



Full wwPDB EM Validation Report ⓘ

Nov 23, 2022 – 05:44 PM JST

PDB ID : 7VB9
EMDB ID : EMD-31875
Title : Rba sphaeroides PufY-KO RC-LH1 dimer type-2
Authors : Bracun, L.; Yamagata, A.; Liu, L.N.; Shirouzu, M.
Deposited on : 2021-08-30
Resolution : 3.45 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

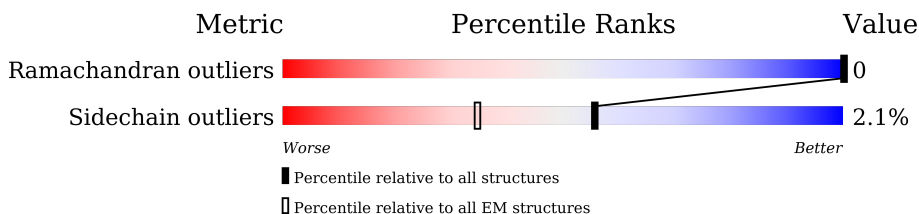
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (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 3.45 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 ≥ 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	L	282	
1	l	282	
2	M	308	
2	m	308	
3	H	260	
3	h	260	
4	5	58	
4	6	58	
4	7	58	

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Mol	Chain	Length	Quality of chain
4	9	58	9% 91% 7%
4	A	58	19% 93% 7%
4	D	58	29% 91% 7%
4	F	58	43% 91% 7%
4	I	58	60% 91% 7%
4	K	58	74% 72% 24%
4	O	58	74% 71% 26%
4	Q	58	91% 7%
4	a	58	93% 7%
4	d	58	90% 7%
4	f	58	9% 91% 7%
4	i	58	21% 91% 7%
4	k	58	34% 91% 7%
4	o	58	31% 91% 7%
4	q	58	19% 91% 7%
4	s	58	16% 90% 7%
4	u	58	24% 91% 7%
4	w	58	19% 71% 26%
4	y	58	57% 69% 28%
5	0	49	14% 88% 10%
5	4	49	73% 73% 27%
5	8	49	14% 88% 10%
5	B	49	27% 88% 10%
5	E	49	27% 86% 12%
5	G	49	51% 86% 10%

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Mol	Chain	Length	Quality of chain
5	J	49	67% 84% 12%
5	N	49	84% 80% 16%
5	aa	49	10% 88% 10%
5	ab	49	88% 10%
5	b	49	88% 10%
5	e	49	86% 12%
5	g	49	18% 88% 10%
5	j	49	24% 86% 12%
5	n	49	18% 76% 22%
5	p	49	22% 78% 20%
5	r	49	27% 86% 12%
5	t	49	16% 84% 14%
5	v	49	16% 76% 24%
5	x	49	57% 84% 14%
5	z	49	73% 76% 22%
6	C	82	26% 76% 22%
6	c	82	20% 79% 17%

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
11	SPO	0	101	-	X	-	-
11	SPO	0	103	-	X	-	-
11	SPO	9	101	-	X	-	-
11	SPO	9	103	-	X	-	-
11	SPO	C	1203	-	X	-	-
11	SPO	D	102	-	X	-	-
11	SPO	E	102	-	X	-	-
11	SPO	F	102	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	SPO	F	103	-	X	-	-
11	SPO	G	102	-	X	-	-
11	SPO	G	103	-	X	-	-
11	SPO	J	102	-	X	-	-
11	SPO	M	404	-	X	-	-
11	SPO	Q	603	-	X	-	-
11	SPO	aa	101	-	X	-	-
11	SPO	ab	102	-	X	-	-
11	SPO	b	101	-	X	-	-
11	SPO	b	103	-	X	-	-
11	SPO	d	102	-	X	-	-
11	SPO	d	103	-	X	-	-
11	SPO	e	102	-	X	-	-
11	SPO	f	102	-	X	-	-
11	SPO	g	101	-	X	-	-
11	SPO	i	103	-	X	-	-
11	SPO	j	101	-	X	-	-
11	SPO	m	405	-	X	-	-
11	SPO	n	102	-	X	-	-
11	SPO	o	102	-	X	-	-
11	SPO	p	102	-	X	-	-
11	SPO	p	103	-	X	-	-
11	SPO	q	102	-	X	-	-
11	SPO	s	101	-	X	-	-
11	SPO	t	102	-	X	-	-
11	SPO	u	101	-	X	-	-
11	SPO	v	102	-	X	-	-
11	SPO	w	102	-	X	-	-

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 36474 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 Reaction center protein L chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	L	268	Total	C	N	O	S	0	0
			2132	1440	338	346	8		
1	l	281	Total	C	N	O	S	0	0
			2232	1507	355	362	8		

- Molecule 2 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	M	305	Total	C	N	O	S	0	0
			2431	1623	397	400	11		
2	m	305	Total	C	N	O	S	0	0
			2431	1623	397	400	11		

- Molecule 3 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	H	260	Total	C	N	O	S	0	0
			1972	1264	335	362	11		
3	h	260	Total	C	N	O	S	0	0
			1972	1264	335	362	11		

- Molecule 4 is a protein called Light-harvesting protein B-875 alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	D	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	F	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	I	54	Total	C	N	O	S	0	0
			455	310	73	69	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	K	44	362	244	60	57	1	0	0
4	O	43	351	235	59	56	1	0	0
4	7	46	392	271	60	58	3	0	0
4	9	54	455	310	73	69	3	0	0
4	a	54	455	310	73	69	3	0	0
4	d	54	455	310	73	69	3	0	0
4	f	54	455	310	73	69	3	0	0
4	i	54	455	310	73	69	3	0	0
4	k	54	455	310	73	69	3	0	0
4	o	54	455	310	73	69	3	0	0
4	q	54	455	310	73	69	3	0	0
4	s	54	455	310	73	69	3	0	0
4	u	54	455	310	73	69	3	0	0
4	w	43	351	235	59	56	1	0	0
4	y	42	343	231	58	53	1	0	0
4	5	42	343	231	58	53	1	0	0
4	6	46	392	271	60	58	3	0	0
4	Q	54	455	310	73	69	3	0	0

- Molecule 5 is a protein called Light-harvesting protein B-875 beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	B	44	359	240	56	62	1	0	0

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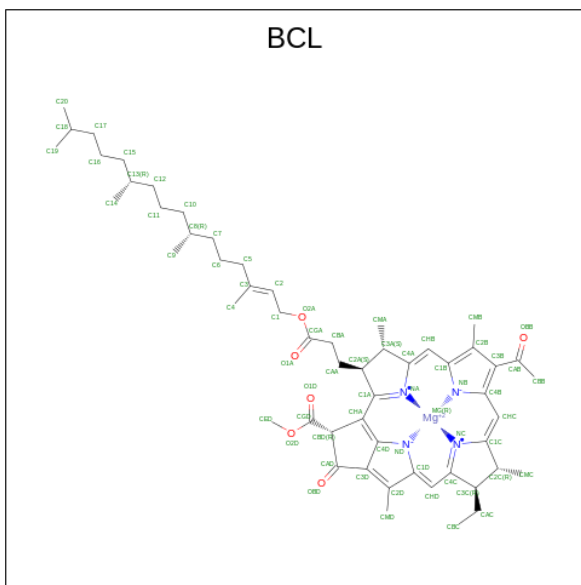
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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	43	351	236	55	59	1	0	0
5	G	44	359	240	56	62	1	0	0
5	J	43	351	236	55	59	1	0	0
5	N	41	339	228	53	57	1	0	0
5	8	44	359	240	56	62	1	0	0
5	0	44	359	240	56	62	1	0	0
5	b	44	359	240	56	62	1	0	0
5	e	43	351	236	55	59	1	0	0
5	g	44	359	240	56	62	1	0	0
5	j	43	351	236	55	59	1	0	0
5	n	38	316	213	50	52	1	0	0
5	p	39	320	215	51	53	1	0	0
5	r	43	351	236	55	59	1	0	0
5	t	42	343	230	54	58	1	0	0
5	v	37	308	207	49	51	1	0	0
5	x	42	343	230	54	58	1	0	0
5	z	38	312	209	50	52	1	0	0
5	4	36	297	198	48	50	1	0	0
5	aa	44	359	240	56	62	1	0	0
5	ab	44	359	240	56	62	1	0	0

- Molecule 6 is a protein called Intrinsic membrane protein PufX.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	64	Total	C	N	O	S	0	0
			500	328	88	81	3		
6	c	68	Total	C	N	O	S	0	0
			529	345	93	88	3		

- Molecule 7 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
7	L	1	Total	C	Mg	N	O	0
			176	143	3	12	18	
7	L	1	Total	C	Mg	N	O	0
			176	143	3	12	18	
7	L	1	Total	C	Mg	N	O	0
			176	143	3	12	18	
7	M	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	B	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	D	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	E	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	F	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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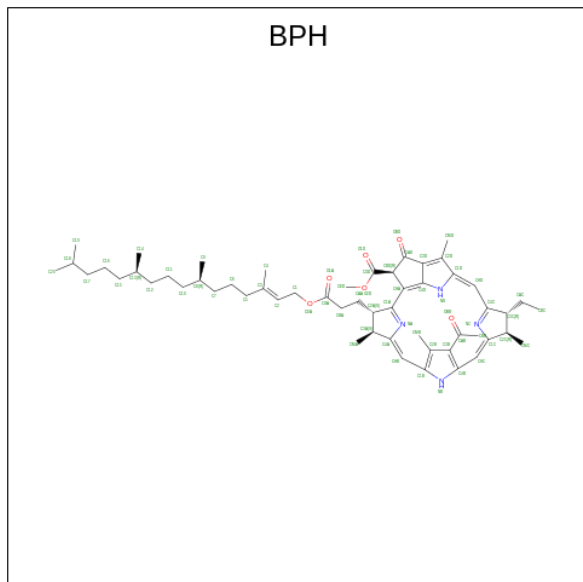
Mol	Chain	Residues	Atoms					AltConf
7	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	I	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	J	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	K	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	O	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
7	8	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	9	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	0	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	C	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
7	l	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
7	l	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
7	m	1	Total	C	Mg	N	O	0
			128	106	2	8	12	
7	m	1	Total	C	Mg	N	O	0
			128	106	2	8	12	
7	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	b	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	d	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	e	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	f	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	i	1	Total	C	Mg	N	O	0
			132	110	2	8	12	

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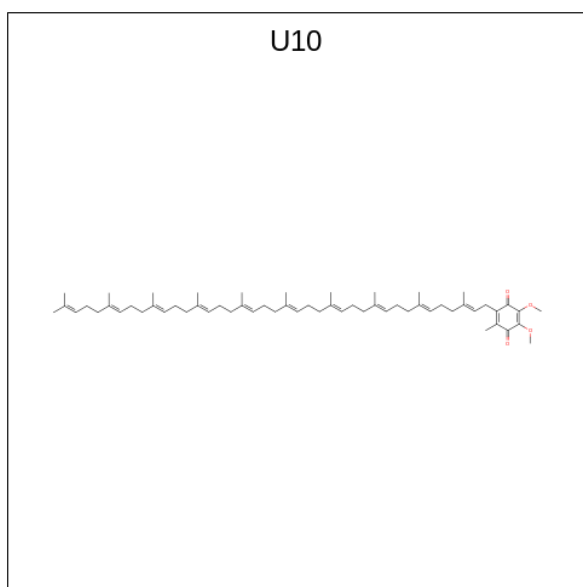
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
7	i	1	Total 132	C 110	Mg 2	N 8	O 12	0
7	k	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	o	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	p	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	q	1	Total 132	C 110	Mg 2	N 8	O 12	0
7	q	1	Total 132	C 110	Mg 2	N 8	O 12	0
7	r	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	s	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	t	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	v	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	w	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	x	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	y	1	Total 46	C 35	Mg 1	N 4	O 6	0
7	z	1	Total 46	C 35	Mg 1	N 4	O 6	0
7	5	1	Total 46	C 35	Mg 1	N 4	O 6	0
7	4	1	Total 46	C 35	Mg 1	N 4	O 6	0
7	aa	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	ab	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	c	1	Total 61	C 50	Mg 1	N 4	O 6	0

- Molecule 8 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
8	L	1	117	97	8	12	0
8	L	1	117	97	8	12	0
8	1	1	117	97	8	12	0
8	1	1	117	97	8	12	0

- Molecule 9 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).

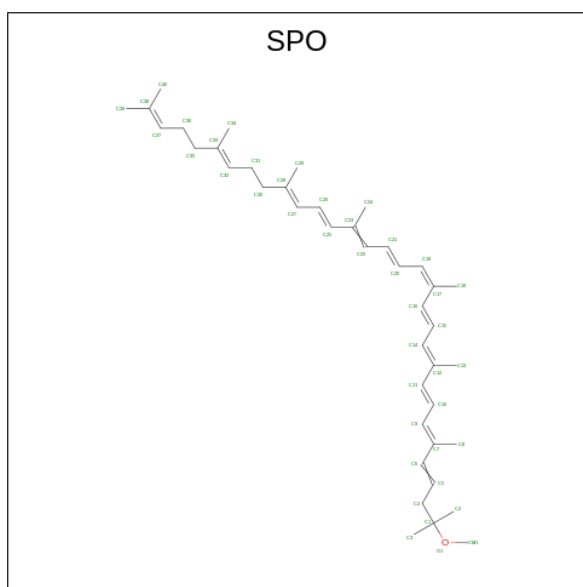


Mol	Chain	Residues	Atoms			AltConf
9	L	1	Total	C	O	0
			43	39	4	
9	M	1	Total	C	O	0
			48	44	4	
9	l	1	Total	C	O	0
			63	59	4	
9	m	1	Total	C	O	0
			48	44	4	

- Molecule 10 is FE (II) ION (three-letter code: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
10	M	1	Total	Fe	0
			1	1	
10	m	1	Total	Fe	0
			1	1	

- Molecule 11 is SPHEROIDENE (three-letter code: SPO) (formula: C₄₁H₆₀O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
11	M	1	Total	C	O	0
			42	41	1	
11	D	1	Total	C	O	0
			42	41	1	
11	E	1	Total	C	O	0
			42	41	1	
11	F	1	Total	C	O	0
			84	82	2	
11	F	1	Total	C	O	0
			84	82	2	
11	G	1	Total	C	O	0
			84	82	2	
11	G	1	Total	C	O	0
			84	82	2	
11	J	1	Total	C	O	0
			42	41	1	
11	9	1	Total	C	O	0
			84	82	2	
11	9	1	Total	C	O	0
			84	82	2	
11	0	1	Total	C	O	0
			84	82	2	
11	0	1	Total	C	O	0
			84	82	2	
11	C	1	Total	C	O	0
			42	41	1	
11	m	1	Total	C	O	0
			42	41	1	

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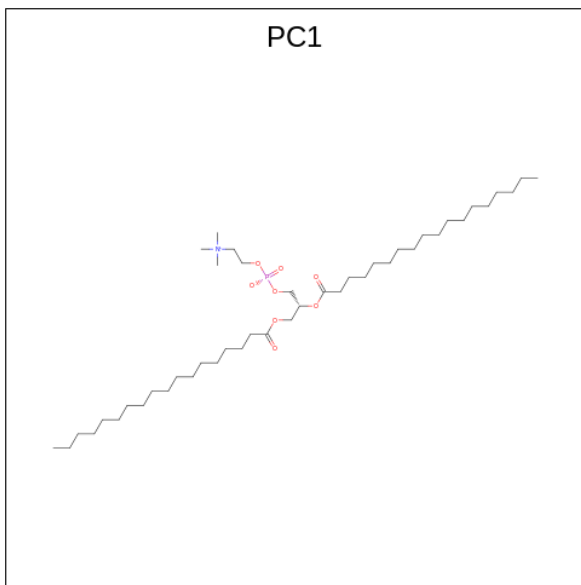
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
11	b	1	84	82	2	0
11	b	1	84	82	2	0
11	d	1	84	82	2	0
11	d	1	84	82	2	0
11	e	1	42	41	1	0
11	f	1	42	41	1	0
11	g	1	42	41	1	0
11	i	1	42	41	1	0
11	j	1	42	41	1	0
11	n	1	42	41	1	0
11	o	1	42	41	1	0
11	p	1	84	82	2	0
11	p	1	84	82	2	0
11	q	1	42	41	1	0
11	s	1	42	41	1	0
11	t	1	42	41	1	0
11	u	1	42	41	1	0
11	v	1	42	41	1	0
11	w	1	42	41	1	0
11	aa	1	42	41	1	0
11	Q	1	42	41	1	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
11	ab	1	42	41	1	0

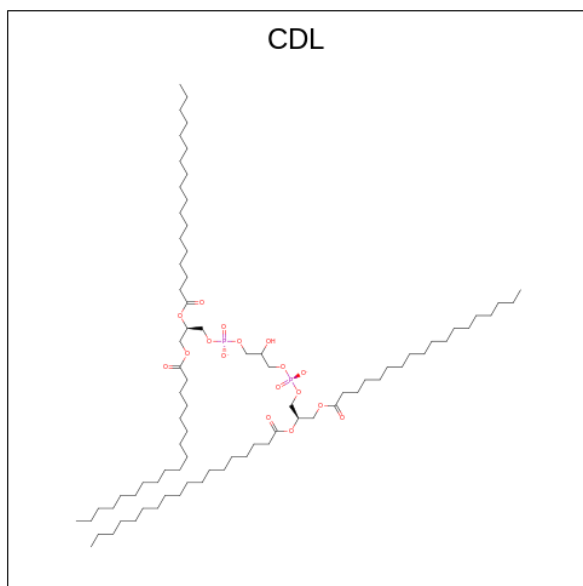
- Molecule 12 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
12	H	1	98	78	2	16	2	0
12	H	1	98	78	2	16	2	0
12	A	1	89	69	2	16	2	0
12	A	1	89	69	2	16	2	0
12	C	1	54	44	1	8	1	0
12	h	1	48	38	1	8	1	0
12	a	1	40	30	1	8	1	0
12	Q	1	54	44	1	8	1	0
12	c	1	48	38	1	8	1	0

- Molecule 13 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled

as "Ligand of Interest" by depositor).

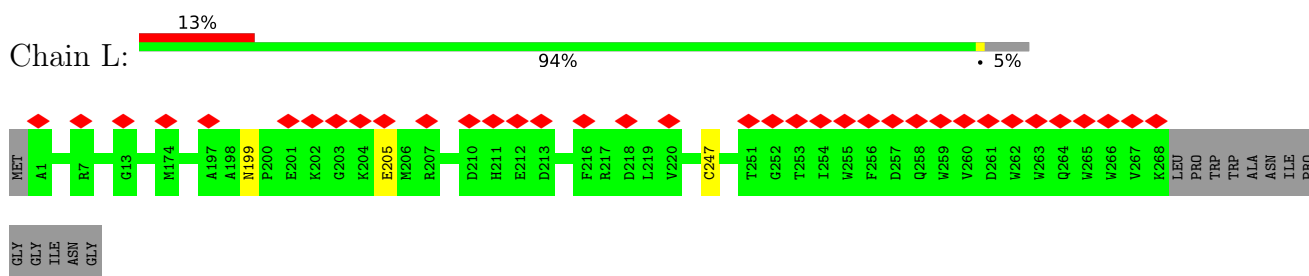


Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
13	m	1	100	81	17	2	0

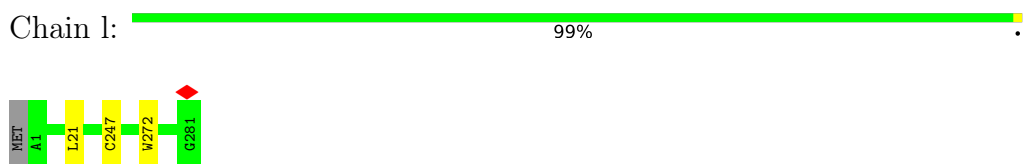
3 Residue-property plots [i](#)

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

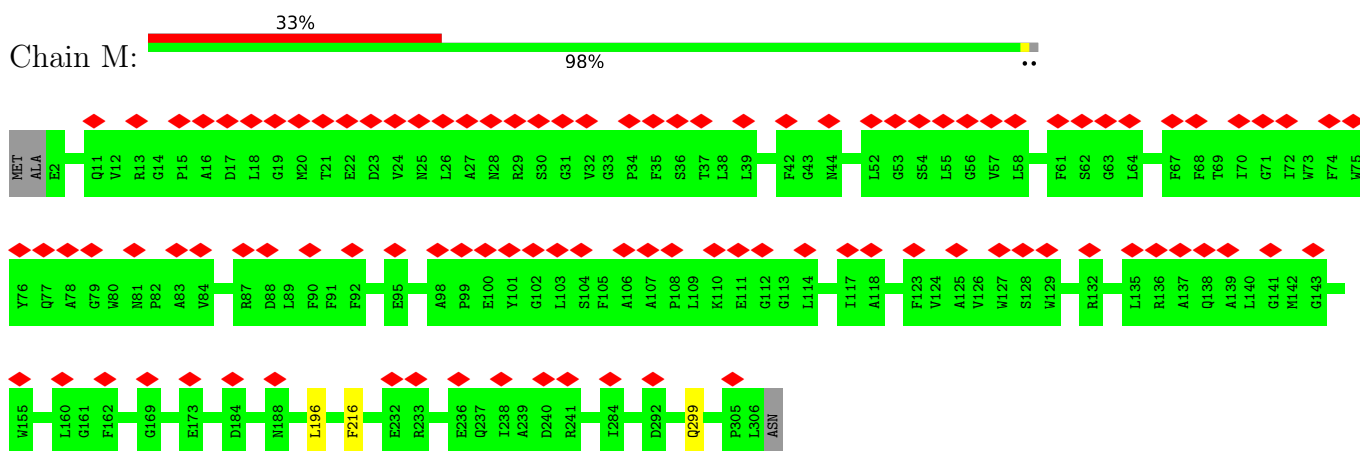
- Molecule 1: Reaction center protein L chain



- Molecule 1: Reaction center protein L chain

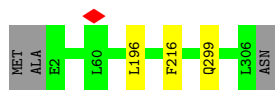


- Molecule 2: Reaction center protein M chain

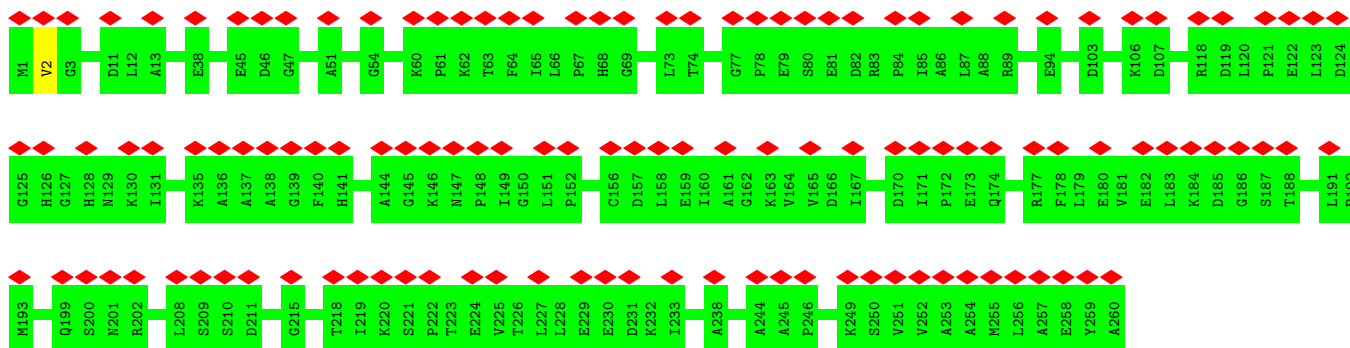


- Molecule 2: Reaction center protein M chain

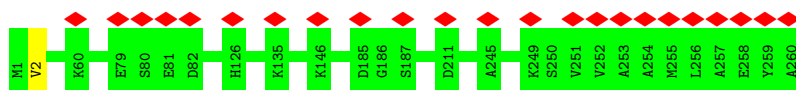




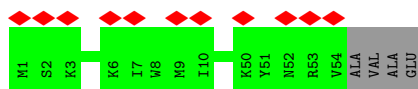
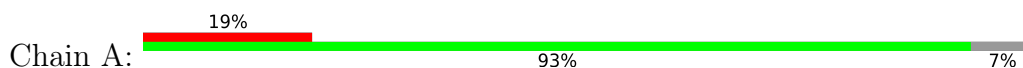
- Molecule 3: Reaction center protein H chain



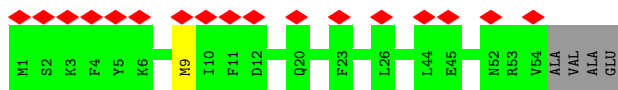
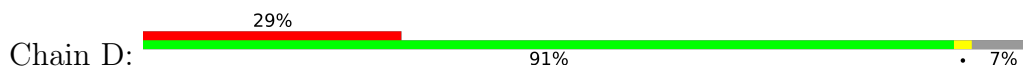
- Molecule 3: Reaction center protein H chain



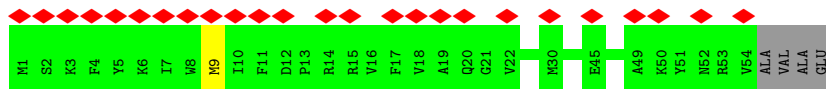
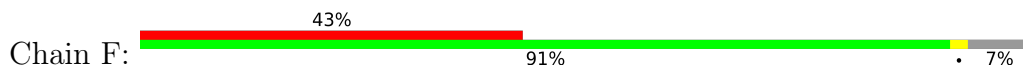
- Molecule 4: Light-harvesting protein B-875 alpha chain



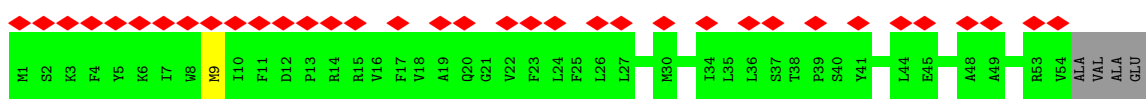
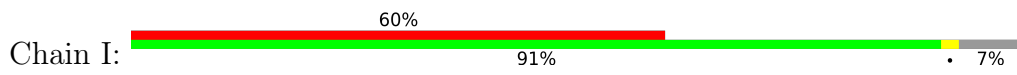
- Molecule 4: Light-harvesting protein B-875 alpha chain



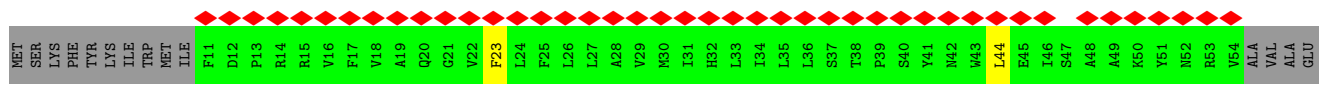
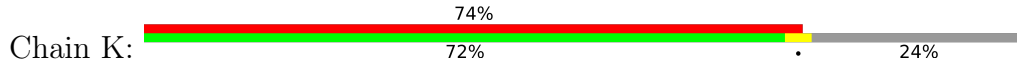
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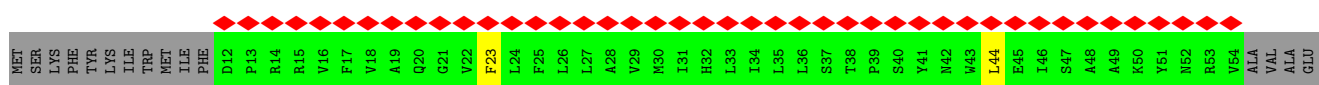
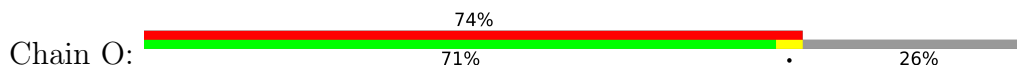
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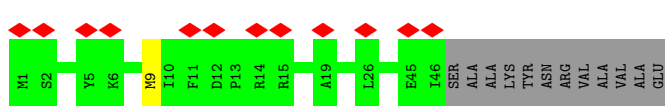
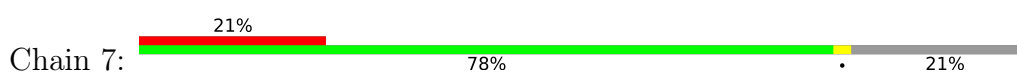
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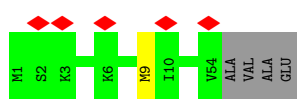
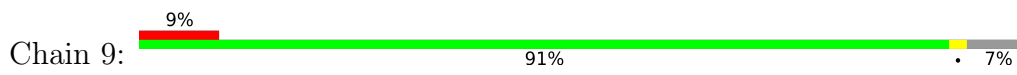
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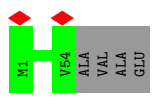
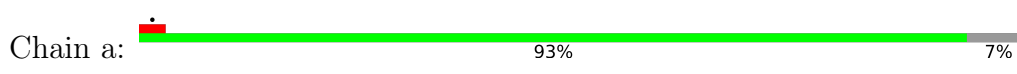
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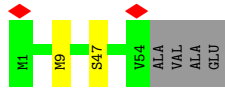
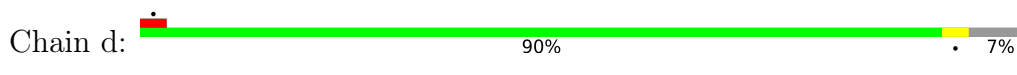
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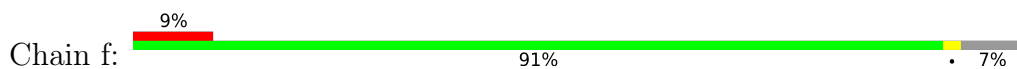
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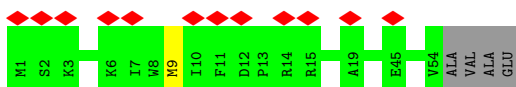
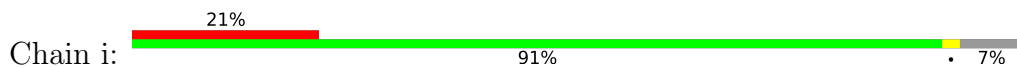
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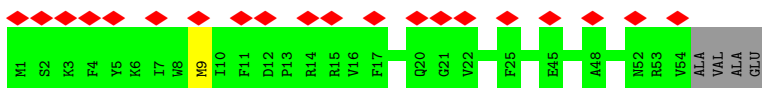
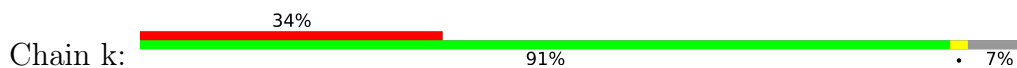
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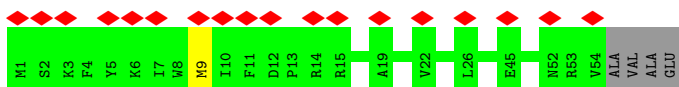
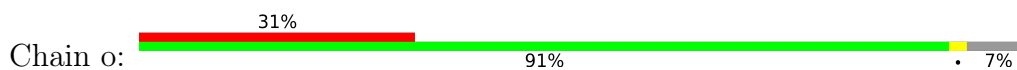
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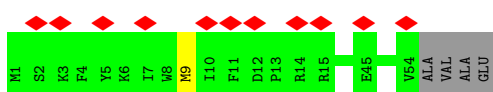
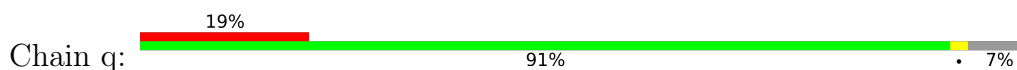
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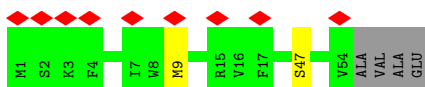
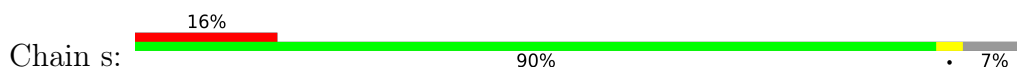
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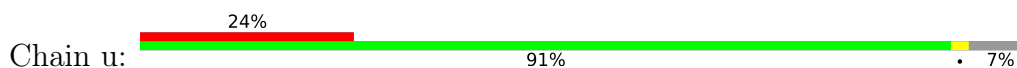
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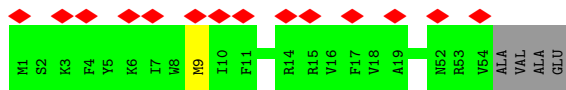


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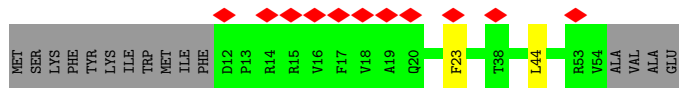
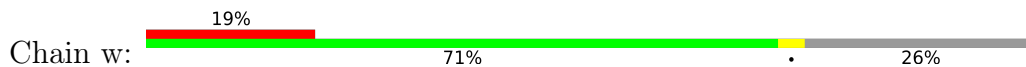


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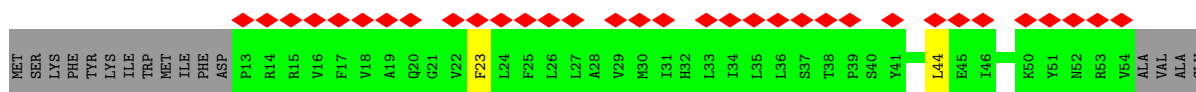




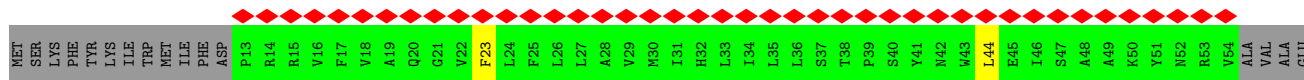
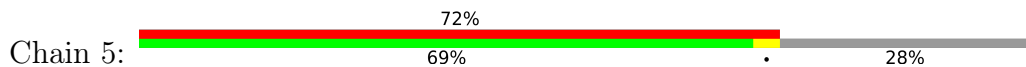
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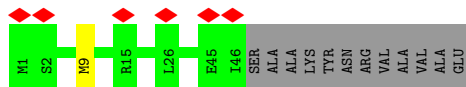
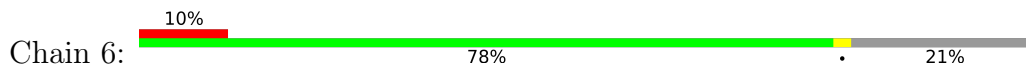
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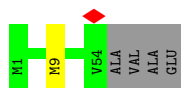
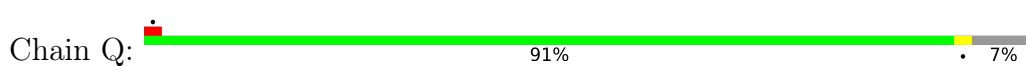
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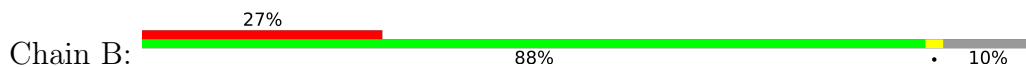
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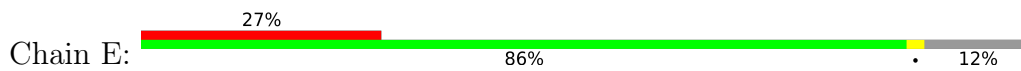
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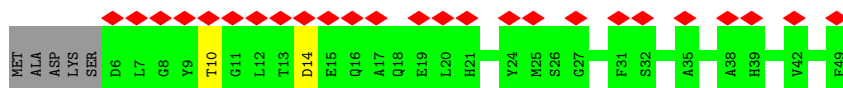
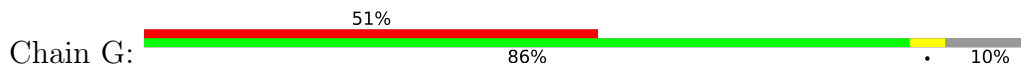
• Molecule 5: Light-harvesting protein B-875 beta chain



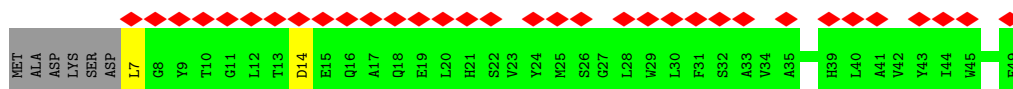
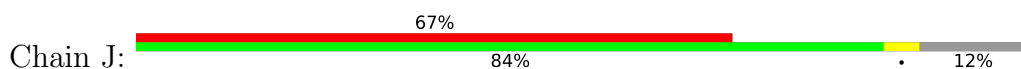
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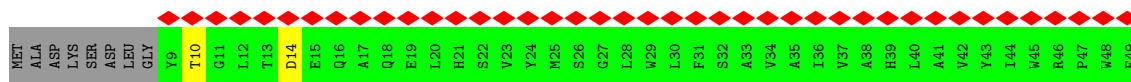
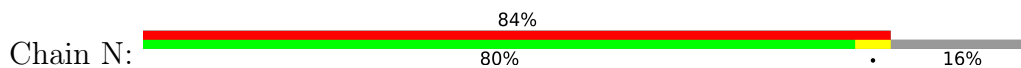
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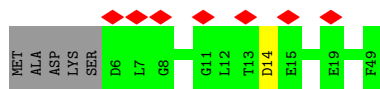
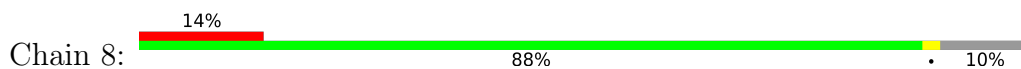
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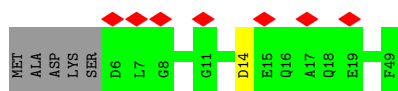
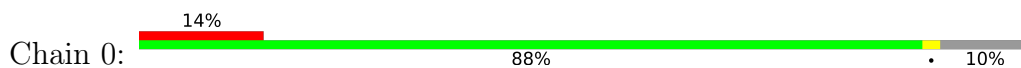
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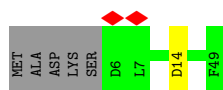
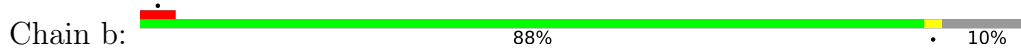
• Molecule 5: Light-harvesting protein B-875 beta chain



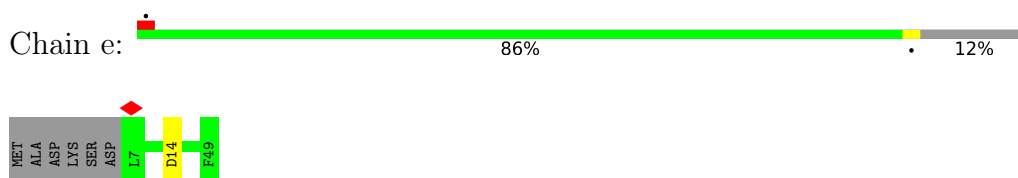
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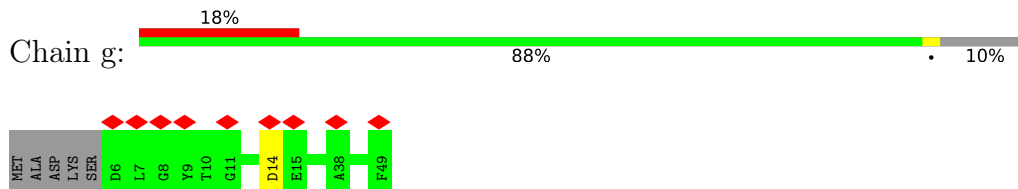
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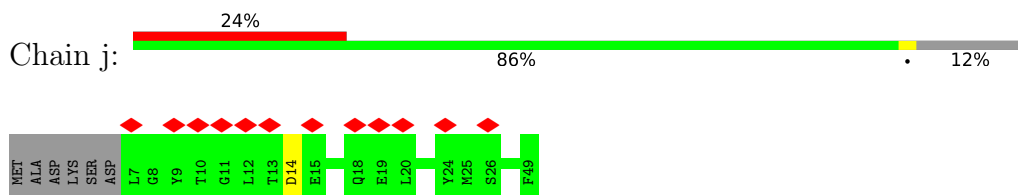
- Molecule 5: Light-harvesting protein B-875 beta chain



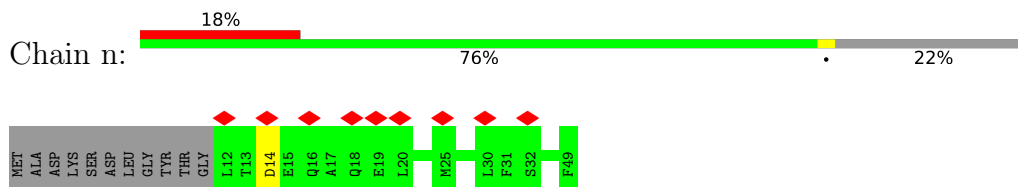
- Molecule 5: Light-harvesting protein B-875 beta chain



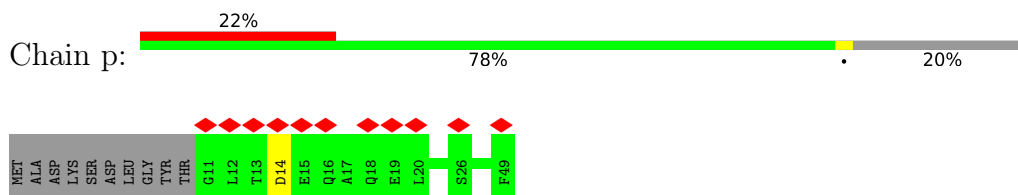
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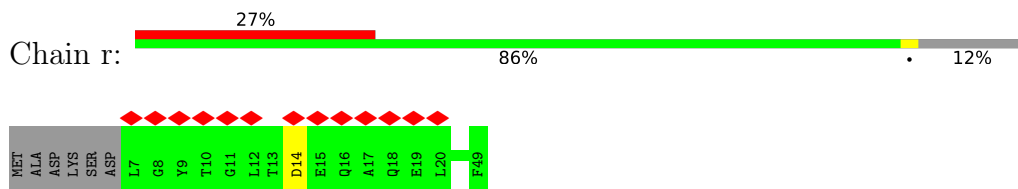
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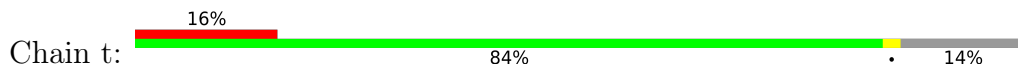
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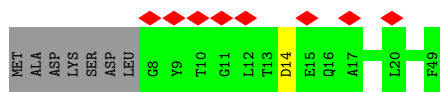


- Molecule 5: Light-harvesting protein B-875 beta chain

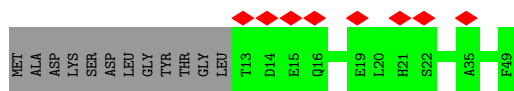
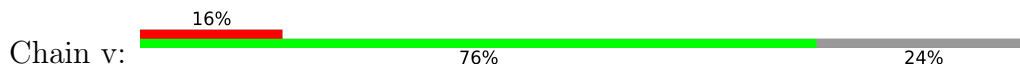


- Molecule 5: Light-harvesting protein B-875 beta chain

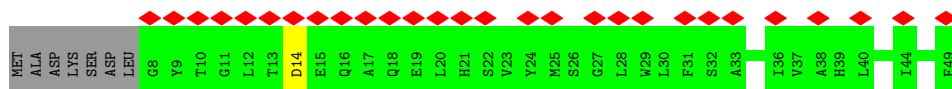
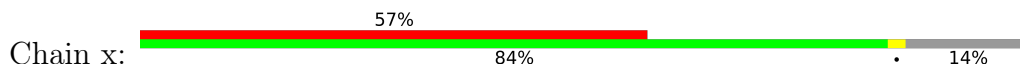




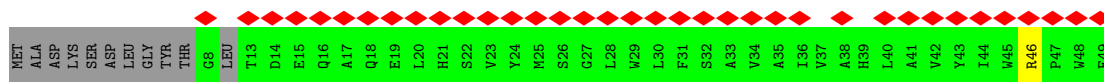
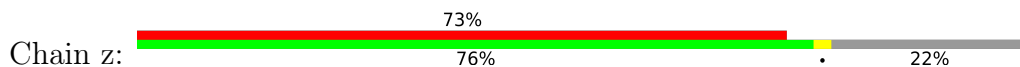
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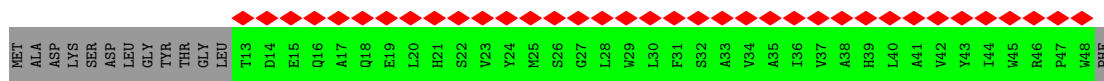
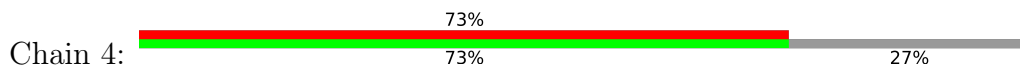
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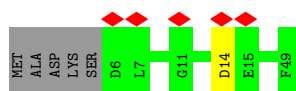
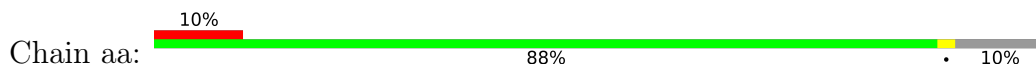
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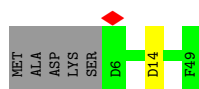
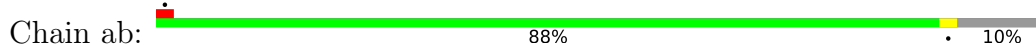
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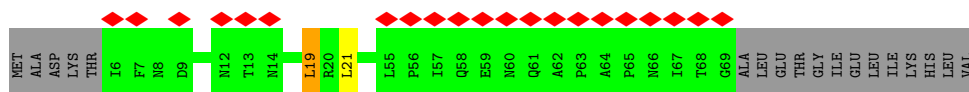
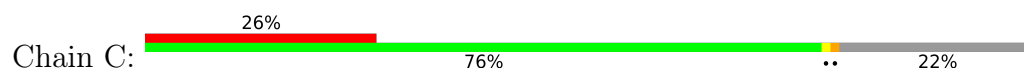
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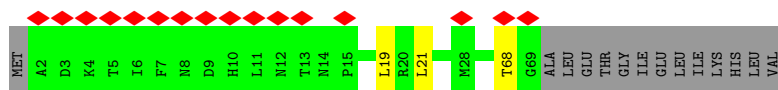
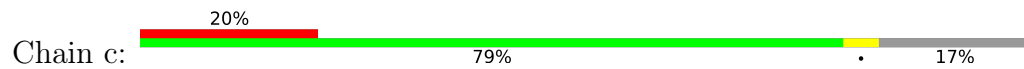
• Molecule 5: Light-harvesting protein B-875 beta chain



• Molecule 6: Intrinsic membrane protein PufX



● Molecule 6: Intrinsic membrane protein PufX



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53830	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.868	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.138	Depositor
Minimum map value	-0.088	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0183	Depositor
Map size (\AA)	289.97498, 289.97498, 289.97498	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.8284999, 0.8284999, 0.8284999	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: BPH, SPO, PC1, BCL, CDL, U10, FE2

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	L	0.39	0/2214	0.46	0/3028
1	l	0.47	0/2320	0.48	1/3175 (0.0%)
2	M	0.37	0/2524	0.43	0/3446
2	m	0.37	0/2524	0.43	0/3446
3	H	0.31	0/2023	0.45	0/2752
3	h	0.31	0/2023	0.45	0/2752
4	5	0.25	0/352	0.39	0/478
4	6	0.35	0/405	0.40	0/549
4	7	0.35	0/405	0.40	0/549
4	9	0.35	0/469	0.41	0/635
4	A	0.36	0/469	0.43	0/635
4	D	0.34	0/469	0.40	0/635
4	F	0.34	0/469	0.39	0/635
4	I	0.35	0/469	0.40	0/635
4	K	0.26	0/372	0.40	0/506
4	O	0.25	0/360	0.39	0/490
4	Q	0.36	0/469	0.40	0/635
4	a	0.36	0/469	0.43	0/635
4	d	0.35	0/469	0.40	0/635
4	f	0.35	0/469	0.40	0/635
4	i	0.35	0/469	0.40	0/635
4	k	0.34	0/469	0.40	0/635
4	o	0.34	0/469	0.40	0/635
4	q	0.36	0/469	0.40	0/635
4	s	0.35	0/469	0.40	0/635
4	u	0.35	0/469	0.40	0/635
4	w	0.25	0/360	0.39	0/490
4	y	0.26	0/352	0.39	0/478
5	0	0.31	0/372	0.39	0/510
5	4	0.25	0/308	0.34	0/423
5	8	0.30	0/372	0.38	0/510
5	B	0.33	0/372	0.38	0/510

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	E	0.31	0/364	0.40	0/499
5	G	0.30	0/372	0.38	0/510
5	J	0.31	0/364	0.39	0/499
5	N	0.30	0/352	0.39	0/483
5	aa	0.32	0/372	0.39	0/510
5	ab	0.34	0/372	0.41	0/510
5	b	0.31	0/372	0.38	0/510
5	e	0.31	0/364	0.40	0/499
5	g	0.31	0/372	0.39	0/510
5	j	0.30	0/364	0.38	0/499
5	n	0.30	0/328	0.37	0/450
5	p	0.30	0/332	0.37	0/455
5	r	0.34	0/364	0.42	0/499
5	t	0.31	0/356	0.39	0/488
5	v	0.31	0/320	0.39	0/439
5	x	0.32	0/356	0.40	0/488
5	z	0.27	0/323	0.36	0/441
6	C	0.36	0/514	0.63	1/697 (0.1%)
6	c	0.41	0/543	0.60	0/736
All	All	0.35	0/31797	0.43	2/43339 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	l	21	LEU	CB-CG-CD1	-5.26	102.05	111.00
6	C	19	LEU	CA-CB-CG	5.17	127.19	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	L	266/282 (94%)	254 (96%)	12 (4%)	0	100	100
1	l	279/282 (99%)	265 (95%)	14 (5%)	0	100	100
2	M	303/308 (98%)	299 (99%)	4 (1%)	0	100	100
2	m	303/308 (98%)	299 (99%)	4 (1%)	0	100	100
3	H	258/260 (99%)	250 (97%)	8 (3%)	0	100	100
3	h	258/260 (99%)	250 (97%)	8 (3%)	0	100	100
4	5	40/58 (69%)	38 (95%)	2 (5%)	0	100	100
4	6	44/58 (76%)	42 (96%)	2 (4%)	0	100	100
4	7	44/58 (76%)	42 (96%)	2 (4%)	0	100	100
4	9	52/58 (90%)	50 (96%)	2 (4%)	0	100	100
4	A	52/58 (90%)	49 (94%)	3 (6%)	0	100	100
4	D	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
4	F	52/58 (90%)	50 (96%)	2 (4%)	0	100	100
4	I	52/58 (90%)	50 (96%)	2 (4%)	0	100	100
4	K	42/58 (72%)	39 (93%)	3 (7%)	0	100	100
4	O	41/58 (71%)	39 (95%)	2 (5%)	0	100	100
4	Q	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
4	a	52/58 (90%)	49 (94%)	3 (6%)	0	100	100
4	d	52/58 (90%)	50 (96%)	2 (4%)	0	100	100
4	f	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
4	i	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
4	k	52/58 (90%)	50 (96%)	2 (4%)	0	100	100
4	o	52/58 (90%)	50 (96%)	2 (4%)	0	100	100
4	q	52/58 (90%)	50 (96%)	2 (4%)	0	100	100
4	s	52/58 (90%)	50 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	u	52/58 (90%)	49 (94%)	3 (6%)	0	100	100
4	w	41/58 (71%)	39 (95%)	2 (5%)	0	100	100
4	y	40/58 (69%)	38 (95%)	2 (5%)	0	100	100
5	0	42/49 (86%)	42 (100%)	0	0	100	100
5	4	34/49 (69%)	34 (100%)	0	0	100	100
5	8	42/49 (86%)	42 (100%)	0	0	100	100
5	B	42/49 (86%)	42 (100%)	0	0	100	100
5	E	41/49 (84%)	41 (100%)	0	0	100	100
5	G	42/49 (86%)	42 (100%)	0	0	100	100
5	J	41/49 (84%)	41 (100%)	0	0	100	100
5	N	39/49 (80%)	38 (97%)	1 (3%)	0	100	100
5	aa	42/49 (86%)	42 (100%)	0	0	100	100
5	ab	42/49 (86%)	42 (100%)	0	0	100	100
5	b	42/49 (86%)	42 (100%)	0	0	100	100
5	e	41/49 (84%)	41 (100%)	0	0	100	100
5	g	42/49 (86%)	42 (100%)	0	0	100	100
5	j	41/49 (84%)	41 (100%)	0	0	100	100
5	n	36/49 (74%)	36 (100%)	0	0	100	100
5	p	37/49 (76%)	37 (100%)	0	0	100	100
5	r	41/49 (84%)	41 (100%)	0	0	100	100
5	t	40/49 (82%)	40 (100%)	0	0	100	100
5	v	35/49 (71%)	34 (97%)	1 (3%)	0	100	100
5	x	40/49 (82%)	40 (100%)	0	0	100	100
5	z	35/49 (71%)	35 (100%)	0	0	100	100
6	C	62/82 (76%)	58 (94%)	4 (6%)	0	100	100
6	c	66/82 (80%)	61 (92%)	5 (8%)	0	100	100
All	All	3704/4169 (89%)	3599 (97%)	105 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	L	211/221 (96%)	208 (99%)	3 (1%)	67	85
1	l	220/221 (100%)	218 (99%)	2 (1%)	78	91
2	M	239/241 (99%)	236 (99%)	3 (1%)	69	86
2	m	239/241 (99%)	236 (99%)	3 (1%)	69	86
3	H	208/208 (100%)	207 (100%)	1 (0%)	88	95
3	h	208/208 (100%)	207 (100%)	1 (0%)	88	95
4	5	37/51 (72%)	35 (95%)	2 (5%)	22	54
4	6	43/51 (84%)	42 (98%)	1 (2%)	50	76
4	7	43/51 (84%)	42 (98%)	1 (2%)	50	76
4	9	49/51 (96%)	48 (98%)	1 (2%)	55	79
4	A	49/51 (96%)	49 (100%)	0	100	100
4	D	49/51 (96%)	48 (98%)	1 (2%)	55	79
4	F	49/51 (96%)	48 (98%)	1 (2%)	55	79
4	I	49/51 (96%)	48 (98%)	1 (2%)	55	79
4	K	39/51 (76%)	37 (95%)	2 (5%)	24	56
4	O	38/51 (74%)	36 (95%)	2 (5%)	22	54
4	Q	49/51 (96%)	48 (98%)	1 (2%)	55	79
4	a	49/51 (96%)	49 (100%)	0	100	100
4	d	49/51 (96%)	47 (96%)	2 (4%)	30	62
4	f	49/51 (96%)	48 (98%)	1 (2%)	55	79
4	i	49/51 (96%)	48 (98%)	1 (2%)	55	79
4	k	49/51 (96%)	48 (98%)	1 (2%)	55	79
4	o	49/51 (96%)	48 (98%)	1 (2%)	55	79
4	q	49/51 (96%)	48 (98%)	1 (2%)	55	79
4	s	49/51 (96%)	47 (96%)	2 (4%)	30	62
4	u	49/51 (96%)	48 (98%)	1 (2%)	55	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	w	38/51 (74%)	36 (95%)	2 (5%)	22	54
4	y	37/51 (72%)	35 (95%)	2 (5%)	22	54
5	0	36/40 (90%)	35 (97%)	1 (3%)	43	72
5	4	30/40 (75%)	30 (100%)	0	100	100
5	8	36/40 (90%)	35 (97%)	1 (3%)	43	72
5	B	36/40 (90%)	35 (97%)	1 (3%)	43	72
5	E	35/40 (88%)	34 (97%)	1 (3%)	42	71
5	G	36/40 (90%)	34 (94%)	2 (6%)	21	53
5	J	35/40 (88%)	33 (94%)	2 (6%)	20	52
5	N	34/40 (85%)	32 (94%)	2 (6%)	19	52
5	aa	36/40 (90%)	35 (97%)	1 (3%)	43	72
5	ab	36/40 (90%)	35 (97%)	1 (3%)	43	72
5	b	36/40 (90%)	35 (97%)	1 (3%)	43	72
5	e	35/40 (88%)	34 (97%)	1 (3%)	42	71
5	g	36/40 (90%)	35 (97%)	1 (3%)	43	72
5	j	35/40 (88%)	34 (97%)	1 (3%)	42	71
5	n	32/40 (80%)	31 (97%)	1 (3%)	40	70
5	p	32/40 (80%)	31 (97%)	1 (3%)	40	70
5	r	35/40 (88%)	34 (97%)	1 (3%)	42	71
5	t	34/40 (85%)	33 (97%)	1 (3%)	42	71
5	v	31/40 (78%)	31 (100%)	0	100	100
5	x	34/40 (85%)	33 (97%)	1 (3%)	42	71
5	z	31/40 (78%)	30 (97%)	1 (3%)	39	69
6	C	51/66 (77%)	49 (96%)	2 (4%)	32	64
6	c	54/66 (82%)	51 (94%)	3 (6%)	21	53
All	All	3161/3434 (92%)	3094 (98%)	67 (2%)	56	78

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	199	ASN
1	L	205	GLU
1	L	247	CYS

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Mol	Chain	Res	Type
2	M	196	LEU
2	M	216	PHE
2	M	299	GLN
3	H	2	VAL
5	B	14	ASP
4	D	9	MET
5	E	14	ASP
4	F	9	MET
5	G	10	THR
5	G	14	ASP
4	I	9	MET
5	J	7	LEU
5	J	14	ASP
4	K	23	PHE
4	K	44	LEU
5	N	10	THR
5	N	14	ASP
4	O	23	PHE
4	O	44	LEU
4	7	9	MET
5	8	14	ASP
4	9	9	MET
5	0	14	ASP
6	C	19	LEU
6	C	21	LEU
1	l	247	CYS
1	l	272	TRP
2	m	196	LEU
2	m	216	PHE
2	m	299	GLN
3	h	2	VAL
5	b	14	ASP
4	d	9	MET
4	d	47	SER
5	e	14	ASP
4	f	9	MET
5	g	14	ASP
4	i	9	MET
5	j	14	ASP
4	k	9	MET
5	n	14	ASP
4	o	9	MET

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Mol	Chain	Res	Type
5	p	14	ASP
4	q	9	MET
5	r	14	ASP
4	s	9	MET
4	s	47	SER
5	t	14	ASP
4	u	9	MET
4	w	23	PHE
4	w	44	LEU
5	x	14	ASP
4	y	23	PHE
4	y	44	LEU
5	z	46	ARG
4	5	23	PHE
4	5	44	LEU
4	6	9	MET
5	aa	14	ASP
4	Q	9	MET
5	ab	14	ASP
6	c	19	LEU
6	c	21	LEU
6	c	68	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
3	H	35	ASN
1	l	166	ASN
3	h	35	ASN
4	f	20	GLN
4	s	20	GLN

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 107 ligands modelled in this entry, 2 are monoatomic - leaving 105 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$
7	BCL	L	305	-	40,56,74	1.41	6 (15%)	47,93,115	1.69	10 (21%)
11	SPO	M	404	-	40,41,41	5.54	17 (42%)	47,50,50	5.64	29 (61%)
7	BCL	f	101	-	58,74,74	1.20	4 (6%)	69,115,115	1.47	11 (15%)
11	SPO	p	103	-	40,41,41	5.78	17 (42%)	47,50,50	5.47	31 (65%)
7	BCL	8	101	-	58,74,74	1.22	3 (5%)	69,115,115	1.44	10 (14%)
11	SPO	n	102	-	40,41,41	5.62	17 (42%)	47,50,50	5.49	31 (65%)
11	SPO	s	101	-	40,41,41	5.64	17 (42%)	47,50,50	5.29	29 (61%)
7	BCL	s	102	-	58,74,74	1.19	4 (6%)	69,115,115	1.45	11 (15%)
7	BCL	I	101	-	58,74,74	1.19	4 (6%)	69,115,115	1.42	10 (14%)
7	BCL	K	101	-	58,74,74	1.17	3 (5%)	69,115,115	1.49	12 (17%)
7	BCL	e	101	-	58,74,74	1.22	3 (5%)	69,115,115	1.44	10 (14%)
11	SPO	G	102	-	40,41,41	5.74	17 (42%)	47,50,50	5.65	29 (61%)
11	SPO	b	103	-	40,41,41	5.51	17 (42%)	47,50,50	5.54	32 (68%)
7	BCL	B	101	-	58,74,74	1.22	3 (5%)	69,115,115	1.45	10 (14%)
7	BCL	c	1202	-	53,69,74	1.24	4 (7%)	63,109,115	1.46	10 (15%)
7	BCL	C	1202	-	53,69,74	1.24	4 (7%)	63,109,115	1.45	10 (15%)
7	BCL	d	101	-	58,74,74	1.19	4 (6%)	69,115,115	1.47	11 (15%)
11	SPO	aa	101	-	40,41,41	5.64	17 (42%)	47,50,50	5.29	29 (61%)
7	BCL	aa	102	-	58,74,74	1.22	3 (5%)	69,115,115	1.45	10 (14%)
7	BCL	q	101	-	58,74,74	1.19	4 (6%)	69,115,115	1.45	10 (14%)
11	SPO	G	103	-	40,41,41	5.78	17 (42%)	47,50,50	5.35	30 (63%)
13	CDL	m	406	-	99,99,99	1.08	7 (7%)	105,111,111	0.88	5 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	SPO	m	405	-	40,41,41	5.54	17 (42%)	47,50,50	5.64	30 (63%)
7	BCL	g	102	-	58,74,74	1.23	3 (5%)	69,115,115	1.45	10 (14%)
11	SPO	C	1203	-	40,41,41	5.65	17 (42%)	47,50,50	5.29	29 (61%)
12	PC1	h	301	-	47,47,53	1.12	3 (6%)	53,55,61	1.03	3 (5%)
11	SPO	j	101	-	40,41,41	5.73	17 (42%)	47,50,50	5.30	29 (61%)
11	SPO	b	101	-	40,41,41	5.61	17 (42%)	47,50,50	5.41	28 (59%)
7	BCL	b	102	-	58,74,74	1.22	3 (5%)	69,115,115	1.44	10 (14%)
8	BPH	L	306	-	41,60,70	1.12	3 (7%)	40,89,101	1.18	5 (12%)
7	BCL	5	101	-	38,54,74	1.40	3 (7%)	45,91,115	1.57	10 (22%)
7	BCL	m	401	-	54,70,74	1.25	4 (7%)	64,110,115	1.46	12 (18%)
7	BCL	Q	602	-	58,74,74	1.76	6 (10%)	69,115,115	2.02	13 (18%)
7	BCL	E	101	-	58,74,74	1.22	3 (5%)	69,115,115	1.44	10 (14%)
7	BCL	q	103	-	58,74,74	1.20	4 (6%)	69,115,115	1.48	12 (17%)
7	BCL	z	101	-	38,54,74	1.40	4 (10%)	45,91,115	1.83	14 (31%)
7	BCL	l	304	-	58,74,74	1.20	6 (10%)	69,115,115	1.47	10 (14%)
12	PC1	A	1703	-	45,45,53	1.16	3 (6%)	51,53,61	1.05	4 (7%)
12	PC1	Q	601	-	53,53,53	1.06	3 (5%)	59,61,61	0.89	3 (5%)
7	BCL	ab	101	-	58,74,74	1.22	3 (5%)	69,115,115	1.45	10 (14%)
7	BCL	A	1702	-	58,74,74	1.21	4 (6%)	69,115,115	1.42	10 (14%)
7	BCL	G	101	-	58,74,74	1.22	3 (5%)	69,115,115	1.44	10 (14%)
11	SPO	ab	102	-	40,41,41	5.45	17 (42%)	47,50,50	5.96	31 (65%)
7	BCL	n	101	-	58,74,74	1.21	3 (5%)	69,115,115	1.44	10 (14%)
11	SPO	i	103	-	40,41,41	5.64	17 (42%)	47,50,50	5.29	29 (61%)
11	SPO	F	102	-	40,41,41	5.64	17 (42%)	47,50,50	5.29	29 (61%)
7	BCL	l	301	-	58,74,74	1.28	6 (10%)	69,115,115	1.50	11 (15%)
7	BCL	a	101	-	58,74,74	1.20	4 (6%)	69,115,115	1.41	10 (14%)
11	SPO	t	102	-	40,41,41	5.75	17 (42%)	47,50,50	5.49	31 (65%)
8	BPH	L	303	-	48,67,70	1.10	4 (8%)	48,97,101	1.12	5 (10%)
8	BPH	l	302	-	48,67,70	1.10	4 (8%)	48,97,101	1.17	6 (12%)
11	SPO	g	101	-	40,41,41	5.64	17 (42%)	47,50,50	5.29	29 (61%)
11	SPO	d	103	-	40,41,41	5.54	17 (42%)	47,50,50	6.04	29 (61%)
7	BCL	k	101	-	58,74,74	1.19	4 (6%)	69,115,115	1.48	12 (17%)
11	SPO	9	103	-	40,41,41	5.64	17 (42%)	47,50,50	5.28	29 (61%)
12	PC1	A	1701	-	42,42,53	1.21	3 (7%)	48,50,61	1.09	4 (8%)
11	SPO	F	103	-	40,41,41	5.64	17 (42%)	47,50,50	5.29	29 (61%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	BCL	i	101	-	58,74,74	1.19	4 (6%)	69,115,115	1.42	10 (14%)
12	PC1	a	102	-	39,39,53	1.21	3 (7%)	45,47,61	1.10	4 (8%)
7	BCL	O	101	-	38,54,74	1.40	3 (7%)	45,91,115	1.57	10 (22%)
7	BCL	M	402	-	58,74,74	1.18	6 (10%)	69,115,115	1.52	12 (17%)
11	SPO	p	102	-	40,41,41	5.68	17 (42%)	47,50,50	5.40	31 (65%)
11	SPO	d	102	-	40,41,41	5.64	17 (42%)	47,50,50	5.28	29 (61%)
11	SPO	0	103	-	40,41,41	5.59	17 (42%)	47,50,50	5.53	30 (63%)
11	SPO	f	102	-	40,41,41	5.64	17 (42%)	47,50,50	5.29	29 (61%)
11	SPO	w	102	-	40,41,41	5.68	17 (42%)	47,50,50	5.55	31 (65%)
9	U10	M	403	-	48,48,63	2.67	14 (29%)	58,61,79	1.68	13 (22%)
11	SPO	e	102	-	40,41,41	5.60	17 (42%)	47,50,50	5.71	30 (63%)
7	BCL	D	101	-	58,74,74	1.19	4 (6%)	69,115,115	1.46	11 (15%)
7	BCL	m	403	-	58,74,74	1.18	6 (10%)	69,115,115	1.52	12 (17%)
7	BCL	x	101	-	58,74,74	1.21	3 (5%)	69,115,115	1.45	10 (14%)
12	PC1	C	1201	-	53,53,53	1.11	3 (5%)	59,61,61	0.93	3 (5%)
7	BCL	9	102	-	58,74,74	1.19	4 (6%)	69,115,115	1.52	11 (15%)
11	SPO	E	102	-	40,41,41	5.75	17 (42%)	47,50,50	5.36	31 (65%)
12	PC1	H	602	-	53,53,53	1.10	3 (5%)	59,61,61	0.98	4 (6%)
7	BCL	p	101	-	58,74,74	1.22	3 (5%)	69,115,115	1.44	10 (14%)
7	BCL	N	101	-	58,74,74	1.22	3 (5%)	69,115,115	1.44	10 (14%)
7	BCL	4	101	-	38,54,74	1.38	4 (10%)	45,91,115	1.62	9 (20%)
7	BCL	t	101	-	58,74,74	1.22	3 (5%)	69,115,115	1.45	10 (14%)
11	SPO	Q	603	-	40,41,41	5.65	17 (42%)	47,50,50	5.29	29 (61%)
7	BCL	o	101	-	58,74,74	1.19	4 (6%)	69,115,115	1.47	12 (17%)
11	SPO	D	102	-	40,41,41	5.65	17 (42%)	47,50,50	5.29	29 (61%)
9	U10	L	304	-	43,43,63	2.74	13 (30%)	52,55,79	1.85	15 (28%)
7	BCL	J	101	-	58,74,74	1.22	3 (5%)	69,115,115	1.44	10 (14%)
7	BCL	0	102	-	58,74,74	1.22	3 (5%)	69,115,115	1.45	10 (14%)
9	U10	m	404	-	48,48,63	2.67	14 (29%)	58,61,79	1.68	13 (22%)
7	BCL	L	302	-	54,70,74	1.24	5 (9%)	64,110,115	1.49	11 (17%)
7	BCL	F	101	-	58,74,74	1.19	4 (6%)	69,115,115	1.46	11 (15%)
11	SPO	o	102	-	40,41,41	5.64	17 (42%)	47,50,50	5.29	29 (61%)
7	BCL	y	101	-	38,54,74	1.39	3 (7%)	45,91,115	1.57	9 (20%)
7	BCL	r	101	-	58,74,74	1.22	3 (5%)	69,115,115	1.44	10 (14%)
12	PC1	H	601	-	43,43,53	1.15	3 (6%)	49,51,61	1.06	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	SPO	u	101	-	40,41,41	5.65	17 (42%)	47,50,50	5.29	29 (61%)
7	BCL	v	101	-	58,74,74	1.19	3 (5%)	69,115,115	1.44	11 (15%)
7	BCL	L	301	-	58,74,74	1.22	4 (6%)	69,115,115	1.52	13 (18%)
7	BCL	i	102	-	58,74,74	1.22	3 (5%)	69,115,115	1.44	10 (14%)
12	PC1	c	1201	-	47,47,53	1.15	3 (6%)	53,55,61	1.02	3 (5%)
11	SPO	0	101	-	40,41,41	5.51	17 (42%)	47,50,50	5.72	31 (65%)
11	SPO	9	101	-	40,41,41	5.61	17 (42%)	47,50,50	5.41	28 (59%)
11	SPO	q	102	-	40,41,41	5.64	17 (42%)	47,50,50	5.29	29 (61%)
9	U10	l	303	-	63,63,63	2.65	16 (25%)	76,79,79	1.93	23 (30%)
7	BCL	w	101	-	58,74,74	1.18	3 (5%)	69,115,115	1.44	11 (15%)
11	SPO	v	102	-	40,41,41	5.63	17 (42%)	47,50,50	5.53	30 (63%)
8	BPH	l	305	-	41,60,70	1.12	3 (7%)	40,89,101	1.19	5 (12%)
11	SPO	J	102	-	40,41,41	5.84	17 (42%)	47,50,50	5.22	30 (63%)

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
7	BCL	L	305	-	-	1/16/116/137	-
11	SPO	M	404	-	-	21/47/47/47	-
7	BCL	f	101	-	-	2/37/137/137	-
11	SPO	p	103	-	-	27/47/47/47	-
7	BCL	8	101	-	-	2/37/137/137	-
11	SPO	n	102	-	-	27/47/47/47	-
11	SPO	s	101	-	-	25/47/47/47	-
7	BCL	s	102	-	-	2/37/137/137	-
7	BCL	I	101	-	-	2/37/137/137	-
7	BCL	K	101	-	-	4/37/137/137	-
7	BCL	e	101	-	-	2/37/137/137	-
11	SPO	G	102	-	-	24/47/47/47	-
11	SPO	b	103	-	-	23/47/47/47	-
7	BCL	B	101	-	-	2/37/137/137	-
7	BCL	c	1202	-	-	2/31/131/137	-
7	BCL	C	1202	-	-	2/31/131/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BCL	d	101	-	-	2/37/137/137	-
11	SPO	aa	101	-	-	25/47/47/47	-
7	BCL	aa	102	-	-	2/37/137/137	-
7	BCL	q	101	-	-	4/37/137/137	-
11	SPO	G	103	-	-	31/47/47/47	-
13	CDL	m	406	-	-	50/110/110/110	-
11	SPO	m	405	-	-	21/47/47/47	-
7	BCL	g	102	-	-	2/37/137/137	-
11	SPO	C	1203	-	-	25/47/47/47	-
12	PC1	h	301	-	-	34/51/51/57	-
11	SPO	j	101	-	-	25/47/47/47	-
11	SPO	b	101	-	-	26/47/47/47	-
7	BCL	b	102	-	-	2/37/137/137	-
8	BPH	L	306	-	-	6/25/93/105	0/5/6/6
7	BCL	5	101	-	-	2/13/113/137	-
7	BCL	m	401	-	-	2/33/133/137	-
7	BCL	Q	602	-	-	4/37/137/137	-
7	BCL	E	101	-	-	2/37/137/137	-
7	BCL	q	103	-	-	2/37/137/137	-
7	BCL	z	101	-	-	8/13/113/137	-
7	BCL	l	304	-	-	3/37/137/137	-
12	PC1	A	1703	-	-	27/49/49/57	-
12	PC1	Q	601	-	-	31/57/57/57	-
7	BCL	ab	101	-	-	2/37/137/137	-
7	BCL	A	1702	-	-	0/37/137/137	-
7	BCL	G	101	-	-	2/37/137/137	-
11	SPO	ab	102	-	-	25/47/47/47	-
7	BCL	n	101	-	-	2/37/137/137	-
11	SPO	i	103	-	-	25/47/47/47	-
11	SPO	F	102	-	-	25/47/47/47	-
7	BCL	l	301	-	-	2/37/137/137	-
7	BCL	a	101	-	-	0/37/137/137	-
11	SPO	t	102	-	-	29/47/47/47	-
8	BPH	L	303	-	-	8/34/102/105	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BPH	l	302	-	-	8/34/102/105	0/5/6/6
11	SPO	g	101	-	-	25/47/47/47	-
11	SPO	d	103	-	-	25/47/47/47	-
7	BCL	k	101	-	-	2/37/137/137	-
11	SPO	9	103	-	-	25/47/47/47	-
12	PC1	A	1701	-	-	21/46/46/57	-
11	SPO	F	103	-	-	25/47/47/47	-
7	BCL	i	101	-	-	5/37/137/137	-
12	PC1	a	102	-	-	22/43/43/57	-
7	BCL	O	101	-	-	2/13/113/137	-
7	BCL	M	402	-	-	2/37/137/137	-
11	SPO	p	102	-	-	28/47/47/47	-
11	SPO	d	102	-	-	25/47/47/47	-
11	SPO	0	103	-	-	23/47/47/47	-
11	SPO	f	102	-	-	25/47/47/47	-
11	SPO	w	102	-	-	23/47/47/47	-
9	U10	M	403	-	-	11/45/69/87	0/1/1/1
11	SPO	e	102	-	-	22/47/47/47	-
7	BCL	D	101	-	-	5/37/137/137	-
7	BCL	m	403	-	-	1/37/137/137	-
7	BCL	x	101	-	-	2/37/137/137	-
12	PC1	C	1201	-	-	34/57/57/57	-
7	BCL	9	102	-	-	4/37/137/137	-
11	SPO	E	102	-	-	31/47/47/47	-
12	PC1	H	602	-	-	27/57/57/57	-
7	BCL	p	101	-	-	2/37/137/137	-
7	BCL	N	101	-	-	2/37/137/137	-
7	BCL	4	101	-	-	5/13/113/137	-
7	BCL	t	101	-	-	2/37/137/137	-
11	SPO	Q	603	-	-	25/47/47/47	-
7	BCL	o	101	-	-	2/37/137/137	-
11	SPO	D	102	-	-	25/47/47/47	-
9	U10	L	304	-	-	21/39/63/87	0/1/1/1
7	BCL	J	101	-	-	2/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BCL	0	102	-	-	2/37/137/137	-
9	U10	m	404	-	-	11/45/69/87	0/1/1/1
7	BCL	L	302	-	-	4/33/133/137	-
7	BCL	F	101	-	-	4/37/137/137	-
11	SPO	o	102	-	-	25/47/47/47	-
7	BCL	y	101	-	-	2/13/113/137	-
7	BCL	r	101	-	-	2/37/137/137	-
12	PC1	H	601	-	-	32/47/47/57	-
11	SPO	u	101	-	-	25/47/47/47	-
7	BCL	v	101	-	-	13/37/137/137	-
7	BCL	L	301	-	-	3/37/137/137	-
7	BCL	i	102	-	-	2/37/137/137	-
12	PC1	c	1201	-	-	21/51/51/57	-
11	SPO	0	101	-	-	30/47/47/47	-
11	SPO	9	101	-	-	26/47/47/47	-
11	SPO	q	102	-	-	25/47/47/47	-
9	U10	l	303	-	-	21/63/87/87	0/1/1/1
7	BCL	w	101	-	-	6/37/137/137	-
11	SPO	v	102	-	-	30/47/47/47	-
8	BPH	l	305	-	-	6/25/93/105	0/5/6/6
11	SPO	J	102	-	-	30/47/47/47	-

All (910) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	G	103	SPO	C27-C28	18.80	1.53	1.34
11	p	103	SPO	C27-C28	18.76	1.53	1.34
11	E	102	SPO	C27-C28	18.62	1.53	1.34
11	p	102	SPO	C27-C28	18.50	1.53	1.34
11	t	102	SPO	C27-C28	18.47	1.53	1.34
11	J	102	SPO	C27-C28	18.30	1.53	1.34
11	G	102	SPO	C27-C28	18.29	1.53	1.34
11	n	102	SPO	C27-C28	18.28	1.53	1.34
11	u	101	SPO	C27-C28	18.28	1.53	1.34
11	j	101	SPO	C27-C28	18.27	1.53	1.34
11	D	102	SPO	C27-C28	18.26	1.53	1.34
11	Q	603	SPO	C27-C28	18.26	1.53	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	w	102	SPO	C27-C28	18.25	1.53	1.34
11	v	102	SPO	C27-C28	18.25	1.53	1.34
11	e	102	SPO	C27-C28	18.25	1.53	1.34
11	o	102	SPO	C27-C28	18.24	1.53	1.34
11	F	102	SPO	C27-C28	18.24	1.53	1.34
11	q	102	SPO	C27-C28	18.23	1.53	1.34
11	d	102	SPO	C27-C28	18.23	1.53	1.34
11	s	101	SPO	C27-C28	18.22	1.53	1.34
11	F	103	SPO	C27-C28	18.22	1.53	1.34
11	9	103	SPO	C27-C28	18.21	1.53	1.34
11	f	102	SPO	C27-C28	18.20	1.53	1.34
11	C	1203	SPO	C27-C28	18.19	1.53	1.34
11	i	103	SPO	C27-C28	18.19	1.53	1.34
11	g	101	SPO	C27-C28	18.17	1.52	1.34
11	aa	101	SPO	C27-C28	18.16	1.52	1.34
11	b	101	SPO	C27-C28	18.12	1.52	1.34
11	d	103	SPO	C27-C28	18.10	1.52	1.34
11	9	101	SPO	C27-C28	18.08	1.52	1.34
11	0	103	SPO	C27-C28	17.86	1.52	1.34
11	ab	102	SPO	C27-C28	17.80	1.52	1.34
11	M	404	SPO	C27-C28	17.76	1.52	1.34
11	0	101	SPO	C27-C28	17.73	1.52	1.34
11	m	405	SPO	C27-C28	17.70	1.52	1.34
11	b	103	SPO	C27-C28	17.41	1.52	1.34
11	J	102	SPO	C14-C12	14.30	1.54	1.35
11	p	103	SPO	C14-C12	14.22	1.54	1.35
11	G	102	SPO	C14-C12	14.16	1.54	1.35
11	t	102	SPO	C14-C12	13.98	1.54	1.35
11	G	103	SPO	C14-C12	13.96	1.54	1.35
11	n	102	SPO	C14-C12	13.95	1.54	1.35
11	j	101	SPO	C14-C12	13.87	1.54	1.35
11	w	102	SPO	C14-C12	13.74	1.54	1.35
11	E	102	SPO	C14-C12	13.70	1.53	1.35
11	v	102	SPO	C14-C12	13.54	1.53	1.35
11	g	101	SPO	C14-C12	13.54	1.53	1.35
11	M	404	SPO	C14-C12	13.53	1.53	1.35
11	m	405	SPO	C14-C12	13.53	1.53	1.35
11	o	102	SPO	C14-C12	13.51	1.53	1.35
11	i	103	SPO	C14-C12	13.51	1.53	1.35
11	F	102	SPO	C14-C12	13.50	1.53	1.35
11	f	102	SPO	C14-C12	13.50	1.53	1.35
11	Q	603	SPO	C14-C12	13.48	1.53	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	102	SPO	C14-C12	13.48	1.53	1.35
11	F	103	SPO	C14-C12	13.47	1.53	1.35
11	u	101	SPO	C14-C12	13.46	1.53	1.35
11	C	1203	SPO	C14-C12	13.46	1.53	1.35
11	9	103	SPO	C14-C12	13.45	1.53	1.35
11	s	101	SPO	C14-C12	13.45	1.53	1.35
11	d	102	SPO	C14-C12	13.43	1.53	1.35
11	q	102	SPO	C14-C12	13.43	1.53	1.35
11	aa	101	SPO	C14-C12	13.42	1.53	1.35
11	9	101	SPO	C14-C12	13.34	1.53	1.35
11	J	102	SPO	C19-C17	13.31	1.53	1.35
11	p	102	SPO	C14-C12	13.31	1.53	1.35
11	J	102	SPO	C22-C23	13.31	1.53	1.35
11	b	101	SPO	C14-C12	13.30	1.53	1.35
11	J	102	SPO	C9-C7	13.27	1.53	1.35
11	C	1203	SPO	C19-C17	13.27	1.53	1.35
11	Q	603	SPO	C19-C17	13.24	1.53	1.35
11	0	103	SPO	C14-C12	13.22	1.53	1.35
11	f	102	SPO	C19-C17	13.22	1.53	1.35
11	D	102	SPO	C19-C17	13.21	1.53	1.35
11	u	101	SPO	C19-C17	13.21	1.53	1.35
11	q	102	SPO	C19-C17	13.20	1.53	1.35
11	o	102	SPO	C19-C17	13.20	1.53	1.35
11	s	101	SPO	C19-C17	13.19	1.53	1.35
11	e	102	SPO	C14-C12	13.19	1.53	1.35
11	aa	101	SPO	C19-C17	13.19	1.53	1.35
11	d	102	SPO	C19-C17	13.18	1.53	1.35
11	G	102	SPO	C19-C17	13.18	1.53	1.35
11	9	103	SPO	C19-C17	13.16	1.53	1.35
11	i	103	SPO	C19-C17	13.16	1.53	1.35
11	F	102	SPO	C19-C17	13.14	1.53	1.35
11	g	101	SPO	C19-C17	13.14	1.53	1.35
11	j	101	SPO	C9-C7	13.13	1.53	1.35
11	E	102	SPO	C22-C23	13.12	1.53	1.35
11	b	103	SPO	C14-C12	13.12	1.53	1.35
11	F	103	SPO	C19-C17	13.11	1.53	1.35
11	t	102	SPO	C22-C23	13.09	1.53	1.35
11	G	103	SPO	C19-C17	13.06	1.53	1.35
11	e	102	SPO	C9-C7	13.06	1.53	1.35
11	v	102	SPO	C9-C7	13.05	1.53	1.35
11	0	103	SPO	C9-C7	13.05	1.53	1.35
11	G	103	SPO	C9-C7	13.05	1.53	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	ab	102	SPO	C14-C12	13.04	1.53	1.35
11	b	103	SPO	C9-C7	13.01	1.53	1.35
11	t	102	SPO	C19-C17	13.01	1.53	1.35
11	w	102	SPO	C19-C17	12.99	1.53	1.35
11	p	103	SPO	C9-C7	12.98	1.53	1.35
11	E	102	SPO	C19-C17	12.98	1.53	1.35
11	d	103	SPO	C14-C12	12.97	1.53	1.35
11	p	103	SPO	C22-C23	12.97	1.53	1.35
11	E	102	SPO	C9-C7	12.96	1.53	1.35
11	G	102	SPO	C22-C23	12.95	1.53	1.35
11	w	102	SPO	C22-C23	12.94	1.52	1.35
11	p	102	SPO	C22-C23	12.93	1.52	1.35
11	j	101	SPO	C19-C17	12.91	1.52	1.35
11	G	103	SPO	C22-C23	12.90	1.52	1.35
11	0	101	SPO	C14-C12	12.89	1.52	1.35
11	9	101	SPO	C22-C23	12.86	1.52	1.35
11	j	101	SPO	C22-C23	12.86	1.52	1.35
11	p	103	SPO	C19-C17	12.86	1.52	1.35
11	t	102	SPO	C9-C7	12.85	1.52	1.35
11	e	102	SPO	C22-C23	12.84	1.52	1.35
11	d	103	SPO	C9-C7	12.84	1.52	1.35
11	p	102	SPO	C9-C7	12.83	1.52	1.35
11	b	101	SPO	C22-C23	12.82	1.52	1.35
11	n	102	SPO	C9-C7	12.82	1.52	1.35
11	0	101	SPO	C19-C17	12.81	1.52	1.35
11	0	101	SPO	C9-C7	12.78	1.52	1.35
11	u	101	SPO	C22-C23	12.76	1.52	1.35
11	C	1203	SPO	C22-C23	12.74	1.52	1.35
11	w	102	SPO	C9-C7	12.73	1.52	1.35
11	m	405	SPO	C19-C17	12.73	1.52	1.35
11	g	101	SPO	C22-C23	12.72	1.52	1.35
11	F	103	SPO	C22-C23	12.72	1.52	1.35
11	Q	603	SPO	C22-C23	12.72	1.52	1.35
11	M	404	SPO	C19-C17	12.72	1.52	1.35
11	G	102	SPO	C9-C7	12.71	1.52	1.35
11	s	101	SPO	C22-C23	12.71	1.52	1.35
11	b	101	SPO	C19-C17	12.71	1.52	1.35
11	d	102	SPO	C22-C23	12.70	1.52	1.35
11	p	102	SPO	C19-C17	12.70	1.52	1.35
11	i	103	SPO	C22-C23	12.70	1.52	1.35
11	aa	101	SPO	C22-C23	12.69	1.52	1.35
11	D	102	SPO	C22-C23	12.69	1.52	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	q	102	SPO	C22-C23	12.68	1.52	1.35
11	F	102	SPO	C22-C23	12.68	1.52	1.35
11	9	101	SPO	C19-C17	12.67	1.52	1.35
11	9	103	SPO	C22-C23	12.66	1.52	1.35
11	f	102	SPO	C22-C23	12.66	1.52	1.35
11	0	103	SPO	C19-C17	12.64	1.52	1.35
11	o	102	SPO	C22-C23	12.62	1.52	1.35
11	0	103	SPO	C22-C23	12.60	1.52	1.35
11	9	101	SPO	C9-C7	12.59	1.52	1.35
11	d	103	SPO	C22-C23	12.59	1.52	1.35
11	b	103	SPO	C22-C23	12.58	1.52	1.35
11	b	101	SPO	C9-C7	12.57	1.52	1.35
11	v	102	SPO	C19-C17	12.57	1.52	1.35
11	m	405	SPO	C22-C23	12.55	1.52	1.35
11	b	103	SPO	C19-C17	12.55	1.52	1.35
11	n	102	SPO	C22-C23	12.51	1.52	1.35
11	M	404	SPO	C22-C23	12.51	1.52	1.35
11	d	103	SPO	C19-C17	12.49	1.52	1.35
11	e	102	SPO	C19-C17	12.46	1.52	1.35
11	m	405	SPO	C9-C7	12.43	1.52	1.35
11	q	102	SPO	C9-C7	12.40	1.52	1.35
11	f	102	SPO	C9-C7	12.39	1.52	1.35
11	o	102	SPO	C9-C7	12.39	1.52	1.35
11	M	404	SPO	C9-C7	12.37	1.52	1.35
11	i	103	SPO	C9-C7	12.37	1.52	1.35
11	aa	101	SPO	C9-C7	12.35	1.52	1.35
11	u	101	SPO	C9-C7	12.35	1.52	1.35
11	v	102	SPO	C22-C23	12.35	1.52	1.35
11	9	103	SPO	C9-C7	12.35	1.52	1.35
11	F	102	SPO	C9-C7	12.35	1.52	1.35
11	C	1203	SPO	C9-C7	12.34	1.52	1.35
11	D	102	SPO	C9-C7	12.34	1.52	1.35
11	d	102	SPO	C9-C7	12.34	1.52	1.35
11	s	101	SPO	C9-C7	12.33	1.52	1.35
11	Q	603	SPO	C9-C7	12.32	1.52	1.35
11	F	103	SPO	C9-C7	12.31	1.52	1.35
11	g	101	SPO	C9-C7	12.31	1.52	1.35
11	ab	102	SPO	C22-C23	12.29	1.52	1.35
11	ab	102	SPO	C9-C7	12.25	1.52	1.35
11	n	102	SPO	C19-C17	12.17	1.51	1.35
11	ab	102	SPO	C19-C17	12.04	1.51	1.35
11	0	101	SPO	C22-C23	11.95	1.51	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	Q	602	BCL	C16-C15	8.88	1.90	1.52
11	C	1203	SPO	C32-C33	8.81	1.54	1.33
11	G	102	SPO	C32-C33	8.81	1.54	1.33
11	9	103	SPO	C32-C33	8.79	1.54	1.33
11	d	102	SPO	C32-C33	8.79	1.54	1.33
11	aa	101	SPO	C32-C33	8.79	1.54	1.33
11	i	103	SPO	C32-C33	8.78	1.54	1.33
11	Q	603	SPO	C32-C33	8.78	1.54	1.33
11	t	102	SPO	C32-C33	8.78	1.54	1.33
11	f	102	SPO	C32-C33	8.78	1.54	1.33
11	p	102	SPO	C32-C33	8.78	1.54	1.33
11	v	102	SPO	C32-C33	8.77	1.54	1.33
11	J	102	SPO	C32-C33	8.77	1.54	1.33
11	s	101	SPO	C32-C33	8.77	1.54	1.33
11	o	102	SPO	C32-C33	8.77	1.54	1.33
11	F	102	SPO	C32-C33	8.77	1.54	1.33
11	g	101	SPO	C32-C33	8.77	1.54	1.33
11	u	101	SPO	C32-C33	8.77	1.54	1.33
11	D	102	SPO	C32-C33	8.76	1.54	1.33
11	q	102	SPO	C32-C33	8.75	1.54	1.33
11	F	103	SPO	C32-C33	8.75	1.54	1.33
11	E	102	SPO	C32-C33	8.71	1.53	1.33
11	0	101	SPO	C32-C33	8.71	1.53	1.33
11	p	103	SPO	C32-C33	8.70	1.53	1.33
11	j	101	SPO	C32-C33	8.70	1.53	1.33
11	9	101	SPO	C32-C33	8.68	1.53	1.33
11	G	103	SPO	C32-C33	8.67	1.53	1.33
11	n	102	SPO	C32-C33	8.66	1.53	1.33
11	b	101	SPO	C32-C33	8.65	1.53	1.33
11	ab	102	SPO	C32-C33	8.64	1.53	1.33
11	b	103	SPO	C32-C33	8.61	1.53	1.33
11	w	102	SPO	C32-C33	8.60	1.53	1.33
11	0	103	SPO	C32-C33	8.45	1.53	1.33
11	M	404	SPO	C32-C33	8.44	1.53	1.33
11	e	102	SPO	C32-C33	8.44	1.53	1.33
11	m	405	SPO	C32-C33	8.44	1.53	1.33
11	d	103	SPO	C32-C33	8.17	1.52	1.33
11	t	102	SPO	C37-C38	7.69	1.54	1.32
11	p	102	SPO	C37-C38	7.69	1.54	1.32
11	9	101	SPO	C37-C38	7.68	1.54	1.32
11	b	101	SPO	C37-C38	7.66	1.54	1.32
11	J	102	SPO	C37-C38	7.60	1.54	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	1203	SPO	C37-C38	7.59	1.54	1.32
11	v	102	SPO	C37-C38	7.58	1.54	1.32
11	g	101	SPO	C37-C38	7.58	1.54	1.32
11	p	103	SPO	C37-C38	7.58	1.54	1.32
11	o	102	SPO	C37-C38	7.58	1.54	1.32
11	f	102	SPO	C37-C38	7.57	1.54	1.32
11	i	103	SPO	C37-C38	7.57	1.54	1.32
11	s	101	SPO	C37-C38	7.57	1.54	1.32
11	9	103	SPO	C37-C38	7.57	1.54	1.32
11	D	102	SPO	C37-C38	7.57	1.54	1.32
11	F	102	SPO	C37-C38	7.57	1.54	1.32
11	Q	603	SPO	C37-C38	7.57	1.54	1.32
11	G	103	SPO	C37-C38	7.57	1.54	1.32
11	u	101	SPO	C37-C38	7.57	1.54	1.32
11	d	102	SPO	C37-C38	7.56	1.54	1.32
11	F	103	SPO	C37-C38	7.56	1.54	1.32
11	aa	101	SPO	C37-C38	7.55	1.54	1.32
11	q	102	SPO	C37-C38	7.54	1.54	1.32
11	G	102	SPO	C37-C38	7.53	1.54	1.32
11	E	102	SPO	C37-C38	7.53	1.54	1.32
11	j	101	SPO	C37-C38	7.52	1.54	1.32
11	0	101	SPO	C37-C38	7.51	1.53	1.32
11	ab	102	SPO	C37-C38	7.49	1.53	1.32
11	n	102	SPO	C37-C38	7.48	1.53	1.32
11	0	103	SPO	C37-C38	7.46	1.53	1.32
11	m	405	SPO	C37-C38	7.44	1.53	1.32
11	M	404	SPO	C37-C38	7.44	1.53	1.32
11	e	102	SPO	C37-C38	7.42	1.53	1.32
11	w	102	SPO	C37-C38	7.38	1.53	1.32
11	b	103	SPO	C37-C38	7.34	1.53	1.32
11	d	103	SPO	C37-C38	7.12	1.52	1.32
9	L	304	U10	C8-C9	6.19	1.47	1.33
9	L	304	U10	C18-C19	6.05	1.47	1.33
9	l	303	U10	C18-C19	5.97	1.47	1.33
9	l	303	U10	C33-C34	5.94	1.47	1.33
9	l	303	U10	C28-C29	5.93	1.47	1.33
9	l	303	U10	C38-C39	5.93	1.47	1.33
9	M	403	U10	C28-C29	5.92	1.47	1.33
9	L	304	U10	C13-C14	5.91	1.47	1.33
9	L	304	U10	C23-C24	5.91	1.47	1.33
9	m	404	U10	C28-C29	5.91	1.47	1.33
9	l	303	U10	C43-C44	5.91	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	L	304	U10	C28-C29	5.85	1.47	1.33
9	m	404	U10	C18-C19	5.83	1.47	1.33
9	L	304	U10	O4-C4	-5.82	1.22	1.36
9	l	303	U10	C23-C24	5.82	1.46	1.33
9	l	303	U10	C48-C49	5.82	1.46	1.33
9	M	403	U10	C18-C19	5.81	1.46	1.33
9	l	303	U10	C13-C14	5.81	1.46	1.33
9	M	403	U10	C33-C34	5.80	1.46	1.33
9	m	404	U10	C33-C34	5.78	1.46	1.33
9	m	404	U10	O3-C3	-5.73	1.22	1.36
9	m	404	U10	C23-C24	5.71	1.46	1.33
9	M	403	U10	O3-C3	-5.70	1.22	1.36
9	m	404	U10	C13-C14	5.69	1.46	1.33
9	M	403	U10	C23-C24	5.68	1.46	1.33
9	M	403	U10	C8-C9	5.67	1.46	1.33
9	M	403	U10	C13-C14	5.67	1.46	1.33
9	l	303	U10	C8-C9	5.66	1.46	1.33
9	m	404	U10	C8-C9	5.66	1.46	1.33
9	M	403	U10	O4-C4	-5.62	1.23	1.36
9	m	404	U10	O4-C4	-5.58	1.23	1.36
9	l	303	U10	O4-C4	-5.51	1.23	1.36
9	L	304	U10	O3-C3	-5.44	1.23	1.36
9	l	303	U10	O3-C3	-5.41	1.23	1.36
9	L	304	U10	C33-C34	5.29	1.47	1.32
9	m	404	U10	C38-C39	5.21	1.47	1.32
9	M	403	U10	C38-C39	5.19	1.47	1.32
9	l	303	U10	C53-C54	5.11	1.47	1.32
8	l	302	BPH	CBD-CGD	-4.86	1.45	1.52
7	4	101	BCL	C1B-NB	4.68	1.39	1.35
7	ab	101	BCL	MG-NA	4.67	2.17	2.06
7	e	101	BCL	MG-NA	4.66	2.17	2.06
7	J	101	BCL	MG-NA	4.66	2.17	2.06
7	g	102	BCL	MG-NA	4.66	2.17	2.06
7	O	101	BCL	C1B-NB	4.66	1.39	1.35
7	x	101	BCL	MG-NA	4.66	2.17	2.06
7	E	101	BCL	MG-NA	4.66	2.17	2.06
7	r	101	BCL	MG-NA	4.66	2.17	2.06
7	b	102	BCL	MG-NA	4.65	2.17	2.06
7	G	101	BCL	MG-NA	4.65	2.17	2.06
7	aa	102	BCL	MG-NA	4.65	2.17	2.06
7	a	101	BCL	MG-NA	4.65	2.17	2.06
7	N	101	BCL	MG-NA	4.65	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	p	101	BCL	MG-NA	4.64	2.17	2.06
7	A	1702	BCL	MG-NA	4.64	2.17	2.06
7	8	101	BCL	MG-NA	4.64	2.17	2.06
7	v	101	BCL	MG-NA	4.64	2.17	2.06
7	0	102	BCL	MG-NA	4.64	2.17	2.06
7	B	101	BCL	MG-NA	4.64	2.17	2.06
7	n	101	BCL	MG-NA	4.64	2.17	2.06
7	t	101	BCL	MG-NA	4.63	2.17	2.06
7	i	102	BCL	MG-NA	4.63	2.17	2.06
7	5	101	BCL	C1B-NB	4.61	1.39	1.35
7	w	101	BCL	C1B-NB	4.61	1.39	1.35
7	K	101	BCL	C1B-NB	4.60	1.39	1.35
7	L	301	BCL	MG-NA	4.60	2.17	2.06
7	z	101	BCL	MG-NA	4.59	2.17	2.06
7	g	102	BCL	C1B-NB	4.55	1.39	1.35
7	d	101	BCL	MG-NA	4.55	2.17	2.06
7	y	101	BCL	C1B-NB	4.55	1.39	1.35
7	o	101	BCL	MG-NA	4.54	2.17	2.06
7	Q	602	BCL	MG-NA	4.54	2.17	2.06
7	D	101	BCL	MG-NA	4.53	2.17	2.06
7	f	101	BCL	MG-NA	4.53	2.17	2.06
7	w	101	BCL	MG-NA	4.53	2.17	2.06
7	e	101	BCL	C1B-NB	4.53	1.39	1.35
7	q	103	BCL	MG-NA	4.52	2.17	2.06
7	9	102	BCL	MG-NA	4.52	2.17	2.06
7	s	102	BCL	MG-NA	4.51	2.17	2.06
7	F	101	BCL	MG-NA	4.51	2.17	2.06
7	I	101	BCL	MG-NA	4.51	2.17	2.06
7	c	1202	BCL	MG-NA	4.51	2.17	2.06
7	C	1202	BCL	MG-NA	4.51	2.17	2.06
7	q	101	BCL	MG-NA	4.51	2.17	2.06
7	k	101	BCL	MG-NA	4.51	2.17	2.06
7	5	101	BCL	MG-NA	4.50	2.17	2.06
7	i	101	BCL	MG-NA	4.50	2.16	2.06
7	y	101	BCL	MG-NA	4.49	2.16	2.06
7	B	101	BCL	C1B-NB	4.48	1.39	1.35
7	G	101	BCL	C1B-NB	4.48	1.39	1.35
7	aa	102	BCL	C1B-NB	4.48	1.39	1.35
7	L	301	BCL	C1B-NB	4.48	1.39	1.35
7	p	101	BCL	C1B-NB	4.48	1.39	1.35
7	K	101	BCL	MG-NA	4.47	2.16	2.06
7	O	101	BCL	MG-NA	4.47	2.16	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	0	102	BCL	C1B-NB	4.47	1.39	1.35
7	i	102	BCL	C1B-NB	4.47	1.39	1.35
7	v	101	BCL	C1B-NB	4.46	1.39	1.35
7	J	101	BCL	C1B-NB	4.46	1.39	1.35
7	t	101	BCL	C1B-NB	4.46	1.39	1.35
7	b	102	BCL	C1B-NB	4.45	1.39	1.35
7	l	301	BCL	MG-NA	4.44	2.16	2.06
7	l	301	BCL	C1B-NB	4.44	1.39	1.35
7	N	101	BCL	C1B-NB	4.43	1.39	1.35
7	ab	101	BCL	C1B-NB	4.43	1.39	1.35
7	8	101	BCL	C1B-NB	4.42	1.39	1.35
7	n	101	BCL	C1B-NB	4.42	1.39	1.35
7	E	101	BCL	C1B-NB	4.40	1.39	1.35
7	r	101	BCL	C1B-NB	4.40	1.39	1.35
7	z	101	BCL	C1B-NB	4.39	1.39	1.35
7	L	302	BCL	MG-NA	4.39	2.16	2.06
7	m	401	BCL	C1B-NB	4.37	1.39	1.35
7	x	101	BCL	C1B-NB	4.37	1.39	1.35
7	M	402	BCL	MG-NA	4.37	2.16	2.06
7	m	403	BCL	MG-NA	4.35	2.16	2.06
8	l	305	BPH	CBD-CGD	-4.35	1.46	1.52
8	L	306	BPH	CBD-CGD	-4.32	1.46	1.52
7	L	305	BCL	C1B-NB	4.30	1.39	1.35
7	q	103	BCL	C1B-NB	4.28	1.39	1.35
7	l	304	BCL	C1B-NB	4.28	1.39	1.35
7	D	101	BCL	C1B-NB	4.26	1.39	1.35
7	l	304	BCL	MG-NA	4.24	2.16	2.06
7	L	305	BCL	MG-NA	4.23	2.16	2.06
7	C	1202	BCL	C1B-NB	4.22	1.39	1.35
7	4	101	BCL	MG-NA	4.21	2.16	2.06
11	J	102	SPO	C11-C12	4.21	1.55	1.45
8	L	303	BPH	CBD-CGD	-4.21	1.46	1.52
7	L	302	BCL	C1B-NB	4.20	1.39	1.35
7	s	102	BCL	C1B-NB	4.19	1.38	1.35
7	f	101	BCL	C1B-NB	4.19	1.38	1.35
7	i	101	BCL	C1B-NB	4.18	1.38	1.35
11	j	101	SPO	C11-C12	4.18	1.54	1.45
7	c	1202	BCL	C1B-NB	4.18	1.38	1.35
7	m	401	BCL	MG-NA	4.17	2.16	2.06
7	F	101	BCL	C1B-NB	4.17	1.38	1.35
7	o	101	BCL	C1B-NB	4.17	1.38	1.35
7	Q	602	BCL	C1B-NB	4.15	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	d	101	BCL	C1B-NB	4.14	1.38	1.35
7	9	102	BCL	C1B-NB	4.14	1.38	1.35
7	k	101	BCL	C1B-NB	4.14	1.38	1.35
7	q	101	BCL	C1B-NB	4.13	1.38	1.35
7	M	402	BCL	C1B-NB	4.13	1.38	1.35
7	Q	602	BCL	C16-C17	4.11	1.69	1.52
7	I	101	BCL	C1B-NB	4.08	1.38	1.35
7	m	403	BCL	C1B-NB	4.07	1.38	1.35
11	J	102	SPO	C15-C14	4.06	1.56	1.43
11	E	102	SPO	C11-C12	4.01	1.54	1.45
11	t	102	SPO	C20-C19	4.01	1.55	1.43
11	p	103	SPO	C20-C19	4.01	1.55	1.43
11	J	102	SPO	C10-C9	4.01	1.55	1.43
11	J	102	SPO	C20-C19	3.99	1.55	1.43
11	G	103	SPO	C20-C19	3.99	1.55	1.43
11	E	102	SPO	C20-C19	3.97	1.55	1.43
11	J	102	SPO	C6-C7	3.96	1.54	1.45
11	G	103	SPO	C11-C12	3.94	1.54	1.45
11	F	102	SPO	C20-C19	3.93	1.55	1.43
11	d	103	SPO	C6-C7	3.93	1.54	1.45
11	j	101	SPO	C15-C14	3.93	1.55	1.43
11	d	102	SPO	C20-C19	3.93	1.55	1.43
11	u	101	SPO	C20-C19	3.92	1.55	1.43
11	q	102	SPO	C20-C19	3.92	1.55	1.43
11	o	102	SPO	C20-C19	3.92	1.55	1.43
11	f	102	SPO	C20-C19	3.92	1.55	1.43
11	F	103	SPO	C20-C19	3.91	1.55	1.43
11	9	103	SPO	C20-C19	3.91	1.55	1.43
11	j	101	SPO	C10-C9	3.91	1.55	1.43
11	aa	101	SPO	C20-C19	3.91	1.55	1.43
11	J	102	SPO	C16-C17	3.91	1.54	1.45
11	D	102	SPO	C20-C19	3.91	1.55	1.43
11	J	102	SPO	C21-C22	3.91	1.55	1.43
11	C	1203	SPO	C20-C19	3.91	1.55	1.43
7	A	1702	BCL	C1B-NB	3.90	1.38	1.35
11	s	101	SPO	C20-C19	3.90	1.55	1.43
11	i	103	SPO	C20-C19	3.90	1.55	1.43
11	j	101	SPO	C20-C19	3.90	1.55	1.43
11	g	101	SPO	C20-C19	3.89	1.55	1.43
11	Q	603	SPO	C20-C19	3.89	1.55	1.43
11	p	103	SPO	C15-C14	3.89	1.55	1.43
11	0	103	SPO	C6-C7	3.88	1.54	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	G	102	SPO	C20-C19	3.87	1.55	1.43
11	w	102	SPO	C20-C19	3.86	1.55	1.43
7	a	101	BCL	C1B-NB	3.86	1.38	1.35
11	b	101	SPO	C20-C19	3.85	1.55	1.43
13	m	406	CDL	OB6-CB5	3.85	1.45	1.34
11	G	102	SPO	C15-C14	3.84	1.55	1.43
11	p	102	SPO	C20-C19	3.84	1.55	1.43
11	9	101	SPO	C15-C14	3.84	1.55	1.43
11	0	103	SPO	C10-C9	3.84	1.55	1.43
11	0	101	SPO	C20-C19	3.84	1.55	1.43
11	v	102	SPO	C10-C9	3.83	1.55	1.43
11	b	101	SPO	C15-C14	3.83	1.55	1.43
11	E	102	SPO	C15-C14	3.83	1.55	1.43
11	9	101	SPO	C20-C19	3.83	1.55	1.43
11	G	102	SPO	C11-C12	3.83	1.54	1.45
11	G	103	SPO	C15-C14	3.83	1.55	1.43
11	G	103	SPO	C6-C7	3.82	1.54	1.45
11	p	103	SPO	C11-C12	3.82	1.54	1.45
11	E	102	SPO	C21-C22	3.82	1.55	1.43
11	n	102	SPO	C15-C14	3.81	1.55	1.43
11	Q	603	SPO	C15-C14	3.81	1.55	1.43
11	F	103	SPO	C15-C14	3.80	1.55	1.43
11	o	102	SPO	C15-C14	3.80	1.55	1.43
11	0	103	SPO	C20-C19	3.80	1.55	1.43
11	q	102	SPO	C15-C14	3.80	1.55	1.43
11	p	103	SPO	C10-C9	3.80	1.55	1.43
11	u	101	SPO	C15-C14	3.80	1.55	1.43
11	G	102	SPO	C21-C22	3.79	1.55	1.43
11	E	102	SPO	C6-C7	3.79	1.54	1.45
11	p	102	SPO	C11-C12	3.79	1.54	1.45
11	D	102	SPO	C15-C14	3.79	1.55	1.43
11	C	1203	SPO	C15-C14	3.79	1.55	1.43
11	m	405	SPO	C20-C19	3.79	1.55	1.43
11	F	102	SPO	C15-C14	3.78	1.55	1.43
11	f	102	SPO	C15-C14	3.78	1.55	1.43
11	s	101	SPO	C15-C14	3.78	1.55	1.43
11	9	103	SPO	C15-C14	3.78	1.55	1.43
11	d	102	SPO	C15-C14	3.78	1.55	1.43
11	aa	101	SPO	C15-C14	3.78	1.55	1.43
11	j	101	SPO	C6-C7	3.78	1.54	1.45
11	e	102	SPO	C10-C9	3.78	1.55	1.43
11	t	102	SPO	C11-C12	3.78	1.54	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	i	103	SPO	C15-C14	3.78	1.55	1.43
11	g	101	SPO	C15-C14	3.77	1.55	1.43
11	t	102	SPO	C15-C14	3.77	1.55	1.43
11	E	102	SPO	C10-C9	3.77	1.55	1.43
11	e	102	SPO	C20-C19	3.76	1.55	1.43
11	9	101	SPO	C10-C9	3.76	1.55	1.43
11	M	404	SPO	C20-C19	3.76	1.55	1.43
11	0	103	SPO	C11-C12	3.75	1.54	1.45
11	w	102	SPO	C15-C14	3.75	1.55	1.43
11	0	103	SPO	C15-C14	3.75	1.55	1.43
11	b	101	SPO	C10-C9	3.75	1.55	1.43
11	p	102	SPO	C10-C9	3.74	1.55	1.43
11	w	102	SPO	C11-C12	3.73	1.54	1.45
11	p	102	SPO	C15-C14	3.73	1.55	1.43
11	p	103	SPO	C21-C22	3.73	1.55	1.43
11	b	101	SPO	C11-C12	3.73	1.54	1.45
11	G	103	SPO	C21-C22	3.73	1.55	1.43
11	t	102	SPO	C21-C22	3.72	1.55	1.43
11	n	102	SPO	C11-C12	3.72	1.53	1.45
11	G	103	SPO	C10-C9	3.72	1.55	1.43
11	w	102	SPO	C21-C22	3.72	1.55	1.43
11	p	102	SPO	C21-C22	3.71	1.55	1.43
11	d	103	SPO	C20-C19	3.71	1.55	1.43
11	t	102	SPO	C6-C7	3.71	1.53	1.45
11	d	102	SPO	C21-C22	3.71	1.54	1.43
11	F	103	SPO	C10-C9	3.71	1.54	1.43
11	F	102	SPO	C10-C9	3.70	1.54	1.43
11	v	102	SPO	C20-C19	3.70	1.54	1.43
11	9	103	SPO	C10-C9	3.70	1.54	1.43
11	D	102	SPO	C21-C22	3.70	1.54	1.43
11	D	102	SPO	C10-C9	3.70	1.54	1.43
11	9	101	SPO	C21-C22	3.70	1.54	1.43
11	ab	102	SPO	C20-C19	3.70	1.54	1.43
11	G	102	SPO	C10-C9	3.70	1.54	1.43
11	b	101	SPO	C21-C22	3.70	1.54	1.43
11	q	102	SPO	C10-C9	3.70	1.54	1.43
11	g	101	SPO	C10-C9	3.69	1.54	1.43
11	C	1203	SPO	C10-C9	3.69	1.54	1.43
11	Q	603	SPO	C21-C22	3.69	1.54	1.43
11	9	103	SPO	C21-C22	3.69	1.54	1.43
11	s	101	SPO	C10-C9	3.69	1.54	1.43
11	M	404	SPO	C15-C14	3.69	1.54	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	o	102	SPO	C21-C22	3.69	1.54	1.43
11	F	103	SPO	C21-C22	3.69	1.54	1.43
11	C	1203	SPO	C21-C22	3.69	1.54	1.43
11	i	103	SPO	C10-C9	3.69	1.54	1.43
11	u	101	SPO	C10-C9	3.69	1.54	1.43
11	aa	101	SPO	C21-C22	3.69	1.54	1.43
11	u	101	SPO	C21-C22	3.69	1.54	1.43
11	aa	101	SPO	C10-C9	3.69	1.54	1.43
11	o	102	SPO	C10-C9	3.69	1.54	1.43
11	d	102	SPO	C10-C9	3.68	1.54	1.43
11	Q	603	SPO	C10-C9	3.68	1.54	1.43
11	m	405	SPO	C15-C14	3.68	1.54	1.43
11	g	101	SPO	C21-C22	3.68	1.54	1.43
11	n	102	SPO	C21-C22	3.68	1.54	1.43
11	i	103	SPO	C21-C22	3.68	1.54	1.43
11	q	102	SPO	C21-C22	3.68	1.54	1.43
11	d	103	SPO	C10-C9	3.68	1.54	1.43
11	t	102	SPO	C16-C17	3.68	1.53	1.45
11	f	102	SPO	C21-C22	3.68	1.54	1.43
11	d	103	SPO	C21-C22	3.67	1.54	1.43
11	f	102	SPO	C10-C9	3.67	1.54	1.43
11	9	101	SPO	C11-C12	3.67	1.53	1.45
11	s	101	SPO	C21-C22	3.67	1.54	1.43
11	0	103	SPO	C21-C22	3.67	1.54	1.43
11	F	102	SPO	C21-C22	3.66	1.54	1.43
11	p	102	SPO	C6-C7	3.66	1.53	1.45
11	j	101	SPO	C21-C22	3.66	1.54	1.43
11	b	103	SPO	C20-C19	3.66	1.54	1.43
11	v	102	SPO	C15-C14	3.65	1.54	1.43
11	b	103	SPO	C10-C9	3.65	1.54	1.43
11	f	102	SPO	C11-C12	3.65	1.53	1.45
11	e	102	SPO	C21-C22	3.65	1.54	1.43
11	ab	102	SPO	C6-C7	3.65	1.53	1.45
11	u	101	SPO	C11-C12	3.64	1.53	1.45
11	t	102	SPO	C10-C9	3.64	1.54	1.43
11	i	103	SPO	C11-C12	3.64	1.53	1.45
11	C	1203	SPO	C11-C12	3.64	1.53	1.45
11	n	102	SPO	C6-C7	3.64	1.53	1.45
11	aa	101	SPO	C11-C12	3.64	1.53	1.45
11	G	103	SPO	C16-C17	3.63	1.53	1.45
11	e	102	SPO	C6-C7	3.63	1.53	1.45
11	m	405	SPO	C10-C9	3.63	1.54	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	q	102	SPO	C11-C12	3.63	1.53	1.45
11	n	102	SPO	C10-C9	3.63	1.54	1.43
11	D	102	SPO	C11-C12	3.62	1.53	1.45
11	w	102	SPO	C6-C7	3.62	1.53	1.45
11	F	103	SPO	C11-C12	3.62	1.53	1.45
11	M	404	SPO	C10-C9	3.62	1.54	1.43
11	e	102	SPO	C15-C14	3.62	1.54	1.43
11	g	101	SPO	C11-C12	3.62	1.53	1.45
11	Q	603	SPO	C11-C12	3.62	1.53	1.45
11	p	103	SPO	C6-C7	3.62	1.53	1.45
9	L	304	U10	C3-C2	-3.61	1.38	1.48
11	s	101	SPO	C11-C12	3.61	1.53	1.45
9	m	404	U10	C3-C2	-3.61	1.38	1.48
11	F	102	SPO	C11-C12	3.61	1.53	1.45
11	0	101	SPO	C6-C7	3.61	1.53	1.45
11	b	103	SPO	C15-C14	3.61	1.54	1.43
9	M	403	U10	C3-C2	-3.61	1.38	1.48
11	n	102	SPO	C20-C19	3.60	1.54	1.43
11	d	102	SPO	C11-C12	3.60	1.53	1.45
11	o	102	SPO	C11-C12	3.60	1.53	1.45
11	w	102	SPO	C16-C17	3.60	1.53	1.45
11	9	103	SPO	C11-C12	3.60	1.53	1.45
11	w	102	SPO	C10-C9	3.60	1.54	1.43
11	G	102	SPO	C6-C7	3.59	1.53	1.45
11	M	404	SPO	C21-C22	3.59	1.54	1.43
11	b	103	SPO	C6-C7	3.58	1.53	1.45
11	v	102	SPO	C11-C12	3.58	1.53	1.45
11	s	101	SPO	C16-C17	3.58	1.53	1.45
11	G	102	SPO	C16-C17	3.57	1.53	1.45
11	m	405	SPO	C21-C22	3.57	1.54	1.43
11	d	102	SPO	C16-C17	3.57	1.53	1.45
11	C	1203	SPO	C16-C17	3.57	1.53	1.45
11	v	102	SPO	C21-C22	3.57	1.54	1.43
11	d	103	SPO	C15-C14	3.56	1.54	1.43
11	F	103	SPO	C16-C17	3.56	1.53	1.45
11	G	103	SPO	C26-C27	3.56	1.54	1.43
11	aa	101	SPO	C16-C17	3.55	1.53	1.45
11	F	102	SPO	C16-C17	3.55	1.53	1.45
11	Q	603	SPO	C16-C17	3.54	1.53	1.45
11	i	103	SPO	C16-C17	3.54	1.53	1.45
11	M	404	SPO	C11-C12	3.54	1.53	1.45
11	g	101	SPO	C16-C17	3.53	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	q	102	SPO	C16-C17	3.53	1.53	1.45
11	o	102	SPO	C16-C17	3.52	1.53	1.45
11	j	101	SPO	C16-C17	3.52	1.53	1.45
11	0	101	SPO	C15-C14	3.52	1.54	1.43
11	J	102	SPO	C26-C27	3.52	1.54	1.43
11	u	101	SPO	C16-C17	3.52	1.53	1.45
11	9	101	SPO	C16-C17	3.52	1.53	1.45
11	0	101	SPO	C21-C22	3.52	1.54	1.43
11	D	102	SPO	C16-C17	3.51	1.53	1.45
11	m	405	SPO	C11-C12	3.51	1.53	1.45
11	d	103	SPO	C11-C12	3.51	1.53	1.45
11	b	101	SPO	C16-C17	3.51	1.53	1.45
11	j	101	SPO	C26-C27	3.51	1.54	1.43
9	L	304	U10	C4-C5	-3.51	1.38	1.48
11	f	102	SPO	C16-C17	3.51	1.53	1.45
11	ab	102	SPO	C21-C22	3.50	1.54	1.43
11	0	101	SPO	C10-C9	3.50	1.54	1.43
11	9	103	SPO	C16-C17	3.50	1.53	1.45
11	p	103	SPO	C16-C17	3.49	1.53	1.45
11	0	101	SPO	C11-C12	3.49	1.53	1.45
11	e	102	SPO	C11-C12	3.48	1.53	1.45
11	G	103	SPO	C25-C23	3.48	1.53	1.45
11	ab	102	SPO	C10-C9	3.48	1.54	1.43
11	9	101	SPO	C26-C27	3.47	1.54	1.43
11	p	103	SPO	C26-C27	3.47	1.54	1.43
11	v	102	SPO	C6-C7	3.47	1.53	1.45
9	l	303	U10	C4-C5	-3.46	1.38	1.48
11	b	103	SPO	C21-C22	3.46	1.54	1.43
11	M	404	SPO	C6-C7	3.46	1.53	1.45
11	m	405	SPO	C6-C7	3.45	1.53	1.45
11	b	101	SPO	C26-C27	3.45	1.54	1.43
11	ab	102	SPO	C15-C14	3.44	1.54	1.43
11	w	102	SPO	C25-C23	3.44	1.53	1.45
9	l	303	U10	C3-C2	-3.44	1.39	1.48
11	j	101	SPO	C25-C23	3.44	1.53	1.45
11	p	103	SPO	C25-C23	3.43	1.53	1.45
11	ab	102	SPO	C11-C12	3.43	1.53	1.45
11	F	103	SPO	C26-C27	3.43	1.54	1.43
11	F	102	SPO	C26-C27	3.43	1.54	1.43
11	o	102	SPO	C26-C27	3.42	1.54	1.43
11	q	102	SPO	C26-C27	3.42	1.54	1.43
11	aa	101	SPO	C26-C27	3.42	1.54	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	i	103	SPO	C26-C27	3.42	1.54	1.43
11	9	103	SPO	C26-C27	3.42	1.54	1.43
11	n	102	SPO	C26-C27	3.42	1.54	1.43
11	b	103	SPO	C11-C12	3.42	1.53	1.45
11	Q	603	SPO	C26-C27	3.42	1.54	1.43
11	D	102	SPO	C6-C7	3.41	1.53	1.45
11	f	102	SPO	C25-C23	3.41	1.53	1.45
11	t	102	SPO	C26-C27	3.41	1.54	1.43
11	C	1203	SPO	C25-C23	3.41	1.53	1.45
11	C	1203	SPO	C26-C27	3.41	1.54	1.43
11	M	404	SPO	C16-C17	3.41	1.53	1.45
11	E	102	SPO	C16-C17	3.41	1.53	1.45
11	m	405	SPO	C16-C17	3.41	1.53	1.45
11	0	103	SPO	C16-C17	3.41	1.53	1.45
11	s	101	SPO	C25-C23	3.41	1.53	1.45
9	m	404	U10	C4-C5	-3.41	1.39	1.48
11	g	101	SPO	C26-C27	3.41	1.54	1.43
11	s	101	SPO	C26-C27	3.41	1.54	1.43
11	Q	603	SPO	C25-C23	3.41	1.53	1.45
11	p	102	SPO	C26-C27	3.41	1.54	1.43
11	u	101	SPO	C25-C23	3.41	1.53	1.45
11	aa	101	SPO	C25-C23	3.40	1.53	1.45
11	f	102	SPO	C26-C27	3.40	1.54	1.43
11	Q	603	SPO	C6-C7	3.40	1.53	1.45
11	d	102	SPO	C26-C27	3.40	1.54	1.43
11	u	101	SPO	C26-C27	3.40	1.54	1.43
11	D	102	SPO	C26-C27	3.40	1.54	1.43
11	s	101	SPO	C6-C7	3.40	1.53	1.45
11	f	102	SPO	C6-C7	3.40	1.53	1.45
11	i	103	SPO	C25-C23	3.39	1.53	1.45
11	d	102	SPO	C6-C7	3.39	1.53	1.45
11	d	102	SPO	C25-C23	3.39	1.53	1.45
11	o	102	SPO	C25-C23	3.39	1.53	1.45
11	F	102	SPO	C6-C7	3.39	1.53	1.45
9	M	403	U10	C4-C5	-3.39	1.39	1.48
11	F	103	SPO	C25-C23	3.39	1.53	1.45
11	e	102	SPO	C26-C27	3.39	1.53	1.43
11	F	103	SPO	C6-C7	3.38	1.53	1.45
11	aa	101	SPO	C6-C7	3.38	1.53	1.45
11	q	102	SPO	C25-C23	3.38	1.53	1.45
11	p	102	SPO	C25-C23	3.38	1.53	1.45
11	0	103	SPO	C26-C27	3.38	1.53	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	102	SPO	C25-C23	3.38	1.53	1.45
11	v	102	SPO	C26-C27	3.37	1.53	1.43
11	o	102	SPO	C6-C7	3.37	1.53	1.45
11	g	101	SPO	C6-C7	3.37	1.53	1.45
11	E	102	SPO	C25-C23	3.37	1.53	1.45
11	9	103	SPO	C25-C23	3.37	1.53	1.45
11	i	103	SPO	C6-C7	3.37	1.53	1.45
11	q	102	SPO	C6-C7	3.37	1.53	1.45
11	u	101	SPO	C6-C7	3.36	1.53	1.45
11	e	102	SPO	C25-C23	3.36	1.53	1.45
11	9	103	SPO	C6-C7	3.36	1.53	1.45
11	g	101	SPO	C25-C23	3.36	1.53	1.45
11	D	102	SPO	C25-C23	3.35	1.53	1.45
11	C	1203	SPO	C6-C7	3.35	1.53	1.45
11	d	103	SPO	C26-C27	3.34	1.53	1.43
11	E	102	SPO	C26-C27	3.34	1.53	1.43
11	G	102	SPO	C25-C23	3.34	1.53	1.45
11	G	102	SPO	C26-C27	3.34	1.53	1.43
11	m	405	SPO	C26-C27	3.33	1.53	1.43
11	b	101	SPO	C6-C7	3.32	1.53	1.45
11	w	102	SPO	C26-C27	3.32	1.53	1.43
11	0	101	SPO	C16-C17	3.31	1.53	1.45
11	M	404	SPO	C26-C27	3.31	1.53	1.43
11	J	102	SPO	C25-C23	3.31	1.53	1.45
11	v	102	SPO	C16-C17	3.28	1.53	1.45
11	d	103	SPO	C25-C23	3.28	1.53	1.45
11	n	102	SPO	C25-C23	3.28	1.53	1.45
11	n	102	SPO	C16-C17	3.28	1.53	1.45
12	C	1201	PC1	O31-C31	3.27	1.42	1.33
11	9	101	SPO	C6-C7	3.27	1.53	1.45
11	0	101	SPO	C26-C27	3.25	1.53	1.43
11	0	101	SPO	C25-C23	3.25	1.52	1.45
11	t	102	SPO	C25-C23	3.25	1.52	1.45
11	9	101	SPO	C25-C23	3.24	1.52	1.45
11	b	103	SPO	C26-C27	3.23	1.53	1.43
11	b	101	SPO	C25-C23	3.23	1.52	1.45
11	ab	102	SPO	C26-C27	3.23	1.53	1.43
11	p	102	SPO	C16-C17	3.22	1.52	1.45
12	A	1701	PC1	O21-C21	3.21	1.43	1.34
7	0	102	BCL	MG-NC	3.20	2.13	2.06
7	G	101	BCL	MG-NC	3.20	2.13	2.06
7	p	101	BCL	MG-NC	3.19	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	0	103	SPO	C25-C23	3.19	1.52	1.45
7	N	101	BCL	MG-NC	3.19	2.13	2.06
7	n	101	BCL	MG-NC	3.19	2.13	2.06
7	8	101	BCL	MG-NC	3.19	2.13	2.06
7	E	101	BCL	MG-NC	3.19	2.13	2.06
7	ab	101	BCL	MG-NC	3.18	2.13	2.06
7	t	101	BCL	MG-NC	3.18	2.13	2.06
7	g	102	BCL	MG-NC	3.18	2.13	2.06
7	aa	102	BCL	MG-NC	3.18	2.13	2.06
7	r	101	BCL	MG-NC	3.18	2.13	2.06
7	B	101	BCL	MG-NC	3.18	2.13	2.06
7	b	102	BCL	MG-NC	3.17	2.13	2.06
7	x	101	BCL	MG-NC	3.17	2.13	2.06
7	e	101	BCL	MG-NC	3.17	2.13	2.06
7	i	102	BCL	MG-NC	3.17	2.13	2.06
7	J	101	BCL	MG-NC	3.17	2.13	2.06
12	A	1701	PC1	O31-C31	3.16	1.42	1.33
11	v	102	SPO	C25-C23	3.15	1.52	1.45
11	b	103	SPO	C16-C17	3.14	1.52	1.45
11	e	102	SPO	C16-C17	3.13	1.52	1.45
12	H	602	PC1	O31-C31	3.12	1.42	1.33
11	b	103	SPO	C25-C23	3.11	1.52	1.45
11	d	103	SPO	C16-C17	3.11	1.52	1.45
12	A	1703	PC1	O31-C31	3.10	1.42	1.33
12	h	301	PC1	O31-C31	3.10	1.42	1.33
13	m	406	CDL	OA6-CA4	-3.09	1.38	1.46
7	l	301	BCL	O1A-CGA	-3.09	1.13	1.22
11	M	404	SPO	C25-C23	3.08	1.52	1.45
12	a	102	PC1	O31-C31	3.08	1.42	1.33
12	c	1201	PC1	O31-C31	3.08	1.42	1.33
13	m	406	CDL	OA8-CA7	3.07	1.42	1.33
11	m	405	SPO	C25-C23	3.07	1.52	1.45
12	H	601	PC1	O31-C31	3.06	1.42	1.33
11	ab	102	SPO	C25-C23	3.05	1.52	1.45
7	4	101	BCL	MG-NC	3.05	2.13	2.06
7	L	301	BCL	MG-NC	2.99	2.13	2.06
12	c	1201	PC1	O21-C21	2.99	1.42	1.34
7	O	101	BCL	MG-NC	2.98	2.13	2.06
7	y	101	BCL	MG-NC	2.98	2.13	2.06
7	A	1702	BCL	MG-NC	2.98	2.13	2.06
12	Q	601	PC1	O31-C31	2.98	1.42	1.33
7	a	101	BCL	MG-NC	2.98	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	w	101	BCL	MG-NC	2.98	2.13	2.06
7	5	101	BCL	MG-NC	2.98	2.13	2.06
7	K	101	BCL	MG-NC	2.97	2.13	2.06
12	Q	601	PC1	O21-C21	2.96	1.42	1.34
12	C	1201	PC1	O21-C21	2.96	1.42	1.34
12	h	301	PC1	O21-C21	2.90	1.42	1.34
7	z	101	BCL	MG-NC	2.88	2.13	2.06
7	i	101	BCL	MG-NC	2.88	2.13	2.06
12	H	601	PC1	O21-C21	2.88	1.42	1.34
7	q	101	BCL	MG-NC	2.87	2.13	2.06
7	C	1202	BCL	MG-NC	2.87	2.13	2.06
7	I	101	BCL	MG-NC	2.86	2.13	2.06
7	q	103	BCL	MG-NC	2.86	2.13	2.06
8	L	303	BPH	O1A-CGA	-2.86	1.14	1.22
7	s	102	BCL	MG-NC	2.85	2.13	2.06
7	c	1202	BCL	MG-NC	2.85	2.13	2.06
7	F	101	BCL	MG-NC	2.84	2.13	2.06
7	f	101	BCL	MG-NC	2.84	2.13	2.06
11	ab	102	SPO	C16-C17	2.84	1.52	1.45
7	d	101	BCL	MG-NC	2.84	2.13	2.06
7	k	101	BCL	MG-NC	2.83	2.13	2.06
7	o	101	BCL	MG-NC	2.83	2.13	2.06
12	a	102	PC1	O21-C21	2.83	1.42	1.34
7	9	102	BCL	MG-NC	2.83	2.13	2.06
12	A	1703	PC1	O21-C21	2.83	1.42	1.34
7	D	101	BCL	MG-NC	2.83	2.13	2.06
9	m	404	U10	C6-C5	-2.82	1.38	1.46
12	H	602	PC1	O21-C2	-2.81	1.39	1.46
9	M	403	U10	C6-C5	-2.81	1.38	1.46
7	Q	602	BCL	MG-NC	2.81	2.12	2.06
7	v	101	BCL	MG-NC	2.80	2.12	2.06
7	l	304	BCL	MG-NC	2.78	2.12	2.06
7	L	305	BCL	MG-NC	2.76	2.12	2.06
12	H	602	PC1	O21-C21	2.75	1.42	1.34
11	d	103	SPO	C4-C5	2.74	1.54	1.50
7	L	302	BCL	MG-NC	2.72	2.12	2.06
7	l	301	BCL	MG-NC	2.72	2.12	2.06
7	m	401	BCL	O1A-CGA	-2.72	1.14	1.22
11	0	103	SPO	C4-C5	2.71	1.54	1.50
11	p	102	SPO	C4-C5	2.71	1.54	1.50
11	G	103	SPO	C4-C5	2.70	1.54	1.50
7	M	402	BCL	MG-NC	2.69	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	m	403	BCL	MG-NC	2.68	2.12	2.06
13	m	406	CDL	OB8-CB7	2.65	1.41	1.33
7	m	401	BCL	MG-NC	2.64	2.12	2.06
9	l	303	U10	C6-C5	-2.64	1.39	1.46
11	J	102	SPO	C4-C5	2.64	1.54	1.50
11	v	102	SPO	C4-C5	2.63	1.54	1.50
7	A	1702	BCL	O1A-CGA	-2.63	1.14	1.22
9	L	304	U10	C6-C5	-2.62	1.39	1.46
12	h	301	PC1	O21-C2	-2.61	1.40	1.46
11	j	101	SPO	C4-C5	2.61	1.54	1.50
13	m	406	CDL	OA6-CA5	2.60	1.41	1.34
7	a	101	BCL	O1A-CGA	-2.60	1.14	1.22
11	G	102	SPO	C4-C5	2.60	1.54	1.50
11	p	103	SPO	C4-C5	2.59	1.54	1.50
12	a	102	PC1	O21-C2	-2.59	1.40	1.46
12	H	601	PC1	O21-C2	-2.59	1.40	1.46
11	E	102	SPO	C4-C5	2.59	1.54	1.50
11	t	102	SPO	C4-C5	2.59	1.54	1.50
12	A	1703	PC1	O21-C2	-2.59	1.40	1.46
12	C	1201	PC1	O21-C2	-2.58	1.40	1.46
12	c	1201	PC1	O21-C2	-2.56	1.40	1.46
7	L	302	BCL	O1A-CGA	-2.53	1.15	1.22
11	n	102	SPO	C4-C5	2.52	1.54	1.50
13	m	406	CDL	C51-CB5	2.52	1.58	1.50
11	m	405	SPO	C4-C5	2.52	1.54	1.50
9	M	403	U10	C1-C2	-2.50	1.38	1.47
9	m	404	U10	C1-C2	-2.49	1.38	1.47
11	M	404	SPO	C4-C5	2.47	1.54	1.50
11	ab	102	SPO	C4-C5	2.46	1.54	1.50
11	o	101	SPO	C4-C5	2.45	1.54	1.50
7	M	402	BCL	O1A-CGA	-2.42	1.15	1.22
7	m	403	BCL	O1A-CGA	-2.41	1.15	1.22
7	z	101	BCL	OBD-CAD	2.41	1.25	1.22
11	b	103	SPO	C4-C5	2.40	1.54	1.50
9	L	304	U10	C1-C2	-2.39	1.38	1.47
8	L	306	BPH	C3A-C2A	-2.37	1.52	1.54
11	w	102	SPO	C4-C5	2.36	1.53	1.50
12	Q	601	PC1	O21-C2	-2.35	1.40	1.46
11	aa	101	SPO	C4-C5	2.32	1.53	1.50
11	b	101	SPO	C4-C5	2.32	1.53	1.50
11	9	103	SPO	C4-C5	2.31	1.53	1.50
8	l	305	BPH	C3A-C2A	-2.31	1.52	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	d	102	SPO	C4-C5	2.30	1.53	1.50
11	f	102	SPO	C4-C5	2.30	1.53	1.50
11	C	1203	SPO	C4-C5	2.29	1.53	1.50
9	l	303	U10	C1-C2	-2.29	1.39	1.47
9	L	304	U10	C6-C1	2.28	1.39	1.35
11	Q	603	SPO	C4-C5	2.28	1.53	1.50
11	e	102	SPO	C4-C5	2.28	1.53	1.50
11	o	102	SPO	C4-C5	2.28	1.53	1.50
11	s	101	SPO	C4-C5	2.28	1.53	1.50
11	9	101	SPO	C4-C5	2.28	1.53	1.50
11	i	103	SPO	C4-C5	2.28	1.53	1.50
11	F	102	SPO	C4-C5	2.27	1.53	1.50
11	q	102	SPO	C4-C5	2.27	1.53	1.50
7	l	301	BCL	C3C-C4C	-2.27	1.48	1.51
11	D	102	SPO	C4-C5	2.26	1.53	1.50
11	g	101	SPO	C4-C5	2.26	1.53	1.50
11	F	103	SPO	C4-C5	2.26	1.53	1.50
7	L	301	BCL	O1A-CGA	-2.26	1.15	1.22
11	u	101	SPO	C4-C5	2.25	1.53	1.50
12	A	1701	PC1	O21-C2	-2.22	1.41	1.46
8	l	302	BPH	O1A-CGA	-2.18	1.16	1.22
8	l	302	BPH	C1C-C2C	-2.17	1.47	1.51
8	L	303	BPH	O2A-CGA	-2.17	1.27	1.33
7	M	402	BCL	CBD-CGD	-2.13	1.45	1.52
7	m	403	BCL	CBD-CGD	-2.11	1.45	1.52
9	M	403	U10	C6-C1	2.11	1.39	1.35
9	m	404	U10	C6-C1	2.10	1.39	1.35
7	I	101	BCL	O1A-CGA	-2.09	1.16	1.22
7	F	101	BCL	O1A-CGA	-2.09	1.16	1.22
8	l	302	BPH	C4A-C3A	-2.09	1.47	1.51
7	s	102	BCL	O1A-CGA	-2.08	1.16	1.22
7	c	1202	BCL	O1A-CGA	-2.07	1.16	1.22
7	C	1202	BCL	O1A-CGA	-2.07	1.16	1.22
7	i	101	BCL	O1A-CGA	-2.07	1.16	1.22
13	m	406	CDL	PA1-OA5	2.07	1.67	1.59
7	D	101	BCL	O1A-CGA	-2.07	1.16	1.22
7	Q	602	BCL	O1A-CGA	-2.07	1.16	1.22
7	l	301	BCL	C3D-CAD	-2.07	1.40	1.46
7	d	101	BCL	O1A-CGA	-2.06	1.16	1.22
7	k	101	BCL	O1A-CGA	-2.06	1.16	1.22
7	q	101	BCL	O1A-CGA	-2.06	1.16	1.22
7	q	103	BCL	O1A-CGA	-2.06	1.16	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	f	101	BCL	O1A-CGA	-2.06	1.16	1.22
7	o	101	BCL	O1A-CGA	-2.06	1.16	1.22
7	L	305	BCL	C3D-CAD	-2.05	1.40	1.46
7	9	102	BCL	O1A-CGA	-2.04	1.16	1.22
7	m	403	BCL	C3C-C4C	-2.04	1.49	1.51
7	l	304	BCL	CBD-CGD	-2.04	1.46	1.52
8	l	305	BPH	O1A-CGA	-2.04	1.16	1.22
7	L	302	BCL	CBD-CGD	-2.03	1.46	1.52
7	l	304	BCL	C3D-CAD	-2.03	1.40	1.46
7	L	305	BCL	O1A-CGA	-2.03	1.16	1.22
7	4	101	BCL	OBD-CAD	2.03	1.25	1.22
7	L	305	BCL	CBD-CGD	-2.03	1.46	1.52
7	l	304	BCL	O1A-CGA	-2.03	1.16	1.22
8	L	303	BPH	C1C-C2C	-2.02	1.48	1.51
7	M	402	BCL	C3C-C4C	-2.02	1.49	1.51
8	L	306	BPH	O1A-CGA	-2.02	1.16	1.22

All (1730) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	ab	102	SPO	C15-C14-C12	-14.64	106.42	127.31
11	G	102	SPO	C10-C9-C7	-14.35	106.83	127.31
11	w	102	SPO	C10-C9-C7	-13.96	107.39	127.31
11	d	103	SPO	C10-C9-C7	-13.76	107.67	127.31
11	0	101	SPO	C20-C19-C17	-13.74	107.70	127.31
11	ab	102	SPO	C20-C19-C17	-13.42	108.16	127.31
11	d	103	SPO	C20-C19-C17	-13.24	108.41	127.31
11	d	103	SPO	C15-C14-C12	-13.06	108.67	127.31
11	p	103	SPO	C20-C19-C17	-12.94	108.85	127.31
11	t	102	SPO	C10-C9-C7	-12.87	108.94	127.31
11	E	102	SPO	C21-C22-C23	-12.53	109.42	127.31
11	J	102	SPO	C15-C14-C12	-12.40	109.61	127.31
11	m	405	SPO	C20-C19-C17	-12.39	109.63	127.31
11	M	404	SPO	C20-C19-C17	-12.38	109.64	127.31
11	G	102	SPO	C15-C14-C12	-12.30	109.75	127.31
11	t	102	SPO	C15-C14-C12	-12.21	109.89	127.31
11	v	102	SPO	C20-C19-C17	-12.08	110.06	127.31
11	ab	102	SPO	C18-C17-C19	-12.06	106.03	122.92
11	e	102	SPO	C10-C9-C7	-11.96	110.24	127.31
11	d	103	SPO	C8-C7-C9	-11.88	106.28	122.92
11	w	102	SPO	C20-C19-C17	-11.84	110.42	127.31
11	w	102	SPO	C15-C14-C12	-11.83	110.43	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	M	404	SPO	C15-C14-C12	-11.78	110.49	127.31
11	m	405	SPO	C15-C14-C12	-11.75	110.55	127.31
11	G	103	SPO	C20-C19-C17	-11.62	110.72	127.31
11	n	102	SPO	C15-C14-C12	-11.57	110.80	127.31
11	p	103	SPO	C10-C9-C7	-11.33	111.14	127.31
11	G	102	SPO	C21-C22-C23	-11.30	111.18	127.31
11	n	102	SPO	C20-C19-C17	-11.28	111.21	127.31
11	t	102	SPO	C20-C19-C17	-11.27	111.23	127.31
11	G	103	SPO	C21-C22-C23	-11.23	111.28	127.31
11	0	103	SPO	C20-C19-C17	-11.22	111.30	127.31
11	M	404	SPO	C21-C22-C23	-11.21	111.31	127.31
11	m	405	SPO	C21-C22-C23	-11.19	111.33	127.31
11	ab	102	SPO	C13-C12-C14	-11.16	107.29	122.92
11	v	102	SPO	C10-C9-C7	-11.13	111.42	127.31
11	0	101	SPO	C15-C14-C12	-11.01	111.60	127.31
11	e	102	SPO	C15-C14-C12	-10.99	111.62	127.31
11	b	103	SPO	C10-C9-C7	-10.98	111.63	127.31
11	e	102	SPO	C18-C17-C19	-10.98	107.55	122.92
11	e	102	SPO	C20-C19-C17	-10.95	111.68	127.31
11	d	103	SPO	C21-C22-C23	-10.95	111.69	127.31
11	0	101	SPO	C24-C23-C22	-10.92	107.63	122.92
11	n	102	SPO	C10-C9-C7	-10.90	111.75	127.31
11	0	103	SPO	C10-C9-C7	-10.85	111.83	127.31
11	e	102	SPO	C21-C22-C23	-10.82	111.86	127.31
11	G	103	SPO	C10-C9-C7	-10.80	111.89	127.31
11	0	101	SPO	C10-C9-C7	-10.79	111.91	127.31
11	E	102	SPO	C10-C9-C7	-10.78	111.92	127.31
11	b	103	SPO	C20-C19-C17	-10.70	112.03	127.31
11	p	103	SPO	C18-C17-C19	-10.67	107.98	122.92
11	p	102	SPO	C20-C19-C17	-10.66	112.09	127.31
11	t	102	SPO	C21-C22-C23	-10.65	112.11	127.31
11	d	103	SPO	C13-C12-C14	-10.64	108.02	122.92
11	J	102	SPO	C13-C12-C14	-10.63	108.04	122.92
11	J	102	SPO	C18-C17-C19	-10.59	108.09	122.92
11	v	102	SPO	C15-C14-C12	-10.55	112.25	127.31
11	j	101	SPO	C10-C9-C7	-10.55	112.25	127.31
11	G	102	SPO	C8-C7-C9	-10.53	108.17	122.92
11	0	103	SPO	C18-C17-C19	-10.49	108.22	122.92
11	ab	102	SPO	C10-C9-C7	-10.45	112.39	127.31
11	q	102	SPO	C10-C9-C7	-10.44	112.40	127.31
11	p	102	SPO	C21-C22-C23	-10.43	112.42	127.31
11	D	102	SPO	C10-C9-C7	-10.43	112.43	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	f	102	SPO	C10-C9-C7	-10.43	112.43	127.31
11	aa	101	SPO	C10-C9-C7	-10.43	112.43	127.31
11	Q	603	SPO	C10-C9-C7	-10.42	112.44	127.31
11	g	101	SPO	C10-C9-C7	-10.41	112.45	127.31
11	F	103	SPO	C10-C9-C7	-10.41	112.45	127.31
11	i	103	SPO	C10-C9-C7	-10.41	112.45	127.31
11	9	101	SPO	C18-C17-C19	-10.41	108.34	122.92
11	b	101	SPO	C18-C17-C19	-10.41	108.34	122.92
11	F	102	SPO	C10-C9-C7	-10.41	112.45	127.31
11	o	102	SPO	C10-C9-C7	-10.41	112.45	127.31
11	u	101	SPO	C10-C9-C7	-10.40	112.46	127.31
11	d	102	SPO	C10-C9-C7	-10.40	112.47	127.31
11	9	103	SPO	C10-C9-C7	-10.40	112.47	127.31
11	s	101	SPO	C10-C9-C7	-10.40	112.47	127.31
11	C	1203	SPO	C10-C9-C7	-10.39	112.47	127.31
11	b	101	SPO	C20-C19-C17	-10.39	112.48	127.31
11	9	101	SPO	C20-C19-C17	-10.39	112.48	127.31
11	j	101	SPO	C13-C12-C14	-10.37	108.39	122.92
11	G	103	SPO	C18-C17-C19	-10.36	108.42	122.92
11	d	103	SPO	C24-C23-C22	-10.31	108.48	122.92
11	d	103	SPO	C18-C17-C19	-10.30	108.50	122.92
11	0	103	SPO	C15-C14-C12	-10.28	112.64	127.31
11	E	102	SPO	C15-C14-C12	-10.26	112.67	127.31
11	p	103	SPO	C21-C22-C23	-10.25	112.68	127.31
11	G	103	SPO	C24-C23-C22	-10.20	108.64	122.92
11	9	101	SPO	C21-C22-C23	-10.15	112.83	127.31
11	t	102	SPO	C18-C17-C19	-10.13	108.73	122.92
11	0	101	SPO	C13-C12-C14	-10.13	108.73	122.92
11	b	101	SPO	C21-C22-C23	-10.10	112.89	127.31
11	p	102	SPO	C18-C17-C19	-10.09	108.79	122.92
11	b	103	SPO	C15-C14-C12	-10.07	112.94	127.31
11	p	103	SPO	C15-C14-C12	-10.06	112.96	127.31
11	M	404	SPO	C24-C23-C22	-10.05	108.84	122.92
11	0	103	SPO	C8-C7-C9	-10.04	108.86	122.92
11	m	405	SPO	C24-C23-C22	-10.03	108.87	122.92
11	0	103	SPO	C13-C12-C14	-10.03	108.87	122.92
11	9	101	SPO	C13-C12-C14	-10.02	108.88	122.92
11	j	101	SPO	C18-C17-C19	-10.02	108.89	122.92
11	b	101	SPO	C13-C12-C14	-10.01	108.90	122.92
11	0	103	SPO	C21-C22-C23	-9.98	113.06	127.31
11	u	101	SPO	C21-C22-C23	-9.97	113.08	127.31
11	C	1203	SPO	C21-C22-C23	-9.97	113.09	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Q	603	SPO	C21-C22-C23	-9.95	113.11	127.31
11	d	102	SPO	C21-C22-C23	-9.95	113.11	127.31
11	D	102	SPO	C21-C22-C23	-9.95	113.12	127.31
11	F	103	SPO	C21-C22-C23	-9.95	113.12	127.31
11	s	101	SPO	C21-C22-C23	-9.94	113.13	127.31
11	aa	101	SPO	C21-C22-C23	-9.94	113.13	127.31
11	f	102	SPO	C21-C22-C23	-9.93	113.13	127.31
11	i	103	SPO	C21-C22-C23	-9.93	113.14	127.31
11	g	101	SPO	C21-C22-C23	-9.93	113.14	127.31
11	o	102	SPO	C21-C22-C23	-9.93	113.14	127.31
11	F	102	SPO	C21-C22-C23	-9.92	113.16	127.31
11	9	103	SPO	C21-C22-C23	-9.91	113.17	127.31
11	q	102	SPO	C21-C22-C23	-9.90	113.18	127.31
11	ab	102	SPO	C8-C7-C9	-9.86	109.11	122.92
11	F	103	SPO	C13-C12-C14	-9.86	109.11	122.92
11	Q	603	SPO	C13-C12-C14	-9.86	109.11	122.92
11	F	102	SPO	C13-C12-C14	-9.86	109.12	122.92
11	o	102	SPO	C13-C12-C14	-9.85	109.13	122.92
11	aa	101	SPO	C13-C12-C14	-9.85	109.13	122.92
11	s	101	SPO	C13-C12-C14	-9.84	109.13	122.92
11	9	103	SPO	C13-C12-C14	-9.84	109.14	122.92
11	i	103	SPO	C13-C12-C14	-9.84	109.14	122.92
11	p	102	SPO	C13-C12-C14	-9.83	109.15	122.92
11	u	101	SPO	C13-C12-C14	-9.83	109.15	122.92
11	C	1203	SPO	C13-C12-C14	-9.82	109.16	122.92
11	g	101	SPO	C13-C12-C14	-9.82	109.17	122.92
11	d	102	SPO	C13-C12-C14	-9.82	109.17	122.92
11	s	101	SPO	C24-C23-C22	-9.81	109.17	122.92
11	q	102	SPO	C13-C12-C14	-9.81	109.18	122.92
11	D	102	SPO	C13-C12-C14	-9.81	109.18	122.92
11	v	102	SPO	C24-C23-C22	-9.81	109.18	122.92
11	f	102	SPO	C13-C12-C14	-9.80	109.19	122.92
11	f	102	SPO	C24-C23-C22	-9.80	109.20	122.92
11	C	1203	SPO	C20-C19-C17	-9.80	113.33	127.31
11	D	102	SPO	C24-C23-C22	-9.79	109.20	122.92
11	g	101	SPO	C24-C23-C22	-9.79	109.21	122.92
11	i	103	SPO	C24-C23-C22	-9.79	109.21	122.92
11	d	102	SPO	C20-C19-C17	-9.79	113.34	127.31
11	aa	101	SPO	C20-C19-C17	-9.79	113.34	127.31
11	e	102	SPO	C8-C7-C9	-9.79	109.22	122.92
11	Q	603	SPO	C24-C23-C22	-9.78	109.22	122.92
11	b	103	SPO	C18-C17-C19	-9.78	109.22	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	aa	101	SPO	C24-C23-C22	-9.78	109.22	122.92
11	Q	603	SPO	C20-C19-C17	-9.78	113.35	127.31
11	F	103	SPO	C24-C23-C22	-9.78	109.22	122.92
11	q	102	SPO	C20-C19-C17	-9.78	113.35	127.31
11	F	102	SPO	C24-C23-C22	-9.78	109.23	122.92
11	C	1203	SPO	C24-C23-C22	-9.78	109.23	122.92
11	F	102	SPO	C20-C19-C17	-9.77	113.36	127.31
11	f	102	SPO	C20-C19-C17	-9.77	113.36	127.31
11	E	102	SPO	C13-C12-C14	-9.77	109.23	122.92
11	u	101	SPO	C20-C19-C17	-9.77	113.37	127.31
11	q	102	SPO	C24-C23-C22	-9.77	109.24	122.92
11	u	101	SPO	C24-C23-C22	-9.77	109.24	122.92
11	s	101	SPO	C20-C19-C17	-9.77	113.37	127.31
11	9	103	SPO	C24-C23-C22	-9.77	109.24	122.92
11	g	101	SPO	C20-C19-C17	-9.76	113.38	127.31
11	D	102	SPO	C20-C19-C17	-9.76	113.38	127.31
11	i	103	SPO	C20-C19-C17	-9.76	113.38	127.31
11	d	102	SPO	C24-C23-C22	-9.76	109.26	122.92
11	9	101	SPO	C8-C7-C9	-9.75	109.26	122.92
11	o	102	SPO	C24-C23-C22	-9.75	109.27	122.92
11	b	101	SPO	C8-C7-C9	-9.75	109.27	122.92
11	9	103	SPO	C20-C19-C17	-9.75	113.40	127.31
11	o	102	SPO	C20-C19-C17	-9.74	113.40	127.31
11	F	103	SPO	C20-C19-C17	-9.74	113.40	127.31
11	G	102	SPO	C20-C19-C17	-9.72	113.44	127.31
11	f	102	SPO	C15-C14-C12	-9.70	113.46	127.31
11	Q	603	SPO	C15-C14-C12	-9.70	113.47	127.31
11	b	103	SPO	C21-C22-C23	-9.70	113.47	127.31
11	u	101	SPO	C15-C14-C12	-9.69	113.48	127.31
11	g	101	SPO	C15-C14-C12	-9.68	113.50	127.31
11	i	103	SPO	C15-C14-C12	-9.68	113.50	127.31
11	D	102	SPO	C15-C14-C12	-9.68	113.50	127.31
11	o	102	SPO	C15-C14-C12	-9.67	113.50	127.31
11	q	102	SPO	C15-C14-C12	-9.67	113.50	127.31
11	v	102	SPO	C21-C22-C23	-9.67	113.51	127.31
11	0	101	SPO	C18-C17-C19	-9.66	109.39	122.92
11	F	102	SPO	C15-C14-C12	-9.66	113.52	127.31
11	C	1203	SPO	C15-C14-C12	-9.66	113.52	127.31
11	F	103	SPO	C15-C14-C12	-9.66	113.53	127.31
11	n	102	SPO	C8-C7-C9	-9.66	109.40	122.92
11	9	103	SPO	C15-C14-C12	-9.65	113.54	127.31
11	aa	101	SPO	C15-C14-C12	-9.65	113.54	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	m	405	SPO	C18-C17-C19	-9.65	109.41	122.92
11	M	404	SPO	C18-C17-C19	-9.64	109.41	122.92
11	d	102	SPO	C15-C14-C12	-9.64	113.55	127.31
11	s	101	SPO	C15-C14-C12	-9.64	113.55	127.31
11	b	101	SPO	C10-C9-C7	-9.64	113.56	127.31
11	v	102	SPO	C13-C12-C14	-9.63	109.43	122.92
11	9	101	SPO	C24-C23-C22	-9.62	109.44	122.92
11	9	101	SPO	C10-C9-C7	-9.62	113.58	127.31
11	j	101	SPO	C8-C7-C9	-9.62	109.45	122.92
11	n	102	SPO	C18-C17-C19	-9.62	109.45	122.92
11	m	405	SPO	C8-C7-C9	-9.62	109.45	122.92
11	b	101	SPO	C24-C23-C22	-9.61	109.46	122.92
11	M	404	SPO	C8-C7-C9	-9.59	109.49	122.92
11	w	102	SPO	C8-C7-C9	-9.57	109.51	122.92
11	p	102	SPO	C10-C9-C7	-9.57	113.65	127.31
11	v	102	SPO	C18-C17-C19	-9.56	109.53	122.92
11	ab	102	SPO	C21-C22-C23	-9.55	113.68	127.31
11	j	101	SPO	C21-C22-C23	-9.55	113.68	127.31
11	e	102	SPO	C13-C12-C14	-9.54	109.56	122.92
11	M	404	SPO	C13-C12-C14	-9.50	109.61	122.92
11	m	405	SPO	C13-C12-C14	-9.50	109.62	122.92
11	j	101	SPO	C20-C19-C17	-9.47	113.79	127.31
11	p	102	SPO	C15-C14-C12	-9.45	113.82	127.31
11	J	102	SPO	C10-C9-C7	-9.44	113.84	127.31
11	w	102	SPO	C18-C17-C19	-9.43	109.72	122.92
11	p	102	SPO	C8-C7-C9	-9.41	109.74	122.92
11	E	102	SPO	C20-C19-C17	-9.40	113.89	127.31
11	t	102	SPO	C8-C7-C9	-9.35	109.82	122.92
11	G	102	SPO	C18-C17-C19	-9.34	109.84	122.92
11	J	102	SPO	C8-C7-C9	-9.32	109.87	122.92
11	0	103	SPO	C24-C23-C22	-9.30	109.89	122.92
11	E	102	SPO	C8-C7-C9	-9.27	109.93	122.92
11	p	103	SPO	C8-C7-C9	-9.27	109.94	122.92
11	n	102	SPO	C13-C12-C14	-9.26	109.95	122.92
11	j	101	SPO	C24-C23-C22	-9.25	109.97	122.92
11	b	103	SPO	C13-C12-C14	-9.23	109.99	122.92
11	e	102	SPO	C24-C23-C22	-9.23	110.00	122.92
11	w	102	SPO	C13-C12-C14	-9.22	110.01	122.92
11	f	102	SPO	C8-C7-C9	-9.19	110.05	122.92
11	q	102	SPO	C8-C7-C9	-9.18	110.06	122.92
11	F	102	SPO	C8-C7-C9	-9.18	110.06	122.92
11	F	103	SPO	C8-C7-C9	-9.17	110.07	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	s	101	SPO	C8-C7-C9	-9.17	110.07	122.92
11	Q	603	SPO	C8-C7-C9	-9.17	110.07	122.92
11	d	102	SPO	C8-C7-C9	-9.17	110.08	122.92
11	aa	101	SPO	C8-C7-C9	-9.17	110.08	122.92
11	g	101	SPO	C8-C7-C9	-9.17	110.08	122.92
11	i	103	SPO	C8-C7-C9	-9.16	110.09	122.92
11	C	1203	SPO	C8-C7-C9	-9.16	110.09	122.92
11	u	101	SPO	C8-C7-C9	-9.16	110.09	122.92
11	o	102	SPO	C8-C7-C9	-9.15	110.10	122.92
11	D	102	SPO	C8-C7-C9	-9.15	110.11	122.92
11	m	405	SPO	C10-C9-C7	-9.15	114.25	127.31
11	M	404	SPO	C10-C9-C7	-9.14	114.26	127.31
11	E	102	SPO	C24-C23-C22	-9.14	110.11	122.92
11	9	103	SPO	C8-C7-C9	-9.13	110.13	122.92
11	n	102	SPO	C24-C23-C22	-9.13	110.14	122.92
11	ab	102	SPO	C24-C23-C22	-9.12	110.15	122.92
11	0	101	SPO	C8-C7-C9	-9.11	110.16	122.92
11	G	103	SPO	C15-C14-C12	-9.09	114.34	127.31
11	G	103	SPO	C8-C7-C9	-9.05	110.24	122.92
11	p	102	SPO	C24-C23-C22	-9.05	110.24	122.92
11	v	102	SPO	C8-C7-C9	-9.03	110.28	122.92
11	w	102	SPO	C24-C23-C22	-9.03	110.28	122.92
11	0	101	SPO	C21-C22-C23	-9.02	114.44	127.31
11	p	103	SPO	C24-C23-C22	-8.96	110.37	122.92
11	E	102	SPO	C18-C17-C19	-8.91	110.44	122.92
11	J	102	SPO	C21-C22-C23	-8.89	114.63	127.31
11	G	102	SPO	C13-C12-C14	-8.88	110.48	122.92
11	b	103	SPO	C24-C23-C22	-8.86	110.51	122.92
11	9	103	SPO	C18-C17-C19	-8.85	110.53	122.92
11	G	102	SPO	C24-C23-C22	-8.85	110.53	122.92
11	D	102	SPO	C18-C17-C19	-8.84	110.54	122.92
11	o	102	SPO	C18-C17-C19	-8.84	110.54	122.92
11	f	102	SPO	C18-C17-C19	-8.83	110.55	122.92
11	q	102	SPO	C18-C17-C19	-8.83	110.55	122.92
11	Q	603	SPO	C18-C17-C19	-8.83	110.55	122.92
11	u	101	SPO	C18-C17-C19	-8.83	110.56	122.92
11	i	103	SPO	C18-C17-C19	-8.82	110.56	122.92
11	g	101	SPO	C18-C17-C19	-8.82	110.57	122.92
11	aa	101	SPO	C18-C17-C19	-8.82	110.57	122.92
11	s	101	SPO	C18-C17-C19	-8.82	110.57	122.92
11	C	1203	SPO	C18-C17-C19	-8.81	110.58	122.92
11	d	102	SPO	C18-C17-C19	-8.81	110.58	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	102	SPO	C18-C17-C19	-8.80	110.59	122.92
11	F	103	SPO	C18-C17-C19	-8.80	110.59	122.92
11	J	102	SPO	C20-C19-C17	-8.77	114.80	127.31
11	j	101	SPO	C15-C14-C12	-8.69	114.91	127.31
7	Q	602	BCL	C16-C17-C18	8.62	156.58	115.98
11	G	103	SPO	C13-C12-C14	-8.60	110.88	122.92
11	n	102	SPO	C21-C22-C23	-8.55	115.11	127.31
11	p	103	SPO	C13-C12-C14	-8.54	110.96	122.92
11	t	102	SPO	C24-C23-C22	-8.53	110.97	122.92
11	b	103	SPO	C8-C7-C9	-8.52	110.98	122.92
11	b	103	SPO	C11-C12-C14	-8.50	105.89	118.94
11	9	101	SPO	C15-C14-C12	-8.50	115.18	127.31
11	b	101	SPO	C15-C14-C12	-8.48	115.20	127.31
11	w	102	SPO	C21-C22-C23	-8.47	115.22	127.31
11	m	405	SPO	C6-C7-C9	-8.46	105.96	118.94
11	M	404	SPO	C6-C7-C9	-8.45	105.97	118.94
11	b	103	SPO	C25-C23-C22	-8.43	106.00	118.94
11	J	102	SPO	C24-C23-C22	-8.42	111.13	122.92
11	t	102	SPO	C13-C12-C14	-8.35	111.23	122.92
11	ab	102	SPO	C18-C17-C16	-8.34	104.94	118.08
11	v	102	SPO	C25-C23-C22	-8.14	106.46	118.94
11	0	101	SPO	C18-C17-C16	-7.96	105.53	118.08
11	p	102	SPO	C11-C12-C14	-7.92	106.79	118.94
11	v	102	SPO	C11-C12-C14	-7.91	106.81	118.94
11	d	103	SPO	C31-C32-C33	-7.80	108.89	127.66
11	n	102	SPO	C16-C17-C19	-7.76	107.03	118.94
11	e	102	SPO	C11-C12-C14	-7.71	107.11	118.94
11	G	102	SPO	C16-C17-C19	-7.71	107.11	118.94
11	0	101	SPO	C6-C7-C9	-7.70	107.13	118.94
11	d	103	SPO	C25-C23-C22	-7.68	107.15	118.94
11	0	101	SPO	C25-C23-C22	-7.67	107.18	118.94
11	j	101	SPO	C16-C17-C19	-7.59	107.30	118.94
11	n	102	SPO	C25-C23-C22	-7.53	107.39	118.94
11	Q	603	SPO	C11-C12-C14	-7.48	107.46	118.94
11	f	102	SPO	C11-C12-C14	-7.48	107.46	118.94
11	i	103	SPO	C11-C12-C14	-7.47	107.47	118.94
11	q	102	SPO	C11-C12-C14	-7.47	107.48	118.94
11	o	102	SPO	C11-C12-C14	-7.46	107.49	118.94
11	g	101	SPO	C11-C12-C14	-7.46	107.50	118.94
11	u	101	SPO	C11-C12-C14	-7.46	107.50	118.94
11	C	1203	SPO	C11-C12-C14	-7.46	107.50	118.94
11	F	103	SPO	C11-C12-C14	-7.45	107.50	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	102	SPO	C11-C12-C14	-7.44	107.52	118.94
11	s	101	SPO	C11-C12-C14	-7.44	107.52	118.94
11	d	102	SPO	C11-C12-C14	-7.44	107.53	118.94
11	D	102	SPO	C11-C12-C14	-7.44	107.53	118.94
11	aa	101	SPO	C11-C12-C14	-7.44	107.53	118.94
11	9	101	SPO	C6-C7-C9	-7.42	107.55	118.94
11	9	103	SPO	C11-C12-C14	-7.42	107.56	118.94
11	b	101	SPO	C6-C7-C9	-7.41	107.57	118.94
11	p	102	SPO	C16-C17-C19	-7.40	107.59	118.94
11	0	101	SPO	C11-C12-C14	-7.35	107.66	118.94
11	b	101	SPO	C16-C17-C19	-7.34	107.67	118.94
11	e	102	SPO	C18-C17-C16	-7.32	106.54	118.08
11	b	103	SPO	C16-C17-C19	-7.32	107.71	118.94
11	p	103	SPO	C18-C17-C16	-7.30	106.57	118.08
11	9	101	SPO	C16-C17-C19	-7.29	107.75	118.94
11	p	102	SPO	C6-C7-C9	-7.29	107.76	118.94
11	0	103	SPO	C11-C12-C14	-7.26	107.80	118.94
11	9	101	SPO	C11-C12-C14	-7.25	107.82	118.94
11	b	101	SPO	C11-C12-C14	-7.23	107.84	118.94
11	C	1203	SPO	C25-C23-C22	-7.21	107.88	118.94
11	d	102	SPO	C25-C23-C22	-7.21	107.88	118.94
11	u	101	SPO	C25-C23-C22	-7.20	107.89	118.94
11	f	102	SPO	C25-C23-C22	-7.20	107.89	118.94
11	s	101	SPO	C25-C23-C22	-7.20	107.89	118.94
11	aa	101	SPO	C25-C23-C22	-7.20	107.90	118.94
11	Q	603	SPO	C25-C23-C22	-7.19	107.90	118.94
11	F	103	SPO	C25-C23-C22	-7.19	107.91	118.94
11	i	103	SPO	C25-C23-C22	-7.19	107.91	118.94
11	D	102	SPO	C25-C23-C22	-7.18	107.92	118.94
11	9	103	SPO	C25-C23-C22	-7.18	107.92	118.94
11	o	102	SPO	C25-C23-C22	-7.18	107.92	118.94
11	F	102	SPO	C25-C23-C22	-7.18	107.92	118.94
11	g	101	SPO	C25-C23-C22	-7.17	107.94	118.94
11	9	101	SPO	C25-C23-C22	-7.17	107.94	118.94
11	q	102	SPO	C25-C23-C22	-7.16	107.95	118.94
11	b	101	SPO	C25-C23-C22	-7.15	107.98	118.94
11	d	103	SPO	C35-C33-C32	-7.11	106.74	121.12
11	M	404	SPO	C25-C23-C22	-7.10	108.04	118.94
11	m	405	SPO	C25-C23-C22	-7.10	108.05	118.94
11	e	102	SPO	C31-C32-C33	-7.04	110.71	127.66
11	n	102	SPO	C6-C7-C9	-6.99	108.22	118.94
11	9	101	SPO	C31-C32-C33	-6.99	110.84	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	G	102	SPO	C25-C23-C22	-6.98	108.23	118.94
11	b	101	SPO	C31-C32-C33	-6.98	110.86	127.66
11	v	102	SPO	C16-C17-C19	-6.96	108.26	118.94
11	ab	102	SPO	C6-C7-C9	-6.96	108.27	118.94
11	F	103	SPO	C6-C7-C9	-6.94	108.30	118.94
11	q	102	SPO	C6-C7-C9	-6.93	108.30	118.94
11	9	103	SPO	C6-C7-C9	-6.93	108.31	118.94
11	o	102	SPO	C6-C7-C9	-6.93	108.31	118.94
11	aa	101	SPO	C6-C7-C9	-6.93	108.31	118.94
11	g	101	SPO	C6-C7-C9	-6.93	108.31	118.94
11	M	404	SPO	C11-C12-C14	-6.93	108.31	118.94
11	F	102	SPO	C6-C7-C9	-6.92	108.31	118.94
11	D	102	SPO	C6-C7-C9	-6.92	108.32	118.94
11	f	102	SPO	C6-C7-C9	-6.92	108.32	118.94
11	i	103	SPO	C6-C7-C9	-6.92	108.32	118.94
11	C	1203	SPO	C6-C7-C9	-6.92	108.33	118.94
11	m	405	SPO	C11-C12-C14	-6.92	108.33	118.94
11	s	101	SPO	C6-C7-C9	-6.91	108.33	118.94
11	u	101	SPO	C6-C7-C9	-6.90	108.35	118.94
11	d	102	SPO	C6-C7-C9	-6.90	108.35	118.94
11	Q	603	SPO	C6-C7-C9	-6.90	108.35	118.94
11	0	103	SPO	C25-C23-C22	-6.88	108.39	118.94
11	j	101	SPO	C25-C23-C22	-6.87	108.40	118.94
11	E	102	SPO	C16-C17-C19	-6.85	108.43	118.94
11	b	103	SPO	C6-C7-C9	-6.84	108.45	118.94
11	C	1203	SPO	C16-C17-C19	-6.82	108.47	118.94
11	s	101	SPO	C16-C17-C19	-6.81	108.49	118.94
11	u	101	SPO	C16-C17-C19	-6.81	108.49	118.94
11	f	102	SPO	C16-C17-C19	-6.81	108.50	118.94
11	q	102	SPO	C16-C17-C19	-6.80	108.50	118.94
11	i	103	SPO	C16-C17-C19	-6.80	108.51	118.94
11	g	101	SPO	C16-C17-C19	-6.79	108.52	118.94
11	F	102	SPO	C16-C17-C19	-6.79	108.53	118.94
11	d	102	SPO	C16-C17-C19	-6.79	108.53	118.94
11	Q	603	SPO	C16-C17-C19	-6.79	108.53	118.94
11	D	102	SPO	C16-C17-C19	-6.79	108.53	118.94
11	aa	101	SPO	C16-C17-C19	-6.78	108.53	118.94
11	F	103	SPO	C16-C17-C19	-6.78	108.54	118.94
11	e	102	SPO	C8-C7-C6	-6.78	107.40	118.08
11	9	103	SPO	C16-C17-C19	-6.77	108.56	118.94
11	o	102	SPO	C16-C17-C19	-6.77	108.56	118.94
11	p	103	SPO	C25-C23-C22	-6.76	108.57	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	G	103	SPO	C31-C32-C33	-6.73	111.45	127.66
11	p	102	SPO	C25-C23-C22	-6.72	108.63	118.94
11	0	103	SPO	C31-C32-C33	-6.69	111.54	127.66
11	ab	102	SPO	C25-C23-C22	-6.68	108.69	118.94
11	j	101	SPO	C11-C12-C14	-6.68	108.69	118.94
11	m	405	SPO	C35-C33-C32	-6.64	107.69	121.12
11	v	102	SPO	C8-C7-C6	-6.62	107.64	118.08
11	b	103	SPO	C35-C33-C32	-6.62	107.72	121.12
11	w	102	SPO	C25-C23-C22	-6.62	108.78	118.94
11	M	404	SPO	C35-C33-C32	-6.62	107.73	121.12
11	d	103	SPO	C18-C17-C16	-6.59	107.69	118.08
11	ab	102	SPO	C11-C12-C14	-6.59	108.83	118.94
11	J	102	SPO	C25-C23-C22	-6.57	108.86	118.94
11	0	103	SPO	C16-C17-C19	-6.53	108.92	118.94
11	p	103	SPO	C13-C12-C11	-6.53	107.79	118.08
11	m	405	SPO	C31-C32-C33	-6.53	111.94	127.66
11	p	102	SPO	C18-C17-C16	-6.52	107.80	118.08
11	M	404	SPO	C31-C32-C33	-6.51	111.99	127.66
11	0	101	SPO	C31-C32-C33	-6.48	112.06	127.66
11	e	102	SPO	C16-C17-C19	-6.47	109.02	118.94
11	t	102	SPO	C25-C23-C22	-6.46	109.03	118.94
11	j	101	SPO	C8-C7-C6	-6.43	107.95	118.08
11	w	102	SPO	C35-C33-C32	-6.41	108.15	121.12
11	ab	102	SPO	C31-C32-C33	-6.40	112.24	127.66
11	d	103	SPO	C13-C12-C11	-6.34	108.09	118.08
11	G	102	SPO	C13-C12-C11	-6.33	108.10	118.08
11	n	102	SPO	C31-C32-C33	-6.30	112.50	127.66
11	b	103	SPO	C18-C17-C16	-6.27	108.19	118.08
11	n	102	SPO	C13-C12-C11	-6.26	108.21	118.08
11	0	103	SPO	C35-C33-C32	-6.26	108.45	121.12
11	p	103	SPO	C31-C32-C33	-6.24	112.64	127.66
11	C	1203	SPO	C31-C32-C33	-6.24	112.64	127.66
11	o	102	SPO	C31-C32-C33	-6.23	112.65	127.66
11	aa	101	SPO	C31-C32-C33	-6.23	112.66	127.66
11	d	102	SPO	C31-C32-C33	-6.23	112.66	127.66
11	Q	603	SPO	C31-C32-C33	-6.23	112.66	127.66
11	9	103	SPO	C31-C32-C33	-6.23	112.67	127.66
11	f	102	SPO	C31-C32-C33	-6.23	112.67	127.66
11	J	102	SPO	C18-C17-C16	-6.22	108.27	118.08
11	F	102	SPO	C31-C32-C33	-6.22	112.68	127.66
11	s	101	SPO	C31-C32-C33	-6.22	112.68	127.66
11	g	101	SPO	C31-C32-C33	-6.22	112.68	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	i	103	SPO	C31-C32-C33	-6.22	112.68	127.66
11	u	101	SPO	C31-C32-C33	-6.22	112.68	127.66
11	q	102	SPO	C31-C32-C33	-6.22	112.69	127.66
11	D	102	SPO	C31-C32-C33	-6.22	112.69	127.66
11	F	103	SPO	C31-C32-C33	-6.22	112.69	127.66
11	b	101	SPO	C34-C33-C32	-6.19	107.80	123.68
11	9	101	SPO	C34-C33-C32	-6.17	107.84	123.68
11	G	103	SPO	C34-C33-C32	-6.17	107.84	123.68
11	p	102	SPO	C31-C32-C33	-6.15	112.84	127.66
11	G	102	SPO	C31-C32-C33	-6.15	112.86	127.66
11	b	103	SPO	C8-C7-C6	-6.14	108.39	118.08
11	j	101	SPO	C35-C33-C32	-6.14	108.69	121.12
11	9	101	SPO	C13-C12-C11	-6.11	108.45	118.08
11	E	102	SPO	C24-C23-C25	-6.11	108.45	118.08
11	b	101	SPO	C13-C12-C11	-6.10	108.46	118.08
11	e	102	SPO	C25-C23-C22	-6.07	109.63	118.94
11	ab	102	SPO	C24-C23-C25	-6.07	108.52	118.08
11	G	102	SPO	C8-C7-C6	-6.06	108.53	118.08
11	J	102	SPO	C24-C23-C25	-6.06	108.53	118.08
11	E	102	SPO	C34-C33-C32	-6.05	108.16	123.68
11	J	102	SPO	C34-C33-C32	-6.04	108.18	123.68
11	G	103	SPO	C6-C7-C9	-6.03	109.69	118.94
11	0	101	SPO	C13-C12-C11	-6.02	108.59	118.08
11	b	101	SPO	C8-C7-C6	-6.02	108.59	118.08
11	9	101	SPO	C8-C7-C6	-5.99	108.63	118.08
11	j	101	SPO	C31-C32-C33	-5.99	113.23	127.66
11	v	102	SPO	C34-C33-C32	-5.99	108.31	123.68
11	M	404	SPO	C18-C17-C16	-5.99	108.64	118.08
11	m	405	SPO	C18-C17-C16	-5.96	108.68	118.08
11	b	103	SPO	C31-C32-C33	-5.94	113.35	127.66
11	E	102	SPO	C11-C12-C14	-5.93	109.84	118.94
11	J	102	SPO	C31-C32-C33	-5.93	113.38	127.66
11	w	102	SPO	C11-C12-C14	-5.93	109.84	118.94
11	t	102	SPO	C6-C7-C9	-5.92	109.85	118.94
11	e	102	SPO	C34-C33-C32	-5.92	108.50	123.68
11	p	103	SPO	C6-C7-C9	-5.91	109.87	118.94
11	w	102	SPO	C16-C17-C19	-5.91	109.87	118.94
11	E	102	SPO	C18-C17-C16	-5.90	108.78	118.08
11	p	103	SPO	C11-C12-C14	-5.90	109.89	118.94
11	p	102	SPO	C35-C33-C32	-5.89	109.19	121.12
11	t	102	SPO	C31-C32-C33	-5.89	113.48	127.66
11	G	103	SPO	C18-C17-C16	-5.89	108.80	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	e	102	SPO	C24-C23-C25	-5.89	108.80	118.08
11	e	102	SPO	C35-C33-C32	-5.88	109.21	121.12
11	E	102	SPO	C8-C7-C6	-5.88	108.81	118.08
11	v	102	SPO	C31-C32-C33	-5.85	113.58	127.66
11	w	102	SPO	C31-C32-C33	-5.84	113.59	127.66
11	s	101	SPO	C35-C33-C32	-5.84	109.30	121.12
7	Q	602	BCL	C17-C16-C15	5.84	140.07	113.24
11	G	102	SPO	C35-C33-C32	-5.84	109.30	121.12
11	u	101	SPO	C35-C33-C32	-5.84	109.31	121.12
11	Q	603	SPO	C35-C33-C32	-5.84	109.31	121.12
11	G	103	SPO	C25-C23-C22	-5.83	109.99	118.94
11	aa	101	SPO	C35-C33-C32	-5.83	109.31	121.12
11	g	101	SPO	C35-C33-C32	-5.83	109.31	121.12
11	f	102	SPO	C35-C33-C32	-5.83	109.32	121.12
11	o	102	SPO	C35-C33-C32	-5.83	109.32	121.12
11	i	103	SPO	C35-C33-C32	-5.83	109.32	121.12
11	C	1203	SPO	C35-C33-C32	-5.83	109.32	121.12
11	F	102	SPO	C35-C33-C32	-5.83	109.33	121.12
11	F	103	SPO	C35-C33-C32	-5.83	109.33	121.12
11	q	102	SPO	C35-C33-C32	-5.83	109.33	121.12
11	D	102	SPO	C35-C33-C32	-5.82	109.33	121.12
11	d	102	SPO	C35-C33-C32	-5.82	109.33	121.12
11	9	103	SPO	C35-C33-C32	-5.82	109.34	121.12
11	v	102	SPO	C6-C7-C9	-5.81	110.02	118.94
11	d	103	SPO	C34-C33-C32	-5.78	108.85	123.68
11	E	102	SPO	C31-C32-C33	-5.77	113.76	127.66
11	u	101	SPO	C13-C12-C11	-5.77	108.98	118.08
11	n	102	SPO	C35-C33-C32	-5.77	109.43	121.12
11	t	102	SPO	C24-C23-C25	-5.76	108.99	118.08
11	q	102	SPO	C13-C12-C11	-5.76	109.00	118.08
11	F	103	SPO	C13-C12-C11	-5.76	109.00	118.08
11	aa	101	SPO	C13-C12-C11	-5.76	109.00	118.08
11	f	102	SPO	C13-C12-C11	-5.76	109.00	118.08
11	Q	603	SPO	C13-C12-C11	-5.76	109.00	118.08
11	d	103	SPO	C16-C17-C19	-5.75	110.11	118.94
11	C	1203	SPO	C13-C12-C11	-5.75	109.02	118.08
11	s	101	SPO	C13-C12-C11	-5.75	109.02	118.08
11	i	103	SPO	C13-C12-C11	-5.75	109.02	118.08
11	d	102	SPO	C13-C12-C11	-5.75	109.02	118.08
11	F	102	SPO	C13-C12-C11	-5.75	109.02	118.08
11	D	102	SPO	C13-C12-C11	-5.75	109.02	118.08
11	G	102	SPO	C29-C28-C27	-5.74	107.78	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	o	102	SPO	C13-C12-C11	-5.74	109.03	118.08
11	g	101	SPO	C13-C12-C11	-5.74	109.03	118.08
11	e	102	SPO	C5-C6-C7	-5.74	117.23	125.89
11	p	103	SPO	C35-C33-C32	-5.73	109.52	121.12
11	d	103	SPO	C6-C7-C9	-5.73	110.15	118.94
11	9	103	SPO	C13-C12-C11	-5.73	109.05	118.08
11	G	103	SPO	C11-C12-C14	-5.65	110.27	118.94
11	F	103	SPO	C18-C17-C16	-5.64	109.19	118.08
11	aa	101	SPO	C18-C17-C16	-5.64	109.19	118.08
11	s	101	SPO	C18-C17-C16	-5.64	109.19	118.08
11	w	102	SPO	C34-C33-C32	-5.64	109.22	123.68
11	g	101	SPO	C18-C17-C16	-5.63	109.20	118.08
11	i	103	SPO	C18-C17-C16	-5.63	109.20	118.08
11	m	405	SPO	C34-C33-C32	-5.63	109.23	123.68
11	u	101	SPO	C18-C17-C16	-5.63	109.20	118.08
11	M	404	SPO	C34-C33-C32	-5.63	109.24	123.68
11	d	102	SPO	C18-C17-C16	-5.63	109.21	118.08
11	F	102	SPO	C18-C17-C16	-5.63	109.21	118.08
11	q	102	SPO	C18-C17-C16	-5.63	109.21	118.08
11	0	103	SPO	C24-C23-C25	-5.62	109.22	118.08
11	D	102	SPO	C18-C17-C16	-5.62	109.22	118.08
11	Q	603	SPO	C18-C17-C16	-5.62	109.23	118.08
11	o	102	SPO	C18-C17-C16	-5.61	109.23	118.08
11	t	102	SPO	C11-C12-C14	-5.61	110.33	118.94
11	C	1203	SPO	C18-C17-C16	-5.61	109.24	118.08
11	0	103	SPO	C6-C7-C9	-5.61	110.33	118.94
11	9	103	SPO	C18-C17-C16	-5.61	109.24	118.08
11	f	102	SPO	C18-C17-C16	-5.61	109.24	118.08
11	9	101	SPO	C24-C23-C25	-5.60	109.25	118.08
7	Q	602	BCL	C16-C15-C13	-5.60	97.83	115.92
11	n	102	SPO	C11-C12-C14	-5.59	110.36	118.94
11	s	101	SPO	C34-C33-C32	-5.59	109.33	123.68
11	9	103	SPO	C34-C33-C32	-5.59	109.34	123.68
11	f	102	SPO	C34-C33-C32	-5.58	109.36	123.68
11	i	103	SPO	C34-C33-C32	-5.58	109.36	123.68
11	F	103	SPO	C34-C33-C32	-5.58	109.36	123.68
11	M	404	SPO	C16-C17-C19	-5.58	110.38	118.94
11	o	102	SPO	C34-C33-C32	-5.58	109.36	123.68
11	C	1203	SPO	C34-C33-C32	-5.58	109.37	123.68
11	d	102	SPO	C34-C33-C32	-5.58	109.37	123.68
11	aa	101	SPO	C34-C33-C32	-5.58	109.37	123.68
11	m	405	SPO	C16-C17-C19	-5.58	110.39	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D	102	SPO	C34-C33-C32	-5.57	109.39	123.68
11	Q	603	SPO	C34-C33-C32	-5.57	109.39	123.68
11	F	102	SPO	C34-C33-C32	-5.57	109.39	123.68
11	g	101	SPO	C34-C33-C32	-5.57	109.39	123.68
11	u	101	SPO	C34-C33-C32	-5.57	109.40	123.68
11	q	102	SPO	C34-C33-C32	-5.56	109.40	123.68
11	G	102	SPO	C34-C33-C32	-5.55	109.43	123.68
11	b	101	SPO	C24-C23-C25	-5.55	109.33	118.08
11	J	102	SPO	C29-C28-C27	-5.54	108.30	122.59
11	J	102	SPO	C6-C7-C9	-5.54	110.45	118.94
11	0	103	SPO	C18-C17-C16	-5.53	109.36	118.08
11	n	102	SPO	C18-C17-C16	-5.53	109.37	118.08
11	M	404	SPO	C13-C12-C11	-5.52	109.38	118.08
11	0	103	SPO	C34-C33-C32	-5.51	109.54	123.68
11	G	102	SPO	C5-C6-C7	-5.51	117.57	125.89
11	w	102	SPO	C5-C6-C7	-5.51	117.57	125.89
11	p	103	SPO	C34-C33-C32	-5.50	109.56	123.68
11	m	405	SPO	C13-C12-C11	-5.49	109.43	118.08
11	j	101	SPO	C34-C33-C32	-5.47	109.64	123.68
11	p	102	SPO	C34-C33-C32	-5.47	109.64	123.68
11	d	103	SPO	C11-C12-C14	-5.47	110.55	118.94
11	w	102	SPO	C6-C7-C9	-5.47	110.55	118.94
11	ab	102	SPO	C34-C33-C32	-5.47	109.66	123.68
11	M	404	SPO	C24-C23-C25	-5.46	109.47	118.08
11	J	102	SPO	C35-C33-C32	-5.45	110.08	121.12
11	m	405	SPO	C24-C23-C25	-5.45	109.48	118.08
11	0	103	SPO	C8-C7-C6	-5.45	109.49	118.08
11	v	102	SPO	C24-C23-C25	-5.44	109.50	118.08
11	G	103	SPO	C13-C12-C11	-5.43	109.52	118.08
11	G	103	SPO	C8-C7-C6	-5.43	109.53	118.08
11	Q	603	SPO	C8-C7-C6	-5.43	109.53	118.08
11	G	103	SPO	C35-C33-C32	-5.42	110.16	121.12
11	q	102	SPO	C8-C7-C6	-5.41	109.55	118.08
11	n	102	SPO	C34-C33-C32	-5.41	109.79	123.68
11	t	102	SPO	C34-C33-C32	-5.41	109.80	123.68
11	o	102	SPO	C8-C7-C6	-5.41	109.56	118.08
11	F	103	SPO	C8-C7-C6	-5.41	109.56	118.08
11	aa	101	SPO	C8-C7-C6	-5.41	109.56	118.08
11	g	101	SPO	C8-C7-C6	-5.40	109.57	118.08
11	s	101	SPO	C8-C7-C6	-5.39	109.58	118.08
11	9	103	SPO	C8-C7-C6	-5.39	109.58	118.08
11	d	102	SPO	C8-C7-C6	-5.39	109.58	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	f	102	SPO	C8-C7-C6	-5.39	109.59	118.08
11	ab	102	SPO	C16-C17-C19	-5.39	110.67	118.94
11	F	102	SPO	C8-C7-C6	-5.39	109.59	118.08
11	D	102	SPO	C8-C7-C6	-5.38	109.59	118.08
11	C	1203	SPO	C8-C7-C6	-5.38	109.60	118.08
11	u	101	SPO	C8-C7-C6	-5.38	109.60	118.08
11	G	103	SPO	C24-C23-C25	-5.37	109.61	118.08
11	i	103	SPO	C8-C7-C6	-5.37	109.62	118.08
11	E	102	SPO	C13-C12-C11	-5.36	109.63	118.08
11	t	102	SPO	C35-C33-C32	-5.36	110.27	121.12
11	j	101	SPO	C18-C17-C16	-5.34	109.67	118.08
11	j	101	SPO	C24-C23-C25	-5.33	109.69	118.08
11	0	101	SPO	C34-C33-C32	-5.32	110.02	123.68
11	0	103	SPO	C29-C28-C27	-5.31	108.89	122.59
11	w	102	SPO	C18-C17-C16	-5.30	109.72	118.08
11	E	102	SPO	C6-C7-C9	-5.30	110.80	118.94
11	b	103	SPO	C13-C12-C11	-5.30	109.72	118.08
11	v	102	SPO	C35-C33-C32	-5.30	110.39	121.12
11	t	102	SPO	C18-C17-C16	-5.28	109.76	118.08
11	ab	102	SPO	C35-C33-C32	-5.28	110.43	121.12
11	ab	102	SPO	C13-C12-C11	-5.27	109.78	118.08
11	b	103	SPO	C24-C23-C25	-5.26	109.79	118.08
11	w	102	SPO	C29-C28-C27	-5.26	109.03	122.59
11	0	101	SPO	C35-C33-C32	-5.25	110.50	121.12
11	M	404	SPO	C8-C7-C6	-5.25	109.81	118.08
11	t	102	SPO	C13-C12-C11	-5.24	109.81	118.08
11	E	102	SPO	C35-C33-C32	-5.24	110.51	121.12
11	t	102	SPO	C16-C17-C19	-5.23	110.91	118.94
11	m	405	SPO	C8-C7-C6	-5.23	109.84	118.08
11	G	103	SPO	C16-C17-C19	-5.22	110.92	118.94
11	n	102	SPO	C8-C7-C6	-5.22	109.85	118.08
11	e	102	SPO	C13-C12-C11	-5.22	109.86	118.08
11	v	102	SPO	C18-C17-C16	-5.22	109.86	118.08
11	0	101	SPO	C29-C28-C27	-5.21	109.15	122.59
11	n	102	SPO	C29-C28-C27	-5.21	109.15	122.59
11	w	102	SPO	C13-C12-C11	-5.20	109.88	118.08
11	ab	102	SPO	C29-C28-C27	-5.18	109.22	122.59
11	0	101	SPO	C8-C7-C6	-5.18	109.92	118.08
11	u	101	SPO	C29-C28-C27	-5.18	109.23	122.59
11	Q	603	SPO	C29-C28-C27	-5.17	109.24	122.59
11	g	101	SPO	C29-C28-C27	-5.17	109.24	122.59
11	D	102	SPO	C29-C28-C27	-5.17	109.25	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	d	102	SPO	C29-C28-C27	-5.17	109.25	122.59
11	9	103	SPO	C29-C28-C27	-5.17	109.26	122.59
11	C	1203	SPO	C29-C28-C27	-5.17	109.26	122.59
11	i	103	SPO	C29-C28-C27	-5.17	109.26	122.59
11	o	102	SPO	C29-C28-C27	-5.17	109.26	122.59
11	f	102	SPO	C29-C28-C27	-5.16	109.27	122.59
11	aa	101	SPO	C29-C28-C27	-5.16	109.28	122.59
11	s	101	SPO	C29-C28-C27	-5.16	109.28	122.59
11	j	101	SPO	C29-C28-C27	-5.16	109.29	122.59
11	F	102	SPO	C29-C28-C27	-5.16	109.29	122.59
11	F	103	SPO	C29-C28-C27	-5.15	109.31	122.59
11	q	102	SPO	C29-C28-C27	-5.15	109.31	122.59
11	m	405	SPO	C29-C28-C27	-5.14	109.32	122.59
11	p	103	SPO	C8-C7-C6	-5.14	109.98	118.08
11	M	404	SPO	C29-C28-C27	-5.14	109.33	122.59
11	e	102	SPO	C29-C28-C27	-5.14	109.33	122.59
11	b	101	SPO	C29-C28-C27	-5.14	109.33	122.59
11	d	103	SPO	C29-C28-C27	-5.13	109.34	122.59
11	9	101	SPO	C29-C28-C27	-5.13	109.35	122.59
11	p	102	SPO	C13-C12-C11	-5.12	110.01	118.08
11	0	103	SPO	C13-C12-C11	-5.11	110.02	118.08
11	G	102	SPO	C11-C12-C14	-5.11	111.10	118.94
11	b	103	SPO	C29-C28-C27	-5.10	109.42	122.59
11	p	102	SPO	C29-C28-C27	-5.10	109.42	122.59
11	J	102	SPO	C11-C12-C14	-5.10	111.11	118.94
11	w	102	SPO	C24-C23-C25	-5.07	110.09	118.08
11	v	102	SPO	C13-C12-C11	-5.06	110.10	118.08
11	j	101	SPO	C13-C12-C11	-5.05	110.12	118.08
11	p	103	SPO	C24-C23-C25	-5.02	110.17	118.08
11	ab	102	SPO	C8-C7-C6	-5.02	110.17	118.08
11	n	102	SPO	C24-C23-C25	-5.01	110.18	118.08
11	G	102	SPO	C18-C17-C16	-5.01	110.18	118.08
11	j	101	SPO	C6-C7-C9	-4.99	111.28	118.94
11	p	103	SPO	C29-C28-C27	-4.98	109.74	122.59
11	b	103	SPO	C34-C33-C32	-4.98	110.91	123.68
11	b	103	SPO	C30-C28-C27	-4.96	106.95	121.98
11	t	102	SPO	C8-C7-C6	-4.92	110.33	118.08
11	e	102	SPO	C6-C7-C9	-4.91	111.40	118.94
11	0	101	SPO	C24-C23-C25	-4.90	110.36	118.08
11	w	102	SPO	C8-C7-C6	-4.87	110.40	118.08
11	s	101	SPO	C24-C23-C25	-4.86	110.42	118.08
11	0	101	SPO	C5-C6-C7	-4.86	118.55	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	102	SPO	C24-C23-C25	-4.85	110.43	118.08
11	C	1203	SPO	C24-C23-C25	-4.85	110.44	118.08
11	u	101	SPO	C24-C23-C25	-4.85	110.44	118.08
11	p	102	SPO	C8-C7-C6	-4.85	110.44	118.08
11	aa	101	SPO	C24-C23-C25	-4.84	110.45	118.08
11	D	102	SPO	C24-C23-C25	-4.84	110.45	118.08
11	Q	603	SPO	C24-C23-C25	-4.84	110.45	118.08
11	o	102	SPO	C24-C23-C25	-4.84	110.45	118.08
11	f	102	SPO	C24-C23-C25	-4.84	110.45	118.08
11	v	102	SPO	C29-C28-C27	-4.84	110.11	122.59
11	9	101	SPO	C18-C17-C16	-4.83	110.46	118.08
11	i	103	SPO	C24-C23-C25	-4.83	110.46	118.08
11	9	103	SPO	C24-C23-C25	-4.82	110.48	118.08
11	F	103	SPO	C24-C23-C25	-4.82	110.48	118.08
11	d	102	SPO	C24-C23-C25	-4.82	110.48	118.08
11	q	102	SPO	C24-C23-C25	-4.82	110.48	118.08
11	G	103	SPO	C29-C28-C27	-4.82	110.16	122.59
11	p	102	SPO	C24-C23-C25	-4.82	110.48	118.08
11	t	102	SPO	C29-C28-C27	-4.81	110.18	122.59
11	g	101	SPO	C24-C23-C25	-4.81	110.50	118.08
11	d	103	SPO	C39-C38-C37	-4.79	108.80	122.65
11	ab	102	SPO	C34-C33-C35	-4.77	107.25	115.27
11	b	101	SPO	C18-C17-C16	-4.77	110.57	118.08
11	0	103	SPO	C36-C37-C38	-4.76	111.47	127.75
7	z	101	BCL	CAD-C3D-C4D	-4.75	105.82	108.47
11	w	102	SPO	C36-C37-C38	-4.74	111.53	127.75
11	J	102	SPO	C8-C7-C6	-4.73	110.62	118.08
11	G	103	SPO	C36-C37-C38	-4.73	111.59	127.75
11	d	103	SPO	C36-C37-C38	-4.71	111.64	127.75
11	0	103	SPO	C30-C28-C27	-4.71	107.73	121.98
11	v	102	SPO	C30-C28-C27	-4.68	107.80	121.98
7	m	401	BCL	CMB-C2B-C1B	-4.65	121.32	128.46
11	J	102	SPO	C13-C12-C11	-4.64	110.77	118.08
7	l	304	BCL	CAD-C3D-C4D	-4.64	105.89	108.47
11	E	102	SPO	C29-C28-C27	-4.63	110.64	122.59
11	p	103	SPO	C5-C6-C7	-4.63	118.90	125.89
11	j	101	SPO	C36-C37-C38	-4.63	111.94	127.75
11	9	101	SPO	C34-C33-C35	-4.62	107.51	115.27
9	l	303	U10	C47-C48-C49	-4.61	116.57	127.66
11	b	101	SPO	C34-C33-C35	-4.60	107.53	115.27
7	L	305	BCL	CAD-C3D-C4D	-4.60	105.90	108.47
11	0	101	SPO	C36-C37-C38	-4.60	112.03	127.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	M	404	SPO	C36-C37-C38	-4.60	112.04	127.75
11	w	102	SPO	C30-C28-C27	-4.59	108.08	121.98
11	m	405	SPO	C36-C37-C38	-4.59	112.06	127.75
11	b	103	SPO	C36-C37-C38	-4.58	112.10	127.75
11	E	102	SPO	C36-C37-C38	-4.57	112.12	127.75
11	E	102	SPO	C5-C6-C7	-4.55	119.01	125.89
11	0	101	SPO	C15-C16-C17	-4.54	113.66	126.42
11	ab	102	SPO	C30-C28-C27	-4.54	108.25	121.98
11	E	102	SPO	C25-C23-C22	-4.53	112.00	118.94
11	M	404	SPO	C30-C28-C27	-4.52	108.28	121.98
11	d	103	SPO	C24-C23-C25	-4.52	110.96	118.08
11	m	405	SPO	C30-C28-C27	-4.51	108.31	121.98
11	ab	102	SPO	C36-C37-C38	-4.50	112.36	127.75
11	b	101	SPO	C35-C33-C32	-4.50	112.01	121.12
11	J	102	SPO	C36-C37-C38	-4.50	112.38	127.75
11	9	101	SPO	C35-C33-C32	-4.49	112.02	121.12
12	A	1703	PC1	O21-C21-C22	4.47	121.13	111.50
12	a	102	PC1	O21-C21-C22	4.46	121.12	111.50
7	M	402	BCL	CMB-C2B-C1B	-4.45	121.62	128.46
11	e	102	SPO	C40-C38-C37	-4.45	109.78	122.65
11	t	102	SPO	C5-C6-C7	-4.45	119.17	125.89
7	m	403	BCL	CMB-C2B-C1B	-4.43	121.66	128.46
11	d	103	SPO	C40-C38-C37	-4.42	109.88	122.65
7	9	102	BCL	C16-C15-C13	4.41	130.16	115.92
11	9	101	SPO	C30-C28-C27	-4.40	108.67	121.98
11	e	102	SPO	C36-C37-C38	-4.39	112.74	127.75
11	b	101	SPO	C30-C28-C27	-4.39	108.69	121.98
11	G	102	SPO	C36-C37-C38	-4.38	112.78	127.75
7	l	301	BCL	CMB-C2B-C1B	-4.38	121.73	128.46
11	G	103	SPO	C30-C28-C27	-4.38	108.72	121.98
11	p	102	SPO	C36-C37-C38	-4.38	112.79	127.75
9	L	304	U10	C6-C1-C2	4.37	122.64	119.18
11	E	102	SPO	C30-C28-C27	-4.36	108.77	121.98
11	p	103	SPO	C39-C38-C37	-4.36	110.04	122.65
11	b	103	SPO	C5-C6-C7	-4.35	119.32	125.89
11	d	103	SPO	C30-C28-C27	-4.35	108.82	121.98
7	L	305	BCL	CMB-C2B-C1B	-4.34	121.80	128.46
7	l	304	BCL	CMB-C2B-C1B	-4.34	121.80	128.46
11	ab	102	SPO	C5-C6-C7	-4.32	119.37	125.89
11	j	101	SPO	C30-C28-C27	-4.31	108.92	121.98
11	b	103	SPO	C40-C38-C37	-4.31	110.18	122.65
11	t	102	SPO	C34-C33-C35	-4.31	108.03	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	s	102	BCL	CMB-C2B-C1B	-4.30	121.86	128.46
11	b	103	SPO	C39-C38-C37	-4.29	110.25	122.65
11	G	102	SPO	C6-C7-C9	-4.29	112.36	118.94
7	d	101	BCL	CMB-C2B-C1B	-4.29	121.88	128.46
11	J	102	SPO	C30-C28-C27	-4.29	109.00	121.98
7	D	101	BCL	CMB-C2B-C1B	-4.29	121.88	128.46
7	F	101	BCL	CMB-C2B-C1B	-4.28	121.88	128.46
7	f	101	BCL	CMB-C2B-C1B	-4.28	121.88	128.46
7	L	301	BCL	CMB-C2B-C1B	-4.28	121.89	128.46
7	c	1202	BCL	CMB-C2B-C1B	-4.28	121.89	128.46
11	p	102	SPO	C30-C28-C27	-4.27	109.04	121.98
7	q	101	BCL	CMB-C2B-C1B	-4.27	121.90	128.46
7	Q	602	BCL	CMB-C2B-C1B	-4.27	121.90	128.46
7	i	101	BCL	CMB-C2B-C1B	-4.26	121.91	128.46
7	q	103	BCL	CMB-C2B-C1B	-4.26	121.91	128.46
7	C	1202	BCL	CMB-C2B-C1B	-4.26	121.92	128.46
11	G	102	SPO	C24-C23-C25	-4.26	111.37	118.08
7	k	101	BCL	CMB-C2B-C1B	-4.25	121.92	128.46
7	o	101	BCL	CMB-C2B-C1B	-4.25	121.93	128.46
7	9	102	BCL	CMB-C2B-C1B	-4.25	121.93	128.46
7	I	101	BCL	CMB-C2B-C1B	-4.24	121.94	128.46
7	z	101	BCL	CMB-C2B-C1B	-4.23	121.96	128.46
7	L	302	BCL	CMB-C2B-C1B	-4.22	121.98	128.46
11	n	102	SPO	C36-C37-C38	-4.22	113.33	127.75
11	e	102	SPO	C39-C38-C37	-4.22	110.45	122.65
7	l	301	BCL	CAD-C3D-C4D	-4.22	106.12	108.47
11	M	404	SPO	C40-C38-C37	-4.21	110.47	122.65
11	m	405	SPO	C40-C38-C37	-4.21	110.47	122.65
11	v	102	SPO	C36-C37-C38	-4.21	113.37	127.75
11	t	102	SPO	C30-C28-C27	-4.19	109.28	121.98
7	K	101	BCL	C1-O2A-CGA	-4.18	105.47	116.44
11	w	102	SPO	C39-C38-C37	-4.18	110.58	122.65
11	0	101	SPO	C30-C28-C27	-4.17	109.37	121.98
12	h	301	PC1	O21-C21-C22	4.16	120.47	111.50
12	c	1201	PC1	O21-C21-C22	4.16	120.47	111.50
12	H	601	PC1	O21-C21-C22	4.16	120.47	111.50
11	ab	102	SPO	C40-C38-C37	-4.15	110.65	122.65
11	G	103	SPO	C39-C38-C37	-4.14	110.67	122.65
11	G	102	SPO	C39-C38-C37	-4.11	110.78	122.65
11	t	102	SPO	C36-C37-C38	-4.09	113.77	127.75
11	0	103	SPO	C40-C38-C37	-4.08	110.86	122.65
11	0	103	SPO	C39-C38-C37	-4.07	110.87	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Q	603	SPO	C36-C37-C38	-4.06	113.87	127.75
11	M	404	SPO	C29-C28-C30	-4.06	108.44	115.27
11	o	102	SPO	C36-C37-C38	-4.06	113.88	127.75
11	s	101	SPO	C36-C37-C38	-4.06	113.88	127.75
11	p	103	SPO	C30-C28-C27	-4.06	109.69	121.98
11	F	103	SPO	C36-C37-C38	-4.06	113.88	127.75
13	m	406	CDL	OA6-CA5-C11	4.06	120.25	111.50
11	u	101	SPO	C36-C37-C38	-4.06	113.89	127.75
11	n	102	SPO	C40-C38-C37	-4.05	110.93	122.65
11	F	102	SPO	C36-C37-C38	-4.05	113.90	127.75
11	d	102	SPO	C36-C37-C38	-4.05	113.90	127.75
11	g	101	SPO	C36-C37-C38	-4.05	113.90	127.75
11	m	405	SPO	C29-C28-C30	-4.05	108.46	115.27
11	i	103	SPO	C36-C37-C38	-4.05	113.91	127.75
11	q	102	SPO	C36-C37-C38	-4.05	113.92	127.75
11	aa	101	SPO	C36-C37-C38	-4.05	113.92	127.75
11	n	102	SPO	C39-C38-C37	-4.05	110.95	122.65
11	f	102	SPO	C36-C37-C38	-4.05	113.92	127.75
11	C	1203	SPO	C36-C37-C38	-4.04	113.93	127.75
11	D	102	SPO	C36-C37-C38	-4.04	113.93	127.75
11	9	103	SPO	C36-C37-C38	-4.04	113.94	127.75
11	w	102	SPO	C40-C38-C37	-4.04	110.97	122.65
11	n	102	SPO	C30-C28-C27	-4.04	109.75	121.98
11	t	102	SPO	C39-C38-C37	-4.02	111.02	122.65
11	n	102	SPO	C20-C21-C22	-4.02	115.23	123.47
11	b	103	SPO	C34-C33-C35	-4.02	108.51	115.27
11	v	102	SPO	C40-C38-C37	-4.02	111.03	122.65
11	J	102	SPO	C40-C38-C37	-4.02	111.03	122.65
11	d	102	SPO	C40-C38-C37	-4.01	111.05	122.65
11	F	103	SPO	C40-C38-C37	-4.01	111.06	122.65
11	g	101	SPO	C40-C38-C37	-4.01	111.06	122.65
11	u	101	SPO	C40-C38-C37	-4.01	111.06	122.65
11	q	102	SPO	C40-C38-C37	-4.01	111.06	122.65
11	Q	603	SPO	C40-C38-C37	-4.01	111.06	122.65
11	s	101	SPO	C40-C38-C37	-4.01	111.07	122.65
11	D	102	SPO	C40-C38-C37	-4.00	111.07	122.65
11	F	102	SPO	C40-C38-C37	-4.00	111.07	122.65
11	o	102	SPO	C40-C38-C37	-4.00	111.07	122.65
12	C	1201	PC1	O21-C21-C22	4.00	120.13	111.50
11	i	103	SPO	C40-C38-C37	-4.00	111.08	122.65
11	aa	101	SPO	C40-C38-C37	-4.00	111.08	122.65
11	f	102	SPO	C40-C38-C37	-4.00	111.08	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	9	103	SPO	C40-C38-C37	-4.00	111.09	122.65
11	C	1203	SPO	C40-C38-C37	-3.99	111.11	122.65
11	e	102	SPO	C30-C28-C27	-3.98	109.92	121.98
11	G	102	SPO	C29-C28-C30	-3.98	108.58	115.27
11	p	103	SPO	C34-C33-C35	-3.97	108.60	115.27
11	M	404	SPO	C39-C38-C37	-3.96	111.21	122.65
11	F	103	SPO	C30-C28-C27	-3.95	110.01	121.98
11	m	405	SPO	C39-C38-C37	-3.95	111.22	122.65
11	9	103	SPO	C30-C28-C27	-3.95	110.01	121.98
11	F	102	SPO	C30-C28-C27	-3.95	110.02	121.98
11	Q	603	SPO	C30-C28-C27	-3.95	110.03	121.98
9	L	304	U10	C7-C8-C9	-3.95	120.22	126.79
11	p	103	SPO	C36-C37-C38	-3.94	114.27	127.75
11	o	102	SPO	C30-C28-C27	-3.94	110.05	121.98
11	s	101	SPO	C30-C28-C27	-3.94	110.06	121.98
11	D	102	SPO	C30-C28-C27	-3.94	110.06	121.98
11	q	102	SPO	C30-C28-C27	-3.94	110.06	121.98
7	a	101	BCL	CMB-C2B-C1B	-3.93	122.42	128.46
11	d	102	SPO	C30-C28-C27	-3.93	110.07	121.98
11	g	101	SPO	C30-C28-C27	-3.93	110.07	121.98
11	i	103	SPO	C30-C28-C27	-3.93	110.07	121.98
11	C	1203	SPO	C30-C28-C27	-3.93	110.08	121.98
9	l	303	U10	C42-C43-C44	-3.93	118.19	127.66
11	u	101	SPO	C30-C28-C27	-3.93	110.08	121.98
11	f	102	SPO	C30-C28-C27	-3.93	110.08	121.98
11	aa	101	SPO	C30-C28-C27	-3.93	110.10	121.98
11	t	102	SPO	C29-C28-C30	-3.92	108.68	115.27
7	A	1702	BCL	CMB-C2B-C1B	-3.91	122.45	128.46
11	ab	102	SPO	C39-C38-C37	-3.90	111.37	122.65
11	j	101	SPO	C39-C38-C37	-3.89	111.39	122.65
11	t	102	SPO	C10-C11-C12	-3.89	115.48	126.42
11	G	102	SPO	C40-C38-C37	-3.89	111.41	122.65
7	m	403	BCL	C4A-NA-C1A	3.88	108.45	106.71
11	G	103	SPO	C40-C38-C37	-3.88	111.43	122.65
12	H	602	PC1	O21-C21-C22	3.87	119.84	111.50
11	j	101	SPO	C40-C38-C37	-3.87	111.47	122.65
11	d	103	SPO	C10-C11-C12	-3.86	115.56	126.42
11	J	102	SPO	C16-C17-C19	-3.86	113.02	118.94
11	E	102	SPO	C39-C38-C37	-3.84	111.55	122.65
7	M	402	BCL	C4A-NA-C1A	3.82	108.42	106.71
9	l	303	U10	C10-C9-C11	3.82	121.70	115.27
11	J	102	SPO	C39-C38-C37	-3.82	111.60	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	p	102	SPO	C5-C6-C7	-3.81	120.13	125.89
7	L	301	BCL	CAD-C3D-C4D	-3.81	106.34	108.47
11	E	102	SPO	C40-C38-C37	-3.80	111.65	122.65
7	D	101	BCL	C4A-NA-C1A	3.80	108.42	106.71
11	b	101	SPO	C36-C37-C38	-3.80	114.75	127.75
11	9	101	SPO	C36-C37-C38	-3.80	114.77	127.75
11	t	102	SPO	C40-C38-C37	-3.79	111.68	122.65
11	p	103	SPO	C16-C17-C19	-3.79	113.13	118.94
7	q	101	BCL	C4A-NA-C1A	3.79	108.41	106.71
7	v	101	BCL	CMB-C2B-C1B	-3.78	122.65	128.46
7	d	101	BCL	C4A-NA-C1A	3.78	108.41	106.71
7	Q	602	BCL	C4A-NA-C1A	3.78	108.40	106.71
7	q	103	BCL	C4A-NA-C1A	3.76	108.40	106.71
7	f	101	BCL	C4A-NA-C1A	3.75	108.39	106.71
11	0	101	SPO	C40-C38-C37	-3.75	111.82	122.65
7	I	101	BCL	C4A-NA-C1A	3.75	108.39	106.71
7	c	1202	BCL	C4A-NA-C1A	3.75	108.39	106.71
11	w	102	SPO	C10-C11-C12	-3.74	115.90	126.42
12	A	1701	PC1	O21-C21-C22	3.73	119.55	111.50
7	m	403	BCL	CAD-C3D-C4D	-3.73	106.39	108.47
7	J	101	BCL	C11-C10-C8	-3.73	103.86	115.92
7	B	101	BCL	C11-C10-C8	-3.73	103.87	115.92
11	p	102	SPO	C34-C33-C35	-3.73	109.00	115.27
7	o	101	BCL	C4A-NA-C1A	3.73	108.38	106.71
11	n	102	SPO	C34-C33-C35	-3.73	109.00	115.27
7	G	101	BCL	C11-C10-C8	-3.72	103.88	115.92
7	n	101	BCL	C11-C10-C8	-3.72	103.88	115.92
11	b	101	SPO	C39-C38-C37	-3.72	111.89	122.65
7	g	102	BCL	C11-C10-C8	-3.72	103.89	115.92
11	9	101	SPO	C39-C38-C37	-3.72	111.90	122.65
7	i	102	BCL	C11-C10-C8	-3.72	103.90	115.92
7	9	102	BCL	C4A-NA-C1A	3.72	108.38	106.71
7	e	101	BCL	C11-C10-C8	-3.72	103.90	115.92
7	8	101	BCL	C11-C10-C8	-3.72	103.90	115.92
7	t	101	BCL	C11-C10-C8	-3.72	103.91	115.92
7	aa	102	BCL	C11-C10-C8	-3.72	103.91	115.92
7	E	101	BCL	C11-C10-C8	-3.72	103.91	115.92
7	x	101	BCL	C11-C10-C8	-3.71	103.92	115.92
7	N	101	BCL	C11-C10-C8	-3.71	103.92	115.92
7	p	101	BCL	C11-C10-C8	-3.71	103.93	115.92
7	r	101	BCL	C11-C10-C8	-3.71	103.93	115.92
7	0	102	BCL	C11-C10-C8	-3.71	103.93	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	b	102	BCL	C11-C10-C8	-3.71	103.94	115.92
7	ab	101	BCL	C11-C10-C8	-3.70	103.95	115.92
7	F	101	BCL	C4A-NA-C1A	3.70	108.37	106.71
11	0	101	SPO	C39-C38-C37	-3.70	111.97	122.65
7	k	101	BCL	C4A-NA-C1A	3.69	108.37	106.71
7	C	1202	BCL	C4A-NA-C1A	3.69	108.36	106.71
11	9	101	SPO	C29-C28-C30	-3.68	109.08	115.27
11	b	101	SPO	C29-C28-C30	-3.68	109.08	115.27
7	i	101	BCL	C4A-NA-C1A	3.67	108.36	106.71
7	M	402	BCL	CAD-C3D-C4D	-3.66	106.43	108.47
7	L	302	BCL	CAD-C3D-C4D	-3.65	106.44	108.47
11	e	102	SPO	C29-C28-C30	-3.64	109.14	115.27
7	s	102	BCL	C4A-NA-C1A	3.64	108.34	106.71
11	i	103	SPO	C39-C38-C37	-3.64	112.13	122.65
11	0	101	SPO	C20-C21-C22	-3.64	116.02	123.47
11	9	103	SPO	C39-C38-C37	-3.64	112.13	122.65
11	C	1203	SPO	C39-C38-C37	-3.64	112.14	122.65
9	l	303	U10	C1M-C1-C6	-3.64	118.47	124.40
11	Q	603	SPO	C39-C38-C37	-3.64	112.14	122.65
11	D	102	SPO	C39-C38-C37	-3.63	112.14	122.65
11	f	102	SPO	C39-C38-C37	-3.63	112.15	122.65
11	F	102	SPO	C39-C38-C37	-3.63	112.15	122.65
11	o	102	SPO	C39-C38-C37	-3.63	112.15	122.65
13	m	406	CDL	OB6-CB5-C51	3.63	119.32	111.50
11	d	102	SPO	C39-C38-C37	-3.62	112.17	122.65
11	q	102	SPO	C39-C38-C37	-3.62	112.17	122.65
11	aa	101	SPO	C39-C38-C37	-3.62	112.18	122.65
11	g	101	SPO	C39-C38-C37	-3.62	112.19	122.65
11	F	103	SPO	C39-C38-C37	-3.62	112.19	122.65
11	u	101	SPO	C39-C38-C37	-3.62	112.19	122.65
11	s	101	SPO	C39-C38-C37	-3.62	112.19	122.65
11	n	102	SPO	C29-C28-C30	-3.61	109.19	115.27
11	ab	102	SPO	C15-C16-C17	-3.61	116.28	126.42
9	m	404	U10	C12-C13-C14	-3.61	118.97	127.66
9	M	403	U10	C12-C13-C14	-3.61	118.98	127.66
7	y	101	BCL	CMB-C2B-C1B	-3.60	122.93	128.46
11	0	103	SPO	C5-C6-C7	-3.60	120.46	125.89
7	O	101	BCL	CMB-C2B-C1B	-3.59	122.95	128.46
7	w	101	BCL	CMB-C2B-C1B	-3.59	122.95	128.46
7	K	101	BCL	CMB-C2B-C1B	-3.58	122.95	128.46
11	p	102	SPO	C39-C38-C37	-3.58	112.29	122.65
7	z	101	BCL	C4A-NA-C1A	3.57	108.31	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	5	101	BCL	CMB-C2B-C1B	-3.57	122.97	128.46
11	J	102	SPO	C15-C16-C17	-3.57	116.38	126.42
7	A	1702	BCL	C4A-NA-C1A	3.57	108.31	106.71
11	v	102	SPO	C39-C38-C37	-3.57	112.34	122.65
9	m	404	U10	C27-C28-C29	-3.57	119.07	127.66
11	0	103	SPO	C29-C28-C30	-3.56	109.28	115.27
11	p	103	SPO	C29-C28-C30	-3.56	109.28	115.27
9	m	404	U10	C25-C24-C26	3.56	121.26	115.27
9	M	403	U10	C27-C28-C29	-3.56	119.09	127.66
7	l	301	BCL	OBD-CAD-CBD	-3.55	120.82	125.89
7	w	101	BCL	C11-C10-C8	3.54	127.37	115.92
9	M	403	U10	C25-C24-C26	3.54	121.23	115.27
7	4	101	BCL	OBD-CAD-CBD	-3.54	120.84	125.89
7	m	401	BCL	OBD-CAD-CBD	-3.53	120.85	125.89
11	J	102	SPO	C5-C6-C7	-3.52	120.57	125.89
11	p	102	SPO	C40-C38-C37	-3.52	112.48	122.65
11	j	101	SPO	C5-C6-C7	-3.51	120.58	125.89
7	b	102	BCL	OBD-CAD-CBD	-3.51	120.88	125.89
7	I	101	BCL	OBD-CAD-CBD	-3.51	120.89	125.89
7	i	102	BCL	OBD-CAD-CBD	-3.51	120.89	125.89
9	l	303	U10	C7-C8-C9	-3.51	120.95	126.79
7	aa	102	BCL	OBD-CAD-CBD	-3.50	120.89	125.89
11	G	102	SPO	C34-C33-C35	-3.50	109.38	115.27
7	q	103	BCL	OBD-CAD-CBD	-3.49	120.90	125.89
7	r	101	BCL	OBD-CAD-CBD	-3.49	120.90	125.89
7	4	101	BCL	CMB-C2B-C1B	-3.49	123.09	128.46
7	t	101	BCL	OBD-CAD-CBD	-3.49	120.91	125.89
7	B	101	BCL	CAD-C3D-C4D	-3.49	106.52	108.47
7	B	101	BCL	OBD-CAD-CBD	-3.49	120.91	125.89
7	0	102	BCL	OBD-CAD-CBD	-3.49	120.91	125.89
11	G	102	SPO	C10-C11-C12	-3.49	116.61	126.42
7	x	101	BCL	CAD-C3D-C4D	-3.49	106.52	108.47
7	g	102	BCL	OBD-CAD-CBD	-3.49	120.91	125.89
7	Q	602	BCL	OBD-CAD-CBD	-3.49	120.91	125.89
7	D	101	BCL	OBD-CAD-CBD	-3.48	120.92	125.89
7	x	101	BCL	OBD-CAD-CBD	-3.48	120.92	125.89
7	G	101	BCL	OBD-CAD-CBD	-3.48	120.92	125.89
7	9	102	BCL	OBD-CAD-CBD	-3.48	120.92	125.89
7	q	101	BCL	OBD-CAD-CBD	-3.48	120.92	125.89
7	J	101	BCL	OBD-CAD-CBD	-3.48	120.92	125.89
7	8	101	BCL	OBD-CAD-CBD	-3.48	120.92	125.89
7	a	101	BCL	OBD-CAD-CBD	-3.48	120.93	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	j	101	SPO	C29-C28-C30	-3.48	109.42	115.27
7	p	101	BCL	OBD-CAD-CBD	-3.47	120.93	125.89
7	ab	101	BCL	OBD-CAD-CBD	-3.47	120.93	125.89
7	i	102	BCL	CAD-C3D-C4D	-3.47	106.53	108.47
7	k	101	BCL	OBD-CAD-CBD	-3.47	120.94	125.89
8	l	305	BPH	OBD-CAD-CBD	-3.47	120.73	125.82
7	F	101	BCL	OBD-CAD-CBD	-3.47	120.94	125.89
7	e	101	BCL	OBD-CAD-CBD	-3.47	120.94	125.89
7	N	101	BCL	OBD-CAD-CBD	-3.47	120.94	125.89
7	i	101	BCL	OBD-CAD-CBD	-3.47	120.94	125.89
7	o	101	BCL	OBD-CAD-CBD	-3.47	120.94	125.89
11	w	102	SPO	C34-C33-C35	-3.47	109.44	115.27
7	v	101	BCL	CAD-C3D-C4D	-3.46	106.54	108.47
7	v	101	BCL	C4A-NA-C1A	3.46	108.26	106.71
7	aa	102	BCL	CAD-C3D-C4D	-3.46	106.54	108.47
7	n	101	BCL	OBD-CAD-CBD	-3.46	120.95	125.89
7	C	1202	BCL	OBD-CAD-CBD	-3.46	120.95	125.89
7	c	1202	BCL	OBD-CAD-CBD	-3.46	120.95	125.89
7	s	102	BCL	OBD-CAD-CBD	-3.46	120.95	125.89
11	0	101	SPO	C34-C33-C35	-3.45	109.46	115.27
7	A	1702	BCL	OBD-CAD-CBD	-3.45	120.96	125.89
7	d	101	BCL	OBD-CAD-CBD	-3.45	120.96	125.89
7	E	101	BCL	OBD-CAD-CBD	-3.45	120.97	125.89
7	v	101	BCL	OBD-CAD-CBD	-3.45	120.97	125.89
7	E	101	BCL	CAD-C3D-C4D	-3.45	106.55	108.47
7	0	102	BCL	CMB-C2B-C1B	-3.45	123.17	128.46
7	b	102	BCL	CAD-C3D-C4D	-3.45	106.55	108.47
7	t	101	BCL	CAD-C3D-C4D	-3.45	106.55	108.47
7	G	101	BCL	CMB-C2B-C1B	-3.44	123.17	128.46
7	f	101	BCL	OBD-CAD-CBD	-3.44	120.98	125.89
7	n	101	BCL	CAD-C3D-C4D	-3.44	106.55	108.47
7	N	101	BCL	CMB-C2B-C1B	-3.43	123.19	128.46
7	g	102	BCL	CMB-C2B-C1B	-3.43	123.19	128.46
8	L	306	BPH	OBD-CAD-CBD	-3.43	120.79	125.82
7	L	301	BCL	OBD-CAD-CBD	-3.43	121.00	125.89
7	x	101	BCL	CMB-C2B-C1B	-3.43	123.20	128.46
7	J	101	BCL	CMB-C2B-C1B	-3.42	123.20	128.46
7	ab	101	BCL	CMB-C2B-C1B	-3.42	123.20	128.46
12	Q	601	PC1	O21-C21-C22	3.42	118.88	111.50
11	d	103	SPO	C29-C28-C30	-3.42	109.52	115.27
7	B	101	BCL	CMB-C2B-C1B	-3.42	123.21	128.46
7	v	101	BCL	C17-C16-C15	3.42	128.94	113.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	a	101	BCL	C4A-NA-C1A	3.42	108.24	106.71
11	j	101	SPO	C34-C33-C35	-3.42	109.52	115.27
9	L	304	U10	C27-C28-C29	-3.41	119.44	127.66
7	N	101	BCL	CAD-C3D-C4D	-3.41	106.57	108.47
7	r	101	BCL	CMB-C2B-C1B	-3.41	123.22	128.46
7	aa	102	BCL	CMB-C2B-C1B	-3.41	123.23	128.46
11	0	103	SPO	C34-C33-C35	-3.41	109.54	115.27
9	L	304	U10	C12-C13-C14	-3.40	119.46	127.66
7	E	101	BCL	CMB-C2B-C1B	-3.40	123.23	128.46
7	r	101	BCL	CAD-C3D-C4D	-3.40	106.57	108.47
7	g	102	BCL	CAD-C3D-C4D	-3.40	106.58	108.47
7	i	102	BCL	CMB-C2B-C1B	-3.40	123.24	128.46
7	8	101	BCL	CMB-C2B-C1B	-3.40	123.24	128.46
7	J	101	BCL	CAD-C3D-C4D	-3.40	106.58	108.47
7	p	101	BCL	CMB-C2B-C1B	-3.40	123.25	128.46
7	t	101	BCL	CMB-C2B-C1B	-3.39	123.25	128.46
11	E	102	SPO	C29-C28-C30	-3.39	109.56	115.27
7	e	101	BCL	CMB-C2B-C1B	-3.39	123.25	128.46
7	b	102	BCL	CMB-C2B-C1B	-3.39	123.25	128.46
7	w	101	BCL	C4A-NA-C1A	3.39	108.23	106.71
7	ab	101	BCL	CAD-C3D-C4D	-3.39	106.58	108.47
11	9	101	SPO	C40-C38-C37	-3.39	112.85	122.65
11	G	103	SPO	C29-C28-C30	-3.39	109.57	115.27
7	n	101	BCL	CMB-C2B-C1B	-3.38	123.26	128.46
11	v	102	SPO	C34-C33-C35	-3.38	109.59	115.27
7	G	101	BCL	CAD-C3D-C4D	-3.38	106.59	108.47
11	s	101	SPO	C29-C28-C30	-3.38	109.59	115.27
11	f	102	SPO	C29-C28-C30	-3.38	109.59	115.27
11	n	102	SPO	C5-C6-C7	-3.37	120.80	125.89
11	C	1203	SPO	C29-C28-C30	-3.37	109.60	115.27
11	d	103	SPO	C15-C16-C17	-3.37	116.95	126.42
11	u	101	SPO	C29-C28-C30	-3.37	109.60	115.27
7	0	102	BCL	CAD-C3D-C4D	-3.37	106.59	108.47
11	b	101	SPO	C40-C38-C37	-3.37	112.92	122.65
11	D	102	SPO	C29-C28-C30	-3.36	109.61	115.27
11	aa	101	SPO	C29-C28-C30	-3.36	109.61	115.27
7	5	101	BCL	C4A-NA-C1A	3.36	108.22	106.71
7	w	101	BCL	OBD-CAD-CBD	-3.36	121.09	125.89
11	F	102	SPO	C29-C28-C30	-3.36	109.62	115.27
7	8	101	BCL	CAD-C3D-C4D	-3.36	106.60	108.47
11	0	101	SPO	C16-C17-C19	-3.36	113.78	118.94
11	d	103	SPO	C20-C21-C22	-3.36	116.59	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	O	101	BCL	OBD-CAD-CBD	-3.36	121.10	125.89
11	F	103	SPO	C29-C28-C30	-3.36	109.63	115.27
11	o	102	SPO	C29-C28-C30	-3.36	109.63	115.27
7	p	101	BCL	CAD-C3D-C4D	-3.36	106.60	108.47
7	K	101	BCL	OBD-CAD-CBD	-3.35	121.10	125.89
11	d	102	SPO	C29-C28-C30	-3.35	109.64	115.27
11	p	103	SPO	C40-C38-C37	-3.35	112.97	122.65
11	g	101	SPO	C29-C28-C30	-3.35	109.64	115.27
7	y	101	BCL	C4A-NA-C1A	3.35	108.21	106.71
11	Q	603	SPO	C29-C28-C30	-3.35	109.64	115.27
11	i	103	SPO	C29-C28-C30	-3.35	109.64	115.27
11	E	102	SPO	C34-C33-C35	-3.35	109.64	115.27
11	n	102	SPO	C10-C11-C12	-3.34	117.02	126.42
11	G	102	SPO	C30-C28-C27	-3.34	111.86	121.98
8	l	302	BPH	OBD-CAD-CBD	-3.34	120.92	125.82
7	Q	602	BCL	CAD-C3D-C4D	-3.34	106.61	108.47
7	L	305	BCL	OBD-CAD-CBD	-3.34	121.13	125.89
7	5	101	BCL	OBD-CAD-CBD	-3.34	121.13	125.89
8	L	303	BPH	OBD-CAD-CBD	-3.34	120.93	125.82
7	e	101	BCL	CAD-C3D-C4D	-3.34	106.61	108.47
11	9	103	SPO	C29-C28-C30	-3.34	109.66	115.27
11	d	103	SPO	C8-C7-C6	-3.34	112.82	118.08
7	I	101	BCL	CAD-C3D-C4D	-3.33	106.61	108.47
7	L	302	BCL	OBD-CAD-CBD	-3.33	121.13	125.89
11	q	102	SPO	C29-C28-C30	-3.33	109.67	115.27
7	l	304	BCL	OBD-CAD-CBD	-3.33	121.14	125.89
7	q	101	BCL	CAD-C3D-C4D	-3.32	106.62	108.47
9	L	304	U10	C30-C29-C31	3.32	120.86	115.27
9	l	303	U10	C22-C23-C24	-3.32	119.67	127.66
7	y	101	BCL	OBD-CAD-CBD	-3.32	121.16	125.89
7	s	102	BCL	CAD-C3D-C4D	-3.31	106.62	108.47
11	E	102	SPO	C26-C25-C23	-3.31	117.11	126.42
7	m	401	BCL	CMB-C2B-C3B	3.30	130.86	124.68
7	4	101	BCL	C2A-C1A-CHA	3.30	129.62	123.86
7	O	101	BCL	C4A-NA-C1A	3.30	108.19	106.71
11	M	404	SPO	C15-C16-C17	-3.30	117.16	126.42
11	m	405	SPO	C15-C16-C17	-3.30	117.16	126.42
9	l	303	U10	C35-C34-C36	3.29	120.81	115.27
7	i	101	BCL	CAD-C3D-C4D	-3.29	106.64	108.47
7	d	101	BCL	CAD-C3D-C4D	-3.29	106.64	108.47
7	K	101	BCL	C4A-NA-C1A	3.28	108.18	106.71
11	ab	102	SPO	C21-C20-C19	-3.28	116.76	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	b	103	SPO	C29-C28-C30	-3.28	109.76	115.27
7	M	402	BCL	CHA-C1A-NA	-3.27	118.90	126.40
9	L	304	U10	C17-C18-C19	-3.27	119.78	127.66
7	D	101	BCL	CAD-C3D-C4D	-3.27	106.65	108.47
7	f	101	BCL	CAD-C3D-C4D	-3.27	106.65	108.47
7	k	101	BCL	CAD-C3D-C4D	-3.27	106.65	108.47
7	m	403	BCL	OBD-CAD-CBD	-3.27	121.22	125.89
7	m	403	BCL	CHA-C1A-NA	-3.27	118.92	126.40
7	o	101	BCL	CAD-C3D-C4D	-3.26	106.65	108.47
7	q	103	BCL	CAD-C3D-C4D	-3.26	106.65	108.47
7	M	402	BCL	OBD-CAD-CBD	-3.26	121.24	125.89
7	y	101	BCL	CHA-C1A-NA	-3.26	118.94	126.40
7	K	101	BCL	CHA-C1A-NA	-3.26	118.94	126.40
7	F	101	BCL	CAD-C3D-C4D	-3.25	106.66	108.47
7	O	101	BCL	CHA-C1A-NA	-3.24	118.97	126.40
7	C	1202	BCL	CAD-C3D-C4D	-3.24	106.66	108.47
9	m	404	U10	C32-C33-C34	-3.24	119.86	127.66
9	M	403	U10	C32-C33-C34	-3.24	119.86	127.66
7	9	102	BCL	CAD-C3D-C4D	-3.24	106.67	108.47
7	5	101	BCL	CHA-C1A-NA	-3.23	118.99	126.40
7	w	101	BCL	CHA-C1A-NA	-3.23	119.00	126.40
7	c	1202	BCL	CAD-C3D-C4D	-3.22	106.68	108.47
11	m	405	SPO	C34-C33-C35	-3.21	109.87	115.27
11	v	102	SPO	C20-C21-C22	-3.21	116.90	123.47
7	z	101	BCL	C2A-C1A-CHA	3.21	129.47	123.86
7	4	101	BCL	C4A-NA-C1A	3.21	108.15	106.71
9	L	304	U10	O5-C5-C4	-3.20	114.13	120.93
7	m	401	BCL	CHA-C1A-NA	-3.19	119.08	126.40
7	L	305	BCL	CMB-C2B-C3B	3.18	130.63	124.68
7	4	101	BCL	CHD-C4C-NC	-3.17	121.55	125.08
11	M	404	SPO	C34-C33-C35	-3.17	109.94	115.27
7	l	304	BCL	CMB-C2B-C3B	3.16	130.58	124.68
11	p	102	SPO	C29-C28-C30	-3.15	109.97	115.27
7	L	302	BCL	C4A-NA-C1A	3.15	108.12	106.71
7	x	101	BCL	CHA-C1A-NA	-3.13	119.22	126.40
7	ab	101	BCL	CHA-C1A-NA	-3.13	119.22	126.40
7	n	101	BCL	CHA-C1A-NA	-3.13	119.23	126.40
7	b	102	BCL	CHA-C1A-NA	-3.13	119.24	126.40
7	aa	102	BCL	CHA-C1A-NA	-3.13	119.24	126.40
7	8	101	BCL	CHA-C1A-NA	-3.13	119.24	126.40
7	g	102	BCL	CHA-C1A-NA	-3.12	119.24	126.40
7	t	101	BCL	CHA-C1A-NA	-3.12	119.24	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	i	102	BCL	CHA-C1A-NA	-3.12	119.24	126.40
7	p	101	BCL	CHA-C1A-NA	-3.12	119.24	126.40
7	J	101	BCL	CHA-C1A-NA	-3.12	119.25	126.40
7	l	301	BCL	CMB-C2B-C3B	3.12	130.52	124.68
7	z	101	BCL	CMB-C2B-C3B	3.12	130.52	124.68
7	N	101	BCL	CHA-C1A-NA	-3.12	119.25	126.40
7	e	101	BCL	CHA-C1A-NA	-3.12	119.26	126.40
7	M	402	BCL	CMB-C2B-C3B	3.12	130.51	124.68
7	B	101	BCL	CHA-C1A-NA	-3.12	119.26	126.40
7	0	102	BCL	CHA-C1A-NA	-3.11	119.27	126.40
11	e	102	SPO	C34-C33-C35	-3.11	110.03	115.27
7	G	101	BCL	CHA-C1A-NA	-3.11	119.27	126.40
7	E	101	BCL	CHA-C1A-NA	-3.11	119.27	126.40
11	t	102	SPO	C15-C16-C17	-3.11	117.68	126.42
7	m	403	BCL	CMB-C2B-C3B	3.10	130.48	124.68
7	d	101	BCL	CMB-C2B-C3B	3.10	130.47	124.68
7	k	101	BCL	CMB-C2B-C3B	3.10	130.47	124.68
7	r	101	BCL	CHA-C1A-NA	-3.10	119.31	126.40
7	L	301	BCL	CMB-C2B-C3B	3.09	130.47	124.68
7	F	101	BCL	CMB-C2B-C3B	3.09	130.47	124.68
7	L	305	BCL	CHA-C1A-NA	-3.09	119.32	126.40
7	q	103	BCL	CMB-C2B-C3B	3.09	130.45	124.68
7	f	101	BCL	CMB-C2B-C3B	3.08	130.45	124.68
9	l	303	U10	C17-C18-C19	-3.08	120.24	127.66
7	a	101	BCL	CHA-C1A-NA	-3.08	119.34	126.40
11	v	102	SPO	C15-C16-C17	-3.08	117.76	126.42
7	i	101	BCL	CMB-C2B-C3B	3.07	130.43	124.68
7	s	102	BCL	CMB-C2B-C3B	3.07	130.43	124.68
7	l	304	BCL	CHA-C1A-NA	-3.07	119.36	126.40
7	o	101	BCL	CHA-C1A-NA	-3.07	119.36	126.40
7	q	101	BCL	CMB-C2B-C3B	3.07	130.43	124.68
7	I	101	BCL	CMB-C2B-C3B	3.07	130.43	124.68
11	0	101	SPO	C29-C28-C30	-3.07	110.10	115.27
7	s	102	BCL	CHA-C1A-NA	-3.07	119.37	126.40
7	o	101	BCL	CMB-C2B-C3B	3.07	130.42	124.68
7	C	1202	BCL	CHA-C1A-NA	-3.07	119.37	126.40
7	Q	602	BCL	CMB-C2B-C3B	3.07	130.42	124.68
9	l	303	U10	C40-C39-C41	3.07	120.44	115.27
7	k	101	BCL	CHA-C1A-NA	-3.07	119.37	126.40
7	A	1702	BCL	CHA-C1A-NA	-3.07	119.37	126.40
7	L	302	BCL	C1-C2-C3	-3.07	120.74	126.04
7	i	101	BCL	CHA-C1A-NA	-3.07	119.38	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	1202	BCL	CMB-C2B-C3B	3.06	130.41	124.68
7	c	1202	BCL	CMB-C2B-C3B	3.06	130.40	124.68
7	D	101	BCL	CMB-C2B-C3B	3.06	130.40	124.68
7	q	103	BCL	CHA-C1A-NA	-3.06	119.39	126.40
7	q	101	BCL	CHA-C1A-NA	-3.06	119.39	126.40
7	F	101	BCL	CHA-C1A-NA	-3.06	119.39	126.40
7	I	101	BCL	CHA-C1A-NA	-3.06	119.39	126.40
7	D	101	BCL	CHA-C1A-NA	-3.06	119.40	126.40
7	c	1202	BCL	CHA-C1A-NA	-3.06	119.40	126.40
7	A	1702	BCL	CAD-C3D-C4D	-3.05	106.77	108.47
7	d	101	BCL	CHA-C1A-NA	-3.05	119.41	126.40
7	9	102	BCL	CMB-C2B-C3B	3.05	130.39	124.68
7	9	102	BCL	CHA-C1A-NA	-3.05	119.41	126.40
7	Q	602	BCL	CHA-C1A-NA	-3.05	119.41	126.40
9	m	404	U10	C22-C23-C24	-3.05	120.32	127.66
7	L	302	BCL	CHA-C1A-NA	-3.05	119.42	126.40
7	f	101	BCL	CHA-C1A-NA	-3.05	119.42	126.40
9	l	303	U10	C15-C14-C16	3.04	120.39	115.27
7	4	101	BCL	CAD-C3D-C4D	-3.04	106.78	108.47
7	v	101	BCL	CHA-C1A-NA	-3.03	119.46	126.40
7	L	302	BCL	CMB-C2B-C3B	3.03	130.34	124.68
9	M	403	U10	C22-C23-C24	-3.02	120.39	127.66
11	ab	102	SPO	C10-C11-C12	-3.02	117.95	126.42
11	J	102	SPO	C34-C33-C35	-3.01	110.21	115.27
7	L	301	BCL	CHA-C1A-NA	-2.99	119.55	126.40
7	a	101	BCL	CAD-C3D-C4D	-2.96	106.82	108.47
9	L	304	U10	C25-C24-C26	2.96	120.25	115.27
7	M	402	BCL	C1-O2A-CGA	2.96	124.21	116.44
7	z	101	BCL	CHA-C1A-NA	-2.95	119.63	126.40
7	m	403	BCL	C1-O2A-CGA	2.95	124.19	116.44
7	ab	101	BCL	C2A-C1A-CHA	2.95	129.02	123.86
7	L	302	BCL	C2A-C1A-CHA	2.95	129.02	123.86
7	l	301	BCL	CHA-C1A-NA	-2.95	119.64	126.40
7	M	402	BCL	C2A-C1A-CHA	2.95	129.01	123.86
8	L	303	BPH	CMB-C2B-C3B	2.94	130.18	124.68
7	m	403	BCL	C2A-C1A-CHA	2.94	129.00	123.86
7	L	301	BCL	C2A-C1A-CHA	2.94	129.00	123.86
7	z	101	BCL	OBD-CAD-CBD	-2.94	121.70	125.89
7	aa	102	BCL	C2A-C1A-CHA	2.93	128.99	123.86
7	l	301	BCL	C2A-C1A-CHA	2.93	128.99	123.86
7	0	102	BCL	C2A-C1A-CHA	2.92	128.97	123.86
7	t	101	BCL	C2A-C1A-CHA	2.92	128.97	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	m	401	BCL	CAD-C3D-C4D	-2.92	106.84	108.47
7	8	101	BCL	C2A-C1A-CHA	2.92	128.96	123.86
7	i	102	BCL	C2A-C1A-CHA	2.92	128.96	123.86
7	J	101	BCL	C2A-C1A-CHA	2.92	128.96	123.86
8	l	302	BPH	CMB-C2B-C3B	2.91	130.13	124.68
7	x	101	BCL	C2A-C1A-CHA	2.91	128.95	123.86
7	g	102	BCL	C2A-C1A-CHA	2.91	128.95	123.86
9	m	404	U10	C10-C9-C11	2.91	120.17	115.27
7	b	102	BCL	C2A-C1A-CHA	2.91	128.95	123.86
7	q	103	BCL	C16-C15-C13	2.91	125.32	115.92
7	E	101	BCL	C2A-C1A-CHA	2.91	128.94	123.86
9	m	404	U10	C35-C34-C36	2.91	120.16	115.27
9	M	403	U10	C35-C34-C36	2.90	120.15	115.27
11	w	102	SPO	C15-C16-C17	-2.90	118.27	126.42
7	B	101	BCL	C2A-C1A-CHA	2.90	128.93	123.86
7	G	101	BCL	C2A-C1A-CHA	2.90	128.93	123.86
11	v	102	SPO	C29-C28-C30	-2.90	110.40	115.27
9	M	403	U10	C17-C18-C19	-2.90	120.69	127.66
7	n	101	BCL	C2A-C1A-CHA	2.89	128.92	123.86
9	m	404	U10	C15-C14-C16	2.89	120.13	115.27
7	e	101	BCL	C2A-C1A-CHA	2.89	128.91	123.86
7	p	101	BCL	C2A-C1A-CHA	2.89	128.91	123.86
9	m	404	U10	C17-C18-C19	-2.89	120.70	127.66
7	N	101	BCL	C2A-C1A-CHA	2.89	128.91	123.86
7	4	101	BCL	CHA-C1A-NA	-2.89	119.79	126.40
7	r	101	BCL	C2A-C1A-CHA	2.89	128.90	123.86
9	M	403	U10	C15-C14-C16	2.88	120.12	115.27
9	M	403	U10	C10-C9-C11	2.88	120.12	115.27
8	l	305	BPH	C1-C2-C3	-2.87	121.08	126.04
7	L	301	BCL	C4A-NA-C1A	2.86	107.99	106.71
7	L	305	BCL	C2A-C1A-CHA	2.86	128.87	123.86
9	l	303	U10	C37-C38-C39	-2.86	120.76	127.66
7	l	304	BCL	C2A-C1A-CHA	2.86	128.86	123.86
8	L	306	BPH	C1-C2-C3	-2.86	121.10	126.04
7	d	101	BCL	C16-C15-C13	2.85	125.13	115.92
7	m	401	BCL	C2A-C1A-CHA	2.84	128.83	123.86
9	l	303	U10	C27-C28-C29	-2.84	120.83	127.66
7	A	1702	BCL	CMB-C2B-C3B	2.83	129.98	124.68
7	w	101	BCL	CAD-C3D-C4D	-2.83	106.89	108.47
12	h	301	PC1	O31-C31-C32	2.82	120.75	111.91
7	a	101	BCL	CMB-C2B-C3B	2.81	129.94	124.68
7	M	402	BCL	C1-C2-C3	-2.81	121.18	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	H	601	PC1	O31-C31-C32	2.81	120.72	111.91
11	b	103	SPO	C20-C21-C22	-2.80	117.73	123.47
12	c	1201	PC1	O31-C31-C32	2.80	120.69	111.91
7	k	101	BCL	C16-C15-C13	2.80	124.97	115.92
9	L	304	U10	C15-C14-C16	2.79	119.97	115.27
11	e	102	SPO	C21-C20-C19	-2.79	117.75	123.47
9	l	303	U10	C32-C33-C34	-2.78	120.96	127.66
11	e	102	SPO	C15-C16-C17	-2.78	118.60	126.42
9	l	303	U10	C25-C24-C26	2.78	119.95	115.27
7	y	101	BCL	CAD-C3D-C4D	-2.78	106.92	108.47
7	m	401	BCL	C1-C2-C3	-2.78	121.24	126.04
7	5	101	BCL	CAD-C3D-C4D	-2.77	106.92	108.47
7	m	403	BCL	C1-C2-C3	-2.77	121.25	126.04
9	l	303	U10	C6-C1-C2	2.75	121.36	119.18
7	K	101	BCL	CAD-C3D-C4D	-2.75	106.94	108.47
11	0	101	SPO	C10-C11-C12	-2.75	118.70	126.42
7	O	101	BCL	CAD-C3D-C4D	-2.73	106.95	108.47
9	l	303	U10	C50-C49-C51	2.73	119.86	115.27
7	z	101	BCL	C4B-C3B-CAB	-2.73	121.86	127.13
11	b	103	SPO	C15-C16-C17	-2.72	118.78	126.42
7	v	101	BCL	CMB-C2B-C3B	2.72	129.76	124.68
9	l	303	U10	C12-C13-C14	-2.71	121.13	127.66
11	ab	102	SPO	C26-C25-C23	-2.71	118.80	126.42
9	l	303	U10	C45-C44-C46	2.70	119.82	115.27
11	0	103	SPO	C10-C11-C12	-2.70	118.83	126.42
7	4	101	BCL	CMD-C2D-C3D	2.69	129.72	124.68
9	M	403	U10	C7-C8-C9	-2.68	122.33	126.79
11	v	102	SPO	C5-C6-C7	-2.67	121.86	125.89
11	E	102	SPO	C10-C11-C12	-2.67	118.92	126.42
9	l	303	U10	C56-C54-C55	2.67	120.50	114.60
11	w	102	SPO	C20-C21-C22	-2.66	118.02	123.47
7	y	101	BCL	CMB-C2B-C3B	2.66	129.66	124.68
7	p	101	BCL	CMD-C2D-C3D	2.66	129.65	124.68
7	O	101	BCL	CMB-C2B-C3B	2.66	129.65	124.68
7	x	101	BCL	CMD-C2D-C3D	2.65	129.64	124.68
9	m	404	U10	C7-C8-C9	-2.65	122.38	126.79
7	n	101	BCL	CMD-C2D-C3D	2.65	129.64	124.68
7	G	101	BCL	CMD-C2D-C3D	2.65	129.63	124.68
7	r	101	BCL	CMD-C2D-C3D	2.65	129.63	124.68
7	ab	101	BCL	CMD-C2D-C3D	2.65	129.63	124.68
7	e	101	BCL	CMD-C2D-C3D	2.65	129.63	124.68
7	l	304	BCL	C4A-NA-C1A	2.65	107.90	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	J	102	SPO	C29-C28-C30	-2.65	110.82	115.27
7	z	101	BCL	CAA-CBA-CGA	2.65	119.53	112.51
7	w	101	BCL	CMB-C2B-C3B	2.65	129.63	124.68
7	B	101	BCL	CMD-C2D-C3D	2.64	129.63	124.68
7	5	101	BCL	CMB-C2B-C3B	2.64	129.63	124.68
7	t	101	BCL	CMD-C2D-C3D	2.64	129.62	124.68
7	8	101	BCL	CMD-C2D-C3D	2.64	129.62	124.68
7	0	102	BCL	CMD-C2D-C3D	2.64	129.62	124.68
7	b	102	BCL	CMD-C2D-C3D	2.64	129.61	124.68
7	J	101	BCL	CMD-C2D-C3D	2.64	129.61	124.68
7	g	102	BCL	C4A-NA-C1A	2.64	107.89	106.71
7	aa	102	BCL	CMD-C2D-C3D	2.64	129.61	124.68
7	g	102	BCL	CMD-C2D-C3D	2.63	129.61	124.68
7	K	101	BCL	CMB-C2B-C3B	2.63	129.60	124.68
7	i	102	BCL	CMD-C2D-C3D	2.63	129.60	124.68
7	N	101	BCL	CMD-C2D-C3D	2.63	129.60	124.68
7	E	101	BCL	CMD-C2D-C3D	2.63	129.60	124.68
7	J	101	BCL	C4A-NA-C1A	2.63	107.89	106.71
7	E	101	BCL	C4A-NA-C1A	2.62	107.89	106.71
12	H	602	PC1	O31-C31-C32	2.62	120.13	111.91
11	t	102	SPO	C26-C25-C23	-2.62	119.06	126.42
7	0	102	BCL	C4A-NA-C1A	2.62	107.88	106.71
7	r	101	BCL	C4A-NA-C1A	2.62	107.88	106.71
7	4	101	BCL	CMB-C2B-C3B	2.61	129.57	124.68
13	m	406	CDL	OA8-CA7-C31	2.61	120.11	111.91
7	G	101	BCL	C4A-NA-C1A	2.61	107.88	106.71
7	8	101	BCL	C4A-NA-C1A	2.61	107.88	106.71
7	ab	101	BCL	C4A-NA-C1A	2.61	107.88	106.71
7	L	301	BCL	C16-C15-C13	2.61	124.34	115.92
7	L	302	BCL	CMD-C2D-C3D	2.60	129.55	124.68
7	x	101	BCL	C4A-NA-C1A	2.60	107.87	106.71
7	t	101	BCL	C4A-NA-C1A	2.59	107.87	106.71
7	B	101	BCL	C4A-NA-C1A	2.59	107.87	106.71
7	l	304	BCL	C4B-C3B-CAB	-2.59	122.13	127.13
7	z	101	BCL	CHD-C4C-NC	-2.59	122.20	125.08
7	e	101	BCL	C4A-NA-C1A	2.58	107.87	106.71
7	v	101	BCL	CMD-C2D-C3D	2.58	129.51	124.68
7	b	102	BCL	C4A-NA-C1A	2.58	107.87	106.71
7	y	101	BCL	C2A-C1A-CHA	2.58	128.37	123.86
12	A	1703	PC1	O31-C31-C32	2.57	119.98	111.91
7	v	101	BCL	C2A-C1A-CHA	2.57	128.35	123.86
7	aa	102	BCL	CBA-CAA-C2A	-2.57	106.29	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	K	101	BCL	C2A-C1A-CHA	2.56	128.34	123.86
12	A	1701	PC1	C13-N-C12	2.56	120.40	109.92
12	a	102	PC1	O31-C31-C32	2.56	119.95	111.91
7	a	101	BCL	CMD-C2D-C3D	2.56	129.47	124.68
7	G	101	BCL	CBA-CAA-C2A	-2.56	106.30	113.86
7	L	305	BCL	C4B-C3B-CAB	-2.56	122.18	127.13
7	r	101	BCL	CBA-CAA-C2A	-2.56	106.31	113.86
7	N	101	BCL	CBA-CAA-C2A	-2.56	106.31	113.86
7	t	101	BCL	CBA-CAA-C2A	-2.55	106.32	113.86
7	ab	101	BCL	CBA-CAA-C2A	-2.55	106.33	113.86
7	x	101	BCL	CBA-CAA-C2A	-2.55	106.33	113.86
7	g	102	BCL	CBA-CAA-C2A	-2.55	106.33	113.86
7	n	101	BCL	CBA-CAA-C2A	-2.55	106.33	113.86
7	b	102	BCL	CBA-CAA-C2A	-2.55	106.33	113.86
7	i	102	BCL	CBA-CAA-C2A	-2.55	106.33	113.86
7	L	305	BCL	C4A-NA-C1A	2.55	107.85	106.71
7	n	101	BCL	C4A-NA-C1A	2.55	107.85	106.71
7	p	101	BCL	CBA-CAA-C2A	-2.55	106.34	113.86
7	A	1702	BCL	CMD-C2D-C3D	2.55	129.45	124.68
7	B	101	BCL	CBA-CAA-C2A	-2.55	106.35	113.86
7	8	101	BCL	CBA-CAA-C2A	-2.55	106.35	113.86
7	O	101	BCL	C2A-C1A-CHA	2.55	128.31	123.86
11	v	102	SPO	C26-C25-C23	-2.55	119.27	126.42
11	d	103	SPO	C34-C33-C35	-2.54	110.99	115.27
7	J	101	BCL	CBA-CAA-C2A	-2.54	106.35	113.86
7	5	101	BCL	C2A-C1A-CHA	2.54	128.30	123.86
7	K	101	BCL	C1-C2-C3	-2.54	121.65	126.04
7	0	102	BCL	CBA-CAA-C2A	-2.54	106.37	113.86
7	e	101	BCL	CBA-CAA-C2A	-2.54	106.37	113.86
7	M	402	BCL	CMD-C2D-C3D	2.54	129.43	124.68
7	E	101	BCL	CBA-CAA-C2A	-2.54	106.38	113.86
7	a	101	BCL	C4B-C3B-CAB	-2.53	122.23	127.13
7	p	101	BCL	C4A-NA-C1A	2.53	107.84	106.71
7	L	302	BCL	OBB-CAB-CBB	-2.53	114.47	120.17
7	m	403	BCL	CMD-C2D-C3D	2.53	129.41	124.68
12	C	1201	PC1	O31-C31-C32	2.53	119.85	111.91
7	w	101	BCL	C2A-C1A-CHA	2.53	128.28	123.86
7	k	101	BCL	CMD-C2D-C3D	2.53	129.40	124.68
11	n	102	SPO	C15-C16-C17	-2.52	119.33	126.42
7	m	401	BCL	OBB-CAB-CBB	-2.52	114.50	120.17
7	9	102	BCL	CMD-C2D-C3D	2.52	129.38	124.68
7	i	101	BCL	CMD-C2D-C3D	2.51	129.38	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	i	102	BCL	C4A-NA-C1A	2.51	107.83	106.71
7	c	1202	BCL	CMD-C2D-C3D	2.51	129.38	124.68
7	aa	102	BCL	C4A-NA-C1A	2.51	107.83	106.71
7	Q	602	BCL	CMD-C2D-C3D	2.51	129.37	124.68
7	A	1702	BCL	C4B-C3B-CAB	-2.51	122.28	127.13
7	s	102	BCL	CMD-C2D-C3D	2.51	129.37	124.68
7	L	302	BCL	C4B-C3B-CAB	-2.51	122.29	127.13
7	I	101	BCL	CMD-C2D-C3D	2.51	129.37	124.68
7	f	101	BCL	CMD-C2D-C3D	2.50	129.36	124.68
7	q	103	BCL	CMD-C2D-C3D	2.50	129.36	124.68
7	F	101	BCL	CMD-C2D-C3D	2.50	129.35	124.68
7	N	101	BCL	C4A-NA-C1A	2.49	107.83	106.71
7	o	101	BCL	CMD-C2D-C3D	2.49	129.34	124.68
7	L	301	BCL	C17-C16-C15	-2.49	101.80	113.24
7	A	1702	BCL	C2A-C1A-CHA	2.49	128.21	123.86
7	C	1202	BCL	CMD-C2D-C3D	2.49	129.33	124.68
7	a	101	BCL	C2A-C1A-CHA	2.49	128.21	123.86
7	c	1202	BCL	C2A-C1A-CHA	2.48	128.20	123.86
7	M	402	BCL	OBB-CAB-CBB	-2.48	114.58	120.17
12	Q	601	PC1	O31-C31-C32	2.48	119.69	111.91
7	D	101	BCL	CMD-C2D-C3D	2.48	129.32	124.68
7	d	101	BCL	CMD-C2D-C3D	2.48	129.31	124.68
7	m	403	BCL	OBB-CAB-CBB	-2.48	114.59	120.17
7	D	101	BCL	C2A-C1A-CHA	2.48	128.19	123.86
7	D	101	BCL	C17-C16-C15	2.48	124.61	113.24
7	o	101	BCL	C2A-C1A-CHA	2.47	128.18	123.86
7	C	1202	BCL	C2A-C1A-CHA	2.47	128.18	123.86
7	q	101	BCL	C2A-C1A-CHA	2.47	128.18	123.86
7	q	101	BCL	CMD-C2D-C3D	2.47	129.30	124.68
7	d	101	BCL	C2A-C1A-CHA	2.47	128.17	123.86
7	I	101	BCL	C2A-C1A-CHA	2.46	128.17	123.86
7	s	102	BCL	C2A-C1A-CHA	2.46	128.17	123.86
12	A	1701	PC1	C11-C12-N	-2.46	107.55	115.78
7	Q	602	BCL	C2A-C1A-CHA	2.46	128.16	123.86
7	k	101	BCL	C2A-C1A-CHA	2.46	128.16	123.86
7	9	102	BCL	C2A-C1A-CHA	2.46	128.16	123.86
7	f	101	BCL	C2A-C1A-CHA	2.46	128.16	123.86
7	q	103	BCL	C2A-C1A-CHA	2.46	128.15	123.86
7	i	101	BCL	C2A-C1A-CHA	2.45	128.15	123.86
7	F	101	BCL	C2A-C1A-CHA	2.45	128.15	123.86
11	p	103	SPO	C10-C11-C12	-2.45	119.54	126.42
11	p	102	SPO	C14-C15-C16	-2.45	115.58	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	G	103	SPO	C15-C16-C17	-2.45	119.55	126.42
7	v	101	BCL	C1C-NC-C4C	2.44	107.80	106.71
9	l	303	U10	C20-C19-C21	2.43	119.36	115.27
11	b	103	SPO	C10-C11-C12	-2.43	119.59	126.42
8	L	306	BPH	CMD-C2D-C3D	2.43	129.22	124.68
9	L	304	U10	C1M-C1-C6	-2.43	120.44	124.40
7	L	301	BCL	OBB-CAB-CBB	-2.43	114.71	120.17
11	j	101	SPO	C21-C20-C19	-2.42	118.52	123.47
12	A	1701	PC1	O31-C31-C32	2.42	119.50	111.91
7	K	101	BCL	CMD-C2D-C3D	2.42	129.20	124.68
7	z	101	BCL	OBB-CAB-CBB	-2.41	114.74	120.17
9	l	303	U10	C30-C29-C31	2.41	119.33	115.27
11	G	103	SPO	C10-C11-C12	-2.41	119.65	126.42
7	5	101	BCL	CMD-C2D-C3D	2.41	129.18	124.68
7	w	101	BCL	CMD-C2D-C3D	2.41	129.18	124.68
11	n	102	SPO	C26-C25-C23	-2.40	119.67	126.42
7	O	101	BCL	CMD-C2D-C3D	2.40	129.16	124.68
7	C	1202	BCL	OBB-CAB-CBB	-2.40	114.78	120.17
7	L	305	BCL	CMD-C2D-C3D	2.39	129.15	124.68
7	y	101	BCL	CMD-C2D-C3D	2.39	129.15	124.68
7	D	101	BCL	OBB-CAB-CBB	-2.39	114.79	120.17
7	Q	602	BCL	OBB-CAB-CBB	-2.39	114.80	120.17
7	I	101	BCL	OBB-CAB-CBB	-2.39	114.80	120.17
7	d	101	BCL	OBB-CAB-CBB	-2.39	114.80	120.17
7	f	101	BCL	OBB-CAB-CBB	-2.38	114.80	120.17
7	l	304	BCL	CMD-C2D-C3D	2.38	129.14	124.68
7	i	101	BCL	OBB-CAB-CBB	-2.38	114.81	120.17
7	q	103	BCL	OBB-CAB-CBB	-2.38	114.81	120.17
7	c	1202	BCL	OBB-CAB-CBB	-2.38	114.82	120.17
7	o	101	BCL	OBB-CAB-CBB	-2.38	114.82	120.17
7	q	101	BCL	OBB-CAB-CBB	-2.38	114.82	120.17
7	s	102	BCL	OBB-CAB-CBB	-2.38	114.82	120.17
7	F	101	BCL	OBB-CAB-CBB	-2.37	114.83	120.17
7	L	301	BCL	CMD-C2D-C3D	2.37	129.12	124.68
7	k	101	BCL	OBB-CAB-CBB	-2.37	114.84	120.17
8	l	305	BPH	CMD-C2D-C3D	2.37	129.11	124.68
8	l	302	BPH	CMD-C2D-C3D	2.37	129.11	124.68
12	Q	601	PC1	C13-N-C12	2.36	119.58	109.92
7	M	402	BCL	C4B-C3B-CAB	-2.36	122.57	127.13
7	l	301	BCL	CMD-C2D-C3D	2.36	129.09	124.68
7	c	1202	BCL	C4B-C3B-CAB	-2.36	122.58	127.13
11	G	103	SPO	C5-C6-C7	-2.36	122.33	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	9	102	BCL	OBB-CAB-CBB	-2.35	114.87	120.17
9	L	304	U10	C36-C34-C35	2.35	119.80	114.60
7	9	102	BCL	C4B-C3B-CAB	-2.35	122.58	127.13
7	F	101	BCL	C4B-C3B-CAB	-2.35	122.59	127.13
7	I	101	BCL	C4B-C3B-CAB	-2.35	122.60	127.13
7	d	101	BCL	C4B-C3B-CAB	-2.34	122.60	127.13
9	l	303	U10	C50-C49-C48	-2.34	117.67	123.68
7	Q	602	BCL	C4B-C3B-CAB	-2.34	122.60	127.13
9	L	304	U10	C32-C33-C34	-2.34	119.75	127.75
7	L	301	BCL	C4B-C3B-CAB	-2.34	122.61	127.13
12	A	1703	PC1	C2-O21-C21	-2.34	112.03	117.79
8	L	306	BPH	CMB-C2B-C3B	2.34	129.05	124.68
7	s	102	BCL	C4B-C3B-CAB	-2.34	122.61	127.13
7	m	403	BCL	C4B-C3B-CAB	-2.34	122.61	127.13
7	L	305	BCL	OBB-CAB-CBB	-2.33	114.92	120.17
8	l	305	BPH	CMB-C2B-C3B	2.33	129.04	124.68
11	b	101	SPO	C14-C15-C16	-2.33	115.94	123.22
7	q	101	BCL	C4B-C3B-CAB	-2.33	122.63	127.13
7	l	304	BCL	OBB-CAB-CBB	-2.33	114.93	120.17
7	o	101	BCL	C4B-C3B-CAB	-2.33	122.64	127.13
12	a	102	PC1	C2-O21-C21	-2.32	112.07	117.79
13	m	406	CDL	OB8-CB7-C71	2.32	119.20	111.91
7	k	101	BCL	C4B-C3B-CAB	-2.32	122.64	127.13
11	9	101	SPO	C14-C15-C16	-2.32	115.97	123.22
7	i	101	BCL	C4B-C3B-CAB	-2.32	122.64	127.13
7	D	101	BCL	C4B-C3B-CAB	-2.32	122.64	127.13
11	e	102	SPO	C26-C25-C23	-2.32	119.90	126.42
7	C	1202	BCL	C4B-C3B-CAB	-2.32	122.65	127.13
7	m	401	BCL	CMD-C2D-C3D	2.32	129.02	124.68
11	G	103	SPO	C34-C33-C35	-2.31	111.38	115.27
7	q	103	BCL	C4B-C3B-CAB	-2.31	122.66	127.13
7	l	301	BCL	C4A-NA-C1A	2.31	107.75	106.71
7	f	101	BCL	C4B-C3B-CAB	-2.31	122.66	127.13
8	L	303	BPH	CMD-C2D-C3D	2.31	129.00	124.68
11	f	102	SPO	C5-C6-C7	-2.31	122.40	125.89
7	0	102	BCL	CMB-C2B-C3B	2.31	129.00	124.68
11	D	102	SPO	C5-C6-C7	-2.31	122.40	125.89
11	b	101	SPO	C5-C6-C7	-2.31	122.40	125.89
7	l	301	BCL	C16-C15-C13	-2.31	108.46	115.92
11	u	101	SPO	C20-C21-C22	-2.31	118.75	123.47
11	s	101	SPO	C5-C6-C7	-2.31	122.41	125.89
7	J	101	BCL	CMB-C2B-C3B	2.30	128.99	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	103	SPO	C20-C21-C22	-2.30	118.76	123.47
11	F	102	SPO	C5-C6-C7	-2.30	122.41	125.89
11	d	102	SPO	C5-C6-C7	-2.30	122.41	125.89
11	d	102	SPO	C20-C21-C22	-2.30	118.76	123.47
7	E	101	BCL	CMB-C2B-C3B	2.30	128.98	124.68
7	x	101	BCL	CMB-C2B-C3B	2.30	128.98	124.68
11	u	101	SPO	C5-C6-C7	-2.30	122.42	125.89
11	b	103	SPO	C21-C20-C19	-2.30	118.77	123.47
11	D	102	SPO	C20-C21-C22	-2.30	118.77	123.47
11	o	102	SPO	C20-C21-C22	-2.30	118.77	123.47
11	m	405	SPO	C5-C6-C7	-2.30	122.42	125.89
7	aa	102	BCL	CMB-C2B-C3B	2.30	128.97	124.68
7	s	102	BCL	C16-C15-C13	2.29	123.34	115.92
11	i	103	SPO	C5-C6-C7	-2.29	122.42	125.89
7	b	102	BCL	CMB-C2B-C3B	2.29	128.97	124.68
11	i	103	SPO	C20-C21-C22	-2.29	118.78	123.47
7	ab	101	BCL	CMB-C2B-C3B	2.29	128.97	124.68
11	aa	101	SPO	C5-C6-C7	-2.29	122.43	125.89
7	g	102	BCL	CMB-C2B-C3B	2.29	128.96	124.68
7	i	102	BCL	CMB-C2B-C3B	2.29	128.96	124.68
11	M	404	SPO	C5-C6-C7	-2.29	122.44	125.89
11	C	1203	SPO	C20-C21-C22	-2.29	118.79	123.47
11	aa	101	SPO	C20-C21-C22	-2.29	118.79	123.47
11	Q	603	SPO	C20-C21-C22	-2.28	118.80	123.47
11	9	103	SPO	C5-C6-C7	-2.28	122.44	125.89
11	g	101	SPO	C20-C21-C22	-2.28	118.80	123.47
7	G	101	BCL	CMB-C2B-C3B	2.28	128.95	124.68
9	M	403	U10	C30-C29-C31	2.28	119.10	115.27
7	F	101	BCL	C16-C15-C13	-2.28	108.55	115.92
11	s	101	SPO	C20-C21-C22	-2.28	118.81	123.47
11	p	102	SPO	C26-C25-C23	-2.28	120.02	126.42
11	q	102	SPO	C20-C21-C22	-2.28	118.81	123.47
7	t	101	BCL	CMB-C2B-C3B	2.28	128.94	124.68
7	N	101	BCL	CMB-C2B-C3B	2.27	128.93	124.68
11	C	1203	SPO	C5-C6-C7	-2.27	122.46	125.89
11	9	103	SPO	C20-C21-C22	-2.27	118.82	123.47
11	o	102	SPO	C5-C6-C7	-2.27	122.46	125.89
7	B	101	BCL	CMB-C2B-C3B	2.27	128.93	124.68
11	j	101	SPO	C26-C25-C23	-2.27	120.04	126.42
11	F	102	SPO	C20-C21-C22	-2.27	118.83	123.47
7	p	101	BCL	CMB-C2B-C3B	2.27	128.92	124.68
7	n	101	BCL	CMB-C2B-C3B	2.27	128.92	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	9	101	SPO	C5-C6-C7	-2.27	122.47	125.89
11	f	102	SPO	C20-C21-C22	-2.27	118.83	123.47
11	Q	603	SPO	C5-C6-C7	-2.27	122.47	125.89
11	0	103	SPO	C20-C21-C22	-2.27	118.83	123.47
7	8	101	BCL	CMB-C2B-C3B	2.26	128.91	124.68
9	m	404	U10	C30-C29-C31	2.26	119.08	115.27
7	w	101	BCL	C4B-C3B-CAB	-2.26	122.76	127.13
12	C	1201	PC1	C13-N-C12	2.26	119.17	109.92
7	z	101	BCL	CMD-C2D-C3D	2.26	128.91	124.68
7	5	101	BCL	C4B-C3B-CAB	-2.26	122.76	127.13
11	q	102	SPO	C34-C33-C35	-2.26	111.47	115.27
11	g	101	SPO	C5-C6-C7	-2.26	122.48	125.89
7	r	101	BCL	CMB-C2B-C3B	2.25	128.90	124.68
9	m	404	U10	C41-C39-C40	2.25	119.58	114.60
7	l	301	BCL	OBB-CAB-CBB	-2.25	115.10	120.17
7	e	101	BCL	CMB-C2B-C3B	2.25	128.89	124.68
7	K	101	BCL	C4B-C3B-CAB	-2.25	122.78	127.13
7	y	101	BCL	C4B-C3B-CAB	-2.25	122.78	127.13
11	F	103	SPO	C34-C33-C35	-2.25	111.49	115.27
11	F	103	SPO	C5-C6-C7	-2.25	122.49	125.89
7	o	101	BCL	C16-C17-C18	-2.25	105.39	115.98
11	o	102	SPO	C34-C33-C35	-2.25	111.49	115.27
11	w	102	SPO	C26-C25-C23	-2.25	120.11	126.42
7	O	101	BCL	C4B-C3B-CAB	-2.24	122.79	127.13
11	q	102	SPO	C5-C6-C7	-2.24	122.50	125.89
11	D	102	SPO	C34-C33-C35	-2.24	111.50	115.27
11	d	102	SPO	C34-C33-C35	-2.24	111.50	115.27
11	i	103	SPO	C34-C33-C35	-2.24	111.51	115.27
11	u	101	SPO	C34-C33-C35	-2.24	111.51	115.27
11	F	102	SPO	C34-C33-C35	-2.24	111.51	115.27
9	L	304	U10	C22-C23-C24	-2.24	122.28	127.66
11	C	1203	SPO	C34-C33-C35	-2.24	111.51	115.27
9	M	403	U10	C41-C39-C40	2.23	119.53	114.60
11	9	103	SPO	C34-C33-C35	-2.23	111.52	115.27
9	m	404	U10	C20-C19-C21	2.23	119.02	115.27
7	a	101	BCL	OBB-CAB-CBB	-2.23	115.16	120.17
11	f	102	SPO	C34-C33-C35	-2.23	111.53	115.27
7	A	1702	BCL	OBB-CAB-CBB	-2.23	115.16	120.17
11	Q	603	SPO	C34-C33-C35	-2.23	111.53	115.27
11	aa	101	SPO	C34-C33-C35	-2.22	111.53	115.27
8	l	302	BPH	C11-C10-C8	-2.22	108.74	115.92
11	g	101	SPO	C34-C33-C35	-2.22	111.54	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	s	101	SPO	C34-C33-C35	-2.22	111.54	115.27
8	L	303	BPH	CBA-CAA-C2A	-2.22	107.34	113.81
12	H	602	PC1	C2-O21-C21	-2.21	112.34	117.79
7	m	401	BCL	C4B-C3B-CAB	-2.21	122.85	127.13
7	z	101	BCL	CHC-C1C-NC	-2.21	121.45	124.51
9	M	403	U10	C20-C19-C21	2.21	118.99	115.27
11	t	102	SPO	C40-C38-C39	-2.21	109.73	114.60
11	b	103	SPO	C26-C25-C23	-2.21	120.22	126.42
11	0	101	SPO	C26-C25-C23	-2.20	120.24	126.42
12	c	1201	PC1	C13-N-C12	2.19	118.90	109.92
12	H	602	PC1	C13-N-C12	2.19	118.89	109.92
9	l	303	U10	C52-C53-C54	-2.19	120.26	127.75
7	m	401	BCL	C4A-NA-C1A	2.19	107.69	106.71
7	k	101	BCL	C16-C17-C18	-2.18	105.69	115.98
11	E	102	SPO	C15-C16-C17	-2.17	120.33	126.42
7	f	101	BCL	C16-C15-C13	2.15	122.88	115.92
7	K	101	BCL	C6-C7-C8	-2.15	108.96	115.92
12	A	1703	PC1	C13-N-C12	2.15	118.69	109.92
12	a	102	PC1	C13-N-C12	2.14	118.69	109.92
12	h	301	PC1	C13-N-C12	2.14	118.68	109.92
13	m	406	CDL	CB6-CB4-CB3	-2.14	106.73	111.79
11	J	102	SPO	C26-C25-C23	-2.13	120.43	126.42
7	L	301	BCL	C1C-NC-C4C	2.13	107.66	106.71
7	q	103	BCL	C17-C16-C15	2.13	123.02	113.24
12	H	601	PC1	C13-N-C12	2.13	118.61	109.92
7	v	101	BCL	O2A-C1-C2	-2.11	103.08	108.64
8	L	303	BPH	OBB-CAB-CBB	-2.11	115.42	120.17
7	w	101	BCL	C1C-NC-C4C	2.11	107.65	106.71
7	m	401	BCL	C11-C10-C8	-2.10	109.13	115.92
7	z	101	BCL	CED-O2D-CGD	2.10	120.69	115.94
11	p	103	SPO	C20-C21-C22	-2.10	119.18	123.47
9	L	304	U10	C20-C19-C21	2.09	118.79	115.27
11	w	102	SPO	C29-C28-C30	-2.09	111.75	115.27
11	u	101	SPO	C15-C16-C17	-2.09	120.55	126.42
11	s	101	SPO	C15-C16-C17	-2.09	120.56	126.42
11	p	103	SPO	C14-C15-C16	-2.09	116.71	123.22
11	F	102	SPO	C15-C16-C17	-2.09	120.56	126.42
11	J	102	SPO	C20-C21-C22	-2.08	119.20	123.47
11	0	103	SPO	C15-C16-C17	-2.08	120.56	126.42
11	q	102	SPO	C15-C16-C17	-2.08	120.56	126.42
11	p	102	SPO	C10-C11-C12	-2.08	120.56	126.42
11	D	102	SPO	C15-C16-C17	-2.08	120.56	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	1203	SPO	C15-C16-C17	-2.08	120.56	126.42
11	i	103	SPO	C15-C16-C17	-2.08	120.56	126.42
11	o	102	SPO	C15-C16-C17	-2.08	120.58	126.42
11	aa	101	SPO	C15-C16-C17	-2.08	120.58	126.42
11	f	102	SPO	C15-C16-C17	-2.08	120.59	126.42
11	9	103	SPO	C15-C16-C17	-2.07	120.59	126.42
11	F	103	SPO	C15-C16-C17	-2.07	120.59	126.42
8	L	306	BPH	CMA-C3A-C4A	-2.07	109.84	114.38
11	d	102	SPO	C15-C16-C17	-2.07	120.60	126.42
11	Q	603	SPO	C15-C16-C17	-2.07	120.60	126.42
8	l	302	BPH	CMA-C3A-C4A	-2.07	109.85	114.38
11	g	101	SPO	C15-C16-C17	-2.07	120.61	126.42
7	o	101	BCL	C16-C15-C13	2.05	122.53	115.92
8	l	305	BPH	CMA-C3A-C4A	-2.05	109.90	114.38
7	l	301	BCL	C4B-C3B-CAB	-2.04	123.18	127.13
9	L	304	U10	C10-C9-C11	2.04	118.69	115.27
11	G	103	SPO	C26-C25-C23	-2.03	120.70	126.42
11	m	405	SPO	C9-C10-C11	-2.03	116.87	123.22
7	O	101	BCL	C1C-NC-C4C	2.03	107.62	106.71
7	5	101	BCL	C1C-NC-C4C	2.03	107.62	106.71
11	ab	102	SPO	C29-C28-C30	-2.03	111.86	115.27
11	E	102	SPO	C40-C38-C39	-2.03	110.13	114.60
11	p	102	SPO	C21-C20-C19	-2.02	119.33	123.47
11	m	405	SPO	C10-C11-C12	-2.02	120.74	126.42
11	p	103	SPO	C27-C26-C25	-2.02	116.92	123.22
8	l	302	BPH	OBB-CAB-CBB	-2.02	115.63	120.17
11	M	404	SPO	C9-C10-C11	-2.02	116.92	123.22
11	G	102	SPO	C40-C38-C39	-2.00	110.19	114.60

There are no chirality outliers.

All (1453) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	w	101	BCL	C4-C3-C5-C6
7	z	101	BCL	CAD-CBD-CGD-O1D
7	z	101	BCL	CAD-CBD-CGD-O2D
7	4	101	BCL	C1A-C2A-CAA-CBA
8	L	303	BPH	C4C-C3C-CAC-CBC
8	L	303	BPH	C2C-C3C-CAC-CBC
8	L	306	BPH	C2-C3-C5-C6
8	L	306	BPH	C4-C3-C5-C6
8	l	302	BPH	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
8	l	305	BPH	C2-C3-C5-C6
8	l	305	BPH	C4-C3-C5-C6
9	L	304	U10	C1-C6-C7-C8
9	L	304	U10	C5-C6-C7-C8
9	L	304	U10	C7-C8-C9-C10
9	L	304	U10	C7-C8-C9-C11
9	L	304	U10	C12-C13-C14-C15
9	L	304	U10	C12-C13-C14-C16
9	L	304	U10	C14-C16-C17-C18
9	L	304	U10	C17-C18-C19-C20
9	L	304	U10	C17-C18-C19-C21
9	L	304	U10	C22-C23-C24-C25
9	L	304	U10	C29-C31-C32-C33
9	M	403	U10	C23-C24-C26-C27
9	M	403	U10	C25-C24-C26-C27
9	l	303	U10	C1-C6-C7-C8
9	l	303	U10	C7-C8-C9-C10
9	l	303	U10	C7-C8-C9-C11
9	l	303	U10	C42-C43-C44-C45
9	l	303	U10	C42-C43-C44-C46
9	l	303	U10	C47-C48-C49-C50
9	l	303	U10	C47-C48-C49-C51
9	l	303	U10	C50-C49-C51-C52
9	m	404	U10	C23-C24-C26-C27
9	m	404	U10	C25-C24-C26-C27
11	M	404	SPO	C2-C1-O1-CM1
11	M	404	SPO	C5-C6-C7-C8
11	M	404	SPO	C5-C6-C7-C9
11	M	404	SPO	C8-C7-C9-C10
11	M	404	SPO	C10-C11-C12-C13
11	M	404	SPO	C10-C11-C12-C14
11	M	404	SPO	C13-C12-C14-C15
11	M	404	SPO	C18-C17-C19-C20
11	M	404	SPO	C21-C22-C23-C24
11	M	404	SPO	C22-C23-C25-C26
11	M	404	SPO	C26-C27-C28-C29
11	M	404	SPO	C31-C32-C33-C34
11	D	102	SPO	C2-C1-C4-C5
11	D	102	SPO	C3-C1-C4-C5
11	D	102	SPO	C1-C4-C5-C6
11	D	102	SPO	C6-C7-C9-C10
11	D	102	SPO	C8-C7-C9-C10

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Mol	Chain	Res	Type	Atoms
11	D	102	SPO	C10-C11-C12-C14
11	D	102	SPO	C13-C12-C14-C15
11	D	102	SPO	C15-C16-C17-C18
11	D	102	SPO	C16-C17-C19-C20
11	D	102	SPO	C21-C22-C23-C24
11	D	102	SPO	C22-C23-C25-C26
11	D	102	SPO	C26-C27-C28-C29
11	D	102	SPO	C34-C33-C35-C36
11	E	102	SPO	C2-C1-O1-CM1
11	E	102	SPO	C3-C1-O1-CM1
11	E	102	SPO	C4-C1-O1-CM1
11	E	102	SPO	C6-C7-C9-C10
11	E	102	SPO	C10-C11-C12-C13
11	E	102	SPO	C10-C11-C12-C14
11	E	102	SPO	C13-C12-C14-C15
11	E	102	SPO	C18-C17-C19-C20
11	E	102	SPO	C17-C19-C20-C21
11	E	102	SPO	C21-C22-C23-C24
11	E	102	SPO	C22-C23-C25-C26
11	E	102	SPO	C26-C27-C28-C30
11	F	102	SPO	C2-C1-C4-C5
11	F	102	SPO	C3-C1-C4-C5
11	F	102	SPO	C1-C4-C5-C6
11	F	102	SPO	C6-C7-C9-C10
11	F	102	SPO	C8-C7-C9-C10
11	F	102	SPO	C10-C11-C12-C14
11	F	102	SPO	C13-C12-C14-C15
11	F	102	SPO	C15-C16-C17-C18
11	F	102	SPO	C16-C17-C19-C20
11	F	102	SPO	C21-C22-C23-C24
11	F	102	SPO	C22-C23-C25-C26
11	F	102	SPO	C26-C27-C28-C29
11	F	102	SPO	C34-C33-C35-C36
11	F	103	SPO	C2-C1-C4-C5
11	F	103	SPO	C3-C1-C4-C5
11	F	103	SPO	C1-C4-C5-C6
11	F	103	SPO	C6-C7-C9-C10
11	F	103	SPO	C8-C7-C9-C10
11	F	103	SPO	C10-C11-C12-C14
11	F	103	SPO	C13-C12-C14-C15
11	F	103	SPO	C15-C16-C17-C18
11	F	103	SPO	C16-C17-C19-C20

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Mol	Chain	Res	Type	Atoms
11	F	103	SPO	C21-C22-C23-C24
11	F	103	SPO	C22-C23-C25-C26
11	F	103	SPO	C26-C27-C28-C29
11	F	103	SPO	C34-C33-C35-C36
11	G	102	SPO	C5-C6-C7-C8
11	G	102	SPO	C8-C7-C9-C10
11	G	102	SPO	C10-C11-C12-C13
11	G	102	SPO	C15-C16-C17-C18
11	G	102	SPO	C18-C17-C19-C20
11	G	102	SPO	C21-C22-C23-C25
11	G	102	SPO	C26-C27-C28-C29
11	G	102	SPO	C27-C28-C30-C31
11	G	102	SPO	C28-C30-C31-C32
11	G	103	SPO	C2-C1-C4-C5
11	G	103	SPO	C3-C1-C4-C5
11	G	103	SPO	C1-C4-C5-C6
11	G	103	SPO	C5-C6-C7-C8
11	G	103	SPO	C5-C6-C7-C9
11	G	103	SPO	C8-C7-C9-C10
11	G	103	SPO	C13-C12-C14-C15
11	G	103	SPO	C18-C17-C19-C20
11	G	103	SPO	C20-C21-C22-C23
11	G	103	SPO	C21-C22-C23-C24
11	G	103	SPO	C25-C26-C27-C28
11	G	103	SPO	C26-C27-C28-C29
11	G	103	SPO	C26-C27-C28-C30
11	G	103	SPO	C27-C28-C30-C31
11	G	103	SPO	C34-C33-C35-C36
11	G	103	SPO	C33-C35-C36-C37
11	J	102	SPO	C8-C7-C9-C10
11	J	102	SPO	C13-C12-C14-C15
11	J	102	SPO	C15-C16-C17-C18
11	J	102	SPO	C15-C16-C17-C19
11	J	102	SPO	C16-C17-C19-C20
11	J	102	SPO	C21-C22-C23-C24
11	J	102	SPO	C24-C23-C25-C26
11	J	102	SPO	C26-C27-C28-C30
11	J	102	SPO	C29-C28-C30-C31
11	J	102	SPO	C31-C32-C33-C34
11	9	101	SPO	O1-C1-C4-C5
11	9	101	SPO	C2-C1-C4-C5
11	9	101	SPO	C3-C1-C4-C5

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Mol	Chain	Res	Type	Atoms
11	9	101	SPO	C5-C6-C7-C9
11	9	101	SPO	C6-C7-C9-C10
11	9	101	SPO	C10-C11-C12-C14
11	9	101	SPO	C11-C12-C14-C15
11	9	101	SPO	C13-C12-C14-C15
11	9	101	SPO	C15-C16-C17-C18
11	9	101	SPO	C18-C17-C19-C20
11	9	101	SPO	C17-C19-C20-C21
11	9	101	SPO	C21-C22-C23-C24
11	9	101	SPO	C22-C23-C25-C26
11	9	101	SPO	C24-C23-C25-C26
11	9	101	SPO	C26-C27-C28-C29
11	9	101	SPO	C28-C30-C31-C32
11	9	101	SPO	C36-C37-C38-C39
11	9	103	SPO	C2-C1-C4-C5
11	9	103	SPO	C3-C1-C4-C5
11	9	103	SPO	C1-C4-C5-C6
11	9	103	SPO	C6-C7-C9-C10
11	9	103	SPO	C8-C7-C9-C10
11	9	103	SPO	C10-C11-C12-C14
11	9	103	SPO	C13-C12-C14-C15
11	9	103	SPO	C15-C16-C17-C18
11	9	103	SPO	C15-C16-C17-C19
11	9	103	SPO	C16-C17-C19-C20
11	9	103	SPO	C21-C22-C23-C24
11	9	103	SPO	C22-C23-C25-C26
11	9	103	SPO	C26-C27-C28-C29
11	9	103	SPO	C34-C33-C35-C36
11	0	101	SPO	C4-C1-O1-CM1
11	0	101	SPO	C2-C1-C4-C5
11	0	101	SPO	C3-C1-C4-C5
11	0	101	SPO	C1-C4-C5-C6
11	0	101	SPO	C5-C6-C7-C8
11	0	101	SPO	C8-C7-C9-C10
11	0	101	SPO	C10-C11-C12-C13
11	0	101	SPO	C13-C12-C14-C15
11	0	101	SPO	C15-C16-C17-C18
11	0	101	SPO	C18-C17-C19-C20
11	0	101	SPO	C17-C19-C20-C21
11	0	101	SPO	C21-C22-C23-C24
11	0	101	SPO	C21-C22-C23-C25
11	0	101	SPO	C22-C23-C25-C26

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Mol	Chain	Res	Type	Atoms
11	0	101	SPO	C26-C27-C28-C29
11	0	101	SPO	C31-C32-C33-C34
11	0	101	SPO	C33-C35-C36-C37
11	0	103	SPO	C8-C7-C9-C10
11	0	103	SPO	C10-C11-C12-C14
11	0	103	SPO	C13-C12-C14-C15
11	0	103	SPO	C12-C14-C15-C16
11	0	103	SPO	C18-C17-C19-C20
11	0	103	SPO	C21-C22-C23-C24
11	0	103	SPO	C26-C27-C28-C29
11	0	103	SPO	C29-C28-C30-C31
11	0	103	SPO	C31-C32-C33-C34
11	0	103	SPO	C32-C33-C35-C36
11	0	103	SPO	C33-C35-C36-C37
11	C	1203	SPO	C2-C1-C4-C5
11	C	1203	SPO	C3-C1-C4-C5
11	C	1203	SPO	C1-C4-C5-C6
11	C	1203	SPO	C6-C7-C9-C10
11	C	1203	SPO	C8-C7-C9-C10
11	C	1203	SPO	C10-C11-C12-C14
11	C	1203	SPO	C13-C12-C14-C15
11	C	1203	SPO	C15-C16-C17-C18
11	C	1203	SPO	C16-C17-C19-C20
11	C	1203	SPO	C21-C22-C23-C24
11	C	1203	SPO	C22-C23-C25-C26
11	C	1203	SPO	C26-C27-C28-C29
11	C	1203	SPO	C34-C33-C35-C36
11	m	405	SPO	C2-C1-O1-CM1
11	m	405	SPO	C5-C6-C7-C8
11	m	405	SPO	C5-C6-C7-C9
11	m	405	SPO	C8-C7-C9-C10
11	m	405	SPO	C10-C11-C12-C13
11	m	405	SPO	C10-C11-C12-C14
11	m	405	SPO	C13-C12-C14-C15
11	m	405	SPO	C18-C17-C19-C20
11	m	405	SPO	C21-C22-C23-C24
11	m	405	SPO	C22-C23-C25-C26
11	m	405	SPO	C26-C27-C28-C29
11	m	405	SPO	C31-C32-C33-C34
11	b	101	SPO	O1-C1-C4-C5
11	b	101	SPO	C2-C1-C4-C5
11	b	101	SPO	C3-C1-C4-C5

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Mol	Chain	Res	Type	Atoms
11	b	101	SPO	C5-C6-C7-C9
11	b	101	SPO	C6-C7-C9-C10
11	b	101	SPO	C10-C11-C12-C14
11	b	101	SPO	C11-C12-C14-C15
11	b	101	SPO	C13-C12-C14-C15
11	b	101	SPO	C15-C16-C17-C18
11	b	101	SPO	C18-C17-C19-C20
11	b	101	SPO	C17-C19-C20-C21
11	b	101	SPO	C21-C22-C23-C24
11	b	101	SPO	C22-C23-C25-C26
11	b	101	SPO	C24-C23-C25-C26
11	b	101	SPO	C26-C27-C28-C29
11	b	101	SPO	C28-C30-C31-C32
11	b	101	SPO	C36-C37-C38-C39
11	b	103	SPO	C5-C6-C7-C9
11	b	103	SPO	C8-C7-C9-C10
11	b	103	SPO	C11-C10-C9-C7
11	b	103	SPO	C13-C12-C14-C15
11	b	103	SPO	C18-C17-C19-C20
11	b	103	SPO	C21-C22-C23-C24
11	b	103	SPO	C25-C26-C27-C28
11	b	103	SPO	C26-C27-C28-C29
11	b	103	SPO	C26-C27-C28-C30
11	b	103	SPO	C31-C32-C33-C34
11	d	102	SPO	C2-C1-C4-C5
11	d	102	SPO	C3-C1-C4-C5
11	d	102	SPO	C1-C4-C5-C6
11	d	102	SPO	C6-C7-C9-C10
11	d	102	SPO	C8-C7-C9-C10
11	d	102	SPO	C10-C11-C12-C14
11	d	102	SPO	C13-C12-C14-C15
11	d	102	SPO	C15-C16-C17-C18
11	d	102	SPO	C16-C17-C19-C20
11	d	102	SPO	C21-C22-C23-C24
11	d	102	SPO	C22-C23-C25-C26
11	d	102	SPO	C26-C27-C28-C29
11	d	102	SPO	C34-C33-C35-C36
11	d	103	SPO	C8-C7-C9-C10
11	d	103	SPO	C11-C10-C9-C7
11	d	103	SPO	C13-C12-C14-C15
11	d	103	SPO	C12-C14-C15-C16
11	d	103	SPO	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
11	d	103	SPO	C15-C16-C17-C19
11	d	103	SPO	C18-C17-C19-C20
11	d	103	SPO	C20-C21-C22-C23
11	d	103	SPO	C21-C22-C23-C25
11	d	103	SPO	C22-C23-C25-C26
11	d	103	SPO	C24-C23-C25-C26
11	d	103	SPO	C26-C27-C28-C29
11	d	103	SPO	C26-C27-C28-C30
11	d	103	SPO	C27-C28-C30-C31
11	d	103	SPO	C31-C32-C33-C35
11	d	103	SPO	C33-C35-C36-C37
11	d	103	SPO	C36-C37-C38-C40
11	e	102	SPO	C5-C6-C7-C9
11	e	102	SPO	C8-C7-C9-C10
11	e	102	SPO	C11-C10-C9-C7
11	e	102	SPO	C10-C11-C12-C14
11	e	102	SPO	C13-C12-C14-C15
11	e	102	SPO	C18-C17-C19-C20
11	e	102	SPO	C25-C26-C27-C28
11	e	102	SPO	C26-C27-C28-C29
11	e	102	SPO	C28-C30-C31-C32
11	e	102	SPO	C31-C32-C33-C35
11	e	102	SPO	C33-C35-C36-C37
11	f	102	SPO	C2-C1-C4-C5
11	f	102	SPO	C3-C1-C4-C5
11	f	102	SPO	C1-C4-C5-C6
11	f	102	SPO	C6-C7-C9-C10
11	f	102	SPO	C8-C7-C9-C10
11	f	102	SPO	C10-C11-C12-C14
11	f	102	SPO	C13-C12-C14-C15
11	f	102	SPO	C15-C16-C17-C18
11	f	102	SPO	C16-C17-C19-C20
11	f	102	SPO	C21-C22-C23-C24
11	f	102	SPO	C22-C23-C25-C26
11	f	102	SPO	C26-C27-C28-C29
11	f	102	SPO	C34-C33-C35-C36
11	g	101	SPO	C2-C1-C4-C5
11	g	101	SPO	C3-C1-C4-C5
11	g	101	SPO	C1-C4-C5-C6
11	g	101	SPO	C6-C7-C9-C10
11	g	101	SPO	C8-C7-C9-C10
11	g	101	SPO	C10-C11-C12-C14

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Mol	Chain	Res	Type	Atoms
11	g	101	SPO	C13-C12-C14-C15
11	g	101	SPO	C15-C16-C17-C18
11	g	101	SPO	C16-C17-C19-C20
11	g	101	SPO	C21-C22-C23-C24
11	g	101	SPO	C22-C23-C25-C26
11	g	101	SPO	C26-C27-C28-C29
11	g	101	SPO	C34-C33-C35-C36
11	i	103	SPO	C2-C1-C4-C5
11	i	103	SPO	C3-C1-C4-C5
11	i	103	SPO	C1-C4-C5-C6
11	i	103	SPO	C6-C7-C9-C10
11	i	103	SPO	C8-C7-C9-C10
11	i	103	SPO	C10-C11-C12-C14
11	i	103	SPO	C13-C12-C14-C15
11	i	103	SPO	C15-C16-C17-C18
11	i	103	SPO	C16-C17-C19-C20
11	i	103	SPO	C21-C22-C23-C24
11	i	103	SPO	C22-C23-C25-C26
11	i	103	SPO	C26-C27-C28-C29
11	i	103	SPO	C34-C33-C35-C36
11	j	101	SPO	O1-C1-C4-C5
11	j	101	SPO	C2-C1-C4-C5
11	j	101	SPO	C3-C1-C4-C5
11	j	101	SPO	C5-C6-C7-C9
11	j	101	SPO	C8-C7-C9-C10
11	j	101	SPO	C10-C11-C12-C14
11	j	101	SPO	C13-C12-C14-C15
11	j	101	SPO	C15-C16-C17-C18
11	j	101	SPO	C18-C17-C19-C20
11	j	101	SPO	C21-C22-C23-C24
11	j	101	SPO	C26-C27-C28-C29
11	j	101	SPO	C31-C32-C33-C34
11	j	101	SPO	C33-C35-C36-C37
11	n	102	SPO	C4-C1-O1-CM1
11	n	102	SPO	C5-C6-C7-C8
11	n	102	SPO	C8-C7-C9-C10
11	n	102	SPO	C10-C11-C12-C13
11	n	102	SPO	C13-C12-C14-C15
11	n	102	SPO	C15-C16-C17-C18
11	n	102	SPO	C15-C16-C17-C19
11	n	102	SPO	C18-C17-C19-C20
11	n	102	SPO	C17-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
11	n	102	SPO	C24-C23-C25-C26
11	n	102	SPO	C26-C27-C28-C29
11	n	102	SPO	C31-C32-C33-C34
11	o	102	SPO	C2-C1-C4-C5
11	o	102	SPO	C3-C1-C4-C5
11	o	102	SPO	C1-C4-C5-C6
11	o	102	SPO	C6-C7-C9-C10
11	o	102	SPO	C8-C7-C9-C10
11	o	102	SPO	C10-C11-C12-C14
11	o	102	SPO	C13-C12-C14-C15
11	o	102	SPO	C15-C16-C17-C18
11	o	102	SPO	C16-C17-C19-C20
11	o	102	SPO	C21-C22-C23-C24
11	o	102	SPO	C22-C23-C25-C26
11	o	102	SPO	C26-C27-C28-C29
11	o	102	SPO	C34-C33-C35-C36
11	p	102	SPO	C8-C7-C9-C10
11	p	102	SPO	C10-C11-C12-C14
11	p	102	SPO	C13-C12-C14-C15
11	p	102	SPO	C15-C16-C17-C18
11	p	102	SPO	C15-C16-C17-C19
11	p	102	SPO	C18-C17-C19-C20
11	p	102	SPO	C21-C22-C23-C24
11	p	102	SPO	C25-C26-C27-C28
11	p	102	SPO	C26-C27-C28-C29
11	p	102	SPO	C31-C32-C33-C35
11	p	102	SPO	C36-C37-C38-C39
11	p	103	SPO	C5-C6-C7-C8
11	p	103	SPO	C5-C6-C7-C9
11	p	103	SPO	C8-C7-C9-C10
11	p	103	SPO	C11-C10-C9-C7
11	p	103	SPO	C13-C12-C14-C15
11	p	103	SPO	C18-C17-C19-C20
11	p	103	SPO	C21-C22-C23-C24
11	p	103	SPO	C22-C23-C25-C26
11	p	103	SPO	C26-C27-C28-C29
11	p	103	SPO	C26-C27-C28-C30
11	p	103	SPO	C31-C32-C33-C34
11	p	103	SPO	C36-C37-C38-C39
11	q	102	SPO	C2-C1-C4-C5
11	q	102	SPO	C3-C1-C4-C5
11	q	102	SPO	C1-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
11	q	102	SPO	C6-C7-C9-C10
11	q	102	SPO	C8-C7-C9-C10
11	q	102	SPO	C10-C11-C12-C14
11	q	102	SPO	C13-C12-C14-C15
11	q	102	SPO	C15-C16-C17-C18
11	q	102	SPO	C16-C17-C19-C20
11	q	102	SPO	C21-C22-C23-C24
11	q	102	SPO	C22-C23-C25-C26
11	q	102	SPO	C26-C27-C28-C29
11	q	102	SPO	C34-C33-C35-C36
11	s	101	SPO	C2-C1-C4-C5
11	s	101	SPO	C3-C1-C4-C5
11	s	101	SPO	C1-C4-C5-C6
11	s	101	SPO	C6-C7-C9-C10
11	s	101	SPO	C8-C7-C9-C10
11	s	101	SPO	C10-C11-C12-C14
11	s	101	SPO	C13-C12-C14-C15
11	s	101	SPO	C15-C16-C17-C18
11	s	101	SPO	C16-C17-C19-C20
11	s	101	SPO	C21-C22-C23-C24
11	s	101	SPO	C22-C23-C25-C26
11	s	101	SPO	C26-C27-C28-C29
11	s	101	SPO	C34-C33-C35-C36
11	t	102	SPO	C8-C7-C9-C10
11	t	102	SPO	C13-C12-C14-C15
11	t	102	SPO	C18-C17-C19-C20
11	t	102	SPO	C21-C22-C23-C24
11	t	102	SPO	C22-C23-C25-C26
11	t	102	SPO	C26-C27-C28-C29
11	t	102	SPO	C31-C32-C33-C34
11	t	102	SPO	C33-C35-C36-C37
11	u	101	SPO	C2-C1-C4-C5
11	u	101	SPO	C3-C1-C4-C5
11	u	101	SPO	C1-C4-C5-C6
11	u	101	SPO	C6-C7-C9-C10
11	u	101	SPO	C8-C7-C9-C10
11	u	101	SPO	C10-C11-C12-C14
11	u	101	SPO	C13-C12-C14-C15
11	u	101	SPO	C15-C16-C17-C18
11	u	101	SPO	C16-C17-C19-C20
11	u	101	SPO	C21-C22-C23-C24
11	u	101	SPO	C22-C23-C25-C26

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Mol	Chain	Res	Type	Atoms
11	u	101	SPO	C26-C27-C28-C29
11	u	101	SPO	C34-C33-C35-C36
11	v	102	SPO	C2-C1-C4-C5
11	v	102	SPO	C3-C1-C4-C5
11	v	102	SPO	C1-C4-C5-C6
11	v	102	SPO	C8-C7-C9-C10
11	v	102	SPO	C13-C12-C14-C15
11	v	102	SPO	C15-C16-C17-C18
11	v	102	SPO	C18-C17-C19-C20
11	v	102	SPO	C21-C22-C23-C24
11	v	102	SPO	C22-C23-C25-C26
11	v	102	SPO	C26-C27-C28-C29
11	v	102	SPO	C29-C28-C30-C31
11	v	102	SPO	C28-C30-C31-C32
11	v	102	SPO	C31-C32-C33-C35
11	w	102	SPO	C1-C4-C5-C6
11	w	102	SPO	C8-C7-C9-C10
11	w	102	SPO	C10-C11-C12-C14
11	w	102	SPO	C13-C12-C14-C15
11	w	102	SPO	C12-C14-C15-C16
11	w	102	SPO	C15-C16-C17-C18
11	w	102	SPO	C18-C17-C19-C20
11	w	102	SPO	C21-C22-C23-C25
11	w	102	SPO	C26-C27-C28-C29
11	w	102	SPO	C29-C28-C30-C31
11	w	102	SPO	C31-C32-C33-C34
11	w	102	SPO	C33-C35-C36-C37
11	aa	101	SPO	C2-C1-C4-C5
11	aa	101	SPO	C3-C1-C4-C5
11	aa	101	SPO	C1-C4-C5-C6
11	aa	101	SPO	C6-C7-C9-C10
11	aa	101	SPO	C8-C7-C9-C10
11	aa	101	SPO	C10-C11-C12-C14
11	aa	101	SPO	C13-C12-C14-C15
11	aa	101	SPO	C15-C16-C17-C18
11	aa	101	SPO	C16-C17-C19-C20
11	aa	101	SPO	C21-C22-C23-C24
11	aa	101	SPO	C22-C23-C25-C26
11	aa	101	SPO	C26-C27-C28-C29
11	aa	101	SPO	C34-C33-C35-C36
11	Q	603	SPO	C2-C1-C4-C5
11	Q	603	SPO	C3-C1-C4-C5

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Mol	Chain	Res	Type	Atoms
11	Q	603	SPO	C1-C4-C5-C6
11	Q	603	SPO	C6-C7-C9-C10
11	Q	603	SPO	C8-C7-C9-C10
11	Q	603	SPO	C10-C11-C12-C14
11	Q	603	SPO	C13-C12-C14-C15
11	Q	603	SPO	C15-C16-C17-C18
11	Q	603	SPO	C16-C17-C19-C20
11	Q	603	SPO	C21-C22-C23-C24
11	Q	603	SPO	C22-C23-C25-C26
11	Q	603	SPO	C26-C27-C28-C29
11	Q	603	SPO	C34-C33-C35-C36
11	ab	102	SPO	C5-C6-C7-C8
11	ab	102	SPO	C5-C6-C7-C9
11	ab	102	SPO	C8-C7-C9-C10
11	ab	102	SPO	C13-C12-C14-C15
11	ab	102	SPO	C12-C14-C15-C16
11	ab	102	SPO	C18-C17-C19-C20
11	ab	102	SPO	C21-C22-C23-C24
11	ab	102	SPO	C22-C23-C25-C26
11	ab	102	SPO	C25-C26-C27-C28
11	ab	102	SPO	C26-C27-C28-C30
11	ab	102	SPO	C28-C30-C31-C32
12	H	601	PC1	C11-O13-P-O12
12	H	601	PC1	C1-O11-P-O14
12	H	601	PC1	C12-C11-O13-P
12	H	601	PC1	C22-C21-O21-C2
12	H	602	PC1	C12-C11-O13-P
12	H	602	PC1	O13-C11-C12-N
12	A	1703	PC1	C11-O13-P-O14
12	A	1703	PC1	C11-O13-P-O11
12	A	1703	PC1	C1-O11-P-O14
12	A	1703	PC1	C1-O11-P-O13
12	A	1703	PC1	C12-C11-O13-P
12	C	1201	PC1	C11-O13-P-O14
12	h	301	PC1	C11-O13-P-O12
12	h	301	PC1	C1-O11-P-O14
12	h	301	PC1	C12-C11-O13-P
12	h	301	PC1	C22-C21-O21-C2
12	a	102	PC1	C11-O13-P-O14
12	a	102	PC1	C11-O13-P-O11
12	a	102	PC1	C1-O11-P-O14
12	a	102	PC1	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
12	a	102	PC1	C12-C11-O13-P
12	c	1201	PC1	C1-O11-P-O14
12	c	1201	PC1	C1-O11-P-O13
13	m	406	CDL	CA2-OA2-PA1-OA3
13	m	406	CDL	OA7-CA5-OA6-CA4
13	m	406	CDL	CB2-OB2-PB2-OB3
13	m	406	CDL	CB2-OB2-PB2-OB4
13	m	406	CDL	OB9-CB7-OB8-CB6
13	m	406	CDL	C71-CB7-OB8-CB6
7	Q	602	BCL	C13-C15-C16-C17
11	G	103	SPO	C36-C37-C38-C39
11	e	102	SPO	C36-C37-C38-C39
11	t	102	SPO	C36-C37-C38-C40
12	H	601	PC1	O32-C31-O31-C3
12	h	301	PC1	O32-C31-O31-C3
12	H	601	PC1	O22-C21-O21-C2
12	h	301	PC1	O22-C21-O21-C2
12	H	601	PC1	C32-C31-O31-C3
12	h	301	PC1	C32-C31-O31-C3
13	m	406	CDL	C11-CA5-OA6-CA4
11	j	101	SPO	C36-C37-C38-C39
11	w	102	SPO	C36-C37-C38-C39
7	w	101	BCL	C2-C3-C5-C6
9	l	303	U10	C48-C49-C51-C52
11	M	404	SPO	C32-C33-C35-C36
11	E	102	SPO	C27-C28-C30-C31
11	m	405	SPO	C32-C33-C35-C36
11	e	102	SPO	C27-C28-C30-C31
11	j	101	SPO	C32-C33-C35-C36
11	p	102	SPO	C32-C33-C35-C36
7	v	101	BCL	C2A-CAA-CBA-CGA
11	b	103	SPO	C36-C37-C38-C39
11	D	102	SPO	C31-C32-C33-C34
11	E	102	SPO	C31-C32-C33-C34
11	F	102	SPO	C31-C32-C33-C34
11	F	103	SPO	C31-C32-C33-C34
11	G	102	SPO	C31-C32-C33-C34
11	G	103	SPO	C31-C32-C33-C34
11	9	101	SPO	C31-C32-C33-C34
11	9	103	SPO	C31-C32-C33-C34
11	C	1203	SPO	C31-C32-C33-C34
11	b	101	SPO	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
11	d	102	SPO	C31-C32-C33-C34
11	f	102	SPO	C31-C32-C33-C34
11	g	101	SPO	C31-C32-C33-C34
11	i	103	SPO	C31-C32-C33-C34
11	o	102	SPO	C31-C32-C33-C34
11	q	102	SPO	C31-C32-C33-C34
11	s	101	SPO	C31-C32-C33-C34
11	u	101	SPO	C31-C32-C33-C34
11	aa	101	SPO	C31-C32-C33-C34
11	Q	603	SPO	C31-C32-C33-C34
11	ab	102	SPO	C31-C32-C33-C34
9	L	304	U10	C22-C23-C24-C26
11	E	102	SPO	C31-C32-C33-C35
11	D	102	SPO	C25-C26-C27-C28
11	E	102	SPO	C12-C14-C15-C16
11	E	102	SPO	C20-C21-C22-C23
11	F	102	SPO	C25-C26-C27-C28
11	F	103	SPO	C25-C26-C27-C28
11	9	103	SPO	C25-C26-C27-C28
11	0	101	SPO	C11-C10-C9-C7
11	0	101	SPO	C20-C21-C22-C23
11	C	1203	SPO	C25-C26-C27-C28
11	d	102	SPO	C25-C26-C27-C28
11	f	102	SPO	C25-C26-C27-C28
11	g	101	SPO	C25-C26-C27-C28
11	i	103	SPO	C25-C26-C27-C28
11	j	101	SPO	C25-C26-C27-C28
11	n	102	SPO	C12-C14-C15-C16
11	o	102	SPO	C25-C26-C27-C28
11	p	102	SPO	C17-C19-C20-C21
11	p	102	SPO	C20-C21-C22-C23
11	p	103	SPO	C20-C21-C22-C23
11	q	102	SPO	C25-C26-C27-C28
11	s	101	SPO	C25-C26-C27-C28
11	t	102	SPO	C17-C19-C20-C21
11	t	102	SPO	C25-C26-C27-C28
11	u	101	SPO	C25-C26-C27-C28
11	aa	101	SPO	C25-C26-C27-C28
11	Q	603	SPO	C25-C26-C27-C28
11	ab	102	SPO	C17-C19-C20-C21
11	M	404	SPO	C36-C37-C38-C39
11	G	102	SPO	C36-C37-C38-C40

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Mol	Chain	Res	Type	Atoms
11	0	101	SPO	C36-C37-C38-C39
11	m	405	SPO	C36-C37-C38-C39
11	ab	102	SPO	C36-C37-C38-C40
12	H	601	PC1	C38-C39-C3A-C3B
12	H	601	PC1	C3A-C3B-C3C-C3D
12	h	301	PC1	C38-C39-C3A-C3B
12	h	301	PC1	C3A-C3B-C3C-C3D
12	H	602	PC1	C26-C27-C28-C29
12	A	1703	PC1	C22-C23-C24-C25
12	C	1201	PC1	C3B-C3C-C3D-C3E
12	Q	601	PC1	C22-C23-C24-C25
12	Q	601	PC1	C38-C39-C3A-C3B
12	a	102	PC1	C22-C23-C24-C25
11	D	102	SPO	C36-C37-C38-C40
11	E	102	SPO	C36-C37-C38-C40
11	F	102	SPO	C36-C37-C38-C40
11	F	103	SPO	C36-C37-C38-C40
11	9	103	SPO	C36-C37-C38-C40
11	C	1203	SPO	C36-C37-C38-C40
11	d	102	SPO	C36-C37-C38-C40
11	f	102	SPO	C36-C37-C38-C40
11	g	101	SPO	C36-C37-C38-C40
11	i	103	SPO	C36-C37-C38-C40
11	n	102	SPO	C36-C37-C38-C39
11	o	102	SPO	C36-C37-C38-C40
11	q	102	SPO	C36-C37-C38-C40
11	s	101	SPO	C36-C37-C38-C40
11	u	101	SPO	C36-C37-C38-C40
11	v	102	SPO	C36-C37-C38-C39
11	aa	101	SPO	C36-C37-C38-C40
11	Q	603	SPO	C36-C37-C38-C40
9	l	303	U10	C35-C34-C36-C37
11	G	103	SPO	C29-C28-C30-C31
11	ab	102	SPO	C29-C28-C30-C31
9	l	303	U10	C33-C34-C36-C37
11	E	102	SPO	C32-C33-C35-C36
11	G	102	SPO	C32-C33-C35-C36
11	J	102	SPO	C32-C33-C35-C36
11	9	101	SPO	C32-C33-C35-C36
11	b	101	SPO	C32-C33-C35-C36
11	p	102	SPO	C27-C28-C30-C31
12	Q	601	PC1	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
9	L	304	U10	C9-C11-C12-C13
9	L	304	U10	C19-C21-C22-C23
9	L	304	U10	C24-C26-C27-C28
9	l	303	U10	C39-C41-C42-C43
11	D	102	SPO	C33-C35-C36-C37
11	F	102	SPO	C33-C35-C36-C37
11	F	103	SPO	C33-C35-C36-C37
11	G	102	SPO	C33-C35-C36-C37
11	9	101	SPO	C33-C35-C36-C37
11	9	103	SPO	C33-C35-C36-C37
11	C	1203	SPO	C33-C35-C36-C37
11	b	101	SPO	C33-C35-C36-C37
11	b	103	SPO	C28-C30-C31-C32
11	d	102	SPO	C33-C35-C36-C37
11	f	102	SPO	C33-C35-C36-C37
11	g	101	SPO	C33-C35-C36-C37
11	i	103	SPO	C33-C35-C36-C37
11	o	102	SPO	C33-C35-C36-C37
11	p	103	SPO	C33-C35-C36-C37
11	q	102	SPO	C33-C35-C36-C37
11	s	101	SPO	C33-C35-C36-C37
11	u	101	SPO	C33-C35-C36-C37
11	w	102	SPO	C28-C30-C31-C32
11	aa	101	SPO	C33-C35-C36-C37
11	Q	603	SPO	C33-C35-C36-C37
11	ab	102	SPO	C33-C35-C36-C37
12	H	602	PC1	C31-C32-C33-C34
11	J	102	SPO	C36-C37-C38-C39
11	0	103	SPO	C36-C37-C38-C40
11	J	102	SPO	C31-C32-C33-C35
12	C	1201	PC1	C3D-C3E-C3F-C3G
12	Q	601	PC1	C32-C31-O31-C3
11	G	102	SPO	C20-C21-C22-C23
11	J	102	SPO	C17-C19-C20-C21
11	b	103	SPO	C12-C14-C15-C16
11	p	102	SPO	C11-C10-C9-C7
11	p	103	SPO	C17-C19-C20-C21
11	v	102	SPO	C11-C10-C9-C7
11	v	102	SPO	C12-C14-C15-C16
11	v	102	SPO	C25-C26-C27-C28
11	ab	102	SPO	C20-C21-C22-C23
12	A	1701	PC1	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
11	G	103	SPO	C36-C37-C38-C40
11	J	102	SPO	C36-C37-C38-C40
12	C	1201	PC1	C2D-C2E-C2F-C2G
7	v	101	BCL	C14-C13-C15-C16
11	M	404	SPO	C15-C16-C17-C18
11	E	102	SPO	C15-C16-C17-C18
11	E	102	SPO	C24-C23-C25-C26
11	G	102	SPO	C24-C23-C25-C26
11	G	103	SPO	C10-C11-C12-C13
11	G	103	SPO	C24-C23-C25-C26
11	J	102	SPO	C5-C6-C7-C8
11	J	102	SPO	C10-C11-C12-C13
11	0	103	SPO	C5-C6-C7-C8
11	0	103	SPO	C10-C11-C12-C13
11	m	405	SPO	C15-C16-C17-C18
11	b	103	SPO	C5-C6-C7-C8
11	d	103	SPO	C5-C6-C7-C8
11	e	102	SPO	C24-C23-C25-C26
11	j	101	SPO	C5-C6-C7-C8
11	p	102	SPO	C5-C6-C7-C8
11	p	102	SPO	C24-C23-C25-C26
11	t	102	SPO	C5-C6-C7-C8
11	t	102	SPO	C10-C11-C12-C13
11	t	102	SPO	C24-C23-C25-C26
11	v	102	SPO	C10-C11-C12-C13
11	v	102	SPO	C24-C23-C25-C26
11	w	102	SPO	C24-C23-C25-C26
11	ab	102	SPO	C10-C11-C12-C13
11	ab	102	SPO	C15-C16-C17-C18
11	ab	102	SPO	C24-C23-C25-C26
11	D	102	SPO	C5-C6-C7-C9
11	D	102	SPO	C15-C16-C17-C19
11	E	102	SPO	C5-C6-C7-C9
11	F	102	SPO	C5-C6-C7-C9
11	F	102	SPO	C15-C16-C17-C19
11	F	103	SPO	C5-C6-C7-C9
11	F	103	SPO	C15-C16-C17-C19
11	J	102	SPO	C22-C23-C25-C26
11	9	103	SPO	C5-C6-C7-C9
11	0	101	SPO	C5-C6-C7-C9
11	0	103	SPO	C22-C23-C25-C26
11	C	1203	SPO	C5-C6-C7-C9

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Mol	Chain	Res	Type	Atoms
11	C	1203	SPO	C15-C16-C17-C19
11	b	103	SPO	C15-C16-C17-C19
11	d	102	SPO	C5-C6-C7-C9
11	d	102	SPO	C15-C16-C17-C19
11	e	102	SPO	C15-C16-C17-C19
11	f	102	SPO	C5-C6-C7-C9
11	f	102	SPO	C15-C16-C17-C19
11	g	101	SPO	C5-C6-C7-C9
11	g	101	SPO	C15-C16-C17-C19
11	i	103	SPO	C5-C6-C7-C9
11	i	103	SPO	C15-C16-C17-C19
11	n	102	SPO	C5-C6-C7-C9
11	n	102	SPO	C22-C23-C25-C26
11	o	102	SPO	C5-C6-C7-C9
11	o	102	SPO	C15-C16-C17-C19
11	p	103	SPO	C15-C16-C17-C19
11	q	102	SPO	C5-C6-C7-C9
11	q	102	SPO	C15-C16-C17-C19
11	s	101	SPO	C5-C6-C7-C9
11	s	101	SPO	C15-C16-C17-C19
11	u	101	SPO	C5-C6-C7-C9
11	u	101	SPO	C15-C16-C17-C19
11	v	102	SPO	C5-C6-C7-C9
11	v	102	SPO	C15-C16-C17-C19
11	w	102	SPO	C5-C6-C7-C9
11	aa	101	SPO	C5-C6-C7-C9
11	aa	101	SPO	C15-C16-C17-C19
11	Q	603	SPO	C5-C6-C7-C9
11	Q	603	SPO	C15-C16-C17-C19
12	Q	601	PC1	O32-C31-O31-C3
12	C	1201	PC1	C32-C31-O31-C3
12	C	1201	PC1	C31-C32-C33-C34
7	v	101	BCL	C13-C15-C16-C17
11	D	102	SPO	C36-C37-C38-C39
11	F	102	SPO	C36-C37-C38-C39
11	F	103	SPO	C36-C37-C38-C39
11	9	103	SPO	C36-C37-C38-C39
11	0	103	SPO	C36-C37-C38-C39
11	C	1203	SPO	C36-C37-C38-C39
11	d	102	SPO	C36-C37-C38-C39
11	f	102	SPO	C36-C37-C38-C39
11	g	101	SPO	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
11	i	103	SPO	C36-C37-C38-C39
11	o	102	SPO	C36-C37-C38-C39
11	q	102	SPO	C36-C37-C38-C39
11	s	101	SPO	C36-C37-C38-C39
11	u	101	SPO	C36-C37-C38-C39
11	aa	101	SPO	C36-C37-C38-C39
11	Q	603	SPO	C36-C37-C38-C39
11	v	102	SPO	C31-C32-C33-C34
12	H	601	PC1	C21-C22-C23-C24
12	A	1703	PC1	C31-C32-C33-C34
12	h	301	PC1	C21-C22-C23-C24
12	a	102	PC1	C31-C32-C33-C34
13	m	406	CDL	CB7-C71-C72-C73
12	H	602	PC1	C38-C39-C3A-C3B
12	H	601	PC1	C31-C32-C33-C34
12	h	301	PC1	C31-C32-C33-C34
12	Q	601	PC1	C31-C32-C33-C34
8	L	303	BPH	C13-C15-C16-C17
11	G	102	SPO	C17-C19-C20-C21
11	G	103	SPO	C11-C10-C9-C7
11	t	102	SPO	C20-C21-C22-C23
11	D	102	SPO	C28-C30-C31-C32
11	F	102	SPO	C28-C30-C31-C32
11	F	103	SPO	C28-C30-C31-C32
11	9	103	SPO	C28-C30-C31-C32
11	C	1203	SPO	C28-C30-C31-C32
11	d	102	SPO	C28-C30-C31-C32
11	f	102	SPO	C28-C30-C31-C32
11	g	101	SPO	C28-C30-C31-C32
11	i	103	SPO	C28-C30-C31-C32
11	o	102	SPO	C28-C30-C31-C32
11	q	102	SPO	C28-C30-C31-C32
11	s	101	SPO	C28-C30-C31-C32
11	u	101	SPO	C28-C30-C31-C32
11	aa	101	SPO	C28-C30-C31-C32
11	Q	603	SPO	C28-C30-C31-C32
12	H	601	PC1	C11-O13-P-O11
12	A	1701	PC1	C1-O11-P-O13
12	C	1201	PC1	C11-O13-P-O11
12	h	301	PC1	C11-O13-P-O11
13	m	406	CDL	CB2-OB2-PB2-OB5
11	d	103	SPO	C29-C28-C30-C31

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Mol	Chain	Res	Type	Atoms
7	D	101	BCL	C13-C15-C16-C17
11	J	102	SPO	C20-C21-C22-C23
11	d	103	SPO	C25-C26-C27-C28
11	n	102	SPO	C25-C26-C27-C28
11	p	103	SPO	C12-C14-C15-C16
12	h	301	PC1	C27-C28-C29-C2A
12	C	1201	PC1	C22-C21-O21-C2
11	E	102	SPO	C8-C7-C9-C10
11	G	102	SPO	C13-C12-C14-C15
11	J	102	SPO	C18-C17-C19-C20
11	9	101	SPO	C8-C7-C9-C10
11	b	101	SPO	C8-C7-C9-C10
11	e	102	SPO	C21-C22-C23-C24
11	n	102	SPO	C21-C22-C23-C24
12	A	1703	PC1	C35-C36-C37-C38
12	Q	601	PC1	C35-C36-C37-C38
12	A	1703	PC1	C23-C24-C25-C26
12	A	1703	PC1	C3B-C3C-C3D-C3E
12	a	102	PC1	C23-C24-C25-C26
12	a	102	PC1	C35-C36-C37-C38
12	Q	601	PC1	C29-C2A-C2B-C2C
12	Q	601	PC1	C3A-C3B-C3C-C3D
12	C	1201	PC1	O22-C21-O21-C2
12	c	1201	PC1	C21-C22-C23-C24
12	Q	601	PC1	C27-C28-C29-C2A
12	Q	601	PC1	C2E-C2F-C2G-C2H
12	c	1201	PC1	C2B-C2C-C2D-C2E
13	m	406	CDL	C75-C76-C77-C78
12	C	1201	PC1	O32-C31-O31-C3
12	H	601	PC1	C25-C26-C27-C28
12	A	1701	PC1	C22-C23-C24-C25
12	A	1703	PC1	C33-C34-C35-C36
12	h	301	PC1	C25-C26-C27-C28
12	a	102	PC1	C33-C34-C35-C36
12	c	1201	PC1	C33-C34-C35-C36
7	K	101	BCL	C3-C5-C6-C7
11	D	102	SPO	C11-C12-C14-C15
11	E	102	SPO	C11-C12-C14-C15
11	F	102	SPO	C11-C12-C14-C15
11	F	103	SPO	C11-C12-C14-C15
11	G	102	SPO	C11-C12-C14-C15
11	G	102	SPO	C16-C17-C19-C20

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Mol	Chain	Res	Type	Atoms
11	G	103	SPO	C6-C7-C9-C10
11	J	102	SPO	C6-C7-C9-C10
11	J	102	SPO	C11-C12-C14-C15
11	9	103	SPO	C11-C12-C14-C15
11	0	101	SPO	C16-C17-C19-C20
11	0	103	SPO	C6-C7-C9-C10
11	C	1203	SPO	C11-C12-C14-C15
11	b	103	SPO	C6-C7-C9-C10
11	d	102	SPO	C11-C12-C14-C15
11	e	102	SPO	C21-C22-C23-C25
11	f	102	SPO	C11-C12-C14-C15
11	g	101	SPO	C11-C12-C14-C15
11	i	103	SPO	C11-C12-C14-C15
11	j	101	SPO	C11-C12-C14-C15
11	n	102	SPO	C16-C17-C19-C20
11	n	102	SPO	C21-C22-C23-C25
11	o	102	SPO	C11-C12-C14-C15
11	p	102	SPO	C16-C17-C19-C20
11	q	102	SPO	C11-C12-C14-C15
11	s	101	SPO	C11-C12-C14-C15
11	u	101	SPO	C11-C12-C14-C15
11	w	102	SPO	C16-C17-C19-C20
11	aa	101	SPO	C11-C12-C14-C15
11	Q	603	SPO	C11-C12-C14-C15
11	ab	102	SPO	C21-C22-C23-C25
13	m	406	CDL	C18-C19-C20-C21
8	l	302	BPH	C4-C3-C5-C6
12	A	1701	PC1	C37-C38-C39-C3A
12	C	1201	PC1	C2B-C2C-C2D-C2E
12	H	601	PC1	C33-C34-C35-C36
12	A	1703	PC1	C39-C3A-C3B-C3C
12	h	301	PC1	C33-C34-C35-C36
11	G	103	SPO	C15-C16-C17-C18
11	9	101	SPO	C5-C6-C7-C8
11	b	101	SPO	C5-C6-C7-C8
11	b	103	SPO	C10-C11-C12-C13
11	b	103	SPO	C24-C23-C25-C26
11	d	103	SPO	C10-C11-C12-C13
11	j	101	SPO	C24-C23-C25-C26
11	p	103	SPO	C10-C11-C12-C13
11	w	102	SPO	C10-C11-C12-C13
11	0	103	SPO	C15-C16-C17-C19

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Mol	Chain	Res	Type	Atoms
11	p	102	SPO	C5-C6-C7-C9
11	t	102	SPO	C10-C11-C12-C14
11	t	102	SPO	C15-C16-C17-C19
13	m	406	CDL	CB5-C51-C52-C53
12	H	602	PC1	C37-C38-C39-C3A
12	A	1703	PC1	C34-C35-C36-C37
12	C	1201	PC1	C37-C38-C39-C3A
12	C	1201	PC1	C39-C3A-C3B-C3C
12	C	1201	PC1	C3C-C3D-C3E-C3F
12	a	102	PC1	C34-C35-C36-C37
12	c	1201	PC1	C2A-C2B-C2C-C2D
7	D	101	BCL	C10-C11-C12-C13
7	F	101	BCL	C10-C11-C12-C13
7	I	101	BCL	C10-C11-C12-C13
7	9	102	BCL	C10-C11-C12-C13
7	C	1202	BCL	C10-C11-C12-C13
7	d	101	BCL	C10-C11-C12-C13
7	f	101	BCL	C10-C11-C12-C13
7	i	101	BCL	C10-C11-C12-C13
7	o	101	BCL	C10-C11-C12-C13
7	q	101	BCL	C10-C11-C12-C13
7	q	103	BCL	C10-C11-C12-C13
7	s	102	BCL	C10-C11-C12-C13
7	Q	602	BCL	C10-C11-C12-C13
7	c	1202	BCL	C10-C11-C12-C13
11	b	103	SPO	C33-C35-C36-C37
11	p	102	SPO	C33-C35-C36-C37
12	Q	601	PC1	C23-C24-C25-C26
12	C	1201	PC1	C21-C22-C23-C24
7	k	101	BCL	C10-C11-C12-C13
7	4	101	BCL	C3A-C2A-CAA-CBA
11	v	102	SPO	C36-C37-C38-C40
11	D	102	SPO	C11-C10-C9-C7
11	F	102	SPO	C11-C10-C9-C7
11	F	103	SPO	C11-C10-C9-C7
11	9	103	SPO	C11-C10-C9-C7
11	C	1203	SPO	C11-C10-C9-C7
11	d	102	SPO	C11-C10-C9-C7
11	f	102	SPO	C11-C10-C9-C7
11	g	101	SPO	C11-C10-C9-C7
11	o	102	SPO	C11-C10-C9-C7
11	q	102	SPO	C11-C10-C9-C7

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Mol	Chain	Res	Type	Atoms
11	s	101	SPO	C11-C10-C9-C7
11	u	101	SPO	C11-C10-C9-C7
11	aa	101	SPO	C11-C10-C9-C7
11	Q	603	SPO	C11-C10-C9-C7
12	H	602	PC1	C25-C26-C27-C28
12	A	1703	PC1	C3E-C3F-C3G-C3H
12	C	1201	PC1	C25-C26-C27-C28
12	Q	601	PC1	C39-C3A-C3B-C3C
12	c	1201	PC1	C29-C2A-C2B-C2C
13	m	406	CDL	C33-C34-C35-C36
12	H	602	PC1	C35-C36-C37-C38
8	L	303	BPH	O2A-C1-C2-C3
12	C	1201	PC1	C33-C34-C35-C36
11	b	103	SPO	C34-C33-C35-C36
11	t	102	SPO	C32-C33-C35-C36
12	H	601	PC1	C2-C3-O31-C31
12	h	301	PC1	C2-C3-O31-C31
12	C	1201	PC1	C26-C27-C28-C29
12	a	102	PC1	C28-C29-C2A-C2B
12	H	602	PC1	C21-C22-C23-C24
12	H	602	PC1	C22-C23-C24-C25
12	Q	601	PC1	C37-C38-C39-C3A
7	M	402	BCL	C2-C1-O2A-CGA
7	m	403	BCL	C2-C1-O2A-CGA
12	A	1703	PC1	C38-C39-C3A-C3B
12	Q	601	PC1	C2A-C2B-C2C-C2D
7	w	101	BCL	C5-C6-C7-C8
12	C	1201	PC1	C24-C25-C26-C27
12	Q	601	PC1	C33-C34-C35-C36
12	c	1201	PC1	C22-C23-C24-C25
12	c	1201	PC1	C32-C33-C34-C35
12	A	1701	PC1	C24-C25-C26-C27
12	Q	601	PC1	C2D-C2E-C2F-C2G
11	n	102	SPO	C34-C33-C35-C36
8	l	302	BPH	C2-C3-C5-C6
8	l	302	BPH	C11-C10-C8-C7
12	C	1201	PC1	C2-C3-O31-C31
11	E	102	SPO	C25-C26-C27-C28
11	9	101	SPO	C25-C26-C27-C28
11	b	101	SPO	C25-C26-C27-C28
11	e	102	SPO	C12-C14-C15-C16
11	i	103	SPO	C11-C10-C9-C7

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Mol	Chain	Res	Type	Atoms
13	m	406	CDL	OB7-CB5-OB6-CB4
12	A	1703	PC1	C21-C22-C23-C24
12	a	102	PC1	C21-C22-C23-C24
12	C	1201	PC1	C29-C2A-C2B-C2C
13	m	406	CDL	C34-C35-C36-C37
12	H	601	PC1	C32-C33-C34-C35
12	h	301	PC1	C32-C33-C34-C35
9	M	403	U10	C34-C36-C37-C38
9	l	303	U10	C34-C36-C37-C38
9	m	404	U10	C34-C36-C37-C38
13	m	406	CDL	C51-CB5-OB6-CB4
12	A	1703	PC1	O11-C1-C2-O21
12	a	102	PC1	O11-C1-C2-O21
13	m	406	CDL	OA5-CA3-CA4-OA6
11	M	404	SPO	C27-C28-C30-C31
11	D	102	SPO	C27-C28-C30-C31
11	F	102	SPO	C27-C28-C30-C31
11	F	103	SPO	C27-C28-C30-C31
11	9	103	SPO	C27-C28-C30-C31
11	C	1203	SPO	C27-C28-C30-C31
11	m	405	SPO	C27-C28-C30-C31
11	d	102	SPO	C27-C28-C30-C31
11	f	102	SPO	C27-C28-C30-C31
11	g	101	SPO	C27-C28-C30-C31
11	i	103	SPO	C27-C28-C30-C31
11	n	102	SPO	C32-C33-C35-C36
11	o	102	SPO	C27-C28-C30-C31
11	s	101	SPO	C27-C28-C30-C31
11	u	101	SPO	C27-C28-C30-C31
11	v	102	SPO	C27-C28-C30-C31
11	aa	101	SPO	C27-C28-C30-C31
11	Q	603	SPO	C27-C28-C30-C31
7	F	101	BCL	C14-C13-C15-C16
7	v	101	BCL	C11-C10-C8-C9
8	L	303	BPH	C11-C10-C8-C9
8	l	302	BPH	C11-C10-C8-C9
12	Q	601	PC1	C26-C27-C28-C29
13	m	406	CDL	C73-C74-C75-C76
12	C	1201	PC1	C22-C23-C24-C25
8	L	306	BPH	C2C-C3C-CAC-CBC
8	l	302	BPH	C2C-C3C-CAC-CBC
8	l	305	BPH	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
11	p	102	SPO	C10-C11-C12-C13
11	p	103	SPO	C15-C16-C17-C18
11	v	102	SPO	C5-C6-C7-C8
12	Q	601	PC1	C3D-C3E-C3F-C3G
11	9	101	SPO	C15-C16-C17-C19
11	b	101	SPO	C15-C16-C17-C19
11	w	102	SPO	C15-C16-C17-C19
11	ab	102	SPO	C10-C11-C12-C14
12	Q	601	PC1	C25-C26-C27-C28
11	M	404	SPO	C25-C26-C27-C28
11	E	102	SPO	C11-C10-C9-C7
11	m	405	SPO	C25-C26-C27-C28
12	H	601	PC1	C1-O11-P-O13
12	h	301	PC1	C1-O11-P-O13
12	H	602	PC1	O11-C1-C2-C3
12	c	1201	PC1	O11-C1-C2-C3
12	Q	601	PC1	C21-C22-C23-C24
12	a	102	PC1	C32-C33-C34-C35
12	A	1703	PC1	C32-C33-C34-C35
13	m	406	CDL	C41-C42-C43-C44
11	p	102	SPO	C1-C4-C5-C6
11	q	102	SPO	C27-C28-C30-C31
12	C	1201	PC1	C3A-C3B-C3C-C3D
13	m	406	CDL	C57-C58-C59-C60
11	J	102	SPO	C4-C1-O1-CM1
11	j	101	SPO	C4-C1-O1-CM1
11	p	102	SPO	C4-C1-O1-CM1
11	t	102	SPO	C4-C1-O1-CM1
12	Q	601	PC1	C2F-C2G-C2H-C2I
11	e	102	SPO	C31-C32-C33-C34
9	L	304	U10	C12-C11-C9-C10
9	L	304	U10	C20-C19-C21-C22
11	p	103	SPO	C29-C28-C30-C31
9	L	304	U10	C12-C11-C9-C8
7	B	101	BCL	C5-C6-C7-C8
7	E	101	BCL	C5-C6-C7-C8
7	G	101	BCL	C5-C6-C7-C8
7	J	101	BCL	C5-C6-C7-C8
7	N	101	BCL	C5-C6-C7-C8
7	8	101	BCL	C5-C6-C7-C8
7	0	102	BCL	C5-C6-C7-C8
7	b	102	BCL	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
7	e	101	BCL	C5-C6-C7-C8
7	g	102	BCL	C5-C6-C7-C8
7	i	102	BCL	C5-C6-C7-C8
7	n	101	BCL	C5-C6-C7-C8
7	p	101	BCL	C5-C6-C7-C8
7	r	101	BCL	C5-C6-C7-C8
7	t	101	BCL	C5-C6-C7-C8
7	x	101	BCL	C5-C6-C7-C8
7	aa	102	BCL	C5-C6-C7-C8
7	ab	101	BCL	C5-C6-C7-C8
11	n	102	SPO	C36-C37-C38-C40
12	H	601	PC1	O21-C21-C22-C23
12	h	301	PC1	O21-C21-C22-C23
7	D	101	BCL	C15-C16-C17-C18
11	J	102	SPO	C2-C1-O1-CM1
11	J	102	SPO	C3-C1-O1-CM1
11	0	101	SPO	C2-C1-O1-CM1
11	0	101	SPO	C3-C1-O1-CM1
11	j	101	SPO	C2-C1-O1-CM1
11	j	101	SPO	C3-C1-O1-CM1
11	n	102	SPO	C3-C1-O1-CM1
11	p	102	SPO	C2-C1-O1-CM1
11	p	103	SPO	C3-C1-O1-CM1
11	t	102	SPO	C3-C1-O1-CM1
11	v	102	SPO	C3-C1-O1-CM1
11	E	102	SPO	C3-C1-C4-C5
11	t	102	SPO	C2-C1-C4-C5
11	t	102	SPO	C3-C1-C4-C5
12	c	1201	PC1	C2D-C2E-C2F-C2G
7	F	101	BCL	C12-C13-C15-C16
7	v	101	BCL	C11-C10-C8-C7
8	L	303	BPH	C11-C10-C8-C7
9	L	304	U10	C18-C19-C21-C22
11	0	103	SPO	C27-C28-C30-C31
11	e	102	SPO	C32-C33-C35-C36
11	n	102	SPO	C27-C28-C30-C31
11	D	102	SPO	O1-C1-C4-C5
11	F	102	SPO	O1-C1-C4-C5
11	F	103	SPO	O1-C1-C4-C5
11	9	103	SPO	O1-C1-C4-C5
11	C	1203	SPO	O1-C1-C4-C5
11	b	103	SPO	O1-C1-C4-C5

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Mol	Chain	Res	Type	Atoms
11	d	102	SPO	O1-C1-C4-C5
11	f	102	SPO	O1-C1-C4-C5
11	g	101	SPO	O1-C1-C4-C5
11	i	103	SPO	O1-C1-C4-C5
11	o	102	SPO	O1-C1-C4-C5
11	q	102	SPO	O1-C1-C4-C5
11	s	101	SPO	O1-C1-C4-C5
11	u	101	SPO	O1-C1-C4-C5
11	v	102	SPO	O1-C1-C4-C5
11	aa	101	SPO	O1-C1-C4-C5
11	Q	603	SPO	O1-C1-C4-C5
11	w	102	SPO	C5-C6-C7-C8
11	G	102	SPO	C10-C11-C12-C14
11	p	103	SPO	C10-C11-C12-C14
11	ab	102	SPO	C15-C16-C17-C19
12	c	1201	PC1	C2E-C2F-C2G-C2H
12	A	1703	PC1	O11-C1-C2-C3
12	C	1201	PC1	O11-C1-C2-C3
12	a	102	PC1	O11-C1-C2-C3
13	m	406	CDL	OA5-CA3-CA4-CA6
11	E	102	SPO	C33-C35-C36-C37
11	J	102	SPO	C28-C30-C31-C32
12	H	601	PC1	C24-C25-C26-C27
12	H	601	PC1	C39-C3A-C3B-C3C
12	h	301	PC1	C24-C25-C26-C27
12	H	601	PC1	C23-C24-C25-C26
12	h	301	PC1	C23-C24-C25-C26
12	h	301	PC1	C39-C3A-C3B-C3C
13	m	406	CDL	C35-C36-C37-C38
7	v	101	BCL	C4-C3-C5-C6
9	l	303	U10	C40-C39-C41-C42
13	m	406	CDL	C82-C83-C84-C85
12	A	1701	PC1	C33-C34-C35-C36
11	0	101	SPO	C25-C26-C27-C28
12	H	602	PC1	C34-C35-C36-C37
13	m	406	CDL	C61-C62-C63-C64
13	m	406	CDL	C51-C52-C53-C54
7	9	102	BCL	C16-C17-C18-C19
7	v	101	BCL	C2-C3-C5-C6
9	l	303	U10	C38-C39-C41-C42
13	m	406	CDL	C44-C45-C46-C47
12	H	602	PC1	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
12	C	1201	PC1	O11-C1-C2-O21
12	c	1201	PC1	O11-C1-C2-O21
9	l	303	U10	C37-C38-C39-C40
12	H	602	PC1	C3F-C3G-C3H-C3I
13	m	406	CDL	C71-C72-C73-C74
13	m	406	CDL	C11-C12-C13-C14
7	w	101	BCL	C10-C11-C12-C13
13	m	406	CDL	C19-C20-C21-C22
11	0	101	SPO	C12-C14-C15-C16
11	E	102	SPO	C36-C37-C38-C39
7	L	302	BCL	C4C-C3C-CAC-CBC
11	n	102	SPO	C10-C11-C12-C14
7	v	101	BCL	C12-C13-C15-C16
12	A	1703	PC1	C26-C27-C28-C29
11	0	103	SPO	C17-C19-C20-C21
11	t	102	SPO	C12-C14-C15-C16
11	w	102	SPO	C25-C26-C27-C28
12	a	102	PC1	C26-C27-C28-C29
12	H	601	PC1	C3B-C3C-C3D-C3E
11	d	103	SPO	C21-C22-C23-C24
12	h	301	PC1	C3B-C3C-C3D-C3E
12	C	1201	PC1	C2A-C2B-C2C-C2D
12	H	602	PC1	C32-C31-O31-C3
12	C	1201	PC1	C32-C33-C34-C35
8	L	303	BPH	CAD-CBD-CGD-O2D
12	c	1201	PC1	C32-C31-O31-C3
12	H	601	PC1	C2-C1-O11-P
12	h	301	PC1	C2-C1-O11-P
13	m	406	CDL	C1-CA2-OA2-PA1
12	A	1701	PC1	O11-C1-C2-O21
7	9	102	BCL	C16-C17-C18-C20
12	c	1201	PC1	O21-C2-C3-O31
12	h	301	PC1	C22-C23-C24-C25
12	H	601	PC1	C22-C23-C24-C25
11	v	102	SPO	C34-C33-C35-C36
12	Q	601	PC1	C3C-C3D-C3E-C3F
7	l	304	BCL	C8-C10-C11-C12
12	c	1201	PC1	C39-C3A-C3B-C3C
13	m	406	CDL	C62-C63-C64-C65
11	E	102	SPO	C15-C16-C17-C19
11	G	103	SPO	C10-C11-C12-C14
11	G	103	SPO	C22-C23-C25-C26

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Mol	Chain	Res	Type	Atoms
11	J	102	SPO	C5-C6-C7-C9
11	0	103	SPO	C5-C6-C7-C9
11	e	102	SPO	C22-C23-C25-C26
12	Q	601	PC1	O22-C21-O21-C2
13	m	406	CDL	C31-CA7-OA8-CA6
13	m	406	CDL	C38-C39-C40-C41
12	H	602	PC1	C1-O11-P-O13
13	m	406	CDL	CA2-OA2-PA1-OA5
12	C	1201	PC1	C35-C36-C37-C38
12	A	1703	PC1	C2-C1-O11-P
12	a	102	PC1	C2-C1-O11-P
12	c	1201	PC1	O32-C31-O31-C3
12	H	601	PC1	C11-O13-P-O14
12	H	601	PC1	C1-O11-P-O12
12	A	1701	PC1	C1-O11-P-O14
12	h	301	PC1	C11-O13-P-O14
12	h	301	PC1	C1-O11-P-O12
12	Q	601	PC1	C11-O13-P-O12
12	A	1703	PC1	C22-C21-O21-C2
12	a	102	PC1	C22-C21-O21-C2
12	A	1701	PC1	C3B-C3C-C3D-C3E
12	A	1703	PC1	C3D-C3E-C3F-C3G
12	C	1201	PC1	C12-C11-O13-P
12	c	1201	PC1	C12-C11-O13-P
12	H	602	PC1	O32-C31-O31-C3
11	9	101	SPO	C1-C4-C5-C6
11	b	101	SPO	C1-C4-C5-C6
11	e	102	SPO	C1-C4-C5-C6
7	q	101	BCL	C12-C13-C15-C16
8	L	306	BPH	C4C-C3C-CAC-CBC
8	l	305	BPH	C4C-C3C-CAC-CBC
12	H	601	PC1	O13-C11-C12-N
12	A	1701	PC1	O13-C11-C12-N
12	h	301	PC1	O13-C11-C12-N
12	c	1201	PC1	O13-C11-C12-N
12	A	1703	PC1	O22-C21-O21-C2
12	a	102	PC1	O22-C21-O21-C2
13	m	406	CDL	OA9-CA7-OA8-CA6
12	Q	601	PC1	O21-C21-C22-C23
13	m	406	CDL	C42-C43-C44-C45
11	v	102	SPO	C4-C1-O1-CM1
11	G	102	SPO	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
11	J	102	SPO	C9-C10-C11-C12
11	d	103	SPO	C23-C25-C26-C27
13	m	406	CDL	C76-C77-C78-C79
12	c	1201	PC1	C27-C28-C29-C2A
9	l	303	U10	C5-C4-O4-C4M
12	H	601	PC1	C37-C38-C39-C3A
12	h	301	PC1	C37-C38-C39-C3A
12	Q	601	PC1	C3-C2-O21-C21
12	C	1201	PC1	C2E-C2F-C2G-C2H
13	m	406	CDL	C37-C38-C39-C40
12	H	602	PC1	C33-C34-C35-C36
12	A	1701	PC1	C3A-C3B-C3C-C3D
12	Q	601	PC1	C22-C21-O21-C2
11	M	404	SPO	C3-C1-O1-CM1
11	0	101	SPO	C28-C30-C31-C32
11	m	405	SPO	C3-C1-O1-CM1
11	d	103	SPO	C16-C17-C19-C20
11	n	102	SPO	C2-C1-O1-CM1
11	p	102	SPO	C3-C1-O1-CM1
11	p	103	SPO	C2-C1-O1-CM1
11	t	102	SPO	C2-C1-O1-CM1
11	v	102	SPO	C2-C1-O1-CM1
13	m	406	CDL	C20-C21-C22-C23
13	m	406	CDL	C78-C79-C80-C81
11	J	102	SPO	C3-C1-C4-C5
11	b	103	SPO	C2-C1-C4-C5
11	p	102	SPO	C31-C32-C33-C34
7	i	101	BCL	C12-C13-C15-C16
13	m	406	CDL	C21-C22-C23-C24
7	q	101	BCL	C14-C13-C15-C16
7	l	304	BCL	C13-C15-C16-C17
11	j	101	SPO	C12-C14-C15-C16
13	m	406	CDL	C36-C37-C38-C39
7	I	101	BCL	C8-C10-C11-C12
7	9	102	BCL	C8-C10-C11-C12
7	f	101	BCL	C8-C10-C11-C12
7	i	101	BCL	C8-C10-C11-C12
7	k	101	BCL	C8-C10-C11-C12
7	q	101	BCL	C8-C10-C11-C12
7	s	102	BCL	C8-C10-C11-C12
7	Q	602	BCL	C8-C10-C11-C12
7	D	101	BCL	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
7	C	1202	BCL	C8-C10-C11-C12
7	d	101	BCL	C8-C10-C11-C12
7	o	101	BCL	C8-C10-C11-C12
7	c	1202	BCL	C8-C10-C11-C12
11	G	103	SPO	O1-C1-C4-C5
11	t	102	SPO	O1-C1-C4-C5
12	H	602	PC1	C2-C1-O11-P
7	q	103	BCL	C8-C10-C11-C12
11	G	103	SPO	C30-C31-C32-C33
11	p	103	SPO	C27-C28-C30-C31
7	F	101	BCL	C8-C10-C11-C12
12	A	1701	PC1	C26-C27-C28-C29
11	M	404	SPO	C12-C14-C15-C16
11	M	404	SPO	C17-C19-C20-C21
11	m	405	SPO	C12-C14-C15-C16
11	m	405	SPO	C17-C19-C20-C21
9	m	404	U10	C14-C16-C17-C18
11	j	101	SPO	C28-C30-C31-C32
9	M	403	U10	C35-C34-C36-C37
13	m	406	CDL	C23-C24-C25-C26
7	z	101	BCL	CAA-CBA-CGA-O1A
7	4	101	BCL	CAA-CBA-CGA-O2A
7	l	301	BCL	C2A-CAA-CBA-CGA
12	H	602	PC1	C32-C33-C34-C35
9	M	403	U10	C5-C4-O4-C4M
9	m	404	U10	C5-C4-O4-C4M
9	m	404	U10	C35-C34-C36-C37
8	L	303	BPH	C11-C12-C13-C14
13	m	406	CDL	C22-C23-C24-C25
11	G	102	SPO	C21-C22-C23-C24
8	l	302	BPH	O2A-C1-C2-C3
9	M	403	U10	C14-C16-C17-C18
13	m	406	CDL	CB3-CB4-OB6-CB5
9	M	403	U10	C30-C29-C31-C32
9	m	404	U10	C30-C29-C31-C32
7	z	101	BCL	CAA-CBA-CGA-O2A
7	4	101	BCL	C2A-CAA-CBA-CGA
12	H	601	PC1	O11-C1-C2-O21
12	h	301	PC1	O11-C1-C2-O21
12	H	601	PC1	O11-C1-C2-C3
12	h	301	PC1	O11-C1-C2-C3
13	m	406	CDL	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
11	p	103	SPO	C34-C33-C35-C36
11	G	102	SPO	C12-C14-C15-C16
12	Q	601	PC1	C28-C29-C2A-C2B
9	l	303	U10	C45-C44-C46-C47
11	d	103	SPO	C34-C33-C35-C36
7	l	304	BCL	C2-C1-O2A-CGA
8	L	306	BPH	C2-C1-O2A-CGA
8	l	305	BPH	C2-C1-O2A-CGA
9	M	403	U10	C33-C34-C36-C37
9	m	404	U10	C33-C34-C36-C37
11	j	101	SPO	C27-C28-C30-C31
7	v	101	BCL	C16-C17-C18-C19
12	A	1703	PC1	C3A-C3B-C3C-C3D
7	4	101	BCL	CAA-CBA-CGA-O1A
12	A	1703	PC1	C3C-C3D-C3E-C3F
12	H	601	PC1	O22-C21-C22-C23
12	h	301	PC1	O22-C21-C22-C23
11	J	102	SPO	C25-C26-C27-C28
11	b	103	SPO	C17-C19-C20-C21
12	A	1701	PC1	C23-C24-C25-C26
11	t	102	SPO	C29-C28-C30-C31
12	H	602	PC1	C36-C37-C38-C39
9	M	403	U10	C28-C29-C31-C32
9	m	404	U10	C28-C29-C31-C32
7	L	305	BCL	C2-C1-O2A-CGA
12	H	601	PC1	C35-C36-C37-C38
12	h	301	PC1	C35-C36-C37-C38
7	L	302	BCL	C4-C3-C5-C6
9	l	303	U10	C25-C24-C26-C27
11	p	103	SPO	C4-C1-O1-CM1
7	L	301	BCL	C5-C6-C7-C8
12	C	1201	PC1	C23-C24-C25-C26
11	t	102	SPO	C11-C10-C9-C7
11	w	102	SPO	C20-C21-C22-C23
7	B	101	BCL	C4-C3-C5-C6
7	E	101	BCL	C4-C3-C5-C6
7	G	101	BCL	C4-C3-C5-C6
7	J	101	BCL	C4-C3-C5-C6
7	N	101	BCL	C4-C3-C5-C6
7	8	101	BCL	C4-C3-C5-C6
7	0	102	BCL	C4-C3-C5-C6
7	b	102	BCL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
7	e	101	BCL	C4-C3-C5-C6
7	g	102	BCL	C4-C3-C5-C6
7	i	102	BCL	C4-C3-C5-C6
7	n	101	BCL	C4-C3-C5-C6
7	p	101	BCL	C4-C3-C5-C6
7	r	101	BCL	C4-C3-C5-C6
7	t	101	BCL	C4-C3-C5-C6
7	x	101	BCL	C4-C3-C5-C6
7	aa	102	BCL	C4-C3-C5-C6
7	ab	101	BCL	C4-C3-C5-C6
9	L	304	U10	C25-C24-C26-C27
11	9	101	SPO	C29-C28-C30-C31
11	b	101	SPO	C29-C28-C30-C31
11	w	102	SPO	C34-C33-C35-C36
11	0	101	SPO	C27-C28-C30-C31
7	i	101	BCL	C14-C13-C15-C16
7	v	101	BCL	C6-C7-C8-C9
7	z	101	BCL	C3A-C2A-CAA-CBA
7	K	101	BCL	CAA-CBA-CGA-O2A
7	w	101	BCL	CAA-CBA-CGA-O2A
12	c	1201	PC1	C23-C24-C25-C26
7	L	302	BCL	CAD-CBD-CGD-O2D
8	L	306	BPH	CAD-CBD-CGD-O2D
8	l	305	BPH	CAD-CBD-CGD-O2D
12	A	1701	PC1	C1-C2-O21-C21
12	H	602	PC1	O31-C31-C32-C33
11	0	101	SPO	C34-C33-C35-C36
11	ab	102	SPO	C34-C33-C35-C36
9	l	303	U10	C43-C44-C46-C47
11	G	102	SPO	C15-C16-C17-C19
7	O	101	BCL	CAA-CBA-CGA-O1A
7	O	101	BCL	CAA-CBA-CGA-O2A
7	y	101	BCL	CAA-CBA-CGA-O2A
7	5	101	BCL	CAA-CBA-CGA-O2A
13	m	406	CDL	OB5-CB3-CB4-OB6
7	y	101	BCL	CAA-CBA-CGA-O1A
7	5	101	BCL	CAA-CBA-CGA-O1A
12	A	1701	PC1	C39-C3A-C3B-C3C
7	D	101	BCL	C16-C17-C18-C19
7	M	402	BCL	CHA-CBD-CGD-O2D
7	m	401	BCL	CHA-CBD-CGD-O1D
7	m	401	BCL	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
7	z	101	BCL	CHA-CBD-CGD-O1D
7	z	101	BCL	CHA-CBD-CGD-O2D
7	L	302	BCL	C2-C3-C5-C6
9	L	304	U10	C23-C24-C26-C27
13	m	406	CDL	C59-C60-C61-C62
11	E	102	SPO	C16-C17-C19-C20
7	K	101	BCL	C8-C10-C11-C12
12	C	1201	PC1	O21-C2-C3-O31
12	C	1201	PC1	C2C-C2D-C2E-C2F
12	Q	601	PC1	C3F-C3G-C3H-C3I
7	v	101	BCL	C8-C10-C11-C12
8	l	302	BPH	CHA-CBD-CGD-O1D
12	Q	601	PC1	C36-C37-C38-C39
11	0	101	SPO	C30-C31-C32-C33
7	v	101	BCL	C6-C7-C8-C10
7	L	301	BCL	CAA-CBA-CGA-O2A
11	G	103	SPO	C35-C36-C37-C38
11	p	103	SPO	C30-C31-C32-C33
12	A	1701	PC1	O21-C21-C22-C23
7	l	301	BCL	C4-C3-C5-C6
12	H	602	PC1	O32-C31-C32-C33
7	v	101	BCL	C1A-C2A-CAA-CBA
7	z	101	BCL	C1A-C2A-CAA-CBA
9	M	403	U10	C16-C17-C18-C19
9	M	403	U10	C26-C27-C28-C29
9	m	404	U10	C16-C17-C18-C19
9	m	404	U10	C26-C27-C28-C29
11	M	404	SPO	C36-C37-C38-C40
11	m	405	SPO	C36-C37-C38-C40
12	h	301	PC1	C3F-C3G-C3H-C3I
12	a	102	PC1	C29-C2A-C2B-C2C
7	w	101	BCL	CAA-CBA-CGA-O1A
7	K	101	BCL	CAA-CBA-CGA-O1A
12	A	1701	PC1	C11-O13-P-O14
12	A	1703	PC1	C11-C12-N-C15
12	a	102	PC1	C11-C12-N-C15
7	L	301	BCL	CAA-CBA-CGA-O1A
11	t	102	SPO	C28-C30-C31-C32
7	Q	602	BCL	C16-C17-C18-C20
12	A	1701	PC1	C31-C32-C33-C34
12	A	1701	PC1	C3-C2-O21-C21
12	H	602	PC1	O21-C21-C22-C23

Continued on next page...

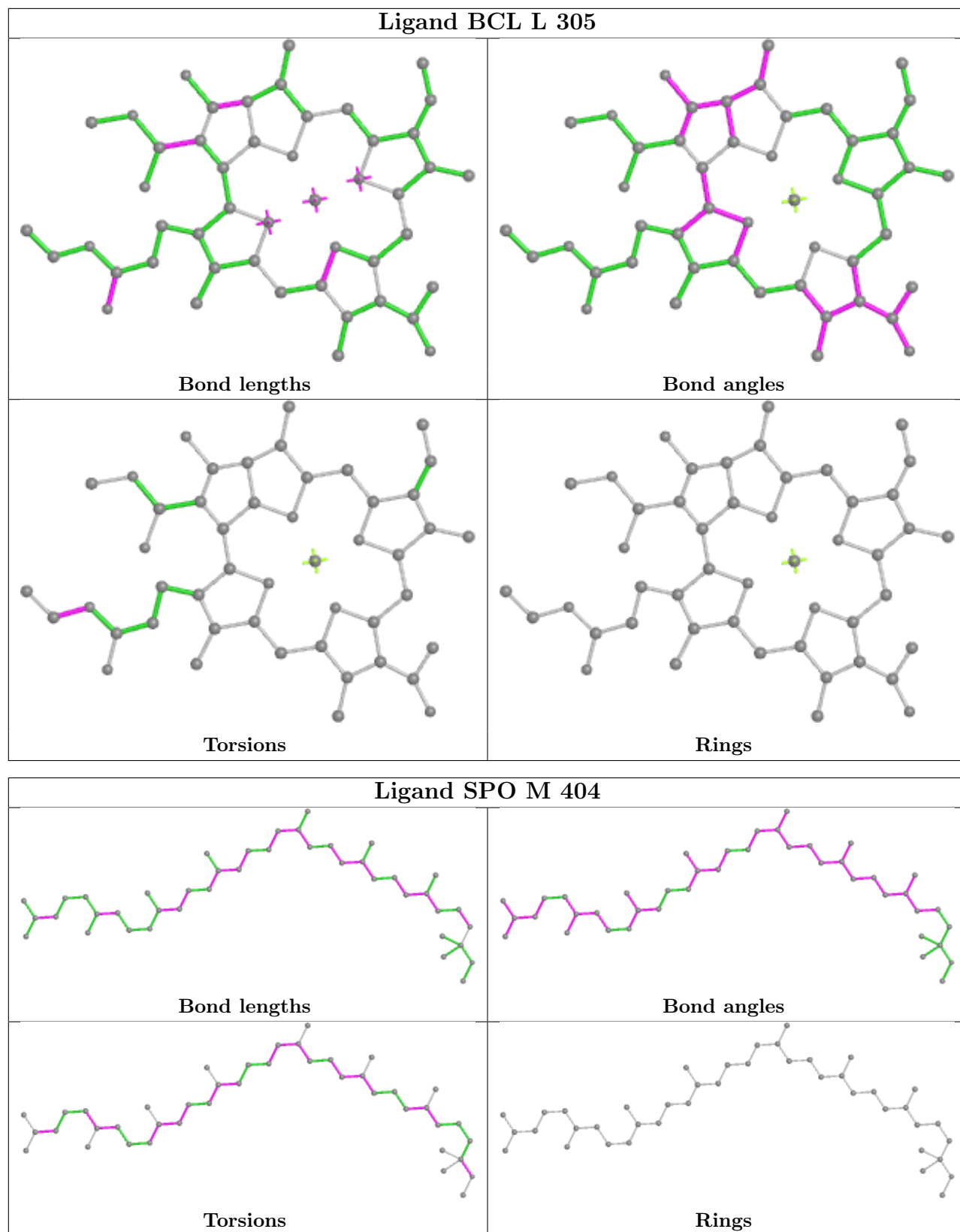
Continued from previous page...

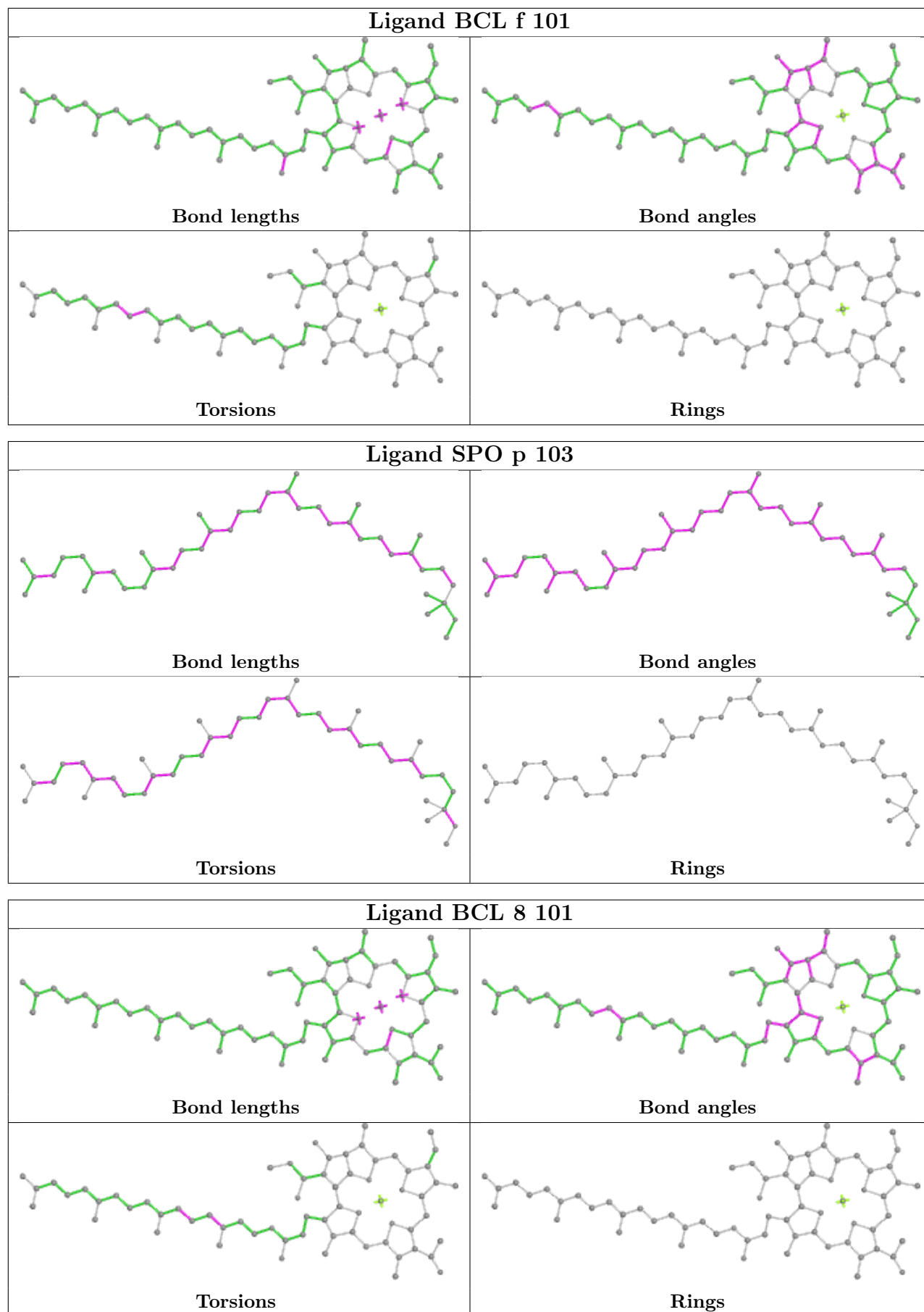
Mol	Chain	Res	Type	Atoms
13	m	406	CDL	C52-C53-C54-C55
11	0	103	SPO	C1-C4-C5-C6
11	t	102	SPO	C1-C4-C5-C6
11	ab	102	SPO	C1-C4-C5-C6
12	H	602	PC1	C2B-C2C-C2D-C2E
11	p	102	SPO	C26-C27-C28-C30
12	A	1701	PC1	O22-C21-C22-C23
12	H	602	PC1	C3B-C3C-C3D-C3E
11	G	103	SPO	C17-C19-C20-C21
12	C	1201	PC1	O31-C31-C32-C33
13	m	406	CDL	C15-C16-C17-C18
11	0	103	SPO	C28-C30-C31-C32
9	l	303	U10	C36-C37-C38-C39
12	H	602	PC1	O22-C21-C22-C23
7	i	101	BCL	C15-C16-C17-C18
12	A	1701	PC1	C2-C3-O31-C31

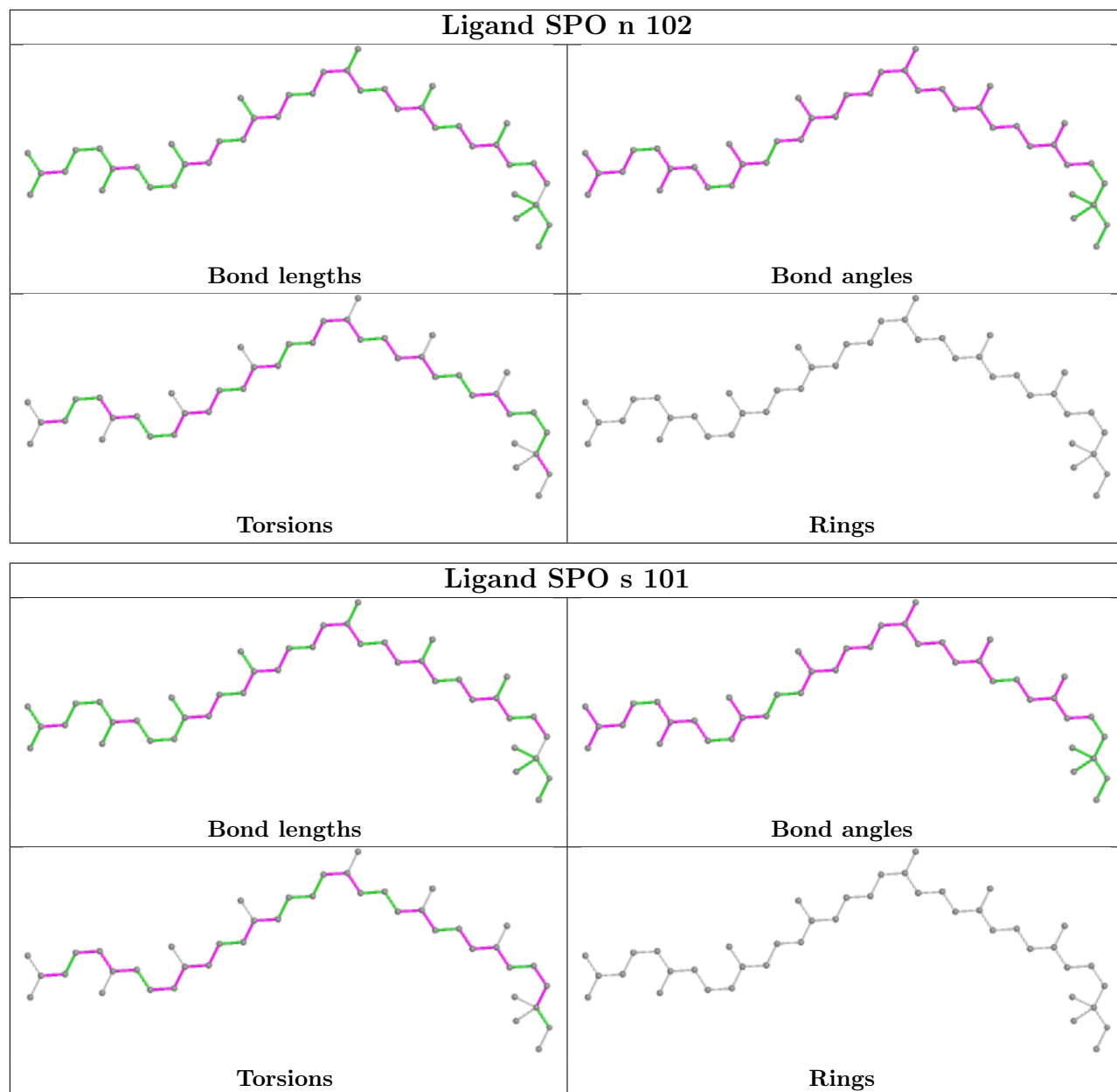
There are no ring outliers.

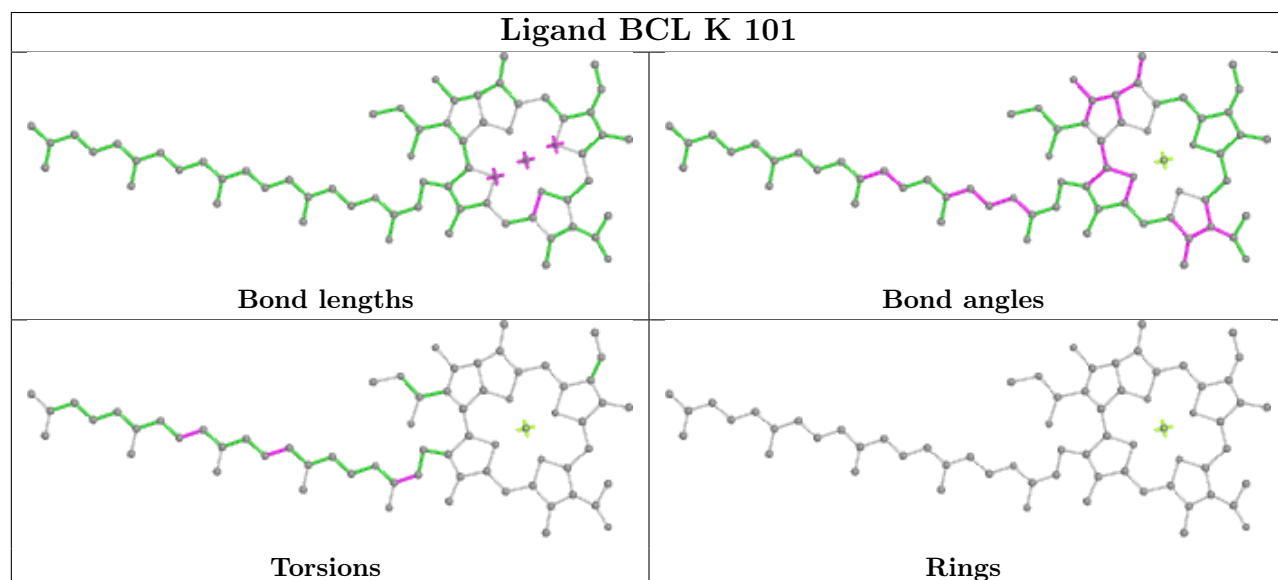
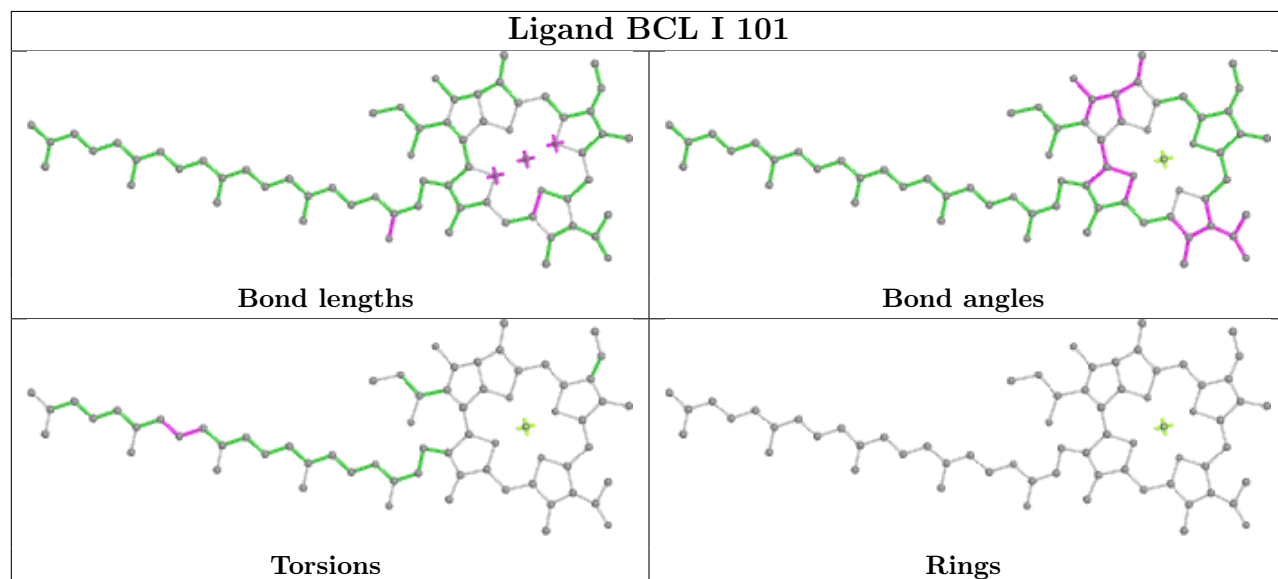
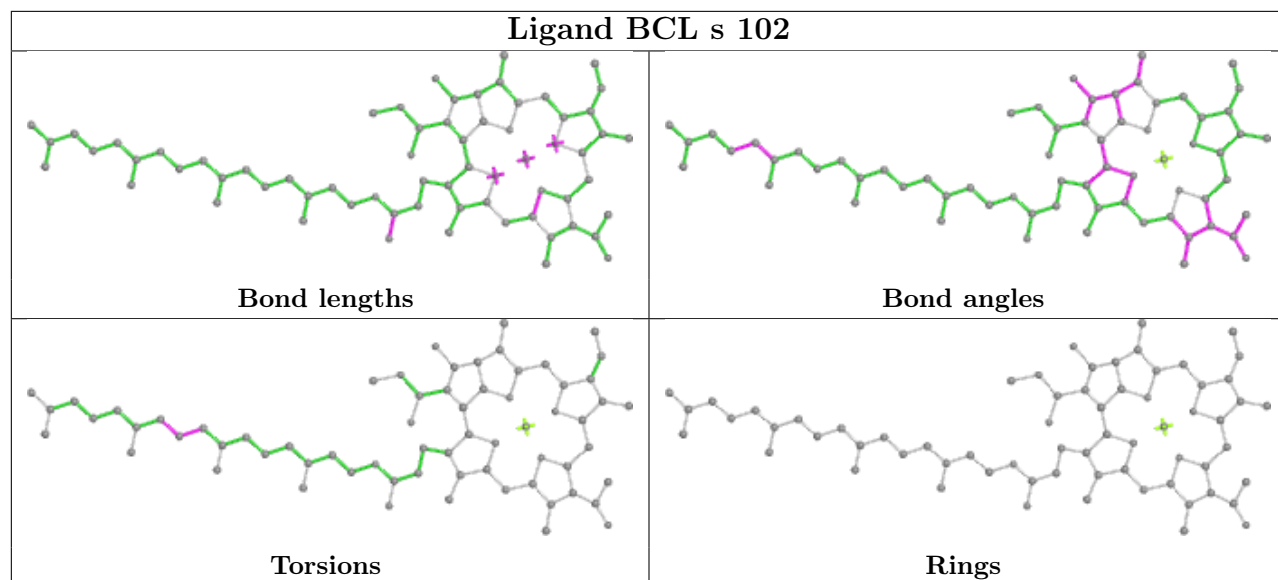
No monomer is involved in short contacts.

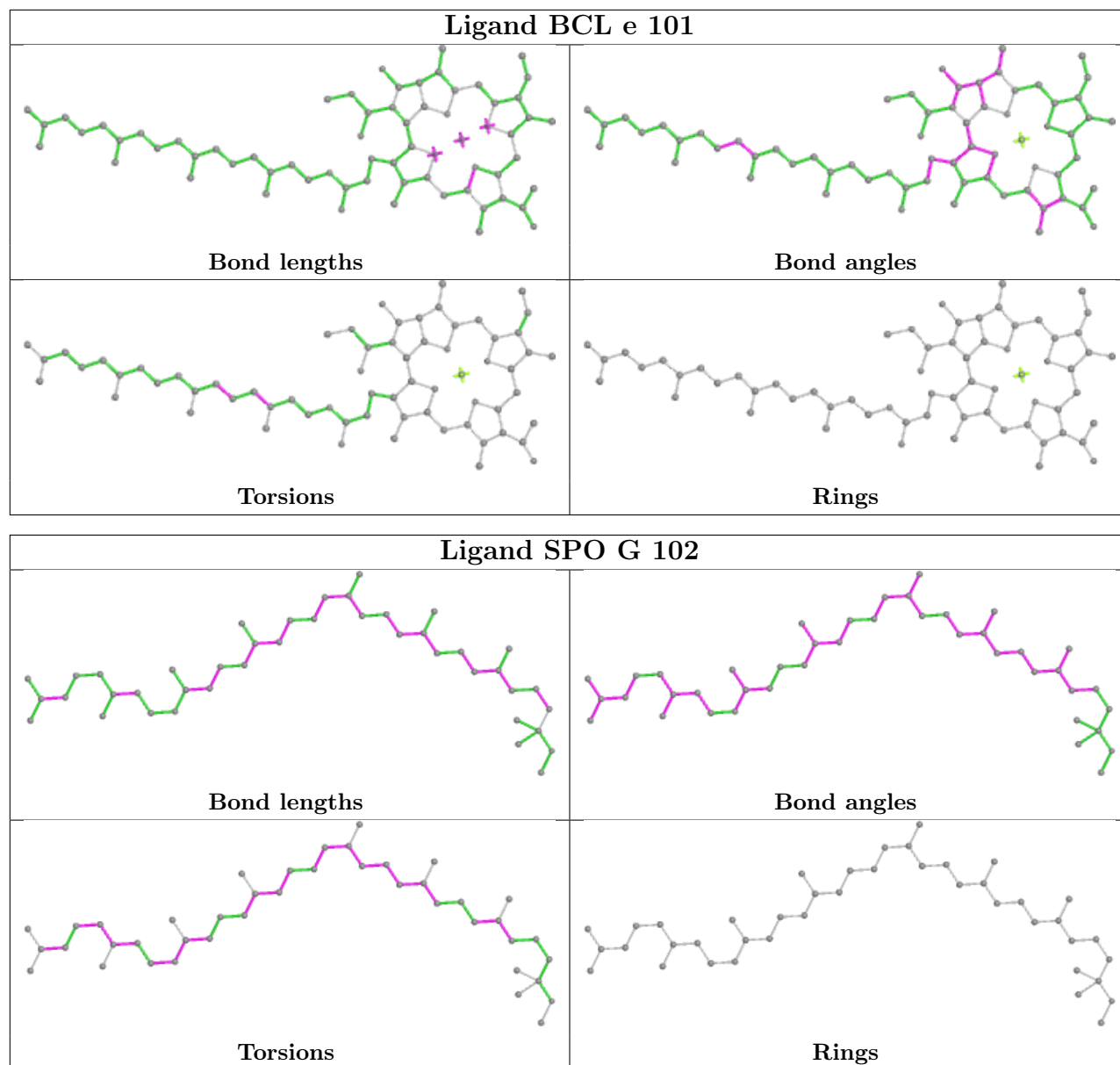
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

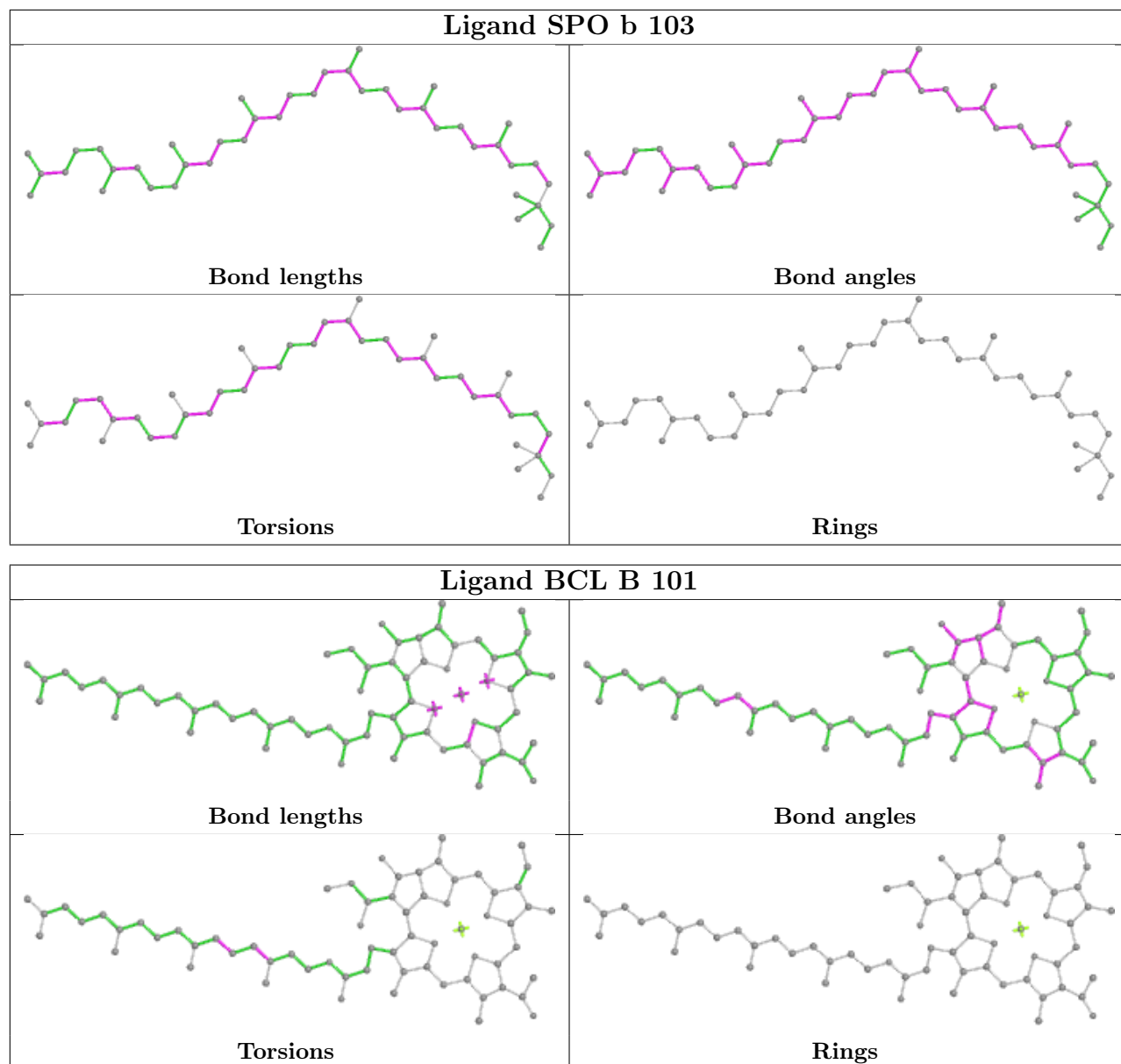


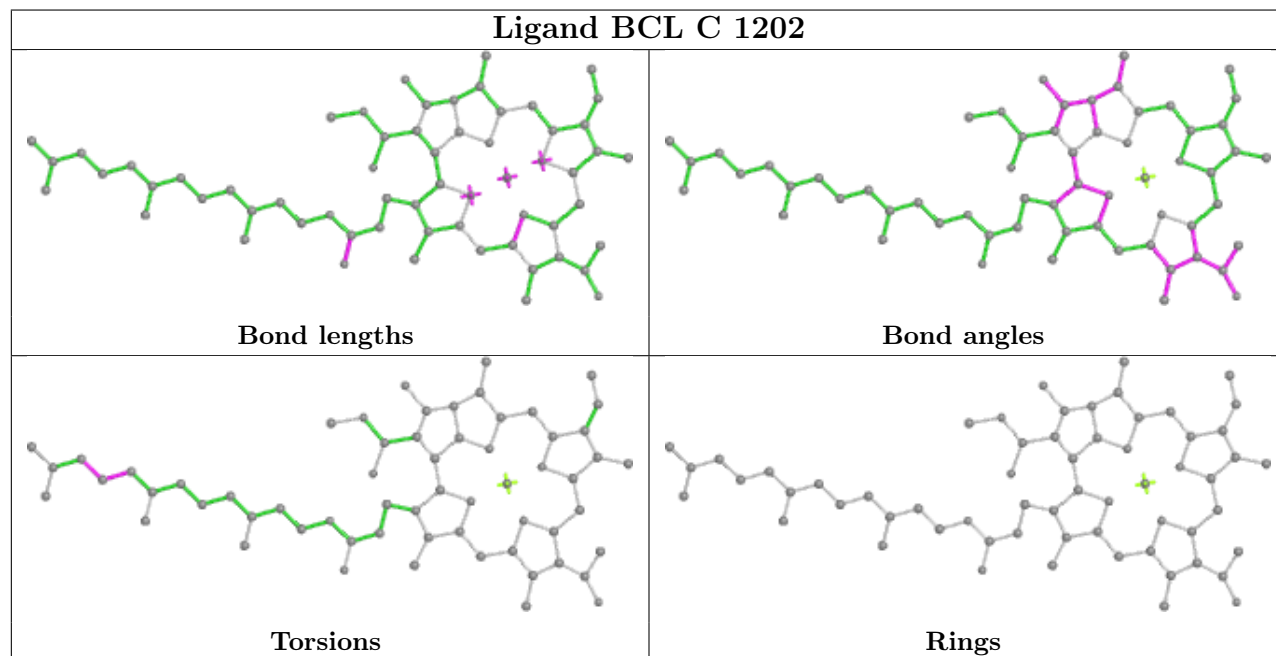
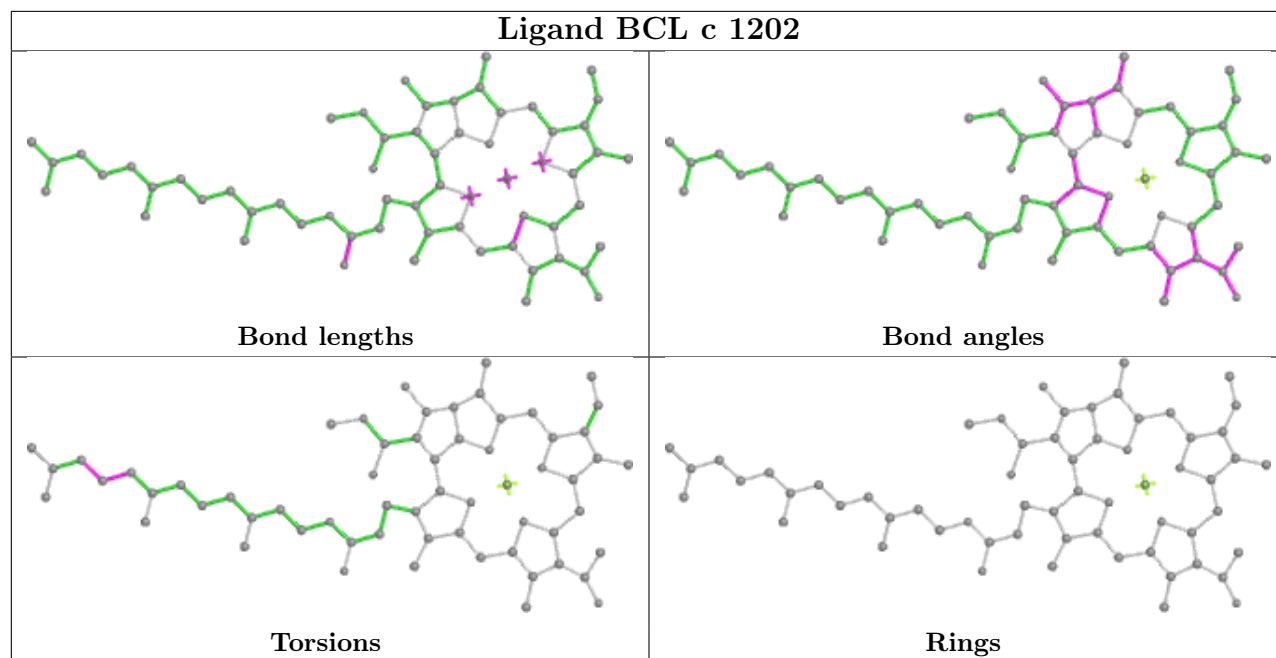


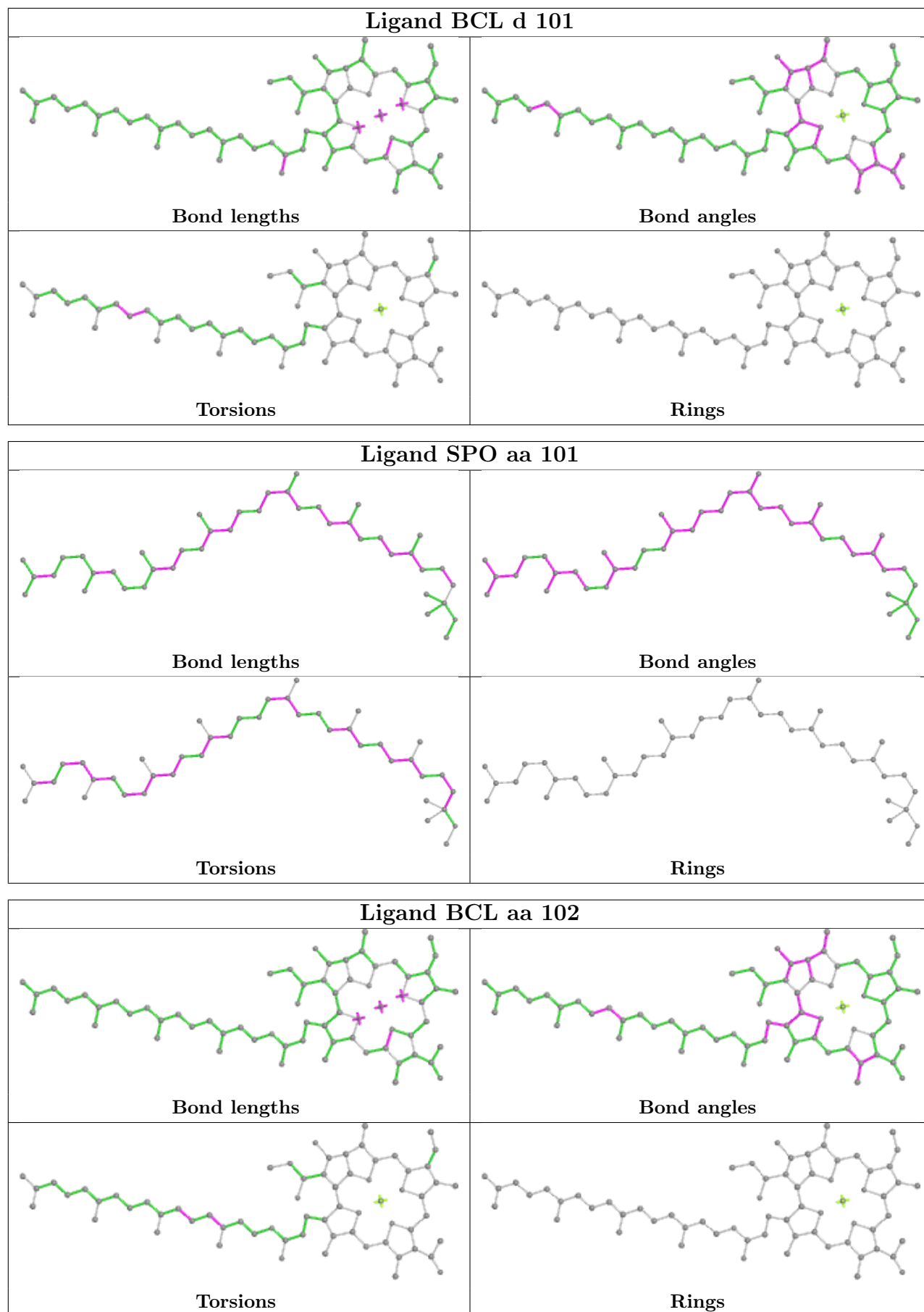


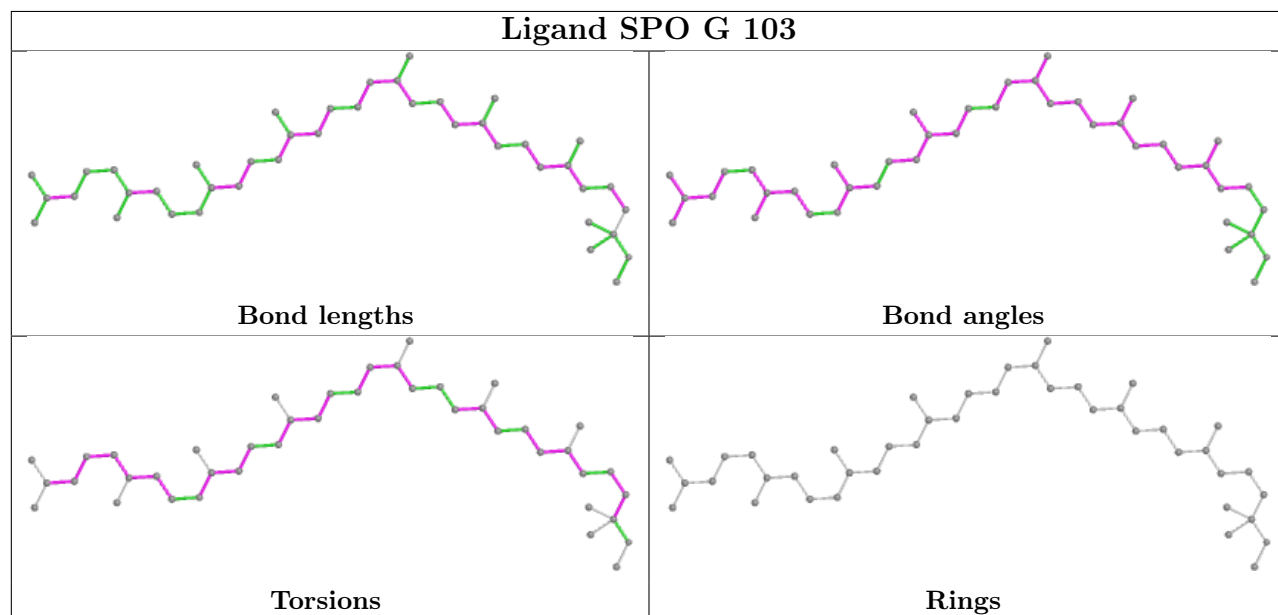
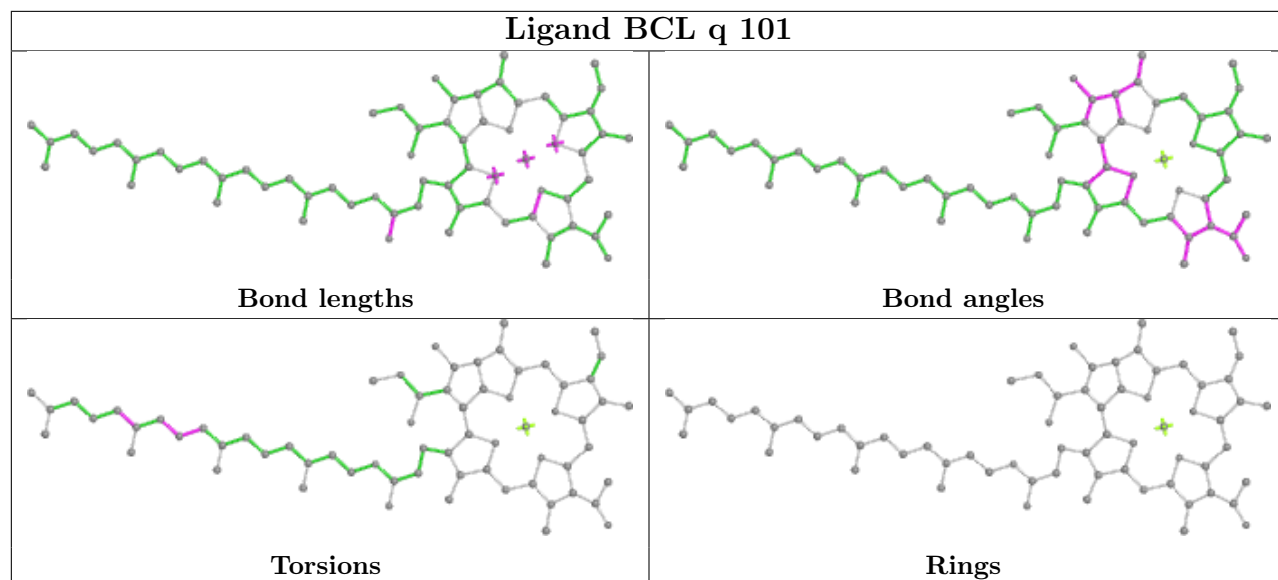


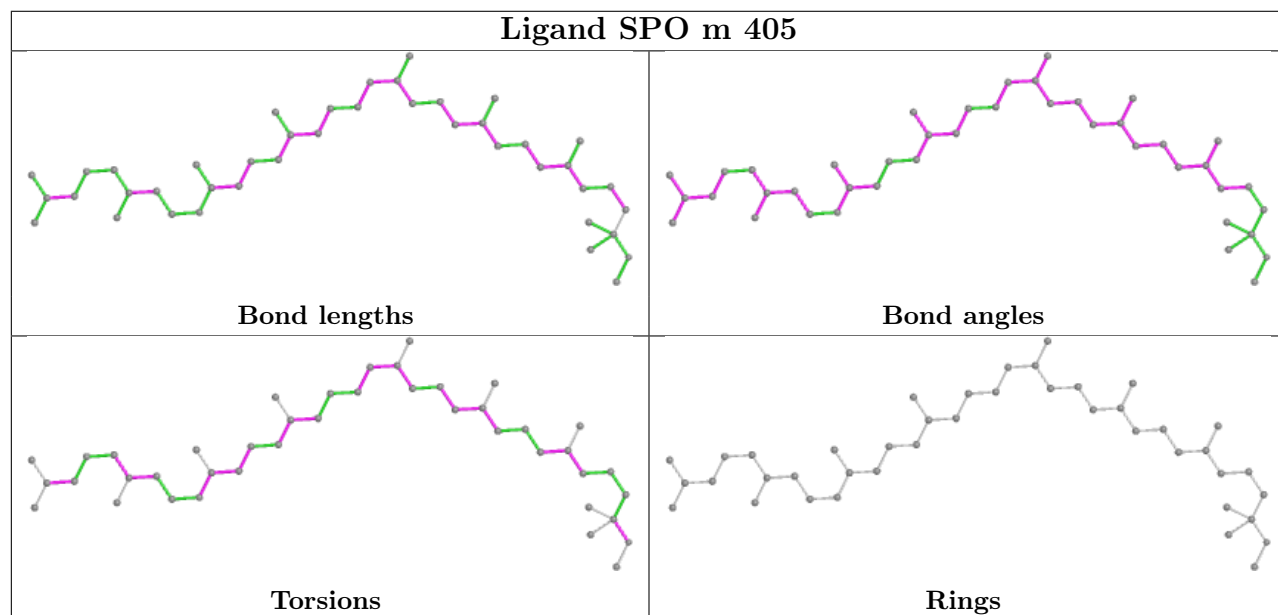
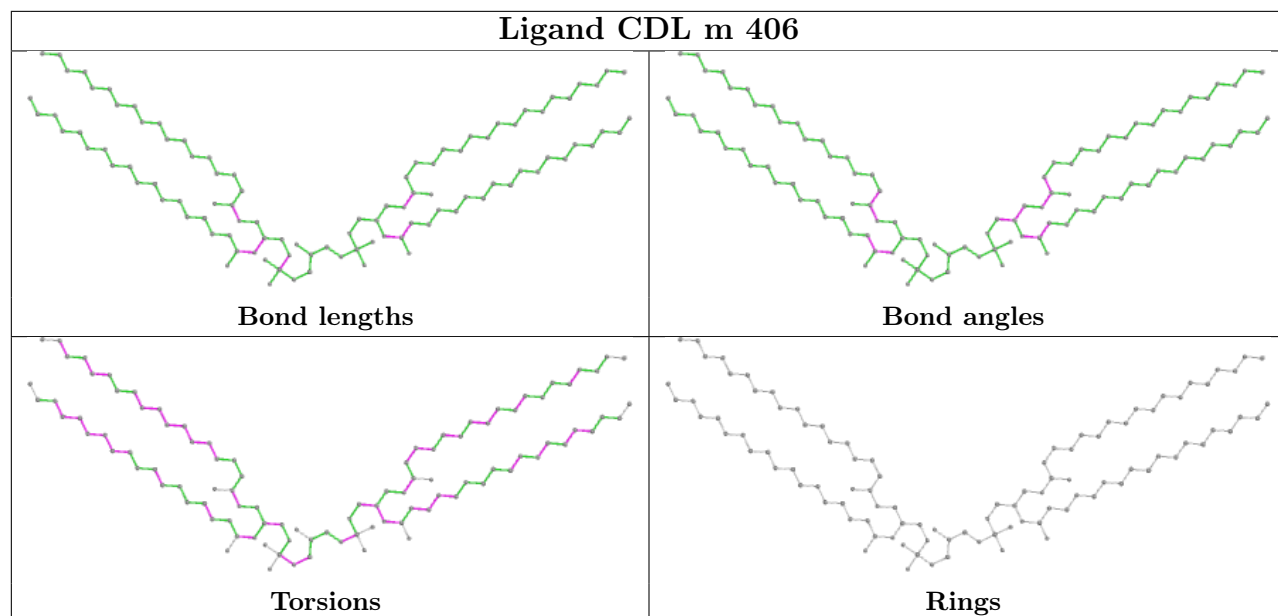


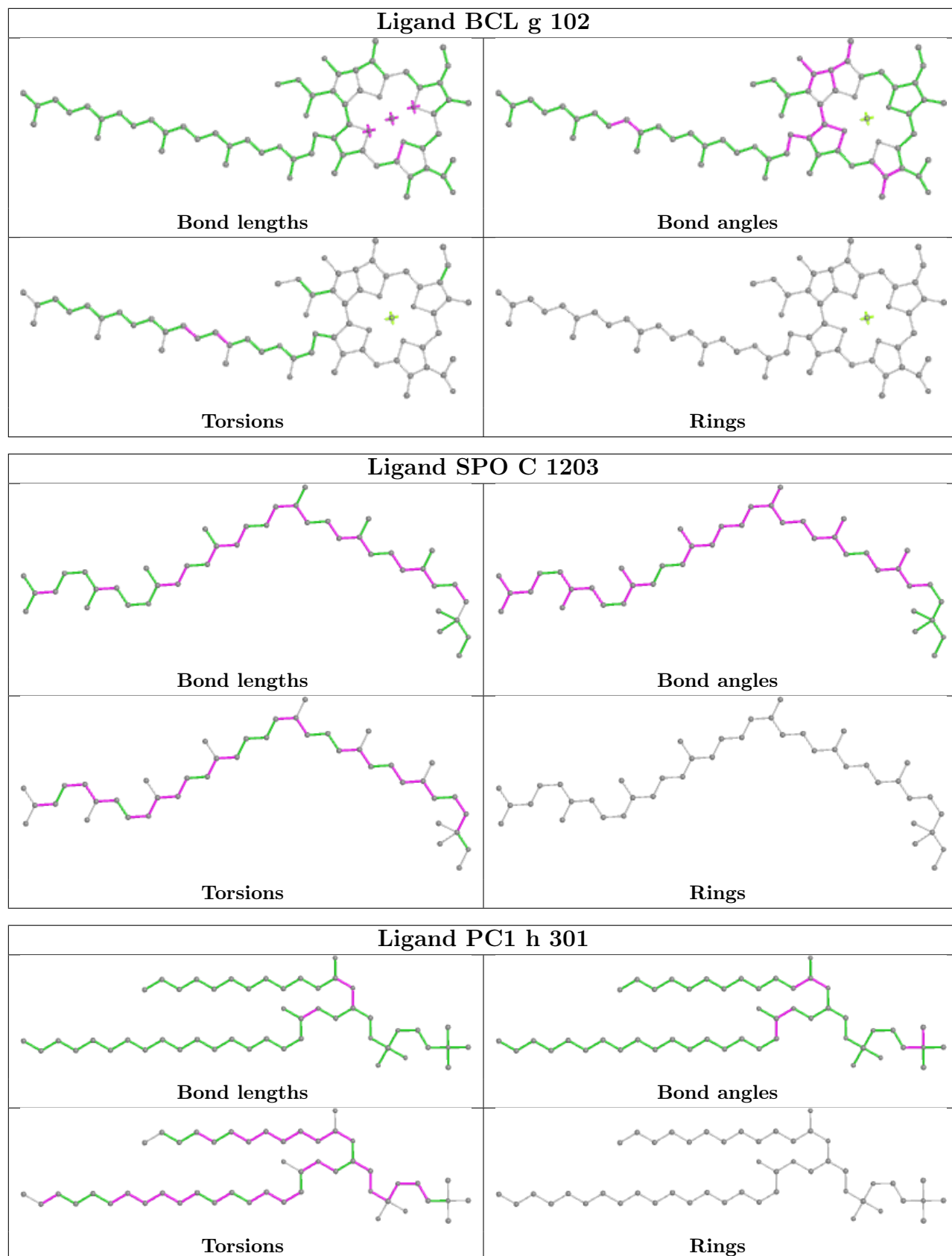


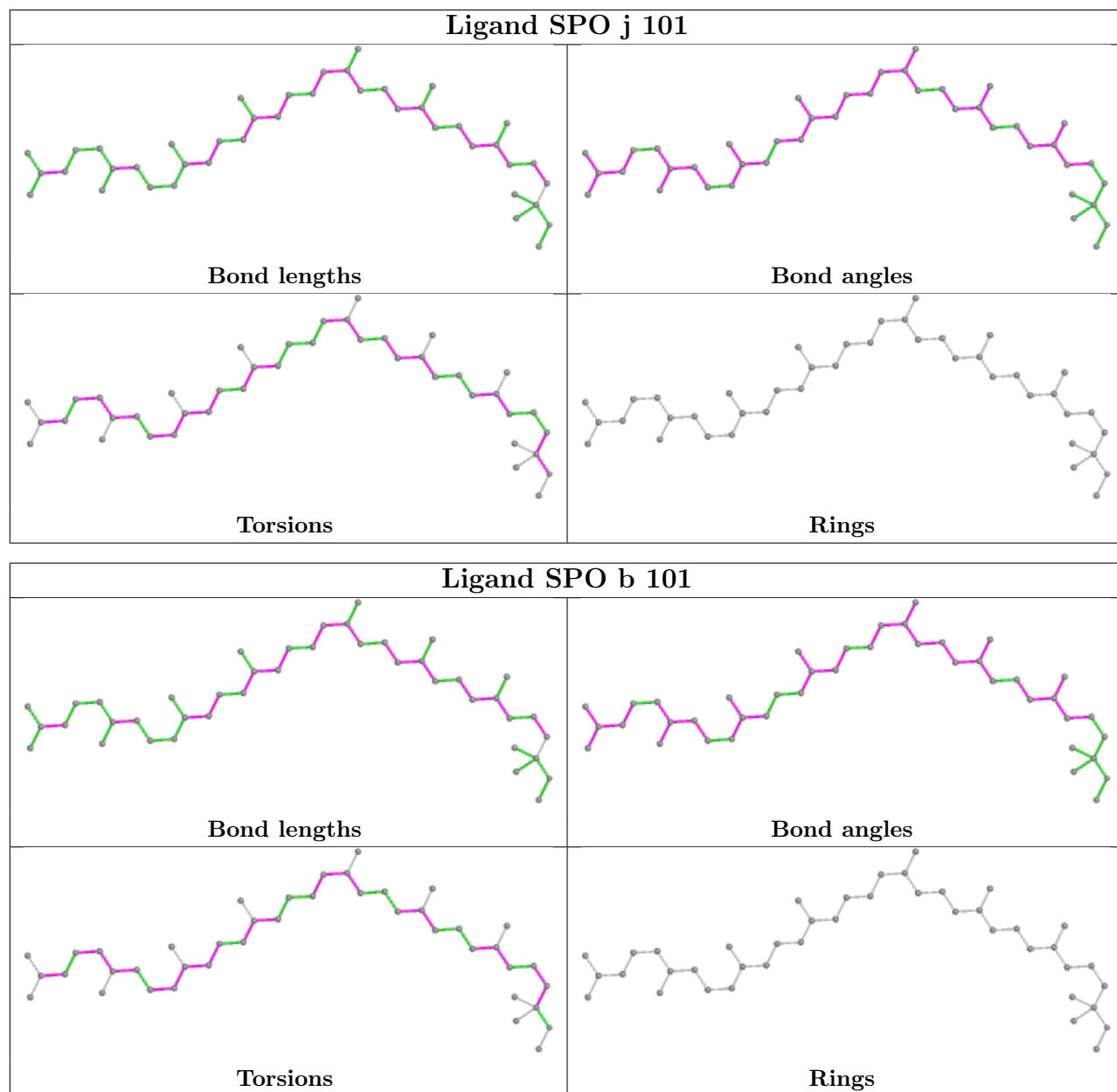


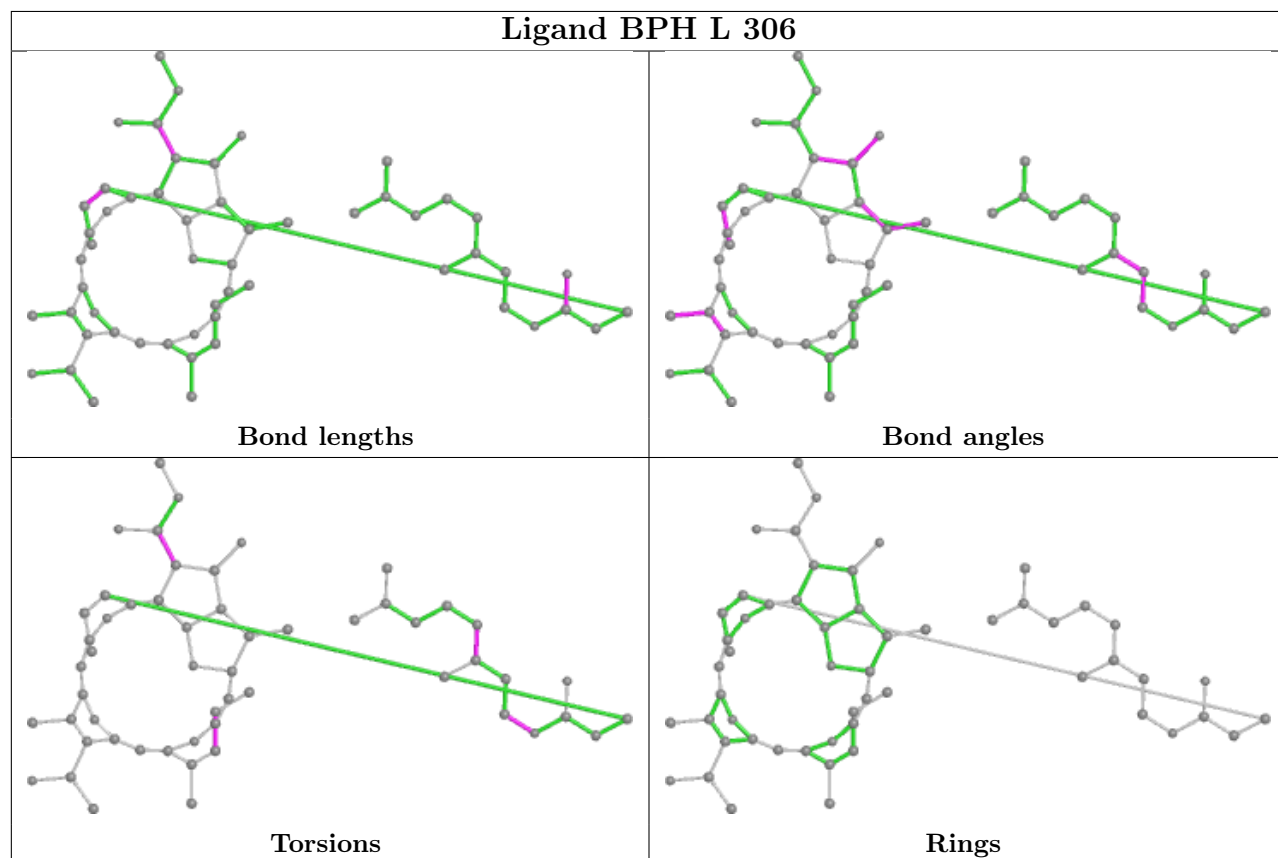
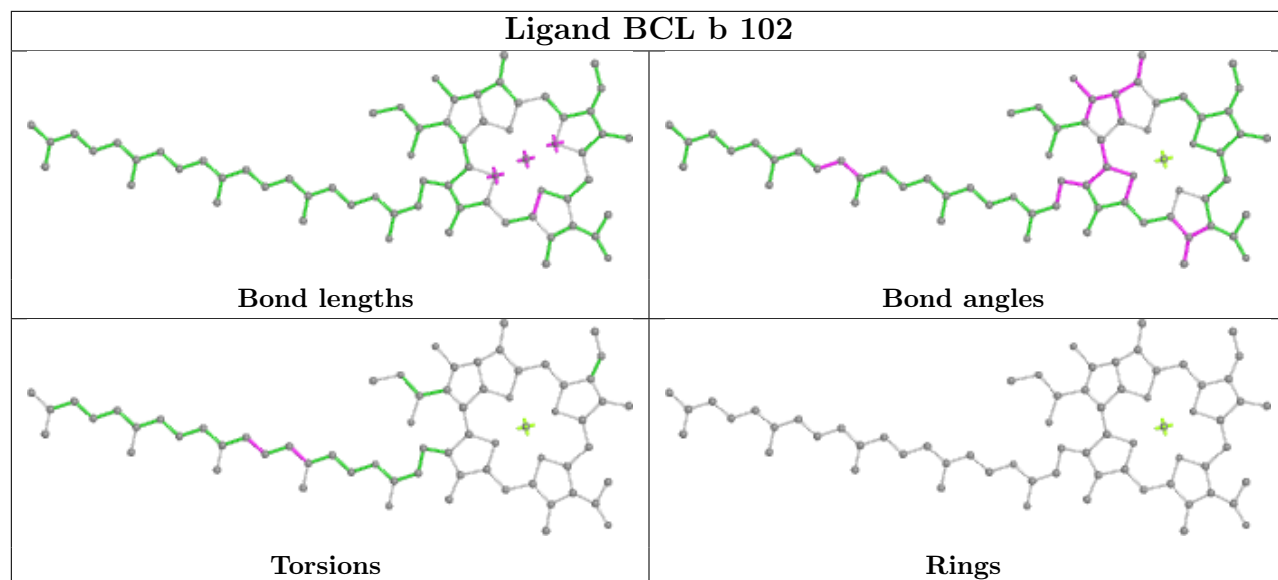


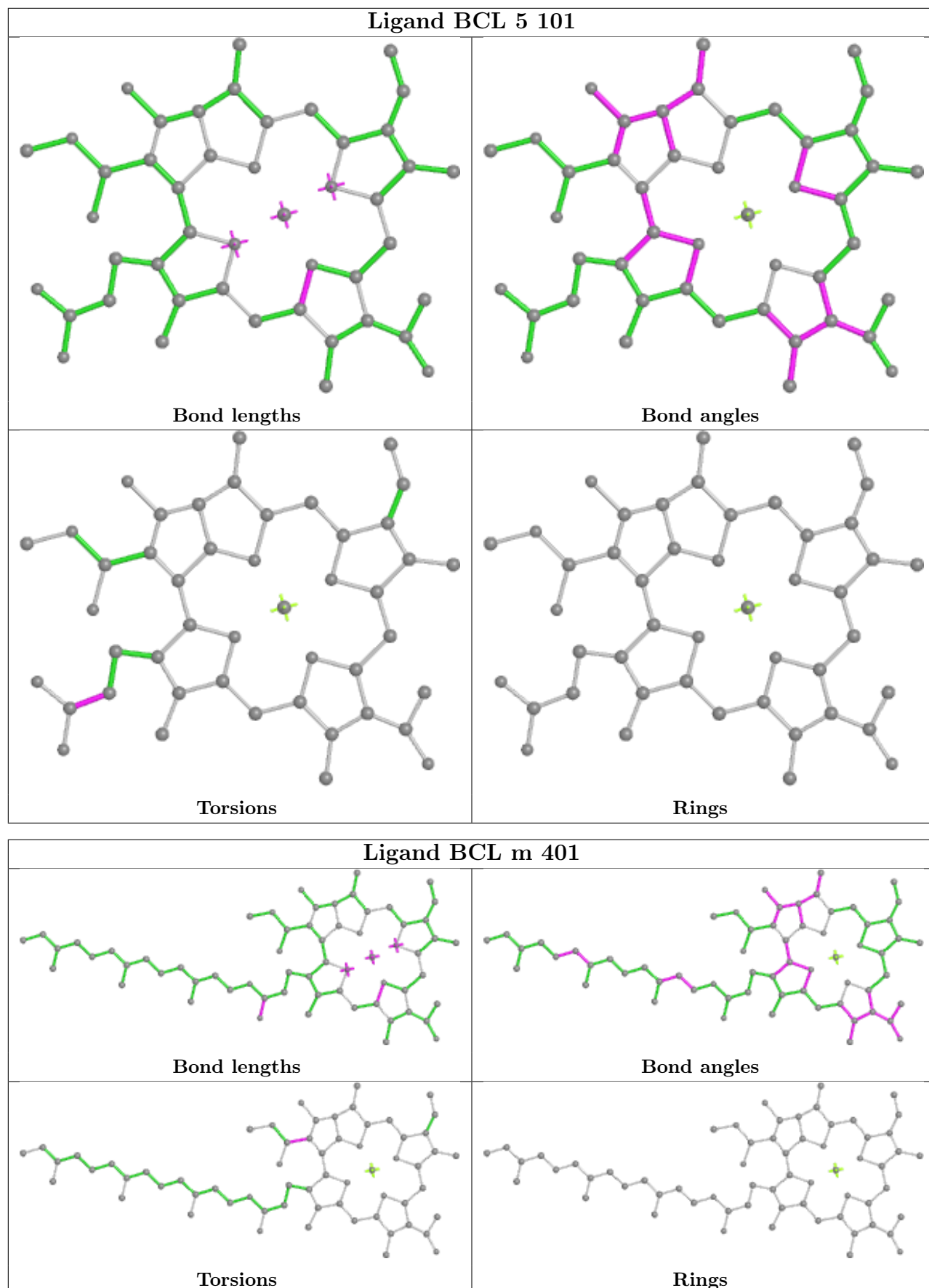


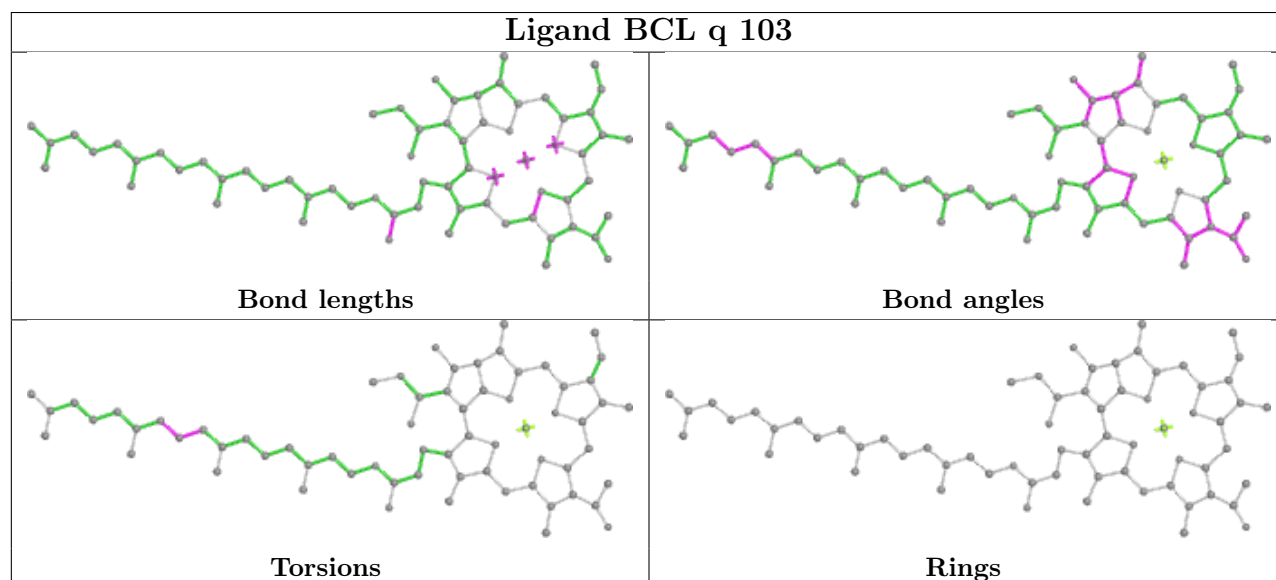
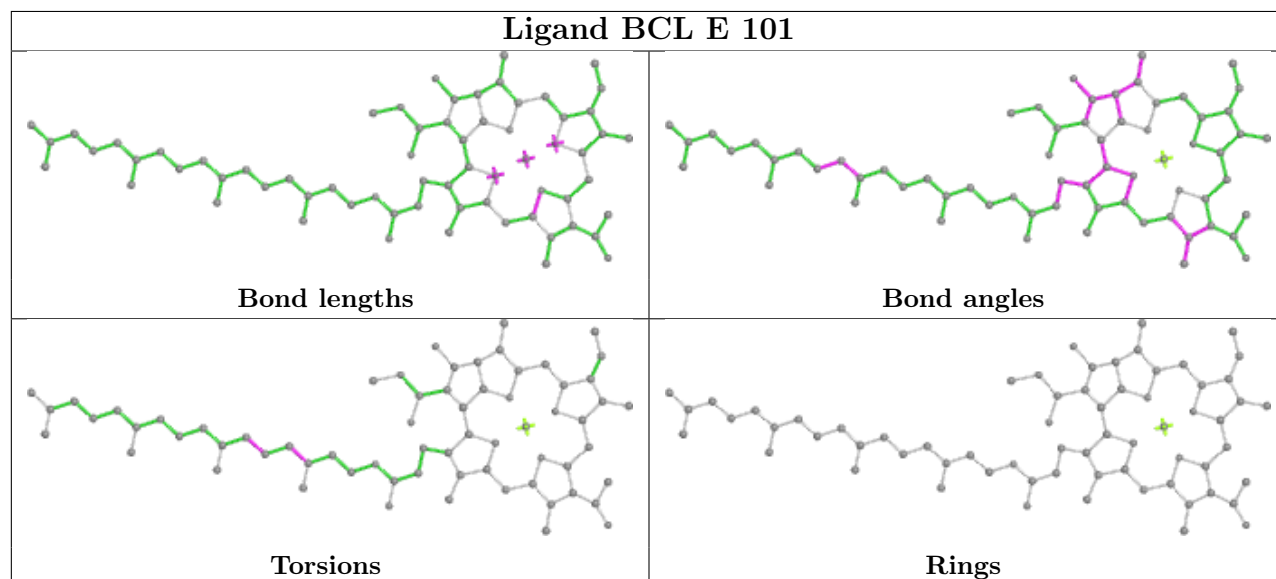
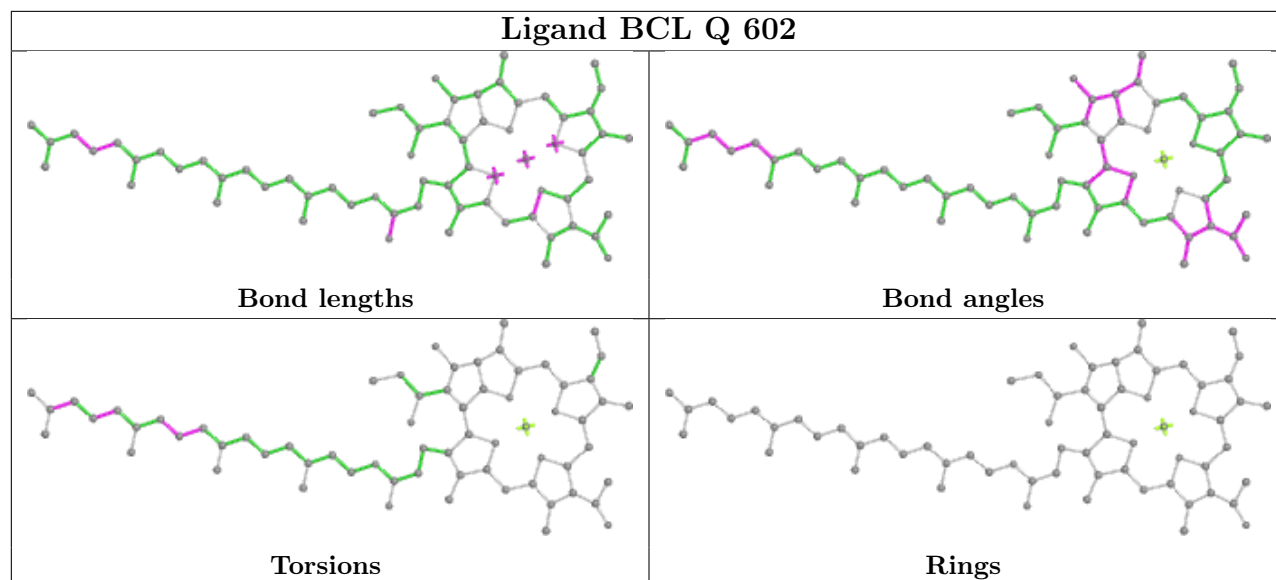


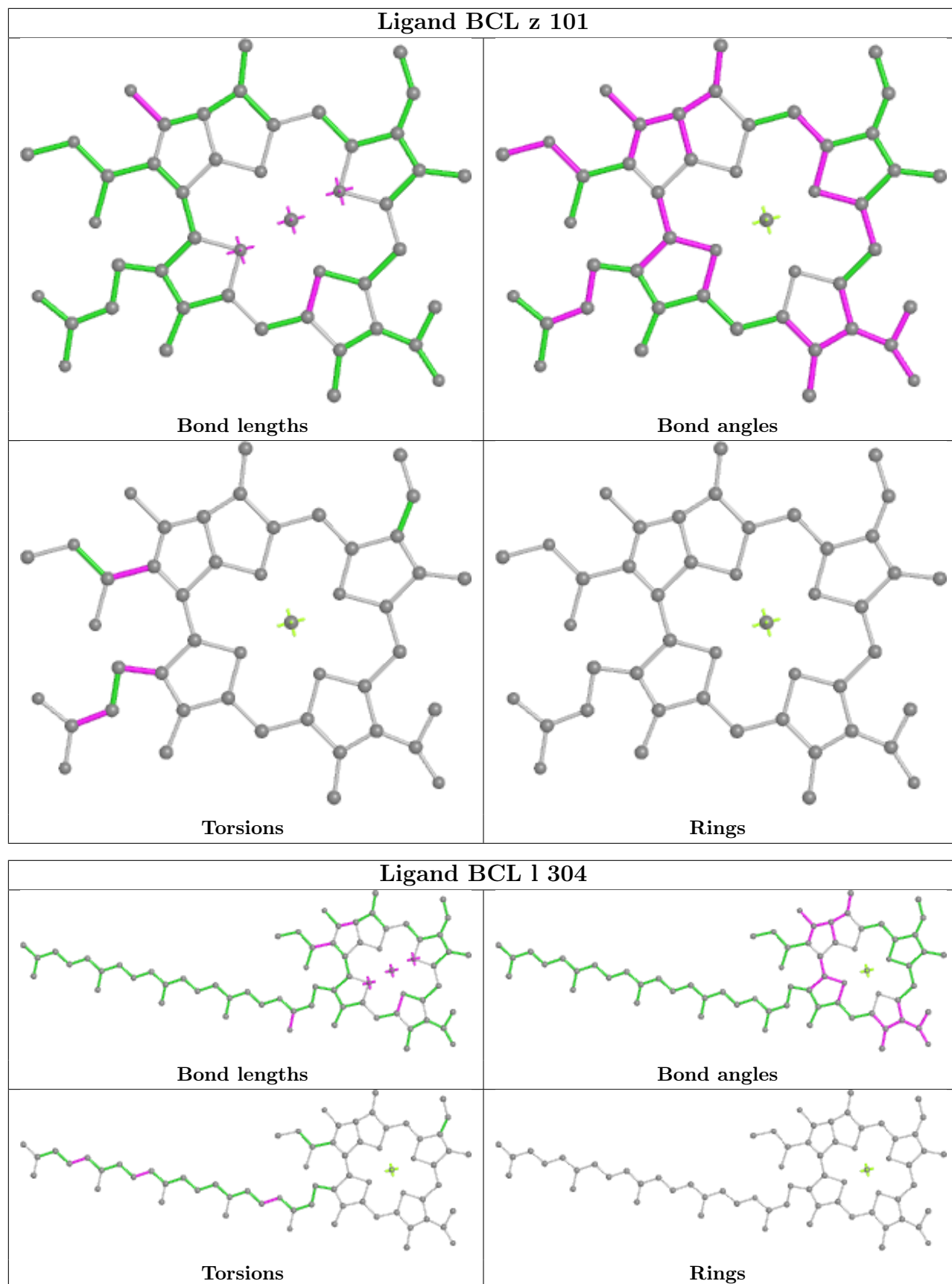


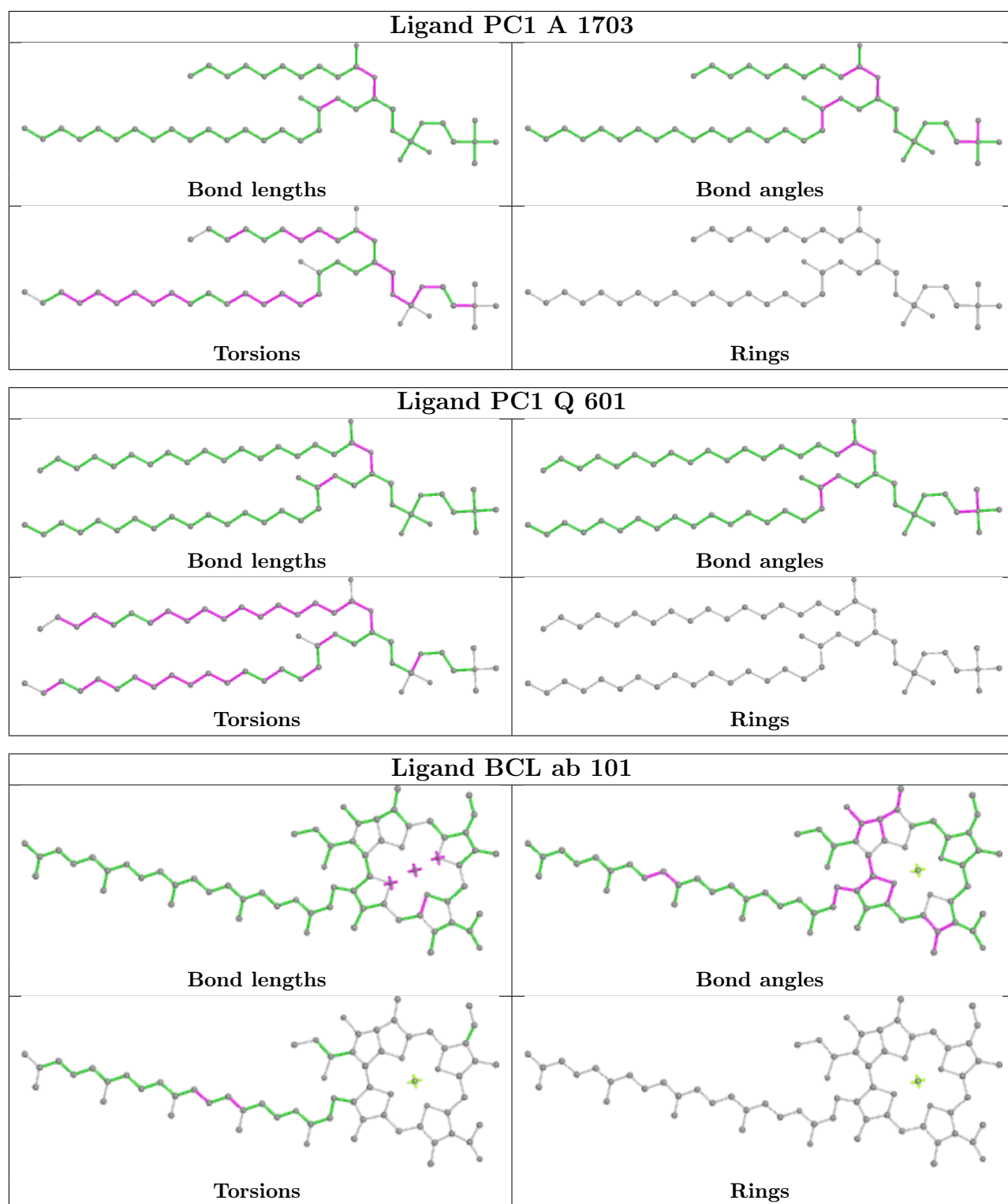


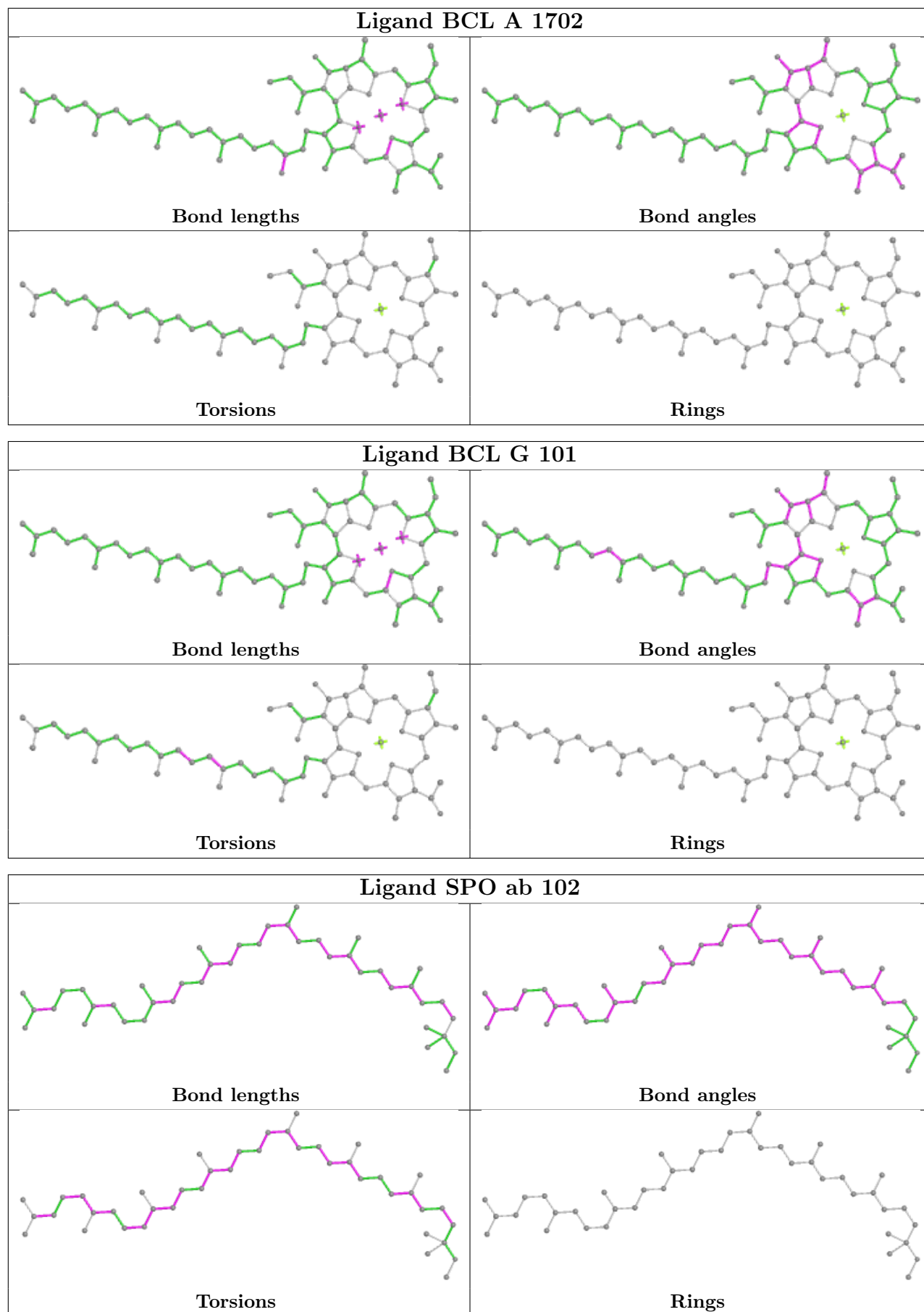


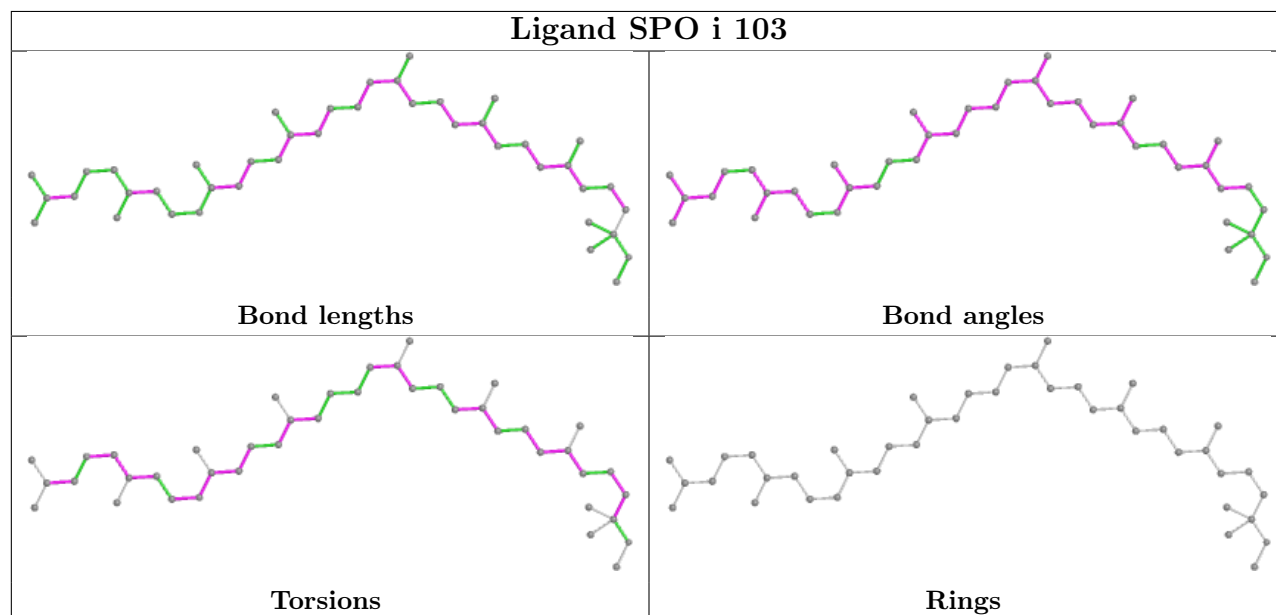
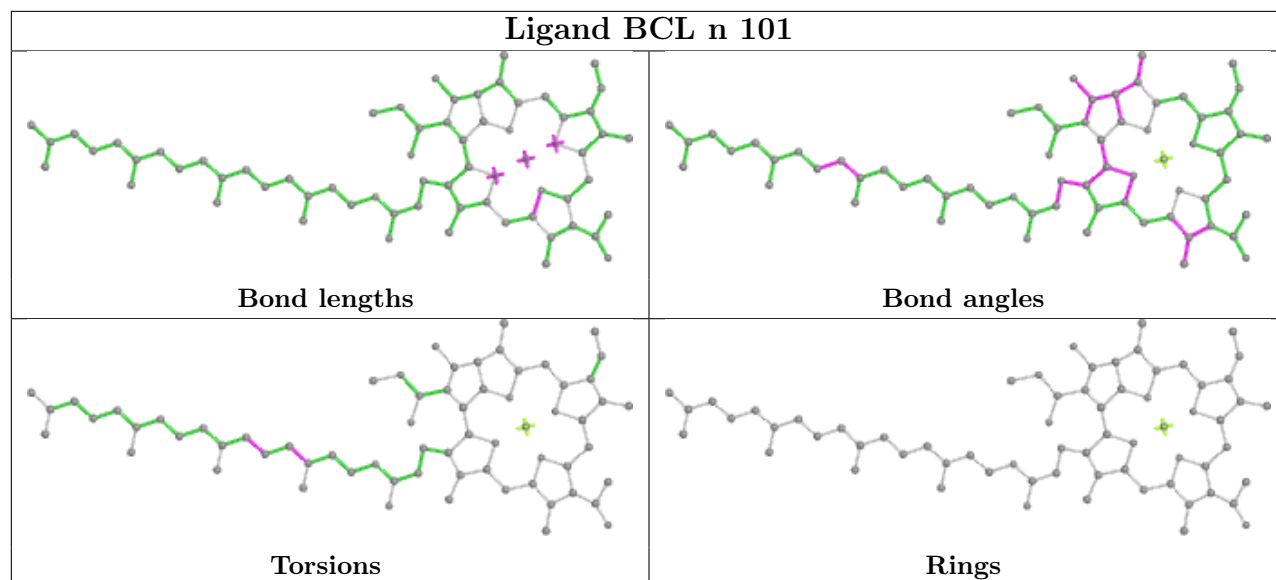


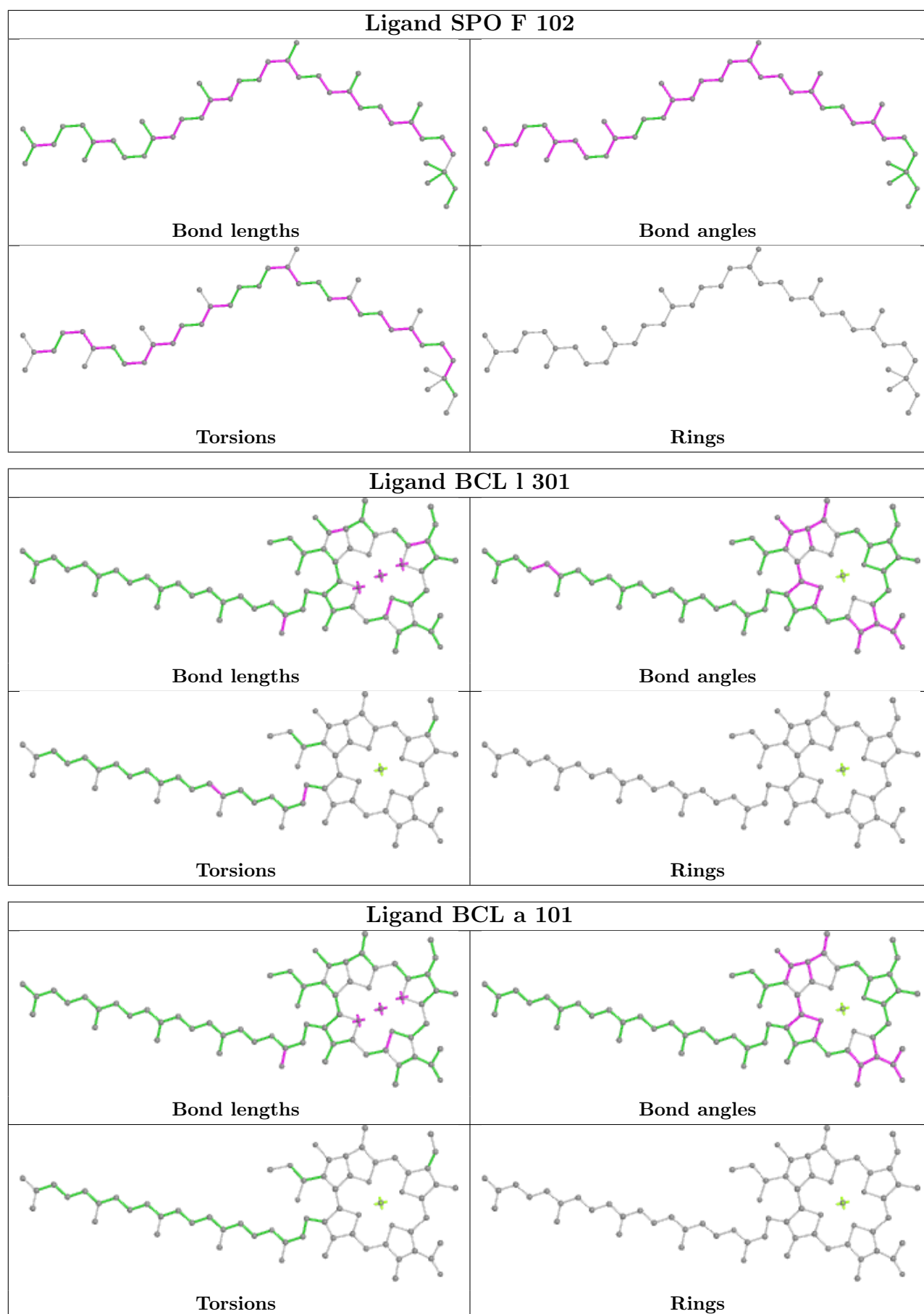


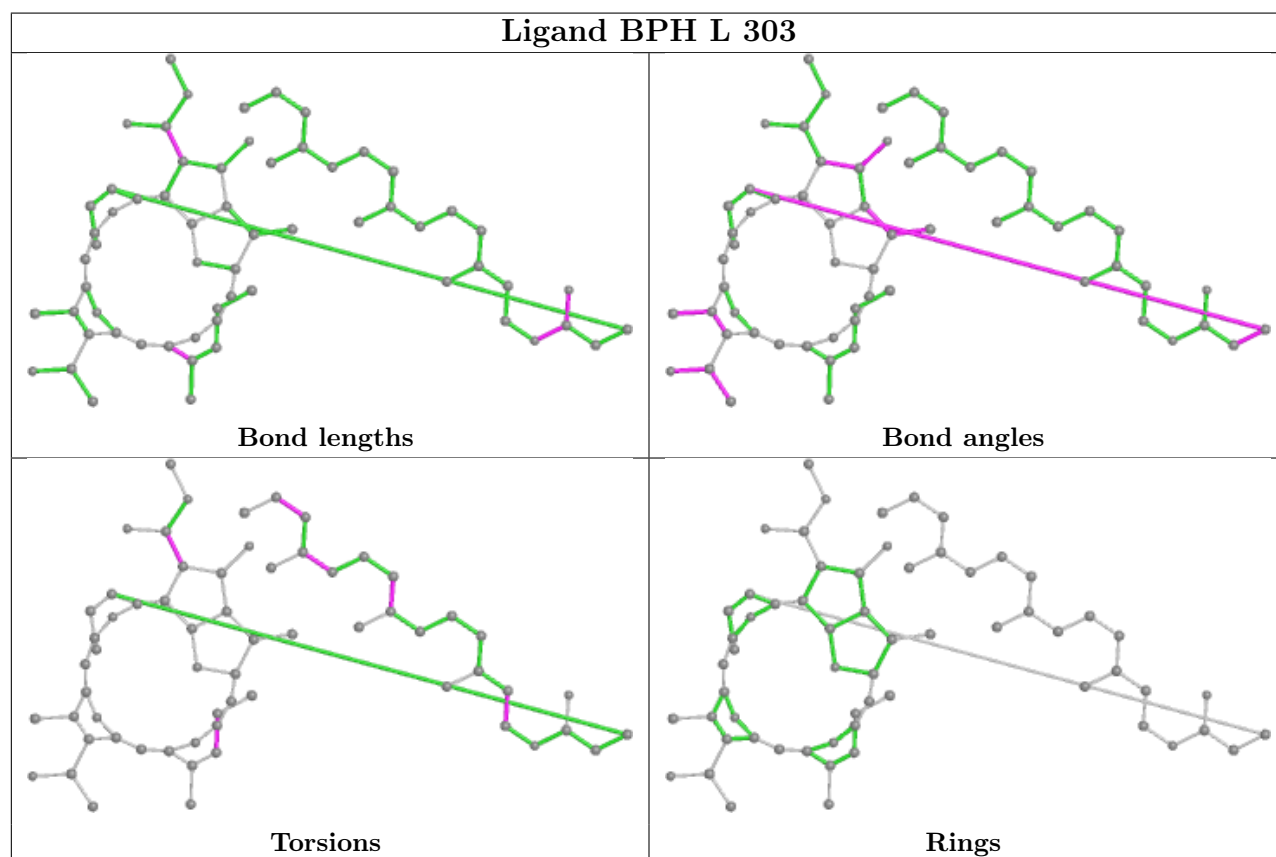
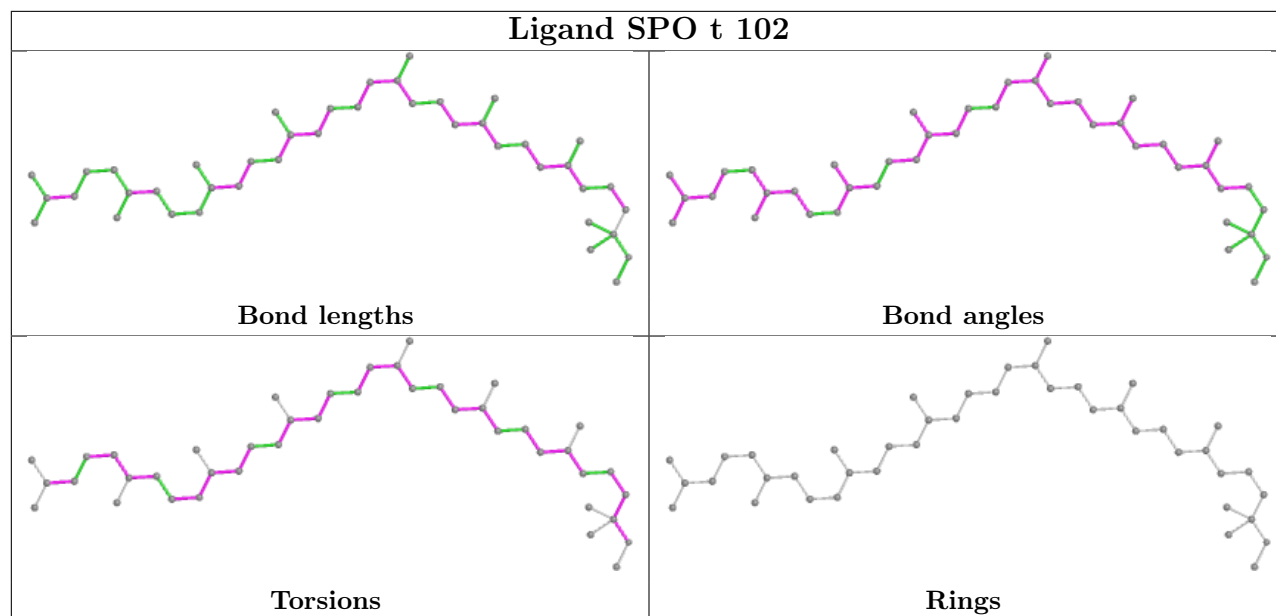


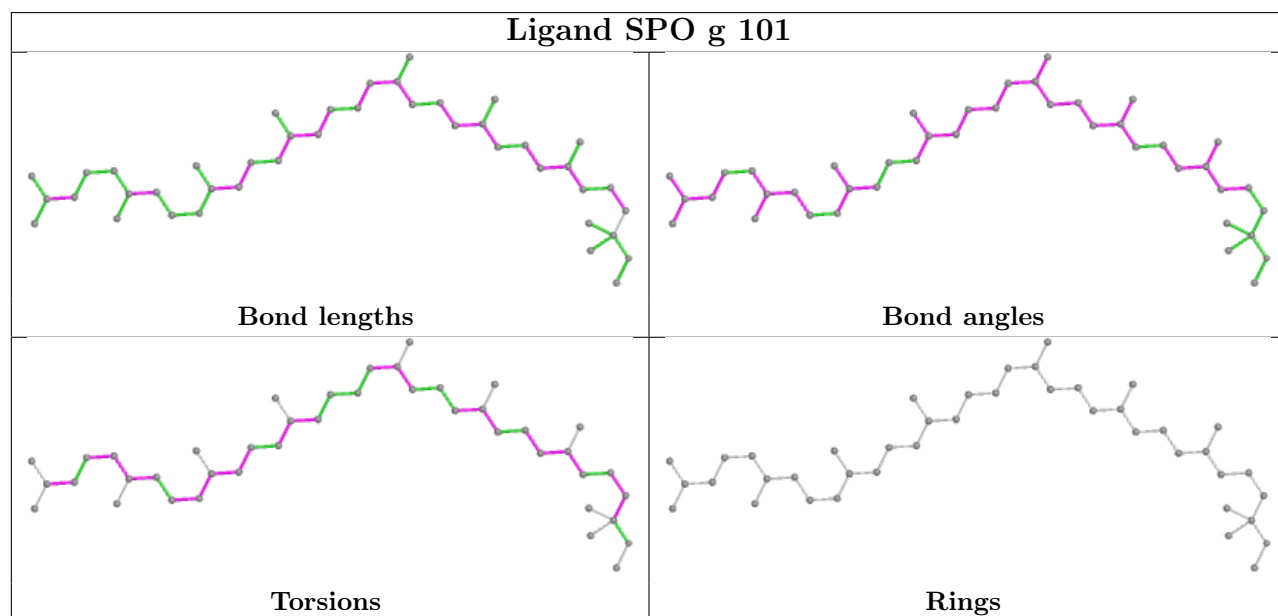
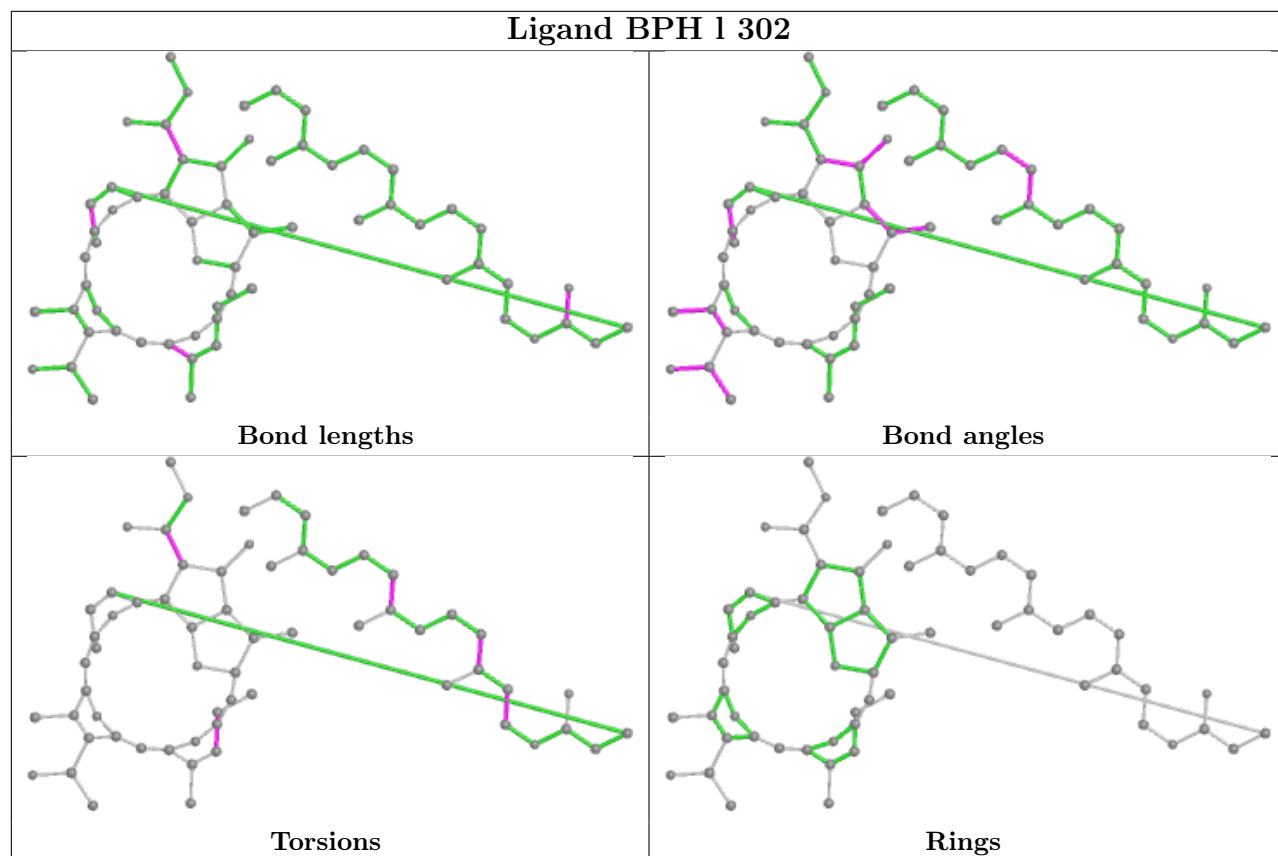


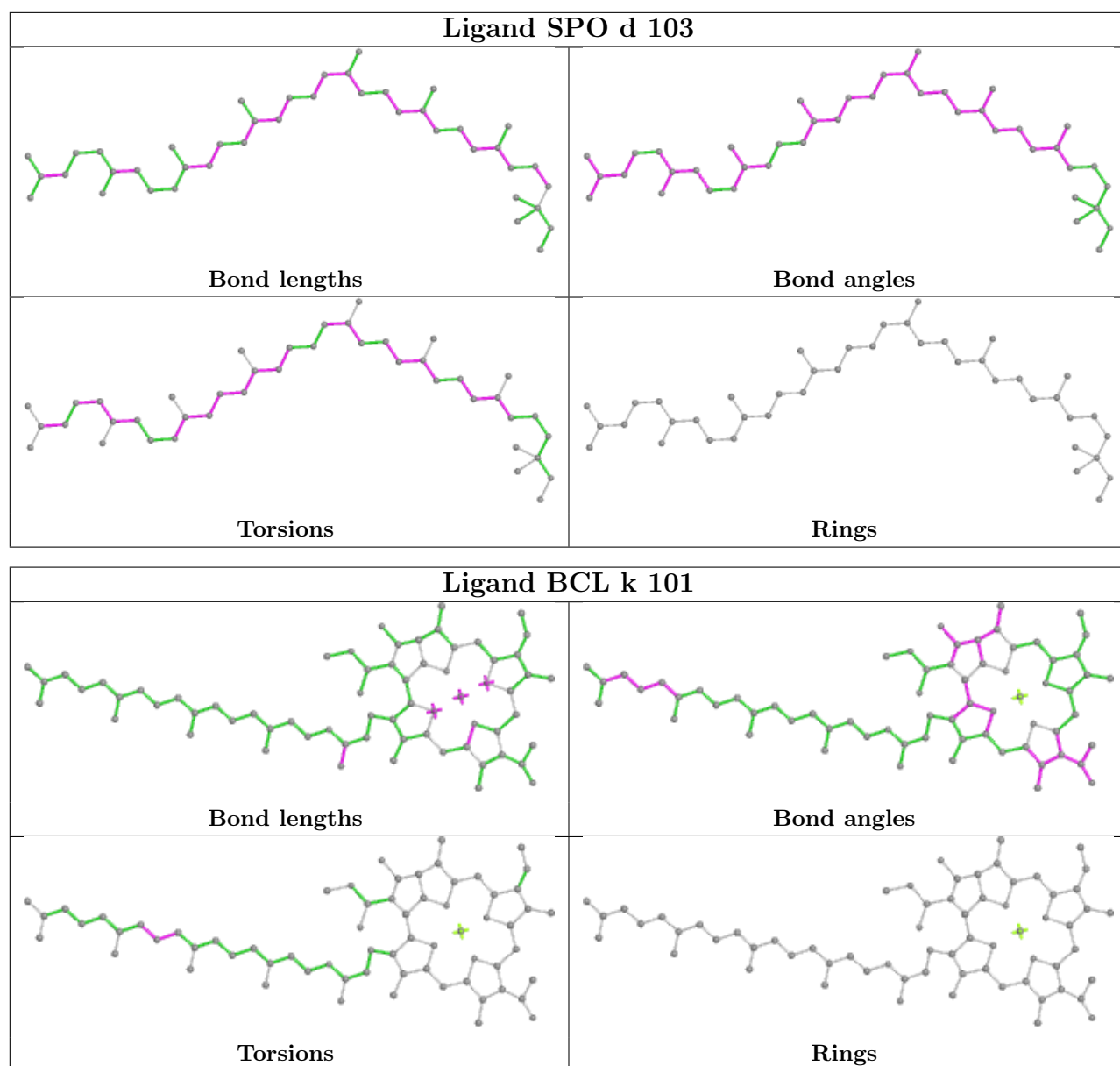


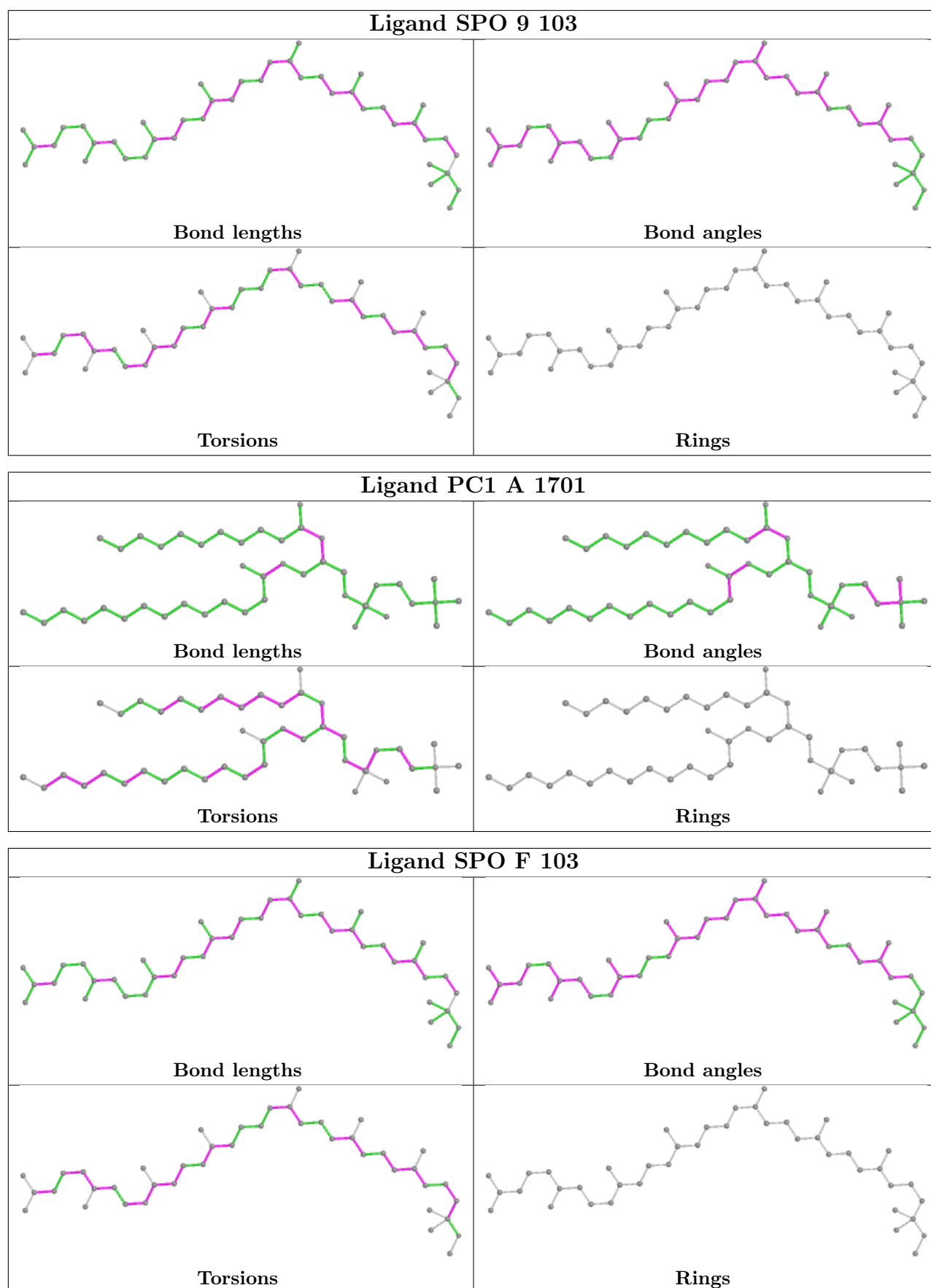


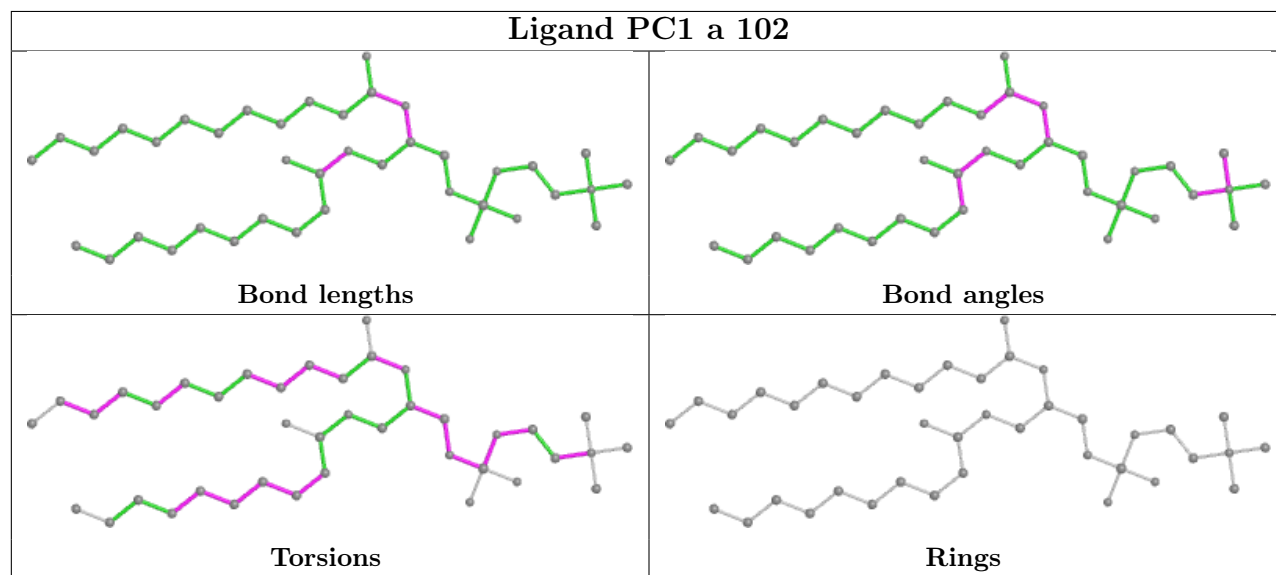
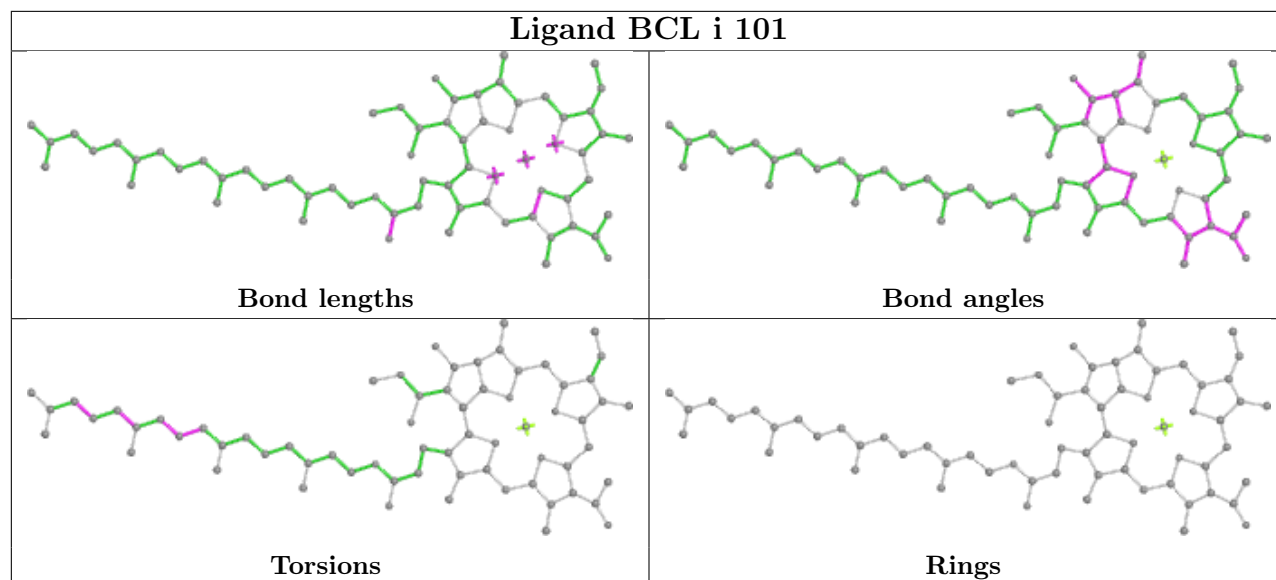


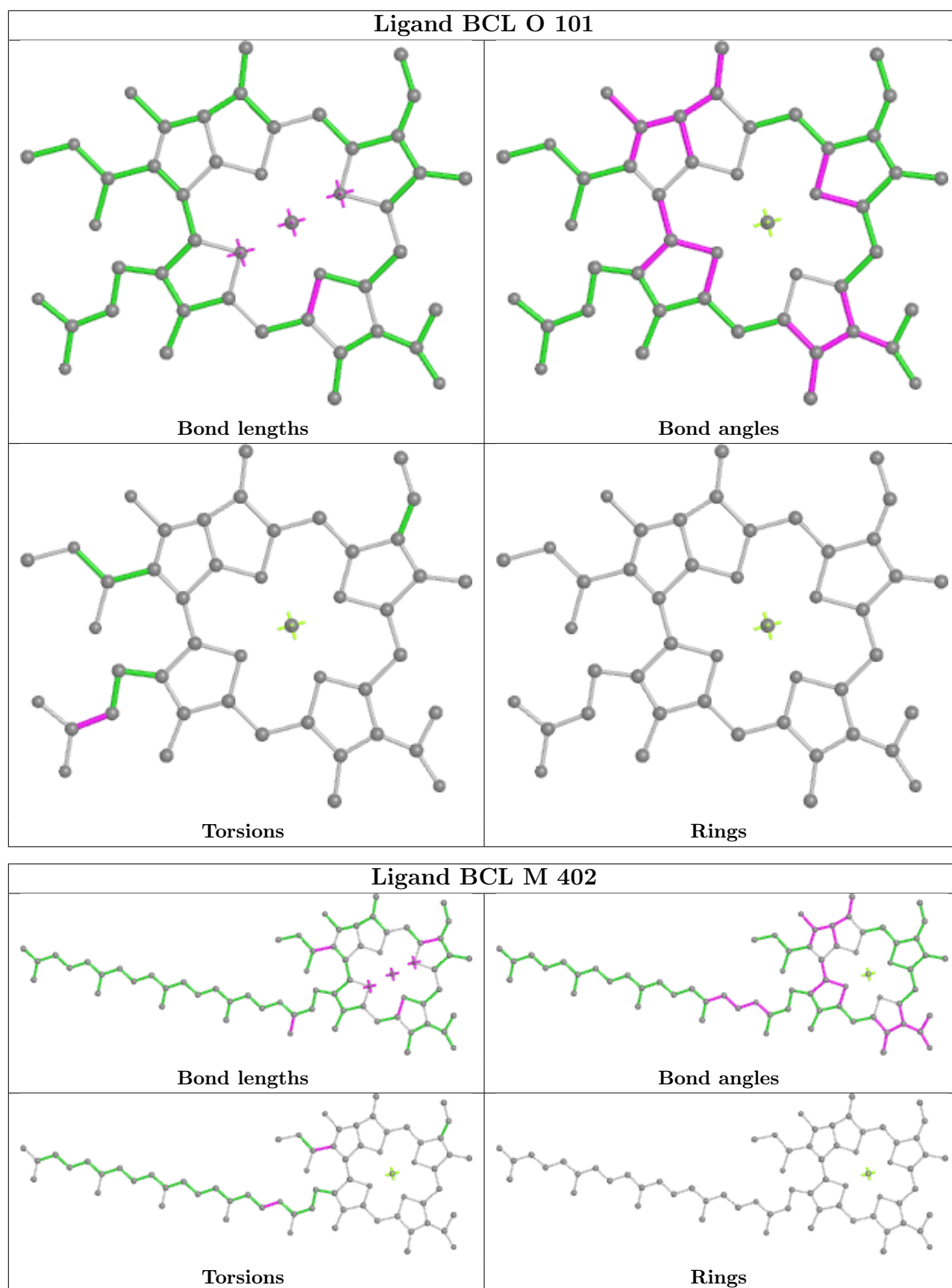


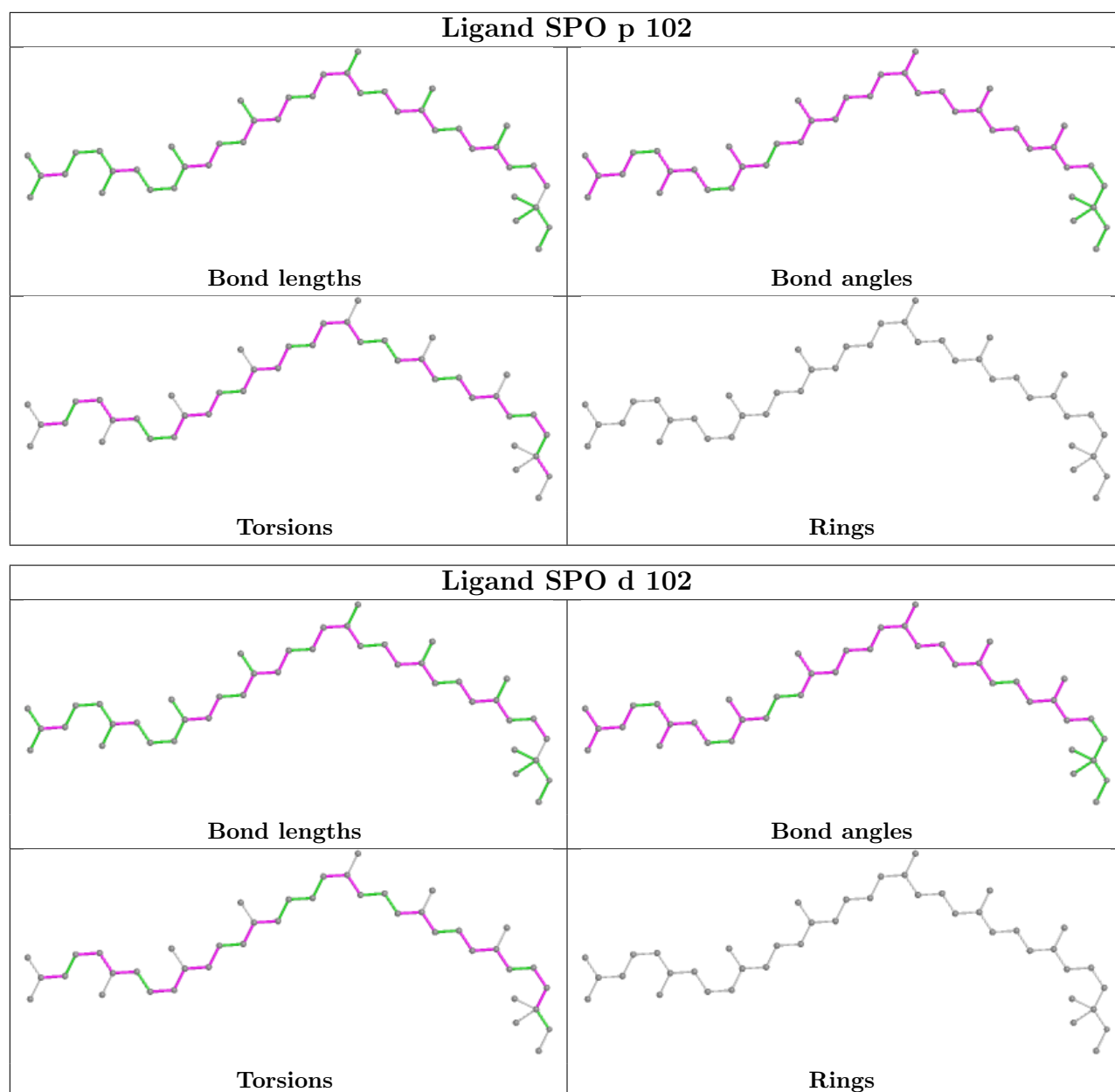


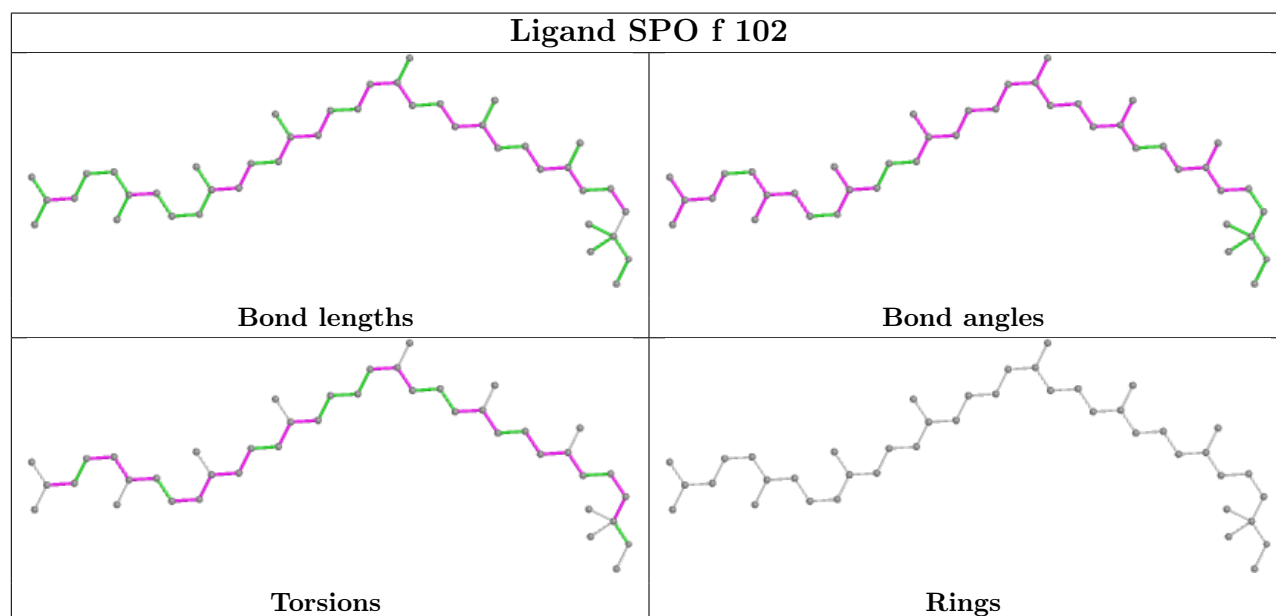
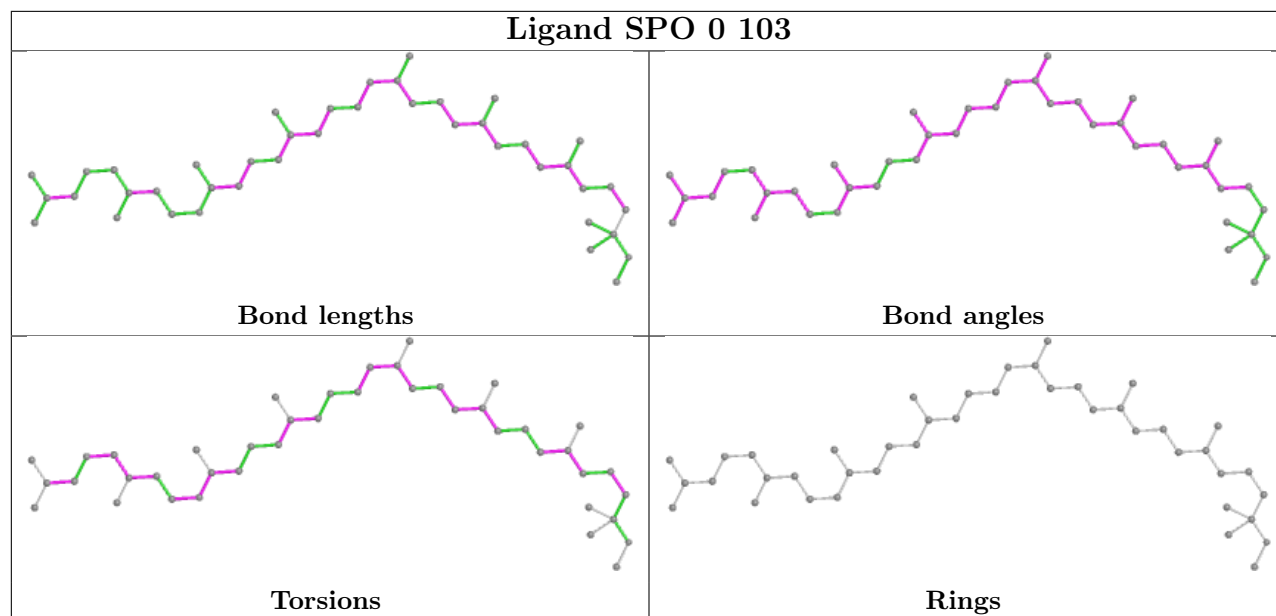


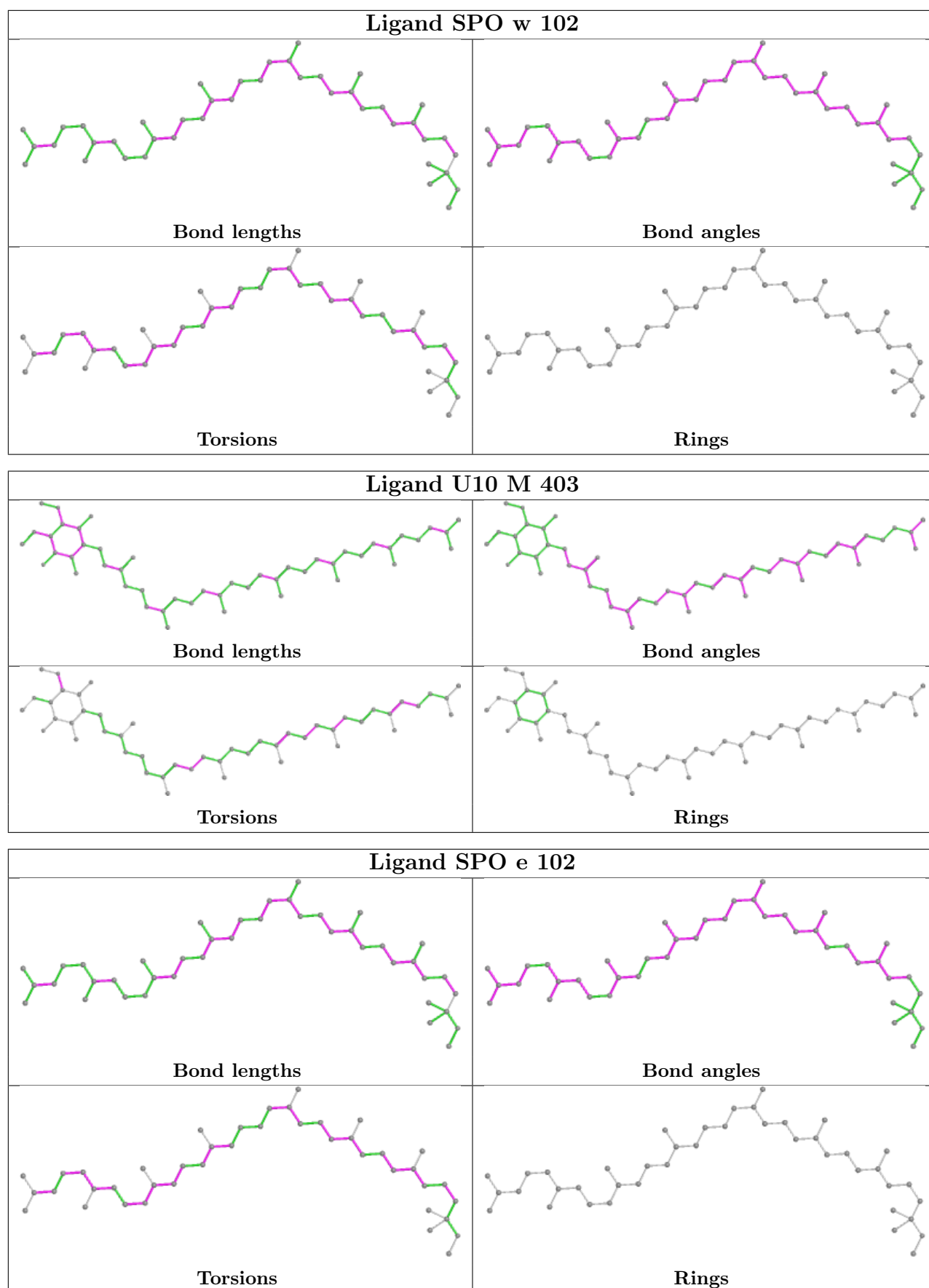


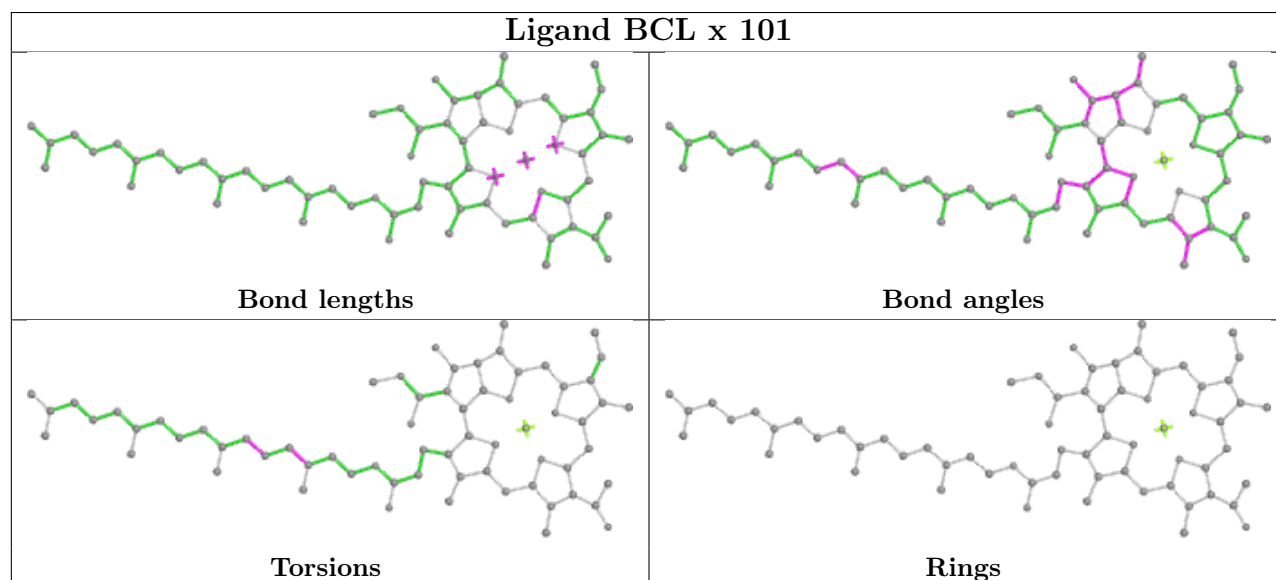
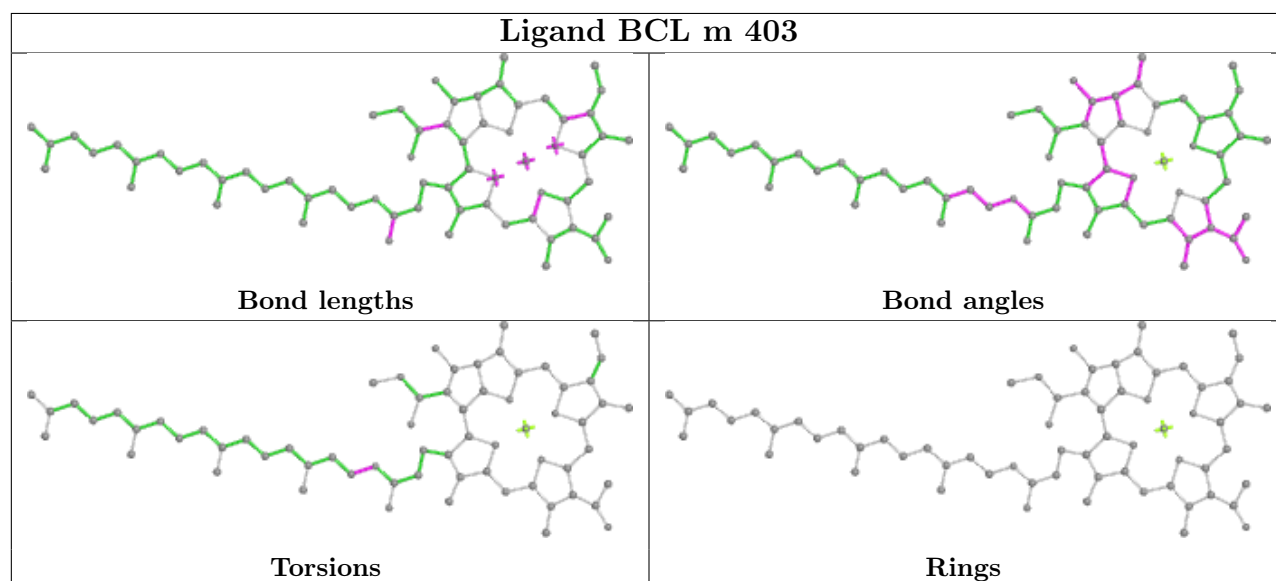
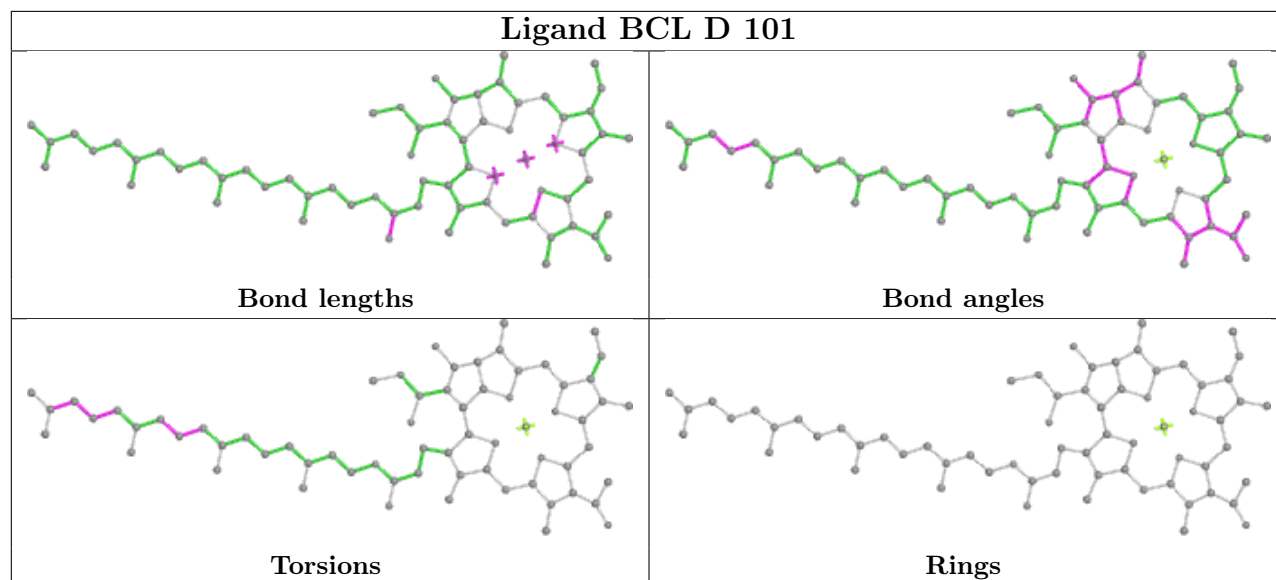


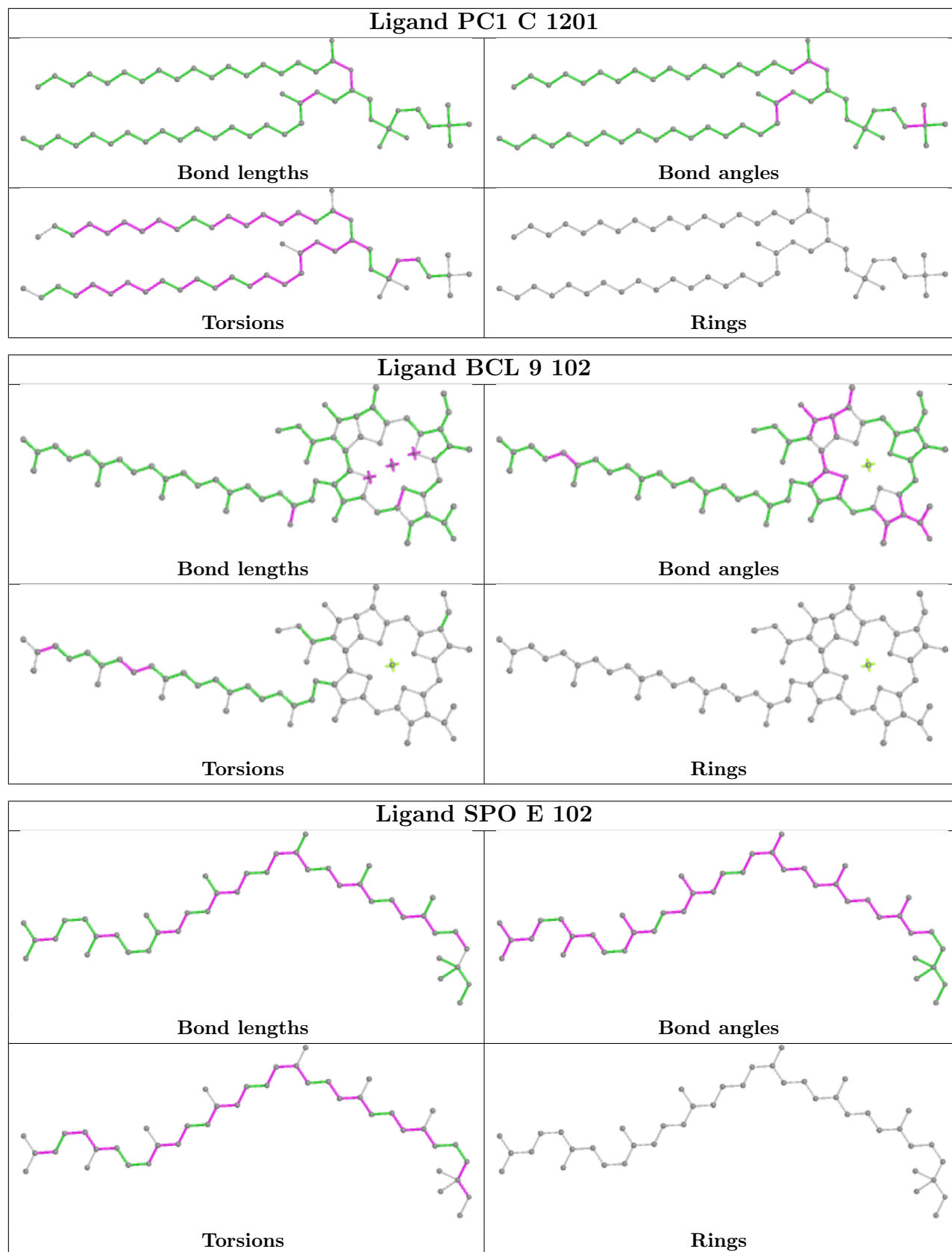


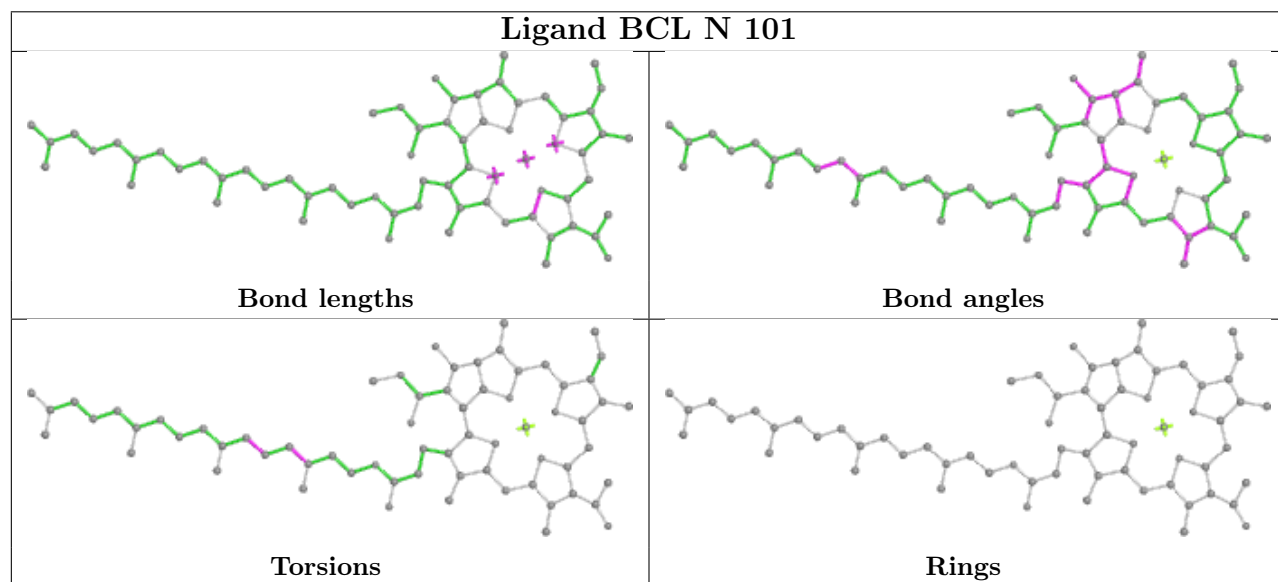
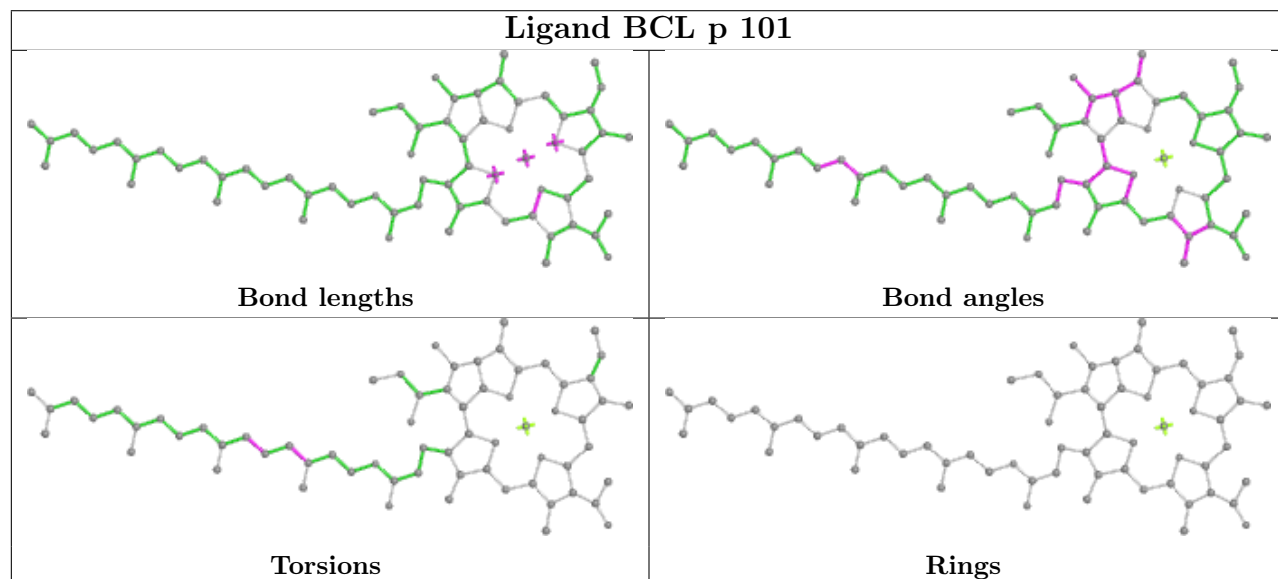
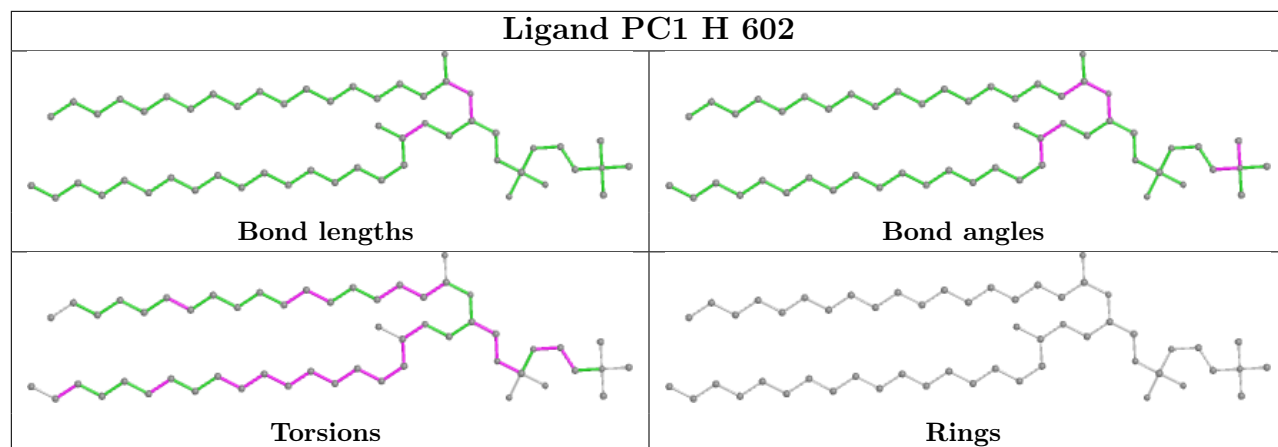


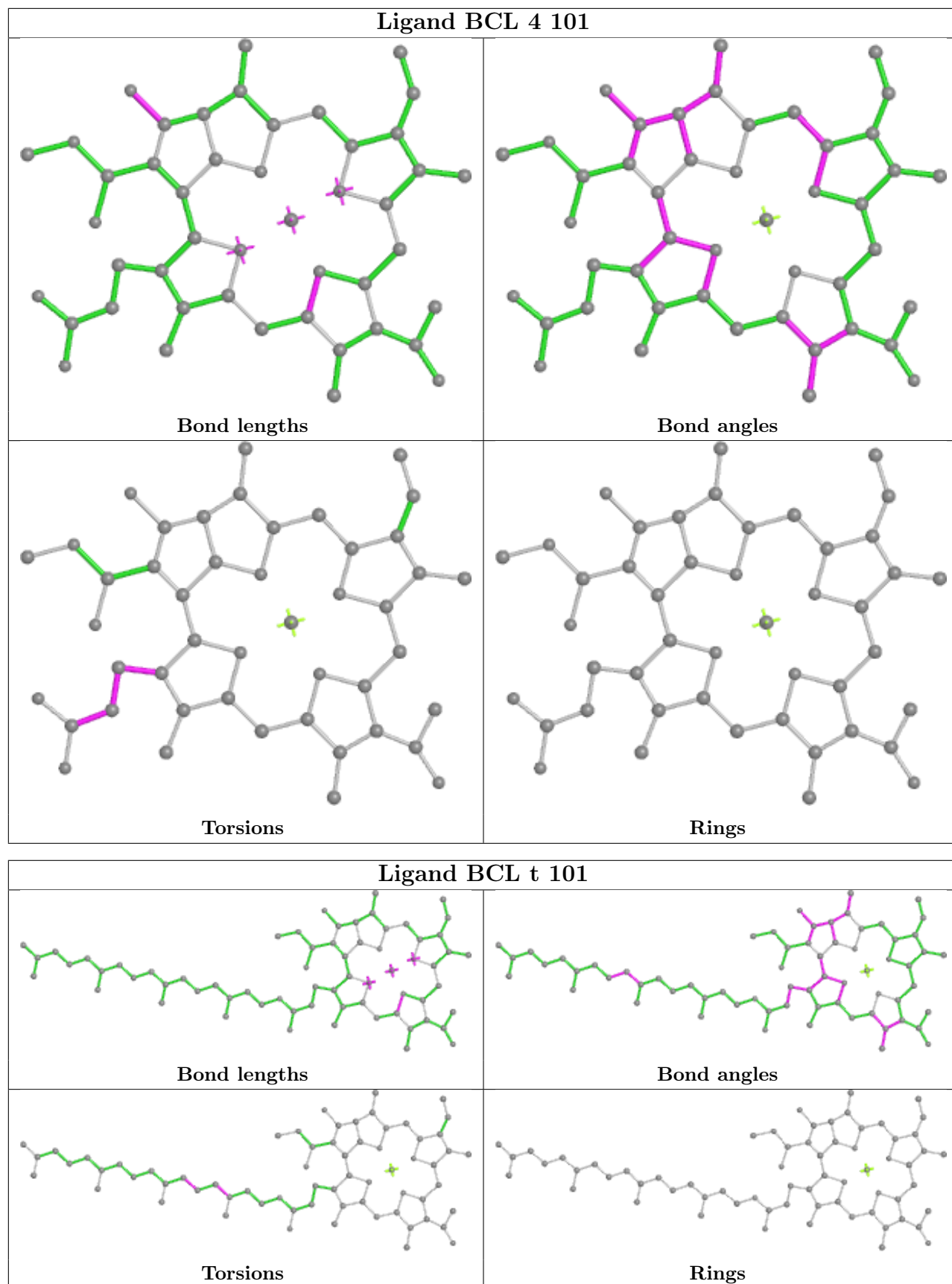


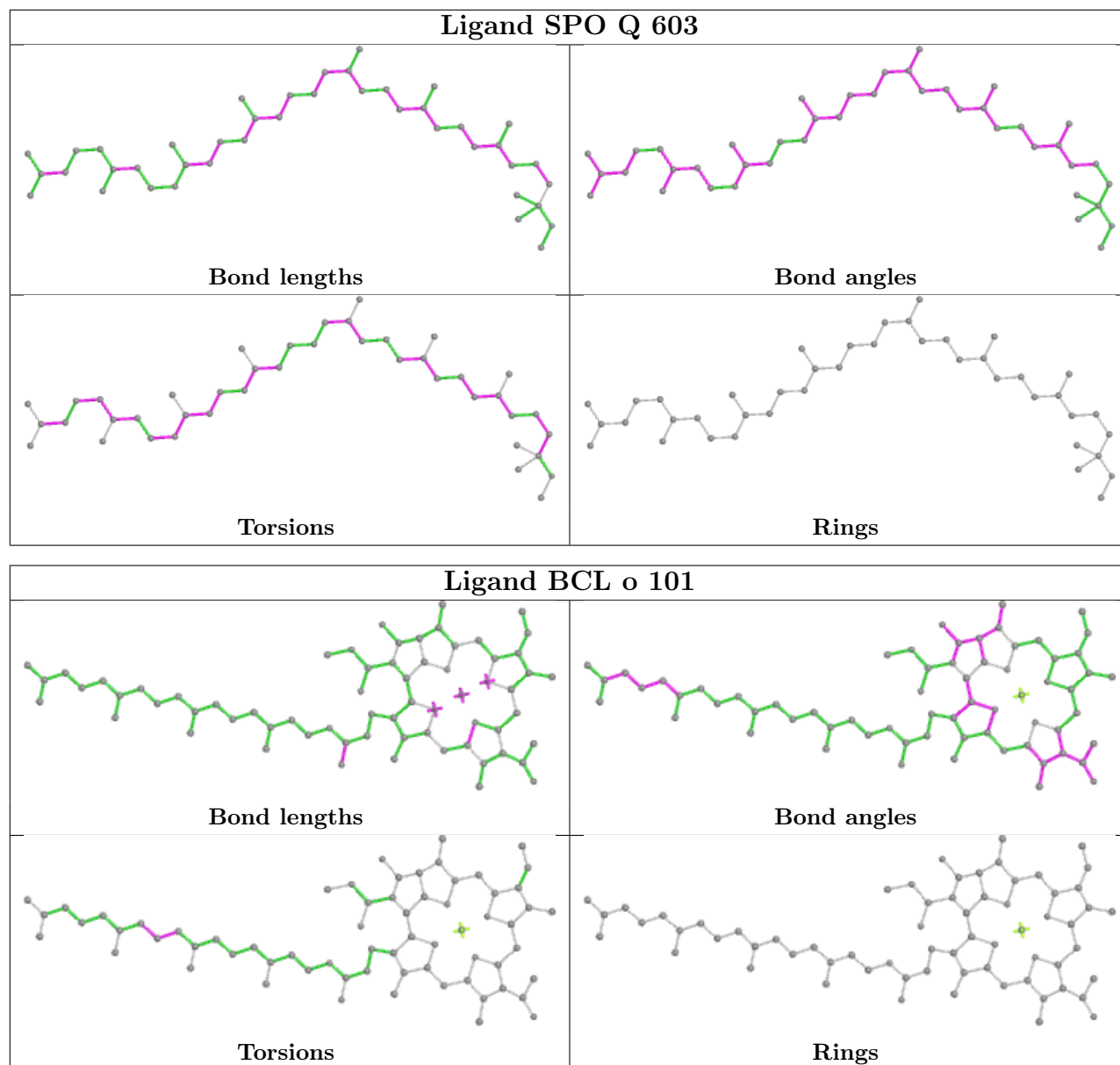


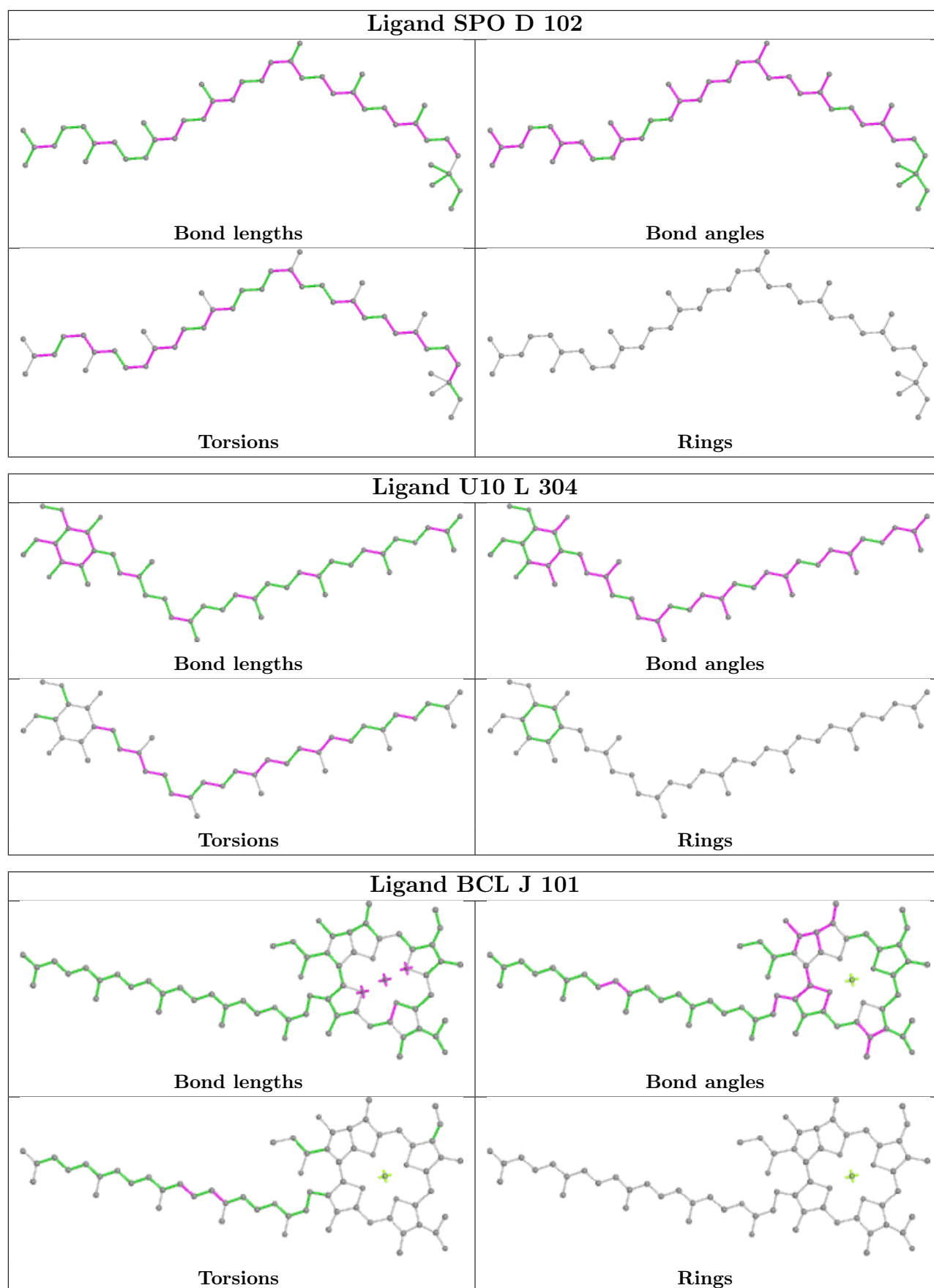


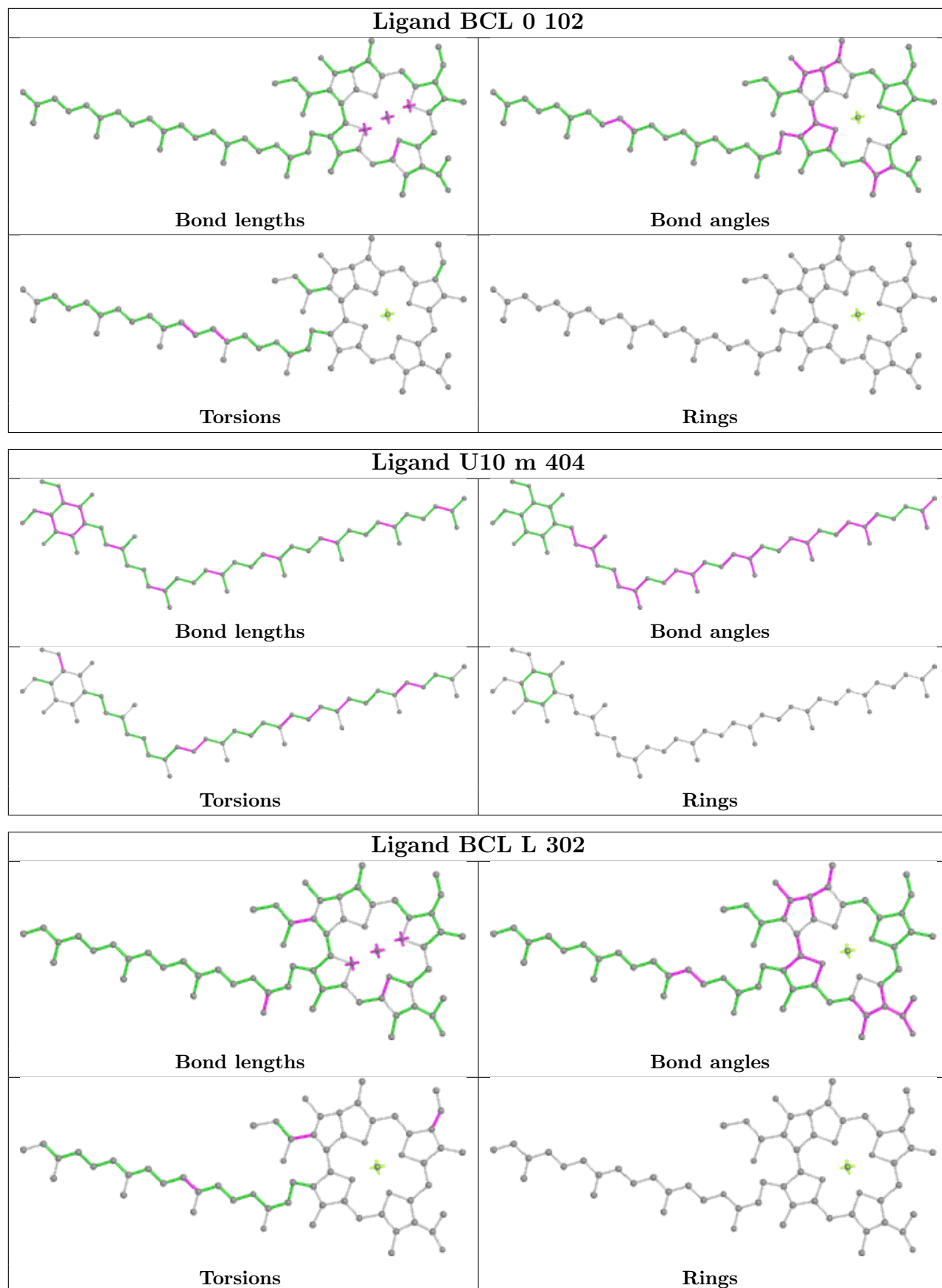


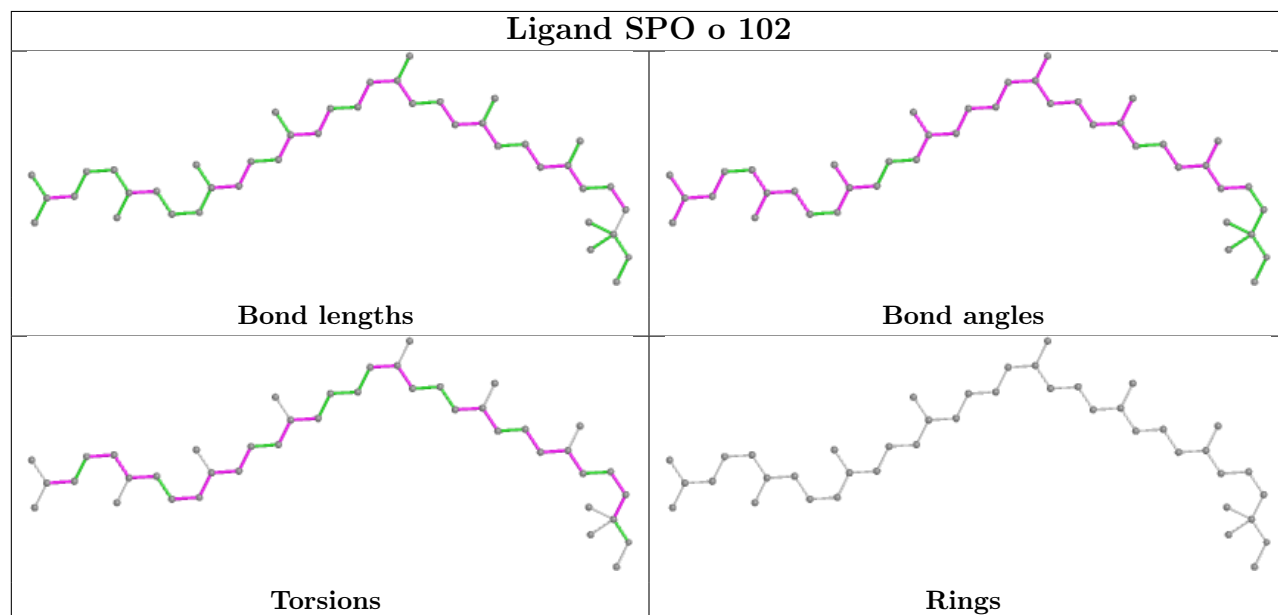
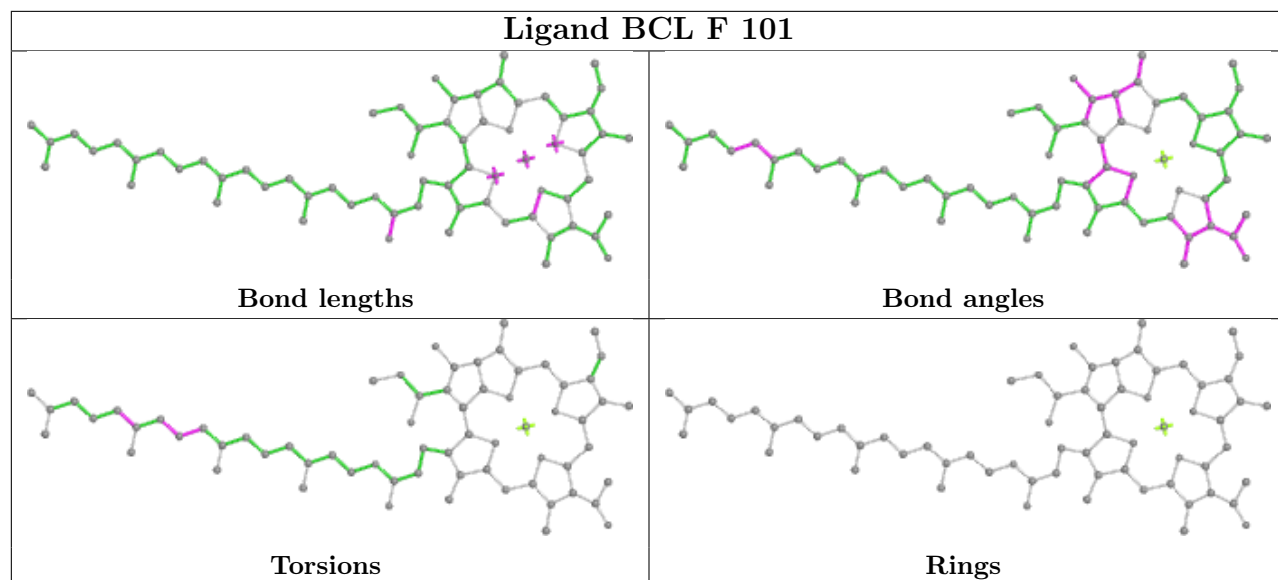


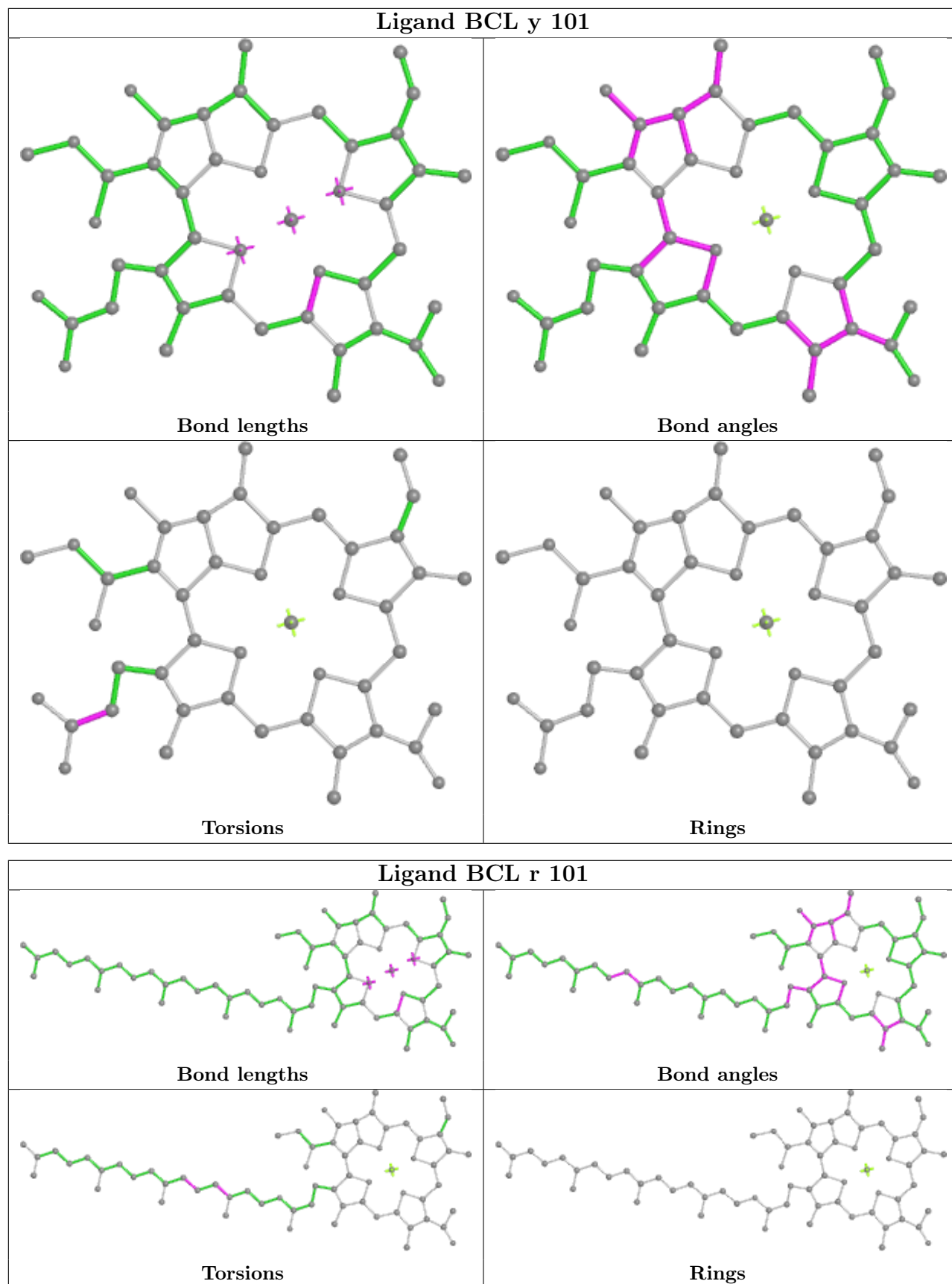


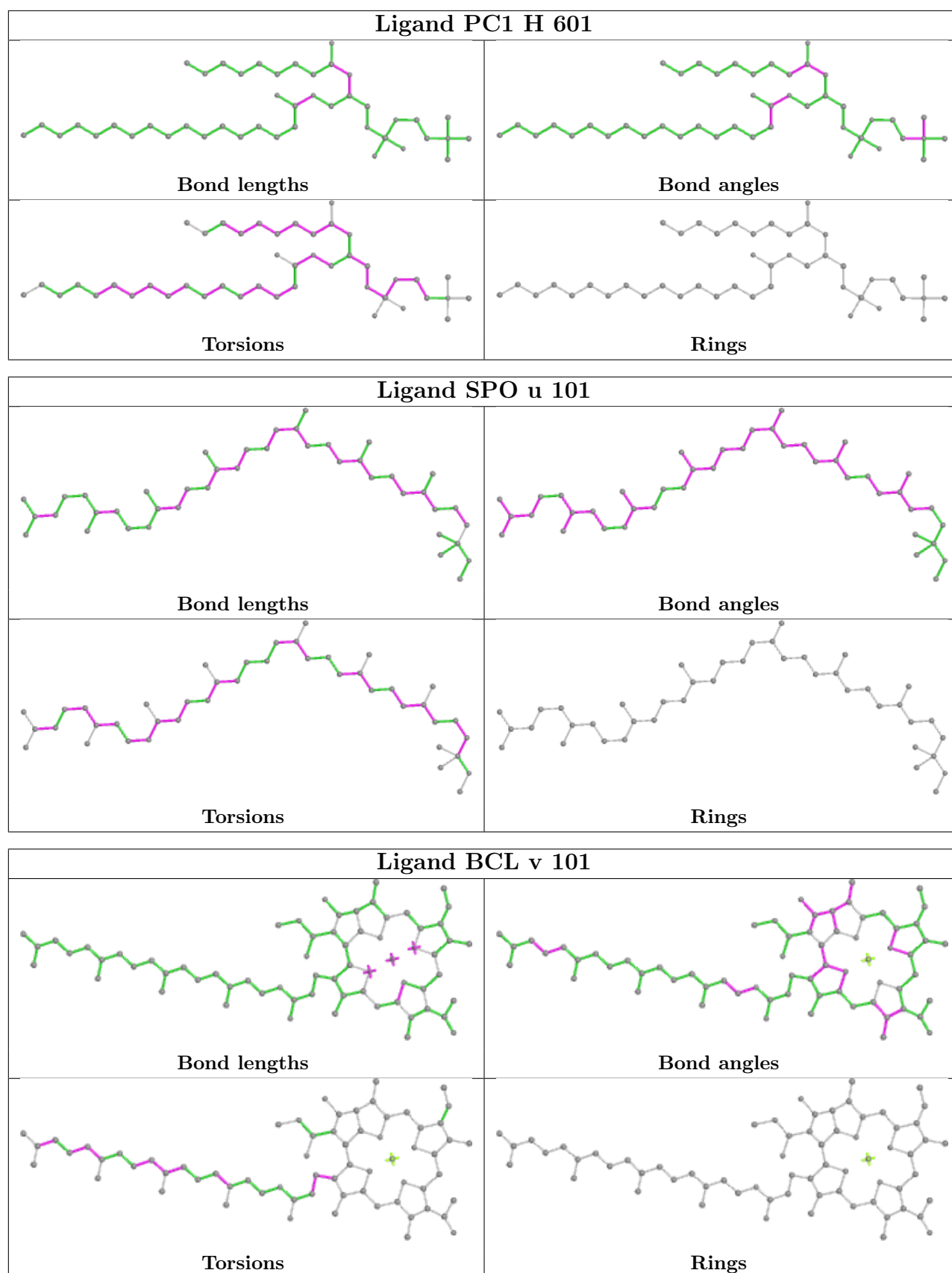


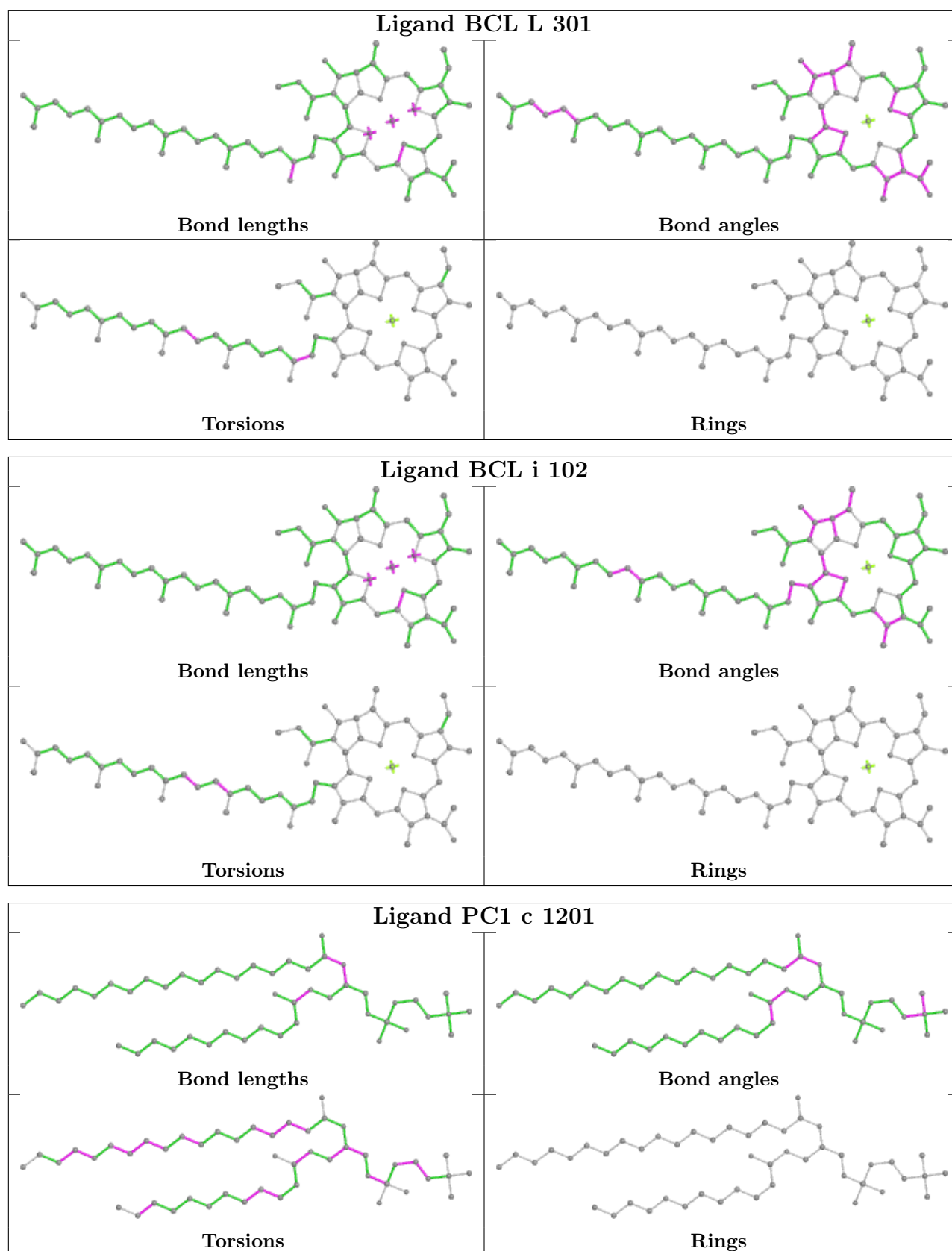


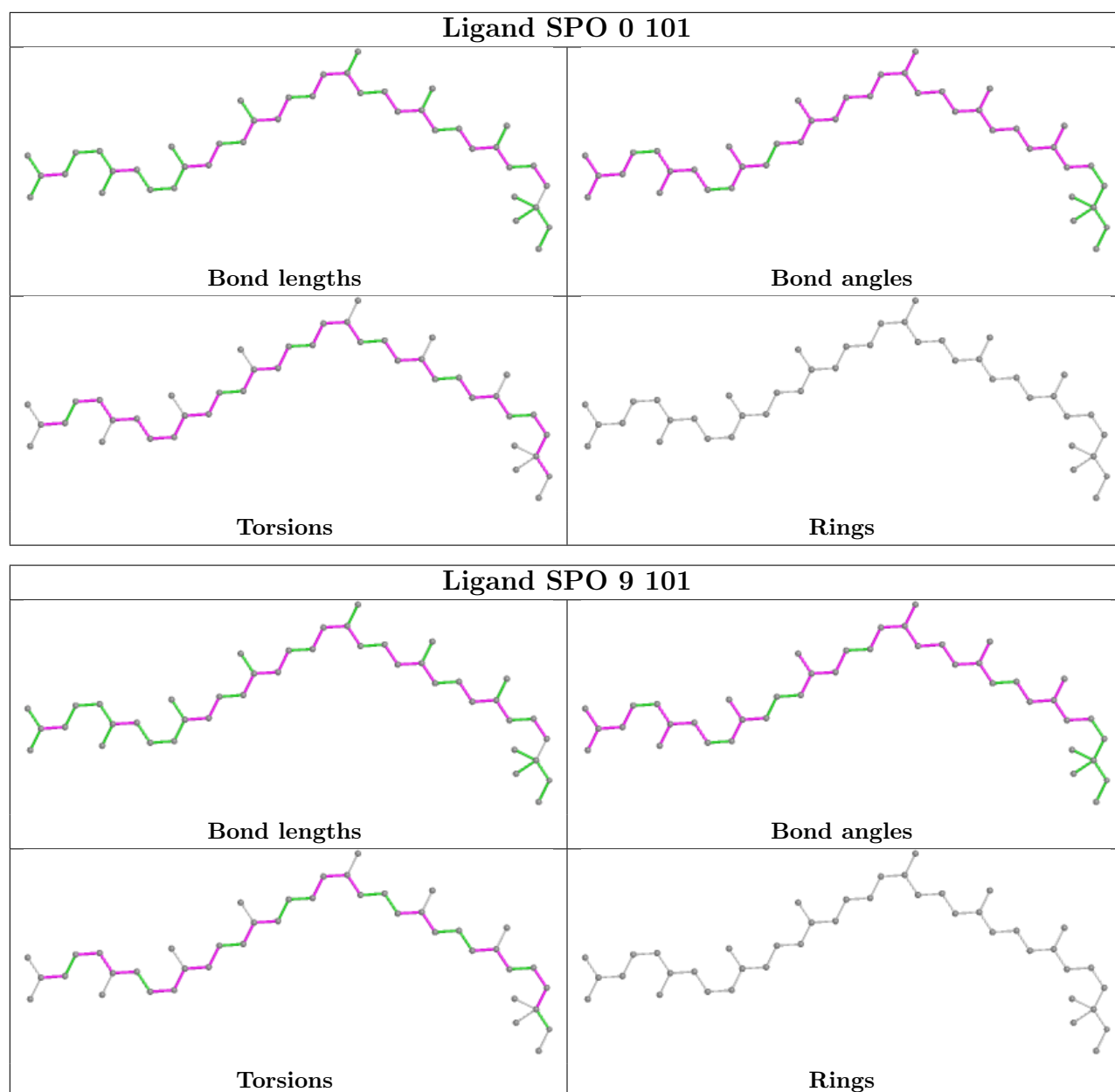


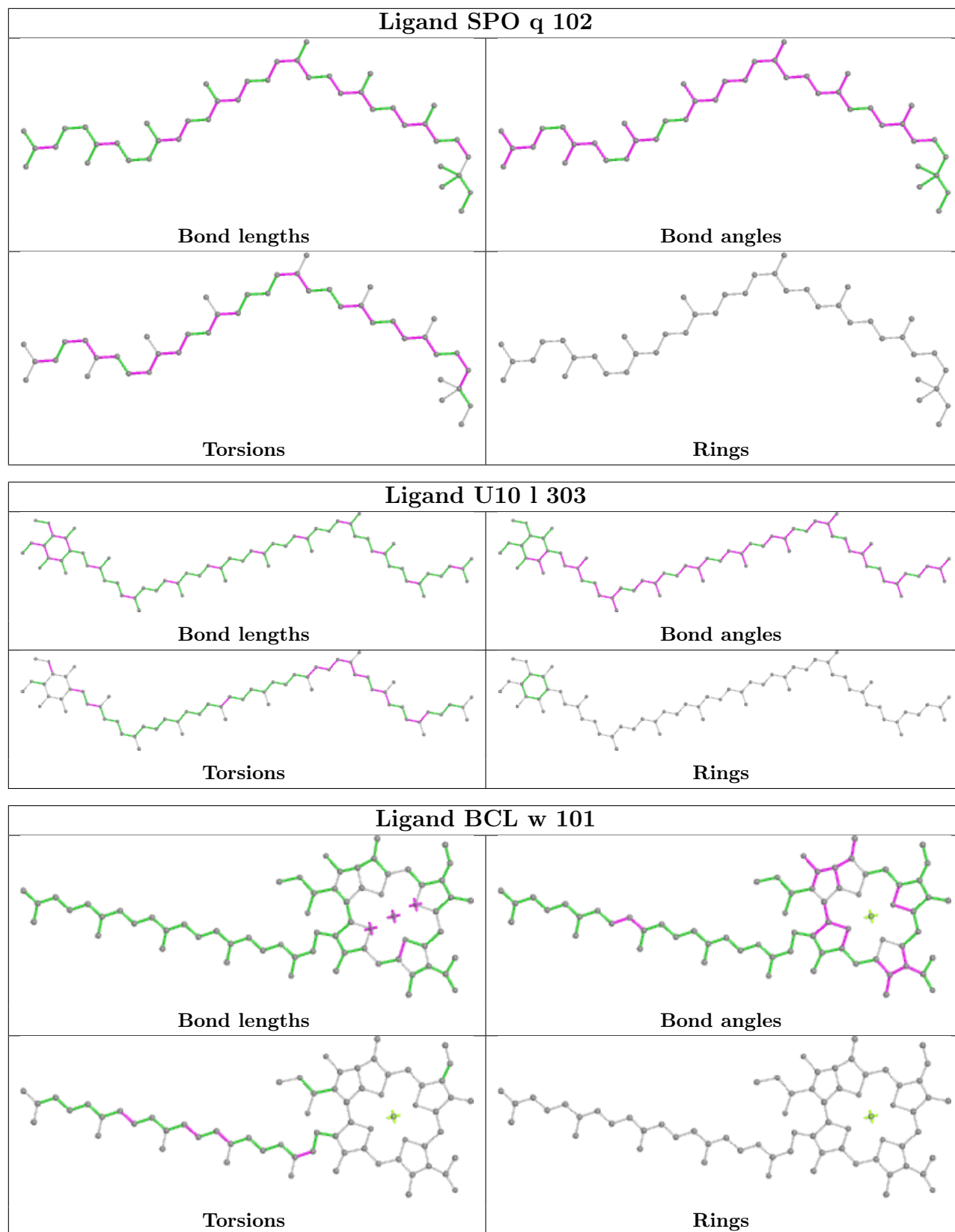


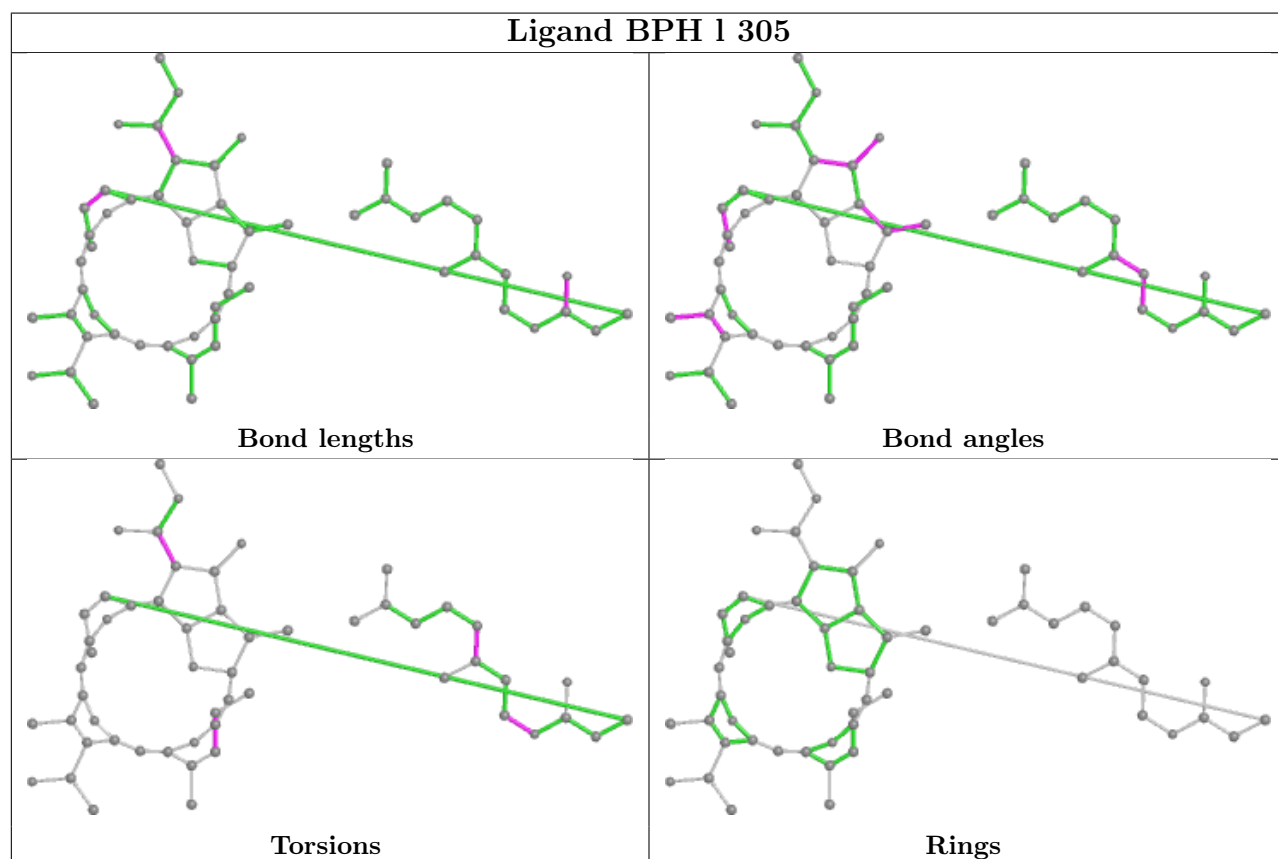
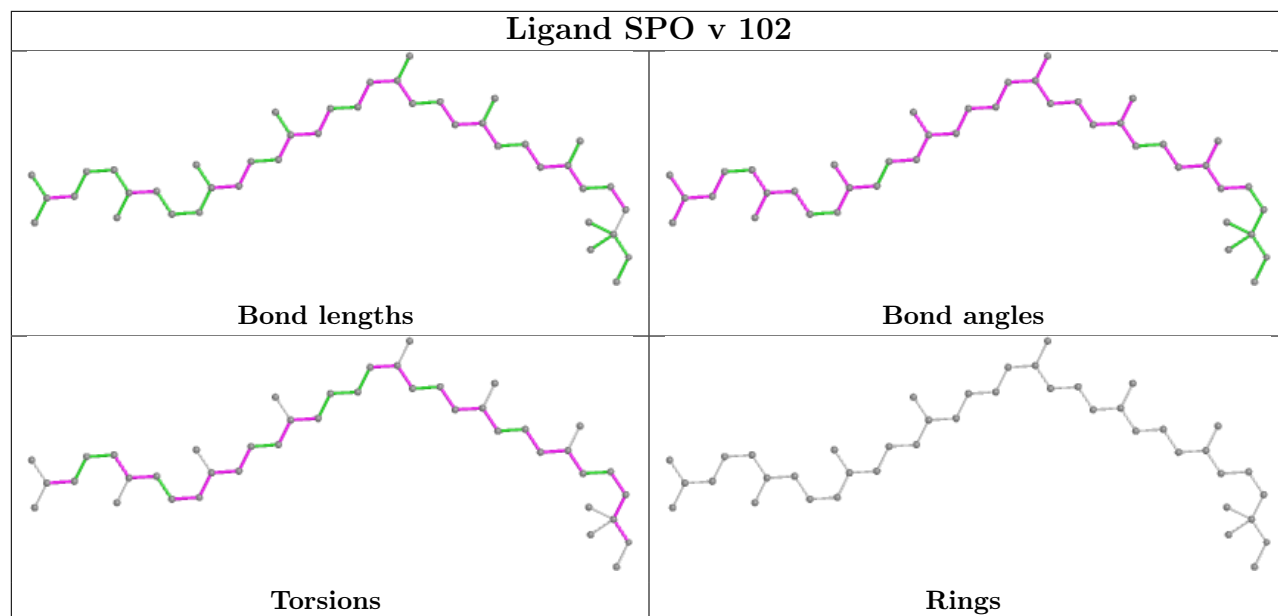


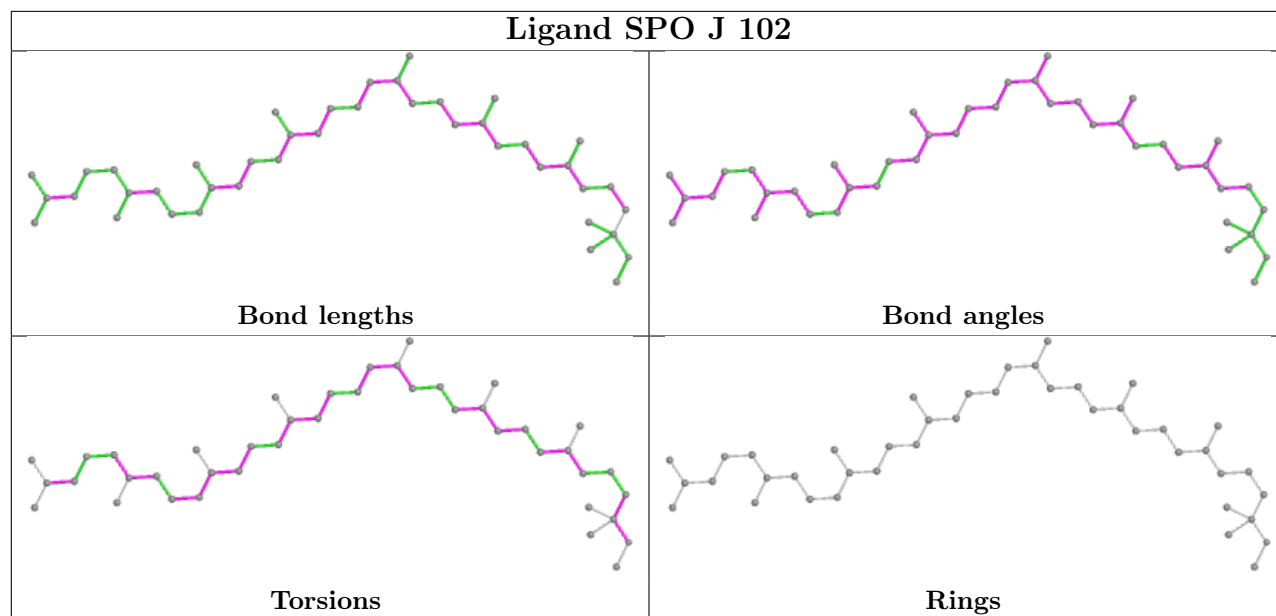












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

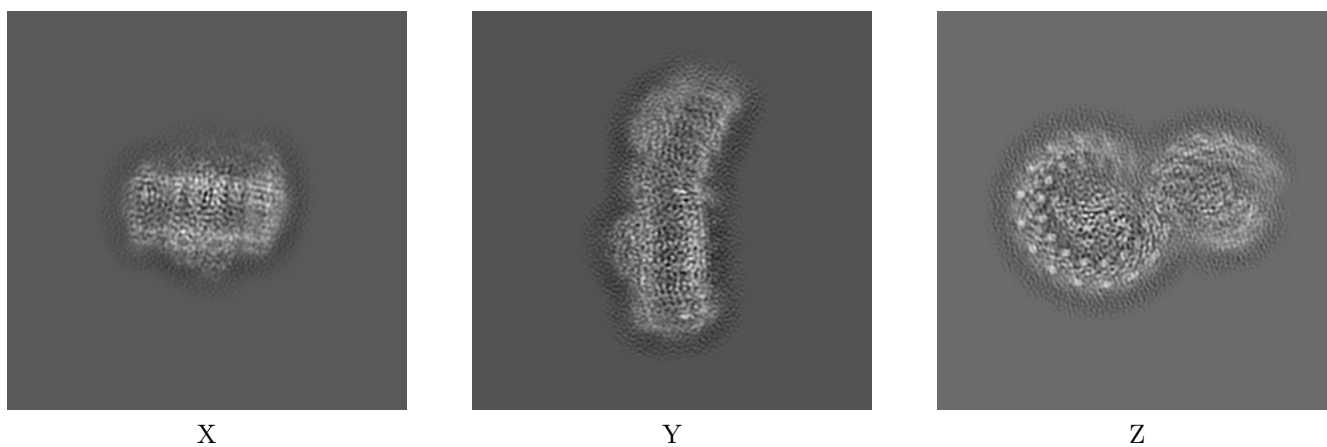
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31875. 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](#)

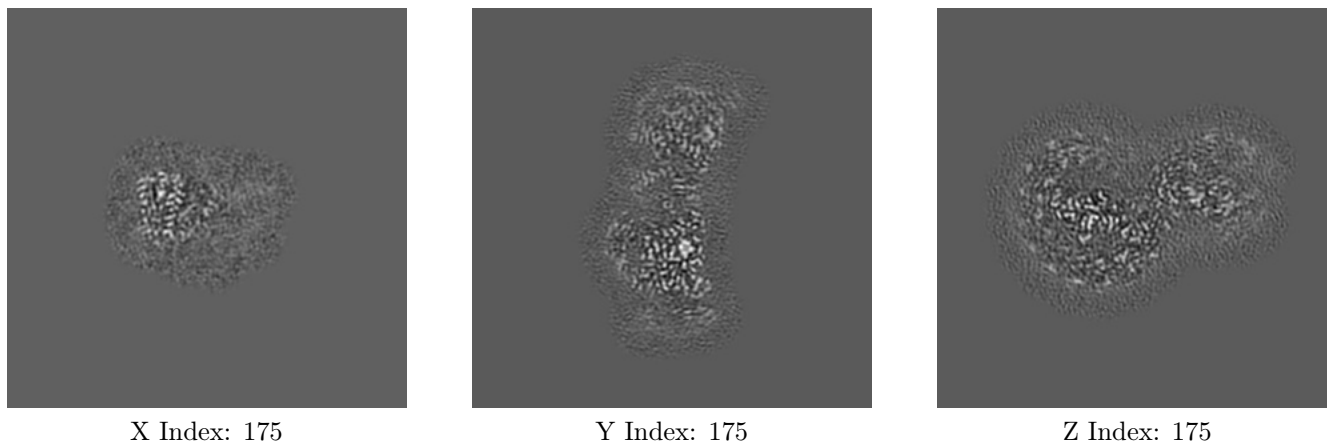
6.1.1 Primary map



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

6.2 Central slices [i](#)

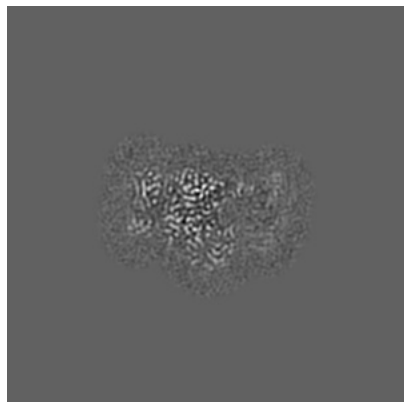
6.2.1 Primary map



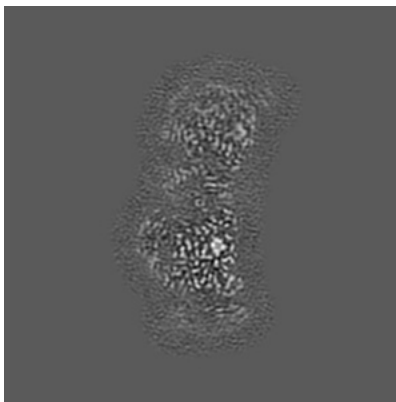
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

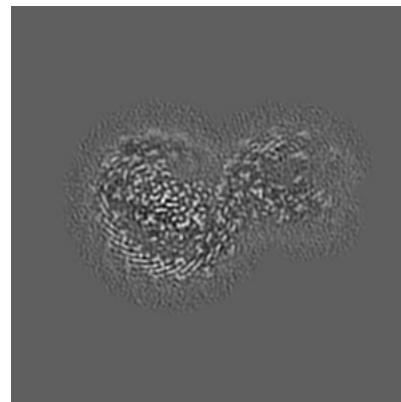
6.3.1 Primary map



X Index: 132



Y Index: 175



Z Index: 190

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

6.4 Orthogonal surface views [i](#)

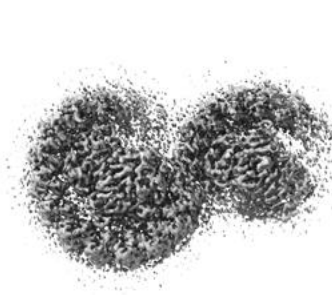
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0183. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

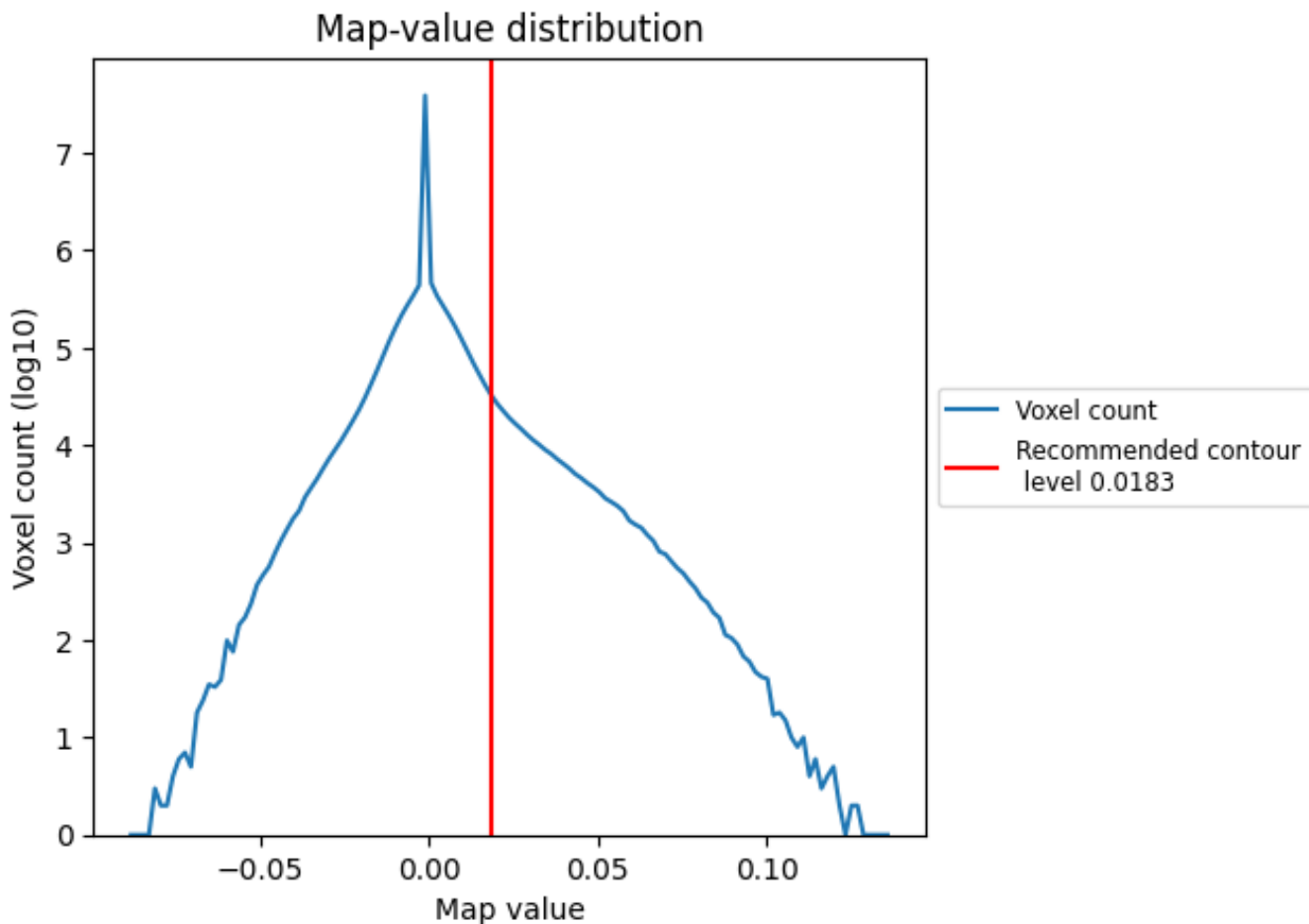
6.5 Mask visualisation

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

7 Map analysis [i](#)

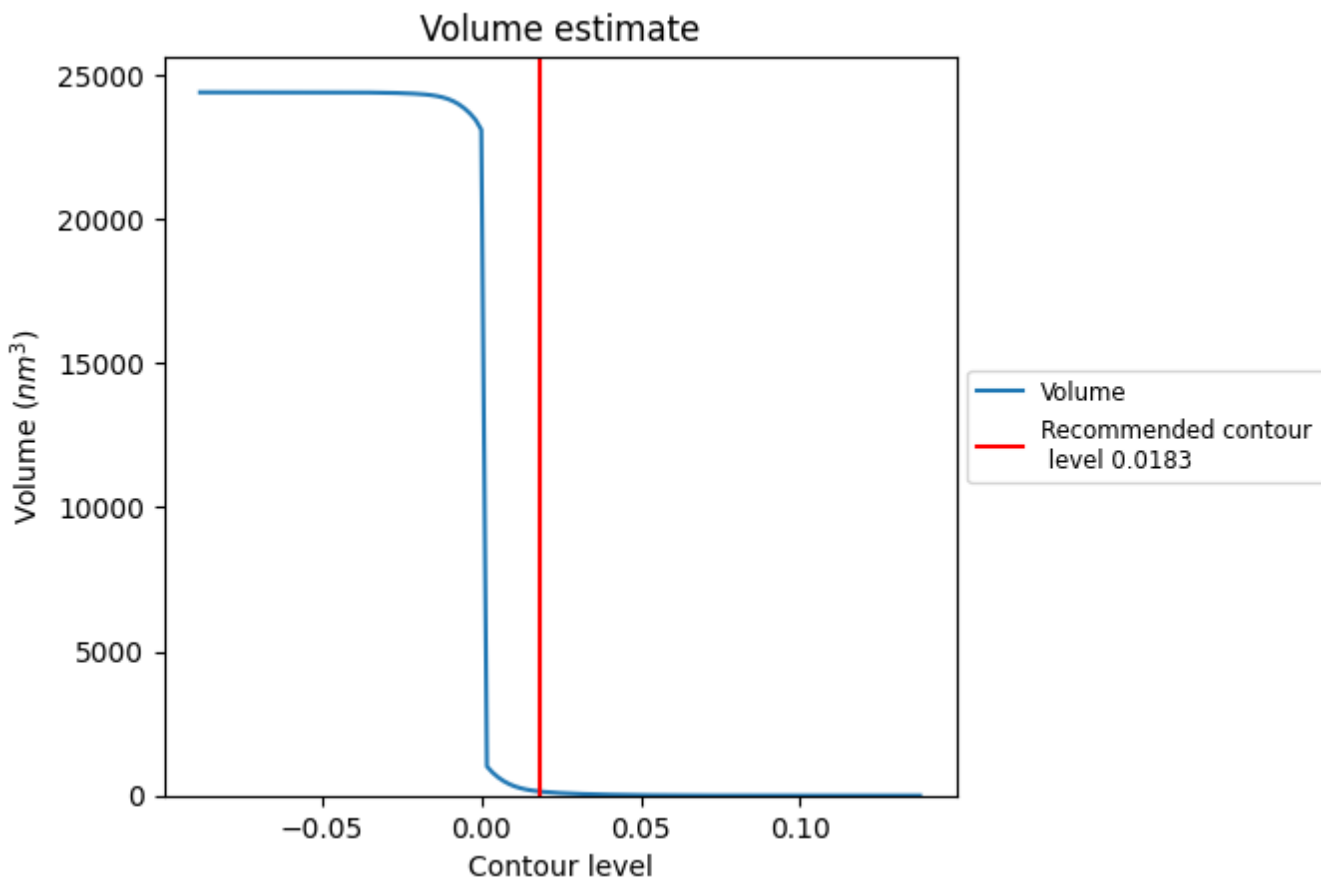
This section contains the results of statistical analysis of the map.

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.

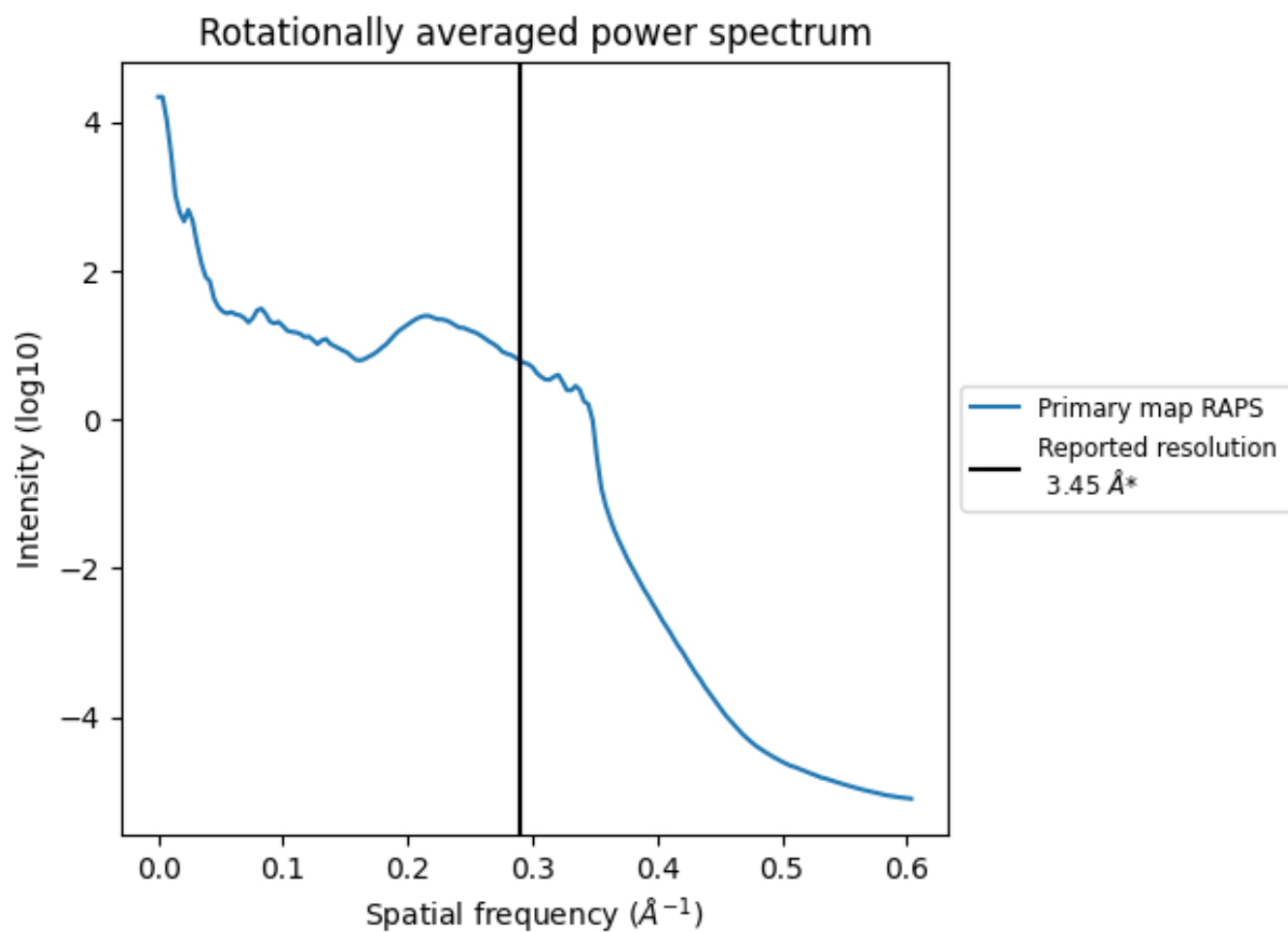
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 142 nm^3 ; this corresponds to an approximate mass of 128 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](#)

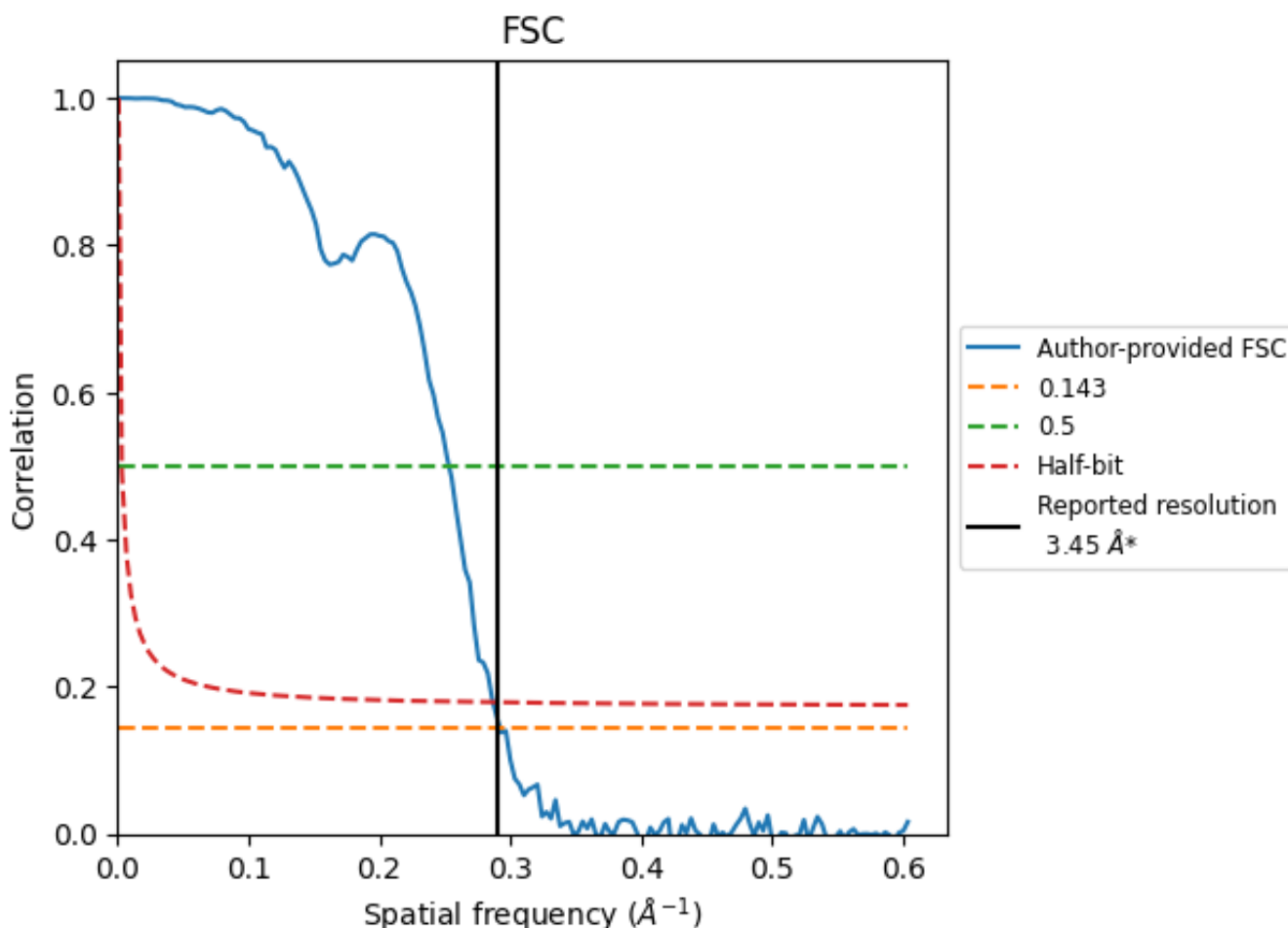


*Reported resolution corresponds to spatial frequency of 0.290\AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.290 Å⁻¹

8.2 Resolution estimates [i](#)

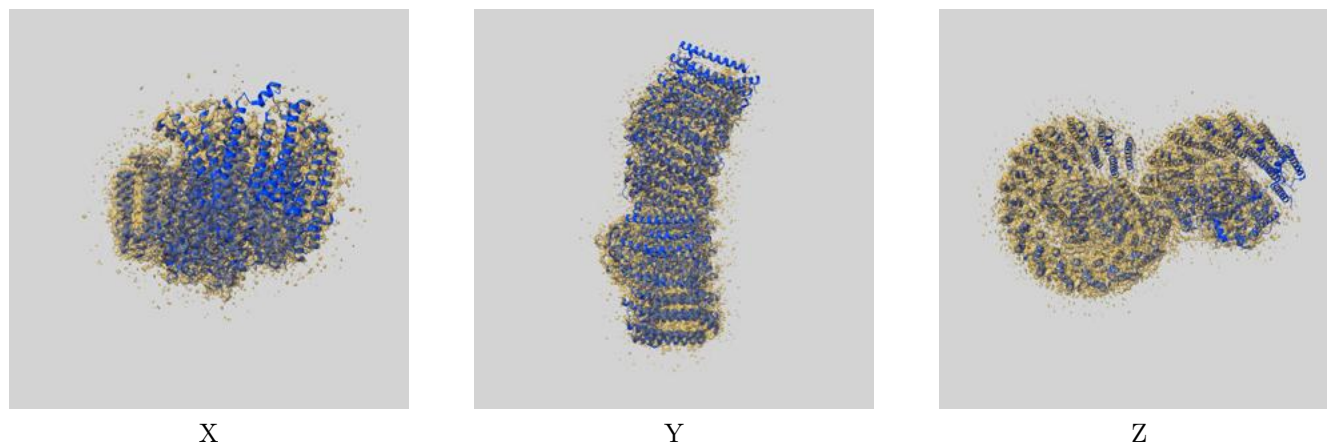
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.45	-	-
Author-provided FSC curve	3.42	3.95	3.49
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

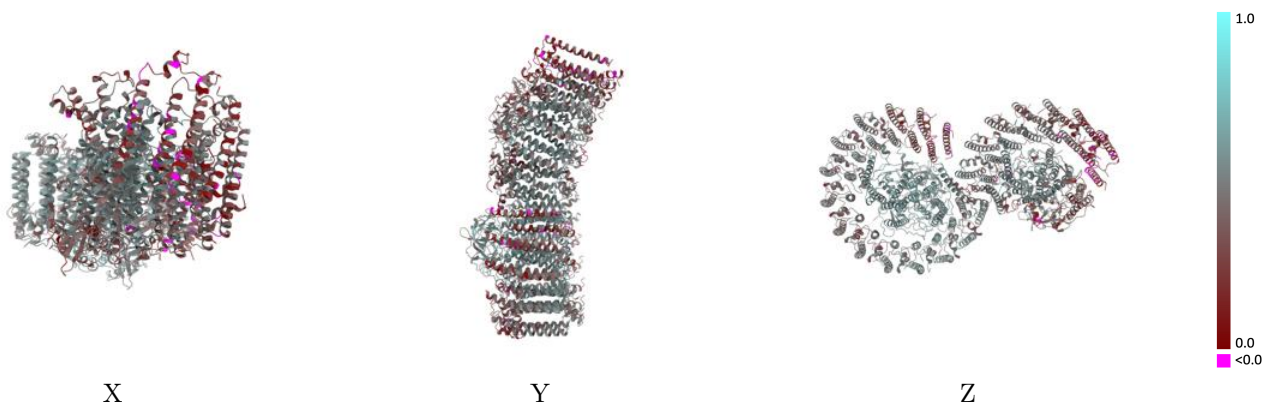
This section contains information regarding the fit between EMDB map EMD-31875 and PDB model 7VB9. Per-residue inclusion information can be found in section 3 on page 18.

9.1 Map-model overlay [i](#)



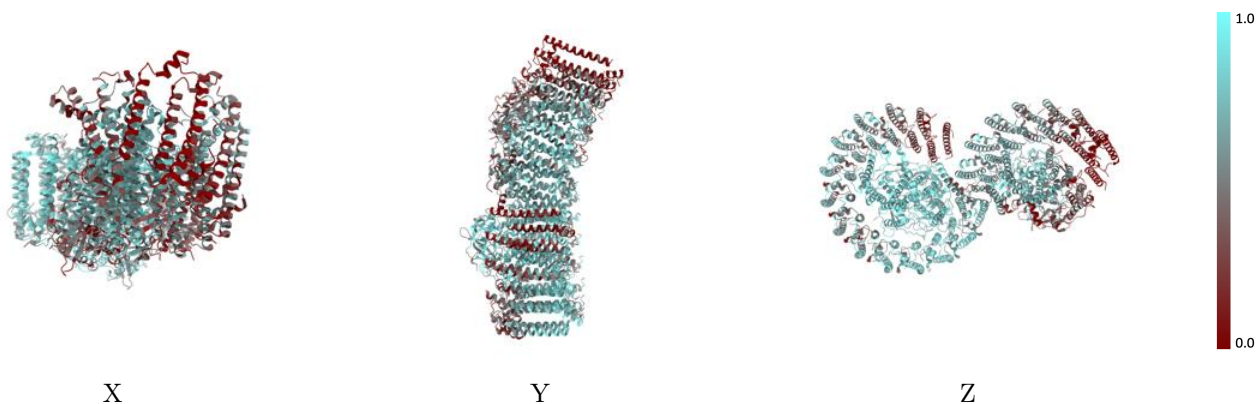
The images above show the 3D surface view of the map at the recommended contour level 0.0183 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



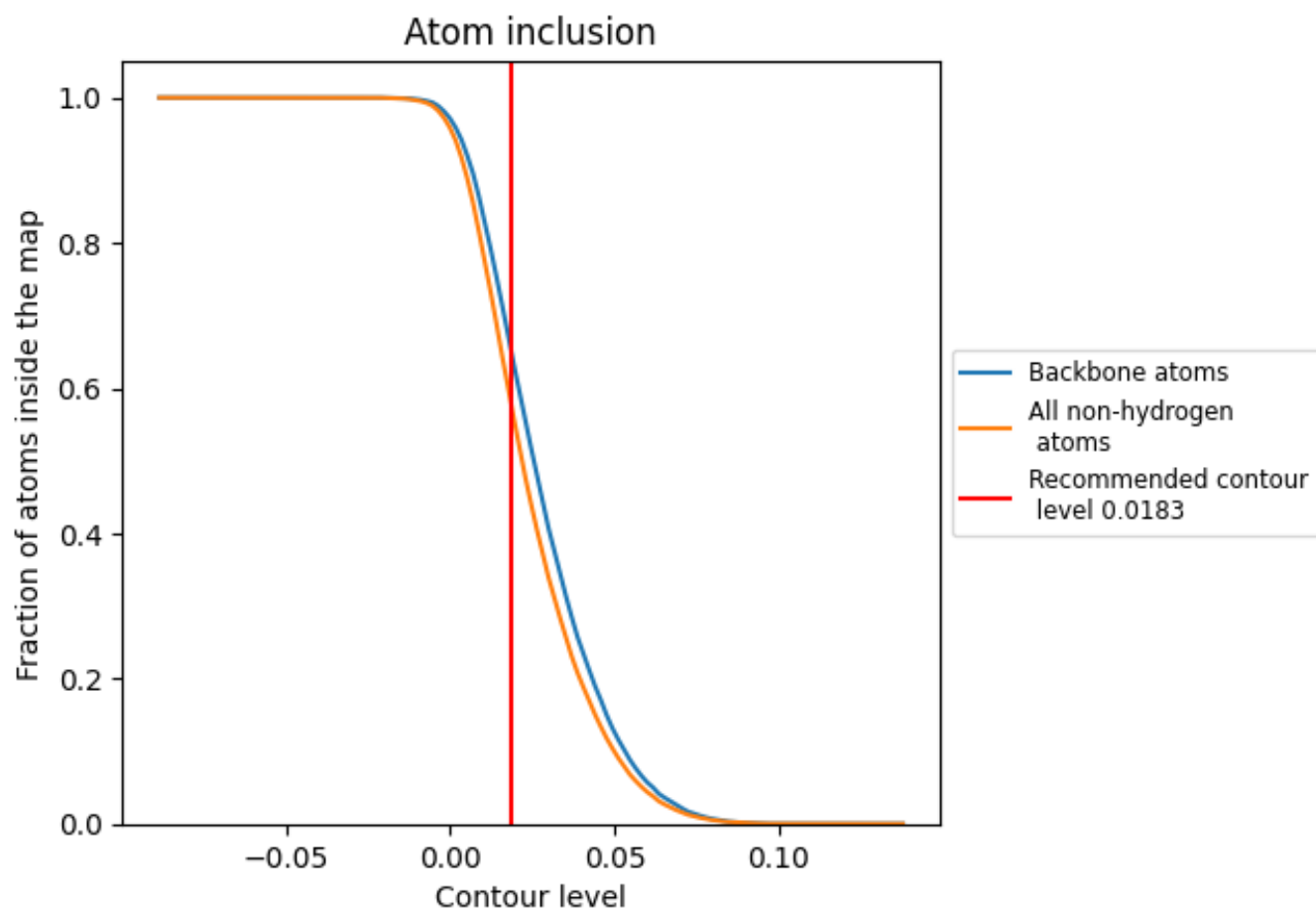
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0183).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 58% 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 (0.0183) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5825	 0.4560
0	 0.5956	 0.4550
4	 0.0753	 0.1650
5	 0.0984	 0.2140
6	 0.6432	 0.3960
7	 0.5964	 0.4010
8	 0.6174	 0.4820
9	 0.6763	 0.4980
A	 0.5505	 0.4550
B	 0.5690	 0.4450
C	 0.5148	 0.4220
D	 0.5420	 0.4370
E	 0.4922	 0.4190
F	 0.3881	 0.3730
G	 0.3481	 0.3640
H	 0.4324	 0.4160
I	 0.3024	 0.3300
J	 0.2192	 0.2690
K	 0.1133	 0.2440
L	 0.6679	 0.5110
M	 0.5243	 0.4540
N	 0.0280	 0.1940
O	 0.0208	 0.1590
Q	 0.7633	 0.5250
a	 0.7821	 0.5420
aa	 0.7275	 0.4960
ab	 0.7692	 0.5280
b	 0.7545	 0.5280
c	 0.5920	 0.4700
d	 0.7508	 0.5110
e	 0.7159	 0.5220
f	 0.6807	 0.4880
g	 0.6593	 0.4670
h	 0.7217	 0.5370
i	 0.5754	 0.4520



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Chain	Atom inclusion	Q-score
j	 0.5403	 0.4230
k	 0.5455	 0.4220
l	 0.8527	 0.5950
m	 0.8446	 0.5820
n	 0.5230	 0.4120
o	 0.5474	 0.4540
p	 0.4815	 0.4110
q	 0.5787	 0.4560
r	 0.5802	 0.4210
s	 0.5967	 0.4470
t	 0.5581	 0.4390
u	 0.5226	 0.3980
v	 0.5333	 0.4340
w	 0.5090	 0.4180
x	 0.3401	 0.3060
y	 0.2819	 0.2910
z	 0.1614	 0.2340