



## Full wwPDB EM Validation Report ⓘ

Dec 7, 2022 – 10:54 AM JST

PDB ID : 5XTI  
EMDB ID : EMD-6776  
Title : Cryo-EM architecture of human respiratory chain megacomplex-I2III2IV2  
Authors : Gu, J.; Wu, M.; Yang, M.  
Deposited on : 2017-06-19  
Resolution : 17.40 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

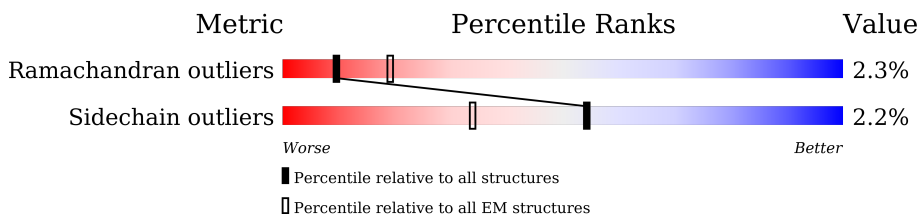
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 17.40 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	431	22% 98%
1	BA	431	98%
2	B	176	99%
2	BB	176	99%
3	BC	156	97%
3	C	156	97%
4	BE	113	97%
4	E	113	97%
5	BF	83	100%

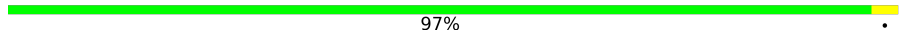
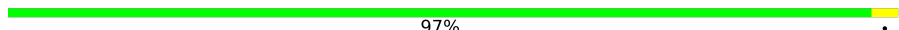
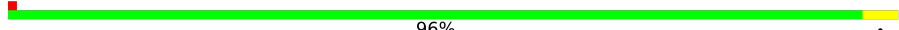
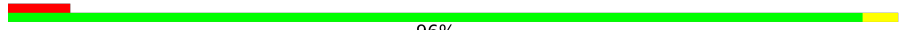
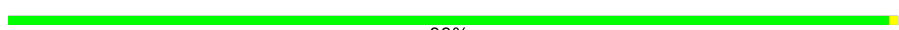





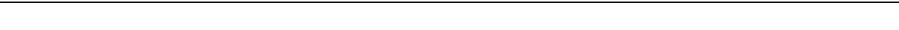

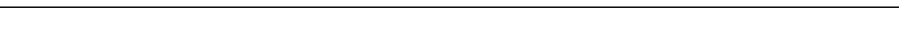
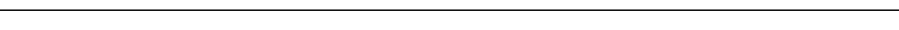
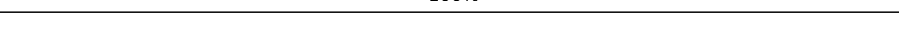
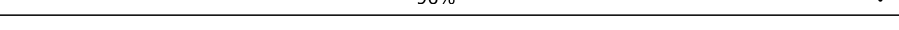
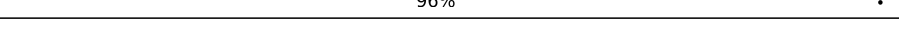


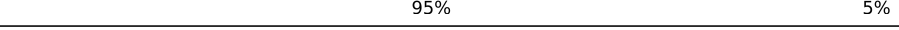
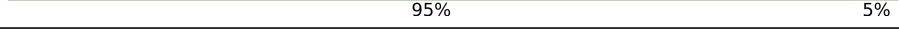
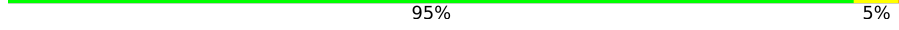
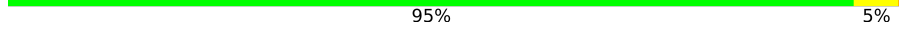
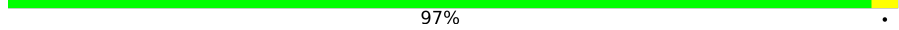
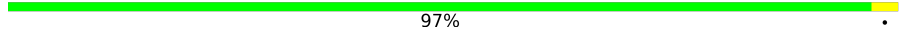
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Mol	Chain	Length	Quality of chain
5	F	83	100%
6	BG	85	26% 98%
6	BX	85	95% 5%
6	G	85	48% 98%
6	X	85	95% 5%
7	BH	112	96%
7	H	112	96%
8	BI	110	81% 5% 14%
8	I	110	81% 5% 14%
9	BJ	337	97%
9	J	337	97%
10	BK	33	91% 9%
10	K	33	91% 9%
11	BL	118	97%
11	L	118	97%
12	BM	687	96%
12	M	687	6% 96%
13	BN	143	95% 5%
13	N	143	95% 5%
14	BO	212	97%
14	O	212	10% 97%
15	BP	208	95% 5%
15	P	208	95% 5%
16	BQ	430	98%
16	Q	430	98%

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Mol	Chain	Length	Quality of chain
17	BS	70	 97%
17	S	70	 97%
18	BT	95	 96%
18	T	95	 96%
19	BU	83	 99%
19	U	83	 99%
20	BV	140	 98%
20	V	140	 98%
21	BW	138	 96%
21	W	138	 96%
22	BY	59	 75% 24%
22	Y	59	 75% 24%
23	BZ	80	 100%
23	Z	80	 100%
24	Ba	138	 96%
24	a	138	 96%
25	Bb	124	 90% 10%
25	b	124	 90% 10%
26	Bc	153	 95% 5%
26	c	153	 95% 5%
27	Bd	171	 95% 5%
27	d	171	 95% 5%
28	Be	97	 97%
28	e	97	 97%
29	Bf	47	 98%

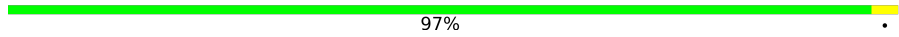
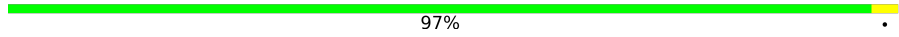


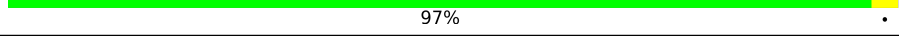
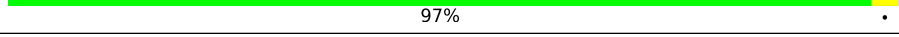
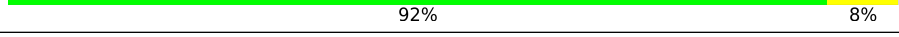
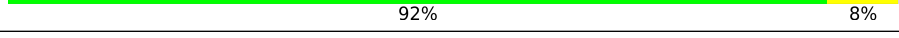
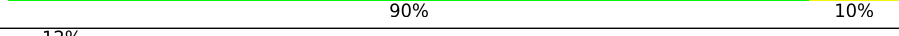

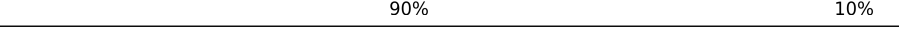
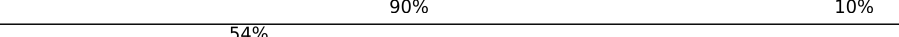
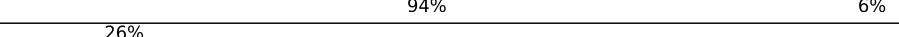
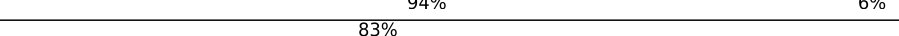
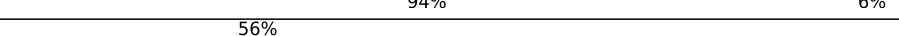
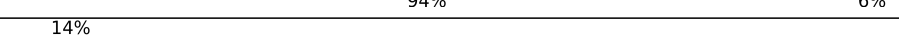
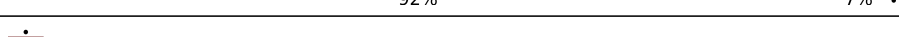
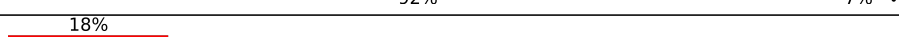
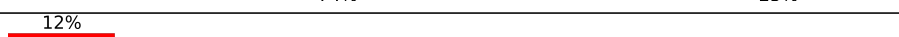






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Mol	Chain	Length	Quality of chain
29	f	47	98% .
30	Bg	119	95% 5%
30	g	119	95% 5%
31	Bh	104	94% 6%
31	h	104	94% 6%
32	Bi	347	98% .
32	i	347	98% .
33	Bj	115	97% .
33	j	115	97% .
34	Bk	97	93% 6% .
34	k	97	93% 6% .
35	Bl	603	95% 5%
35	l	603	95% 5%
36	Bm	174	94% 6%
36	m	174	94% 6%
37	Bn	56	96% .
37	n	56	96% .
38	Bo	128	97% .
38	o	128	97% .
39	Bp	172	98% .
39	p	172	98% .
40	Br	459	98% .
40	r	459	98% .
41	Bs	318	97% .
41	s	318	97% .

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Mol	Chain	Length	Quality of chain
42	Bu	169	 97%
42	u	169	 97%
43	Bv	122	 86% 5% 9%
43	v	122	 86% 5% 9%
44	Bw	320	 97%
44	w	320	 97%
45	Bx	514	 92% 8%
45	x	514	 92% 8%
46	By	227	 90% 10%
46	y	227	 12% 90% 10%
47	Bz	261	 90% 10%
47	z	261	 90% 10%
48	0	144	 54% 94% 6%
48	B0	144	 26% 94% 6%
49	1	109	 83% 94% 6%
49	B1	109	 56% 94% 6%
50	2	98	 14% 92% 7%
50	B2	98	 14% 92% 7%
51	3	84	 18% 74% 25%
51	B3	84	 12% 74% 25%
52	4	75	 16% 87% 13%
52	B4	75	 11% 87% 13%
53	5	73	 51% 93% 7%
53	B5	73	 25% 93% 7%
54	6	56	 88% 9%

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Mol	Chain	Length	Quality of chain
54	B6	56	9% 88% 9%
55	7	49	39% 96%
55	B7	49	96%
56	8	47	96%
56	B8	47	96%
57	9	43	9% 93% 7%
57	B9	43	7% 93% 7%
58	AA	81	90% 10%
58	AN	81	99%
59	AB	57	93% 7%
59	AO	57	88% 12%
60	AC	196	97%
60	AP	196	98%
61	AD	62	100%
61	AQ	62	100%
62	AE	74	96%
62	AR	74	96%
63	AF	106	88% 12%
63	AS	106	100%
64	AG	51	100%
64	AT	51	96%
65	AH	241	99%
65	AU	241	99%
66	AJ	378	98%
66	AV	378	96%

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Mol	Chain	Length	Quality of chain
67	AK	419	 98%
67	AW	419	 98%
68	AL	446	 99%
68	AY	446	 96%

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
79	HEA	Bx	603	X	-	-	-
79	HEA	Bx	604	X	-	-	-
79	HEA	x	603	X	-	-	-
79	HEA	x	604	X	-	-	-



## 2 Entry composition

There are 82 unique types of molecules in this entry. The entry contains 196753 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 protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	431	Total	C	N	O	S	0	0
			3322	2096	594	612	20		
1	BA	431	Total	C	N	O	S	0	0
			3322	2096	594	612	20		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	176	Total	C	N	O	S	0	0
			1420	893	243	271	13		
2	BB	176	Total	C	N	O	S	0	0
			1420	893	243	271	13		

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	156	Total	C	N	O	S	0	0
			1249	794	227	214	14		
3	BC	156	Total	C	N	O	S	0	0
			1249	794	227	214	14		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	113	Total	C	N	O	S	0	0
			968	623	178	162	5		
4	BE	113	Total	C	N	O	S	0	0
			968	623	178	162	5		

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit

2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	83	Total	C	N	O	S	0	0
			670	422	124	122	2		
5	BF	83	Total	C	N	O	S	0	0
			670	422	124	122	2		

- Molecule 6 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	85	Total	C	N	O	S	0	0
			672	434	99	134	5		
6	X	85	Total	C	N	O	S	0	0
			686	442	101	138	5		
6	BG	85	Total	C	N	O	S	0	0
			672	434	99	134	5		
6	BX	85	Total	C	N	O	S	0	0
			686	442	101	138	5		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	112	Total	C	N	O	S	0	0
			922	593	157	169	3		
7	BH	112	Total	C	N	O	S	0	0
			922	593	157	169	3		

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	95	Total	C	N	O	S	0	0
			769	483	146	138	2		
8	BI	95	Total	C	N	O	S	0	0
			769	483	146	138	2		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	337	Total	C	N	O	S	0	0
			2712	1759	482	463	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	BJ	337	Total	C	N	O	S	0	0
			2712	1759	482	463	8		

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	K	33	Total	C	N	O	S	0	0
			274	173	47	53	1		
10	BK	33	Total	C	N	O	S	0	0
			274	173	47	53	1		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	L	118	Total	C	N	O	S	0	0
			964	608	173	179	4		
11	BL	118	Total	C	N	O	S	0	0
			964	608	173	179	4		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	M	687	Total	C	N	O	S	0	0
			5274	3310	917	1009	38		
12	BM	687	Total	C	N	O	S	0	0
			5274	3310	917	1009	38		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	N	143	Total	C	N	O	S	0	0
			1195	770	210	212	3		
13	BN	143	Total	C	N	O	S	0	0
			1195	770	210	212	3		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	212	Total	C	N	O	S	0	0
			1643	1047	276	310	10		
14	BO	212	Total	C	N	O	S	0	0
			1643	1047	276	310	10		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	208	Total	C	N	O	S	0	0
			1730	1117	297	313	3		
15	BP	208	Total	C	N	O	S	0	0
			1730	1117	297	313	3		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	430	Total	C	N	O	S	0	0
			3460	2214	599	624	23		
16	BQ	430	Total	C	N	O	S	0	0
			3460	2214	599	624	23		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	70	Total	C	N	O	S	0	0
			568	367	101	96	4		
17	BS	70	Total	C	N	O	S	0	0
			568	367	101	96	4		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	95	Total	C	N	O	S	0	0
			742	459	138	142	3		
18	BT	95	Total	C	N	O	S	0	0
			742	459	138	142	3		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	83	Total	C	N	O	S	0	0
			647	427	105	113	2		
19	BU	83	Total	C	N	O	S	0	0
			647	427	105	113	2		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	140	Total	C	N	O	S	0	0
			1038	668	178	187	5		
20	BV	140	Total	C	N	O	S	0	0
			1038	668	178	187	5		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	138	Total	C	N	O	S	0	0
			1135	727	202	200	6		
21	BW	138	Total	C	N	O	S	0	0
			1135	727	202	200	6		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	59	Total	C	N	O	S	0	0
			533	354	87	91	1		
22	BY	59	Total	C	N	O	S	0	0
			533	354	87	91	1		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	80	Total	C	N	O	S	0	0
			648	426	110	110	2		
23	BZ	80	Total	C	N	O	S	0	0
			648	426	110	110	2		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	138	Total	C	N	O	S	0	0
			1174	771	199	202	2		
24	Ba	138	Total	C	N	O	S	0	0
			1174	771	199	202	2		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	124	Total	C	N	O	S	0	0
			1059	697	181	176	5		
25	Bb	124	Total	C	N	O	S	0	0
			1059	697	181	176	5		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	153	Total	C	N	O	S	0	0
			1236	795	208	222	11		
26	Bc	153	Total	C	N	O	S	0	0
			1236	795	208	222	11		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	d	171	Total	C	N	O	S	0	0
			1418	885	262	259	12		
27	Bd	171	Total	C	N	O	S	0	0
			1418	885	262	259	12		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	e	97	Total	C	N	O	S	0	0
			810	522	132	152	4		
28	Be	97	Total	C	N	O	S	0	0
			810	522	132	152	4		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	f	47	Total	C	N	O	0	0
			405	269	69	67		
29	Bf	47	Total	C	N	O	0	0
			405	269	69	67		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	g	119	Total	C	N	O	S	0	0
			1004	658	173	169	4		
30	Bg	119	Total	C	N	O	S	0	0
			1004	658	173	169	4		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	h	104	Total	C	N	O	S	0	0
			863	546	161	150	6		
31	Bh	104	Total	C	N	O	S	0	0
			863	546	161	150	6		

- Molecule 32 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	i	347	Total	C	N	O	S	0	0
			2735	1819	421	470	25		
32	Bi	347	Total	C	N	O	S	0	0
			2735	1819	421	470	25		

- Molecule 33 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	j	115	Total	C	N	O	S	0	0
			919	626	132	152	9		
33	Bj	115	Total	C	N	O	S	0	0
			919	626	132	152	9		

- Molecule 34 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	k	97	Total	C	N	O	S	0	0
			740	487	113	127	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
34	Bk	97	Total	C	N	O	S	0	0
			740	487	113	127	13		

- Molecule 35 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	l	603	Total	C	N	O	S	0	0
			4717	3119	742	823	33		
35	Bl	603	Total	C	N	O	S	0	0
			4717	3119	742	823	33		

- Molecule 36 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	174	Total	C	N	O	S	0	0
			1313	879	194	229	11		
36	Bm	174	Total	C	N	O	S	0	0
			1313	879	194	229	11		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	n	56	Total	C	N	O	S	0	0
			473	305	85	80	3		
37	Bn	56	Total	C	N	O	S	0	0
			473	305	85	80	3		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	o	128	Total	C	N	O	S	0	0
			1063	684	191	186	2		
38	Bo	128	Total	C	N	O	S	0	0
			1066	685	192	187	2		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.



Mol	Chain	Residues	Atoms					AltConf	Trace
39	p	172	Total	C	N	O	S	0	0
			1495	961	265	261	8		
39	Bp	172	Total	C	N	O	S	0	0
			1495	961	265	261	8		

- Molecule 40 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	r	459	Total	C	N	O	S	0	0
			3629	2411	569	619	30		
40	Br	459	Total	C	N	O	S	0	0
			3629	2411	569	619	30		

- Molecule 41 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	s	318	Total	C	N	O	S	0	0
			2509	1678	380	435	16		
41	Bs	318	Total	C	N	O	S	0	0
			2509	1678	380	435	16		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	u	169	Total	C	N	O	S	0	0
			1394	886	247	252	9		
42	Bu	169	Total	C	N	O	S	0	0
			1394	886	247	252	9		

- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	v	111	Total	C	N	O	S	0	0
			921	569	187	156	9		
43	Bv	111	Total	C	N	O	S	0	0
			921	569	187	156	9		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	w	320	Total	C	N	O	S	0	0
			2474	1573	429	464	8		
44	Bw	320	Total	C	N	O	S	0	0
			2474	1573	429	464	8		

- Molecule 45 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	x	514	Total	C	N	O	S	0	0
			4025	2690	623	677	35		
45	Bx	514	Total	C	N	O	S	0	0
			4025	2690	623	677	35		

- Molecule 46 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	y	227	Total	C	N	O	S	0	0
			1822	1184	281	339	18		
46	By	227	Total	C	N	O	S	0	0
			1822	1184	281	339	18		

- Molecule 47 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	z	261	Total	C	N	O	S	0	0
			2124	1420	338	353	13		
47	Bz	261	Total	C	N	O	S	0	0
			2124	1420	338	353	13		

- Molecule 48 is a protein called Cytochrome c oxidase subunit 4 isoform 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	0	144	Total	C	N	O	S	0	0
			1195	777	196	218	4		
48	B0	144	Total	C	N	O	S	0	0
			1195	777	196	218	4		

- Molecule 49 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	1	109	Total	C	N	O	S	0	0
			878	558	150	168	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	B1	109	878	558	150	168	2	0	0

- Molecule 50 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	2	98	748	464	134	145	5	0	0
50	B2	98	748	464	134	145	5	0	0

- Molecule 51 is a protein called Cytochrome c oxidase subunit 6A2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	3	84	672	431	129	111	1	0	0
51	B3	84	672	431	129	111	1	0	0

- Molecule 52 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	4	75	628	395	114	114	5	0	0
52	B4	75	628	395	114	114	5	0	0

- Molecule 53 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	5	73	598	388	107	99	4	0	0
53	B5	73	598	388	107	99	4	0	0

- Molecule 54 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	6	56	441	285	73	80	3	0	0
54	B6	56	441	285	73	80	3	0	0

- Molecule 55 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	7	49	Total	C	N	O	S	0	0
			384	250	65	67	2		
55	B7	49	Total	C	N	O	S	0	0
			384	250	65	67	2		

- Molecule 56 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	8	47	Total	C	N	O	S	0	0
			386	257	65	62	2		
56	B8	47	Total	C	N	O	S	0	0
			386	257	65	62	2		

- Molecule 57 is a protein called Cytochrome c oxidase subunit 8B, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
57	9	43	Total	C	N	O	0	0
			335	223	53	59		
57	B9	43	Total	C	N	O	0	0
			335	223	53	59		

- Molecule 58 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	AA	81	Total	C	N	O	S	0	0
			694	450	126	117	1		
58	AN	81	Total	C	N	O	S	0	0
			687	444	126	116	1		

- Molecule 59 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	AB	57	Total	C	N	O	S	0	0
			413	261	75	76	1		
59	AO	57	Total	C	N	O	S	0	0
			409	259	74	75	1		

- Molecule 60 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	AC	196	Total	C	N	O	S	0	0
			1521	960	264	290	7		
60	AP	196	Total	C	N	O	S	0	0
			1521	960	264	290	7		

- Molecule 61 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	AD	62	Total	C	N	O	S	0	0
			509	332	87	89	1		
61	AQ	62	Total	C	N	O	S	0	0
			509	332	87	89	1		

- Molecule 62 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	AE	74	Total	C	N	O	S	0	0
			580	351	108	116	5		
62	AR	74	Total	C	N	O	S	0	0
			580	351	108	116	5		

- Molecule 63 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	AF	106	Total	C	N	O	S	0	0
			921	589	162	168	2		
63	AS	106	Total	C	N	O	S	0	0
			921	589	162	168	2		

- Molecule 64 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
64	AG	51	Total	C	N	O	0	0
			425	287	72	66		
64	AT	51	Total	C	N	O	0	0
			425	287	72	66		

- Molecule 65 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	AH	241	Total	C	N	O	S	0	0
			1924	1231	329	349	15		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	AU	241	Total	C	N	O	S	0	0
			1924	1231	329	349	15		

- Molecule 66 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
66	AJ	378	Total	C	N	O	S	0	0
			3009	2017	467	509	16		
66	AV	378	Total	C	N	O	S	0	0
			3009	2017	467	509	16		

- Molecule 67 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
67	AK	419	Total	C	N	O	S	0	0
			3159	1986	553	610	10		
67	AW	419	Total	C	N	O	S	0	0
			3162	1989	553	610	10		

- Molecule 68 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

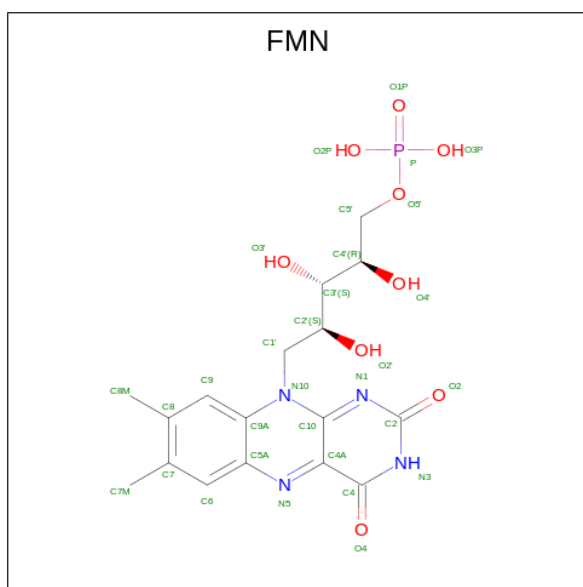
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
68	AL	446	Total	C	N	O	S	0	0
			3442	2160	602	660	20		
68	AY	446	Total	C	N	O	S	0	0
			3428	2147	601	660	20		

- Molecule 69 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



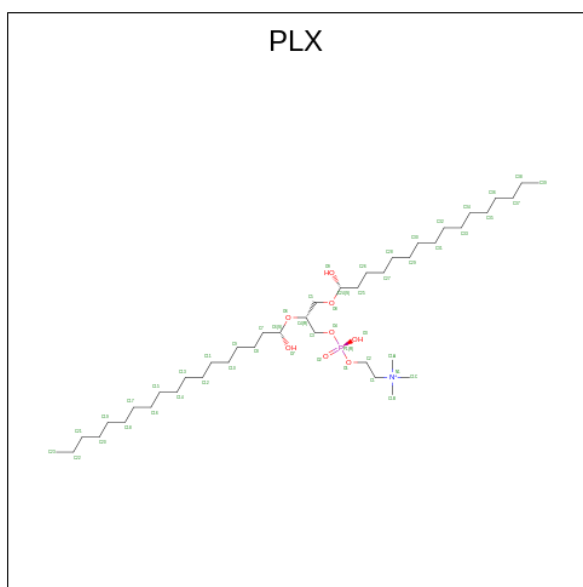
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
69	A	1	8	4	4	0
69	B	1	16	8	8	0
69	B	1	16	8	8	0
69	C	1	8	4	4	0
69	M	1	16	8	8	0
69	M	1	16	8	8	0
69	BA	1	8	4	4	0
69	BB	1	16	8	8	0
69	BB	1	16	8	8	0
69	BC	1	8	4	4	0
69	BM	1	16	8	8	0
69	BM	1	16	8	8	0

- Molecule 70 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P).



Mol	Chain	Residues	Atoms					AltConf
70	A	1	Total	C	N	O	P	0
			31	17	4	9	1	
70	BA	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 71 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (three-letter code: PLX) (formula: C<sub>42</sub>H<sub>89</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					AltConf
71	B	1	Total	C	N	O	P	0
			52	42	1	8	1	

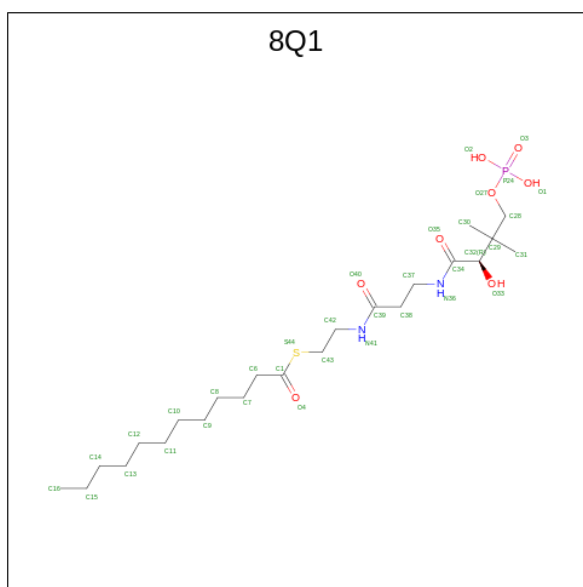
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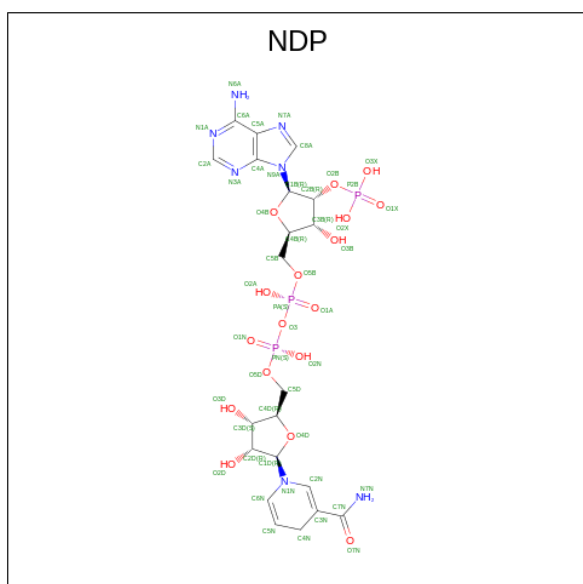
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
71	U	1	Total 52	C 42	N 1	O 8	P 1	0
71	b	1	Total 52	C 42	N 1	O 8	P 1	0
71	g	1	Total 156	C 126	N 3	O 24	P 3	0
71	g	1	Total 156	C 126	N 3	O 24	P 3	0
71	g	1	Total 156	C 126	N 3	O 24	P 3	0
71	r	1	Total 104	C 84	N 2	O 16	P 2	0
71	r	1	Total 104	C 84	N 2	O 16	P 2	0
71	AL	1	Total 52	C 42	N 1	O 8	P 1	0
71	AN	1	Total 52	C 42	N 1	O 8	P 1	0
71	AQ	1	Total 52	C 42	N 1	O 8	P 1	0
71	AT	1	Total 52	C 42	N 1	O 8	P 1	0
71	BB	1	Total 52	C 42	N 1	O 8	P 1	0
71	BU	1	Total 52	C 42	N 1	O 8	P 1	0
71	BV	1	Total 52	C 42	N 1	O 8	P 1	0
71	Bb	1	Total 52	C 42	N 1	O 8	P 1	0
71	Bg	1	Total 156	C 126	N 3	O 24	P 3	0
71	Bg	1	Total 156	C 126	N 3	O 24	P 3	0
71	Bg	1	Total 156	C 126	N 3	O 24	P 3	0
71	Br	1	Total 104	C 84	N 2	O 16	P 2	0
71	Br	1	Total 104	C 84	N 2	O 16	P 2	0

- Molecule 72 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonoxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (three-letter code: 8Q1) (formula: C<sub>23</sub>H<sub>45</sub>N<sub>2</sub>O<sub>8</sub>PS).



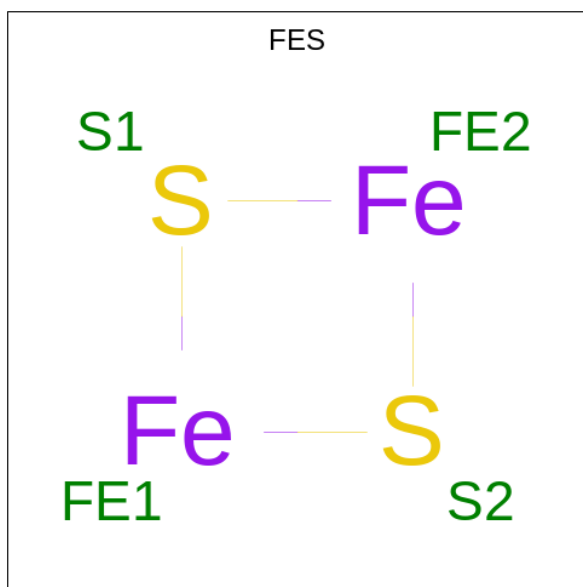
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	N	O	P		S
72	E	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
72	p	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
72	BE	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
72	Bp	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

- Molecule 73 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula:  $C_{21}H_{30}N_7O_{17}P_3$ ).



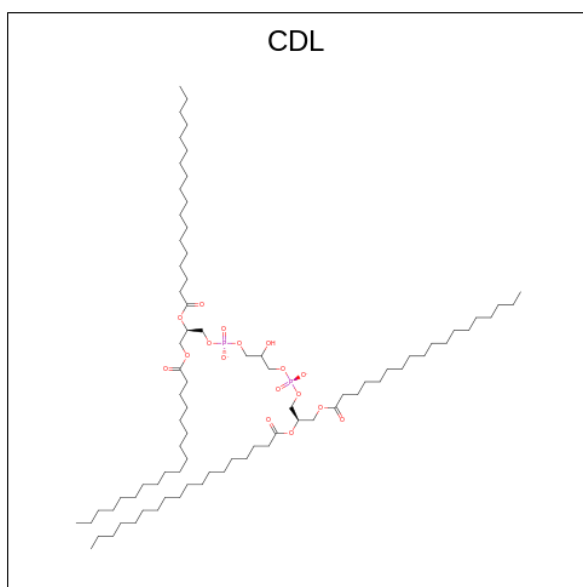
Mol	Chain	Residues	Atoms					AltConf
73	J	1	Total	C	N	O	P	0
			48	21	7	17	3	
73	BJ	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 74 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms			AltConf
74	M	1	Total	Fe	S	0
			4	2	2	
74	O	1	Total	Fe	S	0
			4	2	2	
74	AC	1	Total	Fe	S	0
			4	2	2	
74	AP	1	Total	Fe	S	0
			4	2	2	
74	BM	1	Total	Fe	S	0
			4	2	2	
74	BO	1	Total	Fe	S	0
			4	2	2	

- Molecule 75 is CARDIOLIPIN (three-letter code: CDL) (formula: C<sub>81</sub>H<sub>156</sub>O<sub>17</sub>P<sub>2</sub>).



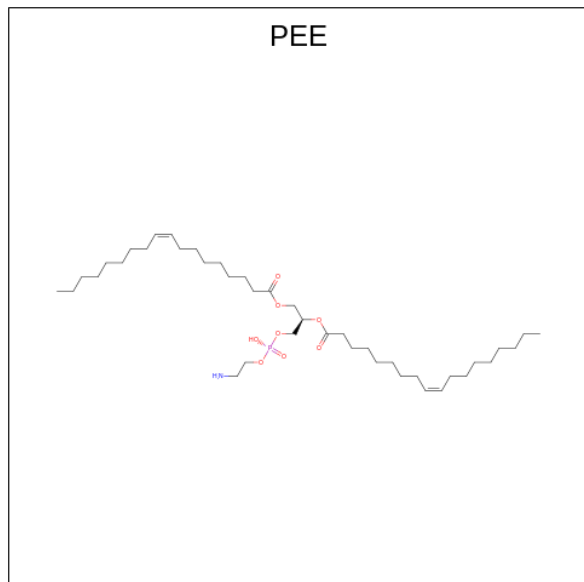
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
75	V	1	63	44	17	2	0
75	i	1	64	45	17	2	0
75	l	1	128	90	34	4	0
75	l	1	128	90	34	4	0
75	n	1	64	45	17	2	0
75	AA	1	64	45	17	2	0
75	AG	1	64	45	17	2	0
75	AH	1	64	45	17	2	0
75	AJ	1	128	90	34	4	0
75	AJ	1	128	90	34	4	0
75	AL	1	64	45	17	2	0
75	AN	1	64	45	17	2	0
75	AU	1	64	45	17	2	0
75	AY	1	64	45	17	2	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
75	BV	1	Total 63	C 44	O 17	P 2	0
75	Bi	1	Total 64	C 45	O 17	P 2	0
75	Bl	1	Total 128	C 90	O 34	P 4	0
75	Bl	1	Total 128	C 90	O 34	P 4	0
75	Bn	1	Total 64	C 45	O 17	P 2	0

- Molecule 76 is 1,2-Dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula:  $C_{41}H_{78}NO_8P$ ).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
76	V	1	Total 51	C 41	N 1	O 8	P 1	0
76	W	1	Total 51	C 41	N 1	O 8	P 1	0
76	l	1	Total 100	C 80	N 2	O 16	P 2	0
76	l	1	Total 100	C 80	N 2	O 16	P 2	0
76	AH	1	Total 49	C 39	N 1	O 8	P 1	0
76	AJ	1	Total 49	C 39	N 1	O 8	P 1	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
76	AL	1	Total 49	C 39	N 1	O 8	P 1	0
76	AU	1	Total 41	C 31	N 1	O 8	P 1	0
76	AV	1	Total 49	C 39	N 1	O 8	P 1	0
76	AY	1	Total 49	C 39	N 1	O 8	P 1	0
76	BV	1	Total 51	C 41	N 1	O 8	P 1	0
76	BW	1	Total 51	C 41	N 1	O 8	P 1	0
76	Bl	1	Total 100	C 80	N 2	O 16	P 2	0
76	Bl	1	Total 100	C 80	N 2	O 16	P 2	0

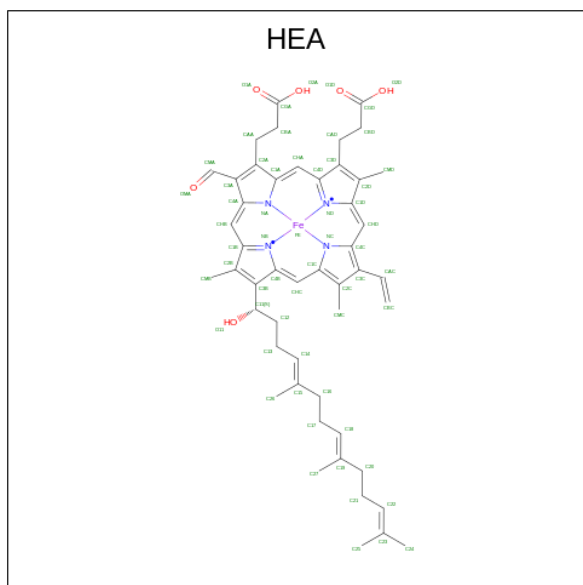
- Molecule 77 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
			Total	Cu	
77	x	1	Total 1	Cu 1	0
77	y	2	Total 2	Cu 2	0
77	Bx	1	Total 1	Cu 1	0
77	By	2	Total 2	Cu 2	0

- Molecule 78 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
78	x	1	Total 1	Mg 1	0
78	Bx	1	Total 1	Mg 1	0

- Molecule 79 is HEME-A (three-letter code: HEA) (formula: C<sub>49</sub>H<sub>56</sub>FeN<sub>4</sub>O<sub>6</sub>).

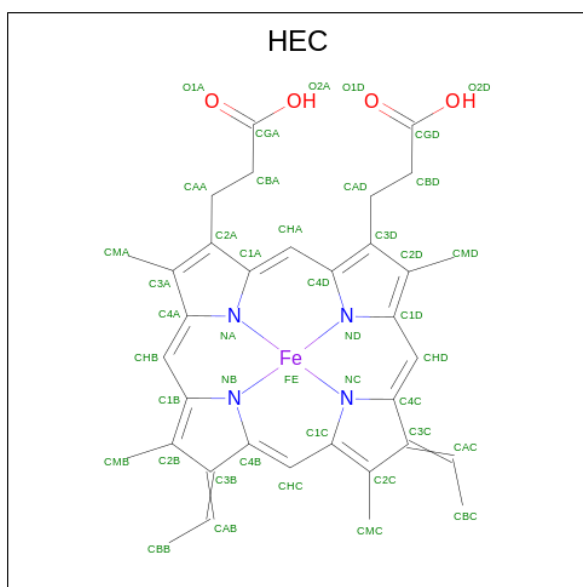


Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Fe	N		O
79	x	1	Total	C	Fe	N	O	0
			120	98	2	8	12	
79	x	1	Total	C	Fe	N	O	0
			120	98	2	8	12	
79	Bx	1	Total	C	Fe	N	O	0
			120	98	2	8	12	
79	Bx	1	Total	C	Fe	N	O	0
			120	98	2	8	12	

- Molecule 80 is ZINC ION (three-letter code: ZN) (formula: Zn).

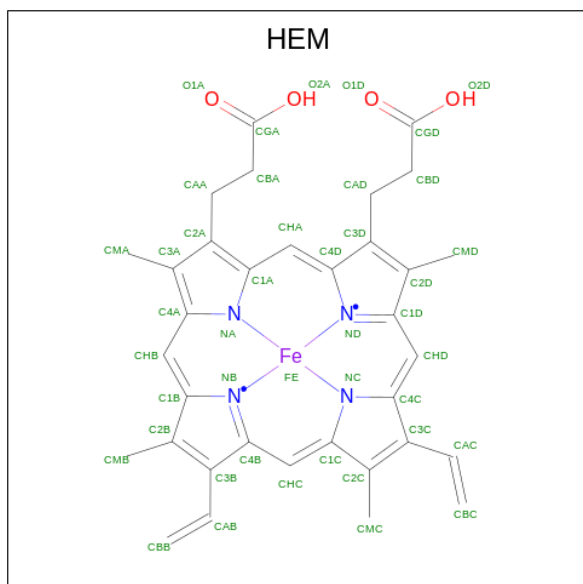
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
80	2	1	Total	Zn	0
			1	1	
80	B2	1	Total	Zn	0
			1	1	

- Molecule 81 is HEME C (three-letter code: HEC) (formula: C<sub>34</sub>H<sub>34</sub>FeN<sub>4</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Fe	N		O
81	AH	1	43	34	1	4	4	0
81	AU	1	43	34	1	4	4	0

- Molecule 82 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Fe	N		O
82	AJ	1	86	68	2	8	8	0

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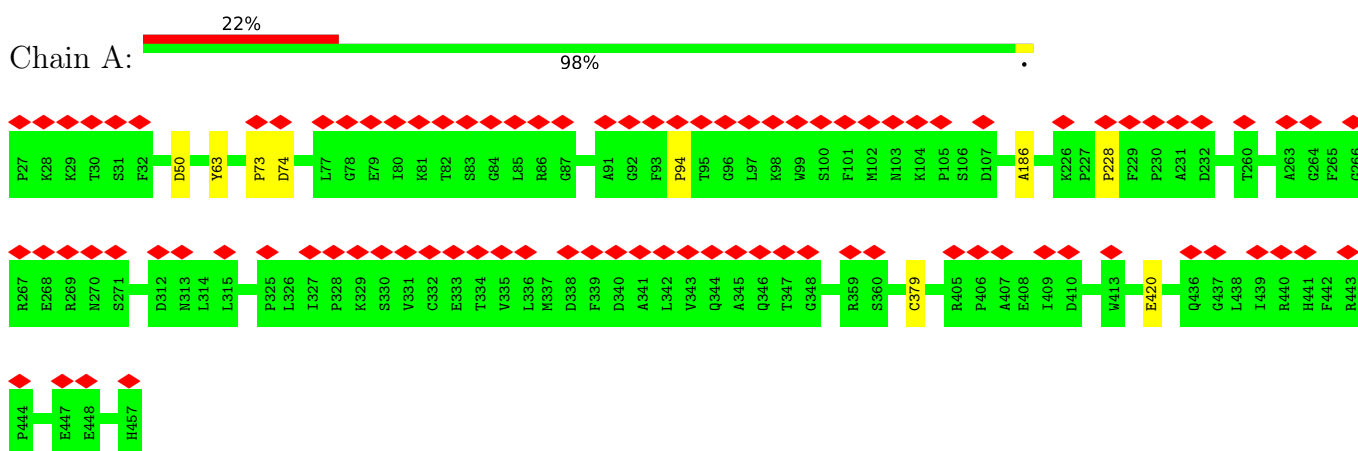
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Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Fe	N		O
82	AJ	1	Total 86	68	2	8	8	0
82	AV	1	Total 86	68	2	8	8	0
82	AV	1	Total 86	68	2	8	8	0

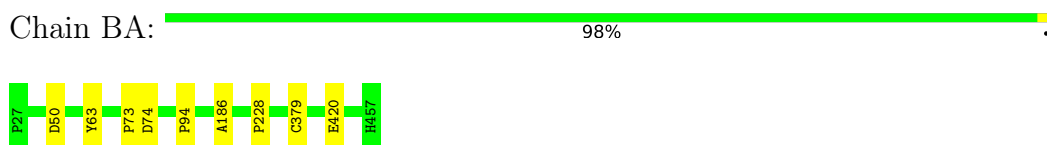
### 3 Residue-property plots

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

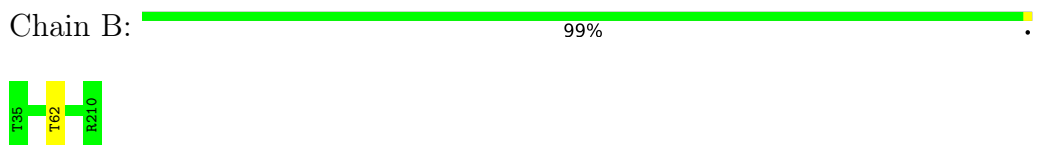
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



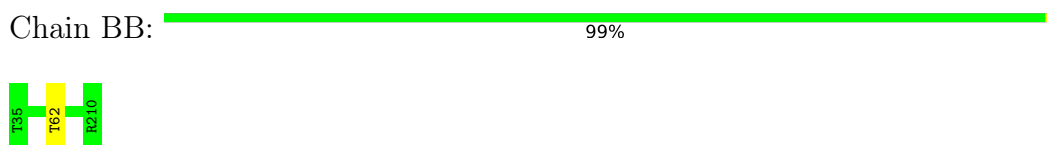
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain C:  97%



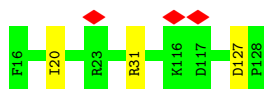
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain BC:  97%



- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain E:  97%



- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain BE:  97%



- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain F:  100%

There are no outlier residues recorded for this chain.

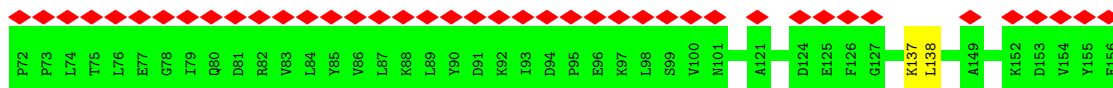
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain BF:  100%

There are no outlier residues recorded for this chain.

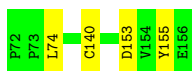
- Molecule 6: Acyl carrier protein, mitochondrial

Chain G:  48%  
98%

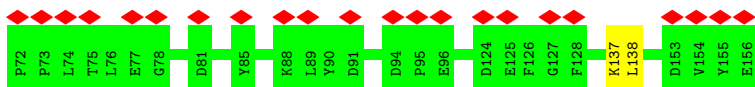


- Molecule 6: Acyl carrier protein, mitochondrial

Chain X:  95% 5%



- Molecule 6: Acyl carrier protein, mitochondrial



- Molecule 6: Acyl carrier protein, mitochondrial



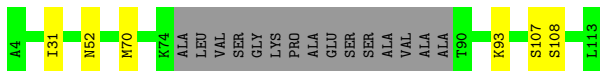
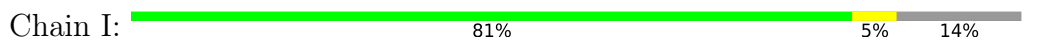
- Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



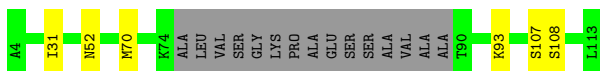
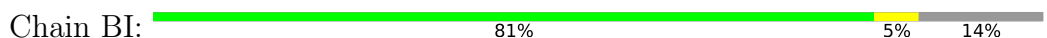
- Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



- Molecule 9: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial





- Molecule 9: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



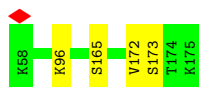
- Molecule 10: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



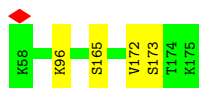
- Molecule 10: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



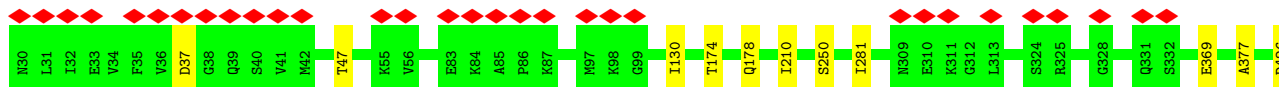
- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

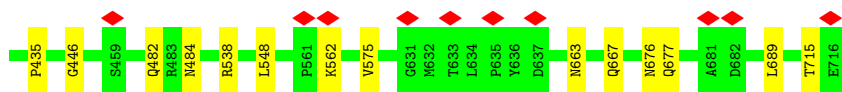


- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial





- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



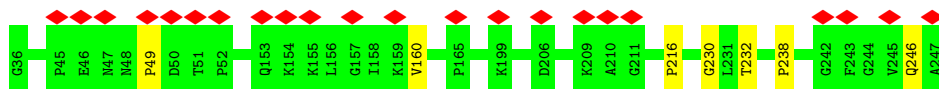
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



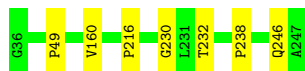
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



- Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



- Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain BP:  95% 5%



- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain Q:  98%



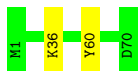
- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain BQ:  98%



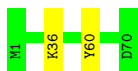
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain S:  97%



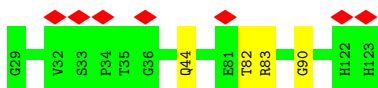
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain BS:  97%



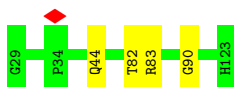
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain T:  7% 96%



- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain BT:  96%



- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain U:  99%



- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain BU:  99%



- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain V:  98%



- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain BV:  98%



- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain W:  96%



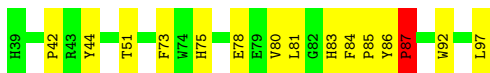
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain BW:  96%




- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

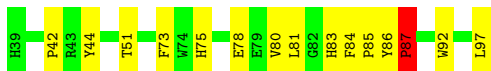
Chain Y:  75%





- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain BY:  75% 24%



- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain Z:  100%

There are no outlier residues recorded for this chain.

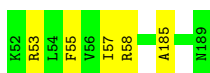
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain BZ:  100%

There are no outlier residues recorded for this chain.

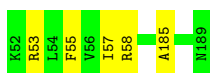
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain a:  96%




- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain Ba:  96%




- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain b:  90% 10%



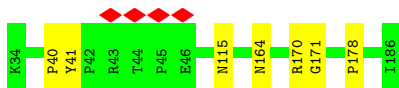
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain Bb:  90% 10%



- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain c:  95% 5%



- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain Bc:  95% 5%



- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain d:  95% 5%



- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain Bd:  95% 5%



- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain e:  97%



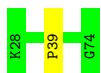
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain Be:  97%



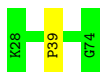
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain f:  98%



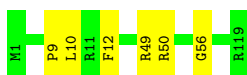
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain Bf:  98%



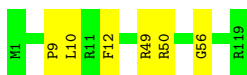
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain g:  95% 5%



- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain Bg:  95% 5%



- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain h:  94% 6%



- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain Bh:  94% 6%



- Molecule 32: NADH-ubiquinone oxidoreductase chain 2

Chain i:  98%



- Molecule 32: NADH-ubiquinone oxidoreductase chain 2

Chain Bi:  98%



- Molecule 33: NADH-ubiquinone oxidoreductase chain 3

Chain j:  97%



- Molecule 33: NADH-ubiquinone oxidoreductase chain 3

Chain Bj:  97%



- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

Chain k:  93% 6%



- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

Chain Bk:  93% 6%



- Molecule 35: NADH-ubiquinone oxidoreductase chain 5

Chain l:  95% 5%



- Molecule 35: NADH-ubiquinone oxidoreductase chain 5

Chain Bl:  95% 5%



- Molecule 36: NADH-ubiquinone oxidoreductase chain 6

Chain m:  94% 6%



- Molecule 36: NADH-ubiquinone oxidoreductase chain 6

Chain Bm:  94% 6%



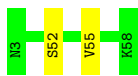
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain n:  96%



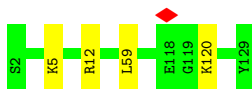
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain Bn:  96%



- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain o:  97%



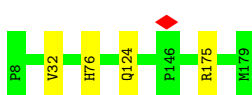
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain Bo:  97%



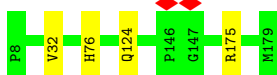
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain p:  98%



- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain Bp:  98%



- Molecule 40: NADH-ubiquinone oxidoreductase chain 4

Chain r:  98%



- Molecule 40: NADH-ubiquinone oxidoreductase chain 4

Chain Br:  98%



- Molecule 41: NADH-ubiquinone oxidoreductase chain 1

Chain s:  97%



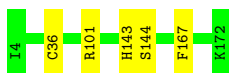
- Molecule 41: NADH-ubiquinone oxidoreductase chain 1

Chain Bs:  97%



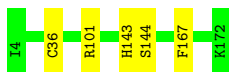
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain u:  97%




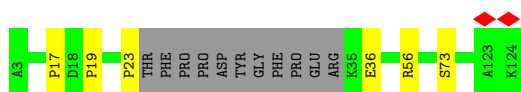
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain Bu:  97%




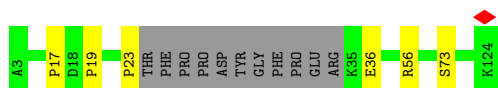
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain v:  86% 5% 9%



- Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain Bv:  86% 5% 9%



- Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain w:  97%



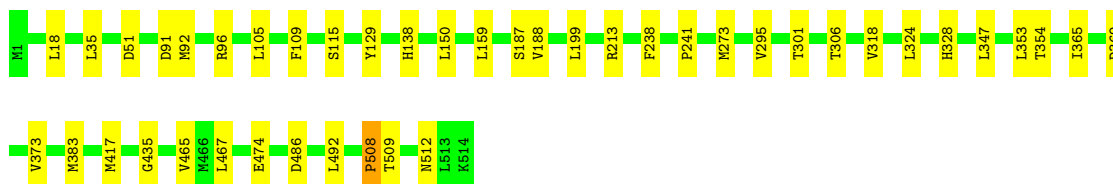
- Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain Bw:  97%



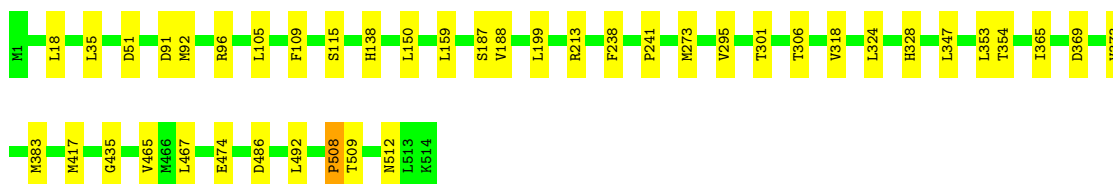
- Molecule 45: Cytochrome c oxidase subunit 1

Chain x:  92% 8%

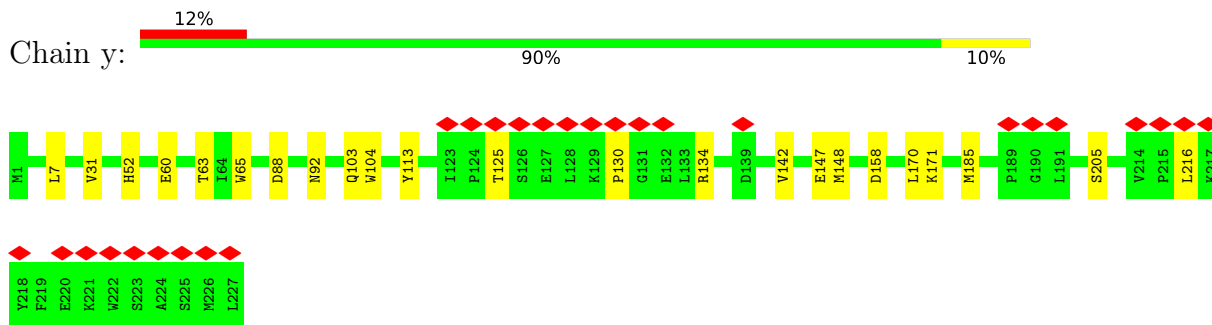


- Molecule 45: Cytochrome c oxidase subunit 1

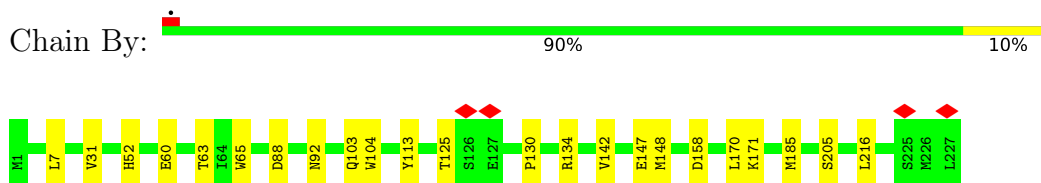
Chain Bx:  92% 8%



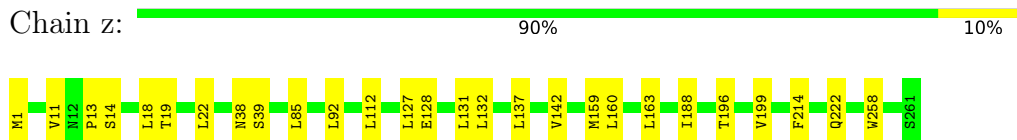
• Molecule 46: Cytochrome c oxidase subunit 2



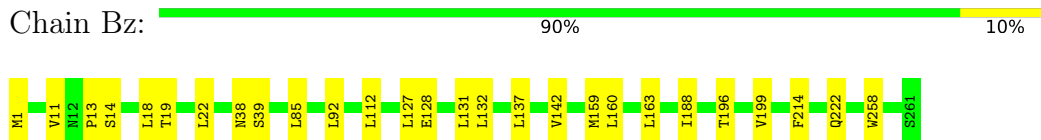
• Molecule 46: Cytochrome c oxidase subunit 2



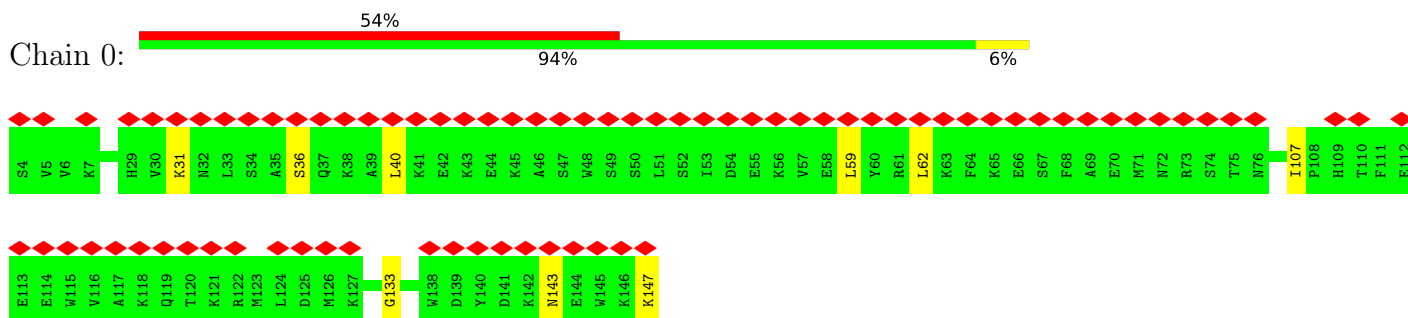
• Molecule 47: Cytochrome c oxidase subunit 3



• Molecule 47: Cytochrome c oxidase subunit 3



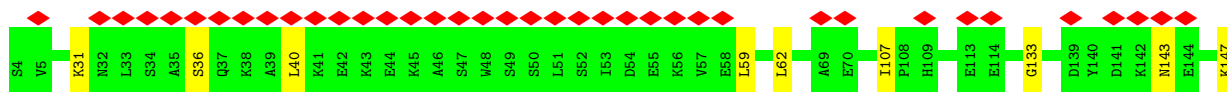
• Molecule 48: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



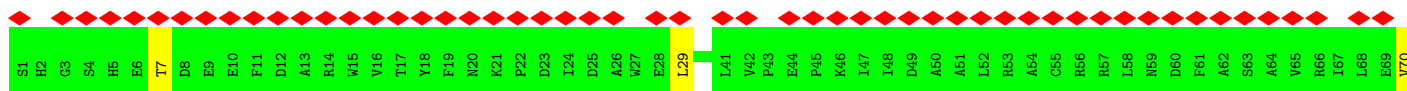
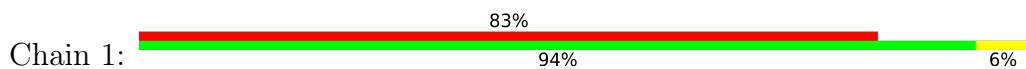
• Molecule 48: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



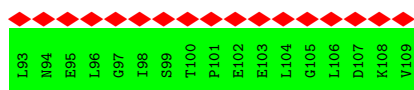
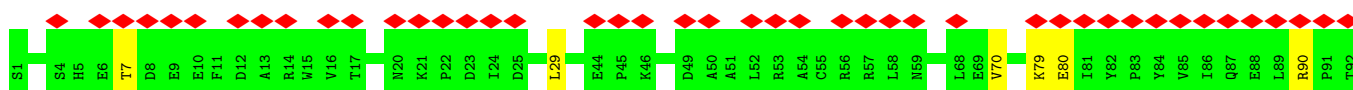




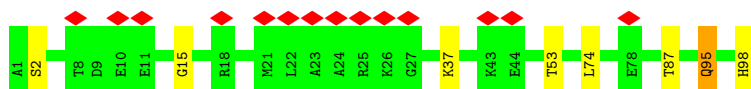
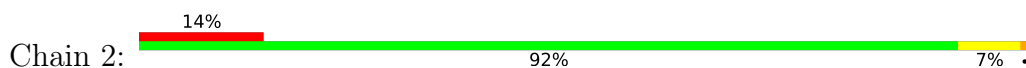
- Molecule 49: Cytochrome c oxidase subunit 5A, mitochondrial



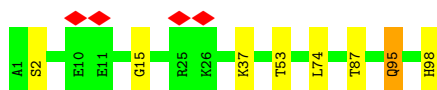
- Molecule 49: Cytochrome c oxidase subunit 5A, mitochondrial



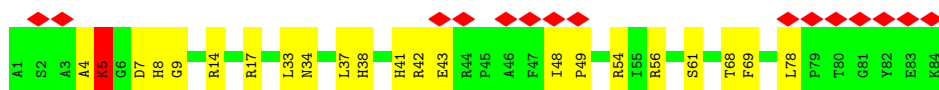
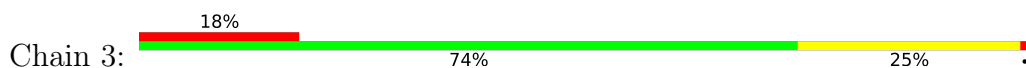
- Molecule 50: Cytochrome c oxidase subunit 5B, mitochondrial



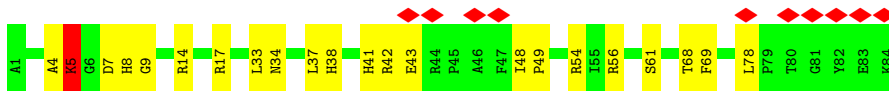
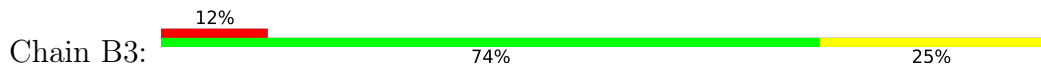
- Molecule 50: Cytochrome c oxidase subunit 5B, mitochondrial



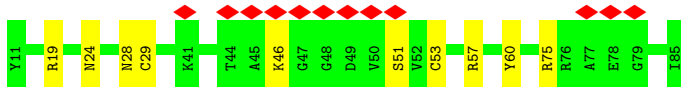
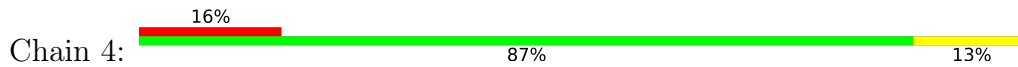
- Molecule 51: Cytochrome c oxidase subunit 6A2, mitochondrial



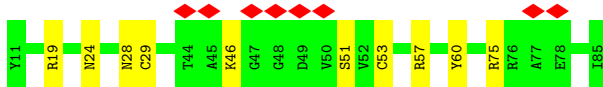
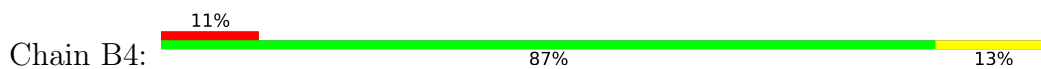
- Molecule 51: Cytochrome c oxidase subunit 6A2, mitochondrial



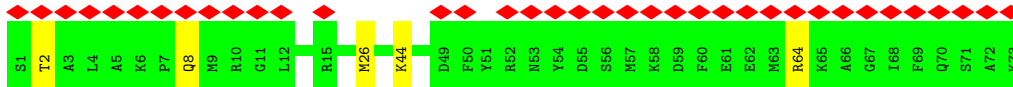
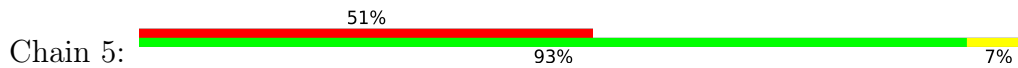
- Molecule 52: Cytochrome c oxidase subunit 6B1



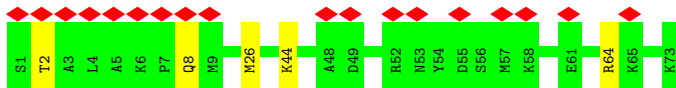
- Molecule 52: Cytochrome c oxidase subunit 6B1



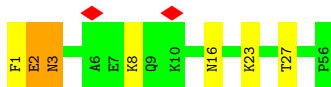
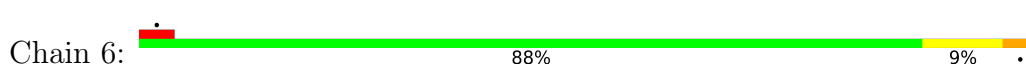
- Molecule 53: Cytochrome c oxidase subunit 6C



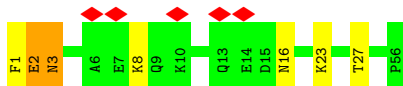
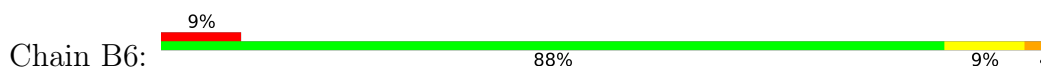
- Molecule 53: Cytochrome c oxidase subunit 6C



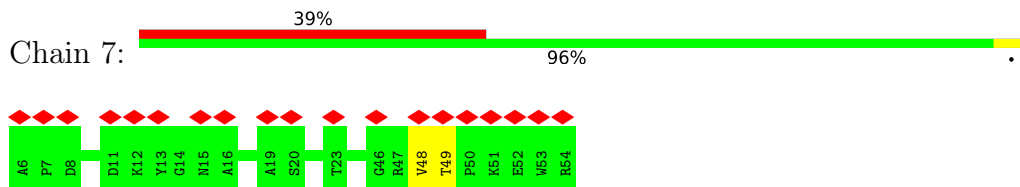
- Molecule 54: Cytochrome c oxidase subunit 7A1, mitochondrial



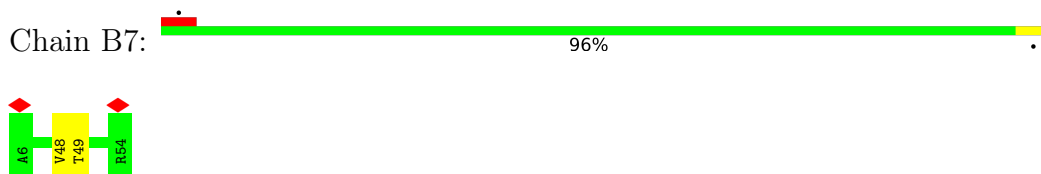
- Molecule 54: Cytochrome c oxidase subunit 7A1, mitochondrial



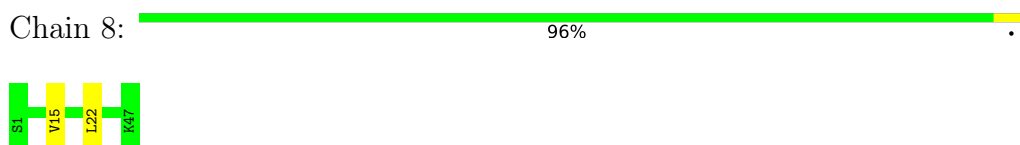
- Molecule 55: Cytochrome c oxidase subunit 7B, mitochondrial



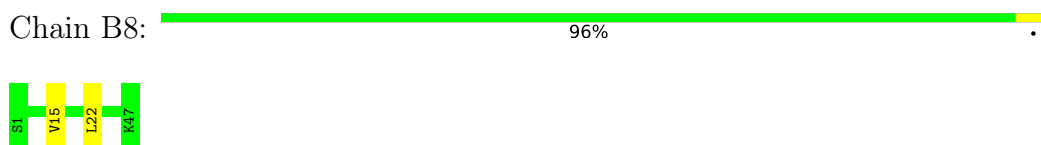
- Molecule 55: Cytochrome c oxidase subunit 7B, mitochondrial



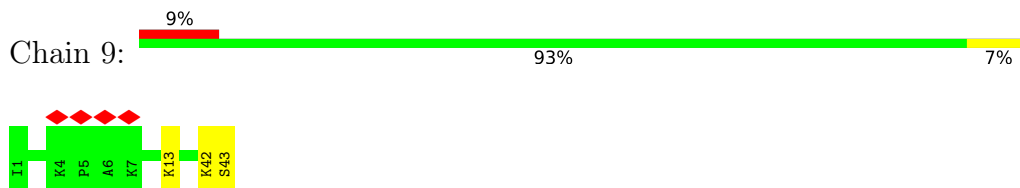
- Molecule 56: Cytochrome c oxidase subunit 7C, mitochondrial



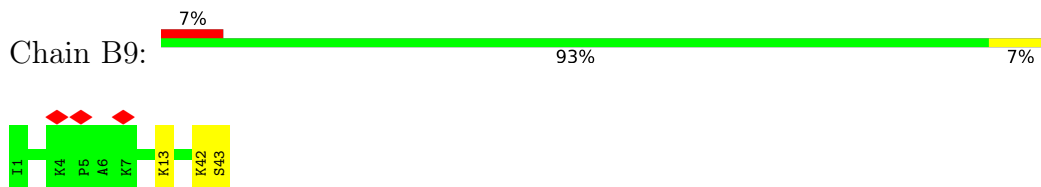
- Molecule 56: Cytochrome c oxidase subunit 7C, mitochondrial



- Molecule 57: Cytochrome c oxidase subunit 8B, mitochondrial



- Molecule 57: Cytochrome c oxidase subunit 8B, mitochondrial

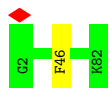


- Molecule 58: Cytochrome b-c1 complex subunit 8

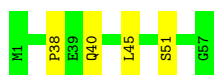




- Molecule 58: Cytochrome b-c1 complex subunit 8



- Molecule 59: Cytochrome b-c1 complex subunit Rieske, mitochondrial



- Molecule 59: Cytochrome b-c1 complex subunit Rieske, mitochondrial



- Molecule 60: Cytochrome b-c1 complex subunit Rieske, mitochondrial



- Molecule 60: Cytochrome b-c1 complex subunit Rieske, mitochondrial



- Molecule 61: Cytochrome b-c1 complex subunit 9



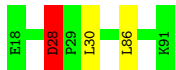
- Molecule 61: Cytochrome b-c1 complex subunit 9



There are no outlier residues recorded for this chain.

- Molecule 62: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain AE:  96%



- Molecule 62: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain AR:  96%



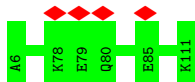
- Molecule 63: Cytochrome b-c1 complex subunit 7

Chain AF:  88% 12%



- Molecule 63: Cytochrome b-c1 complex subunit 7

Chain AS:  100%



- Molecule 64: Cytochrome b-c1 complex subunit 10

Chain AG:  100%

There are no outlier residues recorded for this chain.

- Molecule 64: Cytochrome b-c1 complex subunit 10

Chain AT:  96%



- Molecule 65: Cytochrome c1, heme protein, mitochondrial

Chain AH:  99%



- Molecule 65: Cytochrome c1, heme protein, mitochondrial

Chain AU:  99%



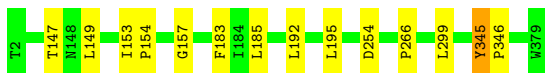
- Molecule 66: Cytochrome b

Chain AJ:  98%



- Molecule 66: Cytochrome b

Chain AV:  96%



- Molecule 67: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain AK:  98%



- Molecule 67: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain AW:  98%



- Molecule 68: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain AL:  99%



- Molecule 68: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain AY:  96%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	8600	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.054	Depositor
Minimum map value	-0.029	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0056	Depositor
Map size ( $\text{\AA}$ )	519.83997, 519.83997, 519.83997	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.083, 1.083, 1.083	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, 8Q1, PEE, NDP, HEM, HEA, HEC, FES, ZN, FMN, PLX, CU, MG, CDL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.30	0/3398	0.49	0/4590
1	BA	0.30	0/3398	0.49	0/4590
2	B	0.50	0/1452	0.57	0/1964
2	BB	0.50	0/1452	0.57	0/1964
3	BC	0.58	0/1280	0.57	0/1732
3	C	0.58	0/1280	0.57	0/1732
4	BE	0.34	0/993	0.54	0/1335
4	E	0.34	0/993	0.54	0/1335
5	BF	0.28	0/682	0.53	0/922
5	F	0.28	0/682	0.53	0/922
6	BG	0.33	0/684	0.53	0/926
6	BX	0.57	0/698	0.61	0/942
6	G	0.33	0/684	0.53	0/926
6	X	0.57	0/698	0.61	0/942
7	BH	0.34	0/941	0.59	0/1275
7	H	0.34	0/941	0.59	0/1275
8	BI	0.29	0/788	0.54	0/1066
8	I	0.29	0/788	0.54	0/1066
9	BJ	0.35	0/2785	0.52	0/3771
9	J	0.35	0/2785	0.52	0/3771
10	BK	0.27	0/282	0.47	0/381
10	K	0.27	0/282	0.47	0/381
11	BL	0.33	0/987	0.53	0/1331
11	L	0.33	0/987	0.53	0/1331
12	BM	0.32	0/5362	0.53	0/7266
12	M	0.32	0/5362	0.53	0/7266
13	BN	0.37	0/1236	0.55	0/1681
13	N	0.37	0/1236	0.55	0/1681
14	BO	0.29	0/1682	0.51	0/2289
14	O	0.29	0/1682	0.51	0/2289
15	BP	0.38	0/1780	0.59	0/2424
15	P	0.38	0/1780	0.59	0/2424



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	BQ	0.43	0/3552	0.59	1/4815 (0.0%)
16	Q	0.43	0/3552	0.59	1/4815 (0.0%)
17	BS	0.60	0/583	0.64	0/785
17	S	0.60	0/583	0.64	0/785
18	BT	0.32	0/755	0.47	0/1017
18	T	0.32	0/755	0.47	0/1017
19	BU	0.52	0/670	0.63	0/920
19	U	0.52	0/670	0.63	0/920
20	BV	0.51	0/1065	0.61	0/1450
20	V	0.51	0/1065	0.61	0/1450
21	BW	0.57	0/1166	0.68	1/1579 (0.1%)
21	W	0.57	0/1166	0.68	1/1579 (0.1%)
22	BY	0.52	0/559	0.73	3/763 (0.4%)
22	Y	0.52	0/559	0.73	3/763 (0.4%)
23	BZ	0.45	0/669	0.53	0/899
23	Z	0.45	0/669	0.53	0/899
24	Ba	0.68	0/1209	0.65	0/1639
24	a	0.69	0/1209	0.65	0/1639
25	Bb	0.59	1/1095 (0.1%)	0.69	4/1480 (0.3%)
25	b	0.59	1/1095 (0.1%)	0.69	4/1480 (0.3%)
26	Bc	0.58	0/1287	0.59	0/1761
26	c	0.58	0/1287	0.58	0/1761
27	Bd	0.63	0/1445	0.65	1/1945 (0.1%)
27	d	0.63	0/1445	0.65	1/1945 (0.1%)
28	Be	0.61	0/835	0.62	0/1134
28	e	0.61	0/835	0.62	0/1134
29	Bf	0.48	0/418	0.58	0/566
29	f	0.48	0/418	0.58	0/566
30	Bg	0.64	0/1035	0.63	0/1398
30	g	0.64	0/1035	0.63	0/1398
31	Bh	0.62	0/884	0.65	0/1182
31	h	0.62	0/884	0.65	0/1182
32	Bi	0.67	0/2808	0.77	2/3843 (0.1%)
32	i	0.67	0/2808	0.77	2/3843 (0.1%)
33	Bj	0.55	0/945	0.70	1/1292 (0.1%)
33	j	0.55	0/945	0.69	1/1292 (0.1%)
34	Bk	0.68	1/751 (0.1%)	0.79	1/1019 (0.1%)
34	k	0.68	1/751 (0.1%)	0.79	1/1019 (0.1%)
35	Bl	0.61	0/4840	0.70	3/6611 (0.0%)
35	l	0.61	1/4840 (0.0%)	0.70	3/6611 (0.0%)
36	Bm	0.68	0/1346	0.67	0/1832
36	m	0.68	0/1346	0.67	0/1832
37	Bn	0.49	0/484	0.62	0/652

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
37	n	0.50	0/484	0.62	0/652
38	Bo	0.54	0/1093	0.61	0/1479
38	o	0.54	0/1090	0.61	0/1475
39	Bp	0.59	0/1549	0.59	0/2098
39	p	0.59	0/1549	0.59	0/2098
40	Br	0.71	0/3723	0.76	2/5089 (0.0%)
40	r	0.71	0/3723	0.76	2/5089 (0.0%)
41	Bs	0.62	0/2580	0.73	0/3539
41	s	0.62	0/2580	0.73	0/3539
42	Bu	0.57	0/1433	0.61	0/1937
42	u	0.57	0/1433	0.61	0/1937
43	Bv	0.49	0/934	0.67	3/1241 (0.2%)
43	v	0.49	0/934	0.67	3/1241 (0.2%)
44	Bw	0.44	0/2533	0.56	0/3440
44	w	0.44	0/2533	0.56	0/3440
45	Bx	0.60	0/4164	0.76	1/5688 (0.0%)
45	x	0.60	0/4164	0.76	2/5688 (0.0%)
46	By	0.58	0/1868	0.80	0/2544
46	y	0.58	0/1868	0.80	0/2544
47	Bz	0.56	0/2211	0.69	0/3023
47	z	0.56	0/2211	0.69	0/3023
48	0	0.57	0/1229	0.65	1/1658 (0.1%)
48	B0	0.57	0/1229	0.65	1/1658 (0.1%)
49	1	0.50	0/898	0.66	0/1218
49	B1	0.50	0/898	0.66	0/1218
50	2	0.56	0/765	0.81	0/1038
50	B2	0.56	0/765	0.81	0/1038
51	3	0.55	0/699	0.73	1/950 (0.1%)
51	B3	0.55	0/699	0.73	1/950 (0.1%)
52	4	0.55	0/648	0.73	0/877
52	B4	0.55	0/648	0.73	0/877
53	5	0.61	0/611	0.64	0/810
53	B5	0.60	0/611	0.65	0/810
54	6	0.60	0/451	0.72	0/610
54	B6	0.60	0/451	0.71	0/610
55	7	0.58	0/398	0.66	0/546
55	B7	0.58	0/398	0.66	0/546
56	8	0.63	0/399	0.62	0/534
56	B8	0.63	0/399	0.62	0/534
57	9	0.51	0/345	0.65	0/470
57	B9	0.52	0/345	0.65	0/470
58	AA	0.31	0/715	0.48	0/964
58	AN	0.27	0/707	0.49	0/953

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
59	AB	0.23	0/421	0.60	1/574 (0.2%)
59	AO	0.25	0/417	0.61	1/569 (0.2%)
60	AC	0.24	0/1554	0.43	0/2104
60	AP	0.24	0/1554	0.42	0/2104
61	AD	0.26	0/521	0.42	0/699
61	AQ	0.27	0/521	0.43	0/699
62	AE	0.35	0/587	0.54	1/789 (0.1%)
62	AR	0.27	0/587	0.46	0/789
63	AF	0.42	0/942	0.52	1/1263 (0.1%)
63	AS	0.27	0/942	0.44	0/1263
64	AG	0.27	0/442	0.48	0/608
64	AT	0.28	0/442	0.49	0/608
65	AH	0.26	0/1983	0.46	0/2691
65	AU	0.27	0/1983	0.45	0/2691
66	AJ	0.31	1/3108 (0.0%)	0.52	1/4254 (0.0%)
66	AV	0.34	2/3108 (0.1%)	0.54	2/4254 (0.0%)
67	AK	0.27	0/3217	0.49	0/4361
67	AW	0.29	1/3220 (0.0%)	0.48	1/4365 (0.0%)
68	AL	0.27	0/3514	0.47	0/4769
68	AY	0.30	1/3499 (0.0%)	0.51	2/4750 (0.0%)
All	All	0.49	10/197905 (0.0%)	0.62	61/268649 (0.0%)

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
44	Bw	0	1
44	w	0	1
All	All	0	2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	AW	448	PRO	N-CD	5.28	1.55	1.47
66	AJ	154	PRO	N-CD	5.24	1.55	1.47
66	AV	154	PRO	N-CD	5.23	1.55	1.47
25	b	118	PRO	N-CD	5.21	1.55	1.47
34	k	2	PRO	N-CD	5.20	1.55	1.47
34	Bk	2	PRO	N-CD	5.19	1.55	1.47
25	Bb	118	PRO	N-CD	5.13	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
68	AY	425	PRO	N-CD	5.12	1.55	1.47
35	l	91	PRO	N-CD	5.04	1.54	1.47
66	AV	346	PRO	N-CD	5.01	1.54	1.47

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	i	323	THR	C-N-CD	-7.38	104.37	120.60
32	Bi	323	THR	C-N-CD	-7.37	104.38	120.60
21	BW	31	SER	N-CA-C	-7.01	92.08	111.00
21	W	31	SER	N-CA-C	-7.00	92.09	111.00
22	BY	92	TRP	N-CA-C	-6.99	92.12	111.00
22	Y	92	TRP	N-CA-C	-6.98	92.15	111.00
27	d	2	PRO	N-CA-CB	6.77	111.42	103.30
27	Bd	2	PRO	N-CA-CB	6.74	111.39	103.30
22	BY	87	PRO	CA-N-CD	-6.55	102.33	111.50
22	Y	87	PRO	CA-N-CD	-6.54	102.34	111.50
48	B0	133	GLY	N-CA-C	6.42	129.15	113.10
48	0	133	GLY	N-CA-C	6.42	129.14	113.10
25	b	36	PRO	C-N-CD	6.19	141.40	128.40
25	Bb	36	PRO	C-N-CD	6.18	141.38	128.40
62	AE	28	ASP	C-N-CD	6.14	141.30	128.40
32	Bi	323	THR	C-N-CA	6.05	147.41	122.00
32	i	323	THR	C-N-CA	6.04	147.39	122.00
43	v	17	PRO	N-CA-CB	5.92	110.40	103.30
43	Bv	17	PRO	N-CA-CB	5.92	110.40	103.30
43	v	23	PRO	N-CA-CB	5.89	110.37	103.30
43	Bv	23	PRO	N-CA-CB	5.88	110.35	103.30
35	Bl	197	ASP	C-N-CD	5.87	140.73	128.40
35	l	197	ASP	C-N-CD	5.87	140.72	128.40
66	AV	345	TYR	C-N-CD	5.80	140.59	128.40
25	b	105	PHE	C-N-CD	5.79	140.56	128.40
66	AV	153	ILE	C-N-CD	5.79	140.56	128.40
25	Bb	105	PHE	C-N-CD	5.78	140.54	128.40
34	k	1	MET	C-N-CD	5.76	140.51	128.40
34	Bk	1	MET	C-N-CD	5.75	140.47	128.40
66	AJ	153	ILE	C-N-CD	5.73	140.43	128.40
35	Bl	90	ILE	C-N-CD	5.73	140.42	128.40
43	Bv	19	PRO	N-CA-CB	5.72	110.17	103.30
35	l	90	ILE	C-N-CD	5.70	140.38	128.40
43	v	19	PRO	N-CA-CB	5.70	110.14	103.30
68	AY	424	ILE	C-N-CD	5.69	140.36	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Bb	117	ILE	C-N-CD	5.69	140.35	128.40
35	l	230	HIS	C-N-CD	5.69	140.35	128.40
25	b	117	ILE	C-N-CD	5.67	140.31	128.40
63	AF	51	LEU	C-N-CD	5.67	140.31	128.40
35	Bl	230	HIS	C-N-CD	5.66	140.28	128.40
16	BQ	97	LEU	CA-CB-CG	5.64	128.27	115.30
67	AW	447	THR	C-N-CD	5.64	140.24	128.40
16	Q	97	LEU	CA-CB-CG	5.63	128.26	115.30
59	AB	45	LEU	CA-CB-CG	5.46	127.86	115.30
33	Bj	98	LEU	CB-CG-CD2	-5.44	101.75	111.00
25	Bb	37	PRO	CA-N-CD	-5.39	103.95	111.50
25	b	37	PRO	CA-N-CD	-5.38	103.96	111.50
33	j	98	LEU	CB-CG-CD2	-5.38	101.85	111.00
68	AY	421	GLY	N-CA-C	-5.37	99.67	113.10
59	AO	45	LEU	CA-CB-CG	5.29	127.47	115.30
51	3	5	LYS	N-CA-C	5.25	125.17	111.00
51	B3	5	LYS	N-CA-C	5.25	125.16	111.00
45	x	435	GLY	N-CA-C	5.24	126.20	113.10
45	Bx	435	GLY	N-CA-C	5.23	126.17	113.10
22	BY	86	TYR	C-N-CD	5.17	139.25	128.40
22	Y	86	TYR	C-N-CD	5.13	139.18	128.40
40	r	238	LEU	CB-CG-CD2	-5.10	102.33	111.00
40	Br	408	LEU	CA-CB-CG	-5.10	103.58	115.30
40	r	408	LEU	CA-CB-CG	-5.09	103.59	115.30
40	Br	238	LEU	CB-CG-CD2	-5.08	102.37	111.00
45	x	129	TYR	CB-CA-C	-5.01	100.39	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
44	Bw	338	LYS	Peptide
44	w	338	LYS	Peptide

## 5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	
1	A	429/431 (100%)	396 (92%)	24 (6%)	9 (2%)	7	36
1	BA	429/431 (100%)	396 (92%)	24 (6%)	9 (2%)	7	36
2	B	174/176 (99%)	163 (94%)	10 (6%)	1 (1%)	25	66
2	BB	174/176 (99%)	163 (94%)	10 (6%)	1 (1%)	25	66
3	BC	154/156 (99%)	136 (88%)	13 (8%)	5 (3%)	4	26
3	C	154/156 (99%)	136 (88%)	13 (8%)	5 (3%)	4	26
4	BE	111/113 (98%)	101 (91%)	8 (7%)	2 (2%)	8	40
4	E	111/113 (98%)	101 (91%)	8 (7%)	2 (2%)	8	40
5	BF	81/83 (98%)	74 (91%)	7 (9%)	0	100	100
5	F	81/83 (98%)	74 (91%)	7 (9%)	0	100	100
6	BG	83/85 (98%)	78 (94%)	3 (4%)	2 (2%)	6	33
6	BX	83/85 (98%)	73 (88%)	6 (7%)	4 (5%)	2	21
6	G	83/85 (98%)	78 (94%)	3 (4%)	2 (2%)	6	33
6	X	83/85 (98%)	73 (88%)	6 (7%)	4 (5%)	2	21
7	BH	110/112 (98%)	100 (91%)	5 (4%)	5 (4%)	2	22
7	H	110/112 (98%)	100 (91%)	5 (4%)	5 (4%)	2	22
8	BI	91/110 (83%)	79 (87%)	6 (7%)	6 (7%)	1	16
8	I	91/110 (83%)	79 (87%)	6 (7%)	6 (7%)	1	16
9	BJ	335/337 (99%)	314 (94%)	14 (4%)	7 (2%)	7	36
9	J	335/337 (99%)	314 (94%)	14 (4%)	7 (2%)	7	36
10	BK	31/33 (94%)	27 (87%)	1 (3%)	3 (10%)	0	10
10	K	31/33 (94%)	27 (87%)	1 (3%)	3 (10%)	0	10
11	BL	116/118 (98%)	104 (90%)	8 (7%)	4 (3%)	3	26
11	L	116/118 (98%)	104 (90%)	8 (7%)	4 (3%)	3	26
12	BM	685/687 (100%)	608 (89%)	54 (8%)	23 (3%)	3	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	M	685/687 (100%)	608 (89%)	54 (8%)	23 (3%)	3	26
13	BN	141/143 (99%)	119 (84%)	15 (11%)	7 (5%)	2	20
13	N	141/143 (99%)	119 (84%)	15 (11%)	7 (5%)	2	20
14	BO	210/212 (99%)	188 (90%)	15 (7%)	7 (3%)	4	26
14	O	210/212 (99%)	188 (90%)	15 (7%)	7 (3%)	4	26
15	BP	206/208 (99%)	173 (84%)	22 (11%)	11 (5%)	2	19
15	P	206/208 (99%)	173 (84%)	22 (11%)	11 (5%)	2	19
16	BQ	428/430 (100%)	398 (93%)	23 (5%)	7 (2%)	9	44
16	Q	428/430 (100%)	398 (93%)	23 (5%)	7 (2%)	9	44
17	BS	68/70 (97%)	61 (90%)	5 (7%)	2 (3%)	4	29
17	S	68/70 (97%)	61 (90%)	5 (7%)	2 (3%)	4	29
18	BT	93/95 (98%)	87 (94%)	2 (2%)	4 (4%)	2	22
18	T	93/95 (98%)	87 (94%)	2 (2%)	4 (4%)	2	22
19	BU	81/83 (98%)	76 (94%)	4 (5%)	1 (1%)	13	50
19	U	81/83 (98%)	76 (94%)	4 (5%)	1 (1%)	13	50
20	BV	138/140 (99%)	129 (94%)	6 (4%)	3 (2%)	6	35
20	V	138/140 (99%)	129 (94%)	6 (4%)	3 (2%)	6	35
21	BW	136/138 (99%)	127 (93%)	4 (3%)	5 (4%)	3	24
21	W	136/138 (99%)	127 (93%)	4 (3%)	5 (4%)	3	24
22	BY	57/59 (97%)	50 (88%)	1 (2%)	6 (10%)	0	8
22	Y	57/59 (97%)	50 (88%)	1 (2%)	6 (10%)	0	8
23	BZ	78/80 (98%)	73 (94%)	5 (6%)	0	100	100
23	Z	78/80 (98%)	73 (94%)	5 (6%)	0	100	100
24	Ba	136/138 (99%)	121 (89%)	12 (9%)	3 (2%)	6	35
24	a	136/138 (99%)	121 (89%)	12 (9%)	3 (2%)	6	35
25	Bb	122/124 (98%)	107 (88%)	10 (8%)	5 (4%)	3	23
25	b	122/124 (98%)	107 (88%)	10 (8%)	5 (4%)	3	23
26	Bc	151/153 (99%)	129 (85%)	15 (10%)	7 (5%)	2	21
26	c	151/153 (99%)	129 (85%)	15 (10%)	7 (5%)	2	21
27	Bd	169/171 (99%)	165 (98%)	3 (2%)	1 (1%)	25	66
27	d	169/171 (99%)	165 (98%)	3 (2%)	1 (1%)	25	66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	Be	95/97 (98%)	83 (87%)	9 (10%)	3 (3%)	4	26
28	e	95/97 (98%)	83 (87%)	9 (10%)	3 (3%)	4	26
29	Bf	45/47 (96%)	43 (96%)	1 (2%)	1 (2%)	6	35
29	f	45/47 (96%)	43 (96%)	1 (2%)	1 (2%)	6	35
30	Bg	117/119 (98%)	105 (90%)	6 (5%)	6 (5%)	2	19
30	g	117/119 (98%)	105 (90%)	6 (5%)	6 (5%)	2	19
31	Bh	102/104 (98%)	86 (84%)	10 (10%)	6 (6%)	1	17
31	h	102/104 (98%)	87 (85%)	9 (9%)	6 (6%)	1	17
32	Bi	345/347 (99%)	324 (94%)	15 (4%)	6 (2%)	9	42
32	i	345/347 (99%)	324 (94%)	15 (4%)	6 (2%)	9	42
33	Bj	113/115 (98%)	103 (91%)	7 (6%)	3 (3%)	5	31
33	j	113/115 (98%)	103 (91%)	7 (6%)	3 (3%)	5	31
34	Bk	95/97 (98%)	88 (93%)	4 (4%)	3 (3%)	4	26
34	k	95/97 (98%)	88 (93%)	4 (4%)	3 (3%)	4	26
35	Bl	601/603 (100%)	553 (92%)	38 (6%)	10 (2%)	9	42
35	l	601/603 (100%)	553 (92%)	38 (6%)	10 (2%)	9	42
36	Bm	172/174 (99%)	150 (87%)	12 (7%)	10 (6%)	1	18
36	m	172/174 (99%)	150 (87%)	12 (7%)	10 (6%)	1	18
37	Bn	54/56 (96%)	50 (93%)	2 (4%)	2 (4%)	3	24
37	n	54/56 (96%)	50 (93%)	2 (4%)	2 (4%)	3	24
38	Bo	126/128 (98%)	113 (90%)	9 (7%)	4 (3%)	4	26
38	o	126/128 (98%)	113 (90%)	9 (7%)	4 (3%)	4	26
39	Bp	170/172 (99%)	158 (93%)	9 (5%)	3 (2%)	8	40
39	p	170/172 (99%)	158 (93%)	9 (5%)	3 (2%)	8	40
40	Br	457/459 (100%)	420 (92%)	28 (6%)	9 (2%)	7	38
40	r	457/459 (100%)	420 (92%)	28 (6%)	9 (2%)	7	38
41	Bs	316/318 (99%)	285 (90%)	22 (7%)	9 (3%)	5	30
41	s	316/318 (99%)	285 (90%)	22 (7%)	9 (3%)	5	30
42	Bu	167/169 (99%)	152 (91%)	10 (6%)	5 (3%)	4	28
42	u	167/169 (99%)	152 (91%)	10 (6%)	5 (3%)	4	28
43	Bv	107/122 (88%)	90 (84%)	14 (13%)	3 (3%)	5	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	v	107/122 (88%)	90 (84%)	14 (13%)	3 (3%)	5	30
44	Bw	318/320 (99%)	281 (88%)	28 (9%)	9 (3%)	5	30
44	w	318/320 (99%)	281 (88%)	28 (9%)	9 (3%)	5	30
45	Bx	512/514 (100%)	479 (94%)	29 (6%)	4 (1%)	19	60
45	x	512/514 (100%)	479 (94%)	29 (6%)	4 (1%)	19	60
46	By	225/227 (99%)	203 (90%)	19 (8%)	3 (1%)	12	48
46	y	225/227 (99%)	203 (90%)	19 (8%)	3 (1%)	12	48
47	Bz	259/261 (99%)	249 (96%)	10 (4%)	0	100	100
47	z	259/261 (99%)	249 (96%)	10 (4%)	0	100	100
48	0	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
48	B0	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
49	1	107/109 (98%)	104 (97%)	3 (3%)	0	100	100
49	B1	107/109 (98%)	104 (97%)	3 (3%)	0	100	100
50	2	96/98 (98%)	86 (90%)	6 (6%)	4 (4%)	3	22
50	B2	96/98 (98%)	86 (90%)	6 (6%)	4 (4%)	3	22
51	3	82/84 (98%)	67 (82%)	10 (12%)	5 (6%)	1	17
51	B3	82/84 (98%)	67 (82%)	10 (12%)	5 (6%)	1	17
52	4	73/75 (97%)	64 (88%)	8 (11%)	1 (1%)	11	46
52	B4	73/75 (97%)	64 (88%)	8 (11%)	1 (1%)	11	46
53	5	71/73 (97%)	65 (92%)	6 (8%)	0	100	100
53	B5	71/73 (97%)	65 (92%)	6 (8%)	0	100	100
54	6	54/56 (96%)	47 (87%)	5 (9%)	2 (4%)	3	24
54	B6	54/56 (96%)	47 (87%)	5 (9%)	2 (4%)	3	24
55	7	47/49 (96%)	41 (87%)	6 (13%)	0	100	100
55	B7	47/49 (96%)	41 (87%)	6 (13%)	0	100	100
56	8	45/47 (96%)	42 (93%)	3 (7%)	0	100	100
56	B8	45/47 (96%)	42 (93%)	3 (7%)	0	100	100
57	9	41/43 (95%)	39 (95%)	2 (5%)	0	100	100
57	B9	41/43 (95%)	39 (95%)	2 (5%)	0	100	100
58	AA	79/81 (98%)	71 (90%)	6 (8%)	2 (2%)	5	32
58	AN	79/81 (98%)	74 (94%)	4 (5%)	1 (1%)	12	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
59	AB	55/57 (96%)	41 (74%)	11 (20%)	3 (6%)	2	19
59	AO	55/57 (96%)	43 (78%)	6 (11%)	6 (11%)	0	8
60	AC	194/196 (99%)	179 (92%)	10 (5%)	5 (3%)	5	31
60	AP	194/196 (99%)	178 (92%)	13 (7%)	3 (2%)	10	46
61	AD	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
61	AQ	60/62 (97%)	55 (92%)	5 (8%)	0	100	100
62	AE	72/74 (97%)	65 (90%)	5 (7%)	2 (3%)	5	30
62	AR	72/74 (97%)	69 (96%)	2 (3%)	1 (1%)	11	46
63	AF	104/106 (98%)	100 (96%)	3 (3%)	1 (1%)	15	55
63	AS	104/106 (98%)	102 (98%)	2 (2%)	0	100	100
64	AG	49/51 (96%)	48 (98%)	1 (2%)	0	100	100
64	AT	49/51 (96%)	47 (96%)	2 (4%)	0	100	100
65	AH	239/241 (99%)	225 (94%)	12 (5%)	2 (1%)	19	60
65	AU	239/241 (99%)	230 (96%)	7 (3%)	2 (1%)	19	60
66	AJ	376/378 (100%)	363 (96%)	10 (3%)	3 (1%)	19	60
66	AV	376/378 (100%)	359 (96%)	14 (4%)	3 (1%)	19	60
67	AK	417/419 (100%)	390 (94%)	22 (5%)	5 (1%)	13	50
67	AW	417/419 (100%)	397 (95%)	15 (4%)	5 (1%)	13	50
68	AL	444/446 (100%)	403 (91%)	35 (8%)	6 (1%)	11	46
68	AY	444/446 (100%)	414 (93%)	22 (5%)	8 (2%)	8	40
All	All	23880/24216 (99%)	21833 (91%)	1487 (6%)	560 (2%)	9	34

All (560) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	TYR
1	A	73	PRO
1	A	379	CYS
2	B	62	THR
12	M	37	ASP
12	M	47	THR
12	M	178	GLN
12	M	210	ILE
12	M	369	GLU
13	N	115	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
14	O	232	THR
14	O	246	GLN
15	P	167	GLU
17	S	60	TYR
18	T	82	THR
19	U	71	GLN
21	W	34	SER
6	X	155	TYR
22	Y	84	PHE
24	a	58	ARG
26	c	115	ASN
26	c	178	PRO
27	d	2	PRO
31	h	20	ILE
32	i	91	ASN
32	i	323	THR
33	j	24	LEU
33	j	26	GLN
34	k	52	HIS
35	l	450	LEU
36	m	115	VAL
36	m	116	VAL
36	m	118	PHE
37	n	55	VAL
40	r	52	CYS
40	r	346	GLN
44	w	57	SER
44	w	282	PRO
44	w	347	VAL
45	x	328	HIS
45	x	508	PRO
50	2	2	SER
50	2	87	THR
50	2	95	GLN
51	3	4	ALA
51	3	9	GLY
52	4	46	LYS
54	6	2	GLU
66	AJ	268	ILE
67	AK	241	ARG
59	AO	23	ALA
60	AP	141	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
68	AY	424	ILE
1	BA	63	TYR
1	BA	73	PRO
1	BA	379	CYS
2	BB	62	THR
12	BM	37	ASP
12	BM	47	THR
12	BM	178	GLN
12	BM	210	ILE
12	BM	369	GLU
13	BN	115	PHE
14	BO	232	THR
14	BO	246	GLN
15	BP	167	GLU
17	BS	60	TYR
18	BT	82	THR
19	BU	71	GLN
21	BW	34	SER
6	BX	155	TYR
22	BY	84	PHE
24	Ba	58	ARG
26	Bc	115	ASN
26	Bc	178	PRO
27	Bd	2	PRO
31	Bh	20	ILE
32	Bi	91	ASN
32	Bi	323	THR
33	Bj	24	LEU
33	Bj	26	GLN
34	Bk	52	HIS
35	Bl	450	LEU
36	Bm	115	VAL
36	Bm	116	VAL
36	Bm	118	PHE
37	Bn	55	VAL
40	Br	52	CYS
40	Br	346	GLN
44	Bw	57	SER
44	Bw	282	PRO
44	Bw	347	VAL
45	Bx	328	HIS
45	Bx	508	PRO

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
50	B2	2	SER
50	B2	87	THR
50	B2	95	GLN
51	B3	4	ALA
51	B3	9	GLY
52	B4	46	LYS
54	B6	2	GLU
3	C	84	PHE
3	C	165	SER
4	E	20	ILE
4	E	127	ASP
6	G	138	LEU
7	H	105	GLU
8	I	31	ILE
8	I	93	LYS
8	I	107	SER
9	J	87	ASP
11	L	173	SER
12	M	250	SER
12	M	482	GLN
12	M	484	ASN
12	M	562	LYS
12	M	663	ASN
12	M	676	ASN
13	N	19	GLY
13	N	76	ASP
14	O	49	PRO
14	O	160	VAL
16	Q	104	GLU
16	Q	117	HIS
18	T	44	GLN
20	V	135	VAL
20	V	140	LYS
21	W	11	PRO
22	Y	44	TYR
22	Y	51	THR
24	a	57	ILE
24	a	185	ALA
25	b	101	LYS
26	c	170	ARG
30	g	9	PRO
31	h	3	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
31	h	24	GLU
31	h	43	CYS
33	j	2	ASN
35	l	73	THR
36	m	122	GLY
37	n	52	SER
40	r	45	ILE
40	r	188	ASN
40	r	250	LEU
40	r	421	HIS
41	s	203	GLY
41	s	213	ILE
41	s	217	ALA
41	s	316	PRO
43	v	56	ARG
44	w	264	GLN
44	w	285	LYS
51	3	5	LYS
60	AC	153	GLU
60	AC	255	PRO
66	AJ	157	GLY
67	AK	176	ASN
59	AO	38	PRO
60	AP	255	PRO
66	AV	157	GLY
66	AV	254	ASP
66	AV	266	PRO
67	AW	244	LEU
68	AY	312	GLY
68	AY	322	VAL
3	BC	84	PHE
3	BC	165	SER
4	BE	20	ILE
4	BE	127	ASP
6	BG	138	LEU
7	BH	105	GLU
8	BI	31	ILE
8	BI	93	LYS
8	BI	107	SER
9	BJ	87	ASP
11	BL	173	SER
12	BM	250	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
12	BM	482	GLN
12	BM	484	ASN
12	BM	562	LYS
12	BM	663	ASN
12	BM	676	ASN
13	BN	19	GLY
13	BN	76	ASP
14	BO	49	PRO
14	BO	160	VAL
16	BQ	104	GLU
16	BQ	117	HIS
18	BT	44	GLN
20	BV	135	VAL
20	BV	140	LYS
21	BW	11	PRO
22	BY	44	TYR
22	BY	51	THR
24	Ba	57	ILE
24	Ba	185	ALA
25	Bb	101	LYS
26	Bc	170	ARG
30	Bg	9	PRO
31	Bh	3	PHE
31	Bh	24	GLU
31	Bh	43	CYS
33	Bj	2	ASN
35	Bl	73	THR
36	Bm	122	GLY
37	Bn	52	SER
40	Br	45	ILE
40	Br	188	ASN
40	Br	250	LEU
40	Br	421	HIS
41	Bs	203	GLY
41	Bs	213	ILE
41	Bs	217	ALA
41	Bs	316	PRO
43	Bv	56	ARG
44	Bw	264	GLN
44	Bw	285	LYS
51	B3	5	LYS
1	A	74	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	H	8	THR
7	H	63	PRO
8	I	52	ASN
9	J	135	GLU
9	J	178	SER
10	K	101	SER
11	L	165	SER
12	M	538	ARG
12	M	677	GLN
12	M	689	LEU
12	M	715	THR
13	N	113	HIS
14	O	238	PRO
15	P	44	ARG
15	P	179	ALA
15	P	214	ASP
15	P	229	GLU
16	Q	36	GLN
16	Q	197	MET
18	T	83	ARG
6	X	140	CYS
22	Y	85	PRO
25	b	37	PRO
25	b	109	THR
26	c	164	ASN
28	e	61	PRO
28	e	111	ASP
30	g	10	LEU
30	g	12	PHE
30	g	50	ARG
32	i	87	THR
34	k	83	ASN
34	k	96	LEU
35	l	65	ASN
35	l	451	LEU
35	l	549	PRO
35	l	554	ASP
35	l	563	PRO
36	m	4	ALA
36	m	76	GLU
36	m	110	ASP
38	o	5	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
38	o	12	ARG
40	r	139	GLN
41	s	38	ASN
42	u	36	CYS
42	u	101	ARG
42	u	143	HIS
43	v	73	SER
44	w	351	TRP
46	y	104	TRP
51	3	61	SER
58	AA	13	HIS
58	AA	29	HIS
59	AB	38	PRO
63	AF	8	SER
65	AH	133	ARG
67	AK	244	LEU
68	AL	180	ARG
68	AL	312	GLY
68	AL	322	VAL
58	AN	46	PHE
59	AO	51	SER
67	AW	241	ARG
67	AW	261	GLN
68	AY	382	SER
1	BA	74	ASP
7	BH	8	THR
7	BH	63	PRO
8	BI	52	ASN
9	BJ	135	GLU
9	BJ	178	SER
10	BK	101	SER
11	BL	165	SER
12	BM	538	ARG
12	BM	677	GLN
12	BM	689	LEU
12	BM	715	THR
13	BN	113	HIS
14	BO	238	PRO
15	BP	44	ARG
15	BP	179	ALA
15	BP	214	ASP
15	BP	229	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
16	BQ	36	GLN
16	BQ	197	MET
18	BT	83	ARG
6	BX	140	CYS
22	BY	85	PRO
25	Bb	37	PRO
25	Bb	109	THR
26	Bc	164	ASN
28	Be	61	PRO
28	Be	111	ASP
30	Bg	10	LEU
30	Bg	12	PHE
30	Bg	50	ARG
32	Bi	87	THR
34	Bk	83	ASN
34	Bk	96	LEU
35	Bl	65	ASN
35	Bl	451	LEU
35	Bl	549	PRO
35	Bl	554	ASP
35	Bl	563	PRO
36	Bm	4	ALA
36	Bm	76	GLU
36	Bm	110	ASP
38	Bo	5	LYS
38	Bo	12	ARG
40	Br	139	GLN
41	Bs	38	ASN
42	Bu	36	CYS
42	Bu	101	ARG
42	Bu	143	HIS
43	Bv	73	SER
44	Bw	351	TRP
46	By	104	TRP
51	B3	61	SER
1	A	50	ASP
1	A	186	ALA
3	C	156	GLY
7	H	76	GLN
8	I	108	SER
9	J	100	LEU
9	J	330	PRO

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
9	J	370	LYS
10	K	78	ASP
11	L	172	VAL
12	M	377	ALA
12	M	426	ASP
13	N	42	ASP
13	N	130	THR
14	O	216	PRO
14	O	230	GLY
15	P	175	GLY
15	P	246	ARG
17	S	36	LYS
21	W	16	TYR
6	X	74	LEU
22	Y	42	PRO
22	Y	87	PRO
25	b	115	GLU
26	c	40	PRO
26	c	41	TYR
30	g	49	ARG
30	g	56	GLY
31	h	32	ARG
31	h	45	HIS
32	i	150	ASN
35	l	249	SER
35	l	387	THR
35	l	562	LEU
38	o	59	LEU
38	o	120	LYS
39	p	76	HIS
40	r	251	ASN
41	s	208	VAL
41	s	288	LEU
41	s	289	LEU
42	u	167	PHE
43	v	36	GLU
45	x	51	ASP
59	AB	51	SER
60	AC	142	ALA
60	AC	204	ARG
60	AC	219	HIS
62	AE	86	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
67	AK	261	GLN
68	AL	193	GLN
62	AR	28	ASP
65	AU	133	ARG
67	AW	144	PRO
67	AW	403	ALA
68	AY	193	GLN
68	AY	461	PRO
1	BA	50	ASP
1	BA	186	ALA
3	BC	156	GLY
7	BH	76	GLN
8	BI	108	SER
9	BJ	100	LEU
9	BJ	330	PRO
9	BJ	370	LYS
10	BK	78	ASP
11	BL	172	VAL
12	BM	377	ALA
12	BM	426	ASP
13	BN	42	ASP
13	BN	130	THR
14	BO	216	PRO
14	BO	230	GLY
15	BP	175	GLY
15	BP	246	ARG
17	BS	36	LYS
21	BW	16	TYR
6	BX	74	LEU
22	BY	42	PRO
22	BY	87	PRO
25	Bb	115	GLU
26	Bc	40	PRO
26	Bc	41	TYR
30	Bg	49	ARG
30	Bg	56	GLY
31	Bh	32	ARG
31	Bh	45	HIS
32	Bi	150	ASN
35	Bl	249	SER
35	Bl	387	THR
35	Bl	562	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
38	Bo	59	LEU
38	Bo	120	LYS
39	Bp	76	HIS
40	Br	251	ASN
41	Bs	208	VAL
41	Bs	288	LEU
41	Bs	289	LEU
42	Bu	167	PHE
43	Bv	36	GLU
45	Bx	51	ASP
1	A	228	PRO
1	A	420	GLU
7	H	103	LEU
9	J	259	ASN
12	M	281	ILE
12	M	548	LEU
12	M	667	GLN
15	P	110	SER
15	P	202	PHE
15	P	239	TRP
15	P	245	TYR
16	Q	102	SER
20	V	48	THR
6	X	153	ASP
26	c	171	GLY
32	i	92	GLN
36	m	113	VAL
39	p	175	ARG
42	u	144	SER
44	w	58	ARG
44	w	121	PRO
44	w	160	GLU
46	y	103	GLN
54	6	3	ASN
59	AB	40	GLN
62	AE	28	ASP
68	AL	463	GLU
59	AO	27	ARG
59	AO	40	GLN
60	AP	204	ARG
65	AU	246	PRO
68	AY	463	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	BA	228	PRO
1	BA	420	GLU
7	BH	103	LEU
9	BJ	259	ASN
12	BM	281	ILE
12	BM	548	LEU
12	BM	667	GLN
15	BP	110	SER
15	BP	202	PHE
15	BP	239	TRP
15	BP	245	TYR
16	BQ	102	SER
20	BV	48	THR
6	BX	153	ASP
26	Bc	171	GLY
32	Bi	92	GLN
36	Bm	113	VAL
39	Bp	175	ARG
42	Bu	144	SER
44	Bw	58	ARG
44	Bw	121	PRO
44	Bw	160	GLU
46	By	103	GLN
54	B6	3	ASN
3	C	102	ASP
6	G	137	LYS
8	I	70	MET
11	L	96	LYS
12	M	446	GLY
13	N	135	GLN
18	T	90	GLY
25	b	41	GLY
29	f	39	PRO
36	m	24	SER
39	p	32	VAL
40	r	205	VAL
45	x	91	ASP
46	y	158	ASP
51	3	49	PRO
65	AH	246	PRO
66	AJ	286	ASN
68	AL	279	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	BC	102	ASP
6	BG	137	LYS
8	BI	70	MET
11	BL	96	LYS
12	BM	446	GLY
13	BN	135	GLN
18	BT	90	GLY
25	Bb	41	GLY
29	Bf	39	PRO
36	Bm	24	SER
39	Bp	32	VAL
40	Br	205	VAL
45	Bx	91	ASP
46	By	158	ASP
51	B3	49	PRO
12	M	435	PRO
21	W	10	MET
41	s	241	ILE
12	BM	435	PRO
21	BW	10	MET
41	Bs	241	ILE
1	A	94	PRO
12	M	575	VAL
21	W	32	GLY
36	m	23	PRO
50	2	15	GLY
59	AO	30	VAL
1	BA	94	PRO
12	BM	575	VAL
36	Bm	23	PRO
50	B2	15	GLY
3	C	144	PRO
16	Q	307	PRO
3	BC	144	PRO
16	BQ	307	PRO
21	BW	32	GLY
16	Q	69	VAL
67	AK	320	PRO
68	AY	267	PRO
16	BQ	69	VAL
10	K	102	GLY
32	i	338	PRO

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Mol	Chain	Res	Type
10	BK	102	GLY
32	Bi	338	PRO
28	e	135	PRO
28	Be	135	PRO

### 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	
1	A	346/346 (100%)	346 (100%)	0	100	100
1	BA	346/346 (100%)	346 (100%)	0	100	100
2	B	151/151 (100%)	151 (100%)	0	100	100
2	BB	151/151 (100%)	151 (100%)	0	100	100
3	BC	132/132 (100%)	132 (100%)	0	100	100
3	C	132/132 (100%)	132 (100%)	0	100	100
4	BE	106/106 (100%)	105 (99%)	1 (1%)	78	87
4	E	106/106 (100%)	105 (99%)	1 (1%)	78	87
5	BF	74/74 (100%)	74 (100%)	0	100	100
5	F	74/74 (100%)	74 (100%)	0	100	100
6	BG	74/79 (94%)	74 (100%)	0	100	100
6	BX	78/79 (99%)	78 (100%)	0	100	100
6	G	74/79 (94%)	74 (100%)	0	100	100
6	X	78/79 (99%)	78 (100%)	0	100	100
7	BH	100/100 (100%)	100 (100%)	0	100	100
7	H	100/100 (100%)	100 (100%)	0	100	100
8	BI	87/96 (91%)	87 (100%)	0	100	100
8	I	87/96 (91%)	87 (100%)	0	100	100
9	BJ	292/292 (100%)	288 (99%)	4 (1%)	67	80
9	J	292/292 (100%)	288 (99%)	4 (1%)	67	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	BK	32/32 (100%)	32 (100%)	0	100	100
10	K	32/32 (100%)	32 (100%)	0	100	100
11	BL	107/107 (100%)	107 (100%)	0	100	100
11	L	107/107 (100%)	107 (100%)	0	100	100
12	BM	576/577 (100%)	574 (100%)	2 (0%)	92	95
12	M	576/577 (100%)	574 (100%)	2 (0%)	92	95
13	BN	129/129 (100%)	129 (100%)	0	100	100
13	N	129/129 (100%)	129 (100%)	0	100	100
14	BO	181/181 (100%)	181 (100%)	0	100	100
14	O	181/181 (100%)	181 (100%)	0	100	100
15	BP	190/190 (100%)	190 (100%)	0	100	100
15	P	190/190 (100%)	190 (100%)	0	100	100
16	BQ	371/371 (100%)	369 (100%)	2 (0%)	88	93
16	Q	371/371 (100%)	369 (100%)	2 (0%)	88	93
17	BS	59/59 (100%)	59 (100%)	0	100	100
17	S	59/59 (100%)	59 (100%)	0	100	100
18	BT	79/79 (100%)	79 (100%)	0	100	100
18	T	79/79 (100%)	79 (100%)	0	100	100
19	BU	72/72 (100%)	72 (100%)	0	100	100
19	U	72/72 (100%)	72 (100%)	0	100	100
20	BV	102/102 (100%)	102 (100%)	0	100	100
20	V	102/102 (100%)	102 (100%)	0	100	100
21	BW	119/119 (100%)	119 (100%)	0	100	100
21	W	119/119 (100%)	119 (100%)	0	100	100
22	BY	57/57 (100%)	49 (86%)	8 (14%)	3	17
22	Y	57/57 (100%)	49 (86%)	8 (14%)	3	17
23	BZ	62/63 (98%)	62 (100%)	0	100	100
23	Z	62/63 (98%)	62 (100%)	0	100	100
24	Ba	124/124 (100%)	122 (98%)	2 (2%)	62	79
24	a	124/124 (100%)	122 (98%)	2 (2%)	62	79
25	Bb	118/118 (100%)	114 (97%)	4 (3%)	37	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	b	118/118 (100%)	114 (97%)	4 (3%)	37	60
26	Bc	124/137 (90%)	124 (100%)	0	100	100
26	c	124/137 (90%)	124 (100%)	0	100	100
27	Bd	145/154 (94%)	137 (94%)	8 (6%)	21	47
27	d	145/154 (94%)	137 (94%)	8 (6%)	21	47
28	Be	90/90 (100%)	90 (100%)	0	100	100
28	e	90/90 (100%)	90 (100%)	0	100	100
29	Bf	43/43 (100%)	43 (100%)	0	100	100
29	f	43/43 (100%)	43 (100%)	0	100	100
30	Bg	105/105 (100%)	105 (100%)	0	100	100
30	g	105/105 (100%)	105 (100%)	0	100	100
31	Bh	90/90 (100%)	90 (100%)	0	100	100
31	h	90/90 (100%)	90 (100%)	0	100	100
32	Bi	314/314 (100%)	314 (100%)	0	100	100
32	i	314/314 (100%)	314 (100%)	0	100	100
33	Bj	102/103 (99%)	102 (100%)	0	100	100
33	j	102/103 (99%)	102 (100%)	0	100	100
34	Bk	85/85 (100%)	82 (96%)	3 (4%)	36	59
34	k	85/85 (100%)	82 (96%)	3 (4%)	36	59
35	Bl	531/532 (100%)	510 (96%)	21 (4%)	31	55
35	l	531/532 (100%)	510 (96%)	21 (4%)	31	55
36	Bm	137/137 (100%)	137 (100%)	0	100	100
36	m	137/137 (100%)	137 (100%)	0	100	100
37	Bn	53/53 (100%)	53 (100%)	0	100	100
37	n	53/53 (100%)	53 (100%)	0	100	100
38	Bo	114/114 (100%)	114 (100%)	0	100	100
38	o	113/114 (99%)	113 (100%)	0	100	100
39	Bp	157/157 (100%)	156 (99%)	1 (1%)	86	92
39	p	157/157 (100%)	156 (99%)	1 (1%)	86	92
40	Br	416/416 (100%)	416 (100%)	0	100	100
40	r	416/416 (100%)	416 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	Bs	278/278 (100%)	278 (100%)	0	100	100
41	s	278/278 (100%)	278 (100%)	0	100	100
42	Bu	153/153 (100%)	153 (100%)	0	100	100
42	u	153/153 (100%)	153 (100%)	0	100	100
43	Bv	89/111 (80%)	89 (100%)	0	100	100
43	v	89/111 (80%)	89 (100%)	0	100	100
44	Bw	249/288 (86%)	249 (100%)	0	100	100
44	w	249/288 (86%)	249 (100%)	0	100	100
45	Bx	427/427 (100%)	389 (91%)	38 (9%)	9	30
45	x	427/427 (100%)	389 (91%)	38 (9%)	9	30
46	By	211/211 (100%)	191 (90%)	20 (10%)	8	27
46	y	211/211 (100%)	191 (90%)	20 (10%)	8	27
47	Bz	226/226 (100%)	199 (88%)	27 (12%)	5	20
47	z	226/226 (100%)	199 (88%)	27 (12%)	5	20
48	0	128/128 (100%)	120 (94%)	8 (6%)	18	43
48	B0	128/128 (100%)	120 (94%)	8 (6%)	18	43
49	1	95/95 (100%)	89 (94%)	6 (6%)	18	43
49	B1	95/95 (100%)	89 (94%)	6 (6%)	18	43
50	2	81/81 (100%)	76 (94%)	5 (6%)	18	43
50	B2	81/81 (100%)	76 (94%)	5 (6%)	18	43
51	3	68/68 (100%)	50 (74%)	18 (26%)	0	3
51	B3	68/68 (100%)	50 (74%)	18 (26%)	0	3
52	4	67/67 (100%)	58 (87%)	9 (13%)	4	17
52	B4	67/67 (100%)	58 (87%)	9 (13%)	4	17
53	5	58/58 (100%)	53 (91%)	5 (9%)	10	32
53	B5	58/58 (100%)	53 (91%)	5 (9%)	10	32
54	6	47/47 (100%)	40 (85%)	7 (15%)	3	15
54	B6	47/47 (100%)	40 (85%)	7 (15%)	3	15
55	7	39/39 (100%)	37 (95%)	2 (5%)	24	48
55	B7	39/39 (100%)	37 (95%)	2 (5%)	24	48
56	8	40/40 (100%)	38 (95%)	2 (5%)	24	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
56	B8	40/40 (100%)	38 (95%)	2 (5%)	24	49
57	9	37/37 (100%)	34 (92%)	3 (8%)	11	35
57	B9	37/37 (100%)	34 (92%)	3 (8%)	11	35
58	AA	74/74 (100%)	68 (92%)	6 (8%)	11	35
58	AN	73/74 (99%)	73 (100%)	0	100	100
59	AB	46/46 (100%)	46 (100%)	0	100	100
59	AO	45/46 (98%)	45 (100%)	0	100	100
60	AC	166/166 (100%)	166 (100%)	0	100	100
60	AP	166/166 (100%)	166 (100%)	0	100	100
61	AD	52/52 (100%)	52 (100%)	0	100	100
61	AQ	52/52 (100%)	52 (100%)	0	100	100
62	AE	61/71 (86%)	59 (97%)	2 (3%)	38	61
62	AR	61/71 (86%)	59 (97%)	2 (3%)	38	61
63	AF	95/95 (100%)	84 (88%)	11 (12%)	5	21
63	AS	95/95 (100%)	95 (100%)	0	100	100
64	AG	42/42 (100%)	42 (100%)	0	100	100
64	AT	42/42 (100%)	40 (95%)	2 (5%)	25	51
65	AH	207/207 (100%)	207 (100%)	0	100	100
65	AU	207/207 (100%)	206 (100%)	1 (0%)	88	93
66	AJ	330/330 (100%)	327 (99%)	3 (1%)	78	87
66	AV	330/330 (100%)	322 (98%)	8 (2%)	49	69
67	AK	334/335 (100%)	331 (99%)	3 (1%)	78	87
67	AW	335/335 (100%)	332 (99%)	3 (1%)	78	87
68	AL	365/367 (100%)	365 (100%)	0	100	100
68	AY	362/367 (99%)	355 (98%)	7 (2%)	57	75
All	All	20773/21008 (99%)	20313 (98%)	460 (2%)	54	71

All (460) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	E	31	ARG
9	J	85	ARG
9	J	91	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
9	J	180	TYR
9	J	212	ARG
12	M	130	ILE
12	M	174	THR
16	Q	268	TRP
16	Q	273	ILE
22	Y	73	PHE
22	Y	75	HIS
22	Y	78	GLU
22	Y	80	VAL
22	Y	81	LEU
22	Y	83	HIS
22	Y	87	PRO
22	Y	97	LEU
24	a	53	ARG
24	a	55	PHE
25	b	21	ARG
25	b	38	GLN
25	b	111	LEU
25	b	112	GLU
27	d	54	ARG
27	d	55	TYR
27	d	57	TYR
27	d	60	ARG
27	d	61	GLN
27	d	113	GLN
27	d	115	TYR
27	d	117	GLN
34	k	1	MET
34	k	3	LEU
34	k	8	ILE
35	l	25	ASN
35	l	59	GLN
35	l	87	MET
35	l	88	MET
35	l	94	LEU
35	l	95	PHE
35	l	97	THR
35	l	99	SER
35	l	191	LEU
35	l	193	SER
35	l	195	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
35	l	196	TRP
35	l	197	ASP
35	l	217	LEU
35	l	218	LEU
35	l	223	LYS
35	l	226	GLN
35	l	447	ASN
35	l	450	LEU
35	l	452	ASN
35	l	513	MET
39	p	124	GLN
45	x	18	LEU
45	x	35	LEU
45	x	92	MET
45	x	96	ARG
45	x	105	LEU
45	x	109	PHE
45	x	115	SER
45	x	138	HIS
45	x	150	LEU
45	x	159	LEU
45	x	187	SER
45	x	188	VAL
45	x	199	LEU
45	x	213	ARG
45	x	238	PHE
45	x	241	PRO
45	x	273	MET
45	x	295	VAL
45	x	301	THR
45	x	306	THR
45	x	318	VAL
45	x	324	LEU
45	x	347	LEU
45	x	353	LEU
45	x	354	THR
45	x	365	ILE
45	x	369	ASP
45	x	373	VAL
45	x	383	MET
45	x	417	MET
45	x	465	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	x	467	LEU
45	x	474	GLU
45	x	486	ASP
45	x	492	LEU
45	x	508	PRO
45	x	509	THR
45	x	512	ASN
46	y	7	LEU
46	y	31	VAL
46	y	52	HIS
46	y	60	GLU
46	y	63	THR
46	y	65	TRP
46	y	88	ASP
46	y	92	ASN
46	y	113	TYR
46	y	125	THR
46	y	130	PRO
46	y	134	ARG
46	y	142	VAL
46	y	147	GLU
46	y	148	MET
46	y	170	LEU
46	y	171	LYS
46	y	185	MET
46	y	205	SER
46	y	216	LEU
47	z	1	MET
47	z	11	VAL
47	z	13	PRO
47	z	14	SER
47	z	18	LEU
47	z	19	THR
47	z	22	LEU
47	z	38	ASN
47	z	39	SER
47	z	85	LEU
47	z	92	LEU
47	z	112	LEU
47	z	127	LEU
47	z	128	GLU
47	z	131	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
47	z	132	LEU
47	z	137	LEU
47	z	142	VAL
47	z	159	MET
47	z	160	LEU
47	z	163	LEU
47	z	188	ILE
47	z	196	THR
47	z	199	VAL
47	z	214	PHE
47	z	222	GLN
47	z	258	TRP
48	0	31	LYS
48	0	36	SER
48	0	40	LEU
48	0	59	LEU
48	0	62	LEU
48	0	107	ILE
48	0	143	ASN
48	0	147	LYS
49	1	7	THR
49	1	29	LEU
49	1	70	VAL
49	1	79	LYS
49	1	80	GLU
49	1	90	ARG
50	2	37	LYS
50	2	53	THR
50	2	74	LEU
50	2	95	GLN
50	2	98	HIS
51	3	5	LYS
51	3	7	ASP
51	3	8	HIS
51	3	14	ARG
51	3	17	ARG
51	3	33	LEU
51	3	34	ASN
51	3	37	LEU
51	3	38	HIS
51	3	41	HIS
51	3	42	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
51	3	43	GLU
51	3	48	ILE
51	3	54	ARG
51	3	56	ARG
51	3	68	THR
51	3	69	PHE
51	3	78	LEU
52	4	19	ARG
52	4	24	ASN
52	4	28	ASN
52	4	29	CYS
52	4	51	SER
52	4	53	CYS
52	4	57	ARG
52	4	60	TYR
52	4	75	ARG
53	5	2	THR
53	5	8	GLN
53	5	26	MET
53	5	44	LYS
53	5	64	ARG
54	6	1	PHE
54	6	2	GLU
54	6	3	ASN
54	6	8	LYS
54	6	16	ASN
54	6	23	LYS
54	6	27	THR
55	7	48	VAL
55	7	49	THR
56	8	15	VAL
56	8	22	LEU
57	9	13	LYS
57	9	42	LYS
57	9	43	SER
58	AA	25	ARG
58	AA	40	ARG
58	AA	48	ARG
58	AA	61	THR
58	AA	64	THR
58	AA	66	GLU
62	AE	28	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
62	AE	30	LEU
63	AF	14	LEU
63	AF	17	ILE
63	AF	29	LYS
63	AF	33	MET
63	AF	34	ARG
63	AF	40	GLU
63	AF	41	ASP
63	AF	49	ARG
63	AF	60	MET
63	AF	71	LEU
63	AF	74	GLN
66	AJ	124	MET
66	AJ	150	LEU
66	AJ	300	ILE
67	AK	49	ILE
67	AK	365	ASN
67	AK	451	ASP
62	AR	78	ARG
62	AR	81	CYS
64	AT	39	ARG
64	AT	40	LEU
65	AU	292	MET
66	AV	147	THR
66	AV	149	LEU
66	AV	183	PHE
66	AV	185	LEU
66	AV	192	LEU
66	AV	195	LEU
66	AV	299	LEU
66	AV	345	TYR
67	AW	254	ARG
67	AW	451	ASP
67	AW	453	LEU
68	AY	92	PHE
68	AY	96	LEU
68	AY	265	LEU
68	AY	416	SER
68	AY	418	LEU
68	AY	422	ARG
68	AY	423	ARG
4	BE	31	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
9	BJ	85	ARG
9	BJ	91	ILE
9	BJ	180	TYR
9	BJ	212	ARG
12	BM	130	ILE
12	BM	174	THR
16	BQ	268	TRP
16	BQ	273	ILE
22	BY	73	PHE
22	BY	75	HIS
22	BY	78	GLU
22	BY	80	VAL
22	BY	81	LEU
22	BY	83	HIS
22	BY	87	PRO
22	BY	97	LEU
24	Ba	53	ARG
24	Ba	55	PHE
25	Bb	21	ARG
25	Bb	38	GLN
25	Bb	111	LEU
25	Bb	112	GLU
27	Bd	54	ARG
27	Bd	55	TYR
27	Bd	57	TYR
27	Bd	60	ARG
27	Bd	61	GLN
27	Bd	113	GLN
27	Bd	115	TYR
27	Bd	117	GLN
34	Bk	1	MET
34	Bk	3	LEU
34	Bk	8	ILE
35	Bl	25	ASN
35	Bl	59	GLN
35	Bl	87	MET
35	Bl	88	MET
35	Bl	94	LEU
35	Bl	95	PHE
35	Bl	97	THR
35	Bl	99	SER
35	Bl	191	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
35	B1	193	SER
35	B1	195	SER
35	B1	196	TRP
35	B1	197	ASP
35	B1	217	LEU
35	B1	218	LEU
35	B1	223	LYS
35	B1	226	GLN
35	B1	447	ASN
35	B1	450	LEU
35	B1	452	ASN
35	B1	513	MET
39	Bp	124	GLN
45	Bx	18	LEU
45	Bx	35	LEU
45	Bx	92	MET
45	Bx	96	ARG
45	Bx	105	LEU
45	Bx	109	PHE
45	Bx	115	SER
45	Bx	138	HIS
45	Bx	150	LEU
45	Bx	159	LEU
45	Bx	187	SER
45	Bx	188	VAL
45	Bx	199	LEU
45	Bx	213	ARG
45	Bx	238	PHE
45	Bx	241	PRO
45	Bx	273	MET
45	Bx	295	VAL
45	Bx	301	THR
45	Bx	306	THR
45	Bx	318	VAL
45	Bx	324	LEU
45	Bx	347	LEU
45	Bx	353	LEU
45	Bx	354	THR
45	Bx	365	ILE
45	Bx	369	ASP
45	Bx	373	VAL
45	Bx	383	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	Bx	417	MET
45	Bx	465	VAL
45	Bx	467	LEU
45	Bx	474	GLU
45	Bx	486	ASP
45	Bx	492	LEU
45	Bx	508	PRO
45	Bx	509	THR
45	Bx	512	ASN
46	By	7	LEU
46	By	31	VAL
46	By	52	HIS
46	By	60	GLU
46	By	63	THR
46	By	65	TRP
46	By	88	ASP
46	By	92	ASN
46	By	113	TYR
46	By	125	THR
46	By	130	PRO
46	By	134	ARG
46	By	142	VAL
46	By	147	GLU
46	By	148	MET
46	By	170	LEU
46	By	171	LYS
46	By	185	MET
46	By	205	SER
46	By	216	LEU
47	Bz	1	MET
47	Bz	11	VAL
47	Bz	13	PRO
47	Bz	14	SER
47	Bz	18	LEU
47	Bz	19	THR
47	Bz	22	LEU
47	Bz	38	ASN
47	Bz	39	SER
47	Bz	85	LEU
47	Bz	92	LEU
47	Bz	112	LEU
47	Bz	127	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
47	Bz	128	GLU
47	Bz	131	LEU
47	Bz	132	LEU
47	Bz	137	LEU
47	Bz	142	VAL
47	Bz	159	MET
47	Bz	160	LEU
47	Bz	163	LEU
47	Bz	188	ILE
47	Bz	196	THR
47	Bz	199	VAL
47	Bz	214	PHE
47	Bz	222	GLN
47	Bz	258	TRP
48	B0	31	LYS
48	B0	36	SER
48	B0	40	LEU
48	B0	59	LEU
48	B0	62	LEU
48	B0	107	ILE
48	B0	143	ASN
48	B0	147	LYS
49	B1	7	THR
49	B1	29	LEU
49	B1	70	VAL
49	B1	79	LYS
49	B1	80	GLU
49	B1	90	ARG
50	B2	37	LYS
50	B2	53	THR
50	B2	74	LEU
50	B2	95	GLN
50	B2	98	HIS
51	B3	5	LYS
51	B3	7	ASP
51	B3	8	HIS
51	B3	14	ARG
51	B3	17	ARG
51	B3	33	LEU
51	B3	34	ASN
51	B3	37	LEU
51	B3	38	HIS

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Mol	Chain	Res	Type
51	B3	41	HIS
51	B3	42	ARG
51	B3	43	GLU
51	B3	48	ILE
51	B3	54	ARG
51	B3	56	ARG
51	B3	68	THR
51	B3	69	PHE
51	B3	78	LEU
52	B4	19	ARG
52	B4	24	ASN
52	B4	28	ASN
52	B4	29	CYS
52	B4	51	SER
52	B4	53	CYS
52	B4	57	ARG
52	B4	60	TYR
52	B4	75	ARG
53	B5	2	THR
53	B5	8	GLN
53	B5	26	MET
53	B5	44	LYS
53	B5	64	ARG
54	B6	1	PHE
54	B6	2	GLU
54	B6	3	ASN
54	B6	8	LYS
54	B6	16	ASN
54	B6	23	LYS
54	B6	27	THR
55	B7	48	VAL
55	B7	49	THR
56	B8	15	VAL
56	B8	22	LEU
57	B9	13	LYS
57	B9	42	LYS
57	B9	43	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (413) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	116	ASN
1	A	164	ASN
1	A	170	GLN
1	A	220	GLN
1	A	284	HIS
1	A	313	ASN
1	A	441	HIS
2	B	184	ASN
3	C	95	HIS
4	E	48	HIS
4	E	49	GLN
4	E	51	GLN
4	E	70	ASN
5	F	62	GLN
5	F	81	ASN
6	G	80	GLN
6	G	101	ASN
7	H	50	GLN
7	H	73	GLN
7	H	76	GLN
7	H	83	GLN
7	H	111	GLN
8	I	73	GLN
9	J	71	ASN
9	J	102	GLN
9	J	183	ASN
10	K	77	HIS
11	L	71	HIS
11	L	86	ASN
12	M	384	ASN
12	M	425	ASN
12	M	444	HIS
12	M	460	HIS
12	M	464	GLN
12	M	498	GLN
12	M	514	ASN
12	M	688	GLN
13	N	91	HIS
13	N	113	HIS
13	N	135	GLN
14	O	69	ASN
14	O	187	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
14	O	189	ASN
14	O	191	ASN
15	P	74	GLN
15	P	82	ASN
15	P	105	ASN
15	P	124	ASN
15	P	247	GLN
16	Q	38	GLN
16	Q	147	ASN
16	Q	182	ASN
16	Q	183	HIS
16	Q	190	HIS
16	Q	233	HIS
16	Q	234	GLN
16	Q	339	GLN
16	Q	431	HIS
16	Q	442	HIS
16	Q	454	GLN
17	S	44	HIS
17	S	68	ASN
18	T	64	ASN
21	W	8	GLN
21	W	61	GLN
21	W	112	HIS
21	W	135	HIS
22	Y	75	HIS
24	a	90	ASN
24	a	189	ASN
25	b	14	GLN
25	b	83	HIS
25	b	89	HIS
25	b	126	GLN
26	c	56	ASN
26	c	84	HIS
26	c	154	GLN
27	d	59	HIS
27	d	61	GLN
27	d	85	GLN
27	d	113	GLN
27	d	117	GLN
27	d	138	GLN
30	g	60	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
30	g	96	HIS
32	i	83	GLN
32	i	112	HIS
32	i	150	ASN
32	i	186	HIS
32	i	222	ASN
33	j	10	ASN
34	k	7	ASN
34	k	94	ASN
35	l	4	HIS
35	l	59	GLN
35	l	139	GLN
35	l	192	HIS
35	l	199	GLN
35	l	205	ASN
35	l	226	GLN
35	l	248	HIS
35	l	274	GLN
35	l	296	ASN
35	l	320	ASN
35	l	332	HIS
35	l	348	HIS
35	l	394	HIS
35	l	400	ASN
35	l	442	ASN
35	l	446	ASN
35	l	534	HIS
35	l	569	HIS
35	l	580	GLN
36	m	45	ASN
36	m	117	ASN
37	n	40	ASN
38	o	62	ASN
38	o	126	HIS
39	p	75	GLN
40	r	48	ASN
40	r	168	HIS
40	r	390	ASN
40	r	415	GLN
40	r	425	ASN
41	s	93	ASN
41	s	169	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
41	s	235	ASN
42	u	30	HIS
42	u	31	HIS
42	u	64	ASN
42	u	77	HIS
42	u	99	HIS
42	u	103	GLN
42	u	104	GLN
42	u	143	HIS
43	v	43	GLN
43	v	61	HIS
43	v	85	HIS
43	v	92	HIS
44	w	85	HIS
44	w	111	ASN
44	w	132	GLN
44	w	149	HIS
44	w	257	GLN
45	x	11	ASN
45	x	12	HIS
45	x	43	GLN
45	x	99	ASN
45	x	170	ASN
45	x	256	HIS
45	x	360	ASN
45	x	413	HIS
45	x	512	ASN
46	y	103	GLN
46	y	203	ASN
47	z	6	HIS
47	z	12	ASN
47	z	133	ASN
47	z	207	HIS
47	z	222	GLN
47	z	232	HIS
48	0	109	HIS
49	1	34	ASN
50	2	66	ASN
51	3	52	HIS
52	4	23	GLN
52	4	24	ASN
52	4	25	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
52	4	28	ASN
52	4	37	HIS
54	6	3	ASN
54	6	16	ASN
55	7	10	HIS
55	7	15	ASN
55	7	41	ASN
57	9	39	ASN
58	AA	29	HIS
59	AB	31	GLN
60	AC	80	HIS
60	AC	135	GLN
60	AC	178	HIS
63	AF	23	ASN
63	AF	70	ASN
63	AF	73	HIS
64	AG	16	ASN
65	AH	107	HIS
65	AH	205	HIS
66	AJ	8	ASN
66	AJ	97	HIS
66	AJ	322	GLN
67	AK	167	GLN
67	AK	178	HIS
67	AK	184	ASN
67	AK	206	HIS
67	AK	212	HIS
67	AK	310	HIS
67	AK	311	GLN
67	AK	327	ASN
67	AK	343	GLN
67	AK	399	GLN
68	AL	87	ASN
68	AL	188	HIS
68	AL	207	ASN
68	AL	239	HIS
68	AL	240	GLN
68	AL	301	ASN
68	AL	308	ASN
60	AP	135	GLN
60	AP	178	HIS
61	AQ	38	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
62	AR	80	HIS
62	AR	84	HIS
63	AS	70	ASN
63	AS	73	HIS
65	AU	284	HIS
66	AV	97	HIS
66	AV	137	GLN
66	AV	255	ASN
66	AV	260	ASN
67	AW	81	HIS
67	AW	139	ASN
67	AW	155	GLN
67	AW	206	HIS
67	AW	212	HIS
67	AW	227	HIS
67	AW	291	HIS
67	AW	298	HIS
67	AW	310	HIS
67	AW	421	ASN
67	AW	446	HIS
68	AY	87	ASN
68	AY	121	ASN
68	AY	152	GLN
68	AY	223	HIS
68	AY	301	ASN
68	AY	342	GLN
1	BA	44	ASN
1	BA	116	ASN
1	BA	164	ASN
1	BA	170	GLN
1	BA	220	GLN
1	BA	284	HIS
1	BA	313	ASN
1	BA	441	HIS
2	BB	184	ASN
3	BC	95	HIS
4	BE	48	HIS
4	BE	49	GLN
4	BE	51	GLN
4	BE	70	ASN
5	BF	62	GLN
5	BF	81	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	BG	80	GLN
6	BG	101	ASN
7	BH	50	GLN
7	BH	73	GLN
7	BH	76	GLN
7	BH	83	GLN
7	BH	111	GLN
8	BI	73	GLN
9	BJ	71	ASN
9	BJ	102	GLN
9	BJ	183	ASN
10	BK	77	HIS
11	BL	86	ASN
12	BM	384	ASN
12	BM	425	ASN
12	BM	444	HIS
12	BM	460	HIS
12	BM	464	GLN
12	BM	498	GLN
12	BM	514	ASN
12	BM	688	GLN
13	BN	91	HIS
13	BN	113	HIS
13	BN	135	GLN
14	BO	69	ASN
14	BO	189	ASN
14	BO	191	ASN
15	BP	74	GLN
15	BP	82	ASN
15	BP	105	ASN
15	BP	124	ASN
15	BP	247	GLN
16	BQ	38	GLN
16	BQ	147	ASN
16	BQ	182	ASN
16	BQ	183	HIS
16	BQ	190	HIS
16	BQ	233	HIS
16	BQ	234	GLN
16	BQ	339	GLN
16	BQ	431	HIS
16	BQ	442	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
16	BQ	454	GLN
17	BS	44	HIS
17	BS	68	ASN
18	BT	64	ASN
21	BW	8	GLN
21	BW	61	GLN
21	BW	112	HIS
21	BW	135	HIS
22	BY	75	HIS
24	Ba	90	ASN
24	Ba	189	ASN
25	Bb	14	GLN
25	Bb	83	HIS
25	Bb	89	HIS
25	Bb	126	GLN
26	Bc	56	ASN
26	Bc	84	HIS
26	Bc	154	GLN
27	Bd	59	HIS
27	Bd	61	GLN
27	Bd	85	GLN
27	Bd	113	GLN
27	Bd	117	GLN
27	Bd	138	GLN
30	Bg	60	GLN
30	Bg	96	HIS
32	Bi	83	GLN
32	Bi	112	HIS
32	Bi	150	ASN
32	Bi	186	HIS
32	Bi	222	ASN
33	Bj	10	ASN
34	Bk	7	ASN
34	Bk	94	ASN
35	Bl	4	HIS
35	Bl	59	GLN
35	Bl	139	GLN
35	Bl	192	HIS
35	Bl	199	GLN
35	Bl	205	ASN
35	Bl	226	GLN
35	Bl	248	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
35	B1	274	GLN
35	B1	296	ASN
35	B1	320	ASN
35	B1	332	HIS
35	B1	348	HIS
35	B1	394	HIS
35	B1	400	ASN
35	B1	442	ASN
35	B1	446	ASN
35	B1	534	HIS
35	B1	569	HIS
35	B1	580	GLN
36	Bm	45	ASN
36	Bm	117	ASN
37	Bn	40	ASN
38	Bo	62	ASN
38	Bo	126	HIS
39	Bp	75	GLN
40	Br	48	ASN
40	Br	168	HIS
40	Br	390	ASN
40	Br	415	GLN
40	Br	425	ASN
41	Bs	93	ASN
41	Bs	169	GLN
41	Bs	235	ASN
42	Bu	30	HIS
42	Bu	31	HIS
42	Bu	64	ASN
42	Bu	77	HIS
42	Bu	99	HIS
42	Bu	104	GLN
42	Bu	143	HIS
43	Bv	43	GLN
43	Bv	61	HIS
43	Bv	85	HIS
43	Bv	92	HIS
44	Bw	85	HIS
44	Bw	111	ASN
44	Bw	132	GLN
44	Bw	149	HIS
44	Bw	257	GLN

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Mol	Chain	Res	Type
45	Bx	11	ASN
45	Bx	12	HIS
45	Bx	43	GLN
45	Bx	99	ASN
45	Bx	170	ASN
45	Bx	256	HIS
45	Bx	360	ASN
45	Bx	413	HIS
45	Bx	512	ASN
46	By	103	GLN
46	By	203	ASN
47	Bz	6	HIS
47	Bz	12	ASN
47	Bz	133	ASN
47	Bz	148	HIS
47	Bz	207	HIS
47	Bz	222	GLN
47	Bz	232	HIS
48	B0	109	HIS
49	B1	34	ASN
50	B2	66	ASN
51	B3	52	HIS
52	B4	23	GLN
52	B4	24	ASN
52	B4	25	GLN
52	B4	28	ASN
52	B4	37	HIS
53	B5	8	GLN
54	B6	3	ASN
54	B6	16	ASN
55	B7	10	HIS
55	B7	15	ASN
55	B7	41	ASN
57	B9	39	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 100 ligands modelled in this entry, 10 are monoatomic - leaving 90 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
76	PEE	AY	502	-	48,48,50	1.39	4 (8%)	51,53,55	0.96	2 (3%)
72	8Q1	Bp	201	-	31,34,34	1.67	5 (16%)	40,43,43	1.56	5 (12%)
71	PLX	r	501	-	51,51,51	0.74	1 (1%)	55,59,59	0.65	1 (1%)
76	PEE	Bl	702	-	50,50,50	1.16	6 (12%)	53,55,55	0.99	2 (3%)
71	PLX	U	101	-	51,51,51	0.74	1 (1%)	55,59,59	0.72	2 (3%)
69	SF4	M	802	12	0,12,12	-	-	-		
69	SF4	BB	302	2	0,12,12	-	-	-		
72	8Q1	BE	201	-	31,34,34	1.64	6 (19%)	40,43,43	1.38	7 (17%)
79	HEA	x	603	45	57,67,67	1.23	6 (10%)	61,103,103	1.47	11 (18%)
75	CDL	V	201	-	61,61,99	1.21	5 (8%)	64,71,111	0.95	3 (4%)
71	PLX	g	203	-	51,51,51	0.78	1 (1%)	55,59,59	0.58	1 (1%)
71	PLX	B	303	-	51,51,51	0.77	1 (1%)	55,59,59	0.68	1 (1%)
76	PEE	V	202	-	50,50,50	1.16	6 (12%)	53,55,55	0.91	2 (3%)
69	SF4	BB	301	2	0,12,12	-	-	-		
76	PEE	AH	401	-	48,48,50	1.35	4 (8%)	51,53,55	0.95	2 (3%)
76	PEE	BW	201	-	50,50,50	1.15	6 (12%)	53,55,55	0.97	2 (3%)
75	CDL	AA	101	-	63,63,99	1.24	5 (7%)	69,75,111	1.07	4 (5%)
71	PLX	b	201	-	51,51,51	0.57	0	55,59,59	0.64	0
73	NDP	BJ	401	-	45,52,52	0.95	2 (4%)	53,80,80	1.32	4 (7%)
81	HEC	AH	402	65	32,50,50	2.23	3 (9%)	24,82,82	1.35	1 (4%)
81	HEC	AU	402	65	32,50,50	2.28	3 (9%)	24,82,82	1.39	2 (8%)
69	SF4	C	301	3	0,12,12	-	-	-		
76	PEE	BV	202	-	50,50,50	1.16	6 (12%)	53,55,55	0.91	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
75	CDL	n	101	-	63,63,99	1.24	5 (7%)	69,75,111	1.07	4 (5%)
71	PLX	AN	101	-	51,51,51	0.78	1 (1%)	55,59,59	0.60	1 (1%)
75	CDL	AH	403	-	63,63,99	1.25	5 (7%)	69,75,111	1.03	4 (5%)
69	SF4	B	301	2	0,12,12	-	-	-	-	-
71	PLX	AQ	101	-	51,51,51	0.77	1 (1%)	55,59,59	0.61	2 (3%)
76	PEE	AU	401	-	40,40,50	1.46	4 (10%)	43,45,55	0.95	3 (6%)
70	FMN	A	502	-	33,33,33	1.39	6 (18%)	48,50,50	1.34	8 (16%)
75	CDL	AJ	405	-	63,63,99	1.13	4 (6%)	69,75,111	1.22	5 (7%)
71	PLX	AT	101	-	51,51,51	0.75	1 (1%)	55,59,59	0.60	1 (1%)
69	SF4	B	302	2	0,12,12	-	-	-	-	-
75	CDL	AN	102	-	63,63,99	1.24	5 (7%)	69,75,111	1.02	4 (5%)
79	HEA	Bx	603	45	57,67,67	1.23	6 (10%)	61,103,103	1.47	10 (16%)
71	PLX	g	201	-	51,51,51	0.81	1 (1%)	55,59,59	0.69	1 (1%)
74	FES	AC	301	60	0,4,4	-	-	-	-	-
71	PLX	Bb	201	-	51,51,51	0.57	0	55,59,59	0.63	0
76	PEE	Bl	701	-	48,48,50	1.34	4 (8%)	51,53,55	0.96	2 (3%)
75	CDL	l	703	-	63,63,99	1.21	5 (7%)	69,75,111	1.08	4 (5%)
76	PEE	W	201	-	50,50,50	1.14	6 (12%)	53,55,55	0.97	2 (3%)
69	SF4	BA	501	1	0,12,12	-	-	-	-	-
69	SF4	BC	301	3	0,12,12	-	-	-	-	-
70	FMN	BA	502	-	33,33,33	1.39	6 (18%)	48,50,50	1.34	8 (16%)
69	SF4	BM	802	12	0,12,12	-	-	-	-	-
75	CDL	l	704	-	63,63,99	1.26	5 (7%)	69,75,111	1.01	4 (5%)
72	8Q1	E	201	-	31,34,34	1.64	6 (19%)	40,43,43	1.39	7 (17%)
71	PLX	Br	502	-	51,51,51	0.64	0	55,59,59	0.67	1 (1%)
79	HEA	Bx	604	45	57,67,67	1.48	6 (10%)	61,103,103	1.47	12 (19%)
71	PLX	BV	203	-	51,51,51	0.77	1 (1%)	55,59,59	0.60	1 (1%)
71	PLX	Br	501	-	51,51,51	0.74	1 (1%)	55,59,59	0.66	1 (1%)
82	HEM	AJ	401	66	41,50,50	1.92	6 (14%)	45,82,82	1.60	5 (11%)
71	PLX	BB	303	-	51,51,51	0.77	1 (1%)	55,59,59	0.68	1 (1%)
82	HEM	AV	401	66	41,50,50	1.97	5 (12%)	45,82,82	1.55	5 (11%)
76	PEE	AJ	403	-	48,48,50	1.32	4 (8%)	51,53,55	0.99	2 (3%)
76	PEE	l	702	-	50,50,50	1.16	6 (12%)	53,55,55	0.99	2 (3%)
69	SF4	A	501	1	0,12,12	-	-	-	-	-
76	PEE	AV	403	-	48,48,50	1.34	4 (8%)	51,53,55	1.04	2 (3%)
75	CDL	Bn	101	-	63,63,99	1.23	5 (7%)	69,75,111	1.07	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
72	8Q1	p	201	-	31,34,34	1.67	5 (16%)	40,43,43	1.56	5 (12%)
76	PEE	l	701	-	48,48,50	1.34	4 (8%)	51,53,55	0.96	2 (3%)
75	CDL	i	401	-	63,63,99	1.21	5 (7%)	69,75,111	1.04	5 (7%)
74	FES	O	301	14	0,4,4	-	-	-	-	-
75	CDL	Bl	704	-	63,63,99	1.26	5 (7%)	69,75,111	1.01	4 (5%)
75	CDL	AL	502	-	63,63,99	1.24	5 (7%)	69,75,111	1.05	4 (5%)
71	PLX	AL	501	-	51,51,51	0.77	1 (1%)	55,59,59	0.63	1 (1%)
74	FES	M	803	-	0,4,4	-	-	-	-	-
71	PLX	Bg	202	-	51,51,51	0.74	1 (1%)	55,59,59	0.61	1 (1%)
75	CDL	AJ	404	-	63,63,99	1.24	5 (7%)	69,75,111	1.03	4 (5%)
79	HEA	x	604	45	57,67,67	1.47	6 (10%)	61,103,103	1.47	12 (19%)
71	PLX	Bg	203	-	51,51,51	0.78	1 (1%)	55,59,59	0.58	1 (1%)
71	PLX	g	202	-	51,51,51	0.74	1 (1%)	55,59,59	0.61	1 (1%)
74	FES	BO	301	14	0,4,4	-	-	-	-	-
76	PEE	AL	503	-	48,48,50	1.37	4 (8%)	51,53,55	0.92	2 (3%)
82	HEM	AJ	402	66	41,50,50	1.89	6 (14%)	45,82,82	1.57	9 (20%)
71	PLX	BU	101	-	51,51,51	0.74	1 (1%)	55,59,59	0.72	2 (3%)
69	SF4	M	801	12	0,12,12	-	-	-	-	-
73	NDP	J	401	-	45,52,52	0.96	2 (4%)	53,80,80	1.31	4 (7%)
82	HEM	AV	402	66	41,50,50	1.90	6 (14%)	45,82,82	1.60	8 (17%)
75	CDL	AG	101	-	63,63,99	1.15	4 (6%)	69,75,111	1.16	6 (8%)
71	PLX	r	502	-	51,51,51	0.64	0	55,59,59	0.67	1 (1%)
75	CDL	BV	201	-	61,61,99	1.21	5 (8%)	64,71,111	0.94	3 (4%)
75	CDL	Bl	703	-	63,63,99	1.21	5 (7%)	69,75,111	1.07	4 (5%)
75	CDL	Bi	401	-	63,63,99	1.21	5 (7%)	69,75,111	1.04	5 (7%)
71	PLX	Bg	201	-	51,51,51	0.82	1 (1%)	55,59,59	0.69	1 (1%)
75	CDL	AU	403	-	63,63,99	1.24	6 (9%)	69,75,111	1.04	4 (5%)
74	FES	BM	803	-	0,4,4	-	-	-	-	-
74	FES	AP	301	60	0,4,4	-	-	-	-	-
69	SF4	BM	801	12	0,12,12	-	-	-	-	-
75	CDL	AY	501	-	63,63,99	1.24	5 (7%)	69,75,111	1.01	4 (5%)

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
76	PEE	AY	502	-	-	20/52/52/54	-
72	8Q1	Bp	201	-	-	19/41/41/41	-
71	PLX	r	501	-	-	28/55/55/55	-
76	PEE	Bl	702	-	-	27/54/54/54	-
71	PLX	U	101	-	-	22/55/55/55	-
69	SF4	M	802	12	-	-	0/6/5/5
69	SF4	BB	302	2	-	-	0/6/5/5
72	8Q1	BE	201	-	-	18/41/41/41	-
79	HEA	x	603	45	3/3/7/16	7/32/76/76	-
75	CDL	V	201	-	-	41/69/69/110	-
71	PLX	g	203	-	-	24/55/55/55	-
71	PLX	B	303	-	-	21/55/55/55	-
76	PEE	V	202	-	-	27/54/54/54	-
69	SF4	BB	301	2	-	-	0/6/5/5
76	PEE	AH	401	-	-	27/52/52/54	-
76	PEE	BW	201	-	-	31/54/54/54	-
75	CDL	AA	101	-	-	35/74/74/110	-
71	PLX	b	201	-	-	27/55/55/55	-
73	NDP	BJ	401	-	-	15/30/77/77	0/5/5/5
81	HEC	AH	402	65	-	2/10/54/54	-
81	HEC	AU	402	65	-	0/10/54/54	-
69	SF4	C	301	3	-	-	0/6/5/5
76	PEE	BV	202	-	-	27/54/54/54	-
75	CDL	n	101	-	-	33/74/74/110	-
71	PLX	AN	101	-	-	26/55/55/55	-
75	CDL	AH	403	-	-	42/74/74/110	-
69	SF4	B	301	2	-	-	0/6/5/5
71	PLX	AQ	101	-	-	25/55/55/55	-
76	PEE	AU	401	-	-	17/44/44/54	-
70	FMN	A	502	-	-	7/18/18/18	0/3/3/3
75	CDL	AJ	405	-	-	28/74/74/110	-
71	PLX	AT	101	-	-	23/55/55/55	-
69	SF4	B	302	2	-	-	0/6/5/5
75	CDL	AN	102	-	-	40/74/74/110	-
79	HEA	Bx	603	45	3/3/7/16	7/32/76/76	-
71	PLX	g	201	-	-	25/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
71	PLX	Bb	201	-	-	27/55/55/55	-
74	FES	AC	301	60	-	-	0/1/1/1
76	PEE	B1	701	-	-	32/52/52/54	-
75	CDL	l	703	-	-	38/74/74/110	-
76	PEE	W	201	-	-	32/54/54/54	-
69	SF4	BA	501	1	-	-	0/6/5/5
69	SF4	BC	301	3	-	-	0/6/5/5
70	FMN	BA	502	-	-	7/18/18/18	0/3/3/3
69	SF4	BM	802	12	-	-	0/6/5/5
75	CDL	l	704	-	-	44/74/74/110	-
72	8Q1	E	201	-	-	18/41/41/41	-
71	PLX	Br	502	-	-	36/55/55/55	-
79	HEA	Bx	604	45	3/3/7/16	5/32/76/76	-
71	PLX	BV	203	-	-	26/55/55/55	-
71	PLX	Br	501	-	-	28/55/55/55	-
82	HEM	AJ	401	66	-	1/12/54/54	-
71	PLX	BB	303	-	-	21/55/55/55	-
82	HEM	AV	401	66	-	3/12/54/54	-
76	PEE	AJ	403	-	-	20/52/52/54	-
76	PEE	l	702	-	-	27/54/54/54	-
69	SF4	A	501	1	-	-	0/6/5/5
76	PEE	AV	403	-	-	30/52/52/54	-
75	CDL	Bn	101	-	-	33/74/74/110	-
72	8Q1	p	201	-	-	20/41/41/41	-
76	PEE	l	701	-	-	32/52/52/54	-
75	CDL	i	401	-	-	39/74/74/110	-
74	FES	O	301	14	-	-	0/1/1/1
75	CDL	B1	704	-	-	44/74/74/110	-
75	CDL	AL	502	-	-	43/74/74/110	-
71	PLX	AL	501	-	-	23/55/55/55	-
74	FES	M	803	-	-	-	0/1/1/1
71	PLX	Bg	202	-	-	25/55/55/55	-
75	CDL	AJ	404	-	-	33/74/74/110	-
79	HEA	x	604	45	3/3/7/16	5/32/76/76	-
71	PLX	Bg	203	-	-	24/55/55/55	-
71	PLX	g	202	-	-	25/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
74	FES	BO	301	14	-	-	0/1/1/1
76	PEE	AL	503	-	-	22/52/52/54	-
82	HEM	AJ	402	66	-	2/12/54/54	-
71	PLX	BU	101	-	-	22/55/55/55	-
69	SF4	M	801	12	-	-	0/6/5/5
73	NDP	J	401	-	-	15/30/77/77	0/5/5/5
82	HEM	AV	402	66	-	4/12/54/54	-
75	CDL	AG	101	-	-	38/74/74/110	-
71	PLX	r	502	-	-	36/55/55/55	-
75	CDL	BV	201	-	-	42/69/69/110	-
75	CDL	Bl	703	-	-	38/74/74/110	-
75	CDL	Bi	401	-	-	39/74/74/110	-
71	PLX	Bg	201	-	-	25/55/55/55	-
75	CDL	AU	403	-	-	48/74/74/110	-
74	FES	BM	803	-	-	-	0/1/1/1
74	FES	AP	301	60	-	-	0/1/1/1
69	SF4	BM	801	12	-	-	0/6/5/5
75	CDL	AY	501	-	-	36/74/74/110	-

All (270) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	AV	402	HEM	C3D-C2D	7.86	1.53	1.36
82	AJ	401	HEM	C3D-C2D	7.86	1.53	1.36
82	AJ	402	HEM	C3D-C2D	7.81	1.53	1.36
82	AV	401	HEM	C3D-C2D	7.73	1.53	1.36
81	AU	402	HEC	C3C-C2C	-6.99	1.33	1.40
81	AU	402	HEC	C2B-C3B	-6.69	1.33	1.40
81	AH	402	HEC	C2B-C3B	-6.57	1.33	1.40
81	AH	402	HEC	C3C-C2C	-6.56	1.33	1.40
79	Bx	604	HEA	C3A-C2A	-6.52	1.31	1.40
79	x	604	HEA	C3A-C2A	-6.51	1.31	1.40
82	AV	401	HEM	C3C-C2C	-5.45	1.32	1.40
81	AU	402	HEC	C3D-C2D	5.43	1.53	1.37
81	AH	402	HEC	C3D-C2D	5.39	1.53	1.37
72	p	201	8Q1	C34-N36	5.33	1.45	1.33
72	Bp	201	8Q1	C34-N36	5.31	1.45	1.33
72	Bp	201	8Q1	C39-N41	5.27	1.45	1.33
72	E	201	8Q1	C34-N36	5.25	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
72	BE	201	8Q1	C34-N36	5.24	1.45	1.33
72	p	201	8Q1	C39-N41	5.23	1.45	1.33
72	BE	201	8Q1	C39-N41	4.91	1.44	1.33
72	E	201	8Q1	C39-N41	4.89	1.44	1.33
70	A	502	FMN	C9A-C5A	4.38	1.48	1.41
70	BA	502	FMN	C9A-C5A	4.37	1.48	1.41
75	Bl	704	CDL	OB8-CB7	4.34	1.46	1.33
75	AH	403	CDL	OA6-CA5	4.33	1.46	1.34
75	AL	502	CDL	OA6-CA5	4.33	1.46	1.34
75	l	704	CDL	OB8-CB7	4.33	1.46	1.33
75	AH	403	CDL	OB8-CB7	4.32	1.46	1.33
76	AY	502	PEE	C39-C38	4.31	1.56	1.31
75	AJ	405	CDL	OA8-CA7	4.30	1.45	1.33
75	Bn	101	CDL	OA6-CA5	4.30	1.46	1.34
75	AU	403	CDL	OA6-CA5	4.29	1.46	1.34
75	AG	101	CDL	OB8-CB7	4.29	1.45	1.33
75	AY	501	CDL	OA6-CA5	4.28	1.46	1.34
75	n	101	CDL	OA6-CA5	4.28	1.46	1.34
76	AU	401	PEE	C39-C38	4.28	1.56	1.31
75	l	703	CDL	OA6-CA5	4.27	1.46	1.34
75	BV	201	CDL	OA6-CA5	4.26	1.46	1.34
75	AJ	404	CDL	OA6-CA5	4.26	1.46	1.34
76	AL	503	PEE	C39-C38	4.26	1.56	1.31
75	V	201	CDL	OA6-CA5	4.25	1.46	1.34
76	AV	403	PEE	C39-C38	4.25	1.56	1.31
75	AU	403	CDL	OB8-CB7	4.25	1.45	1.33
75	Bl	703	CDL	OA6-CA5	4.24	1.46	1.34
76	AJ	403	PEE	C39-C38	4.24	1.56	1.31
75	AG	101	CDL	OA6-CA5	4.23	1.46	1.34
76	AH	401	PEE	C39-C38	4.23	1.56	1.31
76	AL	503	PEE	O3-C30	4.23	1.45	1.33
75	AG	101	CDL	OA8-CA7	4.23	1.45	1.33
75	l	703	CDL	OB8-CB7	4.23	1.45	1.33
75	Bl	703	CDL	OB8-CB7	4.22	1.45	1.33
75	BV	201	CDL	OB8-CB7	4.21	1.45	1.33
75	AL	502	CDL	OB8-CB7	4.21	1.45	1.33
75	AJ	404	CDL	OB8-CB7	4.21	1.45	1.33
76	AY	502	PEE	C19-C18	4.21	1.56	1.31
75	AY	501	CDL	OB8-CB7	4.21	1.45	1.33
76	AH	401	PEE	C19-C18	4.21	1.56	1.31
75	V	201	CDL	OB8-CB7	4.20	1.45	1.33
76	AY	502	PEE	O3-C30	4.20	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
76	AL	503	PEE	C19-C18	4.19	1.56	1.31
76	AH	401	PEE	O3-C30	4.19	1.45	1.33
75	AA	101	CDL	OB8-CB7	4.18	1.45	1.33
75	AA	101	CDL	OA6-CA5	4.18	1.46	1.34
75	Bl	704	CDL	OA6-CA5	4.18	1.46	1.34
76	Bl	701	PEE	C39-C38	4.17	1.55	1.31
76	l	701	PEE	C39-C38	4.17	1.55	1.31
75	AJ	405	CDL	OB8-CB7	4.17	1.45	1.33
75	l	704	CDL	OA8-CA7	4.14	1.45	1.33
76	l	701	PEE	O3-C30	4.14	1.45	1.33
82	AJ	401	HEM	C3C-C2C	-4.14	1.34	1.40
75	Bl	704	CDL	OA8-CA7	4.14	1.45	1.33
76	AJ	403	PEE	C19-C18	4.14	1.55	1.31
76	AV	403	PEE	C19-C18	4.14	1.55	1.31
76	Bl	701	PEE	C19-C18	4.14	1.55	1.31
76	l	701	PEE	C19-C18	4.14	1.55	1.31
75	AN	102	CDL	OB8-CB7	4.13	1.45	1.33
76	Bl	701	PEE	O3-C30	4.13	1.45	1.33
76	AV	403	PEE	O3-C30	4.13	1.45	1.33
75	l	704	CDL	OA6-CA5	4.13	1.45	1.34
75	AN	102	CDL	OA6-CA5	4.12	1.45	1.34
75	n	101	CDL	OB8-CB7	4.12	1.45	1.33
76	AU	401	PEE	O3-C30	4.11	1.45	1.33
75	AJ	405	CDL	OB6-CB5	4.11	1.45	1.34
75	Bn	101	CDL	OB8-CB7	4.08	1.45	1.33
75	i	401	CDL	OB8-CB7	4.08	1.45	1.33
75	Bi	401	CDL	OB8-CB7	4.06	1.45	1.33
76	AU	401	PEE	C19-C18	4.06	1.55	1.28
75	AG	101	CDL	OB6-CB5	4.03	1.45	1.34
75	Bi	401	CDL	OA6-CA5	4.01	1.45	1.34
75	AJ	405	CDL	OA6-CA5	4.00	1.45	1.34
75	i	401	CDL	OA6-CA5	3.99	1.45	1.34
82	AJ	402	HEM	C3C-C2C	-3.99	1.34	1.40
75	AJ	404	CDL	OA8-CA7	3.98	1.45	1.33
82	AV	402	HEM	C3C-C2C	-3.98	1.34	1.40
76	AJ	403	PEE	O3-C30	3.97	1.44	1.33
75	AY	501	CDL	OA8-CA7	3.96	1.44	1.33
79	Bx	604	HEA	C3A-CMA	-3.96	1.37	1.46
75	AU	403	CDL	OA8-CA7	3.95	1.44	1.33
75	AH	403	CDL	OA8-CA7	3.92	1.44	1.33
75	Bn	101	CDL	OA8-CA7	3.92	1.44	1.33
75	AN	102	CDL	OA8-CA7	3.92	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
75	n	101	CDL	OA8-CA7	3.92	1.44	1.33
75	AA	101	CDL	OA8-CA7	3.90	1.44	1.33
79	x	604	HEA	C3A-CMA	-3.89	1.37	1.46
75	AL	502	CDL	OA8-CA7	3.89	1.44	1.33
75	Bl	703	CDL	OA8-CA7	3.84	1.44	1.33
75	l	703	CDL	OA8-CA7	3.83	1.44	1.33
76	V	202	PEE	C19-C18	3.78	1.53	1.31
76	Bl	702	PEE	C19-C18	3.77	1.53	1.31
76	l	702	PEE	C19-C18	3.77	1.53	1.31
82	AV	402	HEM	C3C-CAC	3.76	1.55	1.47
76	BV	202	PEE	C19-C18	3.76	1.53	1.31
76	W	201	PEE	C19-C18	3.74	1.53	1.31
76	BW	201	PEE	C19-C18	3.74	1.53	1.31
75	Bi	401	CDL	OA8-CA7	3.71	1.44	1.33
76	V	202	PEE	C39-C38	3.71	1.53	1.31
82	AJ	401	HEM	C3C-CAC	3.70	1.55	1.47
76	BV	202	PEE	C39-C38	3.70	1.53	1.31
75	i	401	CDL	OA8-CA7	3.69	1.44	1.33
76	Bl	702	PEE	C39-C38	3.68	1.53	1.31
76	BW	201	PEE	C39-C38	3.68	1.53	1.31
76	l	702	PEE	C39-C38	3.68	1.53	1.31
76	W	201	PEE	C39-C38	3.67	1.53	1.31
82	AJ	402	HEM	C3C-CAC	3.55	1.55	1.47
76	AY	502	PEE	O2-C10	3.46	1.44	1.34
76	AL	503	PEE	O2-C10	3.44	1.44	1.34
82	AV	401	HEM	C3C-CAC	3.44	1.54	1.47
75	Bl	704	CDL	OB6-CB5	3.35	1.43	1.34
76	Bl	701	PEE	O2-C10	3.35	1.43	1.34
75	l	704	CDL	OB6-CB5	3.34	1.43	1.34
76	l	701	PEE	O2-C10	3.31	1.43	1.34
75	AY	501	CDL	OB6-CB5	3.29	1.43	1.34
75	Bn	101	CDL	OB6-CB5	3.27	1.43	1.34
75	n	101	CDL	OB6-CB5	3.26	1.43	1.34
75	AJ	404	CDL	OB6-CB5	3.23	1.43	1.34
75	AN	102	CDL	OB6-CB5	3.22	1.43	1.34
75	AH	403	CDL	OB6-CB5	3.21	1.43	1.34
79	Bx	603	HEA	C3C-C2C	-3.21	1.35	1.40
76	AJ	403	PEE	O2-C10	3.21	1.43	1.34
75	Bl	703	CDL	OB6-CB5	3.21	1.43	1.34
75	l	703	CDL	OB6-CB5	3.20	1.43	1.34
76	AU	401	PEE	O2-C10	3.19	1.43	1.34
75	AA	101	CDL	OB6-CB5	3.18	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
75	AU	403	CDL	OB6-CB5	3.17	1.43	1.34
76	AV	403	PEE	O2-C10	3.15	1.43	1.34
79	x	603	HEA	C3C-C2C	-3.15	1.36	1.40
73	J	401	NDP	C6N-C5N	3.13	1.38	1.33
75	V	201	CDL	OB6-CB5	3.12	1.43	1.34
75	AL	502	CDL	OB6-CB5	3.10	1.43	1.34
76	AH	401	PEE	O2-C10	3.10	1.43	1.34
75	i	401	CDL	OB6-CB5	3.09	1.43	1.34
75	BV	201	CDL	OB6-CB5	3.09	1.43	1.34
73	BJ	401	NDP	C6N-C5N	3.07	1.38	1.33
70	BA	502	FMN	C8-C7	3.05	1.48	1.40
75	Bi	401	CDL	OB6-CB5	3.05	1.42	1.34
70	A	502	FMN	C8-C7	3.05	1.48	1.40
70	A	502	FMN	C4-N3	-3.03	1.33	1.38
75	BV	201	CDL	OA8-CA7	3.02	1.45	1.33
75	V	201	CDL	OA8-CA7	3.02	1.45	1.33
70	BA	502	FMN	C4-N3	-3.01	1.33	1.38
82	AJ	402	HEM	CAB-C3B	2.99	1.55	1.47
71	BB	303	PLX	O6-C4	-2.98	1.40	1.44
82	AV	401	HEM	CAB-C3B	2.97	1.55	1.47
71	B	303	PLX	O6-C4	-2.96	1.40	1.44
82	AJ	401	HEM	CAB-C3B	2.95	1.55	1.47
71	g	203	PLX	O6-C4	-2.92	1.40	1.44
82	AV	402	HEM	CAB-C3B	2.90	1.55	1.47
71	Bg	203	PLX	O6-C4	-2.90	1.40	1.44
79	Bx	603	HEA	C3A-CMA	-2.88	1.39	1.46
79	x	603	HEA	C3A-CMA	-2.86	1.39	1.46
79	Bx	604	HEA	C3C-C2C	-2.79	1.36	1.40
75	n	101	CDL	OB6-CB4	-2.77	1.39	1.46
75	Bn	101	CDL	OB6-CB4	-2.75	1.39	1.46
71	Bg	201	PLX	O6-C4	-2.74	1.40	1.44
71	AN	101	PLX	O6-C4	-2.74	1.40	1.44
79	x	604	HEA	C3C-C2C	-2.72	1.36	1.40
71	BV	203	PLX	O6-C4	-2.72	1.41	1.44
71	g	201	PLX	O6-C4	-2.71	1.41	1.44
71	AL	501	PLX	O6-C4	-2.71	1.41	1.44
79	x	603	HEA	C4C-NC	2.70	1.41	1.36
79	Bx	603	HEA	C4C-NC	2.69	1.41	1.36
79	x	604	HEA	C1D-C2D	2.66	1.49	1.44
75	AL	502	CDL	OB6-CB4	-2.65	1.40	1.46
75	AH	403	CDL	OB6-CB4	-2.64	1.40	1.46
75	V	201	CDL	OB6-CB4	-2.64	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
75	AA	101	CDL	OB6-CB4	-2.61	1.40	1.46
75	BV	201	CDL	OB6-CB4	-2.61	1.40	1.46
71	U	101	PLX	O6-C4	-2.60	1.41	1.44
79	Bx	604	HEA	C1D-C2D	2.60	1.49	1.44
82	AV	401	HEM	FE-ND	2.60	2.09	1.96
71	AQ	101	PLX	O6-C4	-2.59	1.41	1.44
79	x	604	HEA	C1D-ND	-2.59	1.35	1.40
79	Bx	604	HEA	C1D-ND	-2.58	1.35	1.40
71	BU	101	PLX	O6-C4	-2.55	1.41	1.44
75	AN	102	CDL	OB6-CB4	-2.53	1.40	1.46
72	p	201	8Q1	O35-C34	-2.52	1.18	1.23
75	i	401	CDL	OB6-CB4	-2.52	1.40	1.46
75	AJ	404	CDL	OB6-CB4	-2.52	1.40	1.46
75	Bi	401	CDL	OB6-CB4	-2.51	1.40	1.46
75	AU	403	CDL	OB6-CB4	-2.51	1.40	1.46
75	AY	501	CDL	OB6-CB4	-2.49	1.40	1.46
72	E	201	8Q1	O35-C34	-2.47	1.18	1.23
72	Bp	201	8Q1	O35-C34	-2.47	1.18	1.23
72	BE	201	8Q1	O35-C34	-2.46	1.18	1.23
71	AT	101	PLX	O6-C4	-2.44	1.41	1.44
71	Bg	202	PLX	O6-C4	-2.43	1.41	1.44
71	r	501	PLX	O6-C4	-2.42	1.41	1.44
71	g	202	PLX	O6-C4	-2.42	1.41	1.44
76	BV	202	PEE	O2-C10	2.39	1.41	1.34
76	l	702	PEE	O2-C10	2.39	1.41	1.34
76	V	202	PEE	O2-C10	2.39	1.41	1.34
71	Br	501	PLX	O6-C4	-2.38	1.41	1.44
76	Bl	702	PEE	O2-C10	2.38	1.41	1.34
75	Bl	704	CDL	OB6-CB4	-2.37	1.40	1.46
75	l	704	CDL	OB6-CB4	-2.36	1.40	1.46
72	Bp	201	8Q1	O40-C39	-2.36	1.18	1.23
72	E	201	8Q1	C1-S44	2.35	1.81	1.76
72	BE	201	8Q1	C1-S44	2.35	1.81	1.76
75	l	703	CDL	OB6-CB4	-2.35	1.40	1.46
76	l	702	PEE	O3-C30	2.34	1.40	1.33
75	Bl	703	CDL	OB6-CB4	-2.34	1.40	1.46
76	Bl	702	PEE	O3-C30	2.33	1.40	1.33
72	BE	201	8Q1	O40-C39	-2.33	1.18	1.23
70	BA	502	FMN	C5A-N5	-2.33	1.35	1.39
72	E	201	8Q1	O40-C39	-2.31	1.18	1.23
72	p	201	8Q1	O40-C39	-2.30	1.18	1.23
70	A	502	FMN	C5A-N5	-2.28	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
76	BV	202	PEE	O2-C2	-2.27	1.40	1.46
76	V	202	PEE	O3-C30	2.27	1.39	1.33
72	Bp	201	8Q1	C1-S44	2.26	1.81	1.76
79	Bx	603	HEA	C1C-NC	2.25	1.40	1.36
76	V	202	PEE	O2-C2	-2.25	1.41	1.46
76	l	702	PEE	O2-C2	-2.25	1.41	1.46
76	Bl	702	PEE	O2-C2	-2.24	1.41	1.46
79	Bx	604	HEA	CMD-C2D	2.24	1.55	1.50
76	BW	201	PEE	O3-C30	2.24	1.39	1.33
72	BE	201	8Q1	C6-C1	2.23	1.53	1.50
76	BV	202	PEE	O3-C30	2.23	1.39	1.33
76	Bl	702	PEE	O3-C3	-2.22	1.40	1.45
79	x	603	HEA	C3A-C2A	-2.22	1.37	1.40
76	W	201	PEE	O3-C30	2.22	1.39	1.33
79	x	604	HEA	CMD-C2D	2.22	1.55	1.50
79	Bx	603	HEA	C3A-C2A	-2.22	1.37	1.40
76	BV	202	PEE	O3-C3	-2.22	1.40	1.45
72	p	201	8Q1	C1-S44	2.22	1.81	1.76
72	E	201	8Q1	C6-C1	2.21	1.53	1.50
79	x	603	HEA	C1C-NC	2.21	1.40	1.36
76	V	202	PEE	O3-C3	-2.21	1.40	1.45
76	BW	201	PEE	O2-C10	2.20	1.40	1.34
76	l	702	PEE	O3-C3	-2.19	1.40	1.45
76	W	201	PEE	O2-C10	2.19	1.40	1.34
76	W	201	PEE	O2-C2	-2.19	1.41	1.46
76	BW	201	PEE	O2-C2	-2.19	1.41	1.46
76	W	201	PEE	O3-C3	-2.17	1.40	1.45
82	AJ	402	HEM	FE-ND	2.17	2.07	1.96
82	AJ	401	HEM	FE-NB	2.17	2.07	1.96
70	BA	502	FMN	C4A-N5	2.16	1.34	1.30
76	BW	201	PEE	O3-C3	-2.15	1.40	1.45
70	A	502	FMN	C4A-N5	2.13	1.34	1.30
82	AJ	402	HEM	CAA-C2A	2.13	1.55	1.52
70	A	502	FMN	C2-N3	-2.09	1.34	1.39
82	AV	402	HEM	CAA-C2A	2.08	1.55	1.52
79	Bx	603	HEA	CHD-C1D	2.05	1.40	1.35
82	AJ	401	HEM	FE-ND	2.05	2.07	1.96
73	BJ	401	NDP	C5A-C4A	2.05	1.46	1.40
75	AU	403	CDL	C11-CA5	2.05	1.56	1.50
73	J	401	NDP	C5A-C4A	2.04	1.46	1.40
70	BA	502	FMN	C2-N3	-2.04	1.34	1.39
79	x	603	HEA	CHD-C1D	2.02	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	AV	402	HEM	FE-ND	2.02	2.06	1.96

All (253) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
82	AV	402	HEM	C4D-ND-C1D	6.19	111.46	105.07
82	AJ	401	HEM	C4D-ND-C1D	6.16	111.43	105.07
82	AJ	402	HEM	C4D-ND-C1D	6.05	111.32	105.07
72	p	201	8Q1	C6-C1-S44	6.01	120.45	113.46
72	Bp	201	8Q1	C6-C1-S44	6.00	120.44	113.46
82	AV	401	HEM	C4D-ND-C1D	5.34	110.59	105.07
73	J	401	NDP	PN-O3-PA	-5.21	114.94	132.83
73	BJ	401	NDP	PN-O3-PA	-5.20	114.97	132.83
72	E	201	8Q1	C6-C1-S44	4.58	118.78	113.46
72	BE	201	8Q1	C6-C1-S44	4.55	118.75	113.46
76	l	702	PEE	O2-C10-C11	4.38	120.94	111.50
76	Bl	702	PEE	O2-C10-C11	4.37	120.92	111.50
75	AJ	405	CDL	OB6-CB5-C51	4.31	120.79	111.50
76	AY	502	PEE	O2-C10-C11	4.31	120.79	111.50
75	AL	502	CDL	OA6-CA5-C11	4.25	120.66	111.50
75	AG	101	CDL	OB6-CB5-C51	4.22	120.59	111.50
75	AY	501	CDL	OA6-CA5-C11	4.21	120.58	111.50
75	l	703	CDL	OA6-CA5-C11	4.20	120.55	111.50
75	Bl	703	CDL	OA6-CA5-C11	4.19	120.53	111.50
75	AH	403	CDL	OA6-CA5-C11	4.16	120.47	111.50
75	AU	403	CDL	OA6-CA5-C11	4.16	120.46	111.50
75	i	401	CDL	OA6-CA5-C11	4.14	120.42	111.50
75	AJ	404	CDL	OA6-CA5-C11	4.13	120.39	111.50
75	Bi	401	CDL	OA6-CA5-C11	4.12	120.39	111.50
75	BV	201	CDL	OB6-CB5-C51	4.11	120.35	111.50
75	V	201	CDL	OB6-CB5-C51	4.10	120.35	111.50
75	l	704	CDL	OA6-CA5-C11	4.09	120.33	111.50
75	n	101	CDL	OB6-CB5-C51	4.08	120.29	111.50
75	Bn	101	CDL	OB6-CB5-C51	4.08	120.29	111.50
75	Bl	704	CDL	OA6-CA5-C11	4.08	120.29	111.50
75	AA	101	CDL	OA6-CA5-C11	4.07	120.28	111.50
75	AU	403	CDL	OB6-CB5-C51	4.05	120.22	111.50
75	AJ	404	CDL	OB6-CB5-C51	4.03	120.19	111.50
76	AJ	403	PEE	O2-C10-C11	4.03	120.18	111.50
76	Bl	701	PEE	O2-C10-C11	4.00	120.13	111.50
75	AA	101	CDL	OB6-CB5-C51	3.99	120.10	111.50
76	l	701	PEE	O2-C10-C11	3.98	120.09	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
75	l	703	CDL	OB6-CB5-C51	3.98	120.08	111.50
79	x	603	HEA	C17-C18-C19	-3.98	118.08	127.66
79	Bx	603	HEA	C17-C18-C19	-3.98	118.09	127.66
75	Bl	703	CDL	OB6-CB5-C51	3.97	120.06	111.50
75	AN	102	CDL	OA6-CA5-C11	3.96	120.03	111.50
75	n	101	CDL	OA6-CA5-C11	3.95	120.01	111.50
75	Bn	101	CDL	OA6-CA5-C11	3.95	120.01	111.50
75	Bl	704	CDL	OB6-CB5-C51	3.94	119.99	111.50
75	l	704	CDL	OB6-CB5-C51	3.94	119.98	111.50
75	AH	403	CDL	OB6-CB5-C51	3.93	119.96	111.50
76	AV	403	PEE	O2-C10-C11	3.92	119.94	111.50
75	AY	501	CDL	OB6-CB5-C51	3.90	119.91	111.50
75	AN	102	CDL	OB6-CB5-C51	3.86	119.82	111.50
75	AL	502	CDL	OB6-CB5-C51	3.86	119.81	111.50
73	BJ	401	NDP	N3A-C2A-N1A	-3.79	122.76	128.68
73	J	401	NDP	N3A-C2A-N1A	-3.72	122.86	128.68
76	BW	201	PEE	O2-C10-C11	3.71	119.50	111.50
76	W	201	PEE	O2-C10-C11	3.70	119.47	111.50
72	p	201	8Q1	O4-C1-C6	-3.67	119.66	123.99
76	BV	202	PEE	O2-C10-C11	3.63	119.32	111.50
72	Bp	201	8Q1	O4-C1-C6	-3.62	119.71	123.99
79	x	604	HEA	C4A-CHB-C1B	3.62	127.33	122.56
76	V	202	PEE	O2-C10-C11	3.61	119.28	111.50
75	AG	101	CDL	OA6-CA5-C11	3.60	119.25	111.50
79	Bx	604	HEA	C4A-CHB-C1B	3.58	127.29	122.56
76	AH	401	PEE	O2-C10-C11	3.55	119.16	111.50
75	AJ	405	CDL	OA6-CA5-C11	3.55	119.15	111.50
76	AL	503	PEE	O2-C10-C11	3.53	119.11	111.50
75	Bi	401	CDL	OB6-CB5-C51	3.50	119.04	111.50
75	i	401	CDL	OB6-CB5-C51	3.49	119.02	111.50
75	V	201	CDL	OA6-CA5-C11	3.46	118.95	111.50
75	BV	201	CDL	OA6-CA5-C11	3.44	118.92	111.50
75	AJ	405	CDL	OB8-CB7-C71	3.25	122.11	111.91
76	AU	401	PEE	O2-C10-C11	3.22	118.44	111.50
79	Bx	603	HEA	C13-C14-C15	-3.14	120.11	127.66
79	x	603	HEA	C13-C14-C15	-3.12	120.14	127.66
82	AV	401	HEM	C4B-CHC-C1C	3.08	126.63	122.56
76	AV	403	PEE	O3-C30-C31	3.06	121.52	111.91
75	l	703	CDL	OA8-CA7-C31	2.99	121.28	111.91
75	Bl	703	CDL	OA8-CA7-C31	2.98	121.26	111.91
75	AA	101	CDL	OA8-CA7-C31	2.97	121.22	111.91
82	AV	401	HEM	CAD-CBD-CGD	-2.95	107.25	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	x	603	HEA	C1B-C2B-C3B	2.95	110.33	106.80
75	AG	101	CDL	CB4-OB6-CB5	-2.91	110.62	117.79
79	Bx	603	HEA	C1B-C2B-C3B	2.90	110.27	106.80
79	Bx	604	HEA	CBA-CAA-C2A	2.87	117.44	112.60
82	AJ	401	HEM	C4C-CHD-C1D	2.87	126.34	122.56
82	AJ	401	HEM	C4B-CHC-C1C	2.86	126.33	122.56
76	V	202	PEE	O3-C30-C31	2.85	120.84	111.91
76	BV	202	PEE	O3-C30-C31	2.85	120.84	111.91
76	Bl	702	PEE	O3-C30-C31	2.85	120.84	111.91
76	l	702	PEE	O3-C30-C31	2.83	120.80	111.91
79	x	604	HEA	CBA-CAA-C2A	2.83	117.38	112.60
70	A	502	FMN	C4-C4A-N5	2.82	122.25	118.23
70	BA	502	FMN	C4-C4A-N5	2.82	122.24	118.23
72	E	201	8Q1	C43-S44-C1	2.80	110.60	101.87
72	BE	201	8Q1	C43-S44-C1	2.79	110.56	101.87
70	A	502	FMN	C4A-C10-N1	-2.76	118.32	124.73
72	E	201	8Q1	C32-C34-N36	2.76	122.08	116.58
82	AV	401	HEM	C4C-CHD-C1D	2.76	126.20	122.56
75	i	401	CDL	OB8-CB7-C71	2.76	120.56	111.91
70	BA	502	FMN	C4A-C10-N1	-2.76	118.34	124.73
75	Bn	101	CDL	OA8-CA7-C31	2.75	120.54	111.91
75	n	101	CDL	OA8-CA7-C31	2.75	120.53	111.91
72	BE	201	8Q1	C32-C34-N36	2.75	122.05	116.58
75	Bi	401	CDL	OB8-CB7-C71	2.74	120.51	111.91
75	AG	101	CDL	OB8-CB7-C71	2.74	120.51	111.91
75	AL	502	CDL	OA8-CA7-C31	2.73	120.47	111.91
72	Bp	201	8Q1	C43-S44-C1	2.72	110.33	101.87
75	l	704	CDL	OA8-CA7-C31	2.72	120.43	111.91
75	Bl	704	CDL	OA8-CA7-C31	2.71	120.43	111.91
72	p	201	8Q1	C43-S44-C1	2.71	110.32	101.87
75	AJ	405	CDL	OA8-CA7-C31	2.71	120.41	111.91
75	l	703	CDL	OB8-CB7-C71	2.70	120.38	111.91
75	AL	502	CDL	OB8-CB7-C71	2.69	120.36	111.91
75	Bn	101	CDL	OB8-CB7-C71	2.69	120.36	111.91
76	W	201	PEE	O3-C30-C31	2.69	120.35	111.91
75	Bl	703	CDL	OB8-CB7-C71	2.69	120.35	111.91
75	n	101	CDL	OB8-CB7-C71	2.69	120.35	111.91
75	AN	102	CDL	OA8-CA7-C31	2.69	120.34	111.91
76	BW	201	PEE	O3-C30-C31	2.68	120.33	111.91
75	l	704	CDL	OB8-CB7-C71	2.68	120.32	111.91
75	Bl	704	CDL	OB8-CB7-C71	2.67	120.30	111.91
75	AU	403	CDL	OA8-CA7-C31	2.67	120.28	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
75	AH	403	CDL	OB8-CB7-C71	2.66	120.27	111.91
82	AV	402	HEM	C4C-CHD-C1D	2.66	126.07	122.56
75	AJ	404	CDL	OA8-CA7-C31	2.66	120.25	111.91
76	AH	401	PEE	O3-C30-C31	2.65	120.23	111.91
79	Bx	604	HEA	CMD-C2D-C1D	2.63	129.04	125.04
79	x	604	HEA	CMD-C2D-C1D	2.62	129.02	125.04
82	AJ	402	HEM	C1B-NB-C4B	2.60	107.76	105.07
79	x	604	HEA	C4D-CHA-C1A	2.60	125.99	122.56
75	AA	101	CDL	OB8-CB7-C71	2.60	120.07	111.91
79	Bx	604	HEA	C4D-CHA-C1A	2.60	125.98	122.56
75	AU	403	CDL	OB8-CB7-C71	2.59	120.03	111.91
75	AG	101	CDL	OA8-CA7-C31	2.57	119.97	111.91
72	Bp	201	8Q1	C38-C39-N41	2.55	120.71	116.42
75	V	201	CDL	OB8-CB7-C71	2.54	119.89	111.91
72	p	201	8Q1	C38-C39-N41	2.54	120.70	116.42
75	BV	201	CDL	OB8-CB7-C71	2.54	119.87	111.91
75	AJ	404	CDL	OB8-CB7-C71	2.53	119.86	111.91
81	AH	402	HEC	CMC-C2C-C1C	-2.53	124.58	128.46
75	AY	501	CDL	OA8-CA7-C31	2.53	119.84	111.91
75	AN	102	CDL	OB8-CB7-C71	2.52	119.82	111.91
72	E	201	8Q1	O4-C1-C6	-2.52	121.01	123.99
75	AY	501	CDL	OB8-CB7-C71	2.52	119.81	111.91
72	BE	201	8Q1	O4-C1-C6	-2.51	121.02	123.99
75	AH	403	CDL	OA8-CA7-C31	2.50	119.75	111.91
82	AV	401	HEM	C1B-NB-C4B	2.49	107.64	105.07
76	AL	503	PEE	O3-C30-C31	2.48	119.69	111.91
82	AV	402	HEM	C1B-NB-C4B	2.47	107.63	105.07
79	Bx	604	HEA	CMC-C2C-C3C	2.46	129.28	124.68
79	x	604	HEA	CMC-C2C-C3C	2.45	129.27	124.68
71	AT	101	PLX	C1C-N1-C1	2.44	119.90	109.92
73	BJ	401	NDP	C4A-C5A-N7A	-2.44	106.86	109.40
73	J	401	NDP	C4A-C5A-N7A	-2.42	106.88	109.40
75	Bi	401	CDL	OA8-CA7-C31	2.42	119.50	111.91
79	x	603	HEA	C17-C16-C15	-2.42	105.02	112.98
75	i	401	CDL	OA8-CA7-C31	2.42	119.50	111.91
70	A	502	FMN	C4A-C10-N10	2.42	120.01	116.48
70	BA	502	FMN	C4A-C10-N10	2.41	120.00	116.48
72	E	201	8Q1	C42-N41-C39	-2.40	118.37	122.84
76	AJ	403	PEE	O3-C30-C31	2.40	119.44	111.91
79	Bx	603	HEA	C17-C16-C15	-2.40	105.09	112.98
79	x	604	HEA	C1D-C2D-C3D	-2.39	104.44	106.96
79	x	604	HEA	CMB-C2B-C3B	-2.39	125.79	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
72	BE	201	8Q1	C42-N41-C39	-2.39	118.41	122.84
82	AJ	401	HEM	CMC-C2C-C3C	2.38	129.14	124.68
79	Bx	604	HEA	C1D-C2D-C3D	-2.38	104.45	106.96
79	Bx	604	HEA	C25-C23-C24	2.38	119.86	114.60
79	x	603	HEA	C16-C17-C18	-2.38	104.07	111.88
79	Bx	603	HEA	C16-C17-C18	-2.37	104.09	111.88
82	AV	402	HEM	CAD-C3D-C4D	2.37	128.79	124.66
71	B	303	PLX	C1C-N1-C1	2.36	119.59	109.92
72	E	201	8Q1	C37-N36-C34	-2.36	118.38	122.59
79	x	603	HEA	C20-C19-C18	2.36	125.89	121.12
71	BB	303	PLX	C1C-N1-C1	2.35	119.54	109.92
72	BE	201	8Q1	C37-N36-C34	-2.35	118.39	122.59
79	Bx	603	HEA	C20-C19-C18	2.35	125.87	121.12
71	AL	501	PLX	C1C-N1-C1	2.35	119.53	109.92
79	x	604	HEA	C25-C23-C24	2.35	119.79	114.60
79	Bx	604	HEA	CMB-C2B-C3B	-2.35	125.86	130.34
82	AJ	402	HEM	C4C-CHD-C1D	2.35	125.66	122.56
70	A	502	FMN	O2-C2-N1	-2.35	117.94	121.83
79	x	603	HEA	CAD-C3D-C4D	2.34	128.74	124.66
79	Bx	603	HEA	CAD-C3D-C4D	2.33	128.74	124.66
71	AN	101	PLX	C1C-N1-C1	2.33	119.44	109.92
71	BV	203	PLX	C1C-N1-C1	2.33	119.43	109.92
76	AU	401	PEE	O3-C30-C31	2.31	119.14	111.91
70	BA	502	FMN	O2-C2-N1	-2.30	118.02	121.83
71	BU	101	PLX	C1C-N1-C1	2.30	119.32	109.92
76	l	701	PEE	O3-C30-C31	2.30	119.11	111.91
71	U	101	PLX	C1C-N1-C1	2.29	119.30	109.92
76	AY	502	PEE	O3-C30-C31	2.29	119.10	111.91
82	AJ	402	HEM	CAD-C3D-C4D	2.28	128.65	124.66
76	Bl	701	PEE	O3-C30-C31	2.28	119.05	111.91
71	Bg	203	PLX	C1C-N1-C1	2.27	119.21	109.92
71	g	203	PLX	C1C-N1-C1	2.26	119.17	109.92
79	x	604	HEA	C13-C14-C15	-2.25	122.24	127.66
79	x	604	HEA	C26-C15-C16	2.24	119.04	115.27
70	BA	502	FMN	C4-N3-C2	-2.24	121.51	125.64
79	Bx	604	HEA	C13-C14-C15	-2.23	122.28	127.66
70	A	502	FMN	C4-N3-C2	-2.23	121.52	125.64
79	x	603	HEA	C4B-C3B-C2B	-2.22	103.62	107.41
75	AJ	405	CDL	OB8-CB7-OB9	-2.22	118.00	123.59
79	Bx	604	HEA	C26-C15-C16	2.21	119.00	115.27
71	Bg	201	PLX	C1C-N1-C1	2.21	118.96	109.92
71	g	201	PLX	C1C-N1-C1	2.21	118.94	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
71	Bg	202	PLX	C1C-N1-C1	2.19	118.89	109.92
71	g	202	PLX	C1C-N1-C1	2.19	118.89	109.92
81	AU	402	HEC	CMB-C2B-C1B	-2.19	125.09	128.46
73	BJ	401	NDP	C3D-C2D-C1D	2.19	105.59	101.43
79	x	603	HEA	C12-C13-C14	-2.19	106.46	112.23
79	Bx	603	HEA	C12-C13-C14	-2.19	106.46	112.23
82	AJ	401	HEM	CAD-CBD-CGD	-2.19	108.90	113.60
73	J	401	NDP	C3D-C2D-C1D	2.18	105.58	101.43
79	Bx	603	HEA	C4B-C3B-C2B	-2.18	103.68	107.41
82	AV	402	HEM	C4A-C3A-C2A	2.18	108.51	107.00
82	AJ	402	HEM	CMC-C2C-C3C	2.18	128.75	124.68
81	AU	402	HEC	C1D-C2D-C3D	-2.18	105.48	107.00
82	AV	402	HEM	CAD-CBD-CGD	-2.17	108.93	113.60
72	E	201	8Q1	O35-C34-N36	-2.16	118.36	122.99
70	A	502	FMN	C4A-C4-N3	2.16	118.67	113.19
82	AJ	402	HEM	C4B-CHC-C1C	2.15	125.40	122.56
70	BA	502	FMN	C4A-C4-N3	2.15	118.64	113.19
72	BE	201	8Q1	O35-C34-N36	-2.15	118.38	122.99
76	AU	401	PEE	C17-C18-C19	-2.14	112.27	126.84
70	BA	502	FMN	C10-N1-C2	2.14	121.19	116.90
70	A	502	FMN	C10-N1-C2	2.13	121.17	116.90
72	Bp	201	8Q1	O4-C1-S44	-2.13	119.85	122.61
70	A	502	FMN	N3-C2-N1	2.13	123.56	119.38
70	BA	502	FMN	N3-C2-N1	2.12	123.54	119.38
82	AJ	402	HEM	C4A-C3A-C2A	2.12	108.47	107.00
82	AV	402	HEM	C4B-CHC-C1C	2.11	125.34	122.56
72	p	201	8Q1	O4-C1-S44	-2.10	119.88	122.61
71	Br	502	PLX	C2-C1-N1	-2.10	108.77	115.78
71	BU	101	PLX	C5-C4-C3	-2.10	106.83	111.79
71	r	502	PLX	C2-C1-N1	-2.09	108.79	115.78
71	U	101	PLX	C5-C4-C3	-2.09	106.85	111.79
82	AV	402	HEM	CMC-C2C-C3C	2.08	128.57	124.68
71	r	501	PLX	C1C-N1-C1	2.07	118.37	109.92
71	Br	501	PLX	C1C-N1-C1	2.07	118.37	109.92
79	x	603	HEA	C27-C19-C18	-2.06	118.40	123.68
79	Bx	603	HEA	C27-C19-C18	-2.05	118.42	123.68
75	AG	101	CDL	OB6-CB5-OB7	-2.05	118.75	123.70
79	Bx	604	HEA	CBD-CAD-C3D	2.04	118.30	112.63
75	i	401	CDL	OA6-CA5-OA7	-2.03	118.78	123.70
79	x	604	HEA	CMC-C2C-C1C	-2.03	125.34	128.46
71	AQ	101	PLX	C2-C1-N1	-2.03	108.99	115.78
79	Bx	604	HEA	CMC-C2C-C1C	-2.03	125.34	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
75	Bi	401	CDL	OA6-CA5-OA7	-2.03	118.80	123.70
71	AQ	101	PLX	C1C-N1-C1	2.03	118.21	109.92
79	x	604	HEA	CBD-CAD-C3D	2.02	118.24	112.63
82	AJ	402	HEM	CHD-C1D-ND	2.02	126.62	124.43
82	AJ	402	HEM	C3B-C2B-C1B	2.01	107.98	106.49
79	x	603	HEA	C4A-CHB-C1B	2.01	125.21	122.56

All (12) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
79	x	603	HEA	NB
79	x	603	HEA	NA
79	x	603	HEA	ND
79	x	604	HEA	NB
79	x	604	HEA	NA
79	x	604	HEA	ND
79	Bx	603	HEA	NB
79	Bx	603	HEA	NA
79	Bx	603	HEA	ND
79	Bx	604	HEA	NB
79	Bx	604	HEA	NA
79	Bx	604	HEA	ND

All (1799) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
70	A	502	FMN	C1'-C2'-C3'-O3'
70	A	502	FMN	C1'-C2'-C3'-C4'
70	A	502	FMN	C3'-C4'-C5'-O5'
70	A	502	FMN	O4'-C4'-C5'-O5'
70	BA	502	FMN	C1'-C2'-C3'-O3'
70	BA	502	FMN	C1'-C2'-C3'-C4'
70	BA	502	FMN	C3'-C4'-C5'-O5'
70	BA	502	FMN	O4'-C4'-C5'-O5'
71	B	303	PLX	C2-O1-P1-O2
71	B	303	PLX	N1-C1-C2-O1
71	U	101	PLX	O7-C6-C7-C8
71	U	101	PLX	O7-C6-O6-C4
71	U	101	PLX	C3-O4-P1-O2
71	U	101	PLX	N1-C1-C2-O1
71	U	101	PLX	O9-C24-C25-C26
71	b	201	PLX	O7-C6-O6-C4

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Mol	Chain	Res	Type	Atoms
71	b	201	PLX	N1-C1-C2-O1
71	b	201	PLX	O9-C24-O8-C5
71	g	201	PLX	O7-C6-C7-C8
71	g	201	PLX	O7-C6-O6-C4
71	g	201	PLX	C3-C4-O6-C6
71	g	202	PLX	C2-O1-P1-O4
71	g	202	PLX	C2-O1-P1-O2
71	g	202	PLX	C2-O1-P1-O3
71	g	202	PLX	O9-C24-O8-C5
71	g	203	PLX	O7-C6-O6-C4
71	g	203	PLX	C2-O1-P1-O2
71	g	203	PLX	C25-C24-O8-C5
71	r	501	PLX	C3-O4-P1-O1
71	r	501	PLX	C3-O4-P1-O2
71	r	501	PLX	C3-O4-P1-O3
71	r	501	PLX	O8-C24-C25-C26
71	r	502	PLX	C7-C6-O6-C4
71	r	502	PLX	C3-O4-P1-O1
71	r	502	PLX	C3-O4-P1-O2
71	r	502	PLX	C3-O4-P1-O3
71	r	502	PLX	C2-O1-P1-O2
71	r	502	PLX	N1-C1-C2-O1
71	r	502	PLX	O9-C24-C25-C26
71	AL	501	PLX	O7-C6-C7-C8
71	AN	101	PLX	O7-C6-C7-C8
71	AN	101	PLX	N1-C1-C2-O1
71	AN	101	PLX	O9-C24-C25-C26
71	AQ	101	PLX	O7-C6-O6-C4
71	AQ	101	PLX	O6-C4-C5-O8
71	AQ	101	PLX	N1-C1-C2-O1
71	AQ	101	PLX	C25-C24-O8-C5
71	AQ	101	PLX	O9-C24-C25-C26
71	AT	101	PLX	C2-O1-P1-O4
71	AT	101	PLX	O9-C24-O8-C5
71	BB	303	PLX	C2-O1-P1-O2
71	BB	303	PLX	N1-C1-C2-O1
71	BU	101	PLX	O7-C6-C7-C8
71	BU	101	PLX	O7-C6-O6-C4
71	BU	101	PLX	C3-O4-P1-O2
71	BU	101	PLX	N1-C1-C2-O1
71	BU	101	PLX	O9-C24-C25-C26
71	BV	203	PLX	O7-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
71	BV	203	PLX	N1-C1-C2-O1
71	BV	203	PLX	O9-C24-C25-C26
71	Bb	201	PLX	O7-C6-O6-C4
71	Bb	201	PLX	N1-C1-C2-O1
71	Bb	201	PLX	O9-C24-O8-C5
71	Bg	201	PLX	O7-C6-C7-C8
71	Bg	201	PLX	O7-C6-O6-C4
71	Bg	201	PLX	C3-C4-O6-C6
71	Bg	202	PLX	C2-O1-P1-O4
71	Bg	202	PLX	C2-O1-P1-O2
71	Bg	202	PLX	C2-O1-P1-O3
71	Bg	202	PLX	O9-C24-O8-C5
71	Bg	203	PLX	O7-C6-O6-C4
71	Bg	203	PLX	C2-O1-P1-O2
71	Bg	203	PLX	C25-C24-O8-C5
71	Br	501	PLX	C3-O4-P1-O1
71	Br	501	PLX	C3-O4-P1-O2
71	Br	501	PLX	C3-O4-P1-O3
71	Br	501	PLX	O8-C24-C25-C26
71	Br	502	PLX	C7-C6-O6-C4
71	Br	502	PLX	C3-O4-P1-O1
71	Br	502	PLX	C3-O4-P1-O2
71	Br	502	PLX	C3-O4-P1-O3
71	Br	502	PLX	C2-O1-P1-O2
71	Br	502	PLX	N1-C1-C2-O1
71	Br	502	PLX	O9-C24-C25-C26
72	E	201	8Q1	C1-C6-C7-C8
72	E	201	8Q1	O4-C1-S44-C43
72	E	201	8Q1	C6-C1-S44-C43
72	E	201	8Q1	C29-C32-C34-N36
72	E	201	8Q1	C29-C32-C34-O35
72	E	201	8Q1	C42-C43-S44-C1
72	E	201	8Q1	C28-O27-P24-O3
72	E	201	8Q1	C28-O27-P24-O2
72	E	201	8Q1	C28-O27-P24-O1
72	p	201	8Q1	C1-C6-C7-C8
72	p	201	8Q1	O4-C1-S44-C43
72	p	201	8Q1	C6-C1-S44-C43
72	p	201	8Q1	C28-C29-C32-C34
72	p	201	8Q1	C28-C29-C32-O33
72	p	201	8Q1	C30-C29-C32-C34
72	p	201	8Q1	C31-C29-C32-C34

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Mol	Chain	Res	Type	Atoms
72	p	201	8Q1	C31-C29-C32-O33
72	p	201	8Q1	C28-O27-P24-O2
72	p	201	8Q1	C28-O27-P24-O1
72	BE	201	8Q1	C1-C6-C7-C8
72	BE	201	8Q1	O4-C1-S44-C43
72	BE	201	8Q1	C6-C1-S44-C43
72	BE	201	8Q1	C29-C32-C34-N36
72	BE	201	8Q1	C29-C32-C34-O35
72	BE	201	8Q1	C42-C43-S44-C1
72	BE	201	8Q1	C28-O27-P24-O3
72	BE	201	8Q1	C28-O27-P24-O2
72	BE	201	8Q1	C28-O27-P24-O1
72	Bp	201	8Q1	C1-C6-C7-C8
72	Bp	201	8Q1	O4-C1-S44-C43
72	Bp	201	8Q1	C6-C1-S44-C43
72	Bp	201	8Q1	C28-C29-C32-C34
72	Bp	201	8Q1	C28-C29-C32-O33
72	Bp	201	8Q1	C30-C29-C32-C34
72	Bp	201	8Q1	C31-C29-C32-C34
72	Bp	201	8Q1	C31-C29-C32-O33
72	Bp	201	8Q1	C28-O27-P24-O2
72	Bp	201	8Q1	C28-O27-P24-O1
73	J	401	NDP	C5B-O5B-PA-O1A
73	J	401	NDP	C5D-O5D-PN-O1N
73	BJ	401	NDP	C5B-O5B-PA-O1A
73	BJ	401	NDP	C5D-O5D-PN-O1N
75	V	201	CDL	CB2-C1-CA2-OA2
75	V	201	CDL	CA2-OA2-PA1-OA3
75	V	201	CDL	CA2-OA2-PA1-OA4
75	V	201	CDL	CA2-OA2-PA1-OA5
75	V	201	CDL	CA3-OA5-PA1-OA3
75	V	201	CDL	CA3-OA5-PA1-OA4
75	V	201	CDL	OA9-CA7-OA8-CA6
75	V	201	CDL	C51-CB5-OB6-CB4
75	i	401	CDL	O1-C1-CA2-OA2
75	i	401	CDL	CB2-C1-CA2-OA2
75	i	401	CDL	CA2-OA2-PA1-OA3
75	i	401	CDL	CA2-OA2-PA1-OA4
75	i	401	CDL	CA2-OA2-PA1-OA5
75	i	401	CDL	CA3-OA5-PA1-OA3
75	i	401	CDL	CA3-OA5-PA1-OA4
75	i	401	CDL	OA6-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
75	i	401	CDL	CB2-OB2-PB2-OB4
75	i	401	CDL	CB3-OB5-PB2-OB3
75	i	401	CDL	CB3-OB5-PB2-OB4
75	l	703	CDL	CA2-OA2-PA1-OA3
75	l	703	CDL	OB7-CB5-OB6-CB4
75	l	704	CDL	CA2-OA2-PA1-OA3
75	l	704	CDL	CA2-OA2-PA1-OA4
75	l	704	CDL	CA3-OA5-PA1-OA2
75	l	704	CDL	CA3-OA5-PA1-OA4
75	l	704	CDL	C11-CA5-OA6-CA4
75	l	704	CDL	CB2-OB2-PB2-OB3
75	n	101	CDL	CA2-OA2-PA1-OA3
75	n	101	CDL	CA2-OA2-PA1-OA4
75	n	101	CDL	CA2-OA2-PA1-OA5
75	n	101	CDL	OA7-CA5-OA6-CA4
75	n	101	CDL	C11-CA5-OA6-CA4
75	n	101	CDL	CB2-OB2-PB2-OB3
75	n	101	CDL	CB2-OB2-PB2-OB4
75	n	101	CDL	C51-CB5-OB6-CB4
75	AA	101	CDL	O1-C1-CB2-OB2
75	AA	101	CDL	CB2-OB2-PB2-OB4
75	AA	101	CDL	CB2-OB2-PB2-OB5
75	AG	101	CDL	OA9-CA7-OA8-CA6
75	AG	101	CDL	CB2-OB2-PB2-OB4
75	AH	403	CDL	CA2-OA2-PA1-OA3
75	AH	403	CDL	CA2-OA2-PA1-OA4
75	AH	403	CDL	CA3-OA5-PA1-OA2
75	AH	403	CDL	C11-CA5-OA6-CA4
75	AH	403	CDL	CB3-OB5-PB2-OB3
75	AH	403	CDL	OB7-CB5-OB6-CB4
75	AJ	404	CDL	CA3-OA5-PA1-OA2
75	AJ	404	CDL	CA3-OA5-PA1-OA3
75	AJ	404	CDL	CA3-OA5-PA1-OA4
75	AJ	404	CDL	C11-CA5-OA6-CA4
75	AJ	404	CDL	CB3-OB5-PB2-OB2
75	AJ	404	CDL	CB3-OB5-PB2-OB3
75	AJ	404	CDL	CB3-OB5-PB2-OB4
75	AJ	405	CDL	CA3-OA5-PA1-OA4
75	AJ	405	CDL	C51-CB5-OB6-CB4
75	AL	502	CDL	O1-C1-CA2-OA2
75	AL	502	CDL	CA3-OA5-PA1-OA2
75	AL	502	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
75	AL	502	CDL	CB2-OB2-PB2-OB3
75	AL	502	CDL	CB2-OB2-PB2-OB4
75	AL	502	CDL	C71-CB7-OB8-CB6
75	AN	102	CDL	CA3-OA5-PA1-OA3
75	AN	102	CDL	OA7-CA5-OA6-CA4
75	AN	102	CDL	C11-CA5-OA6-CA4
75	AN	102	CDL	CB2-OB2-PB2-OB4
75	AN	102	CDL	CB2-OB2-PB2-OB5
75	AU	403	CDL	CA3-OA5-PA1-OA2
75	AU	403	CDL	CA3-OA5-PA1-OA3
75	AU	403	CDL	C11-CA5-OA6-CA4
75	AU	403	CDL	CB3-OB5-PB2-OB2
75	AU	403	CDL	CB3-OB5-PB2-OB3
75	AU	403	CDL	OB7-CB5-OB6-CB4
75	AY	501	CDL	CB2-C1-CA2-OA2
75	AY	501	CDL	C11-CA5-OA6-CA4
75	BV	201	CDL	CB2-C1-CA2-OA2
75	BV	201	CDL	CA2-OA2-PA1-OA3
75	BV	201	CDL	CA2-OA2-PA1-OA4
75	BV	201	CDL	CA2-OA2-PA1-OA5
75	BV	201	CDL	CA3-OA5-PA1-OA3
75	BV	201	CDL	CA3-OA5-PA1-OA4
75	BV	201	CDL	OA9-CA7-OA8-CA6
75	BV	201	CDL	C51-CB5-OB6-CB4
75	Bi	401	CDL	O1-C1-CA2-OA2
75	Bi	401	CDL	CB2-C1-CA2-OA2
75	Bi	401	CDL	CA2-OA2-PA1-OA3
75	Bi	401	CDL	CA2-OA2-PA1-OA4
75	Bi	401	CDL	CA2-OA2-PA1-OA5
75	Bi	401	CDL	CA3-OA5-PA1-OA3
75	Bi	401	CDL	CA3-OA5-PA1-OA4
75	Bi	401	CDL	OA6-CA4-CA6-OA8
75	Bi	401	CDL	CB2-OB2-PB2-OB4
75	Bi	401	CDL	CB3-OB5-PB2-OB3
75	Bi	401	CDL	CB3-OB5-PB2-OB4
75	Bl	703	CDL	CA2-OA2-PA1-OA3
75	Bl	703	CDL	OB7-CB5-OB6-CB4
75	Bl	704	CDL	CA2-OA2-PA1-OA3
75	Bl	704	CDL	CA2-OA2-PA1-OA4
75	Bl	704	CDL	CA3-OA5-PA1-OA2
75	Bl	704	CDL	CA3-OA5-PA1-OA4
75	Bl	704	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
75	B1	704	CDL	CB2-OB2-PB2-OB3
75	Bn	101	CDL	CA2-OA2-PA1-OA3
75	Bn	101	CDL	CA2-OA2-PA1-OA4
75	Bn	101	CDL	CA2-OA2-PA1-OA5
75	Bn	101	CDL	OA7-CA5-OA6-CA4
75	Bn	101	CDL	C11-CA5-OA6-CA4
75	Bn	101	CDL	CB2-OB2-PB2-OB3
75	Bn	101	CDL	CB2-OB2-PB2-OB4
75	Bn	101	CDL	C51-CB5-OB6-CB4
76	V	202	PEE	C2-C1-O3P-P
76	V	202	PEE	O4P-C4-C5-N
76	W	201	PEE	C4-O4P-P-O1P
76	W	201	PEE	C4-O4P-P-O3P
76	l	701	PEE	C11-C10-O2-C2
76	l	701	PEE	C4-O4P-P-O1P
76	l	701	PEE	C4-O4P-P-O2P
76	AH	401	PEE	C4-O4P-P-O2P
76	AJ	403	PEE	C37-C38-C39-C40
76	AL	503	PEE	C11-C10-O2-C2
76	AL	503	PEE	O4-C10-O2-C2
76	AU	401	PEE	C11-C10-O2-C2
76	AU	401	PEE	C1-O3P-P-O1P
76	AU	401	PEE	C1-O3P-P-O2P
76	AU	401	PEE	C4-O4P-P-O2P
76	AV	403	PEE	O4P-C4-C5-N
76	AV	403	PEE	C39-C40-C41-C42
76	AY	502	PEE	C1-O3P-P-O2P
76	AY	502	PEE	C4-O4P-P-O1P
76	AY	502	PEE	C4-O4P-P-O2P
76	AY	502	PEE	C4-O4P-P-O3P
76	BV	202	PEE	C2-C1-O3P-P
76	BV	202	PEE	O4P-C4-C5-N
76	BW	201	PEE	C4-O4P-P-O1P
76	BW	201	PEE	C4-O4P-P-O3P
76	B1	701	PEE	C11-C10-O2-C2
76	B1	701	PEE	C4-O4P-P-O1P
76	B1	701	PEE	C4-O4P-P-O2P
79	x	603	HEA	C12-C11-C3B-C2B
79	Bx	603	HEA	C12-C11-C3B-C2B
82	AJ	402	HEM	C1A-C2A-CAA-CBA
82	AV	402	HEM	C1A-C2A-CAA-CBA
82	AV	402	HEM	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
75	AL	502	CDL	OB9-CB7-OB8-CB6
75	l	704	CDL	OA9-CA7-OA8-CA6
75	l	704	CDL	OB9-CB7-OB8-CB6
75	n	101	CDL	OA9-CA7-OA8-CA6
75	AA	101	CDL	OB9-CB7-OB8-CB6
75	AN	102	CDL	OB9-CB7-OB8-CB6
75	AU	403	CDL	OB9-CB7-OB8-CB6
75	Bl	704	CDL	OA9-CA7-OA8-CA6
75	Bl	704	CDL	OB9-CB7-OB8-CB6
75	Bn	101	CDL	OA9-CA7-OA8-CA6
75	V	201	CDL	OB7-CB5-OB6-CB4
75	l	704	CDL	OA7-CA5-OA6-CA4
75	n	101	CDL	OB7-CB5-OB6-CB4
75	AJ	404	CDL	OA7-CA5-OA6-CA4
75	AJ	405	CDL	OB7-CB5-OB6-CB4
75	AL	502	CDL	OA7-CA5-OA6-CA4
75	AU	403	CDL	OA7-CA5-OA6-CA4
75	AY	501	CDL	OA7-CA5-OA6-CA4
75	AY	501	CDL	OB7-CB5-OB6-CB4
75	BV	201	CDL	OB7-CB5-OB6-CB4
75	Bl	704	CDL	OA7-CA5-OA6-CA4
75	Bn	101	CDL	OB7-CB5-OB6-CB4
76	l	701	PEE	O4-C10-O2-C2
76	AU	401	PEE	O4-C10-O2-C2
76	Bl	701	PEE	O4-C10-O2-C2
75	l	704	CDL	C31-CA7-OA8-CA6
75	l	704	CDL	C71-CB7-OB8-CB6
75	n	101	CDL	C31-CA7-OA8-CA6
75	n	101	CDL	C71-CB7-OB8-CB6
75	AG	101	CDL	C31-CA7-OA8-CA6
75	AN	102	CDL	C71-CB7-OB8-CB6
75	AU	403	CDL	C71-CB7-OB8-CB6
75	Bl	704	CDL	C31-CA7-OA8-CA6
75	Bl	704	CDL	C71-CB7-OB8-CB6
75	Bn	101	CDL	C31-CA7-OA8-CA6
75	Bn	101	CDL	C71-CB7-OB8-CB6
75	l	703	CDL	C51-CB5-OB6-CB4
75	AH	403	CDL	C51-CB5-OB6-CB4
75	AU	403	CDL	C51-CB5-OB6-CB4
75	AY	501	CDL	C51-CB5-OB6-CB4
75	Bl	703	CDL	C51-CB5-OB6-CB4
72	E	201	8Q1	C38-C39-N41-C42

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Mol	Chain	Res	Type	Atoms
72	BE	201	8Q1	C38-C39-N41-C42
75	AA	101	CDL	C71-CB7-OB8-CB6
75	AH	403	CDL	C71-CB7-OB8-CB6
75	AJ	405	CDL	C31-CA7-OA8-CA6
75	AL	502	CDL	C31-CA7-OA8-CA6
76	W	201	PEE	C17-C18-C19-C20
76	l	701	PEE	C37-C38-C39-C40
76	l	702	PEE	C37-C38-C39-C40
76	BW	201	PEE	C17-C18-C19-C20
76	Bl	701	PEE	C37-C38-C39-C40
76	Bl	702	PEE	C37-C38-C39-C40
75	AH	403	CDL	OA7-CA5-OA6-CA4
75	n	101	CDL	OB9-CB7-OB8-CB6
75	Bn	101	CDL	OB9-CB7-OB8-CB6
76	l	702	PEE	O5-C30-O3-C3
76	Bl	702	PEE	O5-C30-O3-C3
71	AL	501	PLX	C2-C1-N1-C1C
75	l	703	CDL	O1-C1-CA2-OA2
75	l	704	CDL	O1-C1-CA2-OA2
75	AG	101	CDL	O1-C1-CB2-OB2
75	AY	501	CDL	O1-C1-CA2-OA2
75	AY	501	CDL	O1-C1-CB2-OB2
75	Bl	703	CDL	O1-C1-CA2-OA2
75	Bl	704	CDL	O1-C1-CA2-OA2
75	AU	403	CDL	C31-CA7-OA8-CA6
75	AH	403	CDL	OB9-CB7-OB8-CB6
75	i	401	CDL	C11-CA5-OA6-CA4
75	AA	101	CDL	C51-CB5-OB6-CB4
75	Bi	401	CDL	C11-CA5-OA6-CA4
76	W	201	PEE	C21-C22-C23-C24
76	AU	401	PEE	C31-C32-C33-C34
76	BW	201	PEE	C21-C22-C23-C24
76	V	202	PEE	C20-C21-C22-C23
76	BV	202	PEE	C20-C21-C22-C23
71	r	502	PLX	C16-C17-C18-C19
71	Br	502	PLX	C16-C17-C18-C19
75	AH	403	CDL	C31-C32-C33-C34
76	l	701	PEE	C32-C33-C34-C35
76	Bl	701	PEE	C32-C33-C34-C35
73	J	401	NDP	O4B-C4B-C5B-O5B
73	J	401	NDP	C3B-C4B-C5B-O5B
73	BJ	401	NDP	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
73	BJ	401	NDP	C3B-C4B-C5B-O5B
76	l	702	PEE	C31-C30-O3-C3
76	Bl	702	PEE	C31-C30-O3-C3
71	r	501	PLX	C10-C11-C12-C13
71	Bg	203	PLX	C26-C27-C28-C29
71	Br	501	PLX	C10-C11-C12-C13
71	b	201	PLX	C4-C3-O4-P1
71	Bb	201	PLX	C4-C3-O4-P1
75	AJ	405	CDL	OA9-CA7-OA8-CA6
75	AL	502	CDL	OA9-CA7-OA8-CA6
75	AU	403	CDL	OA9-CA7-OA8-CA6
71	g	203	PLX	C26-C27-C28-C29
76	W	201	PEE	C32-C33-C34-C35
79	x	603	HEA	C15-C16-C17-C18
79	Bx	603	HEA	C15-C16-C17-C18
71	b	201	PLX	C14-C15-C16-C17
71	g	203	PLX	C30-C31-C32-C33
71	r	502	PLX	C30-C31-C32-C33
71	Bb	201	PLX	C14-C15-C16-C17
71	Bg	203	PLX	C30-C31-C32-C33
71	Br	502	PLX	C30-C31-C32-C33
75	AJ	405	CDL	C71-C72-C73-C74
75	AY	501	CDL	C12-C13-C14-C15
76	BW	201	PEE	C32-C33-C34-C35
73	J	401	NDP	C1B-C2B-O2B-P2B
73	BJ	401	NDP	C1B-C2B-O2B-P2B
71	g	202	PLX	C10-C11-C12-C13
71	Bg	202	PLX	C10-C11-C12-C13
72	E	201	8Q1	O40-C39-N41-C42
72	BE	201	8Q1	O40-C39-N41-C42
75	l	703	CDL	CB2-C1-CA2-OA2
75	AA	101	CDL	CA2-C1-CB2-OB2
75	AJ	404	CDL	CB2-C1-CA2-OA2
75	AL	502	CDL	CB2-C1-CA2-OA2
75	AL	502	CDL	CA2-C1-CB2-OB2
75	Bl	703	CDL	CB2-C1-CA2-OA2
71	r	502	PLX	C12-C13-C14-C15
71	Br	502	PLX	C12-C13-C14-C15
75	i	401	CDL	C31-C32-C33-C34
75	Bi	401	CDL	C31-C32-C33-C34
75	AH	403	CDL	C31-CA7-OA8-CA6
75	AY	501	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
76	W	201	PEE	C31-C30-O3-C3
76	BW	201	PEE	C31-C30-O3-C3
75	l	703	CDL	C73-C74-C75-C76
75	Bl	703	CDL	C73-C74-C75-C76
75	l	703	CDL	OB5-CB3-CB4-OB6
75	Bl	703	CDL	OB5-CB3-CB4-OB6
76	W	201	PEE	C12-C13-C14-C15
76	BW	201	PEE	C12-C13-C14-C15
75	V	201	CDL	O1-C1-CA2-OA2
75	l	703	CDL	O1-C1-CB2-OB2
75	AA	101	CDL	O1-C1-CA2-OA2
75	AJ	404	CDL	O1-C1-CA2-OA2
75	BV	201	CDL	O1-C1-CA2-OA2
75	Bl	703	CDL	O1-C1-CB2-OB2
75	AY	501	CDL	CB5-C51-C52-C53
71	AT	101	PLX	O6-C4-C5-O8
71	r	501	PLX	C12-C13-C14-C15
71	Br	501	PLX	C12-C13-C14-C15
76	l	701	PEE	C34-C35-C36-C37
76	Bl	701	PEE	C34-C35-C36-C37
76	W	201	PEE	O5-C30-O3-C3
76	BW	201	PEE	O5-C30-O3-C3
75	V	201	CDL	C54-C55-C56-C57
75	BV	201	CDL	C54-C55-C56-C57
75	i	401	CDL	OA7-CA5-OA6-CA4
75	Bi	401	CDL	OA7-CA5-OA6-CA4
75	AH	403	CDL	OA9-CA7-OA8-CA6
71	AN	101	PLX	C13-C14-C15-C16
71	BV	203	PLX	C13-C14-C15-C16
75	l	704	CDL	CB5-C51-C52-C53
75	n	101	CDL	CA7-C31-C32-C33
75	AH	403	CDL	CB5-C51-C52-C53
75	AY	501	CDL	CA7-C31-C32-C33
75	Bl	704	CDL	CB5-C51-C52-C53
75	Bn	101	CDL	CA7-C31-C32-C33
76	Bl	702	PEE	C10-C11-C12-C13
76	l	702	PEE	C17-C18-C19-C20
76	AH	401	PEE	C37-C38-C39-C40
76	Bl	702	PEE	C17-C18-C19-C20
75	AN	102	CDL	C71-C72-C73-C74
76	W	201	PEE	C15-C16-C17-C18
76	BW	201	PEE	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
75	i	401	CDL	CA5-C11-C12-C13
75	AJ	404	CDL	CA7-C31-C32-C33
75	AL	502	CDL	CA5-C11-C12-C13
75	AN	102	CDL	CA5-C11-C12-C13
75	AU	403	CDL	CA5-C11-C12-C13
75	Bi	401	CDL	CA5-C11-C12-C13
76	V	202	PEE	C10-C11-C12-C13
76	l	701	PEE	C30-C31-C32-C33
76	l	702	PEE	C10-C11-C12-C13
76	AV	403	PEE	C10-C11-C12-C13
76	BV	202	PEE	C10-C11-C12-C13
71	r	501	PLX	C27-C28-C29-C30
71	Br	501	PLX	C27-C28-C29-C30
75	AL	502	CDL	C52-C53-C54-C55
75	AA	101	CDL	OB7-CB5-OB6-CB4
75	AA	101	CDL	CB7-C71-C72-C73
75	AG	101	CDL	CB7-C71-C72-C73
75	AJ	405	CDL	CB7-C71-C72-C73
82	AJ	401	HEM	C3D-CAD-CBD-CGD
82	AV	401	HEM	C3D-CAD-CBD-CGD
76	Bl	701	PEE	C30-C31-C32-C33
75	n	101	CDL	C31-C32-C33-C34
75	Bn	101	CDL	C31-C32-C33-C34
76	AL	503	PEE	C30-C31-C32-C33
75	AL	502	CDL	O1-C1-CB2-OB2
75	i	401	CDL	C31-CA7-OA8-CA6
75	Bi	401	CDL	C31-CA7-OA8-CA6
73	J	401	NDP	C3B-C2B-O2B-P2B
73	BJ	401	NDP	C3B-C2B-O2B-P2B
75	AN	102	CDL	C14-C15-C16-C17
75	AY	501	CDL	OA9-CA7-OA8-CA6
76	l	701	PEE	C39-C40-C41-C42
76	Bl	701	PEE	C39-C40-C41-C42
76	V	202	PEE	C17-C18-C19-C20
76	l	701	PEE	C17-C18-C19-C20
76	BV	202	PEE	C17-C18-C19-C20
76	Bl	701	PEE	C17-C18-C19-C20
75	AH	403	CDL	C33-C34-C35-C36
71	B	303	PLX	C2-O1-P1-O4
71	U	101	PLX	C3-O4-P1-O1
71	b	201	PLX	C3-O4-P1-O1
71	g	201	PLX	C3-O4-P1-O1

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Mol	Chain	Res	Type	Atoms
71	g	202	PLX	C3-O4-P1-O1
71	g	203	PLX	C2-O1-P1-O4
71	r	502	PLX	C2-O1-P1-O4
71	BB	303	PLX	C2-O1-P1-O4
71	BU	101	PLX	C3-O4-P1-O1
71	Bb	201	PLX	C3-O4-P1-O1
71	Bg	201	PLX	C3-O4-P1-O1
71	Bg	202	PLX	C3-O4-P1-O1
71	Bg	203	PLX	C2-O1-P1-O4
71	Br	502	PLX	C2-O1-P1-O4
75	V	201	CDL	CA3-OA5-PA1-OA2
75	V	201	CDL	CB3-OB5-PB2-OB2
75	i	401	CDL	CA3-OA5-PA1-OA2
75	i	401	CDL	CB2-OB2-PB2-OB5
75	i	401	CDL	CB3-OB5-PB2-OB2
75	l	703	CDL	CB3-OB5-PB2-OB2
75	l	704	CDL	CA2-OA2-PA1-OA5
75	n	101	CDL	CB2-OB2-PB2-OB5
75	AG	101	CDL	CA2-OA2-PA1-OA5
75	AG	101	CDL	CB2-OB2-PB2-OB5
75	AH	403	CDL	CA2-OA2-PA1-OA5
75	AH	403	CDL	CB3-OB5-PB2-OB2
75	AJ	405	CDL	CA3-OA5-PA1-OA2
75	AL	502	CDL	CB2-OB2-PB2-OB5
75	AL	502	CDL	CB3-OB5-PB2-OB2
75	AN	102	CDL	CA3-OA5-PA1-OA2
75	AY	501	CDL	CA3-OA5-PA1-OA2
75	BV	201	CDL	CA3-OA5-PA1-OA2
75	BV	201	CDL	CB3-OB5-PB2-OB2
75	Bi	401	CDL	CA3-OA5-PA1-OA2
75	Bi	401	CDL	CB2-OB2-PB2-OB5
75	Bi	401	CDL	CB3-OB5-PB2-OB2
75	Bl	703	CDL	CB3-OB5-PB2-OB2
75	Bl	704	CDL	CA2-OA2-PA1-OA5
75	Bn	101	CDL	CB2-OB2-PB2-OB5
76	V	202	PEE	C1-O3P-P-O4P
76	W	201	PEE	C1-O3P-P-O4P
76	l	701	PEE	C4-O4P-P-O3P
76	AH	401	PEE	C4-O4P-P-O3P
76	AU	401	PEE	C1-O3P-P-O4P
76	AU	401	PEE	C4-O4P-P-O3P
76	AY	502	PEE	C1-O3P-P-O4P

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Mol	Chain	Res	Type	Atoms
76	BV	202	PEE	C1-O3P-P-O4P
76	BW	201	PEE	C1-O3P-P-O4P
76	Bl	701	PEE	C4-O4P-P-O3P
75	AY	501	CDL	C71-CB7-OB8-CB6
76	V	202	PEE	C31-C30-O3-C3
76	BV	202	PEE	C31-C30-O3-C3
71	AL	501	PLX	C12-C13-C14-C15
75	l	703	CDL	CA2-C1-CB2-OB2
75	AG	101	CDL	CA2-C1-CB2-OB2
75	AY	501	CDL	CA2-C1-CB2-OB2
75	Bl	703	CDL	CA2-C1-CB2-OB2
71	AL	501	PLX	C2-C1-N1-C1A
75	l	703	CDL	C71-CB7-OB8-CB6
75	Bl	703	CDL	C71-CB7-OB8-CB6
71	B	303	PLX	O6-C6-C7-C8
71	U	101	PLX	O6-C6-C7-C8
71	g	203	PLX	O8-C24-C25-C26
71	AQ	101	PLX	O8-C24-C25-C26
71	BB	303	PLX	O6-C6-C7-C8
71	BU	101	PLX	O6-C6-C7-C8
71	Bg	203	PLX	O8-C24-C25-C26
75	n	101	CDL	C13-C14-C15-C16
75	Bn	101	CDL	C13-C14-C15-C16
75	l	704	CDL	C51-CB5-OB6-CB4
75	AG	101	CDL	C51-CB5-OB6-CB4
75	Bl	704	CDL	C51-CB5-OB6-CB4
71	B	303	PLX	C27-C28-C29-C30
71	g	201	PLX	C13-C14-C15-C16
71	g	201	PLX	C7-C8-C9-C10
71	g	202	PLX	C7-C8-C9-C10
71	g	203	PLX	C29-C30-C31-C32
71	AQ	101	PLX	C19-C20-C21-C22
71	AT	101	PLX	C7-C8-C9-C10
71	BB	303	PLX	C27-C28-C29-C30
71	Bg	201	PLX	C13-C14-C15-C16
71	Bg	201	PLX	C7-C8-C9-C10
71	Bg	202	PLX	C7-C8-C9-C10
71	Bg	203	PLX	C29-C30-C31-C32
75	l	704	CDL	C31-C32-C33-C34
75	n	101	CDL	C12-C13-C14-C15
75	AG	101	CDL	C33-C34-C35-C36
75	AJ	405	CDL	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
75	AY	501	CDL	C32-C33-C34-C35
75	Bn	101	CDL	C12-C13-C14-C15
76	W	201	PEE	C14-C15-C16-C17
76	l	701	PEE	C22-C23-C24-C25
76	BW	201	PEE	C14-C15-C16-C17
76	Bl	701	PEE	C22-C23-C24-C25
71	g	203	PLX	C34-C35-C36-C37
71	AT	101	PLX	C9-C10-C11-C12
71	Bg	203	PLX	C34-C35-C36-C37
75	AU	403	CDL	C13-C14-C15-C16
75	Bl	704	CDL	C31-C32-C33-C34
76	l	702	PEE	C20-C21-C22-C23
76	AJ	403	PEE	C20-C21-C22-C23
76	AY	502	PEE	C11-C12-C13-C14
76	Bl	702	PEE	C20-C21-C22-C23
75	AL	502	CDL	CA6-CA4-OA6-CA5
75	l	704	CDL	OB7-CB5-OB6-CB4
75	AG	101	CDL	OB7-CB5-OB6-CB4
75	Bl	704	CDL	OB7-CB5-OB6-CB4
75	n	101	CDL	CB5-C51-C52-C53
75	Bn	101	CDL	CB5-C51-C52-C53
71	AQ	101	PLX	C10-C11-C12-C13
72	p	201	8Q1	C11-C12-C13-C14
72	Bp	201	8Q1	C11-C12-C13-C14
75	AA	101	CDL	C51-C52-C53-C54
76	Bl	701	PEE	C21-C22-C23-C24
75	AJ	404	CDL	C1-CB2-OB2-PB2
75	AY	501	CDL	OA5-CA3-CA4-OA6
71	AQ	101	PLX	C12-C13-C14-C15
75	V	201	CDL	C71-C72-C73-C74
75	AL	502	CDL	C51-C52-C53-C54
75	AU	403	CDL	C54-C55-C56-C57
75	BV	201	CDL	C71-C72-C73-C74
76	l	701	PEE	C21-C22-C23-C24
71	r	501	PLX	C13-C14-C15-C16
71	Br	501	PLX	C13-C14-C15-C16
71	Br	502	PLX	C14-C15-C16-C17
75	AG	101	CDL	C14-C15-C16-C17
75	Bl	704	CDL	C51-C52-C53-C54
76	V	202	PEE	C12-C13-C14-C15
76	BV	202	PEE	C12-C13-C14-C15
75	l	703	CDL	CB7-C71-C72-C73

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Mol	Chain	Res	Type	Atoms
75	l	704	CDL	CB7-C71-C72-C73
75	AA	101	CDL	CA5-C11-C12-C13
75	Bl	703	CDL	CB7-C71-C72-C73
75	Bl	704	CDL	CB7-C71-C72-C73
71	U	101	PLX	C33-C34-C35-C36
71	r	502	PLX	C14-C15-C16-C17
71	AL	501	PLX	C15-C16-C17-C18
71	AL	501	PLX	C13-C14-C15-C16
71	BU	101	PLX	C33-C34-C35-C36
71	Bb	201	PLX	C16-C17-C18-C19
72	p	201	8Q1	C6-C7-C8-C9
72	Bp	201	8Q1	C6-C7-C8-C9
75	l	704	CDL	C51-C52-C53-C54
75	AA	101	CDL	C31-C32-C33-C34
76	V	202	PEE	C40-C41-C42-C43
76	l	702	PEE	C33-C34-C35-C36
76	AJ	403	PEE	C13-C14-C15-C16
76	BV	202	PEE	C40-C41-C42-C43
76	Bl	702	PEE	C33-C34-C35-C36
71	U	101	PLX	C19-C20-C21-C22
71	U	101	PLX	C10-C11-C12-C13
71	U	101	PLX	C35-C36-C37-C38
71	b	201	PLX	C16-C17-C18-C19
71	g	203	PLX	C15-C16-C17-C18
71	r	502	PLX	C11-C12-C13-C14
71	r	502	PLX	C10-C11-C12-C13
71	BU	101	PLX	C19-C20-C21-C22
71	BU	101	PLX	C10-C11-C12-C13
71	BU	101	PLX	C35-C36-C37-C38
71	Bg	203	PLX	C15-C16-C17-C18
71	Br	502	PLX	C11-C12-C13-C14
71	Br	502	PLX	C10-C11-C12-C13
76	AH	401	PEE	C21-C22-C23-C24
76	AJ	403	PEE	C11-C12-C13-C14
75	AN	102	CDL	CB4-CB6-OB8-CB7
71	B	303	PLX	C28-C29-C30-C31
71	U	101	PLX	C12-C13-C14-C15
71	U	101	PLX	C9-C10-C11-C12
71	b	201	PLX	C27-C28-C29-C30
71	b	201	PLX	C29-C30-C31-C32
71	g	202	PLX	C14-C15-C16-C17
71	AN	101	PLX	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
71	AQ	101	PLX	C34-C35-C36-C37
71	BB	303	PLX	C28-C29-C30-C31
71	BU	101	PLX	C12-C13-C14-C15
71	BU	101	PLX	C9-C10-C11-C12
71	BV	203	PLX	C10-C11-C12-C13
71	Bb	201	PLX	C27-C28-C29-C30
71	Bb	201	PLX	C29-C30-C31-C32
72	E	201	8Q1	C12-C13-C14-C15
72	BE	201	8Q1	C12-C13-C14-C15
75	i	401	CDL	C13-C14-C15-C16
75	l	704	CDL	C32-C33-C34-C35
75	Bi	401	CDL	C13-C14-C15-C16
75	Bl	704	CDL	C32-C33-C34-C35
76	l	702	PEE	C40-C41-C42-C43
76	AL	503	PEE	C32-C33-C34-C35
76	Bl	702	PEE	C40-C41-C42-C43
71	B	303	PLX	C9-C10-C11-C12
71	r	502	PLX	C9-C10-C11-C12
71	BB	303	PLX	C9-C10-C11-C12
71	Bg	202	PLX	C14-C15-C16-C17
71	Br	502	PLX	C9-C10-C11-C12
75	AJ	405	CDL	C33-C34-C35-C36
75	AL	502	CDL	C32-C33-C34-C35
75	AU	403	CDL	C31-C32-C33-C34
76	V	202	PEE	C14-C15-C16-C17
76	AH	401	PEE	C11-C12-C13-C14
76	AU	401	PEE	C11-C12-C13-C14
76	BV	202	PEE	C14-C15-C16-C17
71	U	101	PLX	C7-C8-C9-C10
71	b	201	PLX	C18-C19-C20-C21
71	g	201	PLX	C16-C17-C18-C19
71	AL	501	PLX	C10-C11-C12-C13
71	Bb	201	PLX	C18-C19-C20-C21
71	Bg	201	PLX	C16-C17-C18-C19
75	AY	501	CDL	C14-C15-C16-C17
76	l	702	PEE	C34-C35-C36-C37
76	AH	401	PEE	C22-C23-C24-C25
76	AJ	403	PEE	C22-C23-C24-C25
76	AL	503	PEE	C11-C12-C13-C14
76	Bl	702	PEE	C34-C35-C36-C37
76	AV	403	PEE	C35-C36-C37-C38
76	AY	502	PEE	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
75	l	704	CDL	CA7-C31-C32-C33
75	AG	101	CDL	CA5-C11-C12-C13
75	AL	502	CDL	CA7-C31-C32-C33
75	AU	403	CDL	CB7-C71-C72-C73
75	Bl	704	CDL	CA7-C31-C32-C33
71	g	201	PLX	C10-C11-C12-C13
71	AN	101	PLX	C25-C26-C27-C28
71	BU	101	PLX	C7-C8-C9-C10
71	BV	203	PLX	C25-C26-C27-C28
71	Bg	201	PLX	C10-C11-C12-C13
75	l	703	CDL	C51-C52-C53-C54
75	Bl	703	CDL	C51-C52-C53-C54
71	AL	501	PLX	C2-C1-N1-C1B
71	b	201	PLX	C25-C26-C27-C28
71	Bb	201	PLX	C25-C26-C27-C28
75	l	703	CDL	C11-C12-C13-C14
75	Bl	703	CDL	C11-C12-C13-C14
76	l	702	PEE	C21-C22-C23-C24
76	AY	502	PEE	C22-C23-C24-C25
76	Bl	702	PEE	C21-C22-C23-C24
71	g	202	PLX	C9-C10-C11-C12
71	AN	101	PLX	C32-C33-C34-C35
71	BV	203	PLX	C32-C33-C34-C35
75	n	101	CDL	C51-C52-C53-C54
75	AG	101	CDL	C73-C74-C75-C76
75	Bn	101	CDL	C51-C52-C53-C54
75	n	101	CDL	CB7-C71-C72-C73
75	Bn	101	CDL	CB7-C71-C72-C73
71	AQ	101	PLX	C15-C16-C17-C18
71	Bg	202	PLX	C9-C10-C11-C12
76	l	701	PEE	C20-C21-C22-C23
76	Bl	701	PEE	C20-C21-C22-C23
71	r	502	PLX	C32-C33-C34-C35
71	Br	502	PLX	C32-C33-C34-C35
76	AJ	403	PEE	C32-C33-C34-C35
76	AL	503	PEE	C34-C35-C36-C37
72	E	201	8Q1	N41-C42-C43-S44
72	BE	201	8Q1	N41-C42-C43-S44
71	g	203	PLX	C10-C11-C12-C13
71	Bg	203	PLX	C10-C11-C12-C13
75	AU	403	CDL	C14-C15-C16-C17
76	V	202	PEE	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
76	AV	403	PEE	C32-C33-C34-C35
76	BV	202	PEE	C34-C35-C36-C37
76	V	202	PEE	O5-C30-O3-C3
76	BV	202	PEE	O5-C30-O3-C3
71	B	303	PLX	C12-C13-C14-C15
71	g	203	PLX	C17-C18-C19-C20
71	r	502	PLX	C26-C27-C28-C29
71	BB	303	PLX	C12-C13-C14-C15
71	Bg	203	PLX	C17-C18-C19-C20
71	Br	502	PLX	C25-C26-C27-C28
71	Br	502	PLX	C26-C27-C28-C29
75	AG	101	CDL	C72-C73-C74-C75
75	AY	501	CDL	C33-C34-C35-C36
76	W	201	PEE	C37-C38-C39-C40
76	BW	201	PEE	C37-C38-C39-C40
71	g	203	PLX	C7-C8-C9-C10
71	r	502	PLX	C25-C26-C27-C28
71	Bg	203	PLX	C7-C8-C9-C10
76	AH	401	PEE	C32-C33-C34-C35
75	i	401	CDL	C34-C35-C36-C37
75	i	401	CDL	OA9-CA7-OA8-CA6
75	AY	501	CDL	OB9-CB7-OB8-CB6
75	Bi	401	CDL	OA9-CA7-OA8-CA6
75	AL	502	CDL	C51-CB5-OB6-CB4
71	g	202	PLX	C11-C12-C13-C14
71	Bg	202	PLX	C11-C12-C13-C14
72	p	201	8Q1	C7-C8-C9-C10
72	Bp	201	8Q1	C7-C8-C9-C10
75	Bi	401	CDL	C34-C35-C36-C37
71	B	303	PLX	O7-C6-C7-C8
71	g	203	PLX	O9-C24-C25-C26
71	r	501	PLX	O9-C24-C25-C26
71	r	502	PLX	O7-C6-C7-C8
71	AT	101	PLX	O9-C24-C25-C26
71	BB	303	PLX	O7-C6-C7-C8
71	Bg	203	PLX	O9-C24-C25-C26
71	Br	501	PLX	O9-C24-C25-C26
71	Br	502	PLX	O7-C6-C7-C8
71	g	203	PLX	C14-C15-C16-C17
71	r	501	PLX	C7-C8-C9-C10
71	AT	101	PLX	C11-C12-C13-C14
71	Bg	203	PLX	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
71	Br	501	PLX	C7-C8-C9-C10
75	i	401	CDL	C11-C12-C13-C14
75	l	703	CDL	C33-C34-C35-C36
75	AH	403	CDL	C32-C33-C34-C35
75	AU	403	CDL	C53-C54-C55-C56
75	Bi	401	CDL	C11-C12-C13-C14
75	Bl	703	CDL	C33-C34-C35-C36
70	A	502	FMN	O2'-C2'-C3'-O3'
70	BA	502	FMN	O2'-C2'-C3'-O3'
75	i	401	CDL	C32-C33-C34-C35
75	Bi	401	CDL	C32-C33-C34-C35
71	r	501	PLX	C35-C36-C37-C38
71	Br	501	PLX	C35-C36-C37-C38
75	AJ	405	CDL	C52-C53-C54-C55
76	V	202	PEE	C43-C44-C45-C46
75	l	703	CDL	OB9-CB7-OB8-CB6
75	Bl	703	CDL	OB9-CB7-OB8-CB6
75	AJ	404	CDL	C11-C12-C13-C14
75	AJ	404	CDL	C14-C15-C16-C17
75	AY	501	CDL	C13-C14-C15-C16
76	l	701	PEE	C13-C14-C15-C16
76	l	701	PEE	C41-C42-C43-C44
76	BV	202	PEE	C43-C44-C45-C46
76	Bl	701	PEE	C13-C14-C15-C16
76	Bl	701	PEE	C41-C42-C43-C44
75	V	201	CDL	OA7-CA5-OA6-CA4
75	BV	201	CDL	OA7-CA5-OA6-CA4
70	A	502	FMN	O2'-C2'-C3'-C4'
70	BA	502	FMN	O2'-C2'-C3'-C4'
71	AN	101	PLX	C11-C12-C13-C14
71	BV	203	PLX	C11-C12-C13-C14
75	AG	101	CDL	C31-C32-C33-C34
72	p	201	8Q1	C12-C13-C14-C15
72	Bp	201	8Q1	C12-C13-C14-C15
76	W	201	PEE	C23-C24-C25-C26
76	AV	403	PEE	C41-C42-C43-C44
75	i	401	CDL	CB5-C51-C52-C53
76	AV	403	PEE	C30-C31-C32-C33
76	BW	201	PEE	C23-C24-C25-C26
75	l	703	CDL	C31-CA7-OA8-CA6
75	Bl	703	CDL	C31-CA7-OA8-CA6
75	V	201	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
75	BV	201	CDL	C11-CA5-OA6-CA4
76	AH	401	PEE	C11-C10-O2-C2
71	g	201	PLX	C32-C33-C34-C35
71	r	501	PLX	C26-C27-C28-C29
71	Bg	201	PLX	C32-C33-C34-C35
71	Br	501	PLX	C26-C27-C28-C29
75	AA	101	CDL	C33-C34-C35-C36
75	AG	101	CDL	C52-C53-C54-C55
75	V	201	CDL	CB5-C51-C52-C53
75	BV	201	CDL	CB5-C51-C52-C53
75	Bi	401	CDL	CB5-C51-C52-C53
76	AL	503	PEE	C10-C11-C12-C13
75	n	101	CDL	C55-C56-C57-C58
75	AN	102	CDL	C31-C32-C33-C34
75	Bn	101	CDL	C55-C56-C57-C58
76	AV	403	PEE	C12-C13-C14-C15
76	AU	401	PEE	C33-C34-C35-C36
76	AL	503	PEE	C37-C38-C39-C40
71	r	502	PLX	C7-C8-C9-C10
71	r	502	PLX	C36-C37-C38-C39
75	i	401	CDL	C73-C74-C75-C76
75	Bi	401	CDL	C73-C74-C75-C76
76	W	201	PEE	C41-C42-C43-C44
76	BW	201	PEE	C41-C42-C43-C44
76	l	701	PEE	C15-C16-C17-C18
76	l	702	PEE	C19-C20-C21-C22
76	Bl	701	PEE	C15-C16-C17-C18
76	Bl	702	PEE	C19-C20-C21-C22
75	AL	502	CDL	OB7-CB5-OB6-CB4
76	AV	403	PEE	O4-C10-O2-C2
75	AJ	405	CDL	CB5-C51-C52-C53
75	Bi	401	CDL	C71-CB7-OB8-CB6
71	r	502	PLX	C20-C21-C22-C23
71	Br	502	PLX	C7-C8-C9-C10
71	Br	502	PLX	C36-C37-C38-C39
76	V	202	PEE	C31-C32-C33-C34
76	BV	202	PEE	C31-C32-C33-C34
71	AT	101	PLX	C33-C34-C35-C36
71	Br	502	PLX	C20-C21-C22-C23
75	n	101	CDL	C71-C72-C73-C74
75	Bn	101	CDL	C71-C72-C73-C74
76	l	702	PEE	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
76	AY	502	PEE	C20-C21-C22-C23
76	Bl	702	PEE	C31-C32-C33-C34
71	g	202	PLX	C26-C27-C28-C29
76	BW	201	PEE	C43-C44-C45-C46
75	i	401	CDL	C71-CB7-OB8-CB6
71	b	201	PLX	C30-C31-C32-C33
71	Bb	201	PLX	C30-C31-C32-C33
71	Bg	202	PLX	C26-C27-C28-C29
76	W	201	PEE	C43-C44-C45-C46
75	i	401	CDL	C51-CB5-OB6-CB4
75	Bi	401	CDL	C51-CB5-OB6-CB4
76	AV	403	PEE	C11-C10-O2-C2
75	AL	502	CDL	OA5-CA3-CA4-OA6
75	AL	502	CDL	OB5-CB3-CB4-OB6
71	AQ	101	PLX	C13-C14-C15-C16
75	AA	101	CDL	C12-C13-C14-C15
76	AV	403	PEE	C40-C41-C42-C43
76	AH	401	PEE	O4-C10-O2-C2
71	r	502	PLX	C35-C36-C37-C38
71	AQ	101	PLX	C18-C19-C20-C21
71	Br	502	PLX	C35-C36-C37-C38
75	V	201	CDL	C14-C15-C16-C17
71	AL	501	PLX	O6-C4-C5-O8
71	B	303	PLX	C29-C30-C31-C32
71	b	201	PLX	C32-C33-C34-C35
75	AH	403	CDL	C53-C54-C55-C56
75	BV	201	CDL	C14-C15-C16-C17
76	AL	503	PEE	C12-C13-C14-C15
76	AU	401	PEE	C34-C35-C36-C37
71	BB	303	PLX	C29-C30-C31-C32
71	Bb	201	PLX	C32-C33-C34-C35
76	V	202	PEE	C19-C20-C21-C22
76	W	201	PEE	C19-C20-C21-C22
76	AV	403	PEE	C19-C20-C21-C22
76	BV	202	PEE	C19-C20-C21-C22
76	BW	201	PEE	C19-C20-C21-C22
71	g	203	PLX	C35-C36-C37-C38
71	r	501	PLX	C9-C10-C11-C12
71	Bg	203	PLX	C35-C36-C37-C38
71	Br	501	PLX	C9-C10-C11-C12
71	b	201	PLX	C11-C12-C13-C14
71	r	502	PLX	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
71	Bb	201	PLX	C11-C12-C13-C14
71	Bg	202	PLX	C11-C10-C9-C8
75	l	703	CDL	OA9-CA7-OA8-CA6
75	Bl	703	CDL	OA9-CA7-OA8-CA6
71	g	202	PLX	C11-C10-C9-C8
71	AQ	101	PLX	C7-C8-C9-C10
71	Br	502	PLX	C17-C18-C19-C20
75	l	704	CDL	C13-C14-C15-C16
75	AU	403	CDL	C73-C74-C75-C76
75	Bl	704	CDL	C13-C14-C15-C16
76	l	701	PEE	C23-C24-C25-C26
76	l	701	PEE	C40-C41-C42-C43
76	Bl	701	PEE	C23-C24-C25-C26
76	Bl	701	PEE	C40-C41-C42-C43
76	l	701	PEE	C16-C17-C18-C19
76	Bl	701	PEE	C16-C17-C18-C19
71	g	201	PLX	C2-O1-P1-O4
71	Bg	201	PLX	C2-O1-P1-O4
75	l	703	CDL	CA2-OA2-PA1-OA5
75	AL	502	CDL	CA2-OA2-PA1-OA5
75	Bl	703	CDL	CA2-OA2-PA1-OA5
76	AV	403	PEE	C1-O3P-P-O4P
71	B	303	PLX	C15-C16-C17-C18
71	BB	303	PLX	C15-C16-C17-C18
75	n	101	CDL	C34-C35-C36-C37
75	Bn	101	CDL	C34-C35-C36-C37
76	AV	403	PEE	C33-C34-C35-C36
76	AH	401	PEE	C2-C1-O3P-P
71	AL	501	PLX	C7-C8-C9-C10
75	AG	101	CDL	C34-C35-C36-C37
71	AL	501	PLX	O4-C3-C4-C5
75	l	704	CDL	OB5-CB3-CB4-CB6
75	Bl	704	CDL	OB5-CB3-CB4-CB6
76	l	701	PEE	O3P-C1-C2-C3
76	AJ	403	PEE	O3P-C1-C2-C3
76	Bl	701	PEE	O3P-C1-C2-C3
71	r	502	PLX	C15-C16-C17-C18
71	AT	101	PLX	C32-C33-C34-C35
71	Br	502	PLX	C15-C16-C17-C18
75	AG	101	CDL	CA7-C31-C32-C33
75	AY	501	CDL	CB7-C71-C72-C73
71	AQ	101	PLX	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
71	AT	101	PLX	C18-C19-C20-C21
76	l	702	PEE	C42-C43-C44-C45
76	AL	503	PEE	C21-C22-C23-C24
76	Bl	702	PEE	C42-C43-C44-C45
71	B	303	PLX	C11-C10-C9-C8
71	AT	101	PLX	C13-C14-C15-C16
71	AT	101	PLX	C34-C35-C36-C37
71	BB	303	PLX	C11-C10-C9-C8
75	l	704	CDL	CB2-C1-CA2-OA2
75	Bl	704	CDL	CB2-C1-CA2-OA2
75	i	401	CDL	OB7-CB5-OB6-CB4
75	Bi	401	CDL	OB7-CB5-OB6-CB4
75	V	201	CDL	C12-C13-C14-C15
75	BV	201	CDL	C12-C13-C14-C15
75	AL	502	CDL	C14-C15-C16-C17
75	n	101	CDL	C33-C34-C35-C36
75	Bn	101	CDL	C33-C34-C35-C36
76	W	201	PEE	C33-C34-C35-C36
76	BW	201	PEE	C33-C34-C35-C36
71	r	501	PLX	C3-C4-C5-O8
71	Br	501	PLX	C3-C4-C5-O8
75	l	703	CDL	CA3-CA4-CA6-OA8
75	AH	403	CDL	CA3-CA4-CA6-OA8
75	AJ	405	CDL	CB3-CB4-CB6-OB8
75	AL	502	CDL	CA3-CA4-CA6-OA8
75	AL	502	CDL	CB3-CB4-CB6-OB8
75	AN	102	CDL	CB3-CB4-CB6-OB8
75	AU	403	CDL	CA3-CA4-CA6-OA8
75	Bl	703	CDL	CA3-CA4-CA6-OA8
76	AV	403	PEE	C1-C2-C3-O3
75	AL	502	CDL	C13-C14-C15-C16
76	AY	502	PEE	C33-C34-C35-C36
76	BV	202	PEE	C41-C42-C43-C44
75	AJ	404	CDL	CA5-C11-C12-C13
71	r	501	PLX	C18-C19-C20-C21
71	Br	501	PLX	C18-C19-C20-C21
75	AG	101	CDL	C75-C76-C77-C78
76	V	202	PEE	C41-C42-C43-C44
71	Bg	201	PLX	C26-C27-C28-C29
75	AJ	404	CDL	C15-C16-C17-C18
76	W	201	PEE	C44-C45-C46-C47
76	AJ	403	PEE	C41-C42-C43-C44

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Mol	Chain	Res	Type	Atoms
76	BW	201	PEE	C44-C45-C46-C47
71	g	201	PLX	C26-C27-C28-C29
71	U	101	PLX	O8-C24-C25-C26
71	BU	101	PLX	O8-C24-C25-C26
75	AY	501	CDL	C15-C16-C17-C18
76	l	702	PEE	C12-C13-C14-C15
72	p	201	8Q1	C13-C14-C15-C16
75	AH	403	CDL	C55-C56-C57-C58
75	AL	502	CDL	C31-C32-C33-C34
75	AU	403	CDL	C15-C16-C17-C18
76	Bl	702	PEE	C12-C13-C14-C15
76	AJ	403	PEE	C35-C36-C37-C38
76	AJ	403	PEE	C39-C40-C41-C42
76	AU	401	PEE	C15-C16-C17-C18
76	AV	403	PEE	C15-C16-C17-C18
75	i	401	CDL	OB9-CB7-OB8-CB6
75	Bi	401	CDL	OB9-CB7-OB8-CB6
72	Bp	201	8Q1	C13-C14-C15-C16
71	AQ	101	PLX	C36-C37-C38-C39
75	AJ	404	CDL	C74-C75-C76-C77
71	b	201	PLX	C20-C21-C22-C23
71	Bb	201	PLX	C20-C21-C22-C23
76	AY	502	PEE	C42-C43-C44-C45
75	AU	403	CDL	CB5-C51-C52-C53
71	AN	101	PLX	C7-C8-C9-C10
71	AQ	101	PLX	C31-C32-C33-C34
71	BV	203	PLX	C7-C8-C9-C10
75	AN	102	CDL	C55-C56-C57-C58
76	l	701	PEE	C42-C43-C44-C45
75	AJ	404	CDL	CA3-CA4-OA6-CA5
75	AJ	405	CDL	CB6-CB4-OB6-CB5
75	AJ	405	CDL	C55-C56-C57-C58
76	l	702	PEE	C44-C45-C46-C47
76	Bl	701	PEE	C42-C43-C44-C45
76	Bl	702	PEE	C44-C45-C46-C47
76	l	701	PEE	C2-C1-O3P-P
76	Bl	701	PEE	C2-C1-O3P-P
71	AQ	101	PLX	C9-C10-C11-C12
75	V	201	CDL	OA5-CA3-CA4-OA6
75	BV	201	CDL	OA5-CA3-CA4-OA6
71	BU	101	PLX	C26-C27-C28-C29
71	U	101	PLX	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
75	AN	102	CDL	C15-C16-C17-C18
75	AJ	405	CDL	CA7-C31-C32-C33
76	AH	401	PEE	C30-C31-C32-C33
71	AL	501	PLX	C34-C35-C36-C37
75	AH	403	CDL	C32-C31-CA7-OA8
76	W	201	PEE	O2-C2-C3-O3
76	BW	201	PEE	O2-C2-C3-O3
75	l	703	CDL	C75-C76-C77-C78
75	Bl	703	CDL	C75-C76-C77-C78
76	AH	401	PEE	C34-C35-C36-C37
72	p	201	8Q1	C30-C29-C32-O33
72	Bp	201	8Q1	C30-C29-C32-O33
75	i	401	CDL	C52-C51-CB5-OB6
75	Bi	401	CDL	C52-C51-CB5-OB6
71	AN	101	PLX	C16-C17-C18-C19
71	BV	203	PLX	C16-C17-C18-C19
75	AA	101	CDL	C71-C72-C73-C74
76	AV	403	PEE	C13-C14-C15-C16
75	AG	101	CDL	C71-CB7-OB8-CB6
75	V	201	CDL	C72-C73-C74-C75
75	BV	201	CDL	C72-C73-C74-C75
76	AH	401	PEE	C24-C25-C26-C27
75	i	401	CDL	C35-C36-C37-C38
75	AH	403	CDL	C15-C16-C17-C18
75	Bi	401	CDL	C35-C36-C37-C38
71	U	101	PLX	C11-C10-C9-C8
71	BU	101	PLX	C11-C10-C9-C8
76	W	201	PEE	C34-C35-C36-C37
76	BW	201	PEE	C34-C35-C36-C37
75	AJ	405	CDL	C32-C33-C34-C35
71	g	201	PLX	C27-C28-C29-C30
71	AN	101	PLX	C12-C13-C14-C15
71	BV	203	PLX	C12-C13-C14-C15
71	Bg	201	PLX	C17-C18-C19-C20
71	g	201	PLX	C17-C18-C19-C20
71	Bg	201	PLX	C27-C28-C29-C30
75	AJ	404	CDL	C73-C74-C75-C76
75	l	703	CDL	OB5-CB3-CB4-CB6
75	AL	502	CDL	OA5-CA3-CA4-CA6
75	AU	403	CDL	OA5-CA3-CA4-CA6
75	AY	501	CDL	OA5-CA3-CA4-CA6
75	AY	501	CDL	OB5-CB3-CB4-CB6

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Mol	Chain	Res	Type	Atoms
75	Bl	703	CDL	OB5-CB3-CB4-CB6
76	BW	201	PEE	O3P-C1-C2-C3
76	AH	401	PEE	C20-C21-C22-C23
71	AN	101	PLX	C31-C32-C33-C34
75	AJ	404	CDL	C12-C13-C14-C15
75	BV	201	CDL	C52-C53-C54-C55
71	B	303	PLX	C30-C31-C32-C33
71	r	501	PLX	C25-C26-C27-C28
71	BB	303	PLX	C30-C31-C32-C33
71	BV	203	PLX	C31-C32-C33-C34
75	V	201	CDL	C52-C53-C54-C55
71	U	101	PLX	C28-C29-C30-C31
71	b	201	PLX	C13-C14-C15-C16
71	BU	101	PLX	C28-C29-C30-C31
71	Bb	201	PLX	C13-C14-C15-C16
71	Br	501	PLX	C25-C26-C27-C28
76	l	702	PEE	C11-C10-O2-C2
71	b	201	PLX	C11-C10-C9-C8
71	Bb	201	PLX	C11-C10-C9-C8
75	AA	101	CDL	C75-C76-C77-C78
76	AJ	403	PEE	C40-C41-C42-C43
71	U	101	PLX	C27-C28-C29-C30
71	b	201	PLX	C36-C37-C38-C39
71	Bb	201	PLX	C36-C37-C38-C39
71	BU	101	PLX	C27-C28-C29-C30
71	g	201	PLX	C3-C4-C5-O8
71	AL	501	PLX	C3-C4-C5-O8
71	AQ	101	PLX	C3-C4-C5-O8
71	AT	101	PLX	C3-C4-C5-O8
71	Bg	201	PLX	C3-C4-C5-O8
75	V	201	CDL	CB3-CB4-CB6-OB8
75	i	401	CDL	CA3-CA4-CA6-OA8
75	AA	101	CDL	CB3-CB4-CB6-OB8
75	BV	201	CDL	CB3-CB4-CB6-OB8
75	Bi	401	CDL	CA3-CA4-CA6-OA8
76	W	201	PEE	C1-C2-C3-O3
76	BW	201	PEE	C1-C2-C3-O3
71	r	502	PLX	C27-C28-C29-C30
71	Br	502	PLX	C27-C28-C29-C30
72	Bp	201	8Q1	C10-C11-C12-C13
72	p	201	8Q1	C10-C11-C12-C13
72	E	201	8Q1	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
72	BE	201	8Q1	C7-C8-C9-C10
76	AV	403	PEE	C22-C23-C24-C25
71	r	501	PLX	C28-C29-C30-C31
71	Br	501	PLX	C28-C29-C30-C31
76	W	201	PEE	C13-C14-C15-C16
76	BW	201	PEE	C13-C14-C15-C16
76	Bl	702	PEE	C11-C10-O2-C2
71	AQ	101	PLX	C14-C15-C16-C17
75	V	201	CDL	C53-C54-C55-C56
75	BV	201	CDL	C53-C54-C55-C56
71	b	201	PLX	C5-C4-O6-C6
71	g	202	PLX	C5-C4-O6-C6
71	AT	101	PLX	C3-O4-P1-O1
71	Bb	201	PLX	C5-C4-O6-C6
71	Bg	202	PLX	C5-C4-O6-C6
76	AV	403	PEE	C4-O4P-P-O3P
75	AJ	404	CDL	C71-C72-C73-C74
71	r	501	PLX	O7-C6-C7-C8
71	Br	501	PLX	O7-C6-C7-C8
71	b	201	PLX	C35-C36-C37-C38
71	AL	501	PLX	C32-C33-C34-C35
71	Bb	201	PLX	C35-C36-C37-C38
75	AH	403	CDL	C52-C53-C54-C55
75	l	704	CDL	OA5-CA3-CA4-OA6
75	AN	102	CDL	OA5-CA3-CA4-OA6
75	Bl	704	CDL	OA5-CA3-CA4-OA6
76	AJ	403	PEE	O3P-C1-C2-O2
71	AN	101	PLX	C26-C27-C28-C29
71	BV	203	PLX	C26-C27-C28-C29
75	AG	101	CDL	OB9-CB7-OB8-CB6
76	AL	503	PEE	C14-C15-C16-C17
75	l	703	CDL	OA6-CA4-CA6-OA8
75	AG	101	CDL	OB6-CB4-CB6-OB8
75	AH	403	CDL	OB6-CB4-CB6-OB8
75	AL	502	CDL	OA6-CA4-CA6-OA8
75	AL	502	CDL	OB6-CB4-CB6-OB8
75	AU	403	CDL	OA6-CA4-CA6-OA8
75	Bl	703	CDL	OA6-CA4-CA6-OA8
75	V	201	CDL	C12-C11-CA5-OA6
75	BV	201	CDL	C12-C11-CA5-OA6
75	AJ	404	CDL	C31-C32-C33-C34
71	g	201	PLX	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
71	Bg	201	PLX	C20-C21-C22-C23
75	AG	101	CDL	C74-C75-C76-C77
75	AN	102	CDL	C52-C53-C54-C55
71	g	203	PLX	C4-C3-O4-P1
71	r	501	PLX	C4-C3-O4-P1
71	Bg	203	PLX	C4-C3-O4-P1
71	Br	501	PLX	C4-C3-O4-P1
75	AA	101	CDL	C1-CA2-OA2-PA1
75	AA	101	CDL	C1-CB2-OB2-PB2
75	AA	101	CDL	CB4-CB3-OB5-PB2
75	AH	403	CDL	C1-CA2-OA2-PA1
75	AN	102	CDL	CB4-CB3-OB5-PB2
75	l	704	CDL	C73-C74-C75-C76
75	Bl	704	CDL	C73-C74-C75-C76
76	AV	403	PEE	C34-C35-C36-C37
71	r	501	PLX	C19-C20-C21-C22
75	AU	403	CDL	C74-C75-C76-C77
75	Bl	703	CDL	C15-C16-C17-C18
71	Br	501	PLX	C19-C20-C21-C22
75	l	703	CDL	C15-C16-C17-C18
75	n	101	CDL	CA5-C11-C12-C13
75	Bn	101	CDL	CA5-C11-C12-C13
76	W	201	PEE	O4-C10-O2-C2
76	Bl	702	PEE	O4-C10-O2-C2
76	W	201	PEE	C11-C10-O2-C2
76	BW	201	PEE	C11-C10-O2-C2
75	AL	502	CDL	C53-C54-C55-C56
76	AV	403	PEE	C20-C21-C22-C23
75	V	201	CDL	OB5-CB3-CB4-CB6
75	AA	101	CDL	OA5-CA3-CA4-CA6
75	AJ	404	CDL	OB5-CB3-CB4-CB6
75	AN	102	CDL	OA5-CA3-CA4-CA6
75	AU	403	CDL	OB5-CB3-CB4-CB6
75	BV	201	CDL	OB5-CB3-CB4-CB6
76	W	201	PEE	O3P-C1-C2-C3
71	B	303	PLX	C11-C12-C13-C14
71	BB	303	PLX	C11-C12-C13-C14
76	AY	502	PEE	C14-C15-C16-C17
76	AV	403	PEE	C16-C17-C18-C19
76	AH	401	PEE	C39-C40-C41-C42
76	l	702	PEE	O4-C10-O2-C2
76	BW	201	PEE	O4-C10-O2-C2

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Mol	Chain	Res	Type	Atoms
71	BB	303	PLX	C32-C33-C34-C35
75	AA	101	CDL	C35-C36-C37-C38
75	AU	403	CDL	C55-C56-C57-C58
76	AV	403	PEE	C11-C12-C13-C14
71	B	303	PLX	C32-C33-C34-C35
76	l	701	PEE	C31-C32-C33-C34
76	Bl	701	PEE	C31-C32-C33-C34
75	BV	201	CDL	C75-C76-C77-C78
71	r	501	PLX	C30-C31-C32-C33
71	Br	501	PLX	C30-C31-C32-C33
75	V	201	CDL	C75-C76-C77-C78
71	AT	101	PLX	C26-C27-C28-C29
75	AU	403	CDL	C71-C72-C73-C74
75	AJ	405	CDL	CA6-CA4-OA6-CA5
75	AU	403	CDL	CA6-CA4-OA6-CA5
75	AY	501	CDL	CA6-CA4-OA6-CA5
75	AY	501	CDL	CB3-CB4-OB6-CB5
71	g	202	PLX	C30-C31-C32-C33
71	Bg	202	PLX	C30-C31-C32-C33
75	AG	101	CDL	C11-C12-C13-C14
76	AL	503	PEE	C31-C32-C33-C34
75	AA	101	CDL	CA3-CA4-CA6-OA8
75	AH	403	CDL	C1-CB2-OB2-PB2
75	AN	102	CDL	CA3-CA4-CA6-OA8
75	AU	403	CDL	C1-CB2-OB2-PB2
75	AY	501	CDL	CA3-CA4-CA6-OA8
71	g	202	PLX	O4-C3-C4-O6
71	AL	501	PLX	O4-C3-C4-O6
71	AQ	101	PLX	O4-C3-C4-O6
71	Bg	202	PLX	O4-C3-C4-O6
75	V	201	CDL	OB5-CB3-CB4-OB6
75	l	703	CDL	OA5-CA3-CA4-OA6
75	AJ	404	CDL	OB5-CB3-CB4-OB6
75	AU	403	CDL	OA5-CA3-CA4-OA6
75	BV	201	CDL	OB5-CB3-CB4-OB6
75	Bl	703	CDL	OA5-CA3-CA4-OA6
76	BV	202	PEE	C33-C34-C35-C36
71	AL	501	PLX	C6-C7-C8-C9
76	V	202	PEE	C32-C33-C34-C35
76	V	202	PEE	C33-C34-C35-C36
75	AA	101	CDL	C32-C31-CA7-OA8
76	BV	202	PEE	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
71	b	201	PLX	O6-C4-C5-O8
71	r	501	PLX	O6-C4-C5-O8
71	Bb	201	PLX	O6-C4-C5-O8
71	Br	501	PLX	O6-C4-C5-O8
75	V	201	CDL	OA6-CA4-CA6-OA8
75	V	201	CDL	OB6-CB4-CB6-OB8
75	AA	101	CDL	OA6-CA4-CA6-OA8
75	AG	101	CDL	OA6-CA4-CA6-OA8
75	AJ	405	CDL	OA6-CA4-CA6-OA8
75	AJ	405	CDL	OB6-CB4-CB6-OB8
75	AN	102	CDL	OA6-CA4-CA6-OA8
75	BV	201	CDL	OA6-CA4-CA6-OA8
75	BV	201	CDL	OB6-CB4-CB6-OB8
72	E	201	8Q1	C6-C7-C8-C9
72	BE	201	8Q1	C6-C7-C8-C9
75	AH	403	CDL	C12-C13-C14-C15
73	J	401	NDP	C5B-O5B-PA-O3
73	J	401	NDP	C5D-O5D-PN-O3
73	BJ	401	NDP	C5B-O5B-PA-O3
73	BJ	401	NDP	C5D-O5D-PN-O3
75	Bl	704	CDL	C12-C13-C14-C15
76	AH	401	PEE	C15-C16-C17-C18
75	l	704	CDL	C12-C13-C14-C15
76	AJ	403	PEE	O4-C10-O2-C2
71	r	502	PLX	C24-C25-C26-C27
71	Br	502	PLX	C24-C25-C26-C27
75	AJ	404	CDL	C33-C34-C35-C36
71	r	502	PLX	C34-C35-C36-C37
71	Bg	201	PLX	C35-C36-C37-C38
71	g	201	PLX	C35-C36-C37-C38
71	Br	502	PLX	C34-C35-C36-C37
76	Bl	701	PEE	C24-C25-C26-C27
76	Bl	702	PEE	C11-C12-C13-C14
76	l	701	PEE	C24-C25-C26-C27
76	l	702	PEE	C11-C12-C13-C14
75	AL	502	CDL	C11-C12-C13-C14
75	n	101	CDL	C35-C36-C37-C38
75	Bn	101	CDL	C35-C36-C37-C38
75	n	101	CDL	C11-C12-C13-C14
75	Bn	101	CDL	C11-C12-C13-C14
76	BW	201	PEE	C31-C32-C33-C34
75	l	704	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
75	AJ	405	CDL	CB2-OB2-PB2-OB5
75	Bl	704	CDL	CB2-OB2-PB2-OB5
71	r	501	PLX	C31-C32-C33-C34
71	Br	501	PLX	C31-C32-C33-C34
76	W	201	PEE	C31-C32-C33-C34
71	r	502	PLX	C4-C3-O4-P1
71	Br	502	PLX	C4-C3-O4-P1
75	l	704	CDL	CA4-CA3-OA5-PA1
75	AH	403	CDL	CA4-CA3-OA5-PA1
75	AJ	404	CDL	CA4-CA3-OA5-PA1
75	AN	102	CDL	C1-CA2-OA2-PA1
75	AN	102	CDL	C1-CB2-OB2-PB2
75	Bl	704	CDL	CA4-CA3-OA5-PA1
71	b	201	PLX	C3-O4-P1-O2
71	g	201	PLX	C3-O4-P1-O3
71	g	202	PLX	C3-O4-P1-O2
71	g	202	PLX	C3-O4-P1-O3
71	r	502	PLX	C2-O1-P1-O3
71	AQ	101	PLX	C3-O4-P1-O3
71	AT	101	PLX	C2-O1-P1-O3
71	Bb	201	PLX	C3-O4-P1-O2
71	Bg	201	PLX	C3-O4-P1-O3
71	Bg	202	PLX	C3-O4-P1-O2
71	Bg	202	PLX	C3-O4-P1-O3
71	Br	502	PLX	C2-O1-P1-O3
73	J	401	NDP	C5B-O5B-PA-O2A
73	J	401	NDP	C5D-O5D-PN-O2N
73	BJ	401	NDP	C5B-O5B-PA-O2A
73	BJ	401	NDP	C5D-O5D-PN-O2N
75	V	201	CDL	CB3-OB5-PB2-OB4
75	i	401	CDL	CB2-OB2-PB2-OB3
75	l	703	CDL	CA2-OA2-PA1-OA4
75	l	703	CDL	CB3-OB5-PB2-OB4
75	l	704	CDL	CA3-OA5-PA1-OA3
75	n	101	CDL	CA3-OA5-PA1-OA3
75	AA	101	CDL	CB2-OB2-PB2-OB3
75	AG	101	CDL	CA2-OA2-PA1-OA3
75	AG	101	CDL	CB2-OB2-PB2-OB3
75	AL	502	CDL	CA2-OA2-PA1-OA4
75	AL	502	CDL	CB3-OB5-PB2-OB3
75	AL	502	CDL	CB3-OB5-PB2-OB4
75	AN	102	CDL	CA2-OA2-PA1-OA3

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Mol	Chain	Res	Type	Atoms
75	AN	102	CDL	CB2-OB2-PB2-OB3
75	AY	501	CDL	CA3-OA5-PA1-OA4
75	BV	201	CDL	CB3-OB5-PB2-OB4
75	Bi	401	CDL	CB2-OB2-PB2-OB3
75	Bl	703	CDL	CA2-OA2-PA1-OA4
75	Bl	703	CDL	CB3-OB5-PB2-OB4
75	Bl	704	CDL	CA3-OA5-PA1-OA3
75	Bn	101	CDL	CA3-OA5-PA1-OA3
76	V	202	PEE	C1-O3P-P-O1P
76	AH	401	PEE	C4-O4P-P-O1P
76	AU	401	PEE	C4-O4P-P-O1P
76	AV	403	PEE	C1-O3P-P-O1P
76	AV	403	PEE	C1-O3P-P-O2P
76	AY	502	PEE	C1-O3P-P-O1P
76	BV	202	PEE	C1-O3P-P-O1P
71	g	202	PLX	O4-C3-C4-C5
71	AQ	101	PLX	O4-C3-C4-C5
71	Bg	202	PLX	O4-C3-C4-C5
75	V	201	CDL	OA5-CA3-CA4-CA6
75	l	703	CDL	OA5-CA3-CA4-CA6
75	l	704	CDL	OA5-CA3-CA4-CA6
75	AL	502	CDL	OB5-CB3-CB4-CB6
75	BV	201	CDL	OA5-CA3-CA4-CA6
75	Bl	703	CDL	OA5-CA3-CA4-CA6
75	Bl	704	CDL	OA5-CA3-CA4-CA6
71	r	501	PLX	C15-C16-C17-C18
71	Br	501	PLX	C15-C16-C17-C18
75	AL	502	CDL	C33-C34-C35-C36
76	AH	401	PEE	C17-C18-C19-C20
76	AV	403	PEE	C17-C18-C19-C20
71	U	101	PLX	C25-C24-O8-C5
71	b	201	PLX	C1-C2-O1-P1
71	g	203	PLX	C1-C2-O1-P1
71	r	501	PLX	C25-C24-O8-C5
71	AT	101	PLX	C1-C2-O1-P1
71	AT	101	PLX	C25-C24-O8-C5
71	BU	101	PLX	C25-C24-O8-C5
71	Bb	201	PLX	C1-C2-O1-P1
71	Bg	203	PLX	C1-C2-O1-P1
71	Br	501	PLX	C25-C24-O8-C5
76	AH	401	PEE	C5-C4-O4P-P
76	W	201	PEE	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
76	BW	201	PEE	C10-C11-C12-C13
71	AN	101	PLX	C19-C20-C21-C22
71	BV	203	PLX	C19-C20-C21-C22
71	Bg	203	PLX	C19-C20-C21-C22
71	g	203	PLX	C19-C20-C21-C22
75	V	201	CDL	C74-C75-C76-C77
75	BV	201	CDL	C74-C75-C76-C77
75	AN	102	CDL	CA2-C1-CB2-OB2
75	AU	403	CDL	CA2-C1-CB2-OB2
75	l	704	CDL	OB5-CB3-CB4-OB6
75	AU	403	CDL	OB5-CB3-CB4-OB6
75	AY	501	CDL	OB5-CB3-CB4-OB6
75	Bl	704	CDL	OB5-CB3-CB4-OB6
76	l	701	PEE	O3P-C1-C2-O2
76	Bl	701	PEE	O3P-C1-C2-O2
82	AV	401	HEM	C2A-CAA-CBA-CGA
71	AL	501	PLX	C19-C20-C21-C22
76	AJ	403	PEE	C11-C10-O2-C2
71	AN	101	PLX	C14-C15-C16-C17
71	BV	203	PLX	C14-C15-C16-C17
76	AH	401	PEE	C14-C15-C16-C17
71	g	203	PLX	C3-C4-C5-O8
71	r	502	PLX	C3-C4-C5-O8
71	AL	501	PLX	N1-C1-C2-O1
71	Bg	203	PLX	C3-C4-C5-O8
75	AG	101	CDL	CA3-CA4-CA6-OA8
81	AH	402	HEC	C1A-C2A-CAA-CBA
81	AH	402	HEC	C3A-C2A-CAA-CBA
82	AJ	402	HEM	C3A-C2A-CAA-CBA
71	g	203	PLX	O6-C4-C5-O8
71	r	502	PLX	O6-C4-C5-O8
71	Bg	203	PLX	O6-C4-C5-O8
71	Br	502	PLX	O6-C4-C5-O8
75	l	704	CDL	OA6-CA4-CA6-OA8
75	AH	403	CDL	OA6-CA4-CA6-OA8
75	AY	501	CDL	OA6-CA4-CA6-OA8
75	Bl	704	CDL	OA6-CA4-CA6-OA8
76	AV	403	PEE	O2-C2-C3-O3
75	AJ	404	CDL	C55-C56-C57-C58
71	g	201	PLX	C24-C25-C26-C27
71	Bg	201	PLX	C24-C25-C26-C27
75	AJ	404	CDL	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
71	r	502	PLX	O8-C24-C25-C26
71	BV	203	PLX	O6-C6-C7-C8
71	Br	502	PLX	O8-C24-C25-C26
72	E	201	8Q1	O33-C32-C34-O35
72	BE	201	8Q1	O33-C32-C34-O35
71	g	202	PLX	O7-C6-C7-C8
71	Bg	202	PLX	O7-C6-C7-C8
75	Bl	704	CDL	C15-C16-C17-C18
71	B	303	PLX	C20-C21-C22-C23
71	BB	303	PLX	C20-C21-C22-C23
75	l	704	CDL	C15-C16-C17-C18
73	J	401	NDP	O4D-C1D-N1N-C6N
73	BJ	401	NDP	O4D-C1D-N1N-C6N
71	U	101	PLX	C36-C37-C38-C39
71	BU	101	PLX	C36-C37-C38-C39
76	AL	503	PEE	C33-C34-C35-C36
71	r	502	PLX	C11-C10-C9-C8
75	AH	403	CDL	O1-C1-CB2-OB2
71	Br	502	PLX	C11-C10-C9-C8
75	AH	403	CDL	C13-C14-C15-C16
75	AH	403	CDL	C54-C55-C56-C57
75	Bn	101	CDL	C73-C74-C75-C76
71	Bg	201	PLX	C14-C15-C16-C17
75	Bi	401	CDL	C32-C31-CA7-OA8
71	g	201	PLX	C14-C15-C16-C17
75	n	101	CDL	C73-C74-C75-C76
75	V	201	CDL	CA3-CA4-OA6-CA5
75	l	703	CDL	CB6-CB4-OB6-CB5
75	l	704	CDL	CA6-CA4-OA6-CA5
75	AH	403	CDL	CA3-CA4-OA6-CA5
75	BV	201	CDL	CA3-CA4-OA6-CA5
75	Bl	703	CDL	CB6-CB4-OB6-CB5
75	Bl	704	CDL	CA6-CA4-OA6-CA5
76	l	701	PEE	C3-C2-O2-C10
76	l	702	PEE	C3-C2-O2-C10
76	Bl	701	PEE	C3-C2-O2-C10
76	Bl	702	PEE	C3-C2-O2-C10
75	AA	101	CDL	CB2-C1-CA2-OA2
75	V	201	CDL	CB7-C71-C72-C73
75	BV	201	CDL	CB7-C71-C72-C73
75	i	401	CDL	C32-C31-CA7-OA8
75	BV	201	CDL	C55-C56-C57-C58

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Mol	Chain	Res	Type	Atoms
75	AJ	404	CDL	CB4-CB3-OB5-PB2
75	V	201	CDL	C55-C56-C57-C58
75	Bn	101	CDL	C53-C54-C55-C56
75	AA	101	CDL	OA5-CA3-CA4-OA6
75	n	101	CDL	C53-C54-C55-C56
75	l	703	CDL	CA7-C31-C32-C33
75	Bl	703	CDL	CA7-C31-C32-C33
76	AH	401	PEE	C31-C32-C33-C34
76	V	202	PEE	C11-C10-O2-C2
76	BV	202	PEE	C11-C10-O2-C2
75	n	101	CDL	C15-C16-C17-C18
75	Bn	101	CDL	C15-C16-C17-C18
76	AY	502	PEE	C38-C39-C40-C41
75	AN	102	CDL	OB6-CB4-CB6-OB8
71	U	101	PLX	C2-O1-P1-O4
71	g	203	PLX	C3-O4-P1-O1
71	AN	101	PLX	C3-O4-P1-O1
71	BU	101	PLX	C2-O1-P1-O4
71	BV	203	PLX	C3-O4-P1-O1
71	Bg	203	PLX	C3-O4-P1-O1
75	V	201	CDL	CB2-OB2-PB2-OB5
75	l	703	CDL	CB2-OB2-PB2-OB5
75	AG	101	CDL	CB3-OB5-PB2-OB2
75	AJ	405	CDL	CA2-OA2-PA1-OA5
75	AJ	405	CDL	CB3-OB5-PB2-OB2
75	AU	403	CDL	CA2-OA2-PA1-OA5
75	BV	201	CDL	CB2-OB2-PB2-OB5
75	Bl	703	CDL	CB2-OB2-PB2-OB5
76	V	202	PEE	C4-O4P-P-O3P
76	l	701	PEE	C1-O3P-P-O4P
76	l	702	PEE	C4-O4P-P-O3P
76	AH	401	PEE	C1-O3P-P-O4P
76	AL	503	PEE	C4-O4P-P-O3P
76	BV	202	PEE	C4-O4P-P-O3P
76	Bl	701	PEE	C1-O3P-P-O4P
76	Bl	702	PEE	C4-O4P-P-O3P
71	BV	203	PLX	C29-C30-C31-C32
71	AN	101	PLX	C29-C30-C31-C32
71	AN	101	PLX	C3-C4-C5-O8
71	BV	203	PLX	C3-C4-C5-O8
71	Br	502	PLX	C3-C4-C5-O8
75	AG	101	CDL	CB3-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
71	b	201	PLX	C28-C29-C30-C31
71	r	501	PLX	C11-C10-C9-C8
71	Bb	201	PLX	C28-C29-C30-C31
71	Br	501	PLX	C11-C10-C9-C8
82	AV	402	HEM	C4D-C3D-CAD-CBD
76	BV	202	PEE	C23-C24-C25-C26
75	AN	102	CDL	CB5-C51-C52-C53
76	V	202	PEE	C23-C24-C25-C26
76	AY	502	PEE	C40-C41-C42-C43
76	AV	403	PEE	C31-C32-C33-C34
75	l	703	CDL	C34-C35-C36-C37
75	Bl	703	CDL	C34-C35-C36-C37
75	l	704	CDL	C1-CB2-OB2-PB2
75	AG	101	CDL	C1-CA2-OA2-PA1
75	AU	403	CDL	CB4-CB3-OB5-PB2
75	Bl	704	CDL	C1-CB2-OB2-PB2
75	AJ	405	CDL	C14-C15-C16-C17
75	AJ	405	CDL	C34-C35-C36-C37
76	V	202	PEE	O4-C10-O2-C2
76	BV	202	PEE	O4-C10-O2-C2
76	V	202	PEE	C35-C36-C37-C38
76	BV	202	PEE	C35-C36-C37-C38
73	J	401	NDP	C2D-C1D-N1N-C6N
73	BJ	401	NDP	C2D-C1D-N1N-C6N
75	AG	101	CDL	C51-C52-C53-C54
76	Bl	702	PEE	C23-C24-C25-C26
76	l	702	PEE	C23-C24-C25-C26
76	l	701	PEE	O4P-C4-C5-N
76	AY	502	PEE	O4P-C4-C5-N
76	Bl	701	PEE	O4P-C4-C5-N
71	g	202	PLX	C15-C16-C17-C18
71	Bg	202	PLX	C15-C16-C17-C18
75	AL	502	CDL	C54-C55-C56-C57
71	g	201	PLX	C19-C20-C21-C22
71	Bg	201	PLX	C19-C20-C21-C22
75	AJ	405	CDL	C15-C16-C17-C18
75	AY	501	CDL	C52-C53-C54-C55
71	g	201	PLX	O6-C6-C7-C8
71	AN	101	PLX	O6-C6-C7-C8
71	Bg	201	PLX	O6-C6-C7-C8
75	i	401	CDL	C1-CB2-OB2-PB2
75	i	401	CDL	CB4-CB3-OB5-PB2

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Mol	Chain	Res	Type	Atoms
75	l	703	CDL	CA4-CA3-OA5-PA1
75	Bi	401	CDL	C1-CB2-OB2-PB2
75	Bi	401	CDL	CB4-CB3-OB5-PB2
75	Bl	703	CDL	CA4-CA3-OA5-PA1
75	AN	102	CDL	C32-C33-C34-C35
75	AG	101	CDL	C71-C72-C73-C74
76	BW	201	PEE	C11-C12-C13-C14
71	B	303	PLX	C6-C7-C8-C9
71	AN	101	PLX	C6-C7-C8-C9
71	BB	303	PLX	C6-C7-C8-C9
71	BV	203	PLX	C6-C7-C8-C9
71	g	201	PLX	C25-C26-C27-C28
71	Bg	201	PLX	C25-C26-C27-C28
76	W	201	PEE	C11-C12-C13-C14
75	l	703	CDL	CB5-C51-C52-C53
75	Bl	703	CDL	CB5-C51-C52-C53
79	x	603	HEA	CAD-CBD-CGD-O1D
79	Bx	603	HEA	CAD-CBD-CGD-O1D
72	E	201	8Q1	O27-C28-C29-C30
72	p	201	8Q1	O27-C28-C29-C31
72	BE	201	8Q1	O27-C28-C29-C30
72	Bp	201	8Q1	O27-C28-C29-C31
75	AU	403	CDL	CB3-CB4-OB6-CB5
75	BV	201	CDL	C11-C12-C13-C14
71	g	203	PLX	C3-C4-O6-C6
71	r	501	PLX	C5-C4-O6-C6
71	AQ	101	PLX	C5-C4-O6-C6
71	Bg	203	PLX	C3-C4-O6-C6
71	Br	501	PLX	C5-C4-O6-C6
75	AN	102	CDL	CA2-OA2-PA1-OA5
75	V	201	CDL	C11-C12-C13-C14
75	i	401	CDL	C72-C71-CB7-OB8
75	Bi	401	CDL	C72-C71-CB7-OB8
82	AV	402	HEM	C2D-C3D-CAD-CBD
75	AN	102	CDL	C31-CA7-OA8-CA6
76	V	202	PEE	C21-C22-C23-C24
76	AJ	403	PEE	C15-C16-C17-C18
76	AL	503	PEE	C19-C20-C21-C22
75	AH	403	CDL	C51-C52-C53-C54
76	BV	202	PEE	C21-C22-C23-C24
79	x	604	HEA	CAD-CBD-CGD-O1D
79	Bx	604	HEA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
79	Bx	604	HEA	CAD-CBD-CGD-O2D
71	AN	101	PLX	C33-C34-C35-C36
71	BV	203	PLX	C33-C34-C35-C36
72	p	201	8Q1	C42-C43-S44-C1
72	Bp	201	8Q1	C42-C43-S44-C1
71	g	201	PLX	O6-C4-C5-O8
71	Bg	201	PLX	O6-C4-C5-O8
75	AA	101	CDL	OB6-CB4-CB6-OB8
76	AU	401	PEE	C30-C31-C32-C33
79	x	604	HEA	CAD-CBD-CGD-O2D
75	AH	403	CDL	C14-C15-C16-C17
76	AL	503	PEE	C40-C41-C42-C43
76	AV	403	PEE	C14-C15-C16-C17
79	x	603	HEA	CAA-CBA-CGA-O1A
79	Bx	603	HEA	CAA-CBA-CGA-O1A
79	Bx	603	HEA	CAD-CBD-CGD-O2D
76	AL	503	PEE	C16-C17-C18-C19
75	AH	403	CDL	C32-C31-CA7-OA9
75	AN	102	CDL	OA9-CA7-OA8-CA6
79	x	603	HEA	CAD-CBD-CGD-O2D
75	AU	403	CDL	O1-C1-CA2-OA2
71	BB	303	PLX	C7-C8-C9-C10
75	i	401	CDL	C52-C51-CB5-OB7
75	Bi	401	CDL	C52-C51-CB5-OB7
71	B	303	PLX	C7-C8-C9-C10
75	V	201	CDL	C73-C74-C75-C76
75	l	704	CDL	CA3-CA4-CA6-OA8
75	AN	102	CDL	C53-C54-C55-C56
75	BV	201	CDL	C73-C74-C75-C76
75	Bl	704	CDL	CA3-CA4-CA6-OA8
75	AN	102	CDL	C35-C36-C37-C38
71	g	202	PLX	C16-C17-C18-C19
71	Br	502	PLX	C28-C29-C30-C31
71	Bg	202	PLX	C16-C17-C18-C19
71	r	502	PLX	C28-C29-C30-C31
76	AJ	403	PEE	C36-C37-C38-C39
71	g	201	PLX	O4-C3-C4-O6
71	Bg	201	PLX	O4-C3-C4-O6
75	AH	403	CDL	CB7-C71-C72-C73
71	AN	101	PLX	C24-C25-C26-C27
71	BV	203	PLX	C24-C25-C26-C27
75	AY	501	CDL	C72-C71-CB7-OB8

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Mol	Chain	Res	Type	Atoms
71	AL	501	PLX	O6-C6-C7-C8
75	AU	403	CDL	C34-C35-C36-C37
76	AL	503	PEE	C23-C24-C25-C26
76	AU	401	PEE	C14-C15-C16-C17
71	AT	101	PLX	C30-C31-C32-C33
76	AU	401	PEE	C38-C39-C40-C41
76	AY	502	PEE	C36-C37-C38-C39
72	E	201	8Q1	O33-C32-C34-N36
72	BE	201	8Q1	O33-C32-C34-N36
76	AU	401	PEE	C42-C43-C44-C45
75	Bl	704	CDL	C32-C31-CA7-OA8
76	W	201	PEE	C35-C36-C37-C38
76	AJ	403	PEE	C19-C20-C21-C22
76	BW	201	PEE	C35-C36-C37-C38
75	AH	403	CDL	C73-C74-C75-C76
76	BV	202	PEE	C30-C31-C32-C33
75	l	703	CDL	C32-C31-CA7-OA8
75	l	704	CDL	C32-C31-CA7-OA8
75	Bl	703	CDL	C32-C31-CA7-OA8
76	W	201	PEE	C1-C2-O2-C10
76	BW	201	PEE	C1-C2-O2-C10
76	V	202	PEE	C30-C31-C32-C33
71	Bg	202	PLX	C27-C28-C29-C30
75	AA	101	CDL	C15-C16-C17-C18
71	B	303	PLX	C14-C15-C16-C17
71	g	202	PLX	C27-C28-C29-C30
71	BB	303	PLX	C14-C15-C16-C17
76	AH	401	PEE	C40-C41-C42-C43
71	AN	101	PLX	C35-C36-C37-C38
71	BV	203	PLX	C35-C36-C37-C38
75	AJ	404	CDL	C52-C51-CB5-OB6
75	AG	101	CDL	C32-C31-CA7-OA8
76	AV	403	PEE	C36-C37-C38-C39
71	b	201	PLX	C3-C4-C5-O8
71	Bb	201	PLX	C3-C4-C5-O8
72	p	201	8Q1	C28-O27-P24-O3
75	V	201	CDL	CA3-CA4-CA6-OA8
75	AH	403	CDL	CB3-CB4-CB6-OB8
75	AJ	405	CDL	CA3-CA4-CA6-OA8
75	BV	201	CDL	CA3-CA4-CA6-OA8
76	AH	401	PEE	O3P-C1-C2-O2
75	AN	102	CDL	C12-C11-CA5-OA6

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Mol	Chain	Res	Type	Atoms
71	AT	101	PLX	C10-C11-C12-C13
73	J	401	NDP	O4D-C4D-C5D-O5D
73	BJ	401	NDP	O4D-C4D-C5D-O5D
79	x	604	HEA	CAA-CBA-CGA-O2A
79	Bx	604	HEA	CAA-CBA-CGA-O2A
71	Br	502	PLX	C33-C34-C35-C36
71	r	502	PLX	C33-C34-C35-C36
73	J	401	NDP	O4D-C1D-N1N-C2N
73	BJ	401	NDP	O4D-C1D-N1N-C2N
75	l	704	CDL	C35-C36-C37-C38
75	Bl	704	CDL	C35-C36-C37-C38
79	x	604	HEA	CAA-CBA-CGA-O1A
79	Bx	604	HEA	CAA-CBA-CGA-O1A
71	B	303	PLX	O9-C24-C25-C26
71	BB	303	PLX	O9-C24-C25-C26
76	l	701	PEE	C38-C39-C40-C41
76	AH	401	PEE	C36-C37-C38-C39
76	Bl	701	PEE	C38-C39-C40-C41
71	AL	501	PLX	C11-C12-C13-C14
75	AU	403	CDL	O1-C1-CB2-OB2
75	l	703	CDL	C32-C31-CA7-OA9
75	Bl	703	CDL	C32-C31-CA7-OA9
71	AL	501	PLX	C29-C30-C31-C32
76	AL	503	PEE	O2-C10-C11-C12
75	AA	101	CDL	C32-C33-C34-C35
76	l	702	PEE	C18-C19-C20-C21
76	Bl	702	PEE	C18-C19-C20-C21
75	AN	102	CDL	C12-C11-CA5-OA7
75	Bl	703	CDL	C32-C33-C34-C35
75	AG	101	CDL	C32-C31-CA7-OA9
75	l	703	CDL	C32-C33-C34-C35
75	AU	403	CDL	CB3-CB4-CB6-OB8
76	l	702	PEE	C1-C2-C3-O3
76	Bl	702	PEE	C1-C2-C3-O3
71	b	201	PLX	C24-C25-C26-C27
71	Bb	201	PLX	C24-C25-C26-C27
75	AU	403	CDL	C72-C71-CB7-OB8
76	AL	503	PEE	C41-C42-C43-C44
76	Bl	702	PEE	C22-C23-C24-C25
71	AL	501	PLX	C33-C34-C35-C36
71	BV	203	PLX	C17-C18-C19-C20
76	l	701	PEE	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
76	l	702	PEE	C22-C23-C24-C25
75	AN	102	CDL	C72-C71-CB7-OB8
71	B	303	PLX	C4-C3-O4-P1
71	BB	303	PLX	C4-C3-O4-P1
75	AU	403	CDL	C1-CA2-OA2-PA1
75	AG	101	CDL	C15-C16-C17-C18
75	AJ	404	CDL	C52-C51-CB5-OB7
71	AN	101	PLX	C17-C18-C19-C20
79	x	603	HEA	CAA-CBA-CGA-O2A
79	Bx	603	HEA	CAA-CBA-CGA-O2A
71	g	201	PLX	C3-O4-P1-O2
71	AN	101	PLX	C3-O4-P1-O2
71	AT	101	PLX	C3-O4-P1-O3
71	BV	203	PLX	C3-O4-P1-O2
71	Bg	201	PLX	C3-O4-P1-O2
75	l	703	CDL	CA3-OA5-PA1-OA3
75	l	704	CDL	CB3-OB5-PB2-OB3
75	n	101	CDL	CB3-OB5-PB2-OB3
75	AJ	405	CDL	CA2-OA2-PA1-OA3
75	AL	502	CDL	CA2-OA2-PA1-OA3
75	AU	403	CDL	CA2-OA2-PA1-OA3
75	AU	403	CDL	CB2-OB2-PB2-OB3
75	AY	501	CDL	CA2-OA2-PA1-OA3
75	Bl	703	CDL	CA3-OA5-PA1-OA3
75	Bl	704	CDL	CB3-OB5-PB2-OB3
75	Bn	101	CDL	CB3-OB5-PB2-OB3
76	l	702	PEE	C4-O4P-P-O1P
76	AH	401	PEE	C1-O3P-P-O1P
76	AJ	403	PEE	C4-O4P-P-O2P
76	Bl	702	PEE	C4-O4P-P-O1P
75	AU	403	CDL	OB6-CB4-CB6-OB8
75	AU	403	CDL	C75-C76-C77-C78
75	V	201	CDL	C12-C11-CA5-OA7
75	l	704	CDL	C32-C31-CA7-OA9
75	BV	201	CDL	C12-C11-CA5-OA7
75	Bl	704	CDL	C32-C31-CA7-OA9
76	AY	502	PEE	C21-C22-C23-C24
76	Bl	701	PEE	C33-C34-C35-C36
82	AV	401	HEM	CAA-CBA-CGA-O2A
71	AT	101	PLX	C25-C26-C27-C28
76	AJ	403	PEE	O4P-C4-C5-N
75	AA	101	CDL	C12-C11-CA5-OA6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
71	r	501	PLX	C14-C15-C16-C17
71	Br	501	PLX	C14-C15-C16-C17
71	b	201	PLX	C25-C24-O8-C5
71	g	202	PLX	C25-C24-O8-C5
71	AL	501	PLX	C1-C2-O1-P1
71	Bb	201	PLX	C25-C24-O8-C5
71	Bg	202	PLX	C25-C24-O8-C5
76	W	201	PEE	C5-C4-O4P-P
76	BW	201	PEE	C5-C4-O4P-P
75	AY	501	CDL	C51-C52-C53-C54
76	l	702	PEE	C41-C42-C43-C44
76	Bl	702	PEE	C41-C42-C43-C44
76	AJ	403	PEE	C10-C11-C12-C13
73	J	401	NDP	C2D-C1D-N1N-C2N
73	BJ	401	NDP	C2D-C1D-N1N-C2N
75	AG	101	CDL	C52-C51-CB5-OB6
76	V	202	PEE	C39-C40-C41-C42
76	BV	202	PEE	C39-C40-C41-C42
76	Bl	702	PEE	C32-C33-C34-C35
75	l	704	CDL	C74-C75-C76-C77
75	Bl	704	CDL	C74-C75-C76-C77
76	l	702	PEE	C32-C33-C34-C35
75	l	704	CDL	C52-C51-CB5-OB6
75	AH	403	CDL	C12-C11-CA5-OA6
76	AH	401	PEE	O2-C10-C11-C12
76	AL	503	PEE	O3-C30-C31-C32
76	AY	502	PEE	O3-C30-C31-C32
76	l	701	PEE	C11-C12-C13-C14
71	g	202	PLX	C6-C7-C8-C9
71	g	202	PLX	C24-C25-C26-C27
71	AQ	101	PLX	C6-C7-C8-C9
71	Bg	202	PLX	C6-C7-C8-C9
71	Bg	202	PLX	C24-C25-C26-C27
79	x	604	HEA	C26-C15-C16-C17
79	Bx	604	HEA	C26-C15-C16-C17
70	A	502	FMN	N10-C1'-C2'-O2'
70	BA	502	FMN	N10-C1'-C2'-O2'
79	x	603	HEA	O11-C11-C3B-C2B
79	Bx	603	HEA	O11-C11-C3B-C2B
75	AU	403	CDL	C72-C71-CB7-OB9
76	AL	503	PEE	O4-C10-C11-C12
76	Bl	701	PEE	C11-C12-C13-C14

*Continued on next page...*

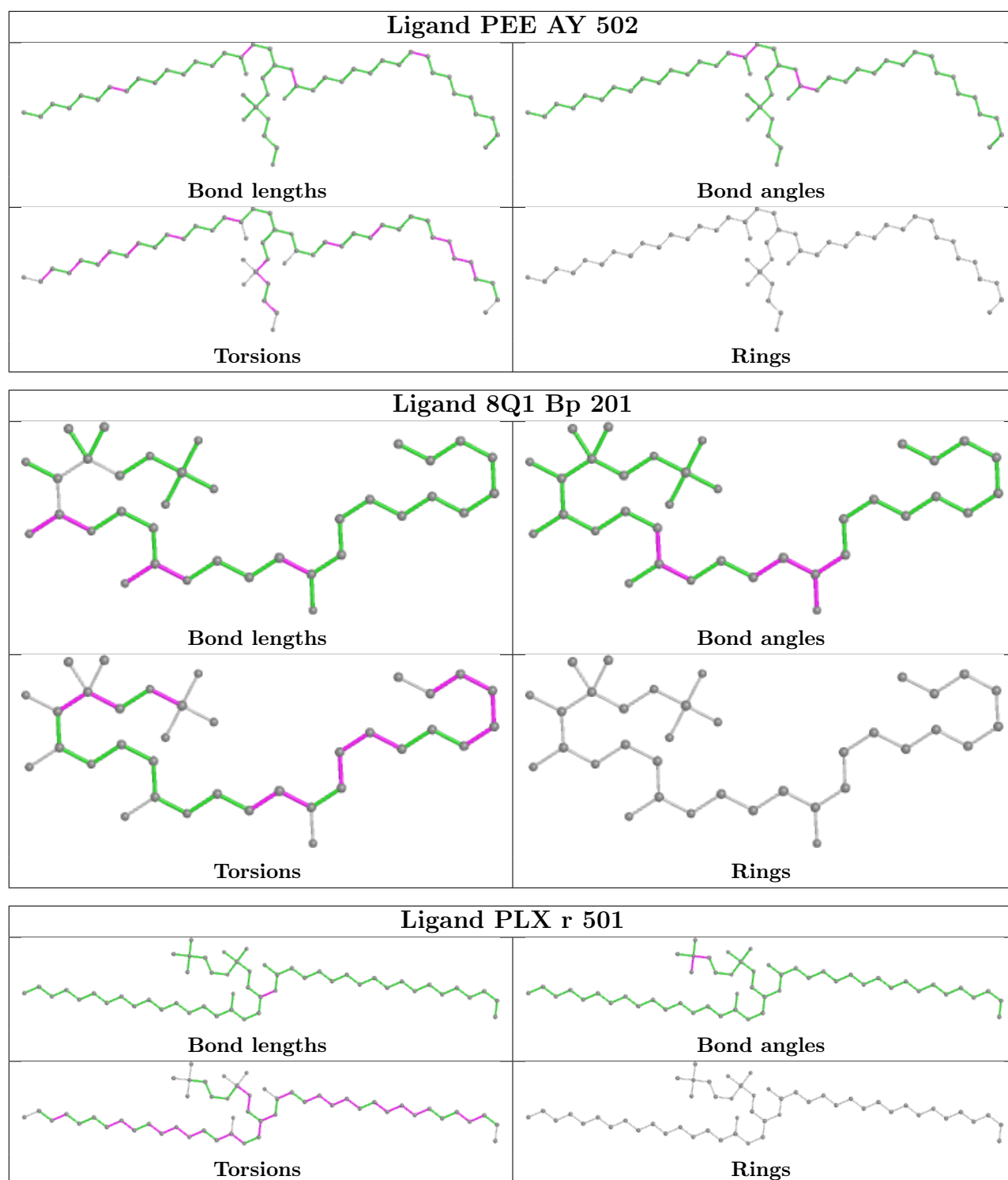
*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
75	AJ	404	CDL	C12-C11-CA5-OA6
75	Bl	704	CDL	C52-C51-CB5-OB6
71	AN	101	PLX	C15-C16-C17-C18
75	l	704	CDL	C52-C51-CB5-OB7
75	AH	403	CDL	C12-C11-CA5-OA7
71	g	203	PLX	C36-C37-C38-C39
71	Bg	203	PLX	C36-C37-C38-C39
75	AA	101	CDL	C12-C11-CA5-OA7
76	AY	502	PEE	O5-C30-C31-C32
71	BV	203	PLX	C15-C16-C17-C18
75	AN	102	CDL	O1-C1-CB2-OB2
75	AJ	404	CDL	C12-C11-CA5-OA7
75	AN	102	CDL	C72-C71-CB7-OB9
75	Bl	704	CDL	C52-C51-CB5-OB7
75	AY	501	CDL	CA5-C11-C12-C13
71	AT	101	PLX	C17-C18-C19-C20
76	W	201	PEE	C42-C43-C44-C45
75	AA	101	CDL	C52-C51-CB5-OB6
75	BV	201	CDL	C52-C51-CB5-OB6

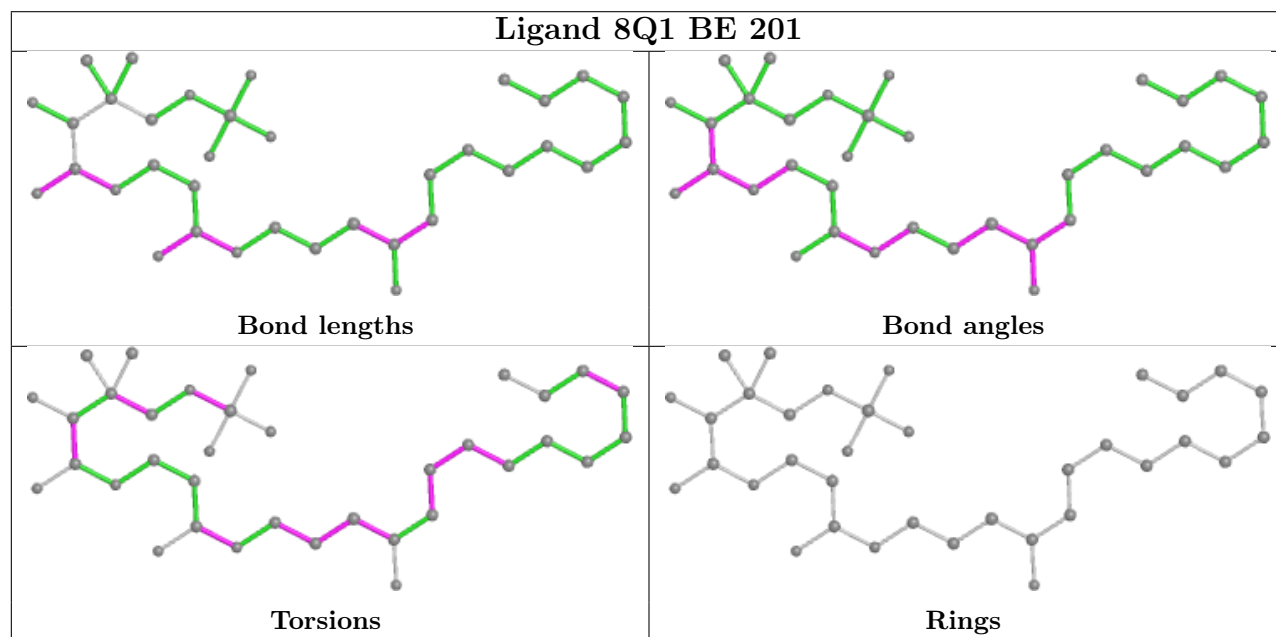
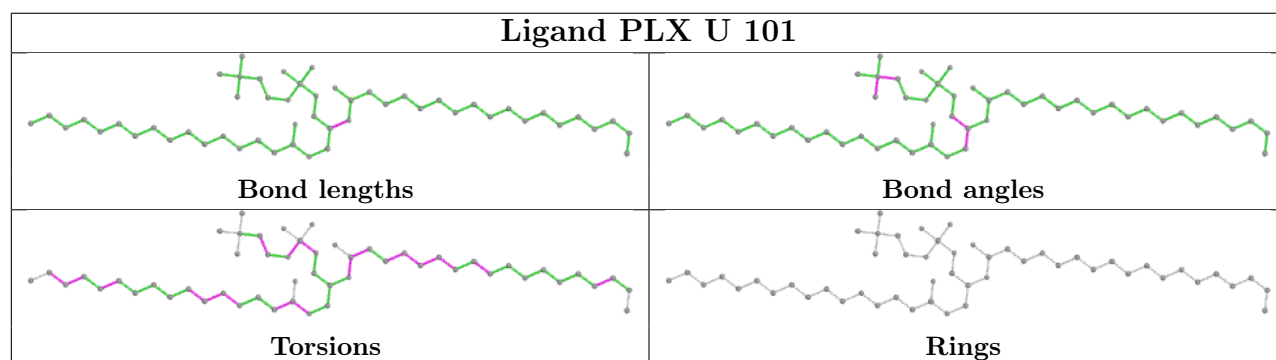
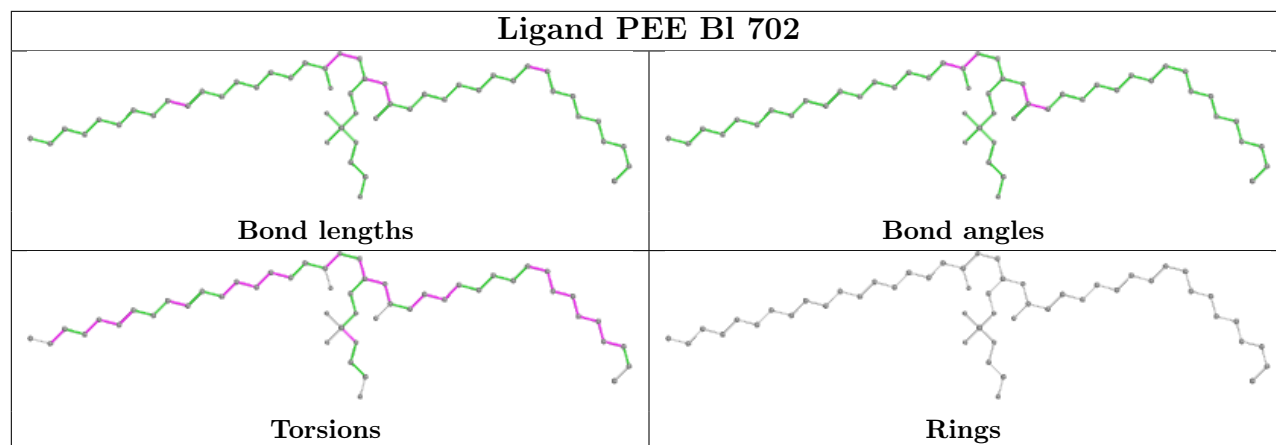
There are no ring outliers.

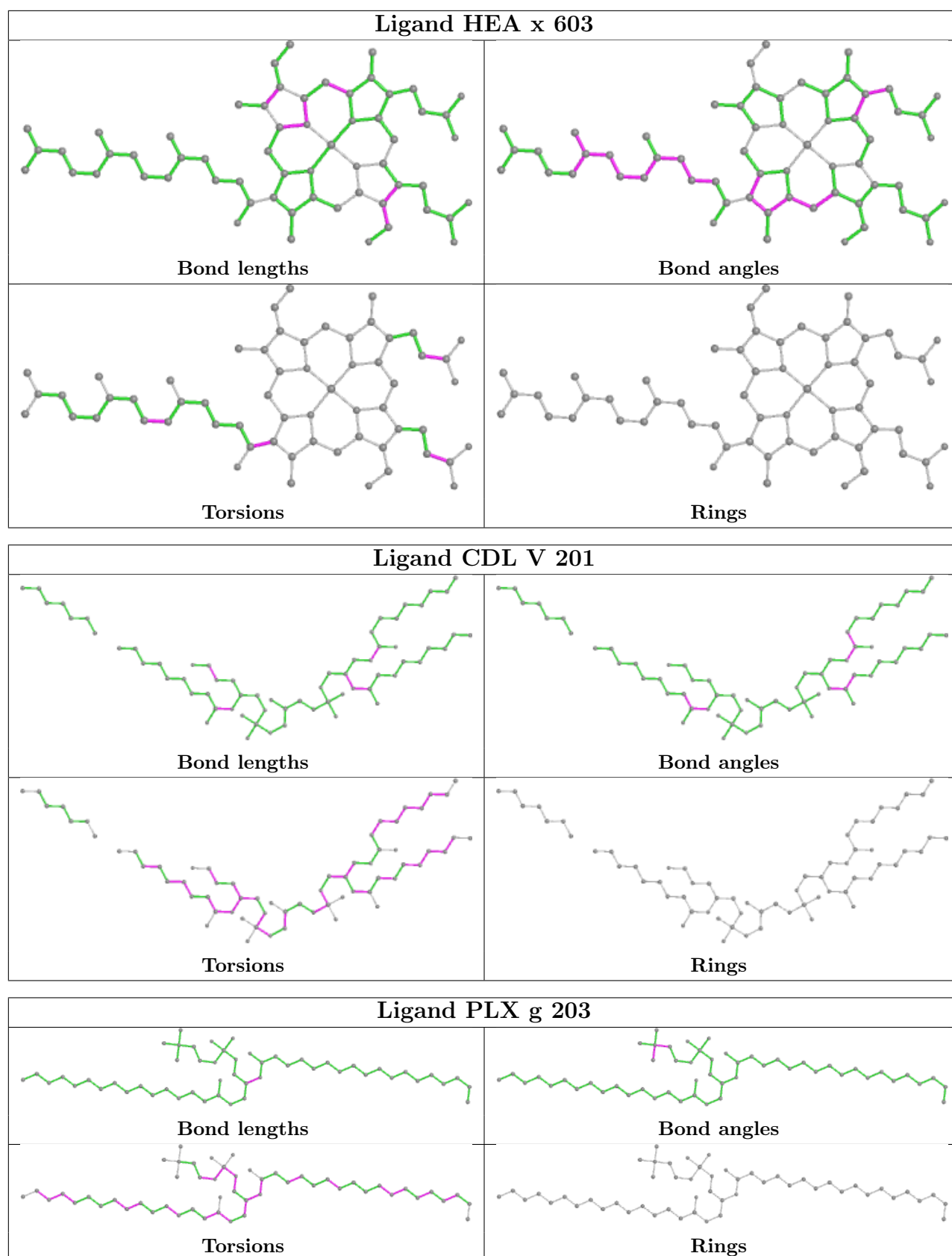
No monomer is involved in short contacts.

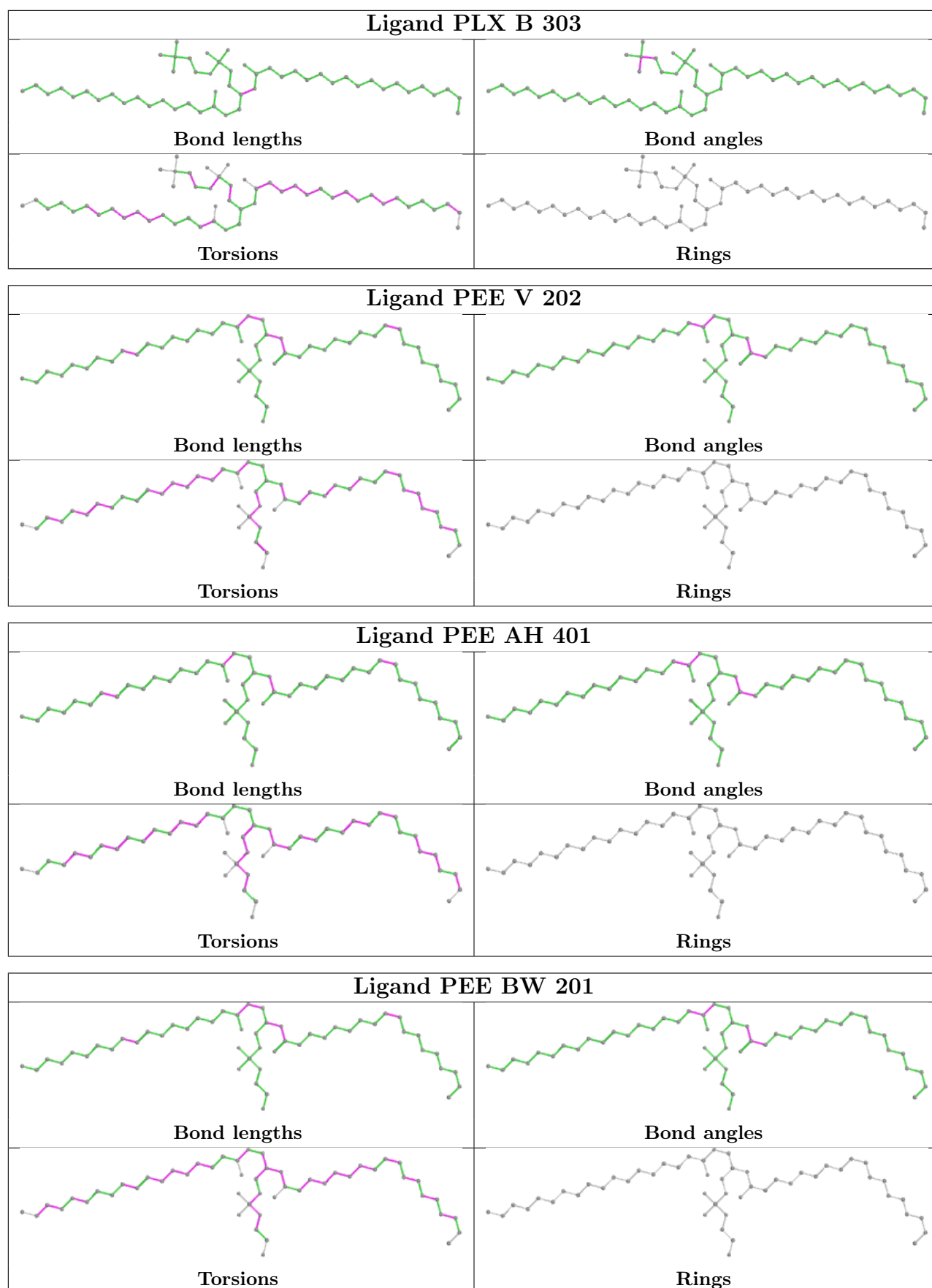
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

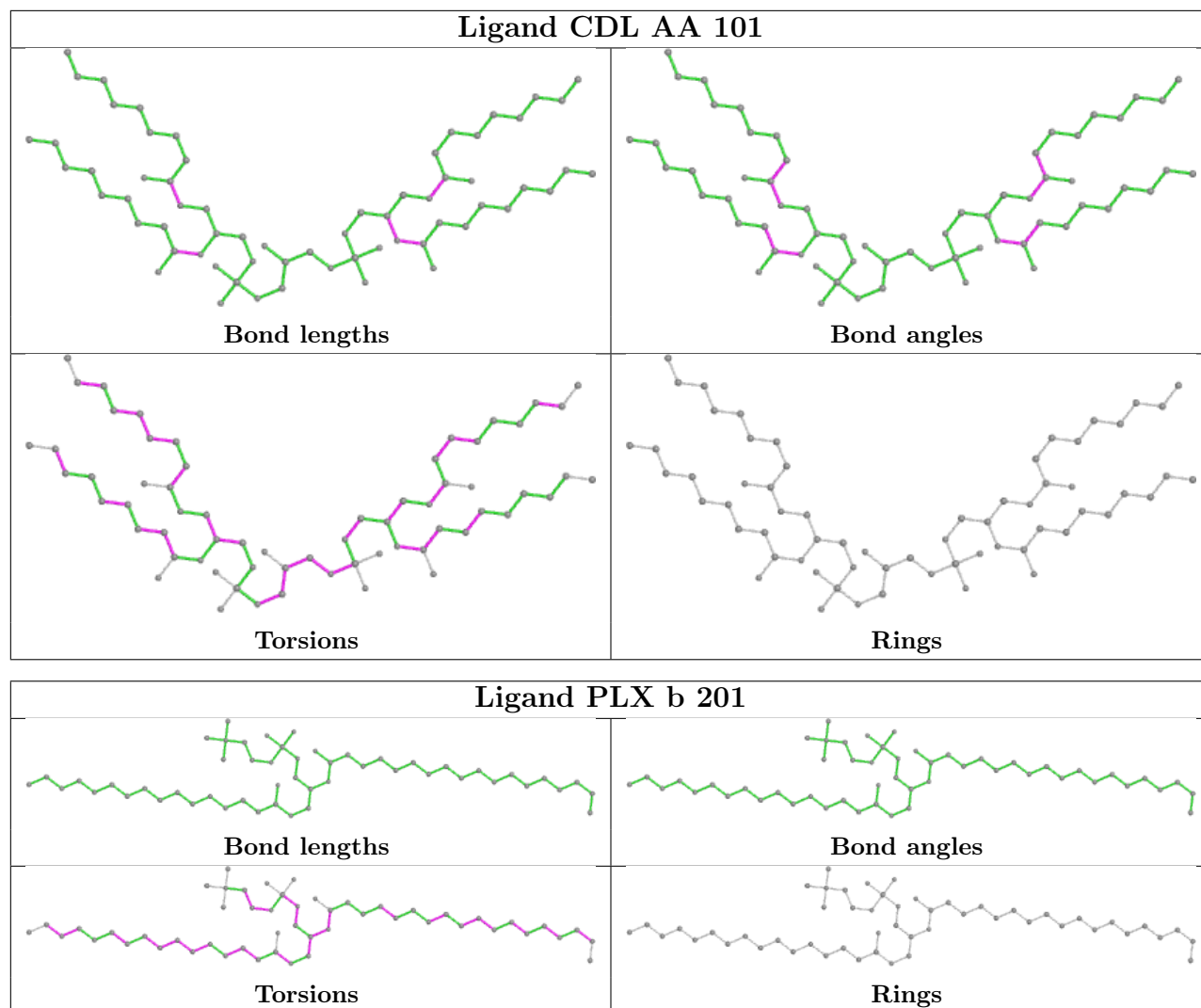


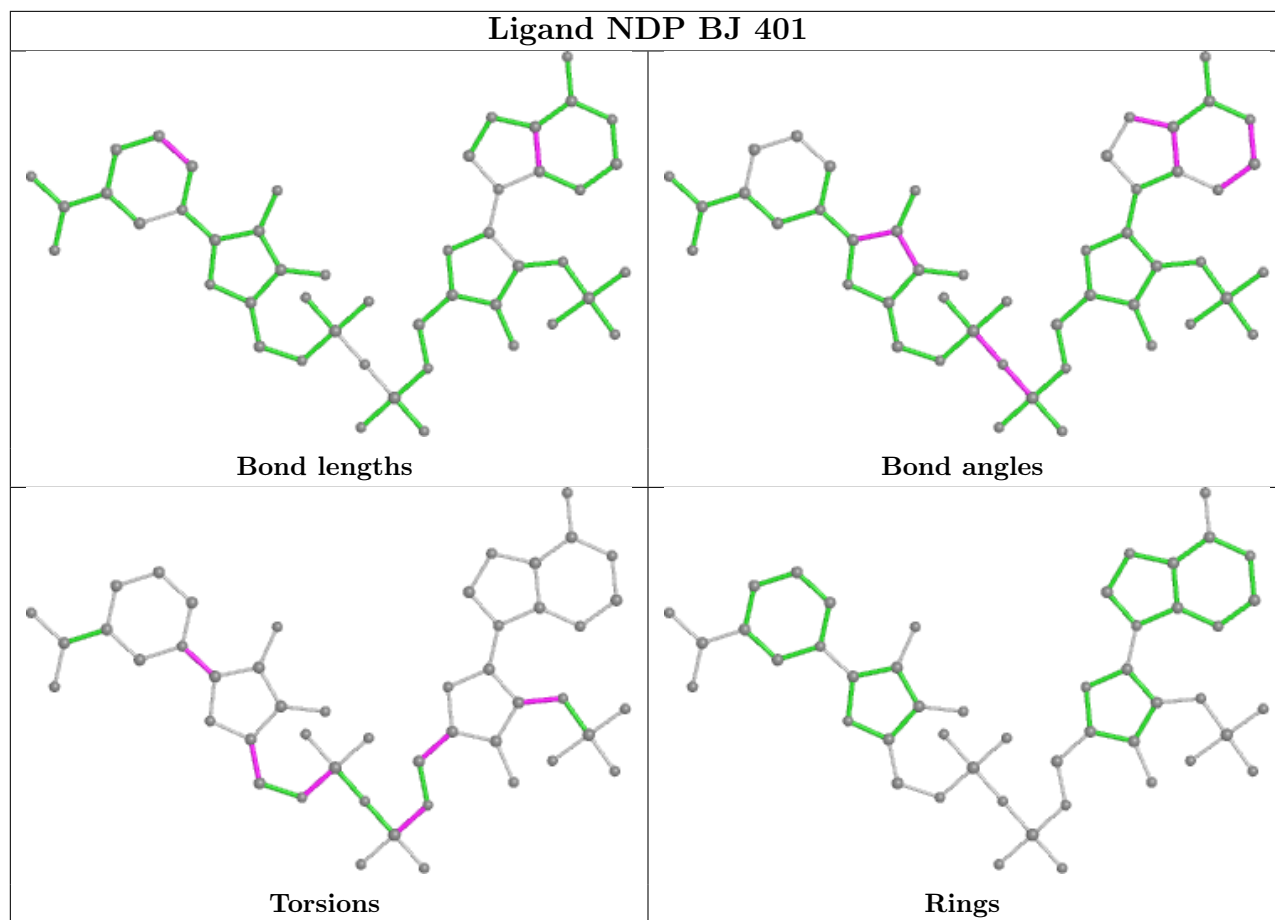


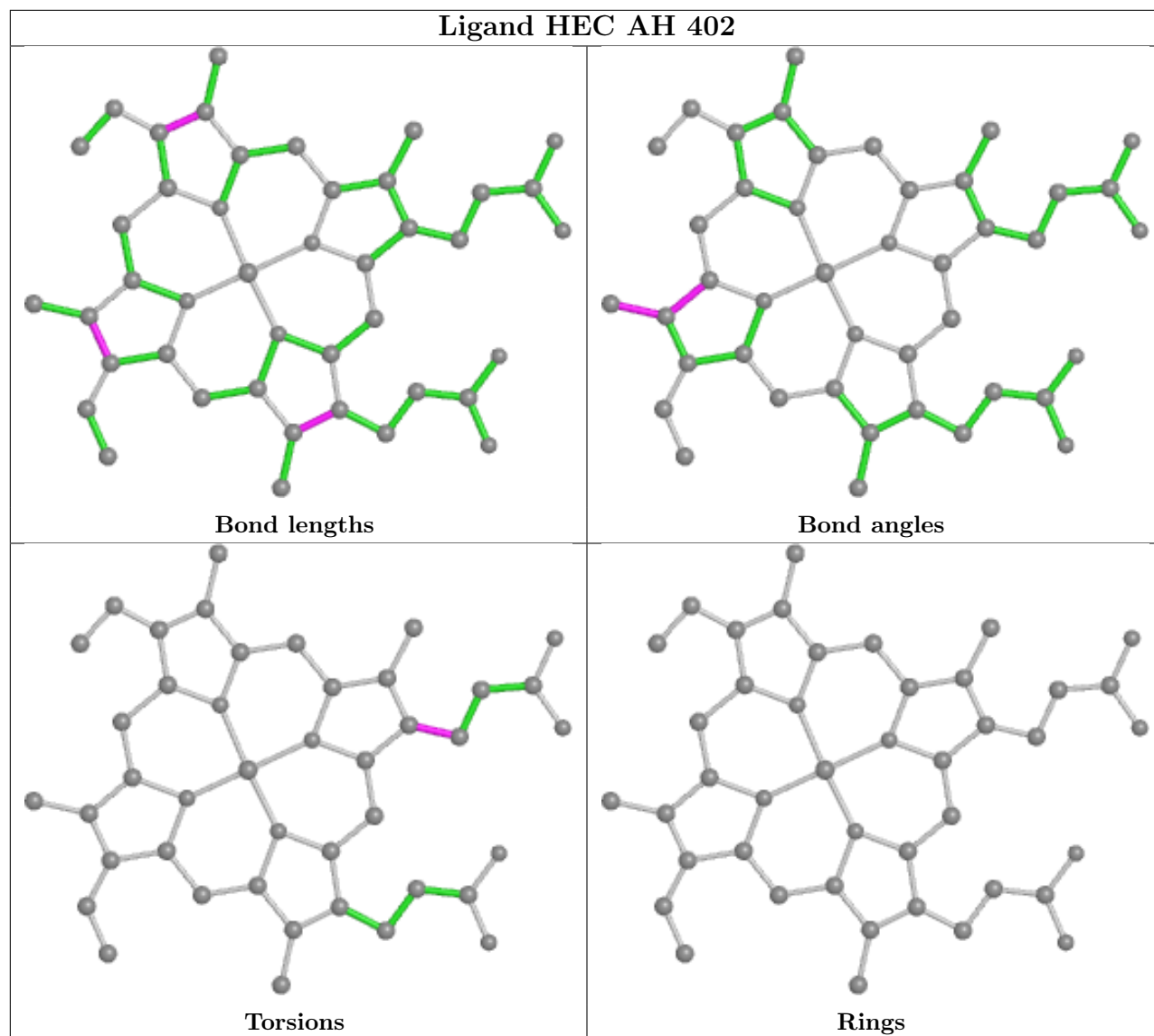


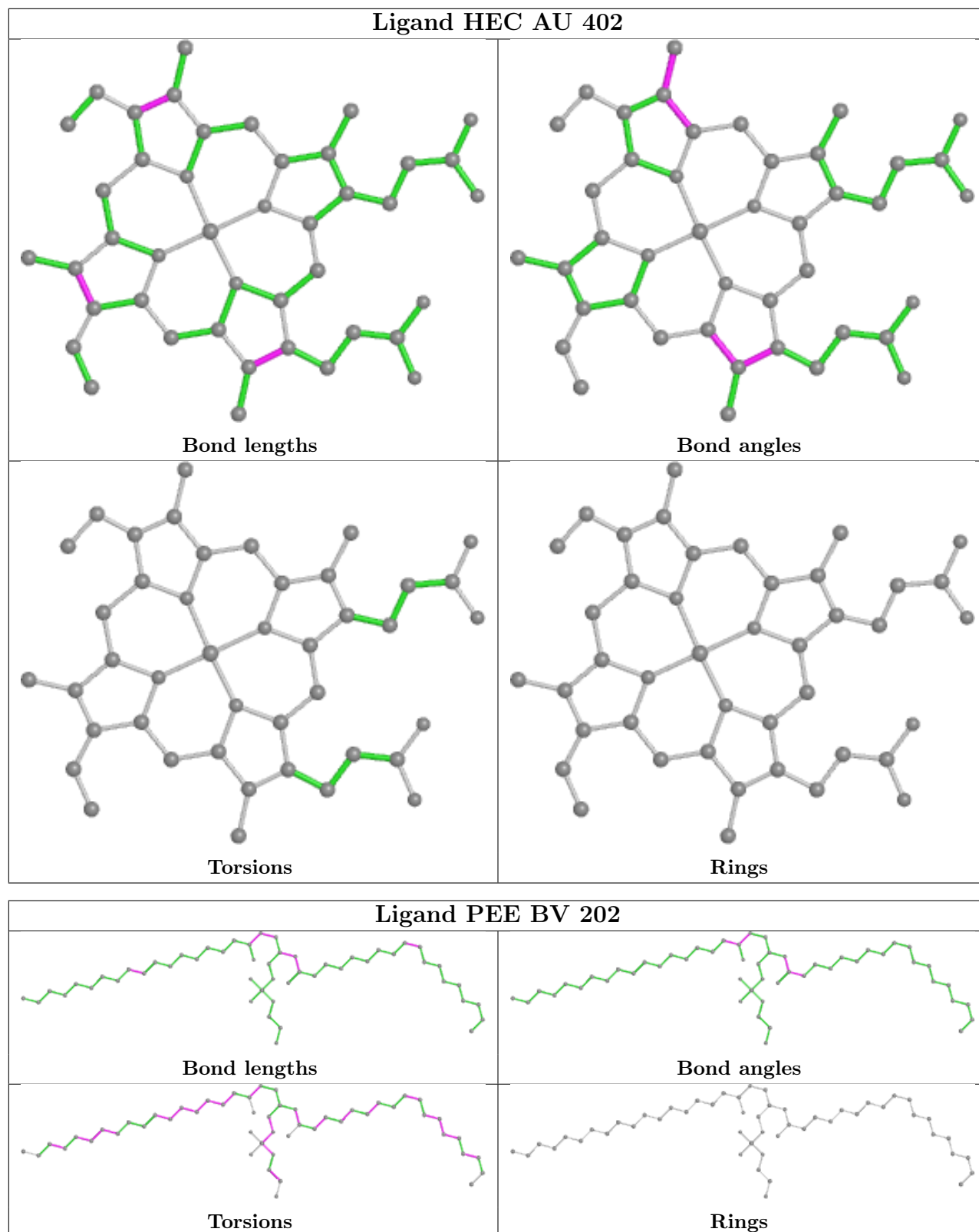


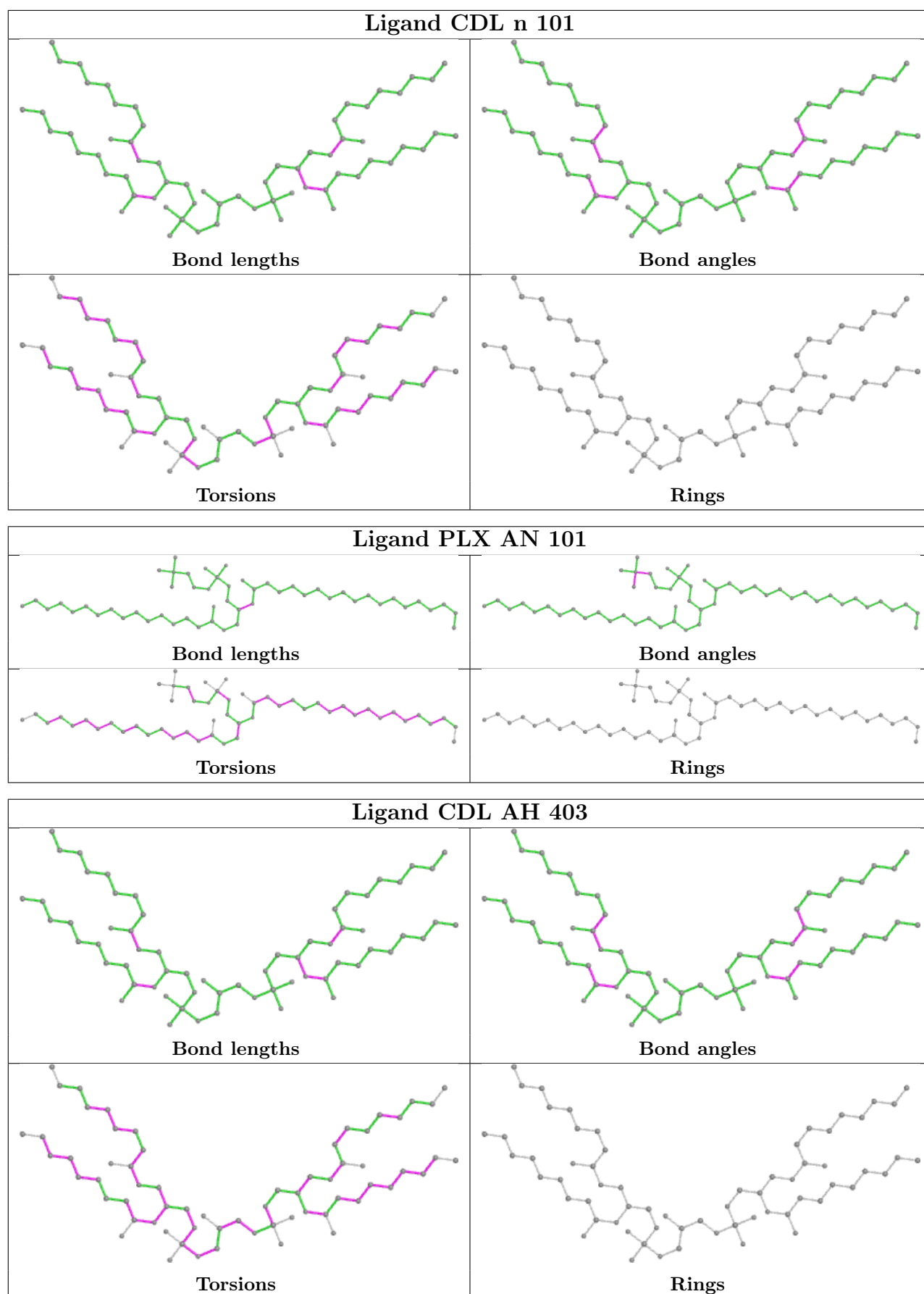




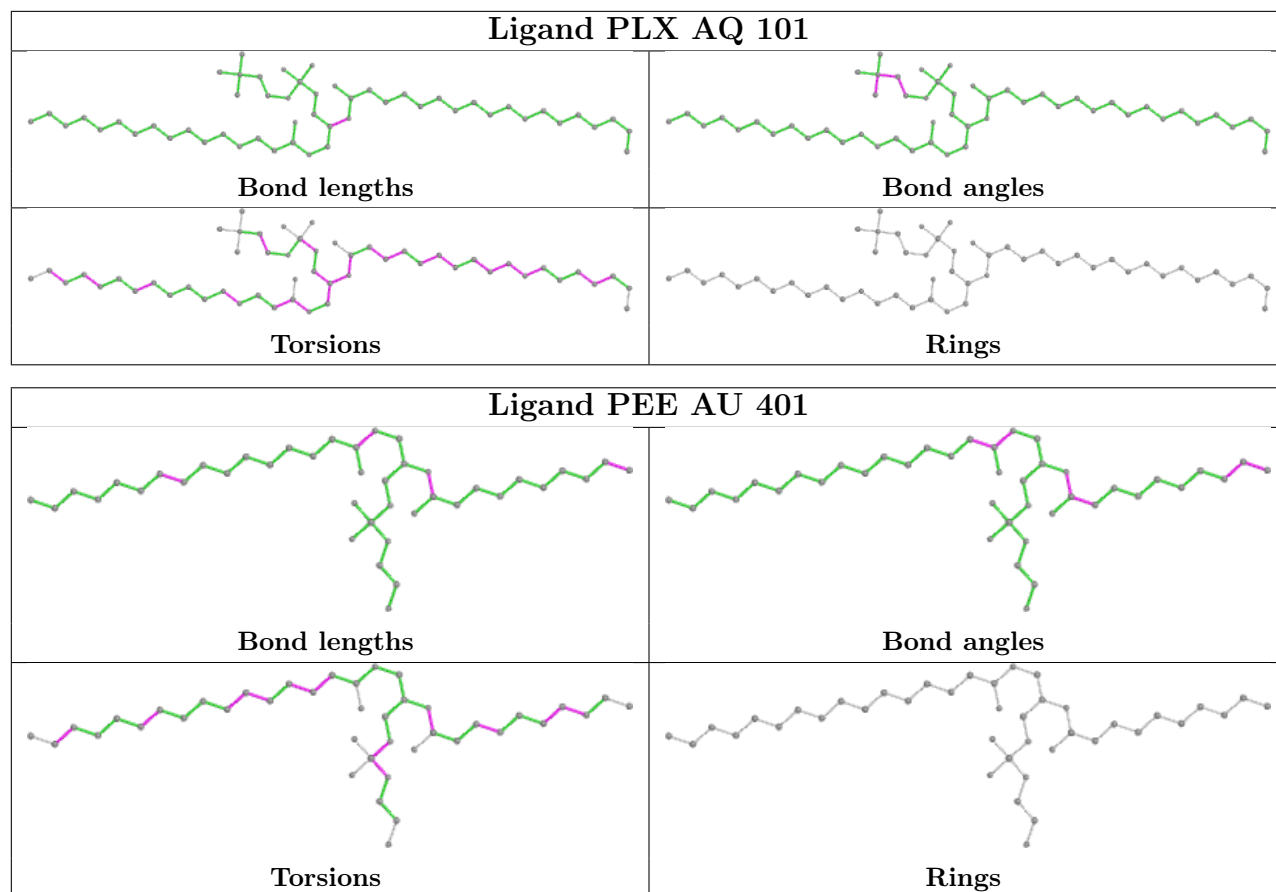


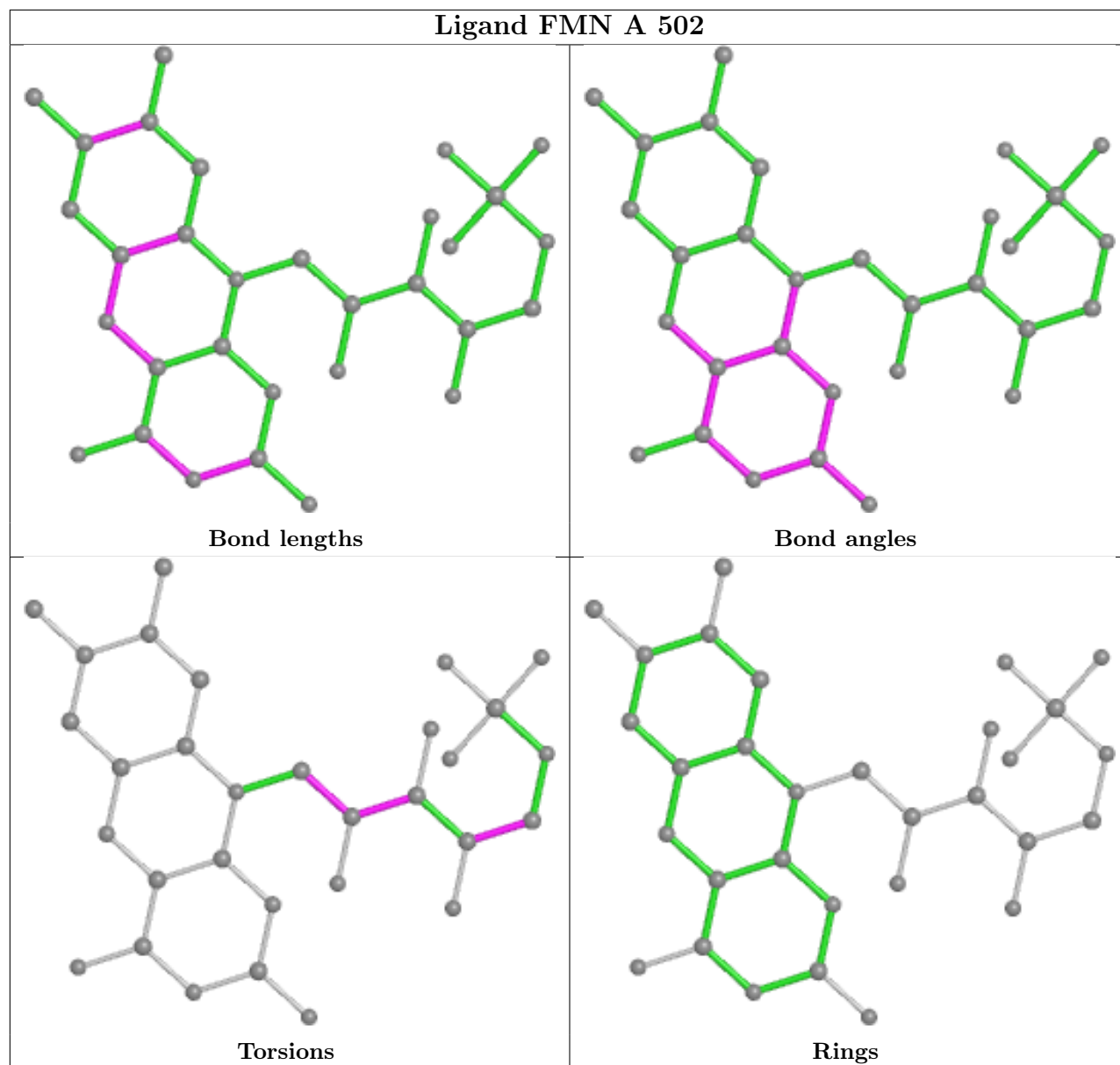


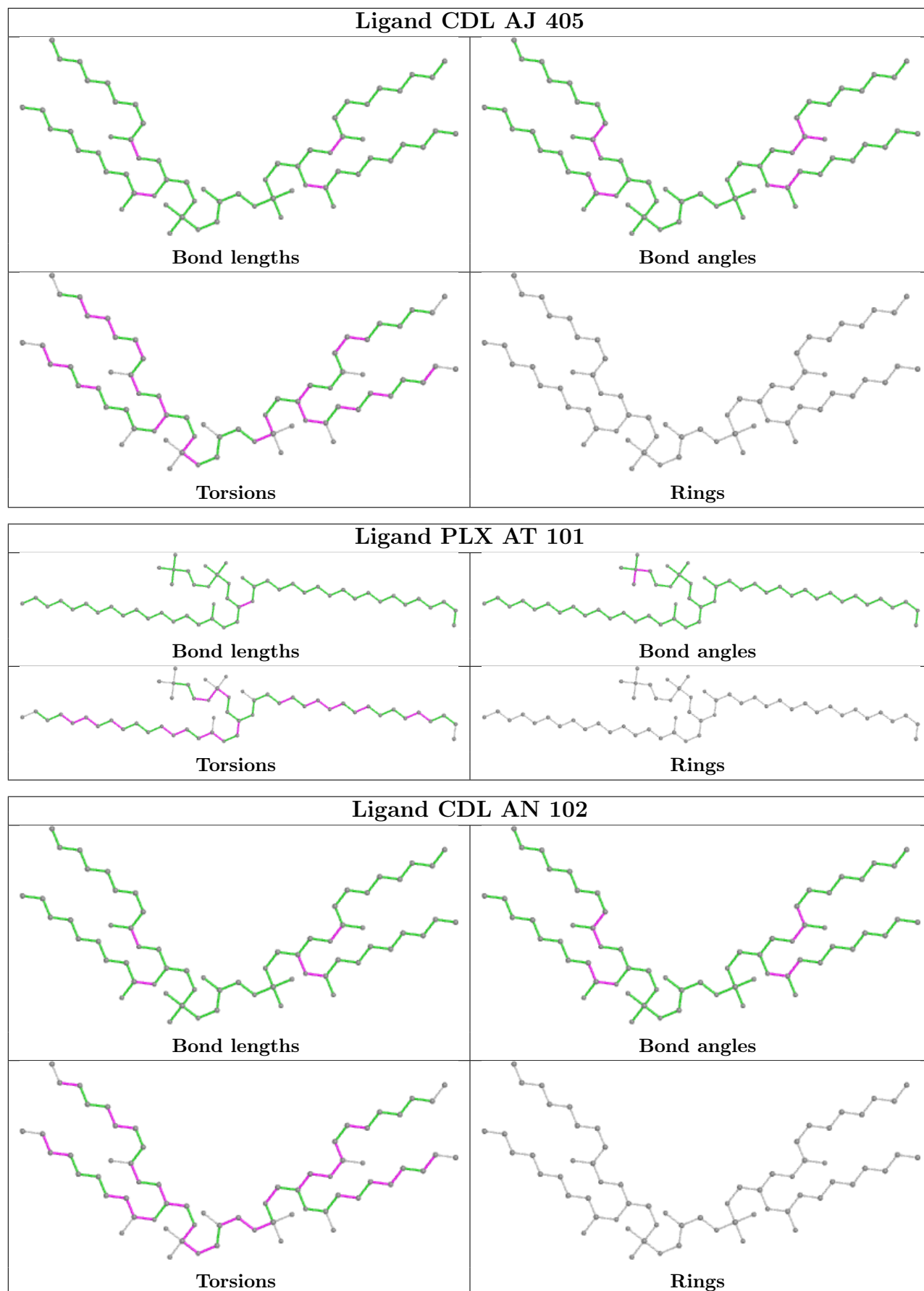


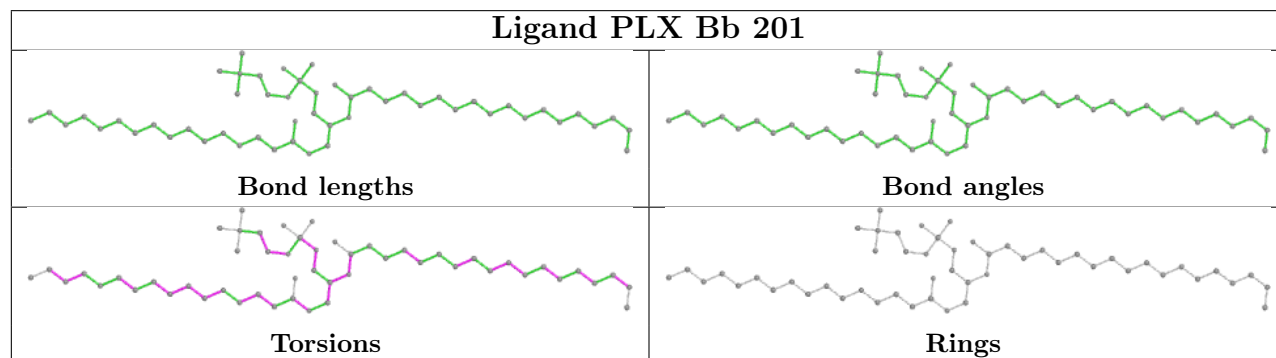
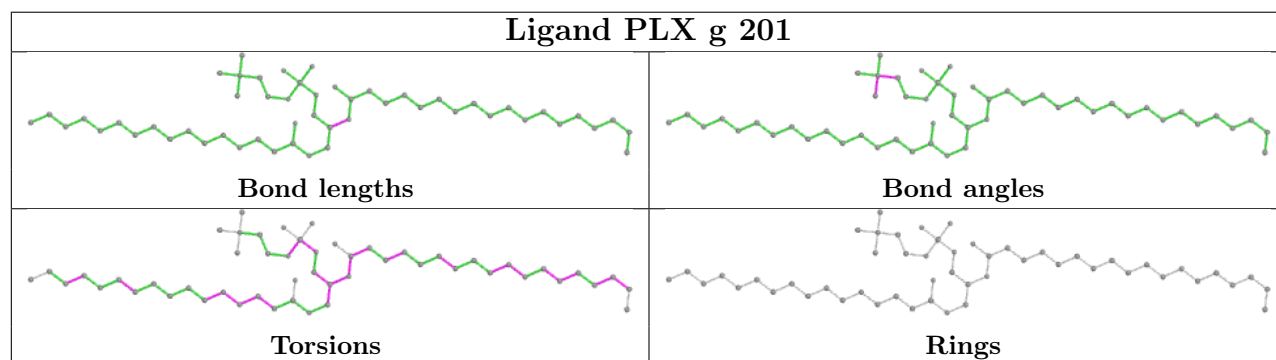
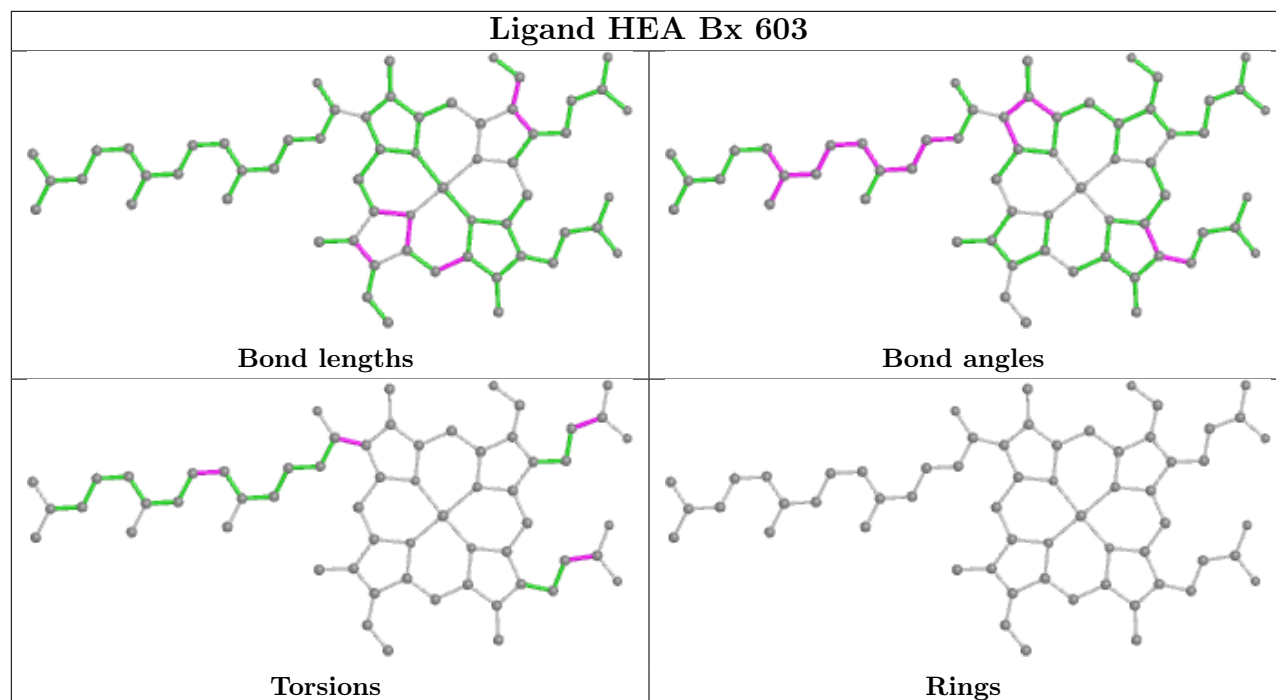


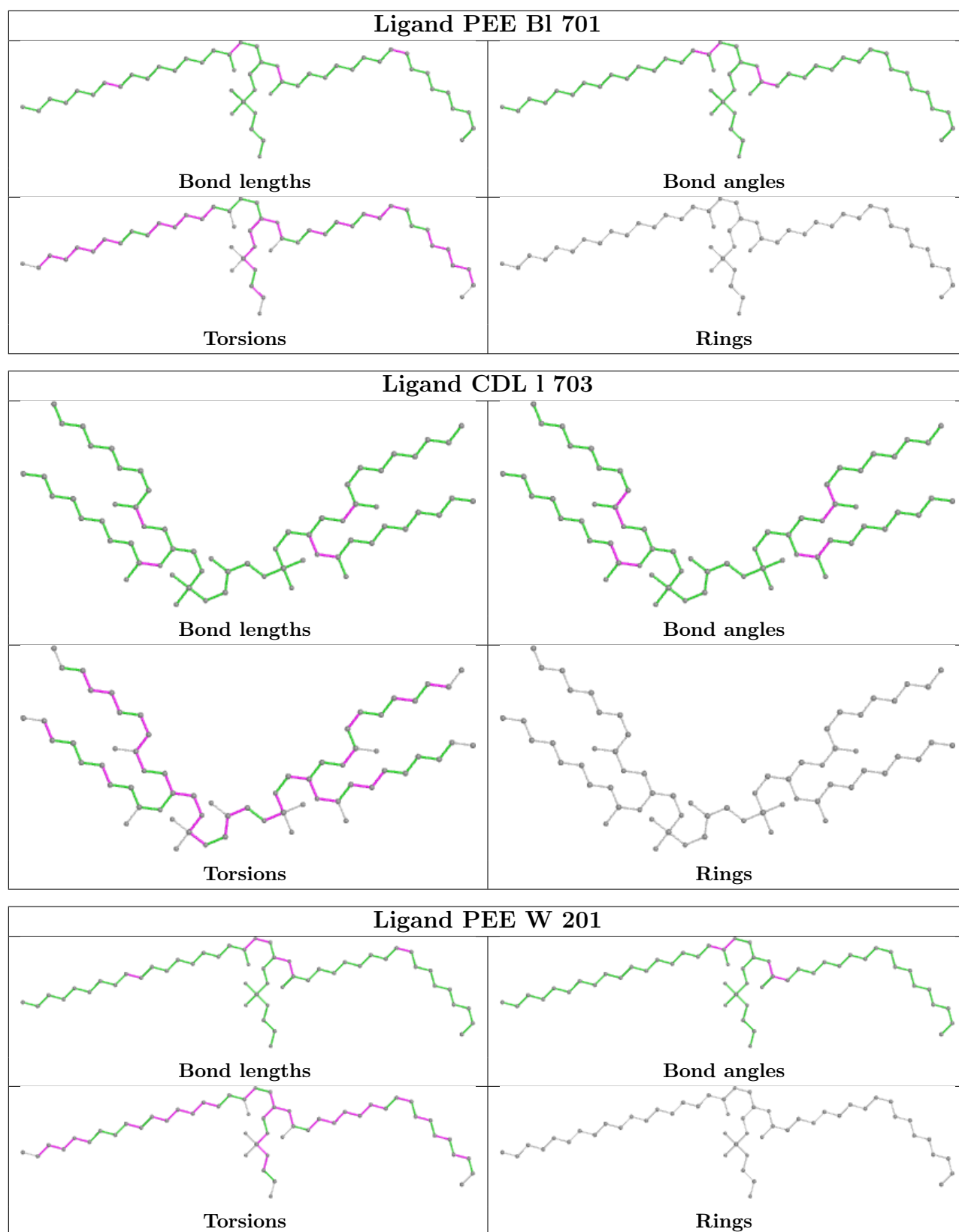


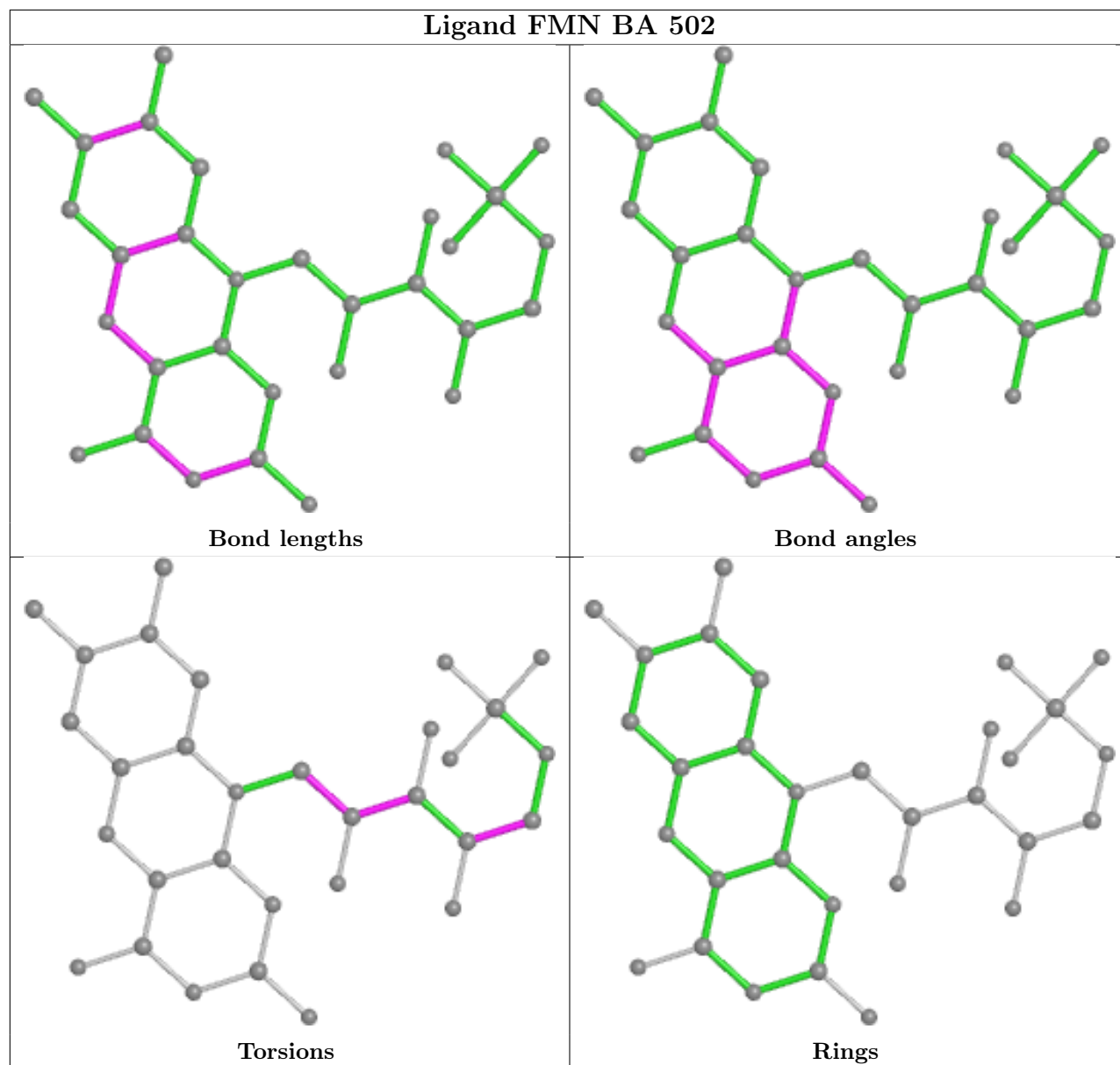


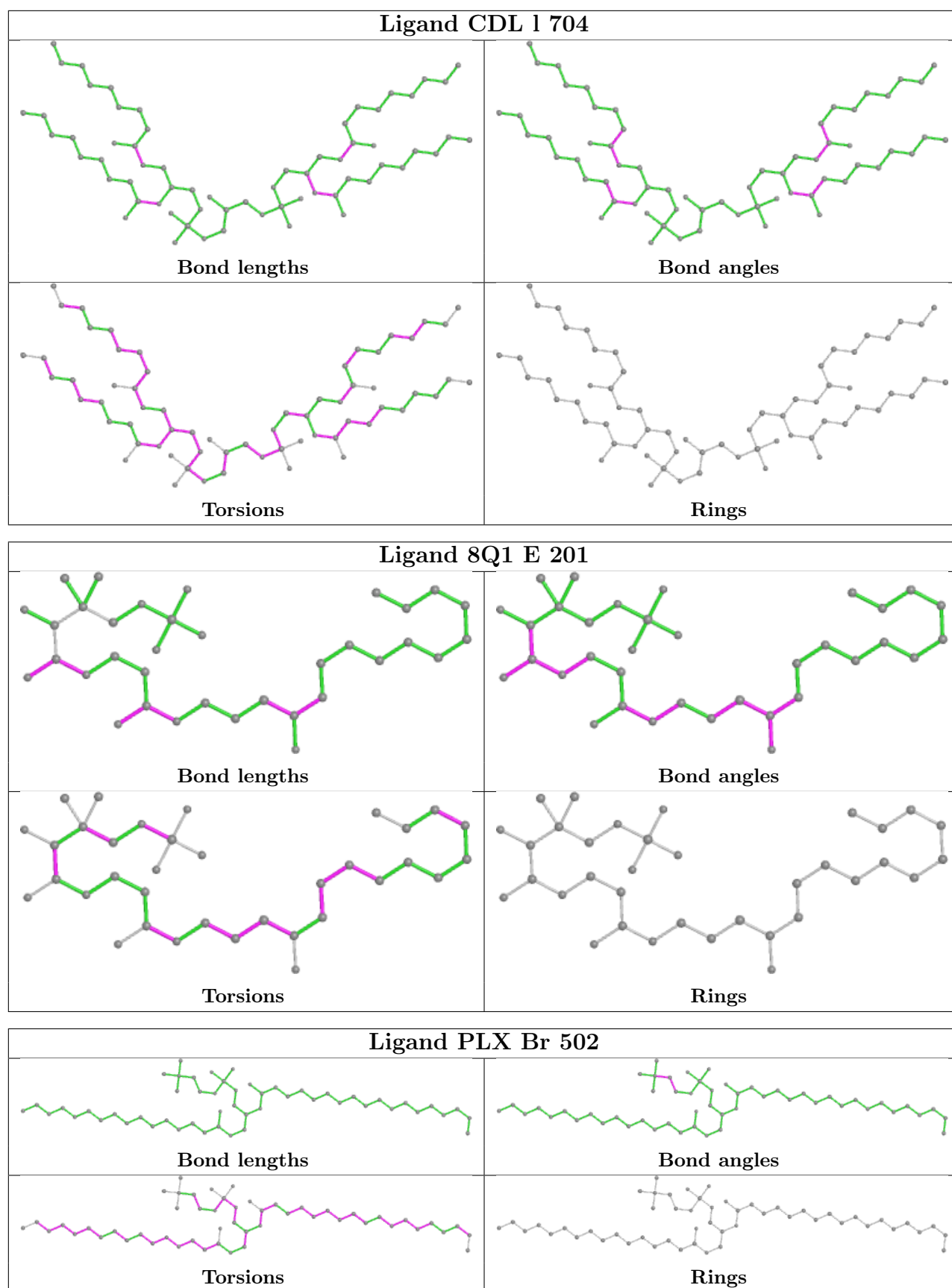


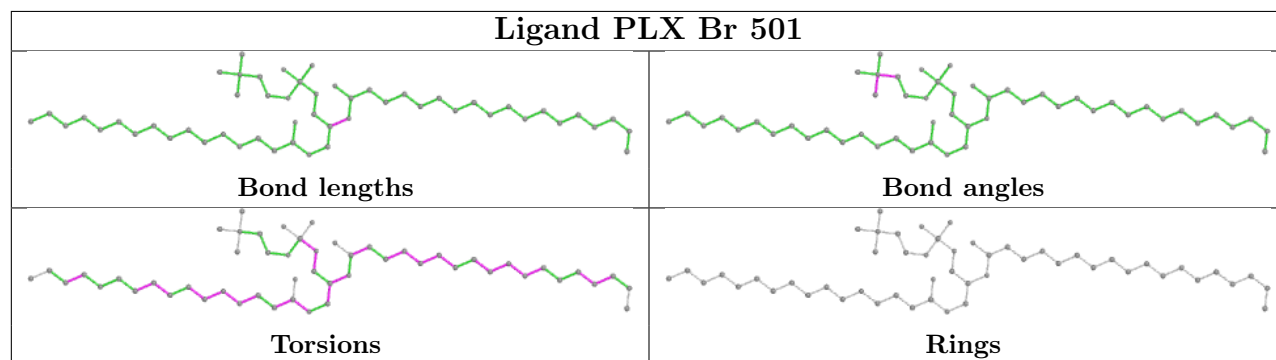
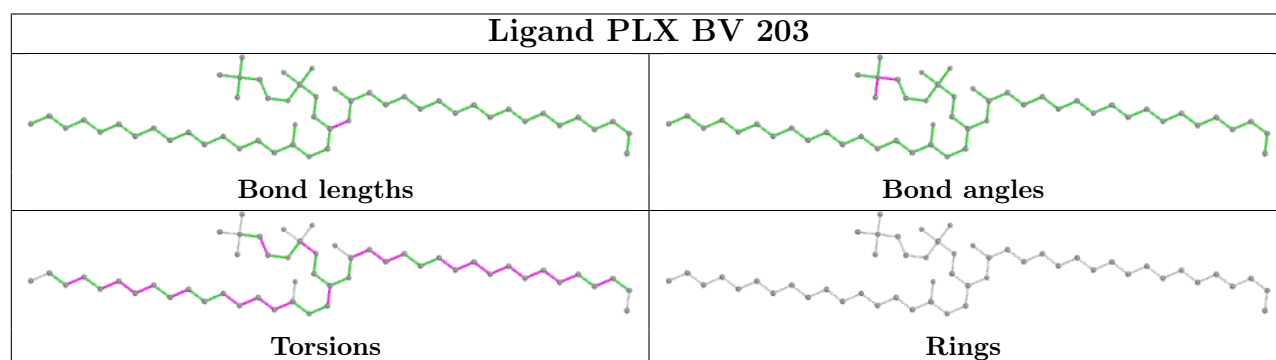
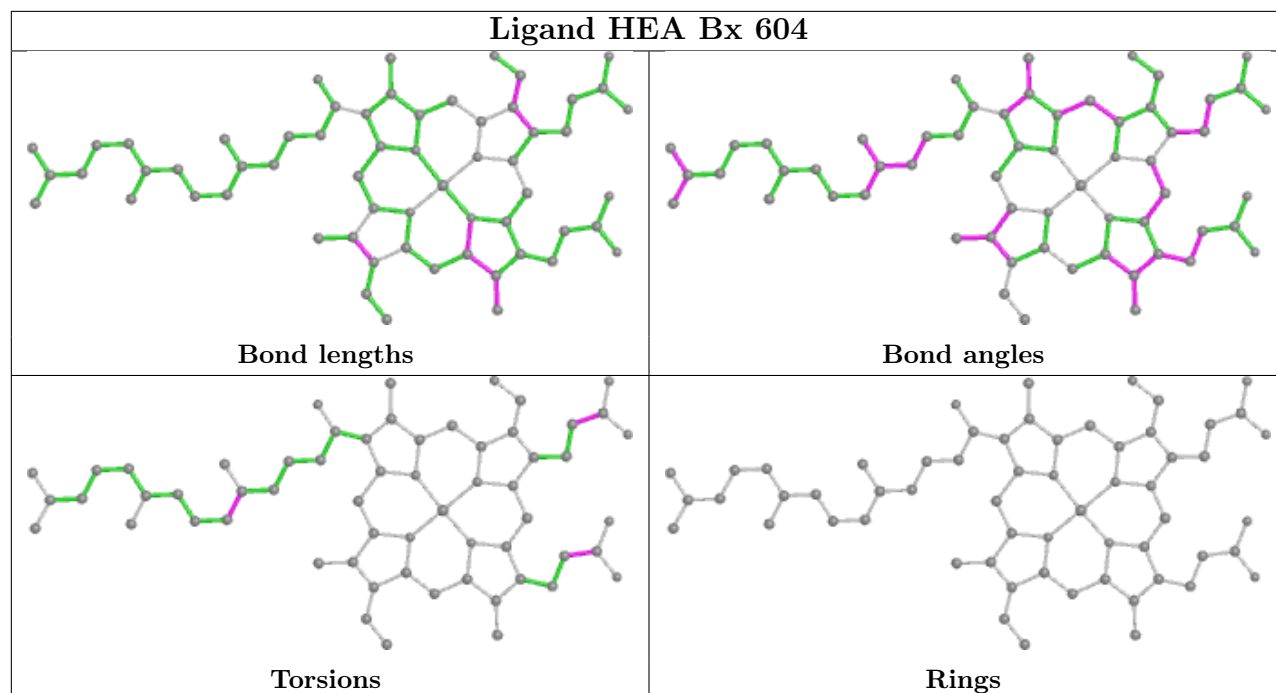




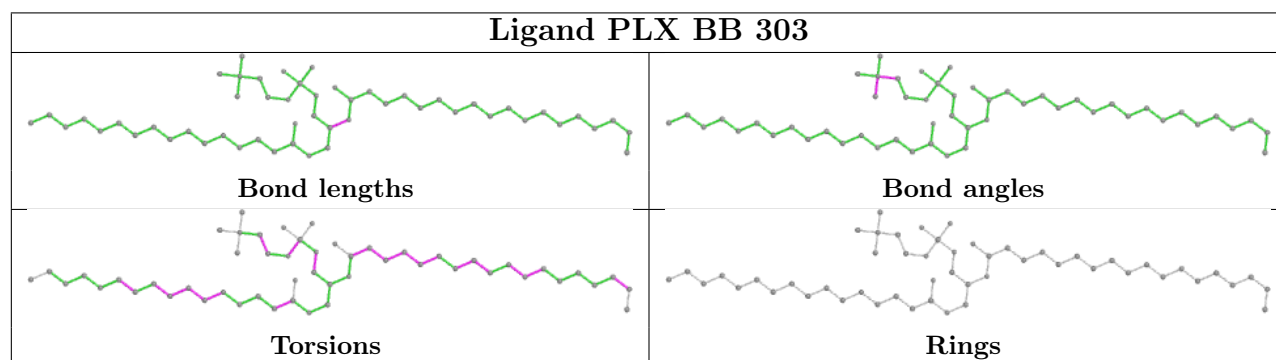
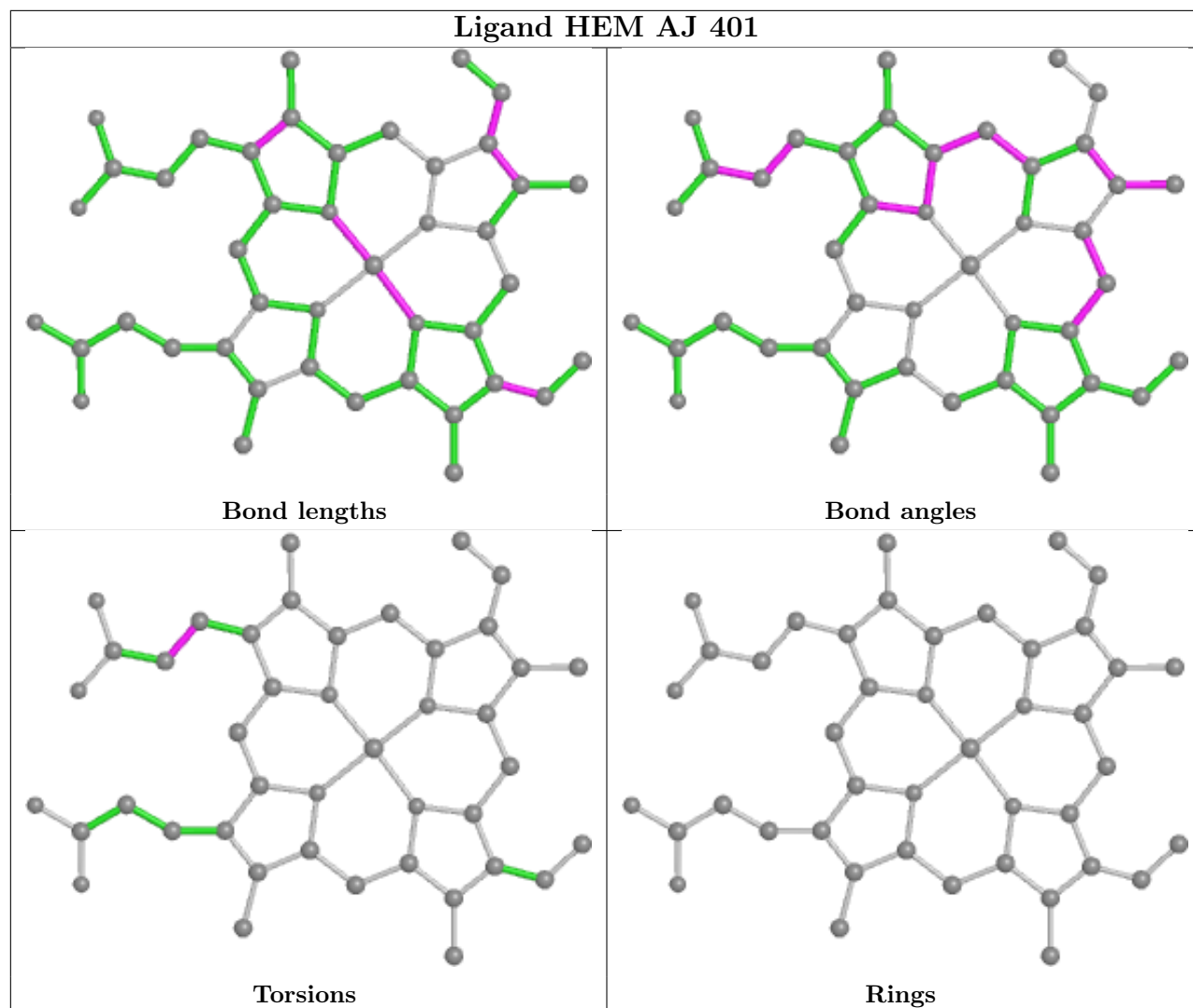


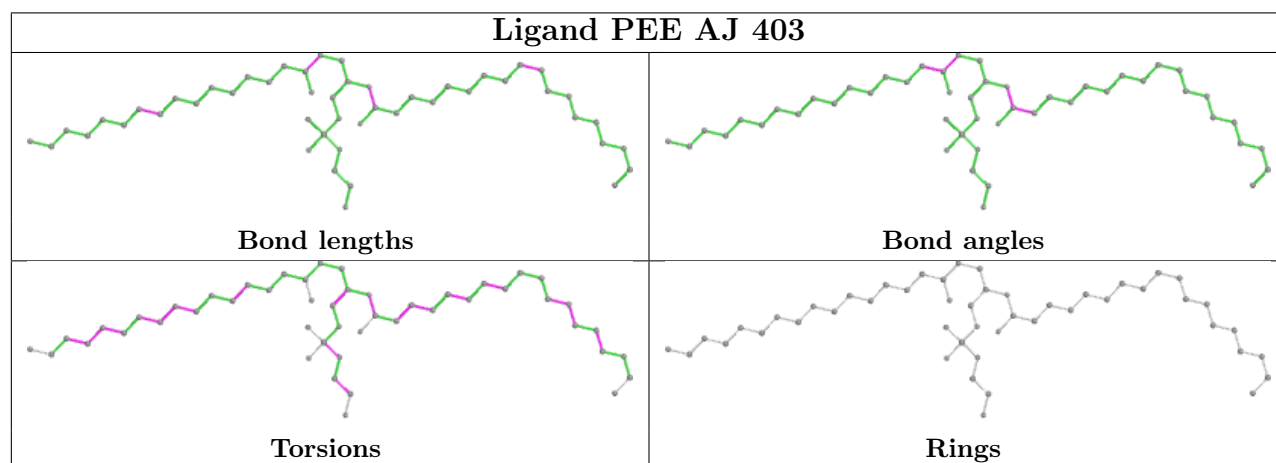
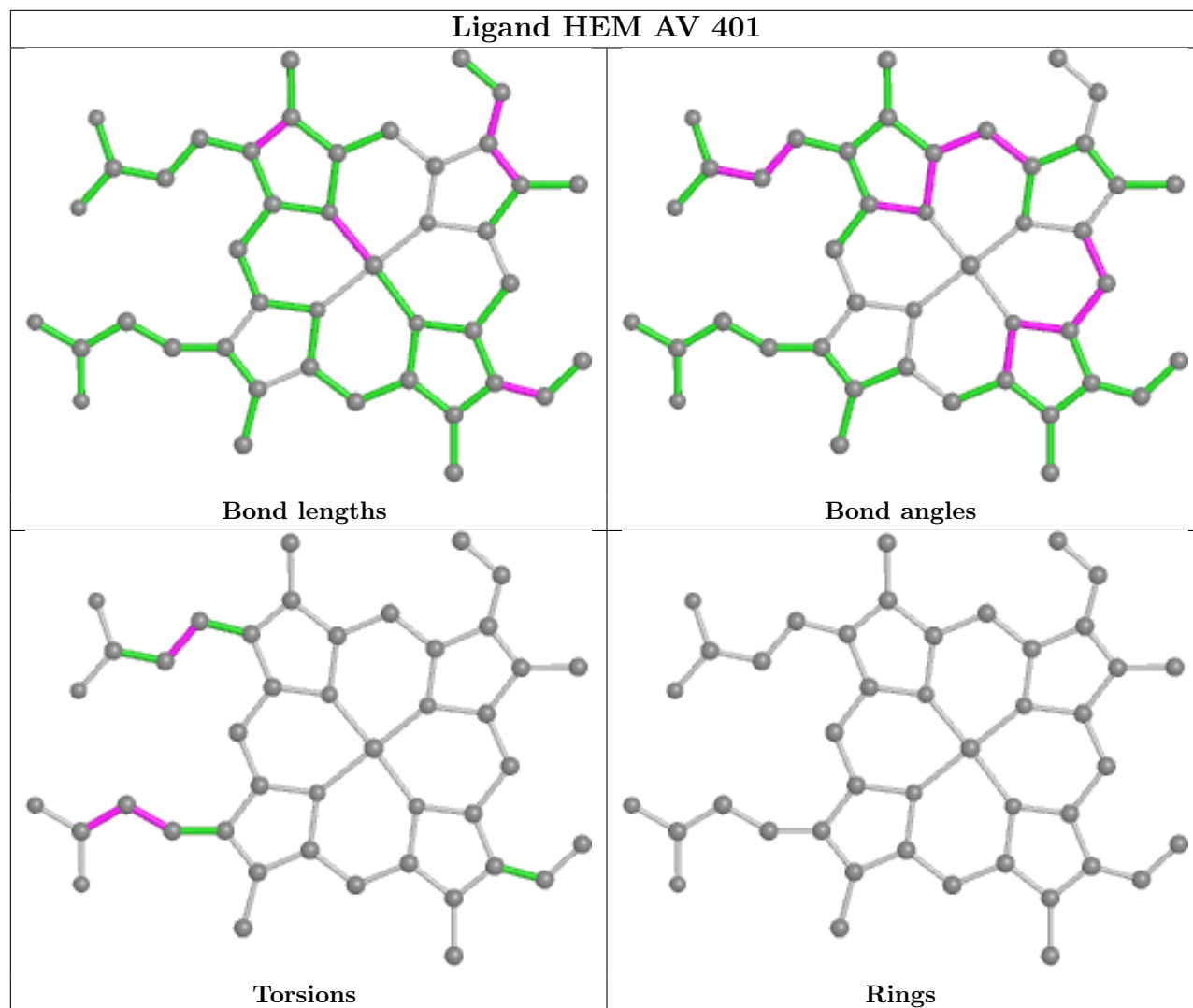


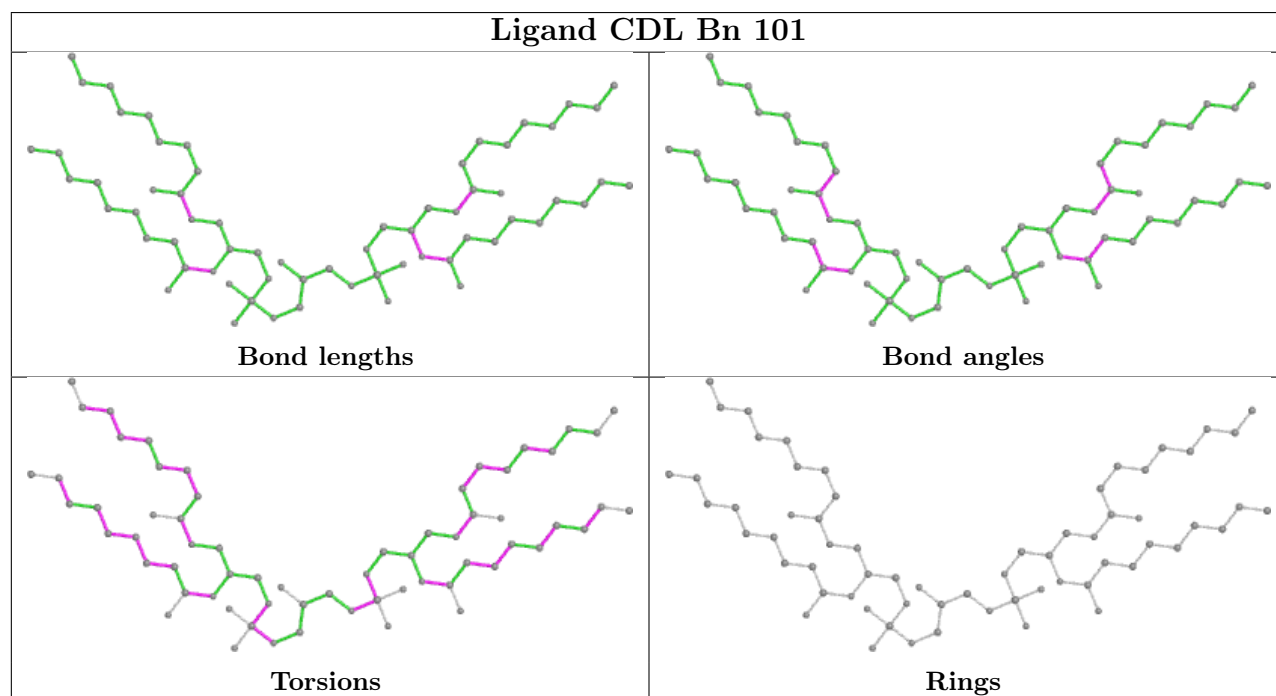
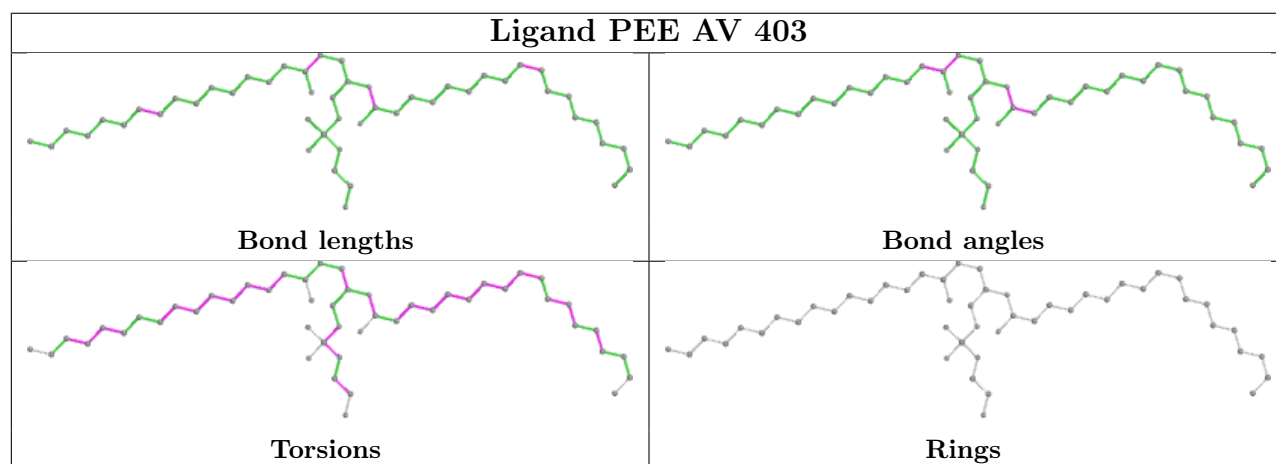
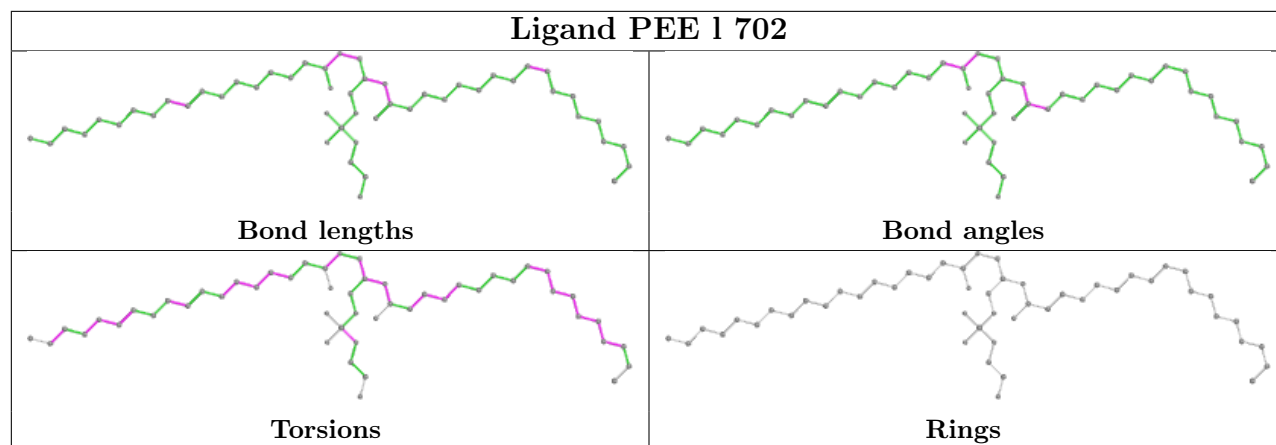


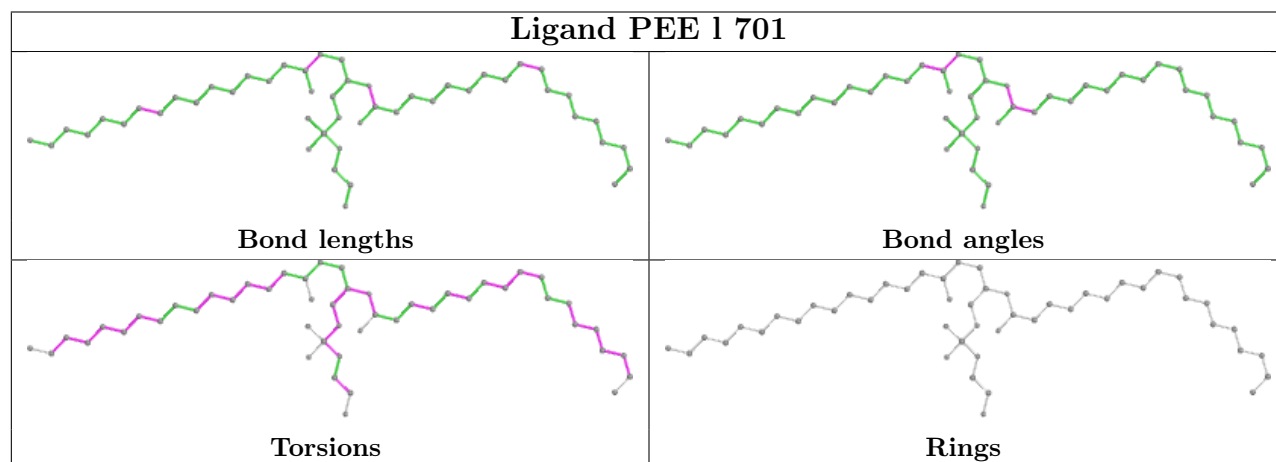
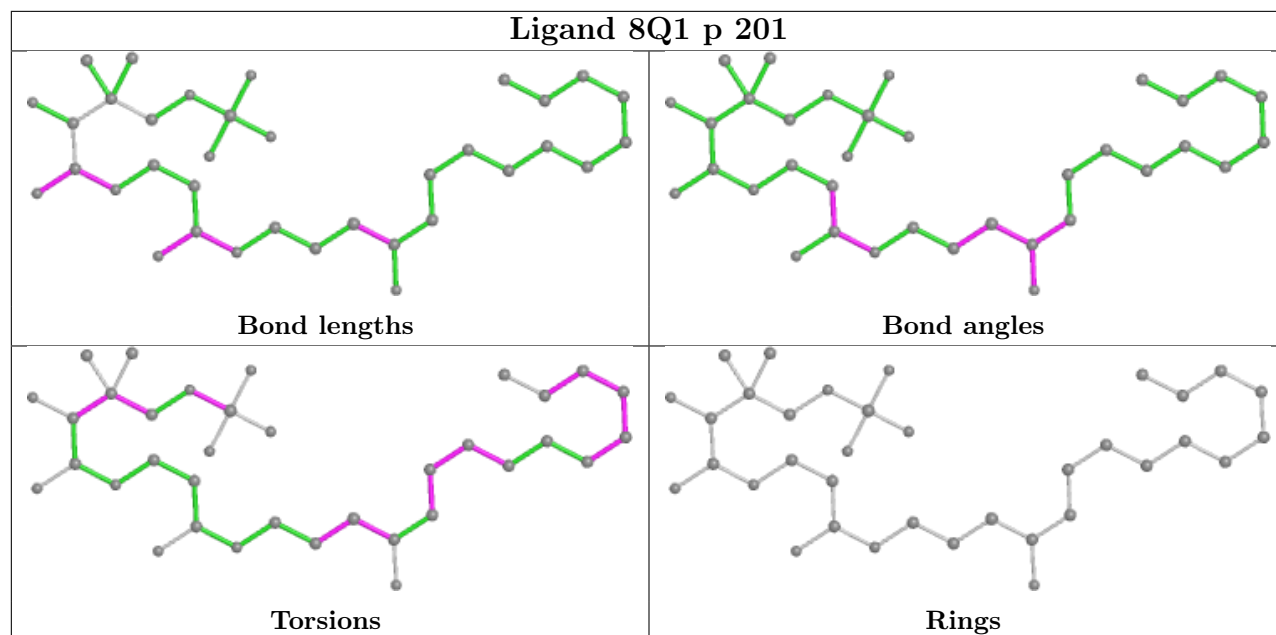


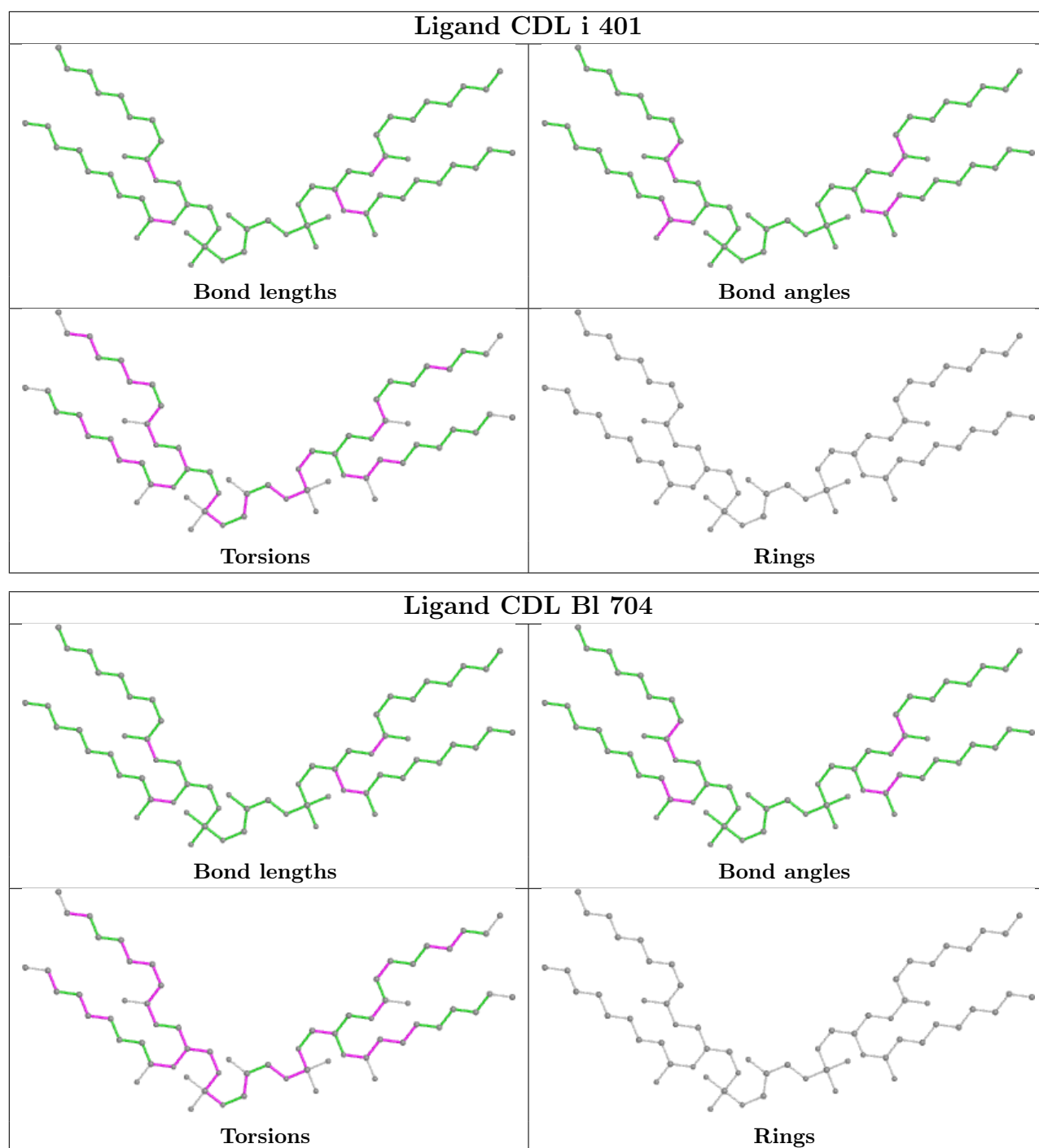


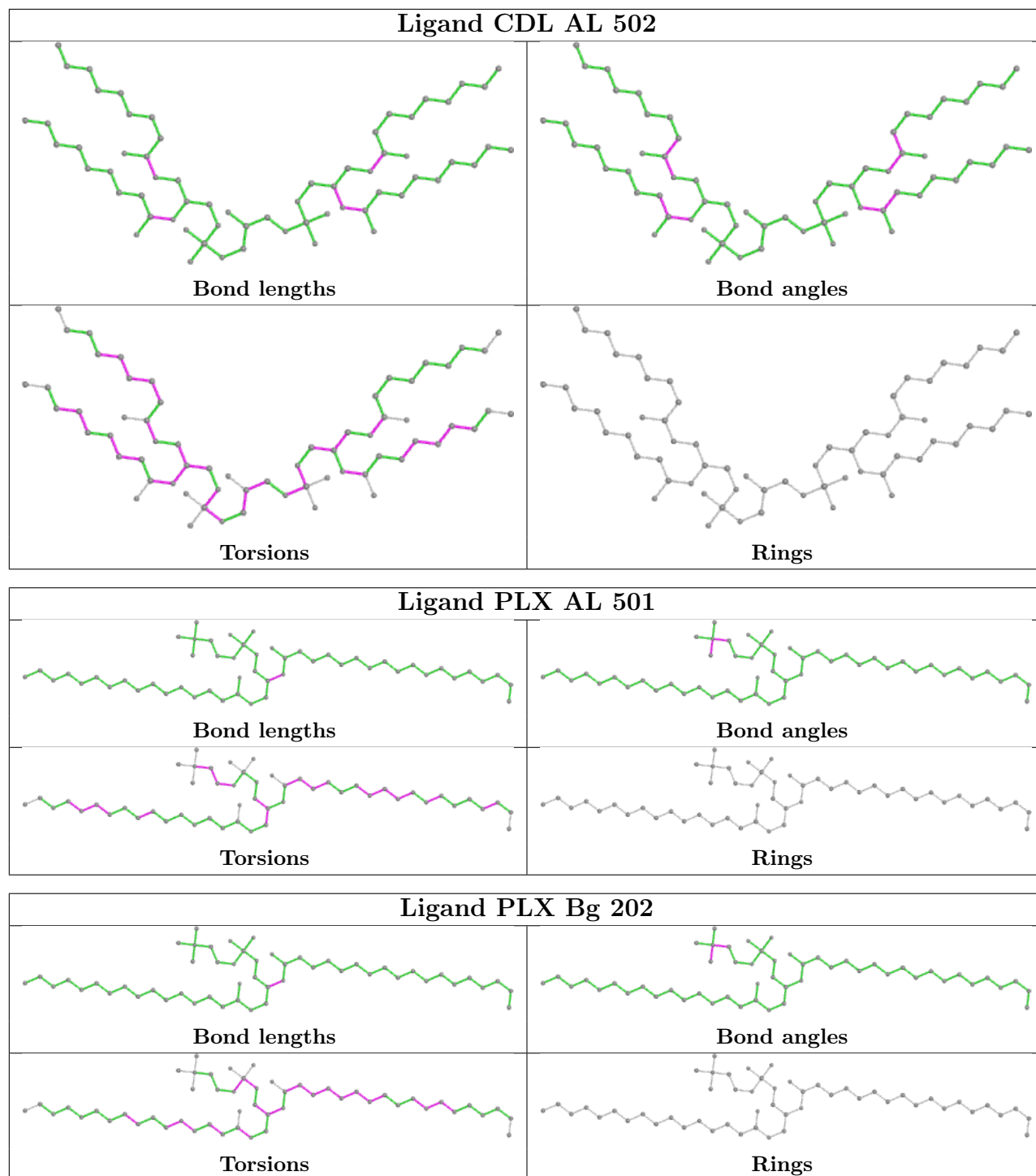


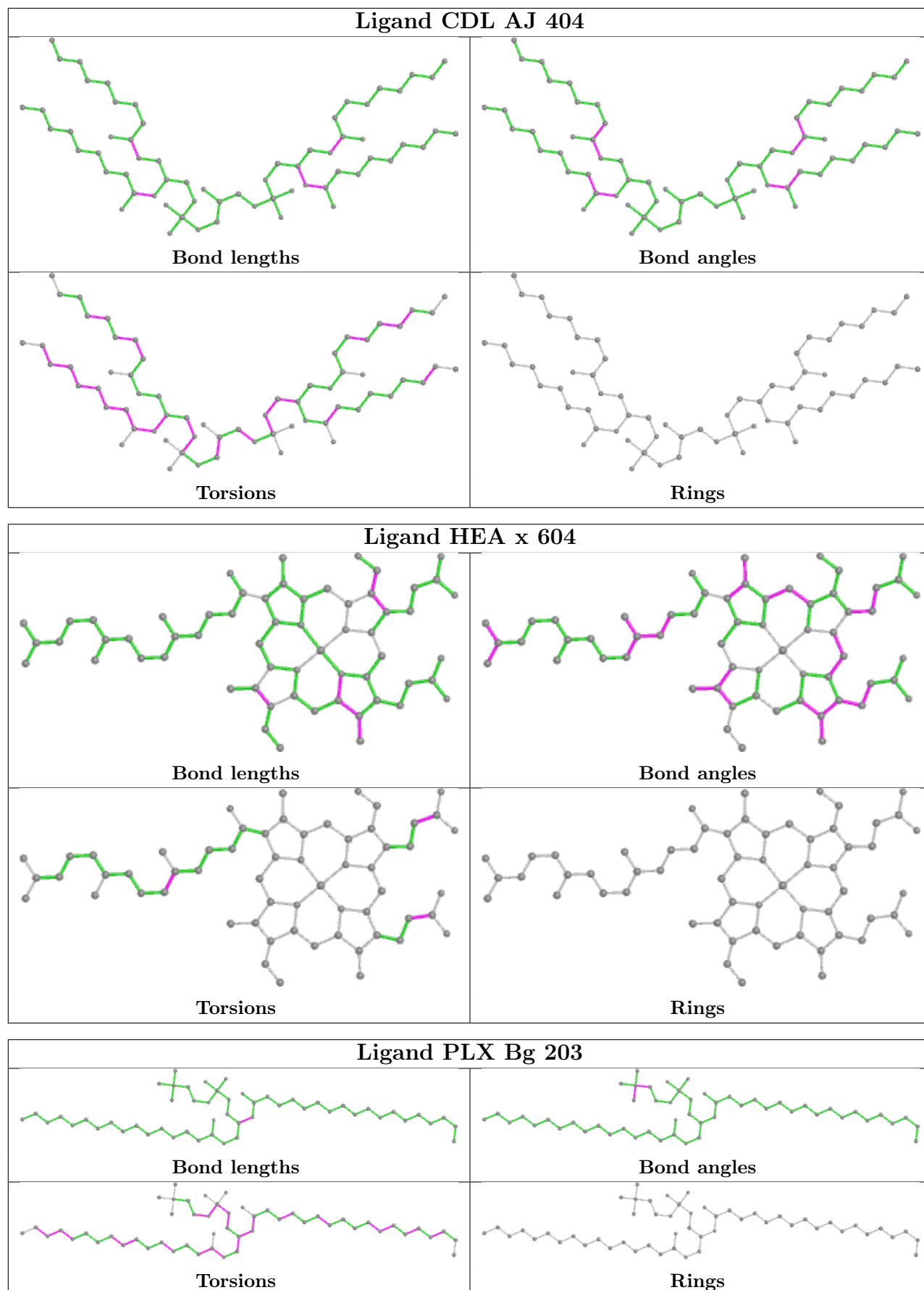


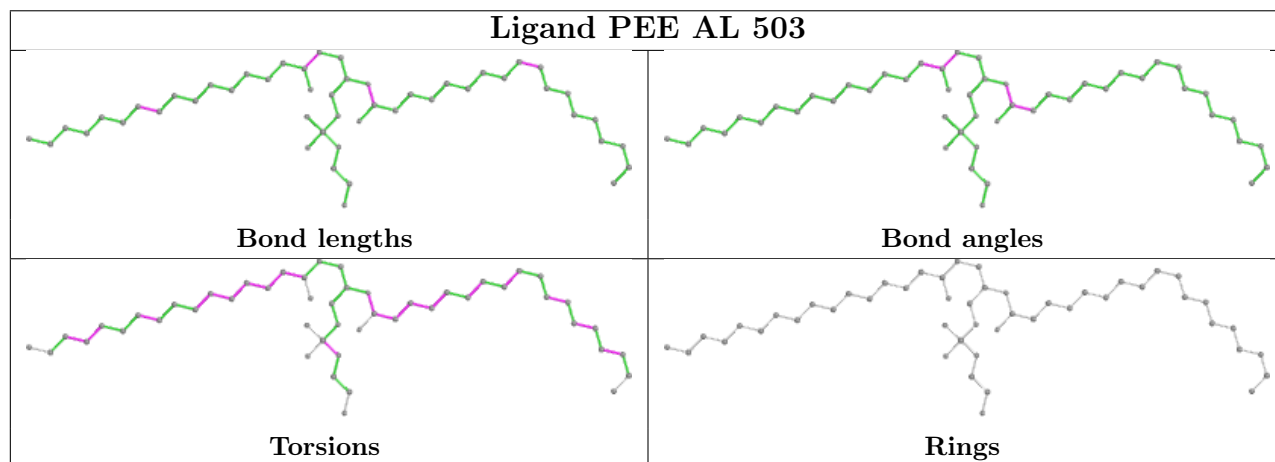
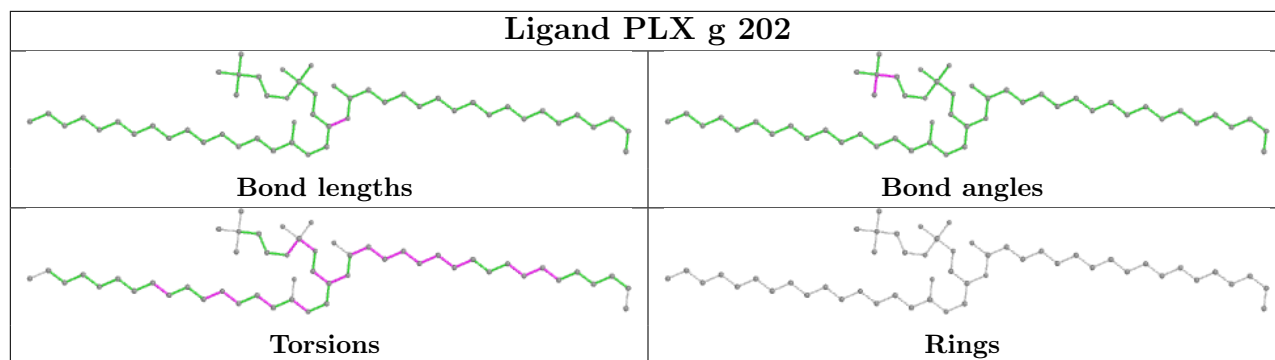




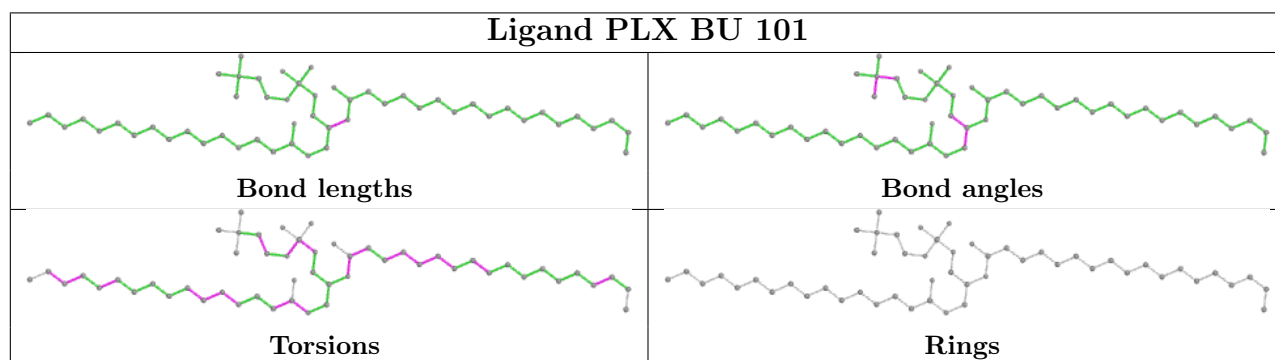
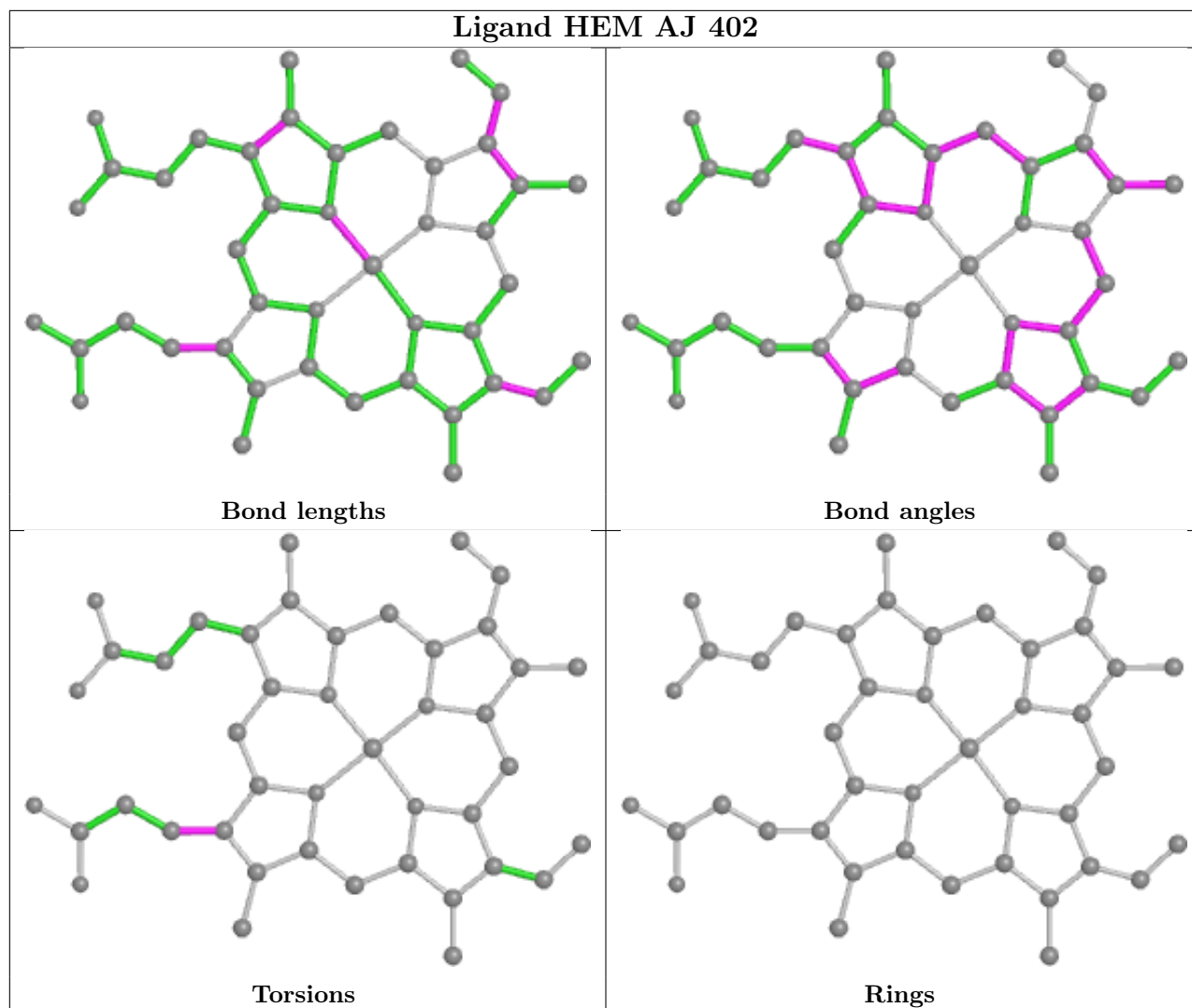


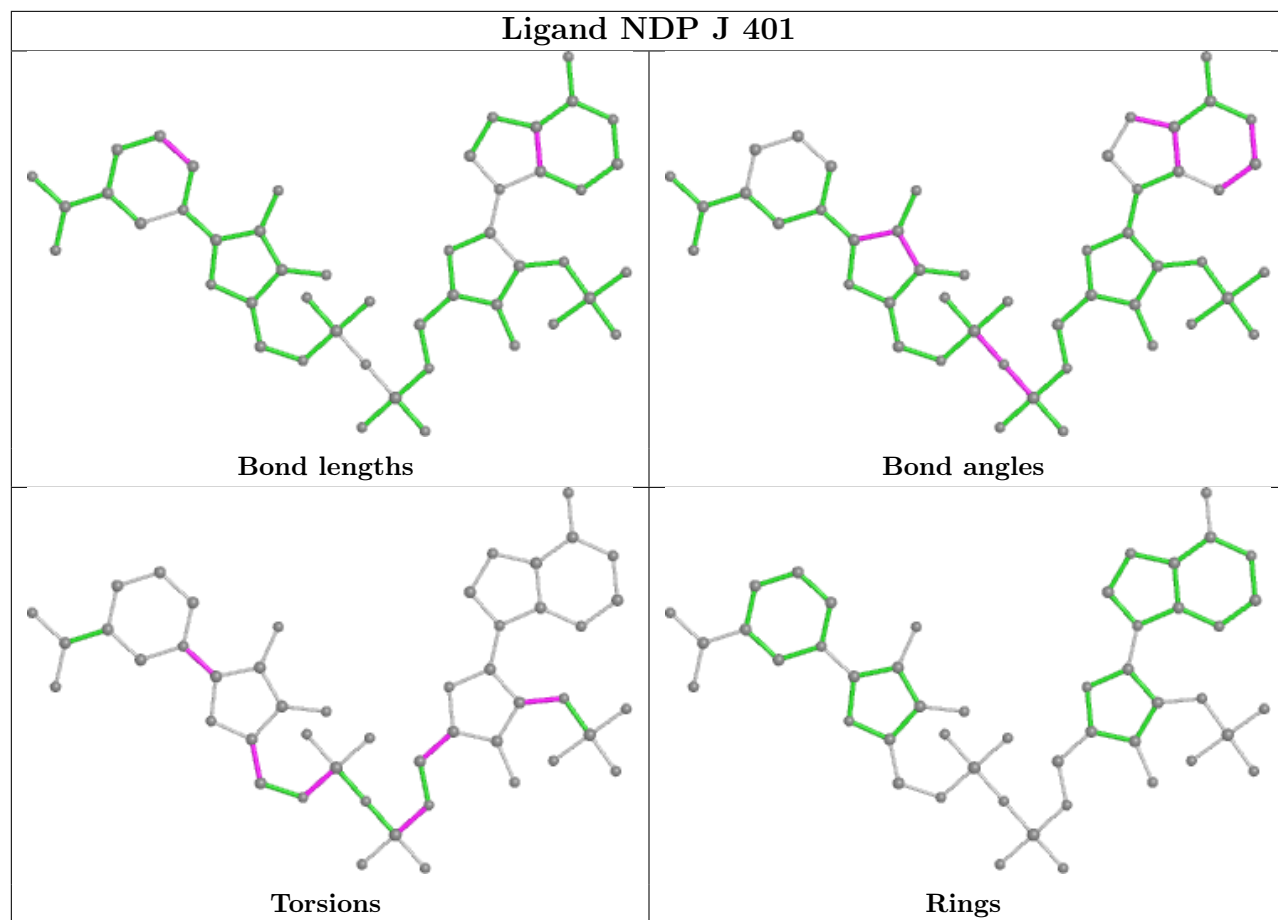


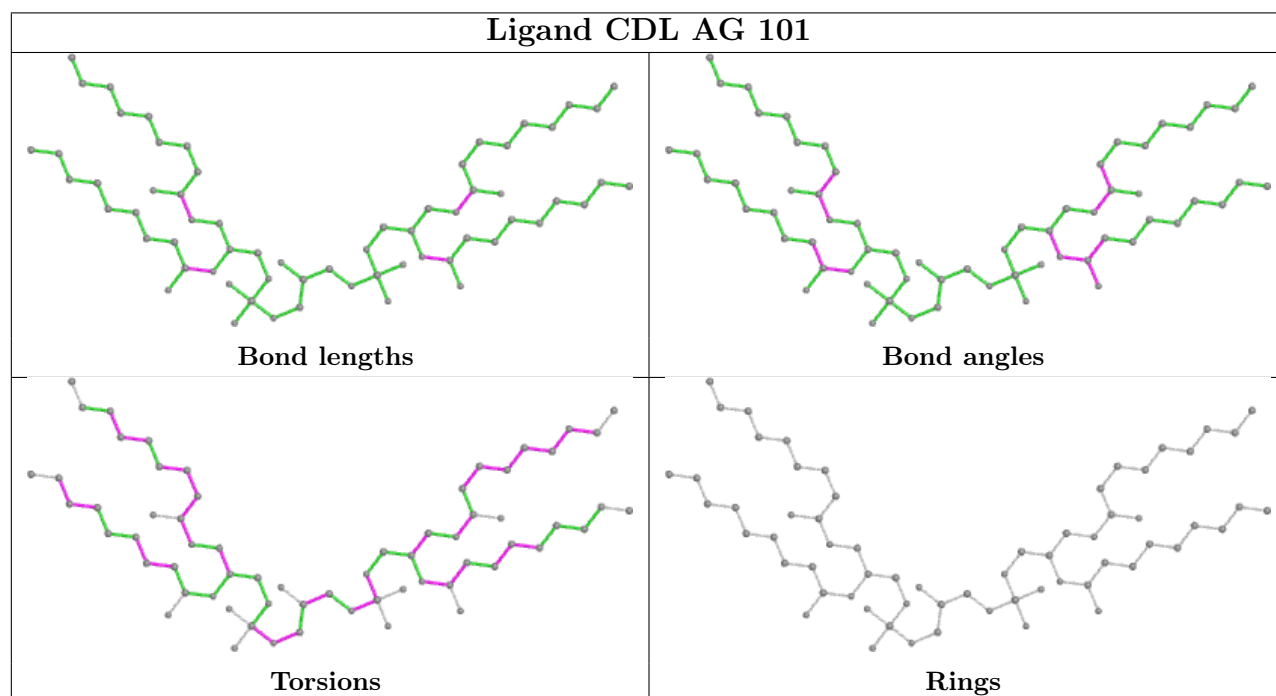
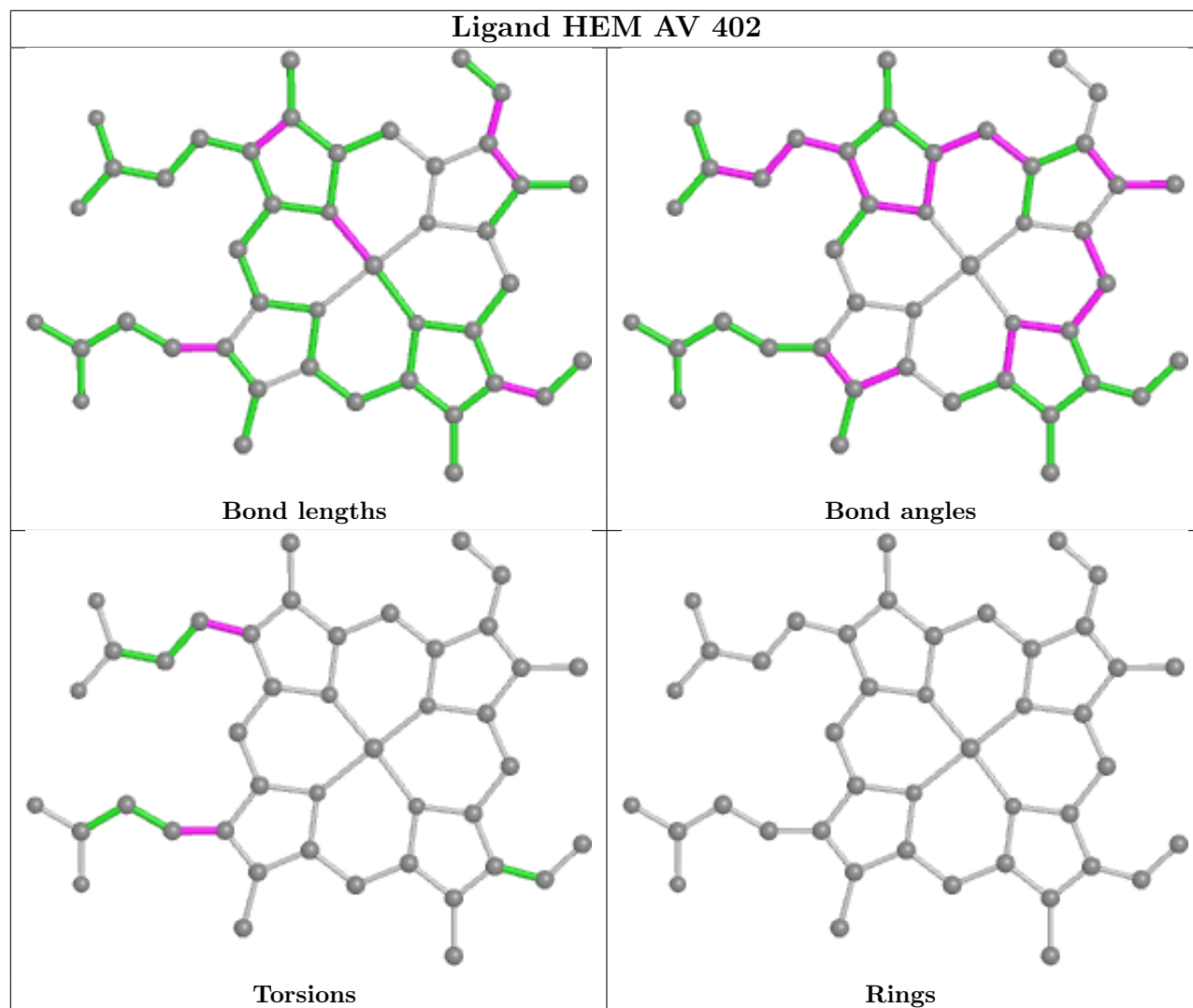


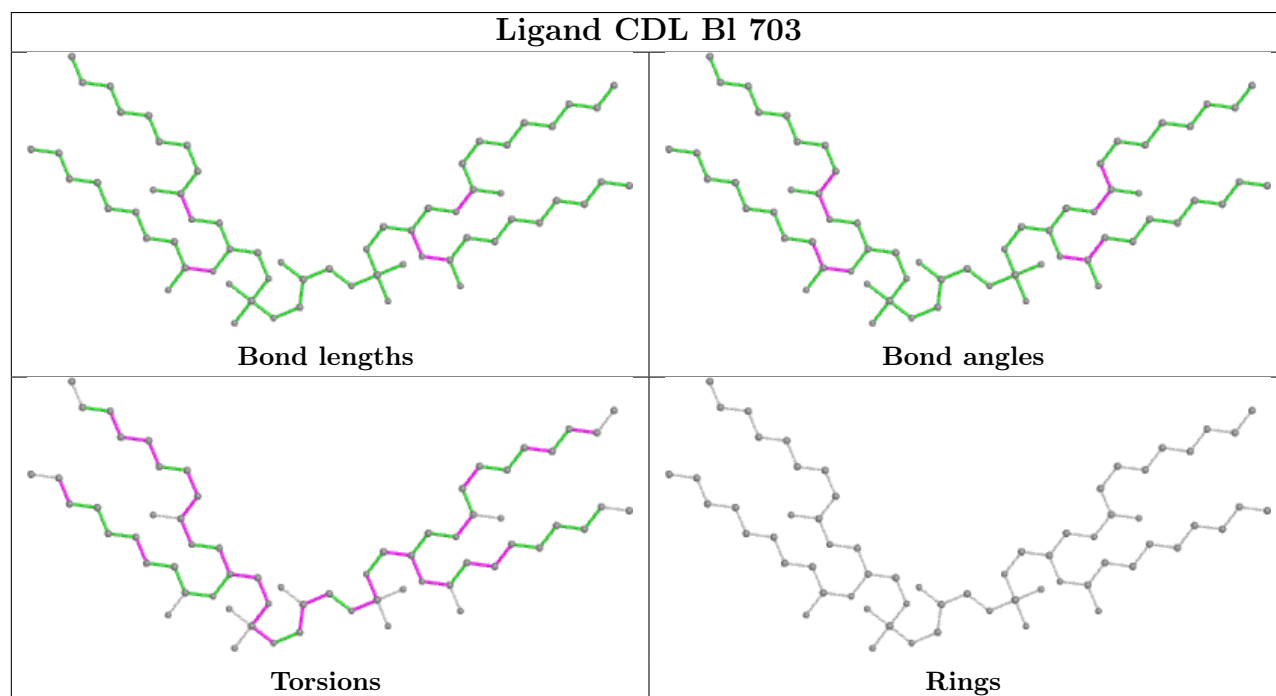
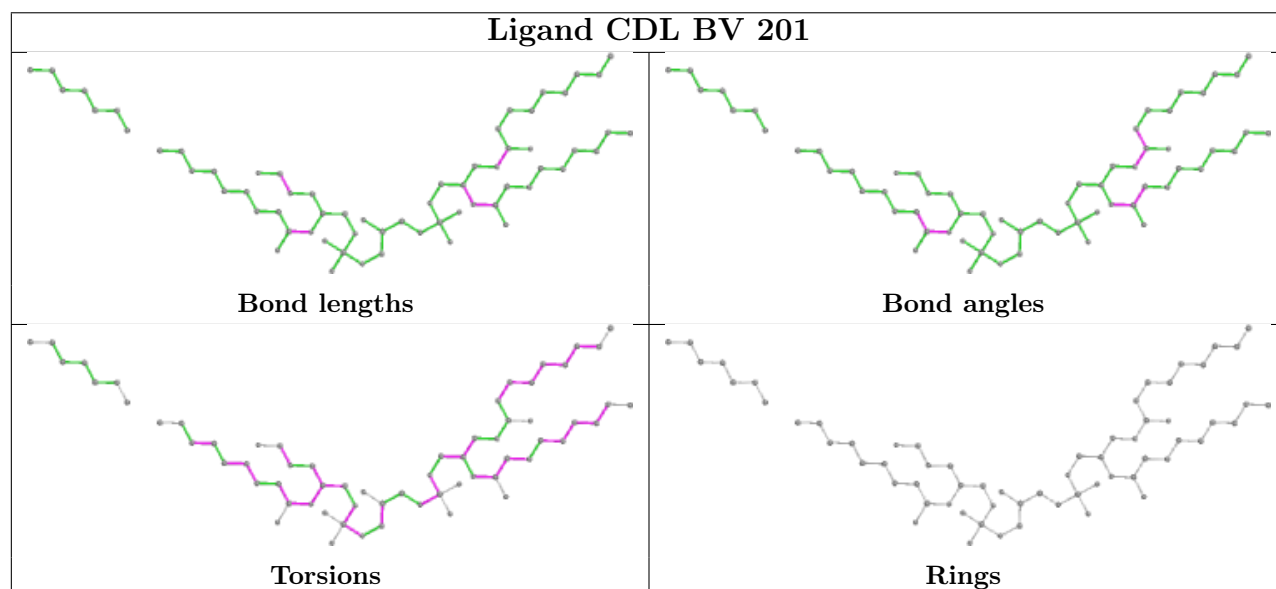
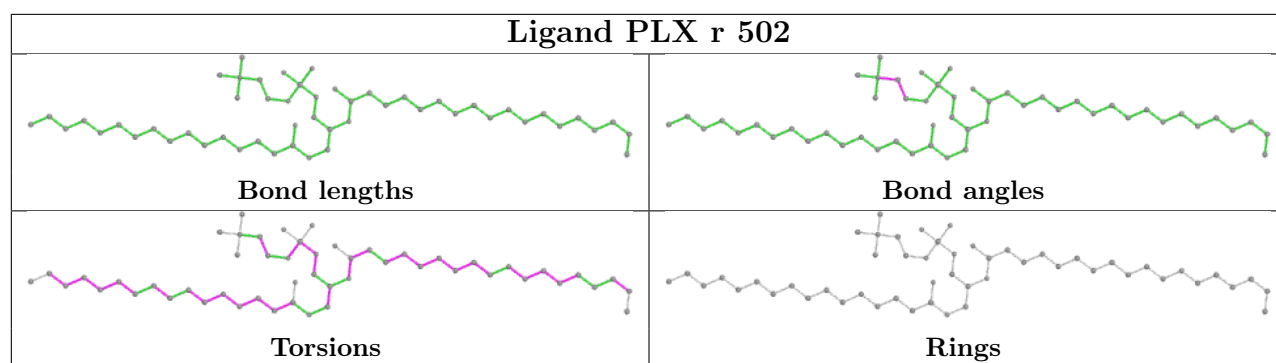


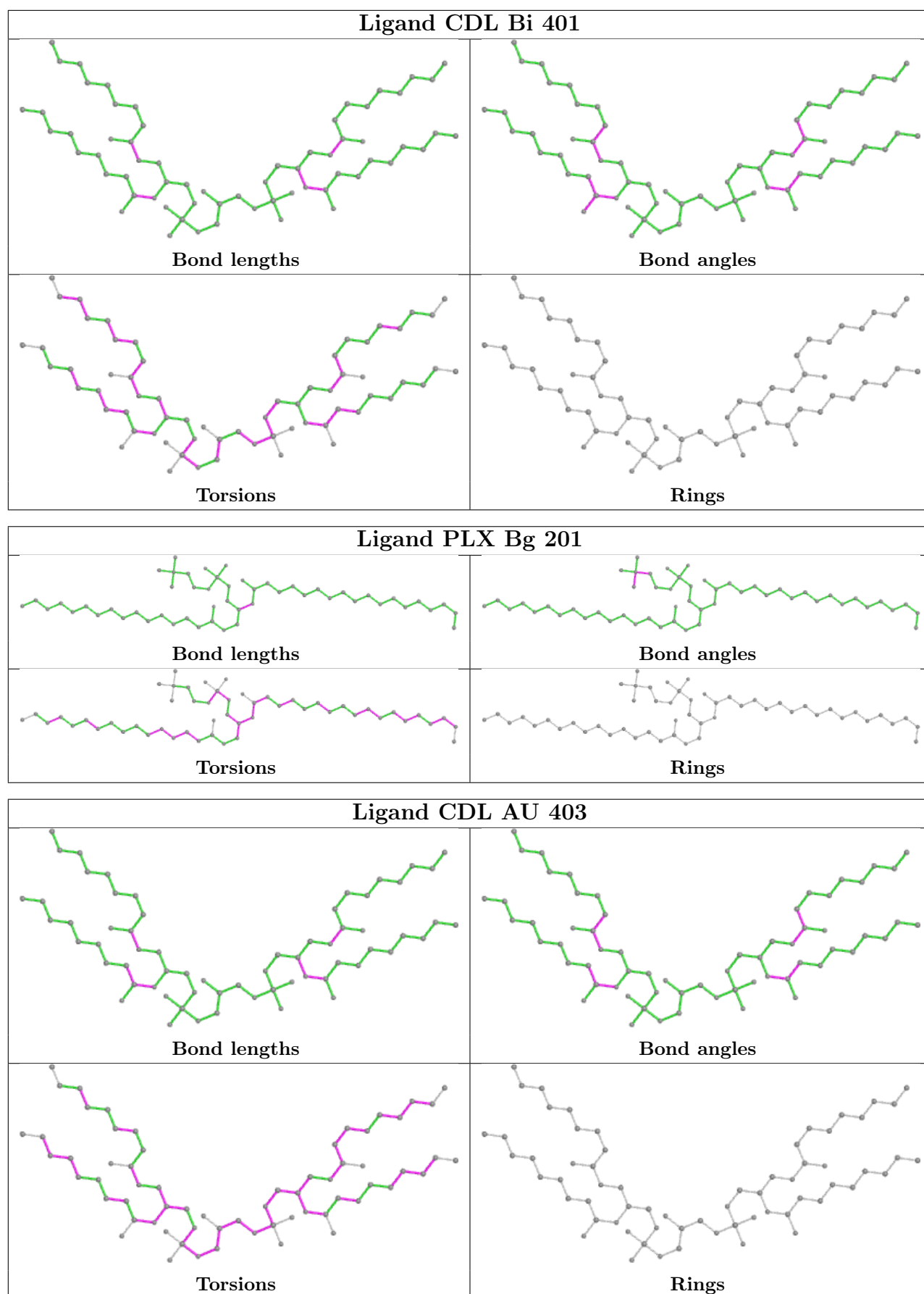


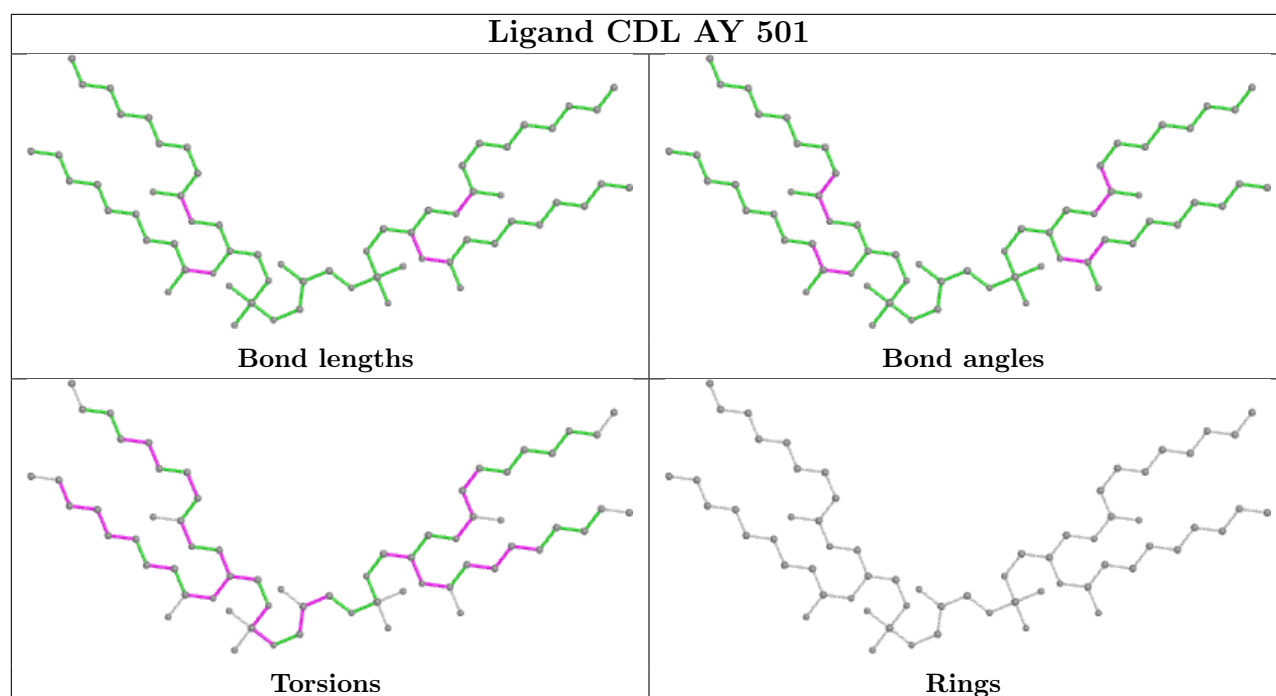












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

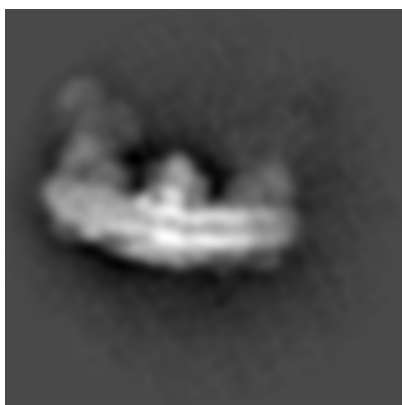
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6776. These allow visual inspection of the internal detail of the map and identification of artifacts.

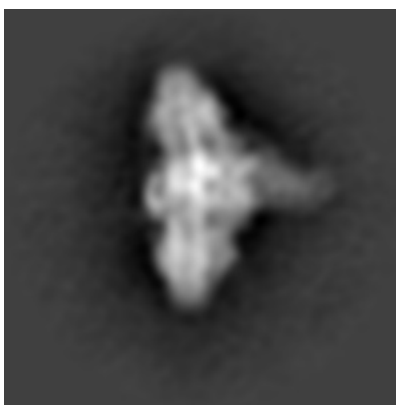
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

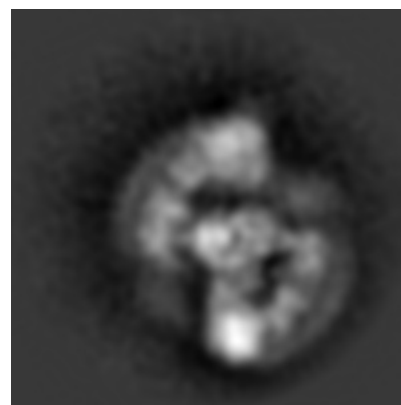
#### 6.1.1 Primary map



X



Y



Z

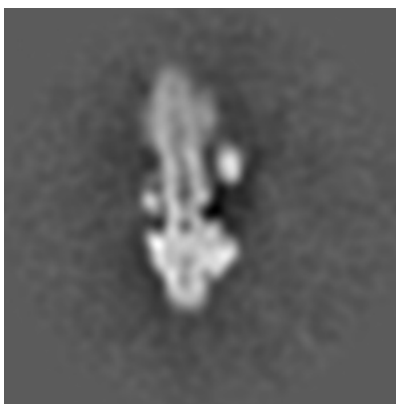
The images above show the map projected in three orthogonal directions.

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

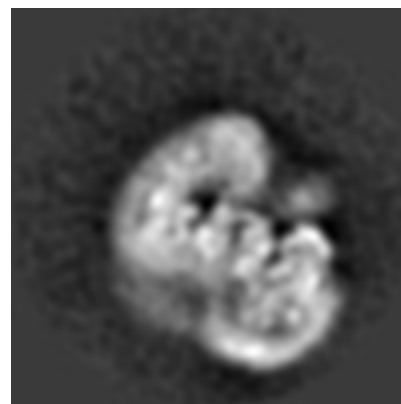
#### 6.2.1 Primary map



X Index: 240



Y Index: 240

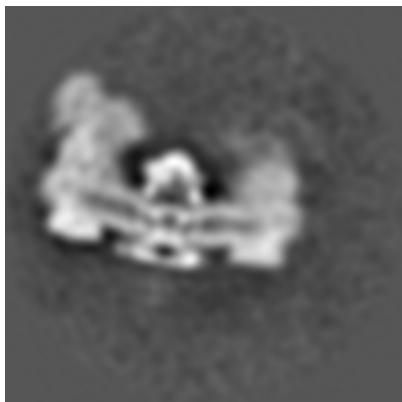


Z Index: 240

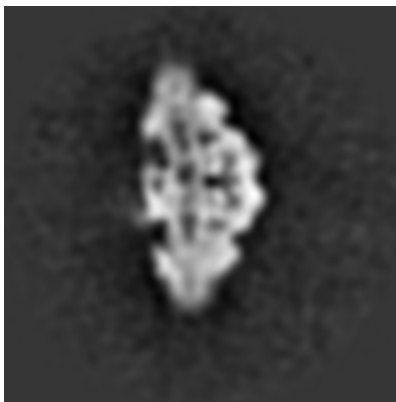
The images above show central slices of the map in three orthogonal directions.

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

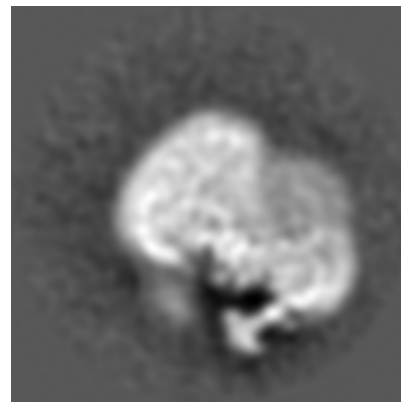
### 6.3.1 Primary map



X Index: 266



Y Index: 204

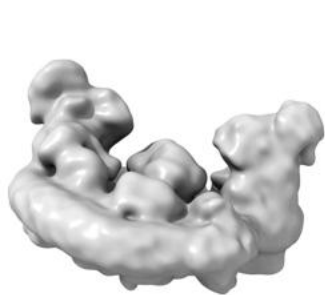


Z Index: 202

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

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

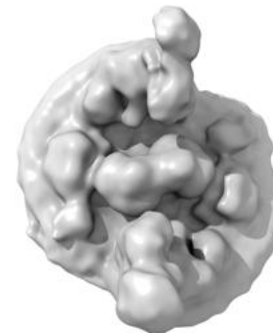
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0056. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



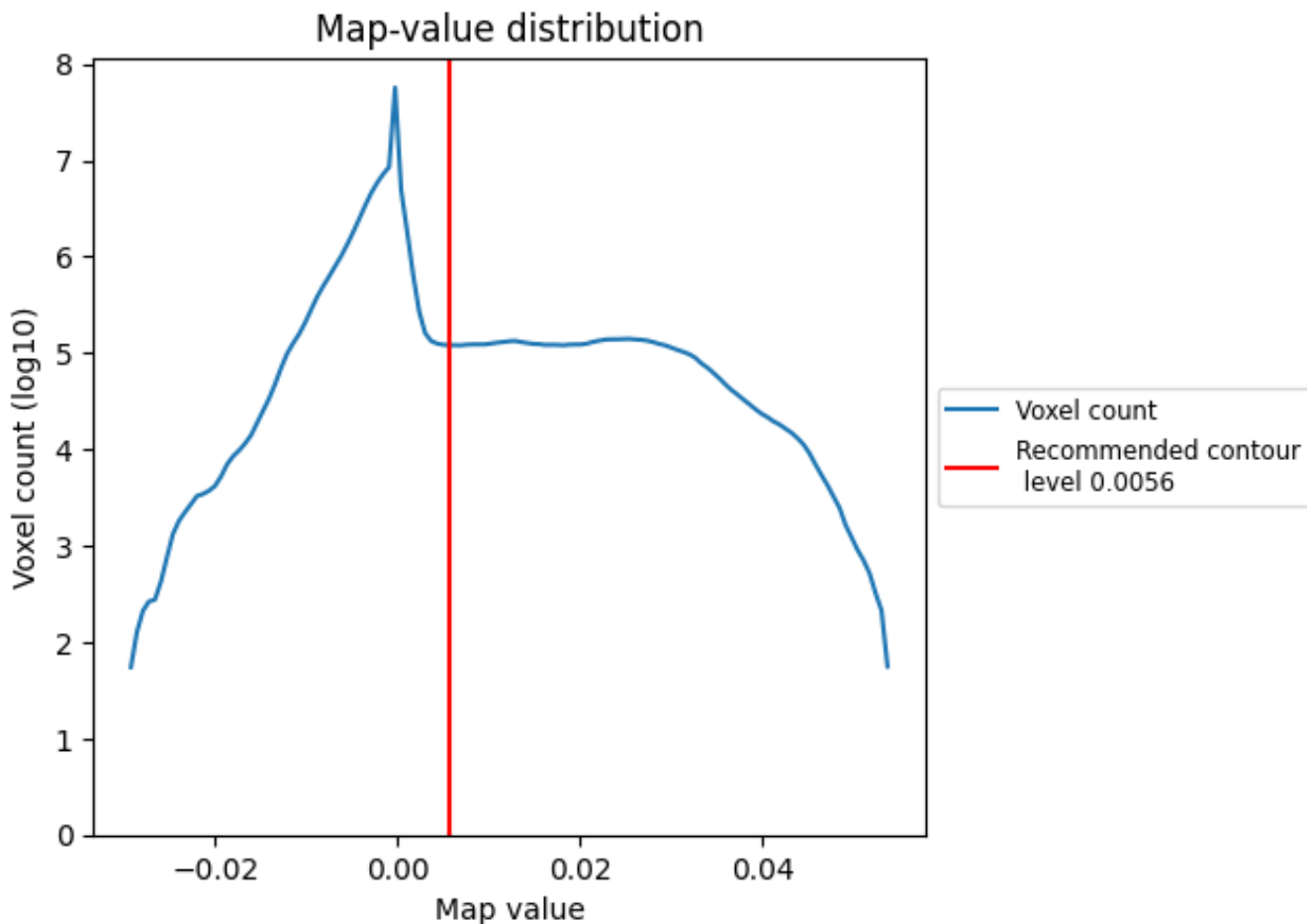
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

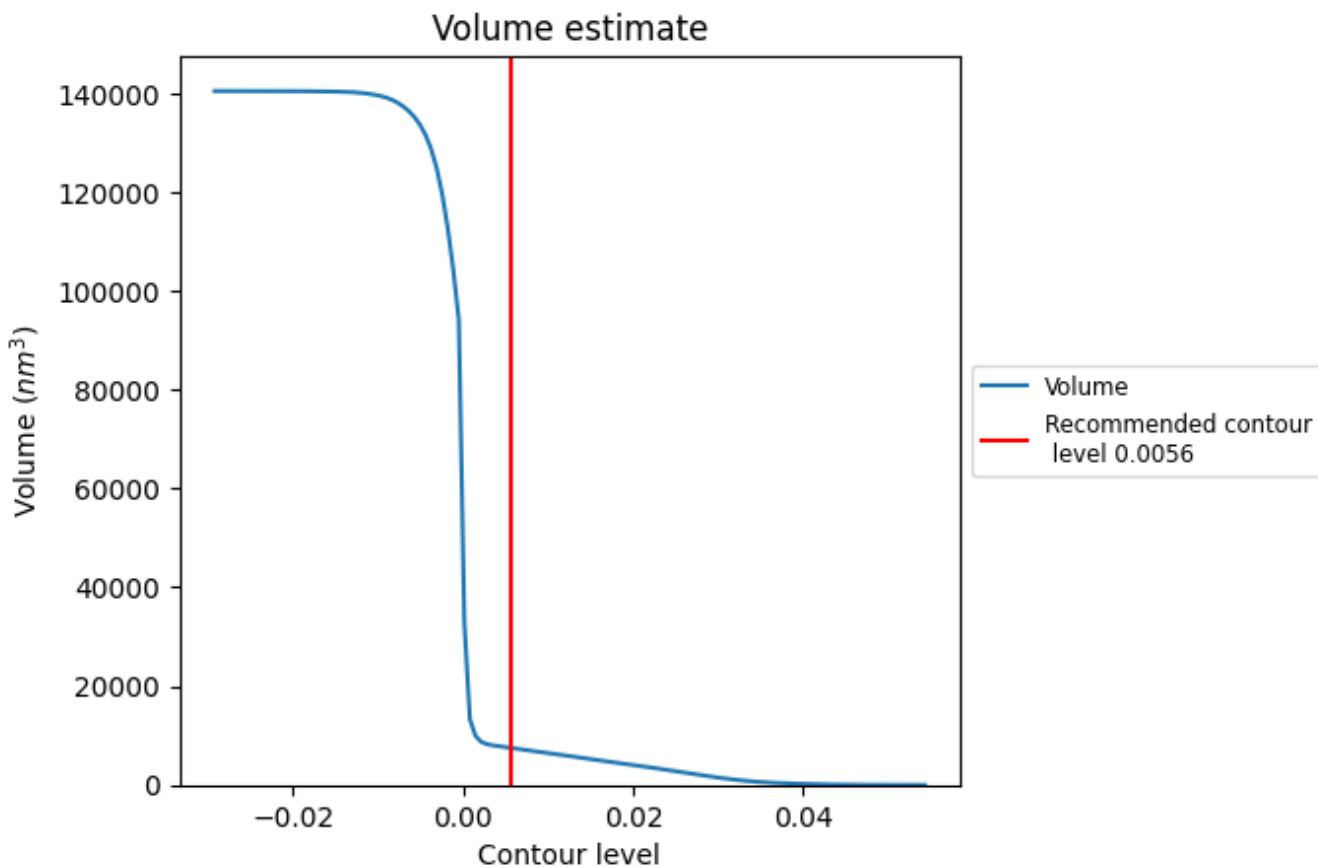
This section contains the results of statistical analysis of the map.

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



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

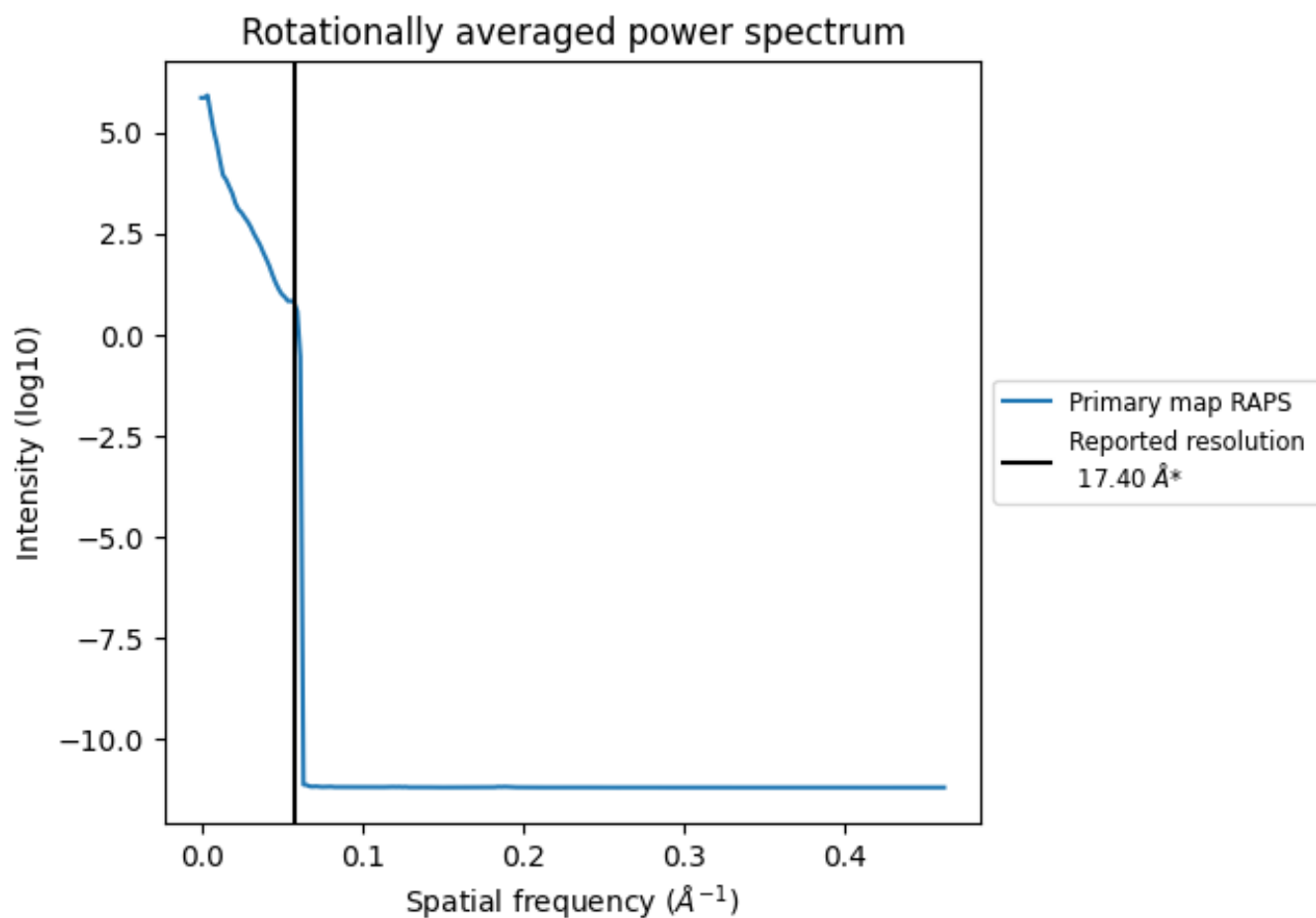
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is  $7506 \text{ nm}^3$ ; this corresponds to an approximate mass of 6780 kDa.

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

### 7.3 Rotationally averaged power spectrum [i](#)



\*Reported resolution corresponds to spatial frequency of 0.057 Å<sup>-1</sup>

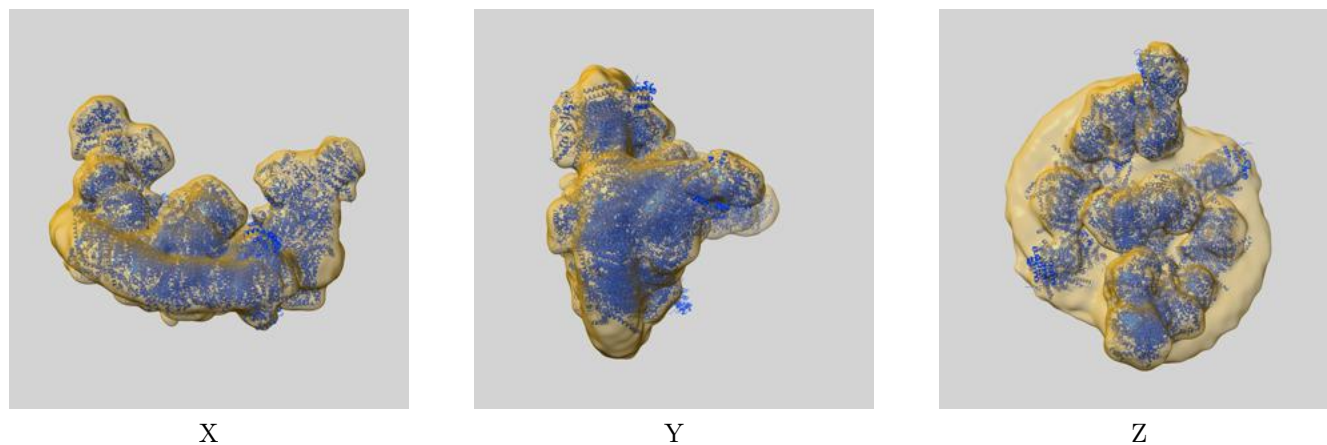
## 8 Fourier-Shell correlation

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

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

This section contains information regarding the fit between EMDB map EMD-6776 and PDB model 5XTI. Per-residue inclusion information can be found in section 3 on page 34.

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

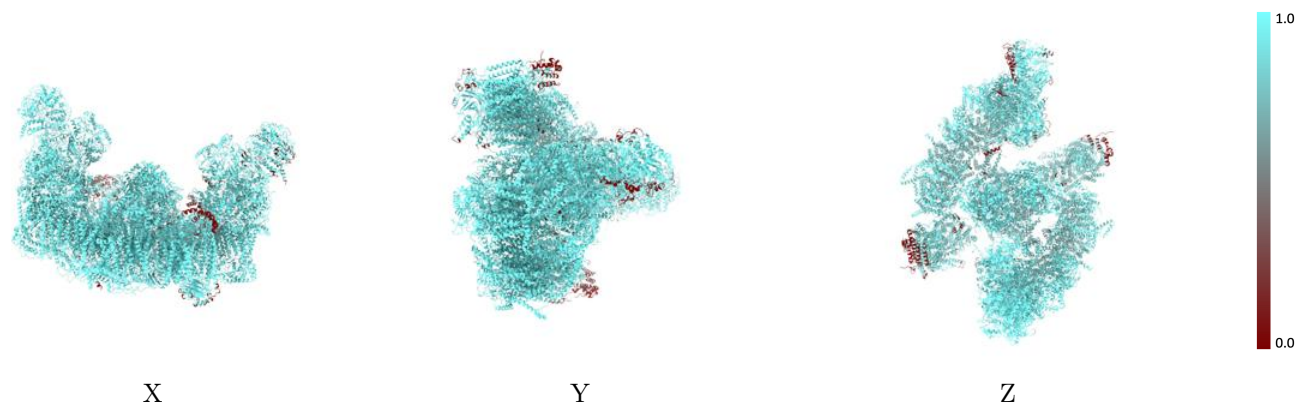


The images above show the 3D surface view of the map at the recommended contour level 0.0056 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

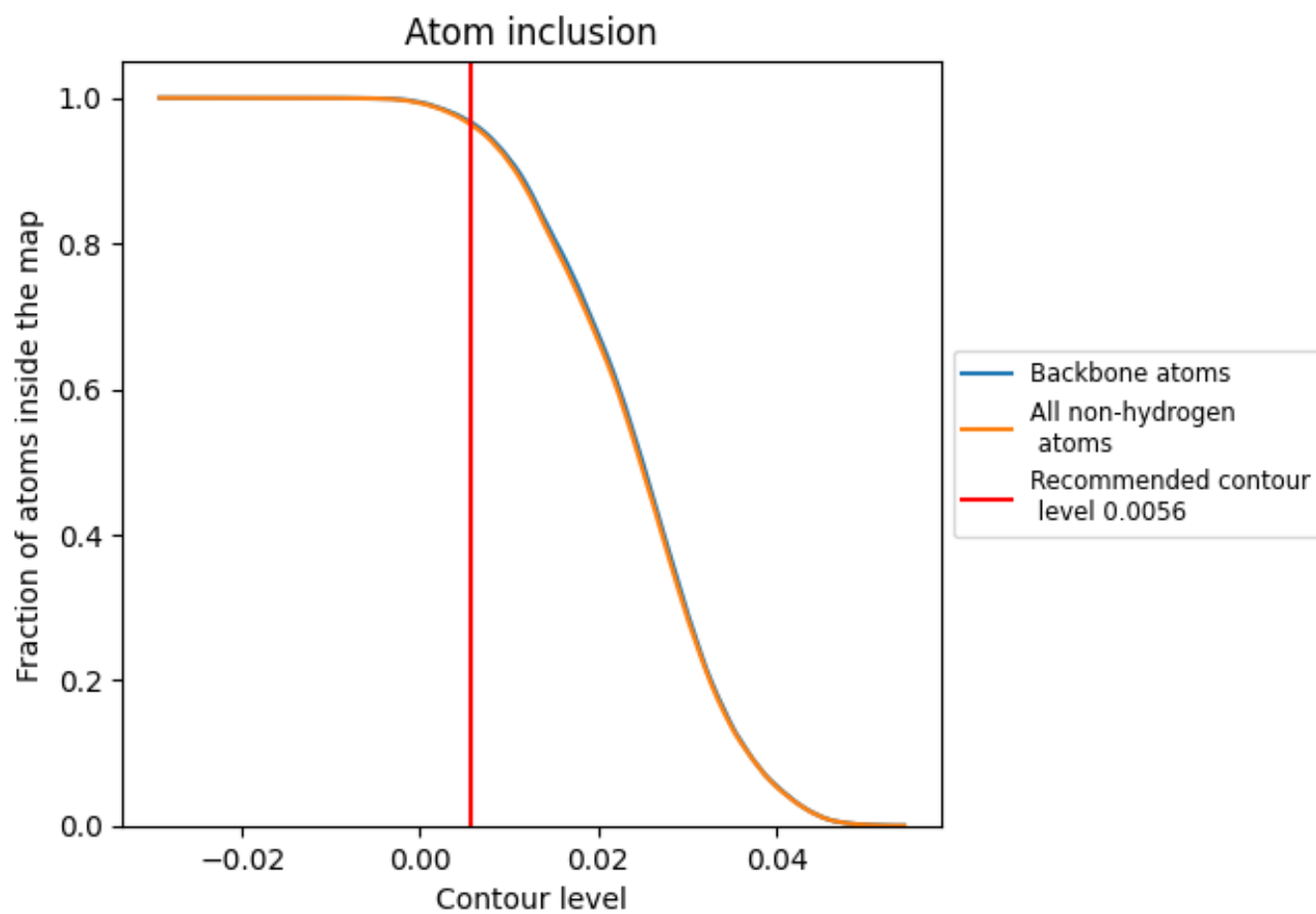
This section was not generated.

## 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 (0.0056).

## 9.4 Atom inclusion [i](#)






































At the recommended contour level, 97% of all backbone atoms, 96% 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 (0.0056) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	 0.9643
0	 0.4386
1	 0.1492
2	 0.8345
3	 0.8147
4	 0.8663
5	 0.4741
6	 0.9607
7	 0.5867
8	 1.0000
9	 0.8976
A	 0.7546
AA	 0.9863
AB	 1.0000
AC	 0.9946
AD	 0.9659
AE	 0.9982
AF	 0.9831
AG	 0.9937
AH	 0.9956
AJ	 0.9988
AK	 0.9994
AL	 0.9958
AN	 0.9949
AO	 1.0000
AP	 0.9900
AQ	 0.9855
AR	 1.0000
AS	 0.9461
AT	 1.0000
AU	 0.9955
AV	 0.9984
AW	 0.9990
AY	 0.9983
B	 1.0000













































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Chain	Atom inclusion
B0	 0.7253
B1	 0.4009
B2	 0.9037
B3	 0.8591
B4	 0.8977
B5	 0.7103
B6	 0.8984
B7	 0.9280
B8	 0.9921
B9	 0.9367
BA	 0.9942
BB	 1.0000
BC	 1.0000
BE	 0.9466
BF	 0.9969
BG	 0.7102
BH	 0.9989
BI	 0.9933
BJ	 0.9800
BK	 1.0000
BL	 0.9862
BM	 0.9856
BN	 0.9845
BO	 0.9963
BP	 0.9887
BQ	 0.9893
BS	 1.0000
BT	 0.9779
BU	 0.9985
BV	 0.9992
BW	 0.9948
BX	 0.9882
BY	 1.0000
BZ	 1.0000
Ba	 0.9974
Bb	 1.0000
Bc	 0.9750
Bd	 0.9715
Be	 0.9848
Bf	 0.9975
Bg	 0.9947
Bh	 0.9976





















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Chain	Atom inclusion
Bi	 1.0000
Bj	 1.0000
Bk	 1.0000
Bl	 0.9998
Bm	 1.0000
Bn	 0.9905
Bo	 0.9893
Bp	 0.9898
Br	 0.9986
Bs	 1.0000
Bu	 0.9934
Bv	 0.9876
Bw	 0.9963
Bx	 0.9998
By	 0.9772
Bz	 1.0000
C	 1.0000
E	 0.9507
F	 0.9708
G	 0.4850
H	 0.9989
I	 0.9866
J	 0.9725
K	 0.9776
L	 0.9841
M	 0.9238
N	 0.9742
O	 0.8668
P	 0.9881
Q	 0.9923
S	 1.0000
T	 0.9061
U	 1.0000
V	 0.9991
W	 0.9991
X	 1.0000
Y	 1.0000
Z	 1.0000
a	 0.9965
b	 1.0000
c	 0.9758
d	 0.9876

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Chain	Atom inclusion
e	 1.0000
f	 1.0000
g	 0.9973
h	 1.0000
i	 1.0000
j	 1.0000
k	 1.0000
l	 1.0000
m	 1.0000
n	 0.9866
o	 0.9873
p	 0.9946
r	 0.9989
s	 1.0000
u	 0.9971
v	 0.9853
w	 0.9992
x	 0.9985
y	 0.8653
z	 1.0000