



Full wwPDB EM Validation Report ⓘ

Apr 15, 2026 – 02:14 AM UTC

PDB ID : 9LTU / pdb_00009ltu
EMDB ID : EMD-63381
Title : Cryo-EM structure of the Dinoroseobacter shibae RC-LH1 supercomplex with incomplete LH1 ring(State 1)
Authors : Liu, Z.K.; Wang, P.; Liu, L.N.
Deposited on : 2025-02-06
Resolution : 2.44 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:

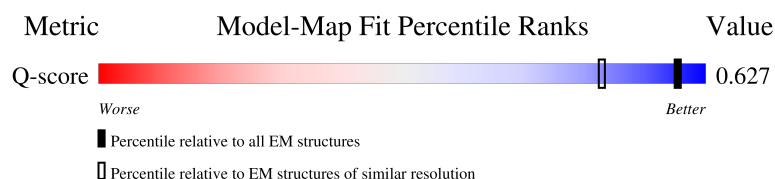
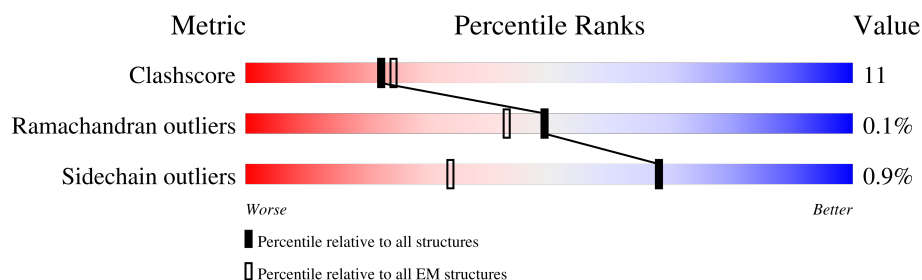
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.44 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	5856 (1.94 - 2.94)

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	0	44	
1	8	44	
1	b	44	
1	d	44	

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Mol	Chain	Length	Quality of chain
1	f	44	
1	h	44	
1	j	44	
1	l	44	
1	n	44	
1	p	44	
2	7	51	
2	9	51	
2	a	51	
2	c	51	
2	e	51	
2	g	51	
2	i	51	
2	k	51	
2	m	51	
2	o	51	
3	C	357	
4	H	255	
5	L	273	
6	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
11	BPH	L	305	-	-	X	-
8	SPN	0	102	-	X	-	-
8	SPN	8	102	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	SPN	9	101	-	X	-	-
8	SPN	a	102	-	X	-	-
8	SPN	a	103	-	X	-	-
8	SPN	e	102	-	X	-	-
8	SPN	f	101	-	X	-	-
8	SPN	g	102	-	X	-	-
8	SPN	i	102	-	X	-	-
8	SPN	l	102	-	X	-	-
8	SPN	m	102	-	X	-	-
8	SPN	n	102	-	X	-	-
8	SPN	p	102	-	X	-	-
8	SPN	p	103	-	X	-	-

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 20306 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 Antenna pigment protein beta chain.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
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		
2	a	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	e	51	Total	C	N	O	S	0	0
			425	291	68	64	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	g	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	k	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		
2	o	51	Total	C	N	O	S	0	0
			425	291	68	64	2		

- Molecule 3 is a protein called Photosynthetic reaction center cytochrome c subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	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 4 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	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 5 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	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

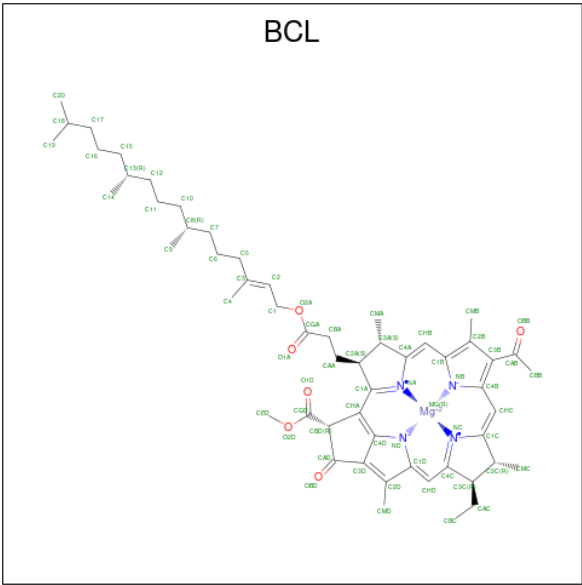
- Molecule 6 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	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 7 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



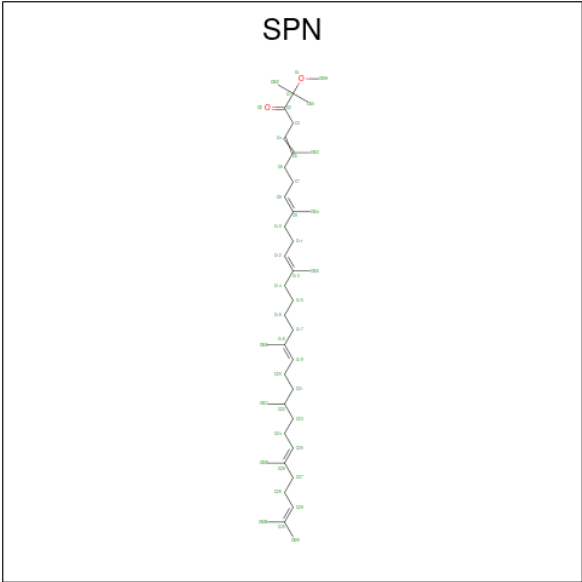
Mol	Chain	Residues	Atoms					AltConf
7	0	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	8	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	9	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	L	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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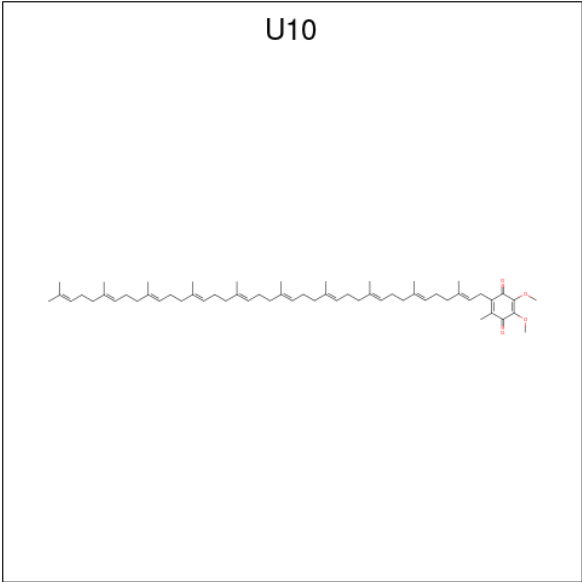
Mol	Chain	Residues	Atoms					AltConf
7	L	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	M	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	M	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	b	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	c	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	d	1	Total	C	Mg	N	O	0
			66	55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

- Molecule 8 is SPEROIDENONE (CCD ID: SPN) (formula: $C_{41}H_{70}O_2$) (labeled as "Ligand of Interest" by depositor).



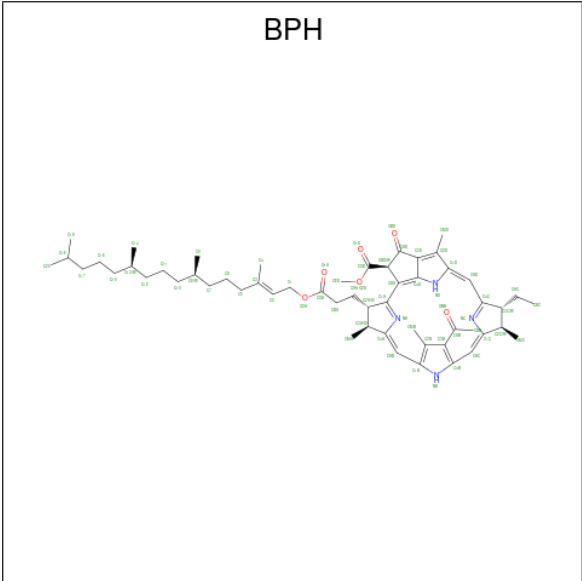
Mol	Chain	Residues	Atoms			AltConf
8	0	1	Total	C	O	0
			43	41	2	
8	8	1	Total	C	O	0
			43	41	2	
8	9	1	Total	C	O	0
			43	41	2	
8	M	1	Total	C	O	0
			43	41	2	
8	a	1	Total	C	O	0
			43	41	2	
8	a	1	Total	C	O	0
			43	41	2	
8	a	1	Total	C	O	0
			43	41	2	
8	e	1	Total	C	O	0
			43	41	2	
8	f	1	Total	C	O	0
			43	41	2	
8	f	1	Total	C	O	0
			43	41	2	
8	g	1	Total	C	O	0
			43	41	2	
8	g	1	Total	C	O	0
			43	41	2	
8	h	1	Total	C	O	0
			43	41	2	
8	i	1	Total	C	O	0
			43	41	2	

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Mol	Chain	Residues	Atoms			AltConf
10	L	1	Total	C	O	0
			38	34	4	
10	M	1	Total	C	O	0
			63	59	4	

- Molecule 11 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



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

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

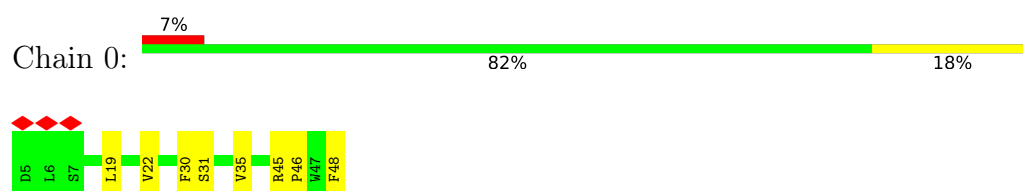
- Molecule 12 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

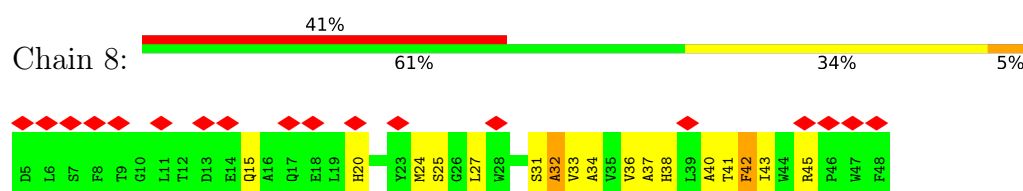
3 Residue-property plots [i](#)

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.

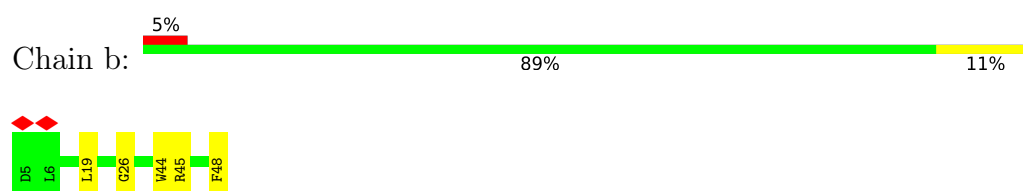
- Molecule 1: Antenna pigment protein beta chain



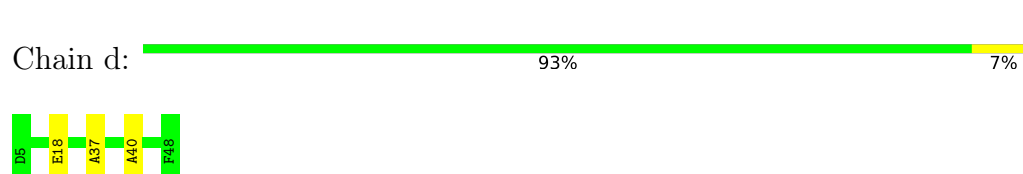
- Molecule 1: Antenna pigment protein beta chain



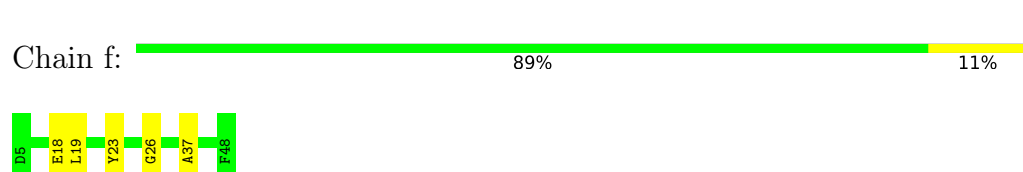
- Molecule 1: Antenna pigment protein beta chain



- Molecule 1: Antenna pigment protein beta chain



- Molecule 1: Antenna pigment protein beta chain

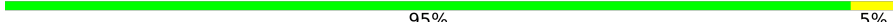


- Molecule 1: Antenna pigment protein beta chain

Chain h:  86% 14%



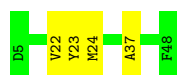
- Molecule 1: Antenna pigment protein beta chain

Chain j:  95% 5%



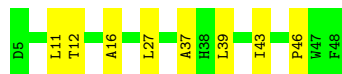
- Molecule 1: Antenna pigment protein beta chain

Chain l:  91% 9%



- Molecule 1: Antenna pigment protein beta chain

Chain n:  82% 18%



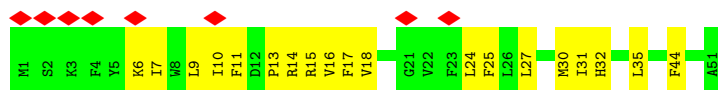
- Molecule 1: Antenna pigment protein beta chain

Chain p:  82% 18%



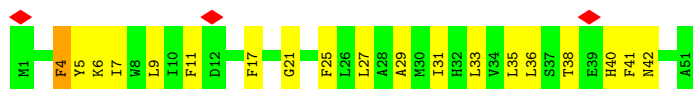
- Molecule 2: Antenna pigment protein alpha chain

Chain 7:  16% 63% 37%



- Molecule 2: Antenna pigment protein alpha chain

Chain 9:  6% 63% 35%



- Molecule 2: Antenna pigment protein alpha chain

Chain a:  73% 27%



- Molecule 2: Antenna pigment protein alpha chain

Chain c:  90% 10%



- Molecule 2: Antenna pigment protein alpha chain

Chain e:  88% 12%



- Molecule 2: Antenna pigment protein alpha chain

Chain g:  90% 10%



- Molecule 2: Antenna pigment protein alpha chain

Chain i:  92% 8%



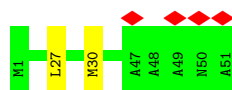
- Molecule 2: Antenna pigment protein alpha chain

Chain k:  98%

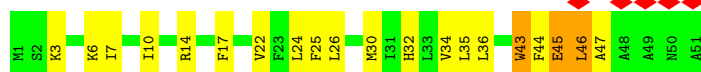


- Molecule 2: Antenna pigment protein alpha chain

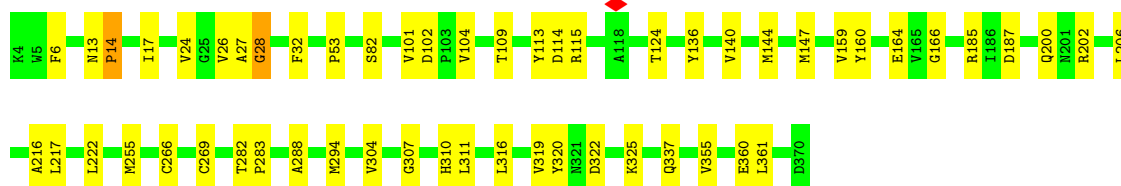
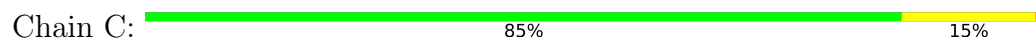
Chain m:  8% 96%



- Molecule 2: Antenna pigment protein alpha chain



- Molecule 3: Photosynthetic reaction center cytochrome c subunit



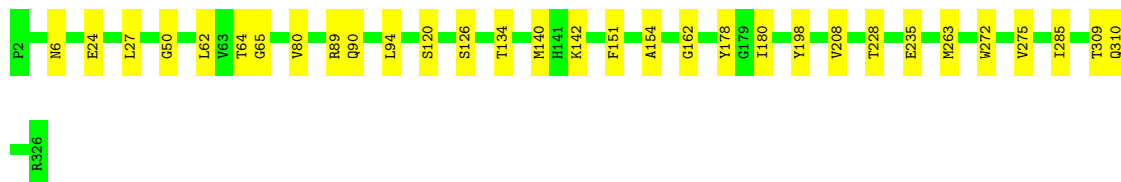
- Molecule 4: Reaction center protein H chain



- Molecule 5: Reaction center protein L chain



- Molecule 6: Reaction center protein M chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, POINT, POINT, POINT, POINT, POINT, POINT, POINT, POINT, POINT	Depositor
Number of particles used	82830, 82830, 82830, 82830, 82830, 82830, 82830, 82830, 82830	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, FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION, 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	2.207	Depositor
Minimum map value	-1.249	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.066	Depositor
Recommended contour level	0.15	Depositor
Map size ($\text{\AA}$)	291.0, 291.0, 291.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.97, 0.97, 0.97	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0	0.32	0/371	0.51	0/508
1	8	0.61	0/371	1.01	3/508 (0.6%)
1	b	0.31	0/371	0.47	0/508
1	d	0.17	0/371	0.27	0/508
1	f	0.18	0/371	0.29	0/508
1	h	0.41	0/371	0.38	0/508
1	j	0.17	0/371	0.26	0/508
1	l	0.19	0/371	0.28	0/508
1	n	0.33	0/371	0.54	1/508 (0.2%)
1	p	0.59	0/371	0.75	2/508 (0.4%)
2	7	0.33	0/439	0.56	0/595
2	9	0.39	0/439	0.70	2/595 (0.3%)
2	a	0.30	0/439	0.41	0/595
2	c	0.14	0/439	0.27	0/595
2	e	0.24	0/439	0.32	0/595
2	g	0.16	0/439	0.27	0/595
2	i	0.20	0/439	0.29	0/595
2	k	0.16	0/439	0.28	0/595
2	m	0.32	0/439	0.50	1/595 (0.2%)
2	o	0.40	0/439	0.74	3/595 (0.5%)
3	C	0.43	1/2864 (0.0%)	0.61	6/3929 (0.2%)
4	H	0.40	1/2065 (0.0%)	0.37	1/2795 (0.0%)
5	L	0.30	0/2261	0.42	1/3097 (0.0%)
6	M	0.36	0/2732	0.45	2/3737 (0.1%)
All	All	0.35	2/18022 (0.0%)	0.49	22/24588 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	54	PRO	N-CD	11.11	1.63	1.47
3	C	27	ALA	CA-C	-5.18	1.46	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	124	THR	N-CA-C	-11.21	91.79	109.72
2	9	4	PHE	N-CA-C	-8.40	103.22	113.97
2	o	45	GLU	N-CA-C	-8.38	103.00	113.55
5	L	165	TYR	N-CA-C	-7.35	101.51	111.87
3	C	6	PHE	N-CA-C	-7.11	104.48	113.72
1	p	8	PHE	N-CA-C	-7.07	104.46	113.23
6	M	272	TRP	N-CA-C	6.81	118.70	111.28
1	8	25	SER	N-CA-C	-6.24	107.51	114.62
2	o	46	LEU	N-CA-C	-6.22	105.17	112.89
1	8	32	ALA	N-CA-C	-6.21	104.44	111.14
2	m	30	MET	N-CA-C	6.21	117.71	111.07
3	C	28	GLY	N-CA-C	-6.07	105.45	112.73
1	p	9	THR	N-CA-C	-6.06	100.31	109.95
1	n	46	PRO	N-CA-C	5.90	120.54	111.57
3	C	102	ASP	N-CA-C	5.63	122.25	109.81
3	C	13	ASN	N-CA-C	5.55	118.29	109.64
3	C	283	PRO	N-CA-C	5.32	120.84	113.98
2	o	43	TRP	N-CA-C	-5.29	106.51	113.17
4	H	57	LEU	N-CA-C	5.26	117.34	110.08
1	8	38	HIS	N-CA-C	5.19	117.02	111.36
2	9	9	LEU	N-CA-C	-5.05	105.83	112.94
6	M	151	PHE	N-CA-C	-5.02	105.51	111.69

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	0	358	0	338	17	0
1	8	358	0	338	14	0
1	b	358	0	338	16	0
1	d	358	0	338	3	0
1	f	358	0	338	6	0
1	h	358	0	338	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	j	358	0	338	5	0
1	l	358	0	338	3	0
1	n	358	0	338	5	0
1	p	358	0	338	10	0
2	7	425	0	433	33	0
2	9	425	0	433	40	0
2	a	425	0	433	18	0
2	c	425	0	433	8	0
2	e	425	0	433	5	0
2	g	425	0	433	6	0
2	i	425	0	433	5	0
2	k	425	0	433	1	0
2	m	425	0	433	1	0
2	o	425	0	433	30	0
3	C	2785	0	2630	64	0
4	H	2015	0	1963	20	0
5	L	2172	0	2113	16	0
6	M	2634	0	2526	29	0
7	0	66	0	74	14	0
7	7	66	0	74	15	0
7	8	66	0	74	13	0
7	9	66	0	74	10	0
7	L	132	0	148	8	0
7	M	132	0	148	18	0
7	a	66	0	74	5	0
7	b	66	0	74	3	0
7	c	66	0	74	3	0
7	d	66	0	74	5	0
7	e	66	0	74	3	0
7	f	66	0	74	10	0
7	g	66	0	74	3	0
7	h	66	0	74	5	0
7	i	66	0	74	4	0
7	j	66	0	74	5	0
7	k	66	0	74	4	0
7	l	66	0	74	5	0
7	m	66	0	74	9	0
7	n	66	0	74	4	0
7	o	66	0	74	4	0
7	p	66	0	74	10	0
8	0	43	0	69	6	0
8	8	43	0	69	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	9	43	0	69	7	0
8	M	43	0	69	11	0
8	a	129	0	207	12	0
8	e	43	0	69	2	0
8	f	86	0	138	10	0
8	g	86	0	138	6	0
8	h	43	0	69	5	0
8	i	86	0	138	5	0
8	l	43	0	69	1	0
8	m	43	0	69	3	0
8	n	43	0	69	2	0
8	p	86	0	138	16	0
9	C	129	0	90	12	0
10	L	38	0	47	0	0
10	M	63	0	90	1	0
11	L	130	0	152	25	0
11	M	65	0	76	15	0
12	M	1	0	0	0	0
All	All	20306	0	20553	465	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 11.

All (465) 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)
3:C:266:CYS:SG	9:C:402:HEM:CAB	2.01	1.46
1:0:45:ARG:HD2	2:9:41:PHE:CE1	1.53	1.44
3:C:266:CYS:SG	9:C:402:HEM:CBB	2.08	1.42
11:L:305:BPH:HBB1	7:M:405:BCL:C20	1.65	1.25
3:C:166:GLY:HA3	3:C:355:VAL:CG2	1.66	1.25
2:a:40:HIS:O	1:b:45:ARG:NH2	1.70	1.23
1:0:45:ARG:CD	2:9:41:PHE:CE1	2.26	1.19
1:0:46:PRO:HB2	1:0:48:PHE:CE2	1.83	1.12
2:i:46:LEU:HD13	1:j:45:ARG:NH2	1.64	1.12
3:C:166:GLY:HA3	3:C:355:VAL:HG21	1.24	1.12
2:9:7:ILE:HD11	2:9:11:PHE:HE2	1.12	1.10
11:L:305:BPH:HMC3	11:M:404:BPH:HMA1	1.11	1.10
11:L:305:BPH:CBB	7:M:405:BCL:C20	2.28	1.09
11:L:305:BPH:HBB1	7:M:405:BCL:H202	1.27	1.09
11:L:305:BPH:HMA3	11:M:404:BPH:H142	1.32	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:7:24:LEU:HD22	7:7:101:BCL:H12	1.33	1.07
4:H:59:LYS:HE3	2:c:15:ARG:NH2	1.70	1.07
2:9:7:ILE:HD11	2:9:11:PHE:CE2	1.91	1.06
3:C:24:VAL:HG23	2:o:22:VAL:HG11	1.34	1.04
11:L:305:BPH:CBB	7:M:405:BCL:H201	1.89	1.02
3:C:32:PHE:CE2	2:o:26:LEU:CD2	2.45	1.00
4:H:117:ARG:HD2	4:H:234:ASP:OD2	1.60	1.00
1:b:44:TRP:CZ3	1:b:45:ARG:HD3	1.97	1.00
3:C:32:PHE:CE2	2:o:26:LEU:HD23	1.98	0.99
11:L:305:BPH:HMC3	11:M:404:BPH:CMA	1.93	0.97
11:L:305:BPH:CMC	11:M:404:BPH:HMA1	1.93	0.97
2:7:7:ILE:O	2:7:11:PHE:HD2	1.47	0.97
2:7:35:LEU:HD11	7:8:101:BCL:HMD3	1.45	0.96
11:L:305:BPH:HMA3	11:M:404:BPH:C14	1.95	0.95
3:C:24:VAL:HG23	2:o:22:VAL:CG1	1.97	0.95
3:C:166:GLY:HA3	3:C:355:VAL:HG23	1.48	0.94
4:H:117:ARG:CD	4:H:234:ASP:OD2	2.15	0.94
2:7:24:LEU:CD2	7:7:101:BCL:H12	1.99	0.93
3:C:24:VAL:CG2	2:o:22:VAL:CG1	2.46	0.93
2:7:35:LEU:HD21	7:8:101:BCL:HAC1	1.49	0.93
1:0:45:ARG:HD2	2:9:41:PHE:HE1	1.26	0.90
2:a:20:GLN:NE2	8:a:103:SPN:H151	1.87	0.89
2:i:46:LEU:CD1	1:j:45:ARG:NH2	2.35	0.89
1:0:45:ARG:HD2	2:9:41:PHE:CD1	2.11	0.85
3:C:32:PHE:CZ	2:o:26:LEU:HD23	2.12	0.84
3:C:24:VAL:CG2	2:o:22:VAL:HG11	2.08	0.83
3:C:266:CYS:SG	9:C:402:HEM:HAB	2.16	0.83
7:M:402:BCL:H171	7:M:402:BCL:H141	1.61	0.83
2:7:35:LEU:CD1	7:8:101:BCL:HMD3	2.09	0.83
11:L:305:BPH:HMB2	11:M:404:BPH:H121	1.61	0.83
3:C:24:VAL:CG2	2:o:22:VAL:HG13	2.08	0.82
3:C:32:PHE:HE2	2:o:26:LEU:CD2	1.93	0.82
1:0:46:PRO:CB	1:0:48:PHE:CE2	2.63	0.82
2:7:10:ILE:O	2:7:10:ILE:HG22	1.79	0.81
7:b:101:BCL:H18	7:b:101:BCL:HBB3	1.63	0.81
2:7:17:PHE:HB3	2:9:11:PHE:HZ	1.45	0.80
1:0:22:VAL:HG11	8:9:101:SPN:HM82	1.63	0.80
11:L:305:BPH:HBB3	7:M:405:BCL:H201	1.65	0.77
3:C:32:PHE:CE2	2:o:26:LEU:HD21	2.18	0.77
3:C:144:MET:HE1	3:C:147:MET:HE1	1.67	0.77
2:a:20:GLN:HE22	8:a:103:SPN:H151	1.48	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:0:101:BCL:HED1	2:9:27:LEU:HG	1.68	0.76
6:M:27:LEU:HD21	6:M:140:MET:HE3	1.67	0.76
1:p:27:LEU:HD13	8:p:103:SPN:H172	1.68	0.76
2:9:40:HIS:CE1	2:9:41:PHE:CE2	2.74	0.75
7:j:101:BCL:HMB1	7:j:101:BCL:HBB2	1.67	0.75
2:7:24:LEU:CD2	7:7:101:BCL:C1	2.64	0.75
11:L:305:BPH:CMB	11:M:404:BPH:H121	2.15	0.75
5:L:220:PHE:CZ	6:M:134:THR:OG1	2.40	0.74
2:i:46:LEU:HD13	1:j:45:ARG:HH21	1.48	0.74
3:C:24:VAL:HG22	2:o:22:VAL:HG13	1.69	0.74
4:H:59:LYS:CE	2:c:15:ARG:NH2	2.49	0.74
7:c:101:BCL:HMB1	7:c:101:BCL:HBB2	1.70	0.74
7:h:101:BCL:HMB1	7:h:101:BCL:HBB2	1.70	0.73
2:a:40:HIS:O	1:b:45:ARG:CZ	2.37	0.73
7:a:101:BCL:HMB1	7:a:101:BCL:HBB3	1.70	0.73
1:0:45:ARG:HD3	2:9:41:PHE:CE1	2.21	0.73
6:M:27:LEU:CD2	6:M:140:MET:HE3	2.18	0.73
7:l:101:BCL:HMB1	7:l:101:BCL:HBB2	1.68	0.73
7:n:101:BCL:HMB1	7:n:101:BCL:HBB2	1.70	0.73
3:C:115:ARG:HH22	3:C:360:GLU:HB2	1.54	0.72
7:m:101:BCL:HMB1	7:m:101:BCL:HBB3	1.70	0.72
6:M:178:TYR:HD1	8:M:406:SPN:H142	1.55	0.71
3:C:17:ILE:O	3:C:17:ILE:HG22	1.89	0.71
1:p:27:LEU:CD1	8:p:103:SPN:H172	2.21	0.71
2:7:25:PHE:HB2	7:7:101:BCL:H62	1.72	0.71
6:M:24:GLU:OE2	6:M:142:LYS:NZ	2.18	0.71
1:f:26:GLY:HA3	8:f:103:SPN:HM73	1.72	0.70
1:8:20:HIS:CE1	1:8:24:MET:HB3	2.27	0.70
7:L:301:BCL:H61	7:L:303:BCL:HBB3	1.74	0.69
2:o:14:ARG:HG3	8:p:103:SPN:HMB1	1.75	0.69
8:a:103:SPN:H211	8:a:103:SPN:HM61	1.72	0.69
2:7:7:ILE:O	2:7:11:PHE:CD2	2.38	0.69
1:h:26:GLY:HA3	8:h:102:SPN:HM73	1.75	0.68
1:n:11:LEU:HD23	1:n:12:THR:O	1.93	0.68
7:8:101:BCL:H2A	7:8:101:BCL:HED2	1.73	0.68
3:C:266:CYS:SG	9:C:402:HEM:C3B	2.86	0.68
2:9:31:ILE:O	2:9:35:LEU:HD13	1.93	0.68
11:L:305:BPH:CBB	7:M:405:BCL:H202	2.06	0.67
7:p:101:BCL:HMB1	7:p:101:BCL:HBB2	1.76	0.67
11:L:305:BPH:CMB	6:M:62:LEU:HD11	2.25	0.67
4:H:85:LEU:HD12	5:L:8:ARG:NH2	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:f:102:BCL:HMB1	7:f:102:BCL:HBB2	1.76	0.67
7:g:101:BCL:HMB1	7:g:101:BCL:HBB2	1.77	0.67
1:8:42:PHE:H	8:8:102:SPN:HM82	1.60	0.66
1:f:23:TYR:HA	8:f:103:SPN:HM72	1.75	0.66
3:C:144:MET:HE2	9:C:401:HEM:NC	2.10	0.66
11:L:305:BPH:CMA	11:M:404:BPH:C14	2.71	0.66
1:b:44:TRP:CH2	1:b:45:ARG:HD3	2.31	0.66
7:i:101:BCL:CBB	7:i:101:BCL:HMB1	2.26	0.65
2:7:6:LYS:HA	2:7:9:LEU:HD13	1.77	0.65
2:9:25:PHE:HB2	7:9:102:BCL:H42	1.78	0.65
7:e:101:BCL:CBB	7:e:101:BCL:HMB1	2.27	0.65
2:o:35:LEU:HD21	7:p:101:BCL:HBC3	1.77	0.65
1:p:47:TRP:CZ3	7:p:101:BCL:HAC2	2.32	0.64
3:C:222:LEU:HD22	3:C:325:LYS:HE2	1.79	0.64
7:0:101:BCL:CED	2:9:27:LEU:HG	2.28	0.64
11:L:305:BPH:HMB1	6:M:62:LEU:HD11	1.80	0.64
3:C:266:CYS:SG	9:C:402:HEM:HBB1	2.30	0.64
3:C:166:GLY:CA	3:C:355:VAL:HG23	2.26	0.64
1:h:12:THR:HG22	1:h:13:ASP:N	2.14	0.63
2:7:17:PHE:HB3	2:9:11:PHE:CZ	2.31	0.63
7:k:101:BCL:HMB1	7:k:101:BCL:CBB	2.29	0.63
4:H:169:ILE:HG22	4:H:176:VAL:HG22	1.79	0.62
6:M:65:GLY:HA3	11:M:404:BPH:H5C1	1.81	0.62
7:a:101:BCL:CHC	7:d:101:BCL:HBB3	2.30	0.62
7:g:101:BCL:HMB1	7:g:101:BCL:CBB	2.29	0.62
4:H:59:LYS:HE3	2:c:15:ARG:HH22	1.63	0.62
2:7:15:ARG:HA	2:7:18:VAL:HG12	1.81	0.62
7:9:102:BCL:HBB2	7:9:102:BCL:HMB1	1.80	0.62
7:0:101:BCL:HED1	2:9:27:LEU:CD2	2.30	0.61
7:9:102:BCL:HMB1	7:9:102:BCL:CBB	2.30	0.61
8:f:103:SPN:HM61	8:f:103:SPN:H211	1.83	0.61
3:C:185:ARG:NE	3:C:187:ASP:OD2	2.29	0.61
5:L:169:HIS:NE2	7:L:301:BCL:HBB2	2.16	0.61
3:C:222:LEU:CD2	3:C:325:LYS:HE2	2.30	0.61
3:C:82:SER:OG	3:C:114:ASP:OD1	2.15	0.61
1:0:45:ARG:HD3	2:9:41:PHE:CZ	2.36	0.61
7:7:101:BCL:HMB2	8:9:101:SPN:H4	1.83	0.60
6:M:162:GLY:HA3	8:M:406:SPN:HM72	1.81	0.60
7:d:101:BCL:HMB1	7:d:101:BCL:HBB2	1.81	0.60
7:8:101:BCL:HMA2	7:8:101:BCL:H12	1.83	0.60
3:C:144:MET:CE	9:C:401:HEM:NC	2.64	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:n:39:LEU:O	1:n:43:ILE:HG12	2.01	0.60
7:f:102:BCL:HMB1	7:f:102:BCL:CBB	2.30	0.60
2:7:17:PHE:CB	2:9:11:PHE:HZ	2.14	0.60
1:h:23:TYR:HA	8:h:102:SPN:HM72	1.83	0.60
1:8:20:HIS:CE1	1:8:24:MET:CG	2.85	0.60
2:a:40:HIS:CG	1:b:45:ARG:NH2	2.70	0.60
2:g:1:MET:HG3	2:g:3:LYS:H	1.67	0.60
5:L:220:PHE:CE1	6:M:134:THR:OG1	2.53	0.60
8:g:103:SPN:H211	8:g:103:SPN:HM61	1.83	0.59
8:i:103:SPN:H211	8:i:103:SPN:HM61	1.84	0.59
1:d:37:ALA:HB1	8:f:101:SPN:HM62	1.84	0.59
2:7:10:ILE:O	2:7:10:ILE:CG2	2.49	0.59
3:C:319:VAL:HG12	3:C:320:TYR:CD2	2.37	0.59
7:0:101:BCL:HED1	2:9:27:LEU:CG	2.33	0.59
8:0:102:SPN:H161	8:0:102:SPN:HM51	1.84	0.59
5:L:186:LEU:HD22	7:M:402:BCL:H41	1.84	0.59
8:n:102:SPN:H19	7:p:101:BCL:H203	1.84	0.58
7:8:101:BCL:HED2	7:8:101:BCL:C2A	2.33	0.58
7:c:101:BCL:HMB1	7:c:101:BCL:CBB	2.33	0.58
7:h:101:BCL:HMB1	7:h:101:BCL:CBB	2.32	0.58
8:i:103:SPN:HM61	8:i:103:SPN:C21	2.34	0.58
8:a:103:SPN:HM81	1:b:19:LEU:HD12	1.86	0.58
2:c:27:LEU:HD23	7:d:101:BCL:HED1	1.86	0.58
6:M:64:THR:OG1	6:M:126:SER:HB2	2.04	0.58
8:e:102:SPN:HM62	1:f:37:ALA:HB1	1.86	0.58
8:g:103:SPN:HM61	8:g:103:SPN:C21	2.34	0.58
4:H:59:LYS:HE3	2:c:15:ARG:HH21	1.63	0.58
2:o:25:PHE:O	2:o:26:LEU:HB2	2.03	0.57
2:7:24:LEU:HD22	7:7:101:BCL:C1	2.20	0.57
11:L:305:BPH:CMA	11:M:404:BPH:H141	2.35	0.57
4:H:165:SER:OG	4:H:180:GLU:OE1	2.23	0.57
1:d:18:GLU:OE2	2:e:6:LYS:HE3	2.05	0.57
2:o:36:LEU:HD21	2:o:43:TRP:CZ2	2.39	0.57
7:M:405:BCL:HAA2	7:M:405:BCL:HBD	1.87	0.57
7:i:101:BCL:HMB1	7:i:101:BCL:HBB3	1.85	0.57
1:p:27:LEU:CD1	8:p:103:SPN:H152	2.35	0.57
7:j:101:BCL:HMB1	7:j:101:BCL:CBB	2.35	0.56
2:7:14:ARG:O	2:7:18:VAL:HG12	2.05	0.56
7:0:101:BCL:HBB2	7:7:101:BCL:HMC3	1.87	0.56
1:8:37:ALA:HA	8:8:102:SPN:HM61	1.87	0.56
3:C:166:GLY:CA	3:C:355:VAL:HG21	2.16	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:46:PRO:CB	1:0:48:PHE:CZ	2.88	0.56
7:9:102:BCL:HMB2	8:a:103:SPN:C4	2.36	0.56
1:b:44:TRP:CH2	1:b:45:ARG:CD	2.89	0.56
8:p:103:SPN:H211	8:p:103:SPN:HM61	1.86	0.56
2:7:35:LEU:CD2	7:8:101:BCL:HAC1	2.31	0.56
4:H:54:PRO:HG2	4:H:55:PHE:CD1	2.41	0.56
8:0:102:SPN:H142	7:9:102:BCL:HMA3	1.88	0.55
7:M:402:BCL:HHC	7:M:402:BCL:HBB2	1.86	0.55
7:b:101:BCL:HHC	7:b:101:BCL:HBB2	1.89	0.55
1:8:42:PHE:CD1	8:8:102:SPN:HM81	2.41	0.55
1:n:11:LEU:CD2	1:n:16:ALA:HB2	2.37	0.55
11:L:305:BPH:HMB2	11:M:404:BPH:H142	1.89	0.55
2:a:40:HIS:CD2	1:b:45:ARG:HH22	2.24	0.55
4:H:59:LYS:CE	2:c:15:ARG:HH22	2.19	0.55
1:p:44:TRP:HB2	8:p:102:SPN:H241	1.89	0.55
2:a:40:HIS:CD2	1:b:45:ARG:NH2	2.76	0.54
2:i:27:LEU:HB3	7:j:101:BCL:HED1	1.88	0.54
2:e:42:ASN:O	2:e:46:LEU:HG	2.06	0.54
2:i:41:PHE:CD1	1:j:45:ARG:HD2	2.42	0.54
8:h:102:SPN:H211	8:h:102:SPN:HM61	1.88	0.54
11:L:305:BPH:HMB2	11:M:404:BPH:C12	2.34	0.54
8:M:406:SPN:H171	8:M:406:SPN:H211	1.89	0.54
3:C:32:PHE:HE2	2:o:26:LEU:HD21	1.62	0.54
5:L:171:ASN:ND2	5:L:248:CYS:SG	2.80	0.54
6:M:120:SER:HB3	8:M:406:SPN:H25	1.90	0.54
7:m:101:BCL:H192	2:o:7:ILE:CD1	2.37	0.54
2:a:20:GLN:NE2	8:a:103:SPN:C15	2.65	0.53
7:m:101:BCL:HMB3	7:p:101:BCL:CHB	2.38	0.53
7:0:101:BCL:CED	2:9:27:LEU:CD2	2.86	0.53
2:7:44:PHE:CE1	2:9:38:THR:CG2	2.91	0.53
11:L:305:BPH:H1C1	6:M:50:GLY:HA3	1.89	0.53
8:M:406:SPN:H211	8:M:406:SPN:C17	2.39	0.53
2:7:44:PHE:CE1	2:9:38:THR:HG21	2.43	0.53
7:0:101:BCL:CBB	7:7:101:BCL:HMC3	2.38	0.53
4:H:36:ARG:NH2	4:H:59:LYS:O	2.42	0.53
3:C:307:GLY:HA2	3:C:311:LEU:HG	1.90	0.53
7:e:101:BCL:HMB1	7:e:101:BCL:HBB3	1.89	0.53
8:p:102:SPN:H141	8:p:102:SPN:H102	1.90	0.53
7:a:101:BCL:HMB1	7:a:101:BCL:CBB	2.36	0.53
7:0:101:BCL:H141	8:8:102:SPN:H25	1.90	0.53
3:C:115:ARG:NH2	3:C:360:GLU:HB2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:g:103:SPN:HM73	8:i:102:SPN:HM21	1.90	0.53
7:l:101:BCL:HMB1	7:l:101:BCL:CBB	2.39	0.52
7:o:101:BCL:HBC3	1:p:41:THR:HG23	1.91	0.52
7:L:301:BCL:HHC	7:L:301:BCL:HBB3	1.91	0.52
8:g:102:SPN:HM62	1:h:37:ALA:HB1	1.90	0.52
1:8:20:HIS:CE1	1:8:24:MET:CB	2.93	0.52
1:8:24:MET:HE2	1:8:27:LEU:HD23	1.92	0.52
8:i:102:SPN:HM62	1:j:37:ALA:HB1	1.90	0.52
6:M:178:TYR:CD1	8:M:406:SPN:H142	2.41	0.52
1:0:19:LEU:HB2	8:9:101:SPN:HM92	1.91	0.52
1:0:46:PRO:HB2	1:0:48:PHE:CD2	2.42	0.52
2:7:24:LEU:HD23	7:7:101:BCL:C1	2.37	0.52
2:7:32:HIS:HB3	8:9:101:SPN:HM21	1.90	0.52
2:a:40:HIS:C	1:b:45:ARG:HH21	2.13	0.52
11:L:305:BPH:HMB3	6:M:62:LEU:CD1	2.40	0.51
6:M:6:ASN:ND2	6:M:228:THR:HG21	2.25	0.51
8:m:102:SPN:HMB3	2:o:10:ILE:HD11	1.92	0.51
1:0:31:SER:O	1:0:35:VAL:HG23	2.10	0.51
1:0:45:ARG:CD	2:9:41:PHE:CZ	2.89	0.51
7:k:101:BCL:HMB1	7:k:101:BCL:HBB3	1.91	0.51
3:C:14:PRO:HD2	2:o:14:ARG:HH21	1.76	0.51
11:L:305:BPH:CMB	6:M:62:LEU:CD1	2.88	0.51
1:n:37:ALA:HB1	8:n:102:SPN:HM62	1.93	0.51
1:h:26:GLY:HA3	8:h:102:SPN:H202	1.92	0.51
7:8:101:BCL:HED2	7:8:101:BCL:C1A	2.40	0.51
6:M:178:TYR:CE1	8:M:406:SPN:H162	2.45	0.51
11:L:305:BPH:HBB3	11:L:305:BPH:HMC2	1.93	0.51
1:0:45:ARG:CD	2:9:41:PHE:CD1	2.83	0.51
7:f:102:BCL:H143	7:f:102:BCL:CHB	2.41	0.51
7:L:301:BCL:H61	7:L:303:BCL:CBB	2.41	0.50
1:b:44:TRP:CE3	1:b:45:ARG:HD3	2.43	0.50
8:0:102:SPN:H242	1:b:48:PHE:CE2	2.46	0.50
2:9:36:LEU:O	2:9:42:ASN:ND2	2.44	0.50
1:h:12:THR:HG22	1:h:13:ASP:H	1.76	0.50
7:m:101:BCL:H192	2:o:7:ILE:HD12	1.92	0.50
6:M:80:VAL:HG22	6:M:80:VAL:O	2.11	0.50
3:C:32:PHE:CZ	2:o:26:LEU:CD2	2.84	0.50
7:f:102:BCL:HMB2	7:f:102:BCL:H141	1.93	0.50
1:p:27:LEU:HD13	8:p:103:SPN:C17	2.37	0.50
7:0:101:BCL:HHC	7:0:101:BCL:HBB3	1.93	0.50
1:f:18:GLU:OE2	2:g:6:LYS:HE3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:305:BPH:H1C1	6:M:50:GLY:CA	2.42	0.50
3:C:144:MET:CE	3:C:147:MET:HE1	2.40	0.50
7:L:303:BCL:HHC	7:L:303:BCL:HBB2	1.92	0.50
8:9:101:SPN:HM81	2:a:6:LYS:HB2	1.94	0.50
2:a:34:VAL:O	2:a:37:SER:OG	2.29	0.50
1:0:46:PRO:HB3	1:0:48:PHE:CZ	2.47	0.49
1:l:23:TYR:HD2	1:l:24:MET:HE2	1.76	0.49
3:C:316:LEU:O	3:C:322:ASP:N	2.45	0.49
3:C:28:GLY:HA2	3:C:32:PHE:CD2	2.48	0.49
3:C:115:ARG:NH2	3:C:361:LEU:HG	2.27	0.49
2:o:17:PHE:CE2	8:p:103:SPN:HM82	2.47	0.49
2:7:24:LEU:HD23	7:7:101:BCL:H11	1.95	0.49
2:a:40:HIS:CG	1:b:45:ARG:HH21	2.30	0.49
8:a:102:SPN:HM21	8:a:103:SPN:HM73	1.94	0.49
1:8:31:SER:HA	1:8:34:ALA:HB3	1.95	0.49
2:9:4:PHE:C	2:9:6:LYS:H	2.21	0.49
3:C:216:ALA:O	3:C:217:LEU:HB2	2.12	0.49
2:a:14:ARG:HG2	2:c:10:ILE:HG23	1.95	0.49
7:c:101:BCL:H3A	7:c:101:BCL:HBA1	1.58	0.48
2:e:27:LEU:HD23	7:f:102:BCL:HED1	1.94	0.48
2:7:27:LEU:HA	2:7:30:MET:HG2	1.95	0.48
7:0:101:BCL:CED	2:9:27:LEU:HD23	2.42	0.48
1:8:42:PHE:N	8:8:102:SPN:HM82	2.25	0.48
3:C:255:MET:HB3	9:C:402:HEM:C4B	2.48	0.48
8:a:103:SPN:H202	1:b:26:GLY:HA3	1.95	0.48
7:9:102:BCL:H3A	7:9:102:BCL:HBA1	1.56	0.48
5:L:21:ASP:HA	5:L:24:ASP:HB2	1.93	0.48
6:M:154:ALA:HB2	11:M:404:BPH:HAC1	1.95	0.48
7:h:101:BCL:HBA1	7:h:101:BCL:H3A	1.66	0.48
2:o:32:HIS:O	2:o:36:LEU:HG	2.13	0.48
7:m:101:BCL:HMB1	7:m:101:BCL:CBB	2.43	0.48
2:7:24:LEU:HD23	2:7:24:LEU:C	2.39	0.48
7:7:101:BCL:HAA2	7:7:101:BCL:HBD	1.95	0.48
3:C:144:MET:HE1	3:C:147:MET:CE	2.42	0.48
4:H:199:VAL:HG12	4:H:208:VAL:HG22	1.95	0.48
3:C:136:TYR:HB2	3:C:310:HIS:HB3	1.96	0.48
4:H:117:ARG:CG	4:H:234:ASP:OD2	2.61	0.48
2:e:32:HIS:CE1	7:f:102:BCL:HMD1	2.48	0.48
2:7:31:ILE:HD12	7:8:101:BCL:HED1	1.95	0.48
7:M:405:BCL:CBB	7:M:405:BCL:HHC	2.44	0.47
1:p:27:LEU:HD13	8:p:103:SPN:H152	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:268:LEU:O	6:M:89:ARG:NH1	2.47	0.47
2:o:30:MET:O	2:o:34:VAL:HG23	2.15	0.47
3:C:200:GLN:O	3:C:202:ARG:N	2.47	0.47
7:L:301:BCL:HHC	7:L:301:BCL:CBB	2.45	0.47
7:a:101:BCL:H121	7:a:101:BCL:H162	1.57	0.47
11:M:404:BPH:H112	11:M:404:BPH:H7C2	1.72	0.47
3:C:144:MET:CE	3:C:147:MET:CE	2.93	0.47
3:C:355:VAL:O	3:C:355:VAL:HG12	2.14	0.47
5:L:174:HIS:HB2	5:L:248:CYS:SG	2.55	0.47
1:b:44:TRP:CZ3	1:b:45:ARG:CD	2.85	0.47
1:l:37:ALA:HB1	8:l:102:SPN:HM62	1.97	0.47
1:8:15:GLN:N	1:8:15:GLN:OE1	2.44	0.47
1:h:12:THR:CG2	1:h:13:ASP:N	2.77	0.47
7:p:101:BCL:H141	7:p:101:BCL:H161	1.75	0.47
5:L:56:GLN:HB3	5:L:82:MET:HE1	1.96	0.47
7:f:102:BCL:HBA1	7:f:102:BCL:H3A	1.67	0.47
8:p:102:SPN:HM43	8:p:102:SPN:H62	1.97	0.47
7:7:101:BCL:H112	7:7:101:BCL:H72	1.47	0.47
2:9:4:PHE:C	2:9:6:LYS:N	2.73	0.47
5:L:133:VAL:HG23	5:L:134:VAL:HG23	1.96	0.46
7:m:101:BCL:CHC	7:p:101:BCL:HBB3	2.45	0.46
7:0:101:BCL:H3A	7:0:101:BCL:H12	1.97	0.46
2:9:29:ALA:O	2:9:33:LEU:HG	2.15	0.46
2:e:30:MET:HE3	2:e:30:MET:HB3	1.86	0.46
6:M:178:TYR:HE1	8:M:406:SPN:H162	1.80	0.46
7:8:101:BCL:H203	7:8:101:BCL:H162	1.79	0.46
7:M:402:BCL:HMC2	8:M:406:SPN:HM61	1.97	0.46
7:b:101:BCL:H203	7:b:101:BCL:H161	1.79	0.46
2:a:8:TRP:HZ3	2:a:16:VAL:HG21	1.81	0.46
1:f:26:GLY:HA3	8:f:103:SPN:H202	1.98	0.46
11:M:404:BPH:HBC3	11:M:404:BPH:HHD	1.98	0.46
7:p:101:BCL:H62	7:p:101:BCL:H41	1.58	0.46
7:d:101:BCL:HBA1	7:d:101:BCL:H3A	1.71	0.45
7:l:101:BCL:H203	7:l:101:BCL:H162	1.78	0.45
7:8:101:BCL:H2A	7:8:101:BCL:CED	2.44	0.45
2:9:21:GLY:O	7:9:102:BCL:H41	2.17	0.45
7:M:402:BCL:H62	7:M:402:BCL:H2	1.64	0.45
7:M:402:BCL:H142	7:M:402:BCL:H111	1.76	0.45
7:m:101:BCL:H143	7:m:101:BCL:H111	1.85	0.45
1:8:42:PHE:CD1	8:8:102:SPN:CM8	2.99	0.45
4:H:85:LEU:HD12	5:L:8:ARG:HH22	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:m:101:BCL:HBA1	7:m:101:BCL:H3A	1.64	0.45
7:8:101:BCL:H91	7:8:101:BCL:H112	1.82	0.45
3:C:14:PRO:CD	2:o:14:ARG:HH21	2.29	0.45
6:M:235:GLU:HG2	6:M:263:MET:SD	2.56	0.45
8:e:102:SPN:H19	7:h:101:BCL:H201	1.97	0.45
8:f:103:SPN:H29	2:g:10:ILE:HD12	1.99	0.45
7:k:101:BCL:H143	7:k:101:BCL:H111	1.76	0.45
6:M:198:TYR:OH	7:M:405:BCL:HBB2	2.15	0.45
7:a:101:BCL:HBA1	7:a:101:BCL:H3A	1.70	0.45
2:o:44:PHE:HA	2:o:47:ALA:HB3	1.99	0.45
2:a:27:LEU:O	2:a:31:ILE:HG13	2.17	0.45
7:j:101:BCL:HBA1	7:j:101:BCL:H3A	1.81	0.45
7:n:101:BCL:H62	7:n:101:BCL:H102	1.78	0.45
2:9:40:HIS:CE1	2:9:41:PHE:CD2	3.05	0.45
1:p:43:ILE:HD13	1:p:43:ILE:HA	1.86	0.45
3:C:159:VAL:O	9:C:403:HEM:HBD2	2.17	0.45
7:f:102:BCL:HMC2	7:f:102:BCL:HHC	1.83	0.45
2:9:7:ILE:HG13	2:9:11:PHE:HD2	1.82	0.44
7:f:102:BCL:H143	7:f:102:BCL:HHB	1.97	0.44
2:7:13:PRO:HA	2:7:16:VAL:HB	1.98	0.44
7:8:101:BCL:H52	7:8:101:BCL:H8	1.58	0.44
3:C:140:VAL:O	3:C:144:MET:HG2	2.17	0.44
8:0:102:SPN:H141	7:9:102:BCL:O1D	2.17	0.44
8:M:406:SPN:C17	8:M:406:SPN:C21	2.96	0.44
2:g:32:HIS:CE1	7:h:101:BCL:HMD1	2.52	0.44
1:h:14:GLU:OE1	1:h:14:GLU:N	2.42	0.44
7:o:101:BCL:HMA3	8:p:102:SPN:H142	1.99	0.44
3:C:109:THR:HG22	3:C:113:TYR:CZ	2.53	0.44
8:a:103:SPN:HM81	8:a:103:SPN:H282	1.46	0.44
8:a:103:SPN:H32	8:a:103:SPN:HM21	1.62	0.44
2:7:7:ILE:HG23	2:7:11:PHE:CE2	2.52	0.43
2:7:44:PHE:CD1	2:9:38:THR:HG21	2.53	0.43
8:0:102:SPN:HM12	2:9:17:PHE:HB3	2.00	0.43
7:0:101:BCL:H93	7:0:101:BCL:H111	1.90	0.43
8:8:102:SPN:H241	8:8:102:SPN:HM71	1.52	0.43
2:9:27:LEU:O	2:9:31:ILE:HG12	2.19	0.43
3:C:337:GLN:HG2	9:C:403:HEM:HAD2	1.99	0.43
7:7:101:BCL:HMB1	7:7:101:BCL:HBB2	1.99	0.43
2:7:14:ARG:HA	2:7:14:ARG:HD3	1.75	0.43
8:9:101:SPN:HM81	8:9:101:SPN:H282	1.67	0.43
5:L:21:ASP:OD1	5:L:21:ASP:N	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:o:24:LEU:HD11	8:p:103:SPN:H162	2.01	0.43
7:j:101:BCL:H192	7:j:101:BCL:H161	1.76	0.43
7:n:101:BCL:HMB1	7:n:101:BCL:CBB	2.43	0.43
1:8:40:ALA:O	8:8:102:SPN:CM7	2.67	0.43
2:9:5:TYR:CE1	2:9:6:LYS:HG3	2.54	0.43
7:9:102:BCL:HMB2	8:a:103:SPN:H4	2.01	0.43
2:g:1:MET:HE3	2:g:3:LYS:HD2	2.01	0.43
8:m:102:SPN:H172	1:n:27:LEU:HD12	2.01	0.43
3:C:53:PRO:HB3	6:M:310:GLN:HB2	2.01	0.42
4:H:44:GLU:HG2	5:L:3:LEU:HD11	2.01	0.42
11:L:304:BPH:HBA1	11:L:304:BPH:H3A	1.79	0.42
7:0:101:BCL:HMC3	7:7:101:BCL:CBB	2.49	0.42
8:a:103:SPN:HM61	8:a:103:SPN:C21	2.42	0.42
3:C:24:VAL:HG22	2:o:22:VAL:CG1	2.34	0.42
4:H:32:THR:HG22	4:H:58:PRO:HB3	2.01	0.42
7:M:405:BCL:H62	7:M:405:BCL:H41	1.60	0.42
8:f:103:SPN:H282	8:f:103:SPN:HM81	1.77	0.42
7:p:101:BCL:HMC2	7:p:101:BCL:HHC	1.86	0.42
7:i:101:BCL:CHC	7:l:101:BCL:HBB3	2.49	0.42
2:o:43:TRP:C	2:o:45:GLU:H	2.27	0.42
3:C:144:MET:CE	9:C:401:HEM:C4C	3.02	0.42
4:H:35:MET:HE2	4:H:57:LEU:HD23	2.00	0.42
10:M:403:U10:H3M3	10:M:403:U10:H4M2	2.01	0.42
8:g:103:SPN:HMB3	2:k:10:ILE:HD11	2.01	0.42
8:p:103:SPN:H211	8:p:103:SPN:CM6	2.47	0.42
2:9:36:LEU:HD23	2:9:36:LEU:HA	1.95	0.42
7:L:303:BCL:HAA1	6:M:208:VAL:HG22	2.01	0.42
1:8:36:VAL:O	1:8:40:ALA:HB3	2.19	0.42
2:9:7:ILE:CD1	2:9:11:PHE:CE2	2.83	0.42
7:0:101:BCL:CED	2:9:27:LEU:CG	2.95	0.42
2:7:15:ARG:HA	2:7:15:ARG:HD3	1.94	0.42
3:C:206:LEU:HD23	3:C:206:LEU:HA	1.82	0.42
1:0:30:PHE:CE1	7:9:102:BCL:HED1	2.55	0.42
3:C:160:TYR:HD1	3:C:164:GLU:HA	1.84	0.42
7:e:101:BCL:HMC2	7:e:101:BCL:HHC	1.89	0.42
1:p:27:LEU:HA	8:p:103:SPN:H19	2.01	0.42
3:C:304:VAL:CG2	3:C:325:LYS:HE3	2.50	0.42
5:L:118:VAL:HB	5:L:119:PRO:HD3	2.01	0.42
7:i:101:BCL:HMB3	7:l:101:BCL:CHB	2.50	0.42
3:C:311:LEU:HD23	3:C:311:LEU:HA	1.90	0.41
7:o:101:BCL:HBA1	7:o:101:BCL:H3A	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:319:VAL:HG12	3:C:320:TYR:N	2.35	0.41
5:L:129:TYR:O	5:L:133:VAL:HG22	2.20	0.41
1:h:12:THR:CG2	1:h:13:ASP:H	2.32	0.41
8:m:102:SPN:HM81	8:m:102:SPN:H282	1.56	0.41
8:8:102:SPN:HM41	8:8:102:SPN:C12	2.51	0.41
2:a:30:MET:HE3	2:a:30:MET:HB3	1.91	0.41
1:f:19:LEU:HA	8:f:103:SPN:HM92	2.02	0.41
7:m:101:BCL:H121	7:m:101:BCL:H162	1.39	0.41
8:0:102:SPN:CM6	8:0:102:SPN:H151	2.50	0.41
2:o:3:LYS:O	2:o:6:LYS:HG3	2.20	0.41
8:9:101:SPN:H29	2:a:10:ILE:HD11	2.02	0.41
8:h:102:SPN:HM71	8:h:102:SPN:H241	1.66	0.41
3:C:294:MET:HE2	3:C:294:MET:HB3	1.92	0.41
7:k:101:BCL:HMC2	7:k:101:BCL:HHC	1.88	0.41
7:7:101:BCL:HAA2	7:7:101:BCL:CBD	2.51	0.41
6:M:90:GLN:O	6:M:94:LEU:HG	2.19	0.41
6:M:285:ILE:HG12	7:M:405:BCL:HED3	2.03	0.41
2:c:14:ARG:HE	2:c:14:ARG:HB2	1.76	0.41
1:d:40:ALA:HA	8:f:101:SPN:H29	2.02	0.41
7:d:101:BCL:H143	7:d:101:BCL:H112	1.78	0.41
7:f:102:BCL:H102	7:f:102:BCL:H142	2.02	0.41
8:f:103:SPN:H29	2:g:10:ILE:CD1	2.51	0.41
3:C:147:MET:HE2	3:C:147:MET:HB3	1.94	0.41
1:b:44:TRP:CD2	1:b:45:ARG:HG3	2.56	0.41
8:i:103:SPN:H272	1:l:22:VAL:HB	2.03	0.41
2:9:7:ILE:HD11	2:9:11:PHE:CD2	2.47	0.40
3:C:269:CYS:HA	3:C:282:THR:OG1	2.21	0.40
4:H:27:ILE:HD13	4:H:27:ILE:HA	1.93	0.40
1:8:32:ALA:O	1:8:36:VAL:HG23	2.21	0.40
7:M:402:BCL:HBC3	7:M:402:BCL:H2C	1.65	0.40
8:M:406:SPN:H241	8:M:406:SPN:HM71	1.32	0.40
7:g:101:BCL:HBA1	8:g:103:SPN:H72	2.03	0.40
4:H:117:ARG:HG3	4:H:234:ASP:OD2	2.21	0.40
2:m:27:LEU:HD23	7:n:101:BCL:HED2	2.03	0.40
2:7:44:PHE:CE1	2:9:38:THR:HG22	2.57	0.40
3:C:288:ALA:HB2	9:C:402:HEM:HBC2	2.02	0.40
2:a:15:ARG:H	2:a:15:ARG:HG3	1.59	0.40
7:L:301:BCL:HMB1	7:L:301:BCL:OBB	2.21	0.40
7:o:101:BCL:H42	8:p:102:SPN:H31	2.04	0.40
7:p:101:BCL:HBA1	7:p:101:BCL:H12	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	42/44 (96%)	42 (100%)	0	0	100	100
1	8	42/44 (96%)	35 (83%)	7 (17%)	0	100	100
1	b	42/44 (96%)	42 (100%)	0	0	100	100
1	d	42/44 (96%)	42 (100%)	0	0	100	100
1	f	42/44 (96%)	42 (100%)	0	0	100	100
1	h	42/44 (96%)	42 (100%)	0	0	100	100
1	j	42/44 (96%)	42 (100%)	0	0	100	100
1	l	42/44 (96%)	42 (100%)	0	0	100	100
1	n	42/44 (96%)	42 (100%)	0	0	100	100
1	p	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
2	7	49/51 (96%)	43 (88%)	6 (12%)	0	100	100
2	9	49/51 (96%)	45 (92%)	4 (8%)	0	100	100
2	a	49/51 (96%)	47 (96%)	2 (4%)	0	100	100
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%)	48 (98%)	1 (2%)	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%)	46 (94%)	3 (6%)	0	100	100
3	C	355/357 (99%)	337 (95%)	17 (5%)	1 (0%)	36	44
4	H	253/255 (99%)	248 (98%)	5 (2%)	0	100	100
5	L	271/273 (99%)	265 (98%)	5 (2%)	1 (0%)	30	36
6	M	323/325 (99%)	318 (98%)	5 (2%)	0	100	100
All	All	2112/2160 (98%)	2054 (97%)	56 (3%)	2 (0%)	49	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	14	PRO
5	L	166	LEU

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	0	37/37 (100%)	37 (100%)	0	100	100
1	8	37/37 (100%)	32 (86%)	5 (14%)	4	3
1	b	37/37 (100%)	37 (100%)	0	100	100
1	d	37/37 (100%)	37 (100%)	0	100	100
1	f	37/37 (100%)	37 (100%)	0	100	100
1	h	37/37 (100%)	37 (100%)	0	100	100
1	j	37/37 (100%)	37 (100%)	0	100	100
1	l	37/37 (100%)	37 (100%)	0	100	100
1	n	37/37 (100%)	37 (100%)	0	100	100
1	p	37/37 (100%)	36 (97%)	1 (3%)	39	52
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%)	42 (98%)	1 (2%)	44	57
2	c	43/43 (100%)	42 (98%)	1 (2%)	44	57
2	e	43/43 (100%)	43 (100%)	0	100	100
2	g	43/43 (100%)	43 (100%)	0	100	100
2	i	43/43 (100%)	42 (98%)	1 (2%)	44	57
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%)	42 (98%)	1 (2%)	44	57
3	C	304/304 (100%)	301 (99%)	3 (1%)	68	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	H	213/213 (100%)	212 (100%)	1 (0%)	81	87
5	L	217/217 (100%)	217 (100%)	0	100	100
6	M	266/266 (100%)	263 (99%)	3 (1%)	65	75
All	All	1800/1800 (100%)	1783 (99%)	17 (1%)	68	80

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	8	33	VAL
1	8	41	THR
1	8	42	PHE
1	8	43	ILE
1	8	45	ARG
3	C	26	VAL
3	C	101	VAL
3	C	104	VAL
4	H	194	VAL
6	M	180	ILE
6	M	275	VAL
6	M	309	THR
2	a	45	GLU
2	c	34	VAL
2	i	18	VAL
2	o	46	LEU
1	p	45	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
2	7	40	HIS
2	7	50	ASN
1	8	20	HIS
2	9	40	HIS
2	9	42	ASN
3	C	176	GLN
3	C	223	ASN
3	C	226	GLN
4	H	94	ASN
4	H	226	ASN
4	H	255	GLN

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Mol	Chain	Res	Type
5	L	171	ASN
5	L	240	ASN
6	M	196	ASN
6	M	267	HIS
2	a	20	GLN
2	a	40	HIS
2	e	40	HIS
2	e	50	ASN
2	g	42	ASN
2	k	42	ASN
2	m	40	HIS
2	o	40	HIS
1	p	15	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 53 ligands modelled in this entry, 1 is monoatomic - leaving 52 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	$\# Z > 2$
8	SPN	i	102	-	42,42,42	3.89	20 (47%)	50,52,52	2.39	21 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	BPH	L	305	-	59,70,70	1.16	4 (6%)	59,101,101	1.60	11 (18%)
11	BPH	L	304	-	59,70,70	1.14	3 (5%)	59,101,101	0.94	4 (6%)
8	SPN	g	102	-	42,42,42	3.90	20 (47%)	50,52,52	2.38	21 (42%)
8	SPN	f	103	-	42,42,42	3.95	20 (47%)	50,52,52	2.54	15 (30%)
7	BCL	d	101	1	69,74,74	0.55	0	79,115,115	1.08	9 (11%)
8	SPN	a	102	-	42,42,42	3.90	20 (47%)	50,52,52	2.39	21 (42%)
10	U10	L	302	-	38,38,63	0.21	0	48,49,79	0.52	1 (2%)
7	BCL	0	101	1	69,74,74	0.55	0	79,115,115	1.01	7 (8%)
8	SPN	f	101	-	42,42,42	3.90	20 (47%)	50,52,52	2.39	21 (42%)
7	BCL	h	101	1	69,74,74	0.62	2 (2%)	79,115,115	0.97	5 (6%)
7	BCL	M	402	6	69,74,74	0.59	1 (1%)	79,115,115	1.11	10 (12%)
7	BCL	f	102	1	69,74,74	0.59	1 (1%)	79,115,115	1.00	9 (11%)
8	SPN	M	406	-	42,42,42	3.97	20 (47%)	50,52,52	2.68	16 (32%)
8	SPN	g	103	-	42,42,42	3.95	20 (47%)	50,52,52	2.53	15 (30%)
8	SPN	i	103	-	42,42,42	3.92	20 (47%)	50,52,52	2.54	16 (32%)
11	BPH	M	404	-	59,70,70	1.12	3 (5%)	59,101,101	0.91	4 (6%)
8	SPN	0	102	-	42,42,42	3.97	20 (47%)	50,52,52	2.52	20 (40%)
8	SPN	m	102	-	42,42,42	3.95	20 (47%)	50,52,52	2.40	18 (36%)
7	BCL	M	405	6	69,74,74	0.66	2 (2%)	79,115,115	0.96	6 (7%)
8	SPN	l	102	-	42,42,42	3.90	20 (47%)	50,52,52	2.39	21 (42%)
9	HEM	C	402	3	50,50,50	0.77	1 (2%)	67,82,82	1.09	4 (5%)
7	BCL	9	102	2	69,74,74	0.57	1 (1%)	79,115,115	1.11	12 (15%)
7	BCL	g	101	2	69,74,74	0.62	2 (2%)	79,115,115	0.99	8 (10%)
7	BCL	o	101	2	69,74,74	0.52	0	79,115,115	1.04	9 (11%)
7	BCL	p	101	1	69,74,74	0.48	0	79,115,115	1.08	11 (13%)
8	SPN	8	102	-	42,42,42	3.94	20 (47%)	50,52,52	2.40	21 (42%)
8	SPN	a	103	-	42,42,42	3.97	20 (47%)	50,52,52	2.48	17 (34%)
7	BCL	a	101	2	69,74,74	0.59	2 (2%)	79,115,115	1.02	10 (12%)
7	BCL	b	101	1	69,74,74	0.55	0	79,115,115	1.08	10 (12%)
8	SPN	e	102	-	42,42,42	3.87	20 (47%)	50,52,52	2.40	21 (42%)
7	BCL	7	101	2	69,74,74	0.52	0	79,115,115	1.11	12 (15%)
8	SPN	a	104	-	42,42,42	3.94	20 (47%)	50,52,52	2.40	17 (34%)
7	BCL	n	101	1	69,74,74	0.51	0	79,115,115	1.07	10 (12%)
9	HEM	C	403	3	50,50,50	0.74	1 (2%)	67,82,82	0.64	0
10	U10	M	403	-	63,63,63	0.18	0	78,79,79	0.42	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	BCL	k	101	2	69,74,74	0.63	2 (2%)	79,115,115	1.00	8 (10%)
7	BCL	L	303	5	69,74,74	0.74	3 (4%)	79,115,115	0.98	7 (8%)
7	BCL	m	101	2	69,74,74	0.62	2 (2%)	79,115,115	1.00	8 (10%)
7	BCL	L	301	5	69,74,74	0.71	3 (4%)	79,115,115	1.07	10 (12%)
7	BCL	i	101	2	69,74,74	0.70	3 (4%)	79,115,115	0.99	9 (11%)
7	BCL	l	101	1	69,74,74	0.55	0	79,115,115	1.03	7 (8%)
8	SPN	p	103	-	42,42,42	3.98	20 (47%)	50,52,52	2.44	18 (36%)
7	BCL	8	101	-	69,74,74	0.52	0	79,115,115	1.18	13 (16%)
8	SPN	9	101	-	42,42,42	3.95	20 (47%)	50,52,52	2.37	19 (38%)
7	BCL	c	101	2	69,74,74	0.60	1 (1%)	79,115,115	1.01	9 (11%)
8	SPN	h	102	-	42,42,42	3.90	20 (47%)	50,52,52	2.56	16 (32%)
9	HEM	C	401	3	50,50,50	0.76	1 (2%)	67,82,82	0.63	0
7	BCL	e	101	2	69,74,74	0.62	1 (1%)	79,115,115	1.00	9 (11%)
8	SPN	p	102	-	42,42,42	3.92	20 (47%)	50,52,52	2.40	19 (38%)
7	BCL	j	101	1	69,74,74	0.62	3 (4%)	79,115,115	1.02	7 (8%)
8	SPN	n	102	-	42,42,42	3.89	20 (47%)	50,52,52	2.37	22 (44%)

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
8	SPN	i	102	-	-	19/50/51/51	-
11	BPH	L	305	-	-	19/37/105/105	0/5/6/6
11	BPH	L	304	-	-	9/37/105/105	0/5/6/6
8	SPN	g	102	-	-	19/50/51/51	-
8	SPN	f	103	-	-	20/50/51/51	-
7	BCL	d	101	1	-	22/41/137/137	-
8	SPN	a	102	-	-	19/50/51/51	-
10	U10	L	302	-	-	5/33/57/87	0/1/1/1
7	BCL	0	101	1	-	23/41/137/137	-
8	SPN	f	101	-	-	20/50/51/51	-
7	BCL	h	101	1	-	14/41/137/137	-
7	BCL	M	402	6	-	16/41/137/137	-
7	BCL	f	102	1	-	17/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	SPN	M	406	-	-	19/50/51/51	-
8	SPN	g	103	-	-	20/50/51/51	-
8	SPN	i	103	-	-	21/50/51/51	-
11	BPH	M	404	-	-	9/37/105/105	0/5/6/6
8	SPN	0	102	-	-	18/50/51/51	-
8	SPN	m	102	-	-	20/50/51/51	-
7	BCL	M	405	6	-	17/41/137/137	-
8	SPN	l	102	-	-	21/50/51/51	-
9	HEM	C	402	3	-	4/14/54/54	-
7	BCL	9	102	2	-	19/41/137/137	-
7	BCL	g	101	2	-	16/41/137/137	-
7	BCL	o	101	2	-	21/41/137/137	-
7	BCL	p	101	1	-	18/41/137/137	-
8	SPN	8	102	-	-	18/50/51/51	-
8	SPN	a	103	-	-	22/50/51/51	-
7	BCL	a	101	2	-	21/41/137/137	-
7	BCL	b	101	1	-	21/41/137/137	-
8	SPN	e	102	-	-	20/50/51/51	-
7	BCL	7	101	2	-	18/41/137/137	-
8	SPN	a	104	-	-	20/50/51/51	-
7	BCL	n	101	1	-	20/41/137/137	-
9	HEM	C	403	3	-	4/14/54/54	-
10	U10	M	403	-	-	14/63/87/87	0/1/1/1
7	BCL	k	101	2	-	16/41/137/137	-
7	BCL	L	303	5	-	18/41/137/137	-
7	BCL	m	101	2	-	21/41/137/137	-
7	BCL	L	301	5	-	15/41/137/137	-
7	BCL	i	101	2	-	14/41/137/137	-
7	BCL	l	101	1	-	16/41/137/137	-
8	SPN	p	103	-	-	21/50/51/51	-
7	BCL	8	101	-	-	22/41/137/137	-
8	SPN	9	101	-	-	22/50/51/51	-
7	BCL	c	101	2	-	15/41/137/137	-
8	SPN	h	102	-	-	20/50/51/51	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	HEM	C	401	3	-	5/14/54/54	-
7	BCL	e	101	2	-	19/41/137/137	-
8	SPN	p	102	-	-	26/50/51/51	-
7	BCL	j	101	1	-	18/41/137/137	-
8	SPN	n	102	-	-	22/50/51/51	-

All (442) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	a	103	SPN	C3-C4	-11.22	1.32	1.50
8	g	103	SPN	C3-C4	-11.19	1.33	1.50
8	p	103	SPN	C3-C4	-11.16	1.33	1.50
8	M	406	SPN	C3-C4	-11.13	1.33	1.50
8	m	102	SPN	C3-C4	-11.12	1.33	1.50
8	f	103	SPN	C3-C4	-11.08	1.33	1.50
8	a	104	SPN	C3-C4	-11.06	1.33	1.50
8	h	102	SPN	C3-C4	-11.05	1.33	1.50
8	0	102	SPN	C3-C4	-11.02	1.33	1.50
8	8	102	SPN	C3-C4	-11.02	1.33	1.50
8	i	103	SPN	C3-C4	-11.01	1.33	1.50
8	9	101	SPN	C3-C4	-11.01	1.33	1.50
8	p	102	SPN	C3-C4	-10.98	1.33	1.50
8	g	102	SPN	C3-C4	-10.90	1.33	1.50
8	i	102	SPN	C3-C4	-10.84	1.33	1.50
8	a	102	SPN	C3-C4	-10.83	1.33	1.50
8	l	102	SPN	C3-C4	-10.83	1.33	1.50
8	f	101	SPN	C3-C4	-10.81	1.33	1.50
8	n	102	SPN	C3-C4	-10.77	1.33	1.50
8	e	102	SPN	C3-C4	-10.76	1.33	1.50
8	M	406	SPN	C10-C9	-7.57	1.35	1.51
8	M	406	SPN	C14-C13	-7.56	1.35	1.51
8	p	103	SPN	C10-C9	-7.52	1.35	1.51
8	p	103	SPN	C6-C5	-7.52	1.35	1.51
8	M	406	SPN	C6-C5	-7.51	1.35	1.51
8	a	103	SPN	C17-C18	-7.51	1.35	1.51
8	a	103	SPN	C6-C5	-7.51	1.35	1.51
8	g	103	SPN	C6-C5	-7.50	1.35	1.51
8	0	102	SPN	C10-C9	-7.50	1.35	1.51
8	f	103	SPN	C6-C5	-7.49	1.35	1.51
8	p	103	SPN	C14-C13	-7.48	1.35	1.51
8	p	102	SPN	C6-C5	-7.46	1.35	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	8	102	SPN	C17-C18	-7.46	1.35	1.51
8	g	103	SPN	C14-C13	-7.46	1.35	1.51
8	a	103	SPN	C10-C9	-7.46	1.35	1.51
8	M	406	SPN	C17-C18	-7.46	1.35	1.51
8	g	102	SPN	C6-C5	-7.46	1.35	1.51
8	g	103	SPN	C17-C18	-7.46	1.35	1.51
8	0	102	SPN	C6-C5	-7.46	1.35	1.51
8	a	104	SPN	C17-C18	-7.45	1.35	1.51
8	m	102	SPN	C10-C9	-7.45	1.35	1.51
8	g	103	SPN	C10-C9	-7.45	1.35	1.51
8	a	103	SPN	C14-C13	-7.45	1.35	1.51
8	8	102	SPN	C14-C13	-7.45	1.35	1.51
8	a	104	SPN	C6-C5	-7.45	1.35	1.51
8	9	101	SPN	C10-C9	-7.44	1.35	1.51
8	f	101	SPN	C14-C13	-7.44	1.35	1.51
8	m	102	SPN	C17-C18	-7.44	1.35	1.51
8	p	103	SPN	C17-C18	-7.44	1.35	1.51
8	9	101	SPN	C17-C18	-7.44	1.36	1.51
8	h	102	SPN	C6-C5	-7.44	1.36	1.51
8	a	104	SPN	C10-C9	-7.43	1.36	1.51
8	f	103	SPN	C17-C18	-7.43	1.36	1.51
8	l	102	SPN	C10-C9	-7.43	1.36	1.51
8	m	102	SPN	C6-C5	-7.43	1.36	1.51
8	9	101	SPN	C6-C5	-7.43	1.36	1.51
8	f	103	SPN	C14-C13	-7.43	1.36	1.51
8	a	102	SPN	C6-C5	-7.43	1.36	1.51
8	8	102	SPN	C6-C5	-7.43	1.36	1.51
8	n	102	SPN	C14-C13	-7.42	1.36	1.51
8	p	102	SPN	C17-C18	-7.42	1.36	1.51
8	l	102	SPN	C17-C18	-7.42	1.36	1.51
8	i	103	SPN	C6-C5	-7.41	1.36	1.51
8	9	101	SPN	C14-C13	-7.41	1.36	1.51
8	p	102	SPN	C10-C9	-7.41	1.36	1.51
8	m	102	SPN	C14-C13	-7.41	1.36	1.51
8	g	102	SPN	C17-C18	-7.41	1.36	1.51
8	f	103	SPN	C10-C9	-7.41	1.36	1.51
8	i	102	SPN	C6-C5	-7.41	1.36	1.51
8	e	102	SPN	C14-C13	-7.40	1.36	1.51
8	i	102	SPN	C17-C18	-7.40	1.36	1.51
8	i	103	SPN	C17-C18	-7.40	1.36	1.51
8	h	102	SPN	C14-C13	-7.40	1.36	1.51
8	0	102	SPN	C14-C13	-7.40	1.36	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	a	104	SPN	C14-C13	-7.40	1.36	1.51
8	i	102	SPN	C14-C13	-7.40	1.36	1.51
8	i	102	SPN	C10-C9	-7.40	1.36	1.51
8	n	102	SPN	C10-C9	-7.40	1.36	1.51
8	n	102	SPN	C17-C18	-7.40	1.36	1.51
8	a	102	SPN	C14-C13	-7.39	1.36	1.51
8	e	102	SPN	C10-C9	-7.39	1.36	1.51
8	a	102	SPN	C10-C9	-7.39	1.36	1.51
8	a	102	SPN	C17-C18	-7.39	1.36	1.51
8	l	102	SPN	C6-C5	-7.39	1.36	1.51
8	h	102	SPN	C10-C9	-7.39	1.36	1.51
8	i	103	SPN	C14-C13	-7.38	1.36	1.51
8	g	102	SPN	C14-C13	-7.38	1.36	1.51
8	i	103	SPN	C10-C9	-7.38	1.36	1.51
8	f	101	SPN	C17-C18	-7.38	1.36	1.51
8	n	102	SPN	C6-C5	-7.38	1.36	1.51
8	g	102	SPN	C10-C9	-7.38	1.36	1.51
8	f	101	SPN	C10-C9	-7.38	1.36	1.51
8	e	102	SPN	C6-C5	-7.38	1.36	1.51
8	l	102	SPN	C14-C13	-7.38	1.36	1.51
8	e	102	SPN	C17-C18	-7.37	1.36	1.51
8	f	101	SPN	C6-C5	-7.36	1.36	1.51
8	h	102	SPN	C17-C18	-7.36	1.36	1.51
8	p	102	SPN	C14-C13	-7.34	1.36	1.51
8	8	102	SPN	C10-C9	-7.27	1.36	1.51
8	0	102	SPN	C17-C18	-7.22	1.36	1.51
8	0	102	SPN	C3-C2	-6.85	1.46	1.52
8	p	103	SPN	C3-C2	-6.55	1.46	1.52
8	M	406	SPN	C3-C2	-6.31	1.46	1.52
8	p	102	SPN	C3-C2	-6.31	1.46	1.52
8	a	103	SPN	C3-C2	-6.30	1.46	1.52
8	f	103	SPN	C3-C2	-6.28	1.46	1.52
8	8	102	SPN	C3-C2	-6.17	1.46	1.52
8	i	103	SPN	C19-C18	5.90	1.46	1.33
8	9	101	SPN	C3-C2	-5.89	1.47	1.52
8	m	102	SPN	C3-C2	-5.88	1.47	1.52
8	g	103	SPN	C19-C18	5.88	1.46	1.33
8	a	103	SPN	C19-C18	5.87	1.46	1.33
8	p	102	SPN	C8-C9	5.86	1.46	1.33
11	L	304	BPH	C1D-C2D	5.86	1.46	1.39
8	M	406	SPN	C19-C18	5.81	1.46	1.33
8	i	103	SPN	C3-C2	-5.80	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	p	102	SPN	C12-C13	5.77	1.46	1.33
8	f	101	SPN	C3-C2	-5.74	1.47	1.52
8	a	104	SPN	C3-C2	-5.71	1.47	1.52
11	M	404	BPH	C1D-C2D	5.70	1.45	1.39
8	f	103	SPN	C19-C18	5.69	1.46	1.33
11	L	305	BPH	C1D-C2D	5.68	1.45	1.39
8	l	102	SPN	C8-C9	5.67	1.46	1.33
8	p	103	SPN	C19-C18	5.66	1.46	1.33
8	l	102	SPN	C3-C2	-5.65	1.47	1.52
8	f	101	SPN	C12-C13	5.64	1.46	1.33
8	e	102	SPN	C12-C13	5.64	1.46	1.33
8	e	102	SPN	C8-C9	5.63	1.46	1.33
8	h	102	SPN	C19-C18	5.63	1.46	1.33
8	i	102	SPN	C4-C5	5.63	1.46	1.33
8	M	406	SPN	C11-C12	-5.63	1.33	1.50
8	e	102	SPN	C4-C5	5.62	1.46	1.33
8	i	102	SPN	C12-C13	5.62	1.46	1.33
8	n	102	SPN	C12-C13	5.62	1.46	1.33
8	n	102	SPN	C8-C9	5.62	1.46	1.33
8	f	101	SPN	C8-C9	5.61	1.46	1.33
8	l	102	SPN	C12-C13	5.61	1.46	1.33
8	g	102	SPN	C12-C13	5.60	1.46	1.33
8	a	102	SPN	C4-C5	5.60	1.46	1.33
8	i	102	SPN	C8-C9	5.60	1.45	1.33
8	g	102	SPN	C4-C5	5.59	1.45	1.33
8	a	102	SPN	C8-C9	5.59	1.45	1.33
8	l	102	SPN	C4-C5	5.59	1.45	1.33
8	g	103	SPN	C4-C5	5.59	1.45	1.33
8	a	102	SPN	C12-C13	5.59	1.45	1.33
8	h	102	SPN	C8-C9	5.58	1.45	1.33
8	i	103	SPN	C12-C13	5.58	1.45	1.33
8	h	102	SPN	C12-C13	5.58	1.45	1.33
8	f	103	SPN	C4-C5	5.57	1.45	1.33
8	l	102	SPN	C19-C18	5.57	1.45	1.33
8	g	102	SPN	C8-C9	5.57	1.45	1.33
8	i	103	SPN	C8-C9	5.57	1.45	1.33
8	p	102	SPN	C4-C5	5.57	1.45	1.33
8	f	101	SPN	C4-C5	5.57	1.45	1.33
8	m	102	SPN	C8-C9	5.57	1.45	1.33
8	a	104	SPN	C8-C9	5.56	1.45	1.33
8	f	103	SPN	C12-C13	5.56	1.45	1.33
8	p	102	SPN	C19-C18	5.56	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	n	102	SPN	C4-C5	5.56	1.45	1.33
8	9	101	SPN	C4-C5	5.55	1.45	1.33
8	g	102	SPN	C19-C18	5.55	1.45	1.33
8	i	103	SPN	C4-C5	5.55	1.45	1.33
8	f	103	SPN	C8-C9	5.55	1.45	1.33
8	a	104	SPN	C4-C5	5.55	1.45	1.33
8	0	102	SPN	C12-C13	5.54	1.45	1.33
8	a	104	SPN	C12-C13	5.54	1.45	1.33
8	h	102	SPN	C4-C5	5.54	1.45	1.33
8	9	101	SPN	C8-C9	5.54	1.45	1.33
8	8	102	SPN	C19-C18	5.54	1.45	1.33
8	e	102	SPN	C19-C18	5.53	1.45	1.33
8	p	103	SPN	C8-C9	5.53	1.45	1.33
8	f	101	SPN	C19-C18	5.53	1.45	1.33
8	m	102	SPN	C19-C18	5.53	1.45	1.33
8	M	406	SPN	C4-C5	5.52	1.45	1.33
8	a	102	SPN	C19-C18	5.52	1.45	1.33
8	m	102	SPN	C4-C5	5.52	1.45	1.33
8	n	102	SPN	C19-C18	5.52	1.45	1.33
8	p	103	SPN	C4-C5	5.52	1.45	1.33
8	0	102	SPN	C8-C9	5.51	1.45	1.33
8	p	103	SPN	C12-C13	5.51	1.45	1.33
8	8	102	SPN	C12-C13	5.51	1.45	1.33
8	9	101	SPN	C12-C13	5.51	1.45	1.33
8	a	102	SPN	C3-C2	-5.51	1.47	1.52
8	0	102	SPN	C4-C5	5.51	1.45	1.33
8	9	101	SPN	C19-C18	5.51	1.45	1.33
8	a	103	SPN	C8-C9	5.50	1.45	1.33
8	a	104	SPN	C19-C18	5.50	1.45	1.33
8	i	102	SPN	C19-C18	5.50	1.45	1.33
8	8	102	SPN	C8-C9	5.49	1.45	1.33
8	a	103	SPN	C12-C13	5.49	1.45	1.33
8	a	103	SPN	C4-C5	5.49	1.45	1.33
8	M	406	SPN	C8-C9	5.49	1.45	1.33
8	m	102	SPN	C12-C13	5.48	1.45	1.33
8	M	406	SPN	C12-C13	5.47	1.45	1.33
8	M	406	SPN	C7-C8	-5.47	1.33	1.50
8	8	102	SPN	C4-C5	5.47	1.45	1.33
8	0	102	SPN	C19-C18	5.47	1.45	1.33
8	g	103	SPN	C8-C9	5.46	1.45	1.33
8	g	103	SPN	C12-C13	5.45	1.45	1.33
8	h	102	SPN	C3-C2	-5.44	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	0	102	SPN	C11-C12	-5.44	1.34	1.50
8	9	101	SPN	C11-C12	-5.39	1.34	1.50
8	p	103	SPN	C7-C8	-5.39	1.34	1.50
8	0	102	SPN	C7-C8	-5.38	1.34	1.50
8	g	103	SPN	C7-C8	-5.37	1.34	1.50
8	g	103	SPN	C3-C2	-5.37	1.47	1.52
8	9	101	SPN	C20-C19	-5.37	1.34	1.50
8	9	101	SPN	C7-C8	-5.36	1.34	1.50
8	a	104	SPN	C20-C19	-5.35	1.34	1.50
8	a	104	SPN	C7-C8	-5.35	1.34	1.50
8	p	103	SPN	C11-C12	-5.34	1.34	1.50
8	a	103	SPN	C7-C8	-5.34	1.34	1.50
8	m	102	SPN	C7-C8	-5.34	1.34	1.50
8	8	102	SPN	C20-C19	-5.34	1.34	1.50
8	m	102	SPN	C11-C12	-5.33	1.34	1.50
8	0	102	SPN	C20-C19	-5.32	1.34	1.50
8	g	102	SPN	C7-C8	-5.30	1.34	1.50
8	f	103	SPN	C7-C8	-5.30	1.34	1.50
8	e	102	SPN	C20-C19	-5.30	1.34	1.50
8	8	102	SPN	C7-C8	-5.30	1.34	1.50
8	i	102	SPN	C11-C12	-5.30	1.34	1.50
8	m	102	SPN	C20-C19	-5.30	1.34	1.50
8	a	103	SPN	C11-C12	-5.30	1.34	1.50
8	h	102	SPN	C7-C8	-5.29	1.34	1.50
8	n	102	SPN	C20-C19	-5.28	1.34	1.50
8	g	102	SPN	C3-C2	-5.28	1.47	1.52
8	a	102	SPN	C20-C19	-5.28	1.34	1.50
8	g	103	SPN	C11-C12	-5.28	1.34	1.50
8	a	104	SPN	C11-C12	-5.28	1.34	1.50
8	i	102	SPN	C20-C19	-5.27	1.34	1.50
8	e	102	SPN	C11-C12	-5.27	1.34	1.50
8	n	102	SPN	C11-C12	-5.26	1.34	1.50
8	8	102	SPN	C11-C12	-5.25	1.34	1.50
8	f	101	SPN	C11-C12	-5.25	1.34	1.50
8	a	102	SPN	C7-C8	-5.25	1.34	1.50
8	g	102	SPN	C11-C12	-5.25	1.34	1.50
8	l	102	SPN	C20-C19	-5.25	1.34	1.50
8	a	102	SPN	C11-C12	-5.24	1.34	1.50
8	i	103	SPN	C7-C8	-5.24	1.34	1.50
8	i	102	SPN	C7-C8	-5.24	1.34	1.50
8	f	101	SPN	C7-C8	-5.24	1.34	1.50
8	f	101	SPN	C20-C19	-5.23	1.34	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	f	103	SPN	C11-C12	-5.23	1.34	1.50
8	l	102	SPN	C7-C8	-5.22	1.34	1.50
8	l	102	SPN	C11-C12	-5.22	1.34	1.50
8	n	102	SPN	C7-C8	-5.22	1.34	1.50
8	i	103	SPN	C11-C12	-5.21	1.34	1.50
8	g	102	SPN	C20-C19	-5.20	1.34	1.50
8	e	102	SPN	C7-C8	-5.20	1.34	1.50
8	n	102	SPN	C3-C2	-5.19	1.47	1.52
8	p	102	SPN	C20-C19	-5.17	1.34	1.50
8	h	102	SPN	C11-C12	-5.17	1.34	1.50
8	p	103	SPN	C20-C19	-5.15	1.34	1.50
8	i	102	SPN	C3-C2	-5.15	1.47	1.52
8	p	102	SPN	C11-C12	-5.04	1.35	1.50
8	h	102	SPN	C20-C19	-4.99	1.35	1.50
8	f	103	SPN	C20-C19	-4.98	1.35	1.50
8	e	102	SPN	C3-C2	-4.89	1.47	1.52
8	g	103	SPN	C20-C19	-4.87	1.35	1.50
8	a	103	SPN	C20-C19	-4.86	1.35	1.50
8	i	103	SPN	C20-C19	-4.78	1.36	1.50
8	p	102	SPN	C7-C8	-4.75	1.36	1.50
8	M	406	SPN	C20-C19	-4.66	1.36	1.50
8	8	102	SPN	C21-C22	-3.75	1.34	1.52
8	p	103	SPN	C21-C22	-3.75	1.34	1.52
8	9	101	SPN	C21-C22	-3.75	1.34	1.52
8	n	102	SPN	C21-C22	-3.75	1.34	1.52
8	0	102	SPN	C21-C22	-3.74	1.34	1.52
8	a	103	SPN	C21-C22	-3.72	1.34	1.52
8	a	102	SPN	C21-C22	-3.71	1.34	1.52
8	a	104	SPN	C21-C22	-3.71	1.34	1.52
8	m	102	SPN	C21-C22	-3.71	1.34	1.52
8	g	103	SPN	C21-C22	-3.70	1.34	1.52
8	e	102	SPN	C21-C22	-3.70	1.34	1.52
8	i	102	SPN	C21-C22	-3.70	1.34	1.52
8	f	101	SPN	C21-C22	-3.69	1.34	1.52
8	l	102	SPN	C21-C22	-3.69	1.34	1.52
8	p	102	SPN	C21-C22	-3.69	1.34	1.52
8	i	103	SPN	C21-C22	-3.68	1.34	1.52
11	L	305	BPH	C3B-C4B	-3.68	1.35	1.41
8	g	102	SPN	C21-C22	-3.68	1.34	1.52
8	M	406	SPN	C21-C22	-3.67	1.34	1.52
8	f	103	SPN	C21-C22	-3.65	1.34	1.52
8	h	102	SPN	C21-C22	-3.61	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	g	103	SPN	C10-C11	-3.34	1.42	1.53
9	C	402	HEM	FE-NB	3.33	2.05	1.94
8	M	406	SPN	C10-C11	-3.31	1.42	1.53
8	m	102	SPN	C10-C11	-3.30	1.42	1.53
8	a	103	SPN	C10-C11	-3.28	1.42	1.53
8	0	102	SPN	C21-C20	-3.28	1.42	1.53
8	8	102	SPN	C16-C15	-3.27	1.35	1.51
8	9	101	SPN	C10-C11	-3.27	1.42	1.53
8	M	406	SPN	C6-C7	-3.26	1.43	1.53
8	g	103	SPN	C16-C15	-3.26	1.35	1.51
8	0	102	SPN	C16-C15	-3.24	1.35	1.51
8	p	103	SPN	C10-C11	-3.24	1.43	1.53
8	g	103	SPN	C6-C7	-3.24	1.43	1.53
8	i	102	SPN	C16-C15	-3.24	1.35	1.51
8	9	101	SPN	C16-C15	-3.24	1.35	1.51
8	i	103	SPN	C21-C20	-3.23	1.42	1.53
8	a	103	SPN	C16-C15	-3.23	1.35	1.51
8	m	102	SPN	C16-C15	-3.22	1.35	1.51
8	g	102	SPN	C16-C15	-3.22	1.35	1.51
8	p	103	SPN	C16-C15	-3.21	1.35	1.51
8	0	102	SPN	C10-C11	-3.21	1.43	1.53
8	0	102	SPN	C6-C7	-3.21	1.43	1.53
8	g	103	SPN	C21-C20	-3.21	1.42	1.53
8	8	102	SPN	C6-C7	-3.20	1.43	1.53
8	l	102	SPN	C16-C15	-3.20	1.35	1.51
8	p	103	SPN	C6-C7	-3.20	1.43	1.53
8	a	104	SPN	C16-C15	-3.20	1.35	1.51
8	9	101	SPN	C6-C7	-3.19	1.43	1.53
8	a	104	SPN	C10-C11	-3.19	1.43	1.53
8	f	101	SPN	C16-C15	-3.19	1.35	1.51
8	f	103	SPN	C16-C15	-3.19	1.35	1.51
8	p	102	SPN	C16-C15	-3.19	1.35	1.51
9	C	401	HEM	FE-NB	3.19	2.04	1.94
8	a	103	SPN	C6-C7	-3.19	1.43	1.53
8	e	102	SPN	C16-C15	-3.19	1.35	1.51
8	n	102	SPN	C16-C15	-3.18	1.36	1.51
8	g	102	SPN	C6-C7	-3.18	1.43	1.53
8	i	103	SPN	C10-C11	-3.17	1.43	1.53
8	a	104	SPN	C21-C20	-3.17	1.43	1.53
8	M	406	SPN	C16-C15	-3.17	1.36	1.51
8	i	103	SPN	C16-C15	-3.17	1.36	1.51
8	8	102	SPN	C21-C20	-3.16	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	m	102	SPN	C21-C20	-3.15	1.43	1.53
8	a	102	SPN	C16-C15	-3.15	1.36	1.51
8	f	103	SPN	C10-C11	-3.15	1.43	1.53
8	h	102	SPN	C16-C15	-3.15	1.36	1.51
8	n	102	SPN	C21-C20	-3.15	1.43	1.53
8	h	102	SPN	C21-C20	-3.14	1.43	1.53
8	m	102	SPN	C6-C7	-3.14	1.43	1.53
8	9	101	SPN	C21-C20	-3.14	1.43	1.53
8	a	104	SPN	C6-C7	-3.12	1.43	1.53
8	f	103	SPN	C6-C7	-3.11	1.43	1.53
11	L	304	BPH	C3B-C2B	3.11	1.45	1.39
8	f	103	SPN	C21-C20	-3.11	1.43	1.53
8	i	102	SPN	C21-C20	-3.10	1.43	1.53
8	h	102	SPN	C10-C11	-3.10	1.43	1.53
8	g	102	SPN	C10-C11	-3.10	1.43	1.53
8	f	101	SPN	C21-C20	-3.08	1.43	1.53
8	a	102	SPN	C21-C20	-3.07	1.43	1.53
8	e	102	SPN	C21-C20	-3.07	1.43	1.53
8	a	103	SPN	C21-C20	-3.07	1.43	1.53
8	p	103	SPN	C21-C20	-3.06	1.43	1.53
8	i	102	SPN	C6-C7	-3.05	1.43	1.53
8	a	102	SPN	C6-C7	-3.04	1.43	1.53
11	M	404	BPH	C3B-C2B	3.04	1.44	1.39
8	p	102	SPN	C10-C11	-3.03	1.43	1.53
7	L	301	BCL	MG-NC	3.03	2.13	2.06
8	g	102	SPN	C21-C20	-3.03	1.43	1.53
11	M	404	BPH	C2C-C3C	3.02	1.57	1.54
8	n	102	SPN	C6-C7	-3.02	1.43	1.53
8	e	102	SPN	C10-C11	-3.02	1.43	1.53
8	i	102	SPN	C10-C11	-3.01	1.43	1.53
8	i	103	SPN	C6-C7	-3.00	1.43	1.53
9	C	403	HEM	FE-NB	3.00	2.04	1.94
8	l	102	SPN	C6-C7	-3.00	1.43	1.53
8	n	102	SPN	C10-C11	-2.99	1.43	1.53
8	h	102	SPN	C6-C7	-2.99	1.43	1.53
8	l	102	SPN	C21-C20	-2.98	1.43	1.53
8	f	101	SPN	C10-C11	-2.98	1.43	1.53
8	l	102	SPN	C10-C11	-2.98	1.43	1.53
8	e	102	SPN	C6-C7	-2.97	1.43	1.53
8	a	102	SPN	C10-C11	-2.97	1.43	1.53
8	f	101	SPN	C6-C7	-2.97	1.43	1.53
8	p	102	SPN	C21-C20	-2.94	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	p	102	SPN	C6-C7	-2.91	1.44	1.53
7	L	303	BCL	C4B-NB	2.86	1.41	1.37
7	i	101	BCL	MG-NC	2.82	2.13	2.06
11	L	304	BPH	C2C-C3C	2.82	1.57	1.54
11	L	305	BPH	C2C-C3C	2.81	1.57	1.54
8	8	102	SPN	C10-C11	-2.78	1.44	1.53
8	M	406	SPN	C15-C14	-2.70	1.42	1.52
8	g	103	SPN	C16-C17	-2.64	1.42	1.52
7	m	101	BCL	MG-NC	2.61	2.12	2.06
7	L	301	BCL	C4B-NB	2.61	1.41	1.37
8	g	103	SPN	C15-C14	-2.60	1.42	1.52
7	c	101	BCL	MG-NC	2.60	2.12	2.06
8	a	103	SPN	C15-C14	-2.60	1.42	1.52
8	f	103	SPN	C16-C17	-2.56	1.42	1.52
11	L	305	BPH	C3B-C2B	2.55	1.44	1.39
7	M	405	BCL	C4B-NB	2.53	1.41	1.37
8	8	102	SPN	C16-C17	-2.53	1.42	1.52
8	f	103	SPN	C15-C14	-2.52	1.43	1.52
8	i	103	SPN	C16-C17	-2.52	1.43	1.52
8	a	103	SPN	C16-C17	-2.52	1.43	1.52
8	a	104	SPN	C15-C14	-2.52	1.43	1.52
8	a	104	SPN	C16-C17	-2.50	1.43	1.52
7	L	303	BCL	MG-NC	2.47	2.12	2.06
8	9	101	SPN	C15-C14	-2.47	1.43	1.52
8	i	103	SPN	C15-C14	-2.47	1.43	1.52
8	p	103	SPN	C16-C17	-2.47	1.43	1.52
8	m	102	SPN	C15-C14	-2.46	1.43	1.52
8	h	102	SPN	C16-C17	-2.46	1.43	1.52
8	m	102	SPN	C16-C17	-2.46	1.43	1.52
8	M	406	SPN	C21-C20	-2.46	1.45	1.53
8	p	103	SPN	C15-C14	-2.46	1.43	1.52
8	8	102	SPN	C15-C14	-2.45	1.43	1.52
7	M	402	BCL	C4B-NB	2.44	1.41	1.37
8	9	101	SPN	C16-C17	-2.44	1.43	1.52
8	h	102	SPN	C15-C14	-2.44	1.43	1.52
8	e	102	SPN	C16-C17	-2.42	1.43	1.52
8	n	102	SPN	C16-C17	-2.42	1.43	1.52
8	i	102	SPN	C16-C17	-2.41	1.43	1.52
7	e	101	BCL	MG-NC	2.39	2.12	2.06
8	0	102	SPN	C15-C14	-2.38	1.43	1.52
8	g	102	SPN	C16-C17	-2.38	1.43	1.52
8	f	101	SPN	C15-C14	-2.37	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	n	102	SPN	C15-C14	-2.37	1.43	1.52
7	j	101	BCL	MG-NC	2.36	2.11	2.06
7	L	303	BCL	C3C-C4C	2.36	1.54	1.51
8	a	102	SPN	C15-C14	-2.35	1.43	1.52
8	a	102	SPN	C16-C17	-2.34	1.43	1.52
8	f	101	SPN	C16-C17	-2.34	1.43	1.52
8	l	102	SPN	C15-C14	-2.34	1.43	1.52
8	i	102	SPN	C15-C14	-2.33	1.43	1.52
8	e	102	SPN	C15-C14	-2.32	1.43	1.52
8	g	102	SPN	C15-C14	-2.32	1.43	1.52
8	l	102	SPN	C16-C17	-2.31	1.43	1.52
7	g	101	BCL	MG-NC	2.29	2.11	2.06
7	h	101	BCL	MG-NC	2.28	2.11	2.06
8	M	406	SPN	C16-C17	-2.24	1.44	1.52
8	p	102	SPN	C16-C17	-2.21	1.44	1.52
8	p	102	SPN	C15-C14	-2.20	1.44	1.52
7	k	101	BCL	MG-NC	2.20	2.11	2.06
7	a	101	BCL	C1D-C2D	-2.19	1.41	1.45
7	i	101	BCL	C4B-NB	2.18	1.40	1.37
7	j	101	BCL	C4B-NB	2.13	1.40	1.37
7	j	101	BCL	C1D-C2D	-2.12	1.41	1.45
7	f	102	BCL	MG-NC	2.12	2.11	2.06
7	m	101	BCL	C3C-C4C	2.12	1.54	1.51
7	h	101	BCL	C4B-NB	2.11	1.40	1.37
8	0	102	SPN	C16-C17	-2.07	1.44	1.52
7	a	101	BCL	MG-NC	2.06	2.11	2.06
7	i	101	BCL	MG-NA	2.05	2.11	2.06
7	M	405	BCL	MG-NC	2.05	2.11	2.06
7	9	102	BCL	C3C-C4C	2.05	1.54	1.51
7	g	101	BCL	C1D-C2D	-2.05	1.41	1.45
7	L	301	BCL	C1D-C2D	-2.05	1.41	1.45
7	k	101	BCL	MG-NA	2.03	2.11	2.06

All (615) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	h	102	SPN	C21-C20-C19	7.15	130.95	112.16
8	f	103	SPN	C21-C20-C19	7.08	130.77	112.16
8	i	103	SPN	C21-C20-C19	6.84	130.15	112.16
8	M	406	SPN	C16-C17-C18	6.84	130.12	113.47
8	g	103	SPN	C21-C20-C19	6.75	129.90	112.16
8	M	406	SPN	C15-C14-C13	6.72	129.83	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	L	305	BPH	C1A-C2A-C3A	-6.48	96.68	102.84
8	0	102	SPN	C15-C14-C13	6.46	129.21	113.47
8	0	102	SPN	C16-C17-C18	6.28	128.76	113.47
8	h	102	SPN	C16-C17-C18	6.24	128.67	113.47
8	i	103	SPN	C16-C17-C18	6.23	128.65	113.47
8	a	103	SPN	C21-C20-C19	6.22	128.52	112.16
8	f	103	SPN	C16-C17-C18	6.21	128.60	113.47
8	g	103	SPN	C16-C17-C18	6.20	128.57	113.47
8	p	103	SPN	C15-C14-C13	6.18	128.51	113.47
8	m	102	SPN	C15-C14-C13	6.03	128.16	113.47
8	e	102	SPN	C15-C14-C13	6.01	128.10	113.47
8	f	101	SPN	C15-C14-C13	6.00	128.08	113.47
8	i	102	SPN	C15-C14-C13	5.98	128.03	113.47
8	a	104	SPN	C15-C14-C13	5.95	127.97	113.47
8	a	103	SPN	C16-C17-C18	5.95	127.97	113.47
8	p	102	SPN	C16-C17-C18	5.94	127.93	113.47
8	l	102	SPN	C15-C14-C13	5.93	127.92	113.47
8	a	102	SPN	C15-C14-C13	5.93	127.91	113.47
8	g	102	SPN	C15-C14-C13	5.92	127.89	113.47
8	n	102	SPN	C15-C14-C13	5.91	127.86	113.47
8	M	406	SPN	C21-C20-C19	5.90	127.66	112.16
8	9	101	SPN	C16-C17-C18	5.84	127.70	113.47
8	a	103	SPN	C15-C14-C13	5.83	127.66	113.47
8	h	102	SPN	C15-C14-C13	5.81	127.62	113.47
8	9	101	SPN	C15-C14-C13	5.81	127.62	113.47
8	a	104	SPN	C16-C17-C18	5.80	127.60	113.47
8	a	102	SPN	C16-C17-C18	5.80	127.59	113.47
8	e	102	SPN	C16-C17-C18	5.79	127.57	113.47
8	f	103	SPN	C15-C14-C13	5.79	127.57	113.47
8	i	103	SPN	C15-C14-C13	5.77	127.52	113.47
8	8	102	SPN	C16-C17-C18	5.77	127.51	113.47
8	g	103	SPN	C15-C14-C13	5.74	127.45	113.47
8	8	102	SPN	C15-C14-C13	5.73	127.44	113.47
8	i	102	SPN	C16-C17-C18	5.72	127.41	113.47
8	m	102	SPN	C16-C17-C18	5.72	127.40	113.47
8	n	102	SPN	C16-C17-C18	5.71	127.39	113.47
8	f	101	SPN	C16-C17-C18	5.70	127.36	113.47
8	g	102	SPN	C16-C17-C18	5.68	127.31	113.47
8	l	102	SPN	C16-C17-C18	5.66	127.26	113.47
8	p	102	SPN	C15-C14-C13	5.66	127.25	113.47
8	p	103	SPN	C16-C17-C18	5.60	127.10	113.47
9	C	402	HEM	CAC-C3C-C4C	5.46	137.87	124.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	406	SPN	CM5-C13-C14	5.25	124.35	115.23
8	p	103	SPN	C21-C20-C19	5.21	125.87	112.16
8	M	406	SPN	C15-C16-C17	5.11	131.92	113.13
8	0	102	SPN	CM5-C13-C14	4.94	123.80	115.23
8	0	102	SPN	CM6-C18-C17	4.91	123.75	115.23
8	8	102	SPN	CM4-C9-C10	4.83	123.61	115.23
8	M	406	SPN	CM6-C18-C17	4.82	123.59	115.23
8	g	103	SPN	CM3-C5-C6	4.80	123.55	115.23
8	M	406	SPN	CM4-C9-C10	4.78	123.52	115.23
8	h	102	SPN	CM3-C5-C6	4.75	123.47	115.23
8	g	103	SPN	CM4-C9-C10	4.74	123.45	115.23
8	M	406	SPN	C11-C10-C9	4.73	128.84	113.19
8	i	103	SPN	CM3-C5-C6	4.72	123.42	115.23
8	p	103	SPN	CM4-C9-C10	4.72	123.42	115.23
8	i	103	SPN	CM4-C9-C10	4.71	123.41	115.23
8	f	103	SPN	CM3-C5-C6	4.71	123.40	115.23
8	8	102	SPN	C11-C10-C9	4.70	128.77	113.19
8	h	102	SPN	C7-C6-C5	4.70	128.75	113.19
8	a	103	SPN	CM4-C9-C10	4.69	123.37	115.23
8	g	103	SPN	C7-C6-C5	4.69	128.73	113.19
8	a	104	SPN	CM4-C9-C10	4.69	123.36	115.23
8	f	103	SPN	CM6-C18-C17	4.69	123.36	115.23
8	p	103	SPN	CM5-C13-C14	4.68	123.36	115.23
8	h	102	SPN	CM6-C18-C17	4.68	123.35	115.23
8	f	103	SPN	CM4-C9-C10	4.67	123.34	115.23
8	a	103	SPN	CM3-C5-C6	4.67	123.33	115.23
8	h	102	SPN	CM4-C9-C10	4.66	123.33	115.23
8	m	102	SPN	CM4-C9-C10	4.66	123.32	115.23
8	i	103	SPN	C7-C6-C5	4.66	128.62	113.19
8	p	103	SPN	CM3-C5-C6	4.64	123.28	115.23
8	a	104	SPN	C7-C6-C5	4.64	128.55	113.19
8	f	103	SPN	C7-C6-C5	4.64	128.55	113.19
8	m	102	SPN	CM3-C5-C6	4.63	123.27	115.23
8	a	104	SPN	CM3-C5-C6	4.63	123.27	115.23
8	p	103	SPN	C11-C10-C9	4.62	128.50	113.19
8	h	102	SPN	C11-C10-C9	4.61	128.46	113.19
8	m	102	SPN	C11-C10-C9	4.61	128.45	113.19
8	i	103	SPN	C11-C10-C9	4.60	128.44	113.19
8	a	104	SPN	C11-C10-C9	4.60	128.43	113.19
8	m	102	SPN	CM5-C13-C14	4.60	123.21	115.23
8	f	103	SPN	C11-C10-C9	4.59	128.40	113.19
8	g	103	SPN	C11-C10-C9	4.59	128.38	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	m	102	SPN	C7-C6-C5	4.59	128.38	113.19
8	p	103	SPN	C7-C6-C5	4.58	128.36	113.19
8	i	103	SPN	CM6-C18-C17	4.58	123.17	115.23
8	a	103	SPN	C7-C6-C5	4.58	128.35	113.19
8	a	104	SPN	CM5-C13-C14	4.57	123.16	115.23
8	M	406	SPN	CM3-C5-C6	4.57	123.15	115.23
8	a	103	SPN	C11-C10-C9	4.55	128.26	113.19
8	g	102	SPN	C21-C20-C19	4.54	124.11	112.16
8	g	103	SPN	CM6-C18-C17	4.54	123.11	115.23
8	e	102	SPN	CM5-C13-C14	4.53	123.08	115.23
8	f	101	SPN	CM5-C13-C14	4.51	123.06	115.23
8	a	102	SPN	CM5-C13-C14	4.49	123.02	115.23
8	0	102	SPN	CM4-C9-C10	4.49	123.02	115.23
8	M	406	SPN	C7-C6-C5	4.49	128.05	113.19
8	a	103	SPN	CM5-C13-C14	4.47	122.99	115.23
8	n	102	SPN	CM5-C13-C14	4.47	122.99	115.23
8	i	102	SPN	CM3-C5-C6	4.47	122.99	115.23
8	g	102	SPN	CM4-C9-C10	4.47	122.98	115.23
8	g	102	SPN	C11-C10-C9	4.46	127.97	113.19
8	i	102	SPN	CM5-C13-C14	4.46	122.97	115.23
8	0	102	SPN	C11-C10-C9	4.46	127.95	113.19
8	8	102	SPN	CM6-C18-C17	4.45	122.96	115.23
8	i	102	SPN	C7-C6-C5	4.45	127.94	113.19
8	l	102	SPN	CM5-C13-C14	4.45	122.95	115.23
8	h	102	SPN	CM5-C13-C14	4.45	122.95	115.23
8	e	102	SPN	C11-C10-C9	4.44	127.91	113.19
8	9	101	SPN	CM3-C5-C6	4.44	122.94	115.23
8	i	102	SPN	CM4-C9-C10	4.44	122.94	115.23
8	9	101	SPN	CM4-C9-C10	4.44	122.94	115.23
8	9	101	SPN	CM6-C18-C17	4.43	122.92	115.23
8	a	102	SPN	CM4-C9-C10	4.43	122.92	115.23
8	f	103	SPN	CM5-C13-C14	4.43	122.92	115.23
8	a	102	SPN	C11-C10-C9	4.43	127.87	113.19
8	8	102	SPN	CM3-C5-C6	4.43	122.92	115.23
8	e	102	SPN	CM4-C9-C10	4.43	122.92	115.23
8	g	102	SPN	CM5-C13-C14	4.43	122.91	115.23
8	9	101	SPN	CM5-C13-C14	4.42	122.91	115.23
8	l	102	SPN	CM3-C5-C6	4.42	122.90	115.23
8	g	102	SPN	CM3-C5-C6	4.42	122.90	115.23
11	L	305	BPH	C4A-C3A-C2A	-4.42	98.64	102.84
8	i	102	SPN	C11-C10-C9	4.42	127.82	113.19
8	f	101	SPN	C11-C10-C9	4.41	127.81	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	a	104	SPN	CM6-C18-C17	4.41	122.89	115.23
8	p	102	SPN	CM3-C5-C6	4.41	122.89	115.23
8	i	103	SPN	CM5-C13-C14	4.41	122.89	115.23
8	f	101	SPN	C21-C20-C19	4.41	123.75	112.16
8	g	103	SPN	CM5-C13-C14	4.40	122.87	115.23
8	i	102	SPN	C21-C20-C19	4.40	123.73	112.16
8	p	102	SPN	CM6-C18-C17	4.40	122.86	115.23
8	l	102	SPN	CM4-C9-C10	4.39	122.85	115.23
8	l	102	SPN	C11-C10-C9	4.39	127.73	113.19
8	p	102	SPN	C11-C10-C9	4.39	127.73	113.19
8	f	101	SPN	CM3-C5-C6	4.39	122.84	115.23
8	n	102	SPN	CM3-C5-C6	4.39	122.84	115.23
8	0	102	SPN	CM3-C5-C6	4.38	122.84	115.23
8	a	102	SPN	CM3-C5-C6	4.38	122.84	115.23
8	n	102	SPN	C11-C10-C9	4.38	127.71	113.19
8	f	101	SPN	CM4-C9-C10	4.38	122.83	115.23
8	e	102	SPN	C7-C6-C5	4.38	127.70	113.19
8	l	102	SPN	C21-C20-C19	4.38	123.68	112.16
8	9	101	SPN	C11-C10-C9	4.38	127.70	113.19
8	9	101	SPN	C7-C6-C5	4.38	127.70	113.19
8	n	102	SPN	C7-C6-C5	4.38	127.69	113.19
8	p	102	SPN	C7-C6-C5	4.38	127.69	113.19
8	g	102	SPN	C7-C6-C5	4.38	127.69	113.19
8	8	102	SPN	C7-C6-C5	4.37	127.67	113.19
8	a	102	SPN	CM6-C18-C17	4.37	122.81	115.23
8	a	102	SPN	C7-C6-C5	4.37	127.66	113.19
8	e	102	SPN	CM3-C5-C6	4.36	122.80	115.23
8	m	102	SPN	CM6-C18-C17	4.36	122.80	115.23
8	l	102	SPN	C7-C6-C5	4.36	127.64	113.19
8	8	102	SPN	CM5-C13-C14	4.36	122.80	115.23
8	n	102	SPN	CM4-C9-C10	4.36	122.79	115.23
8	e	102	SPN	CM6-C18-C17	4.35	122.79	115.23
8	a	103	SPN	CM6-C18-C17	4.34	122.77	115.23
8	i	102	SPN	CM6-C18-C17	4.34	122.76	115.23
8	n	102	SPN	CM6-C18-C17	4.34	122.76	115.23
8	0	102	SPN	C7-C6-C5	4.34	127.56	113.19
8	f	101	SPN	C7-C6-C5	4.33	127.54	113.19
8	n	102	SPN	C21-C20-C19	4.33	123.54	112.16
8	f	101	SPN	CM6-C18-C17	4.32	122.73	115.23
8	e	102	SPN	C21-C20-C19	4.30	123.48	112.16
8	g	102	SPN	CM6-C18-C17	4.29	122.67	115.23
8	l	102	SPN	CM6-C18-C17	4.28	122.65	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	m	102	SPN	C21-C20-C19	4.27	123.39	112.16
8	8	102	SPN	C21-C20-C19	4.25	123.33	112.16
8	p	102	SPN	CM4-C9-C10	4.24	122.59	115.23
8	0	102	SPN	C21-C20-C19	4.24	123.31	112.16
8	a	102	SPN	C21-C20-C19	4.18	123.15	112.16
8	9	101	SPN	C21-C20-C19	4.16	123.11	112.16
8	a	104	SPN	C21-C20-C19	4.16	123.09	112.16
8	p	103	SPN	CM6-C18-C17	4.12	122.38	115.23
8	p	102	SPN	C21-C20-C19	4.07	122.85	112.16
9	C	402	HEM	CAC-C3C-C2C	-3.99	115.46	128.43
7	8	101	BCL	C2C-C3C-C4C	-3.91	95.49	101.34
8	p	102	SPN	CM5-C13-C14	3.89	121.99	115.23
8	M	406	SPN	CM7-C22-C21	3.86	125.04	111.27
11	L	305	BPH	C1-O2A-CGA	3.79	125.83	116.65
11	M	404	BPH	C4D-CHA-CBD	3.79	110.27	108.45
11	L	305	BPH	C4D-CHA-CBD	3.78	110.27	108.45
11	L	304	BPH	C4D-CHA-CBD	3.73	110.25	108.45
8	h	102	SPN	C23-C22-C21	3.71	130.88	112.07
8	f	103	SPN	C23-C22-C21	3.67	130.65	112.07
8	i	103	SPN	CM7-C22-C21	3.64	124.26	111.27
8	g	103	SPN	CM7-C22-C21	3.59	124.07	111.27
8	0	102	SPN	C15-C16-C17	3.51	126.03	113.13
8	0	102	SPN	CM7-C22-C21	3.49	123.72	111.27
8	e	102	SPN	CM7-C22-C21	3.43	123.49	111.27
8	0	102	SPN	C16-C15-C14	3.42	125.69	113.13
8	p	103	SPN	C15-C16-C17	3.41	125.67	113.13
8	p	102	SPN	CM7-C22-C21	3.41	123.42	111.27
8	9	101	SPN	CM7-C22-C21	3.38	123.31	111.27
8	a	102	SPN	CM7-C22-C21	3.36	123.27	111.27
8	a	104	SPN	CM7-C22-C21	3.34	123.19	111.27
8	l	102	SPN	CM7-C22-C21	3.32	123.10	111.27
8	p	102	SPN	C6-C7-C8	3.27	128.19	112.02
11	L	305	BPH	C1-C2-C3	3.27	131.55	126.20
8	i	102	SPN	CM7-C22-C21	3.27	122.92	111.27
7	n	101	BCL	CHC-C1C-NC	3.26	129.10	124.40
8	p	103	SPN	CM7-C22-C21	3.26	122.88	111.27
7	p	101	BCL	CHC-C1C-NC	3.24	129.07	124.40
8	p	102	SPN	C16-C15-C14	3.24	125.02	113.13
8	g	103	SPN	C16-C15-C14	3.22	124.97	113.13
8	i	103	SPN	C16-C15-C14	3.22	124.96	113.13
8	f	101	SPN	CM7-C22-C21	3.20	122.67	111.27
8	l	102	SPN	C15-C16-C17	3.19	124.84	113.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	m	102	SPN	CM7-C22-C21	3.18	122.63	111.27
8	f	101	SPN	C15-C16-C17	3.18	124.80	113.13
8	h	102	SPN	C16-C15-C14	3.15	124.71	113.13
7	d	101	BCL	CHC-C1C-NC	3.14	128.94	124.40
7	7	101	BCL	CHC-C1C-NC	3.14	128.93	124.40
8	f	103	SPN	C16-C15-C14	3.14	124.66	113.13
8	m	102	SPN	C15-C16-C17	3.13	124.61	113.13
7	M	402	BCL	CHC-C1C-NC	3.13	128.91	124.40
7	h	101	BCL	CHC-C1C-NC	3.12	128.90	124.40
8	i	102	SPN	C15-C16-C17	3.09	124.48	113.13
8	g	102	SPN	C15-C16-C17	3.08	124.45	113.13
8	n	102	SPN	C15-C16-C17	3.08	124.44	113.13
7	g	101	BCL	CHC-C1C-NC	3.07	128.83	124.40
8	e	102	SPN	C15-C16-C17	3.05	124.35	113.13
7	L	301	BCL	C2A-C3A-C4A	-3.05	96.94	101.87
7	9	102	BCL	C1C-NC-C4C	-3.04	105.29	106.68
7	l	101	BCL	CHC-C1C-NC	3.03	128.77	124.40
7	c	101	BCL	CHC-C1C-NC	3.03	128.77	124.40
8	n	102	SPN	CM7-C22-C21	3.03	122.06	111.27
7	L	301	BCL	CHC-C1C-NC	3.01	128.75	124.40
8	g	102	SPN	CM7-C22-C21	3.01	122.00	111.27
7	j	101	BCL	CHC-C1C-NC	3.00	128.73	124.40
8	a	103	SPN	CM7-C22-C21	3.00	121.98	111.27
8	a	102	SPN	C15-C16-C17	3.00	124.15	113.13
9	C	402	HEM	CAB-C3B-C2B	-3.00	118.69	128.43
7	8	101	BCL	C1D-CHD-C4C	-2.99	119.41	126.62
8	8	102	SPN	CM7-C22-C21	2.97	121.86	111.27
7	L	303	BCL	CHC-C1C-NC	2.96	128.68	124.40
11	M	404	BPH	C2D-C1D-ND	-2.94	107.30	109.43
8	p	102	SPN	C10-C11-C12	2.94	126.58	112.02
7	b	101	BCL	CHC-C1C-NC	2.94	128.64	124.40
8	a	103	SPN	C16-C15-C14	2.93	123.91	113.13
7	f	102	BCL	CHC-C1C-NC	2.93	128.62	124.40
7	e	101	BCL	CHC-C1C-NC	2.92	128.61	124.40
7	M	402	BCL	C2A-C3A-C4A	-2.91	97.16	101.87
11	L	304	BPH	C2D-C1D-ND	-2.90	107.33	109.43
8	a	104	SPN	C15-C16-C17	2.90	123.77	113.13
8	M	406	SPN	C20-C21-C22	2.87	129.88	114.56
7	M	402	BCL	C1-C2-C3	-2.87	121.50	126.20
7	0	101	BCL	CHC-C4B-NB	-2.86	119.76	124.05
8	8	102	SPN	C15-C16-C17	2.86	123.62	113.13
11	L	305	BPH	C2D-C1D-ND	-2.86	107.37	109.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	i	101	BCL	CHC-C1C-NC	2.85	128.52	124.40
8	8	102	SPN	C16-C15-C14	2.85	123.61	113.13
7	8	101	BCL	CHC-C4B-NB	-2.85	119.77	124.05
8	p	102	SPN	C20-C21-C22	2.85	129.76	114.56
8	9	101	SPN	C16-C15-C14	2.83	123.51	113.13
7	o	101	BCL	CHC-C4B-NB	-2.82	119.82	124.05
7	M	405	BCL	CHC-C1C-NC	2.81	128.45	124.40
7	n	101	BCL	C1D-ND-C4D	2.80	108.28	106.31
8	8	102	SPN	C10-C11-C12	2.79	125.84	112.02
7	o	101	BCL	C4D-CHA-C1A	2.79	124.58	121.24
7	j	101	BCL	CHA-C1A-NA	-2.79	120.07	126.39
7	7	101	BCL	CHC-C4B-NB	-2.77	119.89	124.05
7	7	101	BCL	C2C-C3C-C4C	-2.77	97.19	101.34
7	b	101	BCL	CHC-C4B-NB	-2.77	119.90	124.05
7	n	101	BCL	CHA-C1A-NA	-2.76	120.15	126.39
7	9	102	BCL	CMA-C3A-C4A	-2.75	104.37	111.77
7	l	101	BCL	CHA-C1A-NA	-2.74	120.19	126.39
8	9	101	SPN	C15-C16-C17	2.73	123.17	113.13
7	d	101	BCL	CHA-C1A-NA	-2.71	120.24	126.39
7	k	101	BCL	CHC-C4B-NB	-2.70	119.99	124.05
7	k	101	BCL	CHC-C1C-NC	2.70	128.30	124.40
7	d	101	BCL	CHC-C4B-NB	-2.70	120.01	124.05
7	p	101	BCL	CHA-C1A-NA	-2.69	120.29	126.39
7	9	102	BCL	CHC-C4B-NB	-2.69	120.01	124.05
11	L	305	BPH	C2B-C1B-NB	-2.69	107.48	109.43
7	p	101	BCL	CHC-C4B-NB	-2.69	120.02	124.05
10	L	302	U10	C7-C6-C5	-2.69	115.39	118.52
7	M	402	BCL	CHC-C4B-NB	-2.68	120.02	124.05
7	m	101	BCL	CHC-C4B-NB	-2.67	120.04	124.05
11	L	305	BPH	CMA-C3A-C4A	-2.67	108.86	114.61
8	g	102	SPN	C16-C15-C14	2.66	122.91	113.13
7	p	101	BCL	C1D-ND-C4D	2.66	108.18	106.31
7	b	101	BCL	CHA-C1A-NA	-2.66	120.37	126.39
7	g	101	BCL	CHC-C4B-NB	-2.65	120.07	124.05
10	M	403	U10	C7-C6-C5	-2.65	115.44	118.52
7	l	101	BCL	CHC-C4B-NB	-2.64	120.09	124.05
7	9	102	BCL	CHC-C1C-NC	2.64	128.21	124.40
7	M	405	BCL	CHC-C4B-NB	-2.64	120.09	124.05
7	L	301	BCL	CHC-C4B-NB	-2.64	120.09	124.05
7	a	101	BCL	CHC-C1C-NC	2.64	128.20	124.40
7	c	101	BCL	CHC-C4B-NB	-2.64	120.10	124.05
7	M	402	BCL	C4A-NA-C1A	-2.63	105.48	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	a	101	BCL	CHC-C4B-NB	-2.63	120.11	124.05
8	a	104	SPN	C16-C15-C14	2.63	122.78	113.13
7	n	101	BCL	CHC-C4B-NB	-2.62	120.11	124.05
7	d	101	BCL	CMA-C3A-C4A	-2.62	104.74	111.77
7	8	101	BCL	CHA-C1A-NA	-2.61	120.47	126.39
7	9	102	BCL	C3D-C4D-ND	-2.61	105.74	109.99
7	a	101	BCL	CMA-C3A-C4A	-2.61	104.77	111.77
8	a	103	SPN	O1-C1-C2	2.60	114.23	108.90
8	a	102	SPN	C16-C15-C14	2.60	122.70	113.13
7	m	101	BCL	CMA-C3A-C4A	-2.60	104.78	111.77
8	a	102	SPN	C20-C21-C22	2.60	128.41	114.56
7	8	101	BCL	CMA-C3A-C4A	-2.59	104.80	111.77
8	i	102	SPN	C16-C15-C14	2.59	122.65	113.13
7	c	101	BCL	CMA-C3A-C4A	-2.59	104.82	111.77
7	7	101	BCL	C4D-CHA-C1A	2.58	124.33	121.24
7	m	101	BCL	CHC-C1C-NC	2.58	128.12	124.40
7	f	102	BCL	CHA-C1A-NA	-2.58	120.55	126.39
7	e	101	BCL	CHC-C4B-NB	-2.58	120.18	124.05
8	p	103	SPN	C20-C21-C22	2.57	128.28	114.56
7	o	101	BCL	C1D-ND-C4D	2.57	108.11	106.31
8	n	102	SPN	C16-C15-C14	2.57	122.56	113.13
7	b	101	BCL	CMA-C3A-C4A	-2.57	104.88	111.77
7	o	101	BCL	CHC-C1C-NC	2.56	128.09	124.40
8	e	102	SPN	C16-C15-C14	2.56	122.52	113.13
7	f	102	BCL	CHC-C4B-NB	-2.55	120.22	124.05
7	h	101	BCL	CHC-C4B-NB	-2.55	120.23	124.05
7	M	405	BCL	CHA-C1A-NA	-2.54	120.63	126.39
8	l	102	SPN	C16-C15-C14	2.54	122.47	113.13
7	i	101	BCL	CHC-C4B-NB	-2.54	120.24	124.05
7	k	101	BCL	CHA-C1A-NA	-2.53	120.67	126.39
7	o	101	BCL	CMA-C3A-C4A	-2.53	104.98	111.77
7	a	101	BCL	C3D-C4D-ND	-2.52	105.89	109.99
7	e	101	BCL	C4D-CHA-C1A	2.52	124.25	121.24
7	0	101	BCL	CMA-C3A-C4A	-2.52	105.00	111.77
7	j	101	BCL	CHC-C4B-NB	-2.51	120.28	124.05
8	a	103	SPN	C15-C16-C17	2.51	122.36	113.13
7	g	101	BCL	CMA-C3A-C4A	-2.51	105.03	111.77
7	p	101	BCL	CMA-C3A-C4A	-2.51	105.04	111.77
8	l	102	SPN	C20-C21-C22	2.50	127.92	114.56
8	p	102	SPN	C15-C16-C17	2.50	122.31	113.13
8	9	101	SPN	C20-C21-C22	2.49	127.86	114.56
8	e	102	SPN	C20-C21-C22	2.49	127.86	114.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	301	BCL	CHA-C1A-NA	-2.48	120.77	126.39
7	0	101	BCL	CHC-C1C-NC	2.48	127.98	124.40
7	g	101	BCL	C4D-CHA-C1A	2.47	124.19	121.24
8	a	104	SPN	C20-C21-C22	2.47	127.75	114.56
7	L	303	BCL	CHC-C4B-NB	-2.47	120.35	124.05
7	h	101	BCL	CHA-C1A-NA	-2.47	120.81	126.39
7	i	101	BCL	CHA-C1A-NA	-2.46	120.81	126.39
8	f	101	SPN	C16-C15-C14	2.46	122.17	113.13
7	a	101	BCL	C4D-CHA-C1A	2.46	124.18	121.24
7	m	101	BCL	C4D-CHA-C1A	2.46	124.18	121.24
7	L	303	BCL	C4D-CHA-C1A	2.45	124.16	121.24
7	M	402	BCL	C4D-CHA-C1A	2.45	124.16	121.24
7	9	102	BCL	C2C-C3C-C4C	-2.44	97.69	101.34
7	e	101	BCL	C3C-C4C-CHD	-2.44	118.26	123.39
7	7	101	BCL	CHA-C1A-NA	-2.43	120.88	126.39
8	m	102	SPN	C16-C15-C14	2.43	122.06	113.13
7	0	101	BCL	CHA-C1A-NA	-2.43	120.90	126.39
7	a	101	BCL	CHA-C1A-NA	-2.42	120.90	126.39
7	8	101	BCL	C4D-CHA-C1A	2.42	124.14	121.24
7	M	402	BCL	CHA-C1A-NA	-2.42	120.90	126.39
7	L	301	BCL	C3C-C4C-CHD	-2.42	118.29	123.39
8	m	102	SPN	C20-C21-C22	2.42	127.45	114.56
7	M	405	BCL	C4D-CHA-C1A	2.41	124.12	121.24
7	j	101	BCL	C1D-ND-C4D	2.41	108.00	106.31
7	L	303	BCL	CHA-C1A-NA	-2.41	120.93	126.39
8	f	101	SPN	C6-C7-C8	2.41	123.93	112.02
7	7	101	BCL	CMA-C3A-C4A	-2.41	105.30	111.77
11	M	404	BPH	C2B-C1B-NB	-2.41	107.69	109.43
7	l	101	BCL	CMA-C3A-C4A	-2.41	105.31	111.77
7	c	101	BCL	C4D-CHA-C1A	2.41	124.11	121.24
8	i	102	SPN	C20-C21-C22	2.40	127.39	114.56
7	9	102	BCL	C4D-CHA-C1A	2.40	124.11	121.24
7	l	101	BCL	C3C-C4C-CHD	-2.40	118.34	123.39
8	f	101	SPN	C20-C21-C22	2.40	127.34	114.56
8	0	102	SPN	C20-C21-C22	2.39	127.30	114.56
8	l	102	SPN	C6-C7-C8	2.38	123.80	112.02
8	0	102	SPN	CM6-C18-C19	-2.37	117.54	123.63
8	p	102	SPN	CM5-C13-C12	-2.37	117.54	123.63
7	o	101	BCL	CHA-C1A-NA	-2.36	121.04	126.39
7	b	101	BCL	C1D-ND-C4D	2.36	107.97	106.31
7	L	303	BCL	CMA-C3A-C4A	-2.36	105.42	111.77
7	m	101	BCL	CHA-C1A-NA	-2.36	121.05	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	i	101	BCL	C3D-C4D-ND	-2.36	106.15	109.99
11	L	304	BPH	C2B-C1B-NB	-2.35	107.73	109.43
7	d	101	BCL	C1D-ND-C4D	2.35	107.96	106.31
7	8	101	BCL	C3D-C2D-C1D	-2.34	102.64	105.83
7	c	101	BCL	CHA-C1A-NA	-2.34	121.09	126.39
7	k	101	BCL	CMA-C3A-C4A	-2.34	105.48	111.77
8	g	102	SPN	C6-C7-C8	2.34	123.57	112.02
8	M	406	SPN	CM6-C18-C19	-2.34	117.63	123.63
8	n	102	SPN	C6-C7-C8	2.33	123.57	112.02
7	m	101	BCL	CMD-C2D-C1D	2.33	128.82	124.73
8	e	102	SPN	C6-C7-C8	2.33	123.52	112.02
7	i	101	BCL	CMD-C2D-C1D	2.32	128.82	124.73
7	a	101	BCL	C3D-C2D-C1D	-2.32	102.66	105.83
7	8	101	BCL	CMD-C2D-C1D	2.31	128.80	124.73
8	a	102	SPN	C6-C7-C8	2.31	123.46	112.02
7	9	102	BCL	C3D-C2D-C1D	-2.31	102.68	105.83
8	h	102	SPN	C15-C16-C17	2.31	121.62	113.13
7	g	101	BCL	CHA-C1A-NA	-2.31	121.16	126.39
7	8	101	BCL	CHC-C1C-NC	2.31	127.73	124.40
8	g	102	SPN	C20-C21-C22	2.31	126.88	114.56
7	e	101	BCL	CMA-C3A-C4A	-2.30	105.58	111.77
8	8	102	SPN	CM4-C9-C8	-2.30	117.71	123.63
7	0	101	BCL	C1D-ND-C4D	2.30	107.93	106.31
8	l	102	SPN	CM6-C18-C19	-2.29	117.74	123.63
7	a	101	BCL	CMD-C2D-C1D	2.29	128.76	124.73
7	9	102	BCL	CMD-C2D-C1D	2.29	128.76	124.73
8	i	102	SPN	CM6-C18-C19	-2.29	117.75	123.63
7	e	101	BCL	CHA-C1A-NA	-2.29	121.21	126.39
7	i	101	BCL	C3D-C2D-C1D	-2.28	102.72	105.83
7	k	101	BCL	C4D-CHA-C1A	2.28	123.96	121.24
7	L	301	BCL	CMD-C2D-C1D	2.28	128.74	124.73
7	c	101	BCL	C3C-C4C-CHD	-2.28	118.59	123.39
8	n	102	SPN	C20-C21-C22	2.28	126.72	114.56
9	C	402	HEM	CAB-C3B-C4B	2.28	134.45	124.39
8	a	102	SPN	C4-C3-C2	2.27	122.31	111.68
8	f	103	SPN	C15-C16-C17	2.27	121.47	113.13
8	g	102	SPN	CM6-C18-C19	-2.27	117.80	123.63
7	n	101	BCL	C2A-C1A-CHA	2.27	127.80	123.87
7	b	101	BCL	C2A-C3A-C4A	-2.27	98.21	101.87
8	f	101	SPN	CM6-C18-C19	-2.27	117.81	123.63
7	i	101	BCL	C4D-CHA-C1A	2.27	123.95	121.24
8	l	102	SPN	CM3-C5-C4	-2.26	117.81	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	8	102	SPN	C20-C21-C22	2.26	126.63	114.56
7	7	101	BCL	C1D-ND-C4D	2.26	107.90	106.31
7	b	101	BCL	C2A-C1A-CHA	2.26	127.79	123.87
8	f	101	SPN	CM3-C5-C4	-2.26	117.82	123.63
7	i	101	BCL	C3C-C4C-CHD	-2.26	118.63	123.39
8	0	102	SPN	C6-C7-C8	2.26	123.20	112.02
8	e	102	SPN	CM6-C18-C19	-2.26	117.83	123.63
7	k	101	BCL	CMD-C2D-C1D	2.26	128.70	124.73
8	n	102	SPN	C10-C11-C12	2.26	123.18	112.02
8	8	102	SPN	C6-C7-C8	2.26	123.18	112.02
8	p	102	SPN	CM3-C5-C4	-2.25	117.84	123.63
7	n	101	BCL	CMA-C3A-C4A	-2.25	105.72	111.77
7	j	101	BCL	C3C-C4C-CHD	-2.25	118.65	123.39
8	n	102	SPN	CM6-C18-C19	-2.25	117.85	123.63
8	m	102	SPN	CM6-C18-C19	-2.25	117.86	123.63
7	c	101	BCL	CMD-C2D-C1D	2.24	128.68	124.73
8	a	102	SPN	CM6-C18-C19	-2.24	117.87	123.63
8	a	104	SPN	CM6-C18-C19	-2.24	117.88	123.63
7	9	102	BCL	CHA-C1A-NA	-2.24	121.32	126.39
8	a	102	SPN	CM3-C5-C4	-2.24	117.88	123.63
7	L	301	BCL	C3D-C2D-C1D	-2.24	102.78	105.83
8	l	102	SPN	C4-C3-C2	2.24	122.13	111.68
8	l	102	SPN	C10-C11-C12	2.24	123.08	112.02
7	c	101	BCL	C3D-C2D-C1D	-2.23	102.78	105.83
7	8	101	BCL	CHB-C1B-NB	-2.23	120.70	124.05
7	m	101	BCL	C3D-C2D-C1D	-2.23	102.78	105.83
8	l	102	SPN	CM4-C9-C8	-2.23	117.89	123.63
8	g	102	SPN	CM3-C5-C4	-2.23	117.89	123.63
7	g	101	BCL	C3D-C4D-ND	-2.23	106.36	109.99
7	8	101	BCL	C2A-C3A-C4A	-2.23	98.27	101.87
8	f	101	SPN	C4-C3-C2	2.23	122.09	111.68
8	f	101	SPN	CM4-C9-C8	-2.23	117.91	123.63
8	n	102	SPN	CM3-C5-C4	-2.22	117.91	123.63
7	i	101	BCL	CMA-C3A-C4A	-2.22	105.80	111.77
8	0	102	SPN	O1-C1-C2	2.22	113.45	108.90
8	f	101	SPN	C10-C11-C12	2.22	122.99	112.02
8	9	101	SPN	CM5-C13-C12	-2.22	117.93	123.63
8	9	101	SPN	CM6-C18-C19	-2.22	117.93	123.63
8	e	102	SPN	CM3-C5-C4	-2.22	117.93	123.63
8	0	102	SPN	CM3-C5-C4	-2.21	117.94	123.63
8	g	102	SPN	CM4-C9-C8	-2.21	117.95	123.63
8	8	102	SPN	CM3-C5-C4	-2.21	117.95	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	n	102	SPN	CM4-C9-C8	-2.21	117.95	123.63
8	9	101	SPN	C10-C11-C12	2.21	122.95	112.02
7	j	101	BCL	CMA-C3A-C4A	-2.21	105.84	111.77
8	8	102	SPN	CM5-C13-C12	-2.20	117.97	123.63
8	a	102	SPN	CM4-C9-C8	-2.20	117.97	123.63
8	i	102	SPN	CM4-C9-C8	-2.20	117.97	123.63
8	i	102	SPN	CM3-C5-C4	-2.20	117.97	123.63
8	0	102	SPN	C4-C3-C2	2.20	121.97	111.68
8	i	102	SPN	C10-C11-C12	2.20	122.90	112.02
8	p	102	SPN	CM6-C18-C19	-2.20	117.98	123.63
7	M	402	BCL	C1D-CHD-C4C	-2.20	121.32	126.62
8	f	103	SPN	CM5-C13-C12	-2.20	117.98	123.63
8	g	102	SPN	C4-C3-C2	2.20	121.95	111.68
7	c	101	BCL	C3D-C4D-ND	-2.20	106.41	109.99
7	7	101	BCL	C2A-C3A-C4A	-2.20	98.32	101.87
7	L	301	BCL	CMA-C3A-C4A	-2.20	105.87	111.77
8	h	102	SPN	CM5-C13-C12	-2.19	117.99	123.63
8	f	101	SPN	CM5-C13-C12	-2.19	118.00	123.63
8	i	103	SPN	C15-C16-C17	2.19	121.18	113.13
8	9	101	SPN	CM3-C5-C4	-2.19	118.00	123.63
8	8	102	SPN	CM6-C18-C19	-2.19	118.00	123.63
7	p	101	BCL	C1D-CHD-C4C	-2.19	121.33	126.62
7	L	301	BCL	C4D-CHA-C1A	2.19	123.86	121.24
8	e	102	SPN	CM4-C9-C8	-2.19	118.00	123.63
8	e	102	SPN	C4-C3-C2	2.19	121.91	111.68
7	f	102	BCL	C1D-ND-C4D	2.19	107.85	106.31
8	g	102	SPN	CM5-C13-C12	-2.19	118.01	123.63
8	e	102	SPN	CM5-C13-C12	-2.19	118.02	123.63
7	a	101	BCL	C1D-CHD-C4C	-2.18	121.35	126.62
8	g	103	SPN	CM5-C13-C12	-2.18	118.02	123.63
8	i	102	SPN	C6-C7-C8	2.18	122.80	112.02
8	a	102	SPN	CM5-C13-C12	-2.18	118.03	123.63
8	a	103	SPN	CM5-C13-C12	-2.18	118.03	123.63
8	n	102	SPN	CM5-C13-C12	-2.18	118.03	123.63
8	0	102	SPN	CM4-C9-C8	-2.18	118.04	123.63
8	i	103	SPN	CM5-C13-C12	-2.17	118.04	123.63
8	M	406	SPN	O1-C1-C2	2.17	113.34	108.90
7	k	101	BCL	C3C-C4C-CHD	-2.17	118.82	123.39
8	e	102	SPN	O1-C1-C2	2.17	113.34	108.90
7	9	102	BCL	C1D-CHD-C4C	-2.17	121.39	126.62
7	7	101	BCL	C3D-C4D-ND	-2.17	106.46	109.99
7	p	101	BCL	CMD-C2D-C1D	2.17	128.54	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	g	102	SPN	C10-C11-C12	2.17	122.73	112.02
8	g	103	SPN	C15-C16-C17	2.17	121.08	113.13
8	a	102	SPN	C10-C11-C12	2.17	122.73	112.02
7	d	101	BCL	C3C-C4C-CHD	-2.17	118.83	123.39
7	M	402	BCL	CMD-C2D-C1D	2.17	128.54	124.73
8	M	406	SPN	CM3-C5-C4	-2.16	118.07	123.63
8	a	103	SPN	CM3-C5-C4	-2.16	118.07	123.63
8	9	101	SPN	C6-C7-C8	2.16	122.71	112.02
8	l	102	SPN	CM5-C13-C12	-2.16	118.08	123.63
8	0	102	SPN	CM5-C13-C12	-2.16	118.09	123.63
8	9	101	SPN	CM4-C9-C8	-2.16	118.09	123.63
8	e	102	SPN	C10-C11-C12	2.15	122.67	112.02
7	f	102	BCL	CMD-C2D-C1D	2.15	128.52	124.73
8	m	102	SPN	CM3-C5-C4	-2.15	118.10	123.63
7	7	101	BCL	C1D-CHD-C4C	-2.15	121.43	126.62
7	p	101	BCL	C4D-CHA-C1A	2.15	123.81	121.24
8	h	102	SPN	CM3-C5-C4	-2.15	118.11	123.63
8	i	102	SPN	CM5-C13-C12	-2.15	118.11	123.63
11	L	305	BPH	CMD-C2D-C3D	2.15	128.97	124.68
8	p	103	SPN	CM3-C5-C4	-2.14	118.12	123.63
8	f	103	SPN	CM3-C5-C4	-2.14	118.13	123.63
8	i	103	SPN	CM3-C5-C4	-2.14	118.13	123.63
7	b	101	BCL	C3C-C4C-CHD	-2.14	118.89	123.39
7	h	101	BCL	C3C-C4C-CHD	-2.13	118.89	123.39
8	l	102	SPN	O1-C1-C2	2.13	113.27	108.90
7	0	101	BCL	CMD-C2D-C1D	2.13	128.49	124.73
8	h	102	SPN	O1-C1-C2	2.13	113.26	108.90
11	L	304	BPH	CMD-C2D-C3D	2.13	128.94	124.68
8	i	102	SPN	C4-C3-C2	2.13	121.64	111.68
8	8	102	SPN	C4-C3-C2	2.13	121.64	111.68
8	p	103	SPN	C16-C15-C14	2.13	120.95	113.13
7	g	101	BCL	C3C-C4C-CHD	-2.13	118.90	123.39
8	m	102	SPN	CM5-C13-C12	-2.13	118.16	123.63
7	f	102	BCL	C3C-C4C-CHD	-2.13	118.91	123.39
8	i	103	SPN	O1-C1-C2	2.13	113.25	108.90
11	M	404	BPH	CMD-C2D-C3D	2.13	128.93	124.68
7	e	101	BCL	C3D-C2D-C1D	-2.12	102.93	105.83
11	L	305	BPH	OBD-CAD-CBD	-2.12	122.71	125.82
7	o	101	BCL	C3C-C4C-CHD	-2.12	118.92	123.39
8	a	104	SPN	CM5-C13-C12	-2.12	118.18	123.63
7	0	101	BCL	C4D-CHA-C1A	2.12	123.77	121.24
8	a	104	SPN	CM3-C5-C4	-2.12	118.18	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	405	BCL	C3C-C4C-CHD	-2.12	118.93	123.39
7	d	101	BCL	C4D-CHA-C1A	2.12	123.77	121.24
7	p	101	BCL	C2C-C3C-C4C	-2.12	98.17	101.34
8	g	102	SPN	C23-C22-C21	2.11	122.78	112.07
8	h	102	SPN	CM4-C9-C8	-2.11	118.20	123.63
8	a	103	SPN	C23-C22-C21	2.11	122.77	112.07
11	L	305	BPH	C1C-C2C-C3C	-2.11	100.83	102.84
8	p	103	SPN	CM5-C13-C12	-2.11	118.21	123.63
7	7	101	BCL	CHB-C1B-NB	-2.11	120.89	124.05
7	p	101	BCL	C3C-C4C-CHD	-2.11	118.95	123.39
7	L	303	BCL	CMD-C2D-C1D	2.10	128.43	124.73
8	a	103	SPN	CM4-C9-C8	-2.10	118.23	123.63
7	b	101	BCL	CMD-C2D-C1D	2.10	128.43	124.73
8	g	103	SPN	CM3-C5-C4	-2.10	118.23	123.63
8	f	103	SPN	CM4-C9-C8	-2.10	118.24	123.63
7	f	102	BCL	C4D-CHA-C1A	2.09	123.74	121.24
7	8	101	BCL	C1D-ND-C4D	2.09	107.78	106.31
7	e	101	BCL	CMD-C2D-C1D	2.09	128.41	124.73
8	8	102	SPN	C23-C22-C21	2.09	122.67	112.07
8	p	103	SPN	CM4-C9-C8	-2.09	118.26	123.63
8	a	104	SPN	CM4-C9-C8	-2.09	118.27	123.63
8	n	102	SPN	C23-C22-C21	2.09	122.64	112.07
7	d	101	BCL	CMD-C2D-C1D	2.08	128.40	124.73
8	f	101	SPN	O1-C1-C2	2.08	113.16	108.90
7	n	101	BCL	C3C-C4C-CHD	-2.08	119.01	123.39
7	g	101	BCL	C3D-C2D-C1D	-2.08	102.99	105.83
7	n	101	BCL	C4D-CHA-C1A	2.08	123.72	121.24
8	p	103	SPN	CM6-C18-C19	-2.08	118.29	123.63
7	n	101	BCL	C1D-CHD-C4C	-2.08	121.61	126.62
7	L	303	BCL	C2A-C3A-C4A	-2.07	98.52	101.87
7	d	101	BCL	CHB-C1B-NB	-2.07	120.94	124.05
7	l	101	BCL	C4D-CHA-C1A	2.07	123.71	121.24
7	k	101	BCL	C3D-C2D-C1D	-2.07	103.01	105.83
7	M	405	BCL	CMA-C3A-C4A	-2.06	106.23	111.77
8	i	102	SPN	O1-C1-C2	2.06	113.12	108.90
8	m	102	SPN	CM4-C9-C8	-2.06	118.33	123.63
8	i	103	SPN	CM4-C9-C8	-2.06	118.33	123.63
8	p	102	SPN	C4-C3-C2	2.06	121.31	111.68
8	a	102	SPN	O1-C1-C2	2.06	113.12	108.90
8	n	102	SPN	C4-C3-C2	2.06	121.31	111.68
7	9	102	BCL	C1-C2-C3	-2.06	122.82	126.20
8	g	103	SPN	CM4-C9-C8	-2.06	118.34	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	p	101	BCL	CHB-C1B-NB	-2.06	120.96	124.05
8	n	102	SPN	O1-C1-C2	2.05	113.10	108.90
7	j	101	BCL	C4D-CHA-C1A	2.05	123.69	121.24
8	M	406	SPN	CM4-C9-C8	-2.05	118.36	123.63
7	f	102	BCL	C3D-C2D-C1D	-2.05	103.04	105.83
7	o	101	BCL	CMD-C2D-C1D	2.04	128.32	124.73
7	f	102	BCL	CMA-C3A-C4A	-2.03	106.32	111.77
7	l	101	BCL	C1D-ND-C4D	2.03	107.74	106.31
7	o	101	BCL	CHB-C1B-NB	-2.03	121.00	124.05
7	n	101	BCL	CMD-C2D-C1D	2.03	128.30	124.73
7	m	101	BCL	C3D-C4D-ND	-2.03	106.69	109.99
8	m	102	SPN	O1-C1-C2	2.03	113.05	108.90
7	e	101	BCL	C3D-C4D-ND	-2.03	106.69	109.99
7	M	402	BCL	CMA-C3A-C4A	-2.02	106.35	111.77
7	7	101	BCL	CMD-C2D-C1D	2.01	128.27	124.73
8	p	103	SPN	O1-C1-C2	2.01	113.02	108.90
7	8	101	BCL	C2A-C1A-CHA	2.01	127.36	123.87
7	L	301	BCL	C4A-NA-C1A	-2.01	105.76	106.68
7	h	101	BCL	C4D-CHA-C1A	2.01	123.64	121.24
7	b	101	BCL	CHB-C1B-NB	-2.00	121.04	124.05
7	a	101	BCL	C3C-C4C-CHD	-2.00	119.17	123.39

There are no chirality outliers.

All (913) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	0	101	BCL	C1A-C2A-CAA-CBA
7	0	101	BCL	C2C-C3C-CAC-CBC
7	0	101	BCL	C4C-C3C-CAC-CBC
7	7	101	BCL	C4C-C3C-CAC-CBC
7	7	101	BCL	CBD-CGD-O2D-CED
7	8	101	BCL	CBA-CGA-O2A-C1
7	8	101	BCL	O1A-CGA-O2A-C1
7	8	101	BCL	C2B-C3B-CAB-OB
7	8	101	BCL	C2B-C3B-CAB-CB
7	8	101	BCL	C4B-C3B-CAB-OB
7	8	101	BCL	C4-C3-C5-C6
7	9	102	BCL	C1A-C2A-CAA-CBA
7	9	102	BCL	C3A-C2A-CAA-CBA
7	9	102	BCL	C4C-C3C-CAC-CBC
7	L	301	BCL	C1A-C2A-CAA-CBA
7	L	301	BCL	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
7	L	301	BCL	C1-C2-C3-C5
7	L	303	BCL	C2B-C3B-CAB-OBB
7	L	303	BCL	C2B-C3B-CAB-CBB
7	L	303	BCL	C4B-C3B-CAB-OBB
7	L	303	BCL	C4B-C3B-CAB-CBB
7	M	402	BCL	C1A-C2A-CAA-CBA
7	a	101	BCL	C4C-C3C-CAC-CBC
7	b	101	BCL	C2C-C3C-CAC-CBC
7	b	101	BCL	C4C-C3C-CAC-CBC
7	c	101	BCL	C1A-C2A-CAA-CBA
7	c	101	BCL	C3A-C2A-CAA-CBA
7	c	101	BCL	C4C-C3C-CAC-CBC
7	d	101	BCL	C1A-C2A-CAA-CBA
7	d	101	BCL	C3A-C2A-CAA-CBA
7	d	101	BCL	C1-C2-C3-C5
7	e	101	BCL	C2C-C3C-CAC-CBC
7	e	101	BCL	C4C-C3C-CAC-CBC
7	e	101	BCL	C1-C2-C3-C5
7	e	101	BCL	C11-C12-C13-C14
7	e	101	BCL	C14-C13-C15-C16
7	f	102	BCL	C1A-C2A-CAA-CBA
7	f	102	BCL	C3A-C2A-CAA-CBA
7	f	102	BCL	C2C-C3C-CAC-CBC
7	f	102	BCL	C4C-C3C-CAC-CBC
7	f	102	BCL	O2A-C1-C2-C3
7	f	102	BCL	C1-C2-C3-C5
7	g	101	BCL	C1A-C2A-CAA-CBA
7	g	101	BCL	C3A-C2A-CAA-CBA
7	g	101	BCL	C2C-C3C-CAC-CBC
7	g	101	BCL	C4C-C3C-CAC-CBC
7	h	101	BCL	C1A-C2A-CAA-CBA
7	h	101	BCL	C3A-C2A-CAA-CBA
7	h	101	BCL	O1A-CGA-O2A-C1
7	h	101	BCL	O2A-C1-C2-C3
7	h	101	BCL	C1-C2-C3-C4
7	h	101	BCL	C1-C2-C3-C5
7	i	101	BCL	C4C-C3C-CAC-CBC
7	j	101	BCL	C1-C2-C3-C4
7	j	101	BCL	C1-C2-C3-C5
7	k	101	BCL	C1A-C2A-CAA-CBA
7	k	101	BCL	C3A-C2A-CAA-CBA
7	k	101	BCL	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
7	l	101	BCL	C2C-C3C-CAC-CBC
7	l	101	BCL	C1-C2-C3-C5
7	m	101	BCL	C1A-C2A-CAA-CBA
7	m	101	BCL	C3A-C2A-CAA-CBA
7	m	101	BCL	C2C-C3C-CAC-CBC
7	m	101	BCL	C4C-C3C-CAC-CBC
7	m	101	BCL	C11-C12-C13-C14
7	o	101	BCL	C2B-C3B-CAB-OB
7	o	101	BCL	C2B-C3B-CAB-CBB
7	o	101	BCL	C4B-C3B-CAB-OB
7	o	101	BCL	C4B-C3B-CAB-CBB
7	o	101	BCL	C2C-C3C-CAC-CBC
7	o	101	BCL	C4C-C3C-CAC-CBC
7	o	101	BCL	C6-C7-C8-C9
7	p	101	BCL	C2C-C3C-CAC-CBC
7	p	101	BCL	C4C-C3C-CAC-CBC
8	0	102	SPN	O1-C1-C2-O2
8	0	102	SPN	C20-C21-C22-CM7
8	8	102	SPN	C20-C21-C22-CM7
8	8	102	SPN	CM7-C22-C23-C24
8	9	101	SPN	O1-C1-C2-O2
8	9	101	SPN	CM1-C1-C2-O2
8	9	101	SPN	CM1-C1-C2-C3
8	9	101	SPN	C20-C21-C22-CM7
8	M	406	SPN	C18-C19-C20-C21
8	M	406	SPN	C20-C21-C22-CM7
8	M	406	SPN	C22-C23-C24-C25
8	a	102	SPN	O1-C1-C2-O2
8	a	102	SPN	CM2-C1-C2-O2
8	a	102	SPN	CM2-C1-C2-C3
8	a	102	SPN	C20-C21-C22-CM7
8	a	103	SPN	CM1-C1-O1-CMA
8	a	103	SPN	CM2-C1-O1-CMA
8	a	103	SPN	C18-C19-C20-C21
8	a	103	SPN	C26-C27-C28-C29
8	a	104	SPN	O1-C1-C2-O2
8	a	104	SPN	C20-C21-C22-CM7
8	a	104	SPN	C25-C26-C27-C28
8	a	104	SPN	CM8-C26-C27-C28
8	e	102	SPN	O1-C1-C2-O2
8	e	102	SPN	CM2-C1-C2-O2
8	e	102	SPN	CM2-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
8	e	102	SPN	C20-C21-C22-CM7
8	f	101	SPN	O1-C1-C2-O2
8	f	101	SPN	CM2-C1-C2-O2
8	f	101	SPN	CM2-C1-C2-C3
8	f	101	SPN	C20-C21-C22-CM7
8	f	103	SPN	C2-C1-O1-CMA
8	f	103	SPN	O1-C1-C2-O2
8	f	103	SPN	C18-C19-C20-C21
8	g	102	SPN	O1-C1-C2-O2
8	g	102	SPN	CM2-C1-C2-O2
8	g	102	SPN	CM2-C1-C2-C3
8	g	102	SPN	C20-C21-C22-CM7
8	g	103	SPN	C2-C1-O1-CMA
8	g	103	SPN	O1-C1-C2-O2
8	g	103	SPN	C18-C19-C20-C21
8	h	102	SPN	O1-C1-C2-O2
8	h	102	SPN	C18-C19-C20-C21
8	h	102	SPN	C25-C26-C27-C28
8	h	102	SPN	CM8-C26-C27-C28
8	h	102	SPN	C26-C27-C28-C29
8	i	102	SPN	O1-C1-C2-O2
8	i	102	SPN	CM2-C1-C2-O2
8	i	102	SPN	CM2-C1-C2-C3
8	i	102	SPN	C20-C21-C22-CM7
8	i	103	SPN	O1-C1-C2-O2
8	i	103	SPN	C18-C19-C20-C21
8	l	102	SPN	CM1-C1-C2-C3
8	l	102	SPN	CM2-C1-C2-C3
8	l	102	SPN	C20-C21-C22-CM7
8	m	102	SPN	O1-C1-C2-O2
8	m	102	SPN	C20-C21-C22-CM7
8	n	102	SPN	C20-C21-C22-CM7
8	p	102	SPN	O1-C1-C2-O2
8	p	102	SPN	C6-C7-C8-C9
8	p	102	SPN	C10-C11-C12-C13
8	p	102	SPN	C20-C21-C22-CM7
8	p	102	SPN	C22-C23-C24-C25
8	p	103	SPN	C2-C1-O1-CMA
8	p	103	SPN	O1-C1-C2-O2
8	p	103	SPN	C17-C18-C19-C20
8	p	103	SPN	CM6-C18-C19-C20
8	p	103	SPN	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
11	L	304	BPH	C3A-C2A-CAA-CBA
11	L	305	BPH	C4C-C3C-CAC-CBC
11	L	305	BPH	C2C-C3C-CAC-CBC
11	L	305	BPH	CBA-CGA-O2A-C1
11	L	305	BPH	O1A-CGA-O2A-C1
11	L	305	BPH	C1-C2-C3-C5
7	7	101	BCL	O1D-CGD-O2D-CED
7	8	101	BCL	O1D-CGD-O2D-CED
7	8	101	BCL	CBD-CGD-O2D-CED
7	o	101	BCL	CBD-CGD-O2D-CED
7	j	101	BCL	O1A-CGA-O2A-C1
8	M	406	SPN	C15-C16-C17-C18
7	b	101	BCL	CBA-CGA-O2A-C1
7	j	101	BCL	CBA-CGA-O2A-C1
7	b	101	BCL	O1A-CGA-O2A-C1
7	d	101	BCL	O1A-CGA-O2A-C1
7	f	102	BCL	O1A-CGA-O2A-C1
7	l	101	BCL	O1A-CGA-O2A-C1
7	p	101	BCL	O1A-CGA-O2A-C1
7	0	101	BCL	C3-C5-C6-C7
7	7	101	BCL	C3-C5-C6-C7
7	9	102	BCL	C3-C5-C6-C7
7	h	101	BCL	C3-C5-C6-C7
7	n	101	BCL	C3-C5-C6-C7
7	d	101	BCL	CBA-CGA-O2A-C1
7	h	101	BCL	CBA-CGA-O2A-C1
7	l	101	BCL	CBA-CGA-O2A-C1
7	p	101	BCL	CBA-CGA-O2A-C1
7	M	405	BCL	C4-C3-C5-C6
7	j	101	BCL	C4-C3-C5-C6
8	a	103	SPN	CM8-C26-C27-C28
8	m	102	SPN	CM8-C26-C27-C28
7	8	101	BCL	C2-C3-C5-C6
7	M	405	BCL	C2-C3-C5-C6
8	m	102	SPN	C25-C26-C27-C28
7	M	402	BCL	C3-C5-C6-C7
7	0	101	BCL	CBA-CGA-O2A-C1
7	f	102	BCL	CBA-CGA-O2A-C1
8	p	102	SPN	C11-C12-C13-CM5
8	p	102	SPN	C11-C12-C13-C14
7	o	101	BCL	O1D-CGD-O2D-CED
8	8	102	SPN	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
7	0	101	BCL	O1A-CGA-O2A-C1
8	0	102	SPN	CM3-C5-C6-C7
8	0	102	SPN	C11-C10-C9-CM4
8	0	102	SPN	CM5-C13-C14-C15
8	0	102	SPN	C16-C17-C18-CM6
8	8	102	SPN	CM3-C5-C6-C7
8	8	102	SPN	C11-C10-C9-CM4
8	8	102	SPN	CM5-C13-C14-C15
8	9	101	SPN	CM3-C5-C6-C7
8	9	101	SPN	C11-C10-C9-CM4
8	9	101	SPN	CM5-C13-C14-C15
8	9	101	SPN	C16-C17-C18-CM6
8	9	101	SPN	CM8-C26-C27-C28
8	M	406	SPN	CM3-C5-C6-C7
8	M	406	SPN	C11-C10-C9-CM4
8	M	406	SPN	CM5-C13-C14-C15
8	M	406	SPN	C16-C17-C18-CM6
8	a	102	SPN	CM3-C5-C6-C7
8	a	102	SPN	C11-C10-C9-CM4
8	a	102	SPN	CM5-C13-C14-C15
8	a	102	SPN	C16-C17-C18-CM6
8	a	103	SPN	CM3-C5-C6-C7
8	a	103	SPN	C11-C10-C9-CM4
8	a	103	SPN	CM5-C13-C14-C15
8	a	103	SPN	C16-C17-C18-CM6
8	a	104	SPN	CM3-C5-C6-C7
8	a	104	SPN	C11-C10-C9-CM4
8	a	104	SPN	CM5-C13-C14-C15
8	a	104	SPN	C16-C17-C18-CM6
8	e	102	SPN	CM3-C5-C6-C7
8	e	102	SPN	C11-C10-C9-CM4
8	e	102	SPN	CM5-C13-C14-C15
8	e	102	SPN	C16-C17-C18-CM6
8	f	101	SPN	CM3-C5-C6-C7
8	f	101	SPN	C11-C10-C9-CM4
8	f	101	SPN	CM5-C13-C14-C15
8	f	101	SPN	C16-C17-C18-CM6
8	f	103	SPN	CM3-C5-C6-C7
8	f	103	SPN	C11-C10-C9-CM4
8	f	103	SPN	CM5-C13-C14-C15
8	f	103	SPN	C16-C17-C18-CM6
8	g	102	SPN	CM3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
8	g	102	SPN	C11-C10-C9-CM4
8	g	102	SPN	CM5-C13-C14-C15
8	g	102	SPN	C16-C17-C18-CM6
8	g	103	SPN	CM3-C5-C6-C7
8	g	103	SPN	C11-C10-C9-CM4
8	g	103	SPN	CM5-C13-C14-C15
8	g	103	SPN	C16-C17-C18-CM6
8	g	103	SPN	CM8-C26-C27-C28
8	h	102	SPN	CM3-C5-C6-C7
8	h	102	SPN	C11-C10-C9-CM4
8	h	102	SPN	CM5-C13-C14-C15
8	h	102	SPN	C16-C17-C18-CM6
8	i	102	SPN	CM3-C5-C6-C7
8	i	102	SPN	C11-C10-C9-CM4
8	i	102	SPN	CM5-C13-C14-C15
8	i	102	SPN	C16-C17-C18-CM6
8	i	103	SPN	CM3-C5-C6-C7
8	i	103	SPN	C11-C10-C9-CM4
8	i	103	SPN	CM5-C13-C14-C15
8	i	103	SPN	C16-C17-C18-CM6
8	l	102	SPN	CM3-C5-C6-C7
8	l	102	SPN	C11-C10-C9-CM4
8	l	102	SPN	CM5-C13-C14-C15
8	l	102	SPN	C16-C17-C18-CM6
8	m	102	SPN	CM3-C5-C6-C7
8	m	102	SPN	C11-C10-C9-CM4
8	m	102	SPN	CM5-C13-C14-C15
8	m	102	SPN	C16-C17-C18-CM6
8	n	102	SPN	CM3-C5-C6-C7
8	n	102	SPN	C11-C10-C9-CM4
8	n	102	SPN	CM5-C13-C14-C15
8	n	102	SPN	C16-C17-C18-CM6
8	p	102	SPN	CM3-C5-C6-C7
8	p	102	SPN	C11-C10-C9-CM4
8	p	102	SPN	CM5-C13-C14-C15
8	p	102	SPN	C16-C17-C18-CM6
8	p	102	SPN	CM8-C26-C27-C28
8	p	103	SPN	CM3-C5-C6-C7
8	p	103	SPN	C11-C10-C9-CM4
8	p	103	SPN	CM5-C13-C14-C15
8	p	103	SPN	C16-C17-C18-CM6
7	p	101	BCL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
8	0	102	SPN	C4-C5-C6-C7
8	0	102	SPN	C11-C10-C9-C8
8	0	102	SPN	C12-C13-C14-C15
8	0	102	SPN	C16-C17-C18-C19
8	8	102	SPN	C4-C5-C6-C7
8	8	102	SPN	C11-C10-C9-C8
8	8	102	SPN	C12-C13-C14-C15
8	9	101	SPN	C4-C5-C6-C7
8	9	101	SPN	C11-C10-C9-C8
8	9	101	SPN	C12-C13-C14-C15
8	9	101	SPN	C16-C17-C18-C19
8	M	406	SPN	C4-C5-C6-C7
8	M	406	SPN	C11-C10-C9-C8
8	M	406	SPN	C12-C13-C14-C15
8	M	406	SPN	C16-C17-C18-C19
8	a	102	SPN	C4-C5-C6-C7
8	a	102	SPN	C11-C10-C9-C8
8	a	102	SPN	C12-C13-C14-C15
8	a	102	SPN	C16-C17-C18-C19
8	a	103	SPN	C4-C5-C6-C7
8	a	103	SPN	C11-C10-C9-C8
8	a	103	SPN	C12-C13-C14-C15
8	a	103	SPN	C16-C17-C18-C19
8	a	103	SPN	C25-C26-C27-C28
8	a	104	SPN	C4-C5-C6-C7
8	a	104	SPN	C11-C10-C9-C8
8	a	104	SPN	C12-C13-C14-C15
8	a	104	SPN	C16-C17-C18-C19
8	e	102	SPN	C4-C5-C6-C7
8	e	102	SPN	C11-C10-C9-C8
8	e	102	SPN	C12-C13-C14-C15
8	e	102	SPN	C16-C17-C18-C19
8	f	101	SPN	C4-C5-C6-C7
8	f	101	SPN	C11-C10-C9-C8
8	f	101	SPN	C12-C13-C14-C15
8	f	101	SPN	C16-C17-C18-C19
8	f	103	SPN	C4-C5-C6-C7
8	f	103	SPN	C11-C10-C9-C8
8	f	103	SPN	C12-C13-C14-C15
8	g	102	SPN	C4-C5-C6-C7
8	g	102	SPN	C11-C10-C9-C8
8	g	102	SPN	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
8	g	102	SPN	C16-C17-C18-C19
8	g	103	SPN	C4-C5-C6-C7
8	g	103	SPN	C11-C10-C9-C8
8	g	103	SPN	C12-C13-C14-C15
8	g	103	SPN	C16-C17-C18-C19
8	g	103	SPN	C25-C26-C27-C28
8	h	102	SPN	C4-C5-C6-C7
8	h	102	SPN	C11-C10-C9-C8
8	h	102	SPN	C12-C13-C14-C15
8	i	102	SPN	C4-C5-C6-C7
8	i	102	SPN	C11-C10-C9-C8
8	i	102	SPN	C12-C13-C14-C15
8	i	102	SPN	C16-C17-C18-C19
8	i	103	SPN	C4-C5-C6-C7
8	i	103	SPN	C11-C10-C9-C8
8	i	103	SPN	C12-C13-C14-C15
8	i	103	SPN	C16-C17-C18-C19
8	l	102	SPN	C4-C5-C6-C7
8	l	102	SPN	C11-C10-C9-C8
8	l	102	SPN	C12-C13-C14-C15
8	l	102	SPN	C16-C17-C18-C19
8	m	102	SPN	C4-C5-C6-C7
8	m	102	SPN	C11-C10-C9-C8
8	m	102	SPN	C12-C13-C14-C15
8	m	102	SPN	C16-C17-C18-C19
8	n	102	SPN	C4-C5-C6-C7
8	n	102	SPN	C11-C10-C9-C8
8	n	102	SPN	C12-C13-C14-C15
8	n	102	SPN	C16-C17-C18-C19
8	p	102	SPN	C16-C17-C18-C19
8	p	102	SPN	C25-C26-C27-C28
8	p	103	SPN	C4-C5-C6-C7
8	p	103	SPN	C11-C10-C9-C8
8	p	103	SPN	C12-C13-C14-C15
8	p	103	SPN	C16-C17-C18-C19
7	f	102	BCL	C10-C11-C12-C13
8	a	104	SPN	C26-C27-C28-C29
8	f	101	SPN	C26-C27-C28-C29
8	f	103	SPN	C26-C27-C28-C29
8	g	102	SPN	C26-C27-C28-C29
8	g	103	SPN	C26-C27-C28-C29
8	i	102	SPN	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
8	i	103	SPN	C26-C27-C28-C29
8	l	102	SPN	C26-C27-C28-C29
8	m	102	SPN	C26-C27-C28-C29
8	n	102	SPN	C26-C27-C28-C29
10	M	403	U10	C24-C26-C27-C28
10	M	403	U10	C34-C36-C37-C38
10	M	403	U10	C39-C41-C42-C43
7	k	101	BCL	C2A-CAA-CBA-CGA
7	8	101	BCL	C5-C6-C7-C8
7	L	301	BCL	CBD-CGD-O2D-CED
7	m	101	BCL	CBD-CGD-O2D-CED
7	p	101	BCL	C4-C3-C5-C6
8	i	103	SPN	CM8-C26-C27-C28
7	j	101	BCL	C2-C3-C5-C6
8	9	101	SPN	C25-C26-C27-C28
8	f	103	SPN	C16-C17-C18-C19
8	h	102	SPN	C16-C17-C18-C19
8	i	103	SPN	C25-C26-C27-C28
8	p	102	SPN	C4-C5-C6-C7
8	p	102	SPN	C11-C10-C9-C8
8	p	102	SPN	C12-C13-C14-C15
7	7	101	BCL	C14-C13-C15-C16
7	8	101	BCL	C14-C13-C15-C16
7	9	102	BCL	C11-C10-C8-C9
7	M	402	BCL	C11-C12-C13-C14
7	a	101	BCL	C11-C12-C13-C14
7	d	101	BCL	C11-C12-C13-C14
7	g	101	BCL	C11-C12-C13-C14
7	g	101	BCL	C14-C13-C15-C16
7	k	101	BCL	C11-C12-C13-C14
7	p	101	BCL	C14-C13-C15-C16
8	M	406	SPN	CM7-C22-C23-C24
8	f	103	SPN	C20-C21-C22-CM7
8	f	103	SPN	CM7-C22-C23-C24
8	h	102	SPN	C20-C21-C22-CM7
8	h	102	SPN	CM7-C22-C23-C24
8	p	102	SPN	CM7-C22-C23-C24
8	p	103	SPN	C20-C21-C22-CM7
8	p	103	SPN	CM7-C22-C23-C24
7	L	303	BCL	C2A-CAA-CBA-CGA
7	L	303	BCL	CBA-CGA-O2A-C1
7	j	101	BCL	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
8	h	102	SPN	CM6-C18-C19-C20
7	M	402	BCL	C5-C6-C7-C8
7	i	101	BCL	C15-C16-C17-C18
7	k	101	BCL	C10-C11-C12-C13
8	e	102	SPN	C22-C23-C24-C25
8	i	102	SPN	C22-C23-C24-C25
7	7	101	BCL	C11-C10-C8-C7
7	b	101	BCL	C6-C7-C8-C10
7	c	101	BCL	C11-C12-C13-C15
7	m	101	BCL	C12-C13-C15-C16
7	n	101	BCL	C6-C7-C8-C10
8	a	103	SPN	C20-C21-C22-C23
8	g	103	SPN	C20-C21-C22-C23
8	i	103	SPN	C20-C21-C22-C23
7	h	101	BCL	C10-C11-C12-C13
7	l	101	BCL	C8-C10-C11-C12
8	9	101	SPN	C26-C27-C28-C29
8	p	102	SPN	C26-C27-C28-C29
10	M	403	U10	C29-C31-C32-C33
7	l	101	BCL	C5-C6-C7-C8
7	9	102	BCL	C8-C10-C11-C12
7	a	101	BCL	C15-C16-C17-C18
7	d	101	BCL	C5-C6-C7-C8
7	d	101	BCL	C10-C11-C12-C13
7	d	101	BCL	C15-C16-C17-C18
7	l	101	BCL	C13-C15-C16-C17
7	o	101	BCL	C13-C15-C16-C17
7	L	301	BCL	C2A-CAA-CBA-CGA
7	M	402	BCL	C2A-CAA-CBA-CGA
7	a	101	BCL	C2A-CAA-CBA-CGA
7	c	101	BCL	C2A-CAA-CBA-CGA
7	e	101	BCL	C2A-CAA-CBA-CGA
7	g	101	BCL	C2A-CAA-CBA-CGA
7	m	101	BCL	C2A-CAA-CBA-CGA
7	0	101	BCL	C8-C10-C11-C12
7	8	101	BCL	C10-C11-C12-C13
7	n	101	BCL	C8-C10-C11-C12
11	L	305	BPH	C5-C6-C7-C8
7	9	102	BCL	CBD-CGD-O2D-CED
7	M	405	BCL	C15-C16-C17-C18
7	h	101	BCL	C13-C15-C16-C17
7	i	101	BCL	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
7	m	101	BCL	C13-C15-C16-C17
7	L	303	BCL	O1A-CGA-O2A-C1
7	j	101	BCL	C15-C16-C17-C18
7	0	101	BCL	C5-C6-C7-C8
7	l	101	BCL	C15-C16-C17-C18
7	7	101	BCL	C8-C10-C11-C12
7	k	101	BCL	C13-C15-C16-C17
7	n	101	BCL	C10-C11-C12-C13
7	M	402	BCL	C8-C10-C11-C12
7	8	101	BCL	C15-C16-C17-C18
7	j	101	BCL	C10-C11-C12-C13
7	m	101	BCL	C10-C11-C12-C13
8	p	102	SPN	C7-C8-C9-CM4
7	a	101	BCL	C10-C11-C12-C13
8	e	102	SPN	C26-C27-C28-C29
7	M	405	BCL	C16-C17-C18-C19
7	c	101	BCL	C16-C17-C18-C20
9	C	401	HEM	C3D-CAD-CBD-CGD
7	o	101	BCL	O2A-C1-C2-C3
7	0	101	BCL	C16-C17-C18-C19
7	L	303	BCL	C16-C17-C18-C20
7	a	101	BCL	C16-C17-C18-C20
7	m	101	BCL	C15-C16-C17-C18
7	l	101	BCL	C3-C5-C6-C7
7	M	405	BCL	C16-C17-C18-C20
7	c	101	BCL	C16-C17-C18-C19
7	n	101	BCL	C16-C17-C18-C19
8	9	101	SPN	C22-C23-C24-C25
8	a	103	SPN	C22-C23-C24-C25
7	9	102	BCL	C16-C17-C18-C20
7	m	101	BCL	C16-C17-C18-C20
7	n	101	BCL	C16-C17-C18-C20
7	0	101	BCL	C13-C15-C16-C17
7	n	101	BCL	C13-C15-C16-C17
7	g	101	BCL	C13-C15-C16-C17
7	0	101	BCL	C3A-C2A-CAA-CBA
7	L	301	BCL	C3A-C2A-CAA-CBA
7	M	402	BCL	C3A-C2A-CAA-CBA
7	M	405	BCL	C3A-C2A-CAA-CBA
7	a	101	BCL	C3A-C2A-CAA-CBA
7	n	101	BCL	C3A-C2A-CAA-CBA
7	b	101	BCL	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
7	L	301	BCL	O1D-CGD-O2D-CED
7	m	101	BCL	O1D-CGD-O2D-CED
7	L	303	BCL	C16-C17-C18-C19
8	f	103	SPN	CM6-C18-C19-C20
7	M	405	BCL	C2A-CAA-CBA-CGA
8	n	102	SPN	CM8-C26-C27-C28
8	p	102	SPN	C7-C8-C9-C10
7	n	101	BCL	C14-C13-C15-C16
7	j	101	BCL	C13-C15-C16-C17
7	p	101	BCL	C5-C6-C7-C8
7	M	402	BCL	C10-C11-C12-C13
7	7	101	BCL	C2A-CAA-CBA-CGA
7	p	101	BCL	C13-C15-C16-C17
7	0	101	BCL	C16-C17-C18-C20
10	M	403	U10	C43-C44-C46-C47
11	L	304	BPH	C2A-CAA-CBA-CGA
7	c	101	BCL	C8-C10-C11-C12
7	a	101	BCL	C16-C17-C18-C19
7	m	101	BCL	C16-C17-C18-C19
8	0	102	SPN	C15-C16-C17-C18
8	8	102	SPN	C22-C23-C24-C25
8	l	102	SPN	C22-C23-C24-C25
7	L	303	BCL	C1A-C2A-CAA-CBA
7	M	405	BCL	C1A-C2A-CAA-CBA
7	a	101	BCL	C1A-C2A-CAA-CBA
7	n	101	BCL	C1A-C2A-CAA-CBA
7	0	101	BCL	C12-C13-C15-C16
7	M	405	BCL	C12-C13-C15-C16
7	a	101	BCL	C12-C13-C15-C16
7	b	101	BCL	C11-C12-C13-C15
7	d	101	BCL	C6-C7-C8-C10
7	e	101	BCL	C11-C12-C13-C15
7	g	101	BCL	C11-C12-C13-C15
7	i	101	BCL	C6-C7-C8-C10
7	k	101	BCL	C11-C10-C8-C7
7	m	101	BCL	C11-C10-C8-C7
7	m	101	BCL	C11-C12-C13-C15
8	9	101	SPN	C21-C22-C23-C24
8	g	102	SPN	C21-C22-C23-C24
8	m	102	SPN	C21-C22-C23-C24
8	n	102	SPN	C21-C22-C23-C24
11	L	305	BPH	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
7	7	101	BCL	C2C-C3C-CAC-CBC
7	9	102	BCL	C2C-C3C-CAC-CBC
7	a	101	BCL	C2C-C3C-CAC-CBC
7	c	101	BCL	C2C-C3C-CAC-CBC
7	i	101	BCL	C2C-C3C-CAC-CBC
7	k	101	BCL	C2C-C3C-CAC-CBC
7	n	101	BCL	C4-C3-C5-C6
7	n	101	BCL	C2-C3-C5-C6
10	L	302	U10	C13-C14-C16-C17
11	L	304	BPH	C2-C3-C5-C6
7	8	101	BCL	C4B-C3B-CAB-CBB
7	9	102	BCL	C2A-CAA-CBA-CGA
7	0	101	BCL	C14-C13-C15-C16
7	7	101	BCL	C11-C10-C8-C9
7	9	102	BCL	C6-C7-C8-C9
7	M	405	BCL	C14-C13-C15-C16
7	b	101	BCL	C6-C7-C8-C9
7	b	101	BCL	C11-C12-C13-C14
7	i	101	BCL	C6-C7-C8-C9
7	i	101	BCL	C14-C13-C15-C16
7	j	101	BCL	C11-C12-C13-C14
11	L	305	BPH	C6-C7-C8-C9
8	p	103	SPN	C24-C25-C26-CM8
7	e	101	BCL	C13-C15-C16-C17
7	i	101	BCL	C10-C11-C12-C13
7	o	101	BCL	C10-C11-C12-C13
10	L	302	U10	C15-C14-C16-C17
10	M	403	U10	C45-C44-C46-C47
11	L	304	BPH	C4-C3-C5-C6
7	j	101	BCL	C16-C17-C18-C20
7	L	303	BCL	O2A-C1-C2-C3
7	d	101	BCL	O2A-C1-C2-C3
7	g	101	BCL	C8-C10-C11-C12
8	a	103	SPN	CM6-C18-C19-C20
7	c	101	BCL	C13-C15-C16-C17
7	7	101	BCL	C13-C15-C16-C17
7	f	102	BCL	C4-C3-C5-C6
7	L	303	BCL	C11-C10-C8-C9
7	c	101	BCL	C11-C12-C13-C14
7	d	101	BCL	C6-C7-C8-C9
7	k	101	BCL	C11-C10-C8-C9
7	m	101	BCL	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
7	o	101	BCL	C14-C13-C15-C16
8	i	103	SPN	CM7-C22-C23-C24
11	M	404	BPH	C14-C13-C15-C16
8	m	102	SPN	C22-C23-C24-C25
7	L	303	BCL	C11-C10-C8-C7
7	a	101	BCL	C6-C7-C8-C10
7	e	101	BCL	C12-C13-C15-C16
7	g	101	BCL	C12-C13-C15-C16
7	i	101	BCL	C11-C10-C8-C7
7	j	101	BCL	C11-C12-C13-C15
8	0	102	SPN	C21-C22-C23-C24
8	a	102	SPN	C21-C22-C23-C24
8	e	102	SPN	C21-C22-C23-C24
8	i	102	SPN	C21-C22-C23-C24
8	l	102	SPN	C21-C22-C23-C24
11	M	404	BPH	C12-C13-C15-C16
7	7	101	BCL	C4-C3-C5-C6
7	e	101	BCL	C3A-C2A-CAA-CBA
7	l	101	BCL	C3A-C2A-CAA-CBA
8	n	102	SPN	C25-C26-C27-C28
7	9	102	BCL	O1D-CGD-O2D-CED
8	0	102	SPN	CM1-C1-C2-O2
8	8	102	SPN	CM1-C1-C2-O2
8	8	102	SPN	CM1-C1-C2-C3
8	M	406	SPN	CM2-C1-C2-O2
8	l	102	SPN	CM2-C1-C2-O2
8	n	102	SPN	CM1-C1-C2-O2
8	n	102	SPN	CM1-C1-C2-C3
8	n	102	SPN	CM2-C1-C2-O2
8	n	102	SPN	CM2-C1-C2-C3
7	b	101	BCL	C15-C16-C17-C18
10	L	302	U10	C24-C26-C27-C28
7	l	101	BCL	C16-C17-C18-C20
7	e	101	BCL	C1-C2-C3-C4
7	f	102	BCL	C1-C2-C3-C4
7	k	101	BCL	C1-C2-C3-C4
11	L	304	BPH	C1A-C2A-CAA-CBA
11	L	305	BPH	C1-C2-C3-C4
7	7	101	BCL	C2-C3-C5-C6
7	f	102	BCL	C2-C3-C5-C6
7	j	101	BCL	C5-C6-C7-C8
7	9	102	BCL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
7	j	101	BCL	C16-C17-C18-C19
7	a	101	BCL	C8-C10-C11-C12
7	a	101	BCL	C1-C2-C3-C5
7	c	101	BCL	C1-C2-C3-C5
7	k	101	BCL	C1-C2-C3-C5
7	m	101	BCL	C1-C2-C3-C5
7	n	101	BCL	C1-C2-C3-C5
7	o	101	BCL	C1-C2-C3-C5
7	p	101	BCL	C1-C2-C3-C5
11	L	304	BPH	C1-C2-C3-C5
7	l	101	BCL	C16-C17-C18-C19
7	7	101	BCL	C4B-C3B-CAB-OBB
7	b	101	BCL	C4B-C3B-CAB-OBB
7	b	101	BCL	C4B-C3B-CAB-CBB
7	8	101	BCL	C3-C5-C6-C7
7	d	101	BCL	C14-C13-C15-C16
11	L	305	BPH	C14-C13-C15-C16
7	k	101	BCL	C15-C16-C17-C18
8	a	102	SPN	C26-C27-C28-C29
10	M	403	U10	C19-C21-C22-C23
7	L	301	BCL	C4C-C3C-CAC-CBC
7	L	303	BCL	C4C-C3C-CAC-CBC
8	8	102	SPN	O1-C1-C2-O2
8	l	102	SPN	O1-C1-C2-O2
8	n	102	SPN	O1-C1-C2-O2
7	i	101	BCL	C13-C15-C16-C17
7	o	101	BCL	CBA-CGA-O2A-C1
7	L	301	BCL	C15-C16-C17-C18
7	8	101	BCL	C16-C17-C18-C20
7	p	101	BCL	C16-C17-C18-C19
7	b	101	BCL	C13-C15-C16-C17
7	e	101	BCL	C11-C10-C8-C7
7	g	101	BCL	C11-C10-C8-C7
7	i	101	BCL	C12-C13-C15-C16
7	n	101	BCL	C11-C10-C8-C7
7	o	101	BCL	C11-C10-C8-C7
7	p	101	BCL	C12-C13-C15-C16
8	f	101	SPN	C21-C22-C23-C24
11	M	404	BPH	C6-C7-C8-C10
7	L	301	BCL	CBA-CGA-O2A-C1
10	L	302	U10	C12-C11-C9-C10
7	b	101	BCL	C2B-C3B-CAB-OBB

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Mol	Chain	Res	Type	Atoms
7	b	101	BCL	C2B-C3B-CAB-CBB
11	L	305	BPH	O2A-C1-C2-C3
7	f	102	BCL	C16-C17-C18-C20
9	C	402	HEM	C4B-C3B-CAB-CBB
9	C	402	HEM	C4C-C3C-CAC-CBC
7	M	402	BCL	C6-C7-C8-C9
7	M	402	BCL	C11-C10-C8-C9
7	M	405	BCL	C11-C12-C13-C14
7	n	101	BCL	C11-C10-C8-C9
7	o	101	BCL	C11-C10-C8-C9
11	M	404	BPH	C2C-C3C-CAC-CBC
10	L	302	U10	C12-C11-C9-C8
7	L	303	BCL	C3-C5-C6-C7
7	d	101	BCL	C3-C5-C6-C7
7	L	301	BCL	C16-C17-C18-C20
7	f	102	BCL	C3-C5-C6-C7
7	e	101	BCL	C1A-C2A-CAA-CBA
7	o	101	BCL	O1A-CGA-O2A-C1
7	L	301	BCL	O1A-CGA-O2A-C1
7	8	101	BCL	C12-C13-C15-C16
7	9	102	BCL	C11-C12-C13-C15
7	a	101	BCL	C11-C12-C13-C15
7	o	101	BCL	C12-C13-C15-C16
8	g	103	SPN	C21-C22-C23-C24
11	L	305	BPH	C12-C13-C15-C16
7	h	101	BCL	C2C-C3C-CAC-CBC
7	a	101	BCL	C6-C7-C8-C9
7	a	101	BCL	C11-C10-C8-C9
7	e	101	BCL	C11-C10-C8-C9
7	g	101	BCL	C11-C10-C8-C9
7	n	101	BCL	C6-C7-C8-C9
8	a	103	SPN	CM7-C22-C23-C24
11	M	404	BPH	C6-C7-C8-C9
7	b	101	BCL	C3-C5-C6-C7
10	M	403	U10	C20-C19-C21-C22
7	p	101	BCL	CAD-CBD-CGD-O2D
10	M	403	U10	C5-C4-O4-C4M
8	p	103	SPN	C24-C25-C26-C27
7	0	101	BCL	CHA-CBD-CGD-O1D
7	0	101	BCL	CHA-CBD-CGD-O2D
7	p	101	BCL	CAD-CBD-CGD-O1D
7	8	101	BCL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
7	k	101	BCL	CBD-CGD-O2D-CED
8	a	104	SPN	C22-C23-C24-C25
7	n	101	BCL	C15-C16-C17-C18
7	i	101	BCL	C11-C10-C8-C9
8	g	103	SPN	CM7-C22-C23-C24
7	a	101	BCL	C11-C10-C8-C7
7	d	101	BCL	C12-C13-C15-C16
7	p	101	BCL	C11-C10-C8-C7
10	M	403	U10	C30-C29-C31-C32
7	M	405	BCL	C10-C11-C12-C13
7	b	101	BCL	C16-C17-C18-C20
11	L	305	BPH	C15-C16-C17-C18
8	a	102	SPN	C22-C23-C24-C25
8	f	101	SPN	C22-C23-C24-C25
8	i	103	SPN	C22-C23-C24-C25
7	d	101	BCL	C16-C17-C18-C19
7	a	101	BCL	C13-C15-C16-C17
7	j	101	BCL	C3A-C2A-CAA-CBA
11	L	305	BPH	C3A-C2A-CAA-CBA
11	L	305	BPH	C4-C3-C5-C6
10	M	403	U10	C18-C19-C21-C22
8	0	102	SPN	CM1-C1-C2-C3
8	M	406	SPN	CM2-C1-C2-C3
8	l	102	SPN	CM1-C1-C2-O2
8	m	102	SPN	CM2-C1-C2-O2
8	p	102	SPN	CM2-C1-C2-C3
7	b	101	BCL	C10-C11-C12-C13
7	e	101	BCL	C8-C10-C11-C12
10	M	403	U10	C28-C29-C31-C32
7	f	102	BCL	C16-C17-C18-C19
7	p	101	BCL	C16-C17-C18-C20
8	8	102	SPN	C26-C27-C28-C29
7	0	101	BCL	C11-C10-C8-C9
7	7	101	BCL	C11-C12-C13-C14
7	L	303	BCL	C14-C13-C15-C16
7	d	101	BCL	C11-C10-C8-C9
7	m	101	BCL	C14-C13-C15-C16
11	M	404	BPH	C11-C12-C13-C14
7	0	101	BCL	C2B-C3B-CAB-OBB
7	0	101	BCL	C2B-C3B-CAB-CBB
7	M	402	BCL	C2B-C3B-CAB-OBB
7	M	402	BCL	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
7	b	101	BCL	O2A-C1-C2-C3
7	L	301	BCL	C1-C2-C3-C4
7	a	101	BCL	C1-C2-C3-C4
7	c	101	BCL	C1-C2-C3-C4
7	d	101	BCL	C1-C2-C3-C4
7	l	101	BCL	C1-C2-C3-C4
7	m	101	BCL	C1-C2-C3-C4
7	n	101	BCL	C1-C2-C3-C4
7	o	101	BCL	C1-C2-C3-C4
11	L	304	BPH	C1-C2-C3-C4
7	M	405	BCL	CBA-CGA-O2A-C1
7	j	101	BCL	C1A-C2A-CAA-CBA
7	l	101	BCL	C1A-C2A-CAA-CBA
9	C	402	HEM	CAA-CBA-CGA-O2A
9	C	403	HEM	CAD-CBD-CGD-O2D
8	f	103	SPN	CM8-C26-C27-C28
11	L	305	BPH	C2-C3-C5-C6
9	C	401	HEM	CAA-CBA-CGA-O1A
9	C	401	HEM	CAA-CBA-CGA-O2A
7	M	402	BCL	C11-C12-C13-C15
7	d	101	BCL	C11-C10-C8-C7
7	d	101	BCL	C11-C12-C13-C15
7	h	101	BCL	C6-C7-C8-C10
7	l	101	BCL	C11-C10-C8-C7
7	o	101	BCL	C6-C7-C8-C10
8	i	103	SPN	C21-C22-C23-C24
7	e	101	BCL	C16-C17-C18-C19
9	C	403	HEM	CAD-CBD-CGD-O1D
9	C	402	HEM	CAA-CBA-CGA-O1A
7	0	101	BCL	C4B-C3B-CAB-OBB
7	0	101	BCL	C4B-C3B-CAB-CBB
7	7	101	BCL	C4B-C3B-CAB-CBB
7	L	301	BCL	C11-C10-C8-C9
7	h	101	BCL	C4-C3-C5-C6
7	9	102	BCL	C10-C11-C12-C13
7	l	101	BCL	C10-C11-C12-C13
7	M	405	BCL	O1A-CGA-O2A-C1
9	C	403	HEM	CAA-CBA-CGA-O2A
8	0	102	SPN	C2-C3-C4-C5
8	8	102	SPN	C2-C3-C4-C5
8	9	101	SPN	C2-C3-C4-C5
8	M	406	SPN	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
8	a	102	SPN	C2-C3-C4-C5
8	a	103	SPN	C2-C3-C4-C5
8	a	104	SPN	C2-C3-C4-C5
8	e	102	SPN	C2-C3-C4-C5
8	f	101	SPN	C2-C3-C4-C5
8	f	103	SPN	C2-C3-C4-C5
8	g	102	SPN	C2-C3-C4-C5
8	g	103	SPN	C2-C3-C4-C5
8	h	102	SPN	C2-C3-C4-C5
8	i	102	SPN	C2-C3-C4-C5
8	i	103	SPN	C2-C3-C4-C5
8	l	102	SPN	C2-C3-C4-C5
8	m	102	SPN	C2-C3-C4-C5
8	n	102	SPN	C2-C3-C4-C5
8	p	102	SPN	C2-C3-C4-C5
8	p	103	SPN	C2-C3-C4-C5
7	e	101	BCL	C4-C3-C5-C6
7	h	101	BCL	C2-C3-C5-C6
7	0	101	BCL	C15-C16-C17-C18
7	7	101	BCL	C12-C13-C15-C16
7	L	301	BCL	C11-C10-C8-C7
7	k	101	BCL	O1D-CGD-O2D-CED
8	M	406	SPN	C26-C27-C28-C29
9	C	403	HEM	CAA-CBA-CGA-O1A
7	f	102	BCL	C11-C10-C8-C9
7	g	101	BCL	C2-C1-O2A-CGA
7	m	101	BCL	C2-C1-O2A-CGA
7	7	101	BCL	C2B-C3B-CAB-OB
7	9	102	BCL	C5-C6-C7-C8
7	e	101	BCL	CBA-CGA-O2A-C1
9	C	401	HEM	CAD-CBD-CGD-O1D
7	p	101	BCL	C8-C10-C11-C12
11	L	305	BPH	C13-C15-C16-C17
7	9	102	BCL	C11-C12-C13-C14
7	8	101	BCL	C2A-CAA-CBA-CGA
7	8	101	BCL	C6-C7-C8-C10
7	8	101	BCL	C11-C12-C13-C15
7	9	102	BCL	C11-C10-C8-C7
7	L	303	BCL	C12-C13-C15-C16
7	f	102	BCL	C11-C10-C8-C7
7	k	101	BCL	C11-C12-C13-C15
8	p	102	SPN	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
11	M	404	BPH	C11-C12-C13-C15
7	c	101	BCL	C2-C1-O2A-CGA
7	i	101	BCL	C2-C1-O2A-CGA
7	e	101	BCL	O1A-CGA-O2A-C1
7	M	405	BCL	CAA-CBA-CGA-O2A
11	L	305	BPH	C3-C5-C6-C7
7	9	102	BCL	C4-C3-C5-C6
8	f	103	SPN	C25-C26-C27-C28
7	8	101	BCL	C11-C10-C8-C9
7	a	101	BCL	C14-C13-C15-C16
7	n	101	BCL	CAA-CBA-CGA-O2A
8	8	102	SPN	C6-C7-C8-C9
8	8	102	SPN	C10-C11-C12-C13
8	8	102	SPN	C18-C19-C20-C21
8	9	101	SPN	C18-C19-C20-C21
8	M	406	SPN	C10-C11-C12-C13
8	a	102	SPN	C10-C11-C12-C13
8	a	102	SPN	C18-C19-C20-C21
8	a	104	SPN	C18-C19-C20-C21
8	e	102	SPN	C6-C7-C8-C9
8	e	102	SPN	C10-C11-C12-C13
8	e	102	SPN	C18-C19-C20-C21
8	f	101	SPN	C10-C11-C12-C13
8	f	101	SPN	C18-C19-C20-C21
8	f	103	SPN	C6-C7-C8-C9
8	f	103	SPN	C10-C11-C12-C13
8	g	102	SPN	C18-C19-C20-C21
8	g	103	SPN	C6-C7-C8-C9
8	h	102	SPN	C6-C7-C8-C9
8	h	102	SPN	C10-C11-C12-C13
8	i	102	SPN	C10-C11-C12-C13
8	i	102	SPN	C18-C19-C20-C21
8	i	103	SPN	C10-C11-C12-C13
8	l	102	SPN	C18-C19-C20-C21
8	m	102	SPN	C18-C19-C20-C21
8	n	102	SPN	C18-C19-C20-C21
8	p	102	SPN	C18-C19-C20-C21
8	a	104	SPN	C6-C7-C8-C9
8	e	102	SPN	C23-C24-C25-C26
8	f	101	SPN	C6-C7-C8-C9
8	g	102	SPN	C10-C11-C12-C13
8	i	102	SPN	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
8	i	103	SPN	C6-C7-C8-C9
8	n	102	SPN	C10-C11-C12-C13
7	0	101	BCL	C2-C1-O2A-CGA
11	L	304	BPH	C2-C1-O2A-CGA
7	M	405	BCL	C6-C7-C8-C10
7	c	101	BCL	C11-C10-C8-C7
10	M	403	U10	C3-C4-O4-C4M
7	d	101	BCL	C2C-C3C-CAC-CBC
9	C	401	HEM	CAD-CBD-CGD-O2D
8	0	102	SPN	C6-C7-C8-C9
8	0	102	SPN	C10-C11-C12-C13
8	9	101	SPN	C6-C7-C8-C9
8	9	101	SPN	C10-C11-C12-C13
8	M	406	SPN	C6-C7-C8-C9
8	a	102	SPN	C6-C7-C8-C9
8	a	103	SPN	C6-C7-C8-C9
8	a	103	SPN	C10-C11-C12-C13
8	a	104	SPN	C10-C11-C12-C13
8	g	102	SPN	C6-C7-C8-C9
8	g	103	SPN	C10-C11-C12-C13
8	l	102	SPN	C6-C7-C8-C9
8	l	102	SPN	C10-C11-C12-C13
8	m	102	SPN	C6-C7-C8-C9
8	m	102	SPN	C10-C11-C12-C13
10	M	403	U10	C14-C16-C17-C18
11	M	404	BPH	C10-C11-C12-C13
8	9	101	SPN	CM2-C1-C2-C3
8	a	103	SPN	CM2-C1-C2-O2
8	a	104	SPN	CM1-C1-C2-O2
8	f	101	SPN	CM1-C1-C2-C3
8	g	102	SPN	CM1-C1-C2-C3
8	i	103	SPN	CM2-C1-C2-O2
8	p	102	SPN	CM2-C1-C2-O2
8	p	103	SPN	CM1-C1-C2-O2
8	0	102	SPN	C18-C19-C20-C21
8	h	102	SPN	C23-C24-C25-C26
8	n	102	SPN	C6-C7-C8-C9
8	p	103	SPN	C6-C7-C8-C9
8	p	103	SPN	C10-C11-C12-C13
7	M	402	BCL	C4B-C3B-CAB-CBB
7	n	101	BCL	C2A-CAA-CBA-CGA
8	a	104	SPN	CM7-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
7	M	402	BCL	C2-C3-C5-C6
7	d	101	BCL	C16-C17-C18-C20
7	g	101	BCL	C15-C16-C17-C18
7	M	402	BCL	CAA-CBA-CGA-O2A
7	g	101	BCL	CAD-CBD-CGD-O2D
11	L	304	BPH	CAD-CBD-CGD-O2D
11	M	404	BPH	C4C-C3C-CAC-CBC
7	L	303	BCL	CAA-CBA-CGA-O2A
7	M	405	BCL	C2-C1-O2A-CGA
7	b	101	BCL	C2-C1-O2A-CGA
7	j	101	BCL	C2-C1-O2A-CGA
7	b	101	BCL	C1-C2-C3-C4
7	i	101	BCL	C1-C2-C3-C4
7	p	101	BCL	C1-C2-C3-C4
11	L	305	BPH	C10-C11-C12-C13

There are no ring outliers.

50 monomers are involved in 270 short contacts:

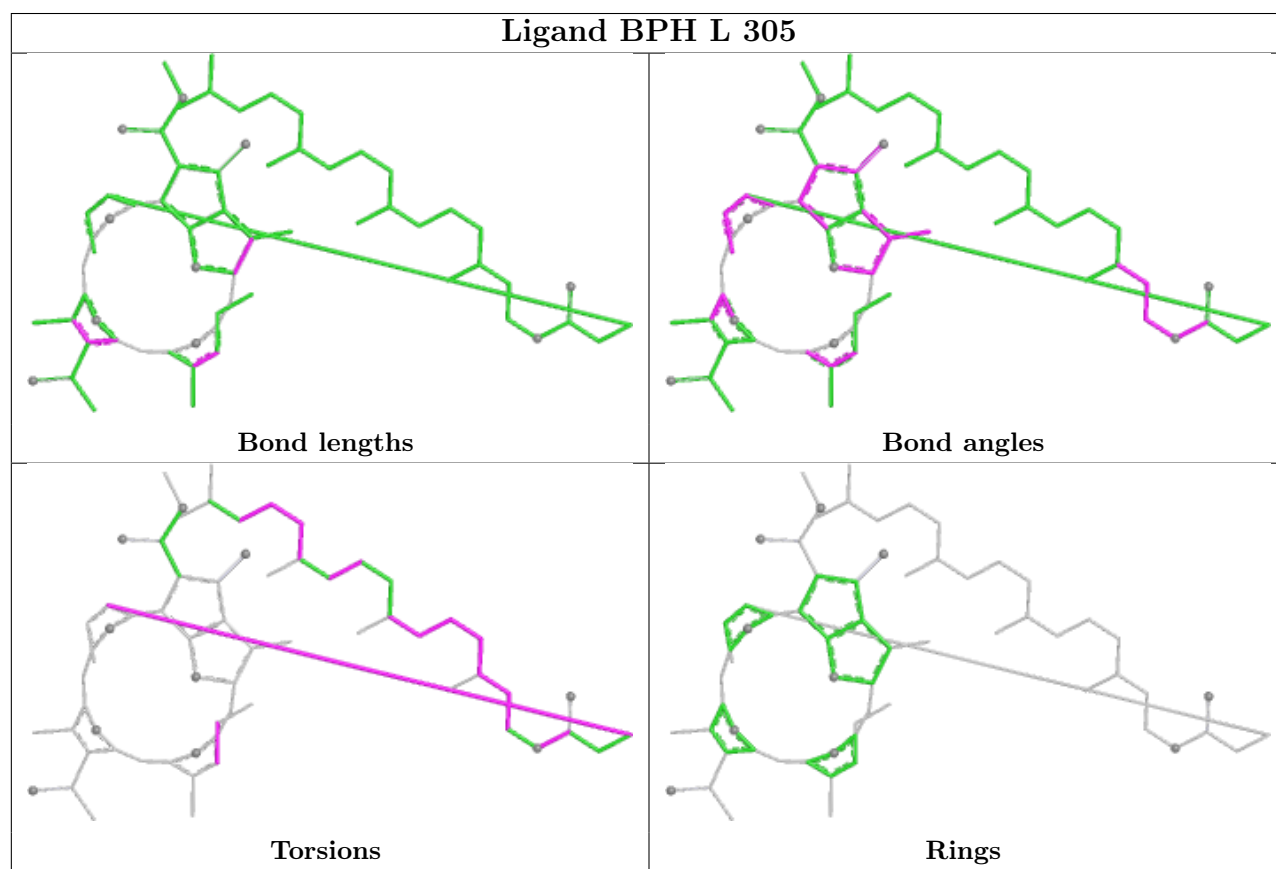
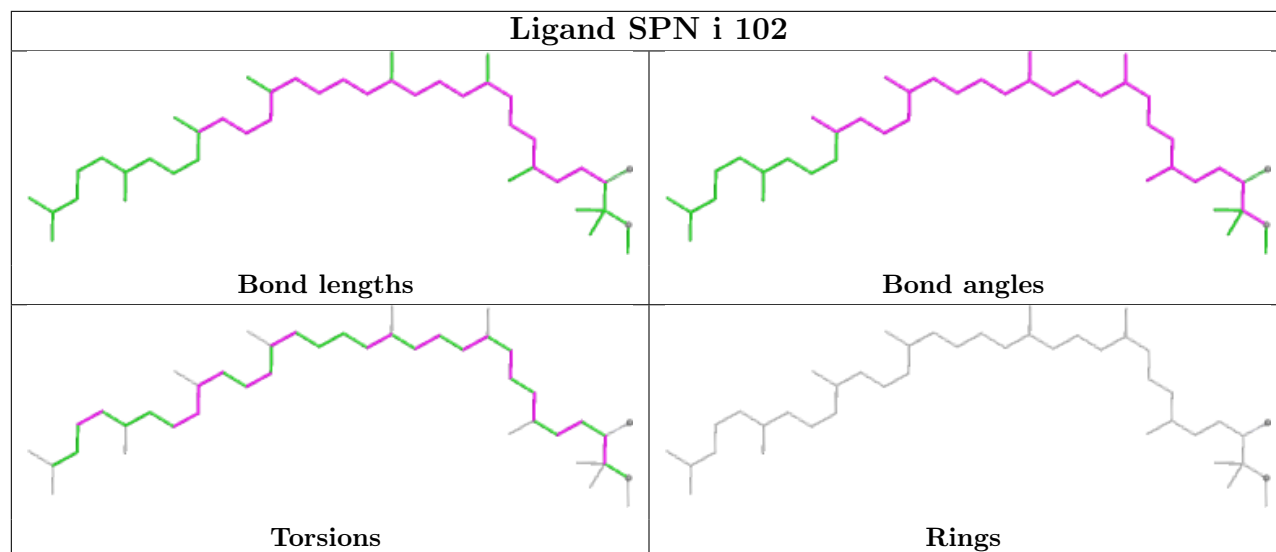
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	i	102	SPN	2	0
11	L	305	BPH	24	0
11	L	304	BPH	1	0
8	g	102	SPN	1	0
8	f	103	SPN	8	0
7	d	101	BCL	5	0
8	a	102	SPN	1	0
7	0	101	BCL	14	0
8	f	101	SPN	2	0
7	h	101	BCL	5	0
7	M	402	BCL	7	0
7	f	102	BCL	10	0
8	M	406	SPN	11	0
8	g	103	SPN	5	0
8	i	103	SPN	3	0
11	M	404	BPH	15	0
8	0	102	SPN	6	0
8	m	102	SPN	3	0
7	M	405	BCL	11	0
8	l	102	SPN	1	0
9	C	402	HEM	7	0
7	9	102	BCL	10	0

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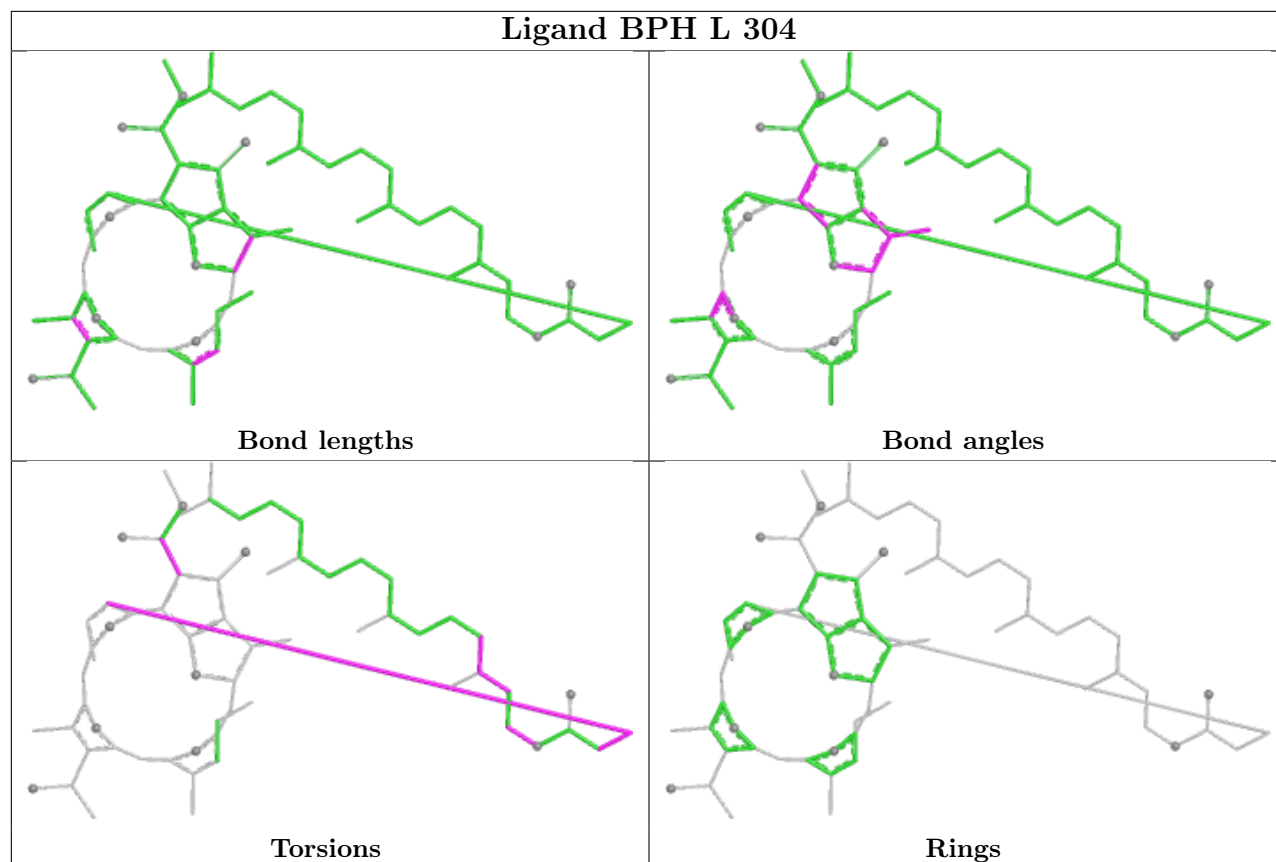
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	g	101	BCL	3	0
7	o	101	BCL	4	0
7	p	101	BCL	10	0
8	8	102	SPN	9	0
8	a	103	SPN	12	0
7	a	101	BCL	5	0
7	b	101	BCL	3	0
8	e	102	SPN	2	0
7	7	101	BCL	15	0
7	n	101	BCL	4	0
9	C	403	HEM	2	0
10	M	403	U10	1	0
7	k	101	BCL	4	0
7	L	303	BCL	4	0
7	m	101	BCL	9	0
7	L	301	BCL	6	0
7	i	101	BCL	4	0
7	l	101	BCL	5	0
8	p	103	SPN	11	0
7	8	101	BCL	13	0
8	9	101	SPN	7	0
7	c	101	BCL	3	0
8	h	102	SPN	5	0
9	C	401	HEM	3	0
7	e	101	BCL	3	0
8	p	102	SPN	5	0
7	j	101	BCL	5	0
8	n	102	SPN	2	0

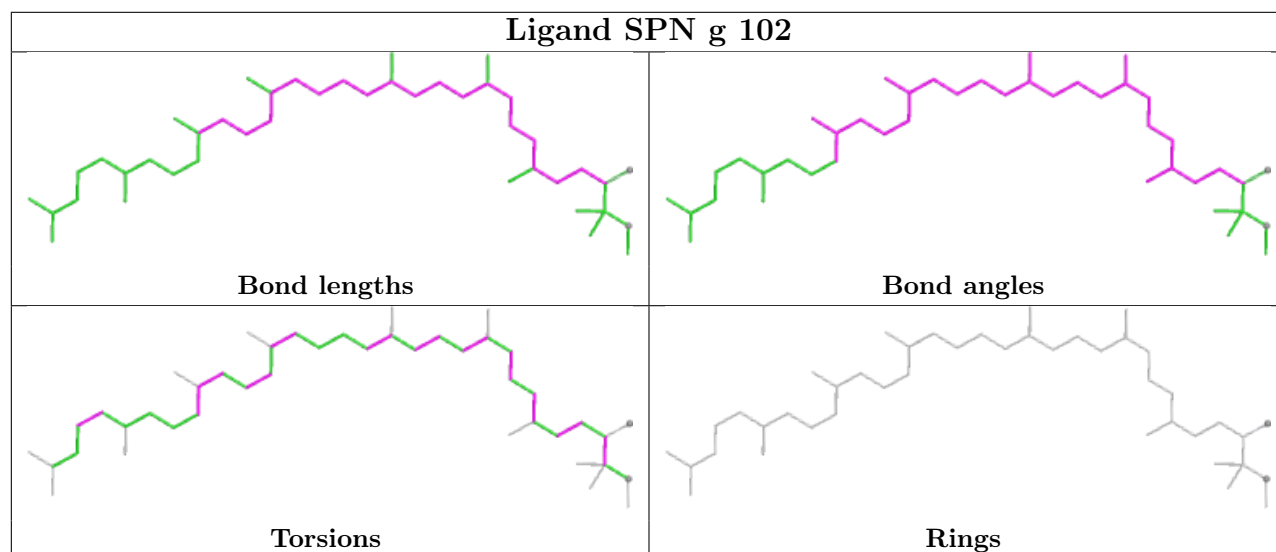
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

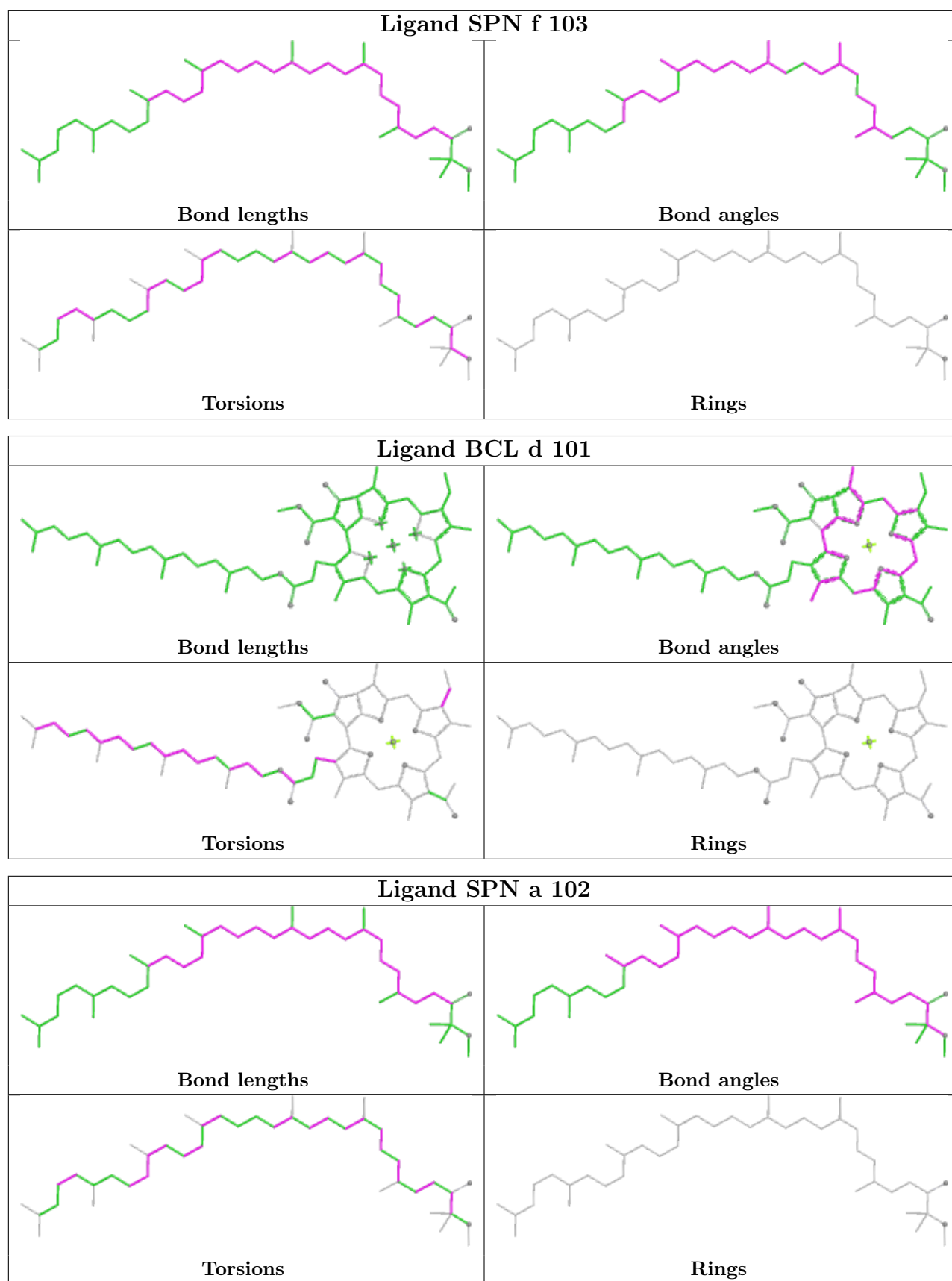


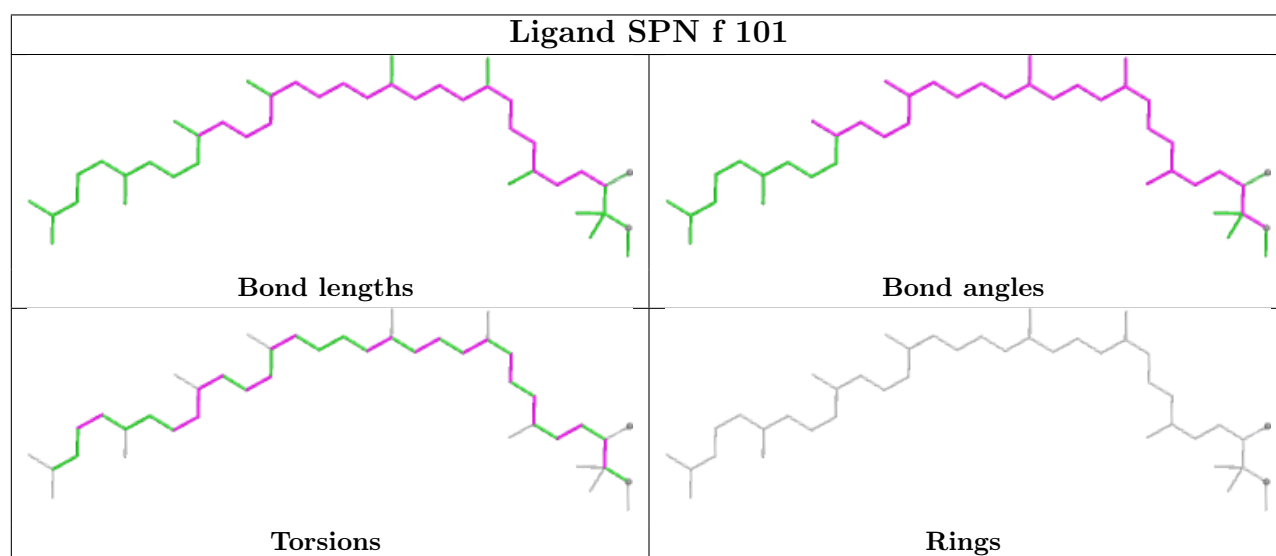
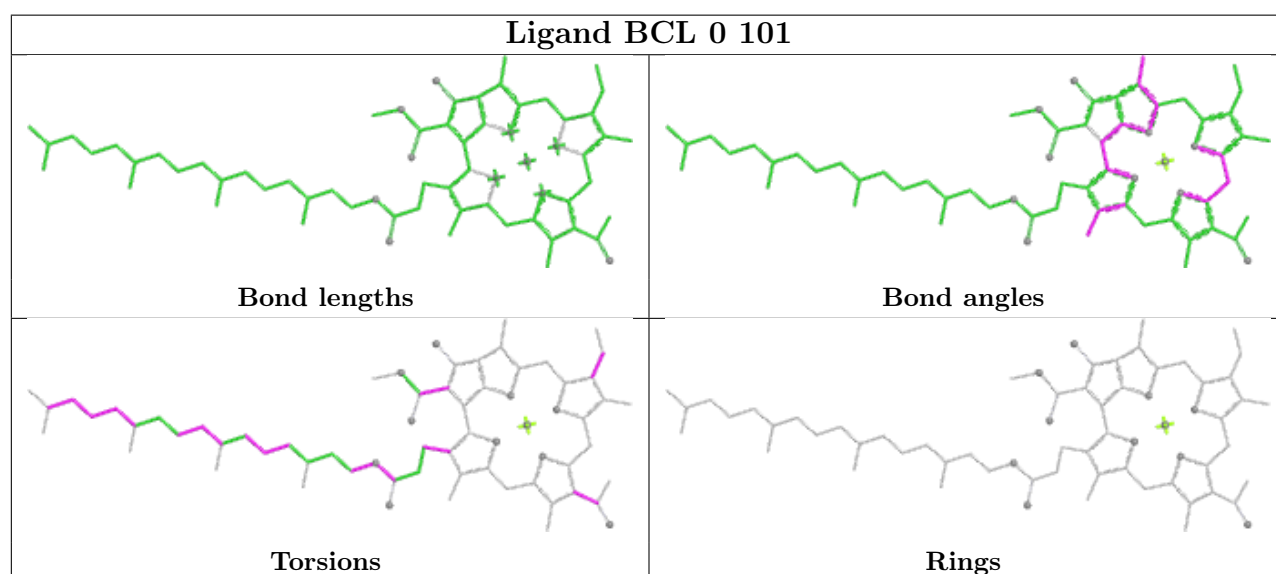
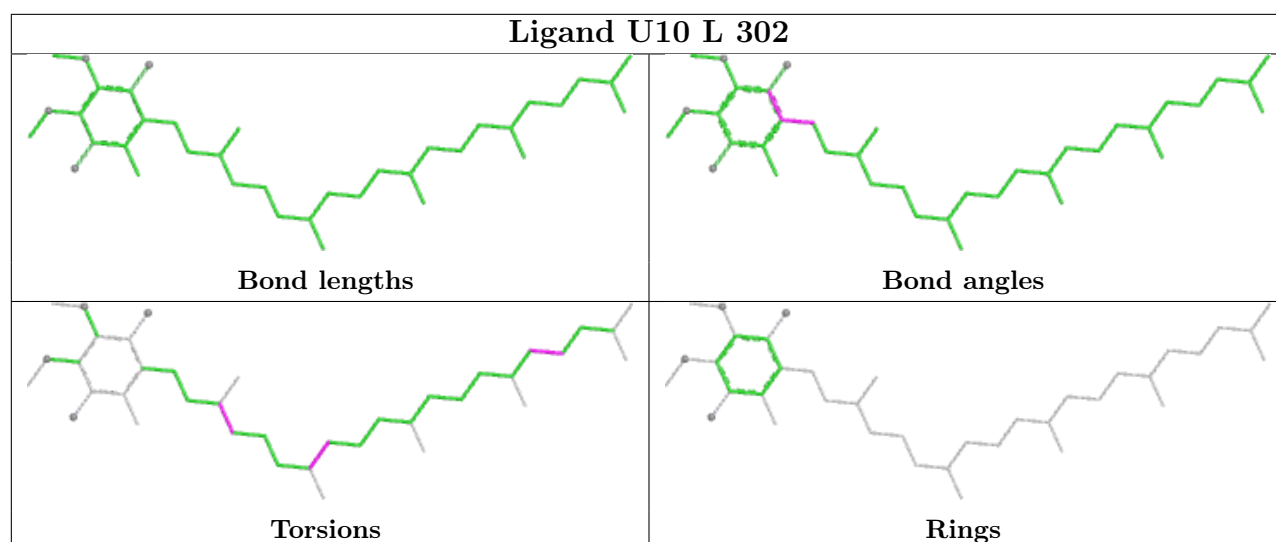
Ligand BPH L 304

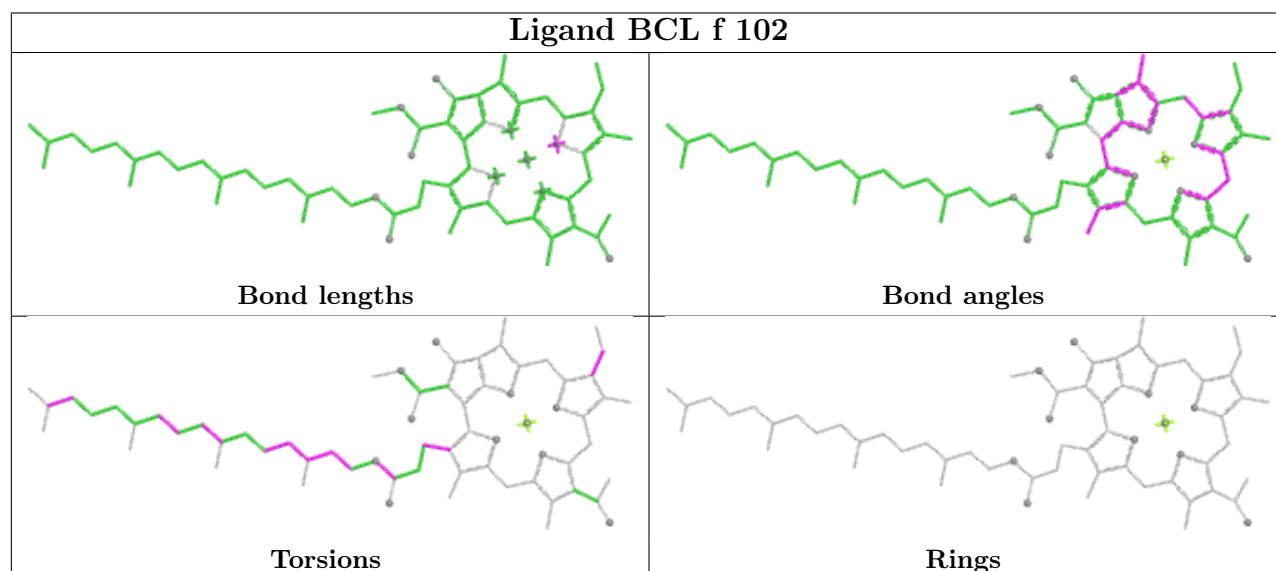
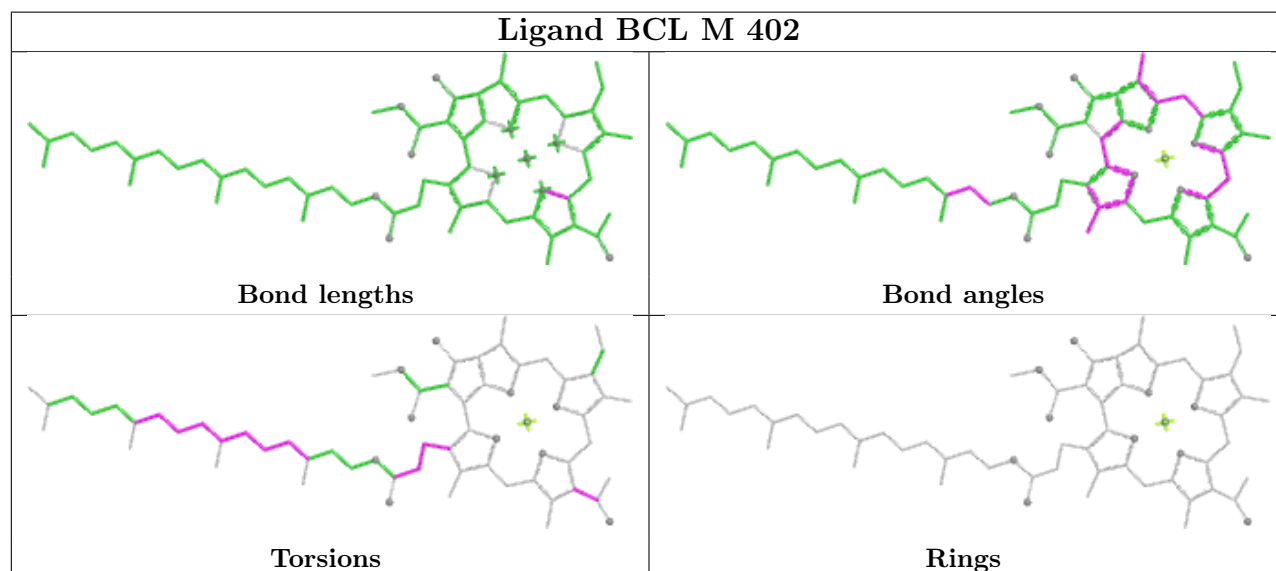
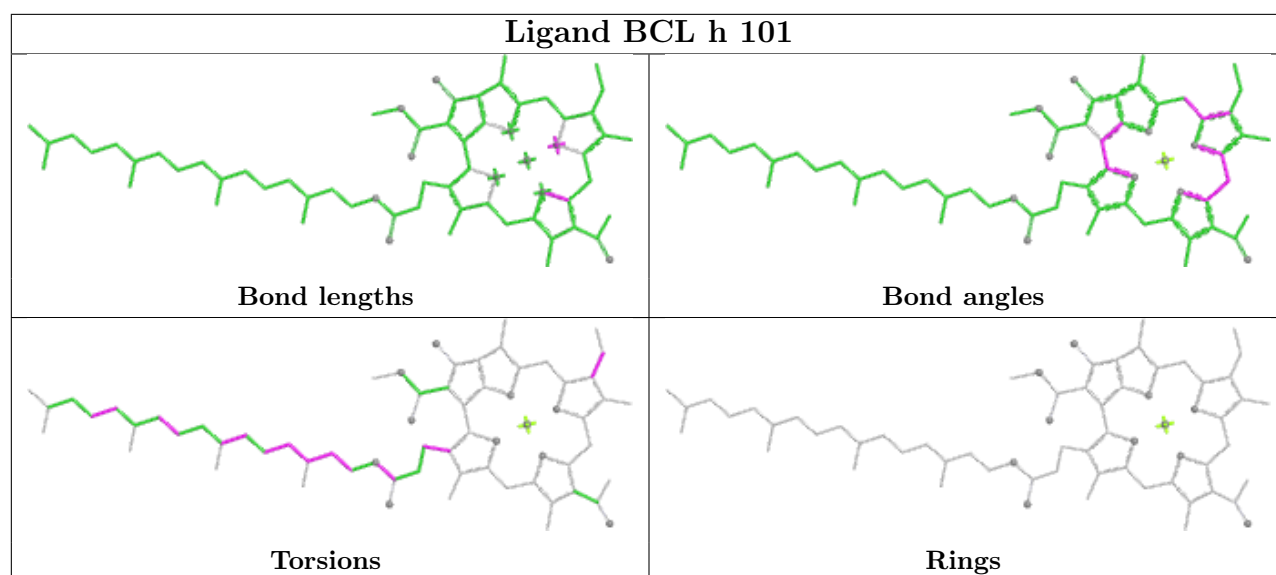


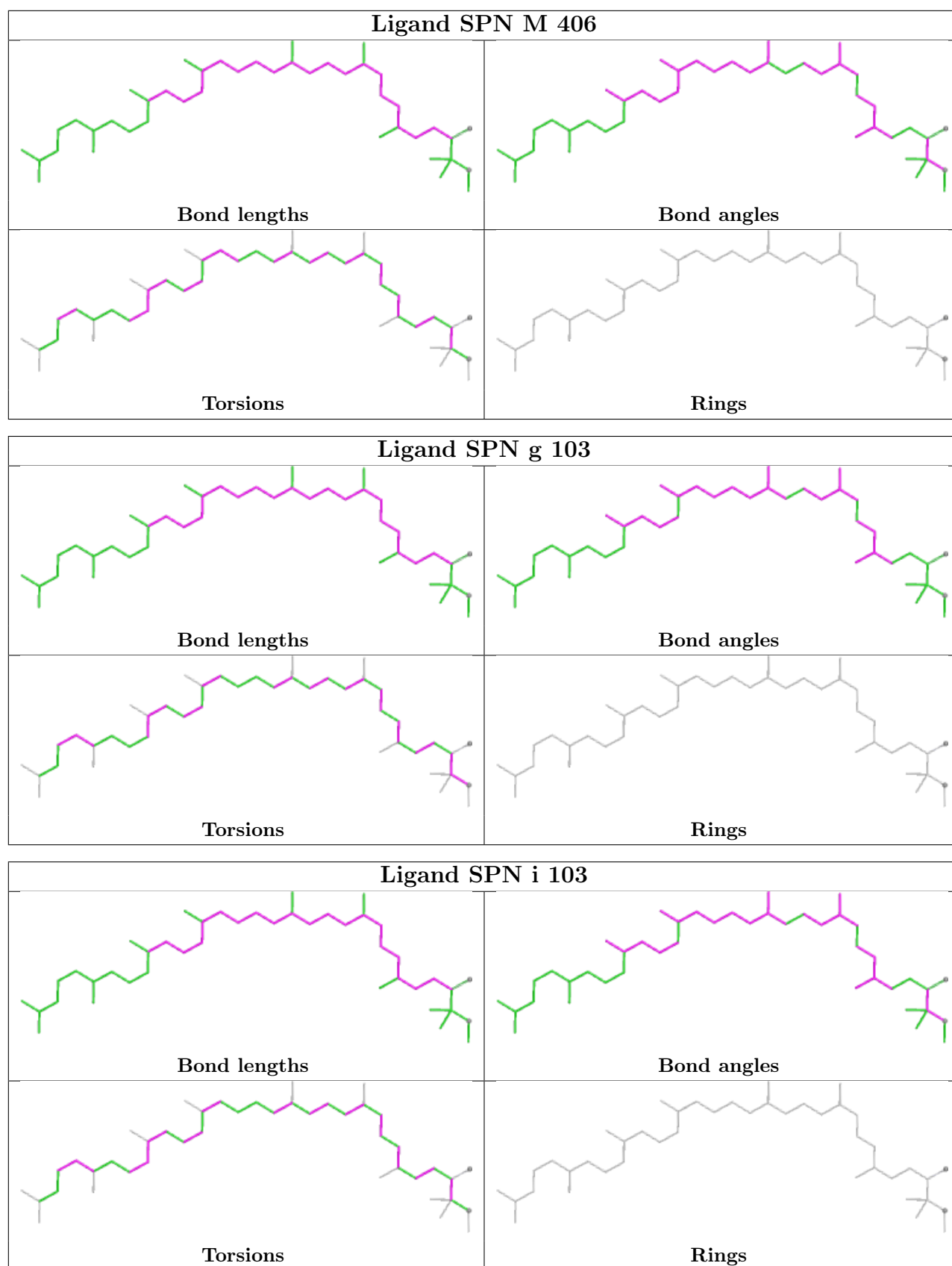
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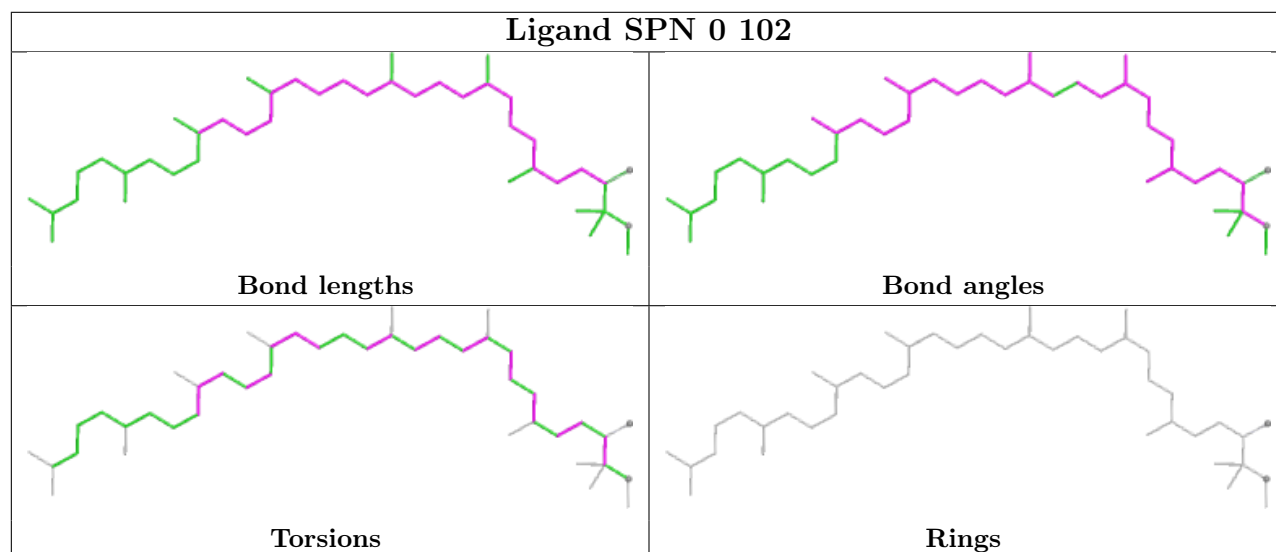
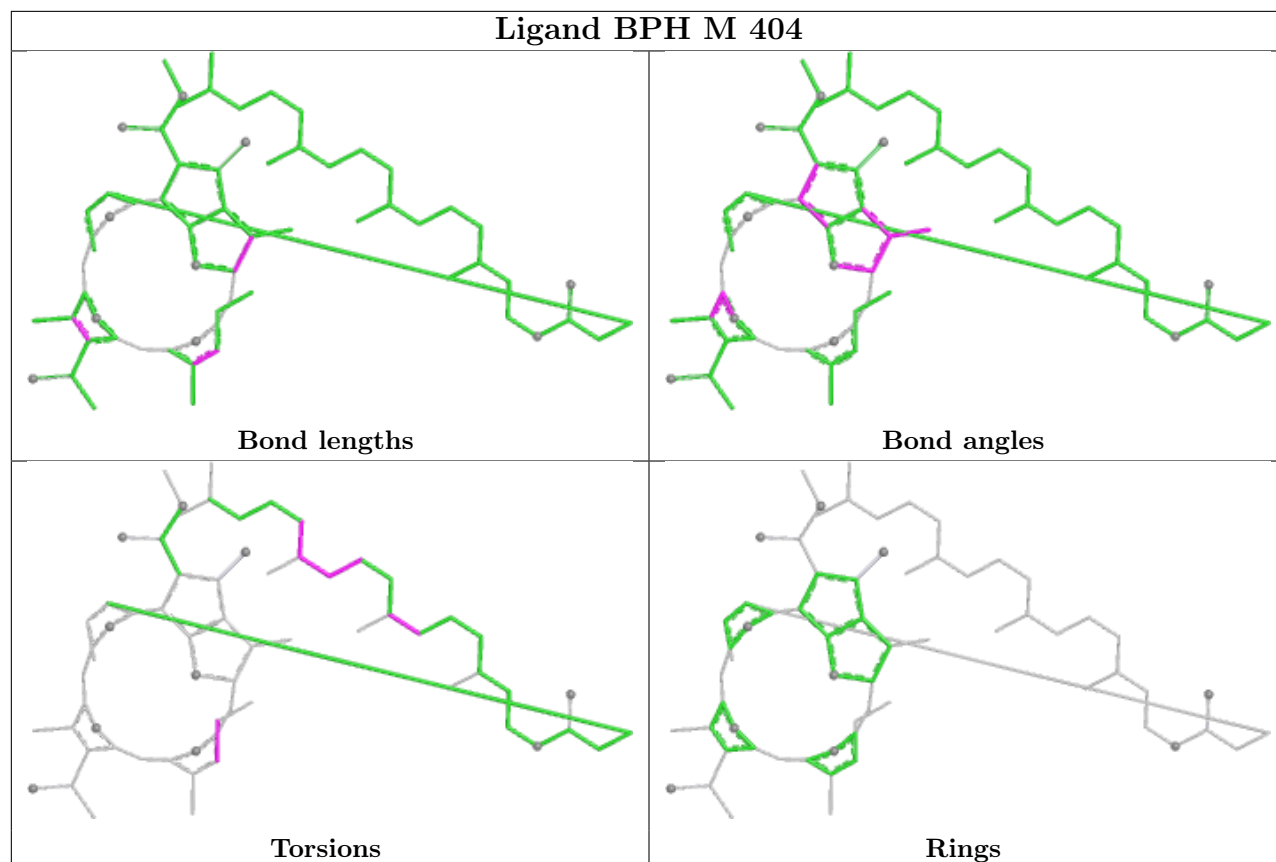


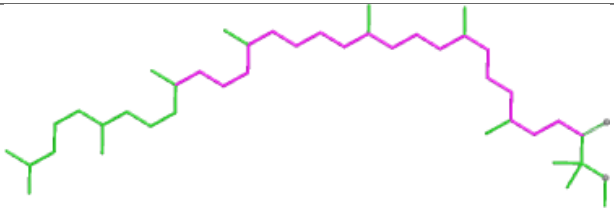
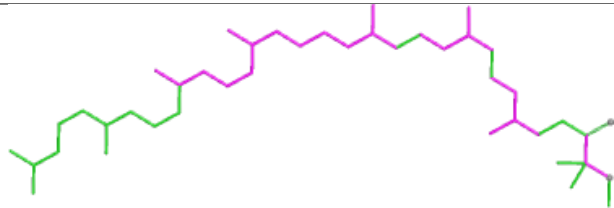
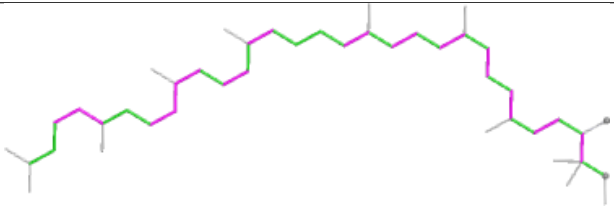
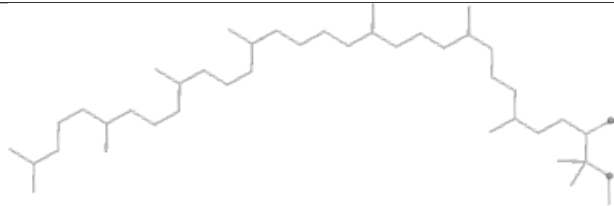


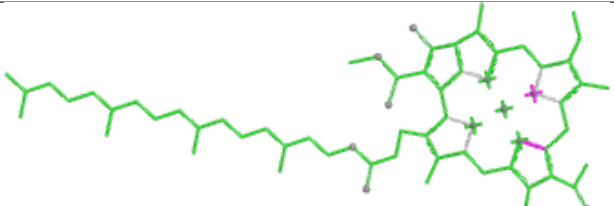
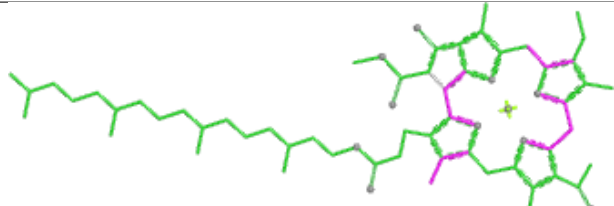
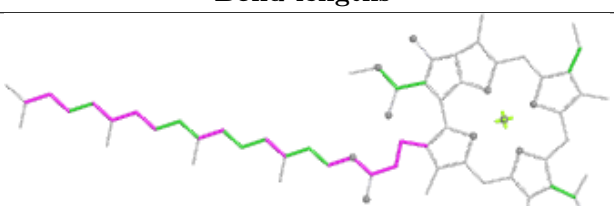
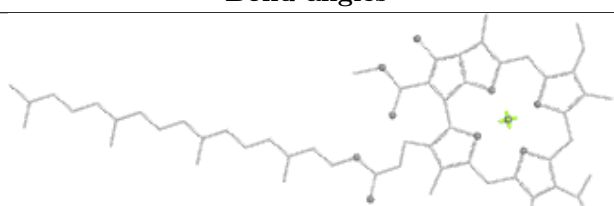


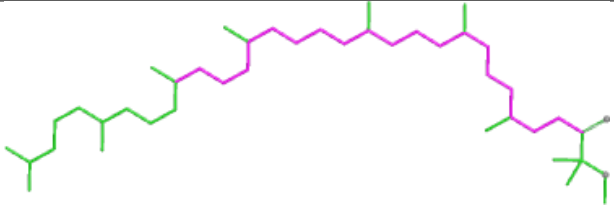
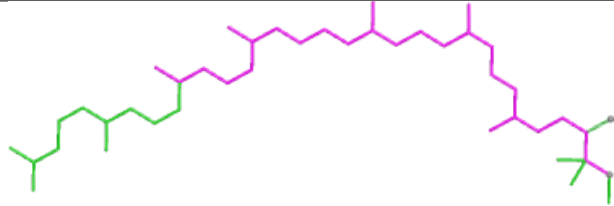
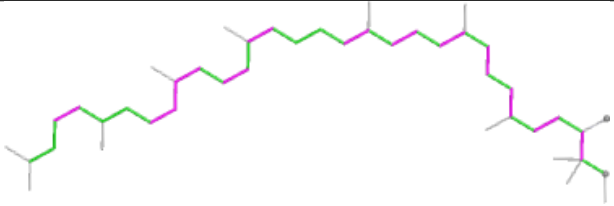
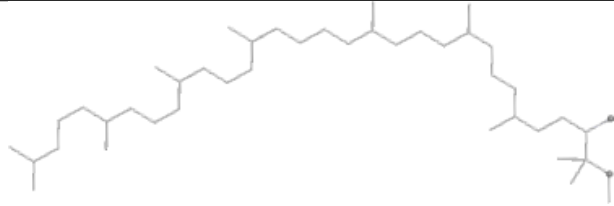


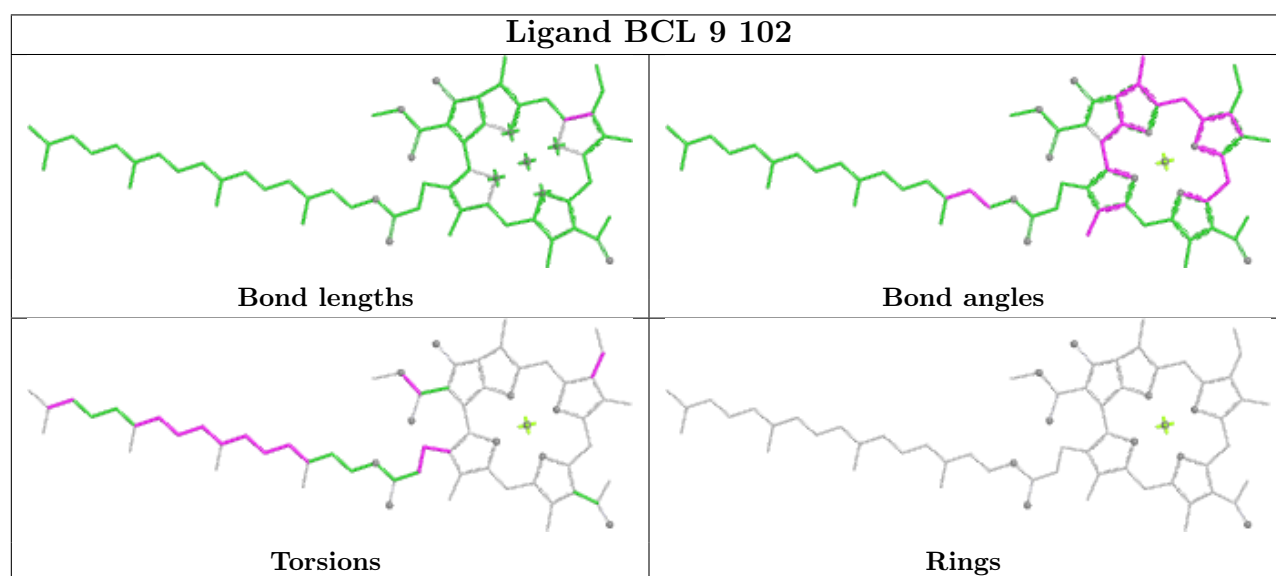
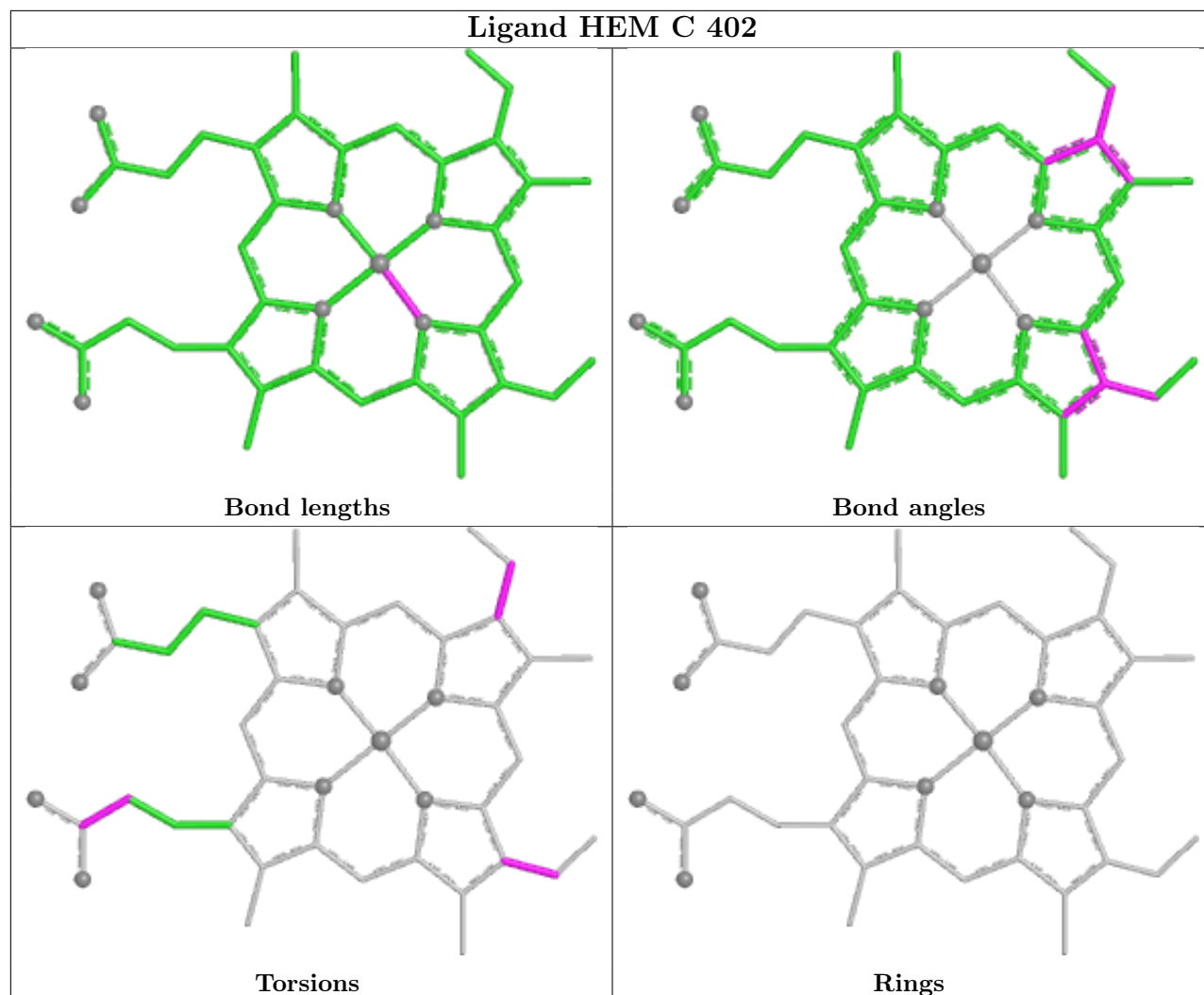


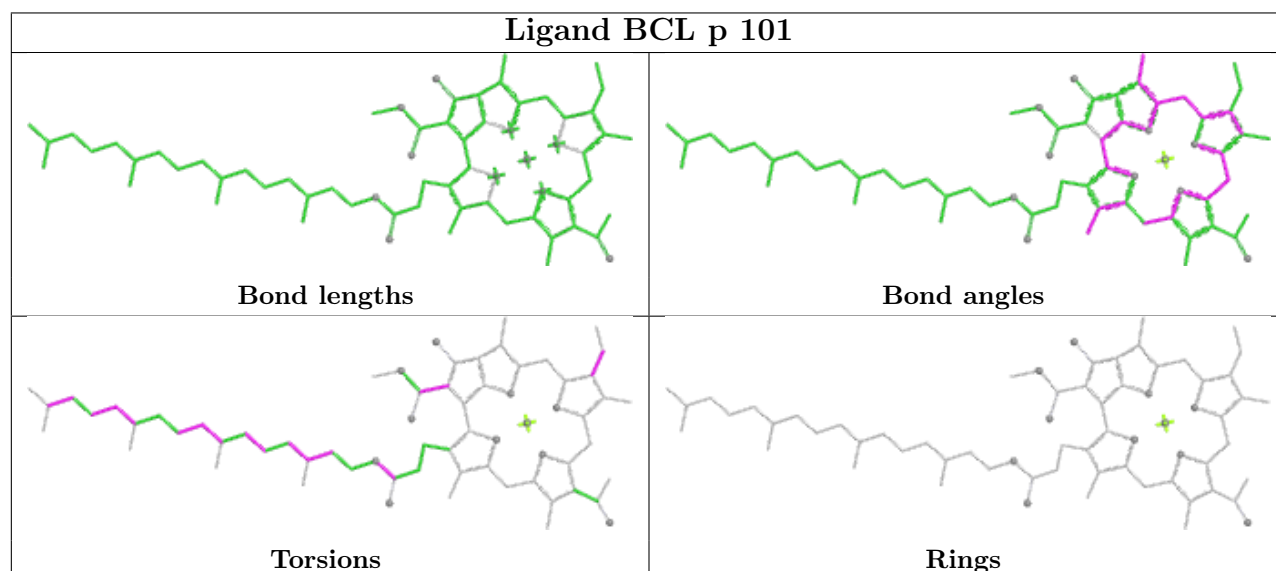
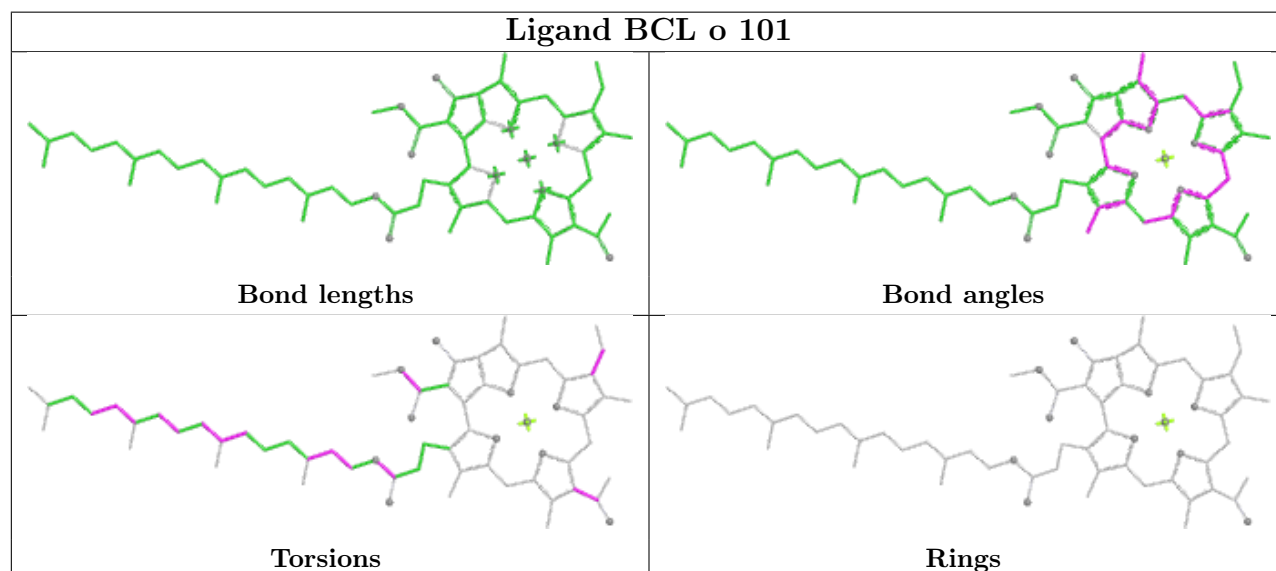
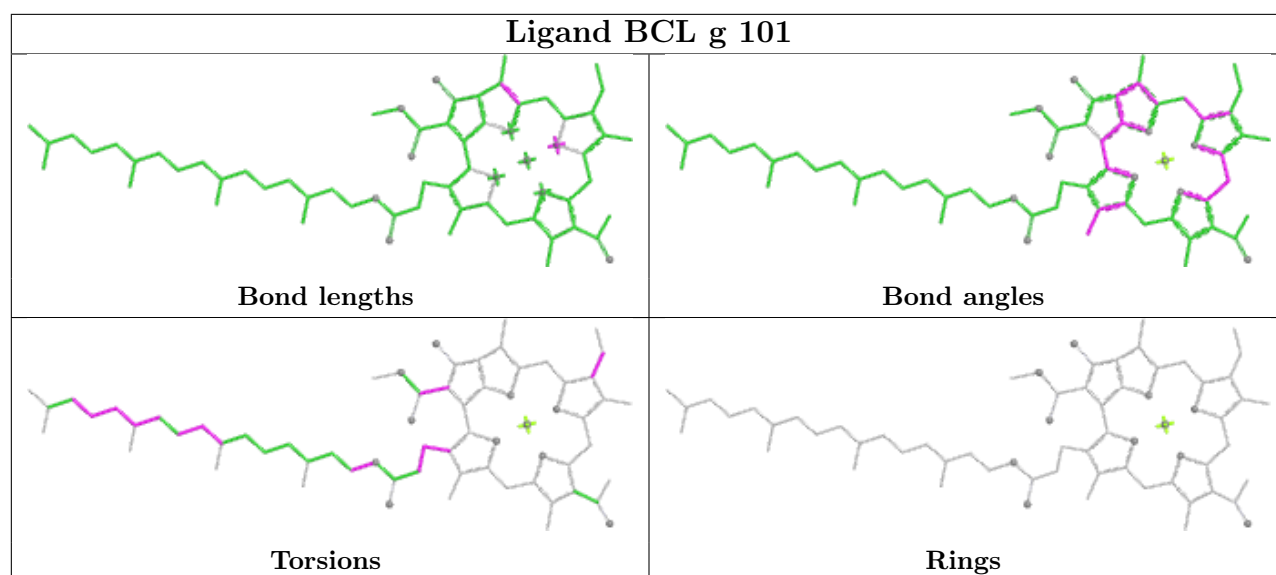


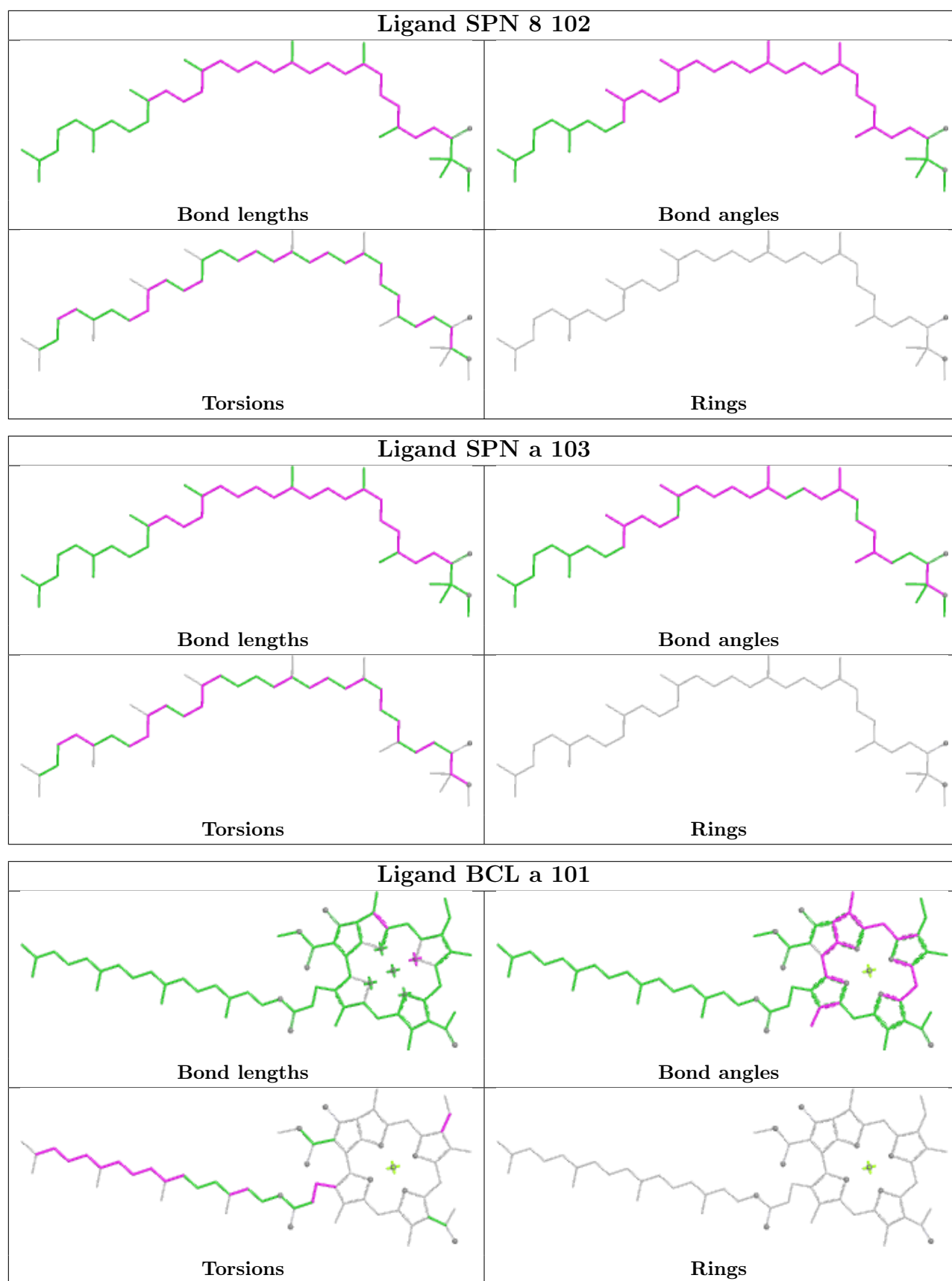
Ligand SPN m 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

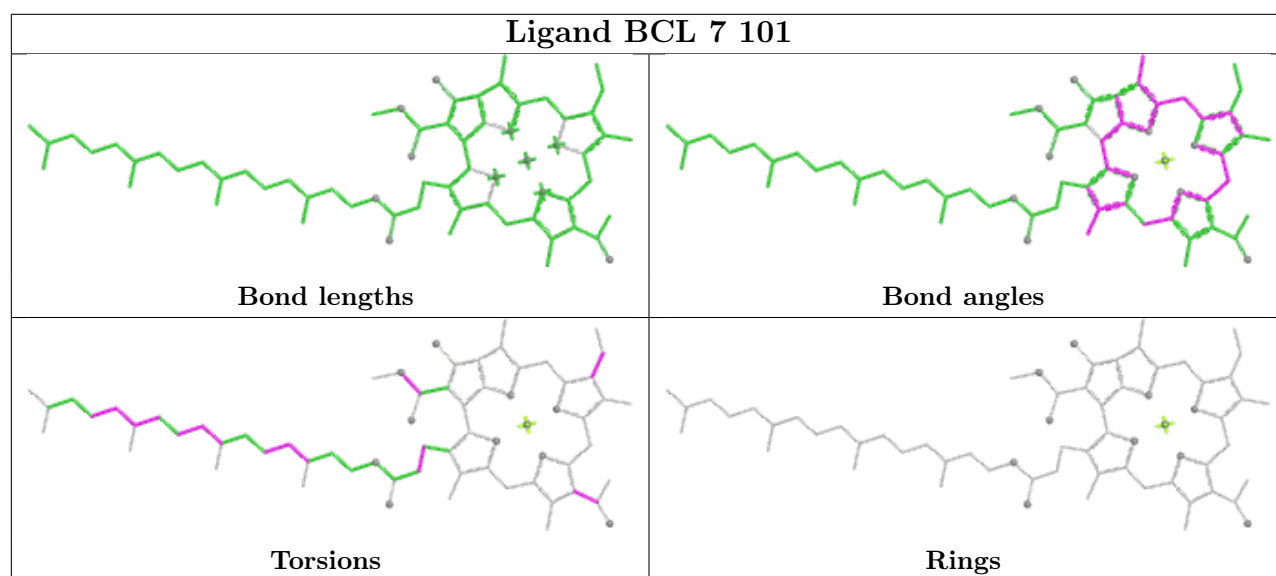
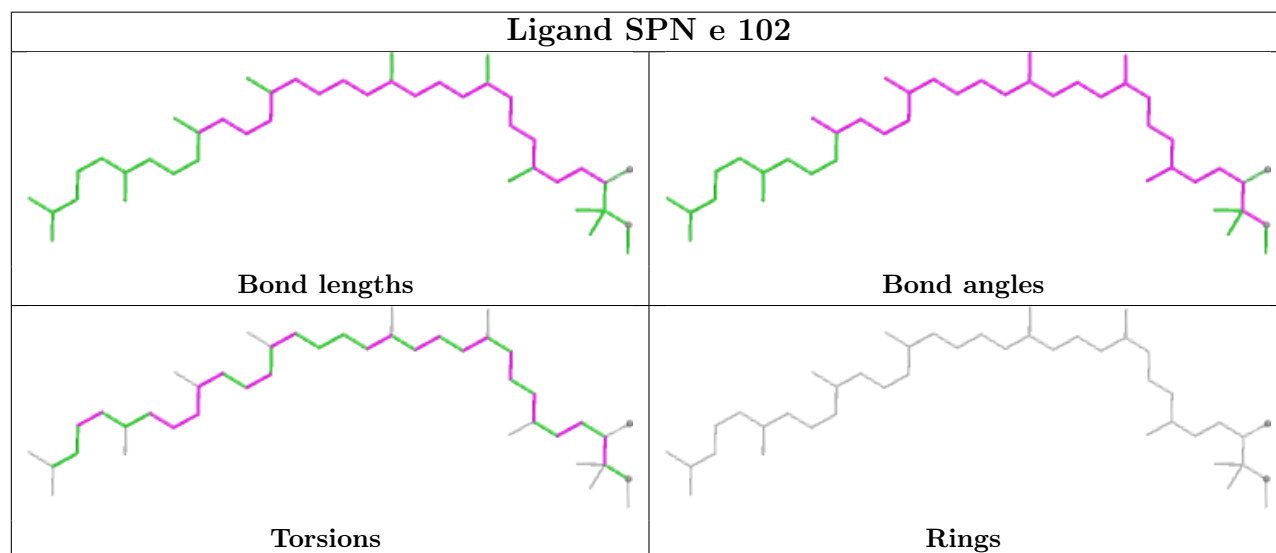
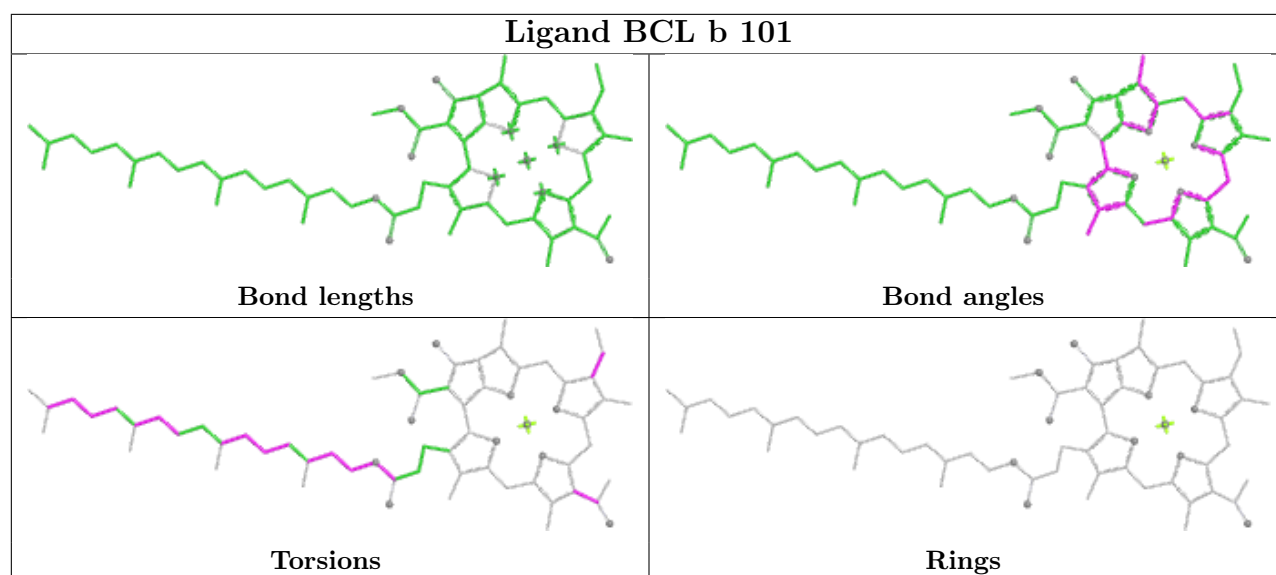
Ligand BCL M 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

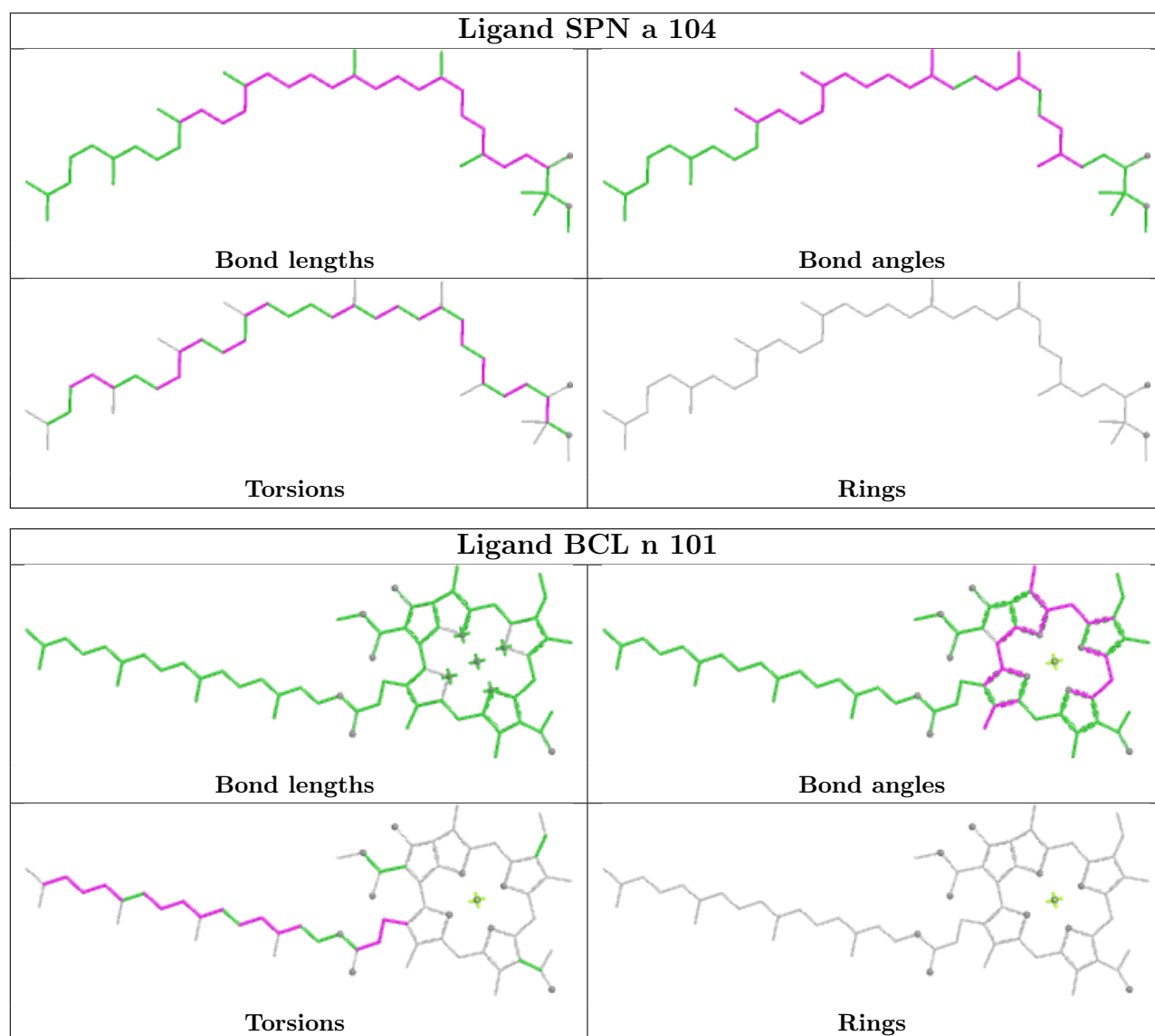
Ligand SPN l 102	
	
Bond lengths	Bond angles
	
Torsions	Rings



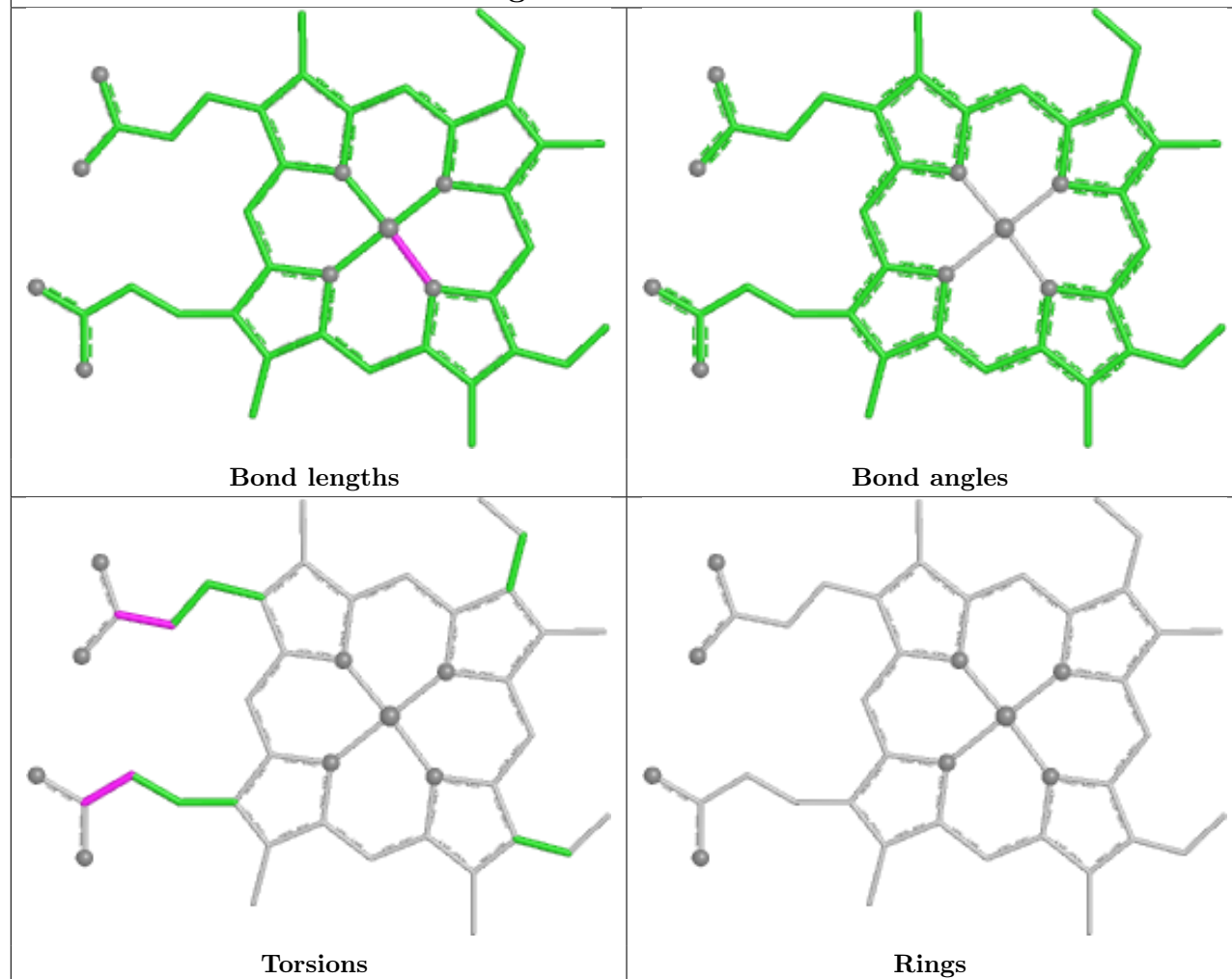




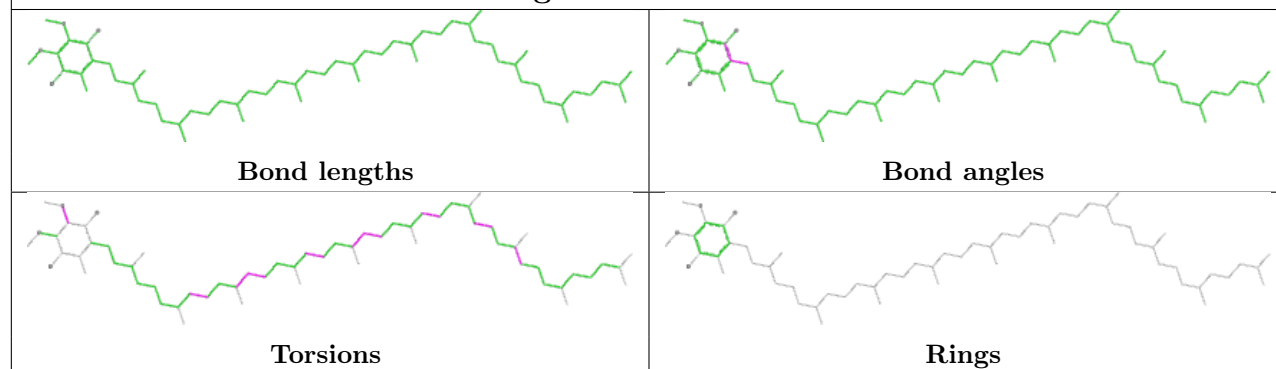


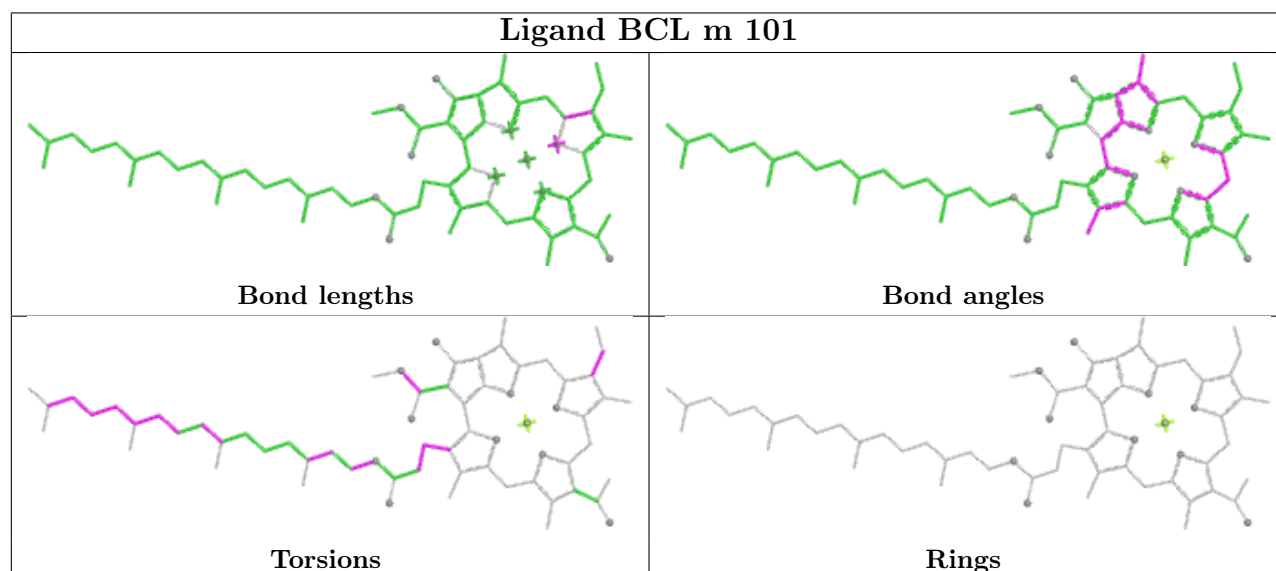
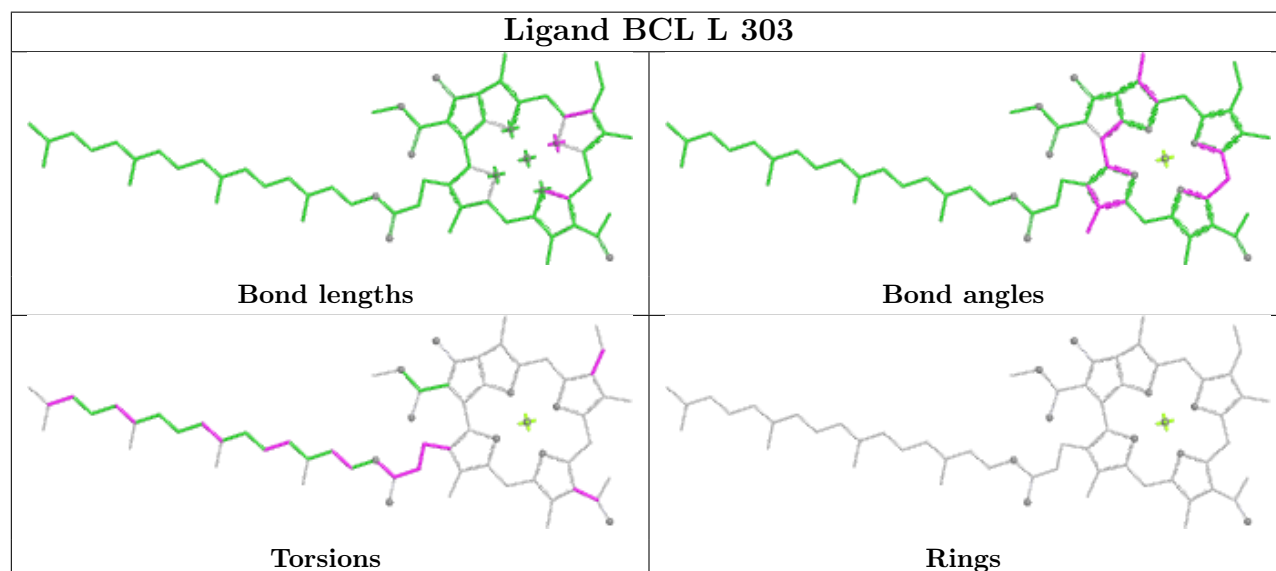
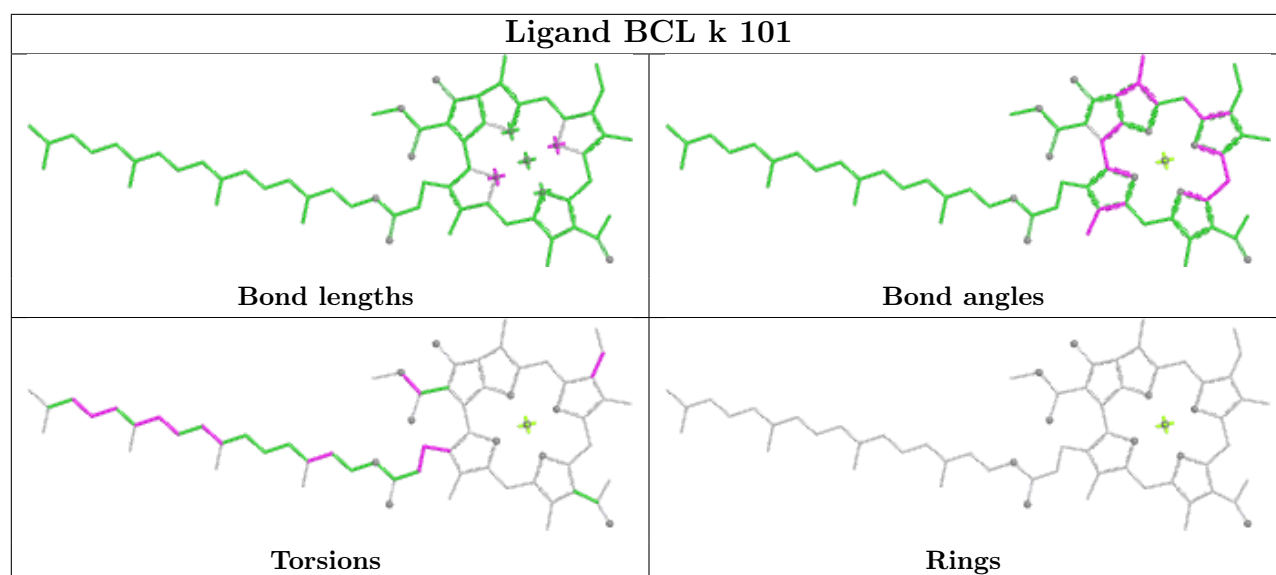


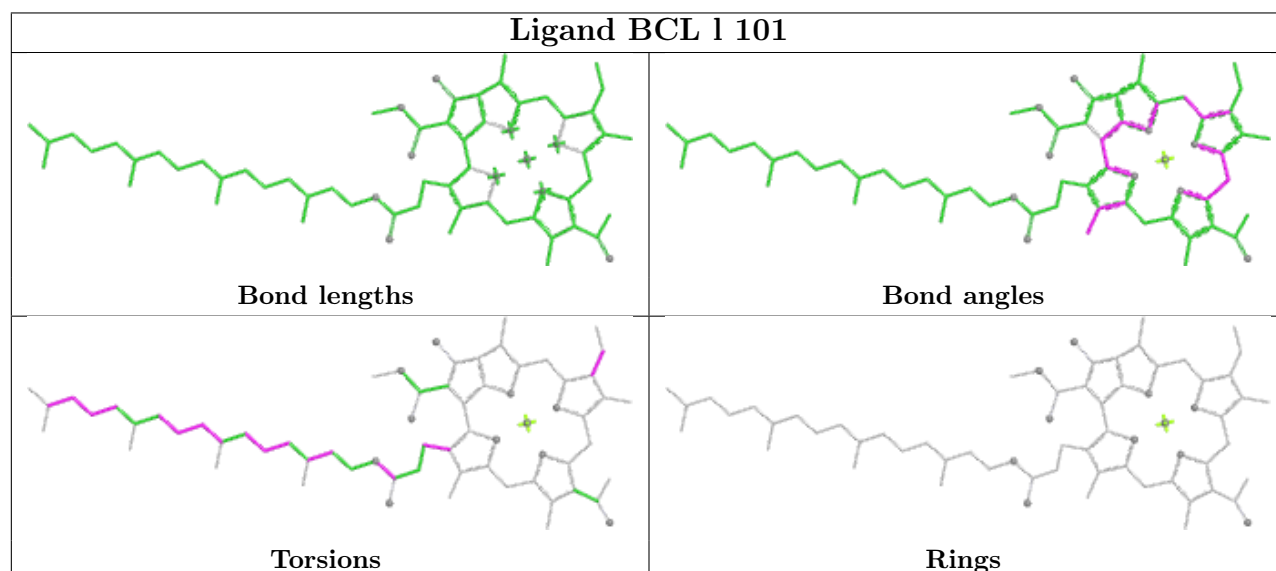
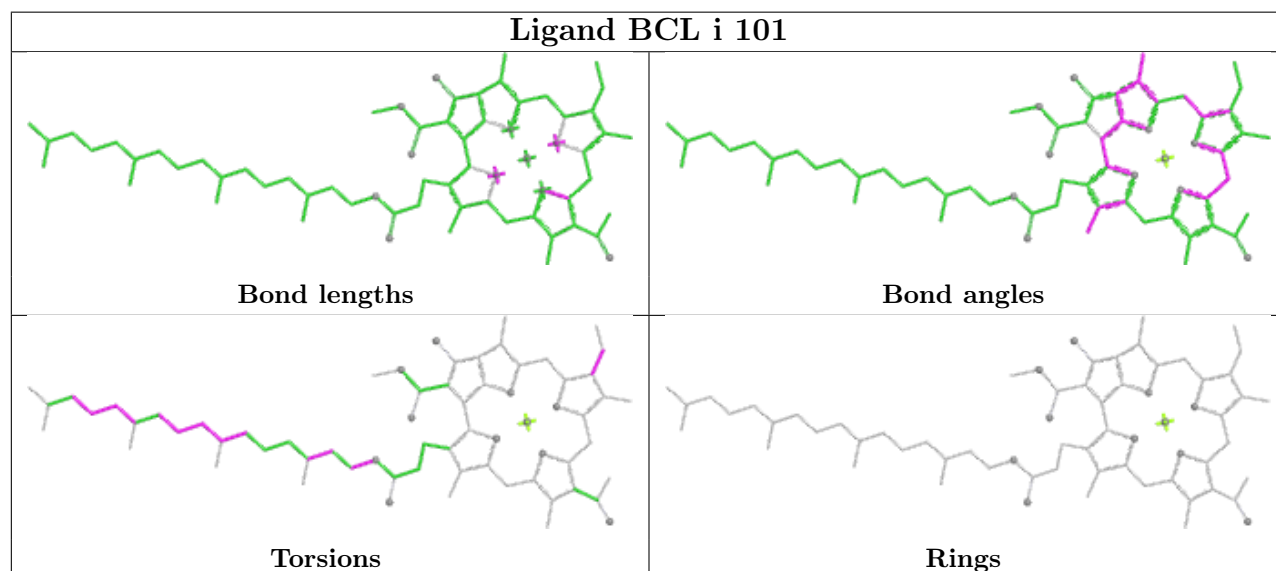
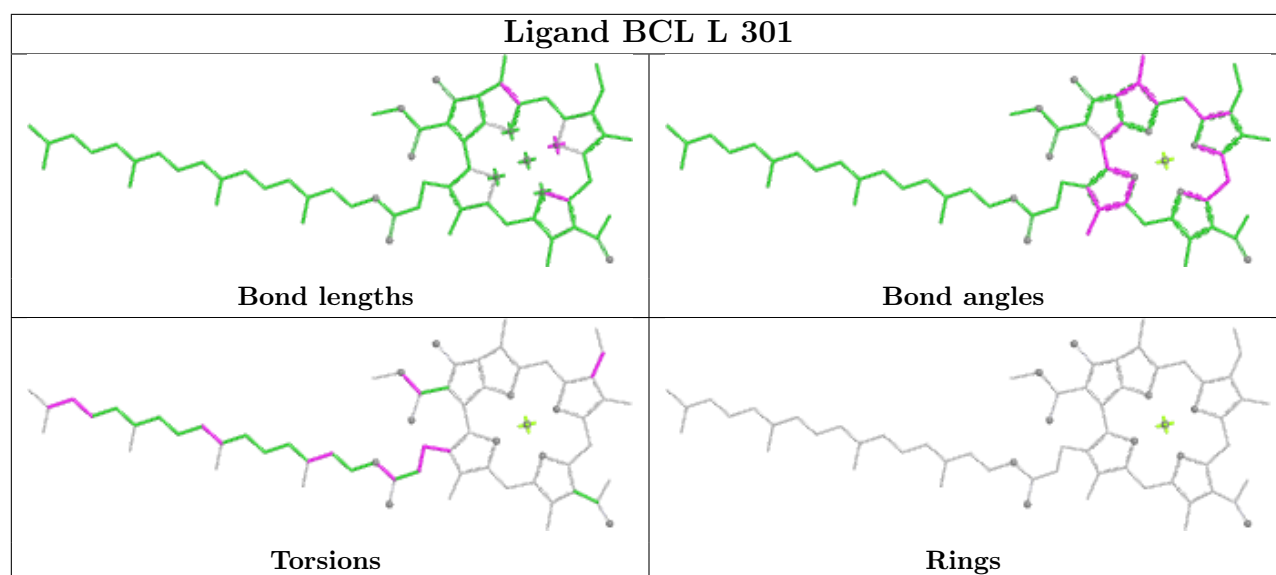
Ligand HEM C 403

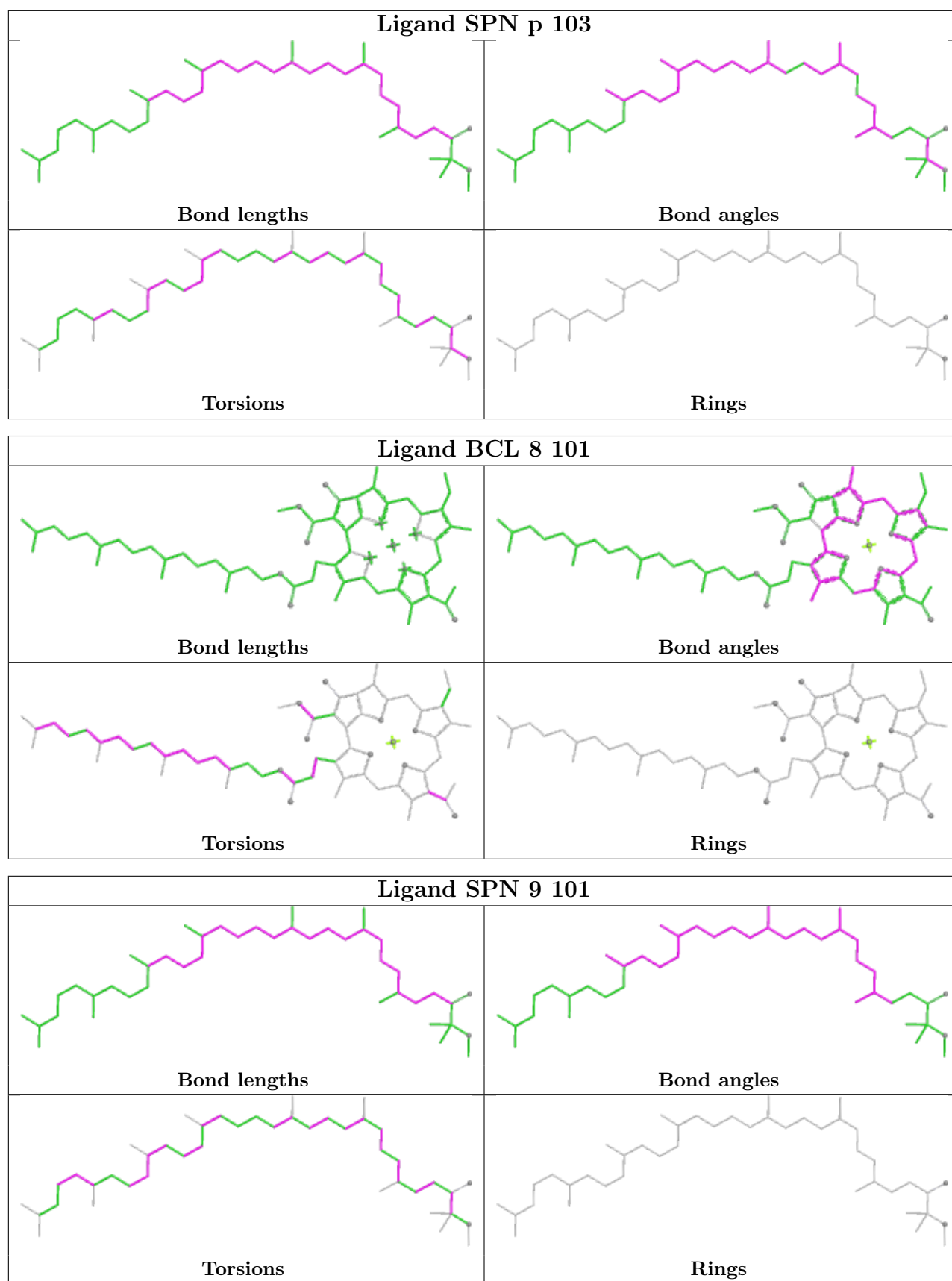


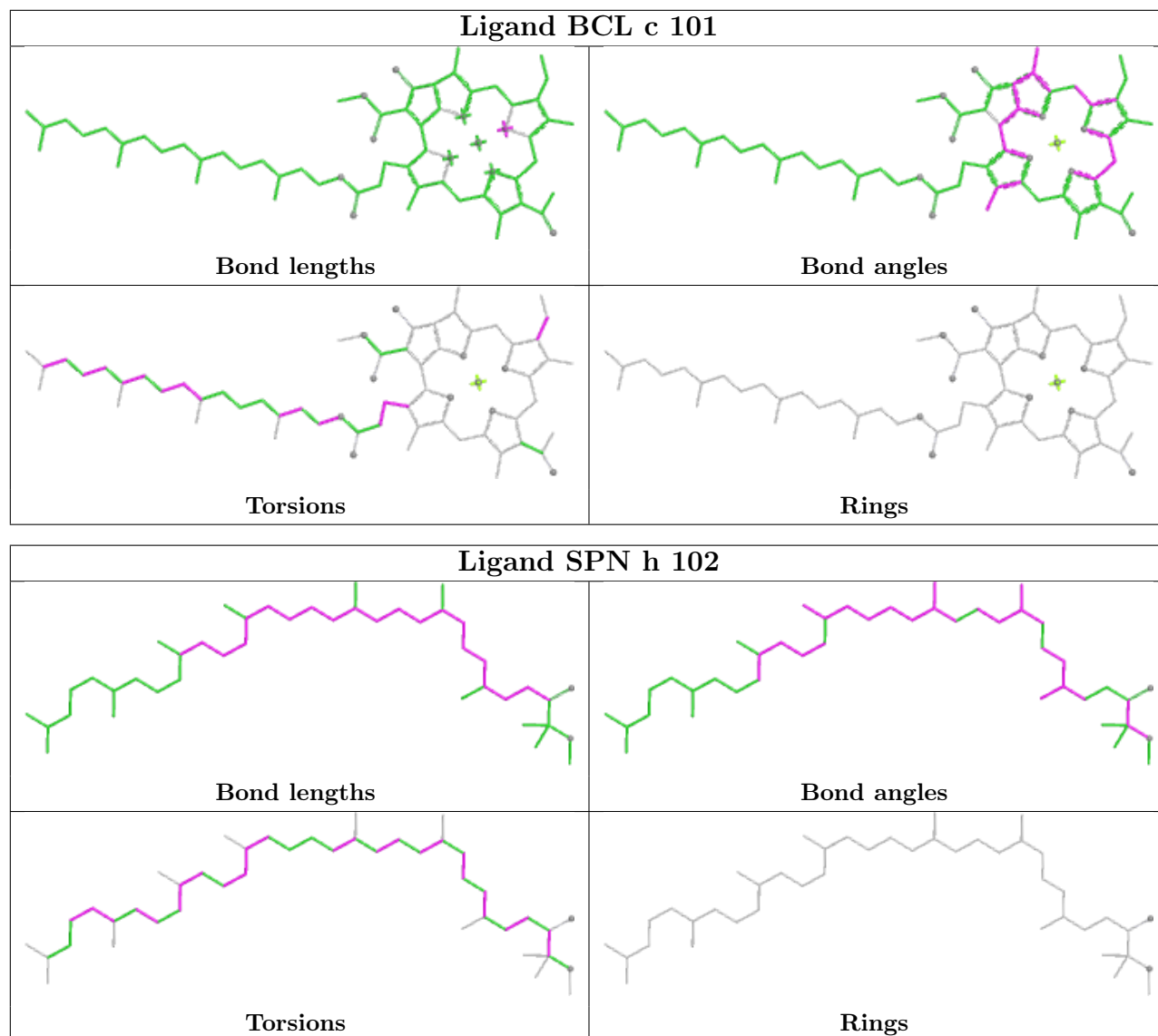
Ligand U10 M 403



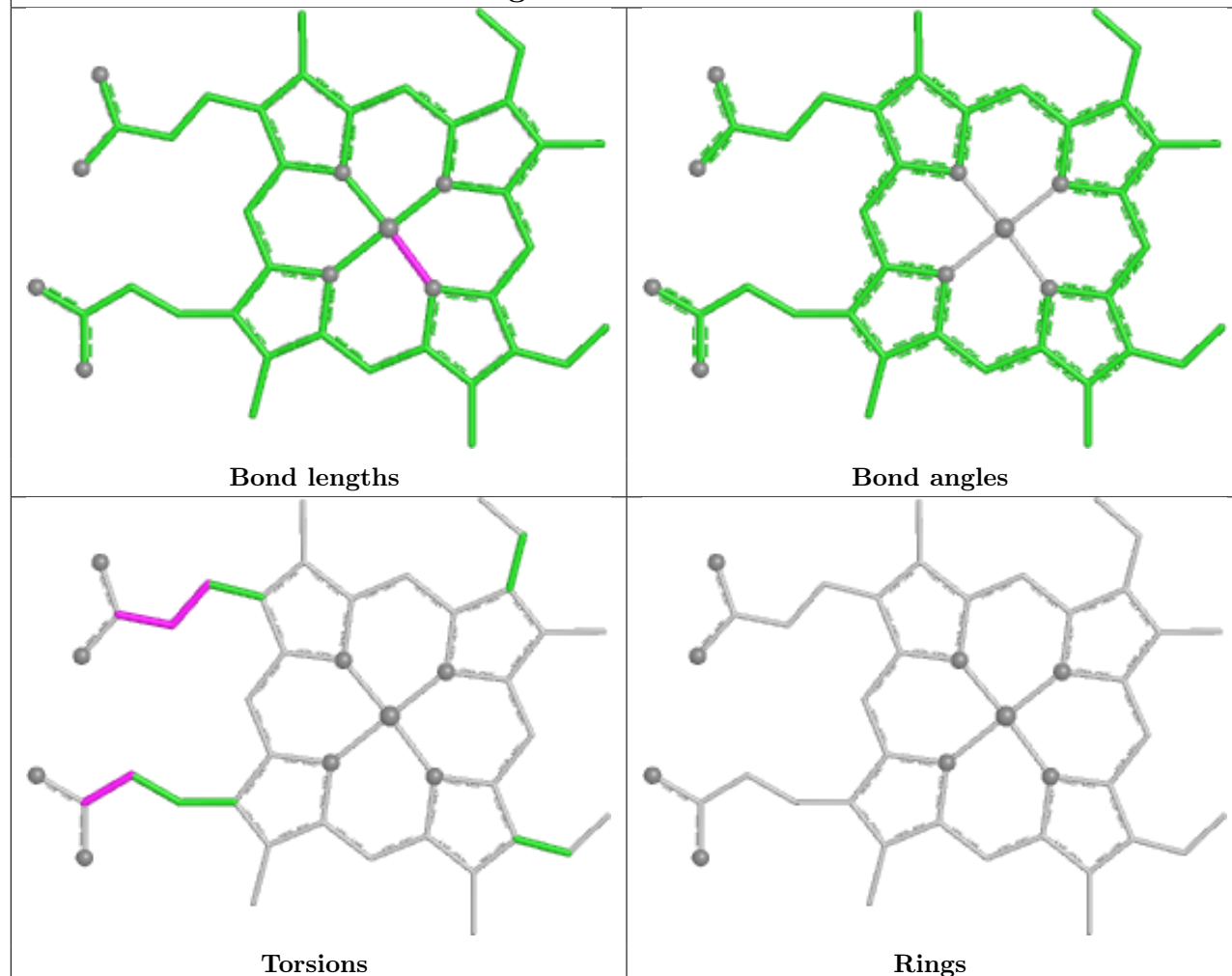




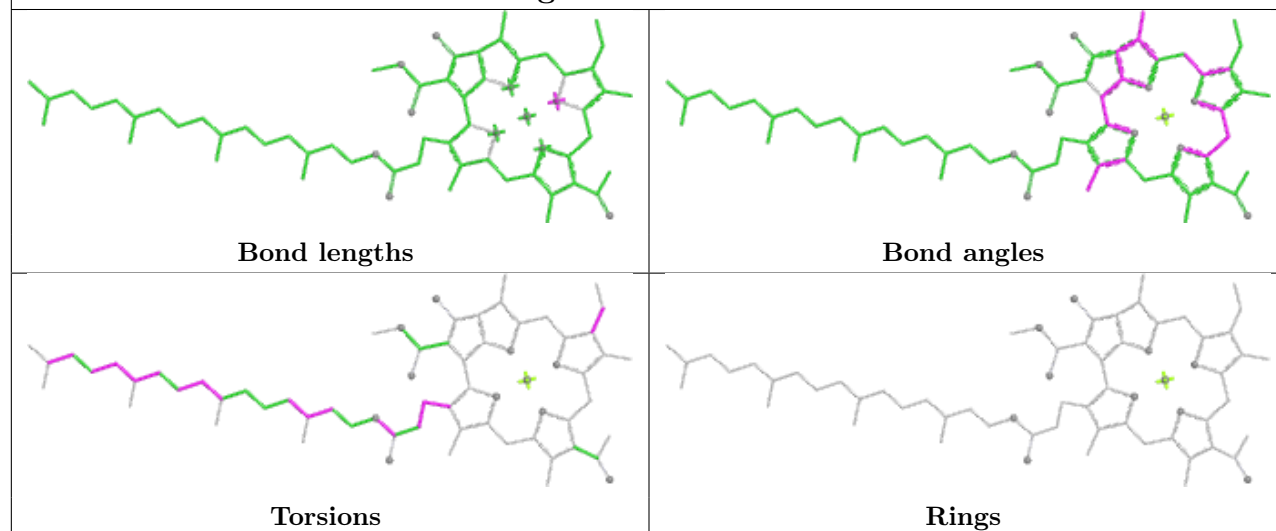


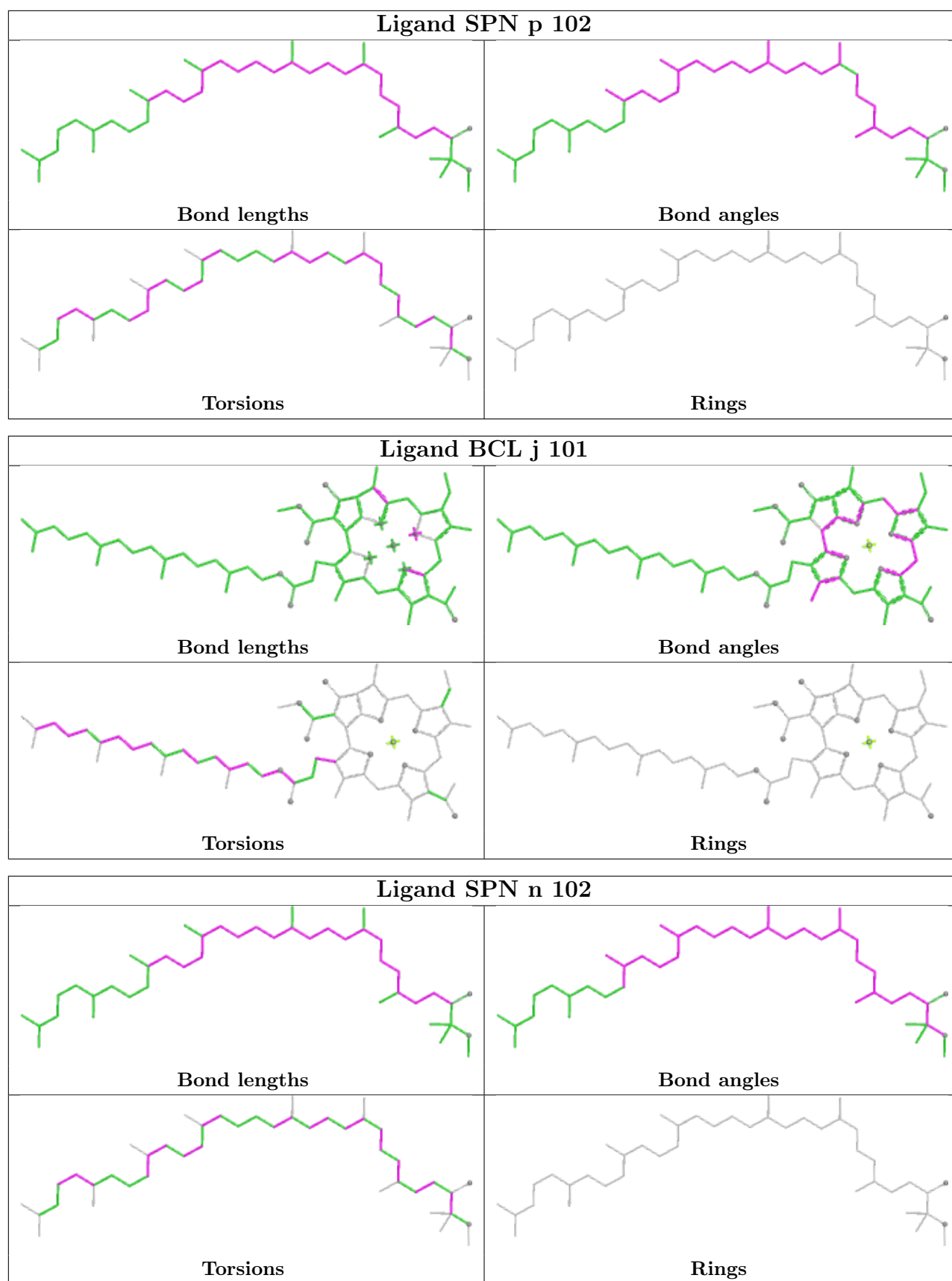


Ligand HEM C 401



Ligand BCL e 101





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

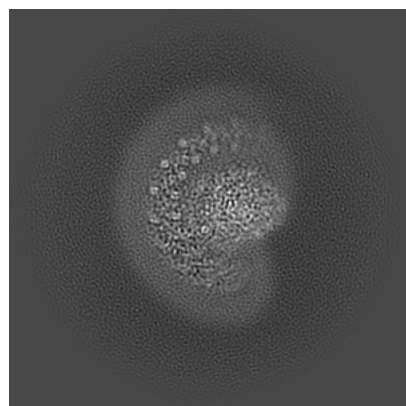
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63381. These allow visual inspection of the internal detail of the map and identification of artifacts.

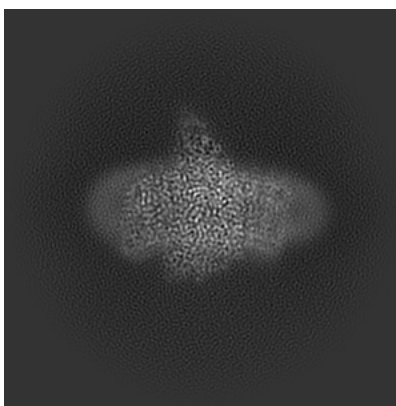
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

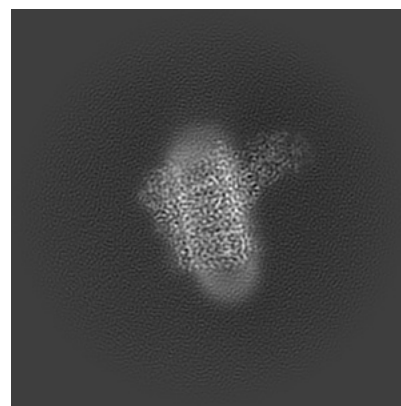
6.1.1 Primary map



X

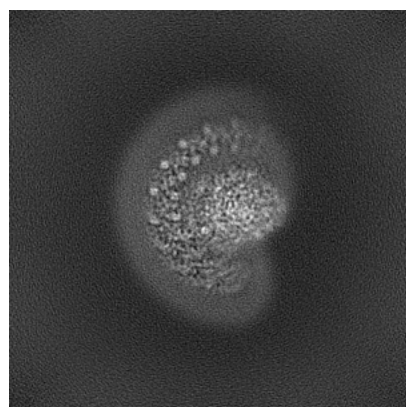


Y

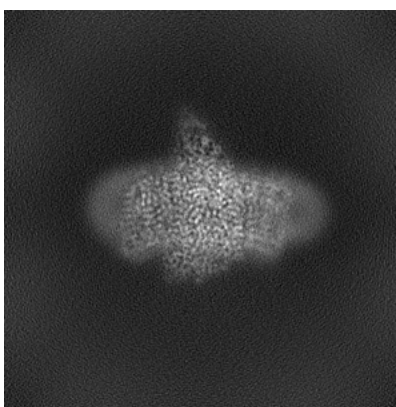


Z

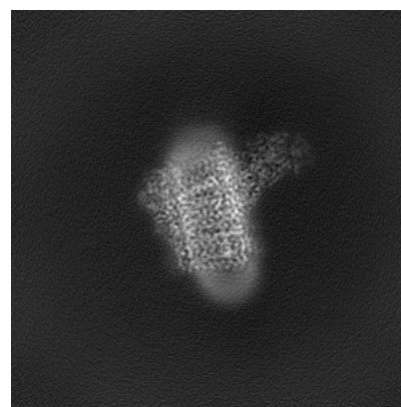
6.1.2 Raw map



X



Y

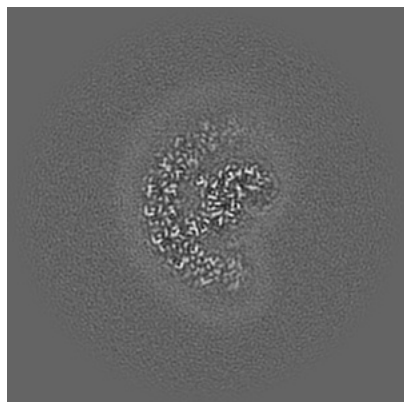


Z

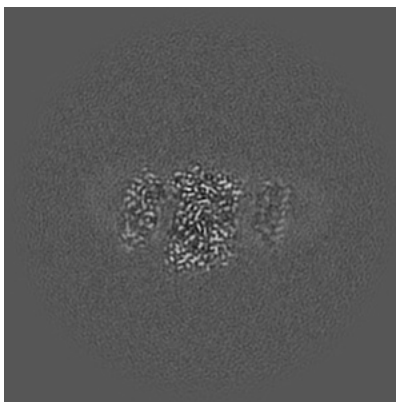
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

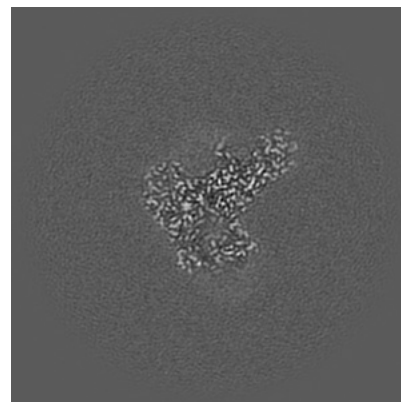
6.2.1 Primary map



X Index: 150

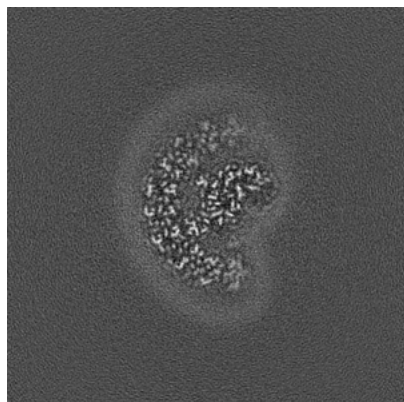


Y Index: 150

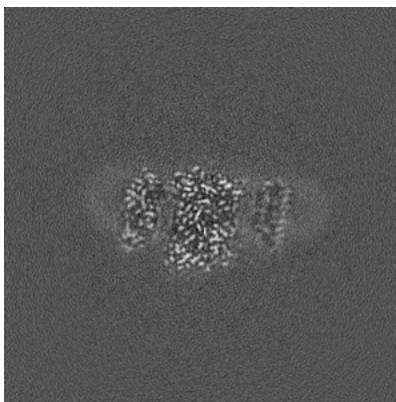


Z Index: 150

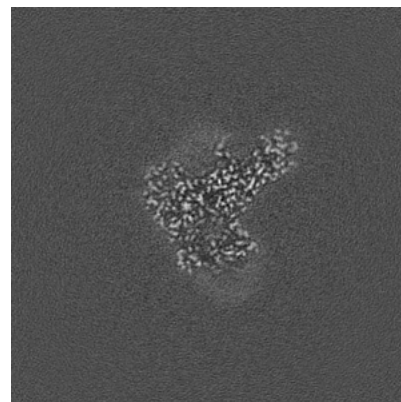
6.2.2 Raw map



X Index: 150



Y Index: 150

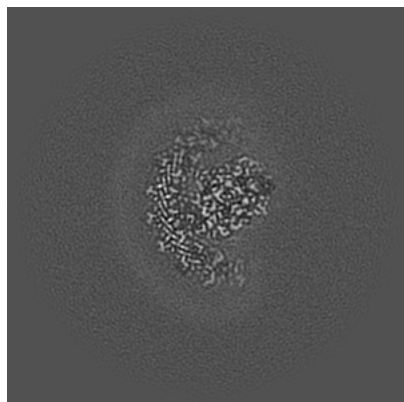


Z Index: 150

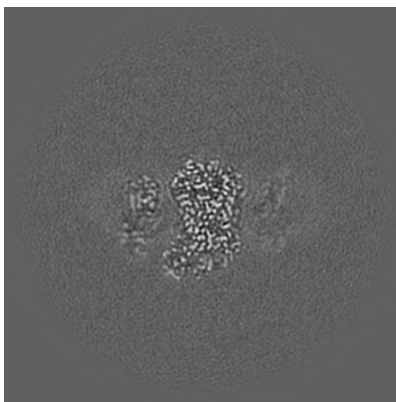
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

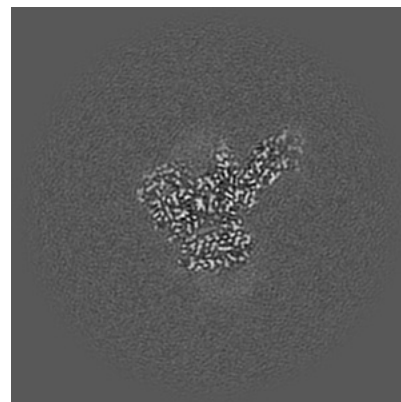
6.3.1 Primary map



X Index: 162

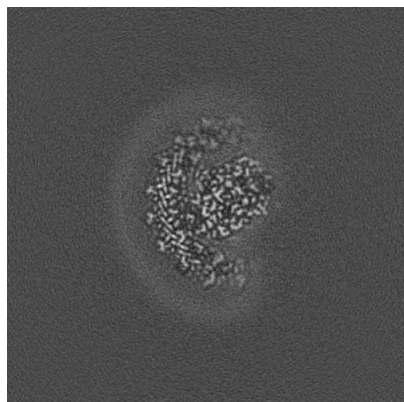


Y Index: 157

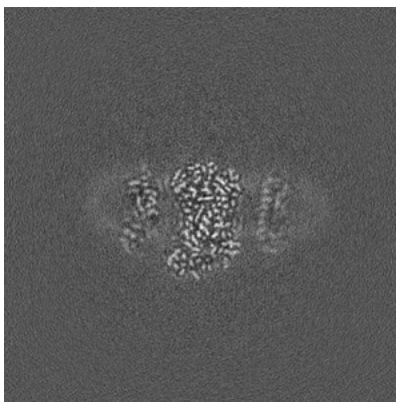


Z Index: 144

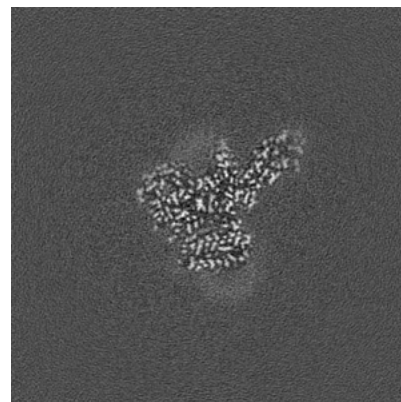
6.3.2 Raw map



X Index: 162



Y Index: 155

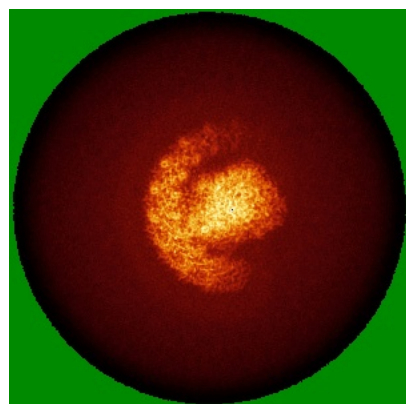


Z Index: 144

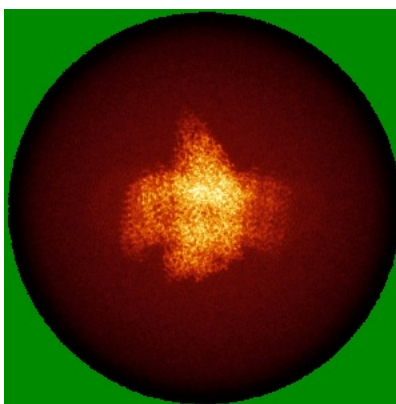
The images above show the largest variance slices of the map in three orthogonal directions.

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

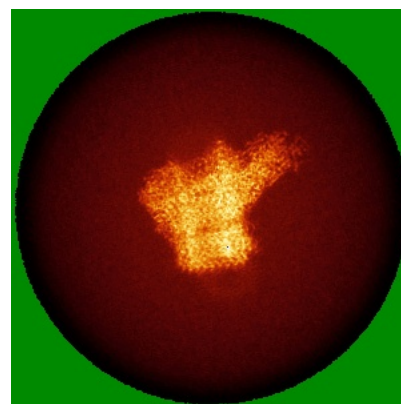
6.4.1 Primary map



X

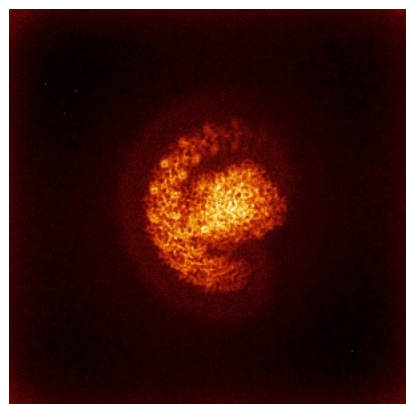


Y

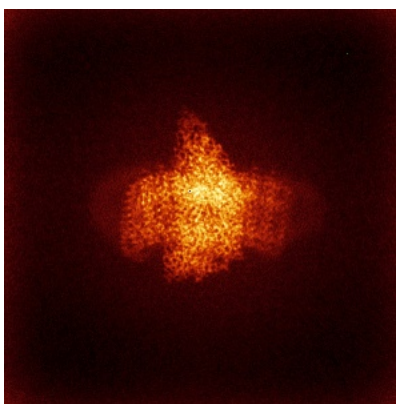


Z

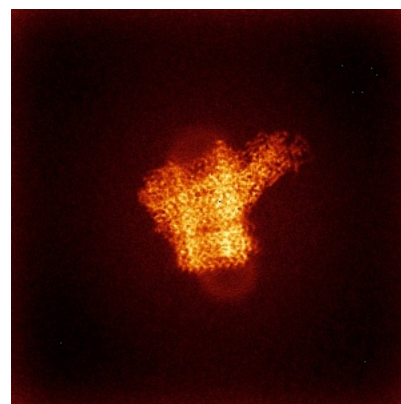
6.4.2 Raw map



X



Y

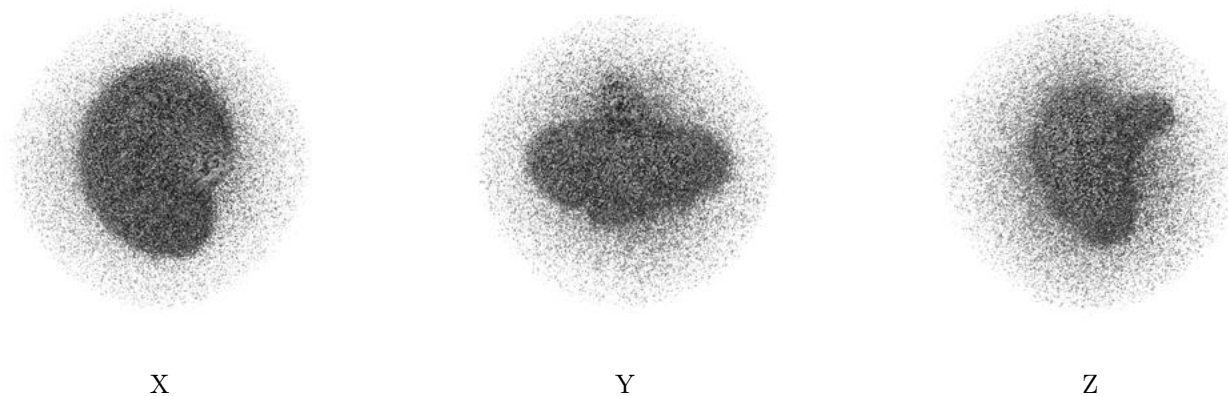


Z

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.

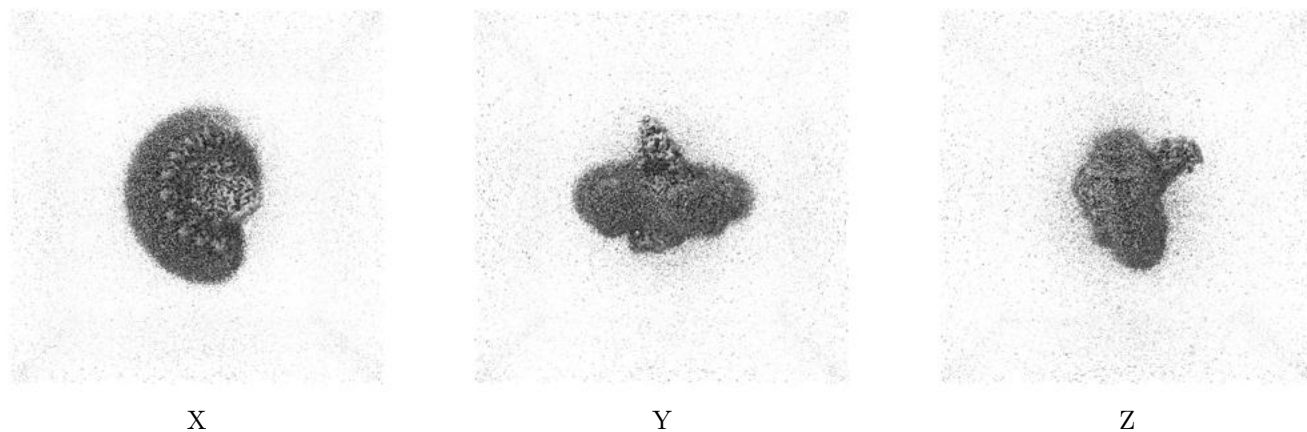
6.5 Orthogonal surface views [i](#)

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.

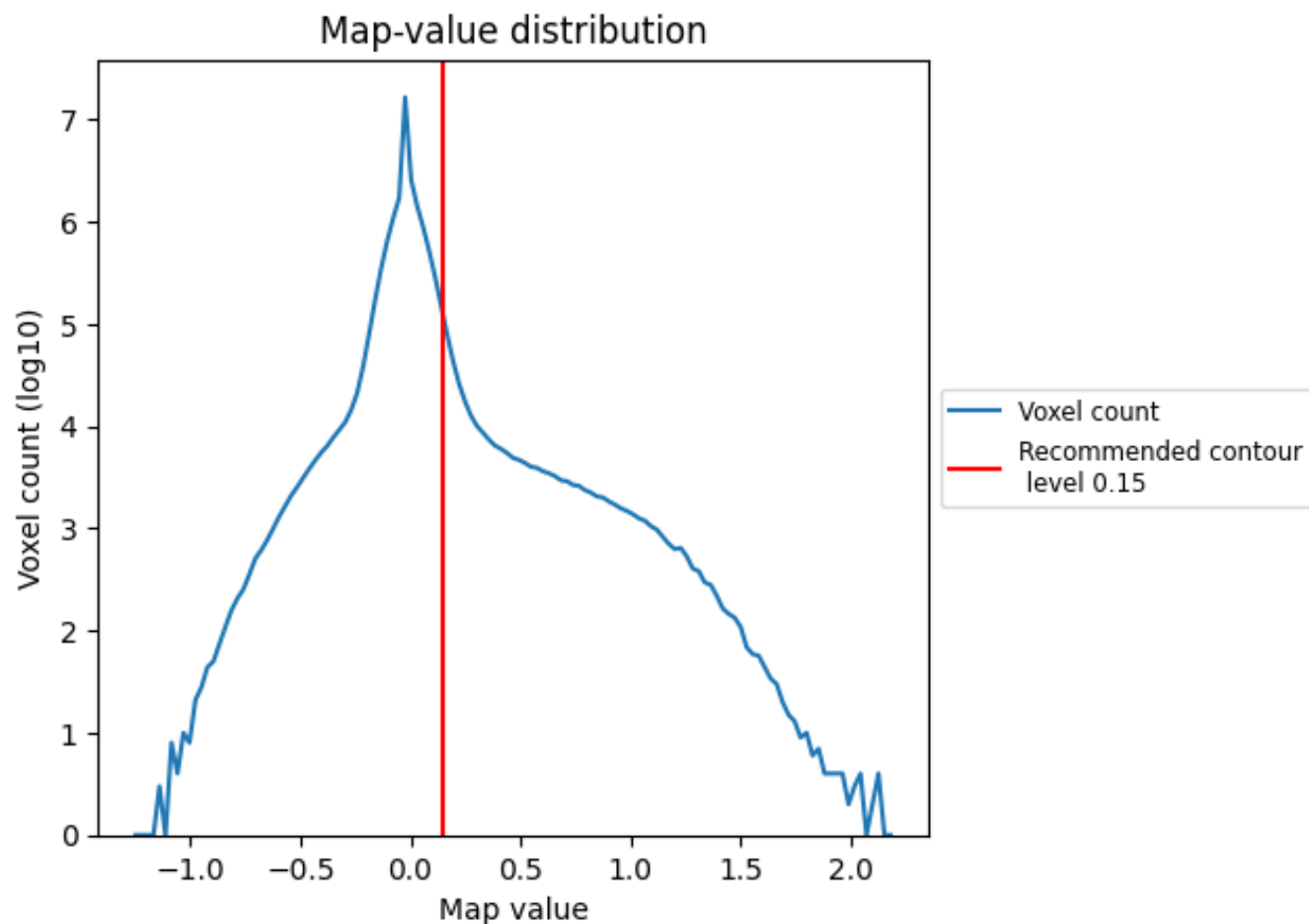
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

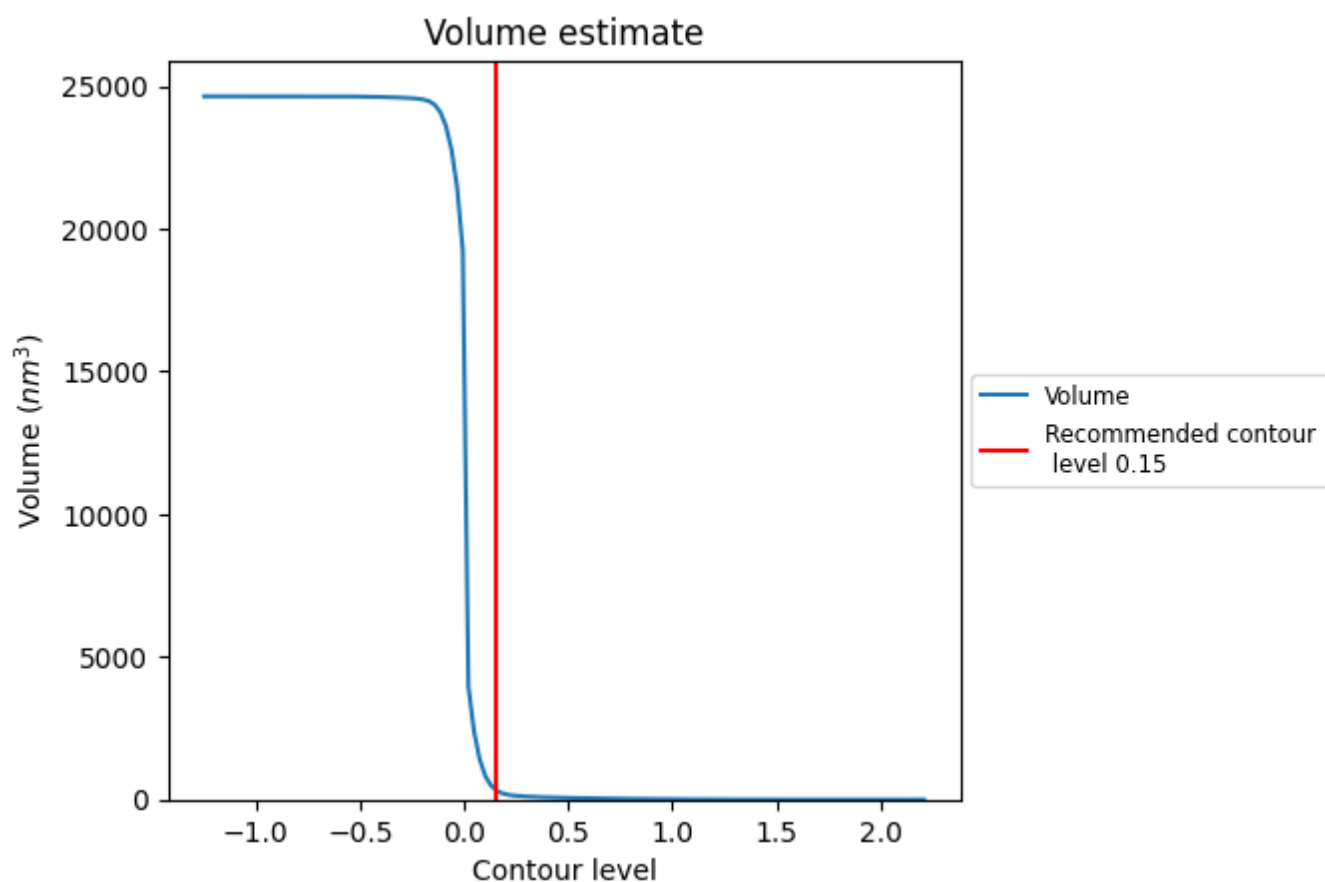
This section contains the results of statistical analysis of the map.

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.

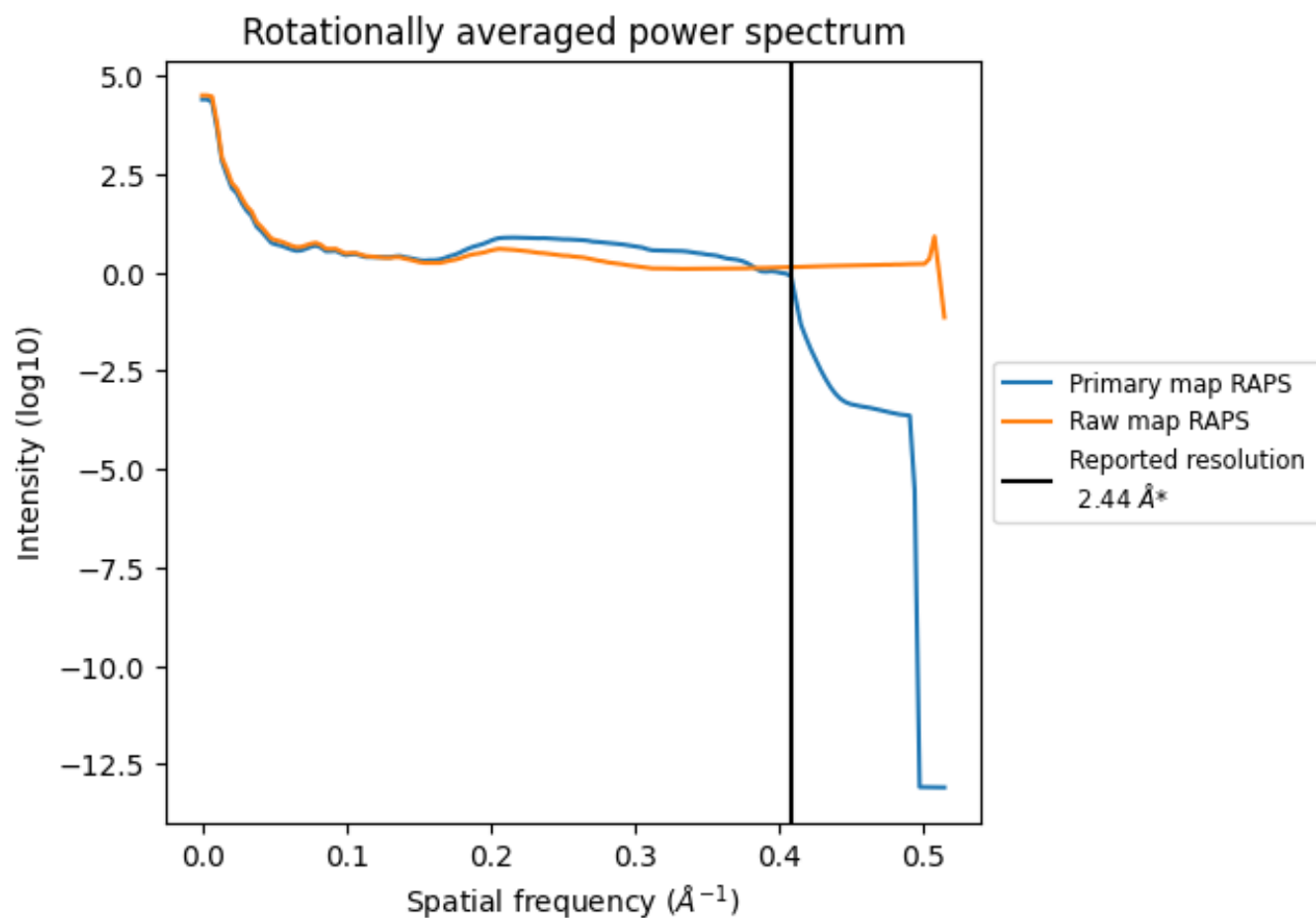
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 350 nm^3 ; this corresponds to an approximate mass of 316 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 ⓘ

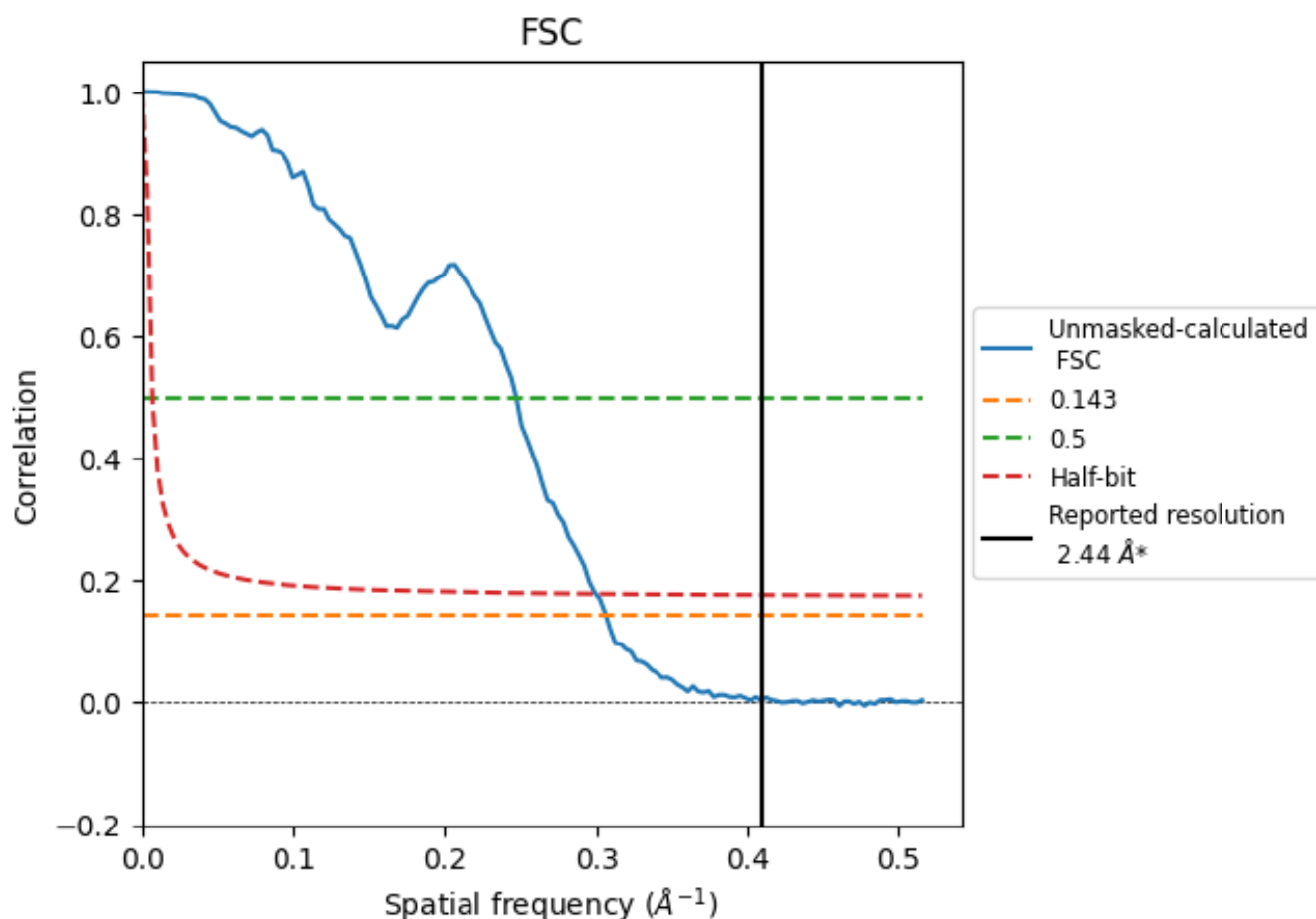


*Reported resolution corresponds to spatial frequency of 0.410 Å⁻¹

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 $0.410 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

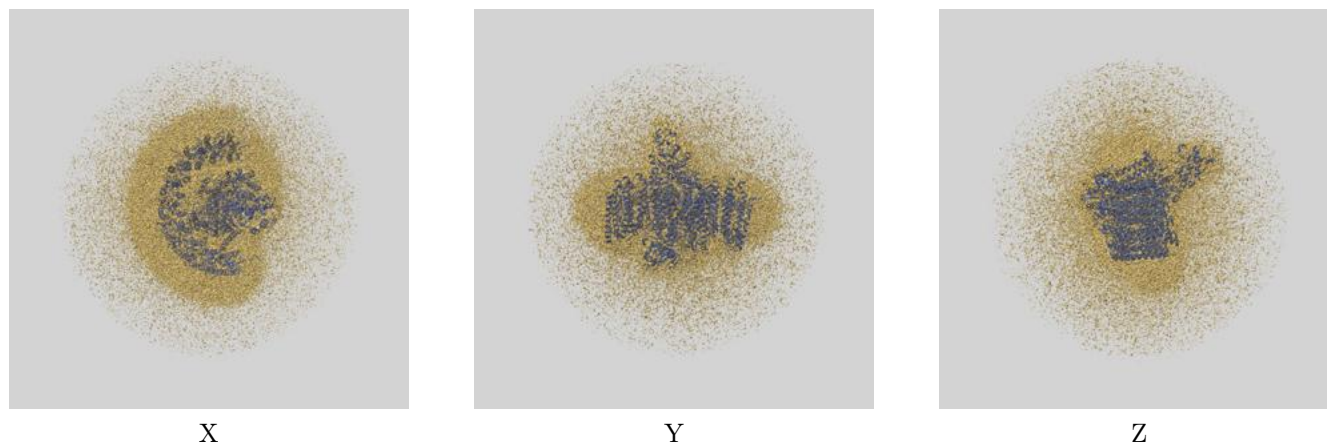
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.26	4.04	3.34

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

9 Map-model fit [i](#)

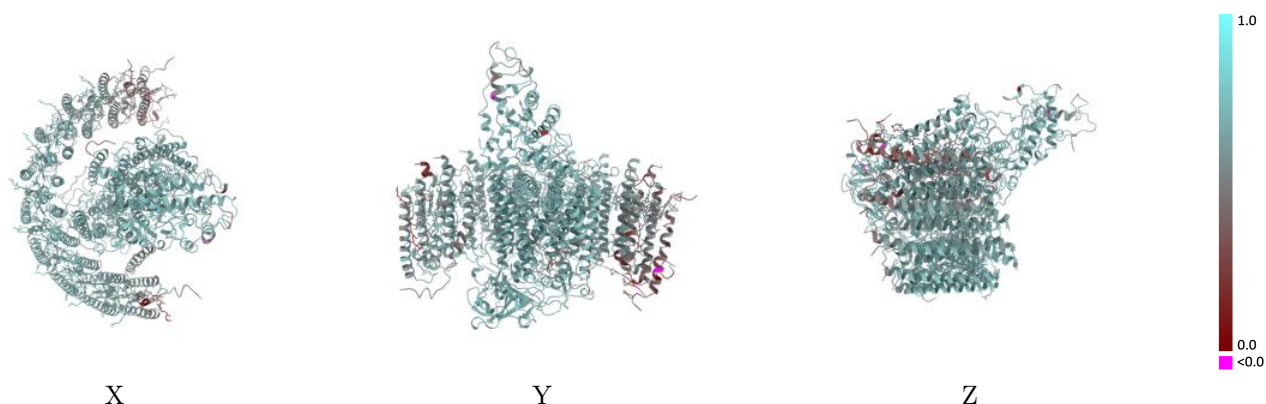
This section contains information regarding the fit between EMDB map EMD-63381 and PDB model 9LTU. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

9.1 Map-model overlay [i](#)



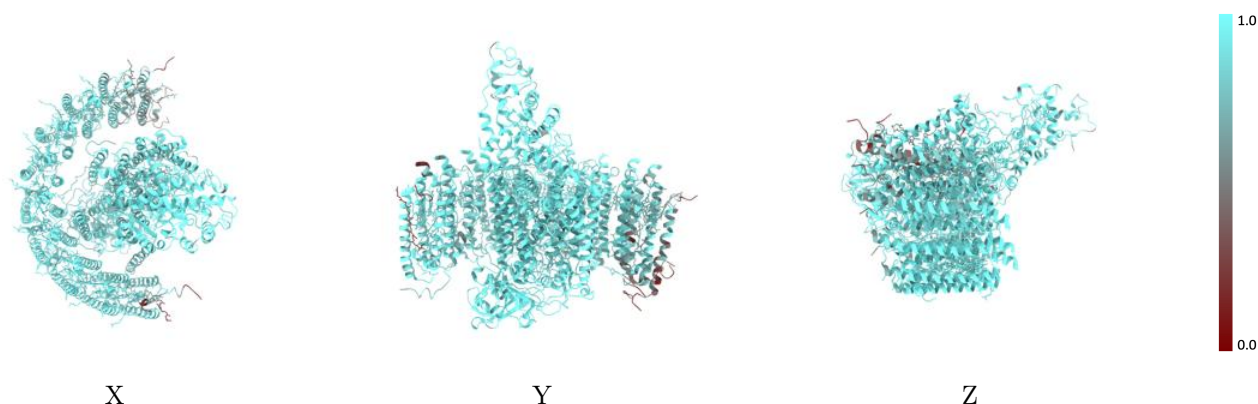
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



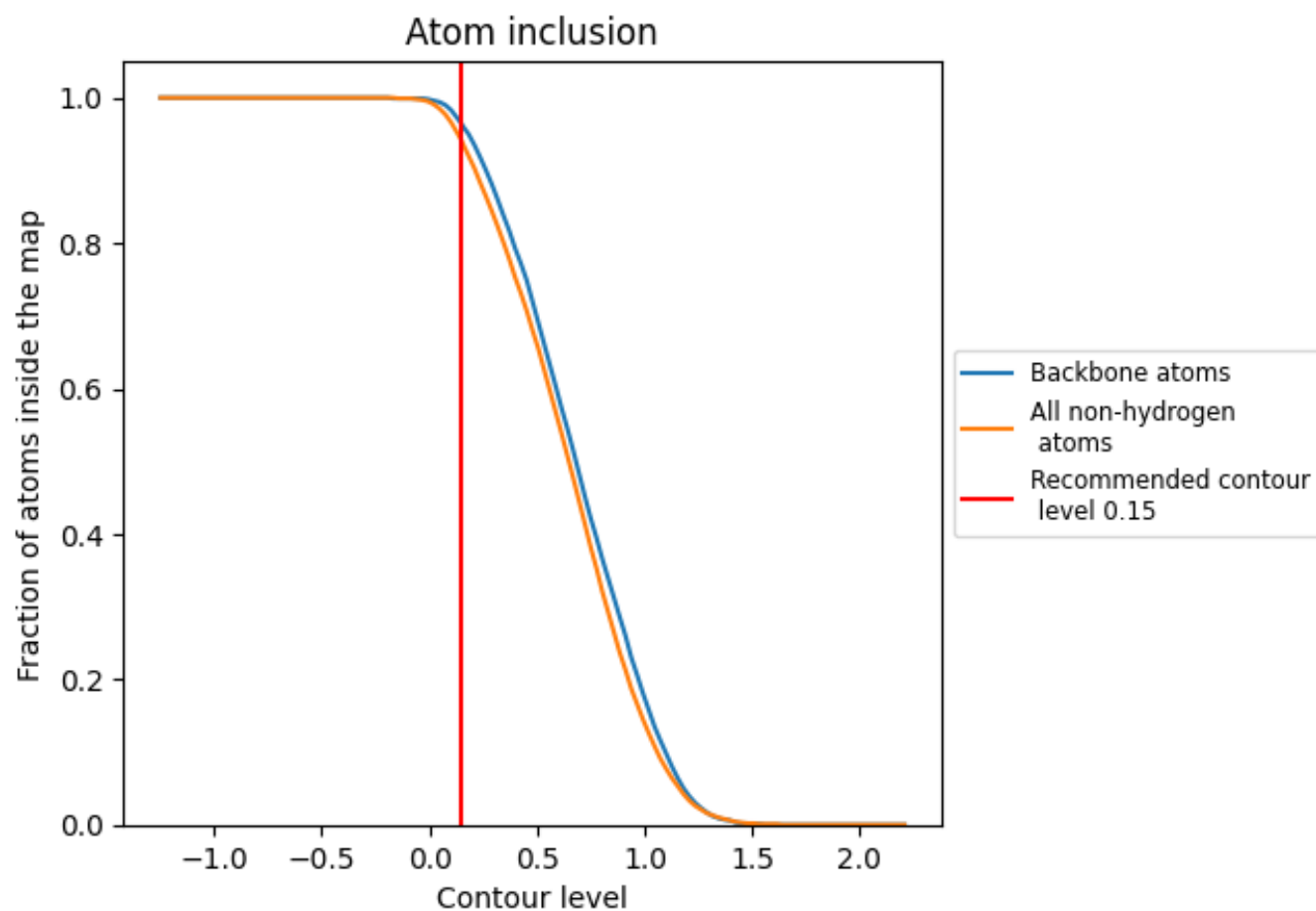
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 96% of all backbone atoms, 94% 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	 0.9410	 0.6270
0	 0.8010	 0.5040
7	 0.6440	 0.4020
8	 0.5120	 0.3630
9	 0.8620	 0.5190
C	 0.9420	 0.6210
H	 0.9760	 0.6510
L	 0.9860	 0.6730
M	 0.9860	 0.6730
a	 0.9640	 0.6200
b	 0.9230	 0.5750
c	 0.9750	 0.6400
d	 0.9590	 0.6350
e	 0.9900	 0.6750
f	 0.9700	 0.6550
g	 0.9880	 0.6760
h	 0.9910	 0.6640
i	 0.9910	 0.6800
j	 0.9830	 0.6580
k	 0.9790	 0.6620
l	 0.9760	 0.6580
m	 0.9450	 0.6210
n	 0.9610	 0.6280
o	 0.8500	 0.5610
p	 0.8660	 0.5430

