	A
27	B8	1523	U
27	B8	1524	G
27	B8	1532	A
27	B8	1535	A
27	B8	1538	G
27	B8	1552	A
27	B8	1560	G
27	B8	1569	A
27	B8	1578	U
27	B8	1583	A
27	B8	1585	C
27	B8	1608	A
27	B8	1609	A
27	B8	1610	A
27	B8	1618	A
27	B8	1634	A
27	B8	1635	A
27	B8	1640	A
27	B8	1647	U
27	B8	1648	U
27	B8	1654	A
27	B8	1674	G
27	B8	1677	A
27	B8	1700	A

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Mol	Chain	Res	Type
27	B8	1714	U
27	B8	1715	G
27	B8	1729	U
27	B8	1730	C
27	B8	1731	G
27	B8	1733	G
27	B8	1738	G
27	B8	1756	G
27	B8	1758	U
27	B8	1761	C
27	B8	1764	C
27	B8	1773	A
27	B8	1776	G
27	B8	1781	U
27	B8	1782	U
27	B8	1784	A
27	B8	1800	C
27	B8	1801	A
27	B8	1808	A
27	B8	1809	A
27	B8	1816	C
27	B8	1819	A
27	B8	1829	A
27	B8	1870	C
27	B8	1896	G
27	B8	1906	G
27	B8	1913	A
27	B8	1914	C
27	B8	1929	G
27	B8	1930	G
27	B8	1940	U
27	B8	1955	U
27	B8	1965	C
27	B8	1966	A
27	B8	1967	C
27	B8	1970	A
27	B8	1971	U
27	B8	1972	G
27	B8	1991	U
27	B8	1993	U
27	B8	1997	C
27	B8	2020	A

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Mol	Chain	Res	Type
27	B8	2022	U
27	B8	2023	C
27	B8	2031	A
27	B8	2033	A
27	B8	2043	C
27	B8	2055	C
27	B8	2056	G
27	B8	2059	A
27	B8	2061	G
27	B8	2062	A
27	B8	2065	C
27	B8	2069	G
27	B8	2077	A
27	B8	2102	G
27	B8	2104	C
27	B8	2111	U
27	B8	2116	G
27	B8	2117	A
27	B8	2118	U
27	B8	2119	A
27	B8	2120	G
27	B8	2128	G
27	B8	2133	G
27	B8	2135	A
27	B8	2136	G
27	B8	2137	U
27	B8	2138	G
27	B8	2145	C
27	B8	2146	C
27	B8	2147	A
27	B8	2148	G
27	B8	2149	U
27	B8	2152	G
27	B8	2153	C
27	B8	2155	U
27	B8	2158	A
27	B8	2164	C
27	B8	2165	C
27	B8	2166	U
27	B8	2167	U
27	B8	2176	A
27	B8	2179	C

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Mol	Chain	Res	Type
27	B8	2181	U
27	B8	2192	U
27	B8	2198	A
27	B8	2199	A
27	B8	2204	G
27	B8	2212	A
27	B8	2213	U
27	B8	2214	C
27	B8	2225	A
27	B8	2238	G
27	B8	2239	G
27	B8	2250	G
27	B8	2251	G
27	B8	2266	A
27	B8	2271	G
27	B8	2278	A
27	B8	2279	G
27	B8	2283	C
27	B8	2286	G
27	B8	2287	A
27	B8	2297	A
27	B8	2305	U
27	B8	2307	G
27	B8	2308	G
27	B8	2311	A
27	B8	2322	A
27	B8	2324	U
27	B8	2325	G
27	B8	2333	A
27	B8	2335	A
27	B8	2336	A
27	B8	2337	G
27	B8	2347	C
27	B8	2357	G
27	B8	2383	G
27	B8	2385	C
27	B8	2396	G
27	B8	2407	A
27	B8	2426	A
27	B8	2429	G
27	B8	2430	A
27	B8	2434	A

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Mol	Chain	Res	Type
27	B8	2441	U
27	B8	2448	A
27	B8	2458	G
27	B8	2472	G
27	B8	2473	U
27	B8	2476	A
27	B8	2478	A
27	B8	2491	U
27	B8	2498	C
27	B8	2505	G
27	B8	2506	U
27	B8	2518	A
27	B8	2529	G
27	B8	2530	A
27	B8	2534	A
27	B8	2535	G
27	B8	2554	U
27	B8	2566	A
27	B8	2567	G
27	B8	2573	C
27	B8	2585	U
27	B8	2586	U
27	B8	2602	A
27	B8	2609	U
27	B8	2613	U
27	B8	2629	U
27	B8	2630	G
27	B8	2689	U
27	B8	2690	U
27	B8	2714	G
27	B8	2726	A
27	B8	2729	G
27	B8	2744	G
27	B8	2748	A
27	B8	2757	A
27	B8	2765	A
27	B8	2778	A
27	B8	2791	G
27	B8	2793	C
27	B8	2799	A
27	B8	2800	A
27	B8	2808	G

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Mol	Chain	Res	Type
27	B8	2809	A
27	B8	2820	A
27	B8	2821	A
27	B8	2832	U
27	B8	2836	U
27	B8	2849	U
27	B8	2850	A
27	B8	2867	G
27	B8	2872	A
27	B8	2873	A
27	B8	2883	A
27	B8	2904	U

All (73) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	51	A
1	AA	60	A
1	AA	85	U
1	AA	243	A
1	AA	279	A
1	AA	328	C
1	AA	366	A
1	AA	372	C
1	AA	428	G
1	AA	429	U
1	AA	484	G
1	AA	653	U
1	AA	700	G
1	AA	960	U
1	AA	1049	U
1	AA	1065	U
1	AA	1159	U
1	AA	1201	A
1	AA	1226	C
1	AA	1300	G
1	AA	1301	U
1	AA	1319	A
1	AA	1541	U
3	AV	16	C
26	B7	14	U
26	B7	66	A

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Mol	Chain	Res	Type
27	B8	91	A
27	B8	241	A
27	B8	320	A
27	B8	329	G
27	B8	507	A
27	B8	670	A
27	B8	792	A
27	B8	827	U
27	B8	858	G
27	B8	876	C
27	B8	880	G
27	B8	890	C
27	B8	891	G
27	B8	973	A
27	B8	984	A
27	B8	1061	U
27	B8	1133	A
27	B8	1205	A
27	B8	1272	A
27	B8	1312	U
27	B8	1608	A
27	B8	1699	G
27	B8	1730	C
27	B8	1786	A
27	B8	1808	A
27	B8	2076	U
27	B8	2116	G
27	B8	2118	U
27	B8	2144	G
27	B8	2145	C
27	B8	2152	G
27	B8	2159	G
27	B8	2164	C
27	B8	2172	U
27	B8	2282	G
27	B8	2286	G
27	B8	2324	U
27	B8	2336	A
27	B8	2402	U
27	B8	2425	A
27	B8	2430	A
27	B8	2491	U

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Mol	Chain	Res	Type
27	B8	2601	C
27	B8	2713	U
27	B8	2756	U
27	B8	2797	U
27	B8	2903	U

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

133 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
60	PEV	BA	527	-	48,48,48	0.82	1 (2%)	51,53,53	0.77	2 (3%)
61	PGV	BA	505	-	50,50,50	1.04	2 (4%)	53,56,56	0.76	2 (3%)
61	PGV	BA	515	-	50,50,50	1.04	2 (4%)	53,56,56	0.72	2 (3%)
60	PEV	A0	307	-	48,48,48	0.81	1 (2%)	51,53,53	0.66	2 (3%)
61	PGV	AZ	205	-	50,50,50	1.05	2 (4%)	53,56,56	0.75	2 (3%)
60	PEV	AZ	203	-	48,48,48	0.81	1 (2%)	51,53,53	0.63	2 (3%)
61	PGV	A0	318	-	50,50,50	1.05	2 (4%)	53,56,56	0.73	2 (3%)
60	PEV	BB	214	-	48,48,48	0.82	1 (2%)	51,53,53	0.71	2 (3%)
60	PEV	BA	520	-	48,48,48	0.82	1 (2%)	51,53,53	0.65	2 (3%)
60	PEV	BA	510	-	48,48,48	0.81	1 (2%)	51,53,53	0.70	2 (3%)
61	PGV	BB	207	-	50,50,50	1.05	2 (4%)	53,56,56	0.76	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
60	PEV	B8	3001	-	48,48,48	0.82	1 (2%)	51,53,53	0.72	2 (3%)
60	PEV	BA	535	-	48,48,48	0.82	1 (2%)	51,53,53	0.68	2 (3%)
60	PEV	BB	211	-	48,48,48	0.81	1 (2%)	51,53,53	0.74	2 (3%)
60	PEV	BA	538	-	48,48,48	0.79	1 (2%)	51,53,53	0.65	2 (3%)
61	PGV	A0	305	-	50,50,50	1.04	2 (4%)	53,56,56	0.73	2 (3%)
60	PEV	BA	537	-	48,48,48	0.84	1 (2%)	51,53,53	0.74	2 (3%)
60	PEV	BB	206	-	48,48,48	0.82	1 (2%)	51,53,53	0.70	2 (3%)
60	PEV	A0	312	-	48,48,48	0.83	1 (2%)	51,53,53	0.61	2 (3%)
60	PEV	A1	317	-	48,48,48	0.82	1 (2%)	51,53,53	0.70	2 (3%)
60	PEV	BB	215	-	48,48,48	0.80	1 (2%)	51,53,53	0.70	2 (3%)
60	PEV	A1	308	-	48,48,48	0.83	1 (2%)	51,53,53	0.66	2 (3%)
60	PEV	BA	529	-	48,48,48	0.84	1 (2%)	51,53,53	0.71	2 (3%)
60	PEV	A0	323	-	48,48,48	0.81	1 (2%)	51,53,53	0.71	2 (3%)
60	PEV	BA	514	-	48,48,48	0.84	1 (2%)	51,53,53	0.76	2 (3%)
60	PEV	A0	329	-	48,48,48	0.82	1 (2%)	51,53,53	0.72	2 (3%)
60	PEV	AZ	202	-	48,48,48	0.81	1 (2%)	51,53,53	0.72	2 (3%)
60	PEV	BA	509	-	48,48,48	0.83	1 (2%)	51,53,53	0.76	2 (3%)
60	PEV	A0	309	-	48,48,48	0.83	1 (2%)	51,53,53	0.70	2 (3%)
60	PEV	A0	311	-	48,48,48	0.82	1 (2%)	51,53,53	0.67	2 (3%)
61	PGV	A0	306	-	50,50,50	1.04	2 (4%)	53,56,56	0.74	2 (3%)
60	PEV	BA	525	-	48,48,48	0.82	1 (2%)	51,53,53	0.75	2 (3%)
61	PGV	B8	3005	-	50,50,50	1.04	2 (4%)	53,56,56	0.71	2 (3%)
61	PGV	BA	522	-	50,50,50	1.05	2 (4%)	53,56,56	0.71	2 (3%)
60	PEV	B8	3007	-	48,48,48	0.81	1 (2%)	51,53,53	0.64	2 (3%)
60	PEV	A1	312	-	48,48,48	0.82	1 (2%)	51,53,53	0.68	2 (3%)
60	PEV	A0	315	-	48,48,48	0.80	1 (2%)	51,53,53	0.64	2 (3%)
60	PEV	A0	313	-	48,48,48	0.84	1 (2%)	51,53,53	0.75	2 (3%)
60	PEV	A1	314	-	48,48,48	0.82	1 (2%)	51,53,53	0.70	2 (3%)
60	PEV	A1	325	-	48,48,48	0.82	1 (2%)	51,53,53	0.67	2 (3%)
61	PGV	BB	213	-	50,50,50	1.05	2 (4%)	53,56,56	0.79	2 (3%)
61	PGV	BB	203	-	50,50,50	1.05	2 (4%)	53,56,56	0.75	2 (3%)
60	PEV	BA	534	-	48,48,48	0.85	1 (2%)	51,53,53	0.76	3 (5%)
60	PEV	BA	504	-	48,48,48	0.83	1 (2%)	51,53,53	0.80	2 (3%)
60	PEV	A0	314	-	48,48,48	0.84	1 (2%)	51,53,53	0.70	2 (3%)
60	PEV	A1	306	-	48,48,48	0.83	1 (2%)	51,53,53	0.63	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
60	PEV	A1	320	-	48,48,48	0.83	1 (2%)	51,53,53	0.72	2 (3%)
60	PEV	A1	321	-	48,48,48	0.82	1 (2%)	51,53,53	0.68	2 (3%)
61	PGV	A1	311	-	50,50,50	1.05	2 (4%)	53,56,56	0.78	2 (3%)
61	PGV	BB	208	-	50,50,50	1.05	2 (4%)	53,56,56	0.72	2 (3%)
60	PEV	A0	322	-	48,48,48	0.82	1 (2%)	51,53,53	0.75	2 (3%)
60	PEV	A0	320	-	48,48,48	0.84	1 (2%)	51,53,53	0.66	2 (3%)
60	PEV	A1	310	-	48,48,48	0.81	1 (2%)	51,53,53	0.73	2 (3%)
60	PEV	B8	3006	-	48,48,48	0.82	1 (2%)	51,53,53	0.67	2 (3%)
61	PGV	A0	332	-	50,50,50	1.06	2 (4%)	53,56,56	0.74	2 (3%)
61	PGV	A1	318	-	50,50,50	1.05	2 (4%)	53,56,56	0.78	2 (3%)
60	PEV	BA	507	-	48,48,48	0.82	1 (2%)	51,53,53	0.69	2 (3%)
60	PEV	BA	508	-	48,48,48	0.82	1 (2%)	51,53,53	0.68	2 (3%)
60	PEV	BA	517	-	48,48,48	0.82	1 (2%)	51,53,53	0.69	2 (3%)
60	PEV	A1	307	-	48,48,48	0.82	1 (2%)	51,53,53	0.70	2 (3%)
60	PEV	A0	302	-	48,48,48	0.81	1 (2%)	51,53,53	0.71	2 (3%)
60	PEV	A1	305	-	48,48,48	0.82	1 (2%)	51,53,53	0.69	2 (3%)
60	PEV	BB	212	-	48,48,48	0.82	1 (2%)	51,53,53	0.67	2 (3%)
61	PGV	BB	217	-	50,50,50	1.04	2 (4%)	53,56,56	0.74	2 (3%)
61	PGV	A0	325	-	50,50,50	1.05	2 (4%)	53,56,56	0.84	2 (3%)
60	PEV	A0	303	-	48,48,48	0.84	1 (2%)	51,53,53	0.70	2 (3%)
61	PGV	BA	540	-	50,50,50	1.03	2 (4%)	53,56,56	0.76	2 (3%)
60	PEV	A0	319	-	48,48,48	0.83	1 (2%)	51,53,53	0.75	2 (3%)
61	PGV	A0	328	-	50,50,50	1.04	2 (4%)	53,56,56	0.75	2 (3%)
60	PEV	A0	326	-	48,48,48	0.80	1 (2%)	51,53,53	0.72	2 (3%)
61	PGV	BA	516	-	50,50,50	1.05	2 (4%)	53,56,56	0.69	2 (3%)
60	PEV	A1	329	-	48,48,48	0.83	1 (2%)	51,53,53	0.73	2 (3%)
60	PEV	A1	313	-	48,48,48	0.81	1 (2%)	51,53,53	0.74	2 (3%)
60	PEV	BA	502	-	48,48,48	0.81	1 (2%)	51,53,53	0.71	2 (3%)
60	PEV	BA	530	-	48,48,48	0.81	1 (2%)	51,53,53	0.67	2 (3%)
60	PEV	BB	201	-	48,48,48	0.83	1 (2%)	51,53,53	0.71	2 (3%)
61	PGV	BA	501	-	50,50,50	1.04	2 (4%)	53,56,56	0.79	2 (3%)
60	PEV	BA	519	-	48,48,48	0.82	1 (2%)	51,53,53	0.75	2 (3%)
60	PEV	BB	210	-	48,48,48	0.81	1 (2%)	51,53,53	0.72	2 (3%)
60	PEV	A0	308	-	48,48,48	0.82	1 (2%)	51,53,53	0.75	2 (3%)
60	PEV	A1	323	-	48,48,48	0.80	1 (2%)	51,53,53	0.67	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
60	PEV	A1	326	-	48,48,48	0.81	1 (2%)	51,53,53	0.69	2 (3%)
60	PEV	A0	301	-	48,48,48	0.82	1 (2%)	51,53,53	0.69	2 (3%)
61	PGV	A0	317	-	50,50,50	1.04	2 (4%)	53,56,56	0.83	2 (3%)
60	PEV	A1	304	-	48,48,48	0.81	1 (2%)	51,53,53	0.63	2 (3%)
60	PEV	BA	503	-	48,48,48	0.83	1 (2%)	51,53,53	0.75	2 (3%)
60	PEV	AZ	206	-	48,48,48	0.82	1 (2%)	51,53,53	0.62	2 (3%)
60	PEV	BA	511	-	48,48,48	0.79	1 (2%)	51,53,53	0.70	2 (3%)
60	PEV	A1	327	-	48,48,48	0.80	1 (2%)	51,53,53	0.69	2 (3%)
60	PEV	B8	3004	-	48,48,48	0.82	1 (2%)	51,53,53	0.71	2 (3%)
60	PEV	BA	521	-	48,48,48	0.81	1 (2%)	51,53,53	0.67	2 (3%)
60	PEV	A0	321	-	48,48,48	0.83	1 (2%)	51,53,53	0.82	3 (5%)
61	PGV	A0	331	-	50,50,50	1.04	2 (4%)	53,56,56	0.76	2 (3%)
60	PEV	A1	309	-	48,48,48	0.82	1 (2%)	51,53,53	0.74	2 (3%)
60	PEV	A1	301	-	48,48,48	0.82	1 (2%)	51,53,53	0.71	2 (3%)
60	PEV	BA	531	-	48,48,48	0.81	1 (2%)	51,53,53	0.66	2 (3%)
60	PEV	A0	310	-	48,48,48	0.83	1 (2%)	51,53,53	0.83	2 (3%)
60	PEV	A1	322	-	48,48,48	0.80	1 (2%)	51,53,53	0.70	2 (3%)
60	PEV	BA	506	-	48,48,48	0.79	1 (2%)	51,53,53	0.70	2 (3%)
60	PEV	BA	528	-	48,48,48	0.82	1 (2%)	51,53,53	0.73	2 (3%)
60	PEV	BB	216	-	48,48,48	0.82	1 (2%)	51,53,53	0.78	2 (3%)
60	PEV	BA	513	-	48,48,48	0.81	1 (2%)	51,53,53	0.68	2 (3%)
60	PEV	BB	202	-	48,48,48	0.82	1 (2%)	51,53,53	0.72	2 (3%)
61	PGV	BB	204	-	50,50,50	1.05	2 (4%)	53,56,56	0.80	2 (3%)
61	PGV	BB	205	-	50,50,50	1.04	2 (4%)	53,56,56	0.78	2 (3%)
60	PEV	AZ	204	-	48,48,48	0.82	1 (2%)	51,53,53	0.68	2 (3%)
60	PEV	BA	539	-	48,48,48	0.82	1 (2%)	51,53,53	0.80	2 (3%)
60	PEV	BA	518	-	48,48,48	0.81	1 (2%)	51,53,53	0.67	2 (3%)
60	PEV	BA	526	-	48,48,48	0.81	1 (2%)	51,53,53	0.69	2 (3%)
60	PEV	A0	316	-	48,48,48	0.83	1 (2%)	51,53,53	0.84	2 (3%)
60	PEV	A1	319	-	48,48,48	0.82	1 (2%)	51,53,53	0.66	1 (1%)
60	PEV	A1	324	-	48,48,48	0.82	1 (2%)	51,53,53	0.65	2 (3%)
60	PEV	BB	218	-	48,48,48	0.81	1 (2%)	51,53,53	0.70	2 (3%)
60	PEV	B8	3003	-	48,48,48	0.82	1 (2%)	51,53,53	0.72	2 (3%)
60	PEV	A0	324	-	48,48,48	0.83	1 (2%)	51,53,53	0.72	2 (3%)
61	PGV	A1	315	-	50,50,50	1.06	2 (4%)	53,56,56	0.78	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	0.82	1 (2%)	51,53,53	0.66	2 (3%)
60	PEV	BA	533	-	48,48,48	3.01	1 (2%)	51,53,53	1.33	2 (3%)
61	PGV	A1	303	-	50,50,50	1.04	2 (4%)	53,56,56	0.74	2 (3%)
60	PEV	A1	302	-	48,48,48	0.83	1 (2%)	51,53,53	0.72	2 (3%)
61	PGV	A0	304	-	50,50,50	1.05	2 (4%)	53,56,56	0.80	2 (3%)
60	PEV	BA	524	-	48,48,48	0.84	1 (2%)	51,53,53	0.71	2 (3%)
60	PEV	BB	209	-	48,48,48	0.80	1 (2%)	51,53,53	0.69	2 (3%)
61	PGV	BA	512	-	50,50,50	1.03	2 (4%)	53,56,56	0.74	2 (3%)
61	PGV	BA	536	-	50,50,50	1.04	2 (4%)	53,56,56	0.72	2 (3%)
60	PEV	A1	316	-	48,48,48	0.82	1 (2%)	51,53,53	0.75	2 (3%)
60	PEV	BA	532	-	48,48,48	0.80	1 (2%)	51,53,53	0.75	2 (3%)
61	PGV	AZ	207	-	50,50,50	1.04	2 (4%)	53,56,56	0.74	2 (3%)
60	PEV	B8	3002	-	48,48,48	0.81	1 (2%)	51,53,53	0.67	2 (3%)
60	PEV	A1	328	-	48,48,48	0.80	1 (2%)	51,53,53	0.68	2 (3%)
61	PGV	A0	327	-	50,50,50	1.06	2 (4%)	53,56,56	0.70	2 (3%)
60	PEV	AZ	201	-	48,48,48	0.79	1 (2%)	51,53,53	0.70	2 (3%)
60	PEV	BA	523	-	48,48,48	0.82	1 (2%)	51,53,53	0.75	2 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	PEV	BA	527	-	-	8/52/52/52	-
61	PGV	BA	505	-	2/2/5/7	7/55/55/55	-
61	PGV	BA	515	-	2/2/5/7	6/55/55/55	-
60	PEV	A0	307	-	-	9/52/52/52	-
61	PGV	AZ	205	-	2/2/5/7	13/55/55/55	-
60	PEV	AZ	203	-	-	7/52/52/52	-
61	PGV	A0	318	-	2/2/5/7	10/55/55/55	-
60	PEV	BB	214	-	-	7/52/52/52	-
60	PEV	BA	520	-	-	5/52/52/52	-
60	PEV	BA	510	-	-	8/52/52/52	-
61	PGV	BB	207	-	2/2/5/7	4/55/55/55	-
60	PEV	B8	3001	-	1/1/4/4	3/52/52/52	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	PEV	BA	535	-	1/1/4/4	8/52/52/52	-
60	PEV	BB	211	-	-	6/52/52/52	-
60	PEV	BA	538	-	1/1/4/4	8/52/52/52	-
61	PGV	A0	305	-	1/1/5/7	10/55/55/55	-
60	PEV	BA	537	-	1/1/4/4	8/52/52/52	-
60	PEV	BB	206	-	1/1/4/4	8/52/52/52	-
60	PEV	A0	312	-	-	6/52/52/52	-
60	PEV	A1	317	-	1/1/4/4	8/52/52/52	-
60	PEV	BB	215	-	-	5/52/52/52	-
60	PEV	A1	308	-	-	11/52/52/52	-
60	PEV	BA	529	-	-	3/52/52/52	-
60	PEV	A0	323	-	1/1/4/4	6/52/52/52	-
60	PEV	BA	514	-	-	8/52/52/52	-
60	PEV	A0	329	-	-	4/52/52/52	-
60	PEV	AZ	202	-	-	7/52/52/52	-
60	PEV	BA	509	-	-	13/52/52/52	-
60	PEV	A0	309	-	-	8/52/52/52	-
60	PEV	A0	311	-	-	7/52/52/52	-
61	PGV	A0	306	-	2/2/5/7	8/55/55/55	-
60	PEV	BA	525	-	-	11/52/52/52	-
61	PGV	B8	3005	-	2/2/5/7	8/55/55/55	-
61	PGV	BA	522	-	2/2/5/7	2/55/55/55	-
60	PEV	B8	3007	-	-	4/52/52/52	-
60	PEV	A1	312	-	-	5/52/52/52	-
60	PEV	A0	315	-	-	9/52/52/52	-
60	PEV	A0	313	-	-	4/52/52/52	-
60	PEV	A1	314	-	-	6/52/52/52	-
60	PEV	A1	325	-	-	11/52/52/52	-
61	PGV	BB	213	-	1/1/5/7	8/55/55/55	-
61	PGV	BB	203	-	2/2/5/7	8/55/55/55	-
60	PEV	BA	534	-	-	5/52/52/52	-
60	PEV	BA	504	-	-	5/52/52/52	-
60	PEV	A0	314	-	1/1/4/4	7/52/52/52	-
61	PGV	A1	311	-	2/2/5/7	7/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	PGV	BB	208	-	2/2/5/7	7/55/55/55	-
60	PEV	A1	306	-	-	6/52/52/52	-
60	PEV	A1	320	-	-	8/52/52/52	-
60	PEV	A1	321	-	-	7/52/52/52	-
60	PEV	A0	322	-	-	5/52/52/52	-
60	PEV	A0	320	-	-	5/52/52/52	-
60	PEV	A1	310	-	-	8/52/52/52	-
60	PEV	B8	3006	-	-	7/52/52/52	-
61	PGV	A0	332	-	2/2/5/7	7/55/55/55	-
61	PGV	A1	318	-	2/2/5/7	10/55/55/55	-
60	PEV	BA	507	-	-	3/52/52/52	-
60	PEV	BA	508	-	1/1/4/4	5/52/52/52	-
60	PEV	BA	517	-	-	4/52/52/52	-
60	PEV	A1	307	-	-	4/52/52/52	-
60	PEV	A0	302	-	-	6/52/52/52	-
60	PEV	A1	305	-	1/1/4/4	6/52/52/52	-
60	PEV	BB	212	-	-	6/52/52/52	-
61	PGV	BB	217	-	2/2/5/7	7/55/55/55	-
61	PGV	A0	325	-	2/2/5/7	6/55/55/55	-
60	PEV	A0	303	-	-	7/52/52/52	-
61	PGV	BA	540	-	2/2/5/7	6/55/55/55	-
60	PEV	A0	319	-	-	7/52/52/52	-
61	PGV	A0	328	-	2/2/5/7	9/55/55/55	-
60	PEV	A0	326	-	-	9/52/52/52	-
61	PGV	BA	516	-	2/2/5/7	5/55/55/55	-
60	PEV	A1	329	-	-	4/52/52/52	-
60	PEV	A1	313	-	1/1/4/4	7/52/52/52	-
60	PEV	BA	502	-	1/1/4/4	8/52/52/52	-
60	PEV	BA	530	-	1/1/4/4	12/52/52/52	-
60	PEV	BB	201	-	-	11/52/52/52	-
61	PGV	BA	501	-	1/1/5/7	6/55/55/55	-
60	PEV	BA	519	-	-	10/52/52/52	-
60	PEV	BB	210	-	-	12/52/52/52	-
60	PEV	A0	308	-	1/1/4/4	5/52/52/52	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	PEV	A1	323	-	-	3/52/52/52	-
60	PEV	A1	326	-	-	4/52/52/52	-
60	PEV	A0	301	-	-	11/52/52/52	-
61	PGV	A0	317	-	2/2/5/7	7/55/55/55	-
60	PEV	A1	304	-	-	4/52/52/52	-
60	PEV	BA	503	-	-	10/52/52/52	-
60	PEV	AZ	206	-	-	4/52/52/52	-
60	PEV	BA	511	-	-	5/52/52/52	-
60	PEV	A1	327	-	-	6/52/52/52	-
60	PEV	B8	3004	-	-	9/52/52/52	-
60	PEV	BA	521	-	-	8/52/52/52	-
60	PEV	A0	321	-	-	11/52/52/52	-
61	PGV	A0	331	-	2/2/5/7	4/55/55/55	-
60	PEV	A1	309	-	-	6/52/52/52	-
60	PEV	A1	301	-	1/1/4/4	12/52/52/52	-
60	PEV	BA	531	-	-	3/52/52/52	-
60	PEV	A0	310	-	-	5/52/52/52	-
60	PEV	A1	322	-	-	4/52/52/52	-
60	PEV	BA	506	-	-	5/52/52/52	-
60	PEV	BA	528	-	-	8/52/52/52	-
60	PEV	BB	216	-	-	4/52/52/52	-
60	PEV	BA	513	-	-	8/52/52/52	-
60	PEV	BB	202	-	1/1/4/4	3/52/52/52	-
61	PGV	BB	204	-	2/2/5/7	9/55/55/55	-
61	PGV	BB	205	-	2/2/5/7	6/55/55/55	-
60	PEV	AZ	204	-	1/1/4/4	7/52/52/52	-
60	PEV	BA	539	-	-	4/52/52/52	-
60	PEV	BA	526	-	1/1/4/4	4/52/52/52	-
60	PEV	BA	518	-	-	7/52/52/52	-
60	PEV	A0	316	-	-	10/52/52/52	-
60	PEV	A1	319	-	-	5/52/52/52	-
60	PEV	A1	324	-	-	5/52/52/52	-
60	PEV	BB	218	-	-	9/52/52/52	-
60	PEV	B8	3003	-	-	13/52/52/52	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	PEV	A0	324	-	-	7/52/52/52	-
61	PGV	A1	315	-	2/2/5/7	13/55/55/55	-
60	PEV	A0	330	-	-	7/52/52/52	-
60	PEV	BA	533	-	-	9/52/52/52	-
61	PGV	A1	303	-	2/2/5/7	5/55/55/55	-
60	PEV	A1	302	-	-	9/52/52/52	-
61	PGV	A0	304	-	2/2/5/7	5/55/55/55	-
60	PEV	BA	524	-	-	10/52/52/52	-
61	PGV	BA	512	-	1/1/5/7	10/55/55/55	-
61	PGV	BA	536	-	2/2/5/7	6/55/55/55	-
60	PEV	BB	209	-	-	8/52/52/52	-
60	PEV	A1	316	-	-	3/52/52/52	-
61	PGV	AZ	207	-	2/2/5/7	7/55/55/55	-
60	PEV	BA	532	-	-	12/52/52/52	-
60	PEV	B8	3002	-	-	4/52/52/52	-
60	PEV	A1	328	-	-	12/52/52/52	-
61	PGV	A0	327	-	2/2/5/7	6/55/55/55	-
60	PEV	AZ	201	-	-	5/52/52/52	-
60	PEV	BA	523	-	-	6/52/52/52	-

All (165) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	BA	533	PEV	C39-C40	20.19	2.52	1.51
61	BA	516	PGV	C9-C10	-4.20	1.34	1.52
61	BB	213	PGV	C9-C10	-4.18	1.34	1.52
61	BA	522	PGV	C9-C10	-4.14	1.34	1.52
61	A1	315	PGV	C9-C10	-4.14	1.34	1.52
61	BB	204	PGV	C9-C10	-4.14	1.34	1.52
61	BA	501	PGV	C9-C10	-4.13	1.34	1.52
61	BB	205	PGV	C9-C10	-4.13	1.34	1.52
61	AZ	207	PGV	C9-C10	-4.12	1.34	1.52
61	BA	515	PGV	C9-C10	-4.12	1.34	1.52
61	A0	327	PGV	C9-C10	-4.11	1.34	1.52
61	A0	331	PGV	C9-C10	-4.11	1.35	1.52
61	A0	318	PGV	C9-C10	-4.11	1.35	1.52
61	BB	208	PGV	C9-C10	-4.10	1.35	1.52
61	BA	540	PGV	C9-C10	-4.10	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	A0	325	PGV	C12-C11	4.10	1.55	1.31
61	A0	305	PGV	C9-C10	-4.10	1.35	1.52
61	AZ	205	PGV	C9-C10	-4.09	1.35	1.52
61	BA	522	PGV	C12-C11	4.09	1.54	1.31
61	BB	207	PGV	C9-C10	-4.09	1.35	1.52
61	BB	203	PGV	C12-C11	4.09	1.54	1.31
61	A1	303	PGV	C9-C10	-4.09	1.35	1.52
61	BA	505	PGV	C12-C11	4.08	1.54	1.31
61	A1	311	PGV	C9-C10	-4.08	1.35	1.52
61	A0	317	PGV	C9-C10	-4.08	1.35	1.52
61	BA	516	PGV	C12-C11	4.08	1.54	1.31
61	BB	213	PGV	C12-C11	4.08	1.54	1.31
61	A1	303	PGV	C12-C11	4.07	1.54	1.31
61	BB	217	PGV	C9-C10	-4.07	1.35	1.52
61	A1	315	PGV	C12-C11	4.07	1.54	1.31
61	BA	512	PGV	C9-C10	-4.07	1.35	1.52
61	A0	328	PGV	C9-C10	-4.07	1.35	1.52
61	BA	536	PGV	C9-C10	-4.06	1.35	1.52
61	A0	327	PGV	C12-C11	4.06	1.54	1.31
61	A0	306	PGV	C9-C10	-4.06	1.35	1.52
61	A0	304	PGV	C9-C10	-4.06	1.35	1.52
61	A0	306	PGV	C12-C11	4.06	1.54	1.31
61	BB	204	PGV	C12-C11	4.05	1.54	1.31
61	B8	3005	PGV	C9-C10	-4.05	1.35	1.52
61	A1	318	PGV	C9-C10	-4.05	1.35	1.52
61	A1	311	PGV	C12-C11	4.05	1.54	1.31
61	A0	332	PGV	C12-C11	4.05	1.54	1.31
61	BA	505	PGV	C9-C10	-4.05	1.35	1.52
61	A0	304	PGV	C12-C11	4.05	1.54	1.31
61	BB	203	PGV	C9-C10	-4.04	1.35	1.52
61	A0	318	PGV	C12-C11	4.04	1.54	1.31
61	A0	332	PGV	C9-C10	-4.04	1.35	1.52
61	BA	536	PGV	C12-C11	4.04	1.54	1.31
61	BB	217	PGV	C12-C11	4.03	1.54	1.31
61	BA	540	PGV	C12-C11	4.03	1.54	1.31
61	A1	318	PGV	C12-C11	4.03	1.54	1.31
61	A0	325	PGV	C9-C10	-4.03	1.35	1.52
61	A0	328	PGV	C12-C11	4.03	1.54	1.31
61	BB	208	PGV	C12-C11	4.02	1.54	1.31
61	A0	317	PGV	C12-C11	4.02	1.54	1.31
61	AZ	205	PGV	C12-C11	4.02	1.54	1.31
61	AZ	207	PGV	C12-C11	4.01	1.54	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	A0	331	PGV	C12-C11	4.01	1.54	1.31
61	BB	207	PGV	C12-C11	4.01	1.54	1.31
61	BA	501	PGV	C12-C11	4.00	1.54	1.31
61	A0	305	PGV	C12-C11	4.00	1.54	1.31
61	BA	512	PGV	C12-C11	3.99	1.54	1.31
61	B8	3005	PGV	C12-C11	3.99	1.54	1.31
61	BA	515	PGV	C12-C11	3.97	1.54	1.31
61	BB	205	PGV	C12-C11	3.97	1.54	1.31
60	A1	319	PEV	C39-C40	-3.42	1.34	1.51
60	B8	3004	PEV	C39-C40	-3.42	1.34	1.51
60	A0	309	PEV	C39-C40	-3.41	1.34	1.51
60	B8	3002	PEV	C39-C40	-3.41	1.34	1.51
60	BA	519	PEV	C39-C40	-3.40	1.34	1.51
60	BA	531	PEV	C39-C40	-3.40	1.34	1.51
60	A1	308	PEV	C39-C40	-3.40	1.34	1.51
60	A1	326	PEV	C39-C40	-3.40	1.34	1.51
60	AZ	204	PEV	C39-C40	-3.39	1.34	1.51
60	A0	314	PEV	C39-C40	-3.39	1.34	1.51
60	A1	301	PEV	C39-C40	-3.39	1.34	1.51
60	A0	308	PEV	C39-C40	-3.39	1.34	1.51
60	B8	3007	PEV	C39-C40	-3.39	1.34	1.51
60	BA	518	PEV	C39-C40	-3.39	1.34	1.51
60	BA	528	PEV	C39-C40	-3.39	1.34	1.51
60	BA	532	PEV	C39-C40	-3.39	1.34	1.51
60	BA	514	PEV	C39-C40	-3.39	1.34	1.51
60	BA	507	PEV	C39-C40	-3.38	1.34	1.51
60	A0	330	PEV	C39-C40	-3.38	1.34	1.51
60	AZ	206	PEV	C39-C40	-3.38	1.35	1.51
60	BA	530	PEV	C39-C40	-3.38	1.35	1.51
60	AZ	202	PEV	C39-C40	-3.38	1.35	1.51
60	A1	323	PEV	C39-C40	-3.38	1.35	1.51
60	BA	534	PEV	C39-C40	-3.38	1.35	1.51
60	A1	310	PEV	C39-C40	-3.38	1.35	1.51
60	A1	305	PEV	C39-C40	-3.38	1.35	1.51
60	A1	322	PEV	C39-C40	-3.38	1.35	1.51
60	BA	521	PEV	C39-C40	-3.38	1.35	1.51
60	A0	310	PEV	C39-C40	-3.38	1.35	1.51
60	BA	539	PEV	C39-C40	-3.38	1.35	1.51
60	BB	211	PEV	C39-C40	-3.38	1.35	1.51
60	A0	322	PEV	C39-C40	-3.37	1.35	1.51
60	A1	324	PEV	C39-C40	-3.37	1.35	1.51
60	A0	315	PEV	C39-C40	-3.37	1.35	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	A1	304	PEV	C39-C40	-3.37	1.35	1.51
60	A1	306	PEV	C39-C40	-3.37	1.35	1.51
60	A1	329	PEV	C39-C40	-3.37	1.35	1.51
60	BB	201	PEV	C39-C40	-3.37	1.35	1.51
60	A0	319	PEV	C39-C40	-3.37	1.35	1.51
60	A0	326	PEV	C39-C40	-3.37	1.35	1.51
60	B8	3006	PEV	C39-C40	-3.37	1.35	1.51
60	A1	328	PEV	C39-C40	-3.37	1.35	1.51
60	BA	517	PEV	C39-C40	-3.37	1.35	1.51
60	BA	504	PEV	C39-C40	-3.37	1.35	1.51
60	BA	535	PEV	C39-C40	-3.37	1.35	1.51
60	A0	313	PEV	C39-C40	-3.36	1.35	1.51
60	A0	329	PEV	C39-C40	-3.36	1.35	1.51
60	AZ	201	PEV	C39-C40	-3.36	1.35	1.51
60	A1	327	PEV	C39-C40	-3.36	1.35	1.51
60	BB	212	PEV	C39-C40	-3.36	1.35	1.51
60	BB	218	PEV	C39-C40	-3.36	1.35	1.51
60	A0	302	PEV	C39-C40	-3.36	1.35	1.51
60	BB	216	PEV	C39-C40	-3.36	1.35	1.51
60	AZ	203	PEV	C39-C40	-3.36	1.35	1.51
60	A0	324	PEV	C39-C40	-3.36	1.35	1.51
60	BA	538	PEV	C39-C40	-3.36	1.35	1.51
60	A0	312	PEV	C39-C40	-3.36	1.35	1.51
60	BA	527	PEV	C39-C40	-3.36	1.35	1.51
60	BB	202	PEV	C39-C40	-3.36	1.35	1.51
60	BA	508	PEV	C39-C40	-3.36	1.35	1.51
60	BB	210	PEV	C39-C40	-3.35	1.35	1.51
60	A1	302	PEV	C39-C40	-3.35	1.35	1.51
60	A1	314	PEV	C39-C40	-3.35	1.35	1.51
60	BA	537	PEV	C39-C40	-3.35	1.35	1.51
60	A0	303	PEV	C39-C40	-3.35	1.35	1.51
60	BA	509	PEV	C39-C40	-3.35	1.35	1.51
60	BB	214	PEV	C39-C40	-3.35	1.35	1.51
60	BA	526	PEV	C39-C40	-3.35	1.35	1.51
60	BA	520	PEV	C39-C40	-3.35	1.35	1.51
60	BA	506	PEV	C39-C40	-3.35	1.35	1.51
60	B8	3003	PEV	C39-C40	-3.35	1.35	1.51
60	A0	301	PEV	C39-C40	-3.34	1.35	1.51
60	BA	513	PEV	C39-C40	-3.34	1.35	1.51
60	A1	321	PEV	C39-C40	-3.34	1.35	1.51
60	BA	503	PEV	C39-C40	-3.34	1.35	1.51
60	BA	529	PEV	C39-C40	-3.34	1.35	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	BA	502	PEV	C39-C40	-3.34	1.35	1.51
60	A0	311	PEV	C39-C40	-3.34	1.35	1.51
60	A0	320	PEV	C39-C40	-3.34	1.35	1.51
60	BA	510	PEV	C39-C40	-3.34	1.35	1.51
60	BA	523	PEV	C39-C40	-3.34	1.35	1.51
60	A1	317	PEV	C39-C40	-3.34	1.35	1.51
60	A1	309	PEV	C39-C40	-3.34	1.35	1.51
60	A1	316	PEV	C39-C40	-3.34	1.35	1.51
60	A0	321	PEV	C39-C40	-3.33	1.35	1.51
60	B8	3001	PEV	C39-C40	-3.33	1.35	1.51
60	A1	320	PEV	C39-C40	-3.33	1.35	1.51
60	A1	307	PEV	C39-C40	-3.33	1.35	1.51
60	BB	209	PEV	C39-C40	-3.33	1.35	1.51
60	A1	312	PEV	C39-C40	-3.33	1.35	1.51
60	BA	525	PEV	C39-C40	-3.33	1.35	1.51
60	A0	307	PEV	C39-C40	-3.33	1.35	1.51
60	A0	323	PEV	C39-C40	-3.32	1.35	1.51
60	A1	313	PEV	C39-C40	-3.32	1.35	1.51
60	BA	524	PEV	C39-C40	-3.32	1.35	1.51
60	BB	206	PEV	C39-C40	-3.32	1.35	1.51
60	A1	325	PEV	C39-C40	-3.31	1.35	1.51
60	BB	215	PEV	C39-C40	-3.31	1.35	1.51
60	BA	511	PEV	C39-C40	-3.29	1.35	1.51
60	A0	316	PEV	C39-C40	-3.28	1.35	1.51

All (267) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	BA	533	PEV	C39-C40-C41	6.09	145.17	114.37
60	BA	533	PEV	C38-C39-C40	5.57	142.55	114.37
60	A0	316	PEV	C38-C39-C40	3.60	132.56	114.37
60	A0	316	PEV	C39-C40-C41	3.22	130.63	114.37
60	A0	321	PEV	C2-O2-C31	3.12	125.27	117.80
61	A0	325	PGV	C8-C9-C10	3.01	128.33	113.86
61	BB	205	PGV	C8-C9-C10	2.94	127.98	113.86
61	A0	332	PGV	C8-C9-C10	2.91	127.84	113.86
61	A1	311	PGV	C8-C9-C10	2.90	127.80	113.86
61	A0	328	PGV	C8-C9-C10	2.90	127.78	113.86
61	BB	213	PGV	C8-C9-C10	2.89	127.73	113.86
61	BA	505	PGV	C8-C9-C10	2.84	127.53	113.86
60	A0	308	PEV	C38-C39-C40	2.83	128.67	114.37
60	BB	211	PEV	C38-C39-C40	2.83	128.67	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	BB	205	PGV	C9-C10-C11	2.83	128.44	112.60
60	BA	532	PEV	C38-C39-C40	2.82	128.64	114.37
60	BA	503	PEV	C38-C39-C40	2.79	128.49	114.37
60	A1	329	PEV	C38-C39-C40	2.79	128.47	114.37
61	BA	512	PGV	C8-C9-C10	2.79	127.27	113.86
61	BB	207	PGV	C9-C10-C11	2.79	128.21	112.60
60	A1	307	PEV	C38-C39-C40	2.78	128.44	114.37
61	BB	203	PGV	C8-C9-C10	2.78	127.24	113.86
61	A0	325	PGV	C9-C10-C11	2.78	128.18	112.60
60	BA	534	PEV	C39-C40-C41	2.78	128.41	114.37
61	A0	304	PGV	C8-C9-C10	2.78	127.21	113.86
60	BA	517	PEV	C38-C39-C40	2.77	128.40	114.37
60	A0	323	PEV	C38-C39-C40	2.77	128.37	114.37
60	BB	210	PEV	C39-C40-C41	2.77	128.37	114.37
61	BA	501	PGV	C8-C9-C10	2.77	127.16	113.86
61	BB	208	PGV	C8-C9-C10	2.76	127.10	113.86
60	BB	211	PEV	C39-C40-C41	2.75	128.28	114.37
60	A0	323	PEV	C39-C40-C41	2.75	128.28	114.37
61	A1	315	PGV	C8-C9-C10	2.75	127.08	113.86
60	BA	503	PEV	C39-C40-C41	2.75	128.25	114.37
61	A0	332	PGV	C9-C10-C11	2.75	127.98	112.60
60	BA	527	PEV	C38-C39-C40	2.74	128.23	114.37
61	A0	318	PGV	C8-C9-C10	2.74	127.03	113.86
60	A1	307	PEV	C39-C40-C41	2.73	128.19	114.37
60	A0	319	PEV	C38-C39-C40	2.73	128.16	114.37
60	BB	210	PEV	C38-C39-C40	2.73	128.16	114.37
61	A0	317	PGV	C8-C9-C10	2.72	126.94	113.86
60	B8	3004	PEV	C39-C40-C41	2.72	128.11	114.37
60	BA	532	PEV	C39-C40-C41	2.72	128.10	114.37
60	BA	506	PEV	C39-C40-C41	2.71	128.08	114.37
61	A0	306	PGV	C8-C9-C10	2.71	126.90	113.86
60	AZ	202	PEV	C39-C40-C41	2.71	128.07	114.37
60	BA	534	PEV	C38-C39-C40	2.71	128.06	114.37
60	BB	206	PEV	C38-C39-C40	2.71	128.06	114.37
61	A1	318	PGV	C8-C9-C10	2.71	126.88	113.86
60	AZ	202	PEV	C38-C39-C40	2.71	128.05	114.37
60	BA	528	PEV	C39-C40-C41	2.71	128.05	114.37
60	A0	329	PEV	C39-C40-C41	2.70	128.00	114.37
60	A0	301	PEV	C39-C40-C41	2.70	128.00	114.37
60	BB	218	PEV	C38-C39-C40	2.70	128.00	114.37
60	B8	3004	PEV	C38-C39-C40	2.69	127.99	114.37
60	BA	526	PEV	C39-C40-C41	2.69	127.98	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	A0	329	PEV	C38-C39-C40	2.69	127.98	114.37
60	BA	506	PEV	C38-C39-C40	2.69	127.95	114.37
61	A1	311	PGV	C9-C10-C11	2.69	127.65	112.60
61	AZ	205	PGV	C8-C9-C10	2.68	126.77	113.86
61	BB	213	PGV	C9-C10-C11	2.68	127.62	112.60
61	BA	540	PGV	C8-C9-C10	2.68	126.73	113.86
60	A1	323	PEV	C38-C39-C40	2.67	127.87	114.37
60	AZ	201	PEV	C38-C39-C40	2.67	127.87	114.37
61	BB	217	PGV	C8-C9-C10	2.67	126.69	113.86
60	A0	319	PEV	C39-C40-C41	2.67	127.85	114.37
60	BA	525	PEV	C38-C39-C40	2.67	127.85	114.37
60	BA	535	PEV	C39-C40-C41	2.67	127.84	114.37
60	BA	525	PEV	C39-C40-C41	2.66	127.83	114.37
60	A1	314	PEV	C39-C40-C41	2.66	127.82	114.37
61	BB	207	PGV	C8-C9-C10	2.66	126.65	113.86
60	A0	308	PEV	C39-C40-C41	2.66	127.81	114.37
60	BA	528	PEV	C38-C39-C40	2.66	127.81	114.37
61	BB	203	PGV	C9-C10-C11	2.66	127.49	112.60
61	A0	331	PGV	C8-C9-C10	2.66	126.63	113.86
60	AZ	201	PEV	C39-C40-C41	2.65	127.79	114.37
61	A0	331	PGV	C9-C10-C11	2.65	127.46	112.60
60	BB	214	PEV	C39-C40-C41	2.65	127.75	114.37
61	AZ	207	PGV	C8-C9-C10	2.64	126.57	113.86
60	BA	517	PEV	C39-C40-C41	2.64	127.73	114.37
60	A1	322	PEV	C39-C40-C41	2.64	127.73	114.37
60	A1	305	PEV	C38-C39-C40	2.64	127.73	114.37
60	BA	507	PEV	C39-C40-C41	2.64	127.73	114.37
60	A0	311	PEV	C39-C40-C41	2.64	127.72	114.37
60	BA	527	PEV	C39-C40-C41	2.64	127.72	114.37
61	A1	303	PGV	C8-C9-C10	2.64	126.54	113.86
60	BA	539	PEV	C38-C39-C40	2.64	127.69	114.37
60	BA	511	PEV	C39-C40-C41	2.64	127.69	114.37
60	A0	326	PEV	C39-C40-C41	2.64	127.69	114.37
60	BA	524	PEV	C39-C40-C41	2.63	127.69	114.37
60	BA	504	PEV	C39-C40-C41	2.63	127.69	114.37
60	BA	514	PEV	C38-C39-C40	2.63	127.68	114.37
60	BA	535	PEV	C38-C39-C40	2.63	127.68	114.37
60	BB	216	PEV	C38-C39-C40	2.63	127.67	114.37
61	BB	208	PGV	C9-C10-C11	2.63	127.34	112.60
60	BA	526	PEV	C38-C39-C40	2.63	127.64	114.37
60	A1	309	PEV	C39-C40-C41	2.62	127.63	114.37
60	BA	510	PEV	C39-C40-C41	2.62	127.63	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	B8	3001	PEV	C39-C40-C41	2.62	127.62	114.37
60	BB	206	PEV	C39-C40-C41	2.62	127.62	114.37
60	A0	326	PEV	C38-C39-C40	2.62	127.62	114.37
60	BB	214	PEV	C38-C39-C40	2.62	127.61	114.37
60	BA	510	PEV	C38-C39-C40	2.62	127.60	114.37
60	A0	320	PEV	C39-C40-C41	2.62	127.60	114.37
61	BA	522	PGV	C9-C10-C11	2.61	127.24	112.60
60	B8	3003	PEV	C39-C40-C41	2.61	127.58	114.37
61	BA	505	PGV	C9-C10-C11	2.61	127.24	112.60
60	A1	314	PEV	C38-C39-C40	2.61	127.58	114.37
60	BA	523	PEV	C39-C40-C41	2.61	127.57	114.37
61	BA	512	PGV	C9-C10-C11	2.61	127.22	112.60
60	A1	309	PEV	C38-C39-C40	2.61	127.56	114.37
60	BA	507	PEV	C38-C39-C40	2.61	127.55	114.37
60	BA	508	PEV	C38-C39-C40	2.61	127.55	114.37
60	BB	212	PEV	C38-C39-C40	2.61	127.55	114.37
61	A0	328	PGV	C9-C10-C11	2.61	127.19	112.60
60	BA	502	PEV	C39-C40-C41	2.60	127.52	114.37
61	BA	536	PGV	C8-C9-C10	2.60	126.34	113.86
60	A1	313	PEV	C39-C40-C41	2.60	127.50	114.37
60	BA	509	PEV	C38-C39-C40	2.60	127.49	114.37
60	A1	325	PEV	C39-C40-C41	2.60	127.49	114.37
60	A1	301	PEV	C38-C39-C40	2.59	127.47	114.37
60	A0	301	PEV	C38-C39-C40	2.59	127.47	114.37
60	A0	320	PEV	C38-C39-C40	2.59	127.47	114.37
61	BB	204	PGV	C8-C9-C10	2.59	126.31	113.86
61	B8	3005	PGV	C8-C9-C10	2.59	126.31	113.86
60	BA	509	PEV	C39-C40-C41	2.59	127.45	114.37
61	BA	540	PGV	C9-C10-C11	2.59	127.09	112.60
61	BA	501	PGV	C9-C10-C11	2.59	127.09	112.60
60	A1	322	PEV	C38-C39-C40	2.59	127.44	114.37
60	A1	328	PEV	C39-C40-C41	2.58	127.43	114.37
60	BA	508	PEV	C39-C40-C41	2.58	127.43	114.37
60	B8	3002	PEV	C39-C40-C41	2.58	127.42	114.37
61	BA	515	PGV	C8-C9-C10	2.58	126.25	113.86
60	BA	539	PEV	C39-C40-C41	2.58	127.40	114.37
60	A0	311	PEV	C38-C39-C40	2.58	127.39	114.37
60	A0	307	PEV	C39-C40-C41	2.58	127.39	114.37
60	A1	328	PEV	C38-C39-C40	2.58	127.39	114.37
60	BA	521	PEV	C38-C39-C40	2.57	127.38	114.37
60	BA	502	PEV	C38-C39-C40	2.57	127.38	114.37
61	AZ	207	PGV	C9-C10-C11	2.57	127.02	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	A0	322	PEV	C39-C40-C41	2.57	127.37	114.37
61	A0	317	PGV	C9-C10-C11	2.57	127.00	112.60
60	B8	3006	PEV	C39-C40-C41	2.57	127.35	114.37
60	A1	313	PEV	C38-C39-C40	2.57	127.35	114.37
61	A1	303	PGV	C9-C10-C11	2.57	126.99	112.60
60	A1	324	PEV	C38-C39-C40	2.57	127.35	114.37
60	A1	327	PEV	C39-C40-C41	2.57	127.35	114.37
60	BA	524	PEV	C38-C39-C40	2.57	127.35	114.37
60	BA	530	PEV	C38-C39-C40	2.57	127.35	114.37
60	A1	329	PEV	C39-C40-C41	2.56	127.33	114.37
60	A0	310	PEV	C38-C39-C40	2.56	127.31	114.37
60	BB	216	PEV	C39-C40-C41	2.56	127.29	114.37
60	A1	325	PEV	C38-C39-C40	2.56	127.29	114.37
60	BB	212	PEV	C39-C40-C41	2.55	127.27	114.37
60	BA	538	PEV	C39-C40-C41	2.55	127.25	114.37
60	BB	202	PEV	C39-C40-C41	2.55	127.25	114.37
60	A1	321	PEV	C39-C40-C41	2.55	127.24	114.37
60	A1	301	PEV	C39-C40-C41	2.55	127.24	114.37
60	A0	307	PEV	C38-C39-C40	2.54	127.23	114.37
61	BA	536	PGV	C9-C10-C11	2.54	126.84	112.60
61	A1	315	PGV	C9-C10-C11	2.54	126.83	112.60
60	BB	202	PEV	C38-C39-C40	2.54	127.20	114.37
60	B8	3006	PEV	C38-C39-C40	2.54	127.19	114.37
60	BA	504	PEV	C38-C39-C40	2.54	127.19	114.37
61	A0	304	PGV	C9-C10-C11	2.54	126.80	112.60
60	BA	521	PEV	C39-C40-C41	2.53	127.18	114.37
60	BA	514	PEV	C39-C40-C41	2.53	127.17	114.37
61	A1	318	PGV	C9-C10-C11	2.53	126.76	112.60
60	B8	3003	PEV	C38-C39-C40	2.53	127.14	114.37
60	A1	321	PEV	C38-C39-C40	2.53	127.14	114.37
60	BA	520	PEV	C38-C39-C40	2.52	127.13	114.37
60	A1	316	PEV	C39-C40-C41	2.52	127.12	114.37
60	B8	3001	PEV	C38-C39-C40	2.52	127.09	114.37
61	A0	306	PGV	C9-C10-C11	2.52	126.70	112.60
60	A0	324	PEV	C39-C40-C41	2.51	127.08	114.37
60	A0	322	PEV	C38-C39-C40	2.51	127.07	114.37
60	BA	519	PEV	C39-C40-C41	2.51	127.06	114.37
60	A0	309	PEV	C39-C40-C41	2.51	127.05	114.37
60	BA	511	PEV	C38-C39-C40	2.51	127.05	114.37
60	A1	310	PEV	C38-C39-C40	2.51	127.04	114.37
60	A0	313	PEV	C38-C39-C40	2.51	127.04	114.37
60	A1	323	PEV	C39-C40-C41	2.51	127.04	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	A0	321	PEV	C39-C40-C41	2.51	127.03	114.37
60	A1	316	PEV	C38-C39-C40	2.50	127.03	114.37
60	BA	523	PEV	C38-C39-C40	2.50	127.01	114.37
60	A0	313	PEV	C39-C40-C41	2.50	127.00	114.37
60	A1	302	PEV	C39-C40-C41	2.50	127.00	114.37
60	BA	513	PEV	C39-C40-C41	2.50	126.99	114.37
60	A1	317	PEV	C39-C40-C41	2.49	126.97	114.37
60	BA	538	PEV	C38-C39-C40	2.49	126.97	114.37
60	A0	315	PEV	C39-C40-C41	2.49	126.96	114.37
60	BB	209	PEV	C39-C40-C41	2.49	126.95	114.37
60	BB	201	PEV	C39-C40-C41	2.49	126.95	114.37
61	A0	327	PGV	C9-C10-C11	2.49	126.54	112.60
61	A0	327	PGV	C8-C9-C10	2.49	125.81	113.86
61	BB	204	PGV	C9-C10-C11	2.49	126.52	112.60
60	A1	317	PEV	C38-C39-C40	2.48	126.92	114.37
60	A0	321	PEV	C38-C39-C40	2.48	126.92	114.37
60	BA	530	PEV	C39-C40-C41	2.48	126.90	114.37
61	BB	217	PGV	C9-C10-C11	2.48	126.48	112.60
60	A0	309	PEV	C38-C39-C40	2.48	126.89	114.37
60	A1	326	PEV	C39-C40-C41	2.48	126.88	114.37
60	A0	303	PEV	C38-C39-C40	2.48	126.88	114.37
60	A1	306	PEV	C38-C39-C40	2.48	126.88	114.37
60	A0	324	PEV	C38-C39-C40	2.47	126.87	114.37
61	AZ	205	PGV	C9-C10-C11	2.47	126.44	112.60
60	B8	3002	PEV	C38-C39-C40	2.47	126.85	114.37
60	BB	209	PEV	C38-C39-C40	2.47	126.85	114.37
60	BA	531	PEV	C39-C40-C41	2.47	126.84	114.37
60	AZ	204	PEV	C39-C40-C41	2.46	126.82	114.37
60	A1	324	PEV	C39-C40-C41	2.46	126.81	114.37
60	A1	327	PEV	C38-C39-C40	2.46	126.80	114.37
60	A1	306	PEV	C39-C40-C41	2.46	126.79	114.37
60	BB	215	PEV	C39-C40-C41	2.45	126.77	114.37
60	A1	326	PEV	C38-C39-C40	2.45	126.75	114.37
60	BA	520	PEV	C39-C40-C41	2.45	126.75	114.37
60	A1	305	PEV	C39-C40-C41	2.45	126.75	114.37
60	A1	320	PEV	C38-C39-C40	2.44	126.71	114.37
60	A1	320	PEV	C39-C40-C41	2.44	126.69	114.37
60	A1	310	PEV	C39-C40-C41	2.44	126.69	114.37
61	A0	318	PGV	C9-C10-C11	2.44	126.26	112.60
60	BA	531	PEV	C38-C39-C40	2.43	126.67	114.37
60	A1	302	PEV	C38-C39-C40	2.43	126.65	114.37
61	BA	515	PGV	C9-C10-C11	2.43	126.20	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	B8	3007	PEV	C39-C40-C41	2.43	126.63	114.37
60	A0	314	PEV	C38-C39-C40	2.43	126.63	114.37
60	A0	315	PEV	C38-C39-C40	2.42	126.61	114.37
60	A1	312	PEV	C39-C40-C41	2.42	126.61	114.37
60	A1	308	PEV	C38-C39-C40	2.41	126.53	114.37
60	A0	303	PEV	C39-C40-C41	2.40	126.49	114.37
60	BB	215	PEV	C38-C39-C40	2.40	126.48	114.37
61	A0	305	PGV	C8-C9-C10	2.39	125.37	113.86
60	BB	201	PEV	C38-C39-C40	2.39	126.47	114.37
60	BA	537	PEV	C38-C39-C40	2.39	126.47	114.37
60	A1	319	PEV	C38-C39-C40	2.39	126.44	114.37
60	A0	314	PEV	C39-C40-C41	2.38	126.41	114.37
60	BA	529	PEV	C39-C40-C41	2.38	126.40	114.37
60	A1	308	PEV	C39-C40-C41	2.38	126.38	114.37
60	BA	518	PEV	C38-C39-C40	2.38	126.38	114.37
60	BA	519	PEV	C38-C39-C40	2.38	126.38	114.37
61	A0	305	PGV	C9-C10-C11	2.37	125.90	112.60
60	A1	312	PEV	C38-C39-C40	2.37	126.37	114.37
60	BB	218	PEV	C39-C40-C41	2.37	126.35	114.37
60	B8	3007	PEV	C38-C39-C40	2.37	126.35	114.37
60	A0	302	PEV	C39-C40-C41	2.37	126.35	114.37
61	BA	516	PGV	C8-C9-C10	2.37	125.25	113.86
61	B8	3005	PGV	C9-C10-C11	2.37	125.86	112.60
60	BA	513	PEV	C38-C39-C40	2.36	126.32	114.37
60	AZ	206	PEV	C39-C40-C41	2.35	126.27	114.37
60	AZ	204	PEV	C38-C39-C40	2.35	126.24	114.37
60	A0	312	PEV	C38-C39-C40	2.35	126.24	114.37
60	A0	302	PEV	C38-C39-C40	2.34	126.22	114.37
60	A0	310	PEV	C39-C40-C41	2.34	126.21	114.37
61	BA	516	PGV	C9-C10-C11	2.32	125.61	112.60
60	BA	537	PEV	C39-C40-C41	2.32	126.11	114.37
60	BA	518	PEV	C39-C40-C41	2.32	126.08	114.37
60	BA	529	PEV	C38-C39-C40	2.31	126.02	114.37
60	A1	304	PEV	C38-C39-C40	2.30	125.99	114.37
60	A0	330	PEV	C39-C40-C41	2.28	125.88	114.37
60	AZ	206	PEV	C38-C39-C40	2.22	125.57	114.37
60	AZ	203	PEV	C39-C40-C41	2.21	125.55	114.37
60	A0	312	PEV	C39-C40-C41	2.18	125.38	114.37
60	A0	330	PEV	C38-C39-C40	2.17	125.34	114.37
60	AZ	203	PEV	C38-C39-C40	2.15	125.25	114.37
60	A1	304	PEV	C39-C40-C41	2.15	125.24	114.37
61	BA	522	PGV	C8-C9-C10	2.15	124.19	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	BA	534	PEV	O3-C3-C2	2.02	114.21	108.40

All (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
60	A1	305	PEV	C2
60	A1	313	PEV	C2
60	A1	317	PEV	C2
60	B8	3001	PEV	C2
60	BA	502	PEV	C2
60	BA	508	PEV	C2
60	BA	526	PEV	C2
60	BA	530	PEV	C2
60	BA	535	PEV	C2
60	BA	537	PEV	C2
60	BA	538	PEV	C2
60	BB	202	PEV	C2
60	BB	206	PEV	C2
61	AZ	205	PGV	C02
61	AZ	205	PGV	C05
61	AZ	207	PGV	C02
61	AZ	207	PGV	C05
61	A0	304	PGV	C02
61	A0	304	PGV	C05
61	A0	305	PGV	C05
61	A0	306	PGV	C02
61	A0	306	PGV	C05
61	A0	317	PGV	C02
61	A0	317	PGV	C05
61	A0	318	PGV	C02
61	A0	318	PGV	C05
61	A0	325	PGV	C02
61	A0	325	PGV	C05
61	A0	327	PGV	C02
61	A0	327	PGV	C05
61	A0	328	PGV	C02
61	A0	328	PGV	C05

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Mol	Chain	Res	Type	Atom
61	A0	331	PGV	C02
61	A0	331	PGV	C05
61	A0	332	PGV	C02
61	A0	332	PGV	C05
61	A1	303	PGV	C02
61	A1	303	PGV	C05
61	A1	311	PGV	C02
61	A1	311	PGV	C05
61	A1	315	PGV	C02
61	A1	315	PGV	C05
61	A1	318	PGV	C02
61	A1	318	PGV	C05
61	B8	3005	PGV	C02
61	B8	3005	PGV	C05
61	BA	501	PGV	C05
61	BA	505	PGV	C02
61	BA	505	PGV	C05
61	BA	512	PGV	C05
61	BA	515	PGV	C02
61	BA	515	PGV	C05
61	BA	516	PGV	C02
61	BA	516	PGV	C05
61	BA	522	PGV	C02
61	BA	522	PGV	C05
61	BA	536	PGV	C02
61	BA	536	PGV	C05
61	BA	540	PGV	C02
61	BA	540	PGV	C05
61	BB	203	PGV	C02
61	BB	203	PGV	C05
61	BB	204	PGV	C02
61	BB	204	PGV	C05
61	BB	205	PGV	C02
61	BB	205	PGV	C05
61	BB	207	PGV	C02
61	BB	207	PGV	C05
61	BB	208	PGV	C02
61	BB	208	PGV	C05
61	BB	213	PGV	C05
61	BB	217	PGV	C02
61	BB	217	PGV	C05

All (931) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	AZ	203	PEV	C4-O4P-P-O3P
60	AZ	203	PEV	C4-O4P-P-O2P
60	A0	301	PEV	C4-O4P-P-O3P
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
60	A0	303	PEV	C1-O3P-P-O2P
60	A0	308	PEV	C1-O3P-P-O2P
60	A0	308	PEV	C1-O3P-P-O4P
60	A0	315	PEV	C1-O3P-P-O4P
60	A0	315	PEV	C4-O4P-P-O2P
60	A0	316	PEV	C4-O4P-P-O3P
60	A0	316	PEV	O11-C11-O3-C3
60	A0	316	PEV	C12-C11-O3-C3
60	A0	319	PEV	C1-O3P-P-O1P
60	A0	319	PEV	C1-O3P-P-O4P
60	A0	321	PEV	C32-C31-O2-C2
60	A0	321	PEV	O31-C31-O2-C2
60	A0	321	PEV	C1-O3P-P-O1P
60	A0	321	PEV	C1-O3P-P-O4P
60	A0	322	PEV	C1-O3P-P-O1P
60	A0	326	PEV	C1-O3P-P-O1P
60	A0	326	PEV	C1-O3P-P-O2P
60	A0	326	PEV	C1-O3P-P-O4P
60	A0	330	PEV	C4-O4P-P-O1P
60	A1	301	PEV	C4-O4P-P-O3P
60	A1	301	PEV	C4-O4P-P-O2P
60	A1	305	PEV	C1-O3P-P-O4P
60	A1	308	PEV	C4-O4P-P-O3P
60	A1	308	PEV	C4-O4P-P-O1P
60	A1	308	PEV	C4-O4P-P-O2P
60	A1	310	PEV	C4-O4P-P-O3P
60	A1	310	PEV	C4-O4P-P-O1P
60	A1	312	PEV	C4-O4P-P-O1P
60	A1	313	PEV	C4-O4P-P-O3P
60	A1	313	PEV	C4-O4P-P-O1P
60	A1	314	PEV	C4-O4P-P-O3P
60	A1	314	PEV	C4-O4P-P-O1P
60	A1	314	PEV	C4-O4P-P-O2P
60	A1	317	PEV	C1-O3P-P-O1P
60	A1	320	PEV	C4-O4P-P-O3P
60	A1	320	PEV	C4-O4P-P-O1P

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Mol	Chain	Res	Type	Atoms
60	A1	321	PEV	C4-O4P-P-O3P
60	A1	321	PEV	C4-O4P-P-O1P
60	A1	325	PEV	O11-C11-O3-C3
60	A1	325	PEV	C12-C11-O3-C3
60	A1	327	PEV	C4-O4P-P-O3P
60	A1	327	PEV	C4-O4P-P-O2P
60	A1	328	PEV	C1-O3P-P-O1P
60	A1	328	PEV	C4-O4P-P-O3P
60	A1	328	PEV	C4-O4P-P-O1P
60	B8	3003	PEV	C1-O3P-P-O2P
60	B8	3004	PEV	C1-O3P-P-O1P
60	B8	3004	PEV	C4-O4P-P-O3P
60	B8	3004	PEV	C4-O4P-P-O2P
60	B8	3006	PEV	C4-O4P-P-O2P
60	BA	502	PEV	C1-O3P-P-O2P
60	BA	502	PEV	C1-O3P-P-O4P
60	BA	503	PEV	C1-O3P-P-O1P
60	BA	503	PEV	C1-O3P-P-O2P
60	BA	503	PEV	C1-O3P-P-O4P
60	BA	509	PEV	C1-O3P-P-O1P
60	BA	509	PEV	C1-O3P-P-O4P
60	BA	510	PEV	C1-O3P-P-O1P
60	BA	510	PEV	C1-O3P-P-O2P
60	BA	510	PEV	C1-O3P-P-O4P
60	BA	514	PEV	C4-O4P-P-O3P
60	BA	521	PEV	C4-O4P-P-O3P
60	BA	521	PEV	C4-O4P-P-O1P
60	BA	521	PEV	C4-O4P-P-O2P
60	BA	524	PEV	C1-O3P-P-O2P
60	BA	524	PEV	C1-O3P-P-O4P
60	BA	525	PEV	C1-O3P-P-O1P
60	BA	525	PEV	C1-O3P-P-O2P
60	BA	525	PEV	C1-O3P-P-O4P
60	BA	525	PEV	C4-O4P-P-O2P
60	BA	527	PEV	C1-O3P-P-O4P
60	BA	527	PEV	C4-O4P-P-O3P
60	BA	527	PEV	C4-O4P-P-O1P
60	BA	528	PEV	C1-O3P-P-O2P
60	BA	528	PEV	C1-O3P-P-O4P
60	BA	528	PEV	C4-O4P-P-O3P
60	BA	530	PEV	C4-O4P-P-O3P
60	BA	530	PEV	C4-O4P-P-O2P

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Mol	Chain	Res	Type	Atoms
60	BA	532	PEV	C4-O4P-P-O3P
60	BA	532	PEV	C4-O4P-P-O1P
60	BA	532	PEV	C4-O4P-P-O2P
60	BA	533	PEV	C1-O3P-P-O4P
60	BA	538	PEV	C1-O3P-P-O1P
60	BA	538	PEV	C4-O4P-P-O3P
60	BB	201	PEV	C4-O4P-P-O3P
60	BB	201	PEV	C4-O4P-P-O1P
60	BB	209	PEV	C1-O3P-P-O2P
60	BB	209	PEV	C1-O3P-P-O4P
60	BB	210	PEV	C1-O3P-P-O1P
60	BB	210	PEV	C1-O3P-P-O2P
60	BB	210	PEV	C1-O3P-P-O4P
60	BB	210	PEV	C4-O4P-P-O3P
60	BB	210	PEV	C4-O4P-P-O1P
60	BB	211	PEV	C4-O4P-P-O1P
60	BB	214	PEV	C4-O4P-P-O3P
60	BB	214	PEV	C4-O4P-P-O1P
60	BB	214	PEV	C4-O4P-P-O2P
60	BB	215	PEV	C1-O3P-P-O1P
60	BB	215	PEV	C1-O3P-P-O4P
60	BB	218	PEV	C1-O3P-P-O1P
60	BB	218	PEV	C1-O3P-P-O4P
60	BB	218	PEV	C4-O4P-P-O2P
61	AZ	205	PGV	C03-O11-P-O13
61	AZ	205	PGV	C04-O12-P-O13
61	AZ	205	PGV	C11-C10-C9-C8
61	AZ	207	PGV	C11-C10-C9-C8
61	A0	304	PGV	C11-C10-C9-C8
61	A0	305	PGV	C04-O12-P-O11
61	A0	305	PGV	C11-C10-C9-C8
61	A0	306	PGV	C03-O11-P-O12
61	A0	306	PGV	C03-O11-P-O14
61	A0	306	PGV	C11-C10-C9-C8
61	A0	317	PGV	C03-O11-P-O13
61	A0	317	PGV	C11-C10-C9-C8
61	A0	318	PGV	C03-O11-P-O12
61	A0	318	PGV	C03-O11-P-O14
61	A0	318	PGV	C11-C10-C9-C8
61	A0	325	PGV	C11-C10-C9-C8
61	A0	327	PGV	C11-C10-C9-C8
61	A0	328	PGV	C03-O11-P-O12

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Mol	Chain	Res	Type	Atoms
61	A0	328	PGV	C03-O11-P-O13
61	A0	328	PGV	C11-C10-C9-C8
61	A0	331	PGV	C11-C10-C9-C8
61	A0	332	PGV	C03-O11-P-O13
61	A0	332	PGV	C11-C10-C9-C8
61	A1	303	PGV	C11-C10-C9-C8
61	A1	311	PGV	C03-O11-P-O12
61	A1	311	PGV	C03-O11-P-O14
61	A1	311	PGV	C11-C10-C9-C8
61	A1	315	PGV	C03-O11-P-O12
61	A1	315	PGV	C03-O11-P-O13
61	A1	315	PGV	C03-O11-P-O14
61	A1	315	PGV	C11-C10-C9-C8
61	A1	318	PGV	C11-C10-C9-C8
61	B8	3005	PGV	C03-O11-P-O12
61	B8	3005	PGV	C03-O11-P-O14
61	B8	3005	PGV	C11-C10-C9-C8
61	BA	501	PGV	C11-C10-C9-C8
61	BA	505	PGV	C11-C10-C9-C8
61	BA	512	PGV	C04-O12-P-O11
61	BA	512	PGV	C04-O12-P-O14
61	BA	512	PGV	C11-C10-C9-C8
61	BA	515	PGV	C11-C10-C9-C8
61	BA	536	PGV	C11-C10-C9-C8
61	BA	540	PGV	C04-O12-P-O11
61	BA	540	PGV	C11-C10-C9-C8
61	BB	203	PGV	C03-O11-P-O12
61	BB	203	PGV	C03-O11-P-O14
61	BB	203	PGV	O04-C19-O03-C01
61	BB	203	PGV	C20-C19-O03-C01
61	BB	203	PGV	C11-C10-C9-C8
61	BB	204	PGV	C11-C10-C9-C8
61	BB	205	PGV	C03-O11-P-O12
61	BB	205	PGV	C03-O11-P-O14
61	BB	205	PGV	C11-C10-C9-C8
61	BB	207	PGV	C11-C10-C9-C8
61	BB	208	PGV	C11-C10-C9-C8
61	BB	213	PGV	C04-O12-P-O11
61	BB	213	PGV	C04-O12-P-O14
61	BB	213	PGV	C11-C10-C9-C8
61	BB	217	PGV	C03-O11-P-O12
61	BB	217	PGV	C03-O11-P-O13

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Mol	Chain	Res	Type	Atoms
61	BB	217	PGV	C03-O11-P-O14
61	BB	217	PGV	C11-C10-C9-C8
60	AZ	201	PEV	C38-C39-C40-C41
60	A0	319	PEV	C38-C39-C40-C41
60	A1	323	PEV	C38-C39-C40-C41
60	BA	514	PEV	C38-C39-C40-C41
60	BB	206	PEV	C38-C39-C40-C41
61	BA	505	PGV	C10-C11-C12-C13
61	BB	204	PGV	C10-C11-C12-C13
60	BA	539	PEV	C38-C39-C40-C41
60	BB	218	PEV	C38-C39-C40-C41
60	A1	316	PEV	C38-C39-C40-C41
60	A1	324	PEV	C38-C39-C40-C41
60	A1	326	PEV	C38-C39-C40-C41
60	BA	527	PEV	C38-C39-C40-C41
60	BB	216	PEV	C38-C39-C40-C41
60	AZ	202	PEV	C38-C39-C40-C41
60	AZ	204	PEV	C38-C39-C40-C41
60	A0	312	PEV	C37-C38-C39-C40
60	A0	316	PEV	C37-C38-C39-C40
60	A0	321	PEV	C38-C39-C40-C41
60	A1	305	PEV	C38-C39-C40-C41
60	A1	320	PEV	C38-C39-C40-C41
60	BA	507	PEV	C38-C39-C40-C41
60	BA	509	PEV	C38-C39-C40-C41
60	BA	510	PEV	C38-C39-C40-C41
60	BA	511	PEV	C38-C39-C40-C41
60	BA	520	PEV	C38-C39-C40-C41
60	BA	524	PEV	C38-C39-C40-C41
60	BA	525	PEV	C38-C39-C40-C41
60	BB	210	PEV	C38-C39-C40-C41
60	BB	214	PEV	C38-C39-C40-C41
60	AZ	206	PEV	C38-C39-C40-C41
60	A0	301	PEV	C38-C39-C40-C41
60	A0	302	PEV	C38-C39-C40-C41
60	A0	303	PEV	C38-C39-C40-C41
60	A0	307	PEV	C38-C39-C40-C41
60	A0	308	PEV	C38-C39-C40-C41
60	A0	310	PEV	C38-C39-C40-C41
60	A0	311	PEV	C38-C39-C40-C41
60	A0	315	PEV	C38-C39-C40-C41
60	A0	323	PEV	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
60	A0	329	PEV	C38-C39-C40-C41
60	A1	301	PEV	C38-C39-C40-C41
60	A1	306	PEV	C38-C39-C40-C41
60	A1	309	PEV	C38-C39-C40-C41
60	A1	312	PEV	C38-C39-C40-C41
60	A1	313	PEV	C38-C39-C40-C41
60	A1	314	PEV	C38-C39-C40-C41
60	A1	321	PEV	C38-C39-C40-C41
60	A1	325	PEV	C38-C39-C40-C41
60	A1	328	PEV	C38-C39-C40-C41
60	B8	3001	PEV	C38-C39-C40-C41
60	B8	3002	PEV	C38-C39-C40-C41
60	B8	3004	PEV	C38-C39-C40-C41
60	BA	503	PEV	C38-C39-C40-C41
60	BA	504	PEV	C38-C39-C40-C41
60	BA	506	PEV	C38-C39-C40-C41
60	BA	517	PEV	C38-C39-C40-C41
60	BA	521	PEV	C38-C39-C40-C41
60	BA	528	PEV	C38-C39-C40-C41
60	BA	530	PEV	C38-C39-C40-C41
60	BA	535	PEV	C38-C39-C40-C41
60	BA	538	PEV	C38-C39-C40-C41
60	BB	201	PEV	C38-C39-C40-C41
60	BB	212	PEV	C38-C39-C40-C41
60	BB	215	PEV	C38-C39-C40-C41
60	A0	320	PEV	C38-C39-C40-C41
60	B8	3007	PEV	C38-C39-C40-C41
60	BA	508	PEV	C38-C39-C40-C41
60	BA	513	PEV	C38-C39-C40-C41
60	A0	326	PEV	C38-C39-C40-C41
60	A1	307	PEV	C38-C39-C40-C41
60	A1	329	PEV	C38-C39-C40-C41
60	B8	3003	PEV	C38-C39-C40-C41
60	BA	502	PEV	C38-C39-C40-C41
60	BA	519	PEV	C38-C39-C40-C41
60	BA	526	PEV	C38-C39-C40-C41
60	BA	534	PEV	C38-C39-C40-C41
60	BB	202	PEV	C38-C39-C40-C41
60	A0	322	PEV	C38-C39-C40-C41
60	A1	308	PEV	C38-C39-C40-C41
60	BA	531	PEV	C38-C39-C40-C41
60	BB	211	PEV	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
60	A0	316	PEV	C38-C39-C40-C41
60	A0	324	PEV	C38-C39-C40-C41
60	A1	302	PEV	C38-C39-C40-C41
60	A1	327	PEV	C38-C39-C40-C41
60	BB	209	PEV	C38-C39-C40-C41
60	A1	310	PEV	C38-C39-C40-C41
60	A0	309	PEV	C38-C39-C40-C41
60	A0	313	PEV	C38-C39-C40-C41
60	A1	317	PEV	C38-C39-C40-C41
60	A1	322	PEV	C38-C39-C40-C41
60	BA	518	PEV	C38-C39-C40-C41
60	BA	529	PEV	C38-C39-C40-C41
60	BA	532	PEV	C38-C39-C40-C41
60	BA	533	PEV	C38-C39-C40-C41
60	BA	537	PEV	C38-C39-C40-C41
60	BA	509	PEV	C2-C1-O3P-P
60	A0	330	PEV	C38-C39-C40-C41
60	B8	3006	PEV	C38-C39-C40-C41
60	AZ	203	PEV	C38-C39-C40-C41
60	A0	314	PEV	C38-C39-C40-C41
60	A1	304	PEV	C38-C39-C40-C41
60	BA	523	PEV	C38-C39-C40-C41
61	A0	325	PGV	C10-C11-C12-C13
61	A1	303	PGV	C10-C11-C12-C13
61	A1	318	PGV	C10-C11-C12-C13
61	BB	208	PGV	C10-C11-C12-C13
61	BA	536	PGV	C10-C11-C12-C13
61	BB	203	PGV	C10-C11-C12-C13
61	A0	332	PGV	C05-C04-O12-P
61	BA	516	PGV	C10-C11-C12-C13
61	A0	318	PGV	C10-C11-C12-C13
61	BB	213	PGV	C10-C11-C12-C13
60	A1	321	PEV	C2-C1-O3P-P
61	BA	516	PGV	C05-C04-O12-P
60	A0	309	PEV	C16-C17-C18-C19
60	A0	312	PEV	C39-C40-C41-C42
60	B8	3001	PEV	C37-C38-C39-C40
60	BA	513	PEV	C39-C40-C41-C42
60	BA	537	PEV	C37-C38-C39-C40
60	BA	538	PEV	C39-C40-C41-C42
61	BA	501	PGV	C7-C8-C9-C10
60	A0	301	PEV	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
60	A0	308	PEV	C39-C40-C41-C42
60	A0	309	PEV	C39-C40-C41-C42
60	A0	310	PEV	C39-C40-C41-C42
60	A0	311	PEV	C39-C40-C41-C42
60	A0	319	PEV	C39-C40-C41-C42
60	A0	320	PEV	C39-C40-C41-C42
60	A1	302	PEV	C39-C40-C41-C42
60	A1	308	PEV	C39-C40-C41-C42
60	A1	309	PEV	C39-C40-C41-C42
60	A1	314	PEV	C39-C40-C41-C42
60	A1	327	PEV	C39-C40-C41-C42
60	BA	503	PEV	C37-C38-C39-C40
60	BA	504	PEV	C39-C40-C41-C42
60	BA	507	PEV	C39-C40-C41-C42
60	BA	524	PEV	C39-C40-C41-C42
60	BA	532	PEV	C37-C38-C39-C40
60	BB	214	PEV	C37-C38-C39-C40
61	A0	304	PGV	C7-C8-C9-C10
61	A0	318	PGV	C7-C8-C9-C10
61	BA	505	PGV	C7-C8-C9-C10
61	BA	536	PGV	C7-C8-C9-C10
61	A0	327	PGV	C10-C11-C12-C13
60	A0	315	PEV	C39-C40-C41-C42
60	A1	312	PEV	C39-C40-C41-C42
60	A1	321	PEV	C37-C38-C39-C40
60	A1	328	PEV	C39-C40-C41-C42
60	BA	507	PEV	C37-C38-C39-C40
60	BA	525	PEV	C37-C38-C39-C40
60	BA	535	PEV	C39-C40-C41-C42
60	BB	212	PEV	C37-C38-C39-C40
61	BA	512	PGV	C7-C8-C9-C10
61	BA	522	PGV	C7-C8-C9-C10
60	AZ	201	PEV	C39-C40-C41-C42
60	A0	303	PEV	C37-C38-C39-C40
60	A0	308	PEV	C37-C38-C39-C40
60	A0	329	PEV	C37-C38-C39-C40
60	A1	313	PEV	C37-C38-C39-C40
60	A1	325	PEV	C44-C45-C46-C47
60	A1	325	PEV	C39-C40-C41-C42
60	B8	3007	PEV	C39-C40-C41-C42
60	BA	511	PEV	C37-C38-C39-C40
60	BA	521	PEV	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
60	BB	201	PEV	C37-C38-C39-C40
60	BB	210	PEV	C37-C38-C39-C40
60	BB	211	PEV	C39-C40-C41-C42
60	BB	216	PEV	C37-C38-C39-C40
60	BB	218	PEV	C37-C38-C39-C40
60	A1	306	PEV	C37-C38-C39-C40
60	BA	504	PEV	C37-C38-C39-C40
60	BA	506	PEV	C37-C38-C39-C40
61	B8	3005	PGV	C19-C20-C21-C22
60	BA	523	PEV	C37-C38-C39-C40
60	BA	528	PEV	C37-C38-C39-C40
60	BA	539	PEV	C37-C38-C39-C40
60	BB	218	PEV	C39-C40-C41-C42
60	A0	302	PEV	C37-C38-C39-C40
60	A0	322	PEV	C37-C38-C39-C40
60	B8	3002	PEV	C39-C40-C41-C42
60	BA	508	PEV	C39-C40-C41-C42
60	BA	530	PEV	C37-C38-C39-C40
60	A0	315	PEV	C37-C38-C39-C40
60	A0	326	PEV	C37-C38-C39-C40
60	A1	324	PEV	C39-C40-C41-C42
60	BB	202	PEV	C39-C40-C41-C42
60	A1	309	PEV	C37-C38-C39-C40
60	A1	317	PEV	C37-C38-C39-C40
60	A1	326	PEV	C39-C40-C41-C42
60	A1	327	PEV	C37-C38-C39-C40
60	A1	328	PEV	C37-C38-C39-C40
60	BA	531	PEV	C37-C38-C39-C40
61	AZ	205	PGV	C7-C8-C9-C10
60	B8	3001	PEV	C39-C40-C41-C42
60	BA	521	PEV	C37-C38-C39-C40
60	BB	206	PEV	C39-C40-C41-C42
60	BB	216	PEV	C39-C40-C41-C42
60	BA	527	PEV	C37-C38-C39-C40
60	A1	301	PEV	C37-C38-C39-C40
60	BA	527	PEV	C39-C40-C41-C42
60	A1	321	PEV	C39-C40-C41-C42
60	B8	3003	PEV	C37-C38-C39-C40
61	BA	540	PGV	C7-C8-C9-C10
60	A0	310	PEV	C37-C38-C39-C40
60	A0	321	PEV	C39-C40-C41-C42
60	A1	302	PEV	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
60	A1	310	PEV	C37-C38-C39-C40
60	AZ	202	PEV	C39-C40-C41-C42
60	A0	321	PEV	C37-C38-C39-C40
60	A1	319	PEV	C37-C38-C39-C40
60	A1	329	PEV	C39-C40-C41-C42
60	BA	506	PEV	C39-C40-C41-C42
60	BA	518	PEV	C37-C38-C39-C40
60	BA	529	PEV	C39-C40-C41-C42
60	BA	538	PEV	C37-C38-C39-C40
61	B8	3005	PGV	C7-C8-C9-C10
60	A0	311	PEV	C37-C38-C39-C40
60	A0	314	PEV	C37-C38-C39-C40
60	A0	326	PEV	C39-C40-C41-C42
60	A1	325	PEV	C37-C38-C39-C40
60	BA	514	PEV	C37-C38-C39-C40
60	BA	534	PEV	C37-C38-C39-C40
60	BB	206	PEV	C37-C38-C39-C40
60	BB	209	PEV	C39-C40-C41-C42
60	BB	214	PEV	C39-C40-C41-C42
60	BA	530	PEV	C39-C40-C41-C42
60	BB	201	PEV	C39-C40-C41-C42
60	BB	209	PEV	C37-C38-C39-C40
61	BA	515	PGV	C7-C8-C9-C10
61	BA	516	PGV	C7-C8-C9-C10
60	AZ	202	PEV	C37-C38-C39-C40
60	AZ	206	PEV	C39-C40-C41-C42
60	A1	313	PEV	C39-C40-C41-C42
60	A1	316	PEV	C37-C38-C39-C40
60	BA	519	PEV	C39-C40-C41-C42
60	BA	535	PEV	C37-C38-C39-C40
60	A1	307	PEV	C11-C12-C13-C14
61	A0	327	PGV	C1-C2-C3-C4
60	A1	301	PEV	C39-C40-C41-C42
61	A1	315	PGV	C10-C11-C12-C13
60	BA	503	PEV	C39-C40-C41-C42
60	BA	514	PEV	C39-C40-C41-C42
60	BA	525	PEV	C39-C40-C41-C42
61	A1	303	PGV	C7-C8-C9-C10
61	BB	217	PGV	C7-C8-C9-C10
60	A0	319	PEV	C37-C38-C39-C40
60	A1	314	PEV	C37-C38-C39-C40
60	A1	323	PEV	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
60	A0	307	PEV	C39-C40-C41-C42
60	A0	324	PEV	C39-C40-C41-C42
60	BA	526	PEV	C39-C40-C41-C42
60	BB	202	PEV	C37-C38-C39-C40
60	BB	210	PEV	C39-C40-C41-C42
60	A0	320	PEV	C37-C38-C39-C40
60	A1	322	PEV	C37-C38-C39-C40
61	AZ	207	PGV	C23-C24-C25-C26
61	A1	315	PGV	C7-C8-C9-C10
60	A1	307	PEV	C39-C40-C41-C42
60	B8	3006	PEV	C37-C38-C39-C40
61	A0	317	PGV	C7-C8-C9-C10
61	A0	325	PGV	C7-C8-C9-C10
61	A1	311	PGV	C7-C8-C9-C10
60	A1	304	PEV	C37-C38-C39-C40
60	AZ	201	PEV	C37-C38-C39-C40
60	A1	307	PEV	C37-C38-C39-C40
60	BA	533	PEV	C37-C38-C39-C40
61	A1	318	PGV	C7-C8-C9-C10
60	A1	319	PEV	C39-C40-C41-C42
60	BA	511	PEV	C39-C40-C41-C42
60	BB	212	PEV	C39-C40-C41-C42
61	A0	332	PGV	C7-C8-C9-C10
60	A0	301	PEV	C37-C38-C39-C40
60	A0	307	PEV	C37-C38-C39-C40
60	A0	323	PEV	C37-C38-C39-C40
60	A1	305	PEV	C37-C38-C39-C40
61	BB	207	PGV	C24-C25-C26-C27
60	A0	330	PEV	C39-C40-C41-C42
60	A1	324	PEV	C37-C38-C39-C40
60	A1	329	PEV	C37-C38-C39-C40
61	AZ	207	PGV	C7-C8-C9-C10
60	BA	533	PEV	C39-C40-C41-C42
60	A1	304	PEV	C39-C40-C41-C42
60	BA	517	PEV	C39-C40-C41-C42
60	AZ	203	PEV	C39-C40-C41-C42
60	A0	313	PEV	C37-C38-C39-C40
60	BA	517	PEV	C37-C38-C39-C40
61	A0	331	PGV	C7-C8-C9-C10
60	BA	502	PEV	C39-C40-C41-C42
60	BA	526	PEV	C37-C38-C39-C40
60	BA	528	PEV	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
60	BB	215	PEV	C39-C40-C41-C42
60	BA	520	PEV	C39-C40-C41-C42
60	BA	537	PEV	C39-C40-C41-C42
60	BB	211	PEV	C37-C38-C39-C40
60	BB	215	PEV	C37-C38-C39-C40
60	A0	310	PEV	C20-C21-C22-C23
61	B8	3005	PGV	C5-C6-C7-C8
60	A0	324	PEV	C37-C38-C39-C40
60	A0	323	PEV	C39-C40-C41-C42
61	BB	205	PGV	C7-C8-C9-C10
60	BA	537	PEV	C18-C19-C20-C21
60	BA	523	PEV	C39-C40-C41-C42
61	AZ	207	PGV	C02-C03-O11-P
61	A1	311	PGV	C02-C03-O11-P
60	B8	3004	PEV	C39-C40-C41-C42
60	BA	523	PEV	C12-C13-C14-C15
60	BA	508	PEV	C37-C38-C39-C40
60	A0	303	PEV	C39-C40-C41-C42
60	A1	308	PEV	C37-C38-C39-C40
61	A0	325	PGV	C20-C21-C22-C23
61	A0	328	PGV	C7-C8-C9-C10
60	A1	312	PEV	C37-C38-C39-C40
60	A1	317	PEV	C39-C40-C41-C42
60	A1	323	PEV	C37-C38-C39-C40
61	A0	305	PGV	C7-C8-C9-C10
60	BA	506	PEV	C35-C36-C37-C38
60	BA	509	PEV	C39-C40-C41-C42
60	BA	510	PEV	C37-C38-C39-C40
60	BA	520	PEV	C21-C22-C23-C24
60	B8	3003	PEV	C39-C40-C41-C42
60	A1	302	PEV	C12-C13-C14-C15
60	A1	322	PEV	C39-C40-C41-C42
60	BA	503	PEV	C41-C42-C43-C44
61	A0	306	PGV	C7-C8-C9-C10
61	A0	305	PGV	C12-C13-C14-C15
60	AZ	203	PEV	C37-C38-C39-C40
60	A0	313	PEV	C39-C40-C41-C42
60	BA	532	PEV	C39-C40-C41-C42
60	A0	309	PEV	C37-C38-C39-C40
60	BB	212	PEV	C44-C45-C46-C47
60	BA	510	PEV	C39-C40-C41-C42
60	B8	3007	PEV	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
60	B8	3004	PEV	C37-C38-C39-C40
60	A0	329	PEV	C39-C40-C41-C42
60	AZ	204	PEV	C39-C40-C41-C42
60	A1	316	PEV	C39-C40-C41-C42
60	A0	322	PEV	C39-C40-C41-C42
60	BA	520	PEV	C37-C38-C39-C40
60	BA	524	PEV	C37-C38-C39-C40
60	A1	319	PEV	C34-C35-C36-C37
61	BB	204	PGV	C7-C8-C9-C10
60	A1	329	PEV	C42-C43-C44-C45
61	A1	311	PGV	C13-C14-C15-C16
61	BB	207	PGV	C7-C8-C9-C10
60	BA	509	PEV	C37-C38-C39-C40
60	A0	326	PEV	C2-C1-O3P-P
61	AZ	205	PGV	C05-C04-O12-P
61	A0	318	PGV	C02-C03-O11-P
61	A1	315	PGV	C02-C03-O11-P
60	A0	316	PEV	C39-C40-C41-C42
60	B8	3002	PEV	C37-C38-C39-C40
60	BA	534	PEV	C39-C40-C41-C42
60	BA	539	PEV	C39-C40-C41-C42
60	A1	320	PEV	C39-C40-C41-C42
61	BB	208	PGV	C7-C8-C9-C10
60	A1	306	PEV	C39-C40-C41-C42
61	A0	305	PGV	C11-C12-C13-C14
60	BA	513	PEV	C37-C38-C39-C40
60	A0	324	PEV	C14-C15-C16-C17
61	AZ	205	PGV	C23-C24-C25-C26
60	A1	320	PEV	C37-C38-C39-C40
60	BA	531	PEV	C39-C40-C41-C42
60	A1	326	PEV	C45-C46-C47-C48
60	BA	532	PEV	C31-C32-C33-C34
60	BA	533	PEV	C40-C41-C42-C43
61	BB	203	PGV	C7-C8-C9-C10
60	BA	502	PEV	C2-C1-O3P-P
60	BA	519	PEV	C2-C1-O3P-P
60	A0	314	PEV	C39-C40-C41-C42
60	BA	504	PEV	C21-C22-C23-C24
60	BA	514	PEV	C32-C33-C34-C35
61	A0	327	PGV	C11-C12-C13-C14
60	A1	313	PEV	C43-C44-C45-C46
60	A1	327	PEV	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
60	A0	330	PEV	C37-C38-C39-C40
61	BB	204	PGV	C22-C23-C24-C25
61	A0	318	PGV	C12-C13-C14-C15
60	A1	328	PEV	C43-C44-C45-C46
60	BA	532	PEV	C32-C33-C34-C35
61	BA	540	PGV	C11-C12-C13-C14
60	A1	310	PEV	C39-C40-C41-C42
60	BA	524	PEV	C15-C16-C17-C18
61	A0	332	PGV	C23-C24-C25-C26
60	BA	533	PEV	C36-C37-C38-C39
61	A0	327	PGV	C7-C8-C9-C10
61	A1	315	PGV	O01-C02-C03-O11
60	BA	513	PEV	C1-C2-C3-O3
60	BA	532	PEV	C42-C43-C44-C45
60	BA	524	PEV	C16-C17-C18-C19
60	A0	301	PEV	C5-C4-O4P-P
60	A0	321	PEV	C5-C4-O4P-P
60	A0	326	PEV	C5-C4-O4P-P
60	B8	3004	PEV	C5-C4-O4P-P
60	BA	509	PEV	C5-C4-O4P-P
60	BA	510	PEV	C5-C4-O4P-P
60	BA	511	PEV	C5-C4-O4P-P
60	BA	514	PEV	C5-C4-O4P-P
60	BA	519	PEV	C5-C4-O4P-P
60	BA	525	PEV	C5-C4-O4P-P
60	BA	530	PEV	C5-C4-O4P-P
60	BB	206	PEV	C5-C4-O4P-P
60	BB	218	PEV	C5-C4-O4P-P
60	BA	502	PEV	C37-C38-C39-C40
61	BB	213	PGV	C7-C8-C9-C10
60	A1	302	PEV	C2-C1-O3P-P
60	A1	322	PEV	C17-C18-C19-C20
60	B8	3006	PEV	C39-C40-C41-C42
60	B8	3003	PEV	C13-C14-C15-C16
61	A1	318	PGV	C4-C5-C6-C7
60	A1	308	PEV	C12-C13-C14-C15
61	A1	315	PGV	C01-C02-C03-O11
60	BA	518	PEV	C39-C40-C41-C42
61	BA	522	PGV	C11-C12-C13-C14
61	BB	205	PGV	C11-C12-C13-C14
60	A0	316	PEV	C2-C1-O3P-P
60	A0	323	PEV	C2-C1-O3P-P

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Mol	Chain	Res	Type	Atoms
60	BB	210	PEV	C2-C1-O3P-P
61	A1	318	PGV	C05-C04-O12-P
61	BA	501	PGV	C02-C03-O11-P
60	BB	206	PEV	C18-C19-C20-C21
61	A0	306	PGV	C11-C12-C13-C14
61	A0	328	PGV	C11-C12-C13-C14
61	BB	204	PGV	C11-C12-C13-C14
60	A1	328	PEV	C12-C13-C14-C15
61	BB	208	PGV	C22-C23-C24-C25
61	B8	3005	PGV	C11-C12-C13-C14
61	BB	203	PGV	C11-C12-C13-C14
60	AZ	204	PEV	C32-C33-C34-C35
60	AZ	202	PEV	C1-O3P-P-O1P
60	AZ	203	PEV	C1-O3P-P-O1P
60	AZ	204	PEV	C1-O3P-P-O4P
60	A0	301	PEV	C1-O3P-P-O1P
60	A0	301	PEV	C4-O4P-P-O1P
60	A0	302	PEV	C4-O4P-P-O1P
60	A0	303	PEV	C1-O3P-P-O4P
60	A0	312	PEV	C4-O4P-P-O1P
60	A0	314	PEV	C1-O3P-P-O1P
60	A0	314	PEV	C4-O4P-P-O1P
60	A0	315	PEV	C1-O3P-P-O1P
60	A0	315	PEV	C4-O4P-P-O3P
60	A0	315	PEV	C4-O4P-P-O1P
60	A0	316	PEV	C4-O4P-P-O1P
60	A0	321	PEV	C1-O3P-P-O2P
60	A0	321	PEV	C4-O4P-P-O1P
60	A0	323	PEV	C1-O3P-P-O1P
60	A0	326	PEV	C4-O4P-P-O1P
60	A0	329	PEV	C1-O3P-P-O1P
60	A0	330	PEV	C1-O3P-P-O4P
60	A1	301	PEV	C1-O3P-P-O1P
60	A1	301	PEV	C1-O3P-P-O2P
60	A1	301	PEV	C1-O3P-P-O4P
60	A1	301	PEV	C4-O4P-P-O1P
60	A1	305	PEV	C1-O3P-P-O1P
60	A1	308	PEV	C1-O3P-P-O1P
60	A1	308	PEV	C1-O3P-P-O2P
60	A1	308	PEV	C1-O3P-P-O4P
60	A1	310	PEV	C4-O4P-P-O2P
60	A1	312	PEV	C4-O4P-P-O3P

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Mol	Chain	Res	Type	Atoms
60	A1	313	PEV	C4-O4P-P-O2P
60	A1	320	PEV	C4-O4P-P-O2P
60	A1	321	PEV	C4-O4P-P-O2P
60	A1	328	PEV	C1-O3P-P-O4P
60	A1	328	PEV	C4-O4P-P-O2P
60	B8	3003	PEV	C1-O3P-P-O4P
60	B8	3003	PEV	C4-O4P-P-O1P
60	B8	3006	PEV	C4-O4P-P-O3P
60	B8	3006	PEV	C4-O4P-P-O1P
60	BA	506	PEV	C4-O4P-P-O1P
60	BA	509	PEV	C4-O4P-P-O1P
60	BA	514	PEV	C4-O4P-P-O1P
60	BA	518	PEV	C4-O4P-P-O1P
60	BA	524	PEV	C1-O3P-P-O1P
60	BA	525	PEV	C4-O4P-P-O3P
60	BA	525	PEV	C4-O4P-P-O1P
60	BA	527	PEV	C1-O3P-P-O1P
60	BA	527	PEV	C4-O4P-P-O2P
60	BA	530	PEV	C4-O4P-P-O1P
60	BA	535	PEV	C1-O3P-P-O1P
60	BA	538	PEV	C4-O4P-P-O1P
60	BB	211	PEV	C1-O3P-P-O1P
60	BB	218	PEV	C4-O4P-P-O3P
60	BB	218	PEV	C4-O4P-P-O1P
61	AZ	205	PGV	C03-O11-P-O12
61	AZ	207	PGV	C03-O11-P-O13
61	AZ	207	PGV	C04-O12-P-O13
61	A0	305	PGV	C04-O12-P-O13
61	A0	306	PGV	C04-O12-P-O13
61	A0	328	PGV	C03-O11-P-O14
61	A0	328	PGV	C04-O12-P-O13
61	A0	332	PGV	C03-O11-P-O12
61	A1	303	PGV	C03-O11-P-O13
61	A1	315	PGV	C04-O12-P-O13
61	A1	318	PGV	C03-O11-P-O13
61	BA	501	PGV	C03-O11-P-O13
61	BA	501	PGV	C04-O12-P-O13
61	BA	515	PGV	C04-O12-P-O13
61	BA	516	PGV	C04-O12-P-O13
61	BA	540	PGV	C04-O12-P-O13
61	BB	205	PGV	C04-O12-P-O13
61	BB	213	PGV	C03-O11-P-O13

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Mol	Chain	Res	Type	Atoms
61	BB	213	PGV	C04-O12-P-O13
61	BA	540	PGV	C12-C13-C14-C15
60	AZ	206	PEV	C2-C1-O3P-P
60	A0	307	PEV	C2-C1-O3P-P
60	A0	324	PEV	C2-C1-O3P-P
60	BA	537	PEV	C2-C1-O3P-P
61	BA	512	PGV	C05-C04-O12-P
60	BA	502	PEV	C18-C19-C20-C21
61	BA	536	PGV	C11-C12-C13-C14
61	BB	213	PGV	C11-C12-C13-C14
60	BB	216	PEV	C31-C32-C33-C34
60	A0	319	PEV	C12-C13-C14-C15
61	A0	325	PGV	C11-C12-C13-C14
61	A1	318	PGV	C11-C12-C13-C14
61	BA	501	PGV	C11-C12-C13-C14
61	BA	512	PGV	C11-C12-C13-C14
60	BB	214	PEV	C20-C21-C22-C23
60	BA	503	PEV	C31-C32-C33-C34
60	A1	305	PEV	C39-C40-C41-C42
61	A0	318	PGV	C11-C12-C13-C14
60	BA	513	PEV	C34-C35-C36-C37
60	A0	330	PEV	C33-C34-C35-C36
61	BB	208	PGV	C13-C14-C15-C16
60	BA	529	PEV	C37-C38-C39-C40
61	B8	3005	PGV	C05-C04-O12-P
61	BB	217	PGV	C05-C04-O12-P
60	BA	518	PEV	C12-C13-C14-C15
61	BA	516	PGV	C11-C12-C13-C14
60	A0	311	PEV	C19-C20-C21-C22
61	BA	515	PGV	C11-C12-C13-C14
60	A1	319	PEV	C43-C44-C45-C46
60	A1	308	PEV	C32-C33-C34-C35
60	BA	518	PEV	C13-C14-C15-C16
61	BA	512	PGV	C02-C03-O11-P
60	BA	533	PEV	C41-C42-C43-C44
60	B8	3003	PEV	C32-C33-C34-C35
61	A0	305	PGV	C2-C3-C4-C5
60	B8	3003	PEV	C1-C2-C3-O3
60	A0	314	PEV	C36-C37-C38-C39
60	A0	310	PEV	C1-C2-O2-C31
60	A0	322	PEV	C1-C2-O2-C31
60	BA	504	PEV	C1-C2-O2-C31

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Mol	Chain	Res	Type	Atoms
60	BA	514	PEV	C1-C2-O2-C31
60	BA	533	PEV	C3-C2-O2-C31
60	BA	537	PEV	C3-C2-O2-C31
60	BA	539	PEV	C1-C2-O2-C31
60	BB	201	PEV	C1-C2-O2-C31
60	A0	307	PEV	C35-C36-C37-C38
61	BB	204	PGV	C4-C5-C6-C7
61	A0	304	PGV	C11-C12-C13-C14
61	A0	332	PGV	C11-C12-C13-C14
60	B8	3003	PEV	C34-C35-C36-C37
61	AZ	205	PGV	C11-C12-C13-C14
61	A0	317	PGV	C11-C12-C13-C14
61	BB	207	PGV	C11-C12-C13-C14
61	BA	536	PGV	C2-C3-C4-C5
61	A0	304	PGV	C05-C04-O12-P
60	A0	315	PEV	C19-C20-C21-C22
60	A1	325	PEV	C32-C33-C34-C35
60	BA	511	PEV	C34-C35-C36-C37
60	BA	519	PEV	C37-C38-C39-C40
60	A0	302	PEV	C39-C40-C41-C42
60	BB	211	PEV	C41-C42-C43-C44
61	A1	315	PGV	C11-C12-C13-C14
60	BB	209	PEV	C14-C15-C16-C17
60	AZ	202	PEV	C33-C34-C35-C36
61	A0	327	PGV	C5-C6-C7-C8
60	B8	3003	PEV	C2-C1-O3P-P
60	BB	209	PEV	C2-C1-O3P-P
60	A1	310	PEV	C42-C43-C44-C45
60	AZ	206	PEV	C17-C18-C19-C20
61	BB	204	PGV	C27-C28-C29-C30
61	A1	303	PGV	C11-C12-C13-C14
60	BA	517	PEV	C32-C33-C34-C35
60	A1	317	PEV	C32-C33-C34-C35
60	BA	513	PEV	C17-C18-C19-C20
60	A1	325	PEV	C31-C32-C33-C34
60	BA	537	PEV	C16-C17-C18-C19
61	A0	331	PGV	C11-C12-C13-C14
60	BA	508	PEV	C2-C1-O3P-P
61	A0	305	PGV	C05-C04-O12-P
60	A0	320	PEV	C35-C36-C37-C38
60	A1	309	PEV	C17-C18-C19-C20
60	BA	509	PEV	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
60	A1	324	PEV	C21-C22-C23-C24
60	BA	524	PEV	C17-C18-C19-C20
60	AZ	204	PEV	C14-C15-C16-C17
60	BA	532	PEV	C36-C37-C38-C39
60	A0	313	PEV	C3-C2-O2-C31
60	A1	309	PEV	C3-C2-O2-C31
60	BA	509	PEV	C3-C2-O2-C31
60	BA	519	PEV	C3-C2-O2-C31
60	BA	523	PEV	C3-C2-O2-C31
61	A0	304	PGV	C01-C02-O01-C1
61	A0	317	PGV	C01-C02-O01-C1
61	A1	311	PGV	C11-C12-C13-C14
61	BA	505	PGV	C11-C12-C13-C14
60	A0	312	PEV	C2-C1-O3P-P
61	BB	217	PGV	C11-C12-C13-C14
60	B8	3006	PEV	C5-C4-O4P-P
60	BA	533	PEV	C15-C16-C17-C18
60	A0	311	PEV	O3-C11-C12-C13
60	B8	3003	PEV	O3-C11-C12-C13
60	A1	302	PEV	O2-C31-C32-C33
60	BB	201	PEV	O2-C31-C32-C33
60	BA	502	PEV	C19-C20-C21-C22
60	BB	212	PEV	C16-C17-C18-C19
60	BB	201	PEV	O3-C11-C12-C13
60	BA	526	PEV	C32-C33-C34-C35
61	BB	208	PGV	C11-C12-C13-C14
61	BA	515	PGV	C28-C29-C30-C31
60	AZ	202	PEV	O3-C11-C12-C13
60	A1	306	PEV	O3-C11-C12-C13
60	A1	328	PEV	O3-C11-C12-C13
60	BA	519	PEV	O2-C31-C32-C33
61	AZ	205	PGV	O03-C19-C20-C21
60	A0	301	PEV	C12-C13-C14-C15
60	A0	307	PEV	O2-C31-C32-C33
61	BA	512	PGV	C4-C5-C6-C7
61	AZ	207	PGV	C11-C12-C13-C14
60	A0	316	PEV	C17-C18-C19-C20
61	BA	512	PGV	O01-C1-C2-C3
60	BA	509	PEV	C16-C17-C18-C19
61	A1	315	PGV	C2-C3-C4-C5
60	AZ	201	PEV	O3-C11-C12-C13
60	A0	307	PEV	O3-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
60	A1	301	PEV	O3-C11-C12-C13
60	BA	530	PEV	O2-C31-C32-C33
60	A0	330	PEV	C32-C33-C34-C35
61	BB	204	PGV	C6-C7-C8-C9
60	A0	314	PEV	C44-C45-C46-C47
60	A1	317	PEV	O2-C31-C32-C33
60	BA	509	PEV	O2-C31-C32-C33
60	BA	535	PEV	O3-C11-C12-C13
60	BA	538	PEV	O3-C11-C12-C13
60	A1	325	PEV	C18-C19-C20-C21
60	BA	520	PEV	C35-C36-C37-C38
60	BA	530	PEV	C15-C16-C17-C18
60	BA	508	PEV	C44-C45-C46-C47
60	BB	210	PEV	O2-C31-C32-C33
60	B8	3002	PEV	C36-C37-C38-C39
60	A1	310	PEV	C17-C18-C19-C20
60	BA	519	PEV	O3-C11-C12-C13
61	A0	317	PGV	O01-C1-C2-C3
60	A0	323	PEV	C13-C14-C15-C16
60	BA	518	PEV	C34-C35-C36-C37
60	A0	302	PEV	C20-C21-C22-C23
61	A0	306	PGV	C21-C22-C23-C24
60	A1	306	PEV	O2-C31-C32-C33
60	BA	521	PEV	O3-C11-C12-C13
60	BA	528	PEV	O3-C11-C12-C13
60	BA	532	PEV	O3-C11-C12-C13
61	AZ	205	PGV	O01-C1-C2-C3
61	A0	305	PGV	O03-C19-C20-C21
61	A0	328	PGV	O01-C1-C2-C3
60	A0	321	PEV	C32-C33-C34-C35
60	BA	537	PEV	O2-C2-C3-O3
61	BA	536	PGV	C3-C4-C5-C6
60	BA	503	PEV	C32-C33-C34-C35
60	A1	320	PEV	O2-C31-C32-C33
60	A0	312	PEV	O2-C31-C32-C33
60	BA	524	PEV	O2-C31-C32-C33
61	AZ	205	PGV	C22-C23-C24-C25
60	A0	311	PEV	C32-C33-C34-C35
60	A1	325	PEV	C15-C16-C17-C18
60	A0	302	PEV	C3-C2-O2-C31
60	A0	303	PEV	C3-C2-O2-C31
60	A0	309	PEV	C3-C2-O2-C31

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Mol	Chain	Res	Type	Atoms
60	A0	319	PEV	C3-C2-O2-C31
60	A0	324	PEV	C1-C2-O2-C31
60	A1	302	PEV	C3-C2-O2-C31
60	A1	320	PEV	C3-C2-O2-C31
60	BA	503	PEV	C3-C2-O2-C31
60	BA	525	PEV	C1-C2-O2-C31
61	A0	325	PGV	C03-C02-O01-C1
61	A1	315	PGV	C03-C02-O01-C1
61	A1	318	PGV	C01-C02-O01-C1
61	A1	318	PGV	C03-C02-O01-C1
60	BB	206	PEV	C32-C33-C34-C35
60	A1	328	PEV	O11-C11-C12-C13
61	BB	204	PGV	C3-C4-C5-C6
60	A0	309	PEV	O2-C31-C32-C33
60	A1	304	PEV	C42-C43-C44-C45
60	A1	324	PEV	C31-C32-C33-C34
61	BB	208	PGV	C05-C04-O12-P
60	BA	530	PEV	O31-C31-C32-C33
60	BA	535	PEV	O11-C11-C12-C13
60	B8	3004	PEV	C14-C15-C16-C17
60	A1	325	PEV	C42-C43-C44-C45
60	A0	307	PEV	O31-C31-C32-C33
61	A0	305	PGV	O04-C19-C20-C21
61	BA	512	PGV	O02-C1-C2-C3
60	BA	535	PEV	C14-C15-C16-C17
61	BA	515	PGV	C24-C25-C26-C27
60	A1	326	PEV	C40-C41-C42-C43
60	BB	206	PEV	O3-C11-C12-C13
60	AZ	201	PEV	O11-C11-C12-C13
60	BA	538	PEV	O11-C11-C12-C13
60	BB	201	PEV	O11-C11-C12-C13
60	BB	210	PEV	O31-C31-C32-C33
60	BA	510	PEV	C20-C21-C22-C23
60	A0	311	PEV	O11-C11-C12-C13
60	A1	301	PEV	O11-C11-C12-C13
60	BA	519	PEV	O31-C31-C32-C33
60	A0	307	PEV	O11-C11-C12-C13
60	B8	3003	PEV	O11-C11-C12-C13
60	BA	528	PEV	O11-C11-C12-C13
60	BA	532	PEV	O11-C11-C12-C13
60	BB	201	PEV	O31-C31-C32-C33
60	BB	201	PEV	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
60	A1	302	PEV	O3-C11-C12-C13
60	AZ	203	PEV	C40-C41-C42-C43
60	A1	302	PEV	O31-C31-C32-C33
61	AZ	205	PGV	O04-C19-C20-C21
60	BA	513	PEV	O2-C2-C3-O3
60	A1	317	PEV	C43-C44-C45-C46
61	A0	318	PGV	C30-C31-C32-C33
60	AZ	202	PEV	O11-C11-C12-C13
60	A1	317	PEV	O31-C31-C32-C33
60	A1	301	PEV	O2-C31-C32-C33
61	BA	505	PGV	O01-C1-C2-C3
60	B8	3004	PEV	C12-C13-C14-C15
60	BB	210	PEV	C12-C13-C14-C15
60	A1	306	PEV	O11-C11-C12-C13
60	A0	320	PEV	C2-C1-O3P-P
60	BA	530	PEV	C2-C1-O3P-P
60	A1	319	PEV	C36-C37-C38-C39
60	BA	509	PEV	O31-C31-C32-C33
60	BA	519	PEV	O11-C11-C12-C13
61	A0	317	PGV	O02-C1-C2-C3
60	AZ	204	PEV	C37-C38-C39-C40
60	A0	309	PEV	C18-C19-C20-C21
60	BA	513	PEV	C32-C33-C34-C35
60	A0	309	PEV	C13-C14-C15-C16
61	AZ	205	PGV	C21-C22-C23-C24
60	AZ	204	PEV	O2-C31-C32-C33
60	A1	305	PEV	O2-C31-C32-C33
61	BA	505	PGV	O03-C19-C20-C21
60	A0	316	PEV	C16-C17-C18-C19
60	B8	3007	PEV	C17-C18-C19-C20
60	BA	530	PEV	C16-C17-C18-C19
60	BA	534	PEV	O3-C11-C12-C13
60	BB	212	PEV	O2-C31-C32-C33
61	A1	318	PGV	O01-C1-C2-C3
61	A0	306	PGV	C29-C30-C31-C32
60	BB	209	PEV	C15-C16-C17-C18
60	BA	534	PEV	O11-C11-C12-C13
60	BB	206	PEV	O11-C11-C12-C13
61	A0	318	PGV	C6-C7-C8-C9
60	BA	523	PEV	C42-C43-C44-C45
60	A1	309	PEV	O2-C31-C32-C33
60	A0	324	PEV	C16-C17-C18-C19

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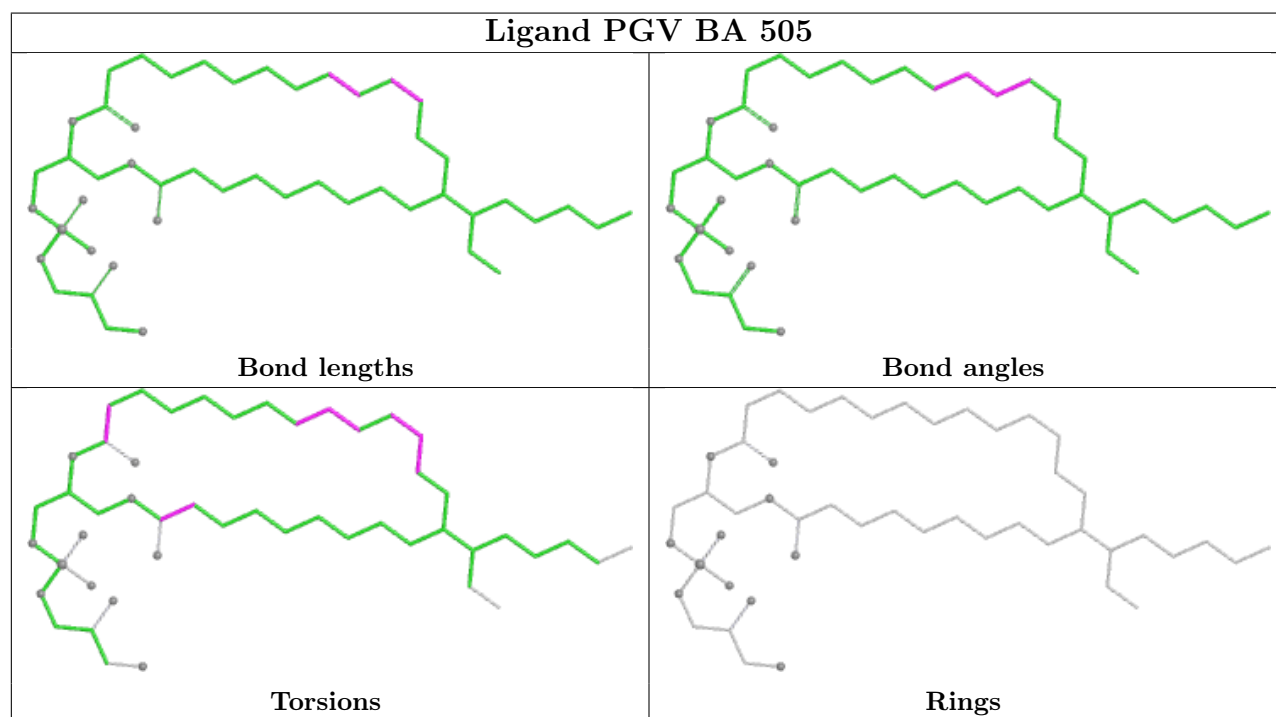
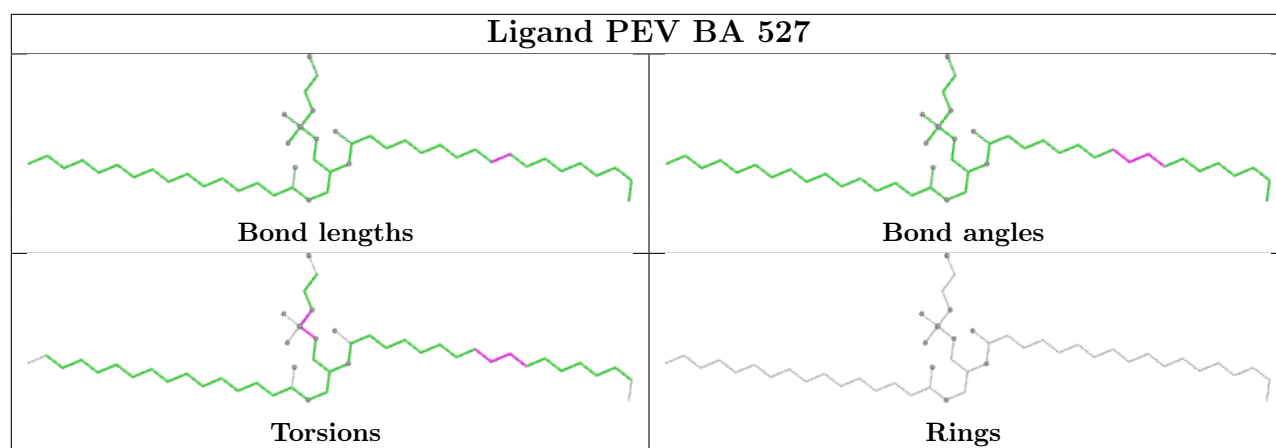
Mol	Chain	Res	Type	Atoms
60	BA	535	PEV	C17-C18-C19-C20
60	A0	312	PEV	O31-C31-C32-C33
60	BA	521	PEV	O11-C11-C12-C13
61	A0	328	PGV	O02-C1-C2-C3
61	BA	505	PGV	O02-C1-C2-C3
61	A0	331	PGV	C20-C21-C22-C23

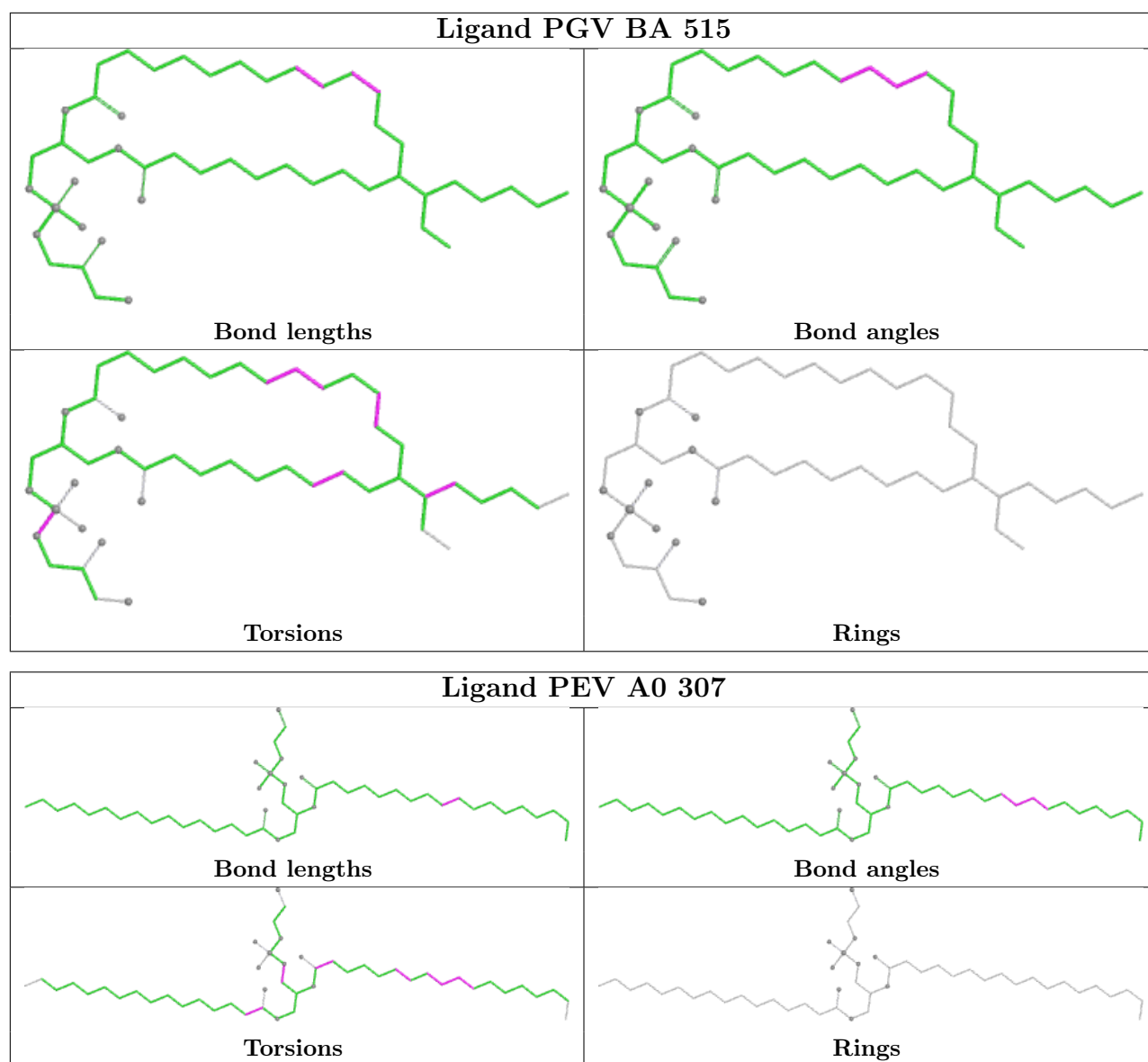
There are no ring outliers.

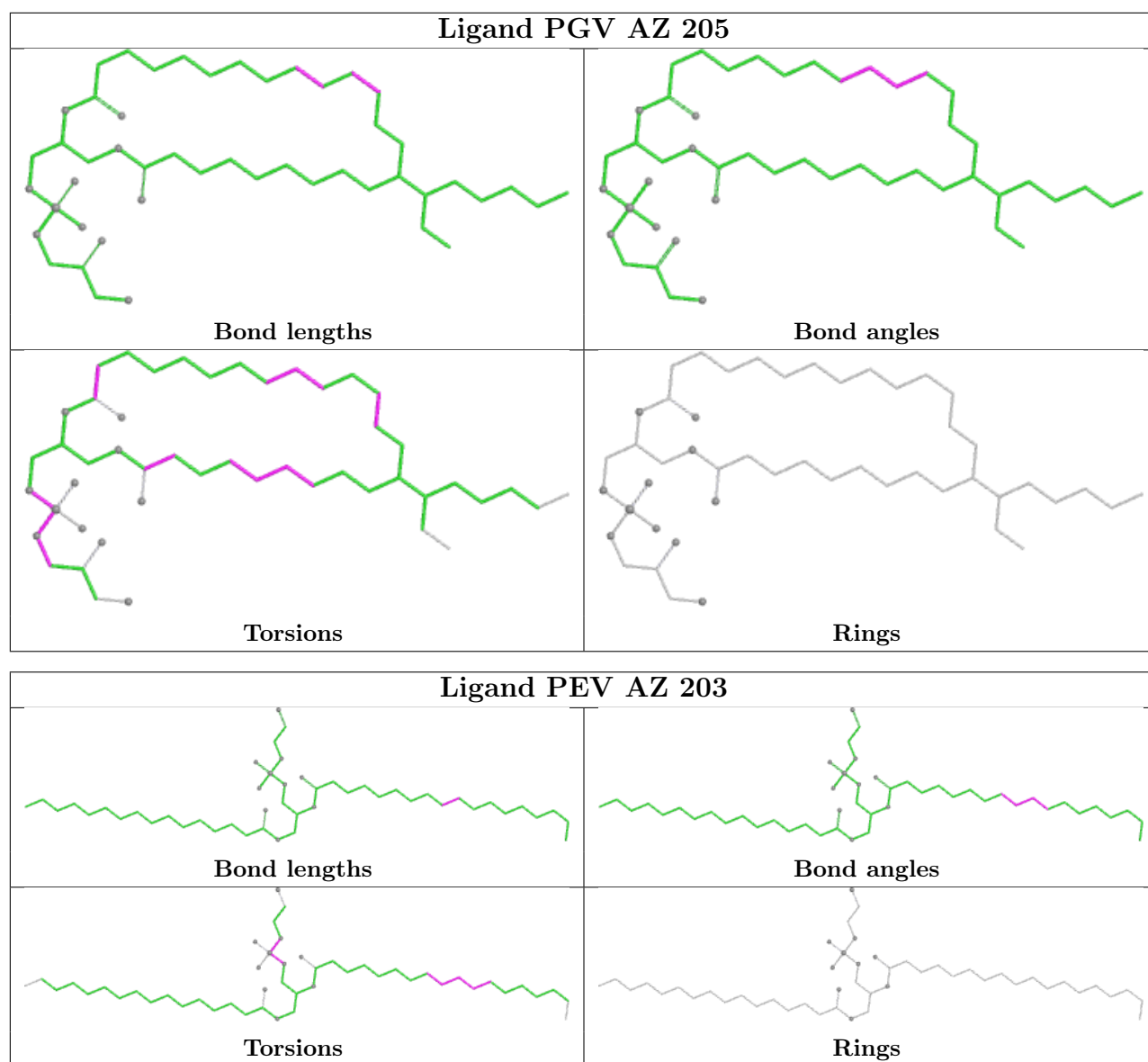
17 monomers are involved in 41 short contacts:

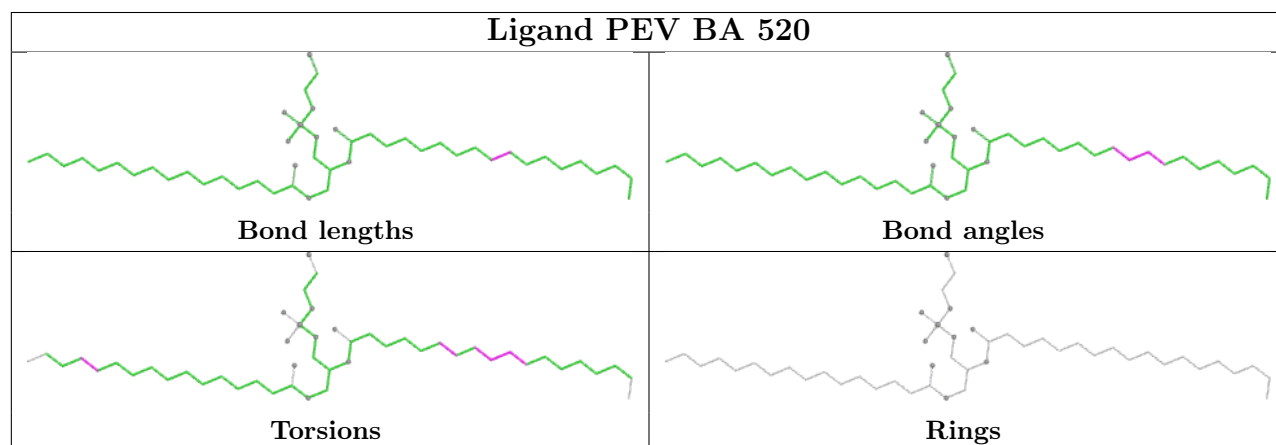
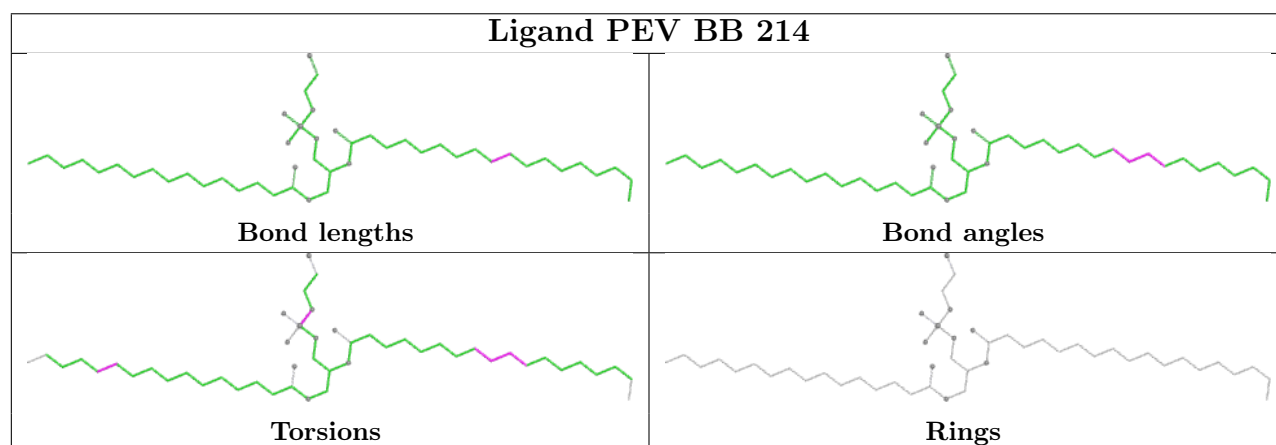
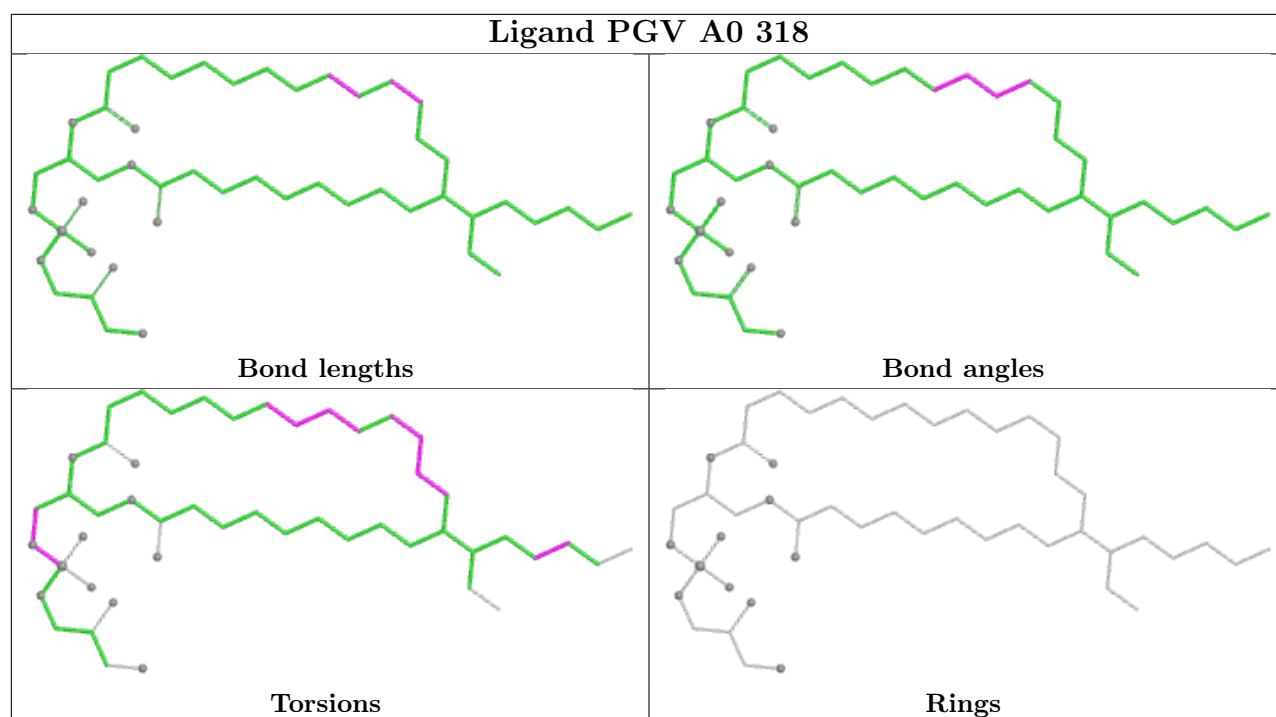
Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	BA	520	PEV	1	0
60	B8	3001	PEV	1	0
60	BA	514	PEV	1	0
60	A0	315	PEV	1	0
60	A1	323	PEV	1	0
60	BA	503	PEV	1	0
60	A1	301	PEV	1	0
60	BA	531	PEV	1	0
60	BA	513	PEV	1	0
60	BA	526	PEV	1	0
60	A1	319	PEV	1	0
61	A1	315	PGV	1	0
60	BA	533	PEV	29	0
61	A1	303	PGV	1	0
60	A1	302	PEV	1	0
61	BA	512	PGV	1	0
60	B8	3002	PEV	2	0

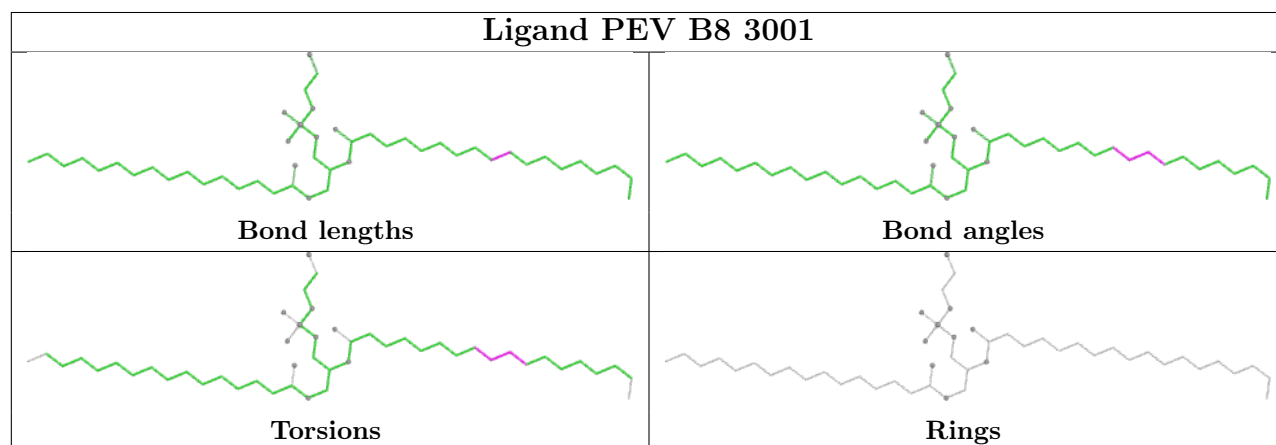
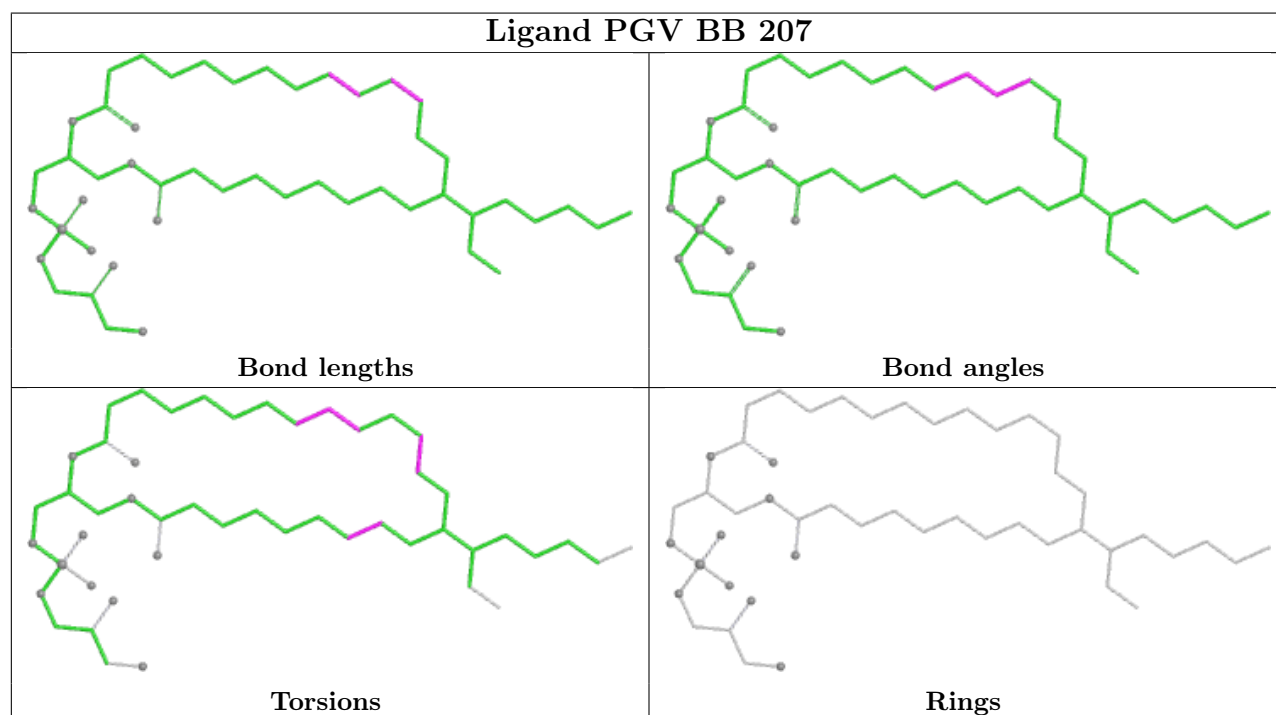
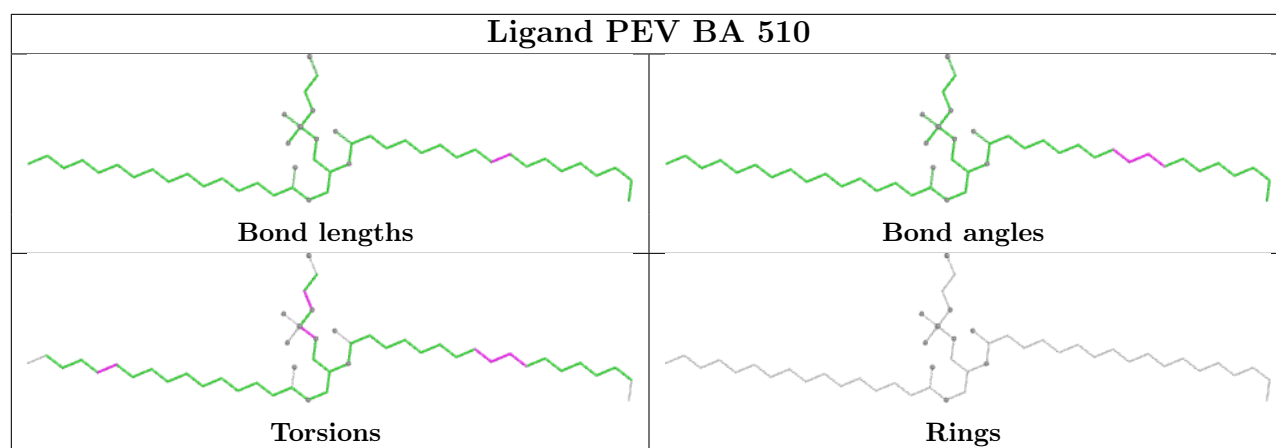
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

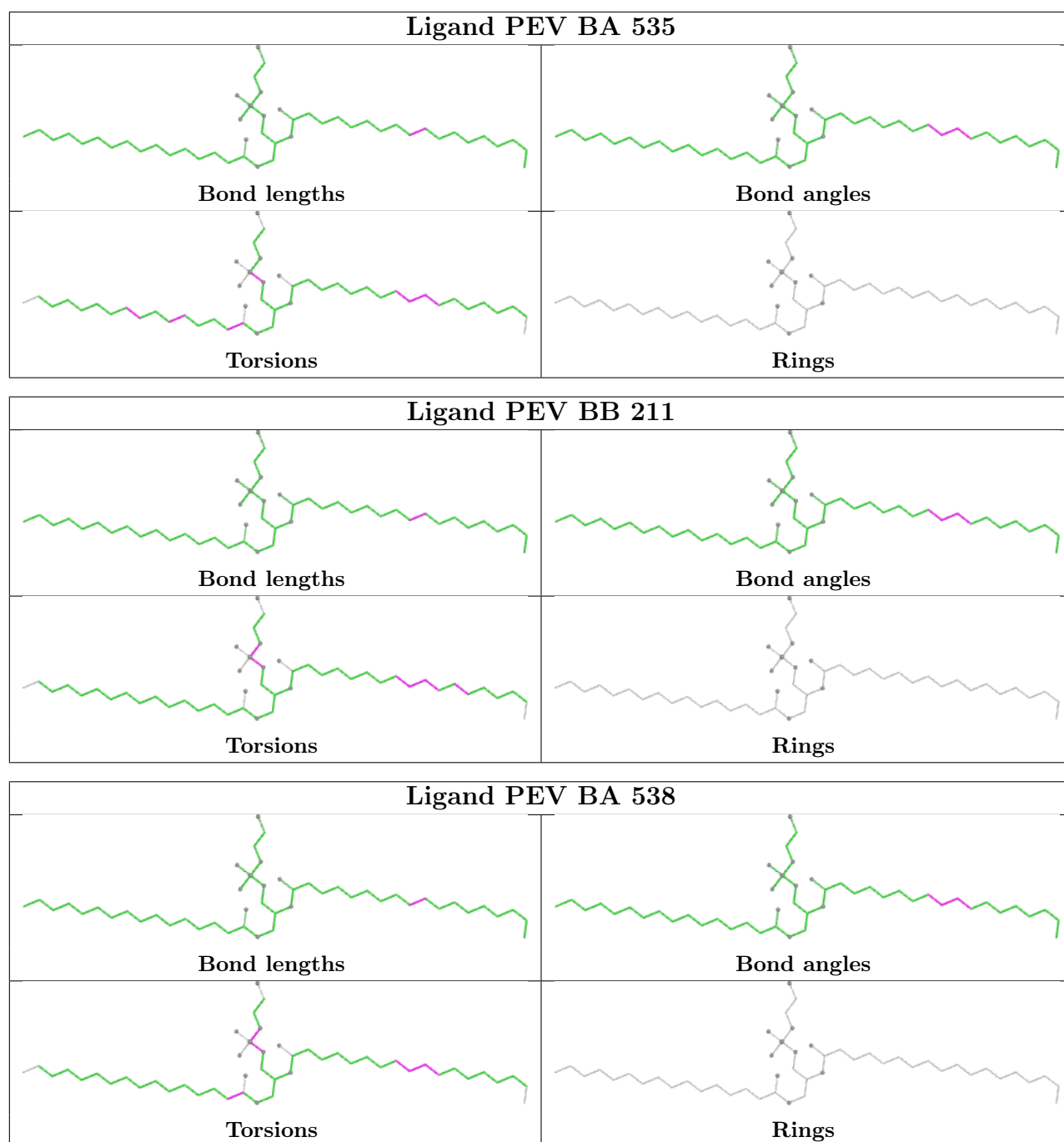


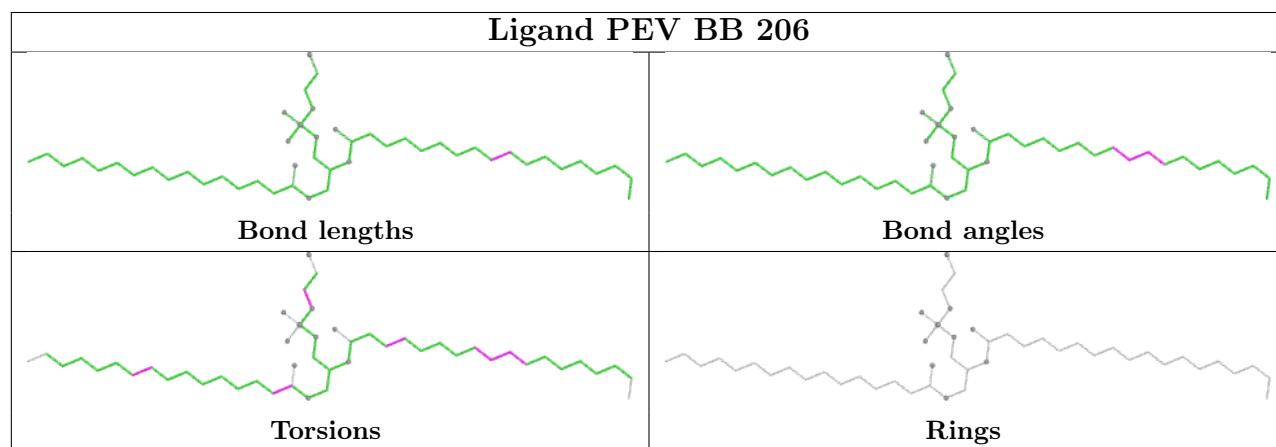
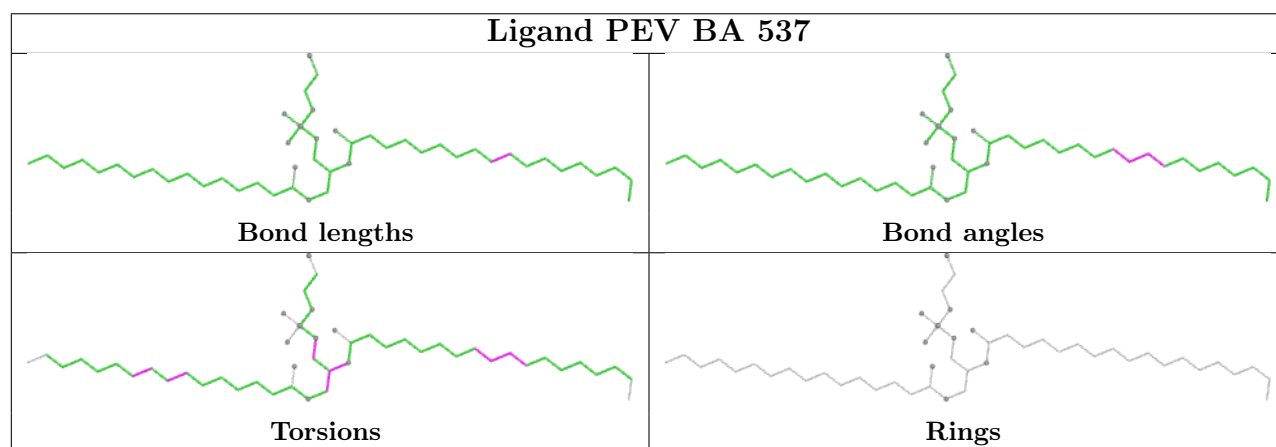
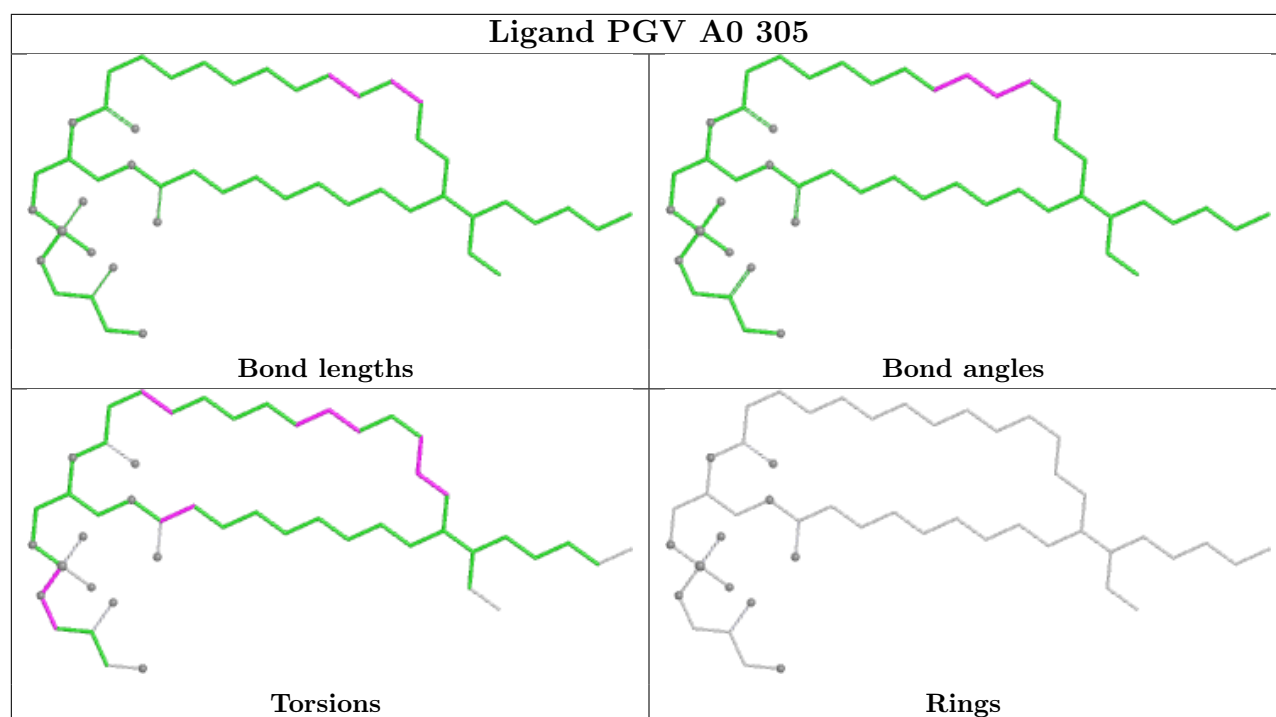


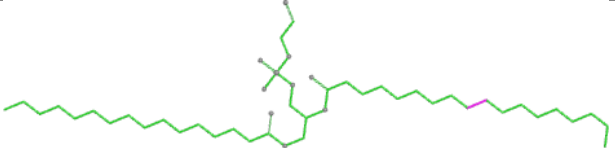
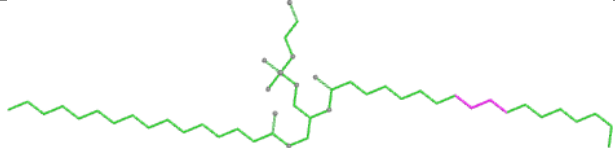
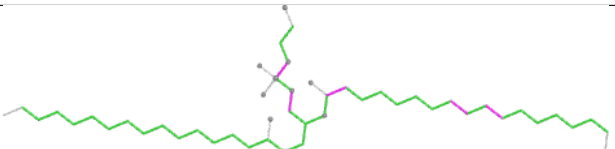
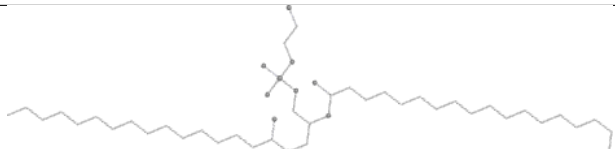
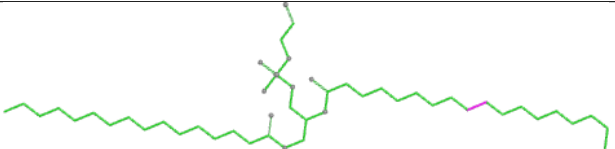
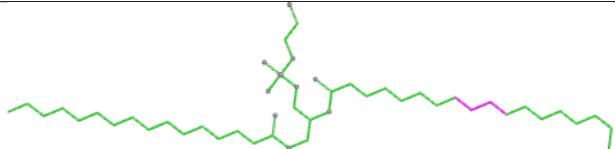
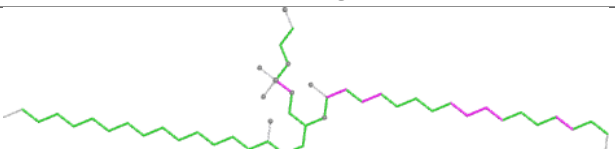
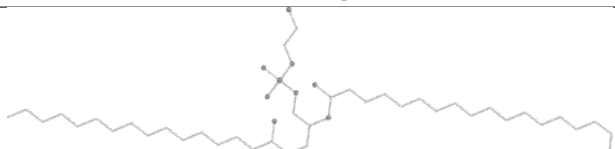
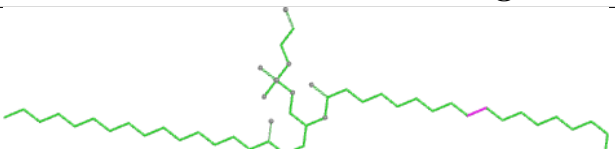
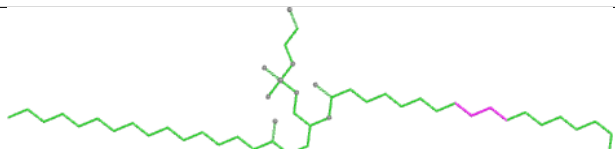
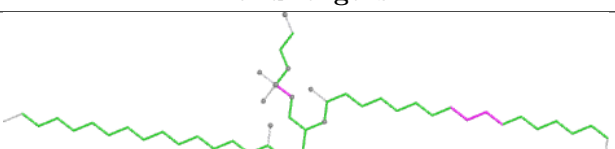
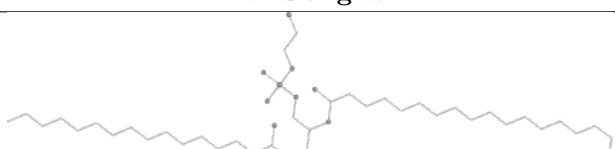


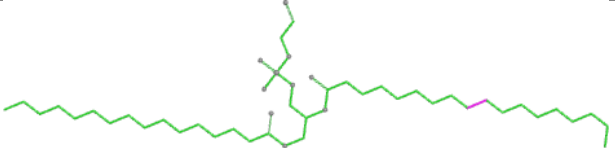
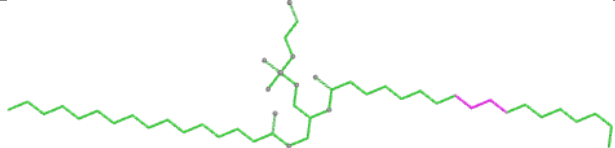
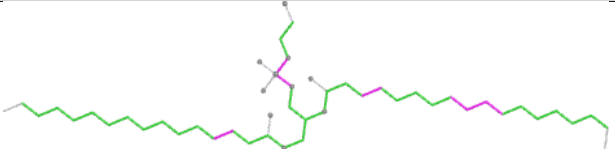
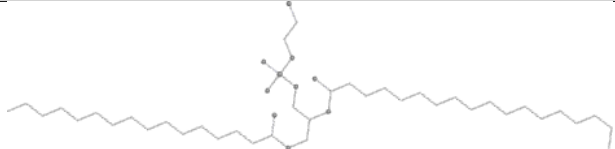
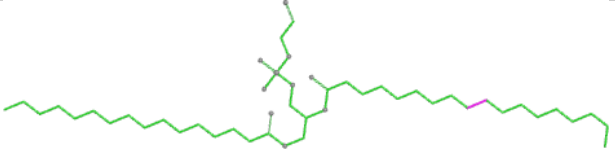
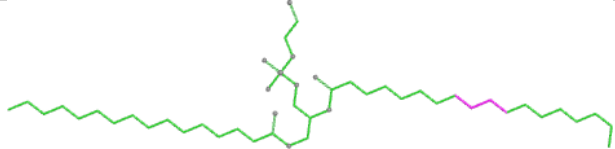
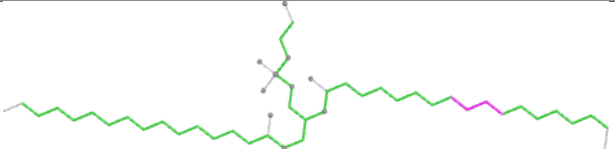
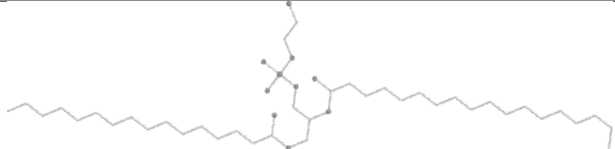
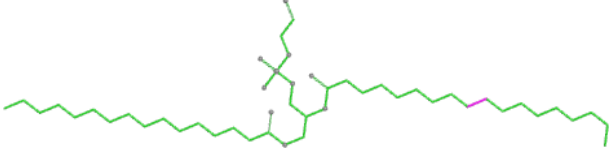
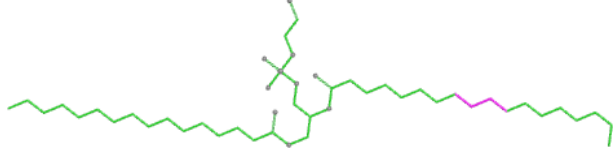
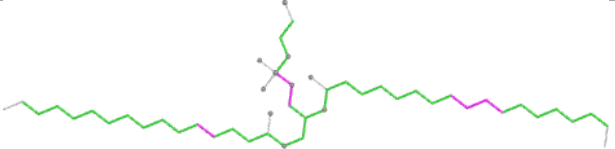
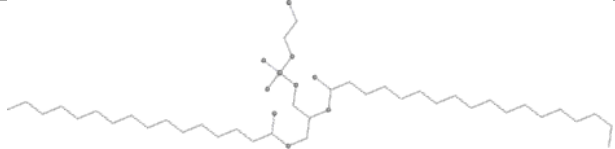


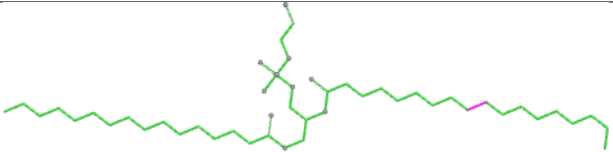
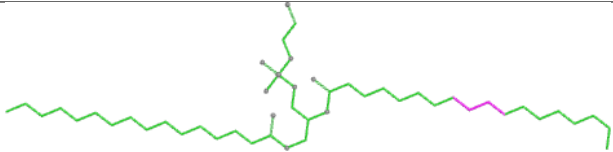
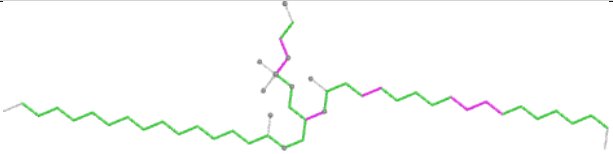
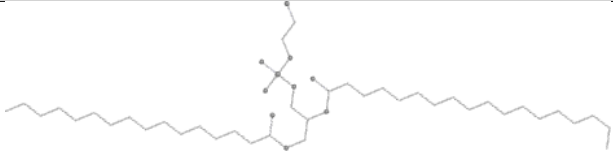
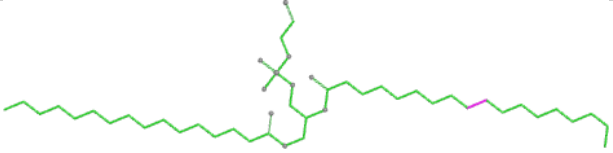
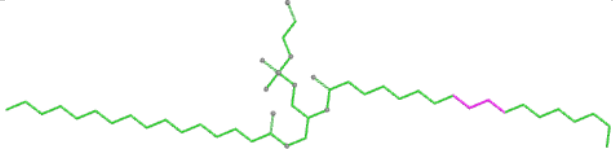
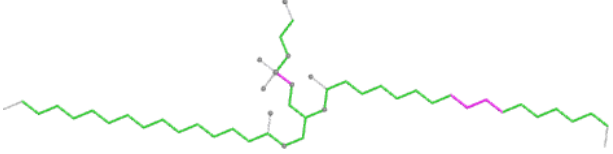
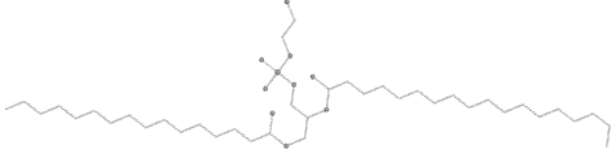
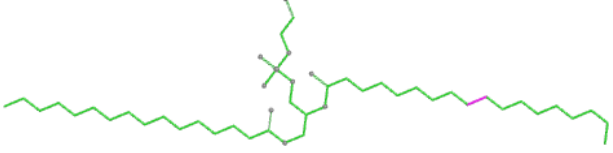
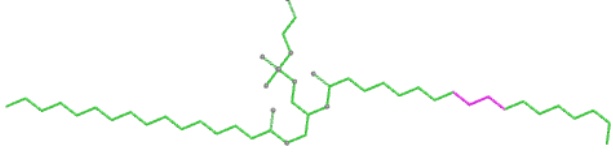
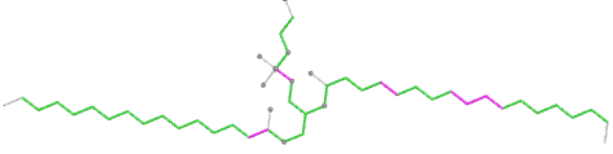
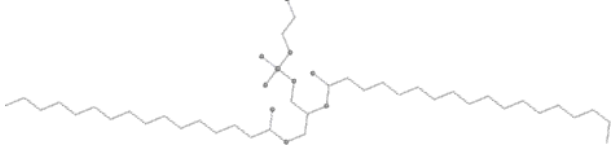


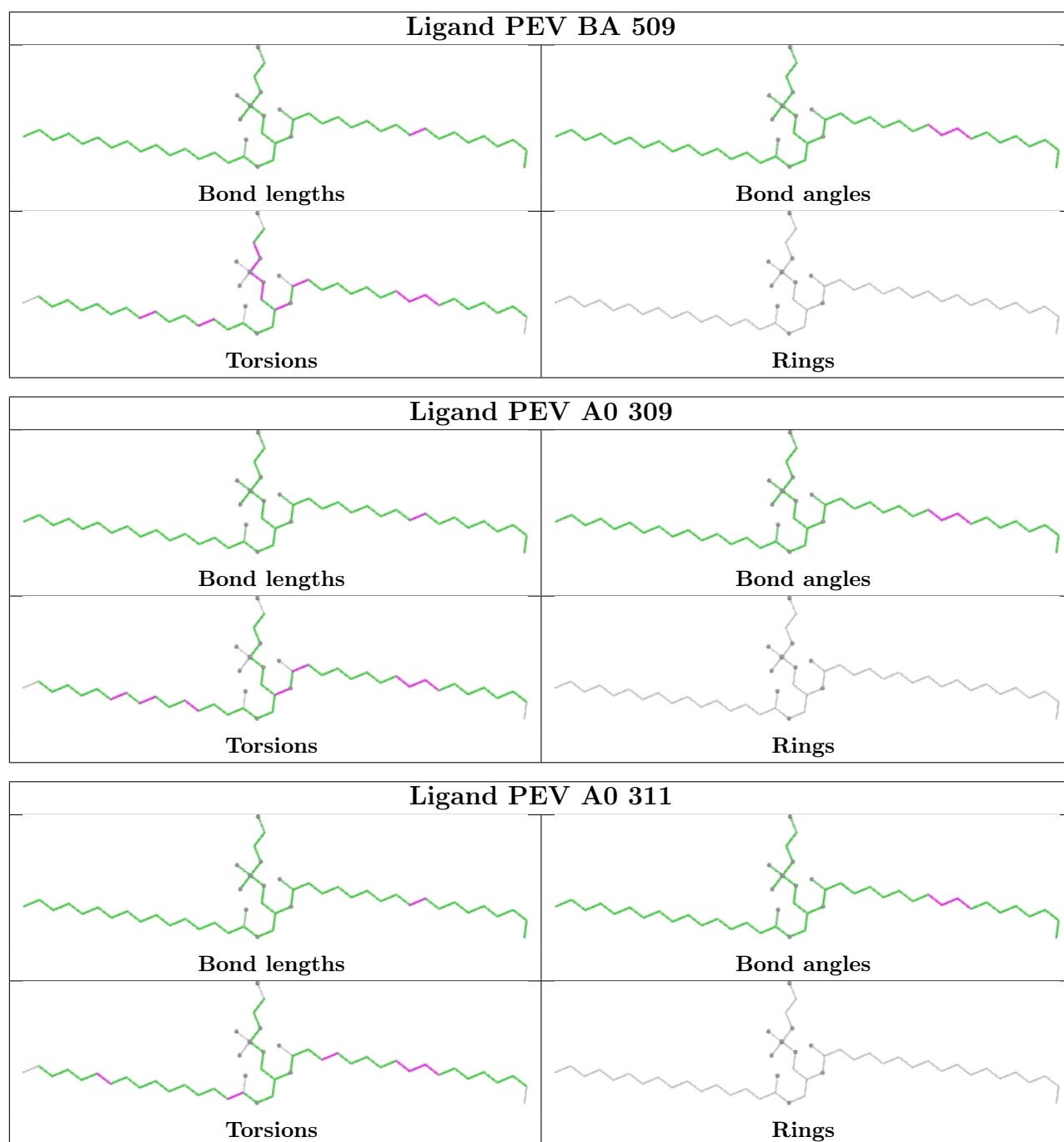


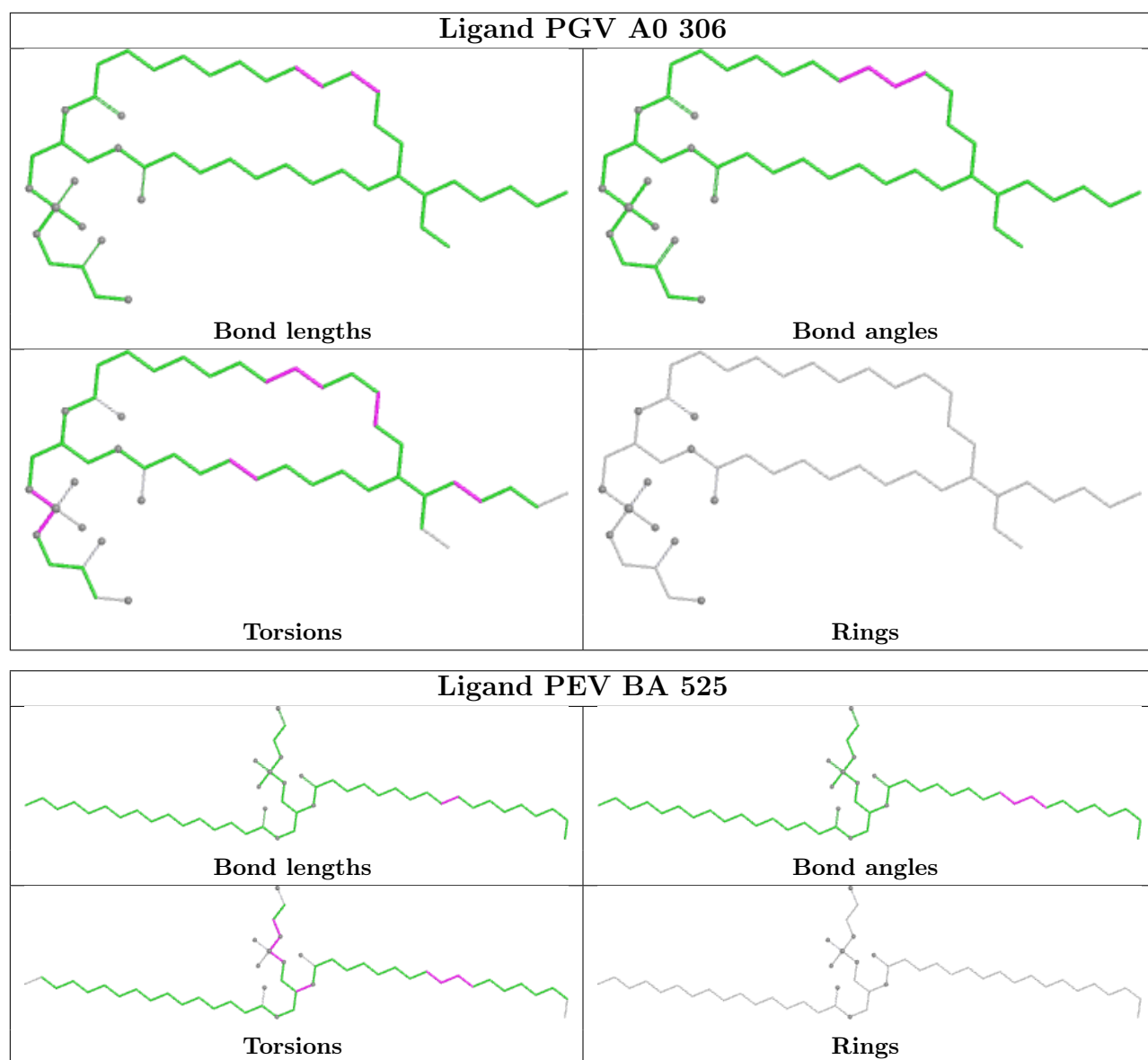


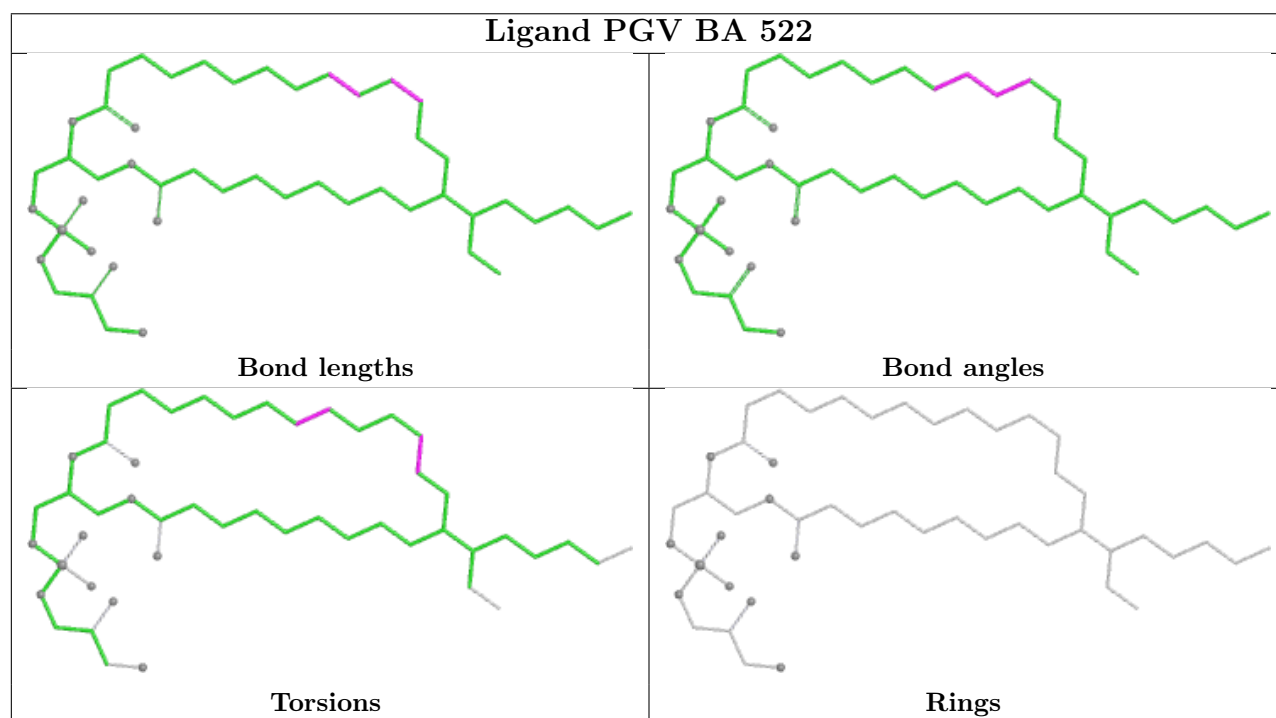
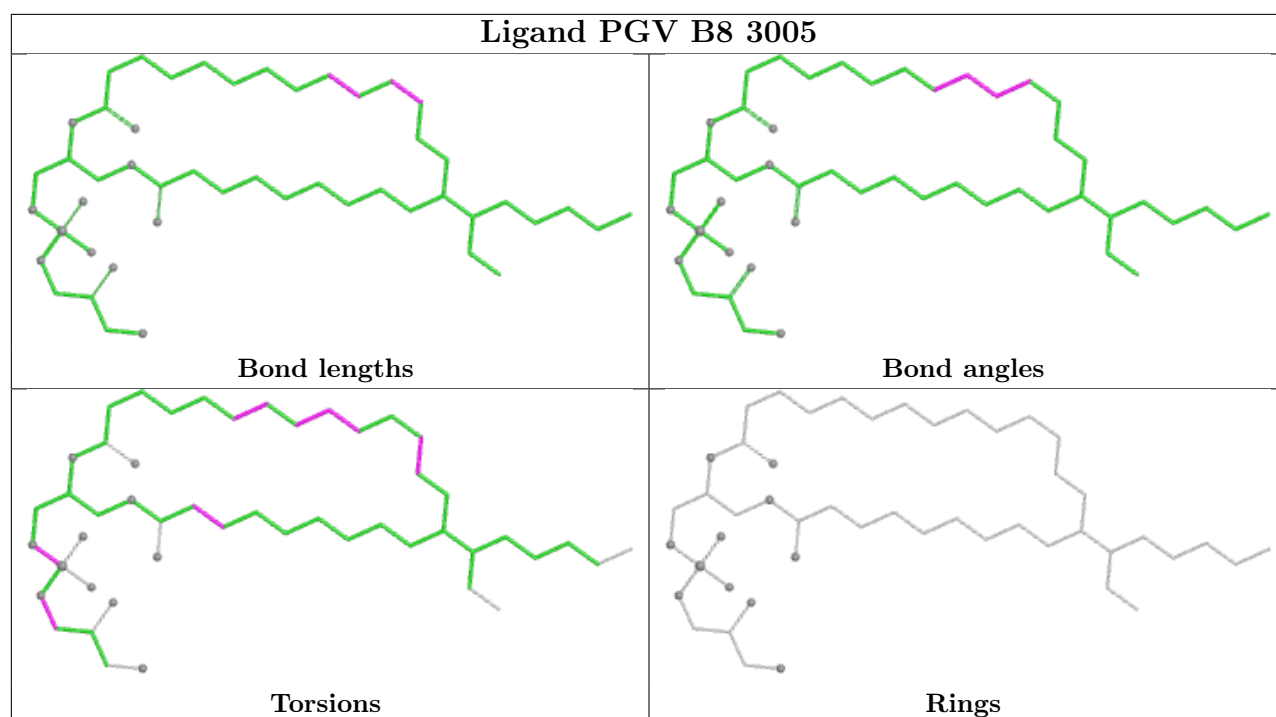
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 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PEV A1 317	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PEV BB 215	
 Bond lengths	 Bond angles
 Torsions	 Rings

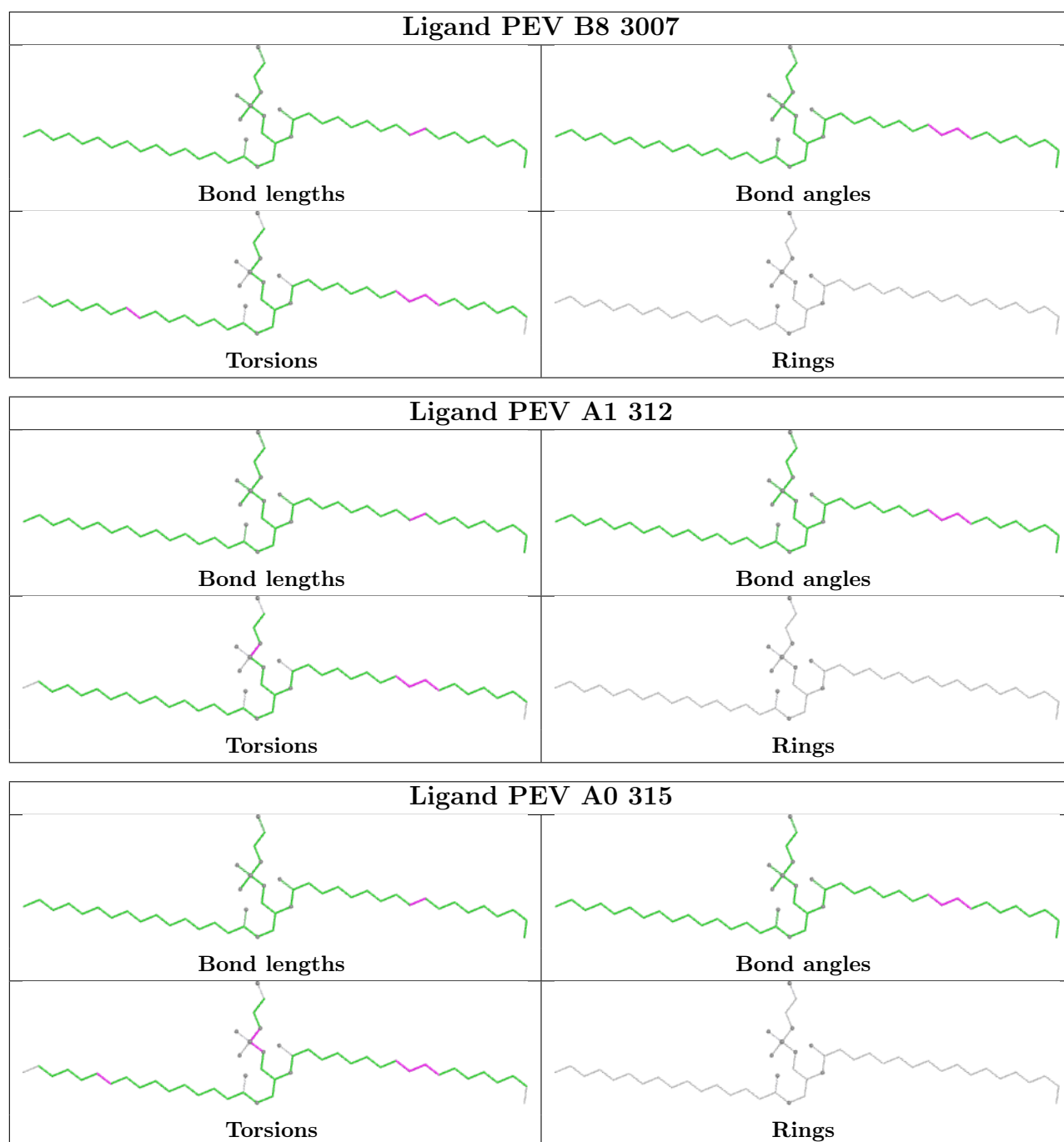
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 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PEV BA 529	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PEV A0 323	
 Bond lengths	 Bond angles
 Torsions	 Rings

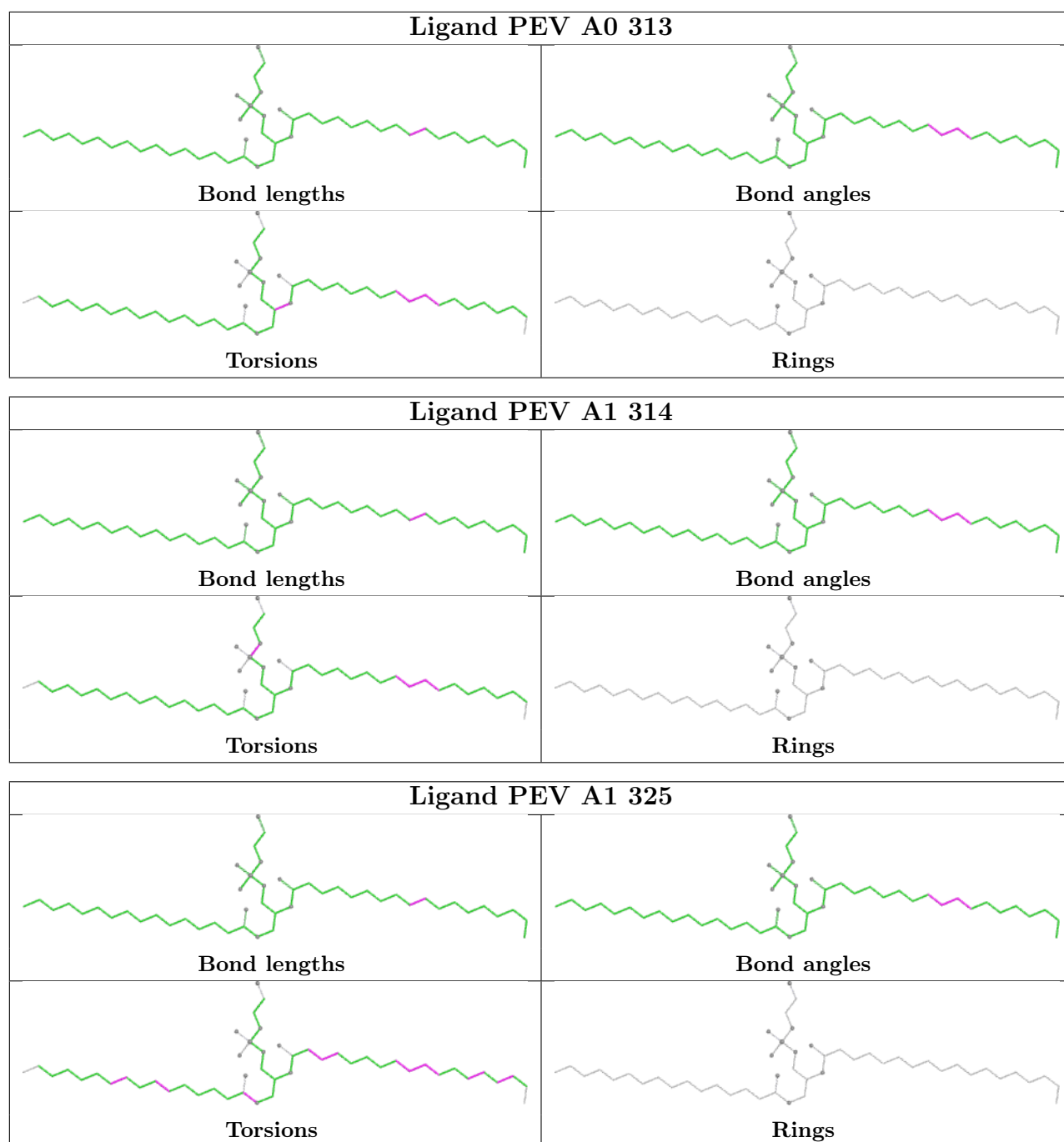
Ligand PEV BA 514	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PEV A0 329	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PEV AZ 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

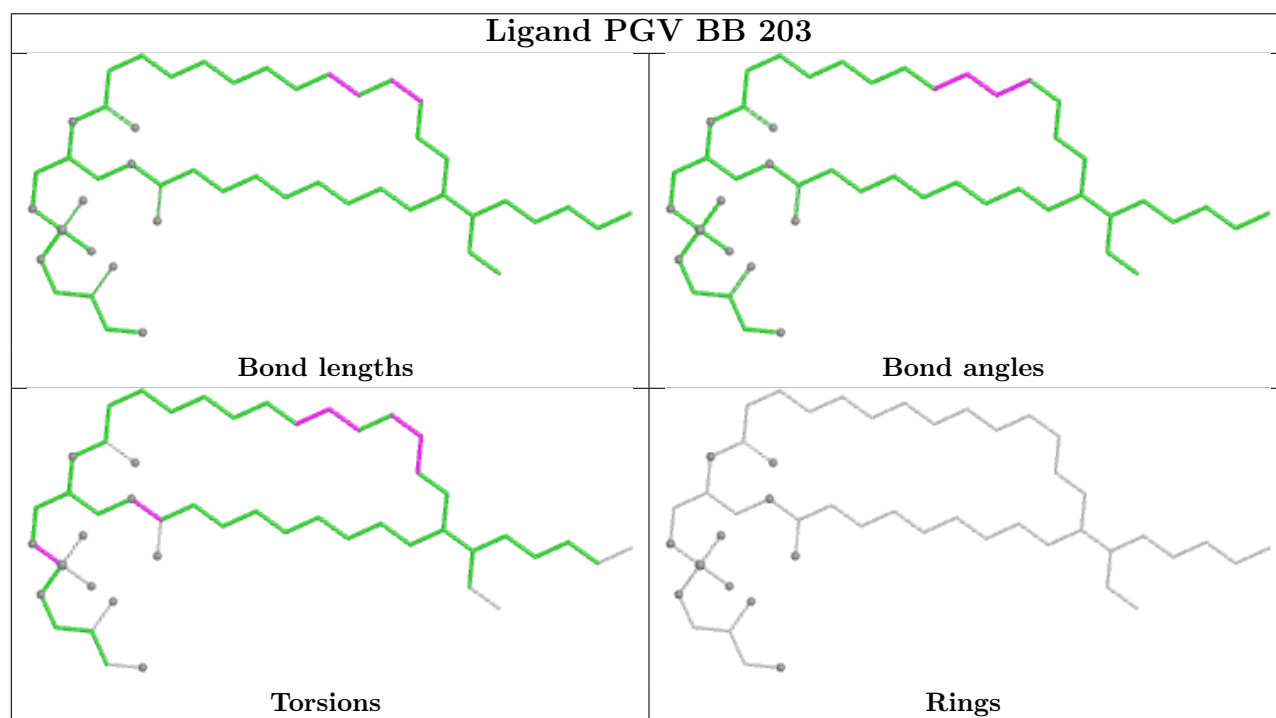
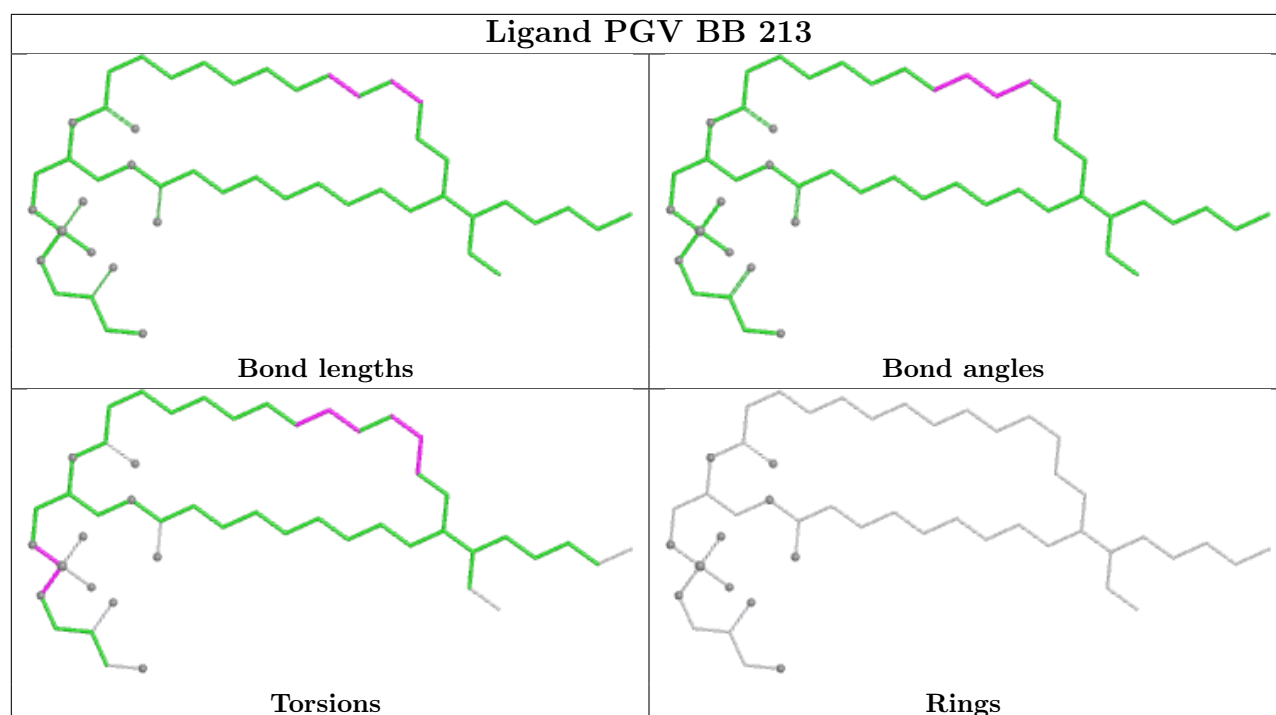


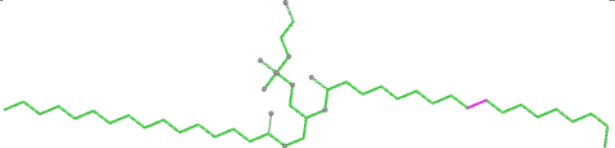
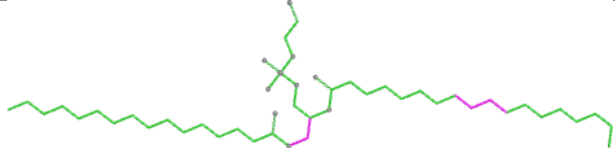
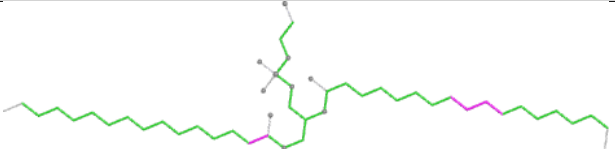
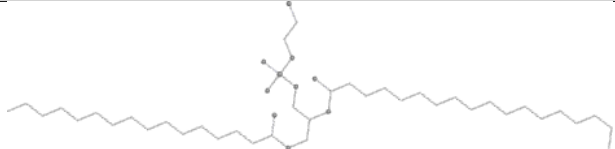
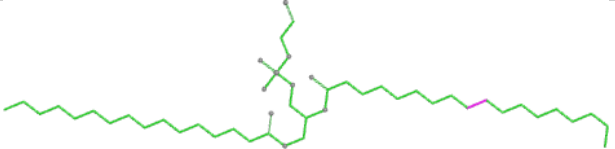
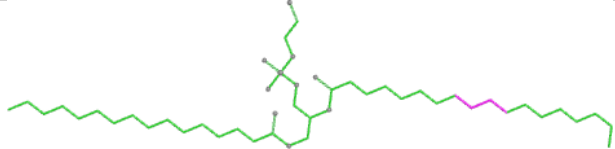
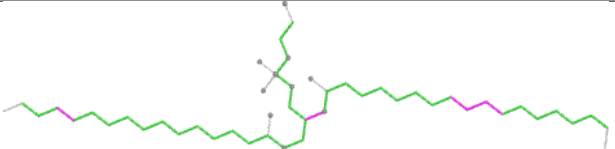
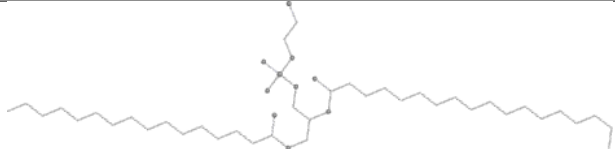
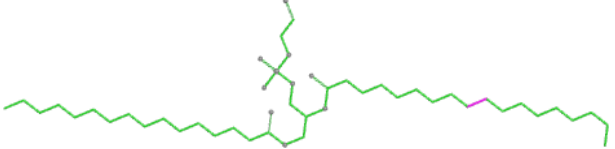
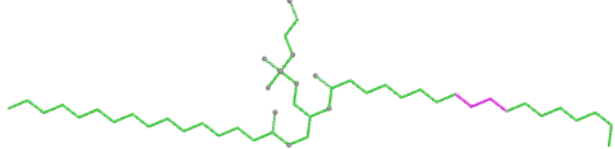
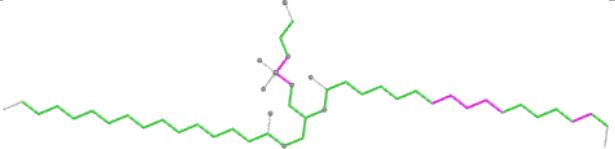
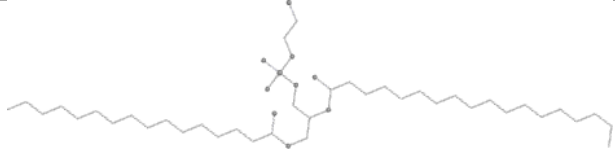


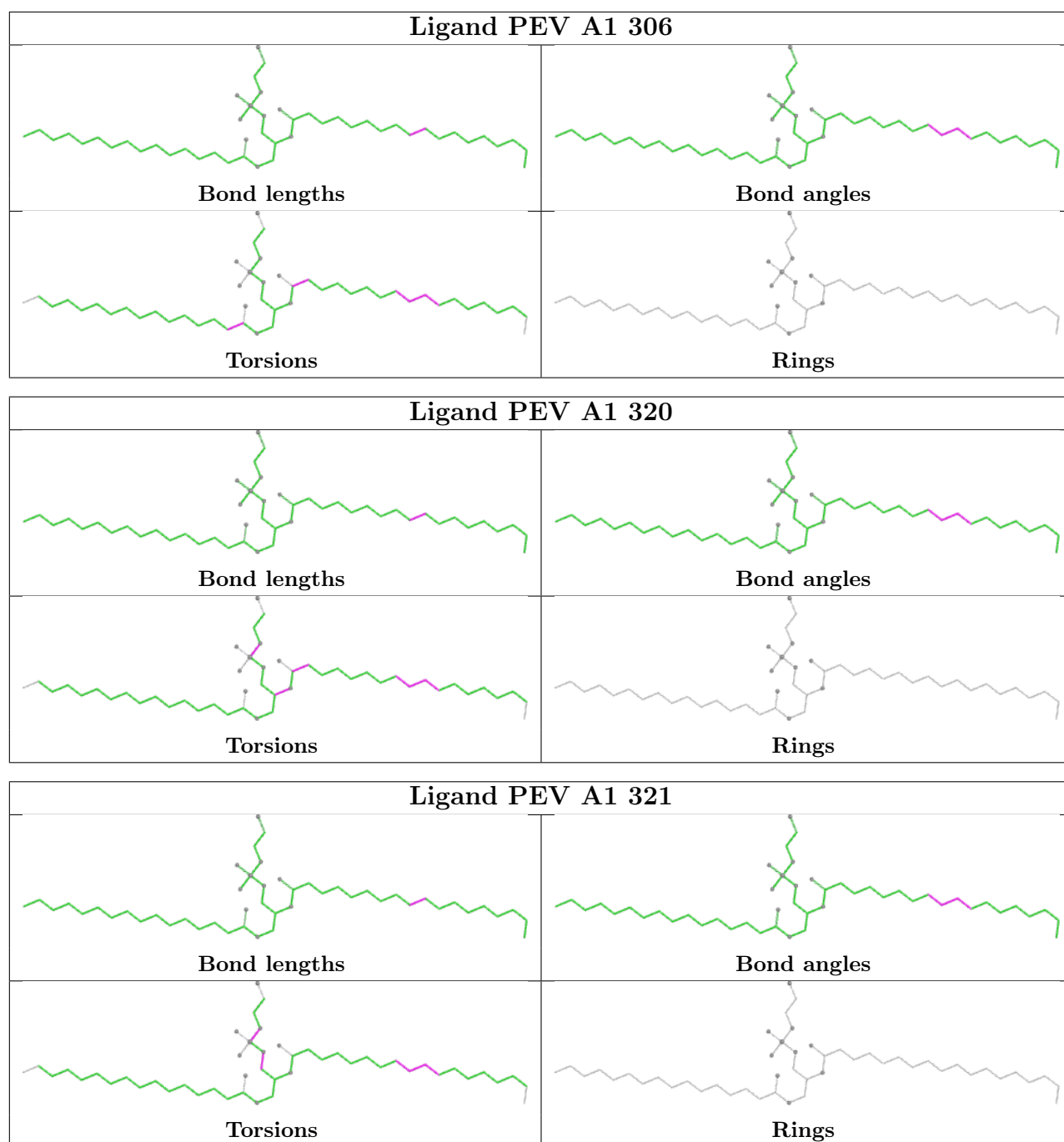


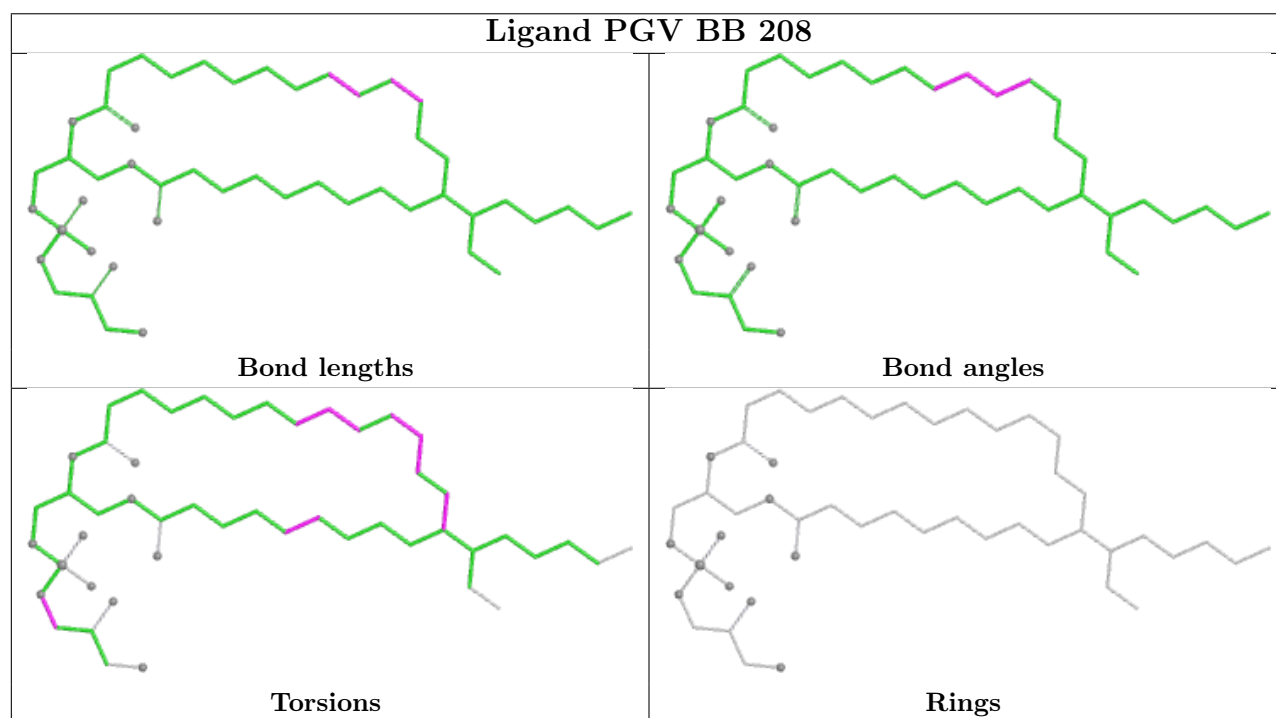
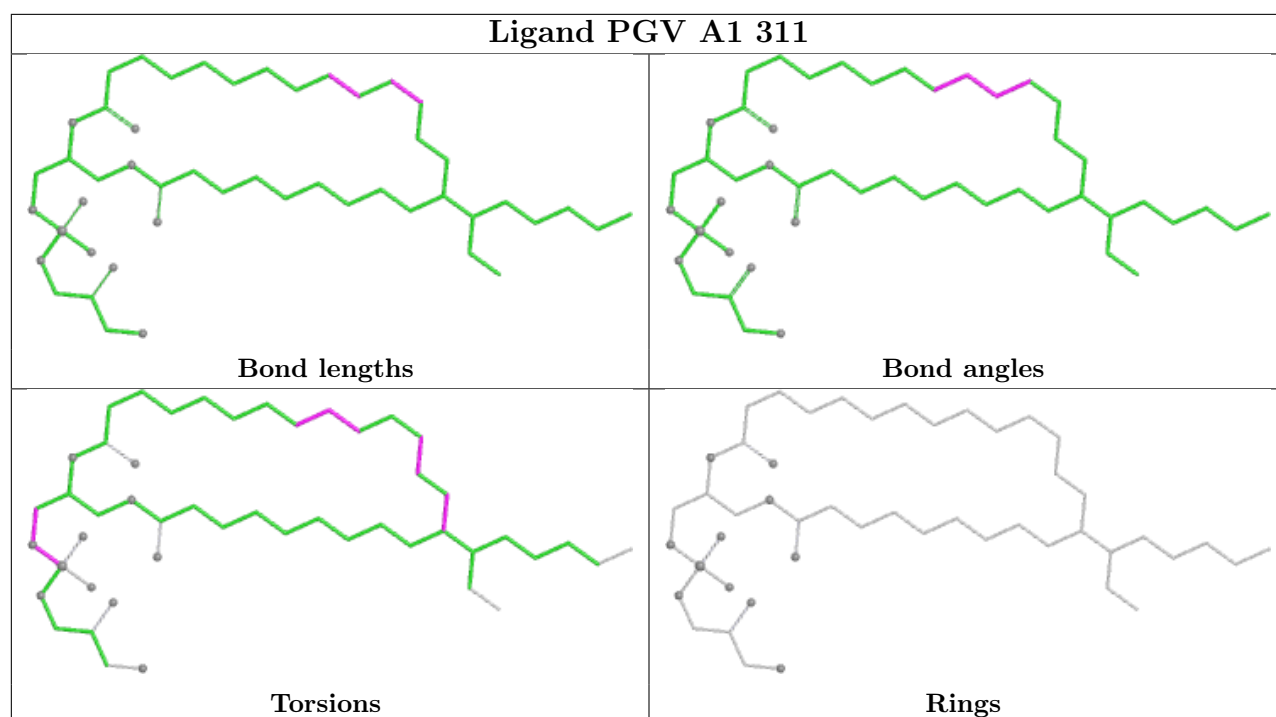


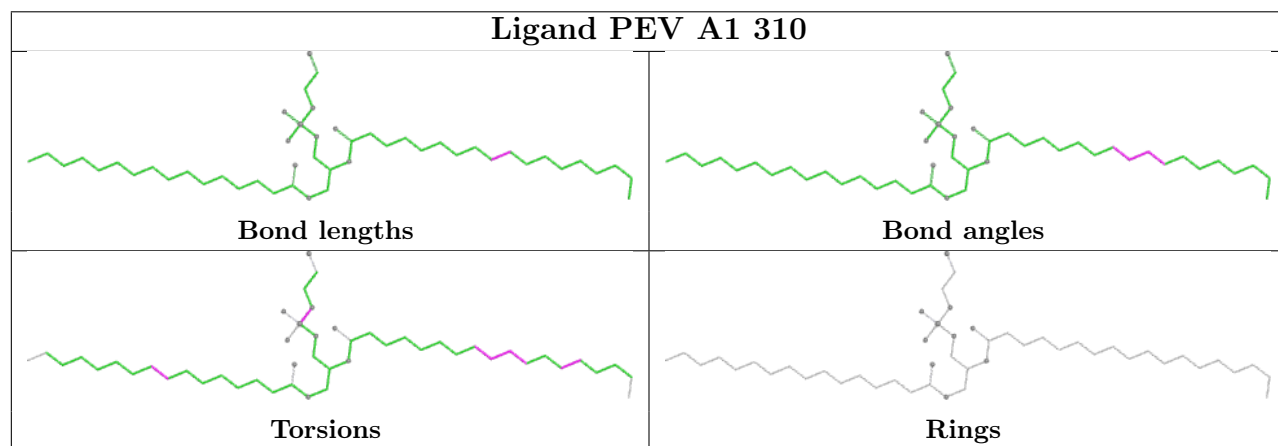
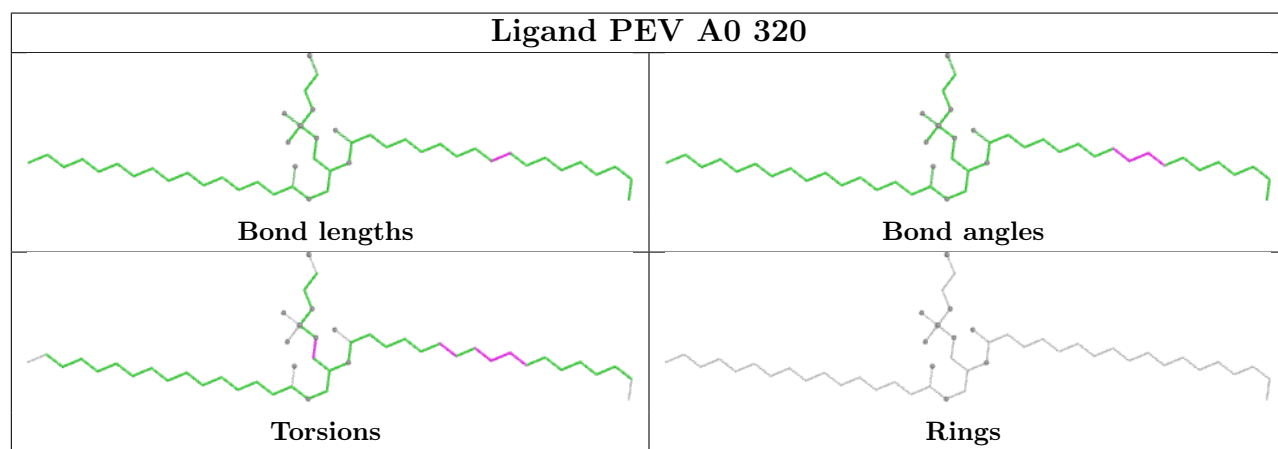
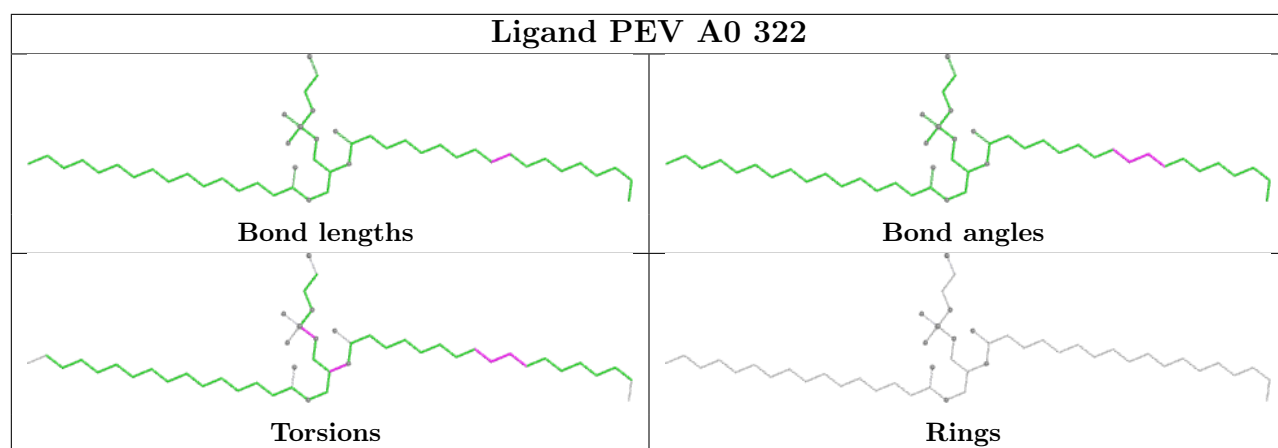


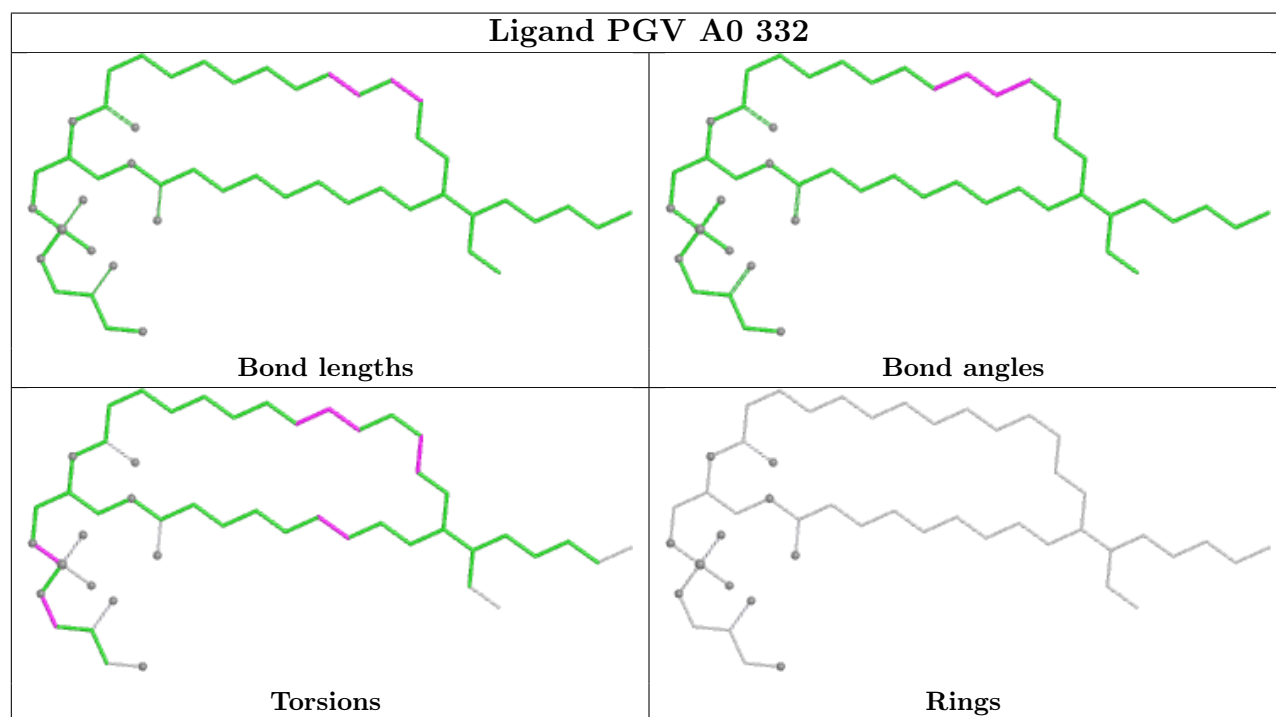
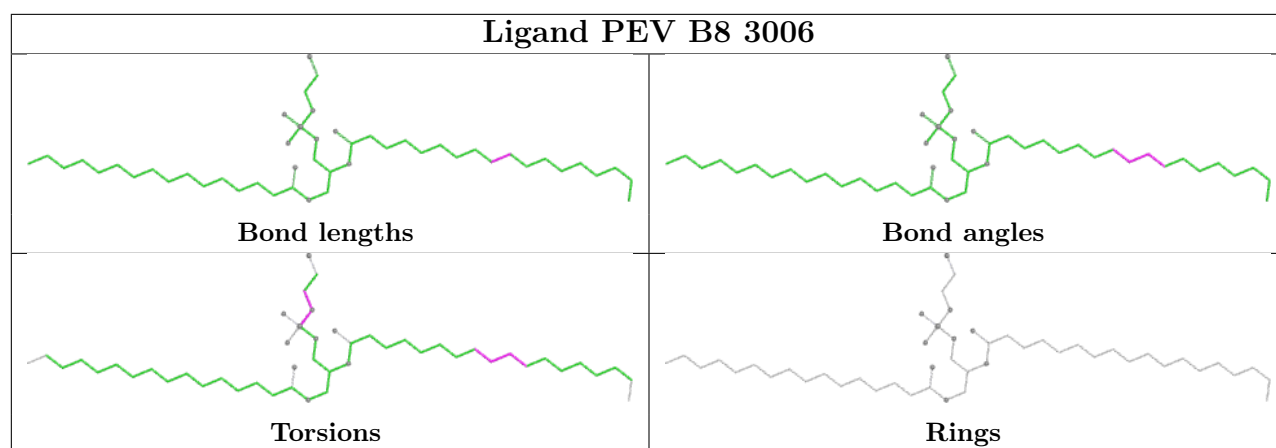


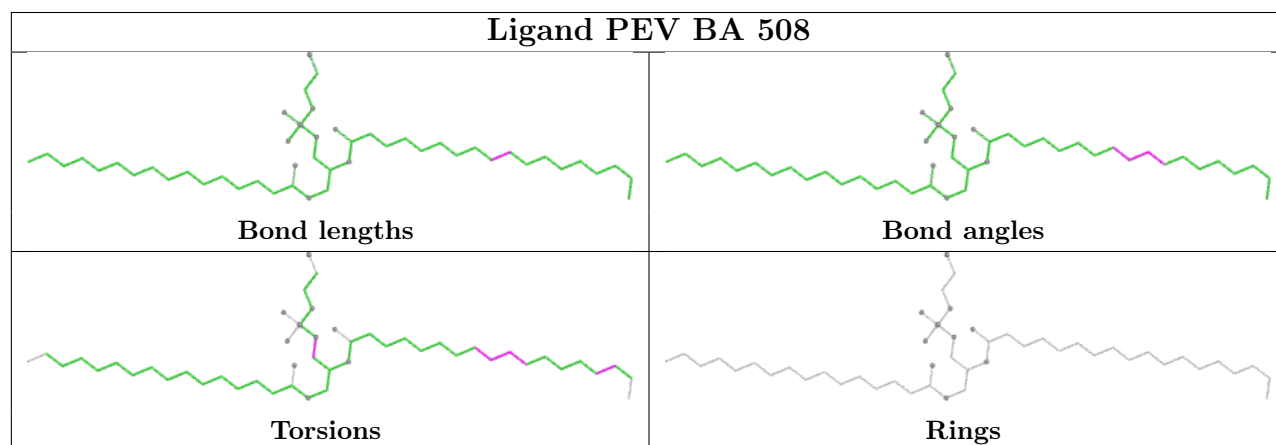
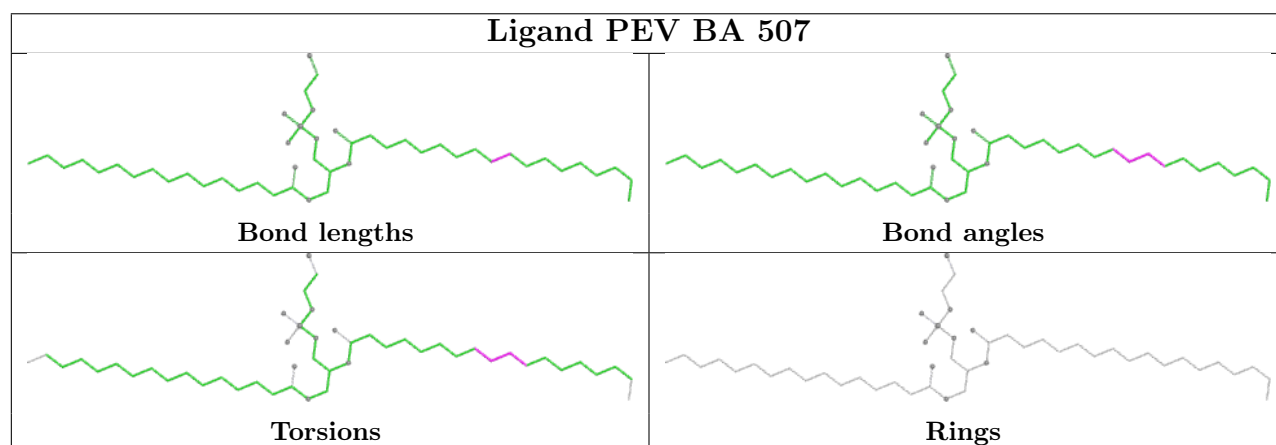
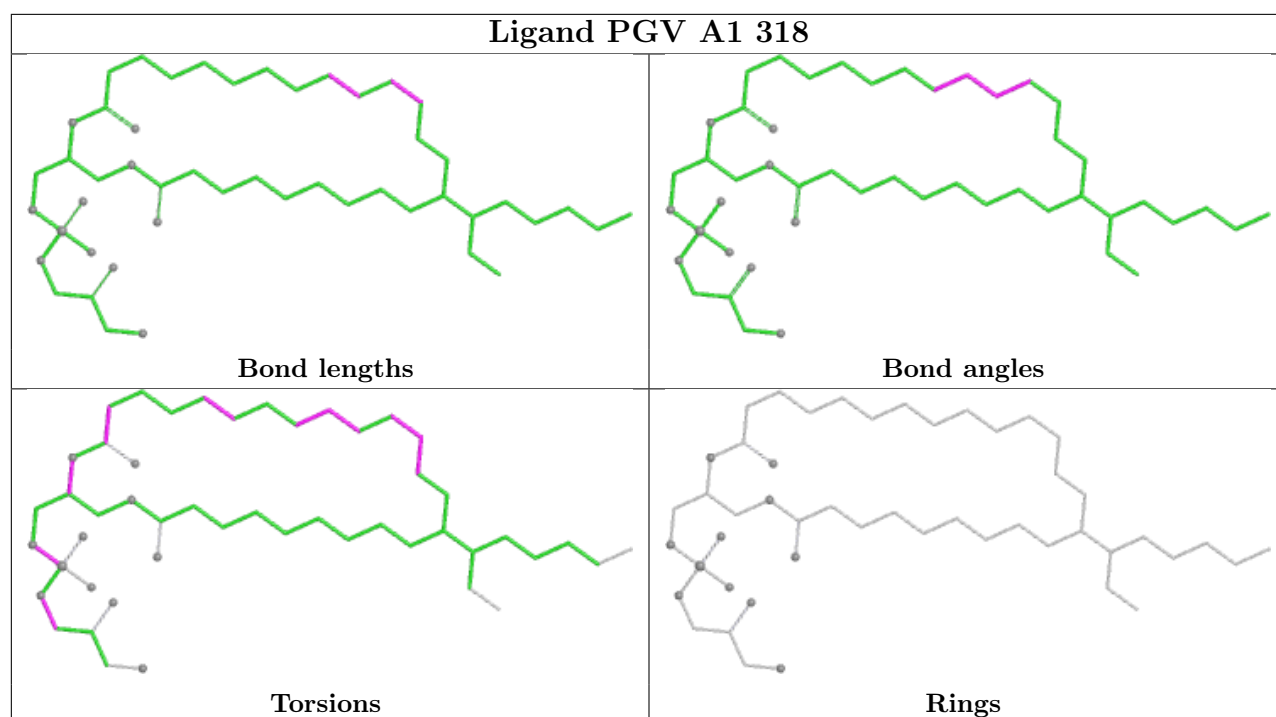
Ligand PEV BA 534	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PEV BA 504	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PEV A0 314	
 Bond lengths	 Bond angles
 Torsions	 Rings

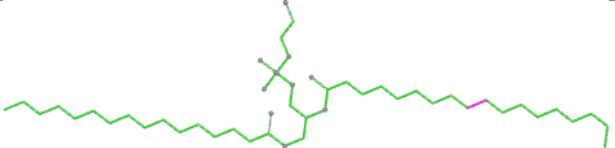
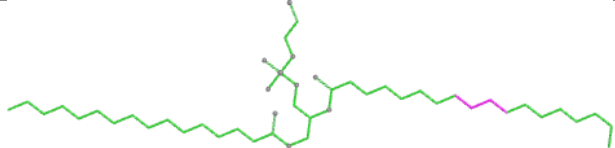
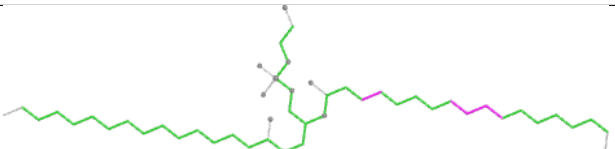
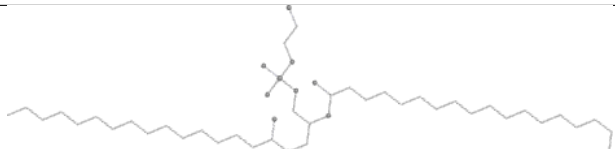
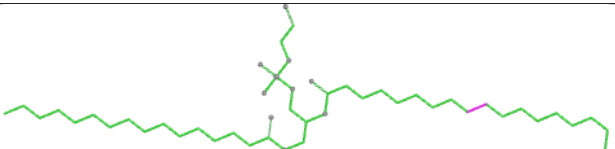
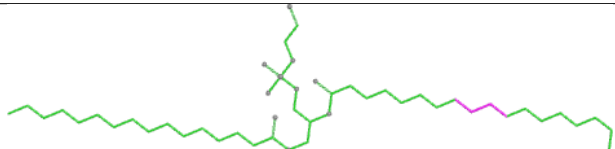
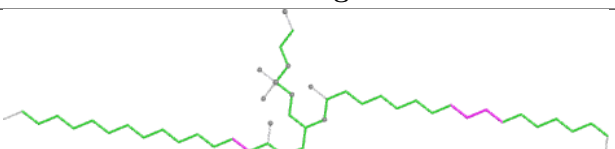
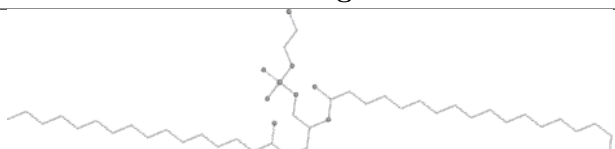
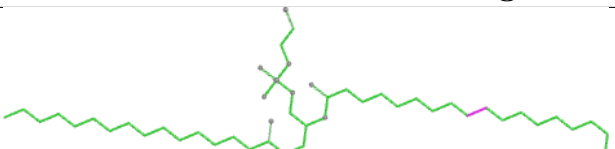
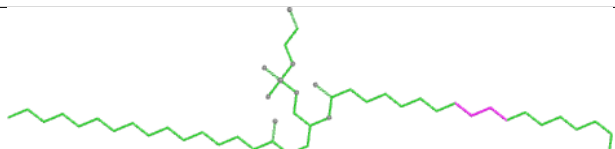
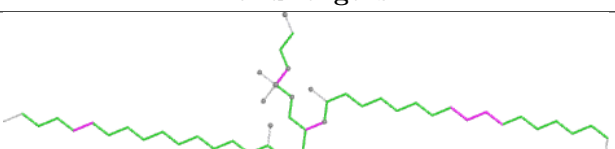
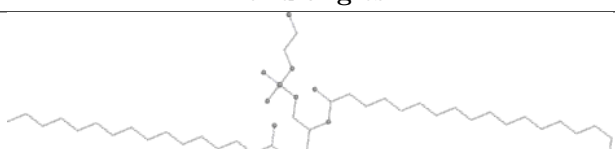


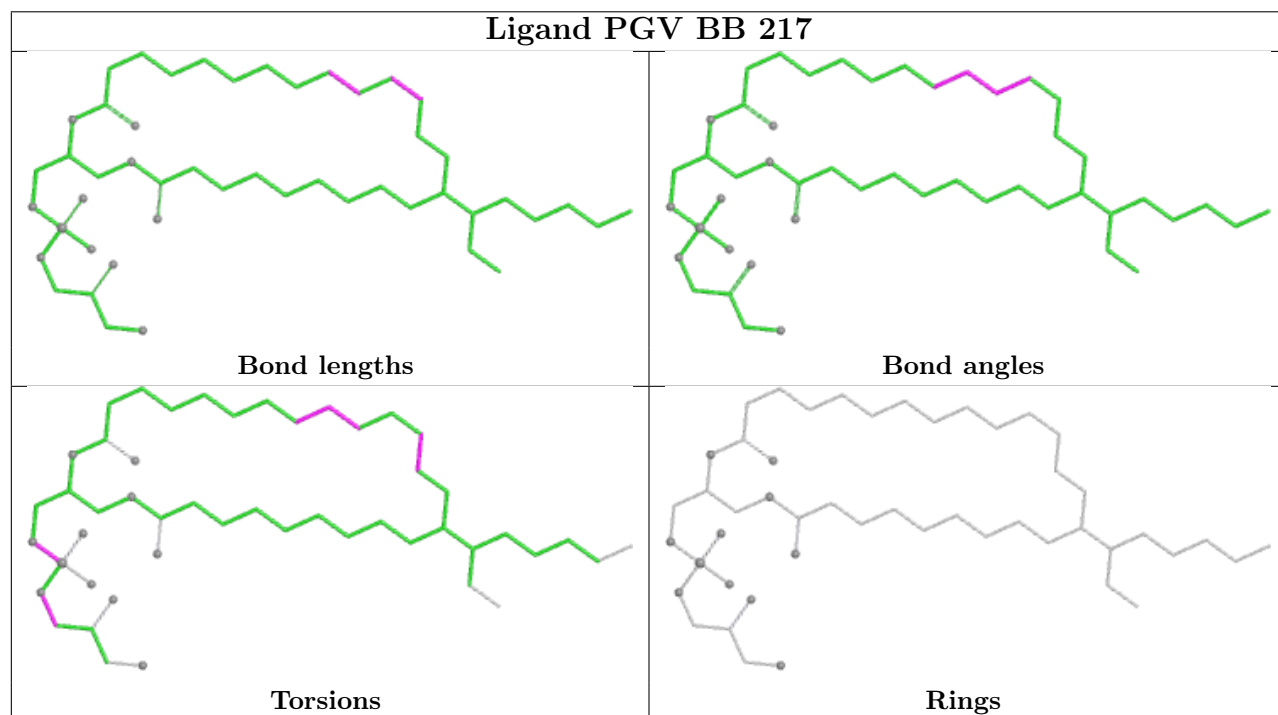
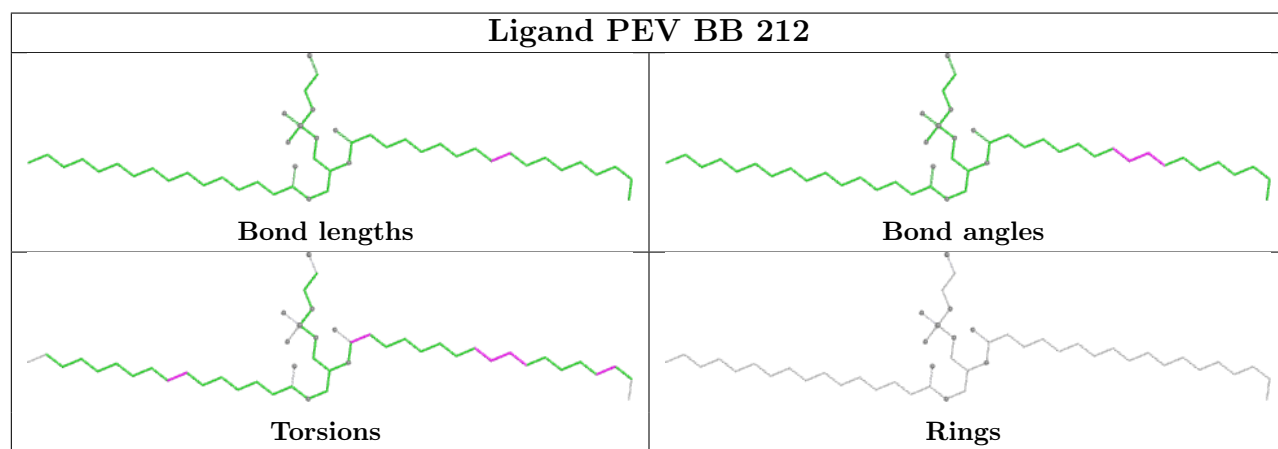
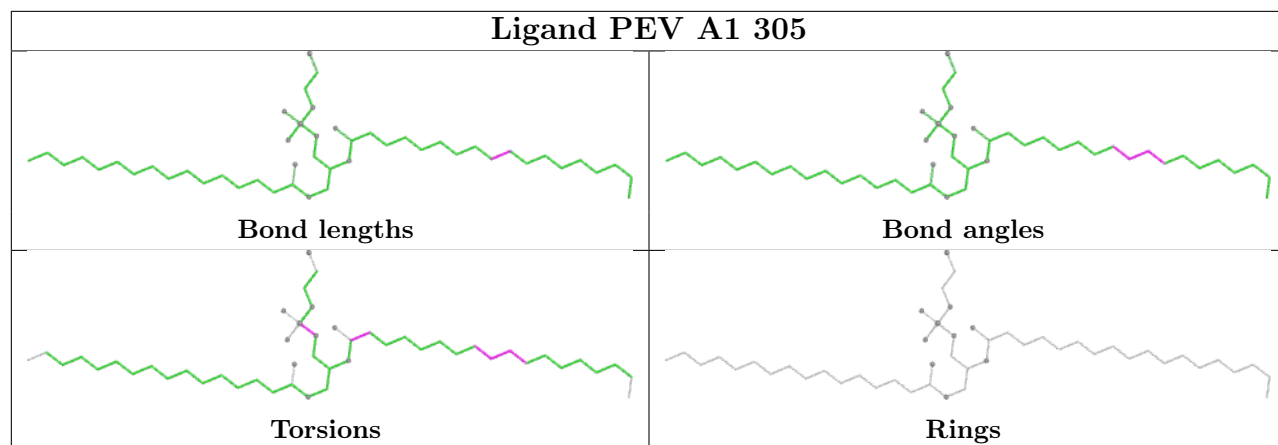


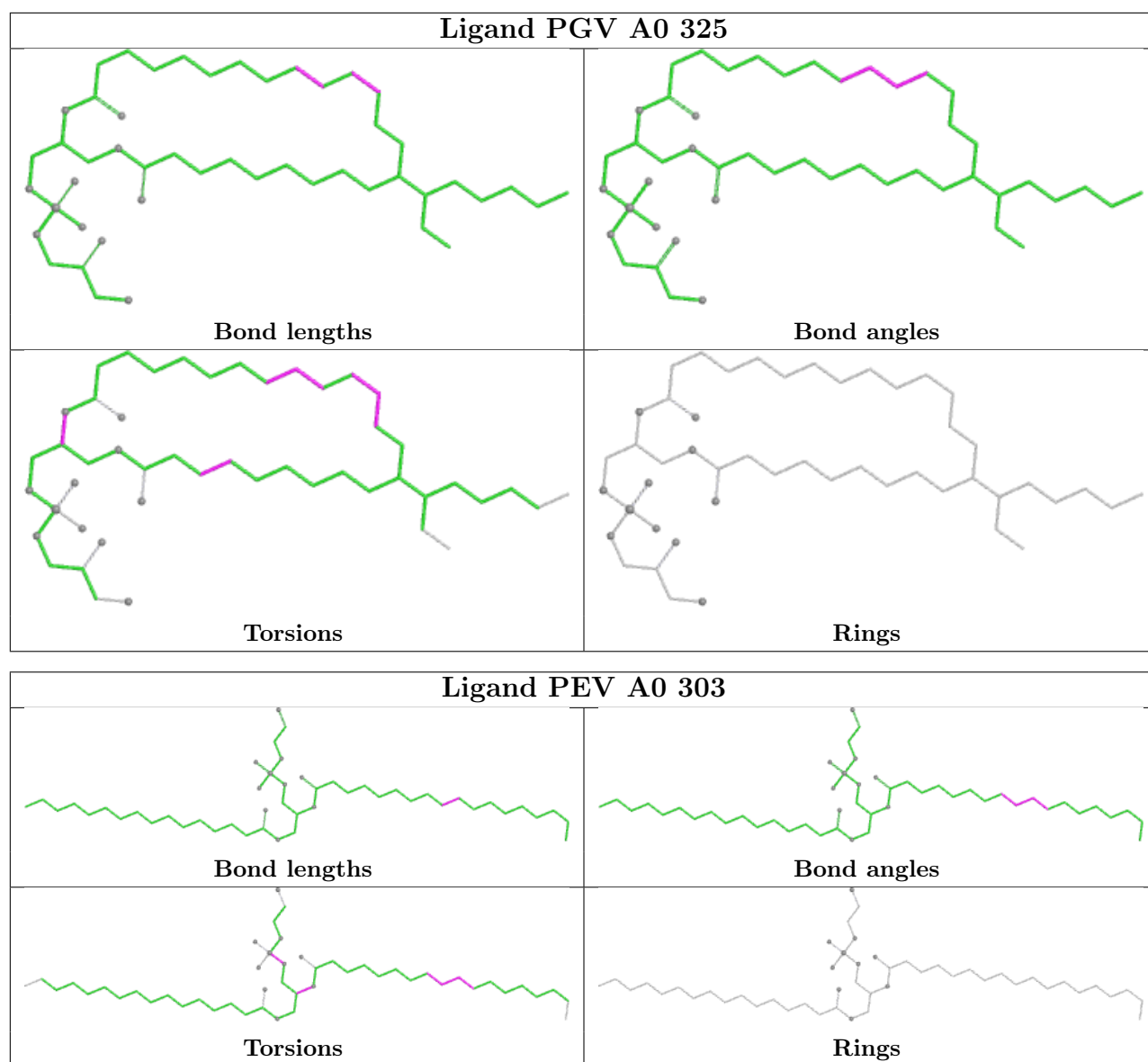


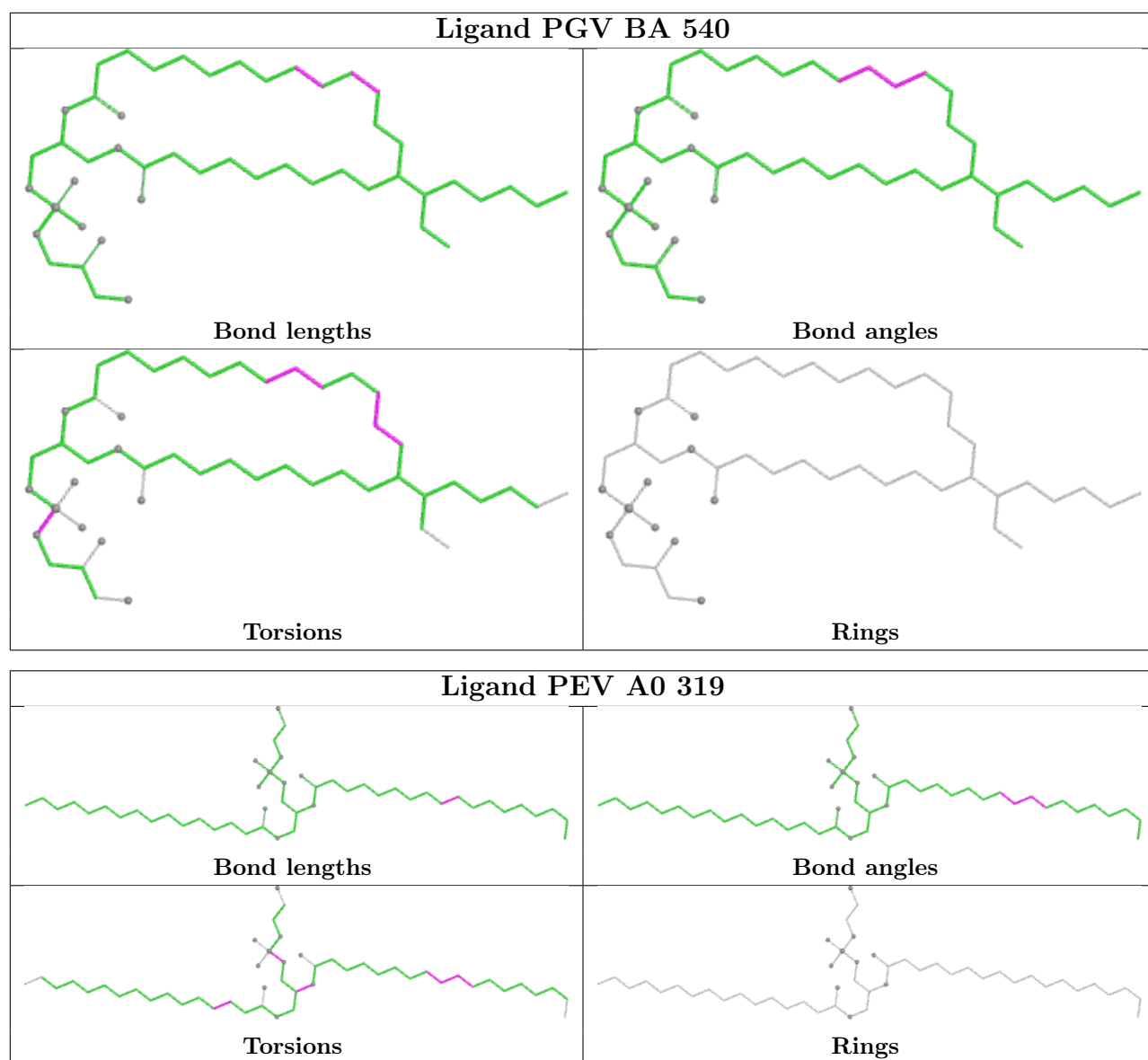


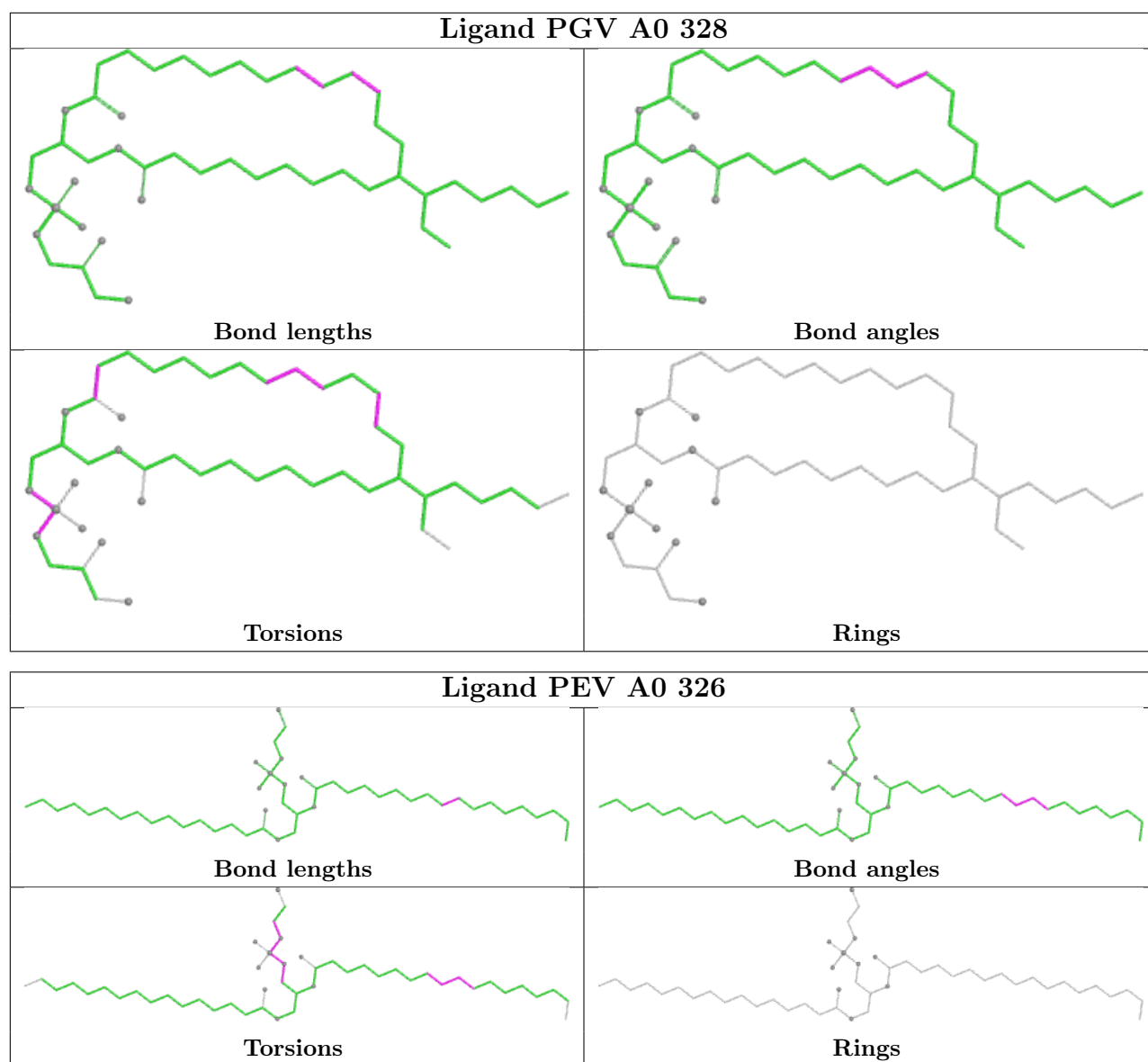


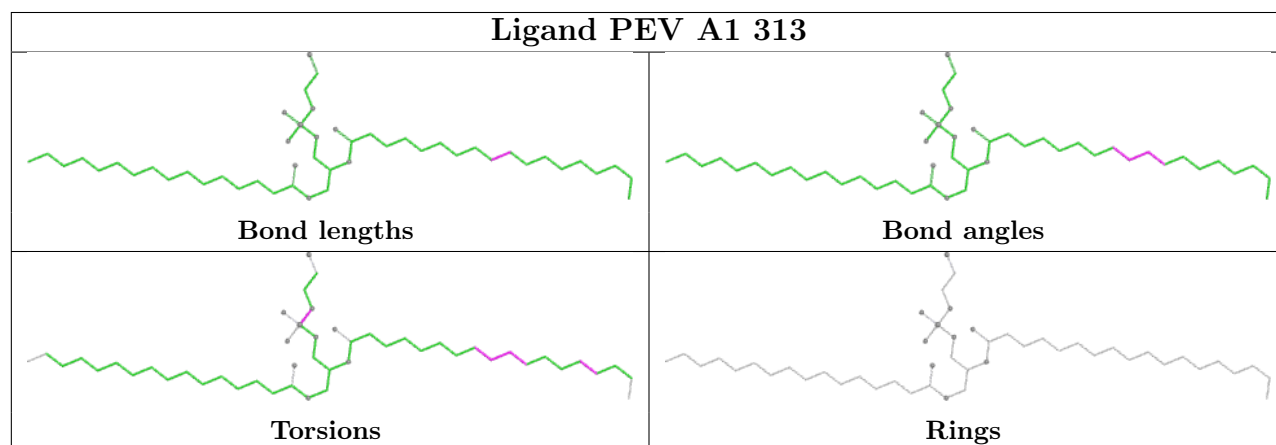
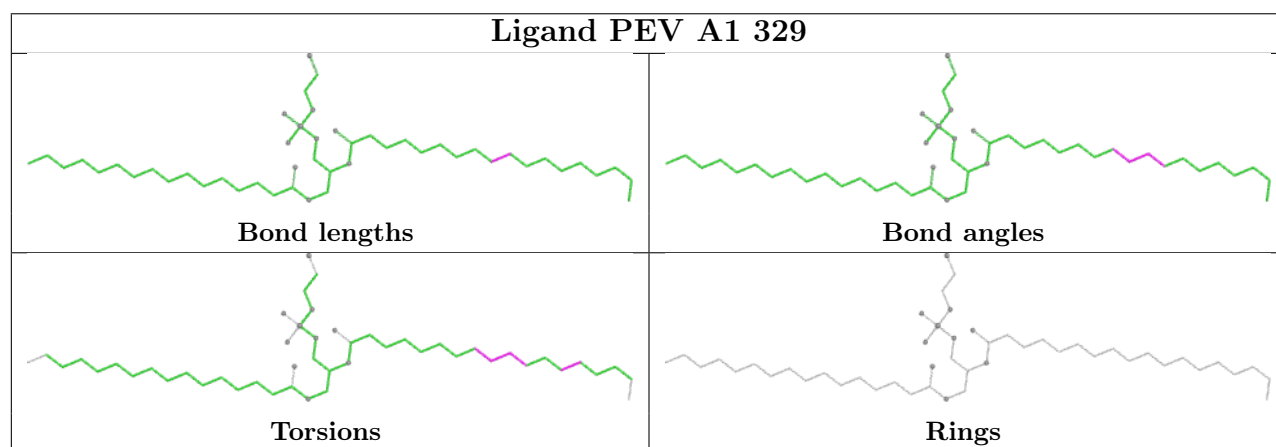
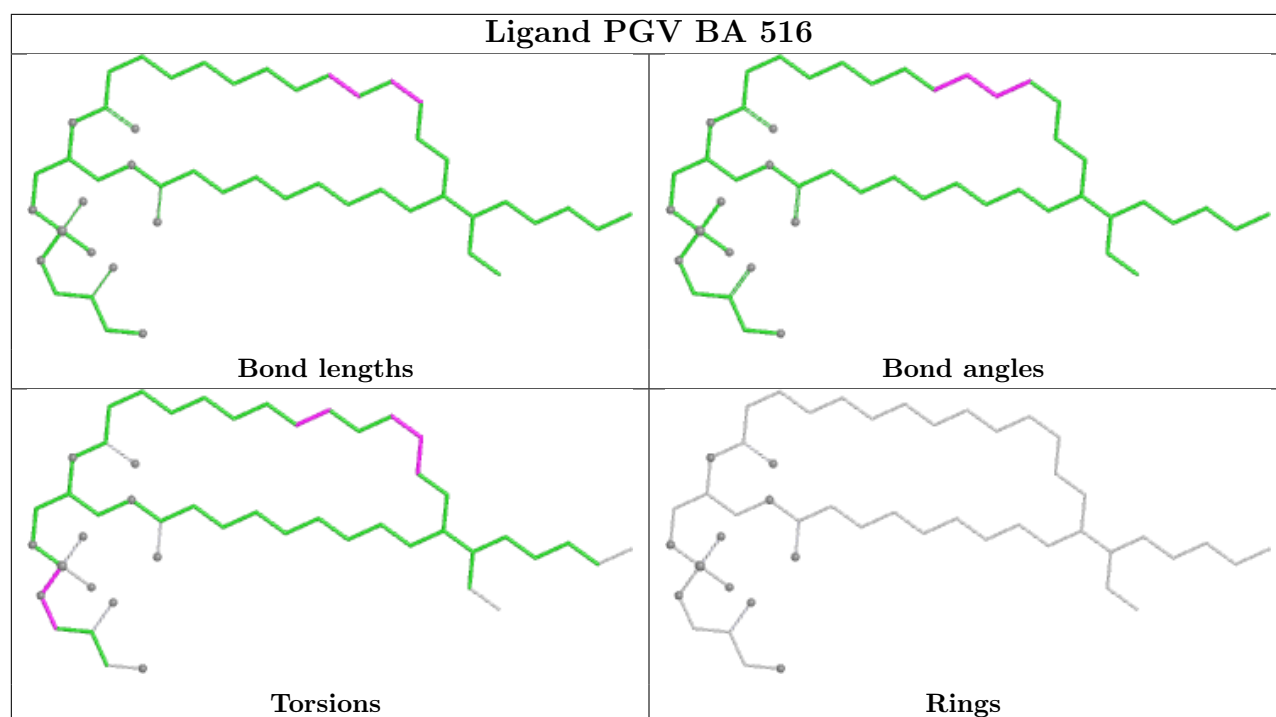
Ligand PEV BA 517	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PEV A1 307	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PEV A0 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

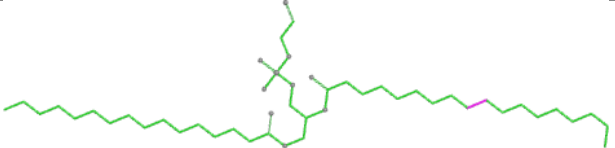
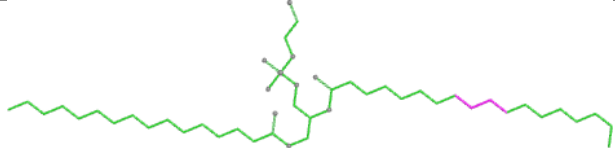
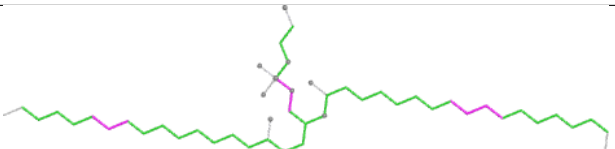
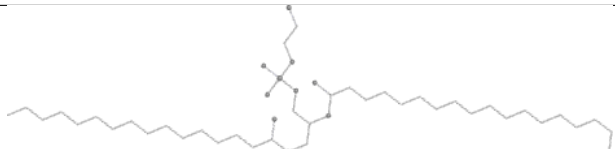
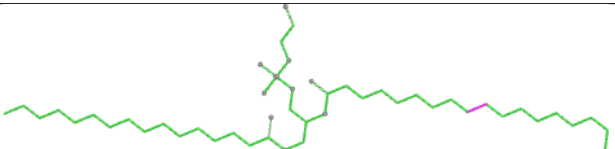
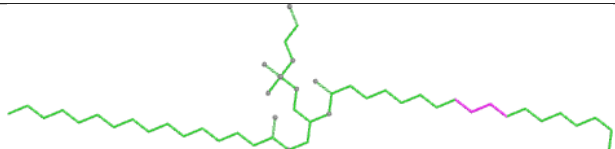
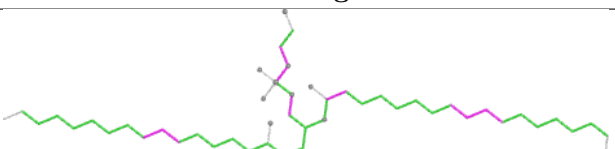
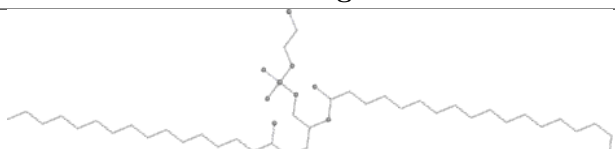
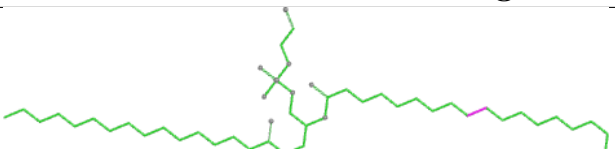
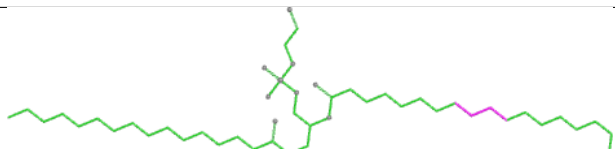
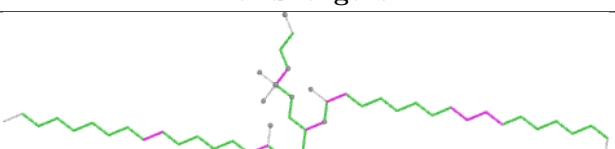
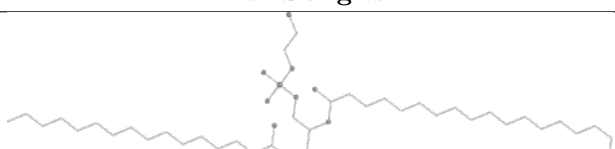


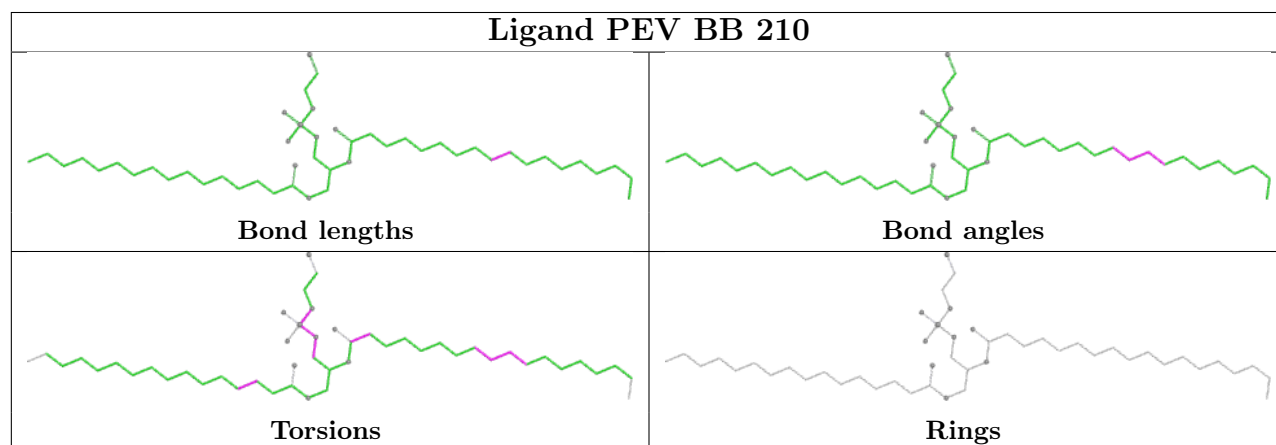
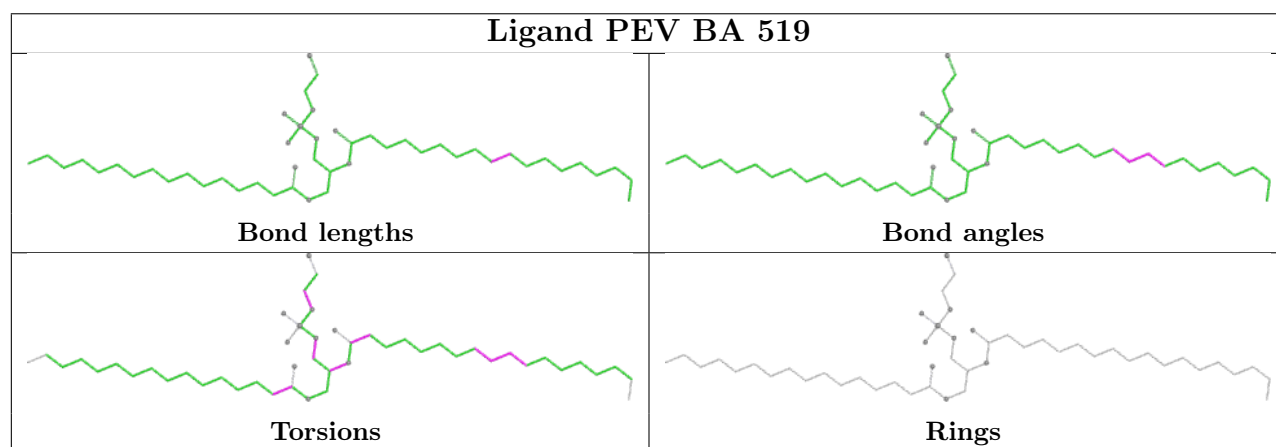
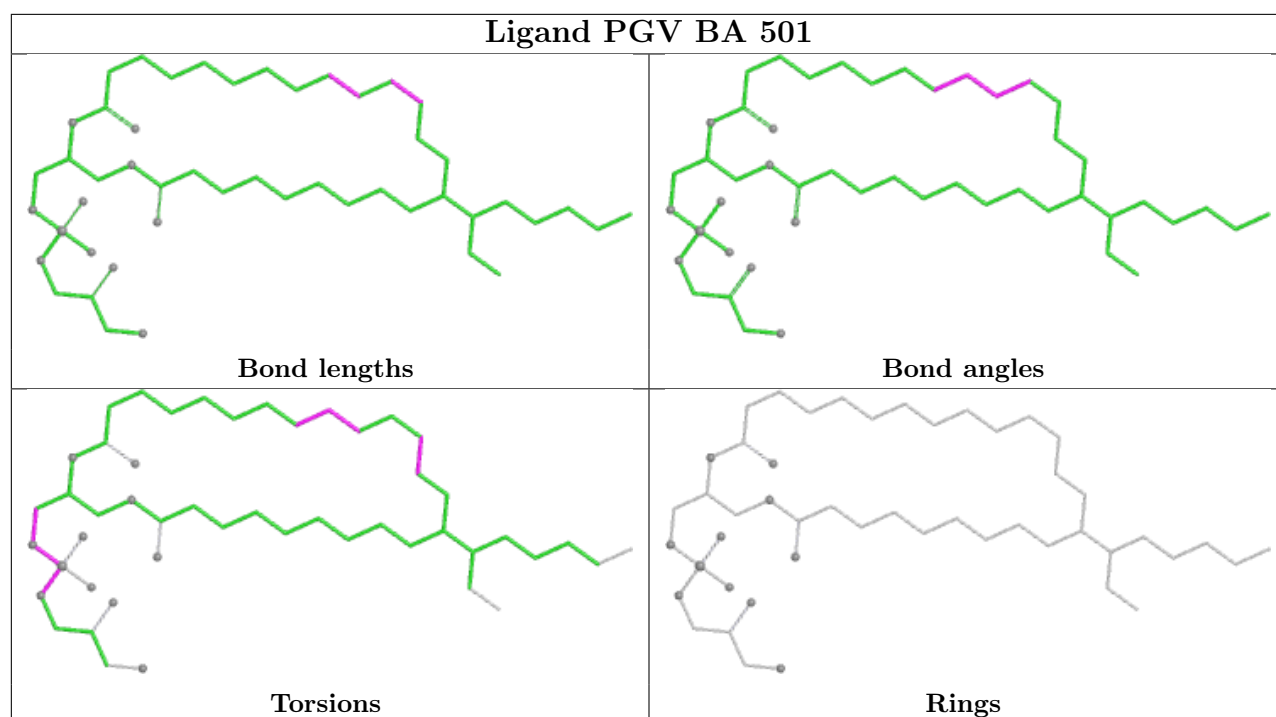


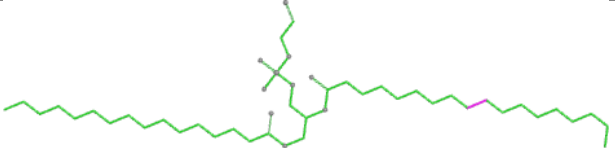
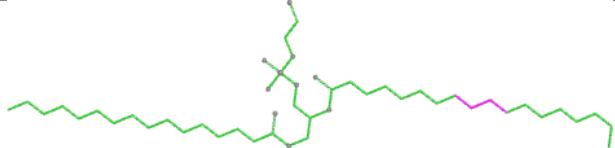
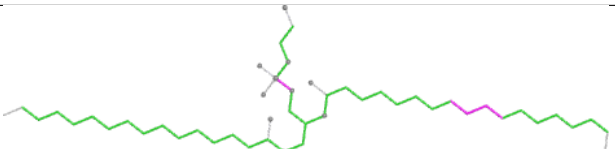
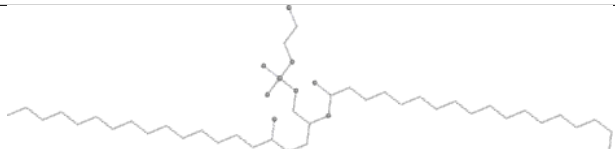
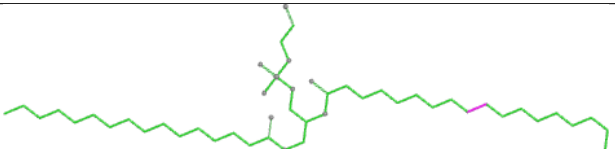
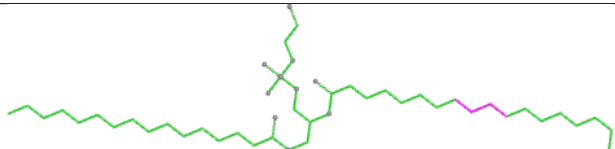
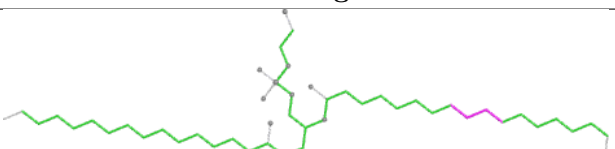
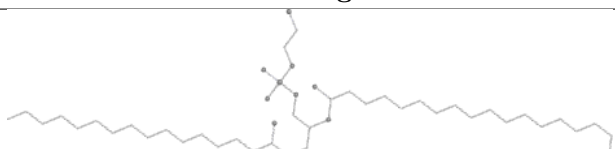
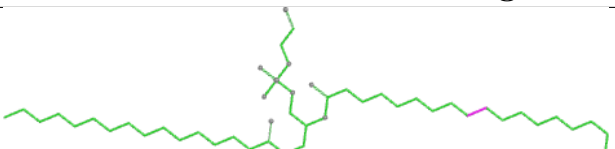
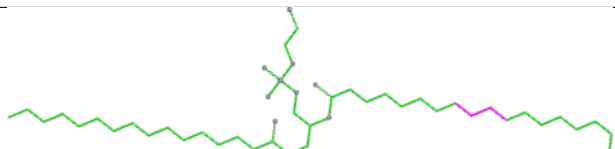
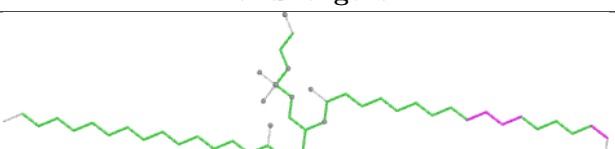
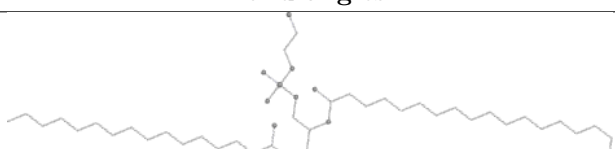


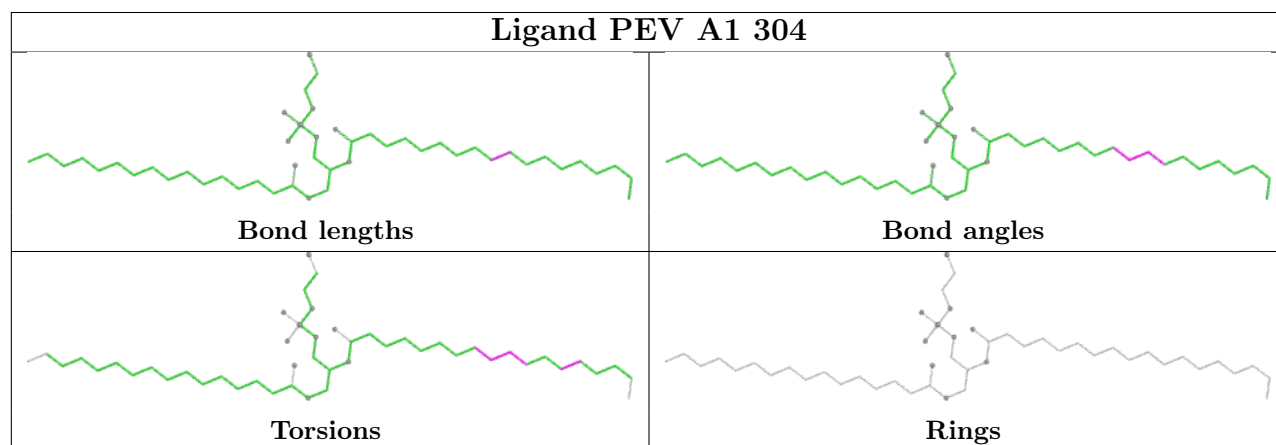
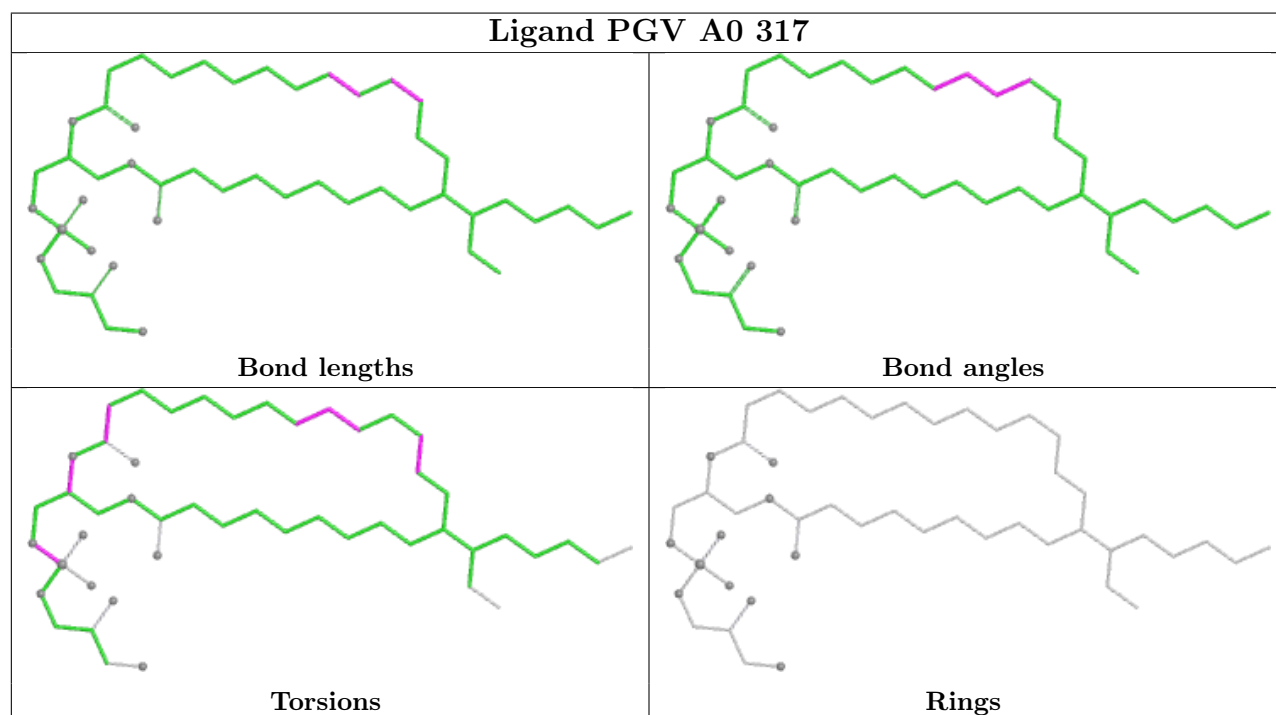
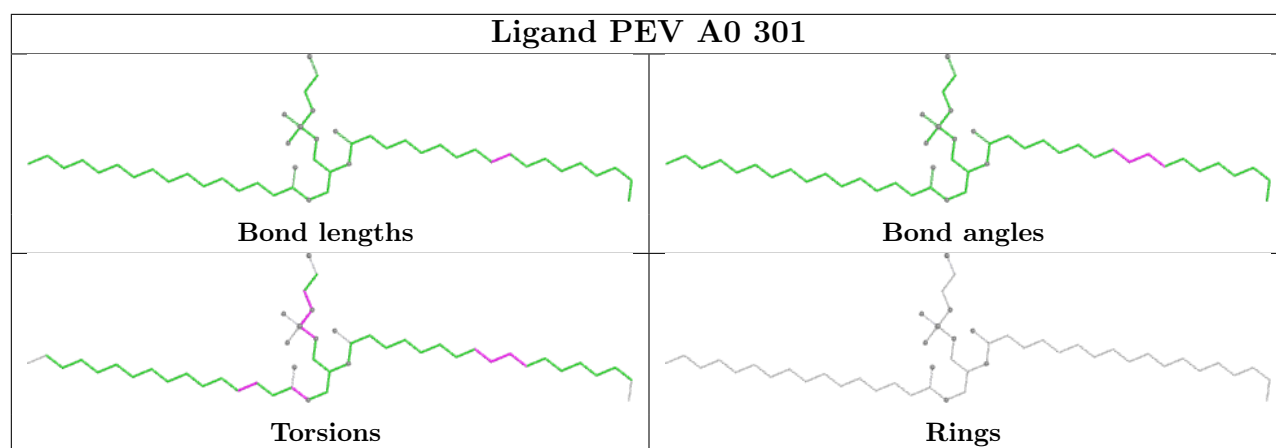


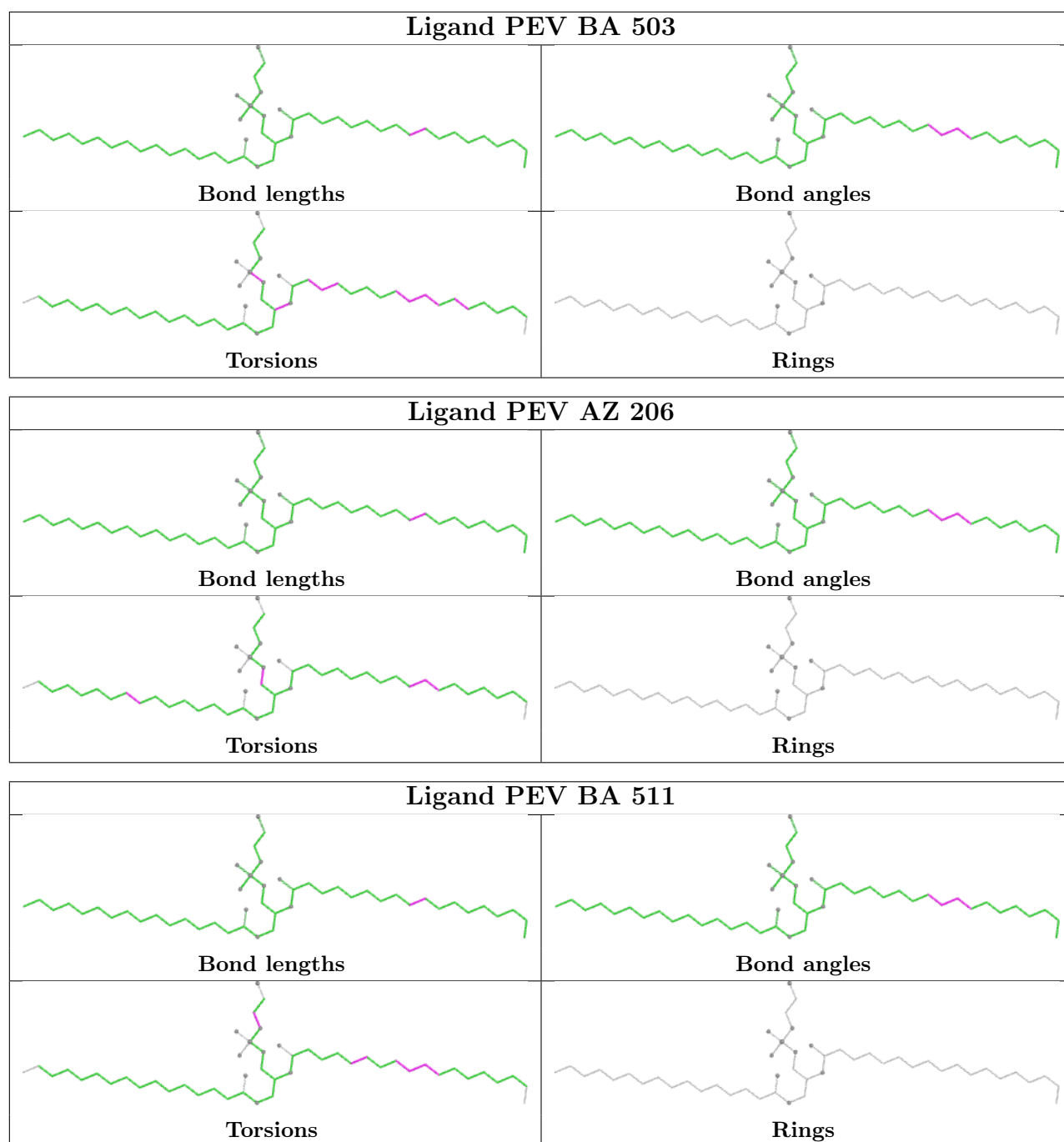


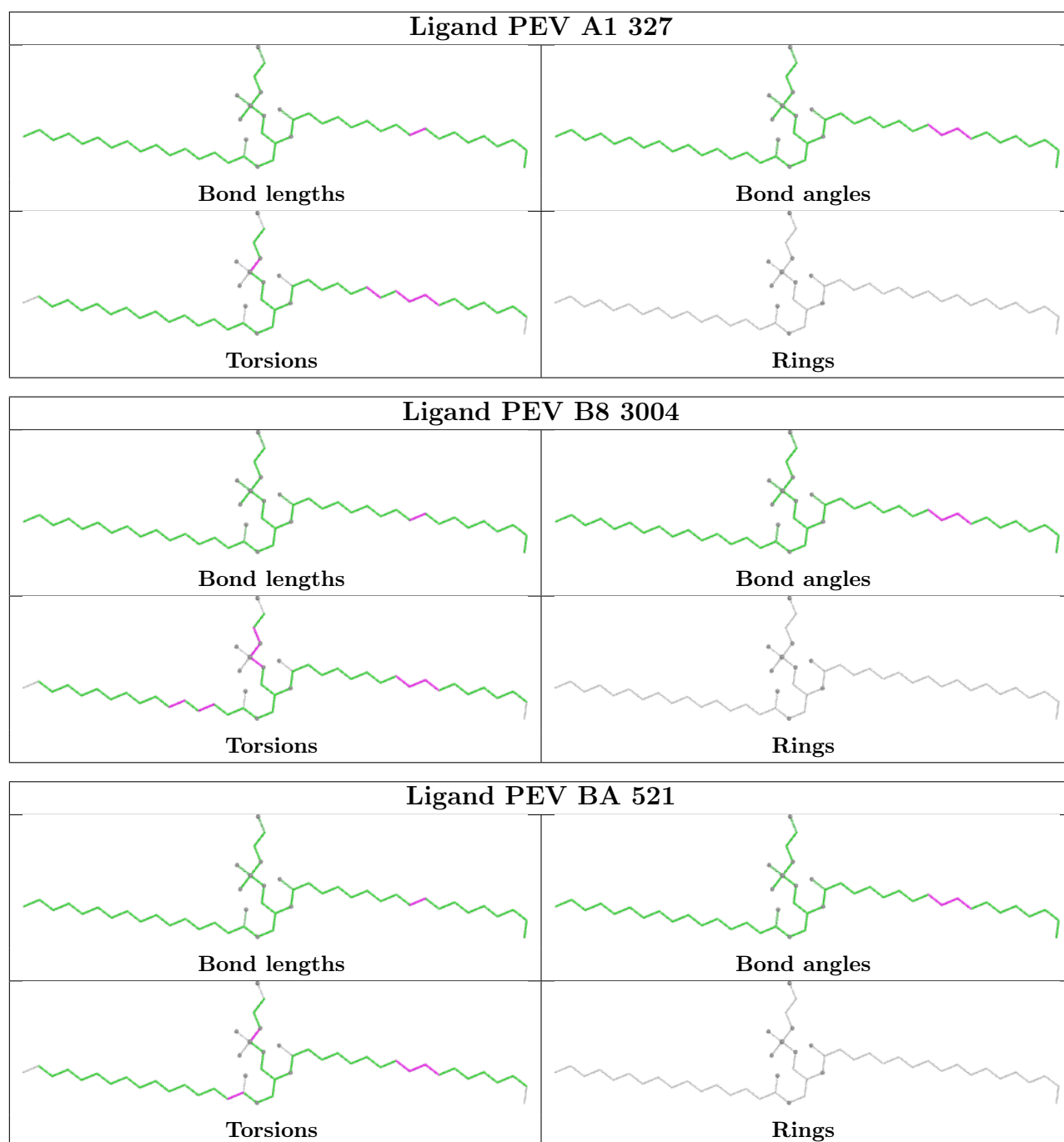
Ligand PEV BA 502	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PEV BA 530	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PEV BB 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

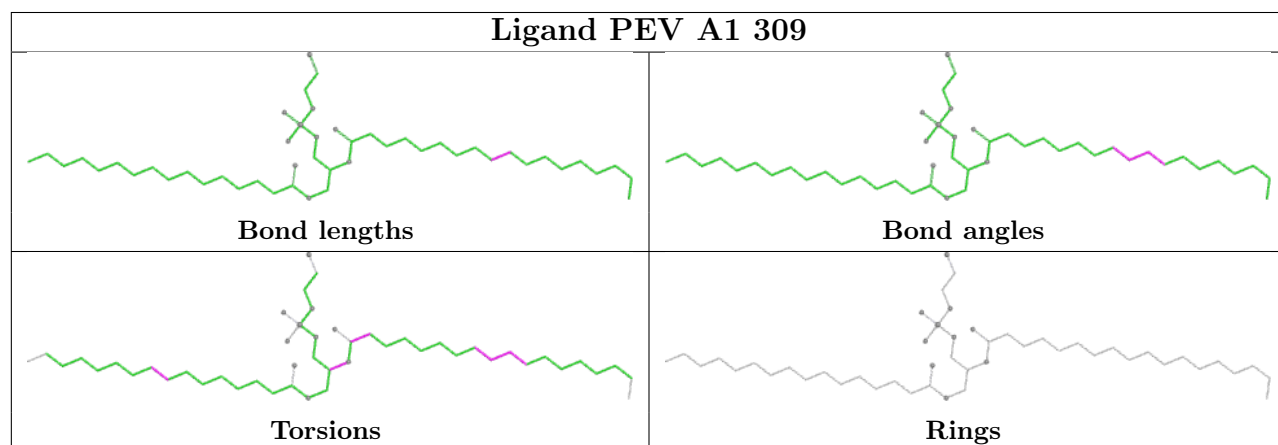
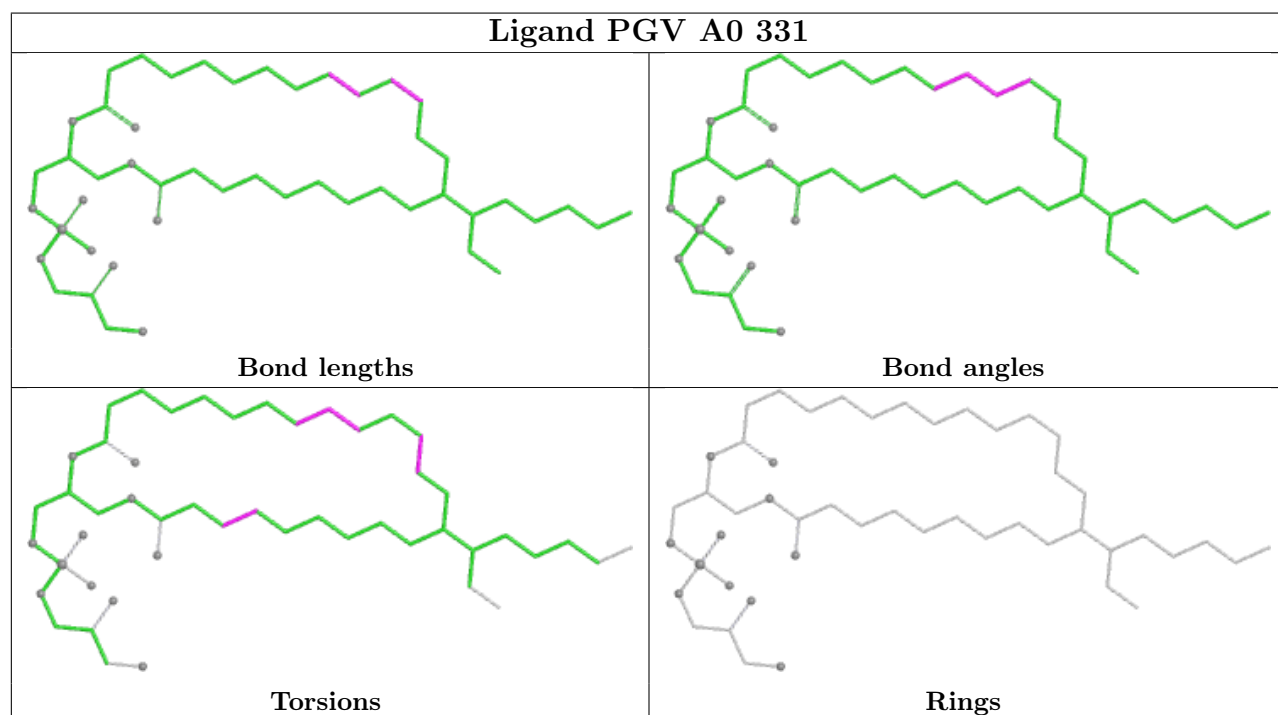
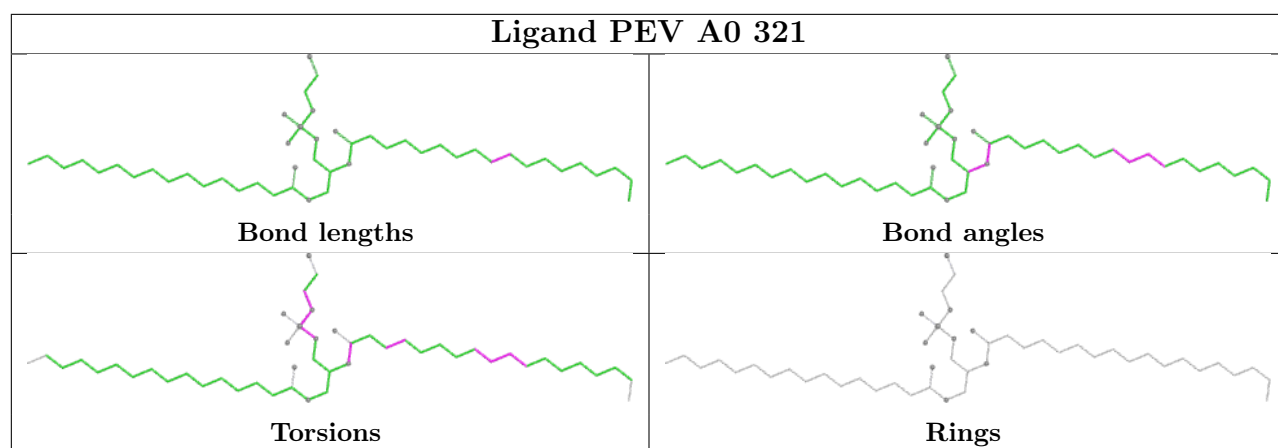


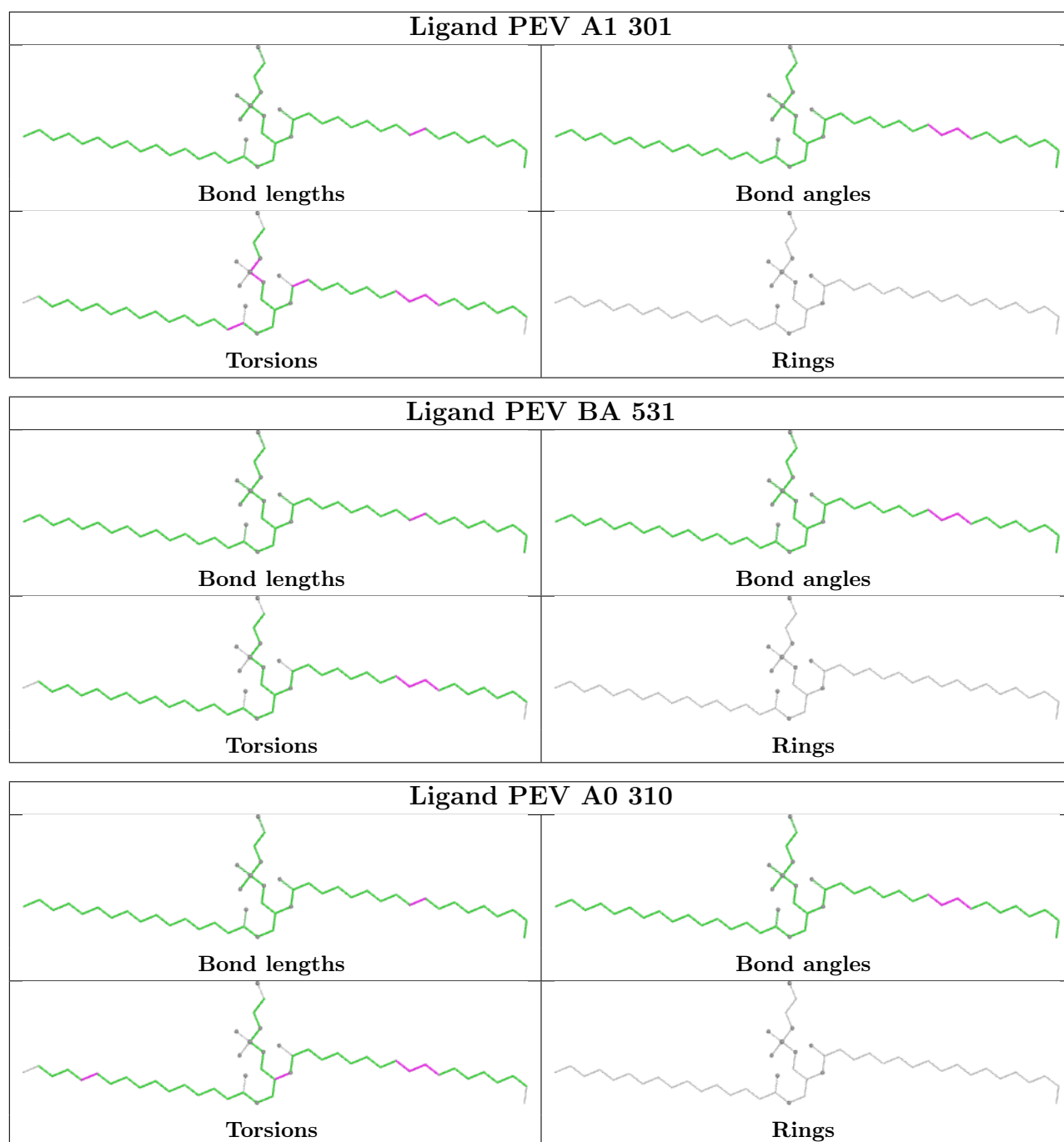
Ligand PEV A0 308	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PEV A1 323	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PEV A1 326	
 Bond lengths	 Bond angles
 Torsions	 Rings

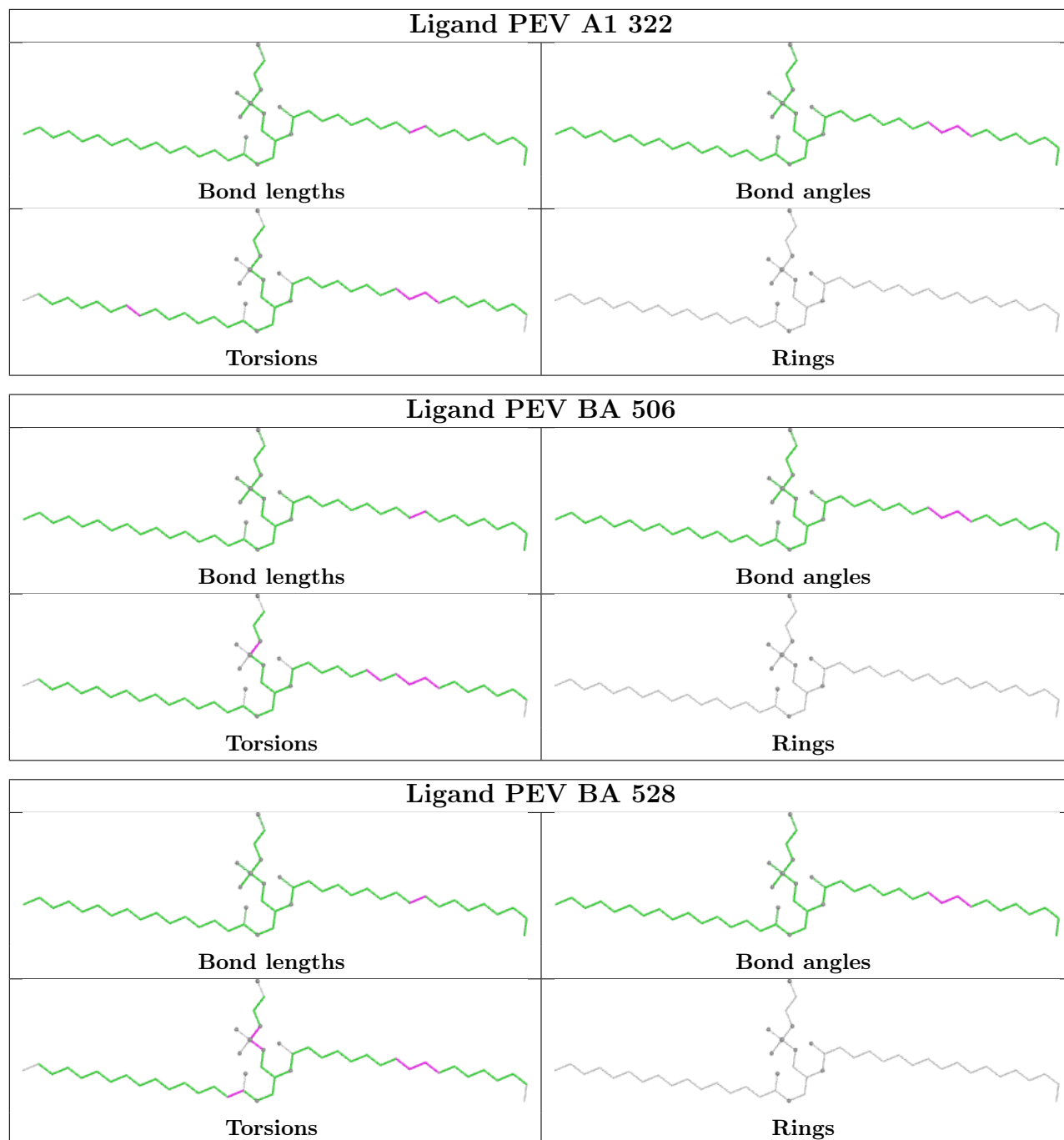


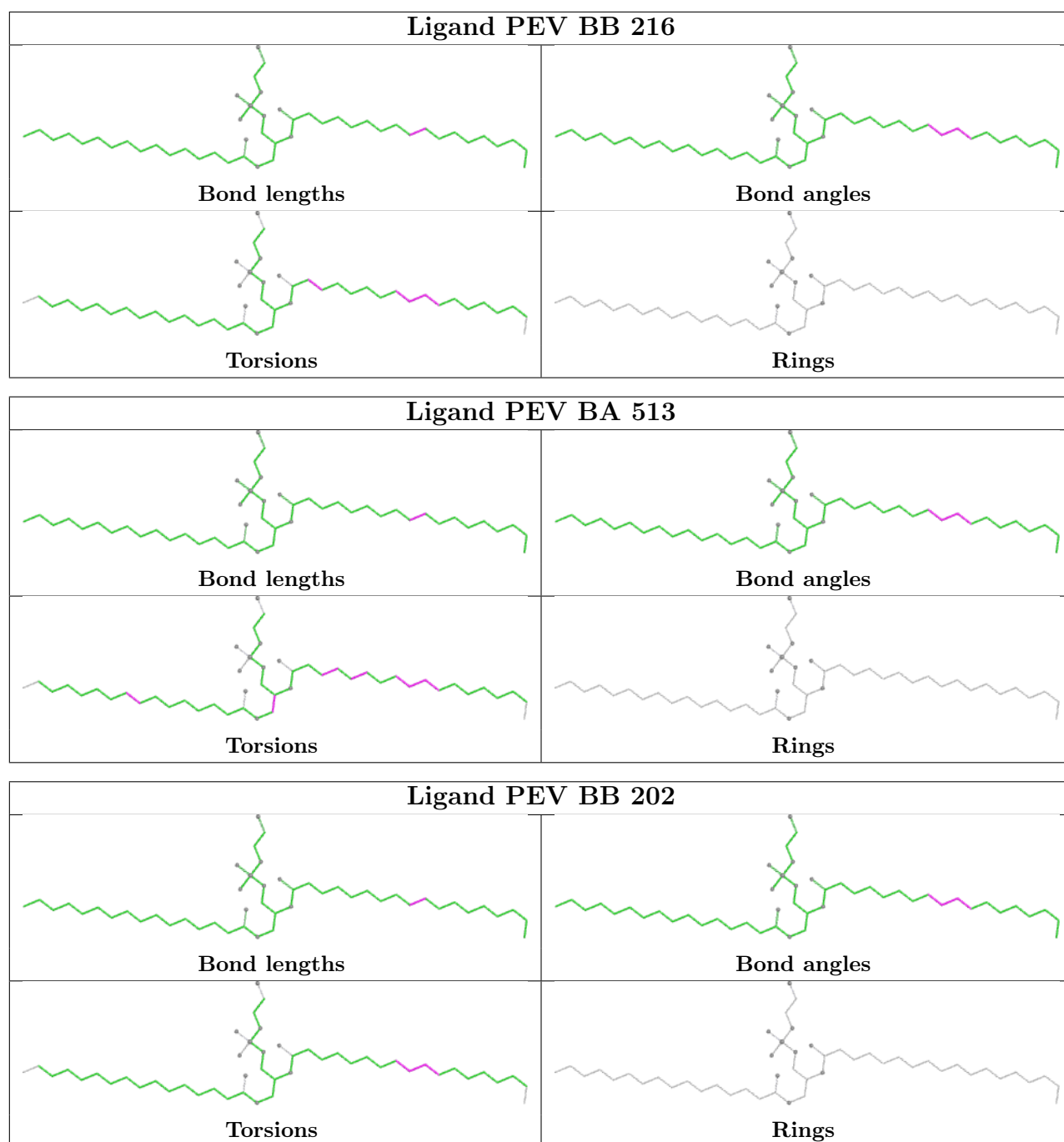


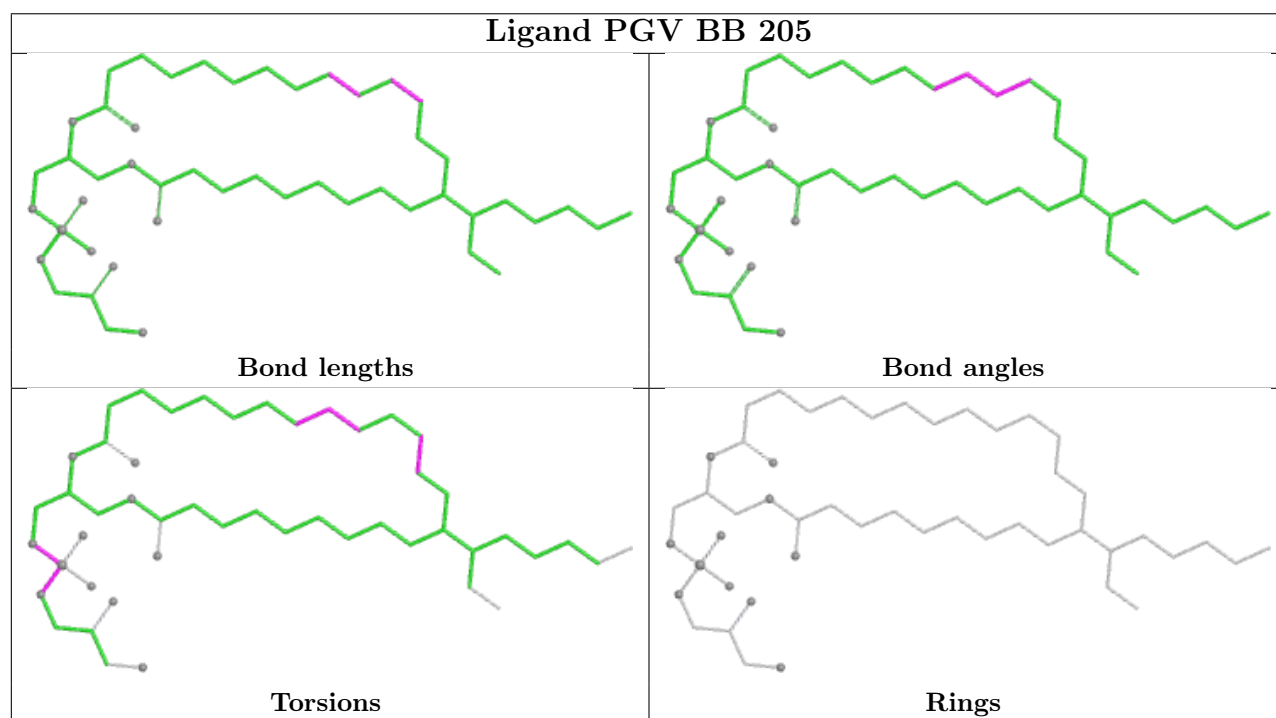
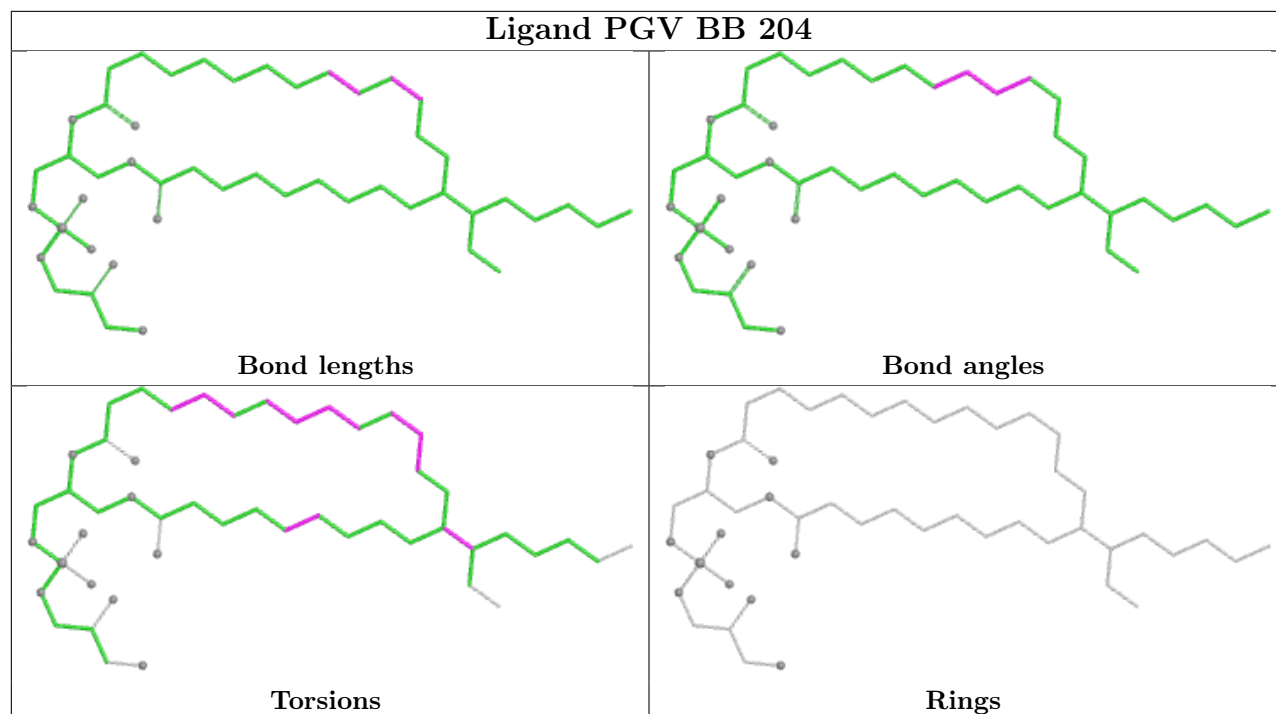


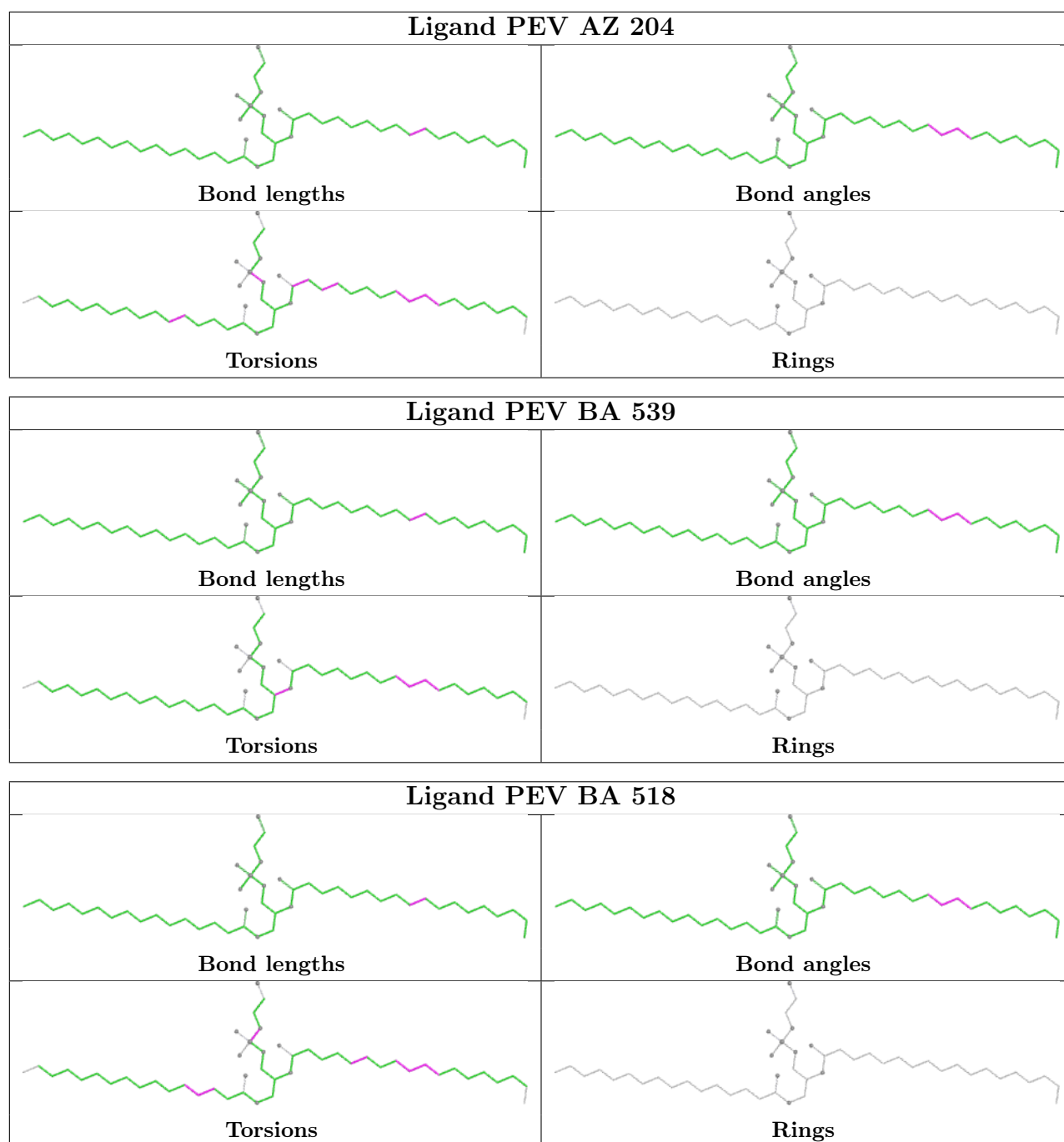


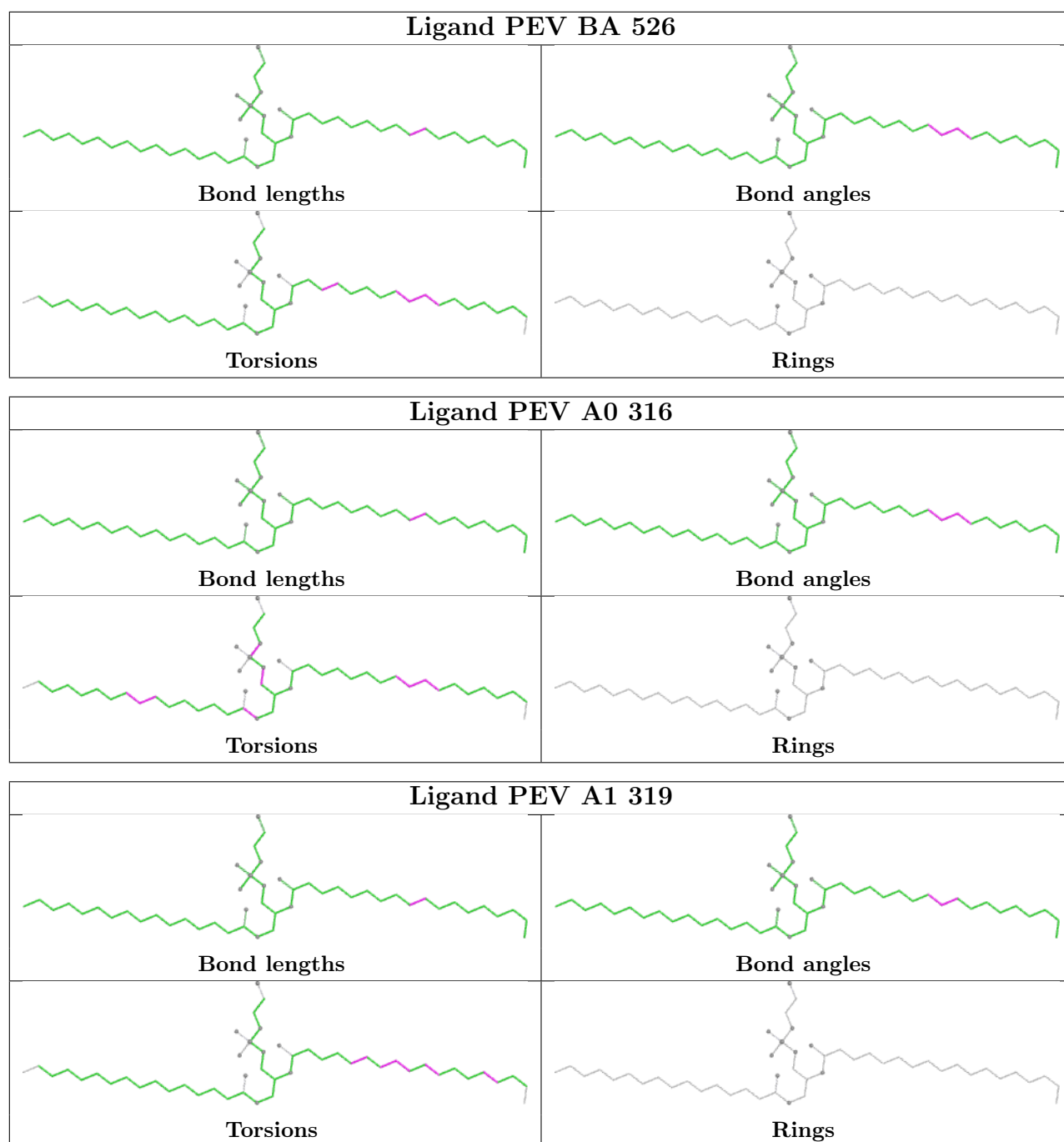


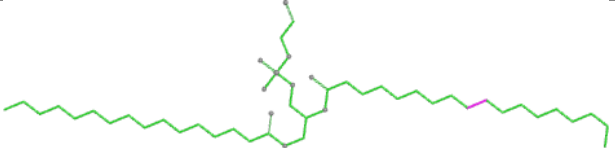
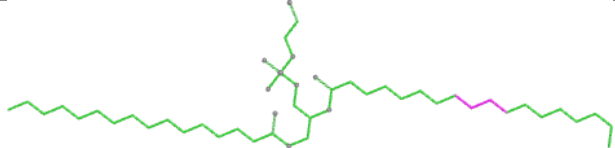
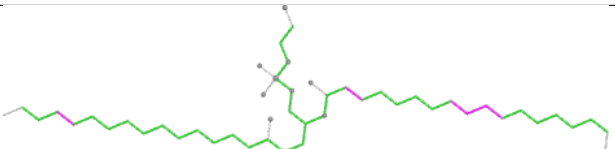
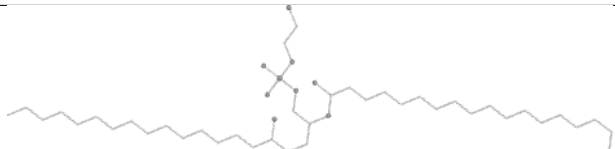
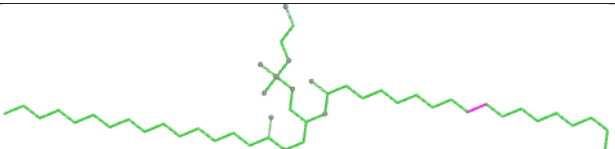
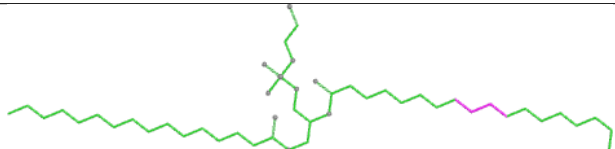
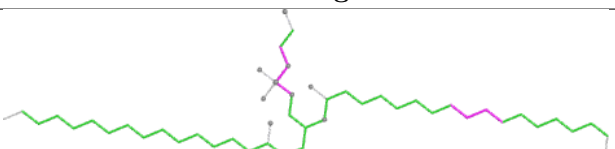
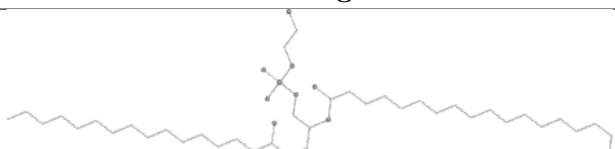
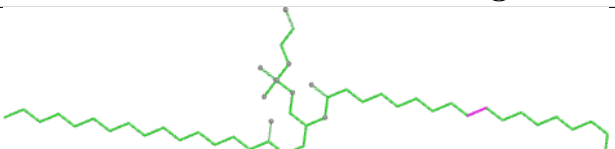
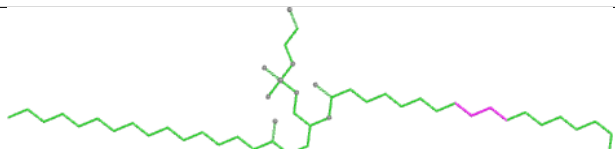
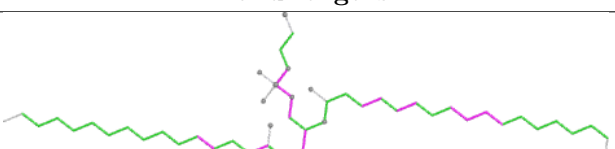
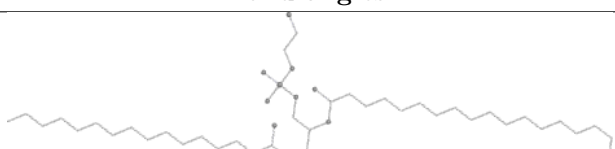


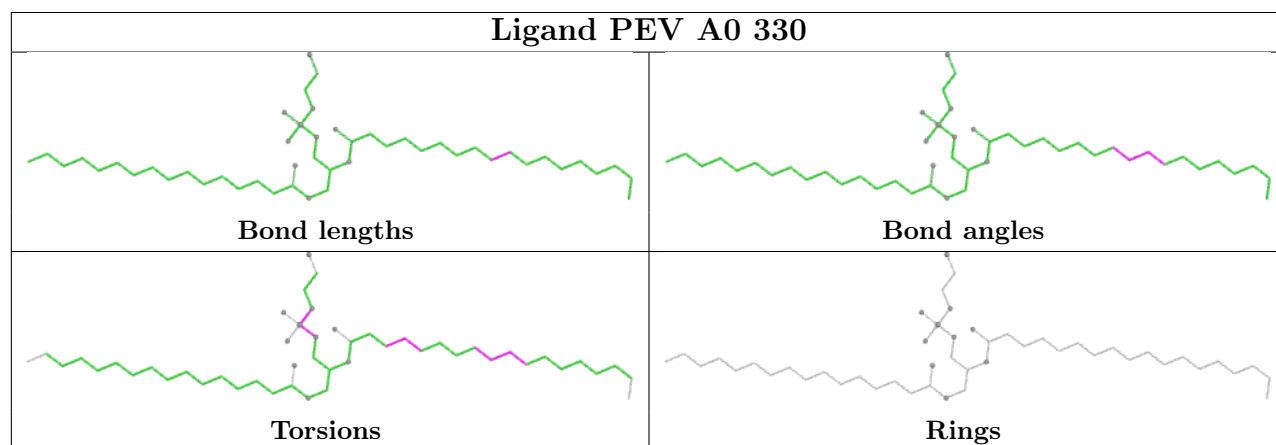
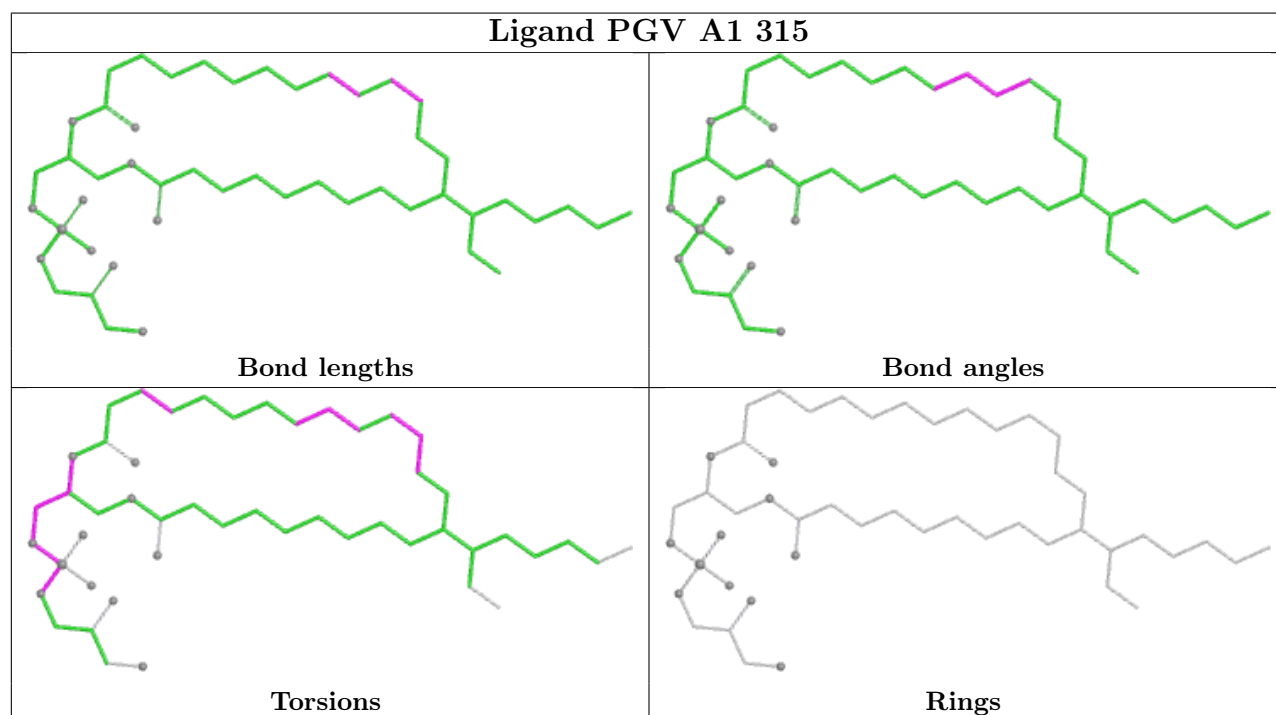
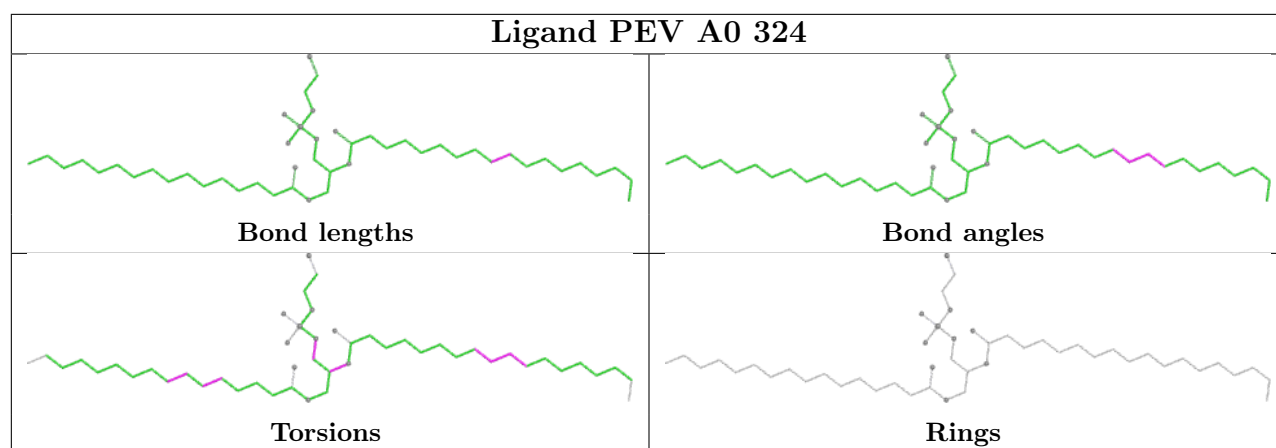


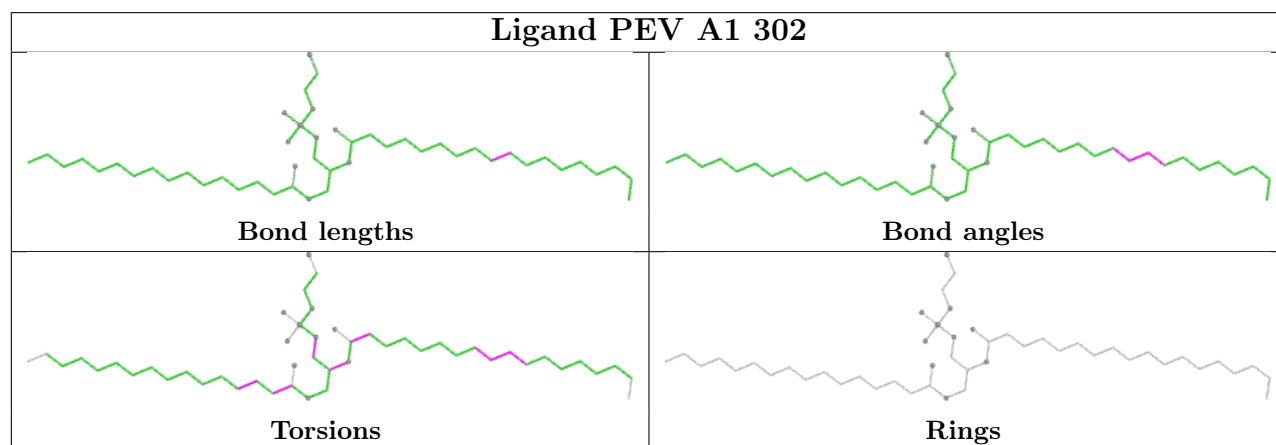
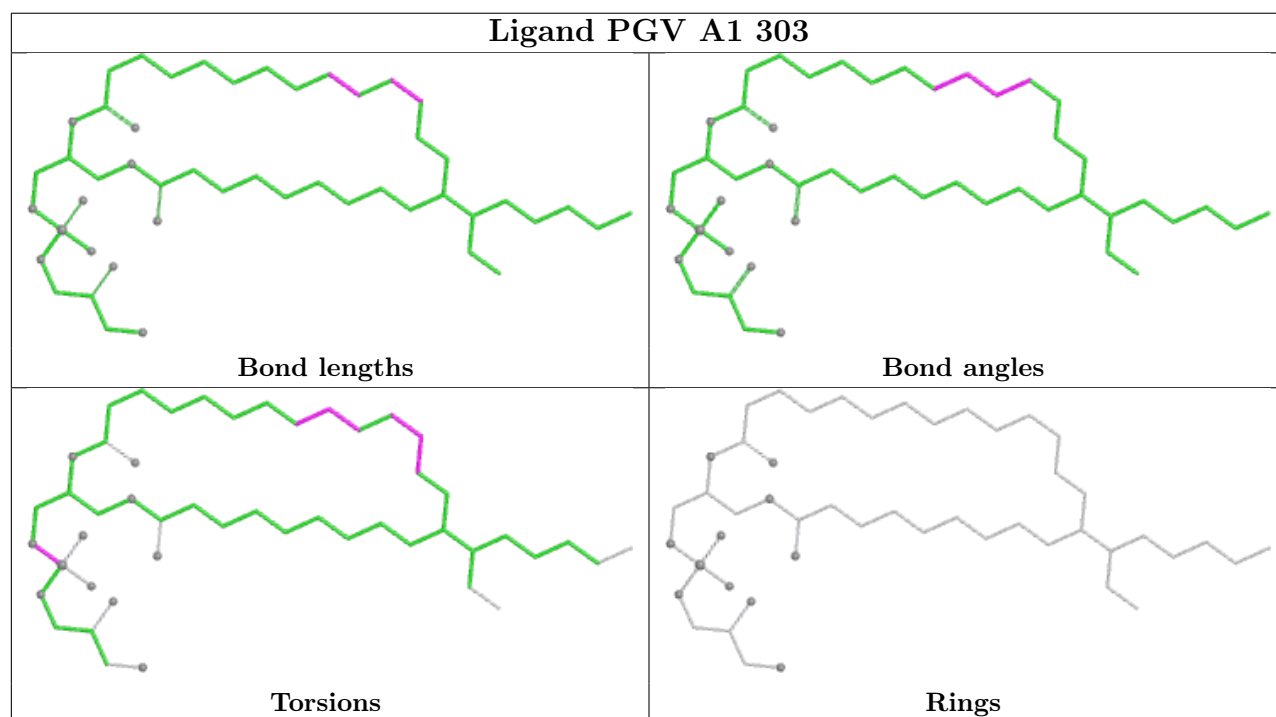
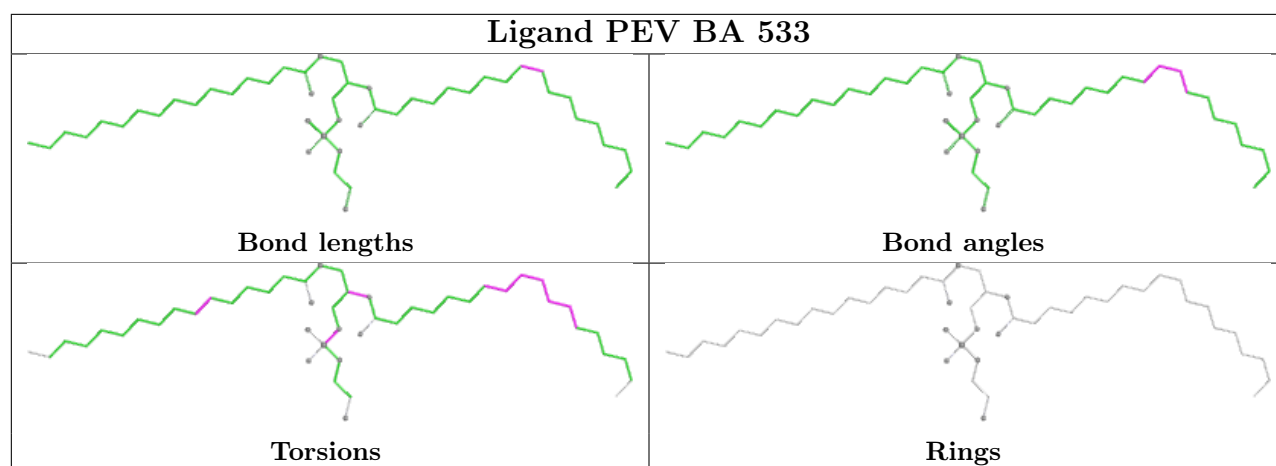


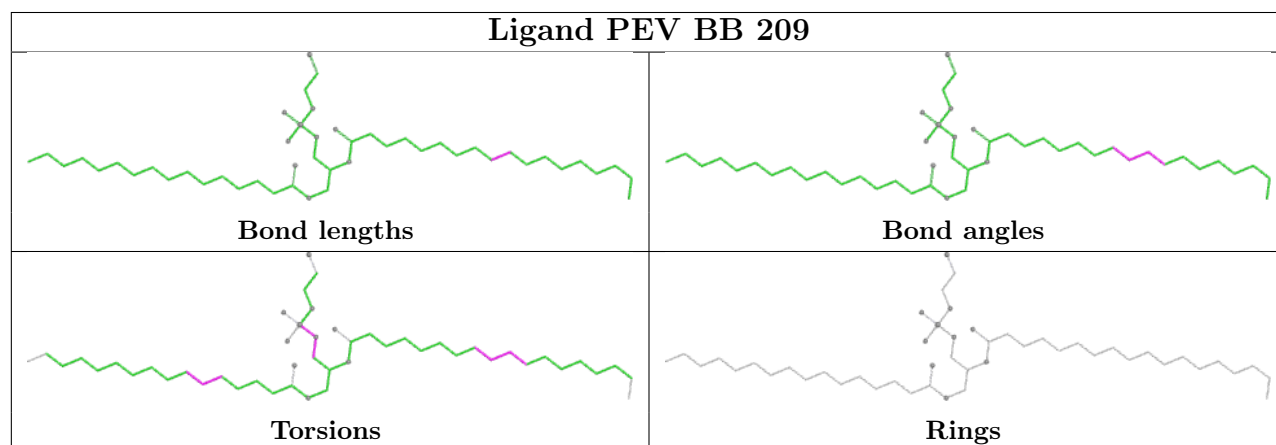
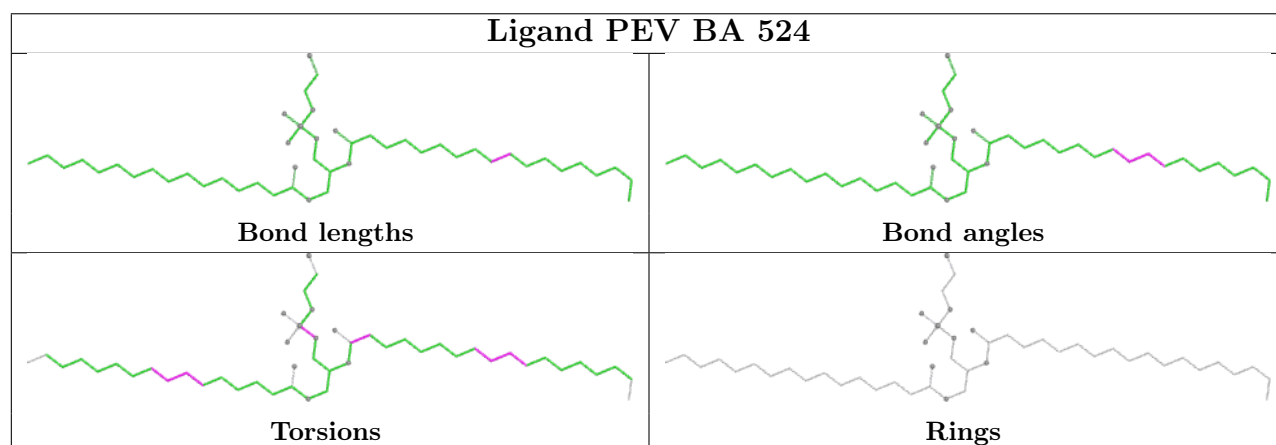
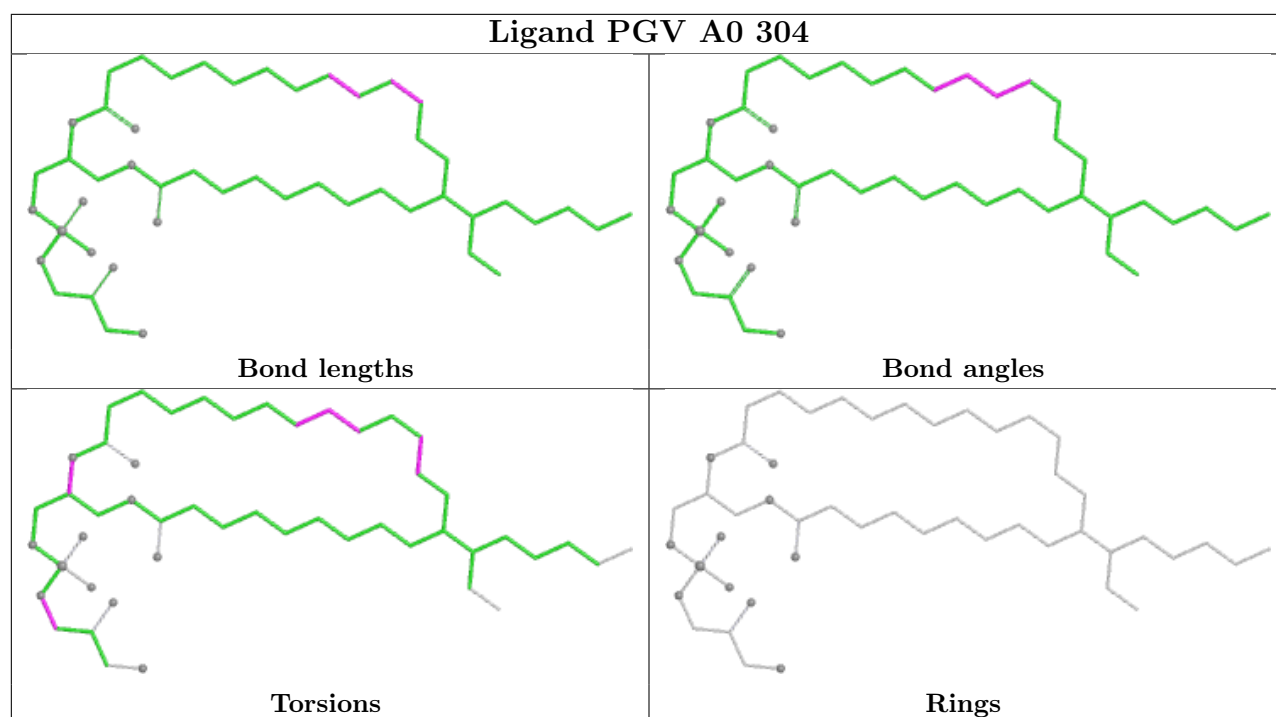


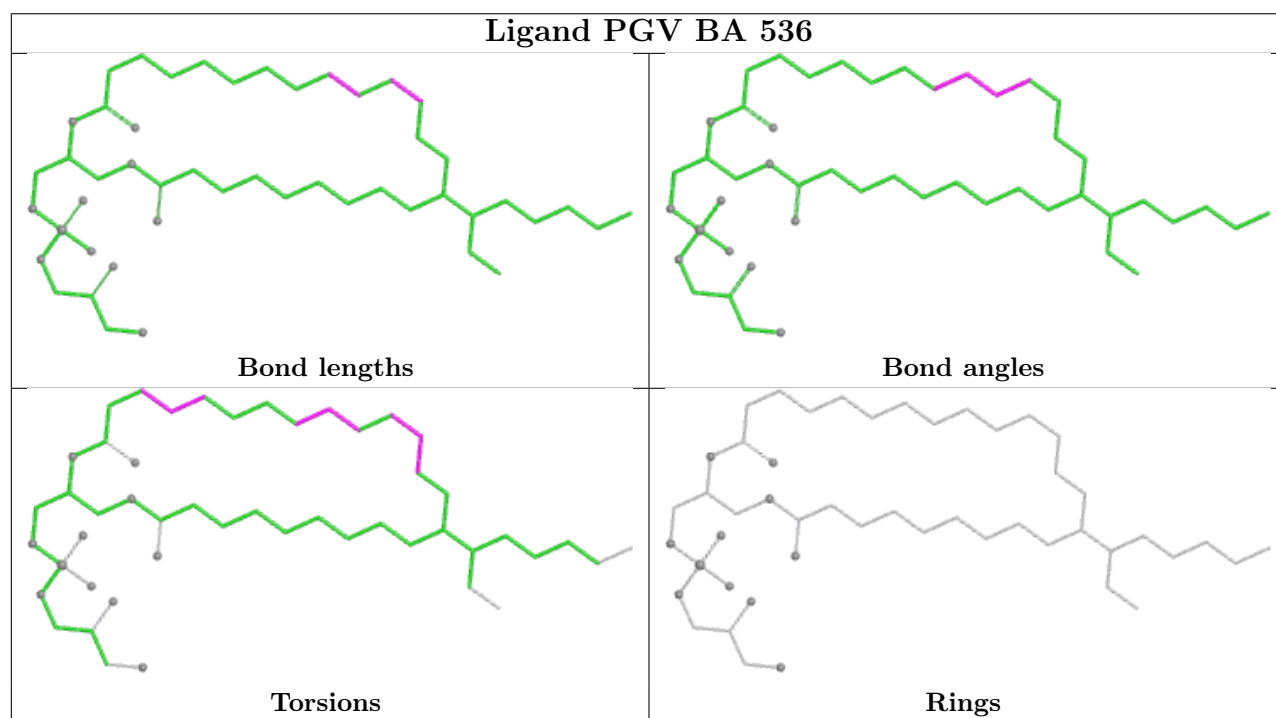
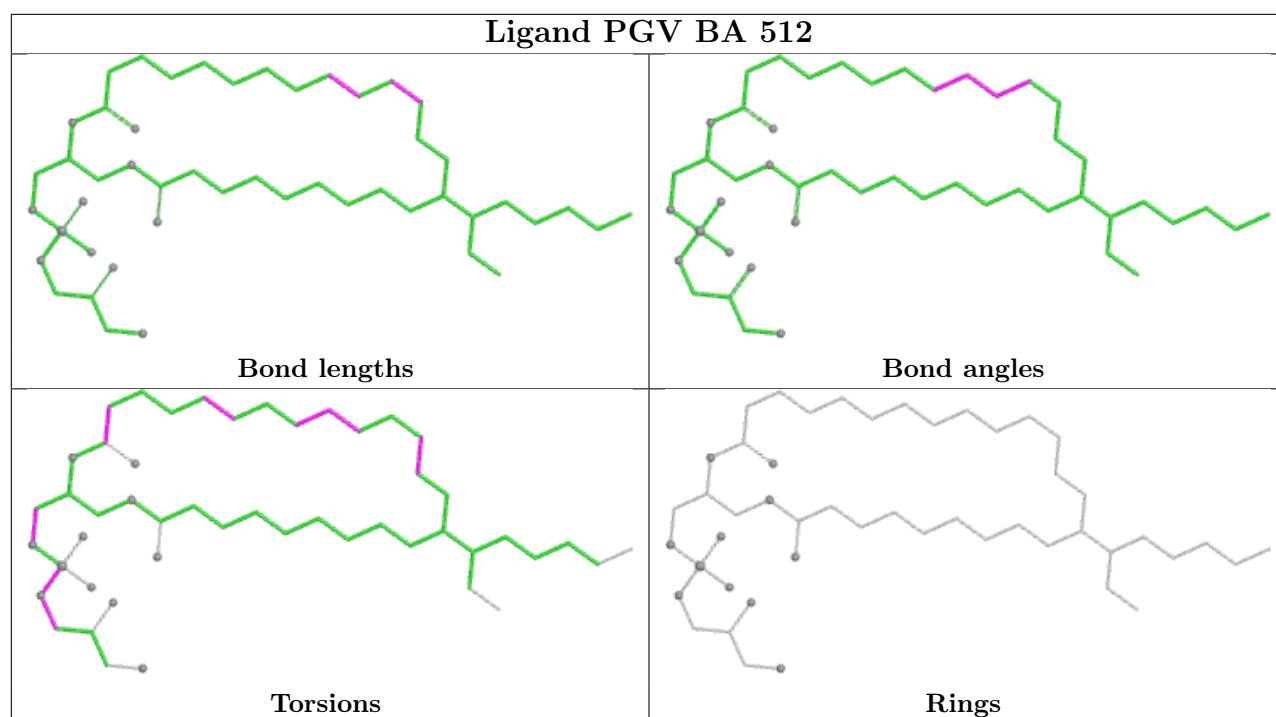


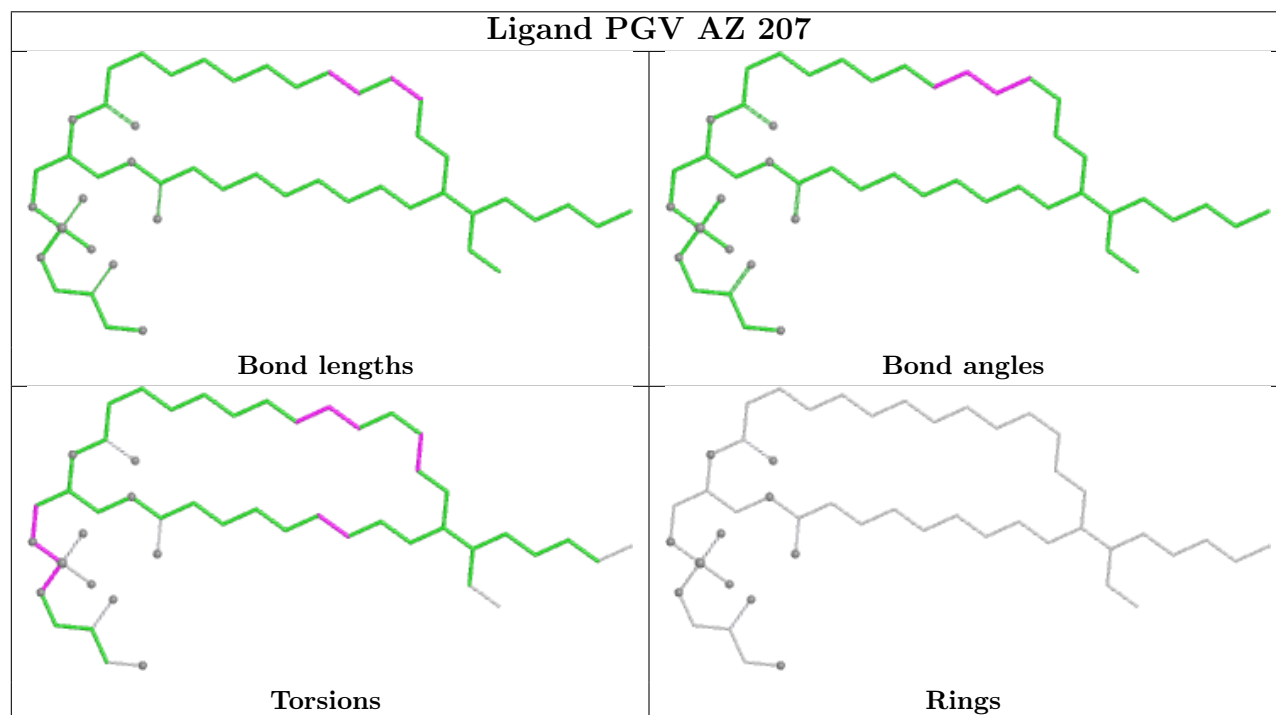
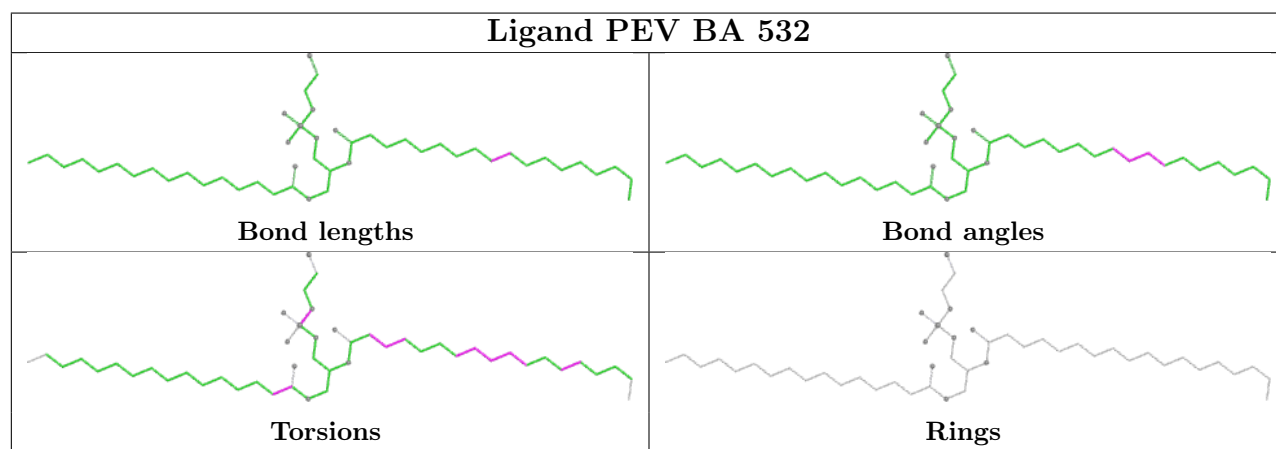
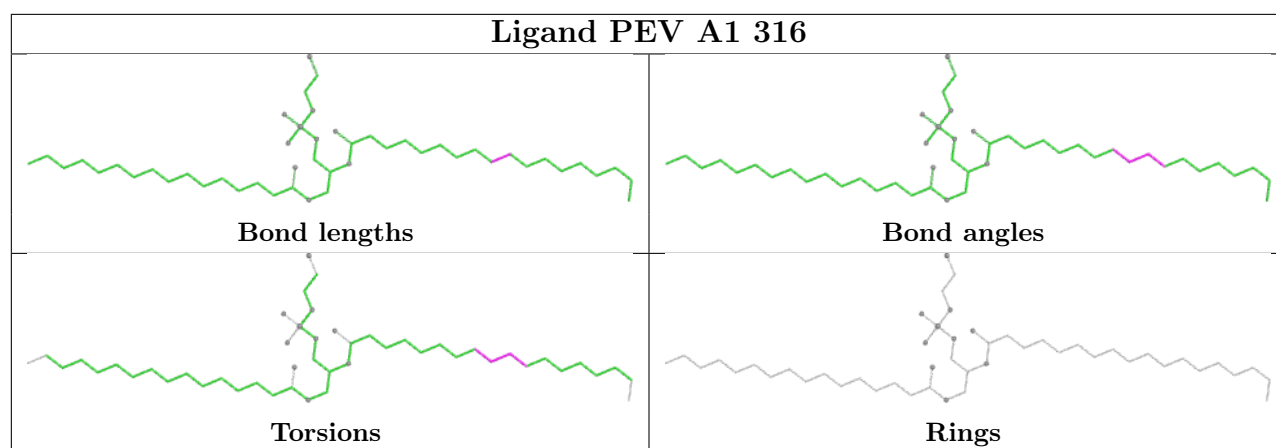
Ligand PEV A1 324	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PEV BB 218	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PEV B8 3003	
 Bond lengths	 Bond angles
 Torsions	 Rings

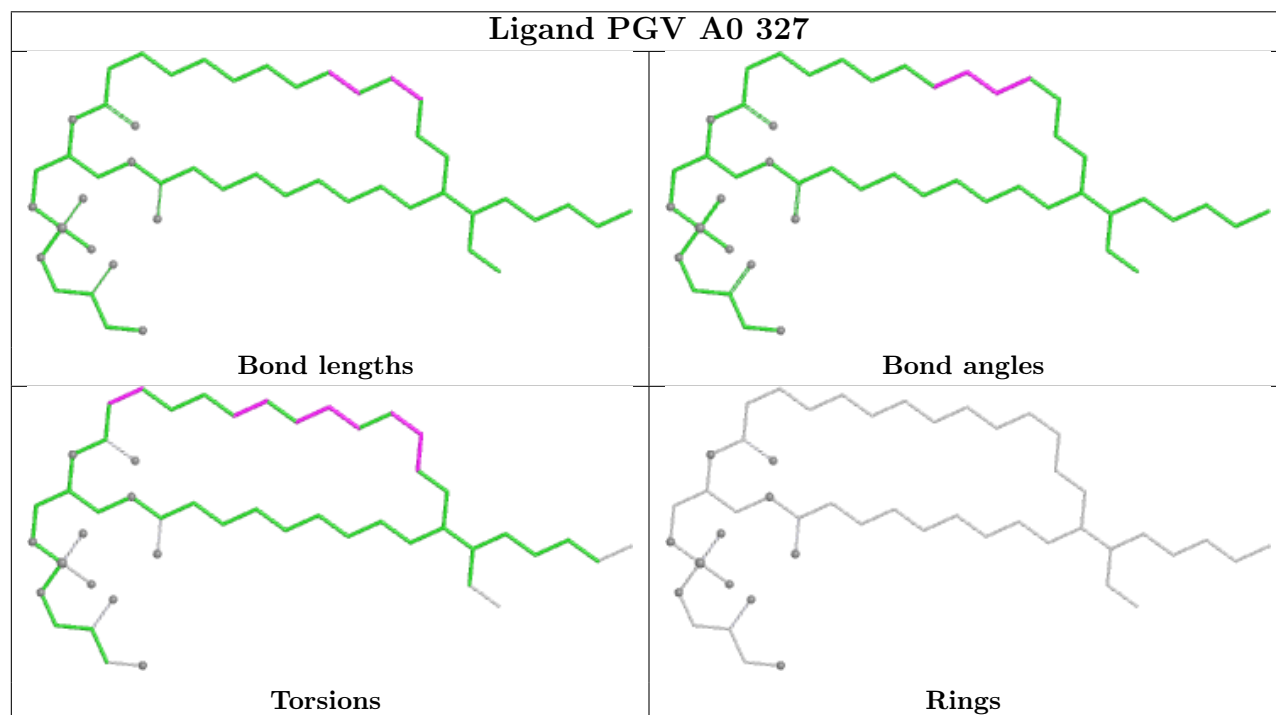
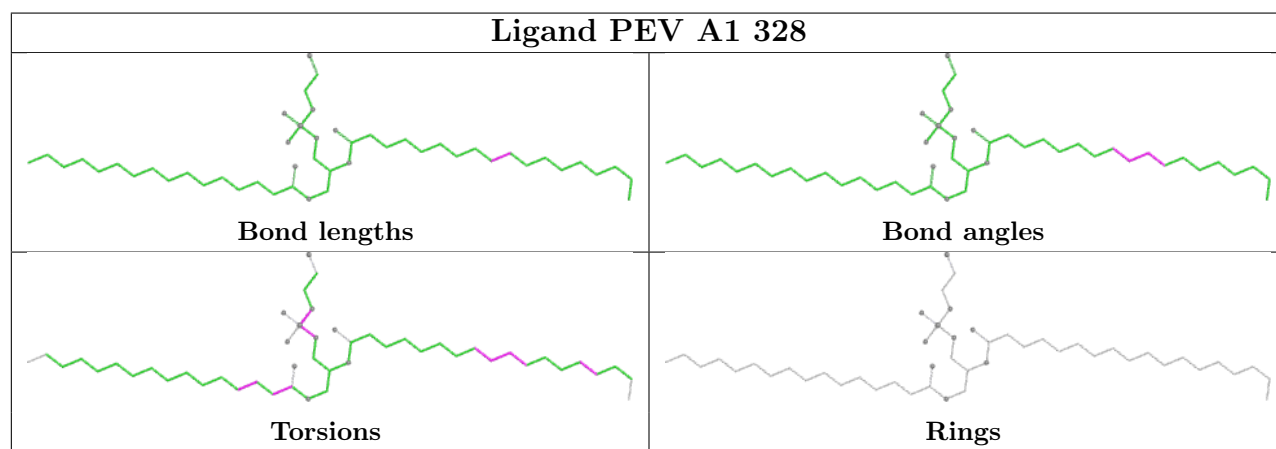
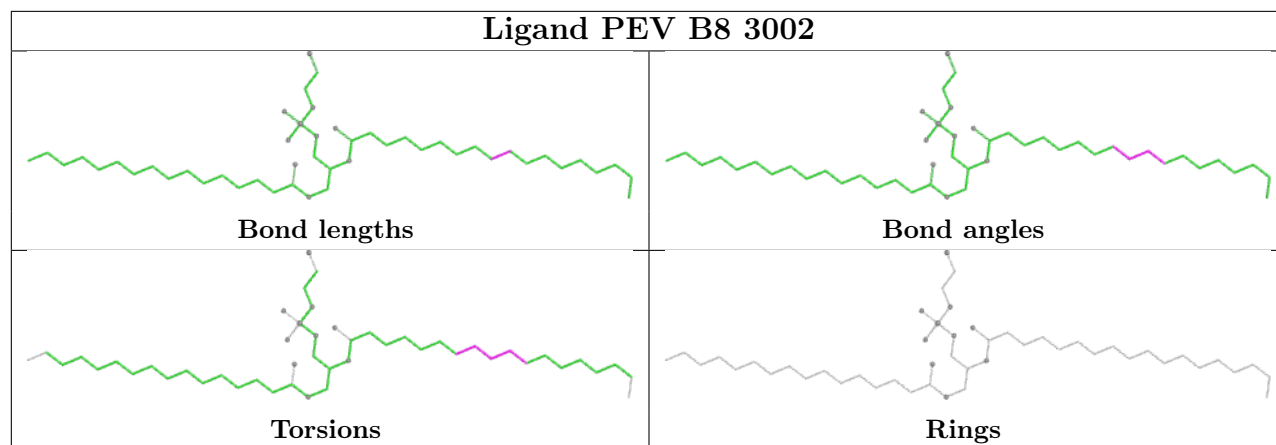


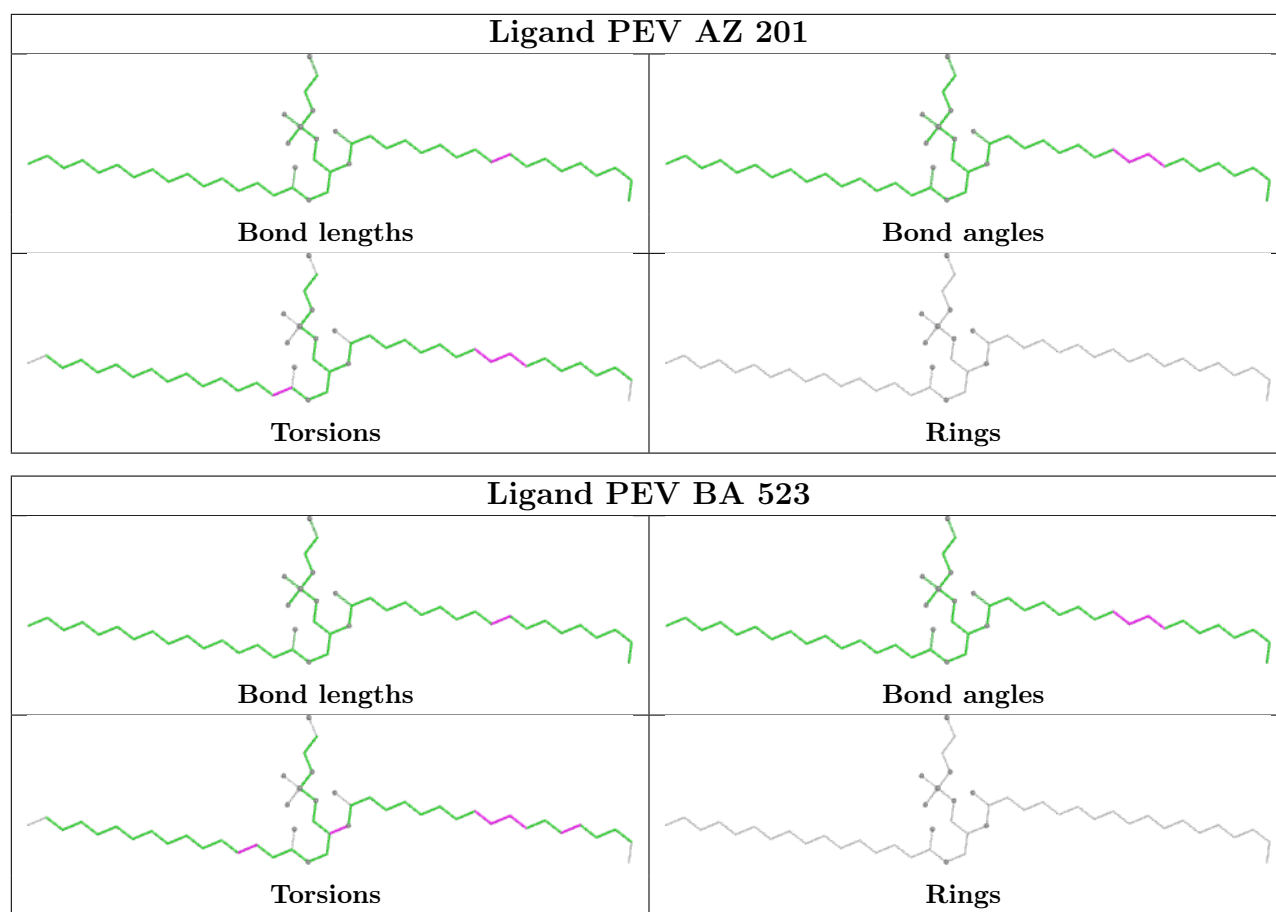












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

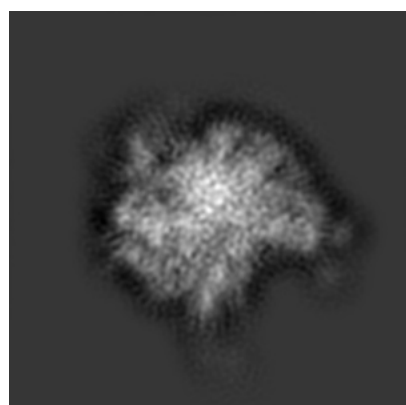
6 Map visualisation [i](#)

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

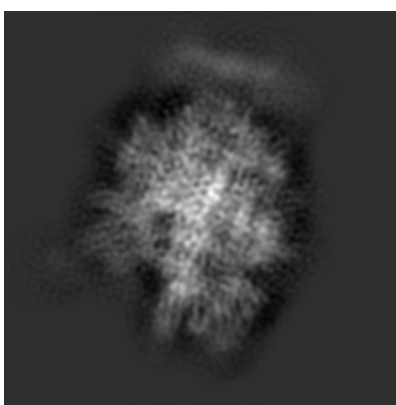
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

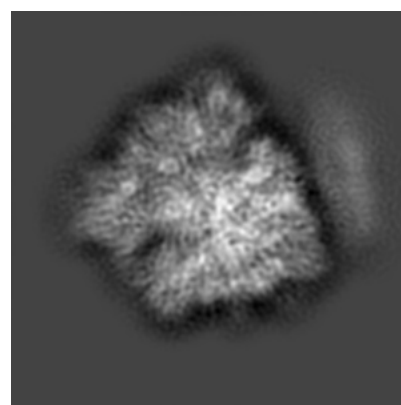
6.1.1 Primary map



X



Y

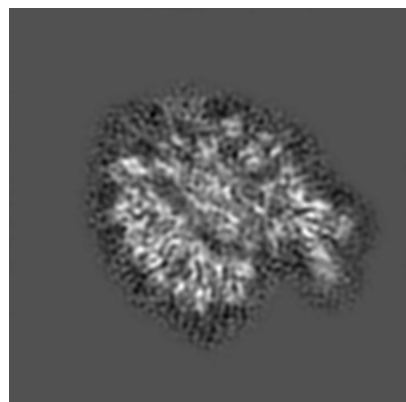


Z

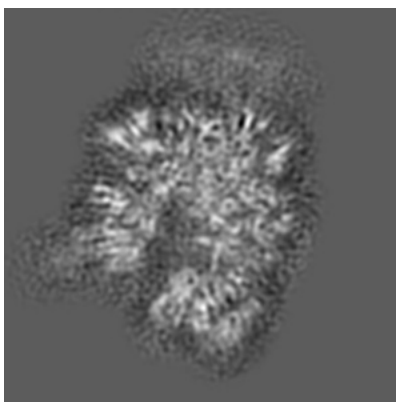
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

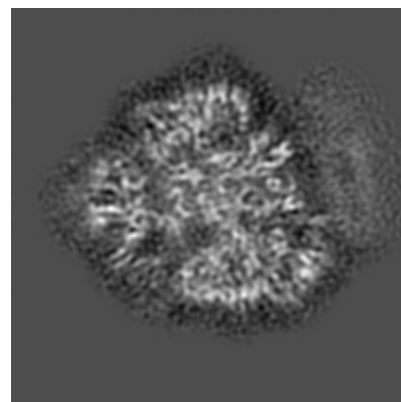
6.2.1 Primary map



X Index: 160



Y Index: 160

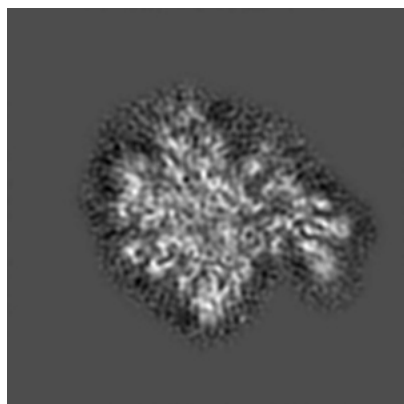


Z Index: 160

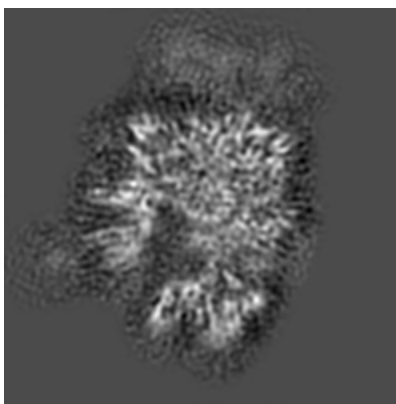
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

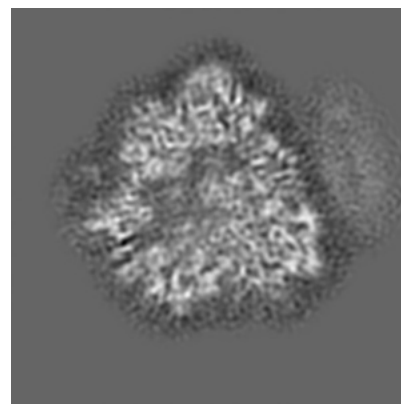
6.3.1 Primary map



X Index: 166



Y Index: 167



Z Index: 146

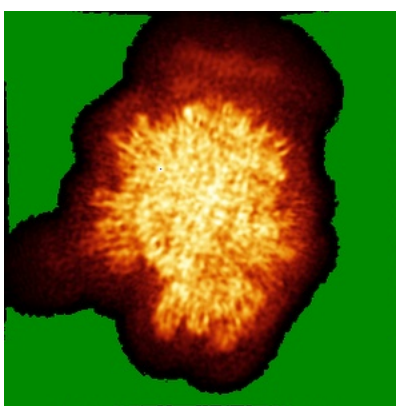
The images above show the largest variance slices of the map in three orthogonal directions.

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

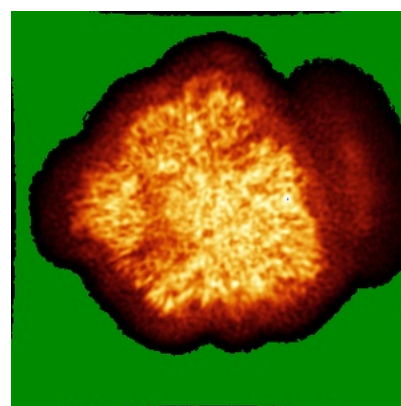
6.4.1 Primary map



X



Y

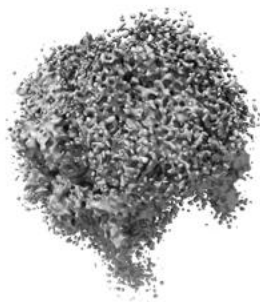


Z

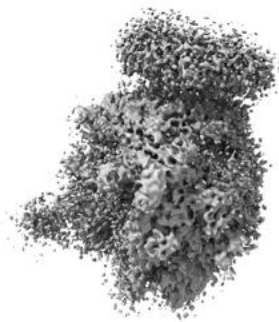
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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.

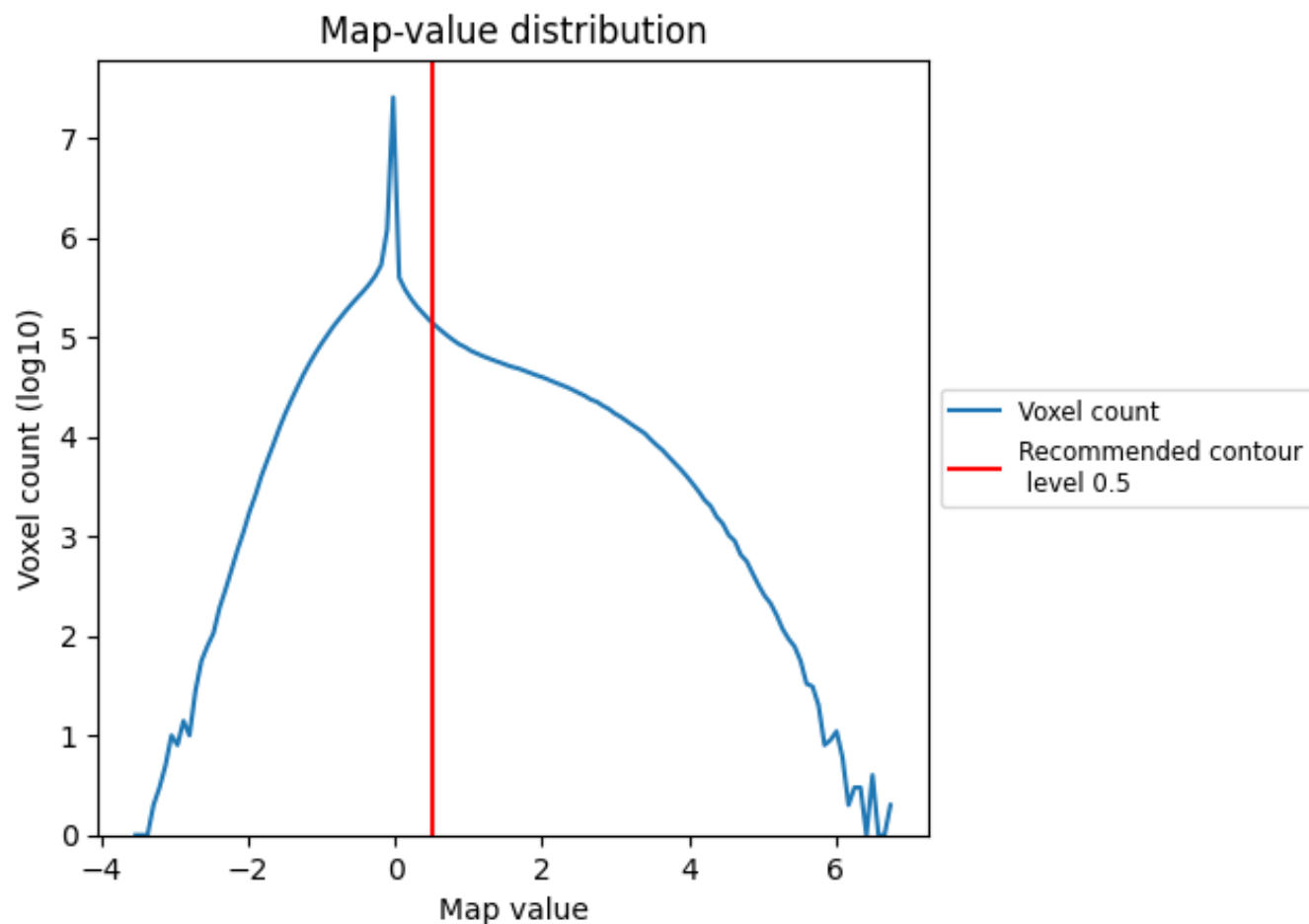
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

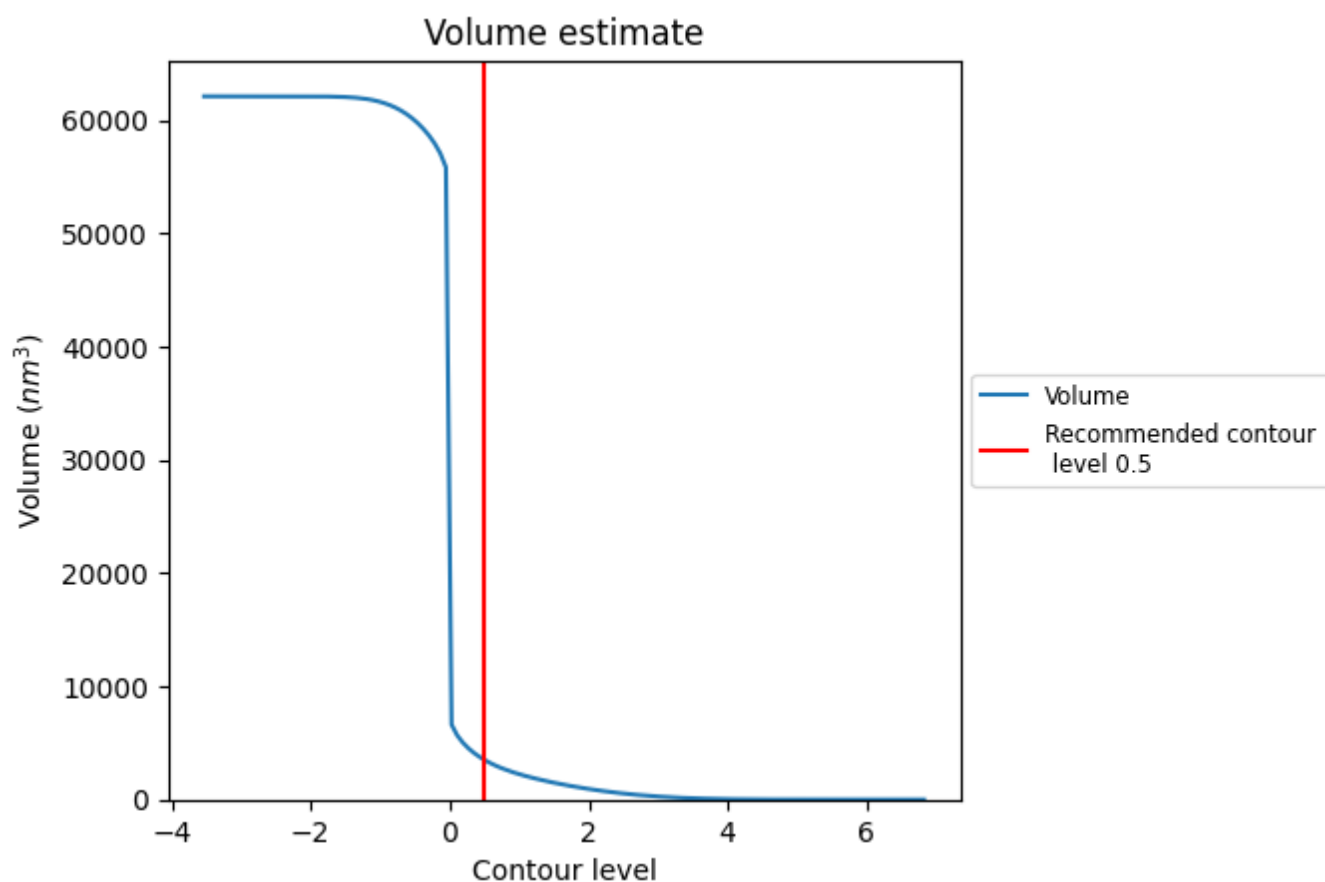
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

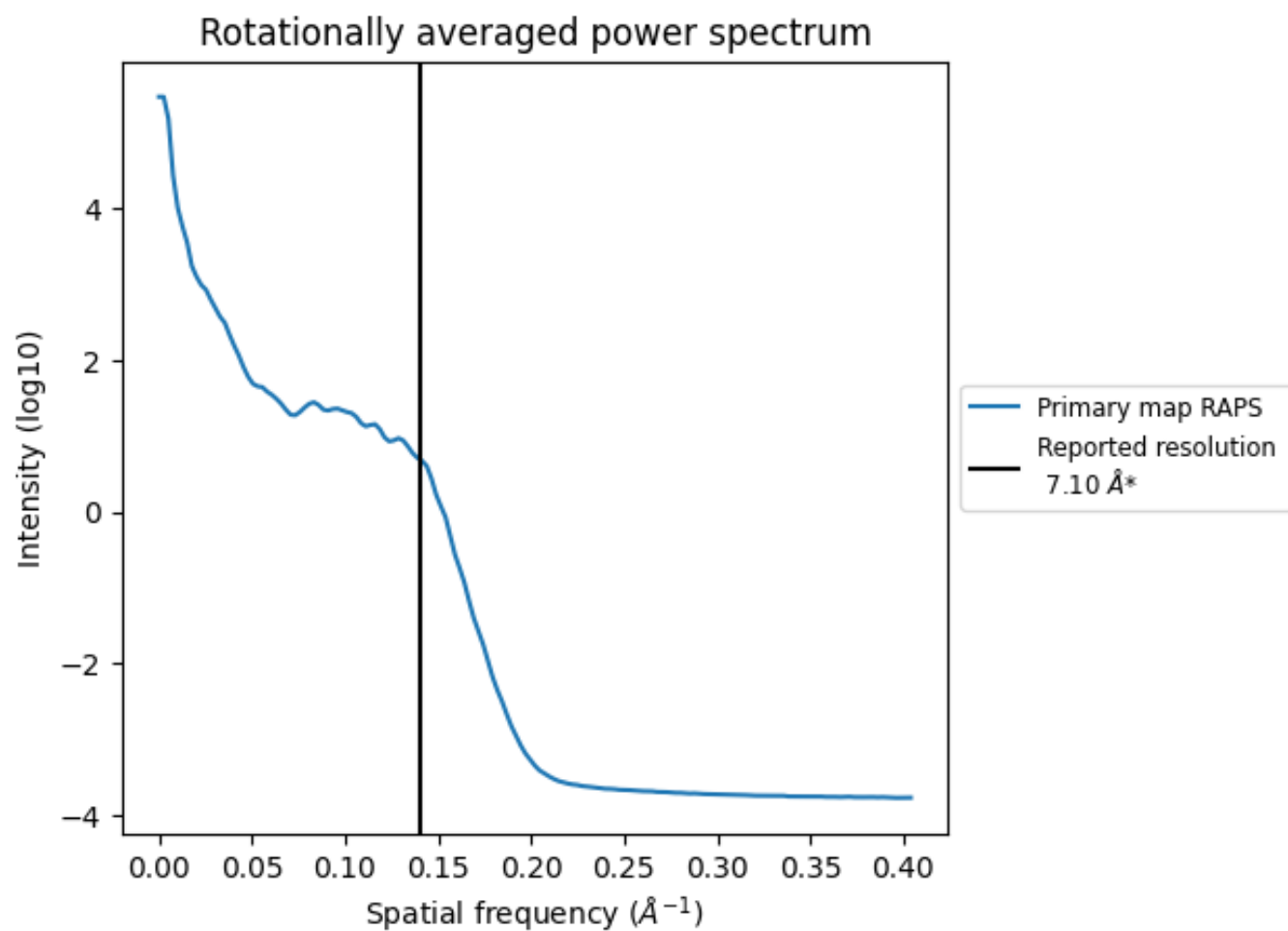
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3504 nm³; this corresponds to an approximate mass of 3166 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



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

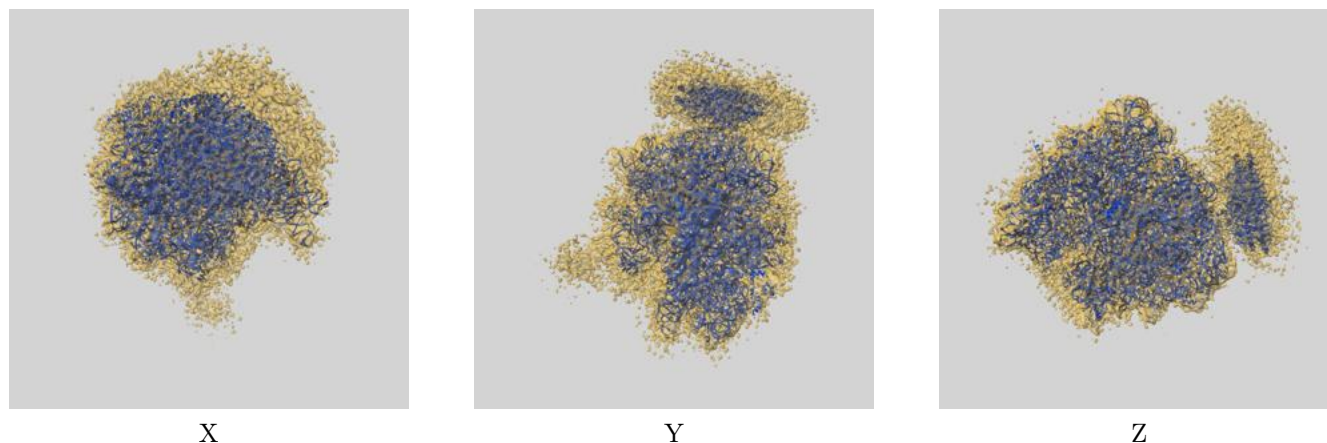
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

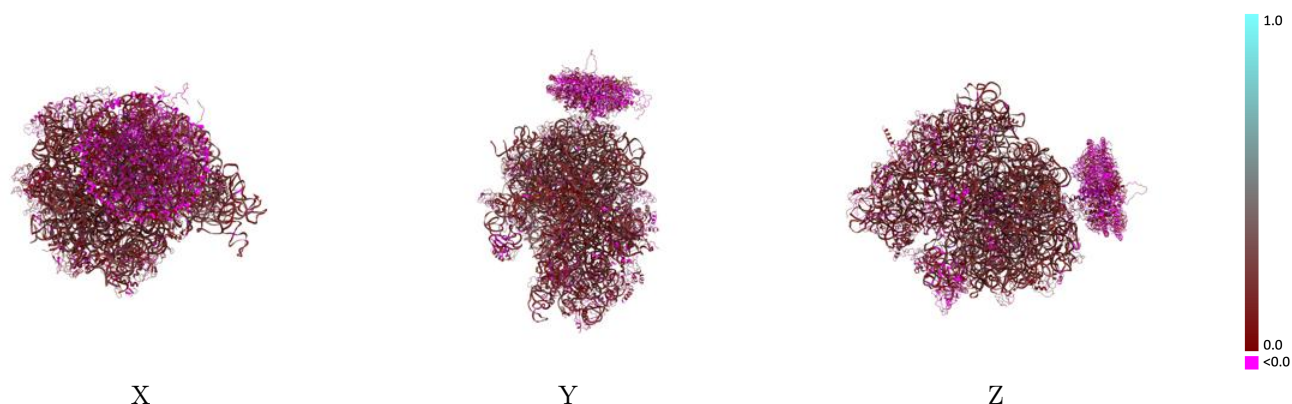
This section contains information regarding the fit between EMDB map EMD-1858 and PDB model 4V6M. Per-residue inclusion information can be found in section 3 on page 24.

9.1 Map-model overlay [i](#)



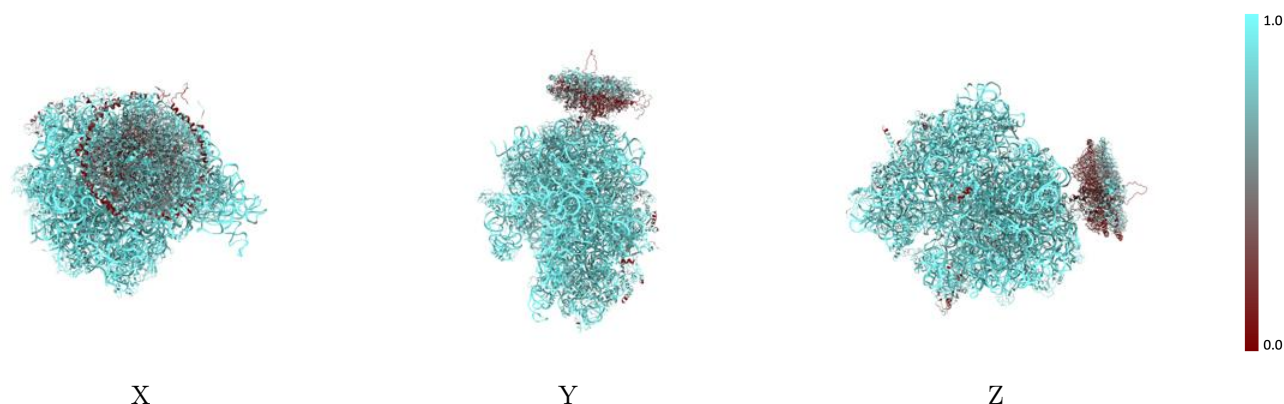
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



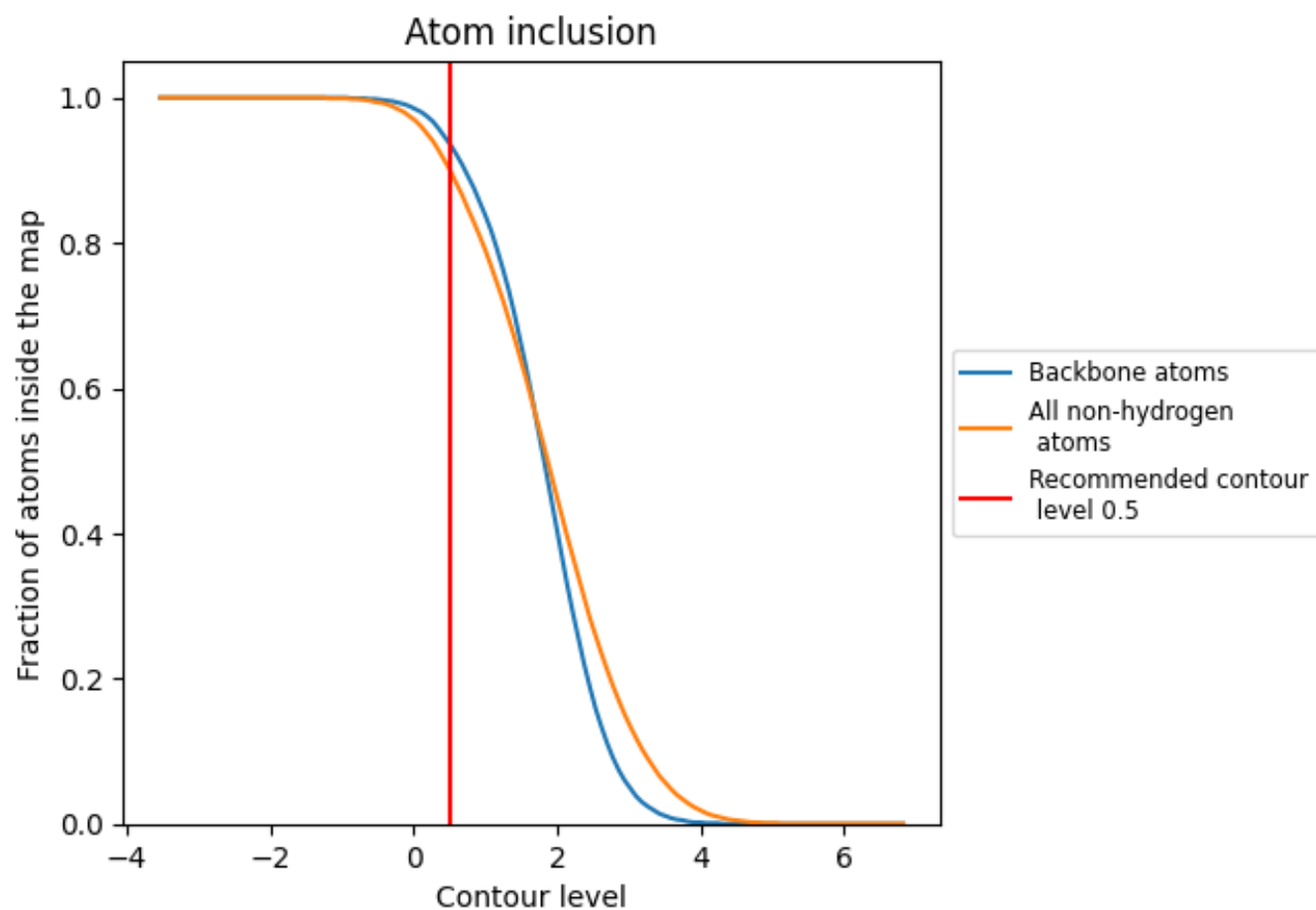
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



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

9.5 Map-model fit summary ⓘ

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

Chain	Atom inclusion	Q-score
All	 0.9010	 0.1450
A0	 0.3260	 0.0170
A1	 0.5620	 0.0090
AA	 0.9850	 0.1740
AB	 0.7510	 0.1210
AC	 0.8280	 0.1200
AD	 0.8390	 0.1240
AE	 0.7780	 0.1190
AF	 0.7180	 0.1060
AG	 0.9090	 0.1350
AH	 0.8540	 0.1350
AI	 0.8730	 0.0980
AJ	 0.8950	 0.0950
AK	 0.8480	 0.1140
AL	 0.9250	 0.1180
AM	 0.8860	 0.1220
AN	 0.8670	 0.1230
AO	 0.9170	 0.1390
AP	 0.8850	 0.1220
AQ	 0.8990	 0.1230
AR	 0.8000	 0.1240
AS	 0.8900	 0.1060
AT	 0.8290	 0.1370
AU	 0.8360	 0.1220
AV	 0.9590	 0.1410
AX	 0.7920	 0.1000
AZ	 0.5150	 0.0640
B0	 0.8550	 0.1190
B1	 0.9420	 0.1170
B2	 0.9270	 0.0860
B3	 0.8960	 0.1220
B4	 0.9140	 0.1000
B5	 0.6780	 0.0570
B6	 0.9290	 0.1300
B7	 0.9880	 0.1840



Continued on next page...

Continued from previous page...

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