



Full wwPDB EM Validation Report ⓘ

Apr 15, 2026 – 02:51 AM UTC

PDB ID : 9LTS / pdb_00009lts
EMDB ID : EMD-63379
Title : Cryo-EM structure of the Dinoroseobacter shibae RC-LH1 supercomplex
Authors : Liu, Z.K.; Wang, P.; Liu, L.N.
Deposited on : 2025-02-06
Resolution : 2.49 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

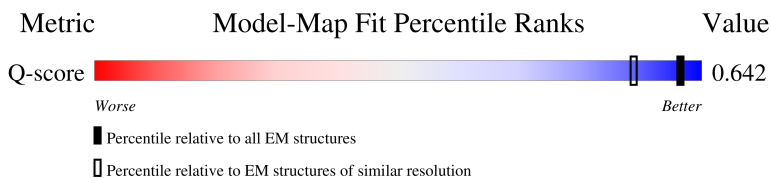
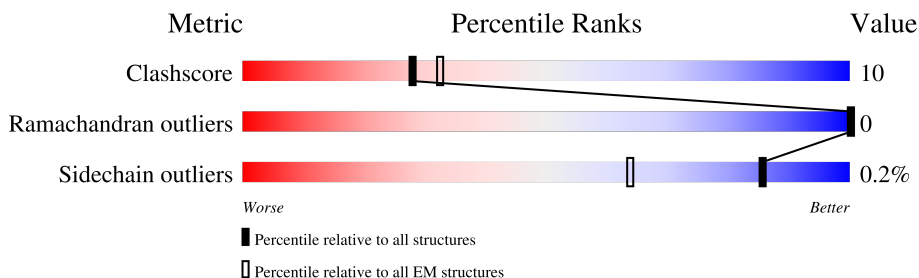
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.49 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



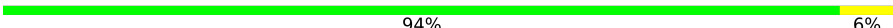
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6237 (2.00 - 2.99)

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	A	76	 76% 21%
2	1	51	 94% 6%
2	3	51	 86% 14%
2	5	51	 86% 14%

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Mol	Chain	Length	Quality of chain
2	7	51	 86% 14%
2	9	51	 90% 10%
2	a	51	 92% 8%
2	c	51	 90% 10%
2	e	51	 84% 16%
2	g	51	 94% 6%
2	i	51	 80% 20%
2	k	51	 82% 18%
2	m	51	 94% 6%
2	o	51	 80% 18%
2	q	51	 84% 16%
2	s	51	 82% 18%
2	u	51	 84% 16%
2	w	51	 92% 8%
3	0	44	 91% 9%
3	2	44	 80% 20%
3	4	44	 86% 14%
3	6	44	 84% 16%
3	8	44	 82% 18%
3	b	44	 80% 20%
3	d	44	 89% 11%
3	f	44	 84% 16%
3	h	44	 70% 27%
3	j	44	 86% 14%
3	l	44	 91% 9%

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Mol	Chain	Length	Quality of chain
3	n	44	
3	p	44	
3	r	44	
3	t	44	
3	v	44	
3	x	44	
4	C	357	
5	H	255	
6	L	273	
7	M	325	

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
10	SPN	1	102	-	X	-	-
10	SPN	1	103	-	X	-	-
10	SPN	1	104	-	X	-	-
10	SPN	1	105	-	X	-	-
10	SPN	3	102	-	X	-	-
10	SPN	5	102	-	X	-	-
10	SPN	5	103	-	X	-	-
10	SPN	7	102	-	X	-	-
10	SPN	7	103	-	X	-	-
10	SPN	9	103	-	X	-	-
10	SPN	a	102	-	X	-	-
10	SPN	a	103	-	X	-	-
10	SPN	c	102	-	X	-	-
10	SPN	c	103	-	X	-	-
10	SPN	e	102	-	X	-	-
10	SPN	h	102	-	X	-	-
10	SPN	i	102	-	X	-	-
10	SPN	j	102	-	X	-	-
10	SPN	k	102	-	X	-	-
10	SPN	m	102	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	SPN	n	102	-	X	-	-
10	SPN	p	102	-	X	-	-
10	SPN	p	103	-	X	-	-
10	SPN	q	102	-	X	-	-
10	SPN	r	102	-	X	-	-
10	SPN	s	102	-	X	-	-
10	SPN	u	102	-	X	-	-
10	SPN	w	102	-	X	-	-

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 28463 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 Protein LRC.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	76	Total	C	N	O	S	0	0
			552	353	95	96	8		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLU	deletion	UNP A8LIU2
A	?	-	THR	deletion	UNP A8LIU2
A	?	-	GLY	deletion	UNP A8LIU2
A	?	-	ARG	deletion	UNP A8LIU2
A	?	-	PRO	deletion	UNP A8LIU2

- Molecule 2 is a protein called Antenna pigment protein alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	51	Total	C	N	O	S	0	0
			425	291	68	64	2		
2	5	51	Total	C	N	O	S	0	0
			425	291	68	64	2		
2	3	51	Total	C	N	O	S	0	0
			425	291	68	64	2		
2	w	51	Total	C	N	O	S	0	0
			425	291	68	64	2		
2	u	51	Total	C	N	O	S	0	0
			425	291	68	64	2		
2	s	51	Total	C	N	O	S	0	0
			425	291	68	64	2		
2	q	51	Total	C	N	O	S	0	0
			425	291	68	64	2		
2	o	51	Total	C	N	O	S	0	0
			425	291	68	64	2		
2	m	51	Total	C	N	O	S	0	0
			425	291	68	64	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	k	51	Total	C	N	O	S	0	0
			425	291	68	64	2		
2	g	51	Total	C	N	O	S	0	0
			425	291	68	64	2		
2	e	51	Total	C	N	O	S	0	0
			425	291	68	64	2		
2	c	51	Total	C	N	O	S	0	0
			425	291	68	64	2		
2	a	51	Total	C	N	O	S	0	0
			425	291	68	64	2		
2	i	51	Total	C	N	O	S	0	0
			425	291	68	64	2		
2	7	51	Total	C	N	O	S	0	0
			425	291	68	64	2		
2	9	51	Total	C	N	O	S	0	0
			425	291	68	64	2		

- Molecule 3 is a protein called Antenna pigment protein beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	44	Total	C	N	O	S	0	0
			358	239	56	62	1		
3	6	44	Total	C	N	O	S	0	0
			358	239	56	62	1		
3	4	44	Total	C	N	O	S	0	0
			358	239	56	62	1		
3	x	44	Total	C	N	O	S	0	0
			358	239	56	62	1		
3	v	44	Total	C	N	O	S	0	0
			358	239	56	62	1		
3	t	44	Total	C	N	O	S	0	0
			358	239	56	62	1		
3	r	44	Total	C	N	O	S	0	0
			358	239	56	62	1		
3	p	44	Total	C	N	O	S	0	0
			358	239	56	62	1		
3	n	44	Total	C	N	O	S	0	0
			358	239	56	62	1		
3	l	44	Total	C	N	O	S	0	0
			358	239	56	62	1		
3	h	44	Total	C	N	O	S	0	0
			358	239	56	62	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	f	44	Total	C	N	O	S	0	0
			358	239	56	62	1		
3	d	44	Total	C	N	O	S	0	0
			358	239	56	62	1		
3	b	44	Total	C	N	O	S	0	0
			358	239	56	62	1		
3	j	44	Total	C	N	O	S	0	0
			358	239	56	62	1		
3	8	44	Total	C	N	O	S	0	0
			358	239	56	62	1		
3	0	44	Total	C	N	O	S	0	0
			358	239	56	62	1		

- Molecule 4 is a protein called Photosynthetic reaction center cytochrome c subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	357	Total	C	N	O	S	0	0
			2785	1761	461	548	15		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	40	MET	TRP	conflict	UNP A8LQ18

- Molecule 5 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	255	Total	C	N	O	S	0	0
			2015	1279	345	383	8		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	44	GLU	ASP	conflict	UNP A8LQ33
H	181	LEU	ILE	conflict	UNP A8LQ33
H	197	GLN	GLU	conflict	UNP A8LQ33

- Molecule 6 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	273	Total	C	N	O	S	0	0
			2172	1466	345	352	9		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	176	LEU	ILE	conflict	UNP A8LQ16

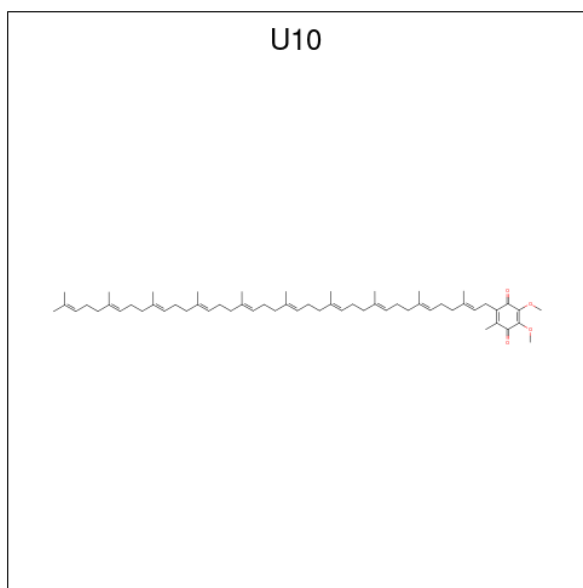
- Molecule 7 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	325	Total	C	N	O	S	0	0
			2634	1753	421	452	8		

There is a discrepancy between the modelled and reference sequences:

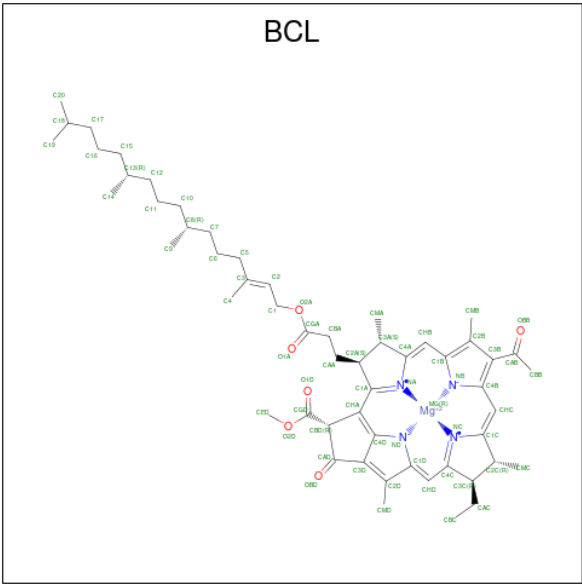
Chain	Residue	Modelled	Actual	Comment	Reference
M	134	THR	SER	conflict	UNP A8LQ17

- Molecule 8 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
8	A	1	Total	C	O	0
			43	39	4	
8	L	1	Total	C	O	0
			38	34	4	
8	L	1	Total	C	O	0
			38	34	4	
8	M	1	Total	C	O	0
			63	59	4	

- Molecule 9 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
9	1	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	2	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	5	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	6	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	3	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	4	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	w	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	x	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	u	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	v	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	s	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	t	1	Total 66	C 55	Mg 1	N 4	O 6	0

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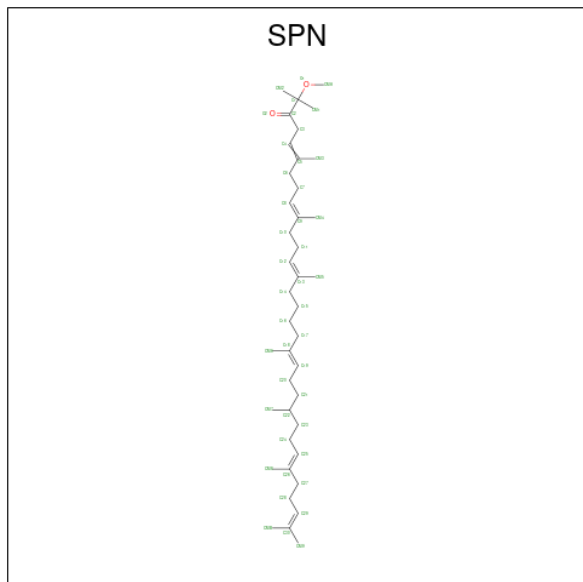
Mol	Chain	Residues	Atoms					AltConf
9	q	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	r	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	o	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	p	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	m	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	k	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	l	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	g	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	h	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	e	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	f	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	c	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	d	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	a	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	b	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	i	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	j	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	7	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	8	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	L	1	Total 66	C 55	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
9	L	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	M	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	M	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	9	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	0	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 10 is SPEROIDENONE (CCD ID: SPN) (formula: $C_{41}H_{70}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
10	1	1	Total	C	O	0
			43	41	2	
10	1	1	Total	C	O	0
			43	41	2	
10	1	1	Total	C	O	0
			43	41	2	
10	1	1	Total	C	O	0
			43	41	2	
10	5	1	Total	C	O	0
			43	41	2	
10	5	1	Total	C	O	0
			43	41	2	

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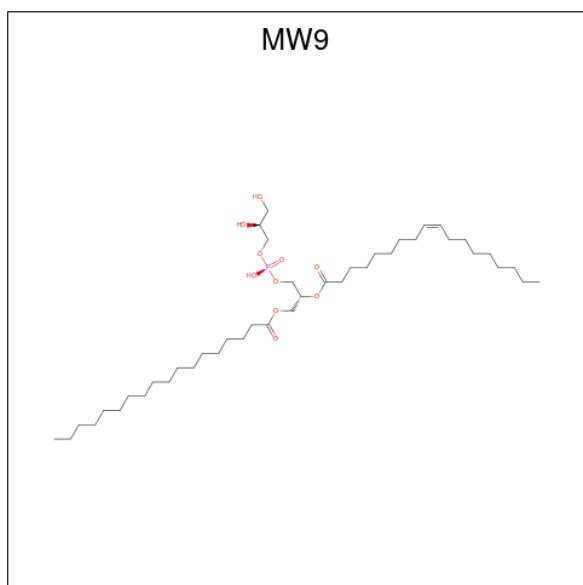
Mol	Chain	Residues	Atoms			AltConf
10	3	1	Total 43	C 41	O 2	0
10	w	1	Total 43	C 41	O 2	0
10	u	1	Total 43	C 41	O 2	0
10	v	1	Total 43	C 41	O 2	0
10	s	1	Total 43	C 41	O 2	0
10	t	1	Total 43	C 41	O 2	0
10	q	1	Total 43	C 41	O 2	0
10	r	1	Total 43	C 41	O 2	0
10	p	1	Total 43	C 41	O 2	0
10	p	1	Total 43	C 41	O 2	0
10	m	1	Total 43	C 41	O 2	0
10	n	1	Total 43	C 41	O 2	0
10	k	1	Total 43	C 41	O 2	0
10	l	1	Total 43	C 41	O 2	0
10	h	1	Total 43	C 41	O 2	0
10	h	1	Total 43	C 41	O 2	0
10	e	1	Total 43	C 41	O 2	0
10	f	1	Total 43	C 41	O 2	0
10	c	1	Total 43	C 41	O 2	0
10	c	1	Total 43	C 41	O 2	0
10	a	1	Total 43	C 41	O 2	0

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Mol	Chain	Residues	Atoms			AltConf
10	a	1	Total	C	O	0
			43	41	2	
10	i	1	Total	C	O	0
			43	41	2	
10	j	1	Total	C	O	0
			43	41	2	
10	7	1	Total	C	O	0
			43	41	2	
10	7	1	Total	C	O	0
			43	41	2	
10	M	1	Total	C	O	0
			43	41	2	
10	9	1	Total	C	O	0
			43	41	2	
10	0	1	Total	C	O	0
			43	41	2	

- Molecule 11 is (21R,24R,27S)-24,27,28-trihydroxy-18,24-dioxo-19,23,25-trioxa-24lambda 5-phosphaoctacosan-21-yl (9Z)-octadec-9-enoate (CCD ID: MW9) (formula: $C_{42}H_{81}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



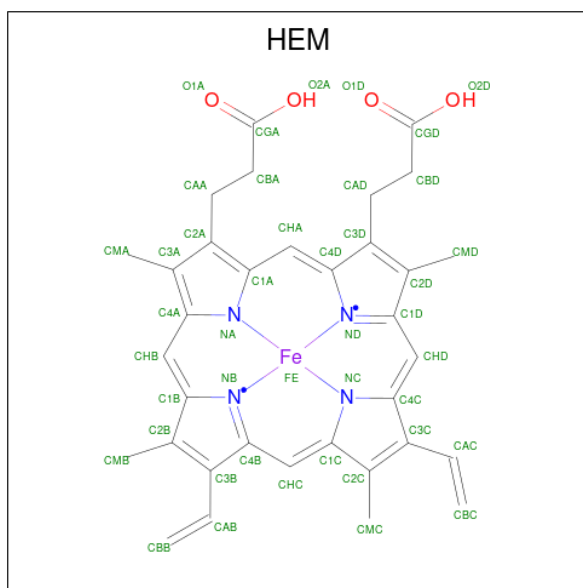
Mol	Chain	Residues	Atoms				AltConf
11	g	1	Total	C	O	P	0
			53	42	10	1	
11	g	1	Total	C	O	P	0
			50	39	10	1	

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Mol	Chain	Residues	Atoms				AltConf
11	H	1	Total	C	O	P	0
			53	42	10	1	
11	H	1	Total	C	O	P	0
			53	42	10	1	
11	H	1	Total	C	O	P	0
			53	42	10	1	
11	H	1	Total	C	O	P	0
			53	42	10	1	
11	M	1	Total	C	O	P	0
			53	42	10	1	
11	M	1	Total	C	O	P	0
			53	42	10	1	
11	9	1	Total	C	O	P	0
			53	42	10	1	

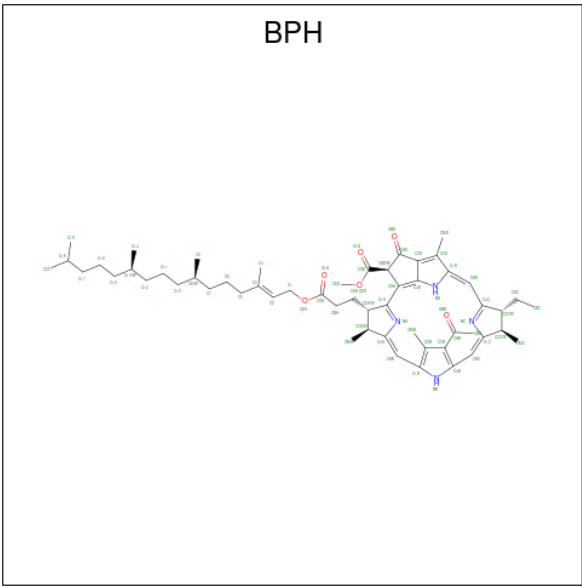
- Molecule 12 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
12	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
12	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
12	C	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 13 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$) (la-

beled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
13	L	1	Total	C	N	O	0
			65	55	4	6	
13	M	1	Total	C	N	O	0
			65	55	4	6	
13	M	1	Total	C	N	O	0
			65	55	4	6	

- Molecule 14 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

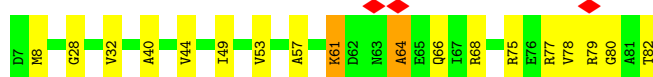
Mol	Chain	Residues	Atoms		AltConf
14	M	1	Total	Fe	0
			1	1	

3 Residue-property plots [i](#)

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

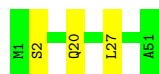
- Molecule 1: Protein LRC

Chain A:  76% 21%



- Molecule 2: Antenna pigment protein alpha chain

Chain 1:  94% 6%



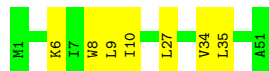
- Molecule 2: Antenna pigment protein alpha chain

Chain 5:  86% 14%

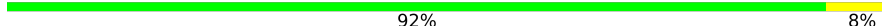


- Molecule 2: Antenna pigment protein alpha chain

Chain 3:  86% 14%



- Molecule 2: Antenna pigment protein alpha chain

Chain w:  92% 8%



- Molecule 2: Antenna pigment protein alpha chain

Chain u:  84% 16%



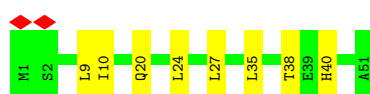
- Molecule 2: Antenna pigment protein alpha chain

Chain s:  82% 18%



- Molecule 2: Antenna pigment protein alpha chain

Chain q:  84% 16%



- Molecule 2: Antenna pigment protein alpha chain

Chain o:  80% 18%



- Molecule 2: Antenna pigment protein alpha chain

Chain m:  94% 6%



- Molecule 2: Antenna pigment protein alpha chain

Chain k:  82% 18%



- Molecule 2: Antenna pigment protein alpha chain

Chain g:  94% 6%



- Molecule 2: Antenna pigment protein alpha chain

Chain e:  84% 16%



- Molecule 2: Antenna pigment protein alpha chain

Chain c:  90% 10%



- Molecule 2: Antenna pigment protein alpha chain

Chain a:  92% 8%



- Molecule 2: Antenna pigment protein alpha chain

Chain i:  80% 20%



- Molecule 2: Antenna pigment protein alpha chain

Chain 7:  86% 14%



- Molecule 2: Antenna pigment protein alpha chain

Chain 9:  90% 10%



- Molecule 3: Antenna pigment protein beta chain

Chain 2:  80% 20%



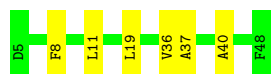
- Molecule 3: Antenna pigment protein beta chain

Chain 6:  84% 16%



- Molecule 3: Antenna pigment protein beta chain

Chain 4:  86% 14%



- Molecule 3: Antenna pigment protein beta chain

Chain x:  91% 9%



- Molecule 3: Antenna pigment protein beta chain

Chain v:  77% 23%



- Molecule 3: Antenna pigment protein beta chain

Chain t:  77% 23%



- Molecule 3: Antenna pigment protein beta chain

Chain r:  7% 82% 18%



- Molecule 3: Antenna pigment protein beta chain

Chain p:  86% 14%



- Molecule 3: Antenna pigment protein beta chain

Chain n:  82% 18%



- Molecule 3: Antenna pigment protein beta chain

Chain l:  91% 9%



- Molecule 3: Antenna pigment protein beta chain

Chain h:  70% 27% .



- Molecule 3: Antenna pigment protein beta chain

Chain f:  84% 16%



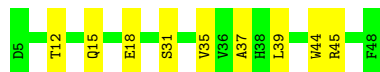
- Molecule 3: Antenna pigment protein beta chain

Chain d:  89% 11%



- Molecule 3: Antenna pigment protein beta chain

Chain b:  80% 20%



- Molecule 3: Antenna pigment protein beta chain

Chain j:  86% 14%



- Molecule 3: Antenna pigment protein beta chain

Chain 8:  82% 18%



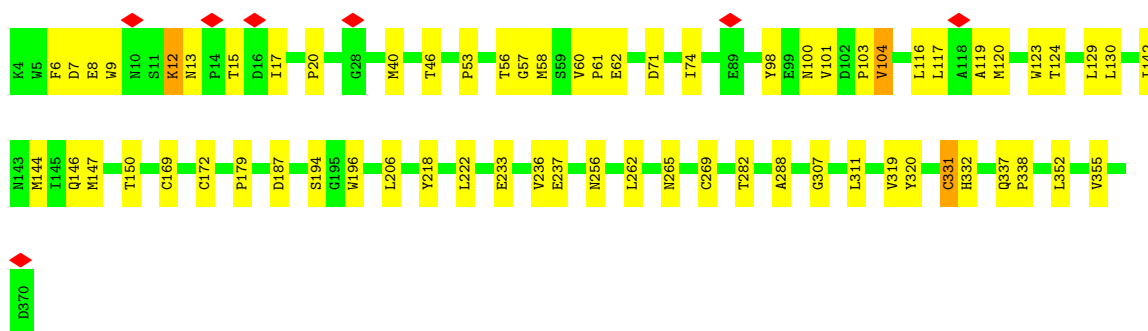
- Molecule 3: Antenna pigment protein beta chain

Chain 0:  91% 9%



- Molecule 4: Photosynthetic reaction center cytochrome c subunit

Chain C:  82% 18%



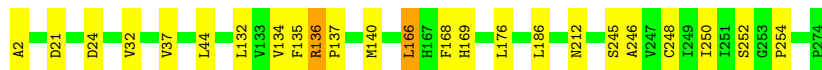
- Molecule 5: Reaction center protein H chain

Chain H:  94% 6%



- Molecule 6: Reaction center protein L chain

Chain L:  91% 8%



- Molecule 7: Reaction center protein M chain

Chain M:  91% 9%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, POINT, POINT, POINT, POINT, POINT, POINT, POINT	Depositor
Number of particles used	123390, 123390, 123390, 123390, 123390, 123390, 123390, 123390	Depositor
Resolution determination method	FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION, PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.00	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.072	Depositor
Minimum map value	-0.968	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.062	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	291.0, 291.0, 291.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.97, 0.97, 0.97	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, MW9, SPN, BCL, BPH, FE, U10

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.90	0/559	1.33	9/757 (1.2%)
2	1	0.51	0/439	0.64	1/595 (0.2%)
2	3	0.75	0/439	0.76	2/595 (0.3%)
2	5	1.02	0/439	0.96	2/595 (0.3%)
2	7	0.55	0/439	0.70	1/595 (0.2%)
2	9	0.49	0/439	0.50	0/595
2	a	0.34	0/439	0.48	0/595
2	c	0.39	0/439	0.39	0/595
2	e	0.22	0/439	0.38	0/595
2	g	0.22	0/439	0.35	0/595
2	i	0.59	0/439	0.68	1/595 (0.2%)
2	k	0.22	0/439	0.31	0/595
2	m	0.57	0/439	0.73	1/595 (0.2%)
2	o	0.68	0/439	0.63	1/595 (0.2%)
2	q	0.42	0/439	0.49	0/595
2	s	0.43	0/439	0.55	0/595
2	u	0.24	0/439	0.32	0/595
2	w	0.13	0/439	0.28	0/595
3	0	0.43	0/371	0.55	1/508 (0.2%)
3	2	0.40	0/371	0.57	1/508 (0.2%)
3	4	0.79	0/371	0.81	1/508 (0.2%)
3	6	0.91	0/371	0.95	2/508 (0.4%)
3	8	0.79	0/371	0.77	2/508 (0.4%)
3	b	0.45	0/371	0.67	1/508 (0.2%)
3	d	0.58	0/371	0.56	0/508
3	f	0.16	0/371	0.31	0/508
3	h	0.38	0/371	0.55	1/508 (0.2%)
3	j	0.72	0/371	0.69	1/508 (0.2%)
3	l	0.18	0/371	0.34	0/508
3	n	0.36	0/371	0.39	0/508
3	p	0.29	0/371	0.48	0/508
3	r	0.59	0/371	0.76	1/508 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	t	0.67	0/371	0.65	0/508
3	v	0.53	0/371	0.63	0/508
3	x	0.25	0/371	0.36	0/508
4	C	0.69	2/2864 (0.1%)	0.93	16/3929 (0.4%)
5	H	0.44	0/2065	0.58	3/2795 (0.1%)
6	L	0.69	3/2261 (0.1%)	0.73	5/3097 (0.2%)
7	M	0.59	2/2732 (0.1%)	0.61	2/3737 (0.1%)
All	All	0.58	7/24251 (0.0%)	0.68	55/33066 (0.2%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	136	ARG	C-O	-5.96	1.18	1.24
7	M	181	PHE	C-N	5.79	1.41	1.33
4	C	117	LEU	CA-C	-5.64	1.45	1.53
7	M	136	GLN	C-O	-5.46	1.17	1.24
6	L	252	SER	CA-C	-5.30	1.46	1.52
4	C	119	ALA	CA-C	-5.24	1.48	1.52
6	L	32	VAL	C-O	-5.03	1.18	1.24

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	187	ASP	N-CA-C	14.22	132.08	112.75
4	C	7	ASP	N-CA-C	-11.51	98.67	113.17
1	A	66	GLN	N-CA-C	-10.86	99.61	113.72
1	A	64	ALA	N-CA-C	-10.59	91.23	108.07
3	6	47	TRP	N-CA-C	-10.28	95.16	109.95
1	A	80	GLY	N-CA-C	-9.59	103.07	114.48
1	A	8	MET	N-CA-C	-9.33	102.03	113.50
4	C	13	ASN	N-CA-C	9.25	124.74	112.35
4	C	124	THR	N-CA-C	-9.02	94.20	108.90
2	i	34	VAL	N-CA-C	-7.74	102.90	110.72
2	5	14	ARG	N-CA-C	-7.73	103.81	113.55
1	A	77	ARG	N-CA-C	-7.72	104.75	114.56
2	m	10	ILE	N-CA-C	-7.71	105.65	111.90
1	A	61	LYS	N-CA-C	-7.26	101.61	111.55
2	o	50	ASN	N-CA-C	-7.16	102.65	112.03
4	C	40	MET	N-CA-C	-7.09	99.43	110.42
2	3	9	LEU	N-CA-C	-6.94	103.21	113.61
3	2	46	PRO	N-CA-C	6.75	121.54	111.41
5	H	207	LYS	N-CA-C	6.67	120.11	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	7	33	LEU	N-CA-C	6.63	120.63	112.54
2	5	50	ASN	N-CA-C	-6.62	105.52	112.93
5	H	60	GLU	N-CA-C	6.58	121.01	109.96
3	r	7	SER	N-CA-C	-6.53	105.61	113.97
1	A	57	ALA	N-CA-C	6.51	118.17	111.14
4	C	116	LEU	N-CA-C	5.96	117.46	110.97
4	C	12	LYS	N-CA-C	-5.87	103.25	110.65
4	C	194	SER	N-CA-C	5.76	123.07	110.80
3	h	43	ILE	O-C-N	-5.72	116.32	121.87
6	L	132	LEU	N-CA-C	5.67	118.40	111.82
3	8	44	TRP	CA-C-N	-5.64	115.98	122.52
3	8	44	TRP	C-N-CA	-5.64	115.98	122.52
3	0	46	PRO	N-CA-C	5.64	120.35	111.38
6	L	168	PHE	N-CA-C	5.59	119.20	112.38
4	C	71	ASP	N-CA-C	-5.55	101.48	109.48
4	C	61	PRO	N-CA-C	5.50	120.72	111.32
6	L	166	LEU	N-CA-C	5.49	122.50	110.80
1	A	78	VAL	N-CA-C	-5.46	105.18	110.42
4	C	196	TRP	N-CA-C	-5.41	106.63	113.18
1	A	75	ARG	N-CA-C	-5.40	105.56	111.82
2	1	2	SER	N-CA-C	-5.39	106.48	113.16
3	j	27	LEU	CA-CB-CG	5.37	135.10	116.30
5	H	210	SER	N-CA-C	5.33	116.77	111.07
6	L	134	VAL	N-CA-C	5.31	115.82	111.62
4	C	331	CYS	CA-CB-SG	-5.31	102.20	114.40
7	M	139	GLU	CA-C-N	-5.28	112.28	120.31
7	M	139	GLU	C-N-CA	-5.28	112.28	120.31
4	C	53	PRO	N-CA-C	5.28	119.61	111.21
3	6	40	ALA	N-CA-C	5.26	117.75	111.71
3	b	39	LEU	N-CA-C	5.17	116.60	111.07
3	4	11	LEU	N-CA-C	-5.12	102.20	110.14
4	C	6	PHE	N-CA-C	5.10	118.61	110.70
2	3	34	VAL	N-CA-C	-5.06	105.61	110.72
6	L	135	PHE	N-CA-C	5.06	116.60	111.14
4	C	120	MET	N-CA-C	5.03	117.50	111.71
4	C	57	GLY	N-CA-C	-5.03	108.30	115.64

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	552	0	570	6	0
2	1	425	0	433	3	0
2	3	425	0	433	7	0
2	5	425	0	433	3	0
2	7	425	0	433	6	0
2	9	425	0	433	6	0
2	a	425	0	433	10	0
2	c	425	0	433	4	0
2	e	425	0	433	8	0
2	g	425	0	433	3	0
2	i	425	0	433	12	0
2	k	425	0	433	10	0
2	m	425	0	433	1	0
2	o	425	0	433	13	0
2	q	425	0	433	13	0
2	s	425	0	433	16	0
2	u	425	0	433	12	0
2	w	425	0	433	6	0
3	0	358	0	338	4	0
3	2	358	0	338	10	0
3	4	358	0	338	8	0
3	6	358	0	338	3	0
3	8	358	0	338	8	0
3	b	358	0	338	13	0
3	d	358	0	338	4	0
3	f	358	0	338	7	0
3	h	358	0	338	18	0
3	j	358	0	338	10	0
3	l	358	0	338	4	0
3	n	358	0	338	8	0
3	p	358	0	338	7	0
3	r	358	0	338	6	0
3	t	358	0	338	18	0
3	v	358	0	338	18	0
3	x	358	0	338	4	0
4	C	2785	0	2631	50	0
5	H	2015	0	1963	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	L	2172	0	2113	17	0
7	M	2634	0	2526	22	0
8	A	43	0	55	0	0
8	L	76	0	94	5	0
8	M	63	0	90	0	0
9	0	66	0	73	7	0
9	1	66	0	74	2	0
9	2	66	0	73	6	0
9	3	66	0	74	7	0
9	4	66	0	73	4	0
9	5	66	0	74	5	0
9	6	66	0	73	4	0
9	7	66	0	74	5	0
9	8	66	0	73	8	0
9	9	66	0	74	5	0
9	L	132	0	148	8	0
9	M	132	0	148	12	0
9	a	66	0	74	4	0
9	b	66	0	73	6	0
9	c	66	0	74	3	0
9	d	66	0	74	6	0
9	e	66	0	74	3	0
9	f	66	0	74	7	0
9	g	66	0	74	3	0
9	h	66	0	74	10	0
9	i	66	0	74	5	0
9	j	66	0	74	7	0
9	k	66	0	74	7	0
9	l	66	0	74	5	0
9	m	66	0	74	6	0
9	n	66	0	74	4	0
9	o	66	0	74	13	0
9	p	66	0	74	11	0
9	q	66	0	74	4	0
9	r	66	0	74	7	0
9	s	66	0	74	7	0
9	t	66	0	74	4	0
9	u	66	0	74	5	0
9	v	66	0	74	7	0
9	w	66	0	74	4	0
9	x	66	0	74	6	0
10	0	43	0	69	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	1	172	0	276	21	0
10	3	43	0	69	4	0
10	5	86	0	138	7	0
10	7	86	0	138	5	0
10	9	43	0	69	1	0
10	M	43	0	69	11	0
10	a	86	0	138	3	0
10	c	86	0	138	3	0
10	e	43	0	69	2	0
10	f	43	0	69	8	0
10	h	86	0	138	16	0
10	i	43	0	69	2	0
10	j	43	0	69	5	0
10	k	43	0	69	2	0
10	l	43	0	69	6	0
10	m	43	0	69	1	0
10	n	43	0	69	4	0
10	p	86	0	138	20	0
10	q	43	0	69	8	0
10	r	43	0	69	1	0
10	s	43	0	69	1	0
10	t	43	0	69	4	0
10	u	43	0	69	3	0
10	v	43	0	69	14	0
10	w	43	0	69	2	0
11	9	53	0	0	0	0
11	H	212	0	0	3	0
11	M	106	0	0	1	0
11	g	103	0	0	0	0
12	C	129	0	90	15	0
13	L	65	0	76	2	0
13	M	130	0	152	2	0
14	M	1	0	0	0	0
All	All	28463	0	28688	550	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (550) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:101:VAL:HG12	4:C:103:PRO:HD2	1.16	1.15
2:s:46:LEU:HD21	3:t:45:ARG:HH12	1.16	1.09
2:k:42:ASN:O	2:k:46:LEU:HD13	1.56	1.04
2:a:40:HIS:CE1	3:b:45:ARG:HH11	1.78	1.02
2:s:40:HIS:CE1	3:t:45:ARG:HD2	1.99	0.96
2:i:40:HIS:CE1	3:j:45:ARG:HH21	1.86	0.94
2:s:46:LEU:HD21	3:t:45:ARG:NH1	1.84	0.93
4:C:101:VAL:CG1	4:C:103:PRO:HD2	2.00	0.91
9:o:101:BCL:H41	10:p:102:SPN:CMA	2.02	0.90
3:v:32:ALA:O	3:v:35:VAL:HG12	1.71	0.89
4:C:101:VAL:HG12	4:C:103:PRO:CD	2.02	0.88
2:q:24:LEU:HD11	10:q:102:SPN:H162	1.56	0.87
6:L:169:HIS:HE1	9:L:301:BCL:HBB2	1.39	0.86
2:o:14:ARG:HH21	4:C:15:THR:HG21	1.40	0.85
2:u:10:ILE:HG22	2:s:14:ARG:HG2	1.57	0.83
9:o:101:BCL:HMA2	10:p:102:SPN:H142	1.60	0.82
4:C:269:CYS:HA	4:C:282:THR:OG1	1.79	0.82
2:a:46:LEU:HD11	3:b:45:ARG:HH22	1.45	0.81
2:i:42:ASN:O	2:i:46:LEU:HD23	1.81	0.81
9:o:101:BCL:CMA	10:p:102:SPN:H142	2.12	0.80
6:L:169:HIS:CE1	9:L:301:BCL:HBB2	2.18	0.79
4:C:218:TYR:CD1	4:C:222:LEU:HD23	2.17	0.78
2:q:9:LEU:HD21	4:C:9:TRP:CE3	2.18	0.78
3:h:26:GLY:HA3	10:h:103:SPN:HM73	1.63	0.78
9:f:101:BCL:H141	9:f:101:BCL:HMB2	1.65	0.77
4:C:172:CYS:SG	12:C:401:HEM:HBC2	2.24	0.77
9:t:101:BCL:HMB1	9:t:101:BCL:HBB2	1.66	0.76
5:H:69:ARG:NH2	5:H:123:LEU:HG	2.01	0.75
3:j:44:TRP:CD2	3:j:45:ARG:HG2	2.21	0.75
4:C:172:CYS:SG	12:C:401:HEM:CBC	2.75	0.75
4:C:256:ASN:OD1	6:L:166:LEU:HD23	1.86	0.75
9:L:301:BCL:H61	9:L:304:BCL:HBB3	1.67	0.74
9:f:101:BCL:HBB2	9:f:101:BCL:HMB1	1.69	0.74
9:j:101:BCL:HMB1	9:j:101:BCL:HBB2	1.70	0.74
9:x:101:BCL:HMB1	9:x:101:BCL:HBB2	1.69	0.74
2:q:35:LEU:HD11	9:r:101:BCL:HHD	1.69	0.74
1:A:64:ALA:HB3	1:A:68:ARG:HG2	1.70	0.74
3:v:6:LEU:HD22	3:t:11:LEU:HD11	1.69	0.74
9:n:101:BCL:HMB1	9:n:101:BCL:HBB2	1.69	0.73
2:k:42:ASN:O	2:k:46:LEU:CD1	2.35	0.73
9:l:101:BCL:HMB1	9:l:101:BCL:HBB2	1.70	0.73
9:u:101:BCL:HMB1	9:u:101:BCL:HBB3	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:q:102:SPN:HMA3	9:o:101:BCL:HBB2	1.70	0.73
9:w:101:BCL:HBB2	9:w:101:BCL:HMB1	1.69	0.73
2:e:42:ASN:HB3	2:e:45:GLU:OE2	1.88	0.73
2:u:6:LYS:NZ	3:t:18:GLU:OE2	2.22	0.73
4:C:331:CYS:SG	12:C:403:HEM:C2C	2.82	0.72
3:t:27:LEU:HD13	10:t:102:SPN:H152	1.71	0.72
9:v:101:BCL:HMB1	9:v:101:BCL:HBB2	1.72	0.72
6:L:176:LEU:HD12	8:L:305:U10:H111	1.71	0.72
2:i:27:LEU:O	2:i:30:MET:HG2	1.90	0.71
9:L:304:BCL:HBA2	7:M:208:VAL:HG22	1.71	0.71
3:f:26:GLY:HA3	10:f:102:SPN:HM73	1.72	0.71
3:h:27:LEU:HB2	10:h:103:SPN:H19	1.73	0.70
2:k:3:LYS:CE	3:j:18:GLU:OE2	2.40	0.70
7:M:178:TYR:HD1	10:M:406:SPN:H142	1.55	0.70
2:q:24:LEU:HD21	10:q:102:SPN:H142	1.73	0.69
9:p:101:BCL:HMB1	9:p:101:BCL:HBB2	1.74	0.69
9:c:101:BCL:HMB1	9:c:101:BCL:HBB2	1.74	0.69
2:a:40:HIS:CE1	3:b:45:ARG:NH1	2.58	0.69
10:q:102:SPN:H231	3:r:23:TYR:HA	1.74	0.69
3:n:11:LEU:HD23	3:n:12:THR:O	1.93	0.69
2:o:14:ARG:NH2	4:C:15:THR:HG21	2.07	0.68
2:o:15:ARG:HG2	4:C:17:ILE:HA	1.75	0.68
3:v:32:ALA:O	3:v:35:VAL:CG1	2.42	0.68
10:v:102:SPN:C4	9:s:101:BCL:HMB2	2.23	0.67
10:3:102:SPN:HM93	3:4:36:VAL:HG12	1.75	0.67
6:L:245:SER:HA	6:L:248:CYS:SG	2.33	0.67
9:x:101:BCL:H201	10:u:102:SPN:H19	1.77	0.67
9:o:101:BCL:HMA3	10:p:102:SPN:H162	1.77	0.67
10:1:103:SPN:H162	3:2:27:LEU:HD12	1.75	0.66
2:a:46:LEU:CD1	3:b:45:ARG:HH22	2.08	0.66
10:1:103:SPN:HMB2	2:3:6:LYS:HB3	1.76	0.66
3:t:13:ASP:OD1	3:t:13:ASP:O	2.13	0.66
2:s:40:HIS:O	3:t:45:ARG:NH2	2.28	0.65
10:u:102:SPN:HM11	10:v:102:SPN:H212	1.78	0.65
10:f:102:SPN:H211	10:f:102:SPN:HM61	1.78	0.65
9:i:101:BCL:HMB1	9:i:101:BCL:HBB2	1.77	0.65
3:b:31:SER:O	3:b:35:VAL:HG23	1.96	0.65
2:a:46:LEU:HD11	3:b:45:ARG:NH2	2.12	0.65
3:j:44:TRP:CE3	3:j:45:ARG:HG2	2.31	0.64
2:o:50:ASN:O	2:o:51:ALA:HB3	1.98	0.64
3:v:32:ALA:C	3:v:35:VAL:HG12	2.23	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:q:20:GLN:CD	10:q:102:SPN:H171	2.23	0.64
9:o:101:BCL:H41	10:p:102:SPN:HMA3	1.79	0.64
9:a:101:BCL:CBB	9:a:101:BCL:HMB1	2.28	0.64
2:i:40:HIS:CE1	3:j:45:ARG:NH2	2.63	0.64
3:v:22:VAL:HG11	10:v:102:SPN:HM92	1.79	0.64
2:q:10:ILE:HD13	10:p:103:SPN:HM92	1.80	0.64
2:9:46:LEU:HD21	2:9:50:ASN:ND2	2.12	0.64
2:u:10:ILE:HG22	2:s:14:ARG:CG	2.27	0.64
9:s:101:BCL:HMB1	9:s:101:BCL:HBB2	1.79	0.63
7:M:271:TRP:O	7:M:275:VAL:HG23	1.99	0.63
9:9:102:BCL:HBB2	9:9:102:BCL:HMB1	1.80	0.63
13:L:303:BPH:H5C1	7:M:65:GLY:HA3	1.81	0.63
2:m:1:MET:HG3	2:m:3:LYS:H	1.64	0.63
9:k:101:BCL:HMB1	9:k:101:BCL:CBB	2.29	0.63
9:e:101:BCL:CBB	9:e:101:BCL:HMB1	2.29	0.63
3:h:12:THR:HG22	3:h:13:ASP:N	2.12	0.62
2:w:10:ILE:HD11	10:v:102:SPN:H29	1.81	0.62
9:m:101:BCL:CBB	9:m:101:BCL:HMB1	2.29	0.62
10:1:103:SPN:H162	3:2:27:LEU:CD1	2.29	0.62
3:t:27:LEU:CD1	10:t:102:SPN:H152	2.29	0.62
2:w:32:HIS:CE1	9:x:101:BCL:HMD1	2.35	0.62
11:H:301:MW9:C9	9:L:304:BCL:HED3	2.29	0.62
2:a:46:LEU:CD1	3:b:45:ARG:NH2	2.63	0.62
3:l:31:SER:O	3:l:35:VAL:HG23	1.99	0.62
10:l:102:SPN:HM61	10:l:102:SPN:H211	1.83	0.61
3:h:39:LEU:HD22	10:h:102:SPN:HMB1	1.80	0.61
2:o:16:VAL:HG12	2:o:20:GLN:HE21	1.65	0.61
9:g:101:BCL:CBB	9:g:101:BCL:HMB1	2.30	0.61
3:h:31:SER:O	3:h:35:VAL:HG23	1.99	0.61
9:9:102:BCL:HMB1	9:9:102:BCL:CBB	2.30	0.61
2:o:14:ARG:HG2	10:p:103:SPN:HMB1	1.81	0.61
2:o:14:ARG:HH21	4:C:15:THR:CG2	2.14	0.61
3:n:31:SER:O	3:n:35:VAL:HG23	2.00	0.61
2:w:10:ILE:CD1	10:v:102:SPN:H29	2.30	0.61
10:p:103:SPN:H211	10:p:103:SPN:HM61	1.82	0.60
2:e:27:LEU:HD23	9:f:101:BCL:HED1	1.83	0.60
4:C:46:THR:OG1	4:C:62:GLU:O	2.18	0.60
7:M:178:TYR:CD1	10:M:406:SPN:H142	2.36	0.60
9:g:101:BCL:HMB1	9:g:101:BCL:HBB2	1.84	0.60
3:h:39:LEU:CD2	10:h:102:SPN:CMB	2.79	0.60
7:M:162:GLY:HA3	10:M:406:SPN:HM72	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:q:9:LEU:CD2	4:C:9:TRP:CE3	2.84	0.60
10:l:102:SPN:HM61	10:l:102:SPN:C21	2.31	0.60
2:w:25:PHE:HB2	9:w:101:BCL:H2	1.83	0.60
10:M:406:SPN:H171	10:M:406:SPN:H211	1.83	0.59
9:v:101:BCL:HMB1	9:v:101:BCL:CBB	2.31	0.59
9:o:101:BCL:H41	10:p:102:SPN:HMA1	1.81	0.59
9:l:101:BCL:H112	10:l:102:SPN:HM32	1.85	0.59
1:A:40:ALA:O	1:A:44:VAL:HG23	2.03	0.59
3:h:6:LEU:HD13	3:f:11:LEU:HD22	1.83	0.59
10:c:102:SPN:HM62	3:d:37:ALA:HB1	1.85	0.59
3:v:12:THR:HG22	3:v:13:ASP:N	2.17	0.58
9:o:101:BCL:C4	10:p:102:SPN:HMA1	2.33	0.58
10:7:102:SPN:HM62	3:8:37:ALA:HB1	1.83	0.58
7:M:6:ASN:HD22	7:M:228:THR:HG21	1.69	0.58
4:C:129:LEU:HG	4:C:130:LEU:HD13	1.86	0.58
7:M:69:PHE:CE1	10:M:406:SPN:H61	2.39	0.58
10:h:103:SPN:H211	10:h:103:SPN:HM61	1.85	0.58
9:c:101:BCL:HMB1	9:c:101:BCL:CBB	2.33	0.58
3:t:27:LEU:HD13	10:t:102:SPN:H172	1.86	0.58
3:d:14:GLU:CD	3:d:14:GLU:H	2.11	0.58
9:h:101:BCL:HMB1	9:h:101:BCL:HBB2	1.86	0.58
2:u:32:HIS:CE1	9:v:101:BCL:HMD1	2.39	0.57
2:s:6:LYS:HE3	3:r:18:GLU:OE2	2.04	0.57
9:h:101:BCL:H201	10:e:102:SPN:H19	1.86	0.57
3:h:39:LEU:CD2	10:h:102:SPN:HMB2	2.34	0.57
9:7:101:BCL:HMB1	9:7:101:BCL:HBB2	1.87	0.57
3:p:32:ALA:O	3:p:36:VAL:HG23	2.05	0.56
9:j:101:BCL:HMB1	9:j:101:BCL:CBB	2.35	0.56
7:M:80:VAL:HG12	7:M:80:VAL:O	2.05	0.56
3:v:32:ALA:HA	3:v:35:VAL:HG12	1.87	0.56
9:o:101:BCL:C4	10:p:102:SPN:CMA	2.81	0.56
2:k:3:LYS:HE2	3:j:18:GLU:OE2	2.05	0.56
9:o:101:BCL:C4D	10:p:102:SPN:HM62	2.35	0.56
10:i:102:SPN:HM62	3:j:37:ALA:HB1	1.88	0.56
3:f:19:LEU:HA	10:f:102:SPN:HM92	1.88	0.56
2:u:10:ILE:CG2	2:s:14:ARG:CG	2.83	0.56
9:7:101:BCL:HMB1	9:7:101:BCL:CBB	2.36	0.56
9:r:101:BCL:H52	9:r:101:BCL:HAA1	1.88	0.56
9:M:402:BCL:H2	9:M:402:BCL:H93	1.87	0.56
3:v:22:VAL:HG11	10:v:102:SPN:CM9	2.36	0.55
3:t:10:GLY:C	3:t:11:LEU:HD22	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:27:LEU:HD23	9:2:101:BCL:HED1	1.88	0.55
4:C:218:TYR:CE1	4:C:222:LEU:HD23	2.41	0.55
10:M:406:SPN:H211	10:M:406:SPN:C17	2.36	0.55
9:q:101:BCL:CBB	9:q:101:BCL:HMB1	2.37	0.55
10:e:102:SPN:HM62	3:f:37:ALA:HB1	1.86	0.55
10:1:103:SPN:HM93	3:2:18:GLU:HG2	1.89	0.55
7:M:109:PRO:HB2	7:M:111:ASP:OD1	2.06	0.55
9:h:101:BCL:HMB2	9:h:101:BCL:H143	1.88	0.55
9:d:101:BCL:HMB1	9:d:101:BCL:HBB2	1.88	0.55
7:M:120:SER:HB3	10:M:406:SPN:H25	1.89	0.55
1:A:49:ILE:O	1:A:53:VAL:HG23	2.07	0.55
9:5:101:BCL:CBB	9:5:101:BCL:HMB1	2.37	0.55
4:C:262:LEU:HD11	12:C:403:HEM:HHB	1.87	0.55
2:q:9:LEU:HD23	2:q:9:LEU:O	2.06	0.54
2:q:40:HIS:HB2	2:o:48:ALA:HB2	1.89	0.54
9:5:101:BCL:HMB1	9:5:101:BCL:HBB2	1.88	0.54
4:C:8:GLU:HG2	4:C:12:LYS:HZ3	1.72	0.54
2:k:35:LEU:HD11	9:l:101:BCL:HHD	1.89	0.54
10:q:102:SPN:HM31	9:o:101:BCL:HBA2	1.89	0.54
4:C:236:VAL:HG12	4:C:237:GLU:N	2.23	0.54
2:u:30:MET:O	2:u:34:VAL:HG23	2.07	0.54
3:b:44:TRP:CD2	3:b:45:ARG:HG2	2.42	0.54
9:u:101:BCL:HMB1	9:u:101:BCL:CBB	2.36	0.54
3:d:5:ASP:OD2	3:d:13:ASP:OD2	2.25	0.54
10:h:103:SPN:HMB3	2:i:10:ILE:HD11	1.89	0.53
12:C:402:HEM:HBB1	6:L:166:LEU:HG	1.90	0.53
2:e:32:HIS:CE1	9:f:101:BCL:HMD1	2.44	0.53
2:c:6:LYS:NZ	3:b:18:GLU:OE2	2.41	0.53
3:r:37:ALA:HB1	10:r:102:SPN:HM62	1.90	0.53
2:u:46:LEU:HD21	3:v:45:ARG:HH22	1.74	0.53
10:s:102:SPN:HM62	3:t:37:ALA:HB1	1.91	0.53
2:9:46:LEU:CD2	2:9:50:ASN:ND2	2.71	0.53
2:s:46:LEU:CD2	3:t:45:ARG:HH12	2.03	0.53
2:k:30:MET:O	2:k:34:VAL:HG23	2.08	0.53
4:C:8:GLU:HG2	4:C:12:LYS:NZ	2.23	0.52
4:C:331:CYS:SG	12:C:403:HEM:C3C	2.89	0.52
2:a:35:LEU:HD11	9:b:101:BCL:HHD	1.91	0.52
2:s:41:PHE:CE1	3:t:45:ARG:HG3	2.44	0.52
9:e:101:BCL:HMB1	9:e:101:BCL:HBB2	1.90	0.52
6:L:21:ASP:HA	6:L:24:ASP:HB2	1.91	0.52
7:M:131:TRP:HA	7:M:134:THR:HG22	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:c:36:LEU:O	2:c:42:ASN:ND2	2.43	0.52
5:H:153:VAL:HG21	5:H:181:LEU:HD13	1.91	0.52
8:L:302:U10:H251	8:L:305:U10:H1M2	1.91	0.52
2:s:1:MET:C	2:s:3:LYS:H	2.17	0.51
9:p:101:BCL:C1B	9:p:101:BCL:H141	2.40	0.51
10:k:102:SPN:HM62	3:l:37:ALA:HB1	1.92	0.51
2:5:43:TRP:HA	2:5:46:LEU:HD12	1.92	0.51
3:h:12:THR:HG22	3:h:13:ASP:H	1.76	0.51
5:H:69:ARG:HH21	5:H:123:LEU:HG	1.73	0.51
2:o:28:ALA:HB2	9:p:101:BCL:HED3	1.92	0.51
3:h:39:LEU:CD2	10:h:102:SPN:HMB1	2.40	0.51
10:v:102:SPN:C21	10:v:102:SPN:HM61	2.41	0.51
9:m:101:BCL:HMB1	9:m:101:BCL:HBB2	1.92	0.51
2:7:43:TRP:HZ2	10:0:102:SPN:HMA1	1.75	0.51
9:f:101:BCL:HMB1	9:f:101:BCL:CBB	2.38	0.51
10:u:102:SPN:HM62	3:v:37:ALA:HB1	1.93	0.51
2:e:1:MET:HE2	2:e:3:LYS:HD3	1.92	0.51
3:f:23:TYR:HA	10:f:102:SPN:HM72	1.92	0.51
9:L:301:BCL:HHC	9:L:301:BCL:HBB3	1.93	0.51
3:h:39:LEU:HD22	10:h:102:SPN:CMB	2.41	0.51
2:c:32:HIS:CE1	9:d:101:BCL:HMD1	2.46	0.51
4:C:179:PRO:HD2	12:C:401:HEM:HBD2	1.91	0.51
3:n:19:LEU:HD12	10:n:102:SPN:H271	1.91	0.50
4:C:74:ILE:HG23	4:C:352:LEU:HD22	1.92	0.50
10:a:102:SPN:HM62	3:b:37:ALA:HB1	1.92	0.50
3:6:24:MET:SD	3:6:27:LEU:HD13	2.51	0.50
9:d:101:BCL:HMB1	9:d:101:BCL:CBB	2.41	0.50
4:C:60:VAL:HG22	4:C:265:ASN:OD1	2.11	0.50
10:9:103:SPN:HM62	3:0:37:ALA:HB1	1.94	0.50
10:1:104:SPN:HM92	3:4:19:LEU:HA	1.94	0.50
3:b:12:THR:OG1	3:b:15:GLN:HG3	2.11	0.50
4:C:104:VAL:O	4:C:104:VAL:HG22	2.10	0.50
3:0:18:GLU:OE1	10:0:102:SPN:HM91	2.11	0.50
3:2:6:LEU:HB2	3:x:15:GLN:HG2	1.92	0.50
2:e:42:ASN:HB3	2:e:45:GLU:HG2	1.94	0.50
3:v:22:VAL:CG1	10:v:102:SPN:HM92	2.41	0.50
2:s:1:MET:HG2	2:s:4:PHE:CE2	2.46	0.50
9:i:101:BCL:HMB1	9:i:101:BCL:CBB	2.42	0.50
5:H:41:LEU:HB3	6:L:2:ALA:HB1	1.92	0.50
10:5:102:SPN:HM62	3:6:37:ALA:HB1	1.92	0.49
2:3:10:ILE:HD12	3:4:8:PHE:HE2	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:f:27:LEU:HB2	10:f:102:SPN:H19	1.94	0.49
2:5:27:LEU:HD23	9:6:101:BCL:HED1	1.94	0.49
4:C:144:MET:HB3	12:C:401:HEM:C3B	2.47	0.49
9:M:402:BCL:H102	9:M:404:BCL:H192	1.92	0.49
9:p:101:BCL:CHB	9:m:101:BCL:HMB3	2.42	0.49
3:p:6:LEU:HD23	3:n:15:GLN:CD	2.37	0.49
4:C:146:GLN:O	4:C:150:THR:HG23	2.12	0.49
6:L:186:LEU:HD13	9:M:402:BCL:H41	1.94	0.49
10:1:103:SPN:H152	3:2:27:LEU:HD11	1.95	0.49
2:u:10:ILE:CG2	2:s:14:ARG:HG3	2.43	0.49
9:k:101:BCL:HMB1	9:k:101:BCL:HBB2	1.95	0.49
11:H:301:MW9:C9	9:L:304:BCL:CED	2.91	0.49
3:v:23:TYR:HA	10:v:102:SPN:HM72	1.96	0.48
2:a:40:HIS:NE2	3:b:45:ARG:NH1	2.59	0.48
5:H:199:VAL:HG12	5:H:208:VAL:HG22	1.94	0.48
4:C:169:CYS:SG	12:C:401:HEM:C3B	3.04	0.48
8:L:305:U10:H171	8:L:305:U10:H151	1.43	0.48
7:M:30:GLU:HB2	7:M:53:TYR:CE2	2.48	0.48
2:s:32:HIS:CE1	9:t:101:BCL:HMD1	2.48	0.48
3:p:40:ALA:HB1	10:p:102:SPN:H232	1.95	0.48
2:7:5:TYR:CE1	3:8:13:ASP:OD1	2.67	0.48
9:x:101:BCL:HMB1	9:x:101:BCL:CBB	2.42	0.48
3:8:34:ALA:HB3	9:8:101:BCL:H91	1.95	0.48
10:h:103:SPN:HMB2	2:i:6:LYS:HB3	1.95	0.48
3:v:32:ALA:CA	3:v:35:VAL:HG12	2.44	0.48
9:r:101:BCL:H62	9:r:101:BCL:H41	1.53	0.48
3:h:15:GLN:HG2	3:j:6:LEU:HB2	1.95	0.48
2:u:27:LEU:HD23	9:v:101:BCL:HED2	1.96	0.48
3:v:12:THR:CG2	3:v:13:ASP:N	2.77	0.48
10:v:102:SPN:HM61	10:v:102:SPN:H211	1.96	0.48
2:e:42:ASN:O	2:e:46:LEU:HG	2.14	0.48
10:1:102:SPN:HM62	3:2:37:ALA:HB1	1.95	0.48
10:5:102:SPN:H19	9:8:101:BCL:C19	2.44	0.48
9:t:101:BCL:HMB1	9:t:101:BCL:CBB	2.40	0.48
9:c:101:BCL:H141	9:c:101:BCL:H162	1.71	0.48
3:8:35:VAL:HG23	9:8:101:BCL:H93	1.96	0.48
10:m:102:SPN:HM62	3:n:37:ALA:HB1	1.96	0.48
9:w:101:BCL:H61	9:w:101:BCL:H102	1.58	0.47
9:l:101:BCL:HBA1	9:l:101:BCL:H3A	1.62	0.47
3:h:12:THR:CG2	3:h:13:ASP:N	2.76	0.47
4:C:319:VAL:HG23	4:C:320:TYR:CD2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:22:VAL:HG12	10:0:102:SPN:H242	1.96	0.47
9:0:101:BCL:H2	9:0:101:BCL:H62	1.45	0.47
2:3:27:LEU:HD23	9:4:101:BCL:HED1	1.96	0.47
6:L:246:ALA:O	6:L:250:ILE:HG22	2.14	0.47
2:9:35:LEU:HD11	9:0:101:BCL:HHD	1.95	0.47
9:x:101:BCL:HBB3	9:u:101:BCL:CHC	2.45	0.47
10:a:103:SPN:H211	10:a:103:SPN:HM61	1.97	0.47
2:1:20:GLN:CD	10:1:103:SPN:H161	2.38	0.47
3:r:11:LEU:HD23	3:r:11:LEU:HA	1.77	0.47
9:h:101:BCL:HMB1	9:h:101:BCL:CBB	2.44	0.47
4:C:147:MET:HE1	12:C:401:HEM:C3C	2.49	0.47
10:1:105:SPN:HMA3	9:u:101:BCL:HBB2	1.96	0.47
2:g:6:LYS:NZ	3:f:18:GLU:OE1	2.34	0.47
2:g:27:LEU:HD23	9:h:101:BCL:HED1	1.96	0.47
1:A:61:LYS:HA	1:A:61:LYS:HD3	1.68	0.47
2:3:35:LEU:HD11	9:4:101:BCL:HHD	1.95	0.47
9:w:101:BCL:HMB1	9:w:101:BCL:CBB	2.40	0.47
4:C:307:GLY:HA2	4:C:311:LEU:HG	1.96	0.47
7:M:56:TRP:HD1	11:M:407:MW9:C21	2.28	0.47
7:M:178:TYR:HE1	10:M:406:SPN:H162	1.80	0.47
10:1:103:SPN:H281	10:1:103:SPN:HM81	1.60	0.47
10:q:102:SPN:HM81	10:q:102:SPN:H282	1.53	0.47
9:r:101:BCL:H62	9:r:101:BCL:H93	1.81	0.47
2:u:10:ILE:CG2	2:s:14:ARG:HG2	2.37	0.47
10:v:102:SPN:H4	9:s:101:BCL:HMB2	1.93	0.47
3:n:19:LEU:CD1	10:n:102:SPN:H271	2.45	0.47
3:j:44:TRP:CE3	3:j:45:ARG:CG	2.97	0.47
10:j:102:SPN:H211	10:j:102:SPN:HM61	1.96	0.47
9:0:101:BCL:H121	9:0:101:BCL:H161	1.47	0.47
9:j:101:BCL:H111	9:j:101:BCL:H72	1.44	0.46
2:7:5:TYR:HE1	3:8:13:ASP:OD1	1.98	0.46
4:C:98:TYR:HB2	4:C:100:ASN:ND2	2.30	0.46
3:p:27:LEU:HB2	10:p:103:SPN:H19	1.97	0.46
9:b:101:BCL:H192	9:b:101:BCL:H162	1.77	0.46
4:C:282:THR:HG22	7:M:312:TYR:HB3	1.96	0.46
2:o:50:ASN:O	2:o:51:ALA:CB	2.63	0.46
3:p:6:LEU:C	3:p:6:LEU:HD12	2.40	0.46
9:p:101:BCL:H172	9:p:101:BCL:C3B	2.45	0.46
10:w:102:SPN:HM62	3:x:37:ALA:HB1	1.97	0.46
3:h:23:TYR:HA	10:h:103:SPN:HM72	1.97	0.46
9:b:101:BCL:HBA1	9:b:101:BCL:H3A	1.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:250:ILE:O	6:L:254:PRO:HD2	2.15	0.46
9:6:101:BCL:H192	9:6:101:BCL:H161	1.51	0.46
3:v:6:LEU:CD2	3:t:11:LEU:HD11	2.42	0.46
9:p:101:BCL:HBB3	9:m:101:BCL:CHC	2.45	0.46
9:g:101:BCL:H61	9:g:101:BCL:H41	1.74	0.46
3:h:37:ALA:HB1	10:h:102:SPN:HM62	1.97	0.46
10:7:103:SPN:H231	3:8:23:TYR:HA	1.97	0.46
7:M:178:TYR:CE1	10:M:406:SPN:H162	2.50	0.46
9:2:101:BCL:H62	9:2:101:BCL:H2	1.58	0.46
9:j:101:BCL:HBA1	9:j:101:BCL:H3A	1.77	0.46
10:5:102:SPN:H19	9:8:101:BCL:H192	1.98	0.46
2:3:10:ILE:HD12	3:4:8:PHE:CE2	2.51	0.46
2:q:10:ILE:HD13	10:p:103:SPN:CM9	2.44	0.46
2:q:27:LEU:CD2	9:r:101:BCL:HED1	2.46	0.46
10:q:102:SPN:CMA	9:o:101:BCL:HBB2	2.44	0.46
10:3:102:SPN:H212	10:3:102:SPN:H272	1.98	0.46
9:2:101:BCL:H112	9:2:101:BCL:H143	1.62	0.45
9:v:101:BCL:HBA1	9:v:101:BCL:H12	1.22	0.45
2:i:22:VAL:CG2	6:L:37:VAL:HG13	2.46	0.45
4:C:56:THR:HG22	4:C:58:MET:HG3	1.98	0.45
7:M:136:GLN:O	7:M:140:MET:HG3	2.15	0.45
9:3:101:BCL:H192	9:3:101:BCL:H161	1.76	0.45
10:3:102:SPN:HM62	3:4:37:ALA:HB1	1.98	0.45
10:p:102:SPN:HM81	10:p:102:SPN:H281	1.37	0.45
2:i:27:LEU:O	2:i:30:MET:CG	2.62	0.45
10:5:102:SPN:H211	9:8:101:BCL:C19	2.46	0.45
3:p:44:TRP:HD1	10:p:102:SPN:H29	1.82	0.45
9:f:101:BCL:HBA1	9:f:101:BCL:H3A	1.68	0.45
2:7:1:MET:HE3	2:7:1:MET:HB2	1.73	0.45
10:1:103:SPN:H232	3:2:23:TYR:HA	1.97	0.45
3:r:18:GLU:O	3:r:22:VAL:HG23	2.16	0.45
9:a:101:BCL:HMB1	9:a:101:BCL:HBB3	1.99	0.45
10:j:102:SPN:HM61	10:j:102:SPN:C21	2.46	0.45
2:o:27:LEU:HB3	9:p:101:BCL:HED1	1.99	0.45
12:C:402:HEM:HMC1	12:C:402:HEM:HAC	1.63	0.45
2:i:27:LEU:HD23	9:j:101:BCL:HED1	1.98	0.45
6:L:245:SER:O	6:L:248:CYS:SG	2.63	0.45
7:M:131:TRP:O	7:M:134:THR:HG22	2.17	0.45
10:j:102:SPN:HM81	10:j:102:SPN:H281	1.47	0.45
3:8:13:ASP:O	3:8:17:GLN:HG3	2.17	0.45
2:k:6:LYS:HB3	10:j:102:SPN:HMB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:288:ALA:CB	12:C:402:HEM:HBC2	2.46	0.45
9:M:402:BCL:H111	9:M:402:BCL:H91	1.49	0.45
2:w:27:LEU:HD23	9:x:101:BCL:HED1	1.99	0.45
9:s:101:BCL:HMB1	9:s:101:BCL:CBB	2.44	0.45
9:n:101:BCL:H152	9:n:101:BCL:H112	1.70	0.45
9:d:101:BCL:CAB	9:d:101:BCL:H192	2.47	0.45
7:M:90:GLN:O	7:M:94:LEU:HG	2.17	0.45
10:v:102:SPN:H241	10:v:102:SPN:HM71	1.76	0.45
9:q:101:BCL:HMB1	9:q:101:BCL:HBB2	1.98	0.45
9:k:101:BCL:HBA1	9:k:101:BCL:H3A	1.68	0.45
9:a:101:BCL:HMB1	9:a:101:BCL:HBB2	1.96	0.45
1:A:79:ARG:HA	1:A:82:THR:HG22	1.99	0.44
9:4:101:BCL:H62	9:4:101:BCL:H2	1.61	0.44
9:M:402:BCL:H143	9:M:402:BCL:H112	1.57	0.44
9:m:101:BCL:H62	9:m:101:BCL:H41	1.53	0.44
9:h:101:BCL:HMB2	9:h:101:BCL:C14	2.47	0.44
9:h:101:BCL:HBB3	9:e:101:BCL:CHC	2.47	0.44
4:C:218:TYR:HD1	4:C:222:LEU:HD23	1.76	0.44
2:q:10:ILE:HG22	4:C:9:TRP:CD1	2.53	0.44
9:n:101:BCL:HMB1	9:n:101:BCL:CBB	2.42	0.44
2:7:39:GLU:HG3	2:7:40:HIS:N	2.32	0.44
3:8:18:GLU:OE2	2:9:6:LYS:NZ	2.50	0.44
9:M:404:BCL:H41	9:M:404:BCL:H62	1.47	0.44
9:5:101:BCL:HBA1	9:5:101:BCL:H3A	1.53	0.44
9:k:101:BCL:H121	9:k:101:BCL:H162	1.61	0.44
10:7:103:SPN:HM93	2:9:10:ILE:HD11	2.00	0.44
10:1:104:SPN:HM61	10:1:104:SPN:C21	2.47	0.44
9:2:101:BCL:H203	9:2:101:BCL:H162	1.59	0.44
10:5:103:SPN:HM31	9:3:101:BCL:HBA2	1.99	0.44
2:a:27:LEU:HD23	9:b:101:BCL:HED1	1.99	0.44
9:b:101:BCL:H101	9:b:101:BCL:H62	1.48	0.44
10:M:406:SPN:C17	10:M:406:SPN:C21	2.95	0.44
13:M:409:BPH:H102	13:M:409:BPH:H6C1	1.68	0.44
2:5:49:ALA:C	2:5:51:ALA:H	2.25	0.44
10:l:102:SPN:H281	10:l:102:SPN:HM81	1.42	0.44
9:v:101:BCL:O1D	9:v:101:BCL:H2A	2.18	0.44
9:i:101:BCL:HMC2	9:i:101:BCL:HHC	1.85	0.44
9:1:101:BCL:HMB3	9:1:101:BCL:HBB2	1.99	0.44
10:1:103:SPN:HM61	10:1:103:SPN:C21	2.47	0.44
3:h:12:THR:CG2	3:h:13:ASP:H	2.31	0.44
3:h:19:LEU:HA	10:h:103:SPN:HM92	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:404:BCL:HAA2	9:M:404:BCL:HBD	2.00	0.44
10:n:102:SPN:C4	9:k:101:BCL:HMB2	2.48	0.44
4:C:288:ALA:HB2	12:C:402:HEM:HBC2	2.00	0.44
4:C:331:CYS:SG	12:C:403:HEM:CMC	3.05	0.44
9:L:304:BCL:HHC	9:L:304:BCL:HBB2	2.00	0.44
9:0:101:BCL:HBA1	9:0:101:BCL:H3A	1.73	0.43
2:1:20:GLN:NE2	10:1:103:SPN:H161	2.33	0.43
3:v:5:ASP:OD1	3:v:5:ASP:O	2.37	0.43
9:s:101:BCL:H143	9:s:101:BCL:H111	1.88	0.43
3:r:32:ALA:O	3:r:36:VAL:HG23	2.18	0.43
8:L:305:U10:H8	9:M:402:BCL:HED1	2.00	0.43
9:9:102:BCL:HBA1	9:9:102:BCL:H3A	1.73	0.43
9:0:101:BCL:H2	9:0:101:BCL:H102	1.99	0.43
10:3:102:SPN:H241	3:4:40:ALA:HB1	2.01	0.43
9:r:101:BCL:H193	9:r:101:BCL:H162	1.81	0.43
9:r:101:BCL:HBB2	9:r:101:BCL:HMB3	2.00	0.43
9:7:101:BCL:HBA1	9:7:101:BCL:H3A	1.60	0.43
9:M:402:BCL:H93	9:M:402:BCL:H62	1.75	0.43
5:H:168:TRP:HB2	5:H:178:TYR:HB2	1.98	0.43
10:1:103:SPN:H29	3:2:19:LEU:HA	2.01	0.43
9:2:101:BCL:HBA1	9:2:101:BCL:H3A	1.68	0.43
10:k:102:SPN:HM11	10:l:102:SPN:H212	2.01	0.43
2:a:46:LEU:HD13	3:b:45:ARG:NH2	2.33	0.43
10:a:103:SPN:HM61	10:a:103:SPN:C21	2.49	0.43
2:i:26:LEU:HD21	6:L:44:LEU:HB3	2.01	0.43
4:C:236:VAL:CG1	4:C:237:GLU:N	2.80	0.43
9:M:402:BCL:HBB2	10:M:406:SPN:CM6	2.49	0.43
9:9:102:BCL:H142	9:9:102:BCL:H111	1.82	0.43
3:v:32:ALA:HA	3:v:35:VAL:CG1	2.48	0.43
9:s:101:BCL:HHH	3:t:41:THR:HG21	2.01	0.43
2:k:5:TYR:CE2	3:l:13:ASP:OD1	2.72	0.43
2:k:5:TYR:HE2	3:l:13:ASP:OD1	2.02	0.43
2:o:15:ARG:HH21	4:C:20:PRO:HD3	1.83	0.43
10:1:105:SPN:H281	10:1:105:SPN:HM81	1.57	0.42
3:2:18:GLU:O	3:2:22:VAL:HG23	2.19	0.42
9:n:101:BCL:H62	9:n:101:BCL:H102	1.73	0.42
9:8:101:BCL:H12	9:8:101:BCL:H52	1.80	0.42
7:M:80:VAL:O	7:M:80:VAL:CG1	2.66	0.42
10:1:105:SPN:HM92	3:x:19:LEU:HA	2.00	0.42
9:t:101:BCL:H142	9:t:101:BCL:H111	1.82	0.42
9:h:101:BCL:H141	9:h:101:BCL:H161	1.70	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:t:23:TYR:HA	10:t:102:SPN:H241	2.01	0.42
9:p:101:BCL:HBA1	9:p:101:BCL:H3A	1.82	0.42
10:h:102:SPN:HM11	10:h:103:SPN:H212	2.01	0.42
10:h:103:SPN:H281	10:h:103:SPN:HM81	1.58	0.42
2:e:27:LEU:CD2	9:f:101:BCL:HED1	2.49	0.42
10:1:104:SPN:HM61	10:1:104:SPN:H211	2.00	0.42
2:3:8:TRP:CE2	3:4:19:LEU:CD2	3.02	0.42
2:3:8:TRP:CE2	3:4:19:LEU:HD22	2.54	0.42
9:4:101:BCL:H62	9:4:101:BCL:H102	1.36	0.42
9:m:101:BCL:H3A	9:m:101:BCL:HBA1	1.76	0.42
10:f:102:SPN:H282	10:f:102:SPN:HM81	1.76	0.42
10:c:103:SPN:H282	10:c:103:SPN:HM81	1.71	0.42
9:l:101:BCL:HMB1	9:l:101:BCL:CBB	2.45	0.42
4:C:337:GLN:HG2	12:C:403:HEM:HAD2	2.01	0.42
2:w:10:ILE:HD12	10:v:102:SPN:H29	2.02	0.42
10:w:102:SPN:HMB2	3:x:43:ILE:HD13	2.01	0.42
3:p:27:LEU:N	10:p:103:SPN:H19	2.34	0.42
9:9:102:BCL:HMC2	9:9:102:BCL:HHC	1.90	0.42
9:q:101:BCL:H41	9:q:101:BCL:H61	1.54	0.42
6:L:212:ASN:HB3	7:M:143:MET:HE2	2.01	0.42
9:0:101:BCL:H62	9:0:101:BCL:H102	1.24	0.42
9:5:101:BCL:H142	9:5:101:BCL:H111	1.84	0.42
2:i:27:LEU:HA	2:i:30:MET:HG2	2.02	0.42
10:7:103:SPN:H281	10:7:103:SPN:HM81	1.86	0.42
9:5:101:BCL:HMC2	9:5:101:BCL:HHC	1.87	0.42
2:u:25:PHE:HB2	9:u:101:BCL:H2	2.02	0.42
2:s:1:MET:C	2:s:3:LYS:N	2.77	0.42
9:s:101:BCL:HBA1	9:s:101:BCL:H3A	1.67	0.42
9:l:101:BCL:H202	9:l:101:BCL:OBB	2.20	0.42
9:d:101:BCL:H192	9:d:101:BCL:OBB	2.20	0.42
9:j:101:BCL:HMC2	9:j:101:BCL:HHC	1.87	0.42
5:H:54:PRO:HD3	11:H:303:MW9:C23	2.50	0.42
9:M:402:BCL:H2	9:M:402:BCL:H62	1.52	0.42
9:M:402:BCL:H111	9:M:402:BCL:H142	1.60	0.42
3:h:43:ILE:HD12	10:h:102:SPN:HMB2	2.02	0.41
9:b:101:BCL:H62	9:b:101:BCL:H2	1.51	0.41
4:C:101:VAL:HG11	4:C:142:ILE:HD12	2.02	0.41
4:C:123:TRP:HE3	4:C:169:CYS:HB2	1.85	0.41
4:C:206:LEU:HD23	4:C:206:LEU:HA	1.82	0.41
3:n:24:MET:HE3	3:n:24:MET:HB3	1.96	0.41
10:i:102:SPN:HM71	10:i:102:SPN:H241	1.70	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:355:VAL:O	4:C:355:VAL:HG22	2.19	0.41
10:f:102:SPN:HM61	10:f:102:SPN:C21	2.48	0.41
10:c:102:SPN:H241	10:c:102:SPN:HM71	1.71	0.41
9:8:101:BCL:H61	9:8:101:BCL:H92	1.79	0.41
10:1:104:SPN:HMA3	10:1:104:SPN:HM12	1.87	0.41
10:5:103:SPN:H72	9:3:101:BCL:HBA1	2.01	0.41
9:3:101:BCL:H121	9:3:101:BCL:H162	1.76	0.41
2:g:32:HIS:CE1	9:h:101:BCL:HMD1	2.55	0.41
10:f:102:SPN:HM71	10:f:102:SPN:H241	1.66	0.41
2:7:27:LEU:HD23	9:8:101:BCL:HED1	2.02	0.41
9:3:101:BCL:CBB	9:3:101:BCL:HMB1	2.50	0.41
10:l:102:SPN:H4	9:i:101:BCL:HMB2	2.03	0.41
1:A:28:GLY:O	1:A:32:VAL:HG23	2.21	0.41
10:1:103:SPN:HM62	3:2:30:PHE:HB2	2.03	0.41
9:3:101:BCL:H142	9:3:101:BCL:H111	1.83	0.41
10:p:103:SPN:H241	10:p:103:SPN:HM71	1.89	0.41
9:7:101:BCL:H121	9:7:101:BCL:H162	1.64	0.41
10:l:102:SPN:C4	9:i:101:BCL:HMB2	2.50	0.41
4:C:332:HIS:CE1	4:C:338:PRO:HD3	2.55	0.41
3:6:32:ALA:O	3:6:36:VAL:HG23	2.20	0.41
2:i:40:HIS:NE2	3:j:45:ARG:NH2	2.67	0.41
4:C:233:GLU:HB2	4:C:236:VAL:CG2	2.50	0.41
2:u:27:LEU:HD11	10:v:102:SPN:H62	2.03	0.41
2:q:38:THR:HG21	2:o:44:PHE:HB3	2.02	0.41
9:o:101:BCL:HBA1	9:o:101:BCL:H3A	1.78	0.41
9:p:101:BCL:H143	9:p:101:BCL:H161	1.90	0.41
9:p:101:BCL:HMC2	9:p:101:BCL:HHC	1.87	0.41
3:n:19:LEU:HD12	10:n:102:SPN:C27	2.51	0.41
2:e:42:ASN:HB3	2:e:45:GLU:CD	2.43	0.41
2:c:46:LEU:HD23	3:d:44:TRP:HZ2	1.86	0.41
8:L:305:U10:H201	8:L:305:U10:H222	1.71	0.41
10:0:102:SPN:HM13	10:0:102:SPN:HMA2	1.85	0.41
10:5:103:SPN:HM53	9:6:101:BCL:H43	2.03	0.41
9:6:101:BCL:H12	9:6:101:BCL:H52	1.64	0.41
3:t:6:LEU:HD23	3:t:6:LEU:HA	1.95	0.41
10:p:102:SPN:HM71	10:p:102:SPN:H242	1.68	0.41
9:k:101:BCL:H143	9:k:101:BCL:H111	1.78	0.41
5:H:35:MET:HE2	5:H:57:LEU:HD23	2.03	0.41
9:k:101:BCL:HMB1	9:k:101:BCL:HBB3	2.02	0.40
9:2:101:BCL:HHH	9:2:101:BCL:HAC1	1.83	0.40
3:v:12:THR:CG2	3:v:13:ASP:H	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:v:101:BCL:HAA1	9:v:101:BCL:H142	2.02	0.40
2:k:10:ILE:HD11	10:j:102:SPN:HMB3	2.03	0.40
9:h:101:BCL:H3A	9:h:101:BCL:HBA1	1.73	0.40
9:a:101:BCL:H142	9:a:101:BCL:H111	1.93	0.40
9:7:101:BCL:H142	9:7:101:BCL:H111	1.84	0.40
10:7:103:SPN:HM92	2:9:6:LYS:HB3	2.03	0.40
6:L:140:MET:HE2	6:L:140:MET:HB3	1.93	0.40
9:0:101:BCL:H193	9:0:101:BCL:H162	1.78	0.40
3:0:18:GLU:O	3:0:22:VAL:HG23	2.21	0.40
9:3:101:BCL:HBA1	9:3:101:BCL:H3A	1.64	0.40
9:q:101:BCL:HMC2	9:q:101:BCL:HHC	1.84	0.40
9:j:101:BCL:H2A	9:j:101:BCL:HED2	2.04	0.40
13:L:303:BPH:H2	13:M:409:BPH:HBB1	2.03	0.40
9:p:101:BCL:H172	9:p:101:BCL:CAB	2.52	0.40
9:d:101:BCL:HBA1	9:d:101:BCL:H3A	1.91	0.40
6:L:136:ARG:HB3	6:L:137:PRO:HD3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
2	1	49/51 (96%)	49 (100%)	0	0	100	100
2	3	49/51 (96%)	49 (100%)	0	0	100	100
2	5	49/51 (96%)	47 (96%)	2 (4%)	0	100	100
2	7	49/51 (96%)	49 (100%)	0	0	100	100
2	9	49/51 (96%)	47 (96%)	2 (4%)	0	100	100
2	a	49/51 (96%)	49 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	c	49/51 (96%)	49 (100%)	0	0	100	100
2	e	49/51 (96%)	49 (100%)	0	0	100	100
2	g	49/51 (96%)	49 (100%)	0	0	100	100
2	i	49/51 (96%)	49 (100%)	0	0	100	100
2	k	49/51 (96%)	49 (100%)	0	0	100	100
2	m	49/51 (96%)	49 (100%)	0	0	100	100
2	o	49/51 (96%)	45 (92%)	4 (8%)	0	100	100
2	q	49/51 (96%)	49 (100%)	0	0	100	100
2	s	49/51 (96%)	48 (98%)	1 (2%)	0	100	100
2	u	49/51 (96%)	49 (100%)	0	0	100	100
2	w	49/51 (96%)	49 (100%)	0	0	100	100
3	0	42/44 (96%)	42 (100%)	0	0	100	100
3	2	42/44 (96%)	42 (100%)	0	0	100	100
3	4	42/44 (96%)	42 (100%)	0	0	100	100
3	6	42/44 (96%)	42 (100%)	0	0	100	100
3	8	42/44 (96%)	42 (100%)	0	0	100	100
3	b	42/44 (96%)	42 (100%)	0	0	100	100
3	d	42/44 (96%)	42 (100%)	0	0	100	100
3	f	42/44 (96%)	42 (100%)	0	0	100	100
3	h	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
3	j	42/44 (96%)	42 (100%)	0	0	100	100
3	l	42/44 (96%)	42 (100%)	0	0	100	100
3	n	42/44 (96%)	42 (100%)	0	0	100	100
3	p	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
3	r	42/44 (96%)	40 (95%)	2 (5%)	0	100	100
3	t	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
3	v	42/44 (96%)	42 (100%)	0	0	100	100
3	x	42/44 (96%)	42 (100%)	0	0	100	100
4	C	355/357 (99%)	338 (95%)	17 (5%)	0	100	100
5	H	253/255 (99%)	248 (98%)	5 (2%)	0	100	100
6	L	271/273 (99%)	266 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	M	323/325 (99%)	317 (98%)	6 (2%)	0	100	100
All	All	2823/2901 (97%)	2772 (98%)	51 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	55/55 (100%)	55 (100%)	0	100	100
2	1	43/43 (100%)	43 (100%)	0	100	100
2	3	43/43 (100%)	43 (100%)	0	100	100
2	5	43/43 (100%)	43 (100%)	0	100	100
2	7	43/43 (100%)	43 (100%)	0	100	100
2	9	43/43 (100%)	43 (100%)	0	100	100
2	a	43/43 (100%)	43 (100%)	0	100	100
2	c	43/43 (100%)	43 (100%)	0	100	100
2	e	43/43 (100%)	42 (98%)	1 (2%)	44	72
2	g	43/43 (100%)	43 (100%)	0	100	100
2	i	43/43 (100%)	43 (100%)	0	100	100
2	k	43/43 (100%)	43 (100%)	0	100	100
2	m	43/43 (100%)	43 (100%)	0	100	100
2	o	43/43 (100%)	43 (100%)	0	100	100
2	q	43/43 (100%)	43 (100%)	0	100	100
2	s	43/43 (100%)	43 (100%)	0	100	100
2	u	43/43 (100%)	43 (100%)	0	100	100
2	w	43/43 (100%)	43 (100%)	0	100	100
3	0	37/37 (100%)	37 (100%)	0	100	100
3	2	37/37 (100%)	37 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	4	37/37 (100%)	37 (100%)	0	100	100
3	6	37/37 (100%)	37 (100%)	0	100	100
3	8	37/37 (100%)	37 (100%)	0	100	100
3	b	37/37 (100%)	37 (100%)	0	100	100
3	d	37/37 (100%)	37 (100%)	0	100	100
3	f	37/37 (100%)	37 (100%)	0	100	100
3	h	37/37 (100%)	37 (100%)	0	100	100
3	j	37/37 (100%)	37 (100%)	0	100	100
3	l	37/37 (100%)	37 (100%)	0	100	100
3	n	37/37 (100%)	37 (100%)	0	100	100
3	p	37/37 (100%)	37 (100%)	0	100	100
3	r	37/37 (100%)	37 (100%)	0	100	100
3	t	37/37 (100%)	37 (100%)	0	100	100
3	v	37/37 (100%)	37 (100%)	0	100	100
3	x	37/37 (100%)	37 (100%)	0	100	100
4	C	304/304 (100%)	303 (100%)	1 (0%)	86	94
5	H	213/213 (100%)	212 (100%)	1 (0%)	81	92
6	L	217/217 (100%)	217 (100%)	0	100	100
7	M	266/266 (100%)	263 (99%)	3 (1%)	65	84
All	All	2415/2415 (100%)	2409 (100%)	6 (0%)	85	95

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	e	15	ARG
4	C	104	VAL
5	H	234	ASP
7	M	117	ILE
7	M	183	HIS
7	M	217	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
3	2	15	GLN
3	6	15	GLN
2	u	40	HIS
2	s	40	HIS
2	s	42	ASN
2	o	20	GLN
2	o	40	HIS
3	n	20	HIS
3	l	20	HIS
2	e	20	GLN
3	f	15	GLN
2	c	20	GLN
2	a	40	HIS
2	i	20	GLN
2	i	40	HIS
4	C	100	ASN
4	C	146	GLN
4	C	223	ASN
4	C	353	ASN
5	H	94	ASN
6	L	56	GLN
6	L	169	HIS
6	L	212	ASN
6	L	231	HIS
7	M	79	GLN
7	M	203	HIS
7	M	267	HIS
7	M	294	ASN
7	M	310	GLN
3	0	20	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 93 ligands modelled in this entry, 1 is monoatomic - leaving 92 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
10	SPN	c	102	-	42,42,42	3.93	20 (47%)	50,52,52	2.39	22 (44%)
11	MW9	M	408	-	52,52,52	0.65	1 (1%)	55,58,58	0.52	2 (3%)
10	SPN	a	103	-	42,42,42	3.98	20 (47%)	50,52,52	2.61	18 (36%)
8	U10	L	305	-	38,38,63	1.33	2 (5%)	48,49,79	2.43	13 (27%)
9	BCL	p	101	3	69,74,74	0.53	1 (1%)	79,115,115	1.04	9 (11%)
9	BCL	7	101	2	69,74,74	0.57	0	79,115,115	1.03	8 (10%)
10	SPN	1	102	-	42,42,42	3.88	20 (47%)	50,52,52	2.38	20 (40%)
9	BCL	L	304	6	69,74,74	0.63	1 (1%)	79,115,115	1.21	11 (13%)
9	BCL	k	101	2	69,74,74	0.57	0	79,115,115	1.02	7 (8%)
9	BCL	M	402	7	69,74,74	1.79	17 (24%)	79,115,115	2.52	29 (36%)
10	SPN	u	102	-	42,42,42	3.94	20 (47%)	50,52,52	2.38	20 (40%)
11	MW9	H	301	-	52,52,52	0.66	1 (1%)	55,58,58	0.62	2 (3%)
9	BCL	w	101	2	69,74,74	0.55	1 (1%)	79,115,115	1.03	7 (8%)
9	BCL	5	101	2	69,74,74	0.56	1 (1%)	79,115,115	1.04	6 (7%)
10	SPN	s	102	-	42,42,42	3.93	20 (47%)	50,52,52	2.38	22 (44%)
11	MW9	9	101	-	52,52,52	0.62	1 (1%)	55,58,58	0.54	2 (3%)
10	SPN	n	102	-	42,42,42	3.96	20 (47%)	50,52,52	2.41	19 (38%)
9	BCL	c	101	2	69,74,74	0.55	0	79,115,115	1.00	9 (11%)
9	BCL	9	102	2	69,74,74	0.58	1 (1%)	79,115,115	0.99	7 (8%)
10	SPN	M	406	-	42,42,42	3.95	20 (47%)	50,52,52	2.69	16 (32%)
10	SPN	h	103	-	42,42,42	3.94	20 (47%)	50,52,52	2.54	15 (30%)
10	SPN	l	102	-	42,42,42	3.95	20 (47%)	50,52,52	2.51	16 (32%)
11	MW9	g	103	-	49,49,52	0.66	1 (2%)	52,55,58	0.66	2 (3%)
11	MW9	H	303	-	52,52,52	0.64	1 (1%)	55,58,58	0.62	2 (3%)
10	SPN	t	102	-	42,42,42	3.95	20 (47%)	50,52,52	2.42	19 (38%)
11	MW9	M	407	-	52,52,52	0.64	1 (1%)	55,58,58	0.84	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	BCL	s	101	2	69,74,74	0.56	2 (2%)	79,115,115	1.08	10 (12%)
9	BCL	j	101	3	69,74,74	0.56	0	79,115,115	1.02	9 (11%)
10	SPN	1	104	-	42,42,42	4.04	20 (47%)	50,52,52	2.61	16 (32%)
9	BCL	x	101	3	69,74,74	0.53	0	79,115,115	1.03	8 (10%)
9	BCL	b	101	3	69,74,74	1.74	18 (26%)	79,115,115	2.55	25 (31%)
10	SPN	p	103	-	42,42,42	3.93	20 (47%)	50,52,52	2.46	18 (36%)
10	SPN	k	102	-	42,42,42	3.93	20 (47%)	50,52,52	2.38	22 (44%)
9	BCL	g	101	2	69,74,74	0.57	0	79,115,115	0.99	10 (12%)
9	BCL	o	101	2	69,74,74	0.60	1 (1%)	79,115,115	1.11	9 (11%)
13	BPH	M	405	-	59,70,70	1.22	4 (6%)	59,101,101	0.94	3 (5%)
12	HEM	C	403	4	50,50,50	0.80	1 (2%)	67,82,82	0.84	2 (2%)
9	BCL	4	101	3	69,74,74	1.74	20 (28%)	79,115,115	2.52	26 (32%)
10	SPN	1	105	-	42,42,42	4.03	20 (47%)	50,52,52	2.39	17 (34%)
9	BCL	t	101	3	69,74,74	0.55	0	79,115,115	1.00	6 (7%)
10	SPN	v	102	-	42,42,42	4.00	20 (47%)	50,52,52	2.55	18 (36%)
9	BCL	h	101	3	69,74,74	0.59	1 (1%)	79,115,115	0.99	7 (8%)
8	U10	L	302	-	38,38,63	0.20	0	48,49,79	0.53	1 (2%)
10	SPN	h	102	-	42,42,42	3.91	20 (47%)	50,52,52	2.38	22 (44%)
10	SPN	c	103	-	42,42,42	4.05	20 (47%)	50,52,52	2.44	18 (36%)
10	SPN	1	103	-	42,42,42	3.89	20 (47%)	50,52,52	2.73	20 (40%)
10	SPN	r	102	-	42,42,42	3.95	20 (47%)	50,52,52	2.37	21 (42%)
9	BCL	v	101	3	69,74,74	0.52	0	79,115,115	1.08	8 (10%)
9	BCL	6	101	3	69,74,74	1.75	19 (27%)	79,115,115	2.54	24 (30%)
10	SPN	a	102	-	42,42,42	3.91	20 (47%)	50,52,52	2.41	19 (38%)
9	BCL	f	101	3	69,74,74	0.56	0	79,115,115	1.03	8 (10%)
10	SPN	p	102	-	42,42,42	3.96	20 (47%)	50,52,52	2.43	19 (38%)
9	BCL	r	101	3	69,74,74	0.56	0	79,115,115	1.07	11 (13%)
10	SPN	7	103	-	42,42,42	3.98	20 (47%)	50,52,52	2.42	17 (34%)
9	BCL	0	101	3	69,74,74	1.75	18 (26%)	79,115,115	2.58	24 (30%)
10	SPN	9	103	-	42,42,42	3.92	20 (47%)	50,52,52	2.39	22 (44%)
11	MW9	g	102	-	52,52,52	0.64	1 (1%)	55,58,58	0.65	2 (3%)
13	BPH	M	409	-	59,70,70	1.08	4 (6%)	59,101,101	1.01	5 (8%)
9	BCL	M	404	7	69,74,74	0.57	0	79,115,115	1.07	7 (8%)
9	BCL	i	101	2	69,74,74	0.61	0	79,115,115	1.05	8 (10%)
9	BCL	l	101	3	69,74,74	0.52	0	79,115,115	1.05	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	U10	M	403	-	63,63,63	1.20	2 (3%)	78,79,79	1.57	16 (20%)
9	BCL	e	101	2	69,74,74	0.58	1 (1%)	79,115,115	1.00	9 (11%)
10	SPN	i	102	-	42,42,42	3.91	20 (47%)	50,52,52	2.39	21 (42%)
12	HEM	C	402	4	50,50,50	0.85	1 (2%)	67,82,82	1.53	5 (7%)
10	SPN	q	102	-	42,42,42	3.98	20 (47%)	50,52,52	2.49	18 (36%)
9	BCL	3	101	2	69,74,74	0.60	0	79,115,115	1.03	8 (10%)
9	BCL	8	101	3	69,74,74	1.74	18 (26%)	79,115,115	2.64	26 (32%)
10	SPN	e	102	-	42,42,42	3.93	20 (47%)	50,52,52	2.39	22 (44%)
11	MW9	H	304	-	52,52,52	0.63	1 (1%)	55,58,58	0.56	2 (3%)
9	BCL	d	101	3	69,74,74	0.55	0	79,115,115	1.01	8 (10%)
9	BCL	a	101	2	69,74,74	0.59	1 (1%)	79,115,115	0.99	8 (10%)
10	SPN	5	102	-	42,42,42	3.89	20 (47%)	50,52,52	2.43	20 (40%)
10	SPN	j	102	-	42,42,42	3.98	20 (47%)	50,52,52	2.61	16 (32%)
9	BCL	u	101	2	69,74,74	0.57	1 (1%)	79,115,115	0.98	7 (8%)
13	BPH	L	303	-	59,70,70	1.17	4 (6%)	59,101,101	1.12	6 (10%)
10	SPN	3	102	-	42,42,42	3.87	20 (47%)	50,52,52	2.41	21 (42%)
10	SPN	0	102	-	42,42,42	3.96	20 (47%)	50,52,52	2.42	16 (32%)
12	HEM	C	401	4	50,50,50	0.88	2 (4%)	67,82,82	0.77	2 (2%)
11	MW9	H	302	-	52,52,52	0.65	1 (1%)	55,58,58	0.73	3 (5%)
10	SPN	w	102	-	42,42,42	3.91	20 (47%)	50,52,52	2.39	21 (42%)
10	SPN	5	103	-	42,42,42	4.01	20 (47%)	50,52,52	2.44	17 (34%)
10	SPN	f	102	-	42,42,42	3.96	20 (47%)	50,52,52	2.53	15 (30%)
9	BCL	1	101	2	69,74,74	0.54	0	79,115,115	1.09	7 (8%)
9	BCL	2	101	3	69,74,74	1.74	18 (26%)	79,115,115	2.57	24 (30%)
10	SPN	m	102	-	42,42,42	3.95	20 (47%)	50,52,52	2.37	21 (42%)
9	BCL	q	101	2	69,74,74	0.61	0	79,115,115	1.06	6 (7%)
9	BCL	n	101	3	69,74,74	0.54	0	79,115,115	1.03	6 (7%)
8	U10	A	101	-	43,43,63	1.31	2 (4%)	54,55,79	1.91	17 (31%)
10	SPN	7	102	-	42,42,42	3.93	20 (47%)	50,52,52	2.38	22 (44%)
9	BCL	m	101	2	69,74,74	0.55	1 (1%)	79,115,115	1.02	7 (8%)
9	BCL	L	301	6	69,74,74	0.65	1 (1%)	79,115,115	1.09	8 (10%)

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
10	SPN	c	102	-	-	20/50/51/51	-
11	MW9	M	408	-	-	25/57/57/57	-
10	SPN	a	103	-	-	20/50/51/51	-
8	U10	L	305	-	-	11/33/57/87	0/1/1/1
9	BCL	p	101	3	-	15/41/137/137	-
9	BCL	7	101	2	-	20/41/137/137	-
10	SPN	1	102	-	-	24/50/51/51	-
9	BCL	L	304	6	-	26/41/137/137	-
9	BCL	k	101	2	-	16/41/137/137	-
9	BCL	M	402	7	-	16/41/137/137	-
10	SPN	u	102	-	-	21/50/51/51	-
11	MW9	H	301	-	-	35/57/57/57	-
9	BCL	w	101	2	-	19/41/137/137	-
9	BCL	5	101	2	-	19/41/137/137	-
10	SPN	s	102	-	-	18/50/51/51	-
11	MW9	9	101	-	-	34/57/57/57	-
10	SPN	n	102	-	-	21/50/51/51	-
9	BCL	c	101	2	-	20/41/137/137	-
9	BCL	9	102	2	-	18/41/137/137	-
10	SPN	M	406	-	-	17/50/51/51	-
10	SPN	h	103	-	-	21/50/51/51	-
10	SPN	l	102	-	-	20/50/51/51	-
11	MW9	g	103	-	-	18/54/54/57	-
11	MW9	H	303	-	-	34/57/57/57	-
10	SPN	t	102	-	-	18/50/51/51	-
11	MW9	M	407	-	-	18/57/57/57	-
9	BCL	s	101	2	-	21/41/137/137	-
9	BCL	j	101	3	-	22/41/137/137	-
10	SPN	1	104	-	-	22/50/51/51	-
9	BCL	x	101	3	-	18/41/137/137	-
9	BCL	b	101	3	-	22/41/137/137	-
10	SPN	p	103	-	-	22/50/51/51	-
10	SPN	k	102	-	-	22/50/51/51	-
9	BCL	g	101	2	-	23/41/137/137	-
9	BCL	o	101	2	-	12/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	BPH	M	405	-	-	9/37/105/105	0/5/6/6
12	HEM	C	403	4	-	4/14/54/54	-
9	BCL	4	101	3	-	19/41/137/137	-
10	SPN	1	105	-	-	22/50/51/51	-
9	BCL	t	101	3	-	18/41/137/137	-
10	SPN	v	102	-	-	18/50/51/51	-
9	BCL	h	101	3	-	19/41/137/137	-
8	U10	L	302	-	-	6/33/57/87	0/1/1/1
10	SPN	h	102	-	-	20/50/51/51	-
10	SPN	c	103	-	-	22/50/51/51	-
10	SPN	1	103	-	-	19/50/51/51	-
10	SPN	r	102	-	-	20/50/51/51	-
9	BCL	v	101	3	-	14/41/137/137	-
9	BCL	6	101	3	-	15/41/137/137	-
10	SPN	a	102	-	-	23/50/51/51	-
9	BCL	f	101	3	-	16/41/137/137	-
10	SPN	p	102	-	-	25/50/51/51	-
9	BCL	r	101	3	-	22/41/137/137	-
10	SPN	7	103	-	-	21/50/51/51	-
9	BCL	0	101	3	-	18/41/137/137	-
10	SPN	9	103	-	-	19/50/51/51	-
11	MW9	g	102	-	-	21/57/57/57	-
13	BPH	M	409	-	-	17/37/105/105	0/5/6/6
9	BCL	M	404	7	-	14/41/137/137	-
9	BCL	i	101	2	-	11/41/137/137	-
9	BCL	l	101	3	-	18/41/137/137	-
8	U10	M	403	-	-	20/63/87/87	0/1/1/1
9	BCL	e	101	2	-	19/41/137/137	-
10	SPN	i	102	-	-	23/50/51/51	-
12	HEM	C	402	4	-	4/14/54/54	-
10	SPN	q	102	-	-	23/50/51/51	-
9	BCL	3	101	2	-	19/41/137/137	-
9	BCL	8	101	3	-	12/41/137/137	-
10	SPN	e	102	-	-	19/50/51/51	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	MW9	H	304	-	-	36/57/57/57	-
9	BCL	d	101	3	-	18/41/137/137	-
9	BCL	a	101	2	-	20/41/137/137	-
10	SPN	5	102	-	-	24/50/51/51	-
10	SPN	j	102	-	-	23/50/51/51	-
9	BCL	u	101	2	-	16/41/137/137	-
13	BPH	L	303	-	-	11/37/105/105	0/5/6/6
10	SPN	3	102	-	-	24/50/51/51	-
10	SPN	0	102	-	-	20/50/51/51	-
12	HEM	C	401	4	-	6/14/54/54	-
11	MW9	H	302	-	-	20/57/57/57	-
10	SPN	w	102	-	-	20/50/51/51	-
10	SPN	5	103	-	-	21/50/51/51	-
10	SPN	f	102	-	-	19/50/51/51	-
9	BCL	1	101	2	-	17/41/137/137	-
9	BCL	2	101	3	-	17/41/137/137	-
10	SPN	m	102	-	-	18/50/51/51	-
9	BCL	q	101	2	-	16/41/137/137	-
9	BCL	n	101	3	-	19/41/137/137	-
8	U10	A	101	-	-	7/39/63/87	0/1/1/1
10	SPN	7	102	-	-	22/50/51/51	-
9	BCL	m	101	2	-	25/41/137/137	-
9	BCL	L	301	6	-	10/41/137/137	-

All (873) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	a	103	SPN	C3-C4	-11.51	1.32	1.50
10	5	103	SPN	C3-C4	-11.50	1.32	1.50
10	c	103	SPN	C3-C4	-11.48	1.32	1.50
10	7	103	SPN	C3-C4	-11.44	1.32	1.50
10	1	104	SPN	C3-C4	-11.37	1.32	1.50
10	q	102	SPN	C3-C4	-11.36	1.32	1.50
10	1	105	SPN	C3-C4	-11.32	1.32	1.50
10	t	102	SPN	C3-C4	-11.26	1.32	1.50
10	1	103	SPN	C3-C4	-11.26	1.32	1.50
10	f	102	SPN	C3-C4	-11.25	1.32	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	0	102	SPN	C3-C4	-11.23	1.32	1.50
10	v	102	SPN	C3-C4	-11.23	1.32	1.50
10	l	102	SPN	C3-C4	-11.19	1.33	1.50
10	n	102	SPN	C3-C4	-11.18	1.33	1.50
10	h	103	SPN	C3-C4	-11.18	1.33	1.50
10	p	102	SPN	C3-C4	-11.15	1.33	1.50
10	M	406	SPN	C3-C4	-11.12	1.33	1.50
10	p	103	SPN	C3-C4	-11.11	1.33	1.50
10	j	102	SPN	C3-C4	-11.10	1.33	1.50
10	k	102	SPN	C3-C4	-11.02	1.33	1.50
10	c	102	SPN	C3-C4	-11.02	1.33	1.50
10	e	102	SPN	C3-C4	-11.01	1.33	1.50
10	r	102	SPN	C3-C4	-11.01	1.33	1.50
10	u	102	SPN	C3-C4	-11.00	1.33	1.50
10	7	102	SPN	C3-C4	-10.99	1.33	1.50
10	m	102	SPN	C3-C4	-10.98	1.33	1.50
10	s	102	SPN	C3-C4	-10.98	1.33	1.50
10	i	102	SPN	C3-C4	-10.96	1.33	1.50
10	w	102	SPN	C3-C4	-10.96	1.33	1.50
10	h	102	SPN	C3-C4	-10.92	1.33	1.50
10	9	103	SPN	C3-C4	-10.89	1.33	1.50
10	1	102	SPN	C3-C4	-10.83	1.33	1.50
10	5	102	SPN	C3-C4	-10.82	1.33	1.50
10	3	102	SPN	C3-C4	-10.82	1.33	1.50
10	a	102	SPN	C3-C4	-10.81	1.33	1.50
10	l	104	SPN	C3-C2	-8.21	1.44	1.52
8	M	403	U10	C6-C1	8.13	1.49	1.35
10	c	103	SPN	C3-C2	-7.74	1.45	1.52
10	p	102	SPN	C17-C18	-7.64	1.35	1.51
10	l	105	SPN	C17-C18	-7.59	1.35	1.51
10	l	105	SPN	C10-C9	-7.56	1.35	1.51
10	M	406	SPN	C14-C13	-7.56	1.35	1.51
10	M	406	SPN	C10-C9	-7.54	1.35	1.51
10	0	102	SPN	C17-C18	-7.52	1.35	1.51
10	l	105	SPN	C14-C13	-7.51	1.35	1.51
10	v	102	SPN	C10-C9	-7.50	1.35	1.51
10	f	102	SPN	C6-C5	-7.50	1.35	1.51
10	c	102	SPN	C6-C5	-7.49	1.35	1.51
10	c	103	SPN	C17-C18	-7.49	1.35	1.51
10	l	105	SPN	C6-C5	-7.49	1.35	1.51
10	M	406	SPN	C6-C5	-7.48	1.35	1.51
10	h	103	SPN	C6-C5	-7.48	1.35	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	m	102	SPN	C10-C9	-7.48	1.35	1.51
10	w	102	SPN	C14-C13	-7.48	1.35	1.51
10	j	102	SPN	C17-C18	-7.48	1.35	1.51
10	p	103	SPN	C6-C5	-7.48	1.35	1.51
10	r	102	SPN	C17-C18	-7.48	1.35	1.51
10	v	102	SPN	C6-C5	-7.47	1.35	1.51
10	l	103	SPN	C6-C5	-7.47	1.35	1.51
10	n	102	SPN	C6-C5	-7.47	1.35	1.51
10	q	102	SPN	C6-C5	-7.47	1.35	1.51
10	s	102	SPN	C10-C9	-7.47	1.35	1.51
10	e	102	SPN	C14-C13	-7.47	1.35	1.51
10	u	102	SPN	C10-C9	-7.47	1.35	1.51
10	n	102	SPN	C17-C18	-7.47	1.35	1.51
10	m	102	SPN	C14-C13	-7.46	1.35	1.51
10	w	102	SPN	C10-C9	-7.46	1.35	1.51
10	m	102	SPN	C17-C18	-7.46	1.35	1.51
10	h	103	SPN	C10-C9	-7.46	1.35	1.51
10	l	102	SPN	C10-C9	-7.46	1.35	1.51
10	v	102	SPN	C14-C13	-7.46	1.35	1.51
10	e	102	SPN	C17-C18	-7.46	1.35	1.51
10	m	102	SPN	C6-C5	-7.45	1.35	1.51
10	7	103	SPN	C17-C18	-7.45	1.35	1.51
10	l	102	SPN	C6-C5	-7.45	1.35	1.51
10	f	102	SPN	C10-C9	-7.45	1.35	1.51
10	c	102	SPN	C10-C9	-7.45	1.35	1.51
10	k	102	SPN	C10-C9	-7.45	1.35	1.51
10	a	102	SPN	C14-C13	-7.45	1.35	1.51
10	c	102	SPN	C14-C13	-7.45	1.35	1.51
10	e	102	SPN	C10-C9	-7.44	1.35	1.51
10	u	102	SPN	C17-C18	-7.44	1.35	1.51
10	9	103	SPN	C14-C13	-7.44	1.35	1.51
10	h	102	SPN	C10-C9	-7.44	1.35	1.51
10	c	103	SPN	C6-C5	-7.44	1.35	1.51
10	9	103	SPN	C6-C5	-7.44	1.35	1.51
10	r	102	SPN	C10-C9	-7.44	1.35	1.51
10	h	102	SPN	C14-C13	-7.44	1.35	1.51
10	h	102	SPN	C6-C5	-7.44	1.35	1.51
10	s	102	SPN	C6-C5	-7.44	1.36	1.51
10	u	102	SPN	C6-C5	-7.44	1.36	1.51
10	p	103	SPN	C10-C9	-7.44	1.36	1.51
10	n	102	SPN	C14-C13	-7.44	1.36	1.51
10	c	103	SPN	C10-C9	-7.43	1.36	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	p	102	SPN	C10-C9	-7.43	1.36	1.51
10	0	102	SPN	C10-C9	-7.43	1.36	1.51
10	u	102	SPN	C14-C13	-7.43	1.36	1.51
10	7	102	SPN	C10-C9	-7.43	1.36	1.51
10	w	102	SPN	C17-C18	-7.43	1.36	1.51
10	5	103	SPN	C17-C18	-7.43	1.36	1.51
10	t	102	SPN	C17-C18	-7.43	1.36	1.51
10	9	103	SPN	C17-C18	-7.43	1.36	1.51
10	r	102	SPN	C14-C13	-7.43	1.36	1.51
10	k	102	SPN	C14-C13	-7.43	1.36	1.51
10	i	102	SPN	C14-C13	-7.43	1.36	1.51
10	c	102	SPN	C17-C18	-7.43	1.36	1.51
10	i	102	SPN	C10-C9	-7.43	1.36	1.51
10	j	102	SPN	C6-C5	-7.43	1.36	1.51
10	w	102	SPN	C6-C5	-7.43	1.36	1.51
10	p	103	SPN	C14-C13	-7.43	1.36	1.51
10	s	102	SPN	C17-C18	-7.43	1.36	1.51
10	p	102	SPN	C14-C13	-7.43	1.36	1.51
10	9	103	SPN	C10-C9	-7.43	1.36	1.51
10	1	104	SPN	C6-C5	-7.43	1.36	1.51
10	n	102	SPN	C10-C9	-7.42	1.36	1.51
10	7	102	SPN	C6-C5	-7.42	1.36	1.51
10	5	103	SPN	C10-C9	-7.42	1.36	1.51
10	k	102	SPN	C17-C18	-7.42	1.36	1.51
10	f	102	SPN	C17-C18	-7.42	1.36	1.51
10	r	102	SPN	C6-C5	-7.42	1.36	1.51
10	M	406	SPN	C17-C18	-7.42	1.36	1.51
10	1	103	SPN	C10-C9	-7.42	1.36	1.51
10	t	102	SPN	C6-C5	-7.42	1.36	1.51
10	j	102	SPN	C10-C9	-7.42	1.36	1.51
10	e	102	SPN	C6-C5	-7.42	1.36	1.51
10	p	102	SPN	C6-C5	-7.41	1.36	1.51
10	1	102	SPN	C14-C13	-7.41	1.36	1.51
10	s	102	SPN	C14-C13	-7.41	1.36	1.51
10	7	102	SPN	C17-C18	-7.41	1.36	1.51
10	7	103	SPN	C10-C9	-7.41	1.36	1.51
10	1	104	SPN	C10-C9	-7.41	1.36	1.51
10	k	102	SPN	C6-C5	-7.41	1.36	1.51
10	7	102	SPN	C14-C13	-7.41	1.36	1.51
10	7	103	SPN	C14-C13	-7.41	1.36	1.51
10	3	102	SPN	C17-C18	-7.40	1.36	1.51
10	l	102	SPN	C14-C13	-7.40	1.36	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	3	102	SPN	C14-C13	-7.40	1.36	1.51
10	1	102	SPN	C17-C18	-7.40	1.36	1.51
10	1	104	SPN	C17-C18	-7.40	1.36	1.51
10	f	102	SPN	C14-C13	-7.40	1.36	1.51
10	0	102	SPN	C14-C13	-7.40	1.36	1.51
10	5	103	SPN	C6-C5	-7.40	1.36	1.51
10	c	103	SPN	C14-C13	-7.39	1.36	1.51
10	h	103	SPN	C17-C18	-7.39	1.36	1.51
10	5	102	SPN	C14-C13	-7.39	1.36	1.51
10	a	102	SPN	C17-C18	-7.39	1.36	1.51
10	1	102	SPN	C10-C9	-7.39	1.36	1.51
10	i	102	SPN	C17-C18	-7.39	1.36	1.51
10	5	103	SPN	C14-C13	-7.39	1.36	1.51
10	l	102	SPN	C17-C18	-7.39	1.36	1.51
10	a	103	SPN	C6-C5	-7.39	1.36	1.51
10	t	102	SPN	C14-C13	-7.39	1.36	1.51
10	7	103	SPN	C6-C5	-7.38	1.36	1.51
10	q	102	SPN	C10-C9	-7.38	1.36	1.51
10	p	103	SPN	C17-C18	-7.38	1.36	1.51
10	h	102	SPN	C17-C18	-7.38	1.36	1.51
10	h	103	SPN	C14-C13	-7.38	1.36	1.51
10	5	102	SPN	C6-C5	-7.38	1.36	1.51
10	a	103	SPN	C17-C18	-7.38	1.36	1.51
10	3	102	SPN	C10-C9	-7.37	1.36	1.51
10	1	102	SPN	C6-C5	-7.37	1.36	1.51
10	i	102	SPN	C6-C5	-7.36	1.36	1.51
10	5	102	SPN	C10-C9	-7.36	1.36	1.51
10	0	102	SPN	C6-C5	-7.36	1.36	1.51
10	q	102	SPN	C17-C18	-7.36	1.36	1.51
10	a	102	SPN	C10-C9	-7.35	1.36	1.51
10	1	104	SPN	C14-C13	-7.35	1.36	1.51
10	3	102	SPN	C6-C5	-7.35	1.36	1.51
10	q	102	SPN	C14-C13	-7.34	1.36	1.51
10	j	102	SPN	C14-C13	-7.34	1.36	1.51
10	1	103	SPN	C14-C13	-7.33	1.36	1.51
10	a	103	SPN	C10-C9	-7.33	1.36	1.51
10	a	102	SPN	C6-C5	-7.32	1.36	1.51
10	t	102	SPN	C10-C9	-7.32	1.36	1.51
10	v	102	SPN	C17-C18	-7.31	1.36	1.51
10	5	102	SPN	C17-C18	-7.31	1.36	1.51
10	a	103	SPN	C14-C13	-7.31	1.36	1.51
8	A	101	U10	C6-C1	7.28	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	a	103	SPN	C3-C2	-7.22	1.45	1.52
10	l	103	SPN	C17-C18	-7.21	1.36	1.51
10	q	102	SPN	C3-C2	-7.17	1.45	1.52
10	5	103	SPN	C3-C2	-6.96	1.46	1.52
10	v	102	SPN	C3-C2	-6.93	1.46	1.52
10	j	102	SPN	C3-C2	-6.79	1.46	1.52
8	L	305	U10	C6-C1	6.71	1.47	1.35
10	p	102	SPN	C3-C2	-6.68	1.46	1.52
10	7	103	SPN	C3-C2	-6.55	1.46	1.52
10	t	102	SPN	C3-C2	-6.54	1.46	1.52
10	l	105	SPN	C3-C2	-6.32	1.46	1.52
10	l	103	SPN	C19-C18	6.20	1.47	1.33
10	a	102	SPN	C3-C2	-6.19	1.46	1.52
10	r	102	SPN	C3-C2	-6.18	1.46	1.52
10	m	102	SPN	C3-C2	-6.15	1.46	1.52
10	p	102	SPN	C8-C9	6.14	1.47	1.33
10	0	102	SPN	C3-C2	-6.07	1.46	1.52
10	M	406	SPN	C3-C2	-6.06	1.46	1.52
13	M	405	BPH	C1D-C2D	6.04	1.46	1.39
10	f	102	SPN	C3-C2	-6.01	1.46	1.52
10	l	102	SPN	C3-C2	-6.00	1.46	1.52
10	j	102	SPN	C19-C18	5.99	1.46	1.33
10	l	102	SPN	C19-C18	5.96	1.46	1.33
10	l	104	SPN	C19-C18	5.95	1.46	1.33
10	a	103	SPN	C19-C18	5.94	1.46	1.33
10	u	102	SPN	C3-C2	-5.91	1.46	1.52
10	v	102	SPN	C19-C18	5.90	1.46	1.33
13	L	303	BPH	C1D-C2D	5.89	1.46	1.39
10	k	102	SPN	C3-C2	-5.86	1.47	1.52
10	M	406	SPN	C19-C18	5.83	1.46	1.33
10	n	102	SPN	C3-C2	-5.83	1.47	1.52
10	s	102	SPN	C3-C2	-5.80	1.47	1.52
10	7	102	SPN	C3-C2	-5.80	1.47	1.52
10	h	103	SPN	C3-C2	-5.78	1.47	1.52
10	5	102	SPN	C3-C2	-5.74	1.47	1.52
10	3	102	SPN	C12-C13	5.68	1.46	1.33
10	f	102	SPN	C19-C18	5.67	1.46	1.33
10	p	102	SPN	C12-C13	5.67	1.46	1.33
10	p	103	SPN	C19-C18	5.67	1.46	1.33
10	c	102	SPN	C3-C2	-5.67	1.47	1.52
10	9	103	SPN	C3-C2	-5.67	1.47	1.52
10	a	102	SPN	C12-C13	5.66	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	t	102	SPN	C12-C13	5.66	1.46	1.33
10	h	103	SPN	C19-C18	5.66	1.46	1.33
10	5	102	SPN	C12-C13	5.65	1.46	1.33
10	3	102	SPN	C8-C9	5.65	1.46	1.33
10	a	103	SPN	C12-C13	5.65	1.46	1.33
10	a	102	SPN	C4-C5	5.64	1.46	1.33
10	1	105	SPN	C20-C19	-5.64	1.33	1.50
10	p	103	SPN	C3-C2	-5.63	1.47	1.52
10	1	102	SPN	C12-C13	5.63	1.46	1.33
10	5	102	SPN	C8-C9	5.63	1.46	1.33
10	q	102	SPN	C12-C13	5.62	1.46	1.33
10	5	102	SPN	C4-C5	5.62	1.46	1.33
10	c	103	SPN	C8-C9	5.61	1.46	1.33
10	u	102	SPN	C8-C9	5.61	1.46	1.33
10	h	102	SPN	C8-C9	5.61	1.46	1.33
10	t	102	SPN	C8-C9	5.60	1.46	1.33
10	e	102	SPN	C12-C13	5.60	1.45	1.33
10	0	102	SPN	C8-C9	5.60	1.45	1.33
10	n	102	SPN	C8-C9	5.59	1.45	1.33
10	h	102	SPN	C12-C13	5.59	1.45	1.33
10	a	102	SPN	C8-C9	5.59	1.45	1.33
10	w	102	SPN	C12-C13	5.59	1.45	1.33
10	h	102	SPN	C4-C5	5.59	1.45	1.33
10	5	103	SPN	C8-C9	5.59	1.45	1.33
10	u	102	SPN	C4-C5	5.59	1.45	1.33
10	i	102	SPN	C8-C9	5.59	1.45	1.33
10	j	102	SPN	C12-C13	5.58	1.45	1.33
10	9	103	SPN	C8-C9	5.58	1.45	1.33
10	k	102	SPN	C4-C5	5.58	1.45	1.33
10	c	102	SPN	C12-C13	5.58	1.45	1.33
10	1	102	SPN	C8-C9	5.58	1.45	1.33
10	1	102	SPN	C4-C5	5.58	1.45	1.33
10	7	102	SPN	C8-C9	5.57	1.45	1.33
10	0	102	SPN	C12-C13	5.57	1.45	1.33
10	e	102	SPN	C8-C9	5.57	1.45	1.33
10	M	406	SPN	C4-C5	5.57	1.45	1.33
10	w	102	SPN	C8-C9	5.57	1.45	1.33
10	n	102	SPN	C4-C5	5.57	1.45	1.33
10	i	102	SPN	C12-C13	5.56	1.45	1.33
10	k	102	SPN	C8-C9	5.56	1.45	1.33
10	t	102	SPN	C19-C18	5.56	1.45	1.33
13	M	409	BPH	C1D-C2D	5.56	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	l	104	SPN	C12-C13	5.56	1.45	1.33
10	k	102	SPN	C12-C13	5.56	1.45	1.33
10	p	103	SPN	C4-C5	5.56	1.45	1.33
10	h	103	SPN	C8-C9	5.56	1.45	1.33
10	f	102	SPN	C4-C5	5.56	1.45	1.33
10	j	102	SPN	C8-C9	5.56	1.45	1.33
10	7	103	SPN	C8-C9	5.56	1.45	1.33
10	s	102	SPN	C8-C9	5.56	1.45	1.33
10	r	102	SPN	C8-C9	5.56	1.45	1.33
10	f	102	SPN	C8-C9	5.55	1.45	1.33
10	w	102	SPN	C4-C5	5.55	1.45	1.33
10	m	102	SPN	C12-C13	5.55	1.45	1.33
10	j	102	SPN	C4-C5	5.55	1.45	1.33
10	c	102	SPN	C8-C9	5.55	1.45	1.33
10	s	102	SPN	C12-C13	5.55	1.45	1.33
10	r	102	SPN	C12-C13	5.55	1.45	1.33
10	l	104	SPN	C8-C9	5.55	1.45	1.33
10	e	102	SPN	C4-C5	5.55	1.45	1.33
10	l	103	SPN	C8-C9	5.55	1.45	1.33
10	p	103	SPN	C12-C13	5.55	1.45	1.33
10	m	102	SPN	C4-C5	5.55	1.45	1.33
10	a	103	SPN	C8-C9	5.55	1.45	1.33
10	s	102	SPN	C4-C5	5.55	1.45	1.33
10	h	103	SPN	C4-C5	5.55	1.45	1.33
10	u	102	SPN	C12-C13	5.54	1.45	1.33
10	l	102	SPN	C4-C5	5.54	1.45	1.33
10	M	406	SPN	C8-C9	5.54	1.45	1.33
10	7	102	SPN	C12-C13	5.54	1.45	1.33
10	9	103	SPN	C4-C5	5.54	1.45	1.33
10	3	102	SPN	C4-C5	5.54	1.45	1.33
10	3	102	SPN	C19-C18	5.54	1.45	1.33
10	m	102	SPN	C8-C9	5.54	1.45	1.33
10	m	102	SPN	C19-C18	5.54	1.45	1.33
10	r	102	SPN	C4-C5	5.54	1.45	1.33
10	c	102	SPN	C19-C18	5.53	1.45	1.33
10	i	102	SPN	C19-C18	5.53	1.45	1.33
10	e	102	SPN	C3-C2	-5.53	1.47	1.52
10	v	102	SPN	C4-C5	5.53	1.45	1.33
10	i	102	SPN	C4-C5	5.53	1.45	1.33
10	q	102	SPN	C8-C9	5.53	1.45	1.33
10	9	103	SPN	C12-C13	5.53	1.45	1.33
10	p	103	SPN	C8-C9	5.52	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	406	SPN	C11-C12	-5.52	1.33	1.50
10	e	102	SPN	C19-C18	5.52	1.45	1.33
10	9	103	SPN	C19-C18	5.52	1.45	1.33
10	s	102	SPN	C19-C18	5.52	1.45	1.33
10	l	102	SPN	C12-C13	5.52	1.45	1.33
10	c	102	SPN	C4-C5	5.52	1.45	1.33
10	a	102	SPN	C19-C18	5.52	1.45	1.33
10	7	102	SPN	C4-C5	5.52	1.45	1.33
10	n	102	SPN	C12-C13	5.52	1.45	1.33
10	1	103	SPN	C4-C5	5.52	1.45	1.33
10	h	102	SPN	C19-C18	5.52	1.45	1.33
10	c	103	SPN	C12-C13	5.51	1.45	1.33
10	7	102	SPN	C19-C18	5.51	1.45	1.33
10	l	102	SPN	C8-C9	5.51	1.45	1.33
10	M	406	SPN	C12-C13	5.51	1.45	1.33
10	5	103	SPN	C12-C13	5.51	1.45	1.33
10	w	102	SPN	C19-C18	5.51	1.45	1.33
10	v	102	SPN	C12-C13	5.51	1.45	1.33
10	n	102	SPN	C19-C18	5.50	1.45	1.33
10	u	102	SPN	C19-C18	5.50	1.45	1.33
10	7	103	SPN	C12-C13	5.50	1.45	1.33
10	r	102	SPN	C19-C18	5.50	1.45	1.33
10	h	103	SPN	C12-C13	5.50	1.45	1.33
10	h	102	SPN	C3-C2	-5.50	1.47	1.52
10	f	102	SPN	C12-C13	5.50	1.45	1.33
10	p	102	SPN	C19-C18	5.49	1.45	1.33
10	k	102	SPN	C19-C18	5.49	1.45	1.33
10	v	102	SPN	C8-C9	5.49	1.45	1.33
10	q	102	SPN	C19-C18	5.48	1.45	1.33
10	p	102	SPN	C4-C5	5.48	1.45	1.33
10	1	105	SPN	C4-C5	5.48	1.45	1.33
10	7	103	SPN	C19-C18	5.47	1.45	1.33
10	0	102	SPN	C19-C18	5.47	1.45	1.33
10	0	102	SPN	C4-C5	5.47	1.45	1.33
10	5	102	SPN	C19-C18	5.46	1.45	1.33
10	5	103	SPN	C4-C5	5.46	1.45	1.33
10	1	105	SPN	C8-C9	5.46	1.45	1.33
10	t	102	SPN	C4-C5	5.46	1.45	1.33
10	a	103	SPN	C4-C5	5.45	1.45	1.33
10	c	103	SPN	C19-C18	5.45	1.45	1.33
10	5	103	SPN	C19-C18	5.45	1.45	1.33
10	1	105	SPN	C7-C8	-5.44	1.34	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	1	104	SPN	C4-C5	5.43	1.45	1.33
10	5	103	SPN	C20-C19	-5.43	1.34	1.50
10	1	102	SPN	C19-C18	5.43	1.45	1.33
10	1	105	SPN	C12-C13	5.43	1.45	1.33
10	c	103	SPN	C20-C19	-5.43	1.34	1.50
10	1	105	SPN	C11-C12	-5.41	1.34	1.50
10	0	102	SPN	C20-C19	-5.41	1.34	1.50
10	q	102	SPN	C4-C5	5.40	1.45	1.33
10	M	406	SPN	C7-C8	-5.40	1.34	1.50
10	1	103	SPN	C12-C13	5.40	1.45	1.33
10	r	102	SPN	C7-C8	-5.39	1.34	1.50
10	c	103	SPN	C4-C5	5.39	1.45	1.33
10	q	102	SPN	C20-C19	-5.38	1.34	1.50
10	7	103	SPN	C4-C5	5.38	1.45	1.33
10	c	103	SPN	C7-C8	-5.36	1.34	1.50
10	p	103	SPN	C7-C8	-5.36	1.34	1.50
10	i	102	SPN	C20-C19	-5.36	1.34	1.50
10	7	103	SPN	C20-C19	-5.36	1.34	1.50
10	c	103	SPN	C11-C12	-5.36	1.34	1.50
10	v	102	SPN	C11-C12	-5.35	1.34	1.50
10	7	103	SPN	C7-C8	-5.35	1.34	1.50
10	v	102	SPN	C7-C8	-5.35	1.34	1.50
10	7	102	SPN	C11-C12	-5.35	1.34	1.50
10	m	102	SPN	C7-C8	-5.34	1.34	1.50
10	n	102	SPN	C7-C8	-5.34	1.34	1.50
10	i	102	SPN	C3-C2	-5.34	1.47	1.52
10	j	102	SPN	C7-C8	-5.34	1.34	1.50
10	f	102	SPN	C7-C8	-5.34	1.34	1.50
10	1	105	SPN	C19-C18	5.33	1.45	1.33
10	n	102	SPN	C20-C19	-5.33	1.34	1.50
10	u	102	SPN	C7-C8	-5.33	1.34	1.50
10	t	102	SPN	C20-C19	-5.33	1.34	1.50
10	7	102	SPN	C7-C8	-5.33	1.34	1.50
10	9	103	SPN	C11-C12	-5.32	1.34	1.50
10	u	102	SPN	C20-C19	-5.32	1.34	1.50
10	m	102	SPN	C11-C12	-5.32	1.34	1.50
10	e	102	SPN	C20-C19	-5.32	1.34	1.50
10	c	102	SPN	C7-C8	-5.32	1.34	1.50
10	r	102	SPN	C20-C19	-5.32	1.34	1.50
10	k	102	SPN	C20-C19	-5.31	1.34	1.50
10	s	102	SPN	C7-C8	-5.31	1.34	1.50
10	n	102	SPN	C11-C12	-5.31	1.34	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	r	102	SPN	C11-C12	-5.31	1.34	1.50
10	h	103	SPN	C7-C8	-5.31	1.34	1.50
10	l	102	SPN	C11-C12	-5.31	1.34	1.50
10	9	103	SPN	C20-C19	-5.31	1.34	1.50
10	1	102	SPN	C20-C19	-5.31	1.34	1.50
10	l	102	SPN	C7-C8	-5.31	1.34	1.50
10	w	102	SPN	C3-C2	-5.30	1.47	1.52
10	h	102	SPN	C20-C19	-5.30	1.34	1.50
10	k	102	SPN	C7-C8	-5.30	1.34	1.50
10	s	102	SPN	C20-C19	-5.29	1.34	1.50
10	j	102	SPN	C11-C12	-5.29	1.34	1.50
10	u	102	SPN	C11-C12	-5.29	1.34	1.50
10	w	102	SPN	C7-C8	-5.29	1.34	1.50
10	7	102	SPN	C20-C19	-5.29	1.34	1.50
10	k	102	SPN	C11-C12	-5.28	1.34	1.50
10	i	102	SPN	C11-C12	-5.28	1.34	1.50
10	c	102	SPN	C20-C19	-5.28	1.34	1.50
10	7	103	SPN	C11-C12	-5.28	1.34	1.50
10	c	102	SPN	C11-C12	-5.28	1.34	1.50
10	p	103	SPN	C11-C12	-5.28	1.34	1.50
10	w	102	SPN	C11-C12	-5.28	1.34	1.50
10	l	104	SPN	C7-C8	-5.28	1.34	1.50
10	e	102	SPN	C11-C12	-5.28	1.34	1.50
10	9	103	SPN	C7-C8	-5.27	1.34	1.50
10	3	102	SPN	C3-C2	-5.27	1.47	1.52
10	h	102	SPN	C7-C8	-5.27	1.34	1.50
10	m	102	SPN	C20-C19	-5.27	1.34	1.50
10	s	102	SPN	C11-C12	-5.27	1.34	1.50
10	l	103	SPN	C7-C8	-5.26	1.34	1.50
10	h	102	SPN	C11-C12	-5.26	1.34	1.50
10	e	102	SPN	C7-C8	-5.26	1.34	1.50
10	f	102	SPN	C11-C12	-5.26	1.34	1.50
10	0	102	SPN	C11-C12	-5.25	1.34	1.50
10	l	102	SPN	C11-C12	-5.25	1.34	1.50
10	p	102	SPN	C11-C12	-5.25	1.34	1.50
10	i	102	SPN	C7-C8	-5.24	1.34	1.50
10	w	102	SPN	C20-C19	-5.24	1.34	1.50
10	a	103	SPN	C7-C8	-5.23	1.34	1.50
10	5	103	SPN	C11-C12	-5.23	1.34	1.50
10	t	102	SPN	C7-C8	-5.22	1.34	1.50
10	a	102	SPN	C7-C8	-5.22	1.34	1.50
10	3	102	SPN	C11-C12	-5.21	1.34	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	h	103	SPN	C11-C12	-5.21	1.34	1.50
10	q	102	SPN	C7-C8	-5.20	1.34	1.50
10	5	102	SPN	C7-C8	-5.20	1.34	1.50
10	5	102	SPN	C20-C19	-5.20	1.34	1.50
10	3	102	SPN	C7-C8	-5.20	1.34	1.50
10	5	103	SPN	C7-C8	-5.19	1.34	1.50
10	1	102	SPN	C7-C8	-5.18	1.34	1.50
10	a	102	SPN	C11-C12	-5.18	1.34	1.50
10	a	102	SPN	C20-C19	-5.18	1.34	1.50
10	0	102	SPN	C7-C8	-5.18	1.34	1.50
10	5	102	SPN	C11-C12	-5.18	1.34	1.50
10	3	102	SPN	C20-C19	-5.18	1.34	1.50
10	q	102	SPN	C11-C12	-5.17	1.34	1.50
10	a	103	SPN	C11-C12	-5.16	1.34	1.50
10	1	102	SPN	C3-C2	-5.14	1.47	1.52
10	1	104	SPN	C11-C12	-5.11	1.35	1.50
10	p	102	SPN	C20-C19	-5.10	1.35	1.50
10	p	103	SPN	C20-C19	-5.08	1.35	1.50
10	1	103	SPN	C3-C2	-5.07	1.47	1.52
10	t	102	SPN	C11-C12	-5.04	1.35	1.50
10	h	103	SPN	C20-C19	-5.03	1.35	1.50
10	f	102	SPN	C20-C19	-5.02	1.35	1.50
10	1	103	SPN	C11-C12	-5.00	1.35	1.50
9	M	402	BCL	C3D-C4D	-4.91	1.33	1.44
10	v	102	SPN	C20-C19	-4.85	1.35	1.50
9	M	402	BCL	C3B-C4B	4.80	1.50	1.41
10	l	102	SPN	C20-C19	-4.71	1.36	1.50
10	1	104	SPN	C20-C19	-4.67	1.36	1.50
10	j	102	SPN	C20-C19	-4.60	1.36	1.50
10	M	406	SPN	C20-C19	-4.56	1.36	1.50
10	a	103	SPN	C20-C19	-4.53	1.36	1.50
9	6	101	BCL	C3B-C4B	4.48	1.50	1.41
9	4	101	BCL	C3D-C4D	-4.47	1.34	1.44
9	0	101	BCL	C3B-C4B	4.47	1.50	1.41
9	0	101	BCL	C3D-C4D	-4.43	1.34	1.44
9	8	101	BCL	C3B-C4B	4.41	1.49	1.41
9	2	101	BCL	C3B-C4B	4.39	1.49	1.41
9	2	101	BCL	C3D-C4D	-4.38	1.34	1.44
9	b	101	BCL	C3D-C4D	-4.37	1.34	1.44
9	6	101	BCL	C3D-C4D	-4.35	1.34	1.44
9	b	101	BCL	C3B-C4B	4.33	1.49	1.41
9	8	101	BCL	C3D-C4D	-4.33	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	p	102	SPN	C7-C8	-4.31	1.37	1.50
9	4	101	BCL	C3B-C4B	4.28	1.49	1.41
10	1	103	SPN	C20-C19	-4.26	1.37	1.50
9	2	101	BCL	O2D-CGD	4.22	1.43	1.33
9	6	101	BCL	O2A-CGA	4.19	1.45	1.33
9	M	402	BCL	O2D-CGD	4.16	1.43	1.33
9	8	101	BCL	O2A-CGA	4.15	1.45	1.33
9	4	101	BCL	O2A-CGA	4.12	1.45	1.33
9	2	101	BCL	O2A-CGA	4.12	1.45	1.33
11	H	301	MW9	C9-C8	-4.10	1.31	1.51
11	M	408	MW9	C9-C8	-4.07	1.31	1.51
13	M	405	BPH	C2C-C3C	4.03	1.58	1.54
9	0	101	BCL	O2A-CGA	4.02	1.45	1.33
11	H	302	MW9	C9-C8	-4.01	1.31	1.51
11	g	103	MW9	C9-C8	-3.99	1.31	1.51
9	b	101	BCL	O2A-CGA	3.98	1.44	1.33
11	9	101	MW9	C9-C8	-3.96	1.32	1.51
11	M	407	MW9	C9-C8	-3.96	1.32	1.51
11	H	304	MW9	C9-C8	-3.95	1.32	1.51
11	H	303	MW9	C9-C8	-3.94	1.32	1.51
9	b	101	BCL	O2D-CGD	3.94	1.42	1.33
11	g	102	MW9	C9-C8	-3.93	1.32	1.51
13	L	303	BPH	C2C-C3C	3.93	1.58	1.54
12	C	402	HEM	FE-NB	3.83	2.06	1.94
9	4	101	BCL	O2D-CGD	3.83	1.42	1.33
9	0	101	BCL	O2D-CGD	3.81	1.42	1.33
10	1	105	SPN	C21-C22	-3.80	1.34	1.52
10	q	102	SPN	C21-C22	-3.76	1.34	1.52
10	n	102	SPN	C21-C22	-3.75	1.34	1.52
10	p	102	SPN	C21-C22	-3.75	1.34	1.52
10	5	103	SPN	C21-C22	-3.74	1.34	1.52
10	r	102	SPN	C21-C22	-3.74	1.34	1.52
10	u	102	SPN	C21-C22	-3.74	1.34	1.52
10	7	103	SPN	C21-C22	-3.74	1.34	1.52
10	5	102	SPN	C21-C22	-3.73	1.34	1.52
10	1	102	SPN	C21-C22	-3.73	1.34	1.52
10	1	104	SPN	C21-C22	-3.73	1.34	1.52
10	7	102	SPN	C21-C22	-3.73	1.34	1.52
10	0	102	SPN	C21-C22	-3.73	1.34	1.52
10	c	103	SPN	C21-C22	-3.72	1.34	1.52
10	m	102	SPN	C21-C22	-3.72	1.34	1.52
10	e	102	SPN	C21-C22	-3.72	1.34	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	c	102	SPN	C21-C22	-3.72	1.34	1.52
10	w	102	SPN	C21-C22	-3.72	1.34	1.52
10	h	102	SPN	C21-C22	-3.71	1.34	1.52
10	j	102	SPN	C21-C22	-3.71	1.34	1.52
8	M	403	U10	C4-C3	3.71	1.49	1.36
10	l	102	SPN	C21-C22	-3.71	1.34	1.52
10	9	103	SPN	C21-C22	-3.70	1.34	1.52
10	f	102	SPN	C21-C22	-3.70	1.34	1.52
10	s	102	SPN	C21-C22	-3.70	1.34	1.52
8	A	101	U10	C4-C3	3.70	1.49	1.36
10	i	102	SPN	C21-C22	-3.70	1.34	1.52
10	k	102	SPN	C21-C22	-3.70	1.34	1.52
10	p	103	SPN	C21-C22	-3.69	1.34	1.52
10	3	102	SPN	C21-C22	-3.69	1.34	1.52
10	M	406	SPN	C21-C22	-3.69	1.34	1.52
8	L	305	U10	C4-C3	3.68	1.49	1.36
10	a	102	SPN	C21-C22	-3.66	1.34	1.52
10	h	103	SPN	C21-C22	-3.66	1.34	1.52
10	t	102	SPN	C21-C22	-3.65	1.34	1.52
9	8	101	BCL	O2D-CGD	3.65	1.42	1.33
9	6	101	BCL	O2D-CGD	3.64	1.42	1.33
10	a	103	SPN	C21-C22	-3.64	1.34	1.52
10	v	102	SPN	C21-C22	-3.63	1.35	1.52
13	M	409	BPH	C3B-C2B	3.56	1.45	1.39
10	1	103	SPN	C21-C22	-3.56	1.35	1.52
10	1	105	SPN	C21-C20	-3.55	1.41	1.53
9	M	402	BCL	CHD-C1D	3.53	1.45	1.38
9	0	101	BCL	C1D-ND	-3.53	1.33	1.37
9	2	101	BCL	CHB-C1B	3.51	1.47	1.39
9	M	402	BCL	O2A-CGA	3.51	1.43	1.33
9	8	101	BCL	CHB-C1B	3.49	1.47	1.39
10	1	105	SPN	C10-C11	-3.46	1.42	1.53
9	b	101	BCL	C1D-ND	-3.45	1.33	1.37
9	M	402	BCL	CHC-C4B	3.40	1.47	1.39
9	4	101	BCL	OBD-CAD	3.39	1.28	1.22
10	1	105	SPN	C16-C15	-3.39	1.34	1.51
10	p	102	SPN	C16-C15	-3.39	1.34	1.51
13	M	405	BPH	C3B-C2B	3.37	1.45	1.39
10	5	103	SPN	C21-C20	-3.36	1.42	1.53
9	4	101	BCL	CHC-C4B	3.35	1.46	1.39
9	8	101	BCL	CHD-C1D	3.34	1.44	1.38
9	8	101	BCL	CHC-C4B	3.34	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	6	101	BCL	CHD-C1D	3.33	1.44	1.38
9	M	402	BCL	CHB-C1B	3.33	1.46	1.39
10	c	103	SPN	C21-C20	-3.32	1.42	1.53
10	1	103	SPN	C10-C11	-3.32	1.42	1.53
9	M	402	BCL	OBD-CAD	3.32	1.28	1.22
9	4	101	BCL	CHB-C1B	3.31	1.46	1.39
10	0	102	SPN	C16-C15	-3.31	1.35	1.51
10	h	103	SPN	C21-C20	-3.30	1.42	1.53
10	1	105	SPN	C6-C7	-3.29	1.42	1.53
9	0	101	BCL	CHC-C4B	3.28	1.46	1.39
10	f	102	SPN	C10-C11	-3.28	1.42	1.53
10	1	104	SPN	C21-C20	-3.28	1.42	1.53
9	0	101	BCL	CHD-C1D	3.27	1.44	1.38
10	0	102	SPN	C21-C20	-3.27	1.42	1.53
10	v	102	SPN	C10-C11	-3.27	1.42	1.53
10	q	102	SPN	C6-C7	-3.26	1.43	1.53
10	l	102	SPN	C10-C11	-3.26	1.43	1.53
10	h	103	SPN	C10-C11	-3.25	1.43	1.53
10	p	102	SPN	C21-C20	-3.25	1.42	1.53
10	v	102	SPN	C6-C7	-3.25	1.43	1.53
9	6	101	BCL	CHC-C4B	3.25	1.46	1.39
10	c	102	SPN	C16-C15	-3.25	1.35	1.51
10	e	102	SPN	C16-C15	-3.25	1.35	1.51
10	n	102	SPN	C6-C7	-3.25	1.43	1.53
10	a	103	SPN	C21-C20	-3.24	1.42	1.53
10	c	103	SPN	C16-C15	-3.24	1.35	1.51
10	n	102	SPN	C10-C11	-3.23	1.43	1.53
9	0	101	BCL	OBD-CAD	3.23	1.28	1.22
10	c	103	SPN	C6-C7	-3.23	1.43	1.53
10	r	102	SPN	C16-C15	-3.23	1.35	1.51
10	7	103	SPN	C6-C7	-3.23	1.43	1.53
10	1	104	SPN	C6-C7	-3.23	1.43	1.53
10	v	102	SPN	C16-C15	-3.22	1.35	1.51
9	b	101	BCL	CHB-C1B	3.22	1.46	1.39
9	0	101	BCL	CHB-C1B	3.22	1.46	1.39
10	w	102	SPN	C16-C15	-3.22	1.35	1.51
10	h	102	SPN	C16-C15	-3.22	1.35	1.51
10	9	103	SPN	C16-C15	-3.22	1.35	1.51
10	1	103	SPN	C6-C7	-3.22	1.43	1.53
10	k	102	SPN	C16-C15	-3.22	1.35	1.51
10	5	103	SPN	C10-C11	-3.22	1.43	1.53
10	1	102	SPN	C21-C20	-3.22	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	l	102	SPN	C16-C15	-3.21	1.35	1.51
10	p	103	SPN	C10-C11	-3.21	1.43	1.53
10	m	102	SPN	C16-C15	-3.21	1.35	1.51
10	n	102	SPN	C16-C15	-3.21	1.35	1.51
10	5	102	SPN	C21-C20	-3.21	1.42	1.53
10	7	103	SPN	C16-C15	-3.21	1.35	1.51
10	7	102	SPN	C16-C15	-3.21	1.35	1.51
10	u	102	SPN	C16-C15	-3.21	1.35	1.51
10	e	102	SPN	C21-C20	-3.20	1.42	1.53
10	5	103	SPN	C6-C7	-3.20	1.43	1.53
10	c	103	SPN	C10-C11	-3.20	1.43	1.53
10	i	102	SPN	C16-C15	-3.20	1.35	1.51
10	j	102	SPN	C10-C11	-3.20	1.43	1.53
10	j	102	SPN	C16-C15	-3.20	1.35	1.51
10	f	102	SPN	C16-C15	-3.20	1.35	1.51
9	4	101	BCL	CHD-C1D	3.20	1.44	1.38
9	2	101	BCL	CHC-C4B	3.19	1.46	1.39
10	j	102	SPN	C6-C7	-3.19	1.43	1.53
10	M	406	SPN	C10-C11	-3.19	1.43	1.53
10	u	102	SPN	C6-C7	-3.19	1.43	1.53
10	a	102	SPN	C16-C15	-3.19	1.35	1.51
10	r	102	SPN	C10-C11	-3.19	1.43	1.53
10	j	102	SPN	C21-C20	-3.18	1.43	1.53
10	f	102	SPN	C6-C7	-3.18	1.43	1.53
10	p	103	SPN	C16-C15	-3.18	1.36	1.51
10	s	102	SPN	C16-C15	-3.18	1.36	1.51
10	f	102	SPN	C21-C20	-3.18	1.43	1.53
9	6	101	BCL	CHB-C1B	3.18	1.46	1.39
10	u	102	SPN	C21-C20	-3.18	1.43	1.53
10	7	103	SPN	C10-C11	-3.17	1.43	1.53
10	1	102	SPN	C16-C15	-3.17	1.36	1.51
10	5	102	SPN	C16-C15	-3.17	1.36	1.51
10	9	103	SPN	C21-C20	-3.17	1.43	1.53
10	M	406	SPN	C6-C7	-3.17	1.43	1.53
10	u	102	SPN	C10-C11	-3.17	1.43	1.53
10	t	102	SPN	C16-C15	-3.17	1.36	1.51
9	b	101	BCL	CHD-C1D	3.17	1.44	1.38
10	5	103	SPN	C16-C15	-3.17	1.36	1.51
9	6	101	BCL	OBD-CAD	3.16	1.27	1.22
9	6	101	BCL	C1D-ND	-3.16	1.33	1.37
10	c	102	SPN	C10-C11	-3.16	1.43	1.53
10	c	102	SPN	C21-C20	-3.16	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	w	102	SPN	C10-C11	-3.16	1.43	1.53
9	8	101	BCL	OBD-CAD	3.16	1.27	1.22
9	4	101	BCL	C1D-ND	-3.16	1.33	1.37
9	2	101	BCL	OBD-CAD	3.15	1.27	1.22
10	l	102	SPN	C6-C7	-3.15	1.43	1.53
10	s	102	SPN	C21-C20	-3.15	1.43	1.53
10	i	102	SPN	C10-C11	-3.15	1.43	1.53
10	h	103	SPN	C16-C15	-3.14	1.36	1.51
10	c	102	SPN	C6-C7	-3.14	1.43	1.53
10	i	102	SPN	C21-C20	-3.14	1.43	1.53
10	1	104	SPN	C10-C11	-3.14	1.43	1.53
10	a	102	SPN	C21-C20	-3.14	1.43	1.53
10	9	103	SPN	C10-C11	-3.13	1.43	1.53
10	9	103	SPN	C6-C7	-3.13	1.43	1.53
10	a	103	SPN	C6-C7	-3.13	1.43	1.53
10	s	102	SPN	C6-C7	-3.13	1.43	1.53
10	7	102	SPN	C21-C20	-3.13	1.43	1.53
10	n	102	SPN	C21-C20	-3.13	1.43	1.53
10	e	102	SPN	C6-C7	-3.12	1.43	1.53
9	b	101	BCL	CHC-C4B	3.12	1.46	1.39
9	b	101	BCL	OBD-CAD	3.12	1.27	1.22
10	r	102	SPN	C6-C7	-3.11	1.43	1.53
10	p	103	SPN	C6-C7	-3.11	1.43	1.53
10	h	102	SPN	C21-C20	-3.11	1.43	1.53
10	1	104	SPN	C16-C15	-3.11	1.36	1.51
10	m	102	SPN	C10-C11	-3.11	1.43	1.53
10	k	102	SPN	C6-C7	-3.11	1.43	1.53
10	k	102	SPN	C21-C20	-3.11	1.43	1.53
10	s	102	SPN	C10-C11	-3.10	1.43	1.53
10	a	103	SPN	C16-C15	-3.10	1.36	1.51
10	q	102	SPN	C21-C20	-3.10	1.43	1.53
10	M	406	SPN	C16-C15	-3.10	1.36	1.51
10	l	102	SPN	C21-C20	-3.10	1.43	1.53
10	m	102	SPN	C6-C7	-3.10	1.43	1.53
10	3	102	SPN	C16-C15	-3.10	1.36	1.51
12	C	401	HEM	FE-NB	3.10	2.04	1.94
10	m	102	SPN	C21-C20	-3.09	1.43	1.53
10	t	102	SPN	C6-C7	-3.09	1.43	1.53
10	h	103	SPN	C6-C7	-3.09	1.43	1.53
10	7	102	SPN	C10-C11	-3.09	1.43	1.53
10	7	103	SPN	C21-C20	-3.09	1.43	1.53
9	M	402	BCL	C3D-C2D	3.09	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	w	102	SPN	C6-C7	-3.09	1.43	1.53
10	7	102	SPN	C6-C7	-3.09	1.43	1.53
10	k	102	SPN	C10-C11	-3.08	1.43	1.53
9	2	101	BCL	CHD-C1D	3.08	1.44	1.38
10	p	103	SPN	C21-C20	-3.07	1.43	1.53
10	0	102	SPN	C10-C11	-3.06	1.43	1.53
10	w	102	SPN	C21-C20	-3.06	1.43	1.53
10	r	102	SPN	C21-C20	-3.05	1.43	1.53
10	h	102	SPN	C6-C7	-3.04	1.43	1.53
10	h	102	SPN	C10-C11	-3.04	1.43	1.53
10	e	102	SPN	C10-C11	-3.04	1.43	1.53
10	v	102	SPN	C21-C20	-3.04	1.43	1.53
9	M	402	BCL	C1D-ND	-3.03	1.33	1.37
10	i	102	SPN	C6-C7	-3.03	1.43	1.53
10	q	102	SPN	C10-C11	-3.03	1.43	1.53
10	3	102	SPN	C21-C20	-3.02	1.43	1.53
10	p	102	SPN	C10-C11	-3.01	1.43	1.53
10	1	103	SPN	C16-C15	-3.01	1.36	1.51
10	0	102	SPN	C6-C7	-3.01	1.43	1.53
9	2	101	BCL	C1D-ND	-3.00	1.33	1.37
10	q	102	SPN	C16-C15	-2.99	1.36	1.51
10	1	102	SPN	C6-C7	-2.99	1.43	1.53
10	t	102	SPN	C10-C11	-2.99	1.43	1.53
10	a	102	SPN	C6-C7	-2.98	1.43	1.53
9	8	101	BCL	C1D-ND	-2.98	1.34	1.37
10	1	102	SPN	C10-C11	-2.97	1.43	1.53
9	6	101	BCL	C3D-C2D	2.97	1.47	1.39
10	3	102	SPN	C10-C11	-2.94	1.44	1.53
9	b	101	BCL	C4B-NB	-2.92	1.34	1.37
10	5	102	SPN	C6-C7	-2.92	1.44	1.53
10	5	102	SPN	C10-C11	-2.91	1.44	1.53
10	a	102	SPN	C10-C11	-2.91	1.44	1.53
9	2	101	BCL	C3D-C2D	2.91	1.46	1.39
10	t	102	SPN	C21-C20	-2.90	1.43	1.53
9	8	101	BCL	C3D-C2D	2.87	1.46	1.39
9	b	101	BCL	C3D-C2D	2.87	1.46	1.39
10	1	105	SPN	C15-C14	-2.84	1.41	1.52
9	0	101	BCL	C3D-C2D	2.82	1.46	1.39
10	3	102	SPN	C6-C7	-2.81	1.44	1.53
10	a	103	SPN	C10-C11	-2.81	1.44	1.53
10	1	105	SPN	C16-C17	-2.78	1.42	1.52
9	0	101	BCL	C1B-NB	-2.78	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	402	BCL	CHD-C4C	2.77	1.47	1.39
9	6	101	BCL	C1B-NB	-2.76	1.34	1.37
9	4	101	BCL	C1B-NB	-2.74	1.34	1.37
9	4	101	BCL	C3D-C2D	2.73	1.46	1.39
10	1	103	SPN	C15-C14	-2.72	1.42	1.52
9	b	101	BCL	C1B-NB	-2.70	1.34	1.37
10	v	102	SPN	C15-C14	-2.68	1.42	1.52
9	6	101	BCL	C4B-NB	-2.67	1.34	1.37
12	C	401	HEM	FE-NC	2.66	2.03	1.95
9	o	101	BCL	MG-NA	-2.64	2.00	2.06
10	1	103	SPN	C21-C20	-2.64	1.44	1.53
10	j	102	SPN	C15-C14	-2.64	1.42	1.52
13	L	303	BPH	C3B-C2B	2.61	1.44	1.39
10	p	102	SPN	C6-C7	-2.61	1.45	1.53
9	8	101	BCL	C4B-NB	-2.61	1.34	1.37
9	0	101	BCL	C4B-NB	-2.58	1.34	1.37
10	v	102	SPN	C16-C17	-2.58	1.42	1.52
9	8	101	BCL	C1B-NB	-2.58	1.34	1.37
13	M	409	BPH	C3B-C4B	-2.56	1.37	1.41
9	6	101	BCL	CHD-C4C	2.55	1.46	1.39
10	M	406	SPN	C15-C14	-2.55	1.42	1.52
10	f	102	SPN	C15-C14	-2.54	1.42	1.52
10	f	102	SPN	C16-C17	-2.54	1.42	1.52
9	2	101	BCL	C4B-NB	-2.52	1.34	1.37
10	h	103	SPN	C16-C17	-2.52	1.43	1.52
10	1	103	SPN	C16-C17	-2.51	1.43	1.52
9	L	301	BCL	C1D-C2D	-2.51	1.40	1.45
10	a	103	SPN	C16-C17	-2.51	1.43	1.52
10	l	102	SPN	C15-C14	-2.51	1.43	1.52
9	M	402	BCL	C1D-C2D	2.50	1.50	1.45
10	n	102	SPN	C16-C17	-2.50	1.43	1.52
10	n	102	SPN	C15-C14	-2.49	1.43	1.52
10	e	102	SPN	C16-C17	-2.49	1.43	1.52
10	7	103	SPN	C15-C14	-2.49	1.43	1.52
9	4	101	BCL	C4B-NB	-2.49	1.34	1.37
10	0	102	SPN	C15-C14	-2.49	1.43	1.52
10	0	102	SPN	C16-C17	-2.49	1.43	1.52
9	8	101	BCL	CHD-C4C	2.48	1.46	1.39
10	p	103	SPN	C16-C17	-2.48	1.43	1.52
10	r	102	SPN	C15-C14	-2.48	1.43	1.52
10	c	103	SPN	C16-C17	-2.48	1.43	1.52
10	j	102	SPN	C16-C17	-2.48	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	r	102	SPN	C16-C17	-2.48	1.43	1.52
9	8	101	BCL	C1B-C2B	2.47	1.48	1.43
9	2	101	BCL	C1B-NB	-2.47	1.34	1.37
10	1	104	SPN	C16-C17	-2.46	1.43	1.52
12	C	403	HEM	FE-NB	2.46	2.02	1.94
9	e	101	BCL	MG-NC	2.45	2.12	2.06
9	0	101	BCL	CHD-C4C	2.45	1.46	1.39
10	m	102	SPN	C15-C14	-2.45	1.43	1.52
10	u	102	SPN	C15-C14	-2.44	1.43	1.52
10	p	103	SPN	C15-C14	-2.44	1.43	1.52
10	l	102	SPN	C16-C17	-2.44	1.43	1.52
10	5	103	SPN	C16-C17	-2.44	1.43	1.52
10	h	103	SPN	C15-C14	-2.44	1.43	1.52
9	M	402	BCL	C1B-NB	-2.44	1.34	1.37
10	c	102	SPN	C15-C14	-2.44	1.43	1.52
9	M	402	BCL	C4B-NB	-2.44	1.34	1.37
9	2	101	BCL	C1B-C2B	2.44	1.48	1.43
10	1	104	SPN	C15-C14	-2.44	1.43	1.52
10	u	102	SPN	C16-C17	-2.43	1.43	1.52
10	s	102	SPN	C15-C14	-2.42	1.43	1.52
10	m	102	SPN	C16-C17	-2.42	1.43	1.52
10	c	103	SPN	C15-C14	-2.42	1.43	1.52
9	4	101	BCL	CHD-C4C	2.42	1.46	1.39
10	7	103	SPN	C16-C17	-2.42	1.43	1.52
9	2	101	BCL	CHD-C4C	2.42	1.46	1.39
10	9	103	SPN	C15-C14	-2.41	1.43	1.52
10	k	102	SPN	C15-C14	-2.40	1.43	1.52
10	7	102	SPN	C16-C17	-2.40	1.43	1.52
10	9	103	SPN	C16-C17	-2.40	1.43	1.52
10	t	102	SPN	C16-C17	-2.40	1.43	1.52
10	3	102	SPN	C15-C14	-2.40	1.43	1.52
10	M	406	SPN	C21-C20	-2.40	1.45	1.53
10	7	102	SPN	C15-C14	-2.39	1.43	1.52
10	e	102	SPN	C15-C14	-2.39	1.43	1.52
10	w	102	SPN	C16-C17	-2.39	1.43	1.52
10	h	102	SPN	C16-C17	-2.39	1.43	1.52
10	i	102	SPN	C16-C17	-2.38	1.43	1.52
10	5	103	SPN	C15-C14	-2.38	1.43	1.52
10	i	102	SPN	C15-C14	-2.37	1.43	1.52
10	c	102	SPN	C16-C17	-2.37	1.43	1.52
13	M	405	BPH	CHA-CBD	2.37	1.54	1.51
10	k	102	SPN	C16-C17	-2.36	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	w	102	SPN	C15-C14	-2.36	1.43	1.52
10	s	102	SPN	C16-C17	-2.34	1.43	1.52
10	p	102	SPN	C15-C14	-2.34	1.43	1.52
10	p	102	SPN	C16-C17	-2.34	1.43	1.52
10	a	103	SPN	C15-C14	-2.31	1.43	1.52
10	h	102	SPN	C15-C14	-2.31	1.43	1.52
10	a	102	SPN	C15-C14	-2.31	1.43	1.52
9	4	101	BCL	MG-NA	-2.30	2.00	2.06
9	0	101	BCL	MG-NA	-2.30	2.00	2.06
9	M	402	BCL	MG-NA	-2.29	2.00	2.06
10	1	102	SPN	C15-C14	-2.28	1.43	1.52
10	t	102	SPN	C15-C14	-2.28	1.43	1.52
9	2	101	BCL	MG-NA	-2.27	2.00	2.06
9	b	101	BCL	CHD-C4C	2.27	1.45	1.39
10	1	102	SPN	C16-C17	-2.26	1.43	1.52
9	b	101	BCL	CHC-C1C	-2.25	1.32	1.37
10	a	102	SPN	C16-C17	-2.25	1.44	1.52
9	8	101	BCL	C1D-C2D	2.24	1.49	1.45
9	u	101	BCL	MG-NC	2.24	2.11	2.06
10	q	102	SPN	C15-C14	-2.21	1.44	1.52
9	5	101	BCL	C1D-C2D	-2.21	1.41	1.45
10	3	102	SPN	C16-C17	-2.21	1.44	1.52
10	5	102	SPN	C16-C17	-2.21	1.44	1.52
9	s	101	BCL	C1D-C2D	-2.20	1.41	1.45
9	0	101	BCL	C1B-C2B	2.20	1.48	1.43
9	6	101	BCL	C1B-C2B	2.19	1.48	1.43
9	8	101	BCL	MG-NC	-2.19	2.01	2.06
10	q	102	SPN	C16-C17	-2.18	1.44	1.52
9	b	101	BCL	MG-NA	-2.18	2.01	2.06
10	5	102	SPN	C15-C14	-2.18	1.44	1.52
9	8	101	BCL	MG-NA	-2.16	2.01	2.06
10	M	406	SPN	C16-C17	-2.15	1.44	1.52
13	M	409	BPH	CHA-CBD	2.15	1.54	1.51
9	2	101	BCL	C3C-C4C	-2.15	1.48	1.51
9	6	101	BCL	MG-NA	-2.14	2.01	2.06
9	0	101	BCL	C1D-C2D	2.13	1.49	1.45
9	6	101	BCL	CHB-C4A	-2.12	1.32	1.37
9	m	101	BCL	C3C-C4C	2.12	1.54	1.51
9	b	101	BCL	C1B-C2B	2.12	1.48	1.43
9	L	304	BCL	C1D-C2D	-2.12	1.41	1.45
9	4	101	BCL	C1B-C2B	2.11	1.48	1.43
9	2	101	BCL	CHC-C1C	-2.11	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	8	101	BCL	CHC-C1C	-2.10	1.32	1.37
13	L	303	BPH	C3B-C4B	-2.10	1.38	1.41
9	6	101	BCL	MG-NC	-2.09	2.01	2.06
9	9	102	BCL	MG-NC	2.09	2.11	2.06
9	6	101	BCL	C1D-C2D	2.09	1.49	1.45
9	M	402	BCL	CHC-C1C	-2.08	1.32	1.37
9	b	101	BCL	C3C-C4C	-2.08	1.49	1.51
9	4	101	BCL	MG-NC	-2.07	2.01	2.06
9	0	101	BCL	CHB-C4A	-2.07	1.32	1.37
9	a	101	BCL	MG-NC	2.07	2.11	2.06
9	0	101	BCL	C4D-CHA	2.07	1.45	1.38
9	p	101	BCL	C3C-C4C	2.06	1.54	1.51
9	6	101	BCL	CHC-C1C	-2.04	1.32	1.37
9	2	101	BCL	C4D-CHA	2.04	1.45	1.38
9	w	101	BCL	MG-NC	2.04	2.11	2.06
9	h	101	BCL	MG-NC	2.04	2.11	2.06
9	4	101	BCL	C1D-C2D	2.03	1.49	1.45
9	b	101	BCL	C1D-C2D	2.03	1.49	1.45
9	4	101	BCL	C4D-CHA	2.03	1.45	1.38
9	s	101	BCL	C1B-NB	-2.01	1.35	1.37
9	4	101	BCL	CHC-C1C	-2.01	1.32	1.37
9	4	101	BCL	C3C-C4C	-2.01	1.49	1.51
9	M	402	BCL	CHB-C4A	-2.00	1.32	1.37

All (1182) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	8	101	BCL	O2D-CGD-CBD	11.13	130.70	111.23
9	0	101	BCL	O2D-CGD-CBD	11.11	130.66	111.23
9	b	101	BCL	O2D-CGD-CBD	10.71	129.95	111.23
9	2	101	BCL	O2D-CGD-CBD	10.41	129.44	111.23
9	6	101	BCL	O2D-CGD-CBD	9.72	128.23	111.23
9	4	101	BCL	O2D-CGD-CBD	9.66	128.12	111.23
8	L	305	U10	C7-C6-C5	9.22	129.22	118.52
8	L	305	U10	C7-C6-C1	-7.89	111.37	124.89
12	C	402	HEM	CAC-C3C-C4C	7.83	143.53	124.82
10	v	102	SPN	C21-C20-C19	7.76	132.56	112.16
10	a	103	SPN	C21-C20-C19	7.61	132.16	112.16
10	1	104	SPN	C21-C20-C19	7.56	132.03	112.16
10	j	102	SPN	C21-C20-C19	7.55	132.00	112.16
9	M	402	BCL	CMD-C2D-C1D	7.50	137.93	124.73
10	1	103	SPN	C21-C20-C19	7.47	131.79	112.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	4	101	BCL	CMD-C2D-C1D	7.18	137.37	124.73
9	6	101	BCL	C2B-C1B-NB	7.14	117.73	110.33
10	h	103	SPN	C21-C20-C19	7.11	130.85	112.16
9	0	101	BCL	C2B-C1B-NB	6.97	117.56	110.33
10	f	102	SPN	C21-C20-C19	6.89	130.28	112.16
10	M	406	SPN	C16-C17-C18	6.83	130.11	113.47
9	M	402	BCL	O2D-CGD-CBD	6.83	123.16	111.23
9	4	101	BCL	C2B-C1B-NB	6.82	117.40	110.33
9	b	101	BCL	C2B-C1B-NB	6.76	117.33	110.33
9	6	101	BCL	CMD-C2D-C1D	6.72	136.56	124.73
10	M	406	SPN	C15-C14-C13	6.71	129.81	113.47
9	2	101	BCL	CMD-C2D-C1D	6.69	136.52	124.73
10	l	102	SPN	C21-C20-C19	6.66	129.66	112.16
9	8	101	BCL	CMD-C2D-C1D	6.64	136.41	124.73
9	0	101	BCL	CMD-C2D-C1D	6.63	136.40	124.73
9	8	101	BCL	C2B-C1B-NB	6.54	117.11	110.33
9	b	101	BCL	CMD-C2D-C1D	6.52	136.21	124.73
9	8	101	BCL	O2D-CGD-O1D	-6.49	111.21	123.85
9	2	101	BCL	C2B-C1B-NB	6.44	117.00	110.33
9	M	402	BCL	C2B-C1B-NB	6.41	116.98	110.33
10	j	102	SPN	C16-C17-C18	6.34	128.91	113.47
9	M	402	BCL	C1-C2-C3	-6.32	115.84	126.20
10	a	103	SPN	C16-C17-C18	6.30	128.81	113.47
10	h	103	SPN	C16-C17-C18	6.29	128.79	113.47
10	1	104	SPN	C16-C17-C18	6.29	128.78	113.47
10	f	102	SPN	C16-C17-C18	6.20	128.57	113.47
10	q	102	SPN	C16-C17-C18	6.18	128.53	113.47
10	5	102	SPN	C15-C14-C13	6.17	128.51	113.47
9	0	101	BCL	O2D-CGD-O1D	-6.16	111.85	123.85
10	3	102	SPN	C15-C14-C13	6.16	128.47	113.47
10	a	102	SPN	C15-C14-C13	6.15	128.45	113.47
10	1	103	SPN	C15-C16-C17	6.14	135.69	113.13
10	1	102	SPN	C15-C14-C13	6.08	128.28	113.47
10	p	103	SPN	C21-C20-C19	6.07	128.11	112.16
10	l	102	SPN	C16-C17-C18	6.06	128.23	113.47
10	q	102	SPN	C15-C14-C13	6.05	128.20	113.47
10	n	102	SPN	C15-C14-C13	6.03	128.15	113.47
10	c	103	SPN	C15-C14-C13	6.02	128.12	113.47
10	p	103	SPN	C15-C14-C13	6.01	128.10	113.47
10	e	102	SPN	C15-C14-C13	5.99	128.06	113.47
10	5	103	SPN	C15-C14-C13	5.99	128.05	113.47
10	i	102	SPN	C15-C14-C13	5.99	128.05	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	7	102	SPN	C15-C14-C13	5.98	128.04	113.47
10	1	105	SPN	C15-C14-C13	5.97	128.00	113.47
10	9	103	SPN	C15-C14-C13	5.96	127.99	113.47
10	h	102	SPN	C15-C14-C13	5.96	127.99	113.47
10	r	102	SPN	C15-C14-C13	5.96	127.98	113.47
10	7	103	SPN	C16-C17-C18	5.95	127.96	113.47
10	0	102	SPN	C15-C14-C13	5.94	127.94	113.47
10	c	102	SPN	C15-C14-C13	5.94	127.94	113.47
10	u	102	SPN	C15-C14-C13	5.94	127.94	113.47
10	w	102	SPN	C15-C14-C13	5.94	127.93	113.47
10	v	102	SPN	C15-C14-C13	5.91	127.87	113.47
10	k	102	SPN	C15-C14-C13	5.91	127.86	113.47
10	a	103	SPN	C15-C14-C13	5.91	127.86	113.47
10	t	102	SPN	C15-C14-C13	5.90	127.85	113.47
10	m	102	SPN	C15-C14-C13	5.90	127.85	113.47
9	b	101	BCL	O2D-CGD-O1D	-5.90	112.36	123.85
10	p	103	SPN	C16-C17-C18	5.89	127.81	113.47
10	s	102	SPN	C15-C14-C13	5.89	127.81	113.47
10	7	103	SPN	C15-C14-C13	5.89	127.80	113.47
10	t	102	SPN	C16-C17-C18	5.88	127.80	113.47
10	v	102	SPN	C16-C17-C18	5.84	127.69	113.47
10	1	104	SPN	C15-C14-C13	5.82	127.64	113.47
10	5	103	SPN	C16-C17-C18	5.82	127.63	113.47
10	M	406	SPN	C21-C20-C19	5.81	127.44	112.16
10	c	103	SPN	C16-C17-C18	5.79	127.58	113.47
10	1	103	SPN	C16-C15-C14	5.79	134.40	113.13
10	u	102	SPN	C16-C17-C18	5.79	127.56	113.47
10	j	102	SPN	C15-C14-C13	5.78	127.56	113.47
10	i	102	SPN	C16-C17-C18	5.78	127.54	113.47
10	s	102	SPN	C16-C17-C18	5.77	127.53	113.47
10	f	102	SPN	C15-C14-C13	5.76	127.50	113.47
10	3	102	SPN	C16-C17-C18	5.76	127.50	113.47
10	l	102	SPN	C15-C14-C13	5.74	127.46	113.47
10	7	102	SPN	C16-C17-C18	5.74	127.45	113.47
12	C	402	HEM	CAC-C3C-C2C	-5.74	109.78	128.43
10	9	103	SPN	C16-C17-C18	5.73	127.43	113.47
10	w	102	SPN	C16-C17-C18	5.73	127.42	113.47
10	n	102	SPN	C16-C17-C18	5.73	127.42	113.47
10	m	102	SPN	C16-C17-C18	5.72	127.41	113.47
10	1	105	SPN	C16-C17-C18	5.72	127.40	113.47
10	r	102	SPN	C16-C17-C18	5.72	127.40	113.47
10	k	102	SPN	C16-C17-C18	5.72	127.39	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	c	102	SPN	C16-C17-C18	5.71	127.38	113.47
10	e	102	SPN	C16-C17-C18	5.70	127.34	113.47
10	h	103	SPN	C15-C14-C13	5.68	127.31	113.47
10	h	102	SPN	C16-C17-C18	5.68	127.30	113.47
10	a	102	SPN	C16-C17-C18	5.68	127.29	113.47
10	5	102	SPN	C16-C17-C18	5.66	127.27	113.47
10	p	102	SPN	C15-C14-C13	5.66	127.27	113.47
10	0	102	SPN	C16-C17-C18	5.66	127.25	113.47
10	1	102	SPN	C16-C17-C18	5.65	127.23	113.47
9	M	402	BCL	CHD-C1D-ND	-5.60	116.92	124.80
10	p	102	SPN	C16-C17-C18	5.56	127.02	113.47
9	4	101	BCL	O2D-CGD-O1D	-5.49	113.17	123.85
9	6	101	BCL	O2D-CGD-O1D	-5.37	113.40	123.85
9	6	101	BCL	CHD-C1D-ND	-5.34	117.29	124.80
9	2	101	BCL	CHD-C1D-ND	-5.28	117.38	124.80
9	8	101	BCL	CHD-C1D-ND	-5.25	117.42	124.80
9	0	101	BCL	CHD-C1D-ND	-5.21	117.47	124.80
10	M	406	SPN	CM5-C13-C14	5.20	124.26	115.23
10	M	406	SPN	C15-C16-C17	5.16	132.07	113.13
10	0	102	SPN	C21-C20-C19	5.15	125.69	112.16
9	b	101	BCL	CHD-C1D-ND	-5.11	117.61	124.80
9	4	101	BCL	CHD-C1D-ND	-5.10	117.62	124.80
9	2	101	BCL	O2D-CGD-O1D	-5.08	113.97	123.85
10	5	103	SPN	CM3-C5-C6	5.07	124.02	115.23
10	1	103	SPN	C15-C14-C13	5.06	125.78	113.47
9	M	402	BCL	O2D-CGD-O1D	-5.04	114.03	123.85
10	7	103	SPN	CM3-C5-C6	5.03	123.97	115.23
9	M	402	BCL	C3D-C2D-C1D	-5.01	99.00	105.83
10	1	103	SPN	C16-C17-C18	4.99	125.63	113.47
10	a	103	SPN	CM3-C5-C6	4.97	123.85	115.23
10	c	103	SPN	CM3-C5-C6	4.96	123.83	115.23
10	0	102	SPN	CM3-C5-C6	4.95	123.82	115.23
10	1	103	SPN	CM3-C5-C6	4.92	123.77	115.23
10	1	104	SPN	CM3-C5-C6	4.92	123.76	115.23
10	q	102	SPN	CM3-C5-C6	4.92	123.76	115.23
12	C	402	HEM	CAB-C3B-C2B	-4.91	112.45	128.43
10	M	406	SPN	CM4-C9-C10	4.90	123.74	115.23
10	t	102	SPN	CM3-C5-C6	4.90	123.74	115.23
10	5	103	SPN	C7-C6-C5	4.90	129.41	113.19
10	1	105	SPN	CM3-C5-C6	4.88	123.69	115.23
9	4	101	BCL	C3D-C2D-C1D	-4.87	99.18	105.83
9	2	101	BCL	C3C-C4C-CHD	-4.87	113.13	123.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	p	102	SPN	CM7-C22-C21	4.82	128.44	111.27
9	M	402	BCL	C4-C3-C5	4.81	123.58	115.23
9	4	101	BCL	C3C-C4C-CHD	-4.80	113.26	123.39
10	M	406	SPN	C11-C10-C9	4.80	129.10	113.19
10	7	103	SPN	C7-C6-C5	4.80	129.10	113.19
10	f	102	SPN	CM3-C5-C6	4.80	123.56	115.23
10	1	103	SPN	C7-C6-C5	4.80	129.09	113.19
10	a	103	SPN	C7-C6-C5	4.80	129.08	113.19
10	0	102	SPN	C7-C6-C5	4.80	129.08	113.19
10	c	103	SPN	C7-C6-C5	4.79	129.05	113.19
10	j	102	SPN	CM3-C5-C6	4.79	123.54	115.23
9	2	101	BCL	C3D-C2D-C1D	-4.78	99.31	105.83
10	M	406	SPN	CM6-C18-C17	4.78	123.52	115.23
10	1	104	SPN	C7-C6-C5	4.76	128.97	113.19
10	q	102	SPN	C7-C6-C5	4.76	128.95	113.19
10	f	102	SPN	CM4-C9-C10	4.74	123.46	115.23
10	1	104	SPN	CM4-C9-C10	4.74	123.45	115.23
9	6	101	BCL	C3D-C2D-C1D	-4.74	99.37	105.83
10	1	105	SPN	C7-C6-C5	4.73	128.87	113.19
10	j	102	SPN	C7-C6-C5	4.73	128.86	113.19
10	q	102	SPN	CM4-C9-C10	4.73	123.44	115.23
10	n	102	SPN	CM4-C9-C10	4.72	123.43	115.23
10	h	103	SPN	CM6-C18-C17	4.72	123.43	115.23
10	t	102	SPN	C7-C6-C5	4.72	128.84	113.19
10	n	102	SPN	CM3-C5-C6	4.72	123.42	115.23
10	t	102	SPN	CM4-C9-C10	4.72	123.42	115.23
10	j	102	SPN	CM4-C9-C10	4.72	123.42	115.23
10	q	102	SPN	CM6-C18-C17	4.71	123.41	115.23
10	7	103	SPN	CM4-C9-C10	4.71	123.40	115.23
10	l	102	SPN	CM3-C5-C6	4.71	123.40	115.23
10	1	103	SPN	CM4-C9-C10	4.70	123.39	115.23
10	h	103	SPN	CM3-C5-C6	4.70	123.38	115.23
10	p	103	SPN	CM4-C9-C10	4.69	123.37	115.23
9	b	101	BCL	C3C-C4C-CHD	-4.69	113.51	123.39
10	h	103	SPN	C7-C6-C5	4.69	128.71	113.19
8	A	101	U10	C7-C8-C9	-4.68	118.76	126.83
10	f	102	SPN	C7-C6-C5	4.68	128.69	113.19
10	n	102	SPN	C7-C6-C5	4.67	128.67	113.19
9	8	101	BCL	C3D-C2D-C1D	-4.67	99.46	105.83
10	h	103	SPN	CM4-C9-C10	4.67	123.33	115.23
10	5	103	SPN	CM4-C9-C10	4.67	123.33	115.23
10	a	103	SPN	CM4-C9-C10	4.66	123.32	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	j	102	SPN	C11-C10-C9	4.66	128.62	113.19
10	l	104	SPN	C11-C10-C9	4.66	128.61	113.19
10	a	103	SPN	C11-C10-C9	4.65	128.61	113.19
9	0	101	BCL	C3D-C2D-C1D	-4.65	99.48	105.83
10	c	103	SPN	CM4-C9-C10	4.65	123.29	115.23
10	7	103	SPN	C11-C10-C9	4.64	128.57	113.19
10	l	105	SPN	CM4-C9-C10	4.64	123.29	115.23
10	f	102	SPN	CM6-C18-C17	4.63	123.27	115.23
10	p	103	SPN	CM3-C5-C6	4.63	123.27	115.23
10	l	102	SPN	CM4-C9-C10	4.63	123.27	115.23
8	L	305	U10	C1M-C1-C6	-4.62	116.85	124.45
10	q	102	SPN	C11-C10-C9	4.62	128.50	113.19
10	5	103	SPN	C11-C10-C9	4.62	128.49	113.19
10	e	102	SPN	C21-C20-C19	4.62	124.30	112.16
10	l	103	SPN	C11-C10-C9	4.62	128.48	113.19
10	n	102	SPN	CM5-C13-C14	4.61	123.24	115.23
10	t	102	SPN	C11-C10-C9	4.61	128.47	113.19
9	0	101	BCL	C3C-C4C-CHD	-4.61	113.67	123.39
10	l	102	SPN	C7-C6-C5	4.61	128.45	113.19
10	v	102	SPN	CM3-C5-C6	4.60	123.22	115.23
10	f	102	SPN	C11-C10-C9	4.60	128.44	113.19
10	p	103	SPN	C11-C10-C9	4.60	128.42	113.19
10	M	406	SPN	CM3-C5-C6	4.60	123.21	115.23
8	A	101	U10	C12-C13-C14	-4.59	117.11	127.62
10	n	102	SPN	C11-C10-C9	4.59	128.40	113.19
10	5	102	SPN	CM5-C13-C14	4.59	123.19	115.23
10	0	102	SPN	CM4-C9-C10	4.59	123.19	115.23
10	0	102	SPN	C11-C10-C9	4.58	128.38	113.19
10	c	103	SPN	C11-C10-C9	4.58	128.37	113.19
10	l	104	SPN	CM6-C18-C17	4.58	123.18	115.23
10	l	105	SPN	C11-C10-C9	4.58	128.37	113.19
10	p	103	SPN	C7-C6-C5	4.58	128.37	113.19
10	l	105	SPN	CM5-C13-C14	4.57	123.17	115.23
10	h	103	SPN	C11-C10-C9	4.56	128.31	113.19
10	j	102	SPN	CM6-C18-C17	4.56	123.14	115.23
9	b	101	BCL	C3D-C2D-C1D	-4.56	99.61	105.83
10	v	102	SPN	CM5-C13-C14	4.56	123.14	115.23
10	c	103	SPN	CM5-C13-C14	4.56	123.14	115.23
10	v	102	SPN	CM4-C9-C10	4.55	123.13	115.23
10	l	102	SPN	C11-C10-C9	4.55	128.27	113.19
10	l	105	SPN	C21-C20-C19	4.55	124.12	112.16
10	a	103	SPN	CM6-C18-C17	4.55	123.12	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	q	102	SPN	CM5-C13-C14	4.55	123.12	115.23
10	t	102	SPN	C21-C20-C19	4.54	124.10	112.16
10	M	406	SPN	C7-C6-C5	4.54	128.24	113.19
10	p	103	SPN	CM5-C13-C14	4.53	123.10	115.23
9	6	101	BCL	C3C-C4C-CHD	-4.53	113.83	123.39
10	1	103	SPN	CM6-C18-C17	4.53	123.09	115.23
10	1	102	SPN	C21-C20-C19	4.53	124.07	112.16
10	h	102	SPN	C21-C20-C19	4.53	124.07	112.16
10	0	102	SPN	CM5-C13-C14	4.53	123.09	115.23
10	5	103	SPN	CM5-C13-C14	4.53	123.09	115.23
10	r	102	SPN	CM5-C13-C14	4.52	123.08	115.23
10	a	102	SPN	CM5-C13-C14	4.52	123.07	115.23
10	v	102	SPN	C7-C6-C5	4.52	128.16	113.19
9	8	101	BCL	C3C-C4C-CHD	-4.52	113.87	123.39
10	c	102	SPN	C21-C20-C19	4.51	124.01	112.16
10	1	102	SPN	CM5-C13-C14	4.51	123.05	115.23
10	3	102	SPN	CM5-C13-C14	4.51	123.05	115.23
10	e	102	SPN	CM5-C13-C14	4.50	123.04	115.23
10	a	102	SPN	C21-C20-C19	4.50	124.00	112.16
10	u	102	SPN	CM5-C13-C14	4.50	123.04	115.23
10	s	102	SPN	CM4-C9-C10	4.50	123.04	115.23
10	m	102	SPN	CM5-C13-C14	4.50	123.04	115.23
10	s	102	SPN	CM5-C13-C14	4.49	123.03	115.23
10	7	103	SPN	CM6-C18-C17	4.49	123.03	115.23
10	7	103	SPN	CM5-C13-C14	4.49	123.02	115.23
10	c	102	SPN	CM4-C9-C10	4.49	123.01	115.23
10	k	102	SPN	C21-C20-C19	4.48	123.95	112.16
10	w	102	SPN	CM5-C13-C14	4.48	123.01	115.23
10	h	102	SPN	CM5-C13-C14	4.48	123.01	115.23
10	7	102	SPN	CM5-C13-C14	4.48	123.01	115.23
10	5	102	SPN	C21-C20-C19	4.48	123.94	112.16
10	i	102	SPN	CM5-C13-C14	4.48	123.01	115.23
10	a	103	SPN	CM5-C13-C14	4.48	123.00	115.23
10	c	102	SPN	CM5-C13-C14	4.48	123.00	115.23
10	5	102	SPN	CM4-C9-C10	4.48	123.00	115.23
10	j	102	SPN	CM5-C13-C14	4.47	122.99	115.23
10	k	102	SPN	CM5-C13-C14	4.47	122.99	115.23
10	u	102	SPN	CM4-C9-C10	4.47	122.98	115.23
10	w	102	SPN	C21-C20-C19	4.47	123.91	112.16
10	c	102	SPN	C11-C10-C9	4.47	127.98	113.19
10	m	102	SPN	C21-C20-C19	4.47	123.90	112.16
10	9	103	SPN	CM5-C13-C14	4.46	122.98	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	3	102	SPN	CM4-C9-C10	4.46	122.97	115.23
10	5	102	SPN	C11-C10-C9	4.46	127.97	113.19
10	e	102	SPN	CM3-C5-C6	4.46	122.97	115.23
10	k	102	SPN	CM4-C9-C10	4.46	122.97	115.23
10	3	102	SPN	C21-C20-C19	4.46	123.88	112.16
10	r	102	SPN	CM4-C9-C10	4.46	122.96	115.23
10	9	103	SPN	C11-C10-C9	4.45	127.95	113.19
10	9	103	SPN	CM4-C9-C10	4.45	122.96	115.23
10	i	102	SPN	C11-C10-C9	4.45	127.94	113.19
10	s	102	SPN	C11-C10-C9	4.45	127.93	113.19
10	u	102	SPN	C11-C10-C9	4.45	127.92	113.19
10	v	102	SPN	C11-C10-C9	4.44	127.91	113.19
10	c	103	SPN	CM6-C18-C17	4.44	122.94	115.23
10	u	102	SPN	CM3-C5-C6	4.44	122.94	115.23
10	k	102	SPN	CM3-C5-C6	4.44	122.94	115.23
10	1	104	SPN	CM5-C13-C14	4.44	122.94	115.23
10	5	103	SPN	CM6-C18-C17	4.44	122.94	115.23
10	w	102	SPN	CM3-C5-C6	4.44	122.93	115.23
10	9	103	SPN	C21-C20-C19	4.44	123.83	112.16
10	3	102	SPN	C11-C10-C9	4.44	127.89	113.19
10	i	102	SPN	CM4-C9-C10	4.43	122.92	115.23
10	k	102	SPN	C11-C10-C9	4.43	127.87	113.19
10	9	103	SPN	CM3-C5-C6	4.43	122.92	115.23
10	e	102	SPN	CM4-C9-C10	4.42	122.91	115.23
10	w	102	SPN	C11-C10-C9	4.42	127.84	113.19
10	1	105	SPN	CM6-C18-C17	4.42	122.90	115.23
10	f	102	SPN	CM5-C13-C14	4.42	122.90	115.23
10	e	102	SPN	C11-C10-C9	4.42	127.83	113.19
10	a	102	SPN	C7-C6-C5	4.42	127.83	113.19
10	h	102	SPN	CM3-C5-C6	4.42	122.90	115.23
10	w	102	SPN	CM4-C9-C10	4.42	122.89	115.23
9	2	101	BCL	C1D-ND-C4D	-4.42	103.21	106.31
10	7	102	SPN	CM4-C9-C10	4.42	122.89	115.23
10	h	102	SPN	CM4-C9-C10	4.42	122.89	115.23
10	p	102	SPN	C7-C6-C5	4.41	127.81	113.19
9	8	101	BCL	C1D-ND-C4D	-4.41	103.22	106.31
10	l	102	SPN	CM5-C13-C14	4.41	122.89	115.23
10	7	102	SPN	C11-C10-C9	4.41	127.81	113.19
10	r	102	SPN	C11-C10-C9	4.41	127.80	113.19
10	m	102	SPN	CM3-C5-C6	4.41	122.88	115.23
10	i	102	SPN	CM6-C18-C17	4.41	122.88	115.23
10	a	102	SPN	C11-C10-C9	4.41	127.78	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	i	102	SPN	CM3-C5-C6	4.41	122.88	115.23
10	w	102	SPN	C7-C6-C5	4.40	127.77	113.19
10	a	102	SPN	CM3-C5-C6	4.40	122.87	115.23
10	h	102	SPN	C11-C10-C9	4.40	127.76	113.19
10	l	102	SPN	CM6-C18-C17	4.40	122.86	115.23
10	s	102	SPN	CM6-C18-C17	4.39	122.85	115.23
10	h	102	SPN	C7-C6-C5	4.39	127.74	113.19
10	r	102	SPN	CM6-C18-C17	4.39	122.85	115.23
10	7	102	SPN	C21-C20-C19	4.39	123.70	112.16
10	s	102	SPN	C21-C20-C19	4.39	123.70	112.16
10	1	102	SPN	CM3-C5-C6	4.39	122.85	115.23
10	c	102	SPN	CM3-C5-C6	4.39	122.85	115.23
10	9	103	SPN	C7-C6-C5	4.39	127.72	113.19
10	3	102	SPN	C7-C6-C5	4.39	127.72	113.19
10	u	102	SPN	CM6-C18-C17	4.39	122.84	115.23
10	s	102	SPN	CM3-C5-C6	4.39	122.84	115.23
10	i	102	SPN	C7-C6-C5	4.38	127.71	113.19
10	u	102	SPN	C7-C6-C5	4.38	127.71	113.19
10	t	102	SPN	CM5-C13-C14	4.38	122.83	115.23
10	v	102	SPN	CM6-C18-C17	4.38	122.83	115.23
10	m	102	SPN	C11-C10-C9	4.38	127.70	113.19
10	c	102	SPN	C7-C6-C5	4.38	127.70	113.19
10	7	102	SPN	CM6-C18-C17	4.38	122.83	115.23
10	k	102	SPN	C7-C6-C5	4.38	127.69	113.19
10	s	102	SPN	C7-C6-C5	4.38	127.69	113.19
10	3	102	SPN	CM3-C5-C6	4.38	122.83	115.23
10	p	102	SPN	CM3-C5-C6	4.38	122.83	115.23
10	n	102	SPN	C21-C20-C19	4.37	123.66	112.16
10	5	102	SPN	CM3-C5-C6	4.37	122.82	115.23
10	e	102	SPN	C7-C6-C5	4.37	127.67	113.19
10	m	102	SPN	CM6-C18-C17	4.37	122.81	115.23
10	1	102	SPN	C7-C6-C5	4.37	127.67	113.19
10	c	102	SPN	CM6-C18-C17	4.37	122.81	115.23
10	p	103	SPN	CM6-C18-C17	4.37	122.81	115.23
10	m	102	SPN	CM4-C9-C10	4.37	122.81	115.23
10	5	102	SPN	C7-C6-C5	4.37	127.65	113.19
10	n	102	SPN	CM6-C18-C17	4.37	122.81	115.23
10	a	102	SPN	CM4-C9-C10	4.37	122.81	115.23
10	7	102	SPN	CM3-C5-C6	4.36	122.80	115.23
9	2	101	BCL	C2D-C1D-ND	4.36	114.44	110.13
10	i	102	SPN	C21-C20-C19	4.36	123.62	112.16
10	9	103	SPN	CM6-C18-C17	4.36	122.79	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	k	102	SPN	CM6-C18-C17	4.36	122.79	115.23
10	h	103	SPN	CM5-C13-C14	4.36	122.79	115.23
10	3	102	SPN	CM6-C18-C17	4.35	122.78	115.23
10	w	102	SPN	CM6-C18-C17	4.35	122.78	115.23
10	t	102	SPN	CM6-C18-C17	4.35	122.77	115.23
10	r	102	SPN	CM3-C5-C6	4.35	122.77	115.23
10	r	102	SPN	C7-C6-C5	4.34	127.57	113.19
10	h	102	SPN	CM6-C18-C17	4.34	122.76	115.23
10	1	102	SPN	C11-C10-C9	4.34	127.57	113.19
10	7	103	SPN	C21-C20-C19	4.33	123.55	112.16
10	7	102	SPN	C7-C6-C5	4.33	127.53	113.19
10	m	102	SPN	C7-C6-C5	4.33	127.52	113.19
10	e	102	SPN	CM6-C18-C17	4.32	122.73	115.23
10	r	102	SPN	C21-C20-C19	4.30	123.46	112.16
10	1	102	SPN	CM6-C18-C17	4.30	122.69	115.23
10	5	103	SPN	C21-C20-C19	4.30	123.45	112.16
10	u	102	SPN	C21-C20-C19	4.29	123.44	112.16
10	1	102	SPN	CM4-C9-C10	4.29	122.67	115.23
9	8	101	BCL	C3B-C4B-NB	4.28	115.40	109.76
10	a	102	SPN	CM6-C18-C17	4.27	122.65	115.23
10	5	102	SPN	CM6-C18-C17	4.27	122.64	115.23
10	c	103	SPN	C21-C20-C19	4.27	123.39	112.16
10	p	102	SPN	C11-C10-C9	4.23	127.19	113.19
10	0	102	SPN	CM6-C18-C17	4.23	122.56	115.23
9	M	402	BCL	CHC-C4B-NB	-4.21	117.74	124.05
9	2	101	BCL	C3B-C4B-NB	4.20	115.30	109.76
9	8	101	BCL	C2D-C1D-ND	4.14	114.22	110.13
9	2	101	BCL	C4A-NA-C1A	4.14	108.57	106.68
9	6	101	BCL	C2D-C1D-ND	4.14	114.22	110.13
9	6	101	BCL	C3B-C4B-NB	4.13	115.21	109.76
8	A	101	U10	C17-C18-C19	-4.12	118.19	127.62
9	4	101	BCL	C3B-C4B-NB	4.11	115.18	109.76
9	4	101	BCL	C2D-C1D-ND	4.07	114.15	110.13
13	L	303	BPH	C1-C2-C3	4.05	132.84	126.20
8	L	305	U10	C6-C1-C2	4.04	122.36	119.17
9	2	101	BCL	O1D-CGD-CBD	-4.03	116.58	124.52
9	6	101	BCL	C1D-ND-C4D	-4.02	103.49	106.31
10	M	406	SPN	CM7-C22-C21	4.02	125.60	111.27
9	b	101	BCL	C2D-C1D-ND	4.02	114.10	110.13
10	j	102	SPN	CM7-C22-C21	4.01	125.56	111.27
9	b	101	BCL	C1D-ND-C4D	-4.00	103.50	106.31
9	0	101	BCL	C2D-C1D-ND	4.00	114.09	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	b	101	BCL	C3B-C4B-NB	3.98	115.01	109.76
8	A	101	U10	C22-C23-C24	-3.97	118.53	127.62
10	5	102	SPN	CM7-C22-C21	3.97	125.42	111.27
9	4	101	BCL	C1D-ND-C4D	-3.95	103.54	106.31
9	0	101	BCL	C1D-ND-C4D	-3.92	103.56	106.31
10	p	102	SPN	CM4-C9-C10	3.91	122.02	115.23
10	1	103	SPN	CM5-C13-C14	3.91	122.01	115.23
10	p	102	SPN	CM5-C13-C14	3.91	122.01	115.23
10	1	104	SPN	CM7-C22-C21	3.86	125.02	111.27
9	0	101	BCL	C3B-C4B-NB	3.85	114.85	109.76
10	p	102	SPN	CM6-C18-C17	3.85	121.91	115.23
10	p	102	SPN	C21-C20-C19	3.84	122.27	112.16
10	q	102	SPN	CM7-C22-C21	3.80	124.83	111.27
9	M	402	BCL	C1D-ND-C4D	-3.80	103.64	106.31
13	M	409	BPH	C4D-CHA-CBD	3.79	110.27	108.45
10	v	102	SPN	C23-C22-C21	3.75	131.06	112.07
10	q	102	SPN	C21-C20-C19	3.73	121.97	112.16
9	M	402	BCL	C3C-C4C-CHD	-3.72	115.55	123.39
9	i	101	BCL	CHC-C1C-NC	3.71	129.76	124.40
9	M	402	BCL	C2D-C1D-ND	3.70	113.79	110.13
12	C	402	HEM	CAB-C3B-C4B	3.69	140.71	124.39
10	p	102	SPN	C6-C7-C8	3.66	130.14	112.02
13	L	303	BPH	C4D-CHA-CBD	3.66	110.21	108.45
9	8	101	BCL	CED-O2D-CGD	-3.66	107.62	115.92
8	M	403	U10	C22-C23-C24	-3.63	119.31	127.62
9	M	402	BCL	C3B-C4B-NB	3.63	114.54	109.76
10	c	103	SPN	CM7-C22-C21	3.62	124.17	111.27
9	o	101	BCL	CHC-C1C-NC	3.62	129.62	124.40
10	a	102	SPN	CM7-C22-C21	3.60	124.11	111.27
10	h	103	SPN	C23-C22-C21	3.59	130.27	112.07
9	0	101	BCL	O1D-CGD-CBD	-3.56	117.49	124.52
9	1	101	BCL	CHC-C1C-NC	3.56	129.53	124.40
8	L	305	U10	C22-C23-C24	-3.52	119.58	127.62
10	l	102	SPN	CM7-C22-C21	3.51	123.80	111.27
12	C	403	HEM	CAC-C3C-C4C	-3.51	116.44	124.82
9	2	101	BCL	CHC-C4B-NB	-3.50	118.80	124.05
9	0	101	BCL	CHC-C4B-NB	-3.50	118.81	124.05
10	f	102	SPN	C23-C22-C21	3.49	129.78	112.07
9	M	402	BCL	C3D-C4D-ND	3.49	115.66	109.99
8	M	403	U10	C4M-O4-C4	3.48	128.71	116.47
10	j	102	SPN	C16-C15-C14	3.48	125.90	113.13
9	b	101	BCL	O1D-CGD-CBD	-3.47	117.68	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	6	101	BCL	CHC-C4B-NB	-3.46	118.86	124.05
9	M	402	BCL	CAA-C2A-C3A	-3.46	103.66	113.00
9	4	101	BCL	CHC-C4B-NB	-3.44	118.89	124.05
9	8	101	BCL	CHC-C4B-NB	-3.41	118.93	124.05
9	b	101	BCL	CED-O2D-CGD	-3.40	108.19	115.92
8	L	305	U10	C10-C9-C11	3.39	121.11	115.23
9	5	101	BCL	CHC-C1C-NC	3.38	129.28	124.40
10	5	102	SPN	C15-C16-C17	3.37	125.51	113.13
9	7	101	BCL	CHC-C1C-NC	3.36	129.25	124.40
10	h	103	SPN	C16-C15-C14	3.35	125.45	113.13
10	p	102	SPN	C20-C21-C22	3.35	132.44	114.56
10	0	102	SPN	C23-C22-C21	3.35	129.03	112.07
9	8	101	BCL	C3D-C4D-ND	3.33	115.39	109.99
8	M	403	U10	C17-C18-C19	-3.31	120.05	127.62
9	k	101	BCL	CHC-C1C-NC	3.31	129.18	124.40
10	5	103	SPN	CM7-C22-C21	3.31	123.06	111.27
13	L	303	BPH	C2D-C1D-ND	-3.30	107.04	109.43
8	M	403	U10	C47-C48-C49	-3.30	120.07	127.62
9	b	101	BCL	CHC-C4B-NB	-3.30	119.11	124.05
13	M	405	BPH	C2D-C1D-ND	-3.29	107.05	109.43
10	1	102	SPN	C15-C16-C17	3.28	125.19	113.13
10	a	102	SPN	C15-C16-C17	3.28	125.18	113.13
9	v	101	BCL	CHC-C1C-NC	3.28	129.13	124.40
9	6	101	BCL	CED-O2D-CGD	-3.27	108.50	115.92
9	6	101	BCL	C3D-C4D-ND	3.26	115.29	109.99
9	8	101	BCL	O1D-CGD-CBD	-3.26	118.08	124.52
9	w	101	BCL	CHC-C1C-NC	3.26	129.10	124.40
10	7	103	SPN	CM7-C22-C21	3.25	122.86	111.27
9	3	101	BCL	CHC-C1C-NC	3.24	129.07	124.40
9	b	101	BCL	C3D-C4D-ND	3.23	115.24	109.99
10	f	102	SPN	C16-C15-C14	3.22	124.96	113.13
9	f	101	BCL	CHC-C1C-NC	3.22	129.04	124.40
10	3	102	SPN	C15-C16-C17	3.22	124.94	113.13
9	s	101	BCL	CHC-C1C-NC	3.21	129.03	124.40
9	0	101	BCL	C3D-C4D-ND	3.21	115.20	109.99
10	p	102	SPN	C10-C11-C12	3.20	127.86	112.02
10	1	104	SPN	C16-C15-C14	3.20	124.88	113.13
9	l	101	BCL	CHC-C1C-NC	3.19	129.00	124.40
10	i	102	SPN	CM7-C22-C21	3.19	122.64	111.27
8	A	101	U10	C4M-O4-C4	3.17	127.63	116.47
9	L	304	BCL	CHC-C1C-NC	3.17	128.97	124.40
9	2	101	BCL	C3D-C4D-ND	3.16	115.13	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	u	102	SPN	CM7-C22-C21	3.16	122.54	111.27
10	e	102	SPN	C15-C16-C17	3.16	124.73	113.13
9	r	101	BCL	CHC-C1C-NC	3.16	128.96	124.40
9	q	101	BCL	CHC-C1C-NC	3.14	128.93	124.40
10	a	103	SPN	C16-C15-C14	3.14	124.65	113.13
9	t	101	BCL	CHC-C1C-NC	3.13	128.92	124.40
9	6	101	BCL	O1D-CGD-CBD	-3.13	118.34	124.52
10	3	102	SPN	CM7-C22-C21	3.13	122.43	111.27
10	l	102	SPN	C16-C15-C14	3.12	124.61	113.13
9	d	101	BCL	CHC-C1C-NC	3.12	128.91	124.40
9	M	404	BCL	CHC-C4B-NB	-3.12	119.37	124.05
10	n	102	SPN	CM7-C22-C21	3.12	122.40	111.27
8	L	305	U10	C17-C18-C19	-3.11	120.51	127.62
10	h	102	SPN	C15-C16-C17	3.11	124.54	113.13
9	h	101	BCL	CHC-C1C-NC	3.10	128.88	124.40
9	0	101	BCL	CED-O2D-CGD	-3.10	108.88	115.92
10	n	102	SPN	C15-C16-C17	3.10	124.52	113.13
9	6	101	BCL	C1-C2-C3	-3.10	121.12	126.20
9	4	101	BCL	CHB-C4A-NA	3.10	128.87	124.40
10	M	406	SPN	C20-C21-C22	3.09	131.05	114.56
8	M	403	U10	C10-C9-C11	3.09	120.59	115.23
10	k	102	SPN	CM7-C22-C21	3.09	122.28	111.27
10	s	102	SPN	CM7-C22-C21	3.08	122.27	111.27
10	7	102	SPN	C15-C16-C17	3.08	124.45	113.13
10	r	102	SPN	CM7-C22-C21	3.07	122.23	111.27
10	5	103	SPN	C15-C16-C17	3.06	124.38	113.13
10	9	103	SPN	C15-C16-C17	3.06	124.38	113.13
10	0	102	SPN	C15-C16-C17	3.06	124.38	113.13
10	7	102	SPN	CM7-C22-C21	3.05	122.15	111.27
10	w	102	SPN	C15-C16-C17	3.05	124.32	113.13
10	p	102	SPN	C16-C15-C14	3.04	124.31	113.13
9	x	101	BCL	CHC-C1C-NC	3.04	128.79	124.40
10	i	102	SPN	C15-C16-C17	3.03	124.25	113.13
9	b	101	BCL	C1-C2-C3	-3.03	121.24	126.20
10	9	103	SPN	CM7-C22-C21	3.03	122.06	111.27
8	A	101	U10	C15-C14-C16	3.03	120.48	115.23
10	r	102	SPN	C15-C16-C17	3.02	124.24	113.13
10	k	102	SPN	C15-C16-C17	3.02	124.22	113.13
10	c	102	SPN	C15-C16-C17	3.02	124.22	113.13
9	s	101	BCL	CMA-C3A-C4A	-3.02	103.66	111.77
9	4	101	BCL	C3D-C4D-ND	3.02	114.89	109.99
9	L	304	BCL	C4D-CHA-C1A	3.01	124.84	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	w	102	SPN	CM7-C22-C21	3.01	122.01	111.27
10	c	102	SPN	CM7-C22-C21	3.01	122.00	111.27
12	C	401	HEM	CAB-C3B-C2B	3.01	138.21	128.43
9	8	101	BCL	O2A-CGA-CBA	3.00	121.00	111.83
10	q	102	SPN	O1-C1-C2	3.00	115.04	108.90
9	6	101	BCL	C4-C3-C5	3.00	120.43	115.23
10	m	102	SPN	C15-C16-C17	3.00	124.14	113.13
9	j	101	BCL	CHC-C1C-NC	3.00	128.72	124.40
9	2	101	BCL	O2A-CGA-CBA	2.99	120.96	111.83
10	1	102	SPN	CM7-C22-C21	2.99	121.94	111.27
10	7	103	SPN	C16-C15-C14	2.99	124.11	113.13
10	t	102	SPN	C16-C15-C14	2.99	124.10	113.13
10	1	105	SPN	C15-C16-C17	2.98	124.07	113.13
10	q	102	SPN	C15-C16-C17	2.97	124.05	113.13
10	c	103	SPN	C15-C16-C17	2.97	124.05	113.13
9	n	101	BCL	CHC-C1C-NC	2.97	128.68	124.40
9	s	101	BCL	CHC-C4B-NB	-2.97	119.60	124.05
9	a	101	BCL	CHC-C1C-NC	2.96	128.68	124.40
9	p	101	BCL	CHC-C1C-NC	2.96	128.67	124.40
10	u	102	SPN	C15-C16-C17	2.96	123.99	113.13
9	M	404	BCL	CHC-C1C-NC	2.95	128.66	124.40
8	A	101	U10	C7-C6-C1	-2.95	119.83	124.89
9	8	101	BCL	CHB-C4A-NA	2.95	128.65	124.40
9	4	101	BCL	O1D-CGD-CBD	-2.95	118.71	124.52
10	h	102	SPN	CM7-C22-C21	2.94	121.74	111.27
8	M	403	U10	C20-C19-C21	2.93	120.31	115.23
9	L	301	BCL	CHC-C4B-NB	-2.93	119.66	124.05
10	s	102	SPN	C15-C16-C17	2.92	123.86	113.13
9	L	304	BCL	C2A-C1A-CHA	2.92	128.94	123.87
9	m	101	BCL	CHC-C1C-NC	2.92	128.61	124.40
9	2	101	BCL	C1-O2A-CGA	2.91	123.70	116.65
9	1	101	BCL	CHC-C4B-NB	-2.91	119.69	124.05
10	1	105	SPN	CM7-C22-C21	2.90	121.62	111.27
10	m	102	SPN	CM7-C22-C21	2.90	121.61	111.27
9	M	404	BCL	CHA-C1A-NA	-2.90	119.83	126.39
13	M	409	BPH	C4A-C3A-C2A	-2.90	100.08	102.84
9	e	101	BCL	CHC-C1C-NC	2.90	128.58	124.40
13	M	409	BPH	C2D-C1D-ND	-2.89	107.34	109.43
8	A	101	U10	C30-C29-C31	2.89	120.24	115.23
9	L	304	BCL	CHA-C1A-NA	-2.88	119.86	126.39
9	i	101	BCL	CHC-C4B-NB	-2.87	119.74	124.05
10	q	102	SPN	C20-C21-C22	2.87	129.86	114.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	p	103	SPN	C15-C16-C17	2.86	123.65	113.13
9	2	101	BCL	CHB-C4A-NA	2.86	128.53	124.40
9	7	101	BCL	CHC-C4B-NB	-2.86	119.76	124.05
10	p	102	SPN	C15-C16-C17	2.86	123.63	113.13
9	0	101	BCL	C4A-NA-C1A	2.86	107.98	106.68
9	5	101	BCL	CHC-C4B-NB	-2.85	119.77	124.05
9	q	101	BCL	CHC-C4B-NB	-2.85	119.78	124.05
11	H	301	MW9	C8-C9-C10	2.84	128.75	114.37
9	3	101	BCL	CHC-C4B-NB	-2.84	119.78	124.05
9	r	101	BCL	CHA-C1A-NA	-2.84	119.97	126.39
9	o	101	BCL	C2A-C3A-C4A	-2.84	97.29	101.87
9	p	101	BCL	CHA-C1A-NA	-2.84	119.97	126.39
9	f	101	BCL	CHA-C1A-NA	-2.83	119.97	126.39
9	c	101	BCL	CHC-C1C-NC	2.83	128.49	124.40
10	e	102	SPN	CM7-C22-C21	2.83	121.36	111.27
9	g	101	BCL	CHC-C1C-NC	2.83	128.48	124.40
8	L	305	U10	C12-C13-C14	-2.82	121.17	127.62
9	n	101	BCL	CHA-C1A-NA	-2.82	120.01	126.39
9	L	301	BCL	C3C-C4C-CHD	-2.81	117.48	123.39
9	m	101	BCL	CHC-C4B-NB	-2.80	119.85	124.05
10	1	103	SPN	C23-C22-C21	2.80	126.24	112.07
13	L	303	BPH	C2B-C1B-NB	-2.80	107.41	109.43
9	M	402	BCL	C11-C12-C13	-2.79	106.71	115.97
10	t	102	SPN	C23-C22-C21	2.78	126.17	112.07
9	L	304	BCL	CHC-C4B-NB	-2.78	119.88	124.05
9	u	101	BCL	C4D-CHA-C1A	2.77	124.55	121.24
9	o	101	BCL	C3C-C4C-CHD	-2.76	117.57	123.39
9	M	402	BCL	O2A-CGA-CBA	2.76	120.26	111.83
9	x	101	BCL	CHA-C1A-NA	-2.76	120.15	126.39
9	g	101	BCL	CHC-C4B-NB	-2.75	119.92	124.05
9	4	101	BCL	C4A-NA-C1A	2.75	107.93	106.68
9	4	101	BCL	O2A-CGA-CBA	2.75	120.21	111.83
9	b	101	BCL	C4A-NA-C1A	2.74	107.93	106.68
9	b	101	BCL	CHB-C4A-NA	2.74	128.35	124.40
9	9	102	BCL	CHC-C1C-NC	2.74	128.35	124.40
10	t	102	SPN	C15-C16-C17	2.74	123.19	113.13
9	u	101	BCL	CHC-C4B-NB	-2.74	119.94	124.05
8	M	403	U10	C15-C14-C16	2.74	119.98	115.23
8	L	305	U10	C20-C19-C21	2.73	119.97	115.23
9	2	101	BCL	C1C-NC-C4C	-2.73	105.43	106.68
9	a	101	BCL	CHC-C4B-NB	-2.73	119.96	124.05
9	L	304	BCL	C2A-C3A-C4A	-2.73	97.46	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	6	101	BCL	CHC-C1C-NC	2.72	128.33	124.40
9	c	101	BCL	CHC-C4B-NB	-2.72	119.97	124.05
9	M	402	BCL	C4-C3-C2	-2.72	116.65	123.63
9	L	301	BCL	CHC-C1C-NC	2.71	128.32	124.40
9	6	101	BCL	O2A-CGA-CBA	2.71	120.11	111.83
9	L	304	BCL	C1D-ND-C4D	2.71	108.21	106.31
9	0	101	BCL	CHB-C4A-NA	2.71	128.31	124.40
9	o	101	BCL	CHC-C4B-NB	-2.71	119.99	124.05
9	9	102	BCL	CHC-C4B-NB	-2.71	119.99	124.05
10	c	103	SPN	C16-C15-C14	2.70	123.06	113.13
11	M	407	MW9	C19-O8-C24	2.70	124.26	117.80
9	4	101	BCL	CMB-C2B-C3B	2.70	134.19	125.67
9	8	101	BCL	C4A-NA-C1A	2.70	107.91	106.68
9	v	101	BCL	CHA-C1A-NA	-2.69	120.30	126.39
10	p	103	SPN	C23-C22-C21	2.68	125.67	112.07
9	p	101	BCL	CHC-C4B-NB	-2.68	120.02	124.05
10	v	102	SPN	C16-C15-C14	2.68	122.98	113.13
9	9	102	BCL	C4D-CHA-C1A	2.68	124.44	121.24
9	4	101	BCL	CED-O2D-CGD	-2.68	109.84	115.92
10	q	102	SPN	C16-C15-C14	2.68	122.97	113.13
9	v	101	BCL	CHC-C4B-NB	-2.67	120.04	124.05
9	s	101	BCL	C4D-CHA-C1A	2.67	124.43	121.24
9	e	101	BCL	CHC-C4B-NB	-2.67	120.04	124.05
9	v	101	BCL	C1D-ND-C4D	2.67	108.18	106.31
9	d	101	BCL	CHA-C1A-NA	-2.67	120.36	126.39
11	M	407	MW9	C8-C9-C10	2.66	127.83	114.37
9	j	101	BCL	CHA-C1A-NA	-2.66	120.36	126.39
9	g	101	BCL	C4D-CHA-C1A	2.66	124.42	121.24
9	w	101	BCL	CHC-C4B-NB	-2.66	120.06	124.05
10	a	103	SPN	C23-C22-C21	2.66	125.54	112.07
10	s	102	SPN	C16-C15-C14	2.66	122.89	113.13
9	k	101	BCL	CHC-C4B-NB	-2.66	120.06	124.05
11	g	102	MW9	C9-C8-C7	2.66	127.79	114.37
8	L	305	U10	C15-C14-C16	2.65	119.83	115.23
8	L	302	U10	C7-C6-C5	-2.65	115.43	118.52
10	p	103	SPN	C16-C15-C14	2.65	122.87	113.13
8	A	101	U10	C12-C11-C9	-2.65	104.41	113.19
9	m	101	BCL	CMA-C3A-C4A	-2.65	104.66	111.77
8	A	101	U10	C25-C24-C26	2.64	119.82	115.23
10	v	102	SPN	C15-C16-C17	2.64	122.84	113.13
11	g	103	MW9	C8-C9-C10	2.64	127.71	114.37
8	M	403	U10	C42-C43-C44	-2.64	121.59	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	5	101	BCL	CMA-C3A-C4A	-2.64	104.69	111.77
9	c	101	BCL	C4D-CHA-C1A	2.64	124.39	121.24
9	e	101	BCL	C4D-CHA-C1A	2.63	124.39	121.24
9	p	101	BCL	C1D-ND-C4D	2.63	108.16	106.31
9	b	101	BCL	CMB-C2B-C3B	2.63	133.96	125.67
11	g	103	MW9	C9-C8-C7	2.63	127.65	114.37
10	k	102	SPN	C16-C15-C14	2.63	122.77	113.13
10	3	102	SPN	C20-C21-C22	2.62	128.56	114.56
10	0	102	SPN	C16-C15-C14	2.62	122.77	113.13
9	n	101	BCL	CHC-C4B-NB	-2.62	120.11	124.05
9	h	101	BCL	CHA-C1A-NA	-2.62	120.45	126.39
10	c	102	SPN	C16-C15-C14	2.62	122.76	113.13
9	l	101	BCL	CHC-C4B-NB	-2.62	120.12	124.05
9	x	101	BCL	CHC-C4B-NB	-2.62	120.12	124.05
10	7	103	SPN	C15-C16-C17	2.62	122.74	113.13
10	5	103	SPN	C16-C15-C14	2.61	122.73	113.13
9	9	102	BCL	CMA-C3A-C4A	-2.61	104.75	111.77
10	u	102	SPN	C16-C15-C14	2.61	122.72	113.13
12	C	403	HEM	CAC-C3C-C2C	2.61	136.92	128.43
9	3	101	BCL	CMD-C2D-C1D	2.61	129.32	124.73
9	q	101	BCL	CMA-C3A-C4A	-2.60	104.78	111.77
9	7	101	BCL	CMA-C3A-C4A	-2.60	104.78	111.77
11	M	407	MW9	C9-C8-C7	2.60	127.51	114.37
10	m	102	SPN	C16-C15-C14	2.60	122.67	113.13
9	n	101	BCL	C1D-ND-C4D	2.60	108.13	106.31
8	A	101	U10	C20-C19-C21	2.60	119.73	115.23
10	i	102	SPN	C16-C15-C14	2.59	122.65	113.13
9	l	101	BCL	CHA-C1A-NA	-2.59	120.52	126.39
9	4	101	BCL	C1-C2-C3	-2.59	121.95	126.20
9	q	101	BCL	C4D-CHA-C1A	2.59	124.33	121.24
9	m	101	BCL	C4D-CHA-C1A	2.59	124.33	121.24
9	t	101	BCL	CHA-C1A-NA	-2.58	120.54	126.39
10	9	103	SPN	C16-C15-C14	2.58	122.61	113.13
9	0	101	BCL	O2A-CGA-CBA	2.58	119.70	111.83
10	r	102	SPN	C16-C15-C14	2.58	122.60	113.13
9	j	101	BCL	CHC-C4B-NB	-2.58	120.18	124.05
9	L	304	BCL	O2A-C1-C2	2.58	118.03	108.11
11	H	301	MW9	C9-C8-C7	2.58	127.39	114.37
10	5	102	SPN	C20-C21-C22	2.57	128.27	114.56
10	7	102	SPN	C16-C15-C14	2.57	122.56	113.13
10	w	102	SPN	C16-C15-C14	2.57	122.56	113.13
9	f	101	BCL	CHC-C4B-NB	-2.56	120.20	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	d	101	BCL	CHC-C4B-NB	-2.56	120.20	124.05
9	c	101	BCL	CMA-C3A-C4A	-2.56	104.89	111.77
9	M	402	BCL	CHC-C1C-NC	2.56	128.09	124.40
9	6	101	BCL	CMB-C2B-C3B	2.56	133.73	125.67
9	q	101	BCL	CHA-C1A-NA	-2.56	120.60	126.39
9	p	101	BCL	CMA-C3A-C4A	-2.55	104.91	111.77
10	l	103	SPN	O1-C1-C2	2.55	114.12	108.90
9	u	101	BCL	CMA-C3A-C4A	-2.55	104.93	111.77
11	H	302	MW9	C8-C9-C10	2.54	127.21	114.37
9	6	101	BCL	CHB-C4A-NA	2.54	128.06	124.40
9	h	101	BCL	CHC-C4B-NB	-2.54	120.24	124.05
10	h	102	SPN	C16-C15-C14	2.53	122.44	113.13
9	t	101	BCL	CHC-C4B-NB	-2.53	120.25	124.05
9	w	101	BCL	C4D-CHA-C1A	2.53	124.26	121.24
9	s	101	BCL	CHA-C1A-NA	-2.53	120.67	126.39
8	M	403	U10	C50-C49-C51	2.53	119.62	115.23
10	a	102	SPN	C20-C21-C22	2.53	128.05	114.56
11	H	302	MW9	C9-C8-C7	2.53	127.14	114.37
8	M	403	U10	C32-C33-C34	-2.53	121.84	127.62
9	k	101	BCL	C4D-CHA-C1A	2.53	124.26	121.24
9	u	101	BCL	CHC-C1C-NC	2.52	128.03	124.40
10	3	102	SPN	C16-C15-C14	2.51	122.34	113.13
9	r	101	BCL	CHC-C4B-NB	-2.51	120.29	124.05
9	a	101	BCL	CMA-C3A-C4A	-2.51	105.04	111.77
10	a	103	SPN	C20-C19-C18	2.51	133.36	127.62
10	j	102	SPN	C20-C19-C18	2.50	133.36	127.62
11	g	102	MW9	C8-C9-C10	2.50	127.01	114.37
9	l	101	BCL	C4D-CHA-C1A	2.50	124.22	121.24
9	l	101	BCL	CMA-C3A-C4A	-2.50	105.07	111.77
10	c	103	SPN	C20-C21-C22	2.49	127.87	114.56
9	x	101	BCL	C1D-ND-C4D	2.49	108.06	106.31
9	5	101	BCL	C3C-C4C-CHD	-2.49	118.14	123.39
9	a	101	BCL	C4D-CHA-C1A	2.49	124.21	121.24
9	2	101	BCL	CAC-C3C-C4C	-2.48	107.07	112.58
9	t	101	BCL	CMA-C3A-C4A	-2.48	105.11	111.77
10	7	103	SPN	C20-C21-C22	2.48	127.77	114.56
9	3	101	BCL	CMA-C3A-C4A	-2.48	105.12	111.77
9	3	101	BCL	C3C-C4C-CHD	-2.47	118.18	123.39
11	H	304	MW9	C8-C9-C10	2.47	126.85	114.37
9	w	101	BCL	CHA-C1A-NA	-2.47	120.80	126.39
9	L	301	BCL	CHA-C1A-NA	-2.47	120.80	126.39
8	M	403	U10	C12-C13-C14	-2.47	121.97	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	i	101	BCL	CHA-C1A-NA	-2.47	120.81	126.39
9	v	101	BCL	C2A-C1A-CHA	2.47	128.15	123.87
9	L	301	BCL	C2A-C1A-CHA	2.47	128.15	123.87
9	0	101	BCL	CMB-C2B-C3B	2.46	133.44	125.67
10	1	103	SPN	CM5-C13-C12	-2.46	117.31	123.63
9	1	101	BCL	C3C-C4C-CHD	-2.46	118.22	123.39
10	1	102	SPN	C16-C15-C14	2.46	122.15	113.13
11	H	303	MW9	C8-C9-C10	2.45	126.77	114.37
9	1	101	BCL	CHA-C1A-NA	-2.45	120.84	126.39
9	x	101	BCL	CMA-C3A-C4A	-2.45	105.18	111.77
9	0	101	BCL	C1-O2A-CGA	2.45	122.58	116.65
9	M	404	BCL	C4D-CHA-C1A	2.45	124.16	121.24
10	e	102	SPN	C16-C15-C14	2.44	122.10	113.13
9	q	101	BCL	C3C-C4C-CHD	-2.44	118.25	123.39
11	H	303	MW9	C9-C8-C7	2.44	126.69	114.37
10	p	102	SPN	CM5-C13-C12	-2.44	117.37	123.63
9	0	101	BCL	CGD-CBD-CAD	2.43	118.72	110.85
9	2	101	BCL	CED-O2D-CGD	-2.43	110.40	115.92
9	c	101	BCL	CHA-C1A-NA	-2.43	120.89	126.39
10	n	102	SPN	C16-C15-C14	2.43	122.04	113.13
11	H	304	MW9	C9-C8-C7	2.42	126.62	114.37
10	l	102	SPN	C15-C16-C17	2.42	122.03	113.13
9	0	101	BCL	CHC-C1C-NC	2.42	127.90	124.40
9	M	404	BCL	CMD-C2D-C1D	2.42	128.99	124.73
10	a	102	SPN	C16-C15-C14	2.42	122.00	113.13
10	1	105	SPN	C16-C15-C14	2.41	122.00	113.13
9	h	101	BCL	CMA-C3A-C4A	-2.41	105.29	111.77
10	1	104	SPN	C20-C19-C18	2.41	133.15	127.62
9	f	101	BCL	C1D-ND-C4D	2.41	108.00	106.31
9	k	101	BCL	CHA-C1A-NA	-2.41	120.94	126.39
9	j	101	BCL	C1D-ND-C4D	2.41	108.00	106.31
9	r	101	BCL	C2A-C3A-C4A	-2.41	97.98	101.87
9	L	301	BCL	C2A-C3A-C4A	-2.40	97.98	101.87
10	1	102	SPN	CM6-C18-C19	-2.40	117.45	123.63
9	7	101	BCL	C3C-C4C-CHD	-2.40	118.32	123.39
10	5	102	SPN	C16-C15-C14	2.40	121.94	113.13
10	5	102	SPN	CM6-C18-C19	-2.39	117.48	123.63
9	i	101	BCL	C3C-C4C-CHD	-2.39	118.35	123.39
10	3	102	SPN	CM6-C18-C19	-2.39	117.48	123.63
10	r	102	SPN	C4-C3-C2	2.39	122.86	111.68
9	8	101	BCL	CMB-C2B-C3B	2.39	133.21	125.67
9	4	101	BCL	CHC-C1C-NC	2.39	127.85	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	e	101	BCL	CHA-C1A-NA	-2.39	120.98	126.39
9	k	101	BCL	CMA-C3A-C4A	-2.39	105.36	111.77
10	1	102	SPN	C6-C7-C8	2.39	123.82	112.02
9	a	101	BCL	CHA-C1A-NA	-2.38	121.00	126.39
9	2	101	BCL	C1D-CHD-C4C	-2.38	120.88	126.62
11	9	101	MW9	C9-C8-C7	2.38	126.40	114.37
10	a	102	SPN	CM6-C18-C19	-2.38	117.51	123.63
9	m	101	BCL	CHA-C1A-NA	-2.38	121.00	126.39
9	n	101	BCL	CMA-C3A-C4A	-2.37	105.39	111.77
9	5	101	BCL	C4D-CHA-C1A	2.37	124.08	121.24
9	L	301	BCL	C4D-CHA-C1A	2.37	124.08	121.24
10	1	103	SPN	C20-C19-C18	2.37	133.06	127.62
10	7	102	SPN	C6-C7-C8	2.37	123.76	112.02
9	8	101	BCL	CHC-C1C-NC	2.37	127.82	124.40
9	9	102	BCL	CHA-C1A-NA	-2.37	121.02	126.39
10	a	102	SPN	C6-C7-C8	2.37	123.74	112.02
10	5	102	SPN	C4-C3-C2	2.37	122.75	111.68
9	8	101	BCL	C11-C10-C8	-2.37	108.10	115.97
10	i	102	SPN	C20-C21-C22	2.36	127.17	114.56
9	b	101	BCL	O2A-CGA-CBA	2.36	119.04	111.83
10	7	102	SPN	C20-C21-C22	2.36	127.14	114.56
9	M	402	BCL	C6-C5-C3	-2.36	107.73	113.47
10	m	102	SPN	C6-C7-C8	2.35	123.65	112.02
10	M	406	SPN	CM6-C18-C19	-2.35	117.59	123.63
9	o	101	BCL	CMD-C2D-C1D	2.35	128.87	124.73
10	a	103	SPN	C15-C16-C17	2.35	121.76	113.13
9	v	101	BCL	CMA-C3A-C4A	-2.35	105.46	111.77
10	9	103	SPN	C4-C3-C2	2.35	122.66	111.68
11	9	101	MW9	C8-C9-C10	2.35	126.23	114.37
9	e	101	BCL	CMA-C3A-C4A	-2.34	105.47	111.77
10	5	102	SPN	C6-C7-C8	2.34	123.62	112.02
10	1	102	SPN	C10-C11-C12	2.34	123.59	112.02
10	p	102	SPN	CM6-C18-C19	-2.34	117.62	123.63
9	8	101	BCL	C4D-CHA-C1A	-2.34	118.46	121.24
10	5	103	SPN	C20-C21-C22	2.34	127.03	114.56
9	w	101	BCL	CMA-C3A-C4A	-2.34	105.50	111.77
10	a	103	SPN	CM7-C22-C21	2.34	119.60	111.27
10	p	102	SPN	O1-C1-C2	2.34	113.68	108.90
9	o	101	BCL	C3D-C2D-C1D	-2.33	102.65	105.83
9	8	101	BCL	CHB-C1B-NB	-2.33	120.55	124.05
9	r	101	BCL	CMA-C3A-C4A	-2.33	105.51	111.77
9	L	304	BCL	CAA-C2A-C1A	2.33	119.61	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	3	102	SPN	C6-C7-C8	2.33	123.54	112.02
10	u	102	SPN	C20-C21-C22	2.33	126.98	114.56
8	A	101	U10	C27-C28-C29	-2.33	122.30	127.62
9	f	101	BCL	CMA-C3A-C4A	-2.33	105.52	111.77
10	r	102	SPN	C20-C21-C22	2.33	126.97	114.56
11	H	302	MW9	O8-C19-C18	-2.32	100.01	108.34
9	4	101	BCL	C4-C3-C5	2.32	119.26	115.23
10	1	103	SPN	C20-C21-C22	2.32	126.93	114.56
9	i	101	BCL	C4D-CHA-C1A	2.32	124.01	121.24
8	M	403	U10	C25-C24-C26	2.32	119.25	115.23
10	0	102	SPN	CM6-C18-C19	-2.32	117.68	123.63
10	h	102	SPN	C6-C7-C8	2.31	123.47	112.02
9	4	101	BCL	C1D-CHD-C4C	-2.31	121.06	126.62
9	M	402	BCL	CAA-C2A-C1A	2.31	119.53	111.97
9	b	101	BCL	CGD-CBD-CAD	2.31	118.31	110.85
9	l	101	BCL	C3C-C4C-CHD	-2.30	118.53	123.39
9	d	101	BCL	CMA-C3A-C4A	-2.30	105.59	111.77
10	e	102	SPN	CM6-C18-C19	-2.30	117.73	123.63
10	p	102	SPN	CM3-C5-C4	-2.29	117.73	123.63
10	w	102	SPN	C6-C7-C8	2.29	123.36	112.02
10	c	102	SPN	C6-C7-C8	2.29	123.36	112.02
10	r	102	SPN	C6-C7-C8	2.29	123.36	112.02
9	3	101	BCL	C3D-C2D-C1D	-2.29	102.70	105.83
9	2	101	BCL	CMB-C2B-C3B	2.29	132.90	125.67
9	g	101	BCL	CMA-C3A-C4A	-2.29	105.63	111.77
8	M	403	U10	C3-C2-C1	2.29	122.62	118.10
10	e	102	SPN	C6-C7-C8	2.28	123.32	112.02
10	9	103	SPN	CM6-C18-C19	-2.28	117.76	123.63
9	8	101	BCL	O2A-CGA-O1A	-2.28	117.92	123.63
10	a	102	SPN	C10-C11-C12	2.28	123.31	112.02
10	h	102	SPN	CM6-C18-C19	-2.28	117.76	123.63
9	7	101	BCL	C4D-CHA-C1A	2.28	123.97	121.24
10	7	102	SPN	C4-C3-C2	2.28	122.34	111.68
9	8	101	BCL	C1-C2-C3	-2.28	122.46	126.20
9	M	402	BCL	C11-C10-C8	-2.28	108.39	115.97
10	c	103	SPN	CM6-C18-C19	-2.28	117.77	123.63
10	m	102	SPN	C4-C3-C2	2.28	122.33	111.68
10	s	102	SPN	C20-C21-C22	2.28	126.72	114.56
10	5	102	SPN	CM3-C5-C4	-2.28	117.78	123.63
10	n	102	SPN	C20-C21-C22	2.28	126.70	114.56
10	3	102	SPN	CM3-C5-C4	-2.27	117.79	123.63
10	c	102	SPN	CM6-C18-C19	-2.27	117.79	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	9	103	SPN	C6-C7-C8	2.27	123.27	112.02
9	4	101	BCL	C4D-C3D-CAD	2.27	110.57	108.11
10	7	103	SPN	CM6-C18-C19	-2.27	117.79	123.63
10	a	102	SPN	CM4-C9-C8	-2.27	117.80	123.63
10	1	105	SPN	CM6-C18-C19	-2.27	117.80	123.63
10	m	102	SPN	CM3-C5-C4	-2.27	117.80	123.63
10	m	102	SPN	CM6-C18-C19	-2.27	117.80	123.63
10	i	102	SPN	CM6-C18-C19	-2.27	117.80	123.63
10	7	102	SPN	CM6-C18-C19	-2.27	117.81	123.63
9	u	101	BCL	CHA-C1A-NA	-2.27	121.26	126.39
10	i	102	SPN	C6-C7-C8	2.27	123.23	112.02
10	w	102	SPN	CM6-C18-C19	-2.27	117.81	123.63
10	9	103	SPN	C20-C21-C22	2.26	126.65	114.56
10	5	103	SPN	CM6-C18-C19	-2.26	117.82	123.63
9	n	101	BCL	C2A-C1A-CHA	2.26	127.79	123.87
10	k	102	SPN	CM6-C18-C19	-2.26	117.82	123.63
10	k	102	SPN	C6-C7-C8	2.26	123.20	112.02
10	9	103	SPN	CM3-C5-C4	-2.26	117.83	123.63
10	7	102	SPN	CM3-C5-C4	-2.26	117.83	123.63
10	u	102	SPN	CM6-C18-C19	-2.26	117.83	123.63
9	8	101	BCL	C4-C3-C5	2.26	119.14	115.23
10	c	102	SPN	C4-C3-C2	2.25	122.22	111.68
10	w	102	SPN	C20-C21-C22	2.25	126.59	114.56
10	r	102	SPN	CM6-C18-C19	-2.25	117.84	123.63
9	d	101	BCL	C3C-C4C-CHD	-2.25	118.64	123.39
10	u	102	SPN	C6-C7-C8	2.25	123.15	112.02
9	M	402	BCL	CAA-CBA-CGA	-2.25	106.82	113.21
9	a	101	BCL	CMD-C2D-C1D	2.25	128.69	124.73
9	j	101	BCL	CMD-C2D-C1D	2.25	128.69	124.73
9	g	101	BCL	CHA-C1A-NA	-2.25	121.30	126.39
10	M	406	SPN	O1-C1-C2	2.25	113.50	108.90
10	e	102	SPN	CM3-C5-C4	-2.25	117.86	123.63
10	1	102	SPN	CM4-C9-C8	-2.24	117.87	123.63
10	n	102	SPN	CM6-C18-C19	-2.24	117.87	123.63
10	k	102	SPN	C20-C21-C22	2.24	126.53	114.56
10	k	102	SPN	CM3-C5-C4	-2.24	117.87	123.63
10	s	102	SPN	CM6-C18-C19	-2.24	117.87	123.63
9	x	101	BCL	C3C-C4C-CHD	-2.24	118.67	123.39
10	s	102	SPN	C6-C7-C8	2.24	123.09	112.02
10	t	102	SPN	CM6-C18-C19	-2.24	117.88	123.63
9	r	101	BCL	CMD-C2D-C1D	2.24	128.67	124.73
10	5	102	SPN	CM4-C9-C8	-2.23	117.89	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	9	103	SPN	O1-C1-C2	2.23	113.47	108.90
9	2	101	BCL	O2A-CGA-O1A	-2.23	118.04	123.63
10	e	102	SPN	C23-C22-C21	2.23	123.38	112.07
9	M	404	BCL	C3C-C4C-CHD	-2.23	118.69	123.39
10	3	102	SPN	CM4-C9-C8	-2.23	117.90	123.63
13	M	409	BPH	C2B-C1B-NB	-2.23	107.82	109.43
9	5	101	BCL	CHA-C1A-NA	-2.23	121.34	126.39
10	c	102	SPN	CM3-C5-C4	-2.23	117.91	123.63
9	j	101	BCL	CMA-C3A-C4A	-2.23	105.79	111.77
9	3	101	BCL	C4D-CHA-C1A	2.23	123.90	121.24
9	b	101	BCL	C4-C3-C5	2.23	119.09	115.23
10	m	102	SPN	CM4-C9-C8	-2.23	117.91	123.63
10	h	102	SPN	CM3-C5-C4	-2.23	117.91	123.63
10	u	102	SPN	CM3-C5-C4	-2.22	117.92	123.63
10	h	103	SPN	CM5-C13-C12	-2.22	117.92	123.63
10	a	102	SPN	CM3-C5-C4	-2.22	117.92	123.63
10	w	102	SPN	CM3-C5-C4	-2.22	117.92	123.63
10	u	102	SPN	CM4-C9-C8	-2.22	117.92	123.63
8	A	101	U10	C36-C34-C35	2.22	119.70	114.59
9	6	101	BCL	CHB-C1B-C2B	-2.22	120.98	127.43
10	r	102	SPN	CM3-C5-C4	-2.22	117.93	123.63
9	l	101	BCL	C1D-ND-C4D	2.22	107.87	106.31
10	1	102	SPN	CM3-C5-C4	-2.22	117.93	123.63
10	w	102	SPN	C10-C11-C12	2.22	122.99	112.02
10	h	102	SPN	CM4-C9-C8	-2.22	117.93	123.63
10	p	103	SPN	O1-C1-C2	2.22	113.44	108.90
9	r	101	BCL	C1D-ND-C4D	2.22	107.87	106.31
10	1	104	SPN	C15-C16-C17	2.22	121.28	113.13
10	3	102	SPN	C10-C11-C12	2.22	122.99	112.02
9	i	101	BCL	CMD-C2D-C1D	2.22	128.63	124.73
10	m	102	SPN	C10-C11-C12	2.22	122.98	112.02
9	o	101	BCL	CMA-C3A-C4A	-2.21	105.82	111.77
9	h	101	BCL	C3C-C4C-CHD	-2.21	118.72	123.39
10	f	102	SPN	C15-C16-C17	2.21	121.26	113.13
10	i	102	SPN	CM3-C5-C4	-2.21	117.95	123.63
9	o	101	BCL	C1-C2-C3	-2.21	122.57	126.20
10	w	102	SPN	CM4-C9-C8	-2.21	117.95	123.63
10	l	102	SPN	CM5-C13-C12	-2.21	117.95	123.63
9	b	101	BCL	C1C-NC-C4C	-2.21	105.67	106.68
11	M	408	MW9	C9-C8-C7	2.21	125.51	114.37
10	1	104	SPN	CM5-C13-C12	-2.20	117.97	123.63
10	9	103	SPN	CM4-C9-C8	-2.20	117.97	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	f	102	SPN	CM5-C13-C12	-2.20	117.97	123.63
10	q	102	SPN	CM6-C18-C19	-2.20	117.97	123.63
10	h	102	SPN	C10-C11-C12	2.20	122.91	112.02
10	5	102	SPN	CM5-C13-C12	-2.20	117.97	123.63
10	c	102	SPN	CM4-C9-C8	-2.20	117.98	123.63
10	7	102	SPN	CM4-C9-C8	-2.20	117.98	123.63
10	e	102	SPN	CM4-C9-C8	-2.20	117.98	123.63
9	t	101	BCL	C3C-C4C-CHD	-2.20	118.76	123.39
10	c	102	SPN	C20-C21-C22	2.20	126.28	114.56
10	k	102	SPN	CM4-C9-C8	-2.20	117.99	123.63
10	m	102	SPN	CM5-C13-C12	-2.20	117.99	123.63
8	A	101	U10	C17-C16-C14	-2.20	105.91	113.19
10	i	102	SPN	CM4-C9-C8	-2.20	117.99	123.63
10	3	102	SPN	C4-C3-C2	2.19	121.94	111.68
10	j	102	SPN	CM5-C13-C12	-2.19	117.99	123.63
10	r	102	SPN	CM4-C9-C8	-2.19	117.99	123.63
9	v	101	BCL	C2A-C3A-C4A	-2.19	98.33	101.87
10	w	102	SPN	CM5-C13-C12	-2.19	118.00	123.63
9	b	101	BCL	CHC-C1C-NC	2.19	127.56	124.40
10	m	102	SPN	C23-C22-C21	2.19	123.17	112.07
10	s	102	SPN	CM3-C5-C4	-2.19	118.00	123.63
10	k	102	SPN	CM5-C13-C12	-2.19	118.01	123.63
10	i	102	SPN	CM5-C13-C12	-2.19	118.01	123.63
10	t	102	SPN	O1-C1-C2	2.19	113.38	108.90
9	M	402	BCL	CHB-C1B-C2B	-2.19	121.08	127.43
9	c	101	BCL	CMD-C2D-C1D	2.19	128.58	124.73
9	1	101	BCL	CMD-C2D-C1D	2.18	128.57	124.73
9	r	101	BCL	C3C-C4C-CHD	-2.18	118.79	123.39
9	3	101	BCL	CHA-C1A-NA	-2.18	121.45	126.39
10	s	102	SPN	CM4-C9-C8	-2.18	118.02	123.63
10	a	103	SPN	CM5-C13-C12	-2.18	118.02	123.63
8	M	403	U10	C56-C54-C55	2.18	119.61	114.59
10	h	102	SPN	CM5-C13-C12	-2.18	118.03	123.63
9	L	301	BCL	C1D-ND-C4D	2.18	107.84	106.31
10	u	102	SPN	CM5-C13-C12	-2.18	118.03	123.63
10	9	103	SPN	CM5-C13-C12	-2.18	118.03	123.63
10	t	102	SPN	CM5-C13-C12	-2.18	118.03	123.63
10	1	105	SPN	C23-C22-C21	2.18	123.10	112.07
10	7	102	SPN	CM5-C13-C12	-2.18	118.03	123.63
10	7	103	SPN	CM5-C13-C12	-2.18	118.04	123.63
10	m	102	SPN	C20-C21-C22	2.18	126.17	114.56
10	h	102	SPN	C20-C21-C22	2.18	126.17	114.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	e	102	SPN	C4-C3-C2	2.17	121.84	111.68
10	l	102	SPN	CM5-C13-C12	-2.17	118.04	123.63
10	r	102	SPN	CM5-C13-C12	-2.17	118.04	123.63
10	5	103	SPN	CM5-C13-C12	-2.17	118.05	123.63
10	s	102	SPN	CM5-C13-C12	-2.17	118.05	123.63
9	j	101	BCL	C3C-C4C-CHD	-2.17	118.82	123.39
9	l	101	BCL	CMD-C2D-C1D	2.17	128.55	124.73
10	e	102	SPN	C10-C11-C12	2.17	122.75	112.02
11	M	408	MW9	C8-C9-C10	2.17	125.33	114.37
10	v	102	SPN	O1-C1-C2	2.17	113.33	108.90
10	c	103	SPN	CM5-C13-C12	-2.17	118.06	123.63
9	M	402	BCL	CMB-C2B-C3B	2.17	132.50	125.67
10	c	102	SPN	CM5-C13-C12	-2.17	118.07	123.63
10	3	102	SPN	CM5-C13-C12	-2.16	118.07	123.63
9	7	101	BCL	C3D-C2D-C1D	-2.16	102.88	105.83
10	0	102	SPN	CM3-C5-C4	-2.16	118.07	123.63
10	v	102	SPN	CM5-C13-C12	-2.16	118.07	123.63
9	r	101	BCL	C2A-C1A-CHA	2.16	127.62	123.87
10	e	102	SPN	O1-C1-C2	2.16	113.33	108.90
10	j	102	SPN	CM3-C5-C4	-2.16	118.08	123.63
10	M	406	SPN	CM3-C5-C4	-2.16	118.08	123.63
13	M	409	BPH	CMD-C2D-C3D	2.16	129.00	124.68
10	h	102	SPN	C4-C3-C2	2.16	121.78	111.68
9	0	101	BCL	CHB-C1B-C2B	-2.16	121.15	127.43
10	7	102	SPN	C10-C11-C12	2.16	122.71	112.02
10	h	102	SPN	C23-C22-C21	2.16	123.01	112.07
10	w	102	SPN	O1-C1-C2	2.16	113.32	108.90
10	p	103	SPN	CM3-C5-C4	-2.16	118.08	123.63
9	e	101	BCL	CMD-C2D-C1D	2.16	128.53	124.73
9	f	101	BCL	C3C-C4C-CHD	-2.16	118.84	123.39
10	5	102	SPN	C10-C11-C12	2.16	122.69	112.02
10	u	102	SPN	C10-C11-C12	2.16	122.68	112.02
10	p	103	SPN	CM5-C13-C12	-2.15	118.09	123.63
10	c	103	SPN	CM3-C5-C4	-2.15	118.10	123.63
10	q	102	SPN	CM3-C5-C4	-2.15	118.10	123.63
10	7	103	SPN	CM3-C5-C4	-2.15	118.10	123.63
9	e	101	BCL	C3C-C4C-CHD	-2.15	118.86	123.39
8	M	403	U10	C3M-O3-C3	2.15	124.02	116.47
10	l	104	SPN	CM3-C5-C4	-2.15	118.11	123.63
10	t	102	SPN	CM4-C9-C8	-2.15	118.11	123.63
10	q	102	SPN	CM5-C13-C12	-2.15	118.11	123.63
10	l	102	SPN	C20-C21-C22	2.15	126.02	114.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	v	102	SPN	CM4-C9-C8	-2.15	118.11	123.63
10	t	102	SPN	CM3-C5-C4	-2.15	118.11	123.63
10	a	102	SPN	CM5-C13-C12	-2.15	118.11	123.63
9	M	402	BCL	CHB-C4A-NA	2.15	127.50	124.40
9	2	101	BCL	CHC-C1C-NC	2.15	127.50	124.40
9	7	101	BCL	CMD-C2D-C1D	2.14	128.50	124.73
10	1	103	SPN	CM7-C22-C21	2.14	118.92	111.27
10	t	102	SPN	CM7-C22-C21	2.14	118.92	111.27
10	0	102	SPN	CM5-C13-C12	-2.14	118.12	123.63
10	c	102	SPN	C10-C11-C12	2.14	122.62	112.02
9	s	101	BCL	C3C-C4C-CHD	-2.14	118.88	123.39
9	w	101	BCL	C3C-C4C-CHD	-2.14	118.88	123.39
12	C	402	HEM	CBC-CAC-C3C	2.14	138.23	127.53
9	1	101	BCL	CMA-C3A-C4A	-2.14	106.02	111.77
10	e	102	SPN	CM5-C13-C12	-2.14	118.13	123.63
10	k	102	SPN	C4-C3-C2	2.14	121.68	111.68
10	a	103	SPN	CM3-C5-C4	-2.14	118.13	123.63
9	6	101	BCL	C11-C12-C13	-2.14	108.85	115.97
10	i	102	SPN	C4-C3-C2	2.14	121.68	111.68
10	l	102	SPN	CM3-C5-C4	-2.14	118.13	123.63
9	u	101	BCL	CMD-C2D-C1D	2.14	128.49	124.73
10	k	102	SPN	C10-C11-C12	2.14	122.60	112.02
9	M	402	BCL	C14-C13-C12	-2.14	103.65	111.27
9	i	101	BCL	C3D-C2D-C1D	-2.14	102.91	105.83
10	p	103	SPN	CM7-C22-C21	2.14	118.89	111.27
9	L	304	BCL	C1C-NC-C4C	2.13	107.65	106.68
10	i	102	SPN	C10-C11-C12	2.13	122.57	112.02
10	1	102	SPN	C23-C22-C21	2.13	122.87	112.07
10	n	102	SPN	CM5-C13-C12	-2.13	118.15	123.63
10	9	103	SPN	C10-C11-C12	2.13	122.56	112.02
9	s	101	BCL	C1D-ND-C4D	2.13	107.81	106.31
8	L	305	U10	C31-C29-C30	2.13	119.49	114.59
9	v	101	BCL	C3C-C4C-CHD	-2.13	118.91	123.39
8	L	305	U10	C25-C24-C26	2.13	118.92	115.23
10	r	102	SPN	C10-C11-C12	2.13	122.54	112.02
9	x	101	BCL	C2A-C1A-CHA	2.13	127.56	123.87
9	M	404	BCL	C2A-C1A-CHA	2.12	127.55	123.87
9	b	101	BCL	CHB-C1B-C2B	-2.12	121.26	127.43
10	l	102	SPN	CM4-C9-C8	-2.12	118.17	123.63
10	t	102	SPN	C20-C21-C22	2.12	125.89	114.56
10	1	105	SPN	CM3-C5-C4	-2.12	118.18	123.63
9	a	101	BCL	C3C-C4C-CHD	-2.12	118.92	123.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	q	102	SPN	CM4-C9-C8	-2.12	118.18	123.63
10	5	103	SPN	CM3-C5-C4	-2.12	118.19	123.63
9	l	101	BCL	C4D-CHA-C1A	2.12	123.77	121.24
9	i	101	BCL	CMA-C3A-C4A	-2.12	106.08	111.77
10	w	102	SPN	C23-C22-C21	2.12	122.80	112.07
10	f	102	SPN	CM3-C5-C4	-2.12	118.19	123.63
10	v	102	SPN	CM3-C5-C4	-2.12	118.19	123.63
10	1	103	SPN	C10-C11-C12	2.11	122.47	112.02
10	c	102	SPN	C23-C22-C21	2.11	122.77	112.07
10	s	102	SPN	C10-C11-C12	2.11	122.44	112.02
9	h	101	BCL	C1D-ND-C4D	2.11	107.79	106.31
10	h	103	SPN	CM3-C5-C4	-2.11	118.22	123.63
12	C	401	HEM	CAB-C3B-C4B	-2.11	115.09	124.39
9	4	101	BCL	C4D-CHA-C1A	-2.10	118.73	121.24
8	A	101	U10	C32-C33-C34	-2.10	120.63	127.64
10	p	103	SPN	CM4-C9-C8	-2.10	118.23	123.63
10	s	102	SPN	O1-C1-C2	2.10	113.20	108.90
10	1	105	SPN	CM5-C13-C12	-2.10	118.23	123.63
9	u	101	BCL	C3D-C2D-C1D	-2.10	102.97	105.83
10	n	102	SPN	CM3-C5-C4	-2.10	118.24	123.63
9	w	101	BCL	CHB-C1B-NB	-2.10	120.90	124.05
10	c	103	SPN	CM4-C9-C8	-2.09	118.25	123.63
10	9	103	SPN	C23-C22-C21	2.09	122.68	112.07
10	0	102	SPN	CM4-C9-C8	-2.09	118.25	123.63
9	c	101	BCL	C3D-C2D-C1D	-2.09	102.97	105.83
9	a	101	BCL	C3D-C2D-C1D	-2.09	102.97	105.83
10	h	103	SPN	CM4-C9-C8	-2.09	118.25	123.63
8	A	101	U10	C10-C9-C11	2.09	118.86	115.23
9	e	101	BCL	C3D-C2D-C1D	-2.09	102.98	105.83
10	f	102	SPN	CM4-C9-C8	-2.09	118.26	123.63
9	m	101	BCL	CHB-C1B-NB	-2.09	120.92	124.05
10	n	102	SPN	CM4-C9-C8	-2.09	118.27	123.63
9	j	101	BCL	C3D-C2D-C1D	-2.09	102.98	105.83
9	e	101	BCL	C3D-C4D-ND	-2.09	106.60	109.99
10	c	103	SPN	O1-C1-C2	2.08	113.17	108.90
10	v	102	SPN	C10-C11-C12	2.08	122.33	112.02
9	r	101	BCL	C3D-C2D-C1D	-2.08	102.99	105.83
10	h	102	SPN	O1-C1-C2	2.08	113.16	108.90
10	u	102	SPN	C4-C3-C2	2.08	121.41	111.68
9	c	101	BCL	C3C-C4C-CHD	-2.08	119.00	123.39
10	v	102	SPN	C20-C19-C18	2.08	132.39	127.62
10	3	102	SPN	C23-C22-C21	2.08	122.61	112.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	8	101	BCL	C1D-CHD-C4C	-2.08	121.60	126.62
9	s	101	BCL	C3D-C2D-C1D	-2.08	102.99	105.83
9	p	101	BCL	C2A-C1A-CHA	2.08	127.48	123.87
9	6	101	BCL	C1D-CHD-C4C	-2.08	121.61	126.62
9	g	101	BCL	C3C-C4C-CHD	-2.08	119.01	123.39
10	h	103	SPN	C15-C16-C17	2.08	120.76	113.13
10	l	103	SPN	CM3-C5-C4	-2.08	118.29	123.63
13	L	303	BPH	OBD-CAD-CBD	-2.08	122.78	125.82
9	b	101	BCL	C1D-CHD-C4C	-2.08	121.61	126.62
10	a	103	SPN	CM4-C9-C8	-2.07	118.30	123.63
10	c	102	SPN	O1-C1-C2	2.07	113.15	108.90
9	M	402	BCL	C1D-CHD-C4C	-2.07	121.62	126.62
10	l	103	SPN	CM4-C9-C8	-2.07	118.31	123.63
8	L	305	U10	C11-C9-C8	-2.07	116.52	121.17
8	M	403	U10	C37-C38-C39	-2.07	122.89	127.62
10	7	102	SPN	C23-C22-C21	2.07	122.54	112.07
10	k	102	SPN	C23-C22-C21	2.06	122.52	112.07
9	c	101	BCL	CHB-C1B-NB	-2.06	120.96	124.05
10	l	104	SPN	CM4-C9-C8	-2.06	118.34	123.63
9	0	101	BCL	C11-C12-C13	-2.06	109.12	115.97
10	j	102	SPN	CM4-C9-C8	-2.06	118.34	123.63
9	k	101	BCL	C3C-C4C-CHD	-2.06	119.06	123.39
9	o	101	BCL	C4D-CHA-C1A	2.05	123.69	121.24
9	g	101	BCL	C3D-C4D-ND	-2.05	106.65	109.99
13	M	405	BPH	C2B-C1B-NB	-2.05	107.95	109.43
9	m	101	BCL	CMD-C2D-C1D	2.05	128.34	124.73
10	s	102	SPN	C4-C3-C2	2.05	121.26	111.68
9	4	101	BCL	O2A-CGA-O1A	-2.05	118.50	123.63
9	L	304	BCL	CMD-C2D-C1D	2.05	128.34	124.73
9	p	101	BCL	CMD-C2D-C1D	2.05	128.34	124.73
10	k	102	SPN	O1-C1-C2	2.05	113.09	108.90
10	l	102	SPN	C10-C11-C12	2.05	122.14	112.02
10	r	102	SPN	C23-C22-C21	2.05	122.44	112.07
9	9	102	BCL	C3C-C4C-CHD	-2.04	119.08	123.39
9	9	102	BCL	CMD-C2D-C1D	2.04	128.33	124.73
9	g	101	BCL	CMD-C2D-C1D	2.04	128.32	124.73
10	s	102	SPN	C23-C22-C21	2.04	122.41	112.07
9	g	101	BCL	C3D-C2D-C1D	-2.04	103.05	105.83
10	M	406	SPN	CM4-C9-C8	-2.04	118.39	123.63
13	L	303	BPH	CMD-C2D-C3D	2.04	128.76	124.68
9	d	101	BCL	C2A-C3A-C4A	-2.04	98.58	101.87
9	f	101	BCL	C2A-C1A-CHA	2.04	127.41	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	1	105	SPN	CM4-C9-C8	-2.04	118.39	123.63
10	a	103	SPN	O1-C1-C2	2.04	113.07	108.90
9	4	101	BCL	CHB-C1B-C2B	-2.04	121.51	127.43
9	d	101	BCL	CMD-C2D-C1D	2.04	128.31	124.73
8	A	101	U10	C22-C21-C19	-2.03	106.45	113.19
9	d	101	BCL	C1D-ND-C4D	2.03	107.74	106.31
9	7	101	BCL	CHA-C1A-NA	-2.03	121.80	126.39
9	0	101	BCL	C1D-CHD-C4C	-2.03	121.73	126.62
9	s	101	BCL	CMD-C2D-C1D	2.03	128.30	124.73
10	n	102	SPN	O1-C1-C2	2.03	113.05	108.90
10	7	103	SPN	CM4-C9-C8	-2.03	118.42	123.63
10	n	102	SPN	C23-C22-C21	2.02	122.33	112.07
9	p	101	BCL	CHB-C1B-NB	-2.02	121.01	124.05
9	x	101	BCL	CHB-C1B-NB	-2.02	121.01	124.05
10	e	102	SPN	C20-C21-C22	2.02	125.34	114.56
9	h	101	BCL	CMD-C2D-C1D	2.02	128.28	124.73
9	l	101	BCL	CHB-C1B-NB	-2.02	121.02	124.05
9	6	101	BCL	CGD-CBD-CAD	2.02	117.38	110.85
9	s	101	BCL	CHB-C1B-NB	-2.02	121.02	124.05
9	p	101	BCL	C3C-C4C-CHD	-2.01	119.15	123.39
9	M	402	BCL	CMD-C2D-C3D	-2.01	123.08	127.69
13	M	405	BPH	CMD-C2D-C3D	2.01	128.70	124.68
9	k	101	BCL	CHB-C1B-NB	-2.01	121.03	124.05
10	i	102	SPN	O1-C1-C2	2.01	113.01	108.90
9	t	101	BCL	C2A-C3A-C4A	-2.01	98.62	101.87
9	j	101	BCL	C4D-CHA-C1A	2.01	123.64	121.24
9	f	101	BCL	CMD-C2D-C1D	2.01	128.26	124.73
9	r	101	BCL	CHB-C1B-NB	-2.01	121.04	124.05
10	5	103	SPN	CM4-C9-C8	-2.01	118.48	123.63
10	7	102	SPN	O1-C1-C2	2.00	113.00	108.90
9	g	101	BCL	CHB-C1B-NB	-2.00	121.05	124.05
10	j	102	SPN	C15-C16-C17	2.00	120.48	113.13
10	p	103	SPN	CM6-C18-C19	-2.00	118.49	123.63

There are no chirality outliers.

All (1746) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	L	305	U10	C1-C6-C7-C8
8	L	305	U10	C5-C6-C7-C8
9	1	101	BCL	C2C-C3C-CAC-CBC
9	1	101	BCL	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
9	1	101	BCL	C11-C12-C13-C14
9	5	101	BCL	C1A-C2A-CAA-CBA
9	5	101	BCL	C3A-C2A-CAA-CBA
9	5	101	BCL	C2C-C3C-CAC-CBC
9	5	101	BCL	C4C-C3C-CAC-CBC
9	3	101	BCL	C1A-C2A-CAA-CBA
9	3	101	BCL	C3A-C2A-CAA-CBA
9	3	101	BCL	C1-C2-C3-C5
9	4	101	BCL	C2C-C3C-CAC-CBC
9	4	101	BCL	C4C-C3C-CAC-CBC
9	w	101	BCL	C2C-C3C-CAC-CBC
9	w	101	BCL	C4C-C3C-CAC-CBC
9	w	101	BCL	C1-C2-C3-C5
9	w	101	BCL	C2-C3-C5-C6
9	w	101	BCL	C4-C3-C5-C6
9	x	101	BCL	C11-C12-C13-C14
9	u	101	BCL	C4C-C3C-CAC-CBC
9	v	101	BCL	CBA-CGA-O2A-C1
9	v	101	BCL	O1A-CGA-O2A-C1
9	v	101	BCL	C2C-C3C-CAC-CBC
9	v	101	BCL	CAD-CBD-CGD-O1D
9	v	101	BCL	CAD-CBD-CGD-O2D
9	s	101	BCL	C2C-C3C-CAC-CBC
9	s	101	BCL	C1-C2-C3-C4
9	t	101	BCL	C1A-C2A-CAA-CBA
9	t	101	BCL	C3A-C2A-CAA-CBA
9	q	101	BCL	C11-C12-C13-C14
9	r	101	BCL	C2C-C3C-CAC-CBC
9	r	101	BCL	C4C-C3C-CAC-CBC
9	o	101	BCL	C2C-C3C-CAC-CBC
9	o	101	BCL	C4C-C3C-CAC-CBC
9	m	101	BCL	C4C-C3C-CAC-CBC
9	m	101	BCL	C1-C2-C3-C4
9	n	101	BCL	C1A-C2A-CAA-CBA
9	n	101	BCL	C3A-C2A-CAA-CBA
9	n	101	BCL	C2C-C3C-CAC-CBC
9	n	101	BCL	C4C-C3C-CAC-CBC
9	k	101	BCL	C1A-C2A-CAA-CBA
9	k	101	BCL	C3A-C2A-CAA-CBA
9	k	101	BCL	C2C-C3C-CAC-CBC
9	l	101	BCL	C1A-C2A-CAA-CBA
9	l	101	BCL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
9	l	101	BCL	C2C-C3C-CAC-CBC
9	l	101	BCL	C1-C2-C3-C4
9	g	101	BCL	C2C-C3C-CAC-CBC
9	g	101	BCL	C4C-C3C-CAC-CBC
9	h	101	BCL	C2C-C3C-CAC-CBC
9	h	101	BCL	C1-C2-C3-C4
9	e	101	BCL	C2C-C3C-CAC-CBC
9	e	101	BCL	C4C-C3C-CAC-CBC
9	e	101	BCL	C1-C2-C3-C4
9	e	101	BCL	C14-C13-C15-C16
9	f	101	BCL	C2C-C3C-CAC-CBC
9	f	101	BCL	C1-C2-C3-C4
9	f	101	BCL	C1-C2-C3-C5
9	c	101	BCL	C1A-C2A-CAA-CBA
9	c	101	BCL	C3A-C2A-CAA-CBA
9	c	101	BCL	C4C-C3C-CAC-CBC
9	c	101	BCL	C1-C2-C3-C5
9	d	101	BCL	CBA-CGA-O2A-C1
9	d	101	BCL	O1A-CGA-O2A-C1
9	d	101	BCL	C1-C2-C3-C4
9	d	101	BCL	C1-C2-C3-C5
9	a	101	BCL	C1A-C2A-CAA-CBA
9	a	101	BCL	C3A-C2A-CAA-CBA
9	a	101	BCL	C4C-C3C-CAC-CBC
9	a	101	BCL	C11-C12-C13-C14
9	b	101	BCL	C11-C10-C8-C9
9	i	101	BCL	C2C-C3C-CAC-CBC
9	i	101	BCL	C4C-C3C-CAC-CBC
9	j	101	BCL	C1A-C2A-CAA-CBA
9	j	101	BCL	C3A-C2A-CAA-CBA
9	j	101	BCL	C2C-C3C-CAC-CBC
9	7	101	BCL	C1A-C2A-CAA-CBA
9	7	101	BCL	C3A-C2A-CAA-CBA
9	7	101	BCL	C2C-C3C-CAC-CBC
9	7	101	BCL	C4C-C3C-CAC-CBC
9	7	101	BCL	C1-C2-C3-C4
9	8	101	BCL	C1A-C2A-CAA-CBA
9	8	101	BCL	C3A-C2A-CAA-CBA
9	8	101	BCL	C2C-C3C-CAC-CBC
9	8	101	BCL	C4C-C3C-CAC-CBC
9	L	301	BCL	C1-C2-C3-C5
9	L	304	BCL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
9	L	304	BCL	C3A-C2A-CAA-CBA
9	L	304	BCL	C4C-C3C-CAC-CBC
9	L	304	BCL	C1-C2-C3-C5
9	9	102	BCL	C1A-C2A-CAA-CBA
9	9	102	BCL	C3A-C2A-CAA-CBA
9	9	102	BCL	C4C-C3C-CAC-CBC
10	1	102	SPN	CM1-C1-O1-CMA
10	1	102	SPN	C2-C1-O1-CMA
10	1	102	SPN	CM1-C1-C2-O2
10	1	102	SPN	CM1-C1-C2-C3
10	1	102	SPN	C20-C21-C22-CM7
10	1	103	SPN	CM1-C1-O1-CMA
10	1	103	SPN	CM2-C1-O1-CMA
10	1	103	SPN	C18-C19-C20-C21
10	1	104	SPN	CM2-C1-O1-CMA
10	1	104	SPN	C2-C1-O1-CMA
10	1	104	SPN	O1-C1-C2-O2
10	1	104	SPN	C18-C19-C20-C21
10	1	105	SPN	CM1-C1-O1-CMA
10	1	105	SPN	CM2-C1-O1-CMA
10	1	105	SPN	C2-C1-O1-CMA
10	1	105	SPN	O1-C1-C2-O2
10	1	105	SPN	C20-C21-C22-CM7
10	1	105	SPN	C25-C26-C27-C28
10	1	105	SPN	CM8-C26-C27-C28
10	5	102	SPN	CM1-C1-O1-CMA
10	5	102	SPN	C2-C1-O1-CMA
10	5	102	SPN	CM1-C1-C2-O2
10	5	102	SPN	CM1-C1-C2-C3
10	5	102	SPN	CM2-C1-C2-C3
10	5	102	SPN	C20-C21-C22-CM7
10	5	102	SPN	C22-C23-C24-C25
10	5	103	SPN	CM1-C1-O1-CMA
10	5	103	SPN	C2-C1-O1-CMA
10	5	103	SPN	C20-C21-C22-CM7
10	3	102	SPN	CM1-C1-O1-CMA
10	3	102	SPN	C2-C1-O1-CMA
10	3	102	SPN	CM1-C1-C2-O2
10	3	102	SPN	CM1-C1-C2-C3
10	3	102	SPN	CM2-C1-C2-C3
10	3	102	SPN	C20-C21-C22-CM7
10	w	102	SPN	CM2-C1-O1-CMA

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Mol	Chain	Res	Type	Atoms
10	w	102	SPN	O1-C1-C2-O2
10	w	102	SPN	CM2-C1-C2-C3
10	w	102	SPN	C20-C21-C22-CM7
10	u	102	SPN	CM1-C1-C2-C3
10	u	102	SPN	CM2-C1-C2-O2
10	u	102	SPN	CM2-C1-C2-C3
10	u	102	SPN	C20-C21-C22-CM7
10	u	102	SPN	C26-C27-C28-C29
10	v	102	SPN	O1-C1-C2-O2
10	v	102	SPN	C18-C19-C20-C21
10	s	102	SPN	O1-C1-C2-O2
10	s	102	SPN	CM2-C1-C2-O2
10	s	102	SPN	CM2-C1-C2-C3
10	s	102	SPN	C20-C21-C22-CM7
10	t	102	SPN	CM2-C1-O1-CMA
10	t	102	SPN	O1-C1-C2-O2
10	t	102	SPN	C20-C21-C22-CM7
10	q	102	SPN	O1-C1-C2-O2
10	q	102	SPN	C20-C21-C22-CM7
10	q	102	SPN	C22-C23-C24-C25
10	r	102	SPN	O1-C1-C2-O2
10	r	102	SPN	CM2-C1-C2-C3
10	r	102	SPN	C20-C21-C22-CM7
10	p	102	SPN	C6-C7-C8-C9
10	p	102	SPN	C10-C11-C12-C13
10	p	102	SPN	C11-C12-C13-CM5
10	p	102	SPN	C11-C12-C13-C14
10	p	102	SPN	C20-C21-C22-CM7
10	p	102	SPN	C22-C23-C24-C25
10	p	103	SPN	O1-C1-C2-O2
10	p	103	SPN	CM2-C1-C2-C3
10	p	103	SPN	CM6-C18-C19-C20
10	p	103	SPN	C18-C19-C20-C21
10	m	102	SPN	C20-C21-C22-CM7
10	n	102	SPN	O1-C1-C2-O2
10	n	102	SPN	C20-C21-C22-CM7
10	n	102	SPN	CM8-C26-C27-C28
10	k	102	SPN	C2-C1-O1-CMA
10	k	102	SPN	C20-C21-C22-CM7
10	l	102	SPN	O1-C1-C2-O2
10	l	102	SPN	C18-C19-C20-C21
10	h	102	SPN	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
10	h	102	SPN	CM1-C1-C2-C3
10	h	102	SPN	CM2-C1-C2-O2
10	h	102	SPN	CM2-C1-C2-C3
10	h	102	SPN	C20-C21-C22-CM7
10	h	103	SPN	O1-C1-C2-O2
10	h	103	SPN	C18-C19-C20-C21
10	e	102	SPN	O1-C1-C2-O2
10	e	102	SPN	CM2-C1-C2-O2
10	e	102	SPN	CM2-C1-C2-C3
10	e	102	SPN	C20-C21-C22-CM7
10	f	102	SPN	O1-C1-C2-O2
10	f	102	SPN	C18-C19-C20-C21
10	c	102	SPN	O1-C1-C2-O2
10	c	102	SPN	CM2-C1-C2-O2
10	c	102	SPN	CM2-C1-C2-C3
10	c	102	SPN	C20-C21-C22-CM7
10	c	103	SPN	CM1-C1-O1-CMA
10	c	103	SPN	CM2-C1-O1-CMA
10	c	103	SPN	O1-C1-C2-O2
10	c	103	SPN	C20-C21-C22-CM7
10	c	103	SPN	C26-C27-C28-C29
10	a	102	SPN	CM1-C1-O1-CMA
10	a	102	SPN	C2-C1-O1-CMA
10	a	102	SPN	O1-C1-C2-O2
10	a	102	SPN	CM2-C1-C2-O2
10	a	102	SPN	CM2-C1-C2-C3
10	a	102	SPN	C20-C21-C22-CM7
10	a	103	SPN	O1-C1-C2-O2
10	a	103	SPN	C18-C19-C20-C21
10	i	102	SPN	CM1-C1-C2-C3
10	i	102	SPN	CM2-C1-C2-O2
10	i	102	SPN	CM2-C1-C2-C3
10	i	102	SPN	C20-C21-C22-CM7
10	j	102	SPN	CM2-C1-O1-CMA
10	j	102	SPN	C2-C1-O1-CMA
10	j	102	SPN	O1-C1-C2-O2
10	j	102	SPN	C18-C19-C20-C21
10	7	102	SPN	CM1-C1-C2-O2
10	7	102	SPN	CM1-C1-C2-C3
10	7	102	SPN	C20-C21-C22-CM7
10	7	103	SPN	CM2-C1-O1-CMA
10	7	103	SPN	C2-C1-O1-CMA

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Mol	Chain	Res	Type	Atoms
10	7	103	SPN	O1-C1-C2-O2
10	7	103	SPN	C20-C21-C22-CM7
10	M	406	SPN	C18-C19-C20-C21
10	M	406	SPN	C20-C21-C22-CM7
10	M	406	SPN	CM7-C22-C23-C24
10	M	406	SPN	C22-C23-C24-C25
10	9	103	SPN	O1-C1-C2-O2
10	9	103	SPN	CM2-C1-C2-O2
10	9	103	SPN	CM2-C1-C2-C3
10	9	103	SPN	C20-C21-C22-CM7
10	0	102	SPN	CM2-C1-O1-CMA
10	0	102	SPN	C2-C1-O1-CMA
10	0	102	SPN	O1-C1-C2-O2
10	0	102	SPN	C20-C21-C22-CM7
11	g	102	MW9	C20-O2-P-O4
11	g	102	MW9	C20-O2-P-O5
11	g	102	MW9	C21-O5-P-O2
11	g	102	MW9	C21-O5-P-O3
11	H	301	MW9	O8-C19-C20-O2
11	H	301	MW9	C21-C22-C23-O6
11	H	301	MW9	C20-O2-P-O3
11	H	302	MW9	C19-C20-O2-P
11	H	302	MW9	C21-C22-C23-O6
11	H	302	MW9	C21-O5-P-O2
11	H	302	MW9	C21-O5-P-O3
11	H	303	MW9	C21-C22-C23-O6
11	H	303	MW9	O7-C22-C23-O6
11	H	303	MW9	C20-O2-P-O3
11	H	303	MW9	C20-O2-P-O4
11	H	303	MW9	C20-O2-P-O5
11	H	303	MW9	C21-O5-P-O2
11	H	303	MW9	C21-O5-P-O4
11	H	304	MW9	O-C17-O1-C18
11	H	304	MW9	C16-C17-O1-C18
11	H	304	MW9	O5-C21-C22-O7
11	H	304	MW9	C21-C22-C23-O6
11	H	304	MW9	C20-O2-P-O3
11	H	304	MW9	C20-O2-P-O4
11	H	304	MW9	C20-O2-P-O5
11	M	407	MW9	C25-C24-O8-C19
11	M	407	MW9	O9-C24-O8-C19
11	9	101	MW9	O7-C22-C23-O6

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Mol	Chain	Res	Type	Atoms
11	9	101	MW9	C20-O2-P-O3
11	9	101	MW9	C20-O2-P-O4
11	9	101	MW9	C20-O2-P-O5
11	9	101	MW9	C21-O5-P-O2
11	9	101	MW9	C21-O5-P-O4
13	L	303	BPH	C1-C2-C3-C5
13	M	405	BPH	C4C-C3C-CAC-CBC
13	M	409	BPH	C1-C2-C3-C4
13	M	409	BPH	C1-C2-C3-C5
9	g	101	BCL	CBD-CGD-O2D-CED
9	2	101	BCL	O1A-CGA-O2A-C1
9	p	101	BCL	O1A-CGA-O2A-C1
9	h	101	BCL	O1A-CGA-O2A-C1
9	0	101	BCL	O1A-CGA-O2A-C1
10	M	406	SPN	C15-C16-C17-C18
9	2	101	BCL	CBA-CGA-O2A-C1
9	p	101	BCL	CBA-CGA-O2A-C1
9	h	101	BCL	CBA-CGA-O2A-C1
9	x	101	BCL	O1A-CGA-O2A-C1
9	f	101	BCL	O1A-CGA-O2A-C1
9	b	101	BCL	O1A-CGA-O2A-C1
9	j	101	BCL	O1A-CGA-O2A-C1
9	b	101	BCL	C3-C5-C6-C7
9	0	101	BCL	C3-C5-C6-C7
13	M	409	BPH	C3-C5-C6-C7
9	r	101	BCL	CBA-CGA-O2A-C1
9	f	101	BCL	CBA-CGA-O2A-C1
9	b	101	BCL	CBA-CGA-O2A-C1
9	j	101	BCL	CBA-CGA-O2A-C1
9	0	101	BCL	CBA-CGA-O2A-C1
9	p	101	BCL	CBD-CGD-O2D-CED
8	L	305	U10	C15-C14-C16-C17
9	s	101	BCL	C4-C3-C5-C6
9	q	101	BCL	C4-C3-C5-C6
9	r	101	BCL	C4-C3-C5-C6
9	d	101	BCL	C4-C3-C5-C6
9	M	404	BCL	C4-C3-C5-C6
10	q	102	SPN	CM8-C26-C27-C28
10	p	102	SPN	CM8-C26-C27-C28
10	l	102	SPN	CM8-C26-C27-C28
10	h	103	SPN	CM8-C26-C27-C28
10	c	103	SPN	CM8-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
10	a	103	SPN	CM8-C26-C27-C28
9	s	101	BCL	C2-C3-C5-C6
9	r	101	BCL	C2-C3-C5-C6
9	d	101	BCL	C2-C3-C5-C6
9	M	404	BCL	C2-C3-C5-C6
10	l	103	SPN	C12-C13-C14-C15
10	p	102	SPN	C25-C26-C27-C28
10	n	102	SPN	C25-C26-C27-C28
10	h	103	SPN	C25-C26-C27-C28
10	c	103	SPN	C25-C26-C27-C28
10	a	103	SPN	C25-C26-C27-C28
9	t	101	BCL	C3-C5-C6-C7
9	p	101	BCL	C3-C5-C6-C7
9	f	101	BCL	C3-C5-C6-C7
9	j	101	BCL	C3-C5-C6-C7
9	x	101	BCL	CBA-CGA-O2A-C1
11	9	101	MW9	C1-C2-C3-C4
10	q	102	SPN	C24-C25-C26-CM8
11	9	101	MW9	C7-C8-C9-C10
11	H	301	MW9	C7-C8-C9-C10
9	r	101	BCL	O1A-CGA-O2A-C1
9	l	101	BCL	O1A-CGA-O2A-C1
11	M	408	MW9	C7-C8-C9-C10
11	H	303	MW9	C7-C8-C9-C10
11	H	304	MW9	C7-C8-C9-C10
11	M	407	MW9	C7-C8-C9-C10
9	2	101	BCL	C3-C5-C6-C7
9	M	402	BCL	C3-C5-C6-C7
9	o	101	BCL	CBD-CGD-O2D-CED
11	H	302	MW9	C7-C8-C9-C10
11	g	103	MW9	O5-C21-C22-O7
9	l	101	BCL	CBA-CGA-O2A-C1
9	g	101	BCL	O1D-CGD-O2D-CED
9	n	101	BCL	C3-C5-C6-C7
8	L	305	U10	C20-C19-C21-C22
9	m	101	BCL	C4-C3-C5-C6
9	g	101	BCL	C4-C3-C5-C6
10	1	102	SPN	CM3-C5-C6-C7
10	1	102	SPN	C11-C10-C9-CM4
10	1	102	SPN	CM5-C13-C14-C15
10	1	102	SPN	C16-C17-C18-CM6
10	1	103	SPN	CM3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
10	1	103	SPN	C11-C10-C9-CM4
10	1	104	SPN	CM3-C5-C6-C7
10	1	104	SPN	C11-C10-C9-CM4
10	1	104	SPN	CM5-C13-C14-C15
10	1	104	SPN	C16-C17-C18-CM6
10	1	105	SPN	CM3-C5-C6-C7
10	1	105	SPN	C11-C10-C9-CM4
10	1	105	SPN	CM5-C13-C14-C15
10	1	105	SPN	C16-C17-C18-CM6
10	5	102	SPN	CM3-C5-C6-C7
10	5	102	SPN	C11-C10-C9-CM4
10	5	102	SPN	CM5-C13-C14-C15
10	5	102	SPN	C16-C17-C18-CM6
10	5	103	SPN	CM3-C5-C6-C7
10	5	103	SPN	C11-C10-C9-CM4
10	5	103	SPN	CM5-C13-C14-C15
10	5	103	SPN	C16-C17-C18-CM6
10	3	102	SPN	CM3-C5-C6-C7
10	3	102	SPN	C11-C10-C9-CM4
10	3	102	SPN	CM5-C13-C14-C15
10	3	102	SPN	C16-C17-C18-CM6
10	w	102	SPN	CM3-C5-C6-C7
10	w	102	SPN	C11-C10-C9-CM4
10	w	102	SPN	CM5-C13-C14-C15
10	w	102	SPN	C16-C17-C18-CM6
10	u	102	SPN	CM3-C5-C6-C7
10	u	102	SPN	C11-C10-C9-CM4
10	u	102	SPN	CM5-C13-C14-C15
10	u	102	SPN	C16-C17-C18-CM6
10	v	102	SPN	CM3-C5-C6-C7
10	v	102	SPN	C11-C10-C9-CM4
10	v	102	SPN	CM5-C13-C14-C15
10	s	102	SPN	CM3-C5-C6-C7
10	s	102	SPN	C11-C10-C9-CM4
10	s	102	SPN	CM5-C13-C14-C15
10	s	102	SPN	C16-C17-C18-CM6
10	t	102	SPN	CM3-C5-C6-C7
10	t	102	SPN	C11-C10-C9-CM4
10	t	102	SPN	CM5-C13-C14-C15
10	t	102	SPN	C16-C17-C18-CM6
10	q	102	SPN	CM3-C5-C6-C7
10	q	102	SPN	C11-C10-C9-CM4

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Mol	Chain	Res	Type	Atoms
10	q	102	SPN	CM5-C13-C14-C15
10	q	102	SPN	C16-C17-C18-CM6
10	r	102	SPN	CM3-C5-C6-C7
10	r	102	SPN	C11-C10-C9-CM4
10	r	102	SPN	CM5-C13-C14-C15
10	r	102	SPN	C16-C17-C18-CM6
10	p	102	SPN	CM3-C5-C6-C7
10	p	102	SPN	C11-C10-C9-CM4
10	p	102	SPN	CM5-C13-C14-C15
10	p	102	SPN	C16-C17-C18-CM6
10	p	103	SPN	CM3-C5-C6-C7
10	p	103	SPN	C11-C10-C9-CM4
10	p	103	SPN	CM5-C13-C14-C15
10	p	103	SPN	C16-C17-C18-CM6
10	m	102	SPN	CM3-C5-C6-C7
10	m	102	SPN	C11-C10-C9-CM4
10	m	102	SPN	CM5-C13-C14-C15
10	m	102	SPN	C16-C17-C18-CM6
10	n	102	SPN	CM3-C5-C6-C7
10	n	102	SPN	C11-C10-C9-CM4
10	n	102	SPN	CM5-C13-C14-C15
10	n	102	SPN	C16-C17-C18-CM6
10	k	102	SPN	CM3-C5-C6-C7
10	k	102	SPN	C11-C10-C9-CM4
10	k	102	SPN	CM5-C13-C14-C15
10	k	102	SPN	C16-C17-C18-CM6
10	l	102	SPN	CM3-C5-C6-C7
10	l	102	SPN	C11-C10-C9-CM4
10	l	102	SPN	CM5-C13-C14-C15
10	l	102	SPN	C16-C17-C18-CM6
10	h	102	SPN	CM3-C5-C6-C7
10	h	102	SPN	C11-C10-C9-CM4
10	h	102	SPN	CM5-C13-C14-C15
10	h	102	SPN	C16-C17-C18-CM6
10	h	103	SPN	CM3-C5-C6-C7
10	h	103	SPN	C11-C10-C9-CM4
10	h	103	SPN	CM5-C13-C14-C15
10	h	103	SPN	C16-C17-C18-CM6
10	e	102	SPN	CM3-C5-C6-C7
10	e	102	SPN	C11-C10-C9-CM4
10	e	102	SPN	CM5-C13-C14-C15
10	e	102	SPN	C16-C17-C18-CM6

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Mol	Chain	Res	Type	Atoms
10	f	102	SPN	CM3-C5-C6-C7
10	f	102	SPN	C11-C10-C9-CM4
10	f	102	SPN	CM5-C13-C14-C15
10	f	102	SPN	C16-C17-C18-CM6
10	c	102	SPN	CM3-C5-C6-C7
10	c	102	SPN	C11-C10-C9-CM4
10	c	102	SPN	CM5-C13-C14-C15
10	c	102	SPN	C16-C17-C18-CM6
10	c	103	SPN	CM3-C5-C6-C7
10	c	103	SPN	C11-C10-C9-CM4
10	c	103	SPN	CM5-C13-C14-C15
10	c	103	SPN	C16-C17-C18-CM6
10	a	102	SPN	CM3-C5-C6-C7
10	a	102	SPN	C11-C10-C9-CM4
10	a	102	SPN	CM5-C13-C14-C15
10	a	102	SPN	C16-C17-C18-CM6
10	a	103	SPN	CM3-C5-C6-C7
10	a	103	SPN	C11-C10-C9-CM4
10	a	103	SPN	CM5-C13-C14-C15
10	a	103	SPN	C16-C17-C18-CM6
10	i	102	SPN	CM3-C5-C6-C7
10	i	102	SPN	C11-C10-C9-CM4
10	i	102	SPN	CM5-C13-C14-C15
10	i	102	SPN	C16-C17-C18-CM6
10	j	102	SPN	CM3-C5-C6-C7
10	j	102	SPN	C11-C10-C9-CM4
10	j	102	SPN	CM5-C13-C14-C15
10	j	102	SPN	C16-C17-C18-CM6
10	j	102	SPN	CM8-C26-C27-C28
10	7	102	SPN	CM3-C5-C6-C7
10	7	102	SPN	C11-C10-C9-CM4
10	7	102	SPN	CM5-C13-C14-C15
10	7	102	SPN	C16-C17-C18-CM6
10	7	103	SPN	CM3-C5-C6-C7
10	7	103	SPN	C11-C10-C9-CM4
10	7	103	SPN	CM5-C13-C14-C15
10	7	103	SPN	C16-C17-C18-CM6
10	7	103	SPN	CM8-C26-C27-C28
10	M	406	SPN	CM3-C5-C6-C7
10	M	406	SPN	C11-C10-C9-CM4
10	M	406	SPN	CM5-C13-C14-C15
10	M	406	SPN	C16-C17-C18-CM6

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Mol	Chain	Res	Type	Atoms
10	9	103	SPN	CM3-C5-C6-C7
10	9	103	SPN	C11-C10-C9-CM4
10	9	103	SPN	CM5-C13-C14-C15
10	9	103	SPN	C16-C17-C18-CM6
10	0	102	SPN	CM3-C5-C6-C7
10	0	102	SPN	C11-C10-C9-CM4
10	0	102	SPN	CM5-C13-C14-C15
10	0	102	SPN	C16-C17-C18-CM6
9	q	101	BCL	C2-C3-C5-C6
9	m	101	BCL	C2-C3-C5-C6
9	g	101	BCL	C2-C3-C5-C6
10	1	102	SPN	C4-C5-C6-C7
10	1	102	SPN	C11-C10-C9-C8
10	1	102	SPN	C12-C13-C14-C15
10	1	102	SPN	C16-C17-C18-C19
10	1	103	SPN	C4-C5-C6-C7
10	1	103	SPN	C11-C10-C9-C8
10	1	104	SPN	C4-C5-C6-C7
10	1	104	SPN	C11-C10-C9-C8
10	1	104	SPN	C12-C13-C14-C15
10	1	104	SPN	C16-C17-C18-C19
10	1	105	SPN	C4-C5-C6-C7
10	1	105	SPN	C11-C10-C9-C8
10	1	105	SPN	C12-C13-C14-C15
10	1	105	SPN	C16-C17-C18-C19
10	5	102	SPN	C4-C5-C6-C7
10	5	102	SPN	C11-C10-C9-C8
10	5	102	SPN	C12-C13-C14-C15
10	5	102	SPN	C16-C17-C18-C19
10	5	103	SPN	C4-C5-C6-C7
10	5	103	SPN	C11-C10-C9-C8
10	5	103	SPN	C12-C13-C14-C15
10	5	103	SPN	C16-C17-C18-C19
10	3	102	SPN	C4-C5-C6-C7
10	3	102	SPN	C11-C10-C9-C8
10	3	102	SPN	C12-C13-C14-C15
10	3	102	SPN	C16-C17-C18-C19
10	w	102	SPN	C4-C5-C6-C7
10	w	102	SPN	C11-C10-C9-C8
10	w	102	SPN	C12-C13-C14-C15
10	w	102	SPN	C16-C17-C18-C19
10	u	102	SPN	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
10	u	102	SPN	C11-C10-C9-C8
10	u	102	SPN	C12-C13-C14-C15
10	u	102	SPN	C16-C17-C18-C19
10	v	102	SPN	C4-C5-C6-C7
10	v	102	SPN	C11-C10-C9-C8
10	v	102	SPN	C12-C13-C14-C15
10	v	102	SPN	C16-C17-C18-C19
10	s	102	SPN	C4-C5-C6-C7
10	s	102	SPN	C11-C10-C9-C8
10	s	102	SPN	C12-C13-C14-C15
10	s	102	SPN	C16-C17-C18-C19
10	t	102	SPN	C4-C5-C6-C7
10	t	102	SPN	C11-C10-C9-C8
10	q	102	SPN	C11-C10-C9-C8
10	q	102	SPN	C12-C13-C14-C15
10	q	102	SPN	C25-C26-C27-C28
10	r	102	SPN	C4-C5-C6-C7
10	r	102	SPN	C11-C10-C9-C8
10	r	102	SPN	C12-C13-C14-C15
10	r	102	SPN	C16-C17-C18-C19
10	p	102	SPN	C4-C5-C6-C7
10	p	102	SPN	C16-C17-C18-C19
10	p	103	SPN	C4-C5-C6-C7
10	p	103	SPN	C11-C10-C9-C8
10	p	103	SPN	C12-C13-C14-C15
10	m	102	SPN	C4-C5-C6-C7
10	m	102	SPN	C11-C10-C9-C8
10	m	102	SPN	C12-C13-C14-C15
10	m	102	SPN	C16-C17-C18-C19
10	n	102	SPN	C4-C5-C6-C7
10	n	102	SPN	C11-C10-C9-C8
10	n	102	SPN	C12-C13-C14-C15
10	n	102	SPN	C16-C17-C18-C19
10	k	102	SPN	C4-C5-C6-C7
10	k	102	SPN	C11-C10-C9-C8
10	k	102	SPN	C12-C13-C14-C15
10	k	102	SPN	C16-C17-C18-C19
10	l	102	SPN	C4-C5-C6-C7
10	l	102	SPN	C11-C10-C9-C8
10	l	102	SPN	C12-C13-C14-C15
10	l	102	SPN	C16-C17-C18-C19
10	l	102	SPN	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
10	h	102	SPN	C4-C5-C6-C7
10	h	102	SPN	C11-C10-C9-C8
10	h	102	SPN	C12-C13-C14-C15
10	h	102	SPN	C16-C17-C18-C19
10	h	103	SPN	C4-C5-C6-C7
10	h	103	SPN	C11-C10-C9-C8
10	h	103	SPN	C12-C13-C14-C15
10	e	102	SPN	C4-C5-C6-C7
10	e	102	SPN	C11-C10-C9-C8
10	e	102	SPN	C12-C13-C14-C15
10	e	102	SPN	C16-C17-C18-C19
10	f	102	SPN	C4-C5-C6-C7
10	f	102	SPN	C11-C10-C9-C8
10	f	102	SPN	C12-C13-C14-C15
10	c	102	SPN	C4-C5-C6-C7
10	c	102	SPN	C11-C10-C9-C8
10	c	102	SPN	C12-C13-C14-C15
10	c	102	SPN	C16-C17-C18-C19
10	c	103	SPN	C4-C5-C6-C7
10	c	103	SPN	C11-C10-C9-C8
10	c	103	SPN	C12-C13-C14-C15
10	c	103	SPN	C16-C17-C18-C19
10	a	102	SPN	C4-C5-C6-C7
10	a	102	SPN	C11-C10-C9-C8
10	a	102	SPN	C12-C13-C14-C15
10	a	102	SPN	C16-C17-C18-C19
10	a	103	SPN	C4-C5-C6-C7
10	a	103	SPN	C11-C10-C9-C8
10	a	103	SPN	C12-C13-C14-C15
10	a	103	SPN	C16-C17-C18-C19
10	i	102	SPN	C4-C5-C6-C7
10	i	102	SPN	C11-C10-C9-C8
10	i	102	SPN	C12-C13-C14-C15
10	i	102	SPN	C16-C17-C18-C19
10	j	102	SPN	C4-C5-C6-C7
10	j	102	SPN	C11-C10-C9-C8
10	j	102	SPN	C12-C13-C14-C15
10	j	102	SPN	C16-C17-C18-C19
10	j	102	SPN	C25-C26-C27-C28
10	7	102	SPN	C4-C5-C6-C7
10	7	102	SPN	C11-C10-C9-C8
10	7	102	SPN	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
10	7	102	SPN	C16-C17-C18-C19
10	7	103	SPN	C4-C5-C6-C7
10	7	103	SPN	C11-C10-C9-C8
10	7	103	SPN	C12-C13-C14-C15
10	7	103	SPN	C16-C17-C18-C19
10	7	103	SPN	C25-C26-C27-C28
10	M	406	SPN	C4-C5-C6-C7
10	M	406	SPN	C11-C10-C9-C8
10	M	406	SPN	C12-C13-C14-C15
10	9	103	SPN	C4-C5-C6-C7
10	9	103	SPN	C11-C10-C9-C8
10	9	103	SPN	C12-C13-C14-C15
10	9	103	SPN	C16-C17-C18-C19
10	0	102	SPN	C4-C5-C6-C7
10	0	102	SPN	C11-C10-C9-C8
8	A	101	U10	C19-C21-C22-C23
8	A	101	U10	C29-C31-C32-C33
8	L	305	U10	C14-C16-C17-C18
8	L	305	U10	C24-C26-C27-C28
8	M	403	U10	C24-C26-C27-C28
8	M	403	U10	C29-C31-C32-C33
8	M	403	U10	C39-C41-C42-C43
10	1	103	SPN	C26-C27-C28-C29
10	5	103	SPN	C26-C27-C28-C29
10	3	102	SPN	C26-C27-C28-C29
10	v	102	SPN	C26-C27-C28-C29
10	s	102	SPN	C26-C27-C28-C29
10	t	102	SPN	C26-C27-C28-C29
10	q	102	SPN	C26-C27-C28-C29
10	r	102	SPN	C26-C27-C28-C29
10	p	102	SPN	C26-C27-C28-C29
10	m	102	SPN	C26-C27-C28-C29
10	n	102	SPN	C26-C27-C28-C29
10	l	102	SPN	C26-C27-C28-C29
10	h	102	SPN	C26-C27-C28-C29
10	h	103	SPN	C26-C27-C28-C29
10	e	102	SPN	C26-C27-C28-C29
10	f	102	SPN	C26-C27-C28-C29
10	c	102	SPN	C26-C27-C28-C29
10	a	103	SPN	C26-C27-C28-C29
10	i	102	SPN	C26-C27-C28-C29
10	j	102	SPN	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
11	g	102	MW9	C7-C8-C9-C10
12	C	401	HEM	C3D-CAD-CBD-CGD
9	g	101	BCL	C2A-CAA-CBA-CGA
10	1	103	SPN	C14-C15-C16-C17
9	5	101	BCL	CBD-CGD-O2D-CED
9	e	101	BCL	CBD-CGD-O2D-CED
11	g	103	MW9	C7-C8-C9-C10
10	q	102	SPN	C24-C25-C26-C27
9	4	101	BCL	C3-C5-C6-C7
11	H	304	MW9	O5-C21-C22-C23
9	q	101	BCL	CBA-CGA-O2A-C1
11	M	408	MW9	C13-C14-C15-C16
11	H	304	MW9	C9-C10-C11-C12
10	1	103	SPN	CM5-C13-C14-C15
10	1	103	SPN	CM8-C26-C27-C28
10	5	103	SPN	CM8-C26-C27-C28
10	v	102	SPN	C16-C17-C18-CM6
8	L	305	U10	C13-C14-C16-C17
8	L	305	U10	C18-C19-C21-C22
10	1	103	SPN	C25-C26-C27-C28
10	5	103	SPN	C25-C26-C27-C28
10	t	102	SPN	C12-C13-C14-C15
10	t	102	SPN	C16-C17-C18-C19
10	q	102	SPN	C4-C5-C6-C7
10	q	102	SPN	C16-C17-C18-C19
10	p	102	SPN	C11-C10-C9-C8
10	p	102	SPN	C12-C13-C14-C15
10	p	103	SPN	C16-C17-C18-C19
10	h	103	SPN	C16-C17-C18-C19
10	f	102	SPN	C16-C17-C18-C19
10	M	406	SPN	C16-C17-C18-C19
10	0	102	SPN	C12-C13-C14-C15
10	0	102	SPN	C16-C17-C18-C19
9	h	101	BCL	C3-C5-C6-C7
9	5	101	BCL	C11-C12-C13-C14
9	6	101	BCL	C11-C12-C13-C14
9	3	101	BCL	C11-C12-C13-C14
9	4	101	BCL	C11-C12-C13-C14
9	w	101	BCL	C11-C12-C13-C14
9	w	101	BCL	C14-C13-C15-C16
9	v	101	BCL	C11-C10-C8-C9
9	s	101	BCL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
9	t	101	BCL	C11-C12-C13-C14
9	r	101	BCL	C6-C7-C8-C9
9	p	101	BCL	C14-C13-C15-C16
9	m	101	BCL	C11-C12-C13-C14
9	k	101	BCL	C11-C12-C13-C14
9	g	101	BCL	C11-C12-C13-C14
9	h	101	BCL	C14-C13-C15-C16
9	e	101	BCL	C11-C12-C13-C14
9	c	101	BCL	C11-C12-C13-C14
9	c	101	BCL	C14-C13-C15-C16
9	d	101	BCL	C11-C12-C13-C14
9	a	101	BCL	C14-C13-C15-C16
9	j	101	BCL	C14-C13-C15-C16
9	7	101	BCL	C11-C12-C13-C14
9	M	402	BCL	C6-C7-C8-C9
9	M	402	BCL	C11-C12-C13-C14
9	9	102	BCL	C11-C12-C13-C14
9	0	101	BCL	C11-C12-C13-C14
10	1	103	SPN	CM7-C22-C23-C24
10	1	104	SPN	CM7-C22-C23-C24
10	v	102	SPN	C20-C21-C22-CM7
10	v	102	SPN	CM7-C22-C23-C24
10	p	102	SPN	CM7-C22-C23-C24
10	p	103	SPN	C20-C21-C22-CM7
10	h	103	SPN	C20-C21-C22-CM7
10	h	103	SPN	CM7-C22-C23-C24
10	f	102	SPN	C20-C21-C22-CM7
10	f	102	SPN	CM7-C22-C23-C24
10	j	102	SPN	CM7-C22-C23-C24
9	p	101	BCL	O1D-CGD-O2D-CED
11	H	304	MW9	C14-C15-C16-C17
9	r	101	BCL	C2A-CAA-CBA-CGA
9	i	101	BCL	C15-C16-C17-C18
9	q	101	BCL	C13-C15-C16-C17
9	h	101	BCL	C10-C11-C12-C13
9	i	101	BCL	C8-C10-C11-C12
9	s	101	BCL	C5-C6-C7-C8
9	o	101	BCL	C10-C11-C12-C13
9	j	101	BCL	C8-C10-C11-C12
9	0	101	BCL	C13-C15-C16-C17
9	0	101	BCL	C15-C16-C17-C18
9	w	101	BCL	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
10	r	102	SPN	C22-C23-C24-C25
10	k	102	SPN	C22-C23-C24-C25
10	a	102	SPN	C22-C23-C24-C25
10	7	102	SPN	C22-C23-C24-C25
10	9	103	SPN	C22-C23-C24-C25
10	0	102	SPN	C22-C23-C24-C25
11	9	101	MW9	C24-C25-C26-C27
9	u	101	BCL	CBD-CGD-O2D-CED
9	4	101	BCL	C6-C7-C8-C10
9	p	101	BCL	C11-C10-C8-C7
9	m	101	BCL	C12-C13-C15-C16
9	n	101	BCL	C6-C7-C8-C10
9	n	101	BCL	C11-C12-C13-C15
9	k	101	BCL	C12-C13-C15-C16
9	j	101	BCL	C11-C10-C8-C7
9	0	101	BCL	C6-C7-C8-C10
10	1	103	SPN	C20-C21-C22-C23
10	1	104	SPN	C20-C21-C22-C23
10	l	102	SPN	C20-C21-C22-C23
10	a	103	SPN	C20-C21-C22-C23
10	j	102	SPN	C20-C21-C22-C23
10	0	102	SPN	C21-C22-C23-C24
13	M	409	BPH	C6-C7-C8-C10
11	g	102	MW9	C5-C6-C7-C8
11	H	304	MW9	C12-C13-C14-C15
11	9	101	MW9	C35-C36-C37-C38
10	f	102	SPN	CM8-C26-C27-C28
11	M	408	MW9	C4-C5-C6-C7
10	1	104	SPN	C26-C27-C28-C29
10	1	105	SPN	C26-C27-C28-C29
10	w	102	SPN	C26-C27-C28-C29
9	M	404	BCL	C3-C5-C6-C7
9	n	101	BCL	C8-C10-C11-C12
9	h	101	BCL	C5-C6-C7-C8
13	M	409	BPH	C5-C6-C7-C8
13	M	409	BPH	C13-C15-C16-C17
9	v	101	BCL	C10-C11-C12-C13
9	c	101	BCL	C13-C15-C16-C17
13	M	409	BPH	C10-C11-C12-C13
9	5	101	BCL	C2A-CAA-CBA-CGA
9	s	101	BCL	C2A-CAA-CBA-CGA
9	m	101	BCL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
9	k	101	BCL	C2A-CAA-CBA-CGA
9	c	101	BCL	C2A-CAA-CBA-CGA
9	a	101	BCL	C2A-CAA-CBA-CGA
9	M	402	BCL	C2A-CAA-CBA-CGA
9	9	102	BCL	C2A-CAA-CBA-CGA
13	M	409	BPH	C2A-CAA-CBA-CGA
9	2	101	BCL	C10-C11-C12-C13
9	2	101	BCL	C15-C16-C17-C18
9	3	101	BCL	C10-C11-C12-C13
9	w	101	BCL	C13-C15-C16-C17
9	t	101	BCL	C5-C6-C7-C8
9	e	101	BCL	C15-C16-C17-C18
9	8	101	BCL	C10-C11-C12-C13
11	H	303	MW9	C24-C25-C26-C27
11	M	407	MW9	C24-C25-C26-C27
9	k	101	BCL	C3-C5-C6-C7
9	1	101	BCL	C10-C11-C12-C13
9	6	101	BCL	C15-C16-C17-C18
9	3	101	BCL	C15-C16-C17-C18
9	s	101	BCL	C8-C10-C11-C12
9	q	101	BCL	C8-C10-C11-C12
9	m	101	BCL	C10-C11-C12-C13
9	b	101	BCL	C10-C11-C12-C13
9	L	301	BCL	C15-C16-C17-C18
11	H	301	MW9	C4-C5-C6-C7
9	q	101	BCL	O1A-CGA-O2A-C1
9	k	101	BCL	C10-C11-C12-C13
9	k	101	BCL	C15-C16-C17-C18
13	L	303	BPH	C15-C16-C17-C18
11	H	301	MW9	C24-C25-C26-C27
9	u	101	BCL	C10-C11-C12-C13
9	q	101	BCL	C15-C16-C17-C18
9	f	101	BCL	C13-C15-C16-C17
13	M	409	BPH	C15-C16-C17-C18
11	H	301	MW9	C11-C12-C13-C14
9	n	101	BCL	C13-C15-C16-C17
9	b	101	BCL	C13-C15-C16-C17
9	3	101	BCL	C2A-CAA-CBA-CGA
9	v	101	BCL	C15-C16-C17-C18
9	q	101	BCL	C10-C11-C12-C13
9	l	101	BCL	C15-C16-C17-C18
9	h	101	BCL	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
9	7	101	BCL	C10-C11-C12-C13
9	7	101	BCL	C15-C16-C17-C18
9	9	102	BCL	C10-C11-C12-C13
9	9	102	BCL	C15-C16-C17-C18
13	M	405	BPH	C8-C10-C11-C12
9	o	101	BCL	O1D-CGD-O2D-CED
9	r	101	BCL	C10-C11-C12-C13
9	r	101	BCL	C13-C15-C16-C17
9	r	101	BCL	C15-C16-C17-C18
9	b	101	BCL	C8-C10-C11-C12
9	3	101	BCL	C8-C10-C11-C12
9	x	101	BCL	C5-C6-C7-C8
9	c	101	BCL	C8-C10-C11-C12
9	j	101	BCL	C5-C6-C7-C8
9	M	402	BCL	C5-C6-C7-C8
9	6	101	BCL	CBA-CGA-O2A-C1
11	g	102	MW9	C14-C15-C16-C17
11	M	408	MW9	C24-C25-C26-C27
9	c	101	BCL	C4-C3-C5-C6
8	M	403	U10	C14-C16-C17-C18
10	1	102	SPN	C26-C27-C28-C29
10	7	102	SPN	C26-C27-C28-C29
10	9	103	SPN	C26-C27-C28-C29
9	p	101	BCL	C16-C17-C18-C20
9	m	101	BCL	C16-C17-C18-C20
9	d	101	BCL	C16-C17-C18-C20
9	r	101	BCL	C5-C6-C7-C8
9	d	101	BCL	C15-C16-C17-C18
9	1	101	BCL	C2A-CAA-CBA-CGA
11	9	101	MW9	C21-C22-C23-O6
9	L	304	BCL	O2A-C1-C2-C3
11	H	301	MW9	C33-C34-C35-C36
9	g	101	BCL	C16-C17-C18-C20
9	n	101	BCL	C15-C16-C17-C18
9	e	101	BCL	C13-C15-C16-C17
9	f	101	BCL	C10-C11-C12-C13
10	f	102	SPN	C25-C26-C27-C28
9	1	101	BCL	C16-C17-C18-C20
9	d	101	BCL	C16-C17-C18-C19
11	M	407	MW9	C4-C5-C6-C7
9	l	101	BCL	C13-C15-C16-C17
13	L	303	BPH	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
11	M	407	MW9	C11-C10-C9-C8
9	e	101	BCL	O1D-CGD-O2D-CED
11	H	303	MW9	C2-C3-C4-C5
11	H	301	MW9	O7-C22-C23-O6
11	H	302	MW9	O7-C22-C23-O6
11	H	304	MW9	O7-C22-C23-O6
10	3	102	SPN	C22-C23-C24-C25
10	t	102	SPN	C22-C23-C24-C25
10	a	103	SPN	C22-C23-C24-C25
10	i	102	SPN	C22-C23-C24-C25
9	9	102	BCL	C13-C15-C16-C17
9	M	404	BCL	C16-C17-C18-C19
10	p	103	SPN	C17-C18-C19-C20
9	o	101	BCL	C2A-CAA-CBA-CGA
9	o	101	BCL	C5-C6-C7-C8
9	M	402	BCL	C8-C10-C11-C12
9	6	101	BCL	C11-C12-C13-C15
9	q	101	BCL	C11-C10-C8-C7
9	b	101	BCL	C6-C7-C8-C10
9	i	101	BCL	C11-C12-C13-C15
9	0	101	BCL	C12-C13-C15-C16
11	M	408	MW9	C14-C15-C16-C17
9	q	101	BCL	C5-C6-C7-C8
11	H	303	MW9	C11-C12-C13-C14
11	H	304	MW9	C26-C27-C28-C29
11	M	408	MW9	C28-C29-C30-C31
9	1	101	BCL	C3A-C2A-CAA-CBA
9	6	101	BCL	C3A-C2A-CAA-CBA
9	4	101	BCL	C3A-C2A-CAA-CBA
9	s	101	BCL	C3A-C2A-CAA-CBA
9	m	101	BCL	C3A-C2A-CAA-CBA
9	f	101	BCL	C3A-C2A-CAA-CBA
9	b	101	BCL	C3A-C2A-CAA-CBA
9	L	301	BCL	C3A-C2A-CAA-CBA
13	M	405	BPH	C3A-C2A-CAA-CBA
11	H	303	MW9	C37-C38-C39-C40
11	M	408	MW9	C27-C28-C29-C30
9	9	102	BCL	CBD-CGD-O2D-CED
9	M	404	BCL	C16-C17-C18-C20
9	6	101	BCL	O1A-CGA-O2A-C1
11	g	102	MW9	C35-C36-C37-C38
11	H	303	MW9	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
9	8	101	BCL	CBA-CGA-O2A-C1
8	L	305	U10	C19-C21-C22-C23
8	M	403	U10	C34-C36-C37-C38
11	g	102	MW9	C1-C2-C3-C4
11	g	102	MW9	C28-C29-C30-C31
11	H	303	MW9	C35-C36-C37-C38
11	9	101	MW9	C34-C35-C36-C37
11	9	101	MW9	C37-C38-C39-C40
9	L	304	BCL	C3-C5-C6-C7
9	5	101	BCL	O1D-CGD-O2D-CED
11	g	103	MW9	C37-C38-C39-C40
11	H	302	MW9	C36-C37-C38-C39
11	M	408	MW9	C11-C10-C9-C8
11	M	408	MW9	C6-C7-C8-C9
9	x	101	BCL	C16-C17-C18-C19
9	s	101	BCL	C16-C17-C18-C20
11	H	304	MW9	C35-C36-C37-C38
11	g	102	MW9	C33-C34-C35-C36
9	7	101	BCL	C2A-CAA-CBA-CGA
11	H	304	MW9	C3-C4-C5-C6
11	M	408	MW9	C25-C26-C27-C28
9	p	101	BCL	C10-C11-C12-C13
9	c	101	BCL	C2-C3-C5-C6
9	m	101	BCL	C16-C17-C18-C19
9	7	101	BCL	C16-C17-C18-C20
11	H	301	MW9	C5-C6-C7-C8
11	9	101	MW9	C2-C3-C4-C5
9	M	402	BCL	C11-C10-C8-C9
11	H	301	MW9	C6-C7-C8-C9
11	9	101	MW9	C28-C29-C30-C31
11	H	302	MW9	C4-C5-C6-C7
9	4	101	BCL	C5-C6-C7-C8
9	n	101	BCL	C10-C11-C12-C13
11	g	103	MW9	C5-C6-C7-C8
11	H	301	MW9	C2-C3-C4-C5
11	H	304	MW9	C10-C11-C12-C13
11	H	303	MW9	C34-C35-C36-C37
9	3	101	BCL	C16-C17-C18-C20
11	M	408	MW9	C2-C3-C4-C5
11	M	407	MW9	C29-C30-C31-C32
9	v	101	BCL	C5-C6-C7-C8
9	p	101	BCL	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
11	H	304	MW9	C24-C25-C26-C27
9	v	101	BCL	C3-C5-C6-C7
13	M	405	BPH	C2A-CAA-CBA-CGA
11	H	302	MW9	C5-C6-C7-C8
11	g	103	MW9	C10-C11-C12-C13
11	H	302	MW9	C37-C38-C39-C40
9	m	101	BCL	C15-C16-C17-C18
11	M	408	MW9	C10-C11-C12-C13
9	8	101	BCL	O1A-CGA-O2A-C1
9	b	101	BCL	C15-C16-C17-C18
11	g	103	MW9	C14-C15-C16-C17
12	C	402	HEM	C4C-C3C-CAC-CBC
9	1	101	BCL	C16-C17-C18-C19
9	g	101	BCL	C16-C17-C18-C19
11	9	101	MW9	C11-C12-C13-C14
11	H	303	MW9	C10-C11-C12-C13
9	2	101	BCL	C8-C10-C11-C12
9	k	101	BCL	C13-C15-C16-C17
9	l	101	BCL	C5-C6-C7-C8
9	8	101	BCL	C3-C5-C6-C7
11	H	303	MW9	C29-C30-C31-C32
11	M	408	MW9	C29-C30-C31-C32
11	9	101	MW9	O1-C18-C19-O8
11	H	301	MW9	C12-C13-C14-C15
9	L	304	BCL	CBA-CGA-O2A-C1
11	H	301	MW9	C36-C37-C38-C39
11	H	304	MW9	C28-C29-C30-C31
9	m	101	BCL	C5-C6-C7-C8
13	M	405	BPH	C2C-C3C-CAC-CBC
9	c	101	BCL	C16-C17-C18-C20
11	9	101	MW9	C27-C28-C29-C30
11	H	304	MW9	C37-C38-C39-C40
9	x	101	BCL	C4-C3-C5-C6
9	s	101	BCL	C3-C5-C6-C7
11	g	103	MW9	O5-C21-C22-C23
11	H	301	MW9	C1-C2-C3-C4
9	L	304	BCL	C2A-CAA-CBA-CGA
11	g	102	MW9	C3-C4-C5-C6
9	5	101	BCL	C8-C10-C11-C12
9	0	101	BCL	C5-C6-C7-C8
11	H	304	MW9	C25-C26-C27-C28
11	M	408	MW9	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
9	s	101	BCL	C15-C16-C17-C18
10	1	102	SPN	C22-C23-C24-C25
10	m	102	SPN	C22-C23-C24-C25
10	n	102	SPN	C22-C23-C24-C25
11	H	302	MW9	C12-C13-C14-C15
9	1	101	BCL	C1A-C2A-CAA-CBA
9	2	101	BCL	C1A-C2A-CAA-CBA
9	6	101	BCL	C1A-C2A-CAA-CBA
9	4	101	BCL	C1A-C2A-CAA-CBA
9	s	101	BCL	C1A-C2A-CAA-CBA
9	m	101	BCL	C1A-C2A-CAA-CBA
9	f	101	BCL	C1A-C2A-CAA-CBA
9	L	301	BCL	C1A-C2A-CAA-CBA
9	4	101	BCL	C8-C10-C11-C12
11	H	304	MW9	C29-C30-C31-C32
11	9	101	MW9	C33-C34-C35-C36
11	H	302	MW9	C18-C19-C20-O2
11	H	303	MW9	C18-C19-C20-O2
9	5	101	BCL	C6-C7-C8-C10
9	5	101	BCL	C11-C10-C8-C7
9	w	101	BCL	C6-C7-C8-C10
9	x	101	BCL	C11-C10-C8-C7
9	x	101	BCL	C12-C13-C15-C16
9	s	101	BCL	C11-C12-C13-C15
9	t	101	BCL	C12-C13-C15-C16
9	p	101	BCL	C12-C13-C15-C16
9	k	101	BCL	C11-C10-C8-C7
9	k	101	BCL	C11-C12-C13-C15
9	l	101	BCL	C6-C7-C8-C10
9	d	101	BCL	C6-C7-C8-C10
9	d	101	BCL	C11-C10-C8-C7
9	a	101	BCL	C6-C7-C8-C10
9	a	101	BCL	C12-C13-C15-C16
9	b	101	BCL	C11-C10-C8-C7
9	7	101	BCL	C11-C10-C8-C7
9	M	402	BCL	C6-C7-C8-C10
9	M	402	BCL	C12-C13-C15-C16
10	k	102	SPN	C21-C22-C23-C24
13	L	303	BPH	C12-C13-C15-C16
9	5	101	BCL	C15-C16-C17-C18
9	6	101	BCL	C2C-C3C-CAC-CBC
9	x	101	BCL	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
9	u	101	BCL	C2C-C3C-CAC-CBC
9	q	101	BCL	C2C-C3C-CAC-CBC
9	m	101	BCL	C2C-C3C-CAC-CBC
9	c	101	BCL	C2C-C3C-CAC-CBC
9	d	101	BCL	C2C-C3C-CAC-CBC
9	a	101	BCL	C2C-C3C-CAC-CBC
9	M	404	BCL	C2C-C3C-CAC-CBC
9	9	102	BCL	C2C-C3C-CAC-CBC
9	5	101	BCL	C10-C11-C12-C13
9	u	101	BCL	C13-C15-C16-C17
9	t	101	BCL	C10-C11-C12-C13
9	n	101	BCL	C4-C3-C5-C6
9	2	101	BCL	C2-C3-C5-C6
9	s	101	BCL	C10-C11-C12-C13
9	5	101	BCL	C11-C10-C8-C9
9	x	101	BCL	C11-C10-C8-C9
9	r	101	BCL	C11-C10-C8-C9
9	m	101	BCL	C14-C13-C15-C16
9	n	101	BCL	C11-C10-C8-C9
9	d	101	BCL	C6-C7-C8-C9
9	d	101	BCL	C11-C10-C8-C9
9	j	101	BCL	C11-C10-C8-C9
9	j	101	BCL	C11-C12-C13-C14
9	L	304	BCL	C11-C10-C8-C9
9	L	304	BCL	C14-C13-C15-C16
9	0	101	BCL	C6-C7-C8-C9
13	L	303	BPH	C14-C13-C15-C16
9	L	304	BCL	C13-C15-C16-C17
10	h	103	SPN	CM6-C18-C19-C20
11	H	303	MW9	O1-C18-C19-C20
11	H	303	MW9	C26-C27-C28-C29
11	H	303	MW9	C4-C5-C6-C7
9	l	101	BCL	C8-C10-C11-C12
9	2	101	BCL	C4-C3-C5-C6
8	M	403	U10	C28-C29-C31-C32
9	x	101	BCL	C2-C3-C5-C6
9	n	101	BCL	C2-C3-C5-C6
9	g	101	BCL	C10-C11-C12-C13
9	c	101	BCL	C15-C16-C17-C18
9	1	101	BCL	C8-C10-C11-C12
11	H	301	MW9	C26-C27-C28-C29
9	w	101	BCL	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
9	f	101	BCL	O2A-C1-C2-C3
11	g	102	MW9	C11-C12-C13-C14
9	9	102	BCL	C8-C10-C11-C12
11	H	304	MW9	C33-C34-C35-C36
11	M	407	MW9	C33-C34-C35-C36
11	H	303	MW9	C36-C37-C38-C39
11	H	304	MW9	C6-C7-C8-C9
9	u	101	BCL	O1D-CGD-O2D-CED
13	L	303	BPH	C10-C11-C12-C13
8	M	403	U10	C30-C29-C31-C32
9	4	101	BCL	C2-C3-C5-C6
9	L	304	BCL	O1A-CGA-O2A-C1
11	M	407	MW9	C-C1-C2-C3
11	H	304	MW9	C32-C33-C34-C35
9	c	101	BCL	C16-C17-C18-C19
9	e	101	BCL	CBA-CGA-O2A-C1
9	M	404	BCL	CBD-CGD-O2D-CED
10	f	102	SPN	CM6-C18-C19-C20
9	l	101	BCL	C10-C11-C12-C13
9	e	101	BCL	C8-C10-C11-C12
9	j	101	BCL	C10-C11-C12-C13
11	M	408	MW9	C38-C39-C40-C41
8	L	302	U10	C15-C14-C16-C17
8	M	403	U10	C40-C39-C41-C42
9	t	101	BCL	CBA-CGA-O2A-C1
9	g	101	BCL	C8-C10-C11-C12
9	a	101	BCL	C8-C10-C11-C12
9	5	101	BCL	C6-C7-C8-C9
9	6	101	BCL	C6-C7-C8-C9
9	s	101	BCL	C14-C13-C15-C16
9	t	101	BCL	C14-C13-C15-C16
9	q	101	BCL	C11-C10-C8-C9
9	o	101	BCL	C11-C10-C8-C9
9	n	101	BCL	C6-C7-C8-C9
9	n	101	BCL	C11-C12-C13-C14
9	k	101	BCL	C11-C10-C8-C9
9	l	101	BCL	C6-C7-C8-C9
9	g	101	BCL	C14-C13-C15-C16
9	f	101	BCL	C11-C10-C8-C9
9	a	101	BCL	C6-C7-C8-C9
9	7	101	BCL	C11-C10-C8-C9
9	M	402	BCL	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
10	1	105	SPN	CM7-C22-C23-C24
10	t	102	SPN	CM7-C22-C23-C24
11	M	408	MW9	C1-C2-C3-C4
9	x	101	BCL	C8-C10-C11-C12
11	9	101	MW9	C13-C14-C15-C16
9	u	101	BCL	C2A-CAA-CBA-CGA
11	H	301	MW9	C28-C29-C30-C31
13	L	303	BPH	C3-C5-C6-C7
11	g	102	MW9	C18-C19-C20-O2
11	H	304	MW9	C18-C19-C20-O2
11	M	408	MW9	C18-C19-C20-O2
9	1	101	BCL	C11-C10-C8-C7
9	2	101	BCL	C11-C10-C8-C7
9	5	101	BCL	C11-C12-C13-C15
9	6	101	BCL	C6-C7-C8-C10
9	w	101	BCL	C11-C10-C8-C7
9	w	101	BCL	C12-C13-C15-C16
9	x	101	BCL	C11-C12-C13-C15
9	u	101	BCL	C6-C7-C8-C10
9	v	101	BCL	C11-C10-C8-C7
9	r	101	BCL	C6-C7-C8-C10
9	r	101	BCL	C11-C10-C8-C7
9	o	101	BCL	C6-C7-C8-C10
9	m	101	BCL	C11-C12-C13-C15
9	n	101	BCL	C11-C10-C8-C7
9	l	101	BCL	C11-C10-C8-C7
9	g	101	BCL	C11-C12-C13-C15
9	h	101	BCL	C6-C7-C8-C10
9	e	101	BCL	C11-C10-C8-C7
9	e	101	BCL	C12-C13-C15-C16
9	f	101	BCL	C11-C10-C8-C7
9	d	101	BCL	C11-C12-C13-C15
9	a	101	BCL	C11-C10-C8-C7
9	a	101	BCL	C11-C12-C13-C15
9	j	101	BCL	C11-C12-C13-C15
9	L	304	BCL	C11-C10-C8-C7
9	M	402	BCL	C11-C12-C13-C15
10	5	102	SPN	C21-C22-C23-C24
10	u	102	SPN	C21-C22-C23-C24
10	m	102	SPN	C21-C22-C23-C24
10	l	102	SPN	C21-C22-C23-C24
10	h	102	SPN	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
10	a	102	SPN	C21-C22-C23-C24
8	L	302	U10	C12-C11-C9-C10
9	2	101	BCL	C3A-C2A-CAA-CBA
9	4	101	BCL	C4-C3-C5-C6
9	u	101	BCL	C3A-C2A-CAA-CBA
9	h	101	BCL	C3A-C2A-CAA-CBA
10	1	102	SPN	CM2-C1-C2-O2
10	1	102	SPN	CM2-C1-C2-C3
10	5	102	SPN	CM2-C1-C2-O2
10	3	102	SPN	CM2-C1-C2-O2
10	w	102	SPN	CM2-C1-C2-O2
10	q	102	SPN	CM2-C1-C2-C3
10	r	102	SPN	CM2-C1-C2-O2
10	p	102	SPN	CM1-C1-C2-O2
10	p	102	SPN	CM1-C1-C2-C3
10	p	103	SPN	CM2-C1-C2-O2
10	m	102	SPN	CM2-C1-C2-O2
10	m	102	SPN	CM2-C1-C2-C3
10	k	102	SPN	CM1-C1-C2-O2
10	k	102	SPN	CM1-C1-C2-C3
10	k	102	SPN	CM2-C1-C2-O2
10	k	102	SPN	CM2-C1-C2-C3
10	7	102	SPN	CM2-C1-C2-O2
10	7	102	SPN	CM2-C1-C2-C3
9	d	101	BCL	C10-C11-C12-C13
9	p	101	BCL	C16-C17-C18-C19
10	a	102	SPN	C26-C27-C28-C29
10	v	102	SPN	C15-C16-C17-C18
11	g	103	MW9	C11-C12-C13-C14
9	s	101	BCL	C16-C17-C18-C19
9	n	101	BCL	C16-C17-C18-C19
9	3	101	BCL	C1-C2-C3-C4
9	w	101	BCL	C1-C2-C3-C4
9	u	101	BCL	C1-C2-C3-C4
9	q	101	BCL	C1-C2-C3-C4
9	g	101	BCL	C1-C2-C3-C4
9	c	101	BCL	C1-C2-C3-C4
9	L	304	BCL	C1-C2-C3-C4
13	L	303	BPH	C1-C2-C3-C4
11	M	407	MW9	C9-C10-C11-C12
11	H	302	MW9	O8-C19-C20-O2
9	w	101	BCL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
11	9	101	MW9	C5-C6-C7-C8
11	g	103	MW9	O1-C18-C19-O8
11	M	407	MW9	O1-C18-C19-O8
11	M	408	MW9	O1-C18-C19-O8
11	H	303	MW9	C3-C4-C5-C6
9	M	402	BCL	C4-C3-C5-C6
8	L	302	U10	C12-C11-C9-C8
8	L	302	U10	C13-C14-C16-C17
9	M	402	BCL	C2-C3-C5-C6
11	H	303	MW9	C13-C14-C15-C16
9	u	101	BCL	C1-C2-C3-C5
9	l	101	BCL	C1-C2-C3-C5
9	h	101	BCL	C1-C2-C3-C5
9	a	101	BCL	C1-C2-C3-C5
11	g	103	MW9	C35-C36-C37-C38
9	1	101	BCL	C11-C10-C8-C9
9	1	101	BCL	C14-C13-C15-C16
9	4	101	BCL	C11-C10-C8-C9
9	w	101	BCL	C11-C10-C8-C9
9	o	101	BCL	C6-C7-C8-C9
9	p	101	BCL	C11-C10-C8-C9
9	a	101	BCL	C11-C10-C8-C9
9	x	101	BCL	C16-C17-C18-C20
10	p	102	SPN	C13-C14-C15-C16
11	g	103	MW9	C24-C25-C26-C27
8	L	302	U10	C24-C26-C27-C28
10	5	102	SPN	C26-C27-C28-C29
9	v	101	BCL	C4C-C3C-CAC-CBC
9	j	101	BCL	C4C-C3C-CAC-CBC
9	M	404	BCL	O1D-CGD-O2D-CED
11	M	407	MW9	O7-C22-C23-O6
9	9	102	BCL	O1D-CGD-O2D-CED
10	e	102	SPN	C22-C23-C24-C25
10	1	102	SPN	O1-C1-C2-O2
10	5	102	SPN	O1-C1-C2-O2
10	3	102	SPN	O1-C1-C2-O2
10	u	102	SPN	O1-C1-C2-O2
10	p	102	SPN	O1-C1-C2-O2
10	k	102	SPN	O1-C1-C2-O2
10	i	102	SPN	O1-C1-C2-O2
10	7	102	SPN	O1-C1-C2-O2
11	H	303	MW9	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
11	H	301	MW9	C18-C19-C20-O2
11	9	101	MW9	C18-C19-C20-O2
9	3	101	BCL	C16-C17-C18-C19
9	7	101	BCL	C16-C17-C18-C19
9	1	101	BCL	C11-C12-C13-C15
9	3	101	BCL	C6-C7-C8-C10
9	4	101	BCL	C11-C10-C8-C7
9	4	101	BCL	C11-C12-C13-C15
9	w	101	BCL	C11-C12-C13-C15
9	s	101	BCL	C11-C10-C8-C7
9	q	101	BCL	C11-C12-C13-C15
9	p	101	BCL	C6-C7-C8-C10
9	m	101	BCL	C11-C10-C8-C7
9	g	101	BCL	C11-C10-C8-C7
9	f	101	BCL	C6-C7-C8-C10
9	c	101	BCL	C11-C10-C8-C7
9	b	101	BCL	C11-C12-C13-C15
9	j	101	BCL	C6-C7-C8-C10
9	M	404	BCL	C12-C13-C15-C16
9	9	102	BCL	C6-C7-C8-C10
9	0	101	BCL	C11-C10-C8-C7
10	w	102	SPN	C21-C22-C23-C24
10	s	102	SPN	C21-C22-C23-C24
10	r	102	SPN	C21-C22-C23-C24
10	e	102	SPN	C21-C22-C23-C24
10	9	103	SPN	C21-C22-C23-C24
9	u	101	BCL	C8-C10-C11-C12
9	L	301	BCL	C2A-CAA-CBA-CGA
8	M	403	U10	C20-C19-C21-C22
9	M	404	BCL	CAA-CBA-CGA-O2A
9	t	101	BCL	O1A-CGA-O2A-C1
9	e	101	BCL	O1A-CGA-O2A-C1
9	a	101	BCL	C15-C16-C17-C18
9	L	304	BCL	C2B-C3B-CAB-OB
9	L	304	BCL	C2B-C3B-CAB-CB
11	H	303	MW9	O8-C19-C20-O2
11	H	304	MW9	O8-C19-C20-O2
11	M	408	MW9	O8-C19-C20-O2
11	9	101	MW9	O8-C19-C20-O2
10	k	102	SPN	C26-C27-C28-C29
11	g	103	MW9	O1-C18-C19-C20
11	H	301	MW9	O1-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
11	M	407	MW9	O1-C18-C19-C20
11	M	408	MW9	O1-C18-C19-C20
11	9	101	MW9	O1-C18-C19-C20
12	C	402	HEM	C4B-C3B-CAB-CBB
9	t	101	BCL	C13-C15-C16-C17
11	H	303	MW9	C1-C2-C3-C4
11	9	101	MW9	C3-C4-C5-C6
11	H	301	MW9	O1-C18-C19-O8
11	H	303	MW9	O1-C18-C19-O8
9	2	101	BCL	C11-C12-C13-C14
9	3	101	BCL	C6-C7-C8-C9
9	p	101	BCL	C6-C7-C8-C9
9	g	101	BCL	C11-C10-C8-C9
9	f	101	BCL	C6-C7-C8-C9
9	b	101	BCL	C14-C13-C15-C16
9	j	101	BCL	C6-C7-C8-C9
9	8	101	BCL	C14-C13-C15-C16
9	0	101	BCL	C11-C10-C8-C9
13	M	409	BPH	C6-C7-C8-C9
9	j	101	BCL	C16-C17-C18-C19
9	6	101	BCL	C16-C17-C18-C19
9	m	101	BCL	C13-C15-C16-C17
8	M	403	U10	C25-C24-C26-C27
10	1	104	SPN	CM8-C26-C27-C28
8	M	403	U10	C18-C19-C21-C22
11	H	302	MW9	C29-C30-C31-C32
11	H	301	MW9	C11-C10-C9-C8
9	m	101	BCL	C3-C5-C6-C7
11	H	304	MW9	C27-C28-C29-C30
9	u	101	BCL	C1A-C2A-CAA-CBA
9	h	101	BCL	C1A-C2A-CAA-CBA
9	b	101	BCL	C1A-C2A-CAA-CBA
9	M	402	BCL	C1A-C2A-CAA-CBA
9	g	101	BCL	C5-C6-C7-C8
9	L	304	BCL	C16-C17-C18-C19
9	m	101	BCL	CBD-CGD-O2D-CED
9	h	101	BCL	C12-C13-C15-C16
9	e	101	BCL	C11-C12-C13-C15
9	b	101	BCL	C12-C13-C15-C16
9	i	101	BCL	C11-C10-C8-C7
9	j	101	BCL	C12-C13-C15-C16
9	7	101	BCL	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
9	L	304	BCL	C12-C13-C15-C16
9	0	101	BCL	C11-C12-C13-C15
10	c	102	SPN	C21-C22-C23-C24
10	i	102	SPN	C21-C22-C23-C24
10	7	102	SPN	C21-C22-C23-C24
13	M	409	BPH	C11-C10-C8-C7
13	M	409	BPH	C11-C12-C13-C15
9	2	101	BCL	C16-C17-C18-C20
9	i	101	BCL	C16-C17-C18-C19
9	9	102	BCL	C16-C17-C18-C19
11	H	304	MW9	C13-C14-C15-C16
9	t	101	BCL	C2C-C3C-CAC-CBC
9	0	101	BCL	C2C-C3C-CAC-CBC
11	H	304	MW9	C4-C5-C6-C7
11	M	407	MW9	C10-C11-C12-C13
9	M	402	BCL	C3A-C2A-CAA-CBA
11	g	102	MW9	O8-C19-C20-O2
9	g	101	BCL	C15-C16-C17-C18
9	2	101	BCL	C11-C10-C8-C9
9	m	101	BCL	C11-C10-C8-C9
9	h	101	BCL	C6-C7-C8-C9
9	e	101	BCL	C11-C10-C8-C9
9	c	101	BCL	C11-C10-C8-C9
9	b	101	BCL	C11-C12-C13-C14
9	M	404	BCL	C14-C13-C15-C16
9	9	102	BCL	C6-C7-C8-C9
11	H	303	MW9	C38-C39-C40-C41
9	6	101	BCL	C8-C10-C11-C12
9	n	101	BCL	C16-C17-C18-C20
9	m	101	BCL	C8-C10-C11-C12
13	M	409	BPH	C8-C10-C11-C12
11	H	303	MW9	C5-C6-C7-C8
9	j	101	BCL	CHA-CBD-CGD-O2D
10	1	102	SPN	CM2-C1-O1-CMA
10	1	104	SPN	CM1-C1-O1-CMA
10	5	102	SPN	CM2-C1-O1-CMA
10	5	103	SPN	CM2-C1-O1-CMA
10	3	102	SPN	CM2-C1-O1-CMA
10	w	102	SPN	CM1-C1-O1-CMA
10	t	102	SPN	CM1-C1-O1-CMA
10	a	102	SPN	CM2-C1-O1-CMA
10	j	102	SPN	CM1-C1-O1-CMA

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Mol	Chain	Res	Type	Atoms
10	7	103	SPN	CM1-C1-O1-CMA
10	0	102	SPN	CM1-C1-O1-CMA
11	H	301	MW9	C20-O2-P-O4
11	H	301	MW9	C20-O2-P-O5
11	H	301	MW9	C21-O5-P-O3
11	H	302	MW9	C21-O5-P-O4
11	H	303	MW9	C21-O5-P-O3
11	H	304	MW9	C21-O5-P-O2
11	H	304	MW9	C21-O5-P-O3
11	H	304	MW9	C21-O5-P-O4
8	L	305	U10	C12-C11-C9-C10
11	g	102	MW9	C19-C20-O2-P
11	H	302	MW9	C22-C21-O5-P
9	t	101	BCL	C16-C17-C18-C20
11	g	102	MW9	C24-C25-C26-C27
10	1	104	SPN	C22-C23-C24-C25
10	l	102	SPN	C22-C23-C24-C25
10	c	103	SPN	C22-C23-C24-C25
11	M	408	MW9	C-C1-C2-C3
9	7	101	BCL	C8-C10-C11-C12
9	5	101	BCL	C14-C13-C15-C16
9	u	101	BCL	C6-C7-C8-C9
9	s	101	BCL	C11-C10-C8-C9
9	l	101	BCL	C11-C10-C8-C9
9	i	101	BCL	C11-C12-C13-C14
10	5	103	SPN	CM7-C22-C23-C24
10	q	102	SPN	CM7-C22-C23-C24
10	p	103	SPN	CM7-C22-C23-C24
10	c	102	SPN	CM7-C22-C23-C24
10	i	102	SPN	CM7-C22-C23-C24
11	9	101	MW9	C12-C13-C14-C15
9	r	101	BCL	C12-C13-C15-C16
11	H	301	MW9	C13-C14-C15-C16
11	H	303	MW9	C30-C31-C32-C33
11	g	102	MW9	C25-C26-C27-C28
9	6	101	BCL	C5-C6-C7-C8
8	M	403	U10	C38-C39-C41-C42
9	r	101	BCL	C2-C1-O2A-CGA
8	A	101	U10	C25-C24-C26-C27
9	L	304	BCL	O1D-CGD-O2D-CED
9	r	101	BCL	C16-C17-C18-C19
9	u	101	BCL	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
9	d	101	BCL	C5-C6-C7-C8
9	t	101	BCL	C4-C3-C5-C6
11	9	101	MW9	C38-C39-C40-C41
11	M	408	MW9	C11-C12-C13-C14
11	9	101	MW9	C25-C26-C27-C28
9	L	304	BCL	C4B-C3B-CAB-OBB
9	a	101	BCL	C16-C17-C18-C19
9	3	101	BCL	C11-C10-C8-C9
9	h	101	BCL	C11-C10-C8-C9
9	b	101	BCL	C6-C7-C8-C9
9	7	101	BCL	C6-C7-C8-C9
9	L	304	BCL	C6-C7-C8-C9
10	3	102	SPN	CM7-C22-C23-C24
10	5	103	SPN	C22-C23-C24-C25
10	j	102	SPN	C22-C23-C24-C25
9	4	101	BCL	CBA-CGA-O2A-C1
11	H	301	MW9	C35-C36-C37-C38
9	M	402	BCL	C15-C16-C17-C18
12	C	403	HEM	C3D-CAD-CBD-CGD
9	g	101	BCL	CBA-CGA-O2A-C1
9	u	101	BCL	O1A-CGA-O2A-C1
8	M	403	U10	C45-C44-C46-C47
9	4	101	BCL	O1A-CGA-O2A-C1
9	g	101	BCL	O1A-CGA-O2A-C1
9	m	101	BCL	O1D-CGD-O2D-CED
9	3	101	BCL	C11-C10-C8-C7
9	h	101	BCL	C11-C10-C8-C7
9	c	101	BCL	C12-C13-C15-C16
9	7	101	BCL	C6-C7-C8-C10
9	r	101	BCL	C16-C17-C18-C20
13	M	409	BPH	C3A-C2A-CAA-CBA
11	M	407	MW9	C37-C38-C39-C40
9	t	101	BCL	C2-C3-C5-C6
10	q	102	SPN	CM2-C1-C2-O2
10	n	102	SPN	CM2-C1-C2-O2
10	n	102	SPN	CM2-C1-C2-C3
10	a	103	SPN	CM1-C1-C2-O2
10	i	102	SPN	CM1-C1-C2-O2
12	C	401	HEM	CAA-CBA-CGA-O2A
9	3	101	BCL	C2-C1-O2A-CGA
11	H	301	MW9	C22-C21-O5-P
11	H	303	MW9	C22-C21-O5-P

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Mol	Chain	Res	Type	Atoms
11	g	103	MW9	C28-C29-C30-C31
8	A	101	U10	C15-C14-C16-C17
8	L	305	U10	C12-C11-C9-C8
8	M	403	U10	C23-C24-C26-C27
8	A	101	U10	C5-C4-O4-C4M
8	M	403	U10	C19-C21-C22-C23
9	8	101	BCL	C11-C12-C13-C14
9	9	102	BCL	C11-C10-C8-C9
10	7	102	SPN	CM7-C22-C23-C24
9	a	101	BCL	C1-C2-C3-C4
9	L	301	BCL	C1-C2-C3-C4
11	H	302	MW9	C26-C27-C28-C29
11	g	102	MW9	C32-C33-C34-C35
11	9	101	MW9	O8-C24-C25-C26
8	A	101	U10	C23-C24-C26-C27
11	H	302	MW9	C27-C28-C29-C30
12	C	401	HEM	CAA-CBA-CGA-O1A
10	c	102	SPN	C22-C23-C24-C25
9	8	101	BCL	C5-C6-C7-C8
9	M	404	BCL	C1A-C2A-CAA-CBA
11	H	301	MW9	C37-C38-C39-C40
9	v	101	BCL	C4-C3-C5-C6
8	A	101	U10	C13-C14-C16-C17
9	2	101	BCL	C12-C13-C15-C16
9	6	101	BCL	C11-C10-C8-C7
9	7	101	BCL	C12-C13-C15-C16
10	1	102	SPN	C21-C22-C23-C24
10	p	103	SPN	C21-C22-C23-C24
10	n	102	SPN	C21-C22-C23-C24
9	2	101	BCL	C13-C15-C16-C17
9	1	101	BCL	C3-C5-C6-C7
11	M	407	MW9	C12-C13-C14-C15
8	M	403	U10	C35-C34-C36-C37
9	1	101	BCL	C13-C15-C16-C17
8	M	403	U10	C43-C44-C46-C47
9	v	101	BCL	C2-C3-C5-C6
9	s	101	BCL	C1-C2-C3-C5
9	q	101	BCL	C1-C2-C3-C5
9	m	101	BCL	C1-C2-C3-C5
9	g	101	BCL	C1-C2-C3-C5
9	e	101	BCL	C1-C2-C3-C5
9	7	101	BCL	C1-C2-C3-C5

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Mol	Chain	Res	Type	Atoms
11	9	101	MW9	C-C1-C2-C3
9	L	304	BCL	C4B-C3B-CAB-CBB
9	3	101	BCL	C3-C5-C6-C7
9	x	101	BCL	C3-C5-C6-C7
9	4	101	BCL	C6-C7-C8-C9
9	x	101	BCL	C6-C7-C8-C9
11	H	302	MW9	C6-C7-C8-C9
9	4	101	BCL	C10-C11-C12-C13
11	g	103	MW9	C3-C4-C5-C6
13	L	303	BPH	C13-C15-C16-C17
11	H	301	MW9	C19-C20-O2-P
11	H	304	MW9	C22-C21-O5-P
10	1	104	SPN	C25-C26-C27-C28
9	L	304	BCL	C16-C17-C18-C20
9	k	101	BCL	C8-C10-C11-C12
9	b	101	BCL	C2A-CAA-CBA-CGA
9	5	101	BCL	C13-C15-C16-C17
10	1	102	SPN	C2-C3-C4-C5
10	1	103	SPN	C2-C3-C4-C5
10	1	104	SPN	C2-C3-C4-C5
10	1	105	SPN	C2-C3-C4-C5
10	5	102	SPN	C2-C3-C4-C5
10	5	103	SPN	C2-C3-C4-C5
10	3	102	SPN	C2-C3-C4-C5
10	w	102	SPN	C2-C3-C4-C5
10	u	102	SPN	C2-C3-C4-C5
10	v	102	SPN	C2-C3-C4-C5
10	s	102	SPN	C2-C3-C4-C5
10	t	102	SPN	C2-C3-C4-C5
10	r	102	SPN	C2-C3-C4-C5
10	p	102	SPN	C2-C3-C4-C5
10	p	103	SPN	C2-C3-C4-C5
10	m	102	SPN	C2-C3-C4-C5
10	n	102	SPN	C2-C3-C4-C5
10	k	102	SPN	C2-C3-C4-C5
10	l	102	SPN	C2-C3-C4-C5
10	h	102	SPN	C2-C3-C4-C5
10	h	103	SPN	C2-C3-C4-C5
10	e	102	SPN	C2-C3-C4-C5
10	f	102	SPN	C2-C3-C4-C5
10	c	102	SPN	C2-C3-C4-C5
10	c	103	SPN	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
10	a	102	SPN	C2-C3-C4-C5
10	a	103	SPN	C2-C3-C4-C5
10	i	102	SPN	C2-C3-C4-C5
10	j	102	SPN	C2-C3-C4-C5
10	7	102	SPN	C2-C3-C4-C5
10	7	103	SPN	C2-C3-C4-C5
10	M	406	SPN	C2-C3-C4-C5
10	9	103	SPN	C2-C3-C4-C5
10	0	102	SPN	C2-C3-C4-C5
11	g	102	MW9	O7-C22-C23-O6
9	4	101	BCL	C16-C17-C18-C20
8	M	403	U10	C5-C4-O4-C4M
11	g	102	MW9	C30-C31-C32-C33
11	H	304	MW9	O8-C24-C25-C26
11	9	101	MW9	C10-C11-C12-C13
9	5	101	BCL	C16-C17-C18-C19
9	l	101	BCL	C16-C17-C18-C20
13	M	409	BPH	C16-C17-C18-C20
9	L	301	BCL	C13-C15-C16-C17
12	C	401	HEM	CAD-CBD-CGD-O1D
9	a	101	BCL	C13-C15-C16-C17
9	t	101	BCL	C6-C7-C8-C10
12	C	402	HEM	CAA-CBA-CGA-O1A
12	C	403	HEM	CAD-CBD-CGD-O2D
11	M	408	MW9	C26-C27-C28-C29
9	L	301	BCL	C11-C10-C8-C9
13	L	303	BPH	C6-C7-C8-C9
12	C	402	HEM	CAA-CBA-CGA-O2A
11	H	301	MW9	C30-C31-C32-C33
9	h	101	BCL	C2-C1-O2A-CGA
9	a	101	BCL	C2-C1-O2A-CGA
9	L	301	BCL	C3-C5-C6-C7
9	w	101	BCL	C3A-C2A-CAA-CBA
9	e	101	BCL	C3A-C2A-CAA-CBA
9	0	101	BCL	C3A-C2A-CAA-CBA
9	l	101	BCL	C3-C5-C6-C7
9	e	101	BCL	C2A-CAA-CBA-CGA
9	L	304	BCL	C15-C16-C17-C18
11	g	103	MW9	C30-C31-C32-C33
11	9	101	MW9	C29-C30-C31-C32
12	C	401	HEM	C4C-C3C-CAC-CBC
11	9	101	MW9	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
11	9	101	MW9	C32-C33-C34-C35
10	p	102	SPN	C15-C16-C17-C18
12	C	403	HEM	CAD-CBD-CGD-O1D
9	2	101	BCL	C14-C13-C15-C16
9	i	101	BCL	C11-C10-C8-C9
9	0	101	BCL	C14-C13-C15-C16
13	M	409	BPH	C11-C10-C8-C9
13	M	409	BPH	C11-C12-C13-C14
11	g	103	MW9	C32-C33-C34-C35
11	M	407	MW9	C32-C33-C34-C35
8	M	403	U10	C33-C34-C36-C37
9	x	101	BCL	C6-C7-C8-C10
9	c	101	BCL	C11-C12-C13-C15
9	9	102	BCL	C11-C10-C8-C7
10	c	103	SPN	C21-C22-C23-C24
10	7	103	SPN	C21-C22-C23-C24
11	H	304	MW9	C2-C3-C4-C5
9	j	101	BCL	O1D-CGD-O2D-CED
11	H	301	MW9	C27-C28-C29-C30
9	o	101	BCL	C2-C1-O2A-CGA
9	9	102	BCL	C2-C1-O2A-CGA
9	b	101	BCL	C4-C3-C5-C6
9	b	101	BCL	C2-C3-C5-C6
13	M	405	BPH	C2-C3-C5-C6
10	p	103	SPN	C24-C25-C26-CM8
9	t	101	BCL	CAA-CBA-CGA-O2A
9	h	101	BCL	C15-C16-C17-C18
11	M	408	MW9	C32-C33-C34-C35
9	i	101	BCL	C5-C6-C7-C8
11	M	408	MW9	C37-C38-C39-C40
9	L	304	BCL	CBD-CGD-O2D-CED
10	q	102	SPN	C2-C3-C4-C5
9	6	101	BCL	C11-C10-C8-C9
10	a	103	SPN	CM7-C22-C23-C24
8	M	403	U10	C44-C46-C47-C48
9	r	101	BCL	C1A-C2A-CAA-CBA
9	0	101	BCL	C1A-C2A-CAA-CBA
12	C	401	HEM	CAD-CBD-CGD-O2D
10	1	102	SPN	C10-C11-C12-C13
10	1	102	SPN	C18-C19-C20-C21
10	1	103	SPN	C23-C24-C25-C26
10	1	104	SPN	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
10	1	105	SPN	C6-C7-C8-C9
10	5	103	SPN	C6-C7-C8-C9
10	5	103	SPN	C18-C19-C20-C21
10	3	102	SPN	C10-C11-C12-C13
10	3	102	SPN	C18-C19-C20-C21
10	w	102	SPN	C6-C7-C8-C9
10	w	102	SPN	C10-C11-C12-C13
10	w	102	SPN	C18-C19-C20-C21
10	u	102	SPN	C6-C7-C8-C9
10	u	102	SPN	C10-C11-C12-C13
10	u	102	SPN	C18-C19-C20-C21
10	s	102	SPN	C10-C11-C12-C13
10	s	102	SPN	C18-C19-C20-C21
10	t	102	SPN	C6-C7-C8-C9
10	r	102	SPN	C6-C7-C8-C9
10	r	102	SPN	C18-C19-C20-C21
10	m	102	SPN	C18-C19-C20-C21
10	n	102	SPN	C6-C7-C8-C9
10	n	102	SPN	C18-C19-C20-C21
10	k	102	SPN	C18-C19-C20-C21
10	l	102	SPN	C6-C7-C8-C9
10	l	102	SPN	C10-C11-C12-C13
10	h	102	SPN	C18-C19-C20-C21
10	h	103	SPN	C6-C7-C8-C9
10	e	102	SPN	C10-C11-C12-C13
10	e	102	SPN	C18-C19-C20-C21
10	f	102	SPN	C6-C7-C8-C9
10	c	102	SPN	C10-C11-C12-C13
10	c	102	SPN	C18-C19-C20-C21
10	c	103	SPN	C6-C7-C8-C9
10	a	102	SPN	C18-C19-C20-C21
10	a	103	SPN	C6-C7-C8-C9
10	i	102	SPN	C18-C19-C20-C21
10	7	102	SPN	C18-C19-C20-C21
10	7	103	SPN	C6-C7-C8-C9
10	7	103	SPN	C18-C19-C20-C21
10	9	103	SPN	C18-C19-C20-C21
9	j	101	BCL	CBD-CGD-O2D-CED
11	H	301	MW9	C15-C16-C17-O1
11	H	301	MW9	C14-C15-C16-C17
10	1	104	SPN	C6-C7-C8-C9
10	5	103	SPN	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
10	3	102	SPN	C6-C7-C8-C9
10	r	102	SPN	C10-C11-C12-C13
10	n	102	SPN	C10-C11-C12-C13
10	h	102	SPN	C10-C11-C12-C13
10	h	103	SPN	C10-C11-C12-C13
10	e	102	SPN	C6-C7-C8-C9
10	i	102	SPN	C6-C7-C8-C9
10	i	102	SPN	C10-C11-C12-C13
10	j	102	SPN	C6-C7-C8-C9
10	7	102	SPN	C6-C7-C8-C9
10	7	102	SPN	C10-C11-C12-C13
10	M	406	SPN	C6-C7-C8-C9
9	b	101	BCL	C5-C6-C7-C8
9	1	101	BCL	C2-C1-O2A-CGA
9	b	101	BCL	C2-C1-O2A-CGA
9	L	304	BCL	C2-C1-O2A-CGA
9	3	101	BCL	C11-C12-C13-C15
13	L	303	BPH	C6-C7-C8-C10
13	M	405	BPH	C6-C7-C8-C10
11	H	302	MW9	C10-C11-C12-C13
9	L	301	BCL	C2C-C3C-CAC-CBC
9	M	404	BCL	CAA-CBA-CGA-O1A
9	g	101	BCL	C13-C15-C16-C17
10	1	103	SPN	C6-C7-C8-C9
10	1	105	SPN	C10-C11-C12-C13
10	1	105	SPN	C18-C19-C20-C21
10	5	102	SPN	C6-C7-C8-C9
10	5	102	SPN	C10-C11-C12-C13
10	5	102	SPN	C18-C19-C20-C21
10	v	102	SPN	C6-C7-C8-C9
10	s	102	SPN	C6-C7-C8-C9
10	q	102	SPN	C18-C19-C20-C21
10	p	103	SPN	C6-C7-C8-C9
10	p	103	SPN	C23-C24-C25-C26
10	m	102	SPN	C6-C7-C8-C9
10	m	102	SPN	C10-C11-C12-C13
10	k	102	SPN	C6-C7-C8-C9
10	k	102	SPN	C10-C11-C12-C13
10	h	102	SPN	C6-C7-C8-C9
10	f	102	SPN	C10-C11-C12-C13
10	c	102	SPN	C6-C7-C8-C9
10	c	103	SPN	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
10	c	103	SPN	C18-C19-C20-C21
10	a	102	SPN	C10-C11-C12-C13
10	a	103	SPN	C10-C11-C12-C13
10	M	406	SPN	C10-C11-C12-C13
10	9	103	SPN	C6-C7-C8-C9
10	9	103	SPN	C10-C11-C12-C13
10	0	102	SPN	C6-C7-C8-C9
8	L	302	U10	C14-C16-C17-C18
9	r	101	BCL	C3A-C2A-CAA-CBA
9	M	404	BCL	C3A-C2A-CAA-CBA
10	i	102	SPN	CM8-C26-C27-C28
9	0	101	BCL	C16-C17-C18-C19
10	1	105	SPN	CM1-C1-C2-O2
10	u	102	SPN	CM1-C1-C2-O2
10	l	102	SPN	CM2-C1-C2-O2
10	h	103	SPN	CM2-C1-C2-O2
10	c	103	SPN	CM1-C1-C2-O2
10	j	102	SPN	CM1-C1-C2-O2
10	7	103	SPN	CM1-C1-C2-O2
10	M	406	SPN	CM2-C1-C2-O2
10	0	102	SPN	CM1-C1-C2-O2
11	M	407	MW9	C35-C36-C37-C38
10	1	102	SPN	C6-C7-C8-C9
10	u	102	SPN	C23-C24-C25-C26
10	v	102	SPN	C10-C11-C12-C13
10	t	102	SPN	C10-C11-C12-C13
10	q	102	SPN	C6-C7-C8-C9
10	q	102	SPN	C10-C11-C12-C13
10	p	102	SPN	C18-C19-C20-C21
10	p	103	SPN	C10-C11-C12-C13
10	a	102	SPN	C6-C7-C8-C9
10	a	102	SPN	C23-C24-C25-C26
10	j	102	SPN	C10-C11-C12-C13
10	7	103	SPN	C10-C11-C12-C13
10	0	102	SPN	C10-C11-C12-C13
9	o	101	BCL	C4B-C3B-CAB-OBB
13	M	405	BPH	C11-C12-C13-C14
10	v	102	SPN	C23-C24-C25-C26
11	g	103	MW9	O7-C22-C23-O6
11	H	303	MW9	C-C1-C2-C3
12	C	403	HEM	CAA-CBA-CGA-O2A
9	x	101	BCL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
11	H	301	MW9	C15-C16-C17-O
10	r	102	SPN	CM8-C26-C27-C28
10	1	103	SPN	C10-C11-C12-C13
10	h	102	SPN	C27-C28-C29-C30
10	h	103	SPN	C23-C24-C25-C26
10	0	102	SPN	C18-C19-C20-C21
9	w	101	BCL	C15-C16-C17-C18
9	7	101	BCL	C13-C15-C16-C17
9	f	101	BCL	CAD-CBD-CGD-O2D
9	8	101	BCL	CAD-CBD-CGD-O2D
13	M	405	BPH	CAD-CBD-CGD-O2D
9	s	101	BCL	C2-C1-O2A-CGA
9	k	101	BCL	C2-C1-O2A-CGA
9	t	101	BCL	CAA-CBA-CGA-O1A
9	r	101	BCL	CAA-CBA-CGA-O2A
9	k	101	BCL	C1-C2-C3-C4
9	i	101	BCL	C1-C2-C3-C4
11	g	103	MW9	C15-C16-C17-O1
9	3	101	BCL	C13-C15-C16-C17
11	H	301	MW9	C9-C10-C11-C12

There are no ring outliers.

83 monomers are involved in 365 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	c	102	SPN	2	0
10	a	103	SPN	2	0
8	L	305	U10	5	0
9	p	101	BCL	11	0
9	7	101	BCL	5	0
10	1	102	SPN	2	0
9	L	304	BCL	5	0
9	k	101	BCL	7	0
9	M	402	BCL	10	0
10	u	102	SPN	3	0
11	H	301	MW9	2	0
9	w	101	BCL	4	0
9	5	101	BCL	5	0
10	s	102	SPN	1	0
10	n	102	SPN	4	0
9	c	101	BCL	3	0
9	9	102	BCL	5	0

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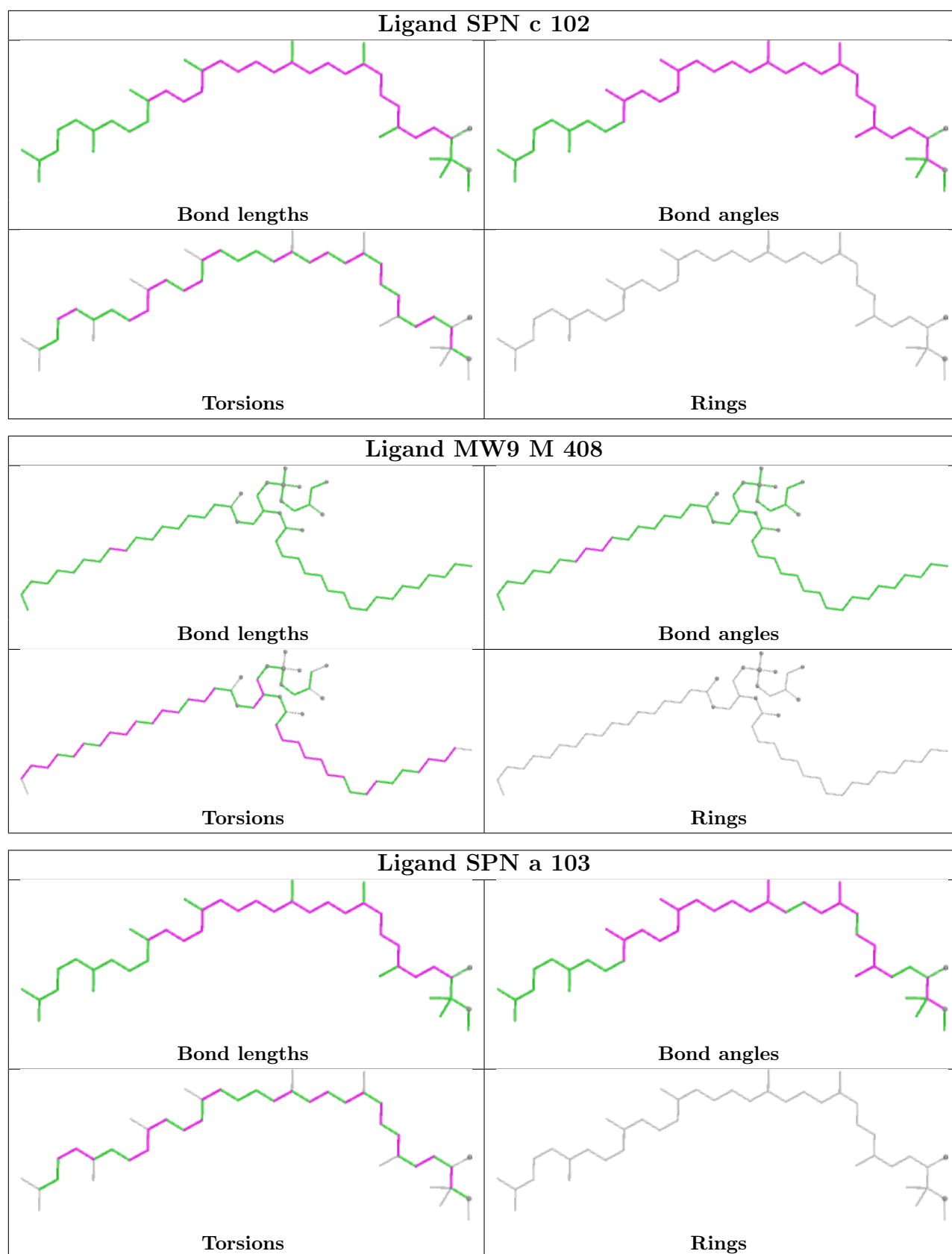
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	M	406	SPN	11	0
10	h	103	SPN	9	0
10	l	102	SPN	6	0
11	H	303	MW9	1	0
10	t	102	SPN	4	0
11	M	407	MW9	1	0
9	s	101	BCL	7	0
9	j	101	BCL	7	0
10	l	104	SPN	4	0
9	x	101	BCL	6	0
9	b	101	BCL	6	0
10	p	103	SPN	7	0
10	k	102	SPN	2	0
9	g	101	BCL	3	0
9	o	101	BCL	13	0
12	C	403	HEM	5	0
9	4	101	BCL	4	0
10	l	105	SPN	3	0
9	t	101	BCL	4	0
10	v	102	SPN	14	0
9	h	101	BCL	10	0
8	L	302	U10	1	0
10	h	102	SPN	8	0
10	c	103	SPN	1	0
10	l	103	SPN	12	0
10	r	102	SPN	1	0
9	v	101	BCL	7	0
9	6	101	BCL	4	0
10	a	102	SPN	1	0
9	f	101	BCL	7	0
10	p	102	SPN	13	0
9	r	101	BCL	7	0
10	7	103	SPN	4	0
9	0	101	BCL	7	0
10	9	103	SPN	1	0
13	M	409	BPH	2	0
9	M	404	BCL	3	0
9	i	101	BCL	5	0
9	l	101	BCL	5	0
9	e	101	BCL	3	0
10	i	102	SPN	2	0
12	C	402	HEM	4	0

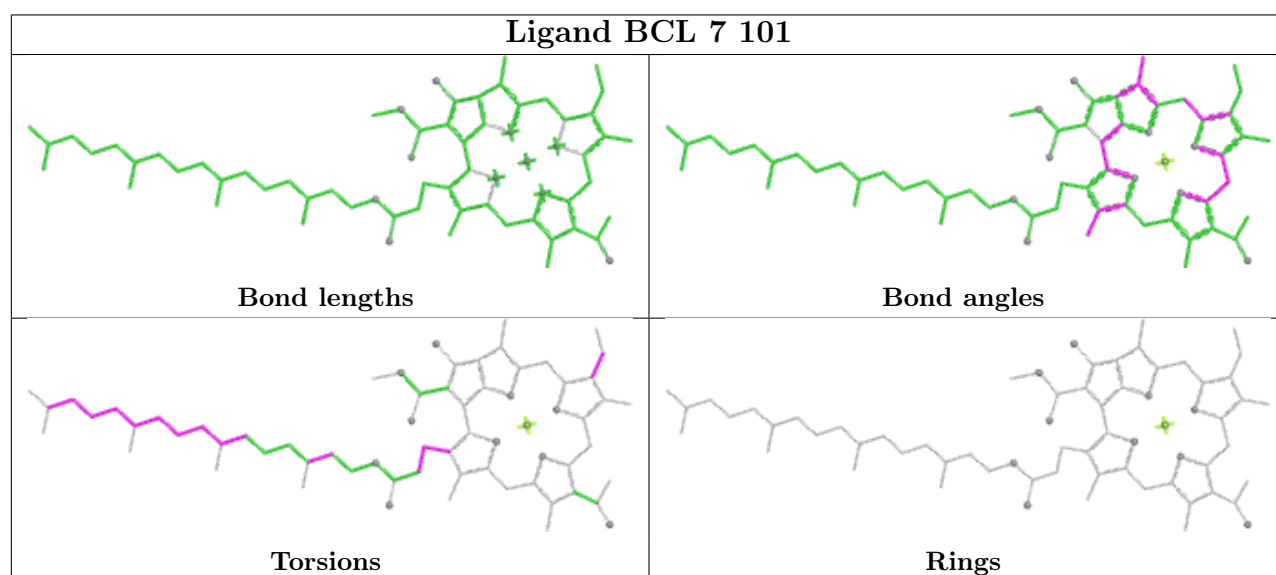
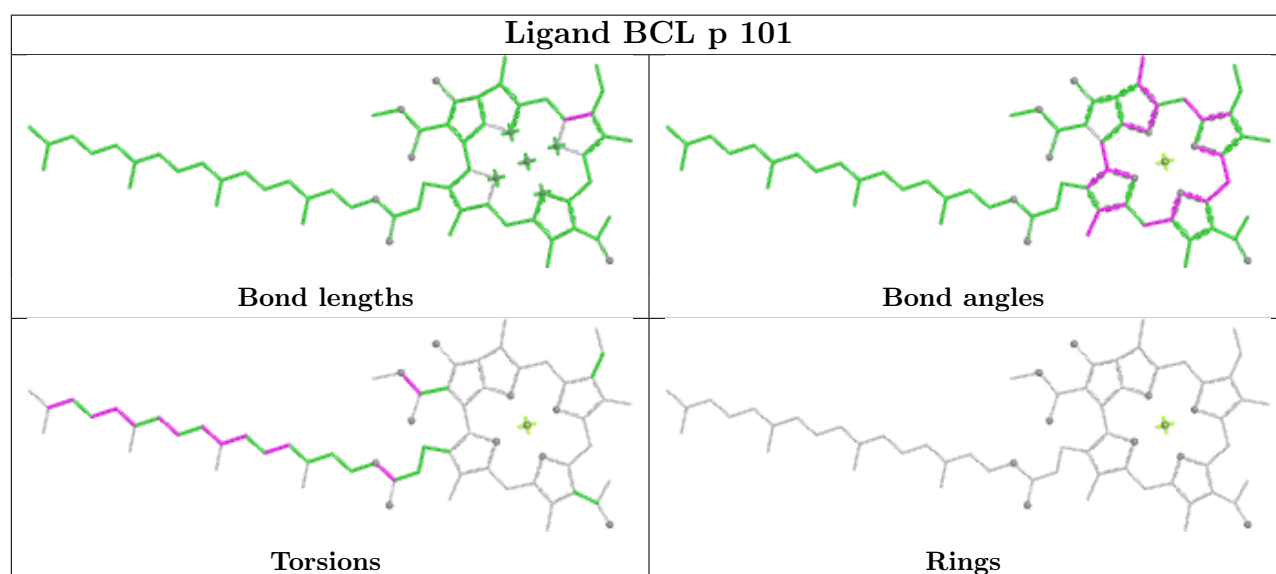
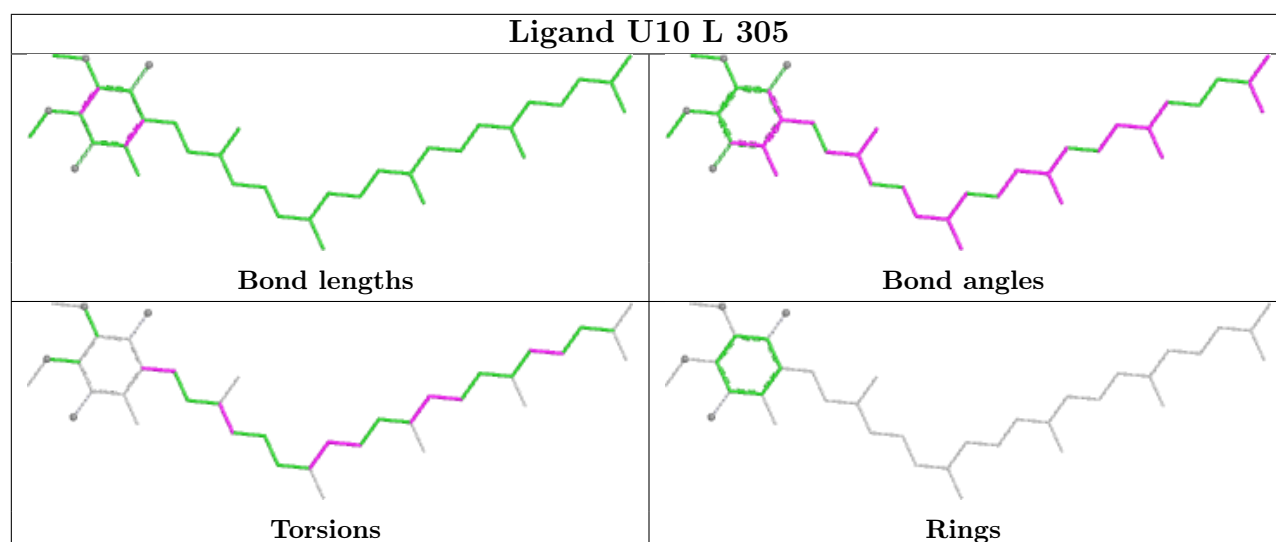
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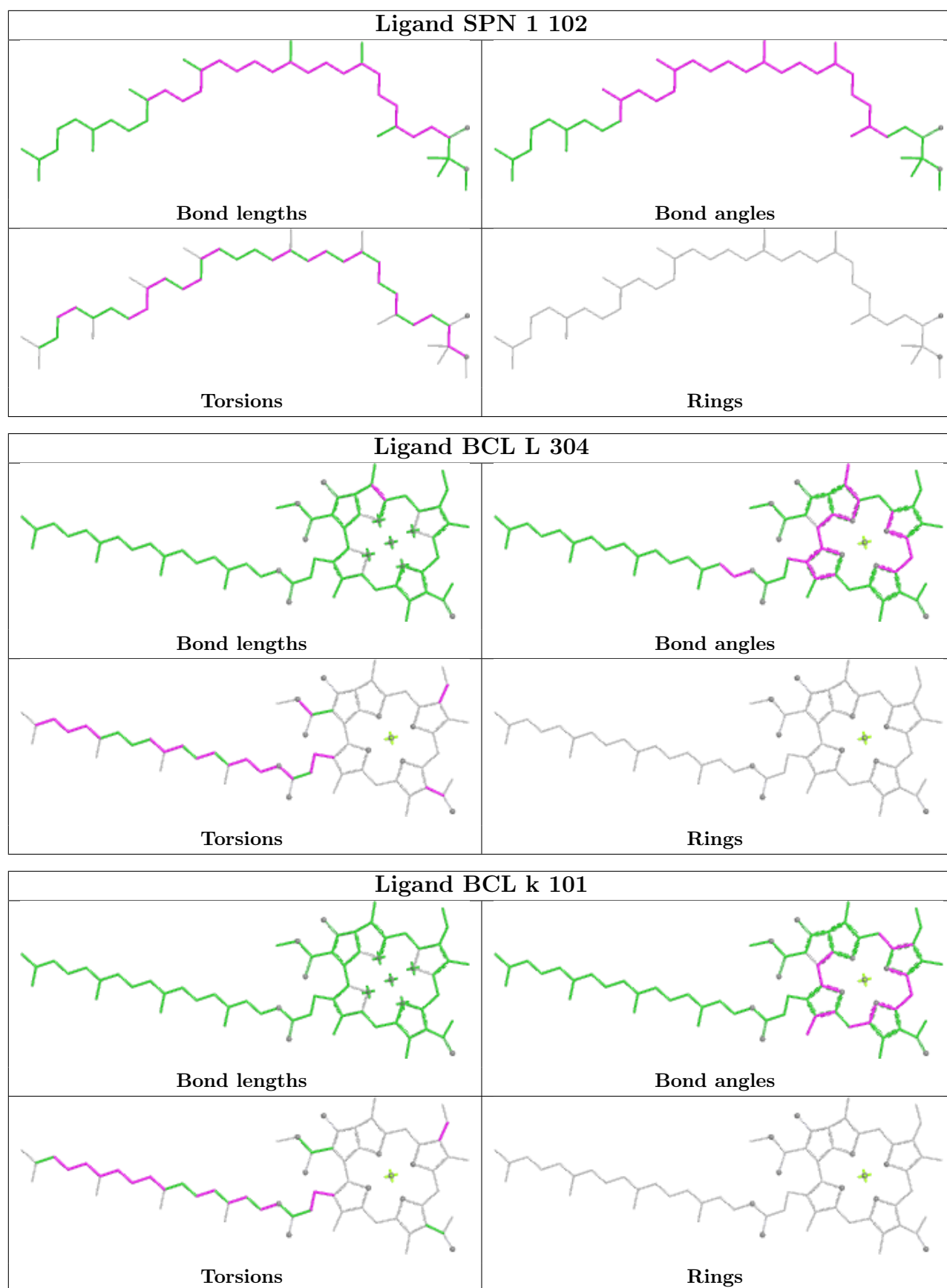
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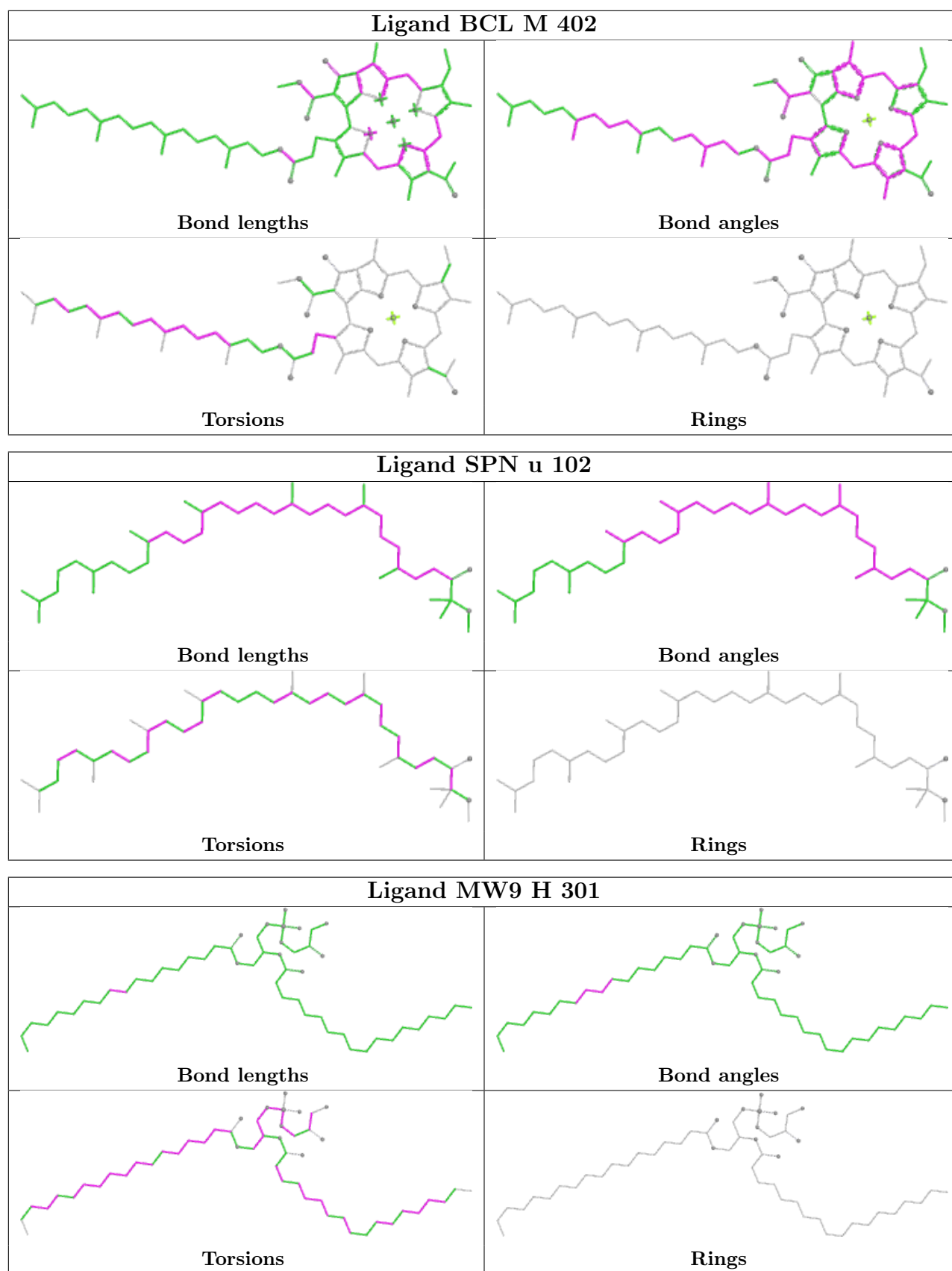
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	q	102	SPN	8	0
9	3	101	BCL	7	0
9	8	101	BCL	8	0
10	e	102	SPN	2	0
9	d	101	BCL	6	0
9	a	101	BCL	4	0
10	5	102	SPN	4	0
10	j	102	SPN	5	0
9	u	101	BCL	5	0
13	L	303	BPH	2	0
10	3	102	SPN	4	0
10	0	102	SPN	4	0
12	C	401	HEM	6	0
10	w	102	SPN	2	0
10	5	103	SPN	3	0
10	f	102	SPN	8	0
9	1	101	BCL	2	0
9	2	101	BCL	6	0
10	m	102	SPN	1	0
9	q	101	BCL	4	0
9	n	101	BCL	4	0
10	7	102	SPN	1	0
9	m	101	BCL	6	0
9	L	301	BCL	4	0

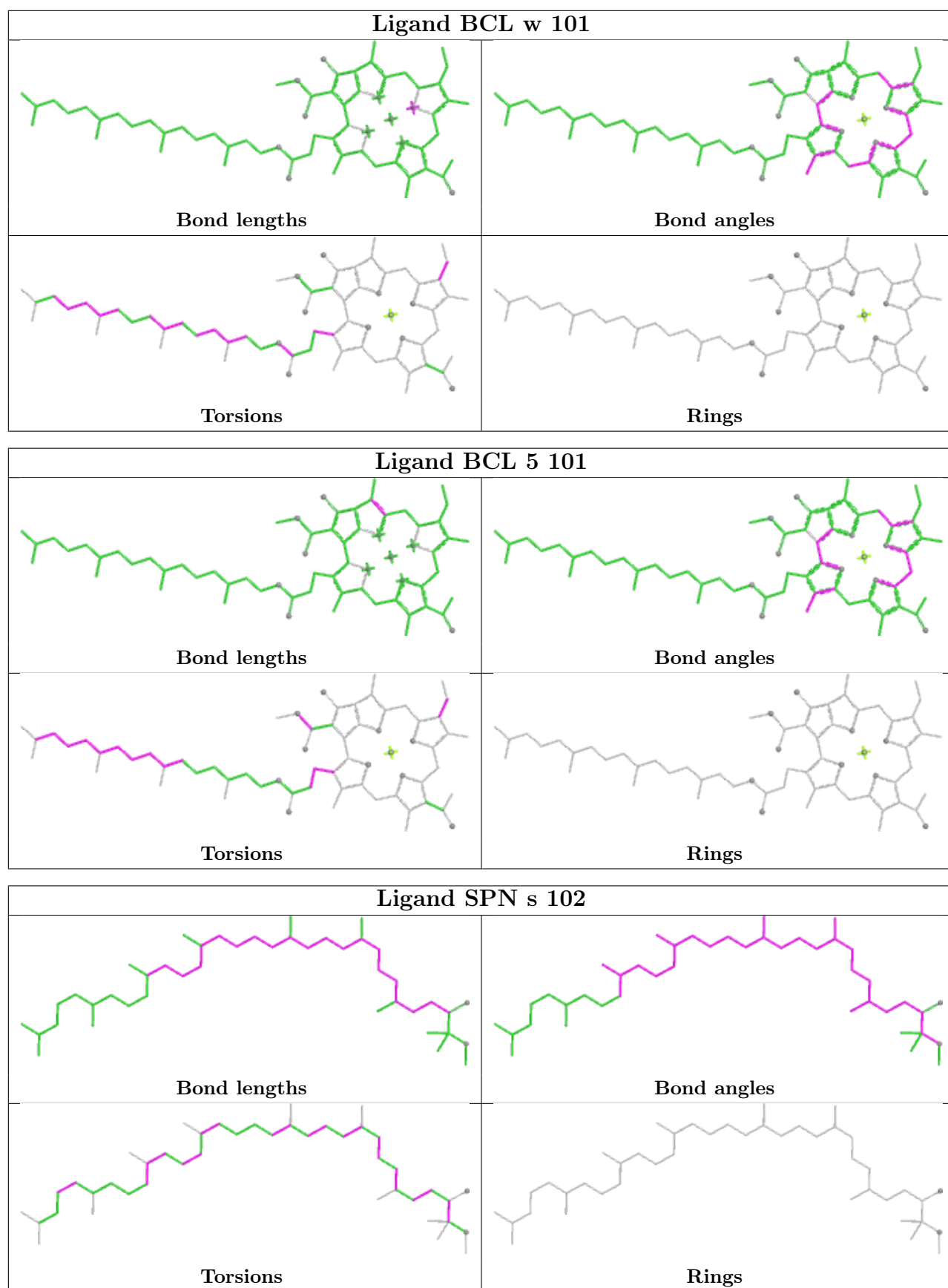
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

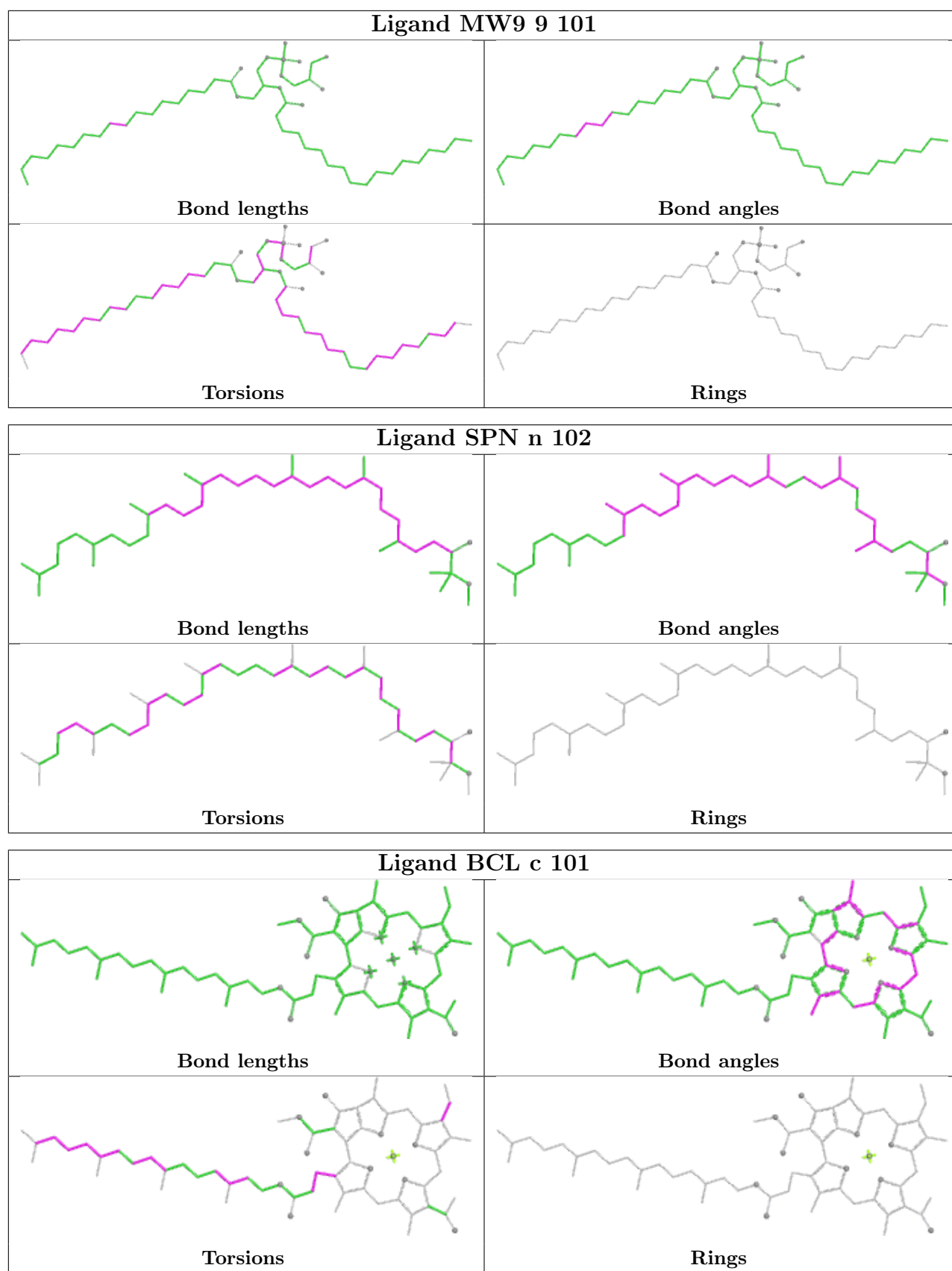


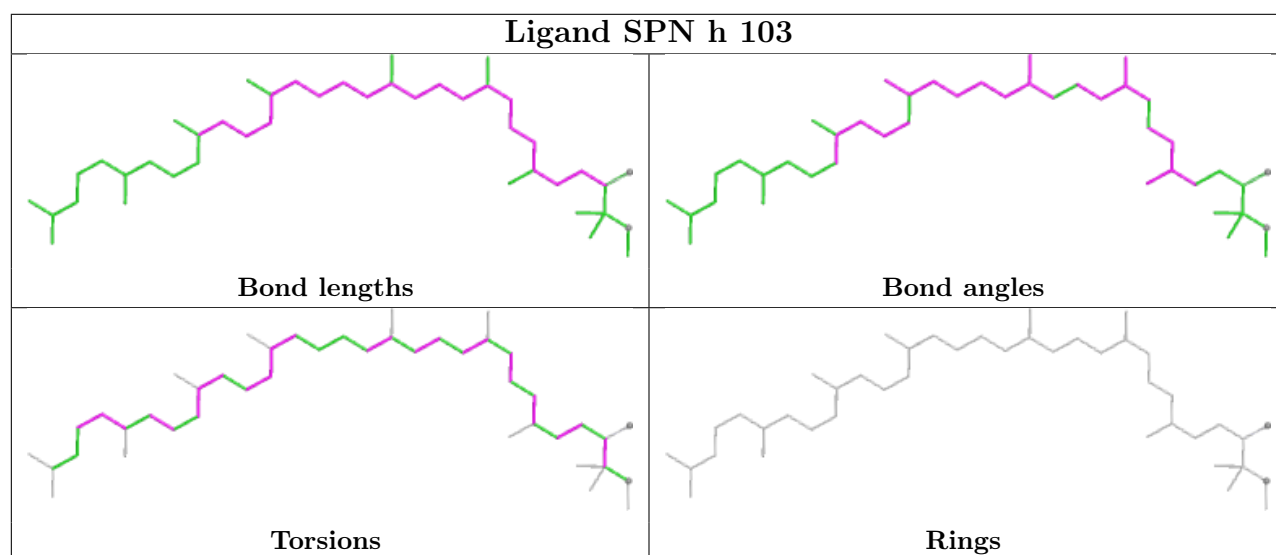
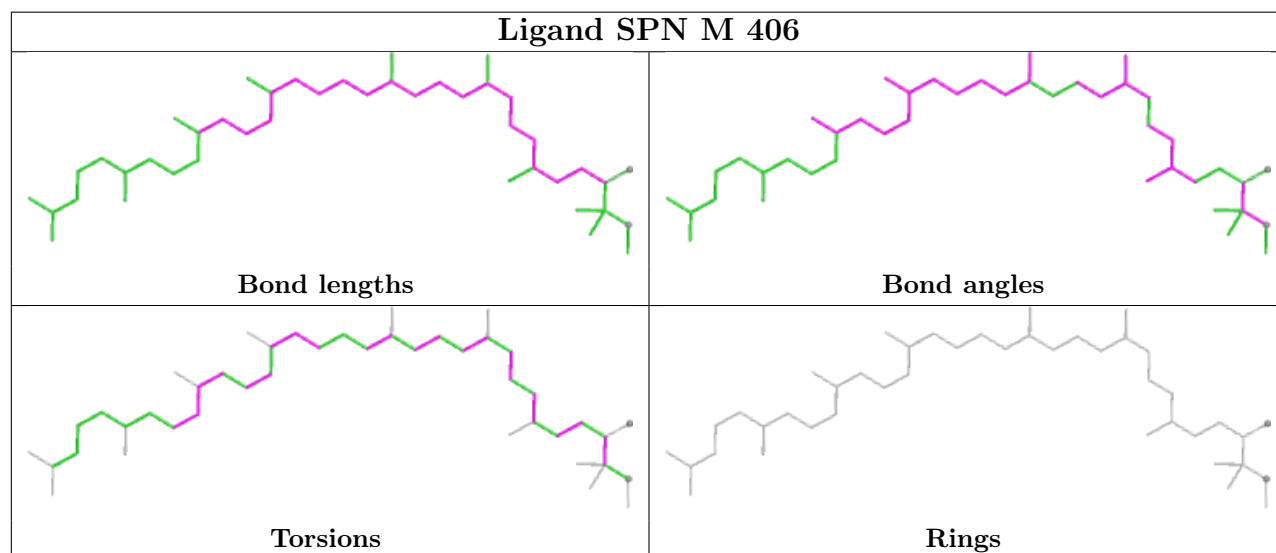
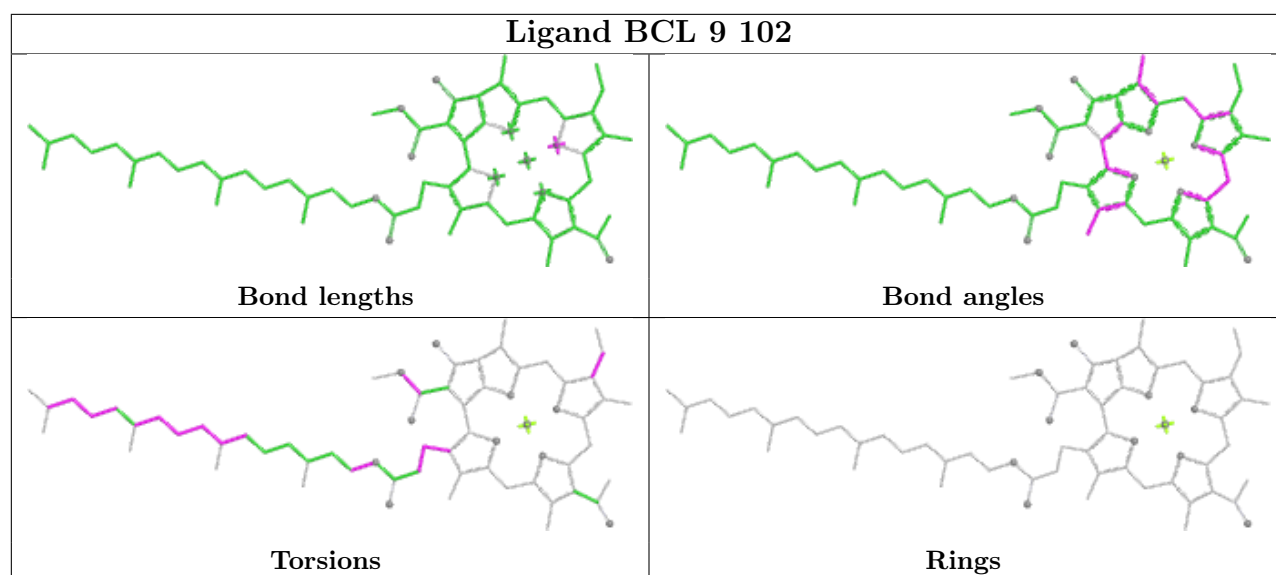


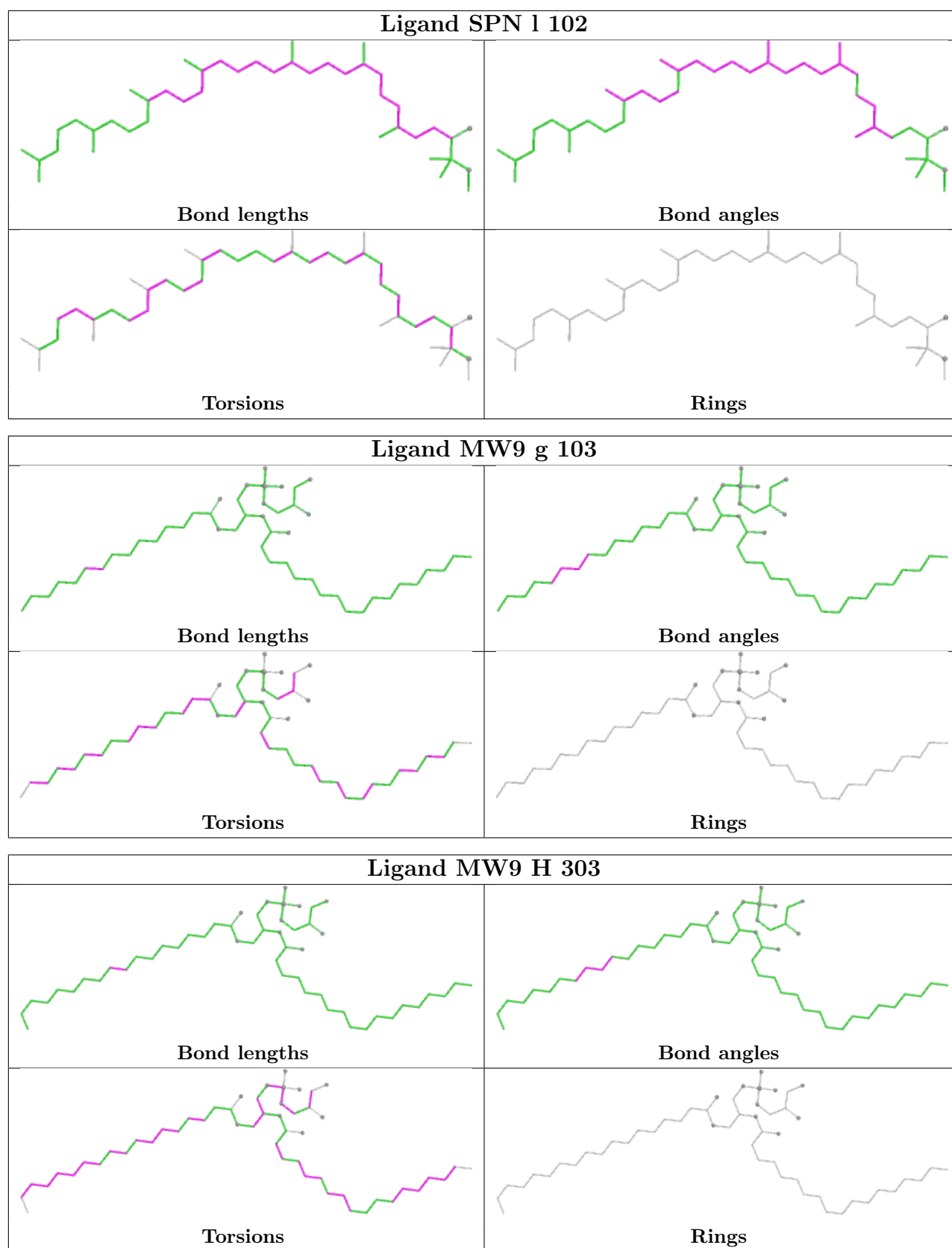


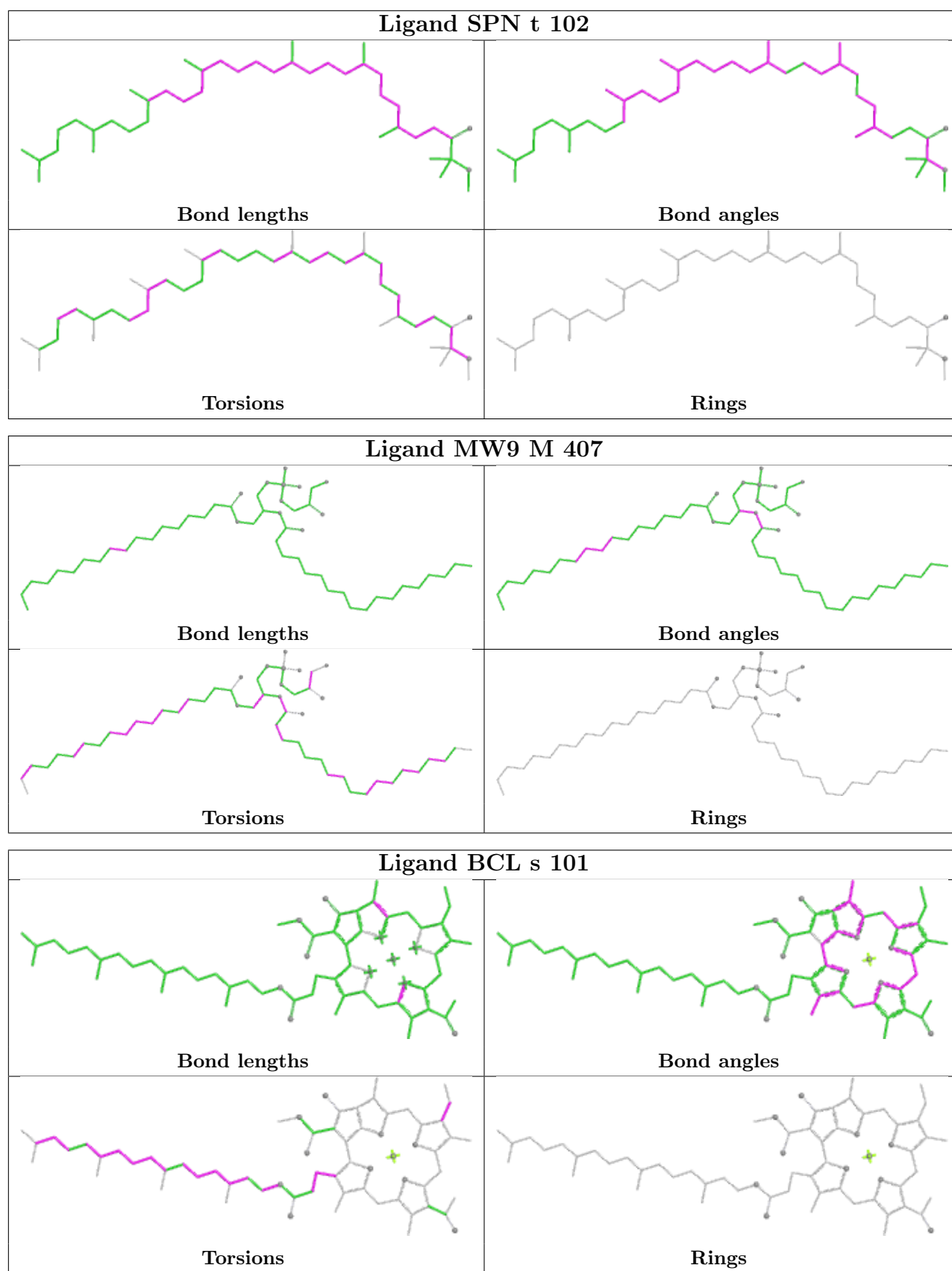


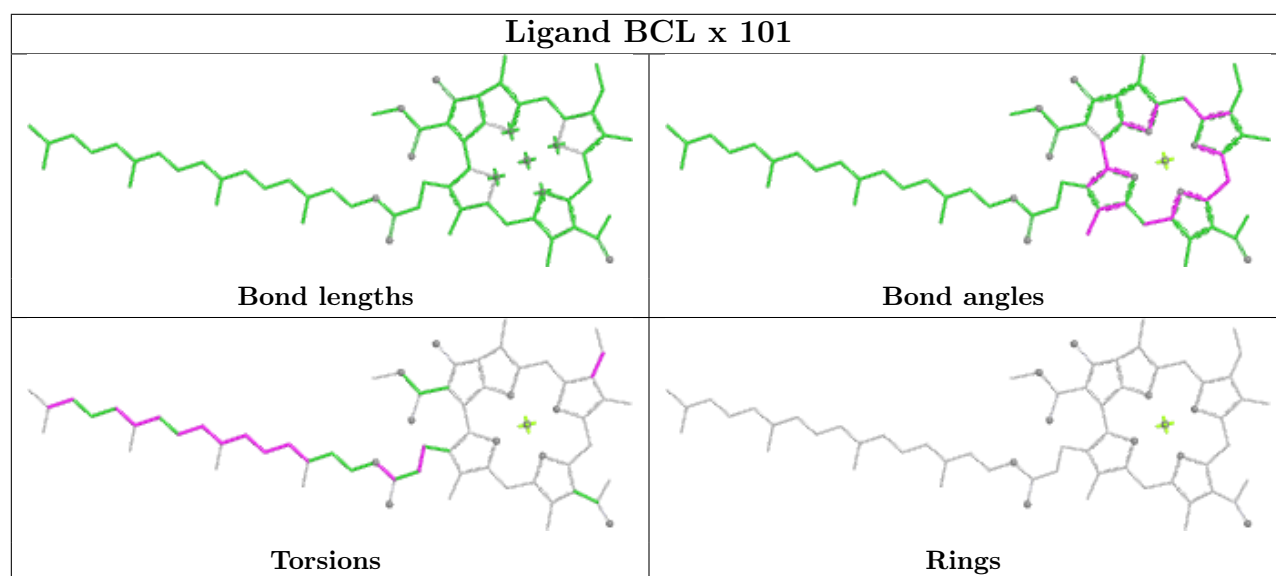
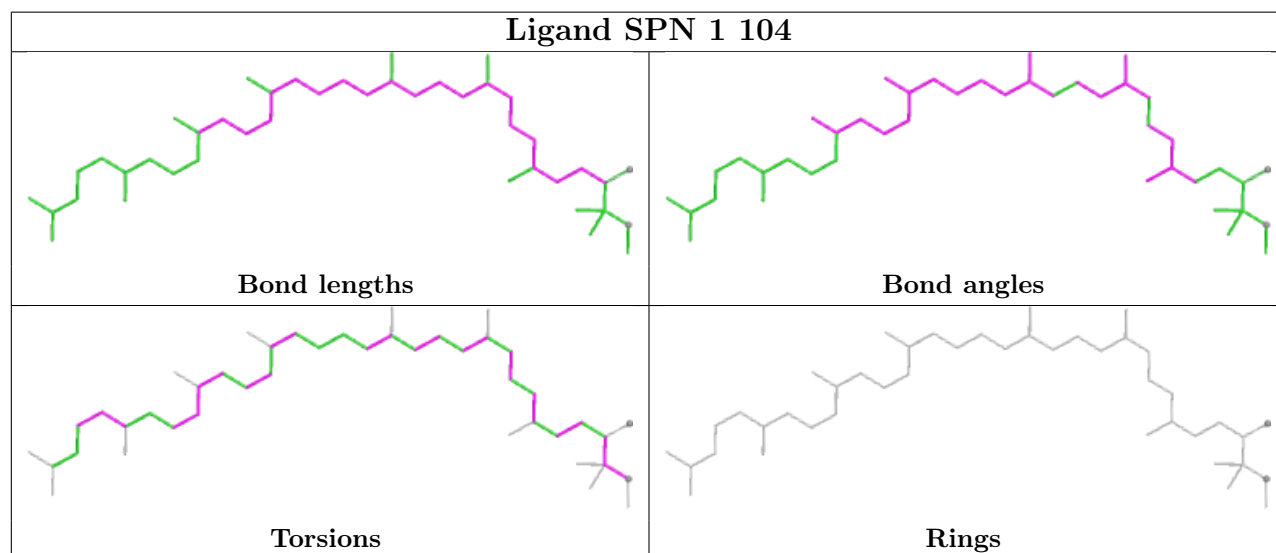
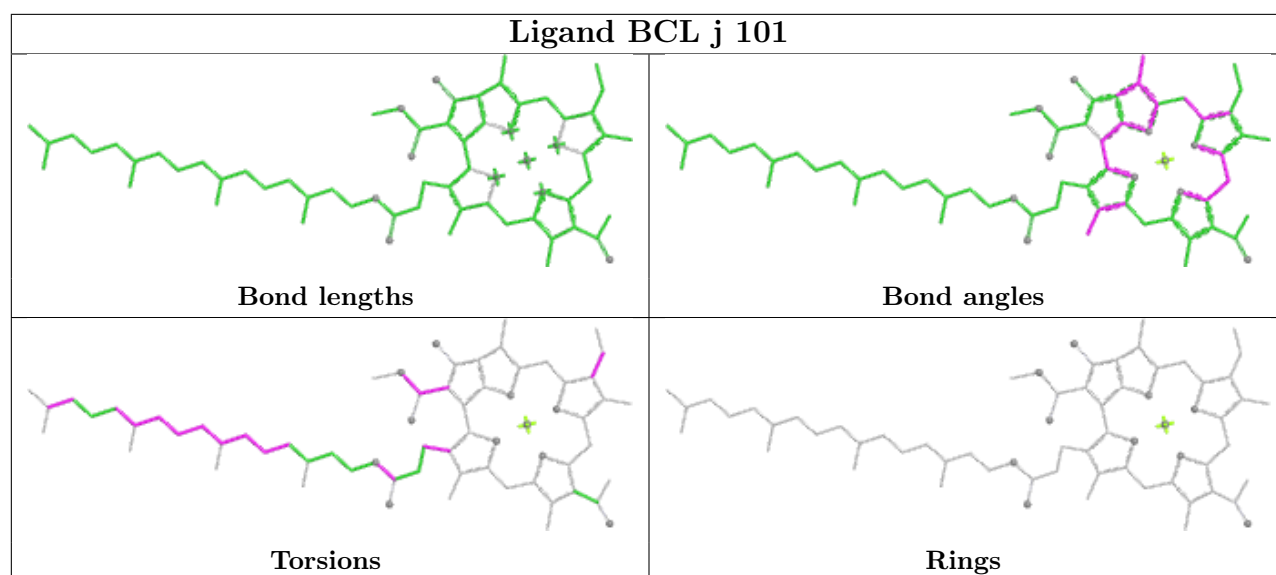


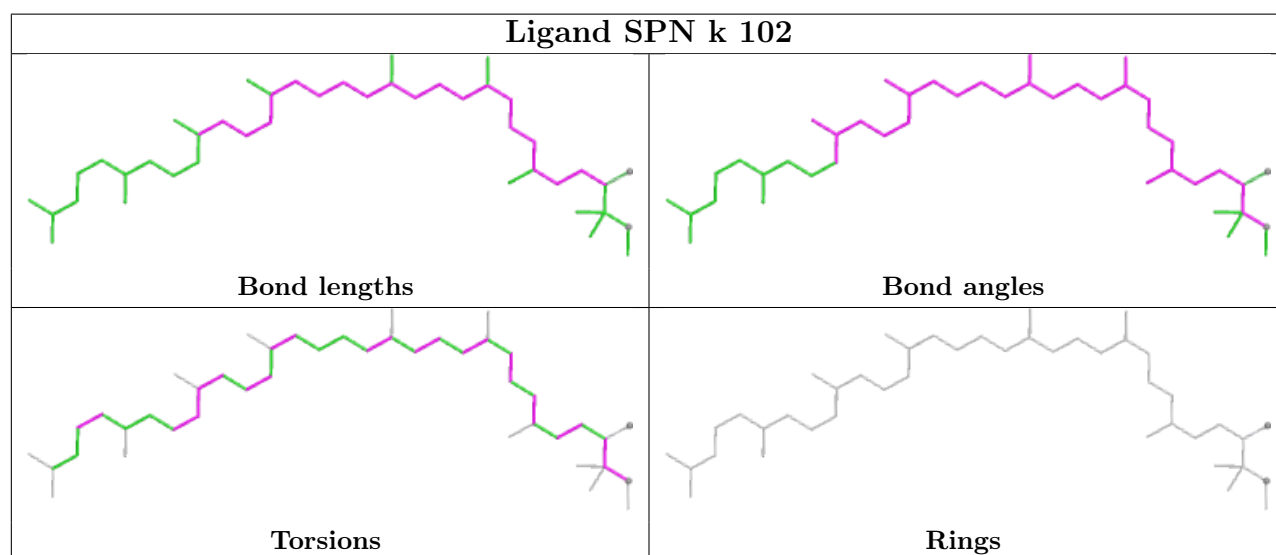
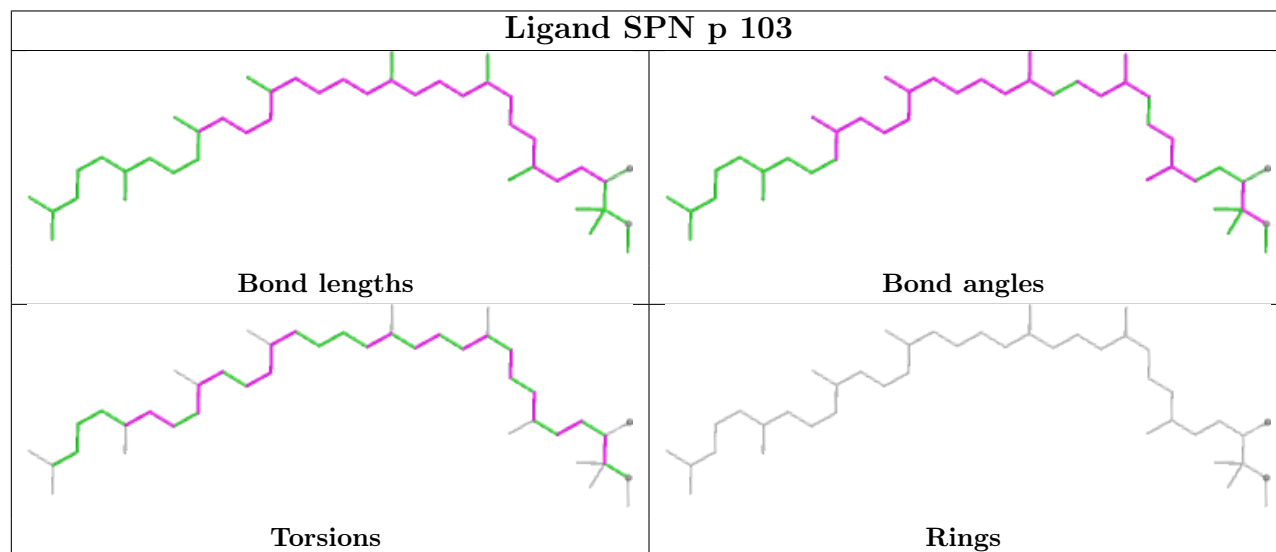
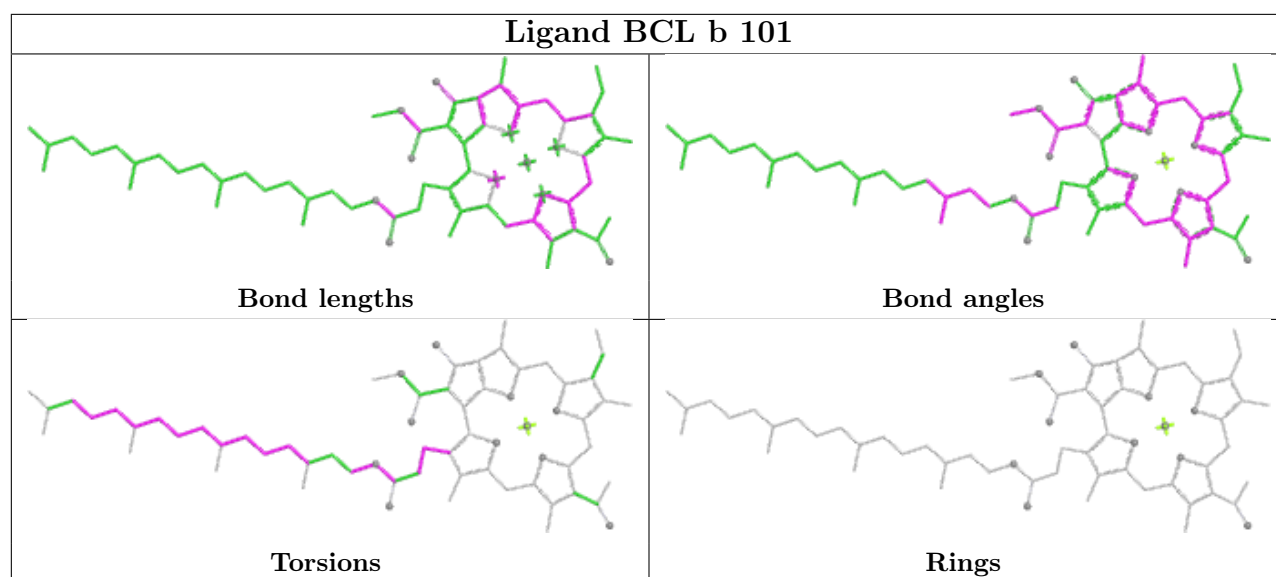


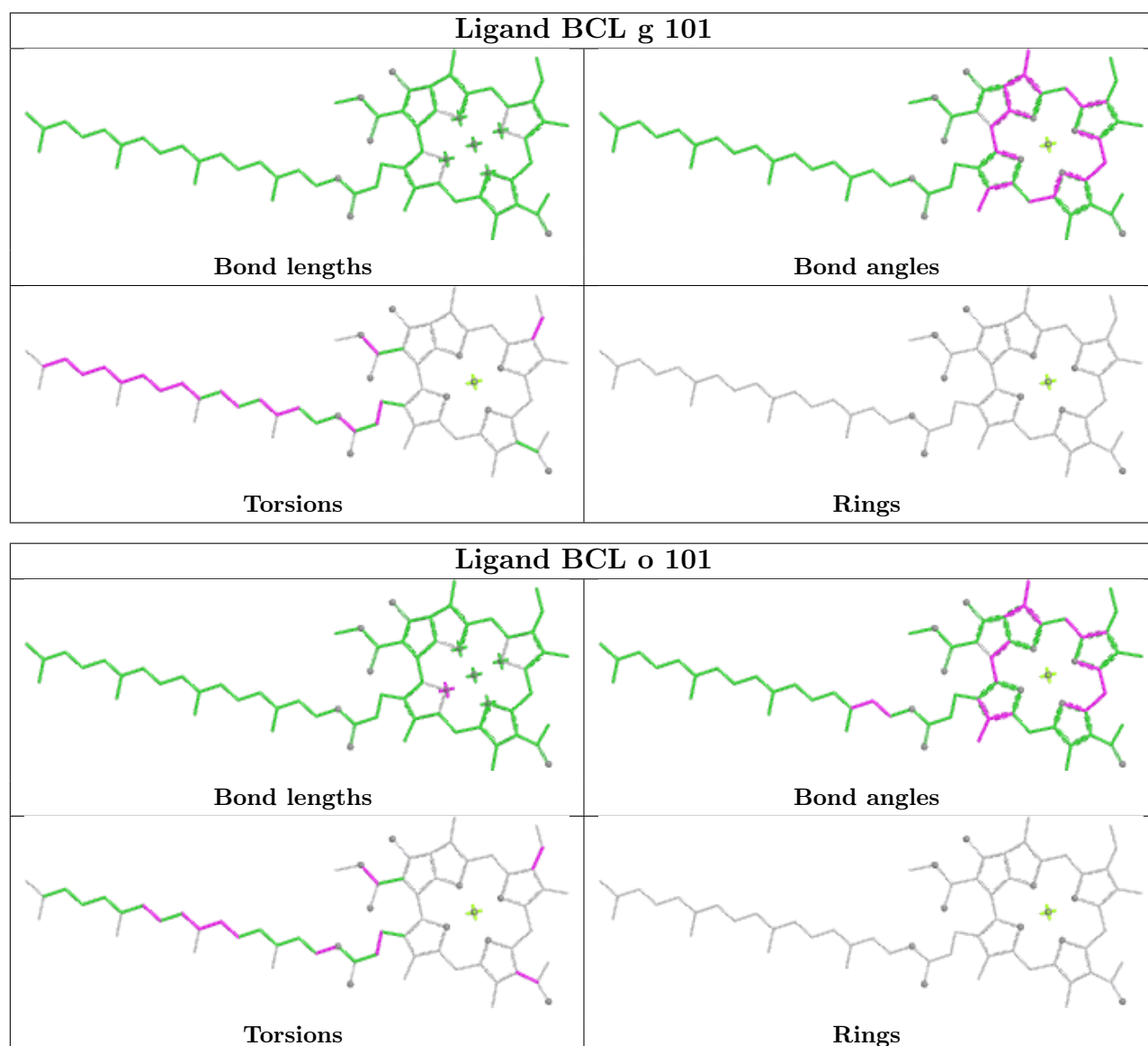


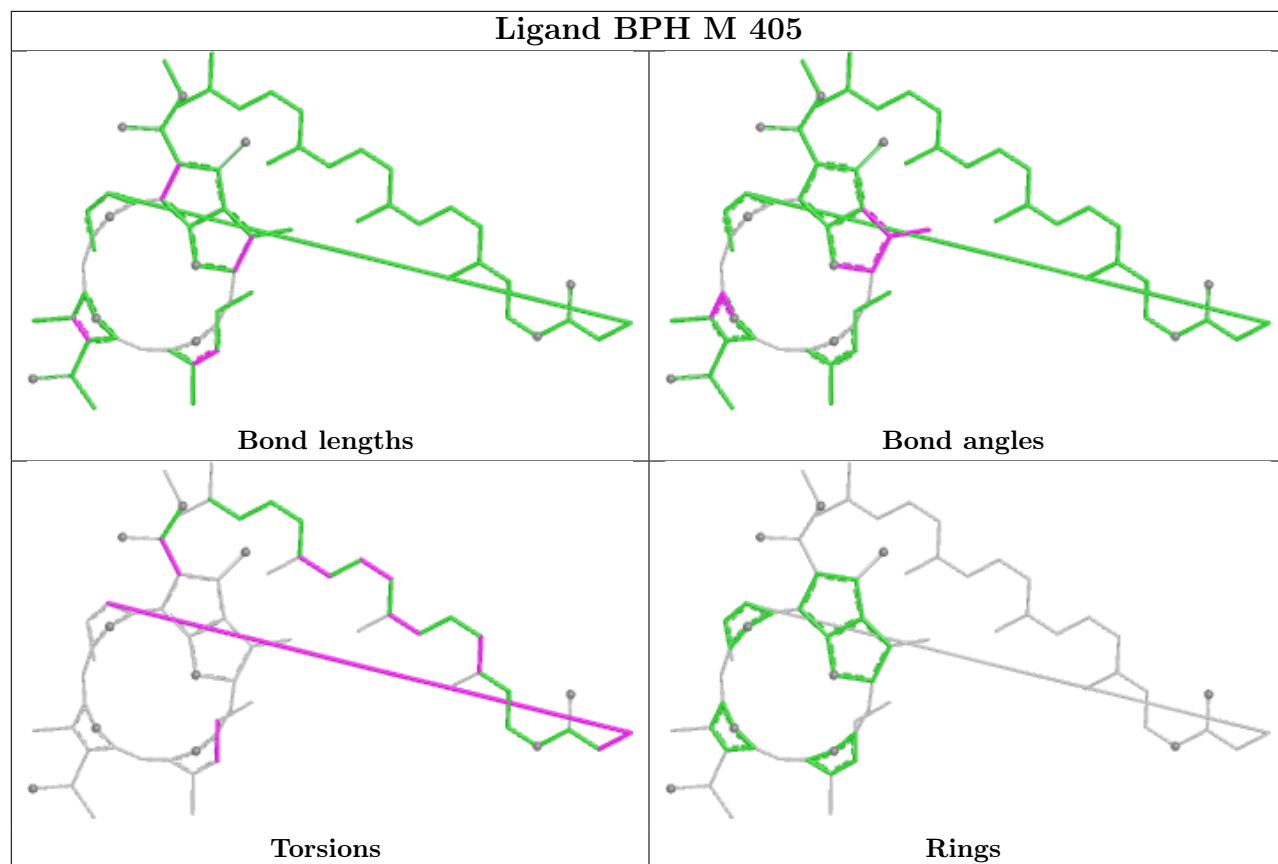


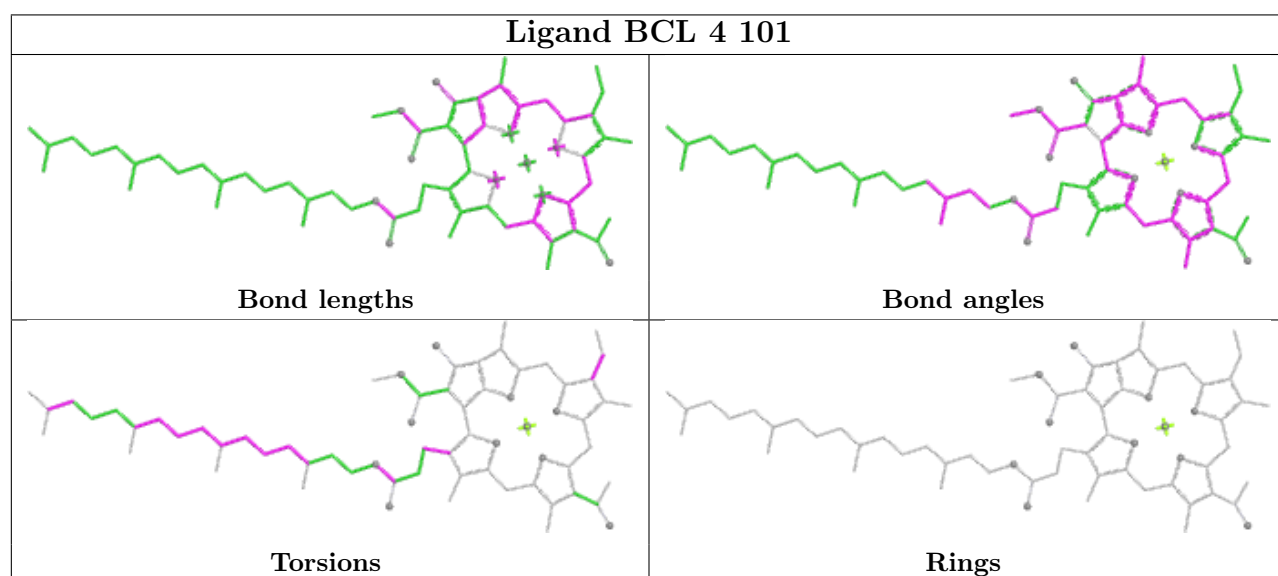
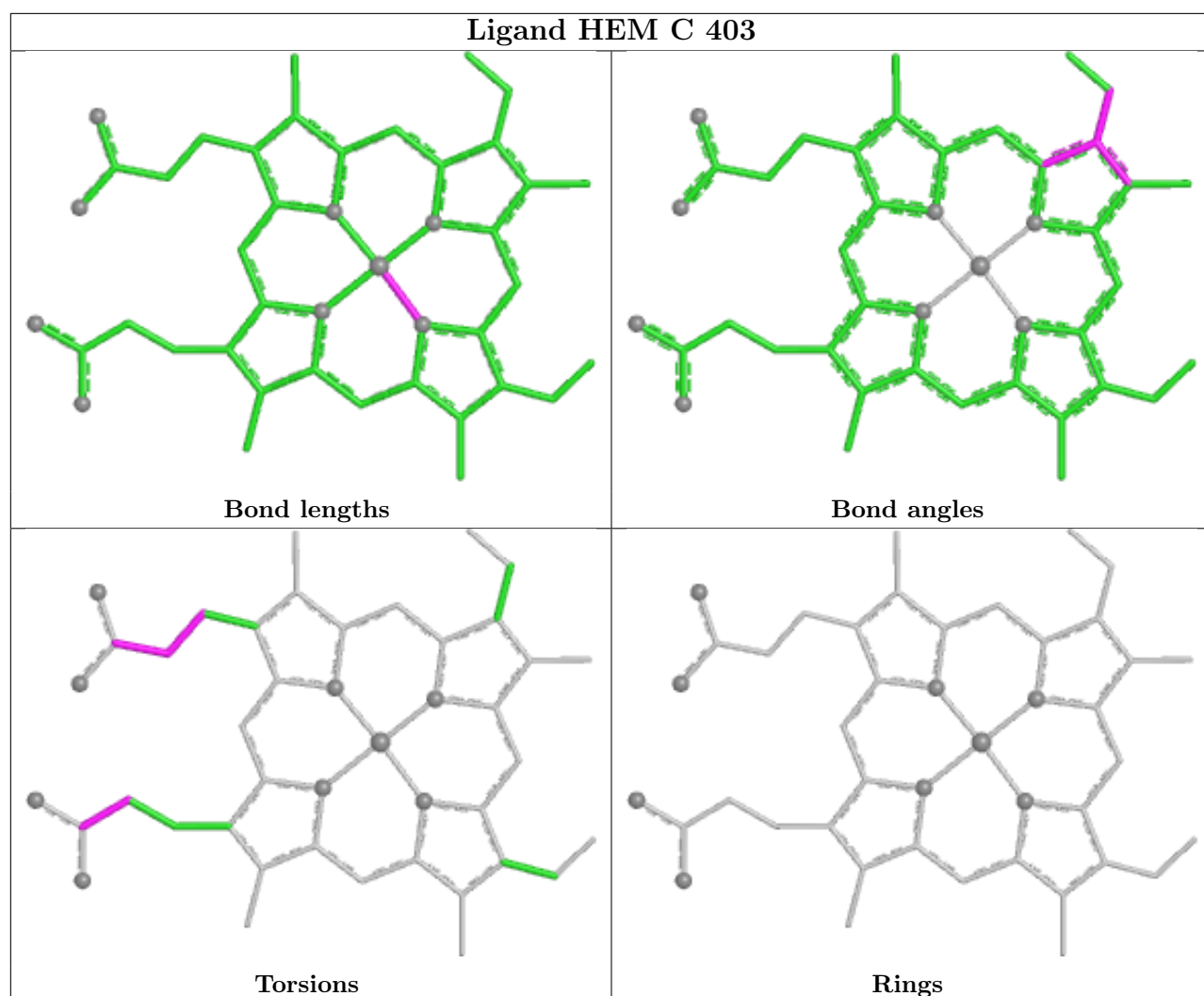


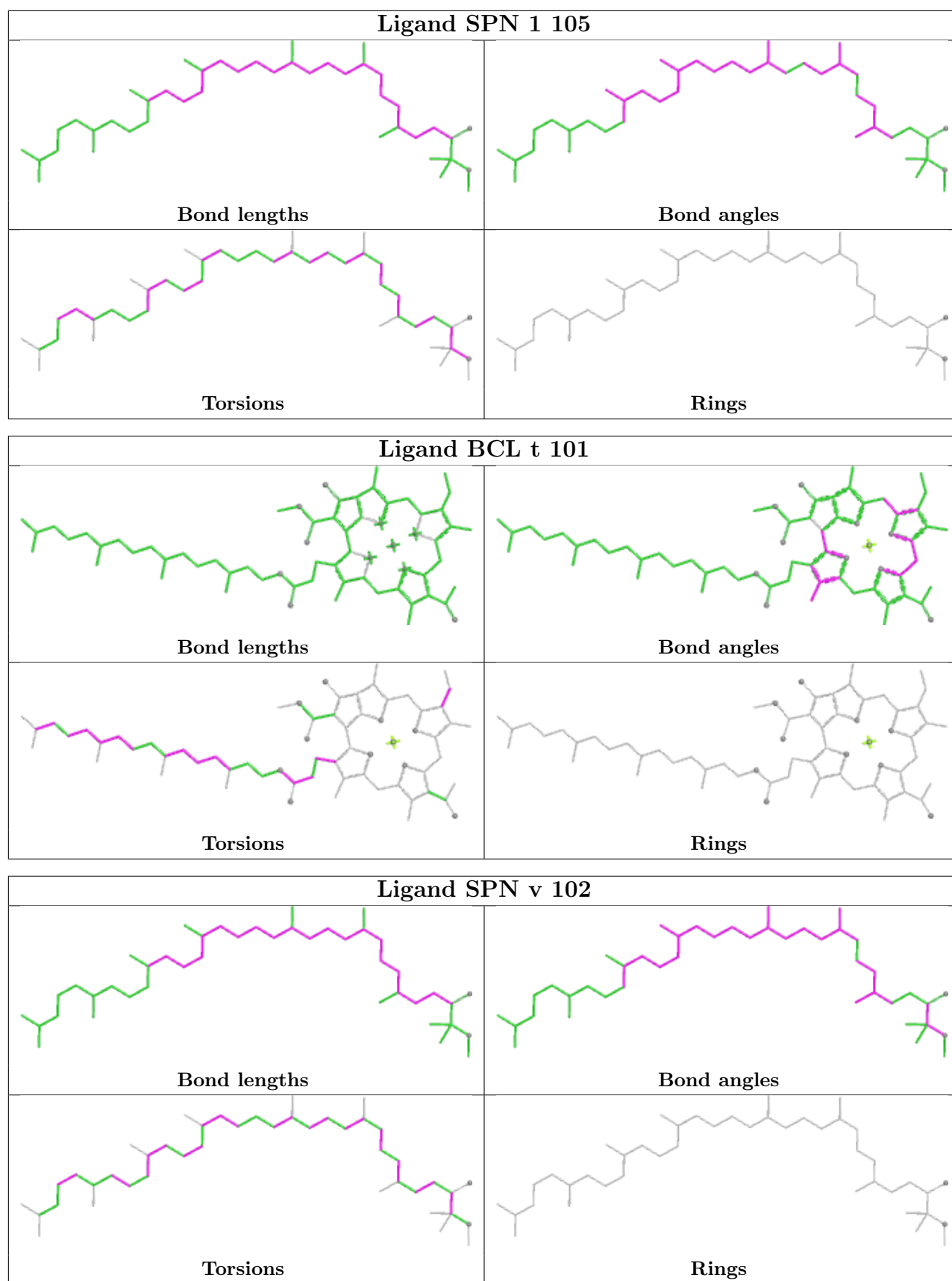


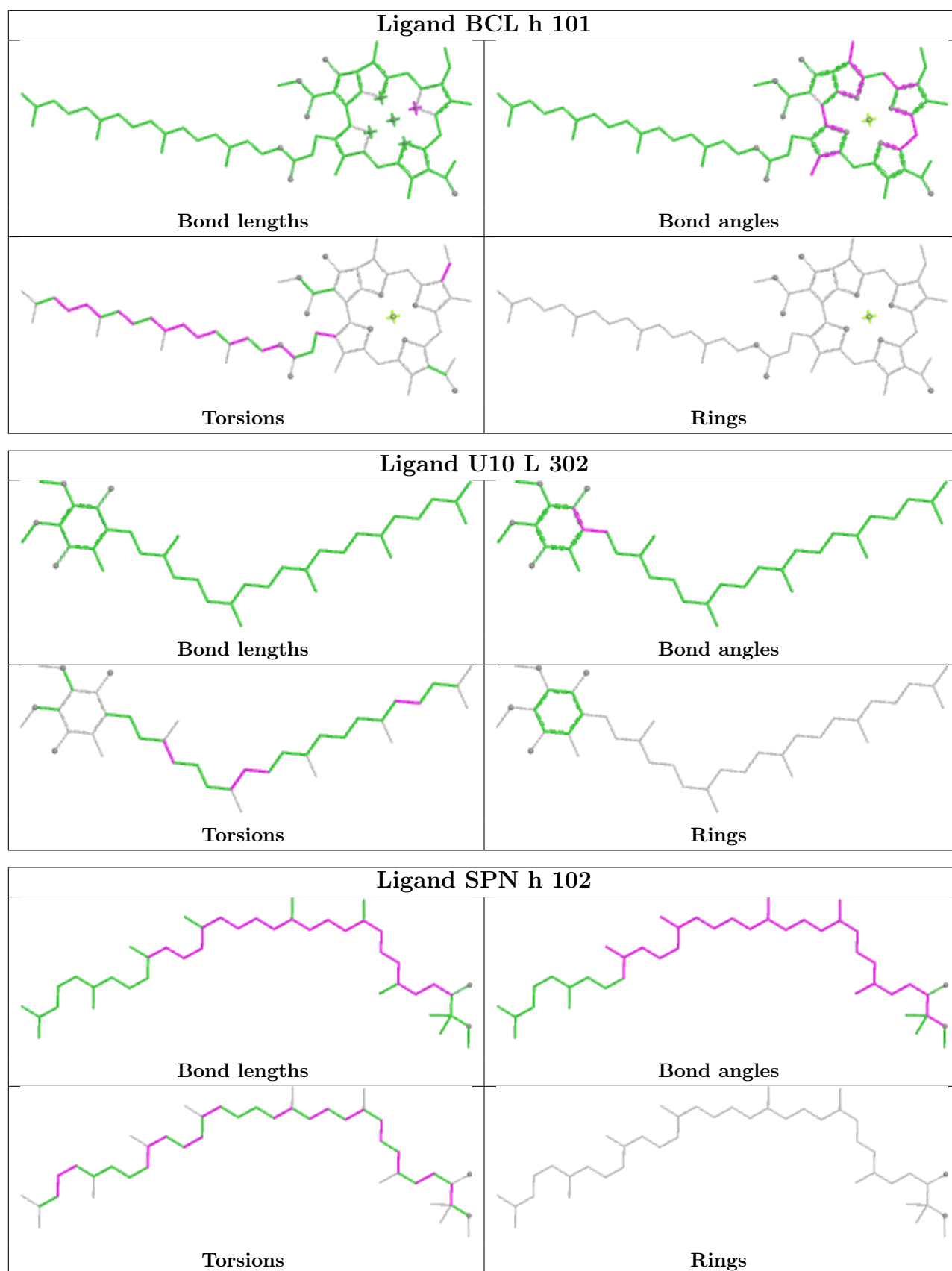


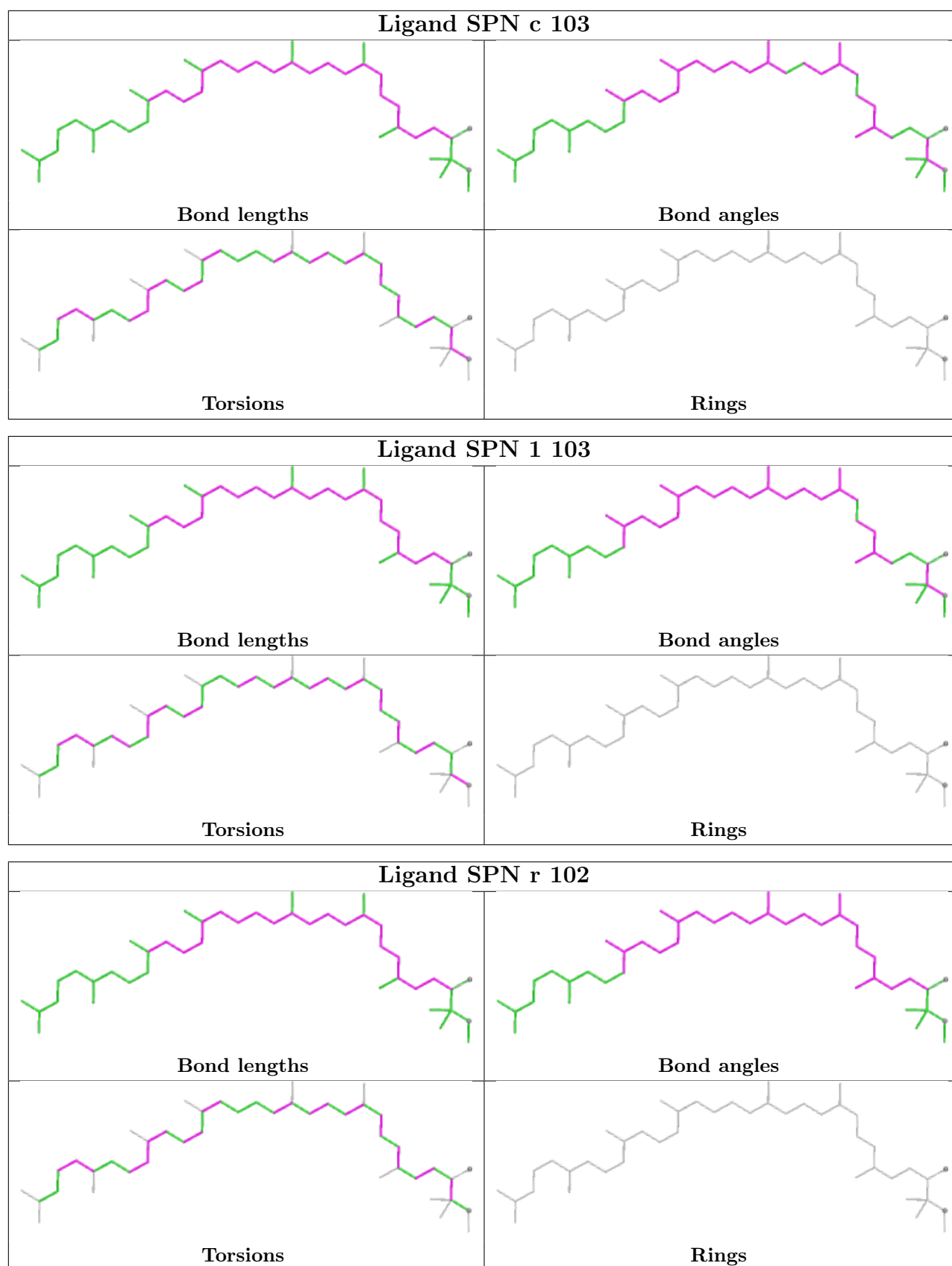


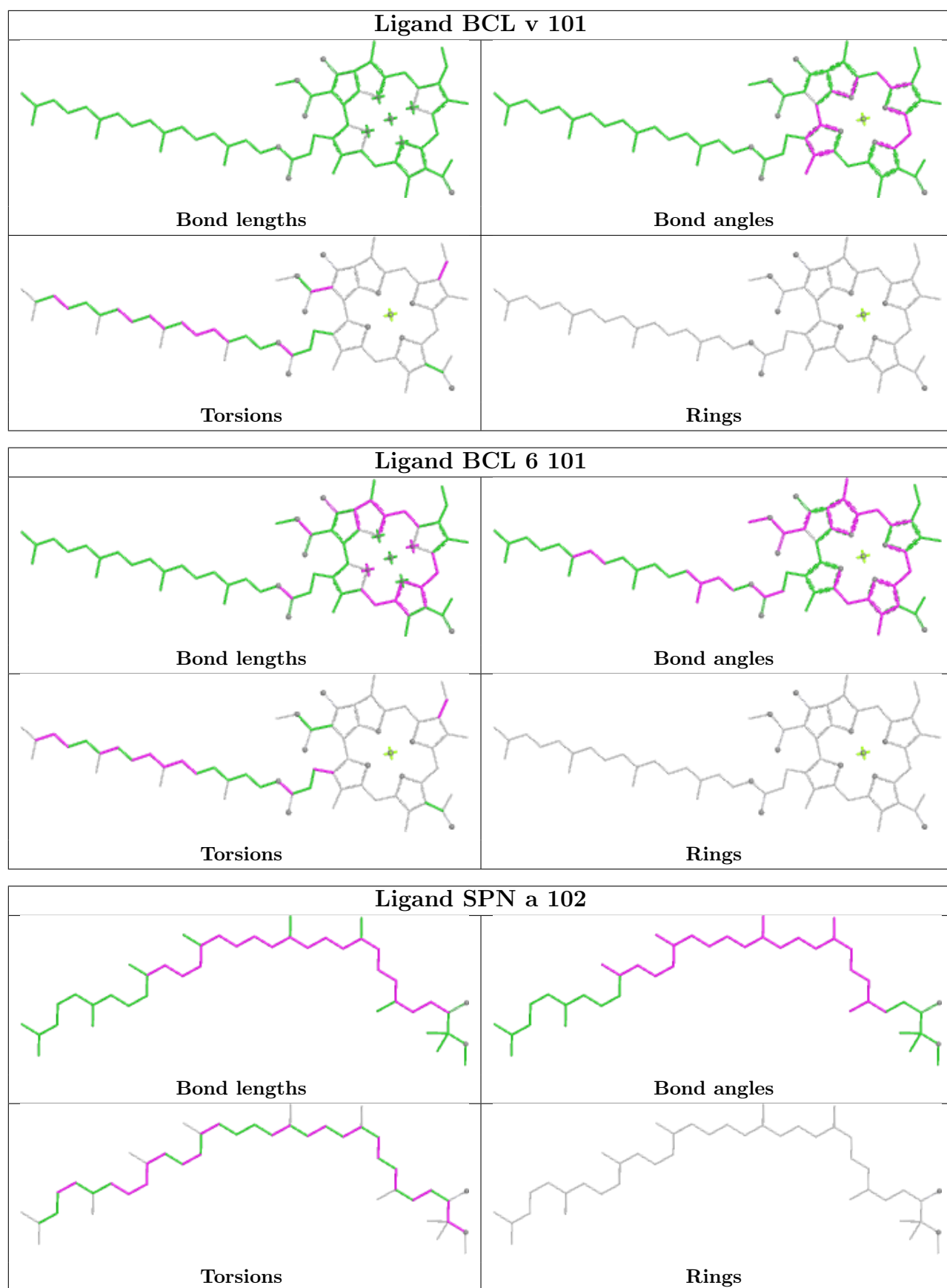


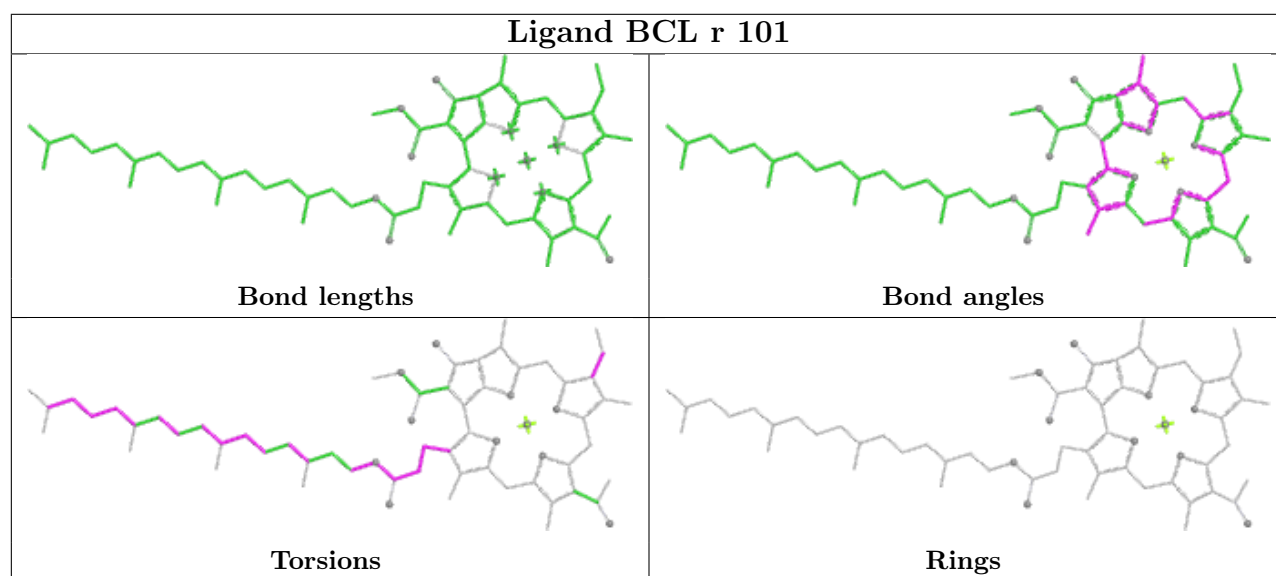
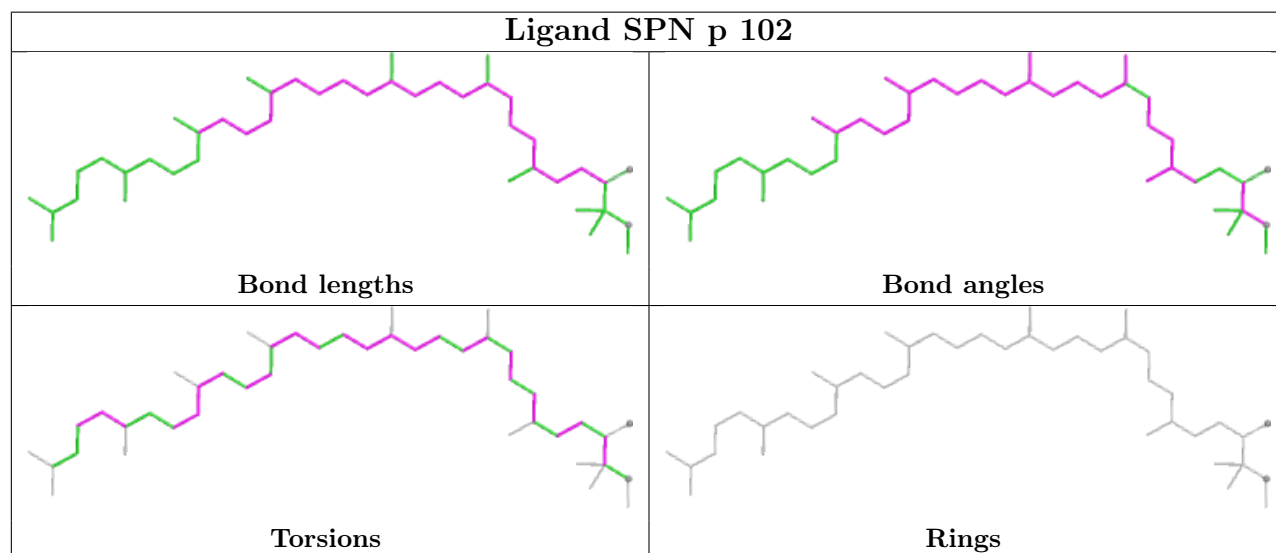
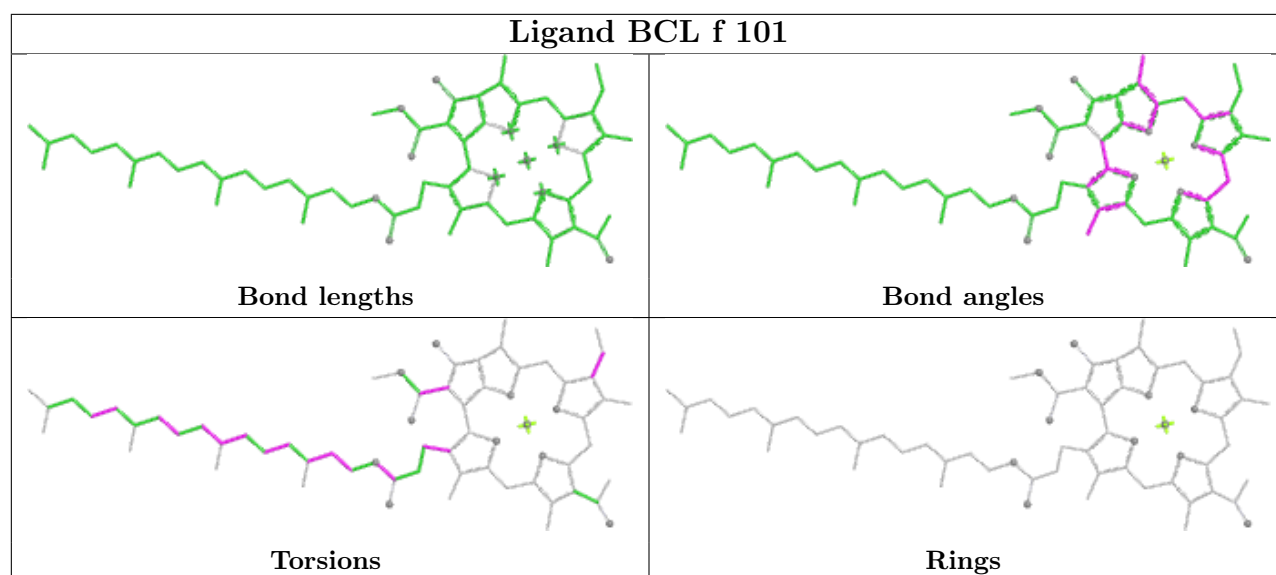


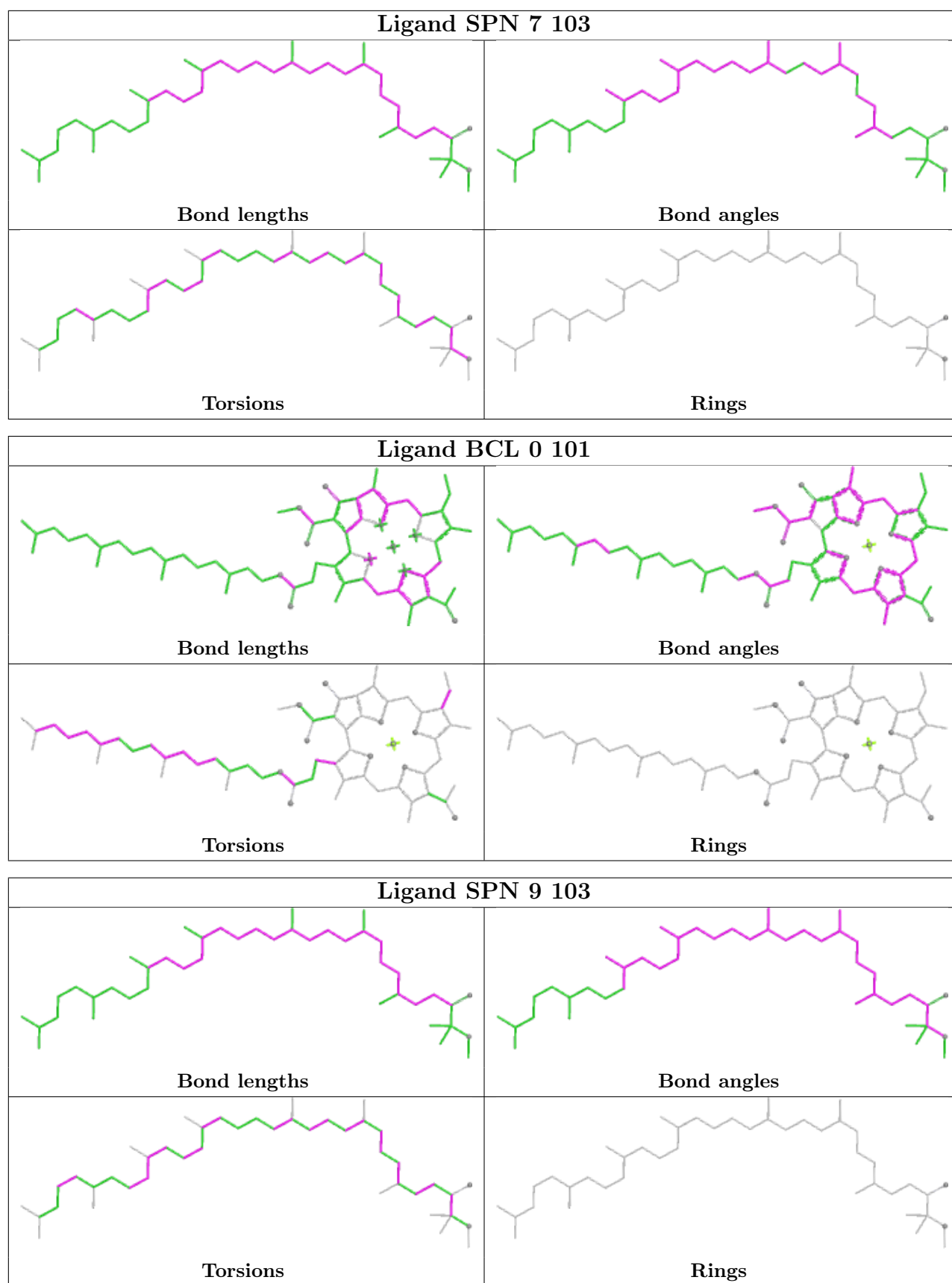


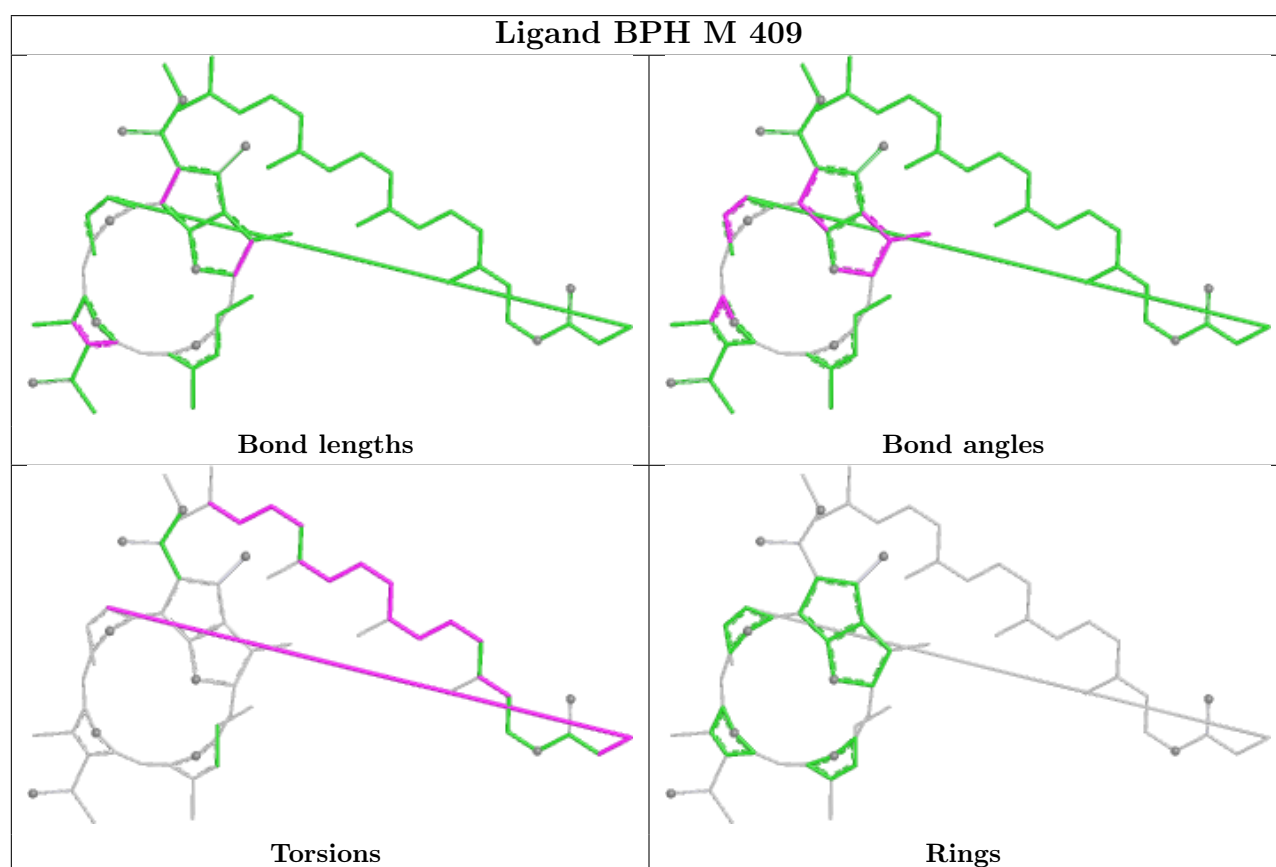
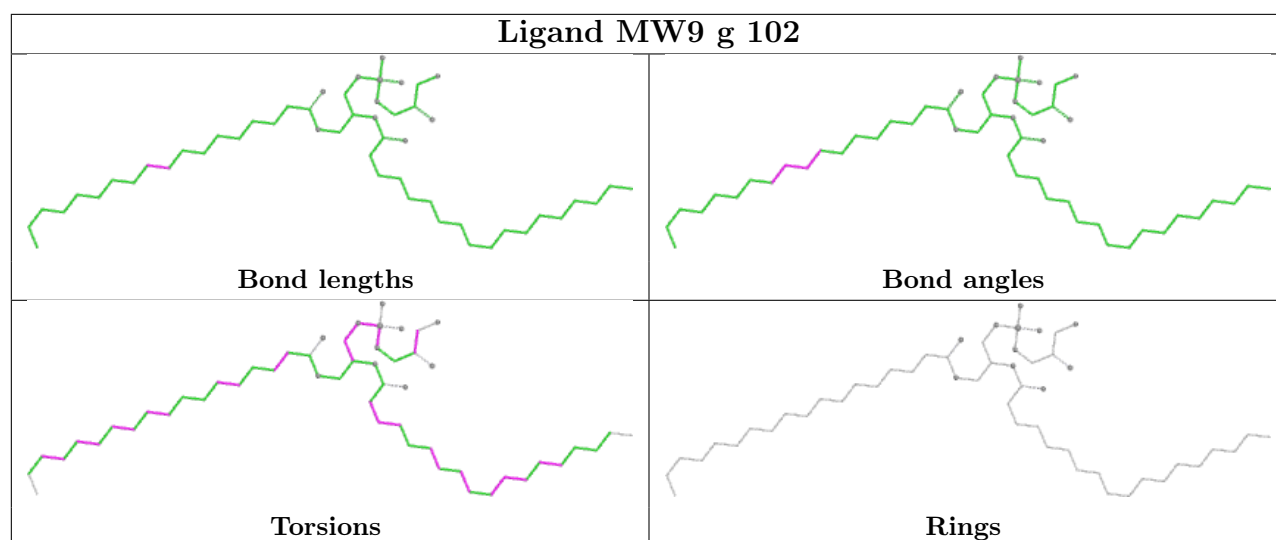


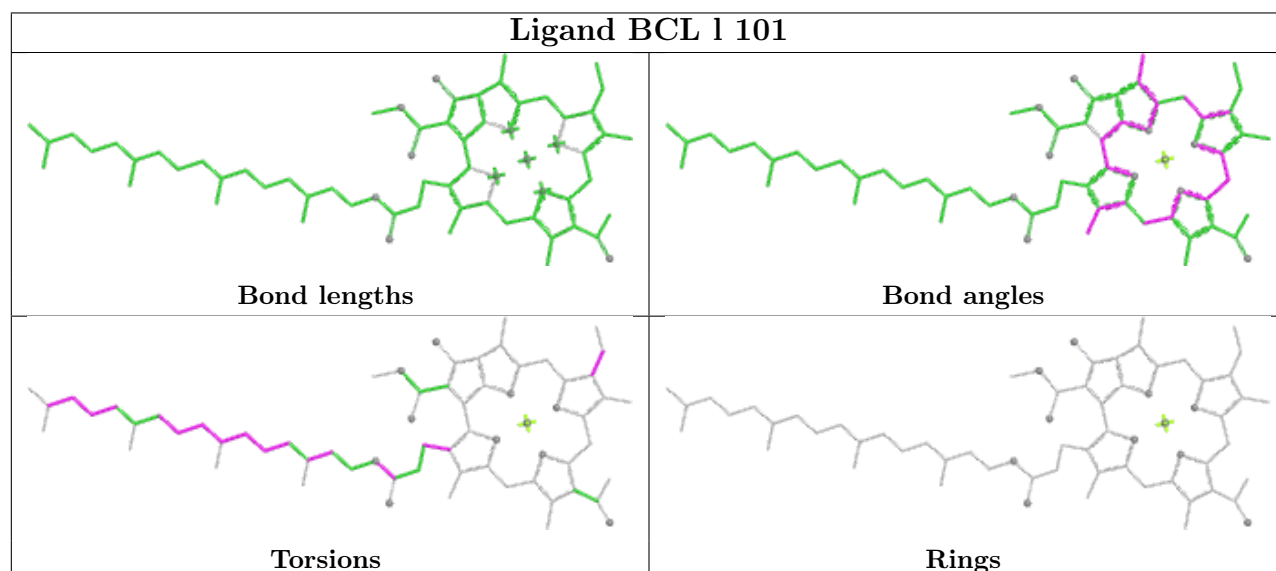
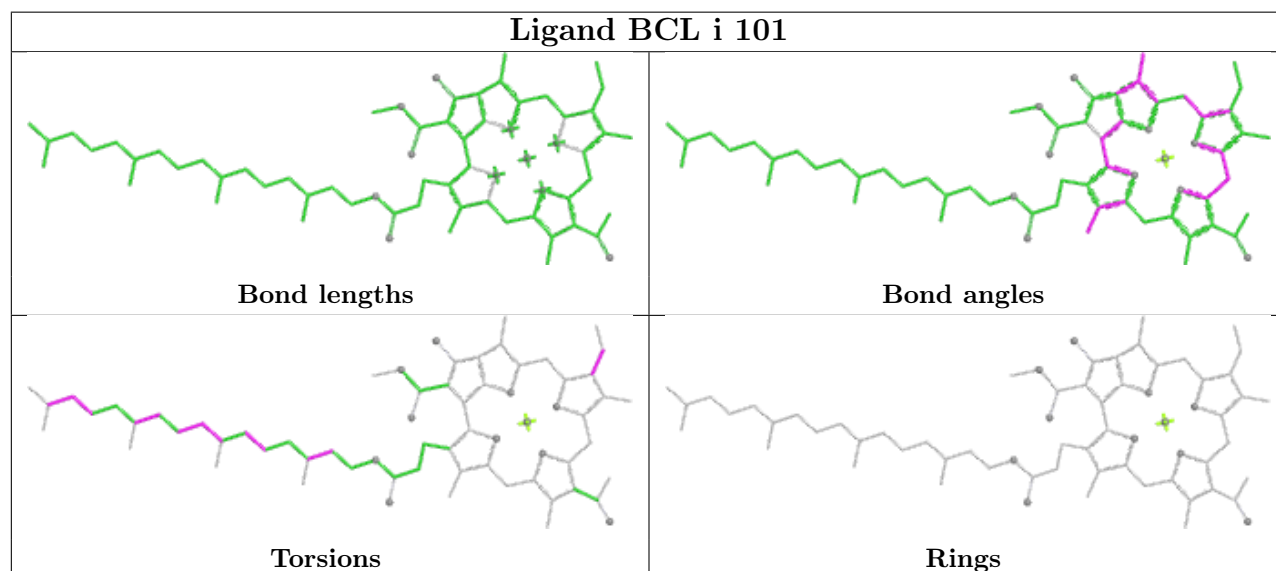
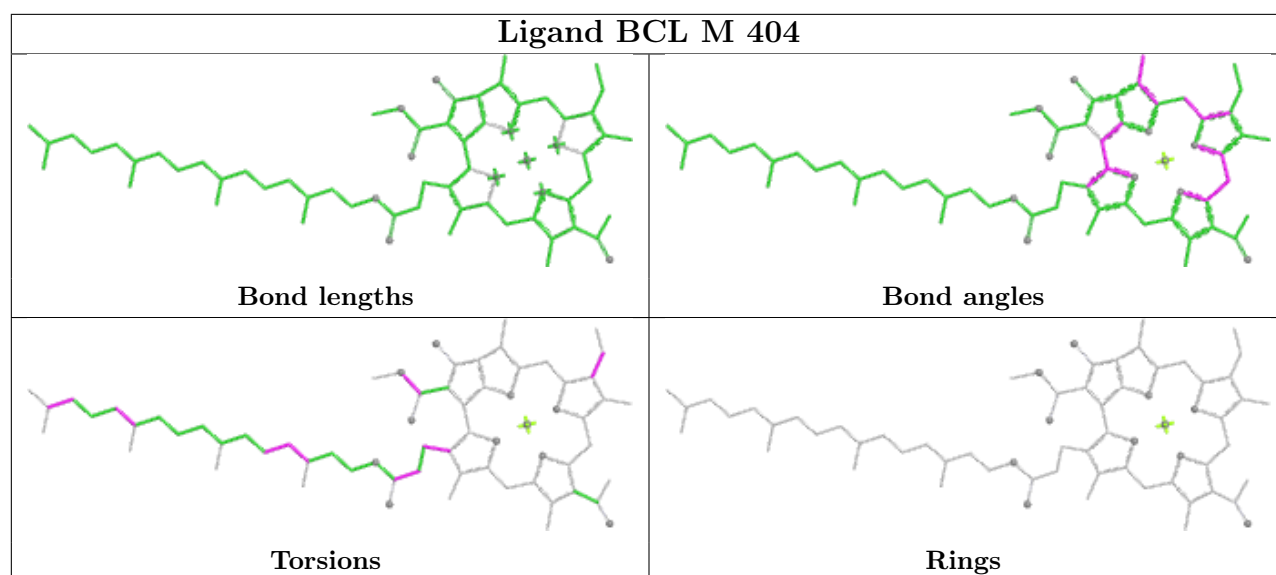


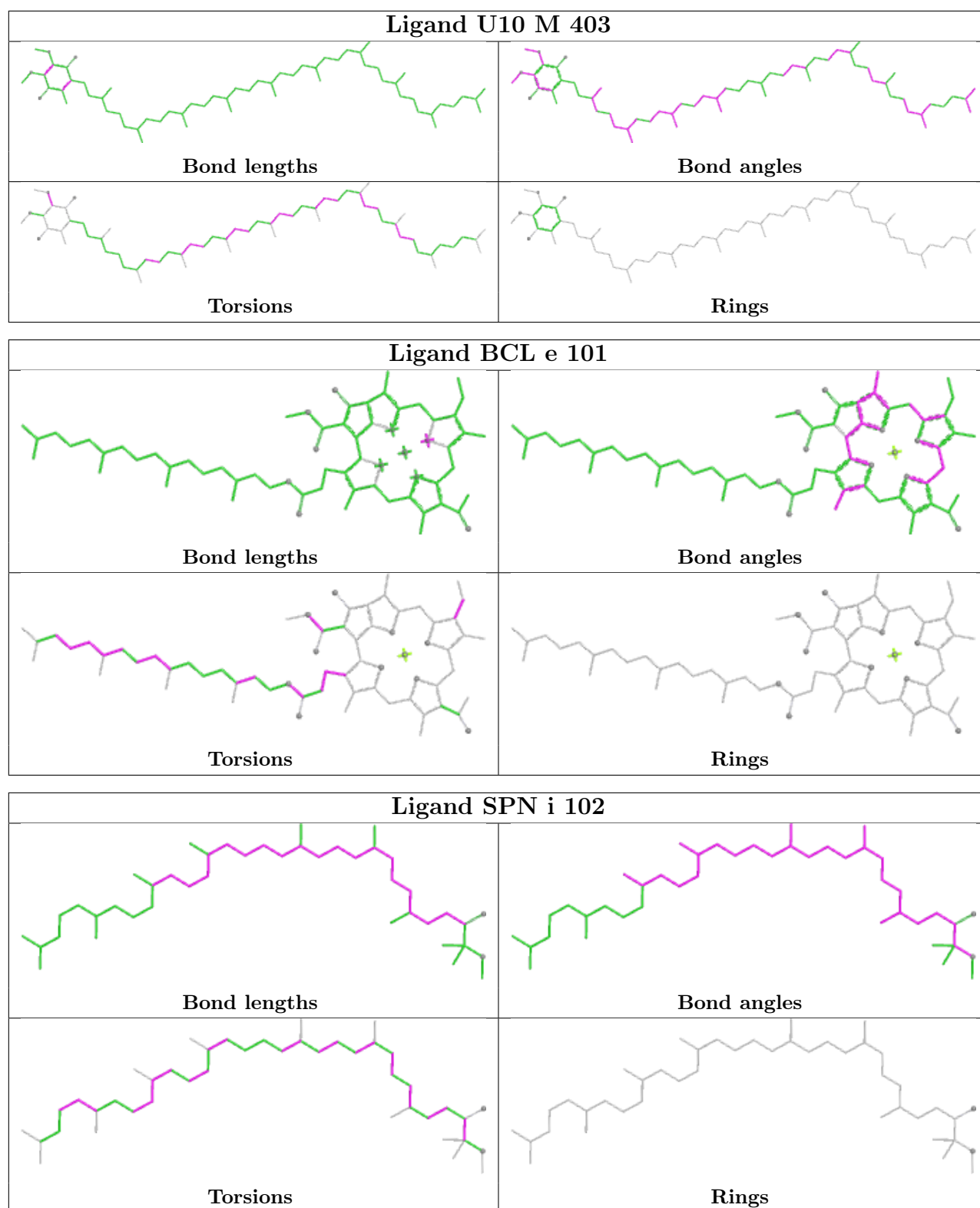


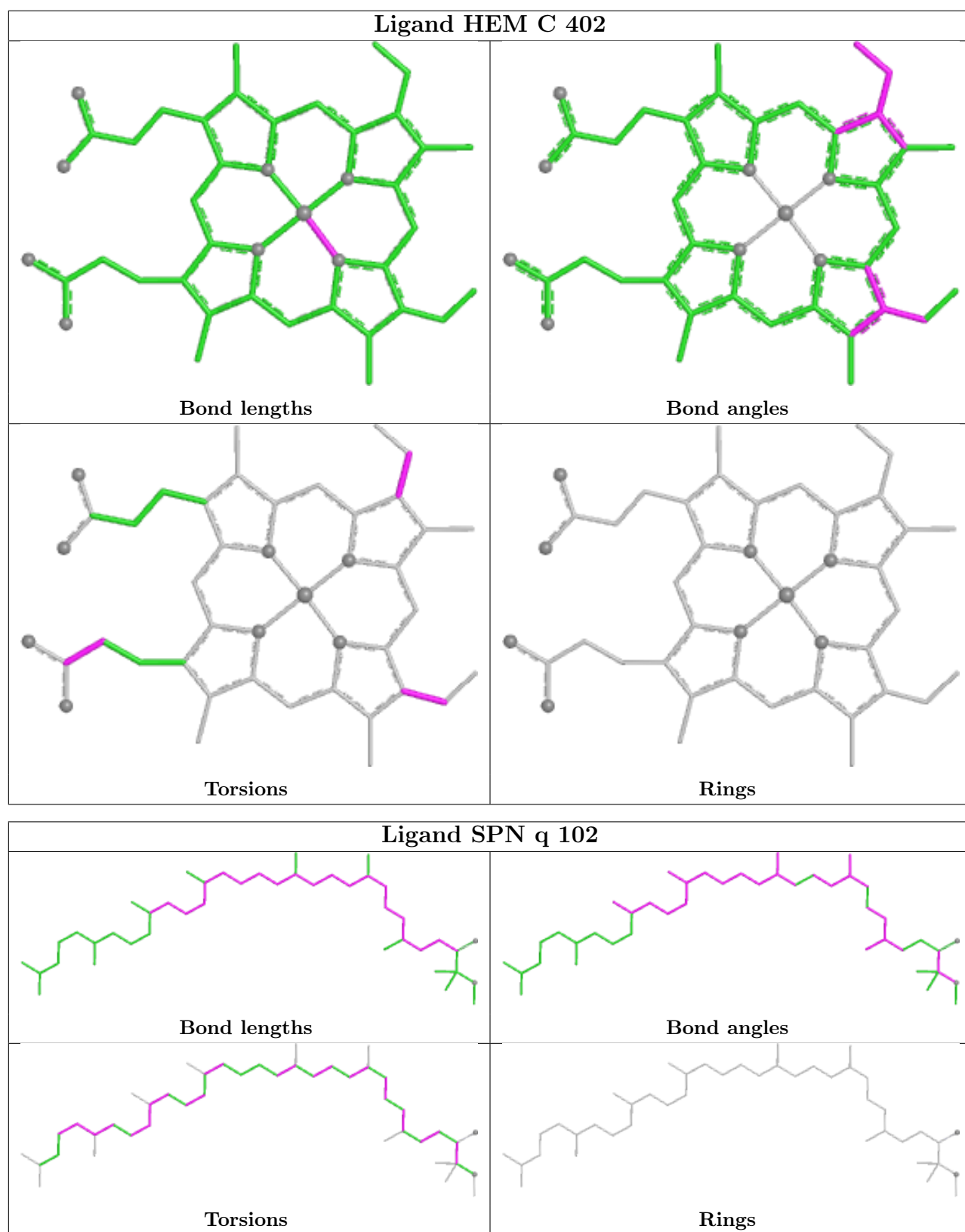


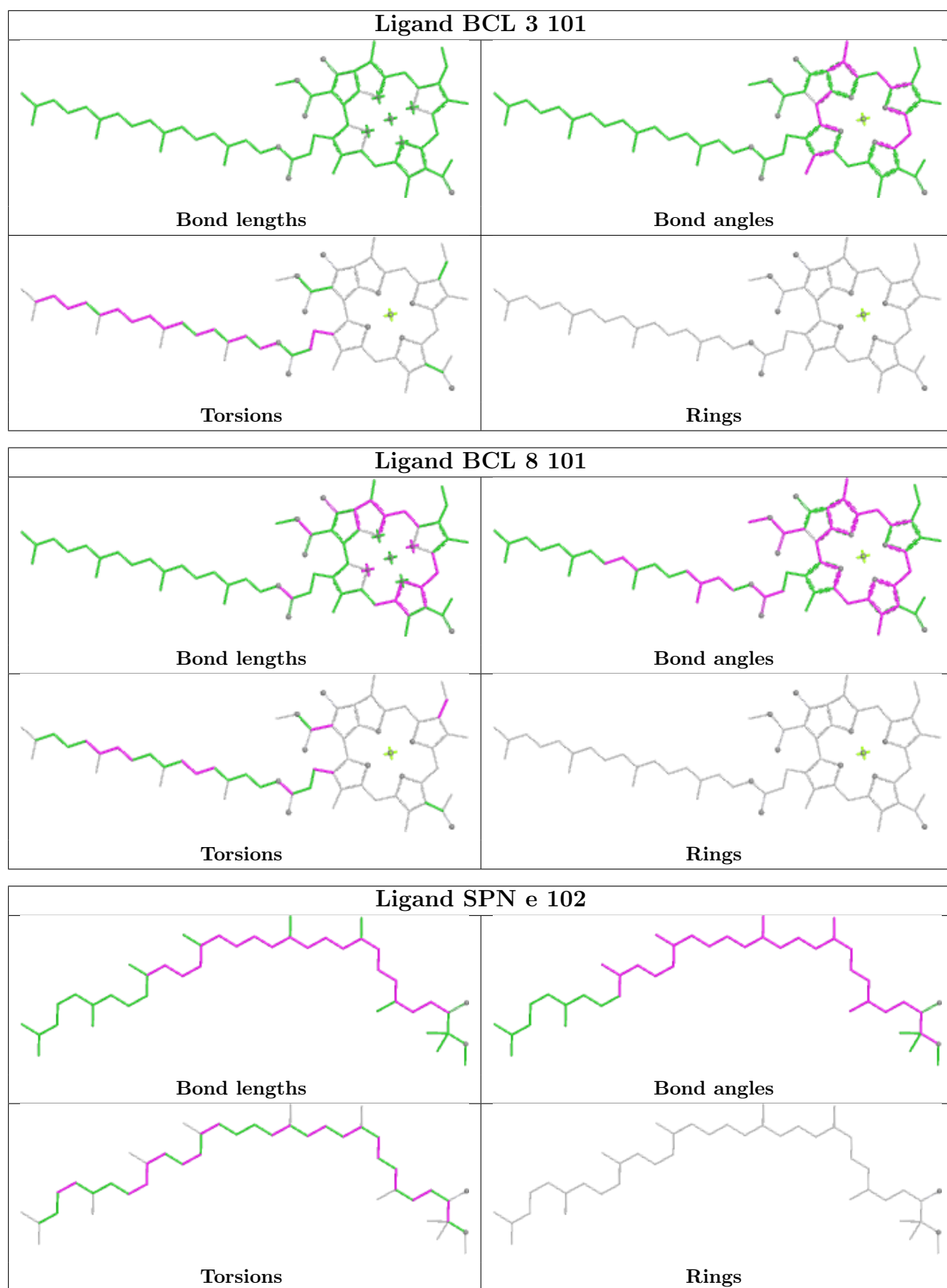


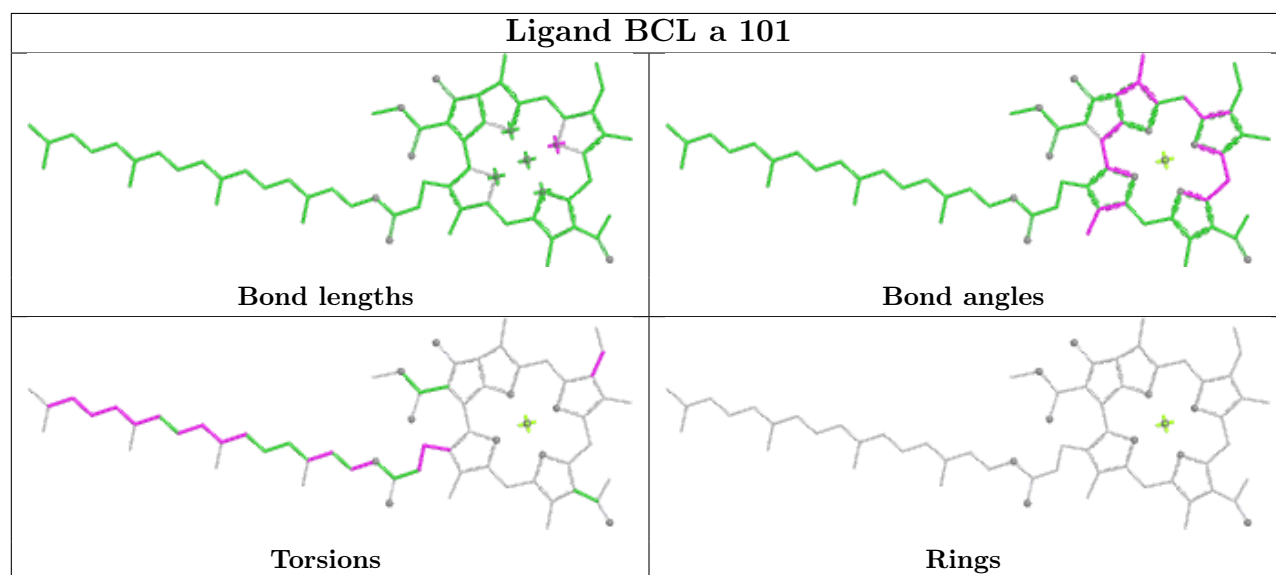
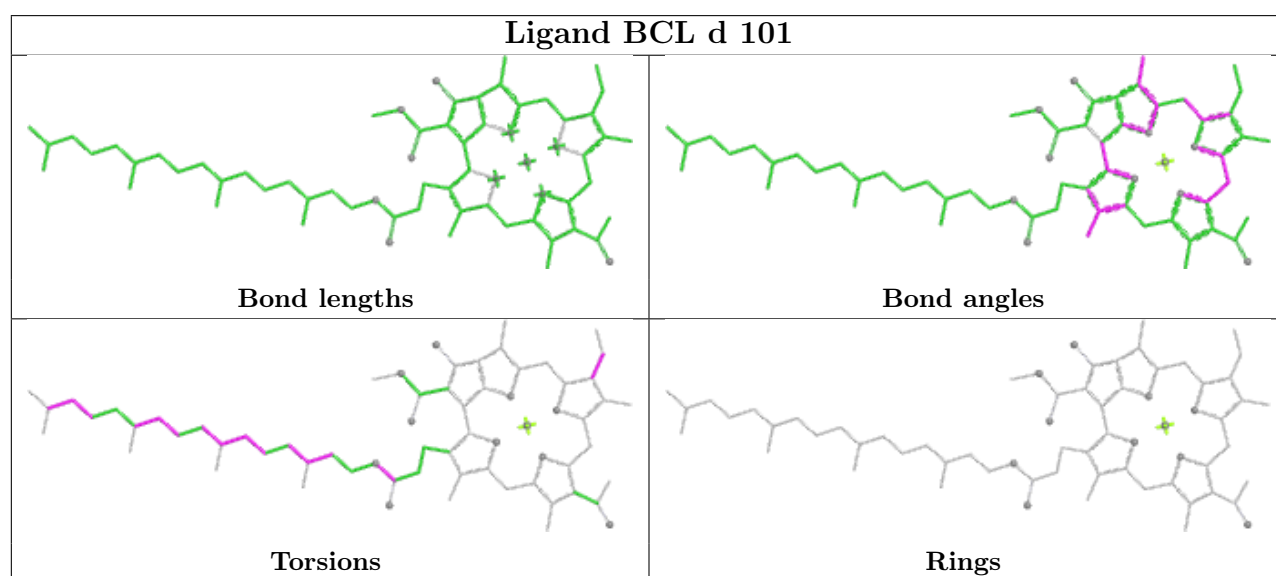
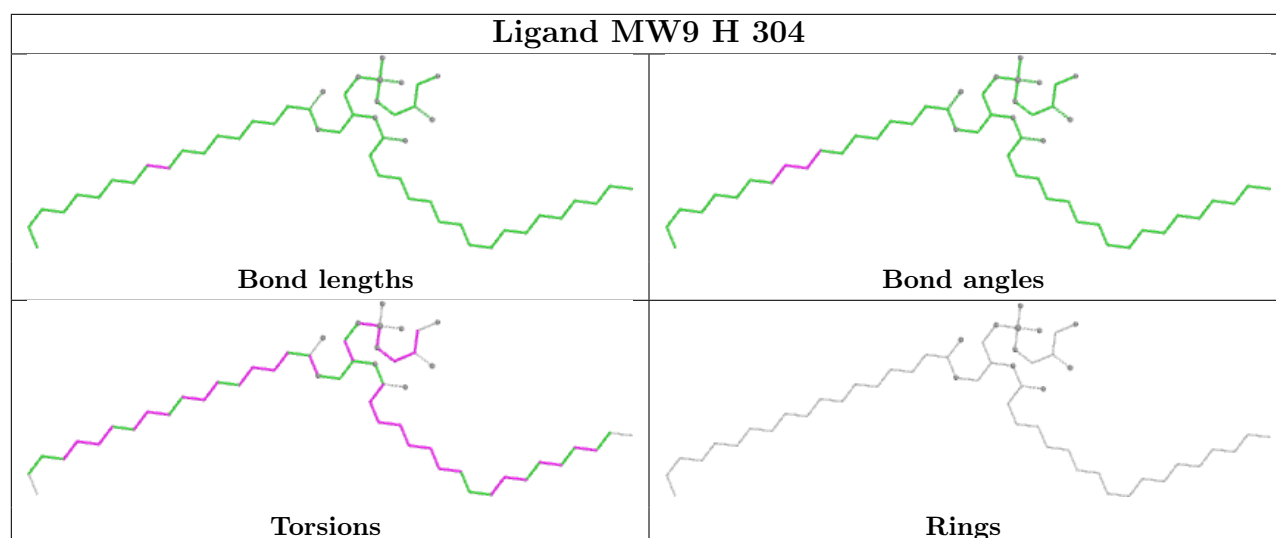


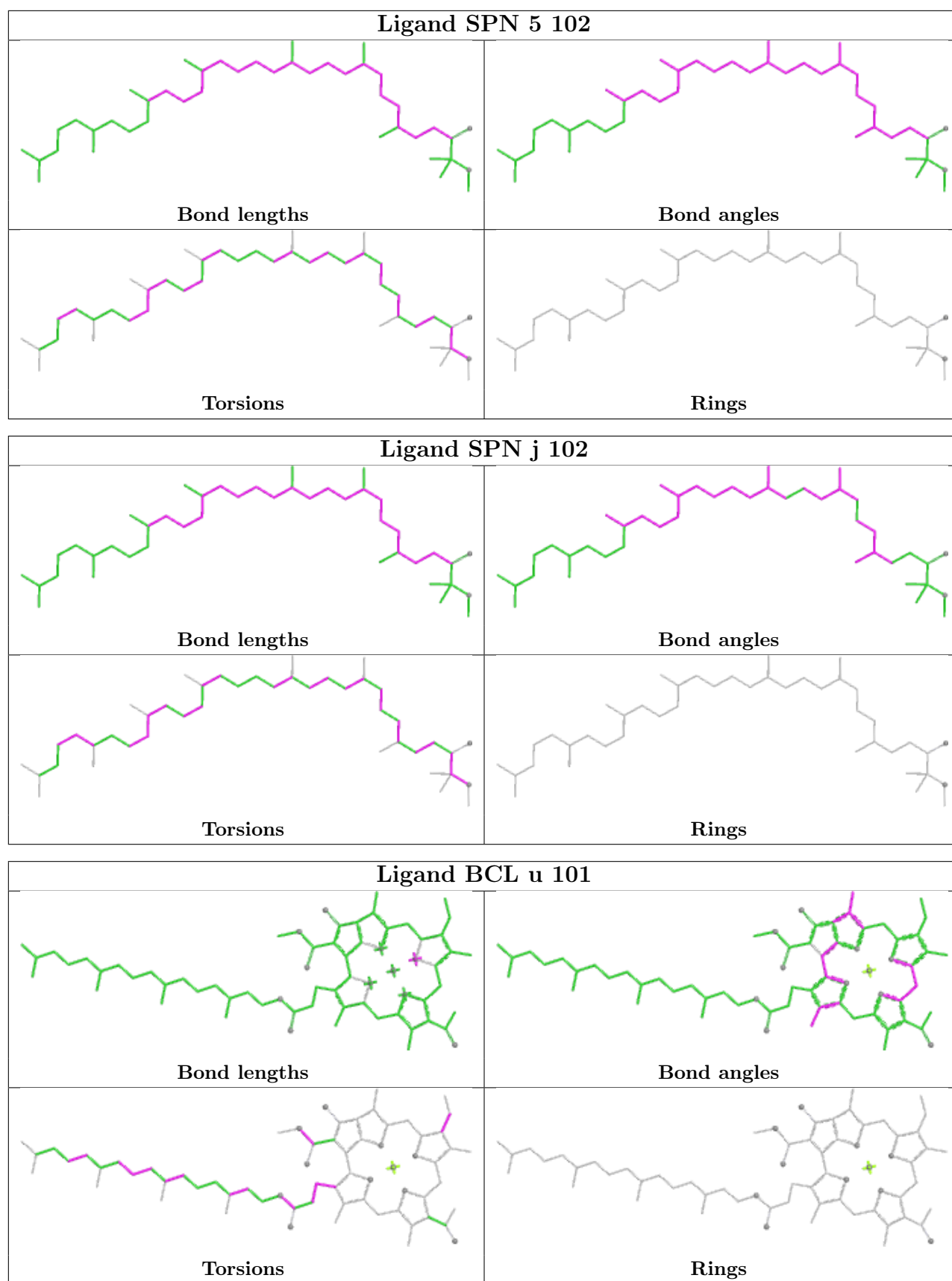




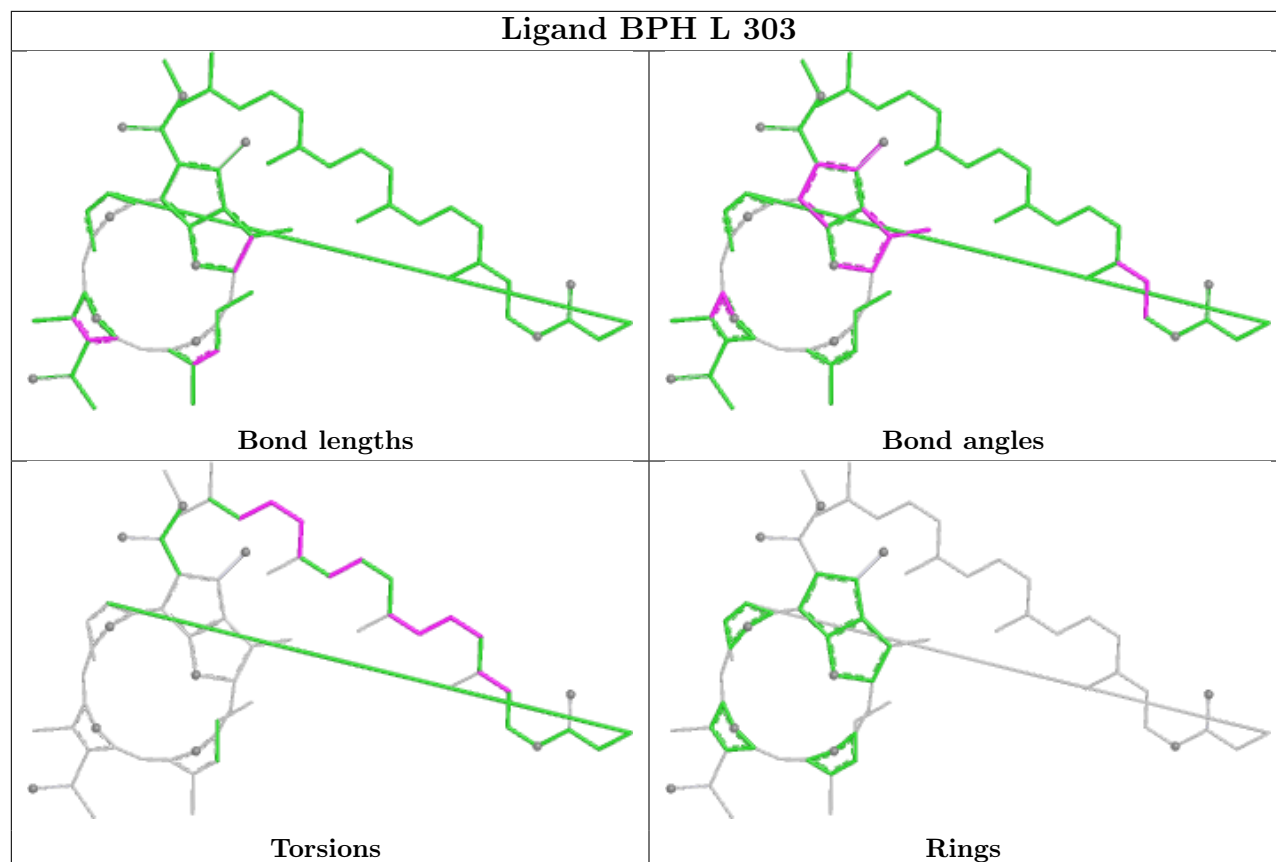




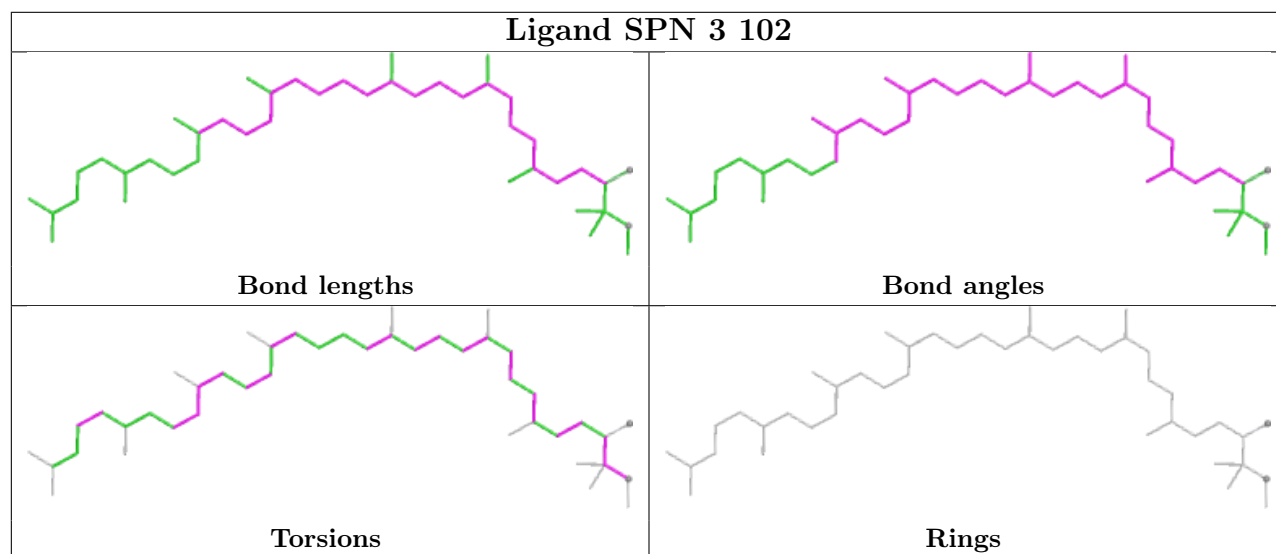


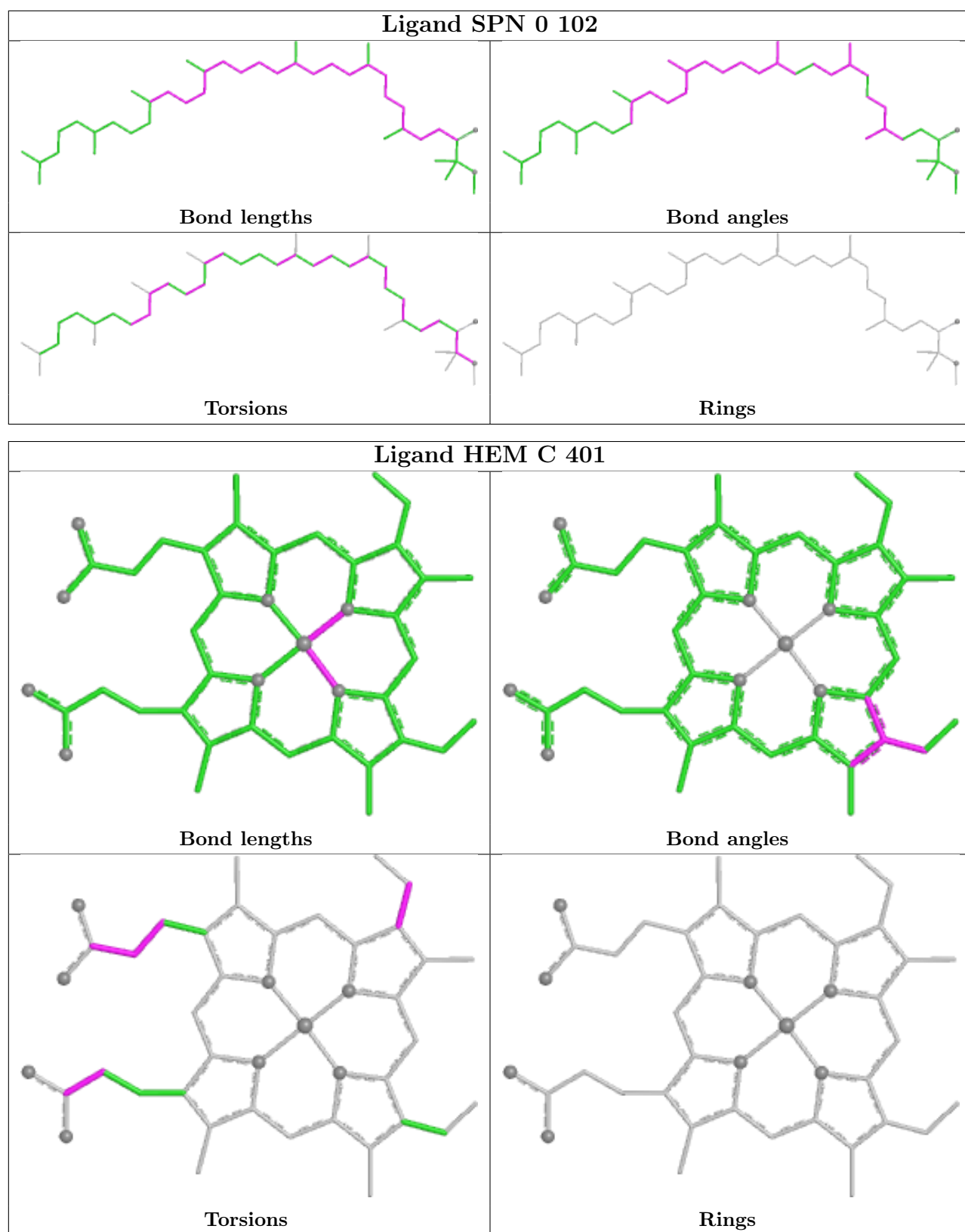


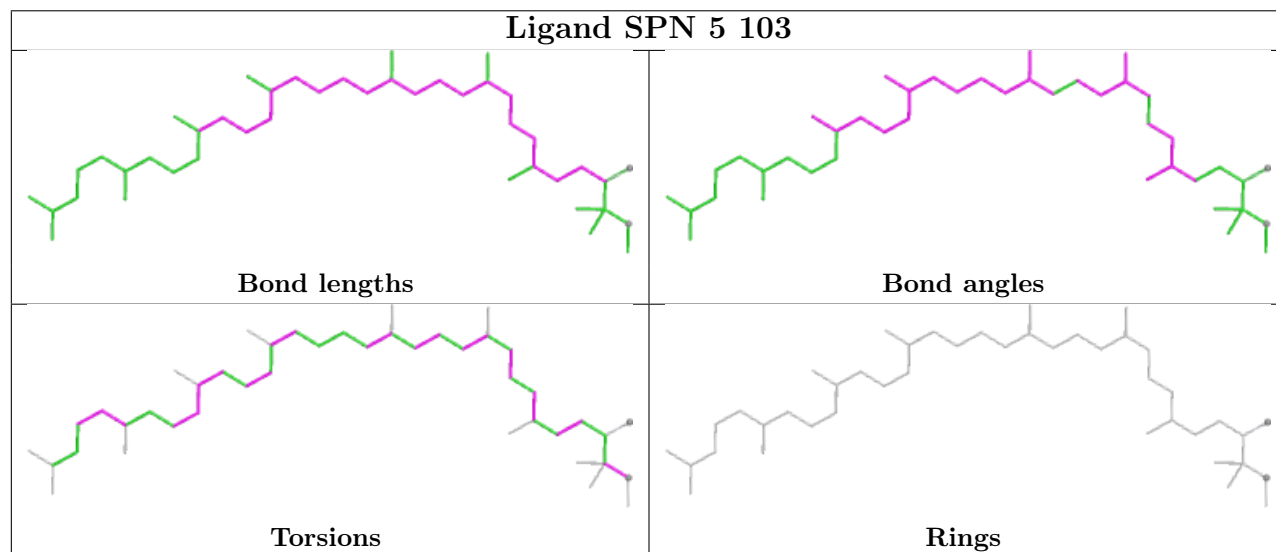
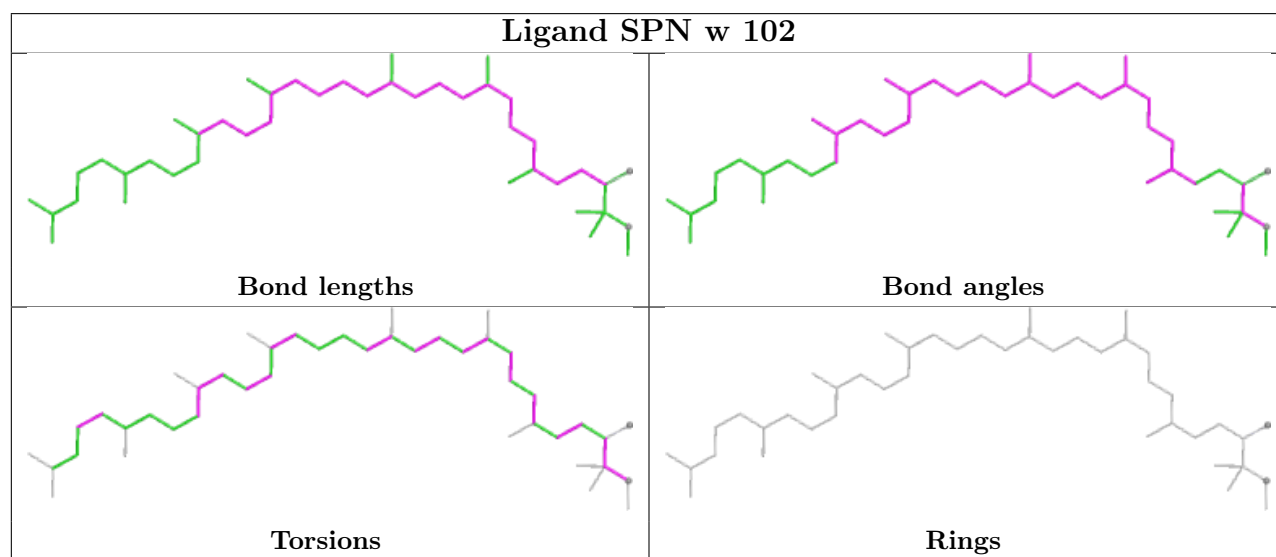
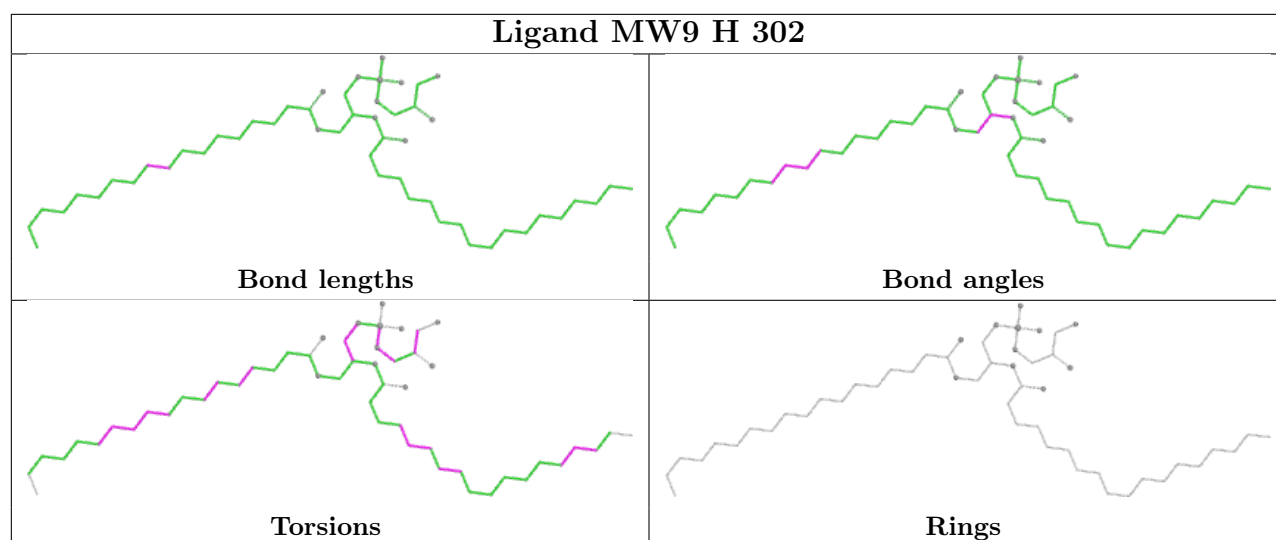
Ligand BPH L 303

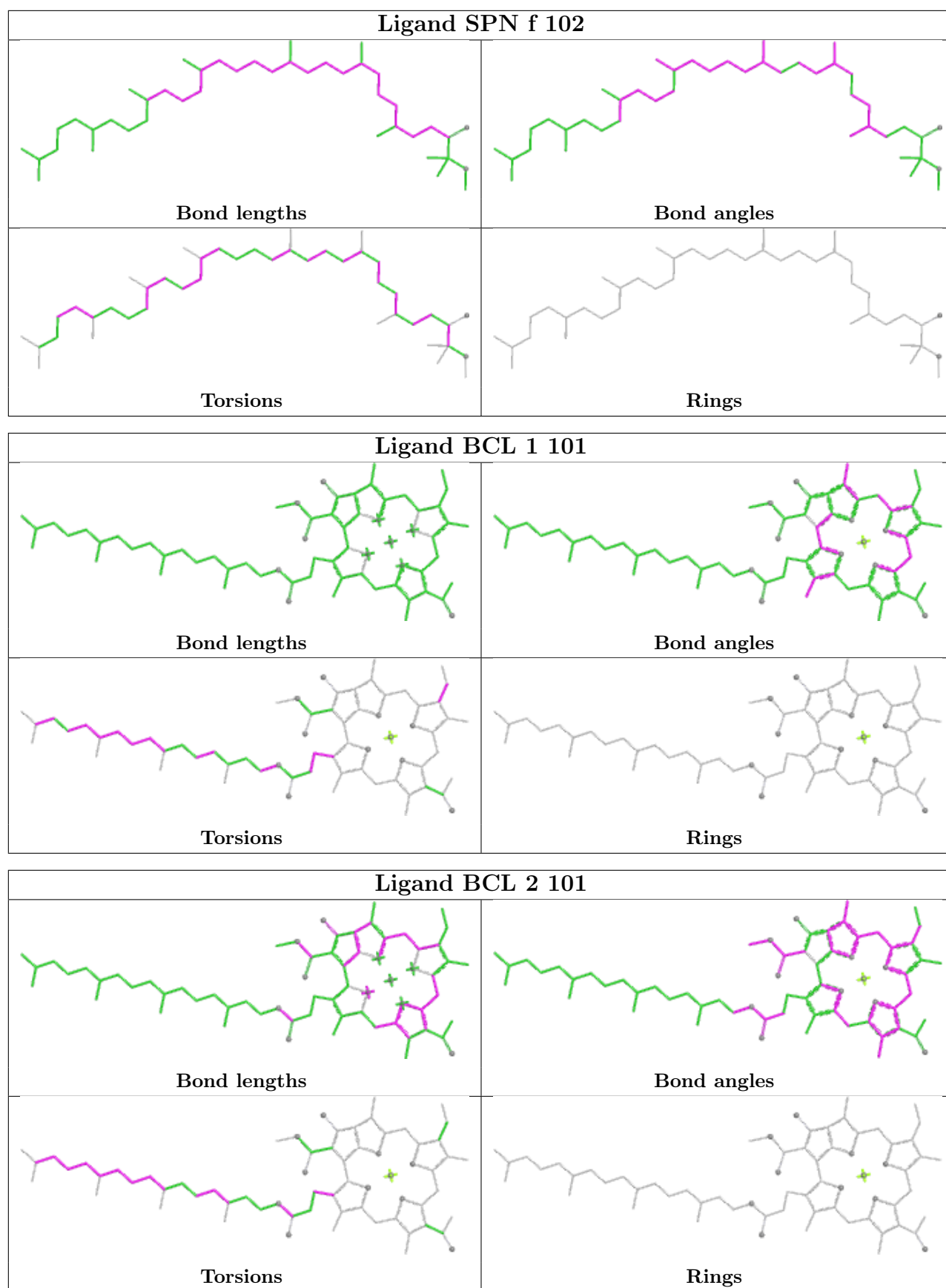


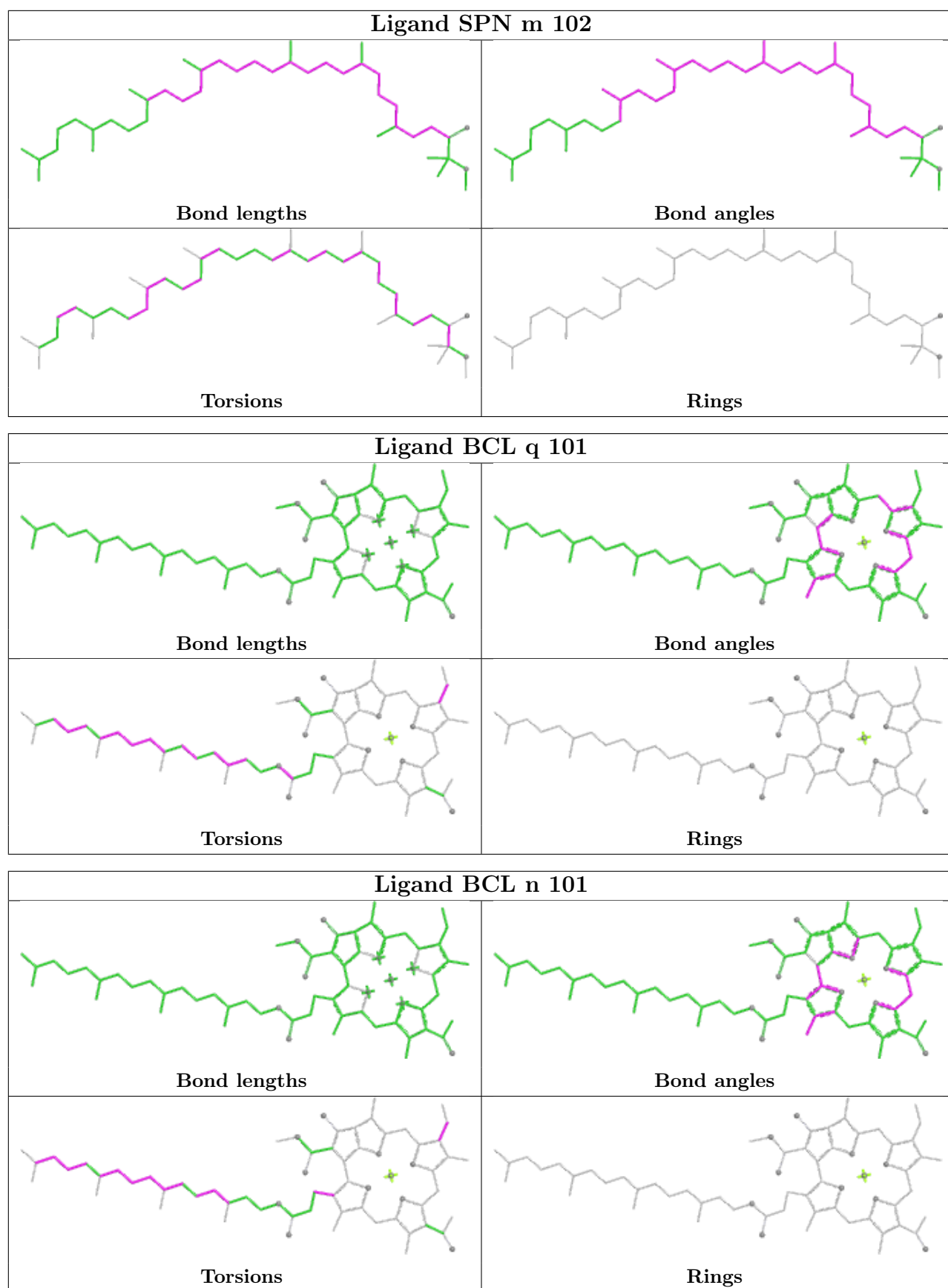
Ligand SPN 3 102

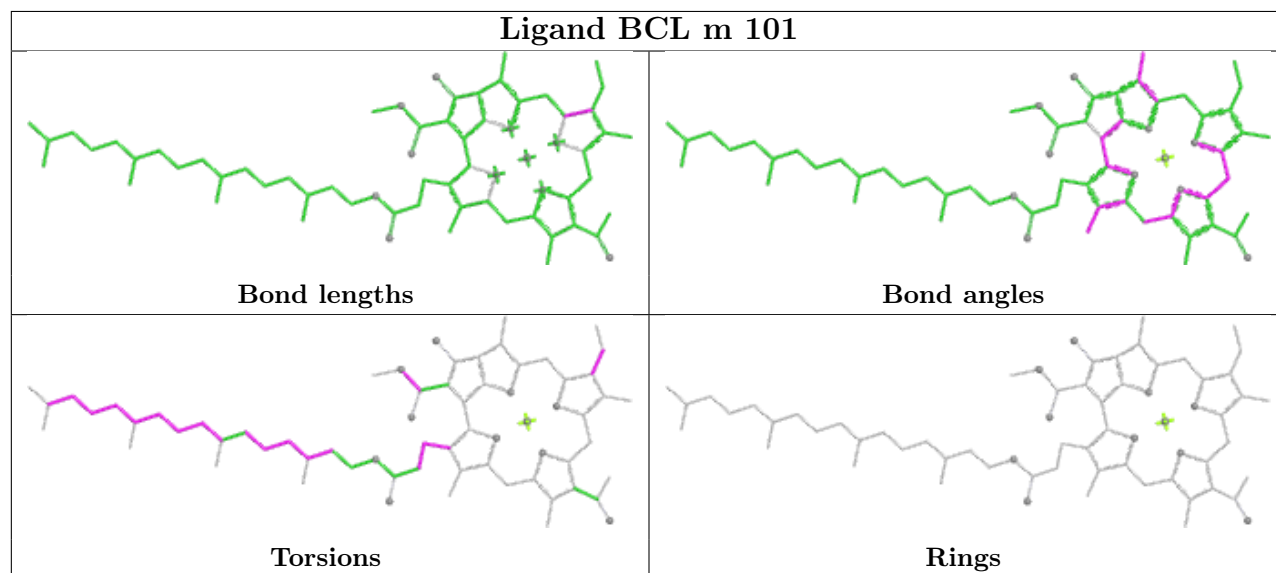
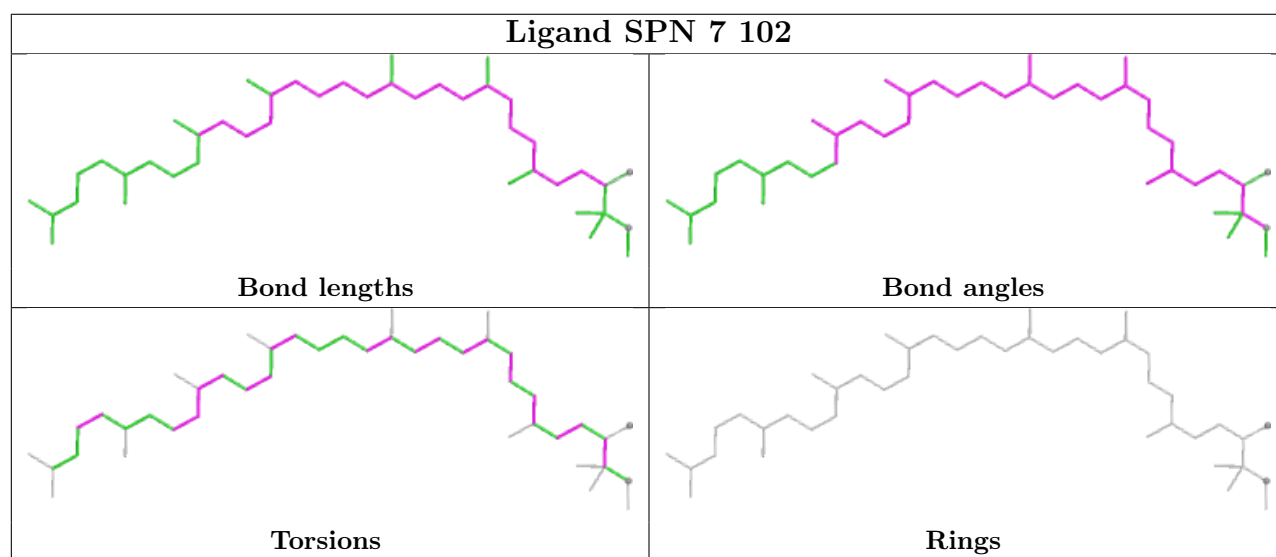
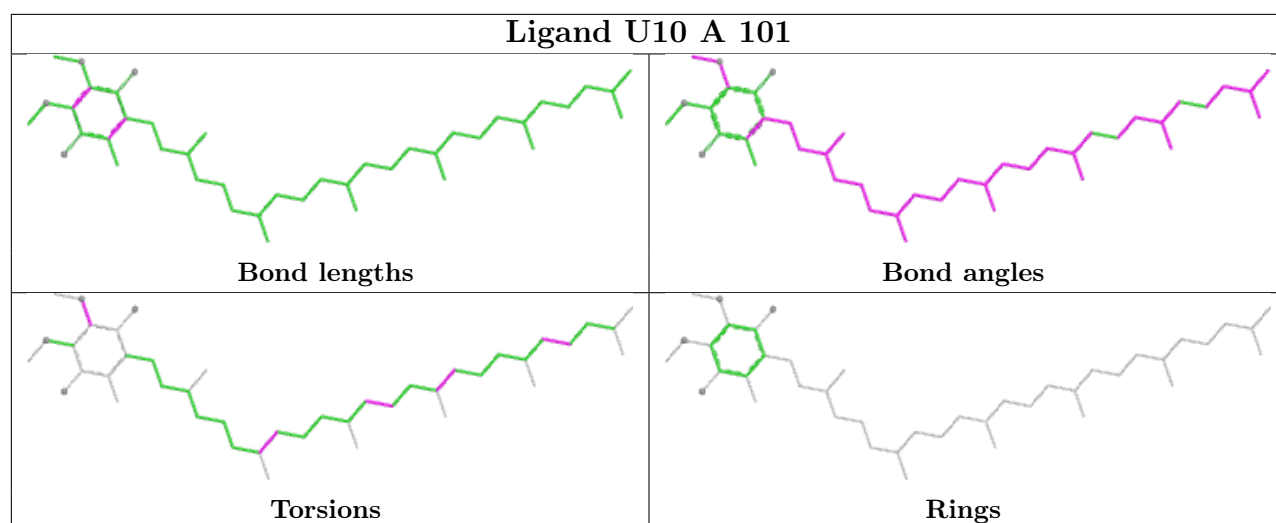


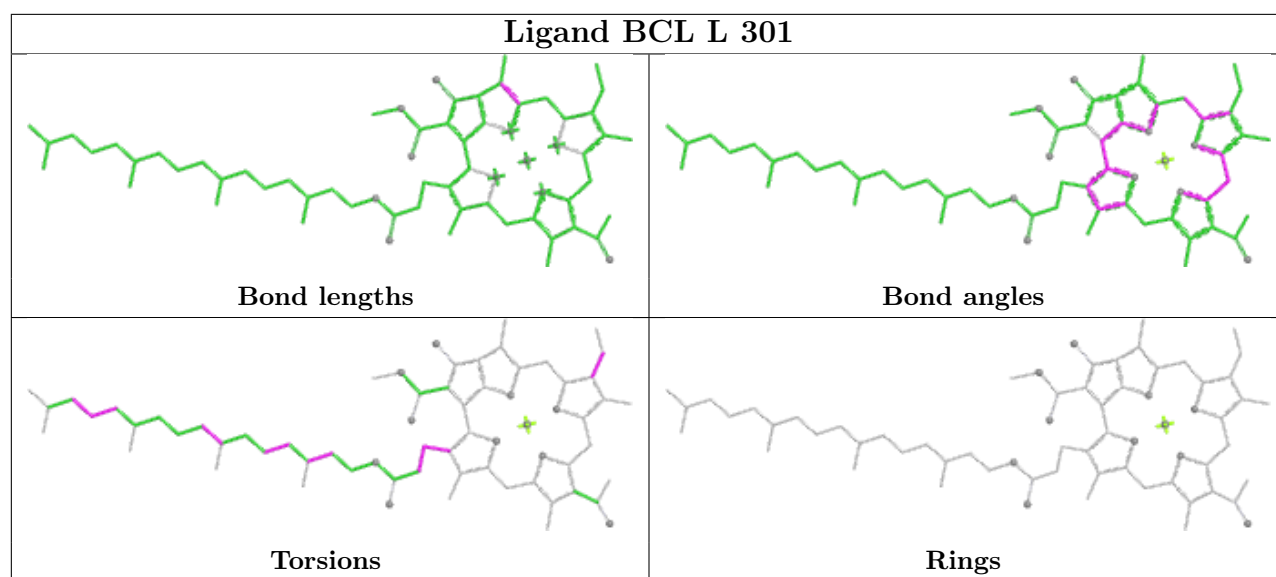












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

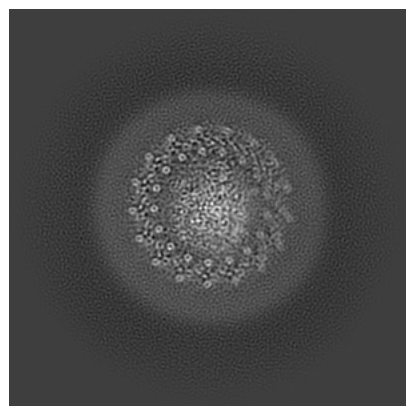
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63379. These allow visual inspection of the internal detail of the map and identification of artifacts.

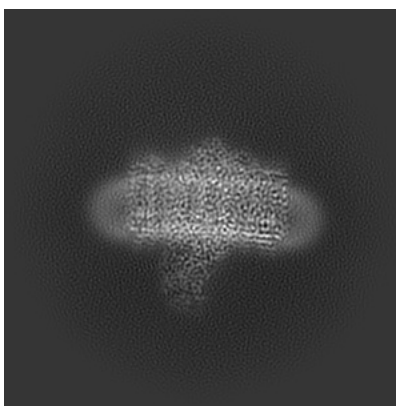
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

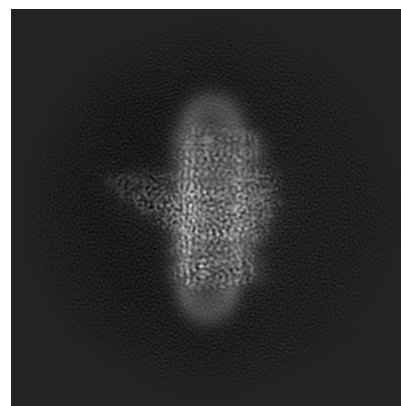
6.1.1 Primary map



X

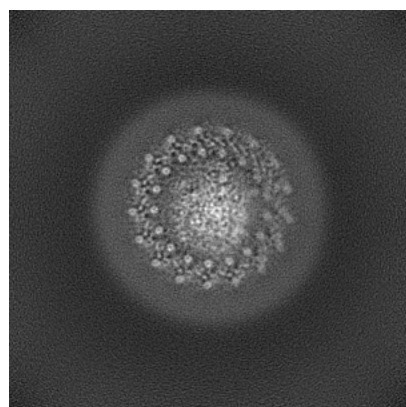


Y

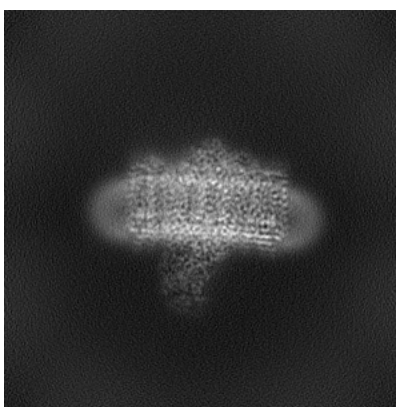


Z

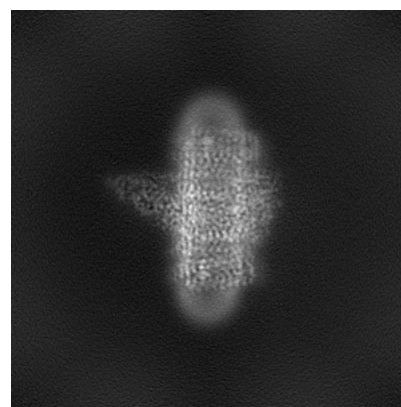
6.1.2 Raw map



X



Y

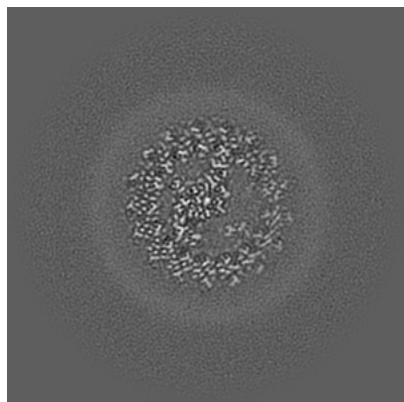


Z

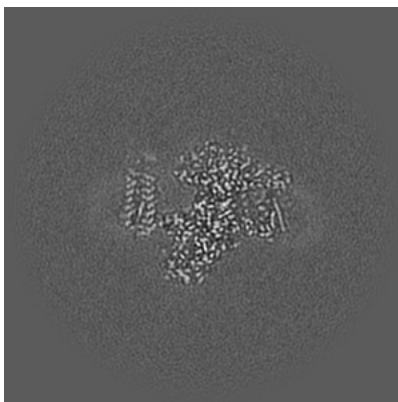
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

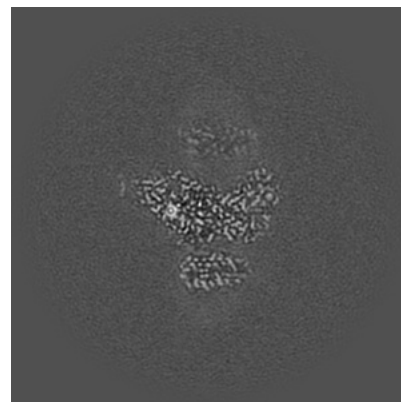
6.2.1 Primary map



X Index: 150

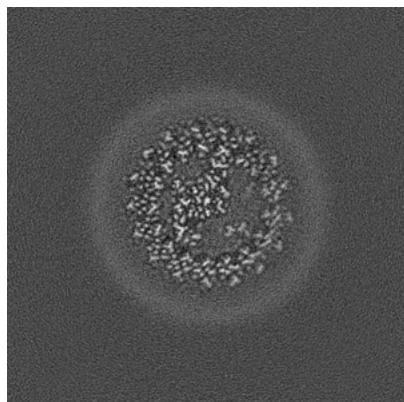


Y Index: 150

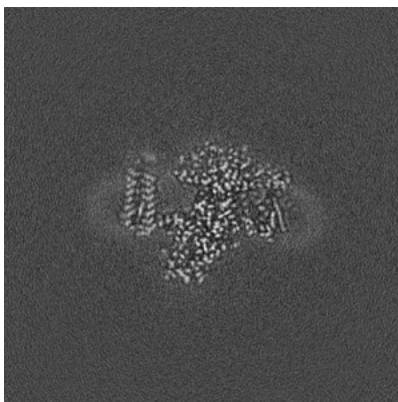


Z Index: 150

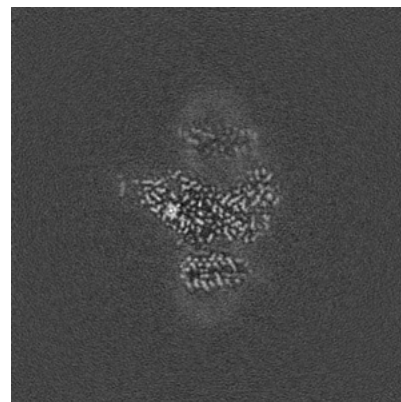
6.2.2 Raw map



X Index: 150



Y Index: 150

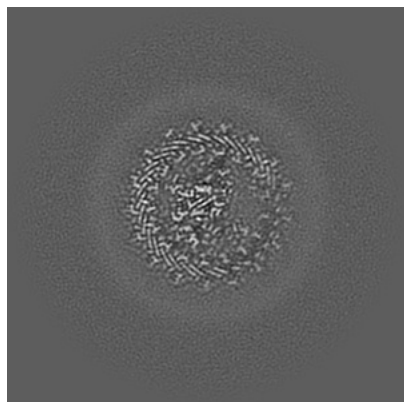


Z Index: 150

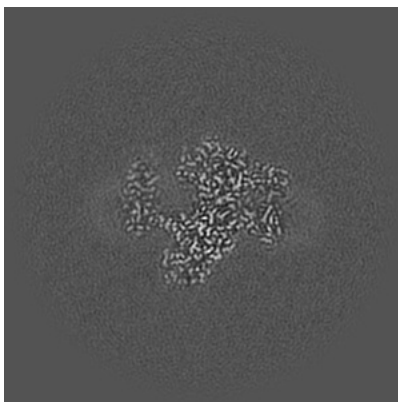
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

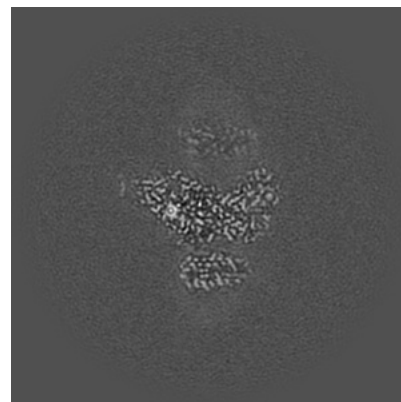
6.3.1 Primary map



X Index: 143

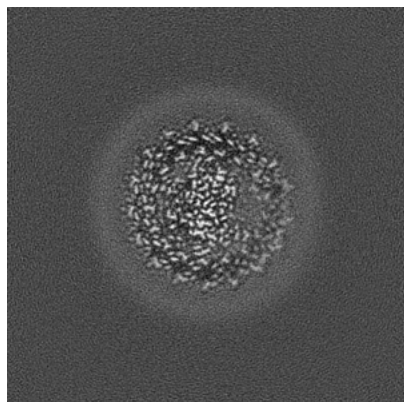


Y Index: 152

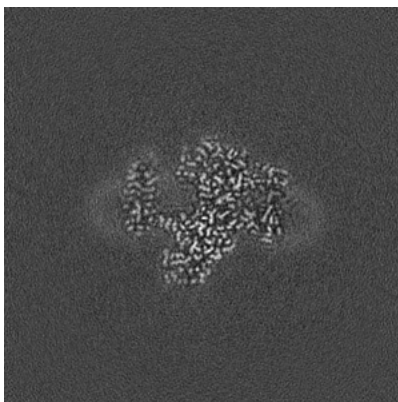


Z Index: 150

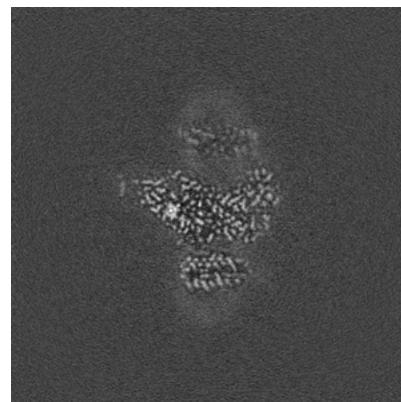
6.3.2 Raw map



X Index: 137



Y Index: 152

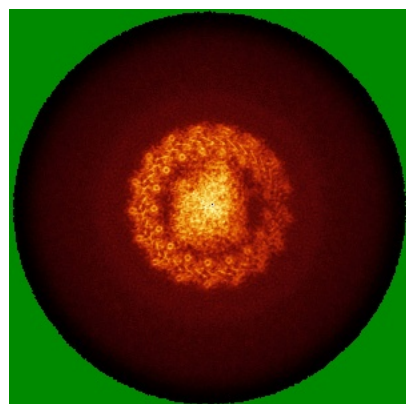


Z Index: 150

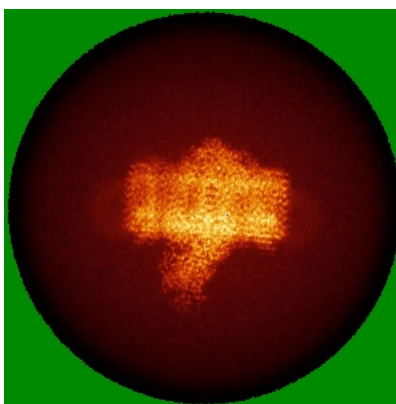
The images above show the largest variance slices of the map in three orthogonal directions.

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

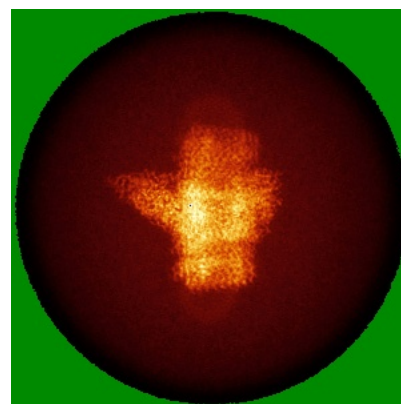
6.4.1 Primary map



X

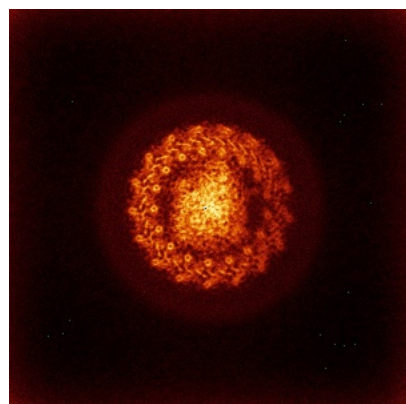


Y

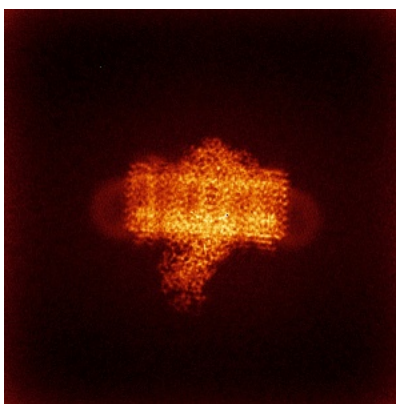


Z

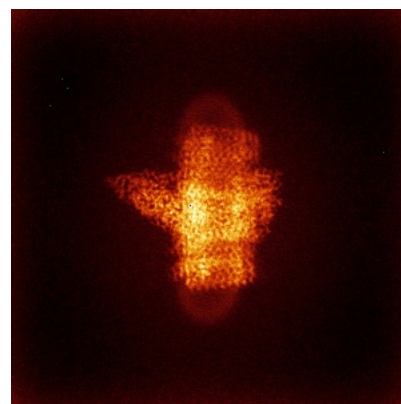
6.4.2 Raw map



X



Y

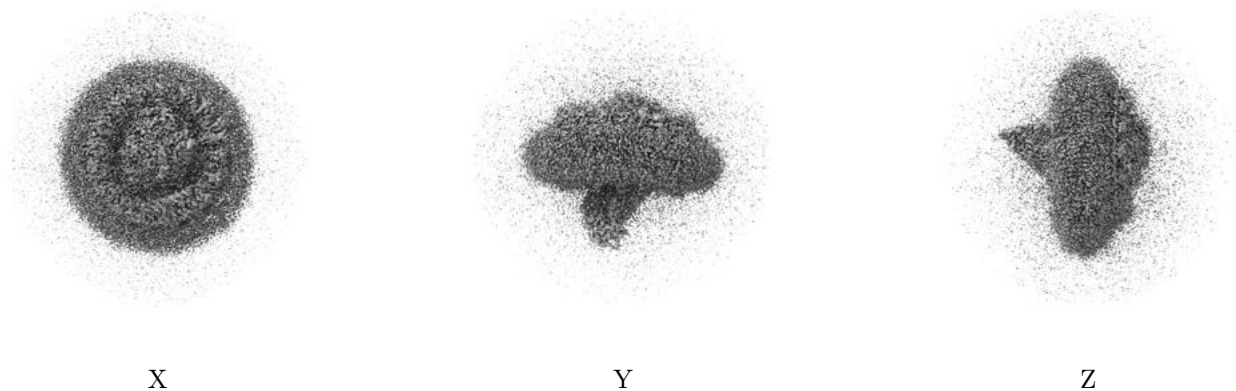


Z

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

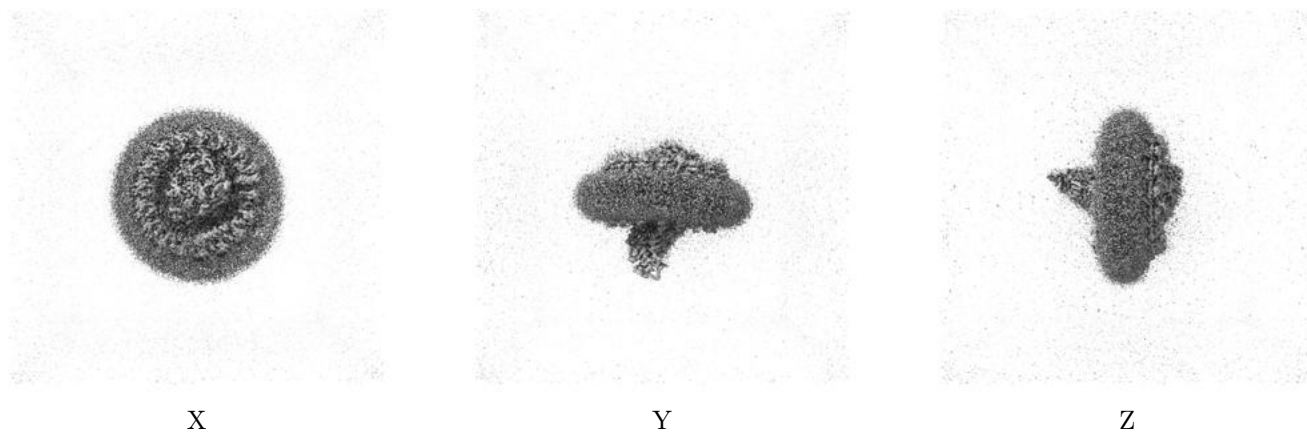
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

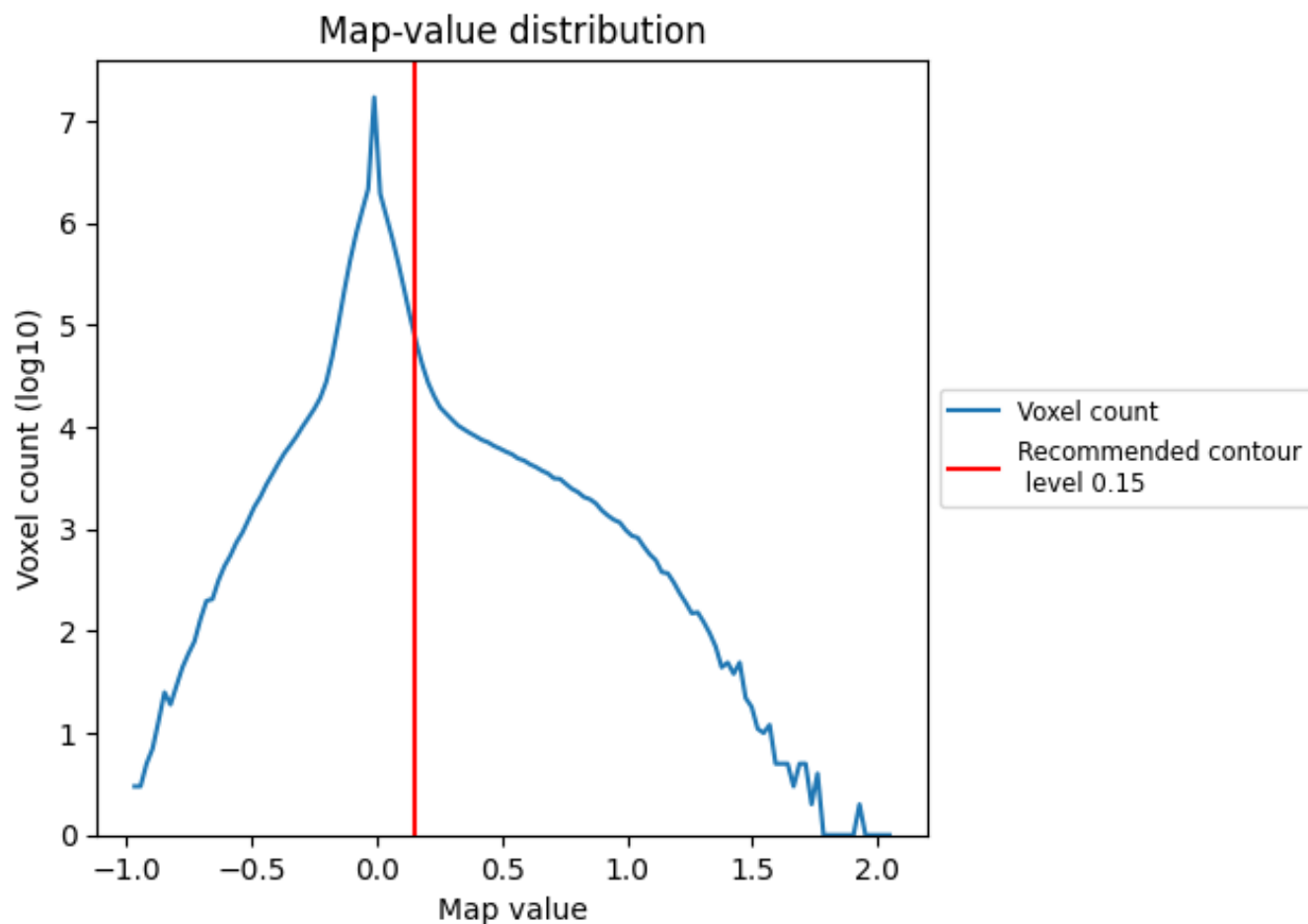
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

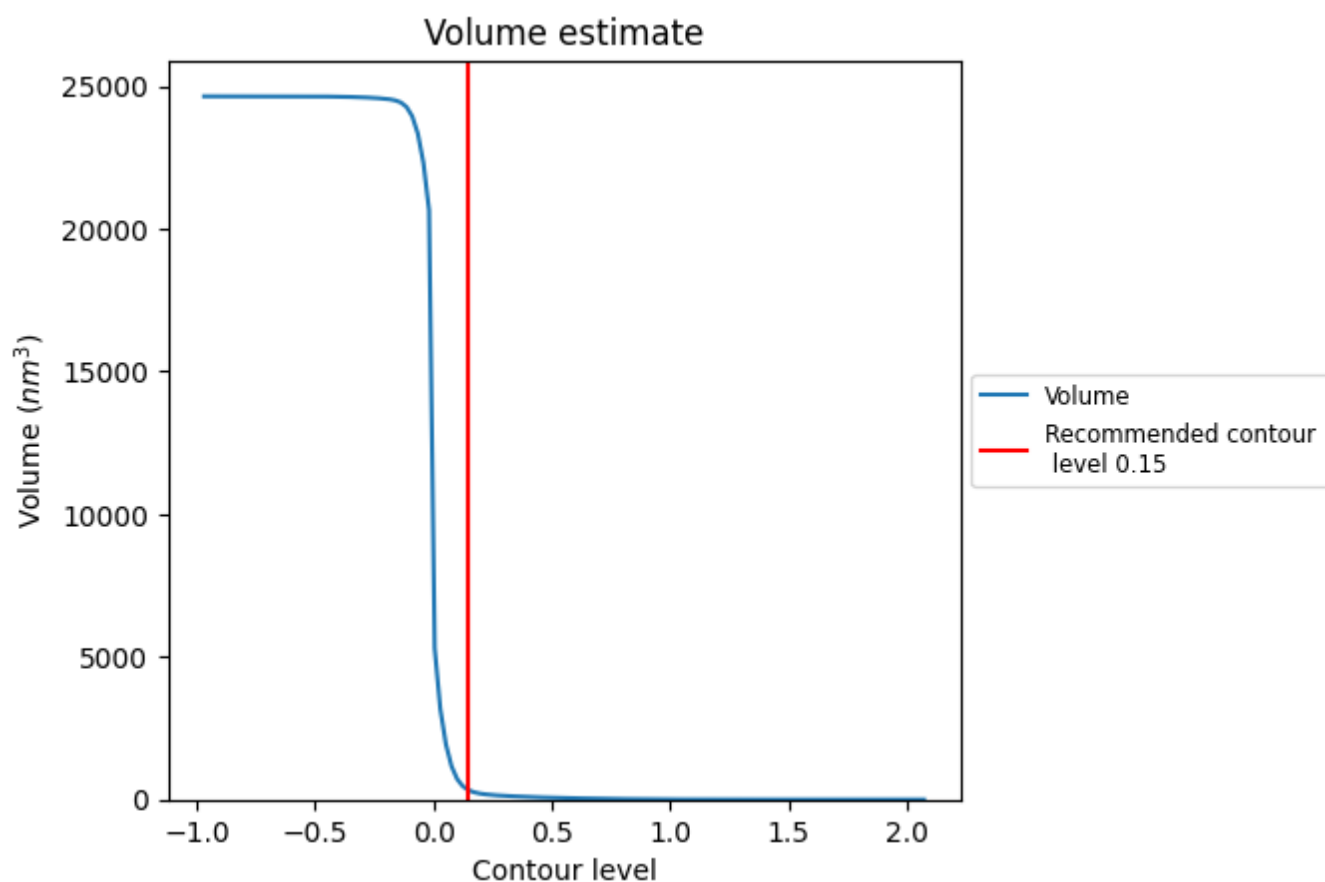
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

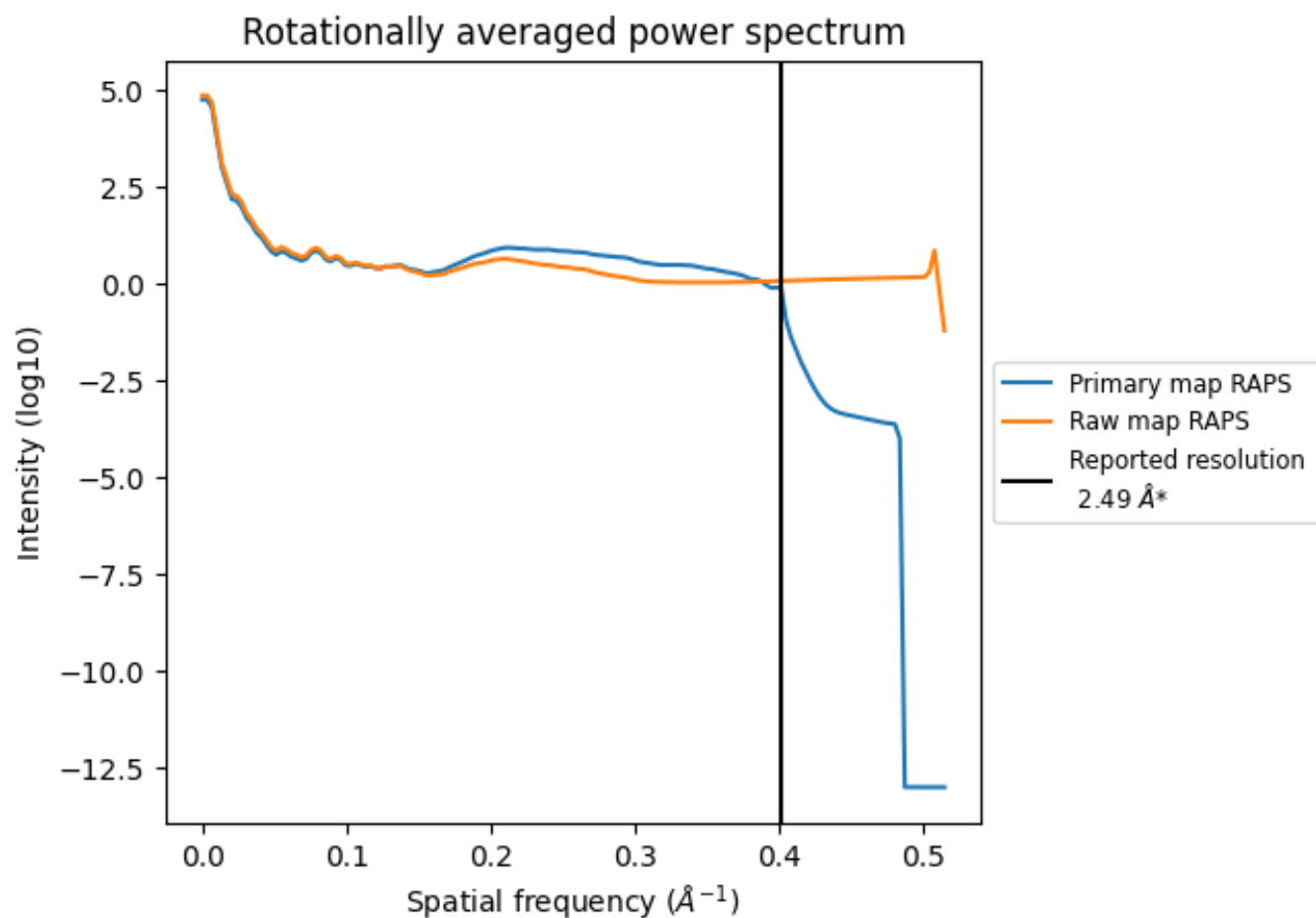
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 326 nm³; this corresponds to an approximate mass of 295 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

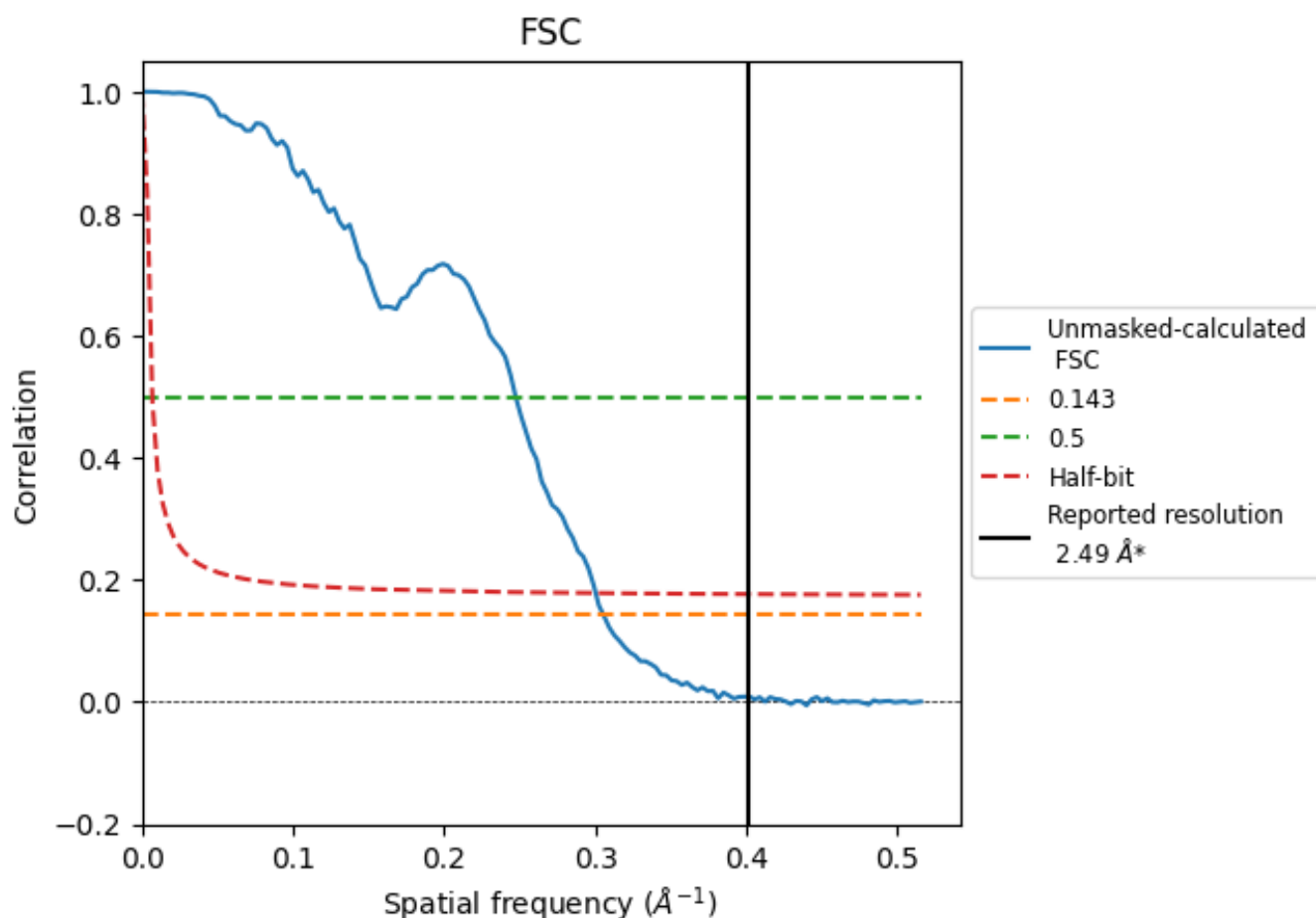


*Reported resolution corresponds to spatial frequency of 0.402 $\text{\AA}^{-1}$

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 0.402 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

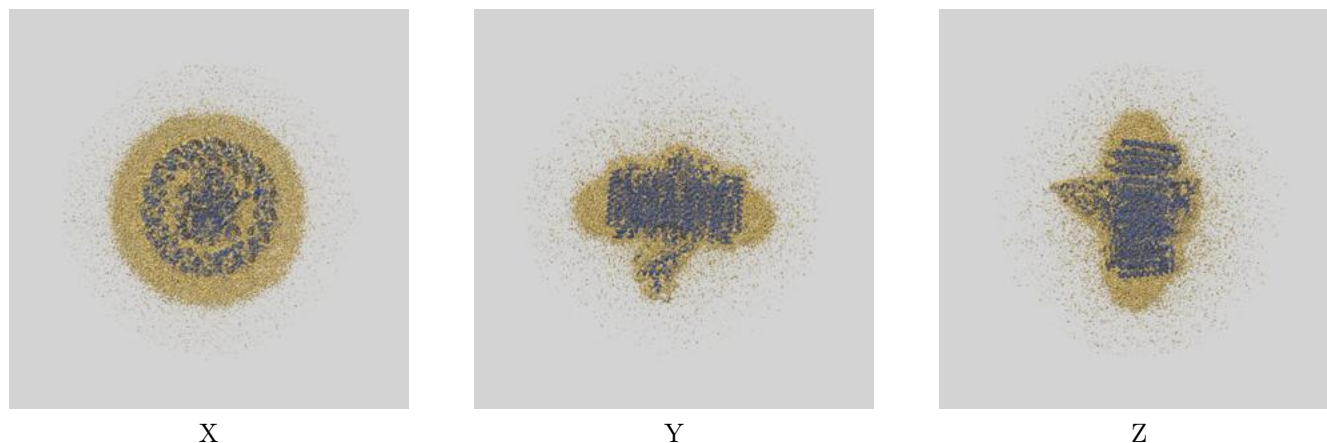
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.27	4.04	3.33

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

9 Map-model fit [i](#)

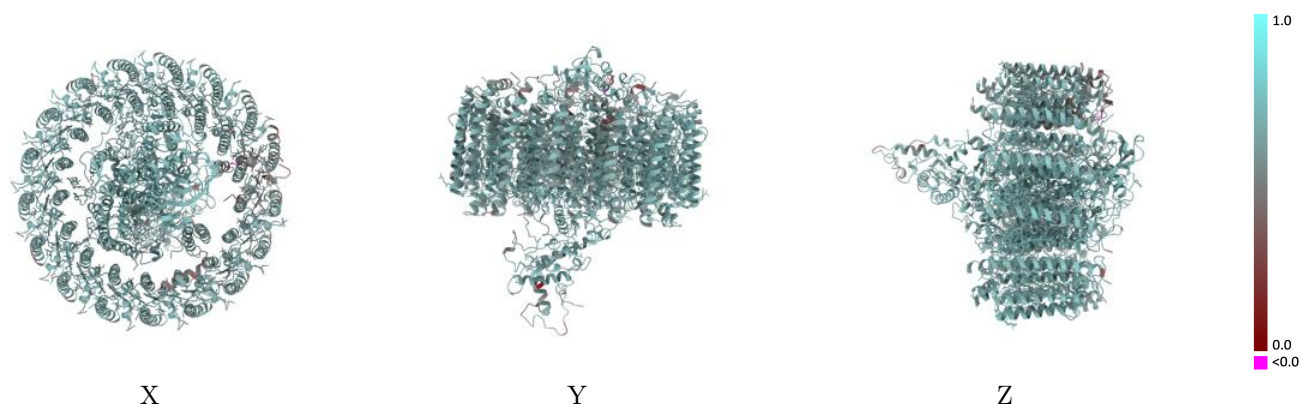
This section contains information regarding the fit between EMDB map EMD-63379 and PDB model 9LTS. Per-residue inclusion information can be found in [section 3](#) on [page 17](#).

9.1 Map-model overlay [i](#)



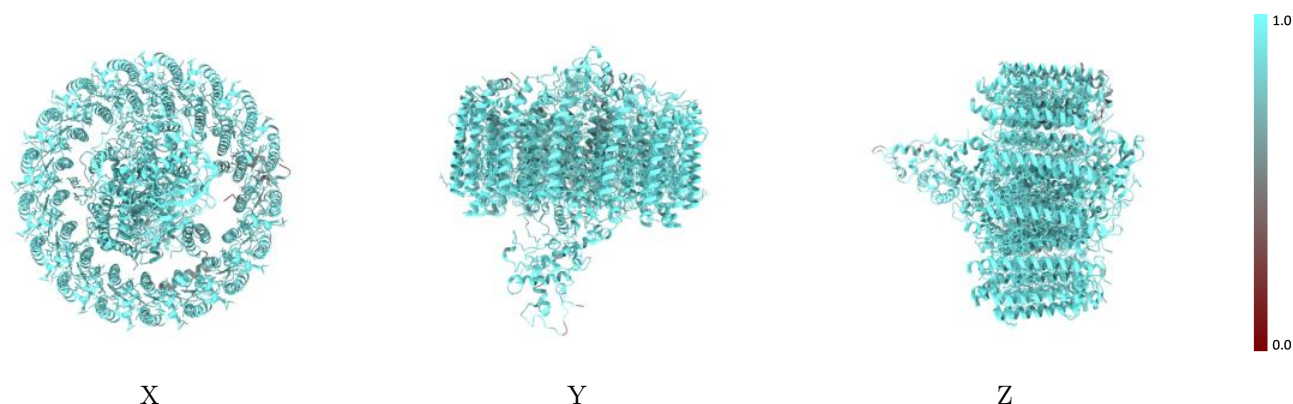
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



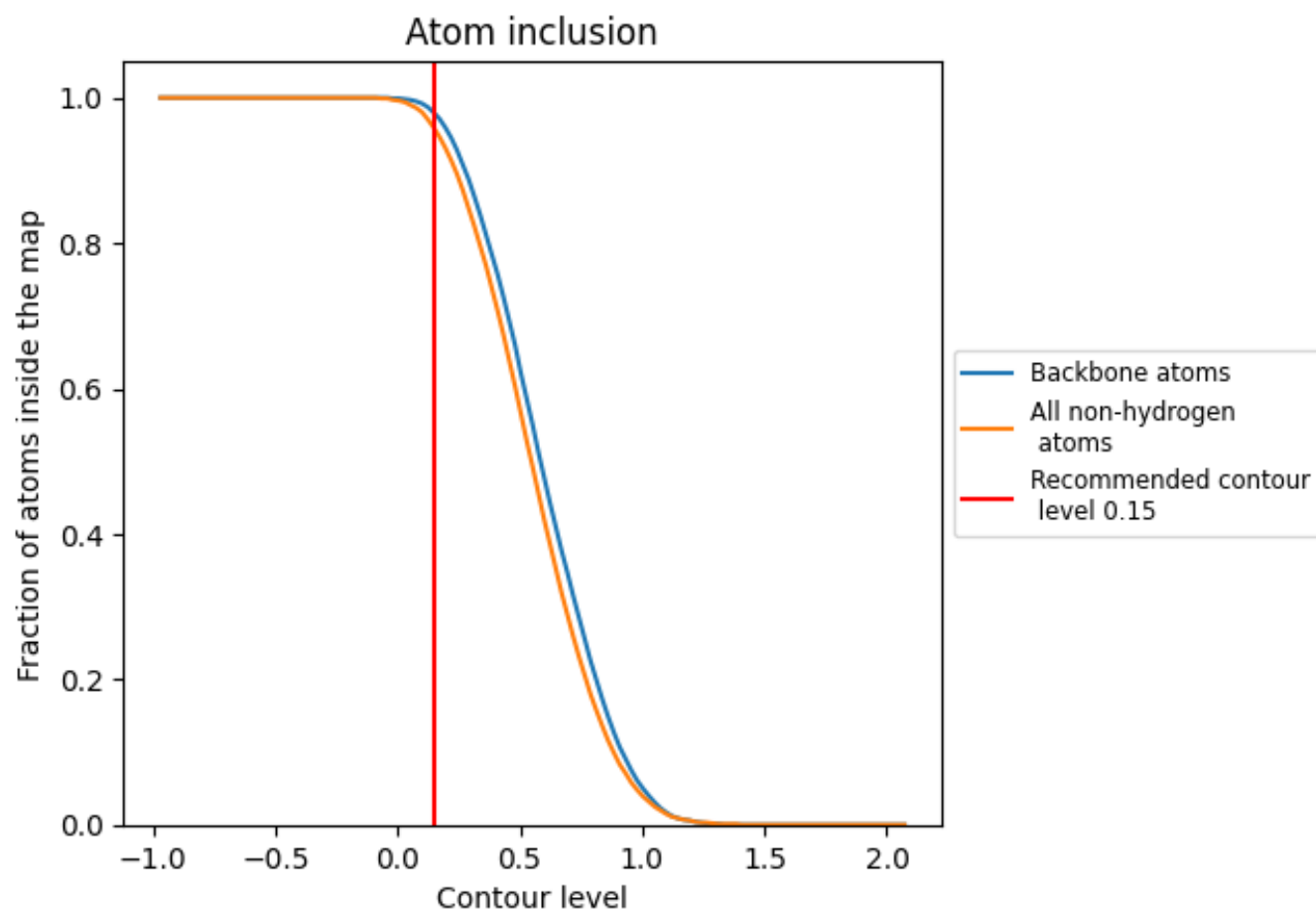
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9580	 0.6420
0	 0.9720	 0.6510
1	 0.9760	 0.6460
2	 0.9520	 0.6300
3	 0.9710	 0.6510
4	 0.9610	 0.6450
5	 0.9810	 0.6680
6	 0.9590	 0.6450
7	 0.9820	 0.6590
8	 0.9640	 0.6360
9	 0.9720	 0.6470
A	 0.8660	 0.5790
C	 0.9400	 0.6240
H	 0.9700	 0.6540
L	 0.9860	 0.6810
M	 0.9860	 0.6750
a	 0.9810	 0.6620
b	 0.9730	 0.6480
c	 0.9840	 0.6620
d	 0.9710	 0.6450
e	 0.9790	 0.6690
f	 0.9720	 0.6420
g	 0.9830	 0.6550
h	 0.9700	 0.6430
i	 0.9710	 0.6580
j	 0.9780	 0.6470
k	 0.9640	 0.6440
l	 0.9630	 0.6390
m	 0.9560	 0.6310
n	 0.9580	 0.6230
o	 0.9150	 0.5820
p	 0.8640	 0.5570
q	 0.8640	 0.5600
r	 0.8270	 0.5610
s	 0.9520	 0.6160



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Chain	Atom inclusion	Q-score
t	 0.9150	 0.5970
u	 0.9560	 0.6270
v	 0.9300	 0.5980
w	 0.9540	 0.6390
x	 0.9470	 0.6240