



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 03:45 AM JST

PDB ID : 9JPB / pdb_00009jpb
EMDB ID : EMD-61695
Title : Cryo-EM structure of a tri-heme cytochrome-associated RC-LH1 complex from a marine photoheterotrophic bacterium, purified with EDTA-containing solutions
Authors : Chen, J.H.; Zheng, Q.; Zhang, X.; Wang, W.; Liu, Y.; Gu, J.
Deposited on : 2024-09-25
Resolution : 2.80 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.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
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) : 2.50

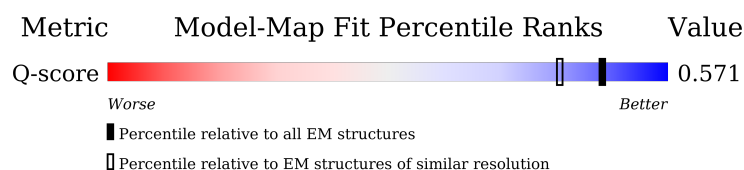
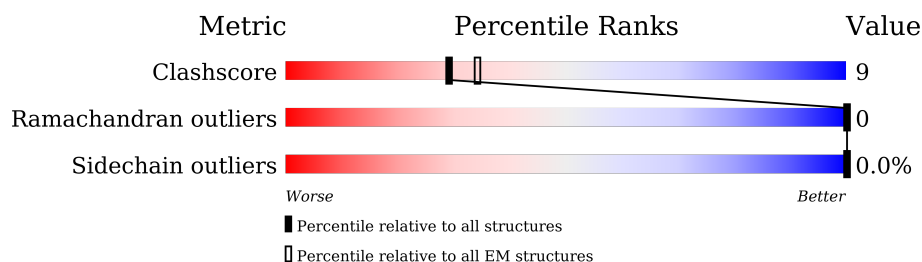
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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	11806 (2.30 - 3.30)

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	1	53	 79% 15% 6%
1	A	53	 72% 25% .
1	B	53	 85% 11% .
1	D	53	 81% 15% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	53	
1	F	53	
1	G	53	
1	I	53	
1	J	53	
1	K	53	
1	N	53	
1	P	53	
1	Q	53	
1	R	53	
1	S	53	
1	T	53	
1	V	53	
2	O	239	
3	2	49	
3	a	49	
3	b	49	
3	d	49	
3	e	49	
3	f	49	
3	g	49	
3	i	49	
3	j	49	
3	k	49	
3	n	49	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	p	49	
3	q	49	
3	r	49	
3	s	49	
3	t	49	
3	v	49	
4	M	330	
5	L	279	
6	H	256	
7	C	360	

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
16	HEC	C	401	X	-	-	-
16	HEC	C	402	X	-	-	-
16	HEC	C	403	X	-	-	-
9	SPN	2	102	-	X	-	-
9	SPN	2	103	-	X	-	-
9	SPN	D	102	-	X	-	-
9	SPN	D	103	-	X	-	-
9	SPN	E	102	-	X	-	-
9	SPN	F	102	-	X	-	-
9	SPN	G	103	-	X	-	-
9	SPN	G	104	-	X	-	-
9	SPN	I	101	-	X	-	-
9	SPN	K	102	-	X	-	-
9	SPN	M	404	-	X	-	-
9	SPN	Q	102	-	X	-	-
9	SPN	R	102	-	X	-	-
9	SPN	S	101	-	X	-	-
9	SPN	S	102	-	X	-	-
9	SPN	V	102	-	X	-	-
9	SPN	a	101	-	X	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	SPN	a	103	-	X	-	-
9	SPN	a	104	-	X	-	-
9	SPN	b	102	-	X	-	-
9	SPN	e	102	-	X	-	-
9	SPN	f	102	-	X	-	-
9	SPN	i	101	-	X	-	-
9	SPN	i	103	-	X	-	-
9	SPN	j	102	-	X	-	-
9	SPN	k	101	-	X	-	-
9	SPN	k	103	-	X	-	-
9	SPN	n	102	-	X	-	-
9	SPN	p	101	-	X	-	-
9	SPN	p	102	-	X	-	-
9	SPN	q	101	-	X	-	-
9	SPN	r	101	-	X	-	-
9	SPN	r	103	-	X	-	-
9	SPN	t	102	-	X	-	-
9	SPN	v	102	-	X	-	-

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 28258 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 alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	P	51	Total	C	N	O	S	0	0
			425	291	68	64	2		
1	V	51	Total	C	N	O	S	0	0
			422	289	68	64	1		
1	S	51	Total	C	N	O	S	0	0
			422	289	68	64	1		
1	T	51	Total	C	N	O	S	0	0
			422	289	68	64	1		
1	Q	51	Total	C	N	O	S	0	0
			422	289	68	64	1		
1	R	51	Total	C	N	O	S	0	0
			422	289	68	64	1		
1	1	50	Total	C	N	O	S	0	0
			417	286	67	63	1		
1	N	51	Total	C	N	O	S	0	0
			422	289	68	64	1		
1	K	51	Total	C	N	O	S	0	0
			422	289	68	64	1		
1	J	50	Total	C	N	O	S	0	0
			417	286	67	63	1		
1	I	51	Total	C	N	O	S	0	0
			422	289	68	64	1		
1	G	51	Total	C	N	O	S	0	0
			422	289	68	64	1		
1	F	51	Total	C	N	O	S	0	0
			422	289	68	64	1		
1	E	51	Total	C	N	O	S	0	0
			422	289	68	64	1		
1	D	51	Total	C	N	O	S	0	0
			422	289	68	64	1		
1	B	51	Total	C	N	O	S	0	0
			422	289	68	64	1		
1	A	51	Total	C	N	O	S	0	0
			422	289	68	64	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	O	52	Total	C	N	O	S	0	0
			371	249	56	59	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	v	40	Total	C	N	O	S	0	0
			321	215	52	53	1		
3	t	43	Total	C	N	O	S	0	0
			346	233	55	57	1		
3	s	44	Total	C	N	O	S	0	0
			354	237	56	60	1		
3	r	43	Total	C	N	O	S	0	0
			350	235	55	59	1		
3	q	44	Total	C	N	O	S	0	0
			354	237	56	60	1		
3	p	44	Total	C	N	O	S	0	0
			354	237	56	60	1		
3	2	44	Total	C	N	O	S	0	0
			354	237	56	60	1		
3	n	44	Total	C	N	O	S	0	0
			354	237	56	60	1		
3	k	43	Total	C	N	O	S	0	0
			346	233	55	57	1		
3	j	43	Total	C	N	O	S	0	0
			346	233	55	57	1		
3	i	43	Total	C	N	O	S	0	0
			346	233	55	57	1		
3	g	44	Total	C	N	O	S	0	0
			354	237	56	60	1		
3	f	44	Total	C	N	O	S	0	0
			354	237	56	60	1		
3	e	44	Total	C	N	O	S	0	0
			354	237	56	60	1		
3	d	44	Total	C	N	O	S	0	0
			354	237	56	60	1		
3	b	44	Total	C	N	O	S	0	0
			358	239	56	62	1		
3	a	44	Total	C	N	O	S	0	0
			358	239	56	62	1		

- Molecule 4 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	325	Total	C	N	O	S	0	0
			2633	1752	421	452	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	274	Total	C	N	O	S	0	0
			2178	1469	346	354	9		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	278	ASP	GLY	conflict	UNP A8LQ16
L	279	CYS	LEU	conflict	UNP A8LQ16

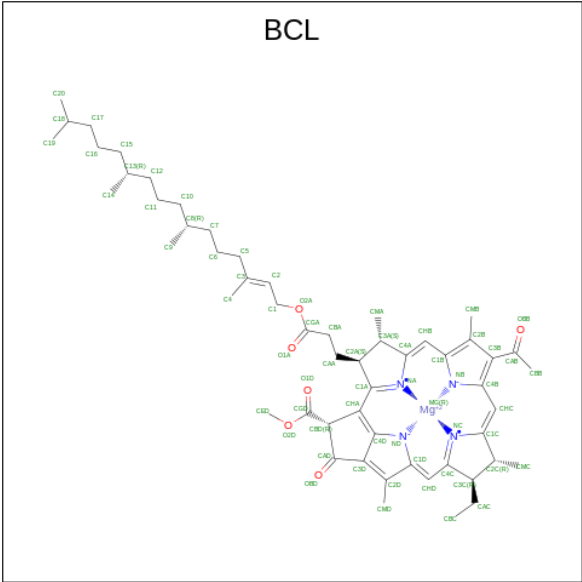
- Molecule 6 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	256	Total	C	N	O	S	0	0
			2022	1283	345	385	9		

- Molecule 7 is a protein called Photosynthetic reaction center cytochrome c subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	352	Total	C	N	O	S	0	0
			2740	1731	455	540	14		

- Molecule 8 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
8	P	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	V	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	v	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	t	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	T	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	s	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	r	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	R	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	R	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	q	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	p	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	2	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	1	1	Total 66	C 55	Mg 1	N 4	O 6	0

Continued on next page...

Continued from previous page...

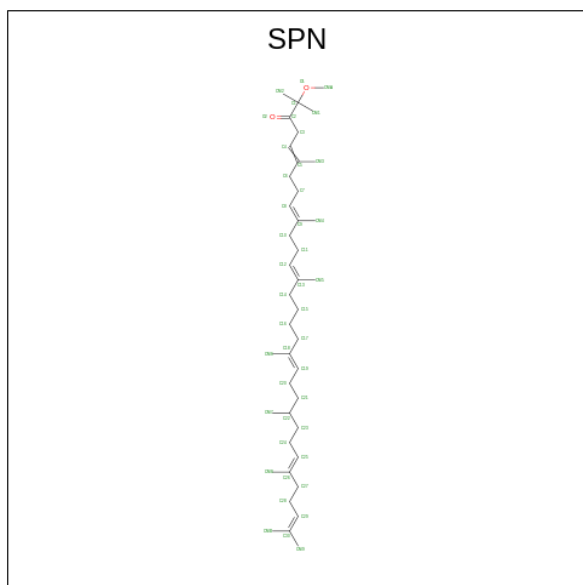
Mol	Chain	Residues	Atoms					AltConf
8	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	k	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	K	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	j	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	J	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	i	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	I	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	f	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	F	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	e	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	E	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	d	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	D	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	b	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	B	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	a	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	M	1	Total 66	C 55	Mg 1	N 4	O 6	0

Continued on next page...

Continued from previous page...

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

- Molecule 9 is SPEROIDENONE (CCD ID: SPN) (formula: $C_{41}H_{70}O_2$).



Mol	Chain	Residues	Atoms			AltConf
9	V	1	Total	C	O	0
			43	41	2	
9	v	1	Total	C	O	0
			43	41	2	
9	S	1	Total	C	O	0
			43	41	2	
9	S	1	Total	C	O	0
			43	41	2	
9	t	1	Total	C	O	0
			43	41	2	
9	Q	1	Total	C	O	0
			43	41	2	
9	r	1	Total	C	O	0
			43	41	2	
9	r	1	Total	C	O	0
			43	41	2	

Continued on next page...

Continued from previous page...

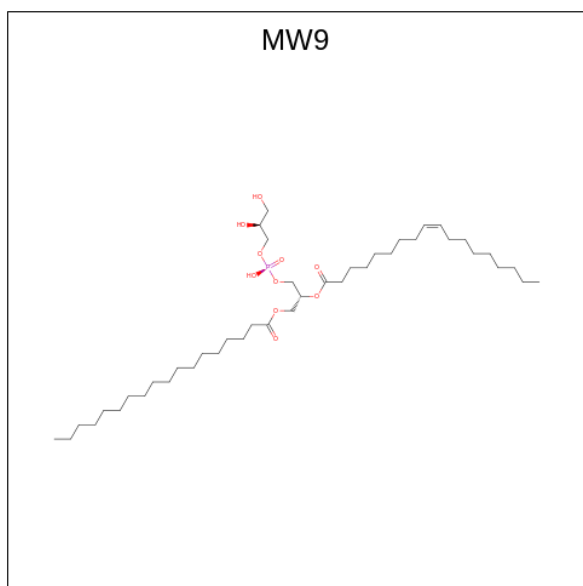
Mol	Chain	Residues	Atoms			AltConf
9	R	1	Total 43	C 41	O 2	0
9	q	1	Total 43	C 41	O 2	0
9	p	1	Total 43	C 41	O 2	0
9	p	1	Total 43	C 41	O 2	0
9	2	1	Total 43	C 41	O 2	0
9	2	1	Total 43	C 41	O 2	0
9	n	1	Total 43	C 41	O 2	0
9	k	1	Total 43	C 41	O 2	0
9	k	1	Total 43	C 41	O 2	0
9	K	1	Total 43	C 41	O 2	0
9	j	1	Total 43	C 41	O 2	0
9	i	1	Total 43	C 41	O 2	0
9	i	1	Total 43	C 41	O 2	0
9	I	1	Total 43	C 41	O 2	0
9	G	1	Total 43	C 41	O 2	0
9	G	1	Total 43	C 41	O 2	0
9	f	1	Total 43	C 41	O 2	0
9	F	1	Total 43	C 41	O 2	0
9	e	1	Total 43	C 41	O 2	0
9	E	1	Total 43	C 41	O 2	0
9	D	1	Total 43	C 41	O 2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
9	D	1	Total	C	O	0
			43	41	2	
9	b	1	Total	C	O	0
			43	41	2	
9	a	1	Total	C	O	0
			43	41	2	
9	a	1	Total	C	O	0
			43	41	2	
9	a	1	Total	C	O	0
			43	41	2	
9	M	1	Total	C	O	0
			43	41	2	

- Molecule 10 is (21R,24R,27S)-24,27,28-trihydroxy-18,24-dioxo-19,23,25-trioxa-24lambda 5 -phosphaoctacosan-21-yl (9Z)-octadec-9-enoate (CCD ID: MW9) (formula: C₄₂H₈₁O₁₀P).



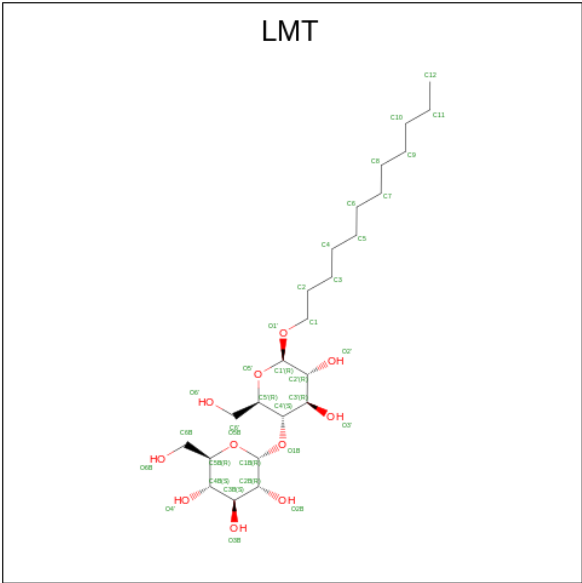
Mol	Chain	Residues	Atoms				AltConf
10	Q	1	Total	C	O	P	0
			45	34	10	1	
10	I	1	Total	C	O	P	0
			40	29	10	1	
10	G	1	Total	C	O	P	0
			49	38	10	1	
10	F	1	Total	C	O	P	0
			43	32	10	1	
10	F	1	Total	C	O	P	0
			48	37	10	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
10	D	1	Total	C	O	0
			27	22	5	
10	B	1	Total	C	O	P
			53	42	10	1
10	M	1	Total	C	O	P
			49	38	10	1
10	M	1	Total	C	O	P
			53	42	10	1
10	L	1	Total	C	O	P
			37	26	10	1
10	L	1	Total	C	O	P
			36	25	10	1
10	H	1	Total	C	O	P
			37	28	8	1

- Molecule 11 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			AltConf
11	E	1	Total	C	O	0
			35	24	11	
11	L	1	Total	C	O	0
			24	18	6	
11	L	1	Total	C	O	0
			24	19	5	
11	H	1	Total	C	O	0
			24	18	6	

Continued on next page...

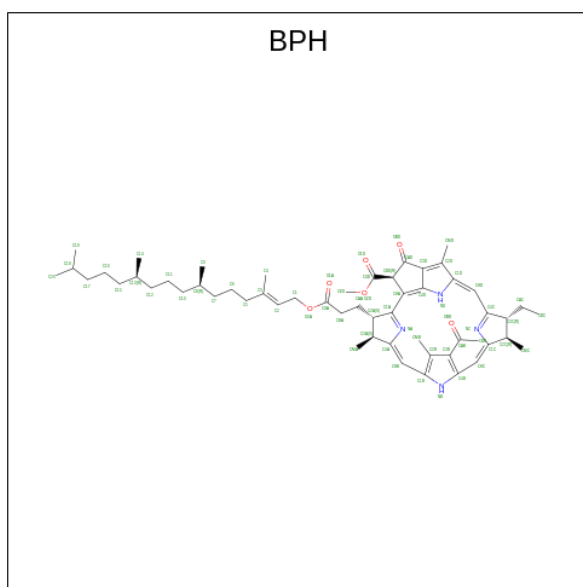
Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
11	C	1	Total	C	O	0
			24	18	6	

- Molecule 12 is FE (III) ION (CCD ID: FE) (formula: Fe).

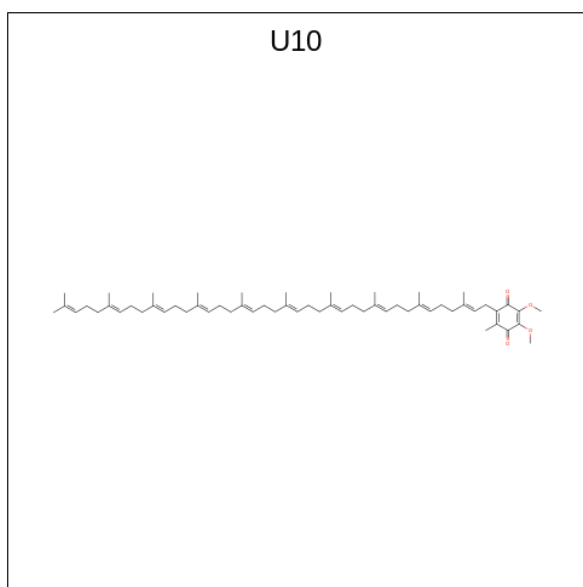
Mol	Chain	Residues	Atoms		AltConf
12	M	1	Total	Fe	0
			1	1	

- Molecule 13 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: C₅₅H₇₆N₄O₆).



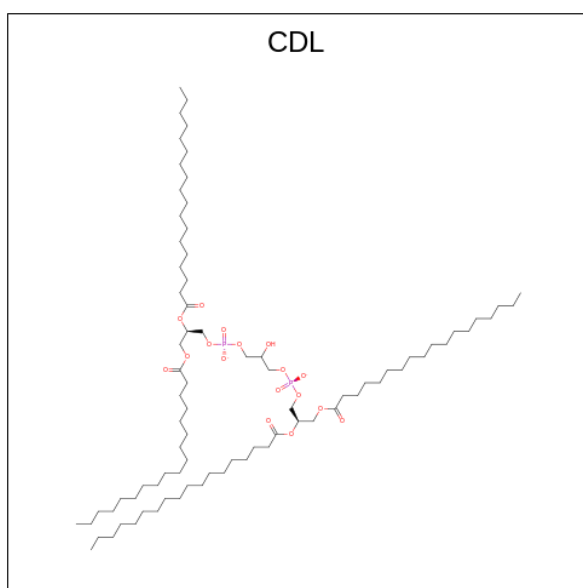
Mol	Chain	Residues	Atoms				AltConf
13	M	1	Total	C	N	O	0
			65	55	4	6	
13	L	1	Total	C	N	O	0
			65	55	4	6	

- Molecule 14 is UBIQUINONE-10 (CCD ID: U10) (formula: C₅₉H₉₀O₄).



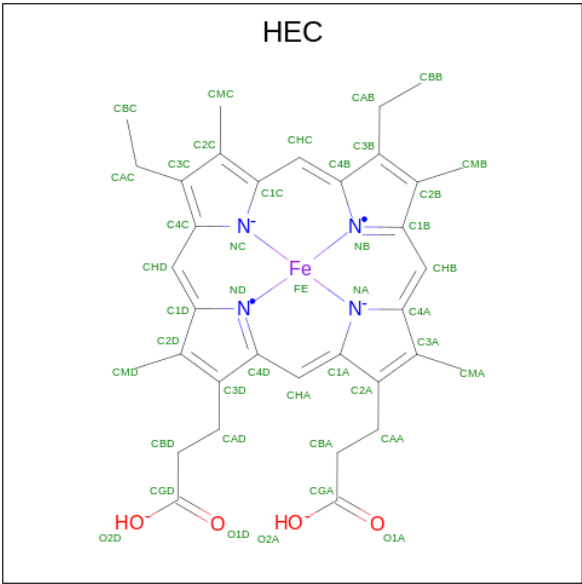
Mol	Chain	Residues	Atoms			AltConf
14	M	1	Total	C	O	0
			63	59	4	
14	L	1	Total	C	O	0
			48	44	4	

- Molecule 15 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
15	H	1	Total	C	O	P	0
			91	72	17	2	
15	H	1	Total	C	O	P	0
			67	48	17	2	

- Molecule 16 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₆FeN₄O₄) (labeled as "Ligand of Interest" by depositor).



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

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.

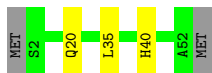
- Molecule 1: Antenna pigment protein alpha chain

Chain P:  75% 21% .



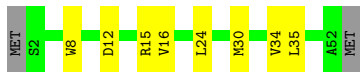
- Molecule 1: Antenna pigment protein alpha chain

Chain V:  91% 6% .



- Molecule 1: Antenna pigment protein alpha chain

Chain S:  81% 15% .



- Molecule 1: Antenna pigment protein alpha chain

Chain T:  77% 19% .



- Molecule 1: Antenna pigment protein alpha chain

Chain Q:  79% 17% .



- Molecule 1: Antenna pigment protein alpha chain

Chain R:  74% 23% .



- Molecule 1: Antenna pigment protein alpha chain

Chain 1:  79% 15% 6%



- Molecule 1: Antenna pigment protein alpha chain

Chain N:  81% 15% .



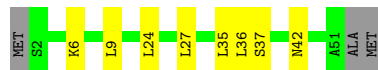
- Molecule 1: Antenna pigment protein alpha chain

Chain K:  87% 9% .



- Molecule 1: Antenna pigment protein alpha chain

Chain J:  79% 15% 6%



- Molecule 1: Antenna pigment protein alpha chain

Chain I:  85% 11% .



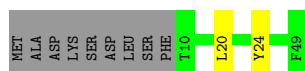
- Molecule 1: Antenna pigment protein alpha chain

Chain G:  81% 15% .



- Molecule 1: Antenna pigment protein alpha chain

Chain v:  78% 18%



• Molecule 3: Antenna pigment protein beta chain

Chain t:  71% 16% 12%



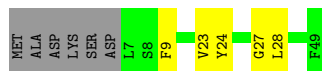
• Molecule 3: Antenna pigment protein beta chain

Chain s:  84% 6% 10%



• Molecule 3: Antenna pigment protein beta chain

Chain r:  78% 10% 12%



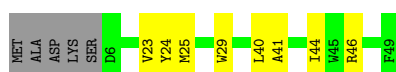
• Molecule 3: Antenna pigment protein beta chain

Chain q:  80% 10% 10%



• Molecule 3: Antenna pigment protein beta chain

Chain p:  73% 16% 10%



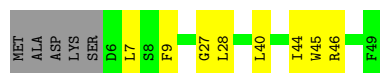
• Molecule 3: Antenna pigment protein beta chain

Chain 2:  82% 8% 10%



• Molecule 3: Antenna pigment protein beta chain

Chain n:  73% 16% 10%



- Molecule 3: Antenna pigment protein beta chain

Chain k:  73% 14% 12%



- Molecule 3: Antenna pigment protein beta chain

Chain j:  76% 12% 12%



- Molecule 3: Antenna pigment protein beta chain

Chain i:  71% 16% 12%



- Molecule 3: Antenna pigment protein beta chain

Chain g:  76% 14% 10%



- Molecule 3: Antenna pigment protein beta chain

Chain f:  76% 14% 10%



- Molecule 3: Antenna pigment protein beta chain

Chain e:  80% 10% 10%



- Molecule 3: Antenna pigment protein beta chain

Chain d:  71% 18% 10%



- Molecule 3: Antenna pigment protein beta chain

Chain b:  82% 8% 10%



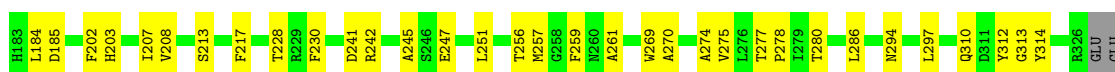
- Molecule 3: Antenna pigment protein beta chain

Chain a:  69% 20% 10%



- Molecule 4: Reaction center protein M chain

Chain M:  79% 19% .



- Molecule 5: Reaction center protein L chain

Chain L:  83% 15% .



- Molecule 6: Reaction center protein H chain

Chain H:  88% 12%

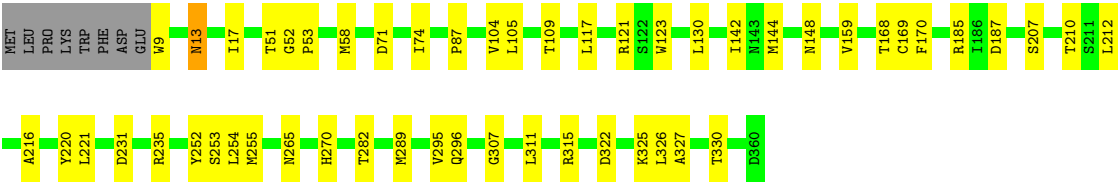


- Molecule 7: Photosynthetic reaction center cytochrome c subunit

Chain C:

83%

14%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	230375	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.280	Depositor
Minimum map value	-0.705	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.042	Depositor
Recommended contour level	0.103	Depositor
Map size ($\text{\AA}$)	307.2, 307.2, 307.2	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.2, 1.2, 1.2	Depositor

5 Model quality

5.1 Standard geometry

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

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	1	0.15	0/431	0.37	0/585
1	A	0.13	0/436	0.27	0/592
1	B	0.12	0/436	0.23	0/592
1	D	0.15	0/436	0.33	0/592
1	E	0.16	0/436	0.29	0/592
1	F	0.17	0/436	0.30	0/592
1	G	0.15	0/436	0.30	0/592
1	I	0.14	0/436	0.28	0/592
1	J	0.13	0/431	0.29	0/585
1	K	0.13	0/436	0.29	0/592
1	N	0.15	0/436	0.32	0/592
1	P	0.14	0/439	0.31	0/595
1	Q	0.13	0/436	0.29	0/592
1	R	0.14	0/436	0.24	0/592
1	S	0.15	0/436	0.32	0/592
1	T	0.12	0/436	0.27	0/592
1	V	0.12	0/436	0.28	0/592
2	O	0.13	0/378	0.26	0/516
3	2	0.10	0/367	0.21	0/503
3	a	0.14	0/371	0.31	0/508
3	b	0.12	0/371	0.24	0/508
3	d	0.15	0/367	0.28	0/503
3	e	0.13	0/367	0.21	0/503
3	f	0.13	0/367	0.21	0/503
3	g	0.14	0/367	0.22	0/503
3	i	0.13	0/359	0.21	0/492
3	j	0.12	0/359	0.29	0/492
3	k	0.14	0/359	0.28	0/492
3	n	0.13	0/367	0.26	0/503
3	p	0.13	0/367	0.27	0/503
3	q	0.11	0/367	0.21	0/503
3	r	0.11	0/363	0.20	0/497

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	s	0.12	0/367	0.25	0/503
3	t	0.12	0/359	0.23	0/492
3	v	0.11	0/333	0.23	0/457
4	M	0.16	0/2731	0.30	0/3735
5	L	0.17	0/2267	0.34	0/3105
6	H	0.13	0/2072	0.24	0/2804
7	C	0.14	0/2818	0.30	0/3868
All	All	0.14	0/23848	0.28	0/32546

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1	417	0	421	8	0
1	A	422	0	426	17	0
1	B	422	0	426	7	0
1	D	422	0	426	7	0
1	E	422	0	426	13	0
1	F	422	0	426	8	0
1	G	422	0	426	7	0
1	I	422	0	426	5	0
1	J	417	0	421	9	0
1	K	422	0	426	4	0
1	N	422	0	426	8	0
1	P	425	0	433	9	0
1	Q	422	0	426	9	0
1	R	422	0	426	9	0
1	S	422	0	426	5	0
1	T	422	0	426	9	0
1	V	422	0	426	3	0
2	O	371	0	393	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	2	354	0	334	5	0
3	a	358	0	338	7	0
3	b	358	0	338	3	0
3	d	354	0	334	9	0
3	e	354	0	334	4	0
3	f	354	0	334	6	0
3	g	354	0	334	7	0
3	i	346	0	330	7	0
3	j	346	0	330	5	0
3	k	346	0	330	5	0
3	n	354	0	334	10	0
3	p	354	0	334	9	0
3	q	354	0	334	4	0
3	r	350	0	334	5	0
3	s	354	0	334	3	0
3	t	346	0	330	9	0
3	v	321	0	305	3	0
4	M	2633	0	2524	61	0
5	L	2178	0	2118	45	0
6	H	2022	0	1971	23	0
7	C	2740	0	2581	45	0
8	1	66	0	74	3	0
8	2	66	0	74	2	0
8	A	66	0	74	6	0
8	B	66	0	74	3	0
8	D	66	0	74	2	0
8	E	66	0	74	4	0
8	F	66	0	74	4	0
8	G	132	0	146	8	0
8	I	66	0	74	7	0
8	J	66	0	74	7	0
8	K	66	0	74	4	0
8	L	132	0	144	9	0
8	M	132	0	144	7	0
8	N	66	0	74	4	0
8	P	66	0	74	4	0
8	Q	66	0	74	5	0
8	R	132	0	145	6	0
8	T	66	0	74	5	0
8	V	66	0	72	5	0
8	a	66	0	74	3	0
8	b	66	0	74	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	d	66	0	74	8	0
8	e	66	0	74	7	0
8	f	66	0	74	9	0
8	i	66	0	74	6	0
8	j	66	0	74	10	0
8	k	66	0	74	4	0
8	n	66	0	74	3	0
8	p	66	0	74	2	0
8	q	66	0	74	5	0
8	r	66	0	74	4	0
8	s	66	0	74	2	0
8	t	66	0	73	9	0
8	v	66	0	74	5	0
9	2	86	0	134	8	0
9	D	86	0	136	6	0
9	E	43	0	68	4	0
9	F	43	0	68	4	0
9	G	86	0	136	8	0
9	I	43	0	65	9	0
9	K	43	0	68	8	0
9	M	43	0	68	3	0
9	Q	43	0	68	3	0
9	R	43	0	68	10	0
9	S	86	0	131	10	0
9	V	43	0	68	9	0
9	a	129	0	197	11	0
9	b	43	0	66	12	0
9	e	43	0	65	4	0
9	f	43	0	68	1	0
9	i	86	0	133	8	0
9	j	43	0	68	4	0
9	k	86	0	131	3	0
9	n	43	0	68	8	0
9	p	86	0	132	15	0
9	q	43	0	65	2	0
9	r	86	0	134	5	0
9	t	43	0	63	3	0
9	v	43	0	68	6	0
10	B	53	0	0	0	0
10	D	27	0	0	0	0
10	F	91	0	0	0	0
10	G	49	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	H	37	0	0	0	0
10	I	40	0	0	0	0
10	L	73	0	0	0	0
10	M	102	0	0	0	0
10	Q	45	0	0	0	0
11	C	24	0	34	0	0
11	E	35	0	46	4	0
11	H	24	0	34	0	0
11	L	48	0	65	1	0
12	M	1	0	0	0	0
13	L	65	0	76	2	0
13	M	65	0	73	2	0
14	L	48	0	63	7	0
14	M	63	0	90	6	0
15	H	158	0	213	6	0
16	C	129	0	89	10	0
All	All	28258	0	28382	526	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 9.

All (526) 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)
7:C:144:MET:SD	16:C:401:HEC:NC	2.17	1.18
7:C:144:MET:SD	16:C:401:HEC:FE	1.52	1.00
7:C:144:MET:SD	16:C:401:HEC:NB	2.51	0.84
5:L:131:THR:HA	5:L:135:PHE:HB2	1.61	0.83
4:M:270:ALA:HB1	5:L:188:LEU:HD11	1.61	0.82
2:O:20:LEU:HD21	1:T:26:LEU:HD11	1.62	0.80
7:C:144:MET:SD	16:C:401:HEC:ND	2.58	0.77
1:A:25:PHE:HB2	8:A:101:BCL:H52	1.67	0.77
4:M:314:TYR:HB3	7:C:51:THR:HG22	1.67	0.75
3:d:48:TRP:CE2	8:d:101:BCL:HHC	2.22	0.75
5:L:225:ILE:HG22	14:L:303:U10:H3M3	1.69	0.73
5:L:80:PRO:HG2	5:L:83:GLU:HB2	1.71	0.73
3:i:13:THR:HB	3:i:16:GLN:HG3	1.73	0.71
5:L:265:ASN:ND2	5:L:269:GLU:OE2	2.24	0.70
7:C:326:LEU:HB2	7:C:330:THR:HG21	1.75	0.69
9:p:101:SPN:HM53	8:p:103:BCL:H12	1.75	0.69
4:M:162:GLY:HA3	9:M:404:SPN:H212	1.73	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:31:TYR:O	5:L:104:ARG:NH1	2.26	0.68
4:M:208:VAL:HG22	8:L:304:BCL:HAA2	1.75	0.68
1:E:38:THR:HG22	1:E:40:HIS:H	1.58	0.68
8:N:101:BCL:HBA2	9:K:102:SPN:HM31	1.77	0.67
9:V:102:SPN:HMB3	3:v:20:LEU:HD12	1.76	0.67
8:1:101:BCL:H3A	9:n:102:SPN:H71	1.77	0.67
4:M:95:ALA:HB2	4:M:182:PRO:HG2	1.77	0.66
4:M:313:GLY:HA2	7:C:282:THR:HG23	1.77	0.66
3:a:19:GLU:OE2	7:C:9:TRP:NE1	2.28	0.66
9:2:103:SPN:HM13	1:1:30:MET:HE3	1.78	0.65
9:F:102:SPN:HM93	1:E:6:LYS:HD3	1.78	0.65
7:C:13:ASN:O	7:C:13:ASN:ND2	2.30	0.64
9:D:103:SPN:HM73	9:b:102:SPN:HM41	1.78	0.64
1:G:36:LEU:O	1:G:42:ASN:ND2	2.30	0.63
1:I:24:LEU:HD11	9:I:101:SPN:H171	1.81	0.63
5:L:225:ILE:HB	14:L:303:U10:H4M2	1.81	0.62
1:P:40:HIS:O	3:p:46:ARG:NH1	2.32	0.62
8:d:101:BCL:H91	8:d:101:BCL:HAA1	1.81	0.62
1:J:6:LYS:HG2	1:J:9:LEU:HD12	1.82	0.62
8:Q:101:BCL:H2	9:p:101:SPN:HM42	1.80	0.62
3:n:46:ARG:HE	1:N:46:LEU:HD11	1.65	0.62
9:a:104:SPN:H72	1:A:27:LEU:HD21	1.82	0.61
8:K:101:BCL:H3A	9:j:102:SPN:H61	1.80	0.61
9:a:103:SPN:HMB2	8:A:101:BCL:H42	1.82	0.61
1:R:38:THR:O	1:R:42:ASN:ND2	2.34	0.61
8:f:101:BCL:HBD	8:F:101:BCL:HBD	1.81	0.61
8:L:301:BCL:H111	8:L:304:BCL:HBB2	1.82	0.61
8:e:101:BCL:HHD	1:E:35:LEU:HD11	1.82	0.61
1:N:36:LEU:O	1:N:42:ASN:ND2	2.34	0.60
8:a:102:BCL:HBC3	1:A:35:LEU:HD21	1.84	0.60
6:H:111:PRO:HB2	6:H:242:GLY:HA2	1.83	0.60
4:M:99:PRO:HB3	4:M:108:PRO:HG3	1.83	0.59
1:P:30:MET:HE3	9:p:101:SPN:HM23	1.83	0.59
3:a:21:HIS:CE1	3:a:25:MET:HE3	2.37	0.59
8:E:101:BCL:H12	9:D:102:SPN:HM42	1.84	0.59
7:C:168:THR:HG23	7:C:170:PHE:H	1.67	0.59
1:E:23:PHE:HE2	9:E:102:SPN:H112	1.66	0.59
4:M:217:PHE:CD1	5:L:188:LEU:HD13	2.38	0.59
1:G:33:LEU:HD21	11:L:305:LMT:H42	1.84	0.59
8:B:101:BCL:H2	9:a:104:SPN:HM41	1.85	0.58
1:A:6:LYS:HA	1:A:9:LEU:HD13	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:261:ALA:HB2	14:M:406:U10:H112	1.85	0.58
3:r:27:GLY:HA3	9:R:102:SPN:H22	1.86	0.58
8:R:101:BCL:H3A	9:R:102:SPN:H61	1.85	0.58
6:H:83:ASP:OD1	6:H:84:ASN:N	2.37	0.58
7:C:207:SER:O	7:C:210:THR:OG1	2.22	0.58
8:V:101:BCL:H3A	9:S:101:SPN:H61	1.85	0.58
6:H:82:ARG:NH1	6:H:108:GLY:O	2.29	0.57
7:C:71:ASP:HB3	7:C:74:ILE:HG13	1.87	0.57
3:t:46:ARG:NH2	1:T:40:HIS:O	2.37	0.57
4:M:256:THR:O	5:L:104:ARG:NH2	2.37	0.57
14:M:406:U10:H421	15:H:303:CDL:H471	1.85	0.57
1:J:37:SER:HB3	6:H:5:PHE:HD1	1.70	0.57
4:M:242:ARG:NH1	4:M:247:GLU:OE2	2.38	0.57
6:H:10:ASP:OD2	7:C:235:ARG:NH1	2.38	0.57
9:V:102:SPN:H271	1:T:7:ILE:HD13	1.88	0.56
3:k:19:GLU:OE2	1:J:6:LYS:NZ	2.38	0.56
9:I:101:SPN:H281	1:G:6:LYS:HG3	1.87	0.56
13:L:302:BPH:HHC	13:L:302:BPH:HBB3	1.85	0.56
3:2:16:GLN:HE21	3:n:7:LEU:HD22	1.71	0.56
1:E:11:PHE:HB3	1:E:16:VAL:HG21	1.87	0.56
1:G:11:PHE:HB3	1:G:16:VAL:HG21	1.88	0.56
9:a:104:SPN:H141	1:A:24:LEU:HD21	1.89	0.55
8:Q:101:BCL:HBA2	9:p:101:SPN:HM31	1.88	0.55
1:E:37:SER:HB3	5:L:82:MET:HE2	1.88	0.55
1:P:20:GLN:HE22	3:p:24:TYR:HE2	1.54	0.55
9:G:103:SPN:HM81	1:F:6:LYS:HG3	1.89	0.55
9:V:102:SPN:HM42	8:A:101:BCL:H51	1.89	0.55
3:n:9:PHE:HB2	1:N:10:ILE:HA	1.87	0.55
5:L:194:LEU:HD21	5:L:213:GLU:HB2	1.87	0.55
1:V:40:HIS:HB2	1:A:48:ALA:HB2	1.86	0.55
9:p:101:SPN:HMB2	1:1:6:LYS:HB3	1.87	0.55
1:Q:38:THR:O	1:Q:42:ASN:ND2	2.40	0.55
1:K:27:LEU:HD11	9:K:102:SPN:H31	1.89	0.54
3:i:13:THR:HG22	3:i:15:GLU:H	1.71	0.54
8:I:102:BCL:H3A	9:G:103:SPN:H61	1.90	0.54
3:t:12:LEU:HD11	3:s:9:PHE:HZ	1.71	0.54
3:b:13:THR:HG23	3:b:16:GLN:H	1.71	0.54
4:M:160:VAL:HA	4:M:164:PHE:HB2	1.88	0.54
3:i:27:GLY:HA3	9:I:101:SPN:H22	1.89	0.54
8:f:101:BCL:HBB2	8:f:101:BCL:H143	1.89	0.54
7:C:322:ASP:OD2	7:C:325:LYS:NZ	2.41	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:4:TYR:HA	6:H:200:ARG:HH21	1.72	0.54
1:P:24:LEU:HD11	9:p:101:SPN:HM63	1.89	0.54
8:N:101:BCL:H3A	9:K:102:SPN:H61	1.90	0.54
4:M:294:ASN:ND2	7:C:231:ASP:O	2.36	0.54
5:L:9:LYS:HD2	6:H:113:SER:HB2	1.90	0.54
4:M:203:HIS:CE1	4:M:207:ILE:HD11	2.43	0.54
9:V:102:SPN:HM21	1:A:32:HIS:HB3	1.89	0.53
8:P:101:BCL:HBA2	9:2:103:SPN:HM31	1.90	0.53
1:R:24:LEU:HD21	9:R:102:SPN:H151	1.89	0.53
3:k:21:HIS:CE1	3:k:25:MET:HE3	2.43	0.53
3:g:46:ARG:HH22	1:G:46:LEU:HD11	1.73	0.53
8:P:101:BCL:HMA3	9:p:102:SPN:H172	1.89	0.53
1:S:35:LEU:HD11	8:s:101:BCL:HHD	1.91	0.53
8:r:102:BCL:H2	8:r:102:BCL:H142	1.91	0.53
3:p:41:ALA:HB1	9:p:102:SPN:H71	1.90	0.53
8:L:304:BCL:H143	8:L:304:BCL:HMA1	1.91	0.53
3:g:45:TRP:HB2	9:G:104:SPN:H61	1.91	0.52
8:f:101:BCL:CBD	8:F:101:BCL:HBD	2.38	0.52
9:a:104:SPN:H171	1:A:24:LEU:HD11	1.90	0.52
8:M:402:BCL:H11	13:M:403:BPH:HBC3	1.91	0.52
1:T:8:TRP:HZ3	1:T:16:VAL:HG11	1.75	0.52
4:M:50:GLY:HA3	5:L:218:ARG:HD3	1.90	0.52
8:J:101:BCL:HHB	9:I:101:SPN:H62	1.92	0.52
3:t:48:TRP:HE1	8:t:101:BCL:HBB2	1.73	0.52
4:M:241:ASP:O	6:H:117:ARG:NH2	2.37	0.52
1:I:11:PHE:HB3	1:I:16:VAL:HG21	1.92	0.52
11:E:103:LMT:H41	5:L:81:LEU:HD11	1.91	0.52
4:M:6:ASN:O	5:L:232:ARG:NE	2.40	0.52
3:q:28:LEU:HA	9:q:101:SPN:H171	1.92	0.52
3:e:9:PHE:HB2	1:E:10:ILE:HA	1.92	0.52
4:M:241:ASP:OD1	6:H:80:GLN:NE2	2.38	0.52
9:S:101:SPN:H151	1:T:24:LEU:HD21	1.91	0.52
3:j:32:SER:HB3	8:j:101:BCL:H72	1.91	0.52
9:i:103:SPN:HM52	9:i:103:SPN:HM41	1.91	0.52
7:C:87:PRO:HB3	7:C:109:THR:HG21	1.91	0.52
4:M:217:PHE:HB2	5:L:188:LEU:HD13	1.93	0.51
8:2:101:BCL:HED1	1:1:27:LEU:HD23	1.92	0.51
3:g:19:GLU:OE2	1:F:6:LYS:NZ	2.44	0.51
3:j:46:ARG:HG3	3:j:46:ARG:HH11	1.75	0.51
5:L:190:LEU:HB2	14:L:303:U10:H1M2	1.92	0.51
6:H:168:TRP:HB2	6:H:178:TYR:HB2	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:231:LEU:HG	6:H:235:LYS:HE3	1.92	0.51
1:S:12:ASP:HB3	1:S:15:ARG:HB3	1.93	0.51
1:S:24:LEU:HD21	9:S:102:SPN:H142	1.92	0.51
9:2:103:SPN:HM81	1:1:17:PHE:CZ	2.46	0.51
9:e:102:SPN:HM93	9:E:102:SPN:HM73	1.91	0.51
4:M:217:PHE:HB2	5:L:188:LEU:HD22	1.91	0.51
5:L:44:LEU:HG	15:H:303:CDL:H431	1.92	0.51
15:H:304:CDL:H331	15:H:304:CDL:H152	1.93	0.51
1:P:20:GLN:OE1	3:p:24:TYR:OH	2.21	0.51
1:Q:27:LEU:HD23	8:q:102:BCL:HED3	1.93	0.51
6:H:2:GLU:HG2	7:C:235:ARG:HB3	1.92	0.51
8:V:101:BCL:C1B	8:t:101:BCL:HMB2	2.41	0.51
9:v:102:SPN:HM52	9:v:102:SPN:HM41	1.93	0.51
3:t:48:TRP:CZ2	8:t:101:BCL:HHC	2.46	0.51
1:S:8:TRP:HZ3	1:S:16:VAL:HG11	1.75	0.50
3:t:24:TYR:HE2	1:T:20:GLN:HE22	1.59	0.50
11:E:103:LMT:H22	1:D:34:VAL:HG13	1.92	0.50
4:M:57:PHE:O	4:M:129:SER:OG	2.28	0.50
6:H:42:GLU:OE2	6:H:81:ARG:NH2	2.36	0.50
3:k:10:THR:HG23	3:k:12:LEU:HD13	1.93	0.50
4:M:217:PHE:CE2	5:L:234:GLY:HA3	2.47	0.50
9:2:103:SPN:H112	1:1:23:PHE:HE2	1.76	0.50
3:a:9:PHE:HB2	1:A:10:ILE:HA	1.94	0.50
4:M:230:PHE:HB2	4:M:245:ALA:HB2	1.93	0.50
5:L:166:LEU:O	7:C:252:TYR:OH	2.25	0.50
1:Q:6:LYS:HG2	1:Q:9:LEU:HD12	1.93	0.50
3:b:24:TYR:HE1	1:B:20:GLN:HE22	1.59	0.50
1:B:8:TRP:HZ3	1:B:16:VAL:HG11	1.77	0.50
3:j:13:THR:OG1	3:j:16:GLN:OE1	2.18	0.50
8:M:402:BCL:H192	8:M:405:BCL:H93	1.92	0.50
9:2:102:SPN:H152	8:n:101:BCL:H143	1.94	0.50
7:C:123:TRP:HE3	7:C:169:CYS:HB3	1.77	0.50
8:j:101:BCL:HHD	1:J:35:LEU:HD11	1.93	0.50
4:M:91:LEU:HD11	9:M:404:SPN:HM31	1.93	0.49
4:M:158:PHE:HB2	8:M:402:BCL:H72	1.93	0.49
8:P:101:BCL:HBD	8:p:103:BCL:HBD	1.93	0.49
9:S:101:SPN:H282	3:t:20:LEU:HG	1.94	0.49
7:C:104:VAL:HG11	7:C:142:ILE:HG23	1.94	0.49
1:N:9:LEU:HD12	1:N:10:ILE:HG23	1.94	0.49
8:i:102:BCL:H11	9:I:101:SPN:H12	1.94	0.49
1:E:27:LEU:HD11	9:E:102:SPN:H71	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:6:LYS:HB3	9:R:102:SPN:HMB2	1.93	0.49
3:2:24:TYR:HA	9:2:103:SPN:HM83	1.93	0.49
9:S:102:SPN:H61	8:T:101:BCL:H3A	1.94	0.49
3:i:24:TYR:HE1	1:I:20:GLN:HE22	1.60	0.49
4:M:6:ASN:HD22	4:M:228:THR:HG21	1.77	0.49
5:L:110:ARG:NH2	15:H:304:CDL:OA3	2.40	0.49
3:q:6:ASP:N	3:q:6:ASP:OD1	2.45	0.49
9:n:102:SPN:HMB1	3:k:7:LEU:HD21	1.95	0.49
8:j:101:BCL:CAD	8:J:101:BCL:HBD	2.42	0.49
8:V:101:BCL:HBB3	8:t:101:BCL:NB	2.28	0.49
5:L:166:LEU:HD21	7:C:265:ASN:HA	1.94	0.49
8:t:101:BCL:HAA1	8:t:101:BCL:H8	1.94	0.48
9:S:102:SPN:H12	8:T:101:BCL:H92	1.95	0.48
3:i:40:LEU:O	3:i:44:ILE:HG12	2.13	0.48
4:M:202:PHE:HD1	4:M:280:THR:HG23	1.78	0.48
1:I:15:ARG:HA	4:M:56:TRP:CZ2	2.49	0.48
1:K:24:LEU:HB2	8:K:101:BCL:H42	1.95	0.48
9:i:101:SPN:HM73	9:I:101:SPN:H101	1.95	0.48
9:i:103:SPN:HM82	8:I:102:BCL:H43	1.94	0.48
1:D:32:HIS:HE1	8:D:101:BCL:NA	2.11	0.48
8:B:101:BCL:HBB2	1:A:31:ILE:HD12	1.95	0.48
9:a:104:SPN:HM23	1:A:30:MET:HE3	1.94	0.48
7:C:144:MET:SD	16:C:401:HEC:NA	2.86	0.48
1:N:7:ILE:HD12	1:N:10:ILE:HD11	1.94	0.48
1:I:36:LEU:O	1:I:42:ASN:ND2	2.43	0.48
3:d:21:HIS:CE1	3:d:25:MET:HE3	2.48	0.48
9:b:102:SPN:H211	9:b:102:SPN:HM63	1.94	0.48
5:L:206:GLU:HA	6:H:64:LYS:HB3	1.96	0.48
7:C:212:LEU:HB3	7:C:253:SER:HB2	1.95	0.48
2:O:8:MET:O	2:O:10:CYS:N	2.46	0.48
3:d:46:ARG:HH11	1:D:40:HIS:CE1	2.32	0.48
3:b:38:ALA:HB1	9:a:101:SPN:HM51	1.96	0.48
3:n:28:LEU:HB2	9:n:102:SPN:H172	1.95	0.48
9:F:102:SPN:HM83	1:E:7:ILE:HB	1.95	0.48
8:B:101:BCL:HBA2	9:a:104:SPN:H61	1.94	0.48
3:a:33:ALA:O	3:a:37:VAL:HG23	2.13	0.48
4:M:277:THR:OG1	4:M:278:PRO:HD3	2.14	0.48
1:G:42:ASN:O	1:G:46:LEU:HD23	2.13	0.48
8:e:101:BCL:H112	8:e:101:BCL:H142	1.55	0.48
1:E:33:LEU:HD21	11:E:103:LMT:H72	1.96	0.48
1:P:27:LEU:O	1:P:31:ILE:HD12	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:v:101:BCL:H41	8:v:101:BCL:H62	1.52	0.48
3:e:34:VAL:HG12	8:E:101:BCL:HED1	1.95	0.48
3:d:24:TYR:OH	1:D:20:GLN:OE1	2.17	0.48
4:M:294:ASN:CG	4:M:297:LEU:HD23	2.39	0.48
1:V:20:GLN:NE2	9:V:102:SPN:HM61	2.29	0.47
4:M:269:TRP:HE1	6:H:34:ASN:ND2	2.11	0.47
1:P:6:LYS:HA	1:P:9:LEU:HD12	1.96	0.47
1:Q:27:LEU:HD21	9:q:101:SPN:H72	1.96	0.47
8:t:101:BCL:HED3	1:T:27:LEU:HD23	1.95	0.47
8:Q:101:BCL:H3A	9:p:101:SPN:H61	1.97	0.47
9:r:101:SPN:HM73	9:R:102:SPN:HM41	1.97	0.47
3:n:27:GLY:HA3	9:n:102:SPN:H22	1.96	0.47
3:f:8:SER:HB2	1:F:9:LEU:HD11	1.96	0.47
8:e:101:BCL:H2C	8:e:101:BCL:HBC3	1.58	0.47
8:d:101:BCL:HHD	1:D:35:LEU:HD22	1.95	0.47
4:M:145:LYS:HB3	4:M:148:ALA:HB3	1.96	0.47
5:L:76:LEU:O	5:L:143:TRP:NE1	2.44	0.47
8:l:101:BCL:H3A	9:n:102:SPN:C7	2.43	0.47
3:j:45:TRP:CD2	3:j:46:ARG:HG2	2.50	0.47
3:j:28:LEU:HD21	8:j:101:BCL:H42	1.97	0.47
4:M:259:PHE:HE1	14:M:406:U10:H262	1.79	0.47
15:H:303:CDL:H801	15:H:303:CDL:H771	1.75	0.47
1:R:11:PHE:HB3	1:R:16:VAL:HG21	1.95	0.47
8:q:102:BCL:H161	8:q:102:BCL:H192	1.73	0.47
8:N:101:BCL:HBC3	8:N:101:BCL:H2C	1.72	0.47
8:j:101:BCL:HED3	1:J:27:LEU:HD23	1.97	0.47
4:M:11:VAL:HA	6:H:145:GLY:HA3	1.95	0.47
5:L:176:ILE:O	5:L:179:THR:HG22	2.14	0.47
9:V:102:SPN:HM82	9:V:102:SPN:H242	1.68	0.47
3:d:49:PHE:HZ	8:d:101:BCL:HBB1	1.80	0.47
3:f:19:GLU:OE1	1:E:6:LYS:NZ	2.40	0.47
4:M:312:TYR:HA	7:C:52:GLY:HA2	1.96	0.47
8:f:101:BCL:HED3	1:F:27:LEU:HD23	1.95	0.46
8:a:102:BCL:HHD	1:A:35:LEU:HD11	1.97	0.46
8:A:101:BCL:H13	8:A:101:BCL:H102	1.72	0.46
4:M:53:TYR:O	4:M:133:ARG:NH1	2.45	0.46
1:R:30:MET:O	1:R:34:VAL:HG23	2.15	0.46
8:i:102:BCL:CAD	8:I:102:BCL:HBD	2.46	0.46
8:G:101:BCL:H112	8:G:101:BCL:H142	1.62	0.46
8:V:101:BCL:H43	9:v:102:SPN:HM82	1.97	0.46
8:M:402:BCL:HAA2	8:M:402:BCL:HBD	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:v:101:BCL:H93	8:v:101:BCL:H111	1.64	0.46
8:T:101:BCL:HBC3	8:T:101:BCL:H2C	1.73	0.46
3:r:9:PHE:CD1	1:R:10:ILE:HG22	2.51	0.46
4:M:257:MET:CE	14:M:406:U10:H13	2.46	0.46
5:L:133:VAL:O	5:L:137:PRO:HG2	2.15	0.46
9:n:102:SPN:H112	9:n:102:SPN:HM42	1.59	0.46
9:i:101:SPN:H4	9:i:101:SPN:HM12	1.97	0.46
9:F:102:SPN:H25	1:E:7:ILE:HD13	1.98	0.46
4:M:160:VAL:HG23	4:M:286:LEU:HD13	1.96	0.46
4:M:185:ASP:OD1	5:L:167:HIS:HE1	1.98	0.46
8:v:101:BCL:HAA1	8:v:101:BCL:H52	1.96	0.46
8:n:101:BCL:H93	8:n:101:BCL:H111	1.63	0.46
9:D:102:SPN:HM81	9:D:102:SPN:H282	1.80	0.46
3:a:16:GLN:HB3	7:C:9:TRP:CZ2	2.51	0.46
14:M:406:U10:H251	15:H:303:CDL:H551	1.97	0.46
7:C:289:MET:SD	16:C:402:HEC:HMD3	2.56	0.46
8:k:102:BCL:H92	8:k:102:BCL:H61	1.79	0.46
8:b:101:BCL:H143	8:b:101:BCL:H161	1.61	0.46
4:M:68:TRP:HD1	4:M:119:ALA:HB1	1.81	0.46
7:C:52:GLY:HA3	7:C:58:MET:HE2	1.96	0.46
9:e:102:SPN:H12	9:e:102:SPN:H151	1.43	0.46
8:r:102:BCL:H2	8:r:102:BCL:H111	1.98	0.46
4:M:270:ALA:HB1	5:L:188:LEU:CD1	2.40	0.46
8:Q:101:BCL:HBD	8:q:102:BCL:HBD	1.98	0.45
11:E:103:LMT:H1B	11:E:103:LMT:H3'	1.77	0.45
1:D:14:ARG:HB3	1:B:10:ILE:HG23	1.97	0.45
7:C:327:ALA:O	7:C:330:THR:HG22	2.16	0.45
1:Q:33:LEU:HD13	4:M:77:LEU:HD21	1.99	0.45
8:A:101:BCL:H41	8:A:101:BCL:H61	1.42	0.45
4:M:275:VAL:O	4:M:278:PRO:HD2	2.16	0.45
6:H:112:ALA:HA	6:H:238:ALA:O	2.17	0.45
7:C:221:LEU:HD13	7:C:295:VAL:HG11	1.98	0.45
3:k:27:GLY:HA3	9:K:102:SPN:H22	1.99	0.45
8:k:102:BCL:HMA2	9:K:102:SPN:HM42	1.97	0.45
8:r:102:BCL:HBD	8:R:103:BCL:HBD	1.99	0.45
1:F:36:LEU:HD13	5:L:52:TRP:CZ3	2.52	0.45
3:g:7:LEU:O	1:G:9:LEU:HD23	2.17	0.45
5:L:23:PHE:CE1	5:L:37:VAL:HG21	2.51	0.45
7:C:216:ALA:HB1	7:C:254:LEU:HB2	1.98	0.45
3:n:7:LEU:HD11	3:n:9:PHE:CE1	2.51	0.45
9:K:102:SPN:HMB3	1:J:6:LYS:HD3	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:24:LEU:HB2	8:J:101:BCL:H42	1.97	0.45
3:i:24:TYR:HA	9:I:101:SPN:H231	1.99	0.45
3:g:38:ALA:HB2	9:G:104:SPN:H152	1.99	0.45
3:d:48:TRP:CZ2	8:d:101:BCL:HHC	2.51	0.45
9:n:102:SPN:H171	9:n:102:SPN:H201	1.76	0.45
9:b:102:SPN:H231	9:a:101:SPN:HM92	1.99	0.45
3:n:45:TRP:HB2	9:k:101:SPN:H71	1.99	0.45
8:i:102:BCL:CBD	8:I:102:BCL:HBD	2.46	0.45
4:M:251:LEU:HD11	5:L:7:GLU:HA	1.97	0.45
8:V:101:BCL:HED3	9:v:102:SPN:H19	1.99	0.44
9:Q:102:SPN:HM73	9:Q:102:SPN:H241	1.80	0.44
8:r:102:BCL:HED3	1:R:27:LEU:HD23	1.99	0.44
8:K:101:BCL:H2	9:j:102:SPN:HM43	1.97	0.44
8:I:102:BCL:H122	8:I:102:BCL:H161	1.73	0.44
8:G:101:BCL:H192	8:G:101:BCL:H143	1.98	0.44
8:M:405:BCL:H91	8:M:405:BCL:H111	1.73	0.44
8:j:101:BCL:HAC2	1:J:35:LEU:HD11	1.99	0.44
8:f:101:BCL:HHD	1:F:35:LEU:HD11	1.98	0.44
9:b:102:SPN:HM32	9:b:102:SPN:H72	1.73	0.44
7:C:159:VAL:O	16:C:403:HEC:HBD2	2.16	0.44
9:v:102:SPN:HM92	9:v:102:SPN:H282	1.80	0.44
3:s:28:LEU:HD21	8:s:101:BCL:H42	1.99	0.44
9:r:103:SPN:HM61	8:q:102:BCL:H72	1.99	0.44
8:J:101:BCL:H162	8:J:101:BCL:H122	1.68	0.44
8:i:102:BCL:H162	8:i:102:BCL:H192	1.80	0.44
4:M:30:GLU:HB2	4:M:53:TYR:CE1	2.51	0.44
4:M:274:ALA:HB1	5:L:189:ALA:HB2	1.99	0.44
5:L:223:TYR:CD2	14:L:303:U10:H4M1	2.51	0.44
6:H:178:TYR:OH	6:H:237:MET:HE3	2.16	0.44
9:V:102:SPN:HM83	3:v:24:TYR:HA	2.00	0.44
3:s:44:ILE:HD12	9:r:101:SPN:HM21	1.98	0.44
8:j:101:BCL:HBD	8:J:101:BCL:HBD	2.00	0.44
9:j:102:SPN:HM71	9:j:102:SPN:H241	1.78	0.44
9:f:102:SPN:H152	8:e:101:BCL:HMB3	1.98	0.44
8:a:102:BCL:H111	8:a:102:BCL:H142	1.70	0.44
9:a:104:SPN:HM53	9:a:104:SPN:H151	1.72	0.44
9:K:102:SPN:HM81	9:K:102:SPN:H281	1.76	0.44
8:G:101:BCL:H11	9:G:103:SPN:H111	2.00	0.44
2:O:24:MET:HE3	1:T:29:ALA:HB1	2.00	0.44
9:S:101:SPN:HM32	9:S:101:SPN:H72	1.69	0.44
4:M:310:GLN:HB2	7:C:53:PRO:HB3	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:R:103:BCL:H192	8:R:103:BCL:H161	1.79	0.44
3:2:38:ALA:HB1	9:2:102:SPN:HM53	1.99	0.44
8:j:101:BCL:CBD	8:J:101:BCL:HBD	2.48	0.44
9:i:101:SPN:HM93	9:i:101:SPN:H281	1.73	0.44
3:t:32:SER:O	3:t:36:VAL:HG23	2.18	0.44
3:r:24:TYR:HE2	1:R:20:GLN:HE22	1.65	0.44
9:p:102:SPN:H8	9:p:102:SPN:HM31	2.00	0.44
8:K:101:BCL:HBC3	8:K:101:BCL:H2C	1.80	0.44
5:L:190:LEU:CB	14:L:303:U10:H1M2	2.48	0.44
1:1:12:ASP:HB2	1:1:15:ARG:HH11	1.83	0.43
8:i:102:BCL:HBD	8:I:102:BCL:HBD	1.99	0.43
1:F:36:LEU:HD13	5:L:52:TRP:HZ3	1.83	0.43
3:d:49:PHE:CZ	8:d:101:BCL:HBB1	2.52	0.43
9:b:102:SPN:HM81	9:b:102:SPN:H281	1.73	0.43
3:a:32:SER:O	3:a:36:VAL:HG23	2.18	0.43
4:M:157:LEU:HA	4:M:160:VAL:HG12	1.99	0.43
8:L:301:BCL:H143	8:L:301:BCL:H161	1.72	0.43
9:S:101:SPN:HM52	9:S:101:SPN:H152	1.80	0.43
3:2:23:VAL:HG12	9:2:103:SPN:H272	2.00	0.43
9:i:103:SPN:H25	8:I:102:BCL:H61	1.99	0.43
8:G:102:BCL:H162	8:G:102:BCL:H122	1.75	0.43
4:M:110:LEU:HA	4:M:114:GLY:HA3	2.00	0.43
4:M:184:LEU:HD13	5:L:169:HIS:HB3	2.00	0.43
4:M:269:TRP:HE1	6:H:34:ASN:HD21	1.66	0.43
3:f:30:LEU:O	3:f:34:VAL:HG23	2.19	0.43
7:C:315:ARG:NE	16:C:401:HEC:O2A	2.49	0.43
3:p:40:LEU:O	3:p:44:ILE:HG12	2.18	0.43
8:1:101:BCL:HBC3	8:1:101:BCL:H2C	1.67	0.43
9:K:102:SPN:HM82	9:K:102:SPN:H241	1.75	0.43
1:I:20:GLN:OE1	9:I:101:SPN:H172	2.18	0.43
8:G:102:BCL:H2C	8:G:102:BCL:HBC3	1.69	0.43
8:E:101:BCL:H61	8:E:101:BCL:H41	1.71	0.43
9:a:103:SPN:HM92	9:a:103:SPN:H281	1.74	0.43
13:M:403:BPH:H151	13:M:403:BPH:H111	1.73	0.43
8:f:101:BCL:HBA1	8:f:101:BCL:H92	2.01	0.43
8:L:301:BCL:H41	8:L:301:BCL:H62	1.48	0.43
9:S:101:SPN:HMB2	3:t:20:LEU:HD12	2.01	0.43
4:M:257:MET:HE1	14:M:406:U10:H13	2.01	0.43
6:H:33:GLU:OE2	6:H:36:ARG:NH2	2.39	0.43
1:P:46:LEU:HD21	3:p:46:ARG:CZ	2.48	0.43
3:q:39:HIS:HA	3:q:42:THR:HG22	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:LEU:O	1:A:31:ILE:HG12	2.19	0.43
4:M:76:MET:HG2	4:M:94:LEU:HB3	2.01	0.43
3:p:25:MET:O	3:p:29:TRP:HD1	2.02	0.43
3:n:46:ARG:NE	1:N:46:LEU:HD11	2.31	0.43
9:I:101:SPN:HM82	9:I:101:SPN:H241	1.75	0.43
3:a:7:LEU:O	1:A:9:LEU:HD23	2.19	0.43
9:M:404:SPN:H72	9:M:404:SPN:H4	1.92	0.43
5:L:126:ILE:O	5:L:130:VAL:HG23	2.19	0.43
6:H:133:PRO:HG3	6:H:168:TRP:CE2	2.53	0.43
9:Q:102:SPN:H111	9:Q:102:SPN:H8	1.52	0.43
3:f:32:SER:OG	8:f:101:BCL:H2	2.19	0.43
9:D:103:SPN:HM51	9:D:103:SPN:H152	1.74	0.43
8:t:101:BCL:H202	8:t:101:BCL:H162	1.83	0.42
9:e:102:SPN:HM73	9:D:102:SPN:HM41	2.01	0.42
1:D:6:LYS:HG2	1:D:9:LEU:HD12	2.00	0.42
5:L:134:VAL:HG23	5:L:143:TRP:CH2	2.54	0.42
3:f:34:VAL:HG12	8:F:101:BCL:HED1	2.00	0.42
5:L:131:THR:HG21	5:L:246:ALA:HB1	2.01	0.42
9:V:102:SPN:H152	9:V:102:SPN:H12	1.72	0.42
3:p:23:VAL:HG21	9:p:101:SPN:HM92	2.01	0.42
5:L:194:LEU:HD22	5:L:217:PHE:CE2	2.53	0.42
7:C:270:HIS:HD2	16:C:402:HEC:NB	2.18	0.42
1:V:35:LEU:HD11	8:v:101:BCL:HBC3	2.01	0.42
8:G:101:BCL:H141	8:G:101:BCL:H162	1.52	0.42
8:e:101:BCL:H143	8:e:101:BCL:H192	2.02	0.42
8:L:304:BCL:H61	8:L:304:BCL:H41	1.70	0.42
9:k:103:SPN:H231	9:j:102:SPN:HM41	2.01	0.42
8:f:101:BCL:CAD	8:F:101:BCL:HBD	2.49	0.42
9:b:102:SPN:HM71	9:b:102:SPN:H241	1.90	0.42
4:M:68:TRP:CD1	4:M:119:ALA:HB1	2.55	0.42
7:C:255:MET:HB3	16:C:402:HEC:C4B	2.50	0.42
9:p:102:SPN:HM73	9:p:102:SPN:H241	1.74	0.42
1:N:6:LYS:O	1:N:9:LEU:HG	2.20	0.42
3:e:13:THR:OG1	3:e:16:GLN:HG3	2.19	0.42
9:Q:102:SPN:HM81	9:Q:102:SPN:H281	1.82	0.42
9:r:101:SPN:HM73	9:r:101:SPN:H241	1.73	0.42
1:K:18:VAL:O	1:K:22:VAL:HG23	2.20	0.42
3:i:49:PHE:CZ	9:i:101:SPN:H61	2.55	0.42
9:b:102:SPN:H8	1:B:23:PHE:CZ	2.55	0.42
9:b:102:SPN:HM53	9:b:102:SPN:H151	1.91	0.42
1:B:48:ALA:HB2	1:A:40:HIS:HB2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:304:BCL:H91	8:L:304:BCL:H112	1.82	0.42
7:C:13:ASN:HD22	7:C:13:ASN:C	2.16	0.42
9:v:102:SPN:HM63	8:t:101:BCL:H52	2.01	0.42
9:v:102:SPN:HM83	9:v:102:SPN:H242	1.85	0.42
1:R:14:ARG:HD2	3:q:9:PHE:CG	2.54	0.42
3:g:20:LEU:HA	9:G:103:SPN:HM92	2.01	0.42
5:L:225:ILE:H	14:L:303:U10:H3M3	1.85	0.42
8:L:304:BCL:H172	8:L:304:BCL:H13	1.89	0.42
8:q:102:BCL:H52	8:q:102:BCL:H8	1.86	0.42
8:j:101:BCL:H112	8:j:101:BCL:H71	1.79	0.42
8:f:101:BCL:H161	8:f:101:BCL:H192	1.75	0.42
3:e:27:GLY:HA3	9:E:102:SPN:H22	2.01	0.42
8:e:101:BCL:CAD	8:E:101:BCL:HBD	2.49	0.42
8:d:101:BCL:H161	8:d:101:BCL:H141	1.82	0.42
9:b:102:SPN:H171	1:B:20:GLN:OE1	2.20	0.42
7:C:104:VAL:HG13	7:C:105:LEU:HG	2.02	0.42
7:C:130:LEU:HD23	7:C:130:LEU:HA	1.85	0.42
7:C:148:ASN:C	7:C:148:ASN:HD22	2.27	0.42
9:t:102:SPN:H202	8:T:101:BCL:HMA2	2.01	0.41
1:R:27:LEU:O	1:R:31:ILE:HG13	2.20	0.41
3:2:16:GLN:NE2	3:n:7:LEU:HB2	2.35	0.41
8:N:101:BCL:H111	8:N:101:BCL:H152	1.80	0.41
9:k:103:SPN:HM81	9:k:103:SPN:H281	1.89	0.41
8:e:101:BCL:H92	8:e:101:BCL:HAA1	2.02	0.41
9:D:103:SPN:H8	9:D:103:SPN:H111	1.57	0.41
8:L:304:BCL:HMB3	8:L:304:BCL:HHB	1.87	0.41
9:p:101:SPN:H201	9:p:101:SPN:H171	1.80	0.41
8:n:101:BCL:H52	8:n:101:BCL:H8	1.88	0.41
8:J:101:BCL:HBC3	8:J:101:BCL:H2C	1.82	0.41
3:d:19:GLU:O	3:d:23:VAL:HG23	2.21	0.41
7:C:117:LEU:HD21	7:C:121:ARG:CZ	2.51	0.41
7:C:220:TYR:O	7:C:296:GLN:NE2	2.38	0.41
6:H:100:PRO:HB3	6:H:109:VAL:HG21	2.02	0.41
8:t:101:BCL:H71	8:t:101:BCL:H112	1.86	0.41
8:2:101:BCL:HMB1	8:2:101:BCL:HHB	1.88	0.41
9:e:102:SPN:H4	9:e:102:SPN:H71	1.51	0.41
1:E:12:ASP:OD1	1:E:14:ARG:HG2	2.20	0.41
9:b:102:SPN:H8	1:B:23:PHE:HZ	1.85	0.41
4:M:133:ARG:NH2	5:L:219:ASP:O	2.53	0.41
9:t:102:SPN:H111	9:t:102:SPN:H8	1.80	0.41
3:d:42:THR:HG23	8:D:101:BCL:HBC3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:101:BCL:H192	8:A:101:BCL:H161	1.69	0.41
7:C:185:ARG:HE	7:C:187:ASP:CG	2.28	0.41
1:1:30:MET:O	1:1:34:VAL:HG23	2.19	0.41
1:S:30:MET:O	1:S:34:VAL:HG23	2.21	0.41
1:Q:42:ASN:HB3	1:Q:45:GLU:HB2	2.03	0.41
3:g:48:TRP:HZ2	8:G:101:BCL:H141	1.86	0.41
4:M:168:LEU:HD12	4:M:286:LEU:HD11	2.02	0.41
4:M:184:LEU:HD11	8:M:405:BCL:HED3	2.02	0.41
7:C:185:ARG:NE	7:C:187:ASP:OD2	2.54	0.41
3:r:28:LEU:HB2	9:R:102:SPN:HM63	2.02	0.41
9:n:102:SPN:HM43	1:N:27:LEU:HD22	2.02	0.41
8:k:102:BCL:HMD1	1:K:32:HIS:CD2	2.55	0.41
8:G:101:BCL:CAD	8:G:102:BCL:HBD	2.50	0.41
8:b:101:BCL:H8	8:b:101:BCL:H52	1.89	0.41
1:P:14:ARG:NH1	1:P:15:ARG:HD2	2.36	0.41
8:v:101:BCL:H141	8:v:101:BCL:H162	1.67	0.41
8:T:101:BCL:H161	8:T:101:BCL:H192	1.72	0.41
1:Q:6:LYS:HD2	9:R:102:SPN:HM93	2.02	0.41
1:Q:11:PHE:HB3	1:Q:16:VAL:HG21	2.02	0.41
3:f:40:LEU:O	3:f:44:ILE:HG12	2.21	0.41
1:F:11:PHE:HB3	1:F:16:VAL:HG21	2.02	0.41
9:b:102:SPN:HMB2	1:A:6:LYS:HB3	2.02	0.41
4:M:137:LEU:HD23	4:M:137:LEU:HA	1.94	0.41
3:t:9:PHE:HD1	1:T:10:ILE:HG22	1.85	0.41
3:r:23:VAL:HG23	9:R:102:SPN:H272	2.03	0.41
8:R:101:BCL:H41	8:R:101:BCL:H62	1.60	0.41
9:p:102:SPN:H281	9:p:102:SPN:HM83	1.86	0.41
9:F:102:SPN:HM43	9:F:102:SPN:H111	1.93	0.41
8:Q:101:BCL:H142	8:Q:101:BCL:H112	1.89	0.40
8:R:103:BCL:H61	8:R:103:BCL:H102	1.86	0.40
3:n:40:LEU:O	3:n:44:ILE:HG12	2.21	0.40
8:k:102:BCL:H92	8:k:102:BCL:HAA1	2.03	0.40
8:M:405:BCL:H152	8:M:405:BCL:H112	1.90	0.40
8:P:101:BCL:H151	8:P:101:BCL:H18	1.86	0.40
9:t:102:SPN:H281	9:t:102:SPN:HM93	1.78	0.40
9:r:101:SPN:HM82	9:r:101:SPN:H242	1.89	0.40
8:j:101:BCL:HBC3	8:j:101:BCL:H2C	1.82	0.40
8:i:102:BCL:H142	8:i:102:BCL:H112	1.81	0.40
9:G:103:SPN:HM92	9:G:103:SPN:H281	1.88	0.40
9:R:102:SPN:H112	9:R:102:SPN:HM42	1.78	0.40
3:p:25:MET:O	3:p:29:TRP:CD1	2.75	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:36:LEU:O	1:J:42:ASN:ND2	2.54	0.40
9:i:101:SPN:H8	9:i:101:SPN:H112	1.91	0.40
8:d:101:BCL:HBC2	8:d:101:BCL:H2C	1.64	0.40
13:L:302:BPH:HBC3	13:L:302:BPH:HHD	2.03	0.40
9:R:102:SPN:HM52	9:R:102:SPN:H152	1.94	0.40
9:p:101:SPN:HM81	9:p:101:SPN:H282	1.88	0.40
1:A:18:VAL:HG21	7:C:17:ILE:O	2.21	0.40
4:M:213:SER:OG	5:L:188:LEU:HD23	2.21	0.40
14:L:303:U10:H321	14:L:303:U10:H362	1.93	0.40
7:C:307:GLY:HA2	7:C:311:LEU:HG	2.04	0.40
9:V:102:SPN:HM92	3:v:20:LEU:HA	2.01	0.40
9:S:102:SPN:HM92	9:S:102:SPN:H281	1.78	0.40
8:R:103:BCL:HBC3	8:R:103:BCL:H2C	1.72	0.40
9:G:104:SPN:HM93	9:G:104:SPN:H282	1.88	0.40
8:b:101:BCL:H11	9:b:102:SPN:H111	2.03	0.40
4:M:217:PHE:CZ	5:L:234:GLY:HA3	2.57	0.40
6:H:78:ASP:OD1	6:H:78:ASP:N	2.46	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	1	48/53 (91%)	46 (96%)	2 (4%)	0	100	100
1	A	49/53 (92%)	49 (100%)	0	0	100	100
1	B	49/53 (92%)	49 (100%)	0	0	100	100
1	D	49/53 (92%)	48 (98%)	1 (2%)	0	100	100
1	E	49/53 (92%)	49 (100%)	0	0	100	100
1	F	49/53 (92%)	49 (100%)	0	0	100	100
1	G	49/53 (92%)	49 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	49/53 (92%)	49 (100%)	0	0	100	100
1	J	48/53 (91%)	48 (100%)	0	0	100	100
1	K	49/53 (92%)	49 (100%)	0	0	100	100
1	N	49/53 (92%)	48 (98%)	1 (2%)	0	100	100
1	P	49/53 (92%)	49 (100%)	0	0	100	100
1	Q	49/53 (92%)	48 (98%)	1 (2%)	0	100	100
1	R	49/53 (92%)	49 (100%)	0	0	100	100
1	S	49/53 (92%)	49 (100%)	0	0	100	100
1	T	49/53 (92%)	49 (100%)	0	0	100	100
1	V	49/53 (92%)	49 (100%)	0	0	100	100
2	O	50/239 (21%)	48 (96%)	2 (4%)	0	100	100
3	2	42/49 (86%)	42 (100%)	0	0	100	100
3	a	42/49 (86%)	41 (98%)	1 (2%)	0	100	100
3	b	42/49 (86%)	42 (100%)	0	0	100	100
3	d	42/49 (86%)	41 (98%)	1 (2%)	0	100	100
3	e	42/49 (86%)	42 (100%)	0	0	100	100
3	f	42/49 (86%)	42 (100%)	0	0	100	100
3	g	42/49 (86%)	42 (100%)	0	0	100	100
3	i	41/49 (84%)	41 (100%)	0	0	100	100
3	j	41/49 (84%)	41 (100%)	0	0	100	100
3	k	41/49 (84%)	41 (100%)	0	0	100	100
3	n	42/49 (86%)	41 (98%)	1 (2%)	0	100	100
3	p	42/49 (86%)	41 (98%)	1 (2%)	0	100	100
3	q	42/49 (86%)	42 (100%)	0	0	100	100
3	r	41/49 (84%)	41 (100%)	0	0	100	100
3	s	42/49 (86%)	42 (100%)	0	0	100	100
3	t	41/49 (84%)	41 (100%)	0	0	100	100
3	v	38/49 (78%)	38 (100%)	0	0	100	100
4	M	323/330 (98%)	313 (97%)	10 (3%)	0	100	100
5	L	272/279 (98%)	261 (96%)	11 (4%)	0	100	100
6	H	254/256 (99%)	246 (97%)	8 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	C	350/360 (97%)	337 (96%)	13 (4%)	0	100	100
All	All	2785/3198 (87%)	2732 (98%)	53 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	42/44 (96%)	42 (100%)	0	100	100
1	A	42/44 (96%)	42 (100%)	0	100	100
1	B	42/44 (96%)	42 (100%)	0	100	100
1	D	42/44 (96%)	42 (100%)	0	100	100
1	E	42/44 (96%)	42 (100%)	0	100	100
1	F	42/44 (96%)	42 (100%)	0	100	100
1	G	42/44 (96%)	42 (100%)	0	100	100
1	I	42/44 (96%)	42 (100%)	0	100	100
1	J	42/44 (96%)	42 (100%)	0	100	100
1	K	42/44 (96%)	42 (100%)	0	100	100
1	N	42/44 (96%)	42 (100%)	0	100	100
1	P	43/44 (98%)	43 (100%)	0	100	100
1	Q	42/44 (96%)	42 (100%)	0	100	100
1	R	42/44 (96%)	42 (100%)	0	100	100
1	S	42/44 (96%)	42 (100%)	0	100	100
1	T	42/44 (96%)	42 (100%)	0	100	100
1	V	42/44 (96%)	42 (100%)	0	100	100
2	O	39/174 (22%)	39 (100%)	0	100	100
3	2	36/41 (88%)	36 (100%)	0	100	100
3	a	37/41 (90%)	37 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	b	37/41 (90%)	37 (100%)	0	100	100
3	d	36/41 (88%)	36 (100%)	0	100	100
3	e	36/41 (88%)	36 (100%)	0	100	100
3	f	36/41 (88%)	36 (100%)	0	100	100
3	g	36/41 (88%)	36 (100%)	0	100	100
3	i	35/41 (85%)	35 (100%)	0	100	100
3	j	35/41 (85%)	35 (100%)	0	100	100
3	k	35/41 (85%)	35 (100%)	0	100	100
3	n	36/41 (88%)	36 (100%)	0	100	100
3	p	36/41 (88%)	36 (100%)	0	100	100
3	q	36/41 (88%)	36 (100%)	0	100	100
3	r	36/41 (88%)	36 (100%)	0	100	100
3	s	36/41 (88%)	36 (100%)	0	100	100
3	t	35/41 (85%)	35 (100%)	0	100	100
3	v	32/41 (78%)	32 (100%)	0	100	100
4	M	266/270 (98%)	266 (100%)	0	100	100
5	L	218/223 (98%)	218 (100%)	0	100	100
6	H	214/214 (100%)	214 (100%)	0	100	100
7	C	298/307 (97%)	297 (100%)	1 (0%)	86	95
All	All	2356/2633 (90%)	2355 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	C	13	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	S	42	ASN
1	S	50	ASN
3	2	16	GLN
1	K	32	HIS
1	K	50	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	42	ASN
1	F	42	ASN
3	e	16	GLN
1	E	42	ASN
3	d	21	HIS
1	B	42	ASN
4	M	5	GLN
4	M	39	GLN
4	M	75	ASN
4	M	260	ASN
5	L	56	GLN
5	L	265	ASN
6	H	34	ASN
6	H	67	HIS
6	H	92	HIS
6	H	218	ASN
7	C	13	ASN
7	C	50	GLN
7	C	143	ASN
7	C	148	ASN
7	C	176	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 100 ligands modelled in this entry, 1 is monoatomic - leaving 99 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
16	HEC	C	401	7	50,50,50	1.32	6 (12%)	68,82,82	1.18	4 (5%)
9	SPN	k	103	3	40,42,42	4.16	14 (35%)	50,52,52	4.61	25 (50%)
8	BCL	R	101	1	69,74,74	1.78	16 (23%)	83,115,115	2.12	27 (32%)
8	BCL	r	102	3	69,74,74	1.78	16 (23%)	83,115,115	2.16	29 (34%)
9	SPN	e	102	3	40,42,42	4.16	14 (35%)	50,52,52	4.64	25 (50%)
9	SPN	S	102	9,1	40,42,42	4.19	14 (35%)	50,52,52	4.63	24 (48%)
8	BCL	R	103	1	69,74,74	1.79	15 (21%)	83,115,115	2.13	28 (33%)
9	SPN	I	101	1	40,42,42	4.18	13 (32%)	50,52,52	4.66	25 (50%)
8	BCL	M	405	4	69,74,74	1.78	15 (21%)	83,115,115	2.11	28 (33%)
9	SPN	a	101	-	40,42,42	4.16	13 (32%)	50,52,52	4.64	25 (50%)
10	MW9	M	407	-	48,48,52	1.48	6 (12%)	51,54,58	1.51	3 (5%)
9	SPN	v	102	-	40,42,42	4.20	14 (35%)	50,52,52	4.59	25 (50%)
8	BCL	s	101	3	69,74,74	1.78	15 (21%)	83,115,115	2.15	28 (33%)
10	MW9	L	307	-	36,36,52	1.47	5 (13%)	39,42,58	1.54	3 (7%)
9	SPN	a	103	3	40,42,42	4.20	15 (37%)	50,52,52	4.52	25 (50%)
8	BCL	e	101	3	69,74,74	1.79	15 (21%)	83,115,115	2.14	27 (32%)
13	BPH	M	403	8,5	59,70,70	1.34	5 (8%)	61,101,101	0.92	5 (8%)
8	BCL	b	101	3	69,74,74	1.79	15 (21%)	83,115,115	2.15	29 (34%)
9	SPN	G	104	-	40,42,42	4.15	13 (32%)	50,52,52	4.69	25 (50%)
8	BCL	G	101	3,1	69,74,74	1.78	15 (21%)	83,115,115	2.14	28 (33%)
16	HEC	C	402	7	50,50,50	1.30	4 (8%)	68,82,82	1.26	7 (10%)
13	BPH	L	302	-	59,70,70	1.05	2 (3%)	61,101,101	0.90	4 (6%)
10	MW9	H	302	-	36,36,52	1.57	7 (19%)	39,41,58	1.86	3 (7%)
14	U10	L	303	-	48,48,63	0.18	0	58,61,79	0.45	1 (1%)
9	SPN	i	101	3	40,42,42	4.17	14 (35%)	50,52,52	4.70	25 (50%)
9	SPN	2	102	-	40,42,42	4.17	13 (32%)	50,52,52	4.65	25 (50%)
9	SPN	K	102	-	40,42,42	4.17	13 (32%)	50,52,52	4.67	25 (50%)
8	BCL	A	101	1	69,74,74	1.78	15 (21%)	83,115,115	2.14	28 (33%)
9	SPN	r	103	3	40,42,42	4.18	13 (32%)	50,52,52	4.61	25 (50%)
8	BCL	p	103	3	69,74,74	1.79	15 (21%)	83,115,115	2.17	27 (32%)
15	CDL	H	303	-	90,90,99	0.91	8 (8%)	96,102,111	1.13	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	BCL	K	101	-	69,74,74	1.79	16 (23%)	83,115,115	2.17	26 (31%)
9	SPN	t	102	3,9	40,42,42	4.18	14 (35%)	50,52,52	4.62	25 (50%)
8	BCL	N	101	1	69,74,74	1.79	16 (23%)	83,115,115	2.19	28 (33%)
11	LMT	H	301	-	24,24,36	1.03	2 (8%)	29,29,47	1.06	1 (3%)
9	SPN	k	101	3	40,42,42	4.17	13 (32%)	50,52,52	4.55	25 (50%)
9	SPN	j	102	-	40,42,42	4.17	13 (32%)	50,52,52	4.61	25 (50%)
10	MW9	F	103	1	42,42,52	1.43	6 (14%)	45,48,58	1.47	3 (6%)
9	SPN	Q	102	-	40,42,42	4.17	14 (35%)	50,52,52	4.65	25 (50%)
10	MW9	G	105	-	48,48,52	1.49	6 (12%)	51,54,58	1.48	4 (7%)
8	BCL	d	101	3	69,74,74	1.81	12 (17%)	83,115,115	2.17	26 (31%)
9	SPN	F	102	-	40,42,42	4.17	14 (35%)	50,52,52	4.58	25 (50%)
10	MW9	I	103	-	39,39,52	1.42	5 (12%)	42,45,58	1.18	3 (7%)
8	BCL	J	101	1	69,74,74	1.80	16 (23%)	83,115,115	2.19	28 (33%)
15	CDL	H	304	-	66,66,99	1.05	8 (12%)	72,78,111	1.15	4 (5%)
8	BCL	Q	101	1	69,74,74	1.79	16 (23%)	83,115,115	2.11	27 (32%)
9	SPN	b	102	3	40,42,42	4.20	15 (37%)	50,52,52	4.59	24 (48%)
8	BCL	T	101	1	69,74,74	1.78	15 (21%)	83,115,115	2.16	27 (32%)
10	MW9	B	102	-	52,52,52	1.45	6 (11%)	55,58,58	1.45	4 (7%)
9	SPN	R	102	-	40,42,42	4.18	14 (35%)	50,52,52	4.59	25 (50%)
8	BCL	q	102	3	69,74,74	1.78	16 (23%)	83,115,115	2.15	30 (36%)
8	BCL	i	102	3	69,74,74	1.80	15 (21%)	83,115,115	2.21	28 (33%)
8	BCL	L	301	8,5	69,74,74	1.76	16 (23%)	83,115,115	2.25	29 (34%)
16	HEC	C	403	7	50,50,50	1.32	6 (12%)	68,82,82	1.17	5 (7%)
8	BCL	a	102	3	69,74,74	1.78	15 (21%)	83,115,115	2.17	28 (33%)
8	BCL	E	101	1	69,74,74	1.79	16 (23%)	83,115,115	2.20	29 (34%)
8	BCL	F	101	1	69,74,74	1.79	16 (23%)	83,115,115	2.19	29 (34%)
8	BCL	v	101	3	69,74,74	1.77	17 (24%)	83,115,115	2.14	27 (32%)
9	SPN	a	104	3	40,42,42	4.17	13 (32%)	50,52,52	4.68	25 (50%)
9	SPN	2	103	3	40,42,42	4.17	13 (32%)	50,52,52	4.60	25 (50%)
14	U10	M	406	-	63,63,63	0.15	0	76,79,79	0.40	1 (1%)
8	BCL	f	101	3	69,74,74	1.79	16 (23%)	83,115,115	2.14	26 (31%)
9	SPN	r	101	-	40,42,42	4.16	14 (35%)	50,52,52	4.60	25 (50%)
9	SPN	G	103	-	40,42,42	4.17	13 (32%)	50,52,52	4.58	25 (50%)
9	SPN	D	102	-	40,42,42	4.18	14 (35%)	50,52,52	4.52	25 (50%)
8	BCL	M	402	4,13	69,74,74	1.78	15 (21%)	83,115,115	2.15	25 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	MW9	Q	103	-	44,44,52	1.47	5 (11%)	47,50,58	1.50	3 (6%)
9	SPN	V	102	-	40,42,42	4.19	13 (32%)	50,52,52	4.65	25 (50%)
10	MW9	L	308	-	35,35,52	1.24	3 (8%)	38,41,58	1.12	2 (5%)
8	BCL	j	101	3	69,74,74	1.79	15 (21%)	83,115,115	2.18	29 (34%)
11	LMT	C	404	-	24,24,36	1.02	2 (8%)	29,29,47	1.06	1 (3%)
9	SPN	M	404	-	40,42,42	4.15	13 (32%)	50,52,52	4.60	25 (50%)
9	SPN	D	103	-	40,42,42	4.18	14 (35%)	50,52,52	4.55	25 (50%)
9	SPN	E	102	-	40,42,42	4.17	14 (35%)	50,52,52	4.58	25 (50%)
9	SPN	S	101	1	40,42,42	4.21	15 (37%)	50,52,52	4.61	25 (50%)
11	LMT	L	305	-	24,24,36	1.04	2 (8%)	29,29,47	1.10	2 (6%)
9	SPN	f	102	-	40,42,42	4.15	13 (32%)	50,52,52	4.64	25 (50%)
9	SPN	i	103	-	40,42,42	4.15	14 (35%)	50,52,52	4.64	25 (50%)
11	LMT	L	306	-	24,24,36	1.04	2 (8%)	29,29,47	1.18	2 (6%)
8	BCL	2	101	3	69,74,74	1.79	16 (23%)	83,115,115	2.19	28 (33%)
8	BCL	1	101	1	69,74,74	1.79	16 (23%)	83,115,115	2.20	28 (33%)
10	MW9	D	104	-	26,26,52	1.41	4 (15%)	28,28,58	1.29	2 (7%)
10	MW9	M	408	-	52,52,52	1.45	6 (11%)	55,58,58	1.47	3 (5%)
11	LMT	E	103	-	36,36,36	1.15	5 (13%)	47,47,47	0.98	1 (2%)
9	SPN	p	102	3	40,42,42	4.17	13 (32%)	50,52,52	4.63	25 (50%)
8	BCL	V	101	8,1	69,74,74	1.77	14 (20%)	83,115,115	2.11	29 (34%)
8	BCL	L	304	8,5	69,74,74	1.76	15 (21%)	83,115,115	2.25	29 (34%)
8	BCL	n	101	3	69,74,74	1.78	15 (21%)	83,115,115	2.16	28 (33%)
8	BCL	B	101	1	69,74,74	1.78	16 (23%)	83,115,115	2.14	27 (32%)
8	BCL	t	101	3,8	69,74,74	1.82	14 (20%)	83,115,115	2.11	25 (30%)
9	SPN	p	101	3	40,42,42	4.19	13 (32%)	50,52,52	4.54	25 (50%)
8	BCL	I	102	1	69,74,74	1.81	16 (23%)	83,115,115	2.22	28 (33%)
9	SPN	n	102	-	40,42,42	4.16	14 (35%)	50,52,52	4.49	25 (50%)
8	BCL	D	101	1	69,74,74	1.79	16 (23%)	83,115,115	2.13	27 (32%)
8	BCL	P	101	1	69,74,74	1.79	16 (23%)	83,115,115	2.13	27 (32%)
8	BCL	G	102	1	69,74,74	1.80	16 (23%)	83,115,115	2.21	28 (33%)
8	BCL	k	102	3	69,74,74	1.78	15 (21%)	83,115,115	2.16	29 (34%)
9	SPN	q	101	3	40,42,42	4.16	13 (32%)	50,52,52	4.63	25 (50%)
10	MW9	F	104	-	47,47,52	1.39	6 (12%)	50,53,58	1.43	3 (6%)

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
16	HEC	C	401	7	1/1/3/7	3/14/54/54	-
9	SPN	k	103	3	-	33/50/51/51	-
8	BCL	R	101	1	-	9/41/137/137	-
8	BCL	r	102	3	-	11/41/137/137	-
9	SPN	e	102	3	-	30/50/51/51	-
9	SPN	S	102	9,1	-	30/50/51/51	-
8	BCL	R	103	1	-	9/41/137/137	-
9	SPN	I	101	1	-	27/50/51/51	-
8	BCL	M	405	4	-	13/41/137/137	-
9	SPN	a	101	-	-	25/50/51/51	-
10	MW9	M	407	-	-	27/53/53/57	-
9	SPN	v	102	-	-	28/50/51/51	-
8	BCL	s	101	3	-	17/41/137/137	-
10	MW9	L	307	-	-	21/41/41/57	-
9	SPN	a	103	3	-	30/50/51/51	-
8	BCL	e	101	3	-	10/41/137/137	-
13	BPH	M	403	8,5	-	14/37/105/105	0/5/6/6
8	BCL	b	101	3	-	9/41/137/137	-
9	SPN	G	104	-	-	26/50/51/51	-
8	BCL	G	101	3,1	-	16/41/137/137	-
16	HEC	C	402	7	1/1/3/7	3/14/54/54	-
13	BPH	L	302	-	-	10/37/105/105	0/5/6/6
10	MW9	H	302	-	-	24/38/38/57	-
14	U10	L	303	-	-	10/45/69/87	0/1/1/1
9	SPN	i	101	3	-	25/50/51/51	-
9	SPN	2	102	-	-	29/50/51/51	-
9	SPN	K	102	-	-	23/50/51/51	-
8	BCL	A	101	1	-	14/41/137/137	-
9	SPN	r	103	3	-	36/50/51/51	-
8	BCL	p	103	3	-	16/41/137/137	-
15	CDL	H	303	-	-	44/101/101/110	-
8	BCL	K	101	-	-	9/41/137/137	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	SPN	t	102	3,9	-	30/50/51/51	-
8	BCL	N	101	1	-	13/41/137/137	-
11	LMT	H	301	-	-	6/15/35/61	0/1/1/2
9	SPN	k	101	3	-	32/50/51/51	-
9	SPN	j	102	-	-	29/50/51/51	-
10	MW9	F	103	1	-	29/47/47/57	-
9	SPN	Q	102	-	-	29/50/51/51	-
10	MW9	G	105	-	-	26/53/53/57	-
8	BCL	d	101	3	-	19/41/137/137	-
9	SPN	F	102	-	-	26/50/51/51	-
10	MW9	I	103	-	-	31/44/44/57	-
8	BCL	J	101	1	-	10/41/137/137	-
15	CDL	H	304	-	-	43/77/77/110	-
8	BCL	Q	101	1	-	15/41/137/137	-
9	SPN	b	102	3	-	27/50/51/51	-
8	BCL	T	101	1	-	10/41/137/137	-
10	MW9	B	102	-	-	32/57/57/57	-
9	SPN	R	102	-	-	31/50/51/51	-
8	BCL	q	102	3	-	16/41/137/137	-
8	BCL	i	102	3	-	18/41/137/137	-
8	BCL	L	301	8,5	-	14/41/137/137	-
16	HEC	C	403	7	1/1/3/7	3/14/54/54	-
8	BCL	a	102	3	-	17/41/137/137	-
8	BCL	E	101	1	-	9/41/137/137	-
8	BCL	F	101	1	-	9/41/137/137	-
8	BCL	v	101	3	-	20/41/137/137	-
9	SPN	a	104	3	-	28/50/51/51	-
9	SPN	2	103	3	-	26/50/51/51	-
14	U10	M	406	-	-	8/63/87/87	0/1/1/1
8	BCL	f	101	3	-	17/41/137/137	-
9	SPN	r	101	-	-	27/50/51/51	-
9	SPN	G	103	-	-	29/50/51/51	-
9	SPN	D	102	-	-	27/50/51/51	-
8	BCL	M	402	4,13	-	17/41/137/137	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	MW9	Q	103	-	-	31/49/49/57	-
9	SPN	V	102	-	-	30/50/51/51	-
10	MW9	L	308	-	-	17/40/40/57	-
8	BCL	j	101	3	-	13/41/137/137	-
11	LMT	C	404	-	-	4/15/35/61	0/1/1/2
9	SPN	M	404	-	-	28/50/51/51	-
9	SPN	D	103	-	-	29/50/51/51	-
9	SPN	E	102	-	-	28/50/51/51	-
9	SPN	S	101	1	-	24/50/51/51	-
11	LMT	L	305	-	-	5/15/35/61	0/1/1/2
9	SPN	f	102	-	-	26/50/51/51	-
9	SPN	i	103	-	-	21/50/51/51	-
11	LMT	L	306	-	-	7/15/35/61	0/1/1/2
8	BCL	2	101	3	-	18/41/137/137	-
8	BCL	1	101	1	-	12/41/137/137	-
10	MW9	D	104	-	-	13/28/28/57	-
10	MW9	M	408	-	-	39/57/57/57	-
11	LMT	E	103	-	-	8/21/61/61	0/2/2/2
9	SPN	p	102	3	-	27/50/51/51	-
8	BCL	V	101	8,1	-	11/41/137/137	-
8	BCL	L	304	8,5	-	18/41/137/137	-
8	BCL	n	101	3	-	9/41/137/137	-
8	BCL	B	101	1	-	17/41/137/137	-
8	BCL	t	101	3,8	-	10/41/137/137	-
9	SPN	p	101	3	-	32/50/51/51	-
8	BCL	I	102	1	-	17/41/137/137	-
9	SPN	n	102	-	-	24/50/51/51	-
8	BCL	D	101	1	-	12/41/137/137	-
8	BCL	P	101	1	-	12/41/137/137	-
8	BCL	G	102	1	-	14/41/137/137	-
8	BCL	k	102	3	-	11/41/137/137	-
9	SPN	q	101	3	-	28/50/51/51	-
10	MW9	F	104	-	-	28/52/52/57	-

All (1178) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	q	101	SPN	C3-C4	-11.22	1.34	1.50
9	G	103	SPN	C3-C4	-11.18	1.34	1.50
9	p	101	SPN	C3-C4	-11.17	1.34	1.50
9	v	102	SPN	C3-C4	-11.11	1.34	1.50
9	S	102	SPN	C3-C4	-11.10	1.34	1.50
9	D	102	SPN	C3-C4	-11.08	1.34	1.50
9	p	102	SPN	C3-C4	-11.08	1.34	1.50
9	e	102	SPN	C3-C4	-11.08	1.34	1.50
9	R	102	SPN	C3-C4	-11.08	1.34	1.50
9	I	101	SPN	C3-C4	-11.08	1.34	1.50
9	E	102	SPN	C3-C4	-11.07	1.34	1.50
9	f	102	SPN	C3-C4	-11.07	1.34	1.50
9	j	102	SPN	C3-C4	-11.06	1.34	1.50
9	t	102	SPN	C3-C4	-11.05	1.34	1.50
9	2	103	SPN	C3-C4	-11.04	1.34	1.50
9	a	103	SPN	C3-C4	-11.04	1.34	1.50
9	a	104	SPN	C3-C4	-11.04	1.34	1.50
9	D	103	SPN	C3-C4	-11.03	1.34	1.50
9	k	101	SPN	C3-C4	-11.03	1.34	1.50
9	M	404	SPN	C3-C4	-11.03	1.34	1.50
9	2	102	SPN	C3-C4	-11.02	1.34	1.50
9	i	101	SPN	C3-C4	-11.02	1.34	1.50
9	r	103	SPN	C3-C4	-11.01	1.34	1.50
9	k	103	SPN	C3-C4	-11.01	1.34	1.50
9	r	101	SPN	C3-C4	-11.00	1.34	1.50
9	Q	102	SPN	C3-C4	-10.99	1.34	1.50
9	a	101	SPN	C3-C4	-10.98	1.34	1.50
9	b	102	SPN	C3-C4	-10.97	1.34	1.50
9	K	102	SPN	C3-C4	-10.96	1.34	1.50
9	F	102	SPN	C3-C4	-10.96	1.34	1.50
9	S	101	SPN	C3-C4	-10.95	1.34	1.50
9	V	102	SPN	C3-C4	-10.94	1.34	1.50
9	G	104	SPN	C3-C4	-10.94	1.34	1.50
9	n	102	SPN	C3-C4	-10.89	1.34	1.50
9	i	103	SPN	C3-C4	-10.85	1.35	1.50
9	i	101	SPN	C12-C13	9.34	1.55	1.33
9	I	101	SPN	C12-C13	9.29	1.55	1.33
9	a	103	SPN	C12-C13	9.28	1.55	1.33
9	S	101	SPN	C12-C13	9.26	1.55	1.33
9	F	102	SPN	C12-C13	9.25	1.55	1.33
9	b	102	SPN	C12-C13	9.25	1.55	1.33
9	S	102	SPN	C12-C13	9.23	1.55	1.33
9	a	104	SPN	C12-C13	9.22	1.55	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	103	SPN	C12-C13	9.19	1.55	1.33
9	E	102	SPN	C8-C9	9.19	1.55	1.33
9	V	102	SPN	C12-C13	9.19	1.55	1.33
9	R	102	SPN	C12-C13	9.19	1.55	1.33
9	j	102	SPN	C12-C13	9.19	1.55	1.33
9	k	101	SPN	C12-C13	9.19	1.55	1.33
9	E	102	SPN	C12-C13	9.18	1.55	1.33
9	r	103	SPN	C12-C13	9.18	1.55	1.33
9	a	103	SPN	C8-C9	9.17	1.55	1.33
9	D	102	SPN	C8-C9	9.16	1.55	1.33
9	k	103	SPN	C12-C13	9.16	1.54	1.33
9	n	102	SPN	C12-C13	9.16	1.54	1.33
9	2	103	SPN	C12-C13	9.15	1.54	1.33
9	t	102	SPN	C12-C13	9.15	1.54	1.33
9	b	102	SPN	C19-C18	9.15	1.54	1.33
9	p	102	SPN	C12-C13	9.15	1.54	1.33
9	D	102	SPN	C12-C13	9.15	1.54	1.33
9	e	102	SPN	C12-C13	9.14	1.54	1.33
9	Q	102	SPN	C8-C9	9.14	1.54	1.33
9	Q	102	SPN	C12-C13	9.14	1.54	1.33
9	G	103	SPN	C12-C13	9.13	1.54	1.33
9	2	103	SPN	C8-C9	9.12	1.54	1.33
9	K	102	SPN	C12-C13	9.12	1.54	1.33
9	V	102	SPN	C8-C9	9.12	1.54	1.33
9	S	101	SPN	C8-C9	9.12	1.54	1.33
9	v	102	SPN	C12-C13	9.12	1.54	1.33
9	p	101	SPN	C12-C13	9.12	1.54	1.33
9	t	102	SPN	C8-C9	9.11	1.54	1.33
9	2	102	SPN	C12-C13	9.11	1.54	1.33
9	a	104	SPN	C8-C9	9.11	1.54	1.33
9	M	404	SPN	C12-C13	9.11	1.54	1.33
9	q	101	SPN	C12-C13	9.10	1.54	1.33
9	a	101	SPN	C12-C13	9.10	1.54	1.33
9	r	101	SPN	C12-C13	9.09	1.54	1.33
9	j	102	SPN	C8-C9	9.09	1.54	1.33
9	f	102	SPN	C12-C13	9.08	1.54	1.33
9	K	102	SPN	C8-C9	9.08	1.54	1.33
9	r	103	SPN	C8-C9	9.07	1.54	1.33
9	p	101	SPN	C8-C9	9.06	1.54	1.33
9	p	101	SPN	C25-C26	9.06	1.54	1.33
9	D	103	SPN	C8-C9	9.06	1.54	1.33
9	F	102	SPN	C8-C9	9.06	1.54	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	v	102	SPN	C8-C9	9.06	1.54	1.33
9	2	102	SPN	C8-C9	9.06	1.54	1.33
9	S	102	SPN	C8-C9	9.06	1.54	1.33
9	r	101	SPN	C8-C9	9.06	1.54	1.33
9	G	104	SPN	C12-C13	9.06	1.54	1.33
9	R	102	SPN	C8-C9	9.05	1.54	1.33
9	M	404	SPN	C8-C9	9.05	1.54	1.33
9	e	102	SPN	C8-C9	9.05	1.54	1.33
9	V	102	SPN	C25-C26	9.05	1.54	1.33
9	i	101	SPN	C8-C9	9.04	1.54	1.33
9	k	101	SPN	C8-C9	9.04	1.54	1.33
9	a	101	SPN	C8-C9	9.04	1.54	1.33
9	b	102	SPN	C8-C9	9.04	1.54	1.33
9	R	102	SPN	C25-C26	9.04	1.54	1.33
9	G	103	SPN	C8-C9	9.03	1.54	1.33
9	a	104	SPN	C25-C26	9.03	1.54	1.33
9	n	102	SPN	C8-C9	9.03	1.54	1.33
9	i	103	SPN	C12-C13	9.03	1.54	1.33
9	I	101	SPN	C8-C9	9.03	1.54	1.33
9	i	103	SPN	C8-C9	9.02	1.54	1.33
9	S	101	SPN	C25-C26	9.02	1.54	1.33
9	G	104	SPN	C8-C9	9.01	1.54	1.33
9	p	102	SPN	C8-C9	9.01	1.54	1.33
9	v	102	SPN	C25-C26	8.99	1.54	1.33
9	K	102	SPN	C25-C26	8.97	1.54	1.33
9	k	103	SPN	C8-C9	8.97	1.54	1.33
9	q	101	SPN	C25-C26	8.96	1.54	1.33
9	2	102	SPN	C25-C26	8.96	1.54	1.33
9	f	102	SPN	C8-C9	8.95	1.54	1.33
9	M	404	SPN	C25-C26	8.93	1.54	1.33
9	j	102	SPN	C25-C26	8.93	1.54	1.33
9	q	101	SPN	C8-C9	8.93	1.54	1.33
9	I	101	SPN	C25-C26	8.92	1.54	1.33
9	a	103	SPN	C25-C26	8.92	1.54	1.33
9	t	102	SPN	C25-C26	8.91	1.54	1.33
9	S	102	SPN	C25-C26	8.91	1.54	1.33
9	k	101	SPN	C25-C26	8.90	1.54	1.33
9	p	102	SPN	C25-C26	8.89	1.54	1.33
9	G	103	SPN	C25-C26	8.89	1.54	1.33
9	r	103	SPN	C25-C26	8.89	1.54	1.33
9	E	102	SPN	C25-C26	8.89	1.54	1.33
9	D	102	SPN	C25-C26	8.89	1.54	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	103	SPN	C25-C26	8.88	1.54	1.33
9	b	102	SPN	C25-C26	8.88	1.54	1.33
9	n	102	SPN	C25-C26	8.87	1.54	1.33
9	a	101	SPN	C25-C26	8.87	1.54	1.33
9	F	102	SPN	C25-C26	8.87	1.54	1.33
9	i	103	SPN	C25-C26	8.87	1.54	1.33
9	f	102	SPN	C25-C26	8.86	1.54	1.33
9	i	103	SPN	C4-C5	8.86	1.54	1.33
9	Q	102	SPN	C25-C26	8.86	1.54	1.33
9	k	103	SPN	C25-C26	8.85	1.54	1.33
9	G	104	SPN	C25-C26	8.85	1.54	1.33
9	2	103	SPN	C25-C26	8.85	1.54	1.33
9	r	101	SPN	C25-C26	8.84	1.54	1.33
9	i	101	SPN	C25-C26	8.84	1.54	1.33
9	S	101	SPN	C4-C5	8.84	1.54	1.33
9	n	102	SPN	C4-C5	8.82	1.54	1.33
9	r	103	SPN	C4-C5	8.81	1.54	1.33
9	e	102	SPN	C25-C26	8.80	1.54	1.33
9	b	102	SPN	C4-C5	8.80	1.54	1.33
9	G	104	SPN	C4-C5	8.79	1.54	1.33
9	k	103	SPN	C4-C5	8.79	1.54	1.33
9	S	102	SPN	C4-C5	8.78	1.54	1.33
9	a	103	SPN	C4-C5	8.78	1.54	1.33
9	v	102	SPN	C4-C5	8.78	1.54	1.33
9	r	101	SPN	C4-C5	8.78	1.54	1.33
9	2	103	SPN	C4-C5	8.77	1.54	1.33
9	D	103	SPN	C4-C5	8.77	1.54	1.33
9	V	102	SPN	C4-C5	8.77	1.54	1.33
9	t	102	SPN	C4-C5	8.77	1.54	1.33
9	Q	102	SPN	C4-C5	8.76	1.54	1.33
9	k	101	SPN	C4-C5	8.76	1.54	1.33
9	E	102	SPN	C4-C5	8.76	1.54	1.33
9	I	101	SPN	C4-C5	8.75	1.54	1.33
9	e	102	SPN	C4-C5	8.75	1.54	1.33
9	f	102	SPN	C4-C5	8.75	1.54	1.33
9	p	102	SPN	C4-C5	8.74	1.53	1.33
9	a	101	SPN	C4-C5	8.73	1.53	1.33
9	F	102	SPN	C4-C5	8.73	1.53	1.33
9	K	102	SPN	C4-C5	8.73	1.53	1.33
9	2	102	SPN	C4-C5	8.73	1.53	1.33
9	D	102	SPN	C4-C5	8.72	1.53	1.33
9	R	102	SPN	C4-C5	8.72	1.53	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	i	101	SPN	C4-C5	8.72	1.53	1.33
9	M	404	SPN	C4-C5	8.71	1.53	1.33
9	j	102	SPN	C4-C5	8.71	1.53	1.33
9	p	101	SPN	C4-C5	8.70	1.53	1.33
9	a	104	SPN	C4-C5	8.66	1.53	1.33
9	q	101	SPN	C4-C5	8.64	1.53	1.33
9	G	103	SPN	C4-C5	8.64	1.53	1.33
9	S	101	SPN	C19-C18	8.64	1.53	1.33
9	v	102	SPN	C19-C18	8.63	1.53	1.33
9	V	102	SPN	C19-C18	8.60	1.53	1.33
9	r	103	SPN	C19-C18	8.55	1.53	1.33
9	a	103	SPN	C19-C18	8.55	1.53	1.33
9	F	102	SPN	C19-C18	8.55	1.53	1.33
9	t	102	SPN	C19-C18	8.54	1.53	1.33
9	p	102	SPN	C19-C18	8.54	1.53	1.33
9	D	103	SPN	C19-C18	8.53	1.53	1.33
9	p	101	SPN	C19-C18	8.53	1.53	1.33
9	Q	102	SPN	C19-C18	8.53	1.53	1.33
9	r	101	SPN	C19-C18	8.52	1.53	1.33
9	D	102	SPN	C19-C18	8.51	1.53	1.33
9	E	102	SPN	C19-C18	8.51	1.53	1.33
9	a	101	SPN	C19-C18	8.50	1.53	1.33
9	S	102	SPN	C19-C18	8.49	1.53	1.33
9	I	101	SPN	C19-C18	8.48	1.53	1.33
9	G	103	SPN	C19-C18	8.48	1.53	1.33
9	K	102	SPN	C19-C18	8.48	1.53	1.33
9	R	102	SPN	C19-C18	8.47	1.53	1.33
9	i	101	SPN	C19-C18	8.47	1.53	1.33
9	i	103	SPN	C19-C18	8.47	1.53	1.33
9	2	103	SPN	C19-C18	8.46	1.53	1.33
9	k	103	SPN	C19-C18	8.46	1.53	1.33
9	j	102	SPN	C19-C18	8.45	1.53	1.33
9	2	102	SPN	C19-C18	8.45	1.53	1.33
9	n	102	SPN	C19-C18	8.45	1.53	1.33
9	e	102	SPN	C19-C18	8.44	1.53	1.33
9	G	104	SPN	C19-C18	8.44	1.53	1.33
9	M	404	SPN	C19-C18	8.44	1.53	1.33
9	f	102	SPN	C19-C18	8.43	1.53	1.33
9	k	101	SPN	C19-C18	8.41	1.53	1.33
9	a	104	SPN	C19-C18	8.41	1.53	1.33
9	q	101	SPN	C19-C18	8.40	1.53	1.33
9	S	101	SPN	C29-C30	8.37	1.56	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	p	101	SPN	C29-C30	8.24	1.56	1.32
9	n	102	SPN	C29-C30	8.22	1.56	1.32
9	v	102	SPN	C29-C30	8.21	1.56	1.32
9	I	101	SPN	C29-C30	8.19	1.55	1.32
9	D	102	SPN	C29-C30	8.17	1.55	1.32
9	S	102	SPN	C29-C30	8.17	1.55	1.32
9	K	102	SPN	C29-C30	8.17	1.55	1.32
9	a	103	SPN	C29-C30	8.16	1.55	1.32
9	r	103	SPN	C29-C30	8.16	1.55	1.32
9	V	102	SPN	C29-C30	8.15	1.55	1.32
9	M	404	SPN	C29-C30	8.15	1.55	1.32
9	j	102	SPN	C29-C30	8.15	1.55	1.32
9	2	103	SPN	C29-C30	8.14	1.55	1.32
9	R	102	SPN	C29-C30	8.14	1.55	1.32
9	G	103	SPN	C29-C30	8.14	1.55	1.32
9	D	103	SPN	C29-C30	8.13	1.55	1.32
9	b	102	SPN	C29-C30	8.13	1.55	1.32
9	t	102	SPN	C29-C30	8.12	1.55	1.32
9	F	102	SPN	C29-C30	8.12	1.55	1.32
9	p	102	SPN	C29-C30	8.11	1.55	1.32
9	2	102	SPN	C29-C30	8.11	1.55	1.32
9	q	101	SPN	C29-C30	8.11	1.55	1.32
9	i	101	SPN	C29-C30	8.10	1.55	1.32
9	a	104	SPN	C29-C30	8.10	1.55	1.32
9	k	103	SPN	C29-C30	8.10	1.55	1.32
9	k	101	SPN	C29-C30	8.10	1.55	1.32
9	Q	102	SPN	C29-C30	8.09	1.55	1.32
9	i	103	SPN	C29-C30	8.08	1.55	1.32
9	r	101	SPN	C29-C30	8.07	1.55	1.32
9	G	104	SPN	C29-C30	8.07	1.55	1.32
9	f	102	SPN	C29-C30	8.06	1.55	1.32
9	a	101	SPN	C29-C30	8.06	1.55	1.32
9	E	102	SPN	C29-C30	8.04	1.55	1.32
9	e	102	SPN	C29-C30	8.03	1.55	1.32
13	M	403	BPH	C1D-C2D	6.22	1.46	1.39
13	L	302	BPH	C1D-C2D	6.12	1.46	1.39
8	t	101	BCL	MG-ND	-6.10	1.93	2.05
8	d	101	BCL	MG-ND	-6.03	1.93	2.05
13	M	403	BPH	C2C-C3C	5.87	1.60	1.54
8	I	102	BCL	MG-ND	-5.85	1.94	2.05
8	F	101	BCL	MG-ND	-5.83	1.94	2.05
8	j	101	BCL	MG-ND	-5.80	1.94	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	101	BCL	MG-ND	-5.79	1.94	2.05
8	G	102	BCL	MG-ND	-5.78	1.94	2.05
8	e	101	BCL	MG-ND	-5.78	1.94	2.05
8	E	101	BCL	MG-ND	-5.77	1.94	2.05
8	M	405	BCL	MG-ND	-5.76	1.94	2.05
8	i	102	BCL	MG-ND	-5.75	1.94	2.05
8	l	101	BCL	MG-ND	-5.74	1.94	2.05
8	T	101	BCL	MG-ND	-5.73	1.94	2.05
8	A	101	BCL	MG-ND	-5.73	1.94	2.05
8	D	101	BCL	MG-ND	-5.71	1.94	2.05
8	R	103	BCL	MG-ND	-5.70	1.94	2.05
8	Q	101	BCL	MG-ND	-5.70	1.94	2.05
8	b	101	BCL	MG-ND	-5.70	1.94	2.05
8	P	101	BCL	MG-ND	-5.69	1.94	2.05
8	r	102	BCL	MG-ND	-5.69	1.94	2.05
8	N	101	BCL	MG-ND	-5.69	1.94	2.05
8	p	103	BCL	MG-ND	-5.69	1.94	2.05
8	K	101	BCL	MG-ND	-5.68	1.94	2.05
8	q	102	BCL	MG-ND	-5.68	1.94	2.05
8	f	101	BCL	MG-ND	-5.68	1.94	2.05
8	a	102	BCL	MG-ND	-5.67	1.94	2.05
8	s	101	BCL	MG-ND	-5.65	1.94	2.05
8	k	102	BCL	MG-ND	-5.65	1.94	2.05
8	G	101	BCL	MG-ND	-5.64	1.94	2.05
8	B	101	BCL	MG-ND	-5.64	1.94	2.05
8	R	101	BCL	MG-ND	-5.64	1.94	2.05
8	V	101	BCL	MG-ND	-5.63	1.94	2.05
8	n	101	BCL	MG-ND	-5.62	1.94	2.05
8	2	101	BCL	MG-ND	-5.62	1.94	2.05
8	L	304	BCL	MG-ND	-5.60	1.94	2.05
8	M	402	BCL	MG-ND	-5.57	1.94	2.05
8	v	101	BCL	MG-ND	-5.57	1.94	2.05
8	L	301	BCL	MG-ND	-5.44	1.95	2.05
8	t	101	BCL	MG-NB	-4.97	1.95	2.05
8	d	101	BCL	MG-NB	-4.94	1.96	2.05
8	e	101	BCL	MG-NB	-4.84	1.96	2.05
8	Q	101	BCL	MG-NB	-4.81	1.96	2.05
8	R	103	BCL	MG-NB	-4.79	1.96	2.05
8	I	102	BCL	MG-NB	-4.78	1.96	2.05
8	i	102	BCL	MG-NB	-4.78	1.96	2.05
8	V	101	BCL	MG-NB	-4.78	1.96	2.05
8	D	101	BCL	MG-NB	-4.78	1.96	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	j	101	BCL	MG-NB	-4.77	1.96	2.05
8	t	101	BCL	OBD-CAD	4.74	1.30	1.22
8	F	101	BCL	MG-NB	-4.74	1.96	2.05
8	E	101	BCL	MG-NB	-4.73	1.96	2.05
8	b	101	BCL	MG-NB	-4.73	1.96	2.05
8	k	102	BCL	OBD-CAD	4.72	1.30	1.22
8	P	101	BCL	MG-NB	-4.72	1.96	2.05
8	1	101	BCL	MG-NB	-4.72	1.96	2.05
8	B	101	BCL	MG-NB	-4.72	1.96	2.05
8	v	101	BCL	OBD-CAD	4.71	1.30	1.22
8	a	102	BCL	MG-NB	-4.71	1.96	2.05
8	M	405	BCL	MG-NB	-4.71	1.96	2.05
8	N	101	BCL	MG-NB	-4.71	1.96	2.05
8	P	101	BCL	OBD-CAD	4.71	1.30	1.22
8	s	101	BCL	OBD-CAD	4.70	1.30	1.22
8	J	101	BCL	MG-NB	-4.70	1.96	2.05
8	R	101	BCL	MG-NB	-4.70	1.96	2.05
8	G	102	BCL	MG-NB	-4.70	1.96	2.05
8	K	101	BCL	MG-NB	-4.69	1.96	2.05
8	f	101	BCL	MG-NB	-4.69	1.96	2.05
8	p	103	BCL	OBD-CAD	4.69	1.30	1.22
8	G	101	BCL	MG-NB	-4.69	1.96	2.05
8	q	102	BCL	OBD-CAD	4.69	1.30	1.22
8	K	101	BCL	OBD-CAD	4.69	1.30	1.22
8	A	101	BCL	MG-NB	-4.68	1.96	2.05
8	r	102	BCL	MG-NB	-4.68	1.96	2.05
8	Q	101	BCL	OBD-CAD	4.67	1.30	1.22
8	R	101	BCL	OBD-CAD	4.67	1.30	1.22
8	F	101	BCL	OBD-CAD	4.67	1.30	1.22
8	i	102	BCL	OBD-CAD	4.67	1.30	1.22
8	2	101	BCL	MG-NB	-4.67	1.96	2.05
8	2	101	BCL	OBD-CAD	4.66	1.30	1.22
8	p	103	BCL	MG-NB	-4.66	1.96	2.05
8	n	101	BCL	MG-NB	-4.66	1.96	2.05
9	k	103	SPN	C7-C8	-4.66	1.35	1.50
8	t	101	BCL	C4D-ND	-4.66	1.31	1.37
9	q	101	SPN	C7-C8	-4.65	1.35	1.50
9	f	102	SPN	C7-C8	-4.65	1.35	1.50
8	k	102	BCL	MG-NB	-4.65	1.96	2.05
8	T	101	BCL	MG-NB	-4.65	1.96	2.05
8	L	301	BCL	OBD-CAD	4.65	1.30	1.22
8	J	101	BCL	OBD-CAD	4.65	1.30	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	101	BCL	OBD-CAD	4.65	1.30	1.22
8	q	102	BCL	MG-NB	-4.65	1.96	2.05
8	s	101	BCL	MG-NB	-4.65	1.96	2.05
8	n	101	BCL	OBD-CAD	4.65	1.30	1.22
8	I	102	BCL	OBD-CAD	4.65	1.30	1.22
8	a	102	BCL	OBD-CAD	4.64	1.30	1.22
8	N	101	BCL	OBD-CAD	4.64	1.30	1.22
8	B	101	BCL	OBD-CAD	4.64	1.30	1.22
9	i	103	SPN	C7-C8	-4.63	1.35	1.50
9	p	101	SPN	C7-C8	-4.63	1.35	1.50
8	R	103	BCL	OBD-CAD	4.63	1.30	1.22
8	M	402	BCL	OBD-CAD	4.63	1.30	1.22
9	D	103	SPN	C7-C8	-4.63	1.35	1.50
9	v	102	SPN	C7-C8	-4.63	1.35	1.50
8	G	102	BCL	OBD-CAD	4.63	1.30	1.22
8	V	101	BCL	OBD-CAD	4.63	1.30	1.22
8	T	101	BCL	OBD-CAD	4.63	1.30	1.22
8	r	102	BCL	OBD-CAD	4.63	1.30	1.22
8	d	101	BCL	OBD-CAD	4.62	1.30	1.22
8	f	101	BCL	OBD-CAD	4.62	1.30	1.22
9	G	104	SPN	C7-C8	-4.62	1.35	1.50
8	j	101	BCL	OBD-CAD	4.61	1.30	1.22
9	2	102	SPN	C7-C8	-4.61	1.35	1.50
9	G	103	SPN	C7-C8	-4.61	1.35	1.50
9	r	101	SPN	C7-C8	-4.61	1.35	1.50
8	b	101	BCL	OBD-CAD	4.61	1.30	1.22
9	a	101	SPN	C7-C8	-4.60	1.35	1.50
8	D	101	BCL	OBD-CAD	4.60	1.30	1.22
9	r	103	SPN	C7-C8	-4.60	1.35	1.50
8	l	101	BCL	OBD-CAD	4.60	1.30	1.22
8	E	101	BCL	OBD-CAD	4.59	1.30	1.22
9	V	102	SPN	C7-C8	-4.59	1.35	1.50
9	2	103	SPN	C20-C19	-4.58	1.35	1.50
9	i	101	SPN	C20-C19	-4.58	1.35	1.50
9	p	102	SPN	C7-C8	-4.58	1.35	1.50
9	e	102	SPN	C20-C19	-4.58	1.35	1.50
9	2	103	SPN	C7-C8	-4.57	1.35	1.50
8	e	101	BCL	OBD-CAD	4.57	1.30	1.22
9	t	102	SPN	C7-C8	-4.57	1.35	1.50
9	M	404	SPN	C7-C8	-4.57	1.35	1.50
9	Q	102	SPN	C7-C8	-4.57	1.35	1.50
9	k	101	SPN	C7-C8	-4.57	1.35	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	d	101	BCL	C4D-ND	-4.57	1.31	1.37
9	k	101	SPN	C20-C19	-4.57	1.35	1.50
9	R	102	SPN	C7-C8	-4.56	1.35	1.50
9	i	101	SPN	C7-C8	-4.56	1.35	1.50
9	I	101	SPN	C7-C8	-4.55	1.35	1.50
9	p	102	SPN	C20-C19	-4.55	1.35	1.50
8	v	101	BCL	MG-NB	-4.55	1.96	2.05
9	j	102	SPN	C7-C8	-4.55	1.35	1.50
9	K	102	SPN	C20-C19	-4.55	1.35	1.50
9	e	102	SPN	C7-C8	-4.55	1.35	1.50
9	b	102	SPN	C7-C8	-4.54	1.35	1.50
8	M	402	BCL	MG-NB	-4.54	1.96	2.05
9	p	101	SPN	C20-C19	-4.54	1.35	1.50
9	a	104	SPN	C20-C19	-4.54	1.35	1.50
9	D	102	SPN	C7-C8	-4.54	1.35	1.50
9	q	101	SPN	C20-C19	-4.53	1.35	1.50
9	M	404	SPN	C20-C19	-4.53	1.35	1.50
9	n	102	SPN	C20-C19	-4.53	1.35	1.50
9	S	102	SPN	C7-C8	-4.53	1.35	1.50
9	i	103	SPN	C20-C19	-4.53	1.35	1.50
9	Q	102	SPN	C20-C19	-4.53	1.35	1.50
9	F	102	SPN	C20-C19	-4.53	1.35	1.50
9	f	102	SPN	C20-C19	-4.53	1.35	1.50
9	n	102	SPN	C7-C8	-4.53	1.35	1.50
9	G	104	SPN	C20-C19	-4.53	1.35	1.50
8	E	101	BCL	C4D-ND	-4.52	1.31	1.37
9	a	103	SPN	C7-C8	-4.52	1.35	1.50
9	I	101	SPN	C20-C19	-4.52	1.35	1.50
9	F	102	SPN	C7-C8	-4.52	1.35	1.50
9	V	102	SPN	C20-C19	-4.52	1.35	1.50
8	L	304	BCL	MG-NB	-4.52	1.96	2.05
9	K	102	SPN	C7-C8	-4.52	1.35	1.50
9	D	103	SPN	C20-C19	-4.52	1.35	1.50
9	2	102	SPN	C20-C19	-4.51	1.35	1.50
9	r	101	SPN	C20-C19	-4.51	1.35	1.50
10	G	105	MW9	C35-C34	-4.51	1.34	1.52
8	M	405	BCL	OBD-CAD	4.51	1.30	1.22
9	E	102	SPN	C20-C19	-4.51	1.35	1.50
9	a	104	SPN	C7-C8	-4.51	1.35	1.50
9	v	102	SPN	C20-C19	-4.51	1.35	1.50
9	S	101	SPN	C7-C8	-4.51	1.35	1.50
8	G	101	BCL	OBD-CAD	4.51	1.30	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	G	103	SPN	C20-C19	-4.51	1.35	1.50
9	a	101	SPN	C20-C19	-4.50	1.35	1.50
9	r	103	SPN	C20-C19	-4.50	1.35	1.50
9	k	103	SPN	C20-C19	-4.50	1.35	1.50
10	M	408	MW9	C35-C34	-4.49	1.34	1.52
9	S	102	SPN	C20-C19	-4.49	1.35	1.50
10	M	407	MW9	C35-C34	-4.49	1.34	1.52
9	a	103	SPN	C20-C19	-4.49	1.35	1.50
8	L	301	BCL	MG-NB	-4.49	1.96	2.05
9	D	102	SPN	C20-C19	-4.49	1.35	1.50
9	j	102	SPN	C20-C19	-4.49	1.35	1.50
9	E	102	SPN	C7-C8	-4.48	1.35	1.50
10	B	102	MW9	C35-C34	-4.48	1.34	1.52
9	t	102	SPN	C20-C19	-4.48	1.35	1.50
8	L	304	BCL	OBD-CAD	4.48	1.30	1.22
10	Q	103	MW9	C35-C34	-4.46	1.34	1.52
9	R	102	SPN	C20-C19	-4.45	1.35	1.50
8	G	102	BCL	C4D-ND	-4.45	1.31	1.37
9	S	101	SPN	C20-C19	-4.45	1.35	1.50
8	b	101	BCL	C4D-ND	-4.43	1.31	1.37
8	i	102	BCL	C4D-ND	-4.43	1.31	1.37
8	F	101	BCL	C4D-ND	-4.42	1.31	1.37
8	I	102	BCL	C4D-ND	-4.41	1.31	1.37
8	M	402	BCL	C4D-ND	-4.41	1.31	1.37
8	J	101	BCL	C4D-ND	-4.38	1.31	1.37
8	M	405	BCL	C4D-ND	-4.37	1.31	1.37
8	n	101	BCL	C4D-ND	-4.36	1.31	1.37
8	e	101	BCL	C4D-ND	-4.36	1.31	1.37
8	v	101	BCL	C4D-ND	-4.35	1.31	1.37
8	D	101	BCL	C4D-ND	-4.32	1.31	1.37
8	V	101	BCL	C4D-ND	-4.32	1.31	1.37
8	j	101	BCL	C4D-ND	-4.31	1.31	1.37
8	R	103	BCL	C4D-ND	-4.30	1.31	1.37
8	K	101	BCL	C4D-ND	-4.30	1.31	1.37
8	a	102	BCL	C4D-ND	-4.30	1.31	1.37
8	2	101	BCL	C4D-ND	-4.29	1.31	1.37
8	N	101	BCL	C4D-ND	-4.29	1.31	1.37
8	B	101	BCL	C4D-ND	-4.28	1.31	1.37
8	f	101	BCL	C4D-ND	-4.28	1.31	1.37
8	s	101	BCL	C4D-ND	-4.28	1.31	1.37
8	p	103	BCL	C4D-ND	-4.27	1.31	1.37
8	Q	101	BCL	C4D-ND	-4.27	1.31	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	T	101	BCL	C4D-ND	-4.27	1.31	1.37
8	k	102	BCL	C4D-ND	-4.27	1.31	1.37
8	q	102	BCL	C4D-ND	-4.26	1.31	1.37
9	K	102	SPN	C11-C12	-4.26	1.36	1.50
8	R	101	BCL	C4D-ND	-4.25	1.31	1.37
9	i	103	SPN	C11-C12	-4.25	1.36	1.50
9	G	104	SPN	C11-C12	-4.25	1.36	1.50
9	q	101	SPN	C11-C12	-4.25	1.36	1.50
8	l	101	BCL	C4D-ND	-4.24	1.31	1.37
9	2	103	SPN	C11-C12	-4.23	1.36	1.50
8	r	102	BCL	C4D-ND	-4.23	1.31	1.37
9	f	102	SPN	C11-C12	-4.23	1.36	1.50
9	k	101	SPN	C11-C12	-4.22	1.36	1.50
9	a	101	SPN	C11-C12	-4.22	1.36	1.50
9	2	102	SPN	C11-C12	-4.22	1.36	1.50
9	e	102	SPN	C11-C12	-4.22	1.36	1.50
8	P	101	BCL	C4D-ND	-4.22	1.31	1.37
9	Q	102	SPN	C11-C12	-4.21	1.36	1.50
9	r	103	SPN	C11-C12	-4.21	1.36	1.50
9	G	103	SPN	C11-C12	-4.21	1.36	1.50
9	p	102	SPN	C11-C12	-4.21	1.36	1.50
9	k	103	SPN	C11-C12	-4.20	1.36	1.50
8	A	101	BCL	C4D-ND	-4.20	1.31	1.37
9	r	101	SPN	C11-C12	-4.19	1.36	1.50
9	p	101	SPN	C11-C12	-4.19	1.36	1.50
9	t	102	SPN	C11-C12	-4.18	1.36	1.50
9	M	404	SPN	C11-C12	-4.18	1.36	1.50
9	a	104	SPN	C11-C12	-4.18	1.36	1.50
9	D	103	SPN	C11-C12	-4.17	1.36	1.50
9	V	102	SPN	C11-C12	-4.17	1.36	1.50
9	v	102	SPN	C11-C12	-4.16	1.36	1.50
9	b	102	SPN	C20-C19	-4.16	1.36	1.50
9	S	102	SPN	C11-C12	-4.16	1.36	1.50
9	D	102	SPN	C11-C12	-4.16	1.36	1.50
8	L	304	BCL	C4D-ND	-4.15	1.32	1.37
9	R	102	SPN	C11-C12	-4.15	1.36	1.50
9	I	101	SPN	C11-C12	-4.14	1.36	1.50
9	n	102	SPN	C11-C12	-4.14	1.36	1.50
10	F	103	MW9	C33-C32	4.13	1.55	1.31
8	G	101	BCL	C4D-ND	-4.13	1.32	1.37
9	a	103	SPN	C11-C12	-4.13	1.37	1.50
9	E	102	SPN	C11-C12	-4.13	1.37	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	102	MW9	C33-C32	4.13	1.55	1.31
9	j	102	SPN	C11-C12	-4.12	1.37	1.50
10	Q	103	MW9	C33-C32	4.12	1.55	1.31
10	M	407	MW9	C33-C32	4.12	1.55	1.31
10	H	302	MW9	C33-C32	4.11	1.55	1.31
10	L	307	MW9	C33-C32	4.11	1.55	1.31
10	F	104	MW9	C33-C32	4.11	1.55	1.31
10	M	408	MW9	C33-C32	4.11	1.55	1.31
10	G	105	MW9	C33-C32	4.11	1.55	1.31
9	b	102	SPN	C11-C12	-4.11	1.37	1.50
9	i	101	SPN	C11-C12	-4.11	1.37	1.50
8	L	304	BCL	O1D-CGD	-4.10	1.10	1.21
9	F	102	SPN	C11-C12	-4.10	1.37	1.50
8	M	405	BCL	O1D-CGD	-4.08	1.11	1.21
8	l	101	BCL	O1D-CGD	-4.08	1.11	1.21
8	R	103	BCL	O1D-CGD	-4.08	1.11	1.21
9	S	101	SPN	C11-C12	-4.07	1.37	1.50
8	d	101	BCL	O1D-CGD	-4.07	1.11	1.21
8	R	101	BCL	O1D-CGD	-4.06	1.11	1.21
8	b	101	BCL	O1D-CGD	-4.06	1.11	1.21
8	e	101	BCL	O1D-CGD	-4.06	1.11	1.21
8	j	101	BCL	O1D-CGD	-4.06	1.11	1.21
8	n	101	BCL	O1D-CGD	-4.06	1.11	1.21
8	M	402	BCL	O1D-CGD	-4.05	1.11	1.21
8	f	101	BCL	O1D-CGD	-4.05	1.11	1.21
8	a	102	BCL	O1D-CGD	-4.05	1.11	1.21
8	K	101	BCL	O1D-CGD	-4.05	1.11	1.21
8	k	102	BCL	O1D-CGD	-4.04	1.11	1.21
8	I	102	BCL	O1D-CGD	-4.03	1.11	1.21
8	N	101	BCL	O1D-CGD	-4.03	1.11	1.21
8	L	301	BCL	O1D-CGD	-4.03	1.11	1.21
8	T	101	BCL	O1D-CGD	-4.03	1.11	1.21
8	2	101	BCL	O1D-CGD	-4.03	1.11	1.21
8	F	101	BCL	O1D-CGD	-4.02	1.11	1.21
8	P	101	BCL	O1D-CGD	-4.02	1.11	1.21
8	A	101	BCL	O1D-CGD	-4.02	1.11	1.21
8	p	103	BCL	O1D-CGD	-4.02	1.11	1.21
8	i	102	BCL	O1D-CGD	-4.02	1.11	1.21
8	E	101	BCL	O1D-CGD	-4.02	1.11	1.21
8	G	102	BCL	O1D-CGD	-4.02	1.11	1.21
8	q	102	BCL	O1D-CGD	-4.02	1.11	1.21
8	Q	101	BCL	O1D-CGD	-4.01	1.11	1.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	I	103	MW9	C33-C32	4.01	1.55	1.28
8	B	101	BCL	O1D-CGD	-4.01	1.11	1.21
8	J	101	BCL	O1D-CGD	-4.00	1.11	1.21
8	D	101	BCL	O1D-CGD	-4.00	1.11	1.21
8	L	301	BCL	C4D-ND	-3.99	1.32	1.37
8	v	101	BCL	O1D-CGD	-3.99	1.11	1.21
8	V	101	BCL	O1D-CGD	-3.99	1.11	1.21
8	s	101	BCL	O1D-CGD	-3.99	1.11	1.21
8	r	102	BCL	O1D-CGD	-3.97	1.11	1.21
8	G	101	BCL	O1D-CGD	-3.95	1.11	1.21
8	t	101	BCL	O1D-CGD	-3.95	1.11	1.21
8	G	101	BCL	O2D-CED	3.64	1.53	1.45
8	d	101	BCL	O2D-CED	3.47	1.53	1.45
8	p	103	BCL	O2D-CED	3.46	1.53	1.45
8	2	101	BCL	O2D-CED	3.46	1.53	1.45
8	N	101	BCL	O2D-CED	3.45	1.53	1.45
8	Q	101	BCL	O2D-CED	3.45	1.53	1.45
8	s	101	BCL	O2D-CED	3.44	1.53	1.45
8	I	102	BCL	O2D-CED	3.43	1.53	1.45
8	G	102	BCL	O2D-CED	3.43	1.53	1.45
8	A	101	BCL	O2D-CED	3.43	1.53	1.45
8	l	101	BCL	O2D-CED	3.43	1.53	1.45
8	j	101	BCL	O2D-CED	3.42	1.53	1.45
8	J	101	BCL	O2D-CED	3.42	1.53	1.45
8	i	102	BCL	O2D-CED	3.42	1.53	1.45
8	a	102	BCL	O2D-CED	3.42	1.53	1.45
8	F	101	BCL	O2D-CED	3.42	1.53	1.45
8	k	102	BCL	O2D-CED	3.42	1.53	1.45
8	t	101	BCL	O2D-CED	3.41	1.53	1.45
8	q	102	BCL	O2D-CED	3.41	1.53	1.45
8	r	102	BCL	O2D-CED	3.41	1.53	1.45
8	E	101	BCL	O2D-CED	3.40	1.53	1.45
8	R	103	BCL	O2D-CED	3.40	1.53	1.45
8	D	101	BCL	O2D-CED	3.39	1.53	1.45
8	M	402	BCL	O2D-CED	3.39	1.53	1.45
8	f	101	BCL	O2D-CED	3.39	1.53	1.45
8	R	101	BCL	O2D-CED	3.39	1.53	1.45
8	P	101	BCL	O2D-CED	3.38	1.53	1.45
8	b	101	BCL	O2D-CED	3.38	1.53	1.45
8	K	101	BCL	O2D-CED	3.38	1.53	1.45
8	L	301	BCL	O2D-CED	3.38	1.53	1.45
8	V	101	BCL	O2D-CED	3.37	1.53	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	n	101	BCL	O2D-CED	3.37	1.53	1.45
8	T	101	BCL	O2D-CED	3.36	1.53	1.45
8	v	101	BCL	O2D-CED	3.35	1.53	1.45
8	e	101	BCL	O2D-CED	3.35	1.53	1.45
8	B	101	BCL	O2D-CED	3.35	1.53	1.45
8	L	304	BCL	O2D-CED	3.35	1.53	1.45
16	C	401	HEC	CBC-CAC	-3.31	1.36	1.51
16	C	403	HEC	CBC-CAC	-3.30	1.36	1.51
16	C	402	HEC	CBC-CAC	-3.28	1.36	1.51
8	M	405	BCL	O2D-CED	3.18	1.52	1.45
10	M	407	MW9	C7-C6	-3.14	1.33	1.51
10	F	104	MW9	C7-C6	-3.13	1.34	1.51
10	M	408	MW9	C7-C6	-3.12	1.34	1.51
10	D	104	MW9	C7-C6	-3.12	1.34	1.51
10	B	102	MW9	C7-C6	-3.12	1.34	1.51
10	G	105	MW9	C7-C6	-3.09	1.34	1.51
8	1	101	BCL	O2A-CGA	-3.07	1.24	1.33
8	G	102	BCL	O2A-CGA	-3.06	1.24	1.33
10	M	408	MW9	O1-C17	3.06	1.42	1.33
8	D	101	BCL	O2A-CGA	-3.06	1.24	1.33
10	H	302	MW9	P-O5	3.05	1.66	1.54
10	L	307	MW9	O1-C17	3.05	1.42	1.33
8	M	402	BCL	O2A-CGA	-3.05	1.24	1.33
8	J	101	BCL	O2A-CGA	-3.04	1.24	1.33
8	L	304	BCL	O2A-CGA	-3.04	1.24	1.33
8	P	101	BCL	O2A-CGA	-3.03	1.24	1.33
8	B	101	BCL	O2A-CGA	-3.03	1.24	1.33
8	K	101	BCL	O2A-CGA	-3.03	1.24	1.33
8	I	102	BCL	O2D-CGD	-3.02	1.25	1.33
10	G	105	MW9	O1-C17	3.02	1.42	1.33
10	Q	103	MW9	O1-C17	3.02	1.42	1.33
8	I	102	BCL	O2A-CGA	-3.02	1.24	1.33
8	N	101	BCL	O2A-CGA	-3.02	1.24	1.33
8	2	101	BCL	O2D-CGD	-3.01	1.25	1.33
8	G	102	BCL	O2D-CGD	-3.01	1.25	1.33
8	q	102	BCL	O2A-CGA	-3.01	1.24	1.33
8	R	103	BCL	O2A-CGA	-3.00	1.24	1.33
8	M	405	BCL	O2D-CGD	-3.00	1.25	1.33
10	F	103	MW9	O1-C17	3.00	1.42	1.33
8	F	101	BCL	O2D-CGD	-3.00	1.25	1.33
10	D	104	MW9	O1-C17	3.00	1.42	1.33
8	t	101	BCL	O2A-CGA	-2.99	1.24	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	s	101	BCL	O2A-CGA	-2.99	1.24	1.33
8	i	102	BCL	O2D-CGD	-2.99	1.25	1.33
8	E	101	BCL	O2D-CGD	-2.99	1.25	1.33
8	2	101	BCL	O2A-CGA	-2.99	1.24	1.33
8	M	405	BCL	O2A-CGA	-2.99	1.24	1.33
8	Q	101	BCL	O2A-CGA	-2.99	1.24	1.33
8	i	102	BCL	O2A-CGA	-2.99	1.24	1.33
10	M	407	MW9	O1-C17	2.98	1.42	1.33
8	J	101	BCL	O2D-CGD	-2.98	1.25	1.33
8	d	101	BCL	O2A-CGA	-2.98	1.24	1.33
10	H	302	MW9	O1-C17	2.98	1.42	1.33
8	d	101	BCL	O2D-CGD	-2.98	1.25	1.33
8	f	101	BCL	O2A-CGA	-2.98	1.24	1.33
10	I	103	MW9	O1-C17	2.98	1.42	1.33
8	b	101	BCL	O2A-CGA	-2.98	1.24	1.33
10	L	308	MW9	O1-C17	2.97	1.42	1.33
8	L	301	BCL	O2A-CGA	-2.97	1.24	1.33
8	n	101	BCL	O2A-CGA	-2.97	1.24	1.33
8	r	102	BCL	O2A-CGA	-2.97	1.24	1.33
8	R	101	BCL	O2A-CGA	-2.97	1.24	1.33
8	a	102	BCL	O2A-CGA	-2.97	1.24	1.33
8	T	101	BCL	O2A-CGA	-2.96	1.24	1.33
8	V	101	BCL	O2A-CGA	-2.96	1.24	1.33
10	B	102	MW9	O1-C17	2.96	1.42	1.33
8	v	101	BCL	O2A-CGA	-2.96	1.24	1.33
8	E	101	BCL	O2A-CGA	-2.95	1.24	1.33
8	j	101	BCL	O2A-CGA	-2.95	1.24	1.33
8	v	101	BCL	O2D-CGD	-2.95	1.26	1.33
8	G	101	BCL	O2A-CGA	-2.95	1.24	1.33
8	k	102	BCL	O2A-CGA	-2.94	1.24	1.33
8	A	101	BCL	O2A-CGA	-2.94	1.24	1.33
8	e	101	BCL	O2A-CGA	-2.94	1.24	1.33
8	L	304	BCL	O2D-CGD	-2.93	1.26	1.33
8	n	101	BCL	O2D-CGD	-2.93	1.26	1.33
8	p	103	BCL	O2D-CGD	-2.93	1.26	1.33
8	D	101	BCL	O2D-CGD	-2.92	1.26	1.33
8	J	101	BCL	O1A-CGA	-2.92	1.13	1.22
8	N	101	BCL	O2D-CGD	-2.92	1.26	1.33
8	e	101	BCL	O2D-CGD	-2.92	1.26	1.33
8	Q	101	BCL	O2D-CGD	-2.92	1.26	1.33
8	F	101	BCL	O2A-CGA	-2.92	1.24	1.33
8	p	103	BCL	O2A-CGA	-2.91	1.24	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	K	101	BCL	O2D-CGD	-2.91	1.26	1.33
8	b	101	BCL	O2D-CGD	-2.91	1.26	1.33
8	B	101	BCL	O2D-CGD	-2.90	1.26	1.33
8	L	301	BCL	O2D-CGD	-2.90	1.26	1.33
8	P	101	BCL	O2D-CGD	-2.90	1.26	1.33
10	F	104	MW9	O1-C17	2.90	1.41	1.33
8	I	102	BCL	O1A-CGA	-2.90	1.13	1.22
8	j	101	BCL	O2D-CGD	-2.90	1.26	1.33
8	A	101	BCL	O2D-CGD	-2.89	1.26	1.33
8	D	101	BCL	O1A-CGA	-2.89	1.14	1.22
8	G	102	BCL	O1A-CGA	-2.89	1.14	1.22
8	R	103	BCL	O1A-CGA	-2.89	1.14	1.22
8	a	102	BCL	O2D-CGD	-2.88	1.26	1.33
8	M	402	BCL	O2D-CGD	-2.88	1.26	1.33
8	k	102	BCL	O2D-CGD	-2.88	1.26	1.33
8	T	101	BCL	O1A-CGA	-2.88	1.14	1.22
8	t	101	BCL	O2D-CGD	-2.88	1.26	1.33
8	V	101	BCL	O2D-CGD	-2.87	1.26	1.33
8	V	101	BCL	O1A-CGA	-2.87	1.14	1.22
8	L	304	BCL	O1A-CGA	-2.87	1.14	1.22
8	l	101	BCL	O2D-CGD	-2.87	1.26	1.33
9	G	104	SPN	C16-C15	-2.87	1.35	1.51
8	q	102	BCL	O2D-CGD	-2.87	1.26	1.33
8	B	101	BCL	O1A-CGA	-2.87	1.14	1.22
8	L	301	BCL	O1A-CGA	-2.87	1.14	1.22
8	T	101	BCL	O2D-CGD	-2.86	1.26	1.33
8	l	101	BCL	O1A-CGA	-2.86	1.14	1.22
9	i	101	SPN	C16-C15	-2.86	1.35	1.51
9	e	102	SPN	C16-C15	-2.86	1.35	1.51
8	f	101	BCL	O2D-CGD	-2.86	1.26	1.33
9	p	102	SPN	C16-C15	-2.86	1.35	1.51
8	R	101	BCL	O2D-CGD	-2.86	1.26	1.33
8	N	101	BCL	O1A-CGA	-2.85	1.14	1.22
8	q	102	BCL	O1A-CGA	-2.85	1.14	1.22
8	s	101	BCL	O2D-CGD	-2.85	1.26	1.33
8	R	103	BCL	O2D-CGD	-2.85	1.26	1.33
8	r	102	BCL	O2D-CGD	-2.84	1.26	1.33
9	k	101	SPN	C16-C15	-2.84	1.35	1.51
8	f	101	BCL	O1A-CGA	-2.84	1.14	1.22
8	k	102	BCL	O1A-CGA	-2.84	1.14	1.22
8	M	405	BCL	O1A-CGA	-2.83	1.14	1.22
8	G	101	BCL	O1A-CGA	-2.83	1.14	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	n	101	BCL	O1A-CGA	-2.83	1.14	1.22
8	R	101	BCL	O1A-CGA	-2.83	1.14	1.22
9	Q	102	SPN	C16-C15	-2.83	1.35	1.51
9	2	102	SPN	C16-C15	-2.83	1.35	1.51
9	K	102	SPN	C16-C15	-2.83	1.35	1.51
9	M	404	SPN	C16-C15	-2.83	1.35	1.51
8	a	102	BCL	O1A-CGA	-2.83	1.14	1.22
8	M	402	BCL	O1A-CGA	-2.83	1.14	1.22
9	i	103	SPN	C16-C15	-2.83	1.35	1.51
9	t	102	SPN	C16-C15	-2.82	1.35	1.51
9	a	104	SPN	C16-C15	-2.82	1.35	1.51
9	D	103	SPN	C16-C15	-2.82	1.35	1.51
9	k	103	SPN	C16-C15	-2.82	1.35	1.51
9	v	102	SPN	C16-C15	-2.82	1.35	1.51
9	2	103	SPN	C16-C15	-2.82	1.35	1.51
9	p	101	SPN	C16-C15	-2.82	1.35	1.51
8	2	101	BCL	O1A-CGA	-2.82	1.14	1.22
8	K	101	BCL	O1A-CGA	-2.82	1.14	1.22
8	A	101	BCL	O1A-CGA	-2.82	1.14	1.22
8	Q	101	BCL	O1A-CGA	-2.82	1.14	1.22
9	r	101	SPN	C16-C15	-2.82	1.35	1.51
8	i	102	BCL	O1A-CGA	-2.81	1.14	1.22
8	P	101	BCL	O1A-CGA	-2.81	1.14	1.22
8	e	101	BCL	O1A-CGA	-2.81	1.14	1.22
9	r	103	SPN	C16-C15	-2.81	1.35	1.51
8	v	101	BCL	O1A-CGA	-2.81	1.14	1.22
9	a	101	SPN	C16-C15	-2.81	1.35	1.51
8	d	101	BCL	O1A-CGA	-2.81	1.14	1.22
8	j	101	BCL	O1A-CGA	-2.81	1.14	1.22
9	V	102	SPN	C16-C15	-2.80	1.35	1.51
9	E	102	SPN	C16-C15	-2.80	1.35	1.51
9	q	101	SPN	C16-C15	-2.80	1.35	1.51
8	r	102	BCL	O1A-CGA	-2.80	1.14	1.22
9	G	103	SPN	C16-C15	-2.80	1.35	1.51
9	f	102	SPN	C16-C15	-2.80	1.35	1.51
8	d	101	BCL	C3B-CAB	2.80	1.55	1.46
9	n	102	SPN	C16-C15	-2.80	1.35	1.51
8	b	101	BCL	O1A-CGA	-2.80	1.14	1.22
8	p	103	BCL	O1A-CGA	-2.79	1.14	1.22
8	t	101	BCL	O1A-CGA	-2.79	1.14	1.22
9	a	103	SPN	C16-C15	-2.79	1.35	1.51
9	D	102	SPN	C16-C15	-2.78	1.36	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	s	101	BCL	O1A-CGA	-2.78	1.14	1.22
9	I	101	SPN	C16-C15	-2.78	1.36	1.51
9	R	102	SPN	C16-C15	-2.78	1.36	1.51
9	S	102	SPN	C16-C15	-2.78	1.36	1.51
9	j	102	SPN	C16-C15	-2.77	1.36	1.51
16	C	401	HEC	CAC-C3C	2.77	1.58	1.51
16	C	403	HEC	CAC-C3C	2.76	1.58	1.51
9	F	102	SPN	C16-C15	-2.76	1.36	1.51
11	L	305	LMT	O3'-C3'	-2.76	1.36	1.43
9	S	101	SPN	C16-C15	-2.76	1.36	1.51
10	B	102	MW9	O8-C24	2.75	1.42	1.34
8	G	101	BCL	O2D-CGD	-2.75	1.26	1.33
16	C	402	HEC	CAC-C3C	2.74	1.58	1.51
10	M	408	MW9	O8-C24	2.74	1.42	1.34
9	b	102	SPN	C16-C15	-2.72	1.36	1.51
10	D	104	MW9	O8-C24	2.71	1.41	1.34
10	L	308	MW9	O8-C24	2.70	1.41	1.34
10	G	105	MW9	O8-C24	2.70	1.41	1.34
10	I	103	MW9	O8-C24	2.69	1.41	1.34
10	Q	103	MW9	O8-C24	2.68	1.41	1.34
11	H	301	LMT	O3'-C3'	-2.67	1.36	1.43
10	L	307	MW9	O8-C24	2.66	1.41	1.34
10	H	302	MW9	O8-C24	2.65	1.41	1.34
10	F	103	MW9	O8-C24	2.63	1.41	1.34
11	L	306	LMT	O3'-C3'	-2.62	1.36	1.43
10	F	104	MW9	O8-C24	2.62	1.41	1.34
11	C	404	LMT	O3'-C3'	-2.62	1.36	1.43
10	M	407	MW9	O8-C24	2.61	1.41	1.34
10	F	104	MW9	O8-C19	-2.61	1.40	1.46
8	t	101	BCL	C3B-CAB	2.61	1.54	1.46
15	H	303	CDL	OB6-CB4	-2.61	1.40	1.46
11	E	103	LMT	O3'-C3'	-2.60	1.36	1.43
10	M	407	MW9	O8-C19	-2.59	1.40	1.46
10	F	103	MW9	O8-C19	-2.56	1.40	1.46
10	I	103	MW9	O8-C19	-2.56	1.40	1.46
10	D	104	MW9	O8-C19	-2.55	1.40	1.46
10	G	105	MW9	O8-C19	-2.54	1.40	1.46
8	v	101	BCL	C3B-CAB	2.54	1.54	1.46
8	n	101	BCL	OBB-CAB	-2.54	1.17	1.23
8	L	301	BCL	C3B-CAB	2.52	1.54	1.46
8	F	101	BCL	O1A-CGA	-2.52	1.15	1.22
10	B	102	MW9	O8-C19	-2.52	1.40	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	L	302	BPH	C3B-C2B	2.52	1.43	1.39
8	N	101	BCL	OBB-CAB	-2.52	1.17	1.23
8	q	102	BCL	OBB-CAB	-2.52	1.17	1.23
8	k	102	BCL	OBB-CAB	-2.51	1.17	1.23
8	E	101	BCL	O1A-CGA	-2.51	1.15	1.22
8	L	301	BCL	OBB-CAB	-2.51	1.17	1.23
8	i	102	BCL	OBB-CAB	-2.51	1.17	1.23
8	G	102	BCL	OBB-CAB	-2.51	1.17	1.23
8	L	304	BCL	OBB-CAB	-2.51	1.17	1.23
8	M	402	BCL	OBB-CAB	-2.51	1.17	1.23
10	H	302	MW9	O8-C19	-2.51	1.40	1.46
8	B	101	BCL	C3B-CAB	2.51	1.54	1.46
10	H	302	MW9	C6-C7	-2.51	1.33	1.51
8	r	102	BCL	OBB-CAB	-2.51	1.17	1.23
8	f	101	BCL	OBB-CAB	-2.50	1.17	1.23
8	R	103	BCL	C3B-CAB	2.50	1.54	1.46
8	I	102	BCL	C3B-CAB	2.50	1.54	1.46
8	J	101	BCL	OBB-CAB	-2.50	1.17	1.23
8	T	101	BCL	OBB-CAB	-2.50	1.17	1.23
8	G	101	BCL	OBB-CAB	-2.50	1.17	1.23
11	L	305	LMT	O2'-C2'	-2.50	1.37	1.43
10	Q	103	MW9	O8-C19	-2.50	1.40	1.46
8	M	402	BCL	C3B-CAB	2.50	1.54	1.46
8	P	101	BCL	C3B-CAB	2.50	1.54	1.46
8	G	102	BCL	C3B-CAB	2.50	1.54	1.46
8	Q	101	BCL	OBB-CAB	-2.50	1.17	1.23
8	R	101	BCL	OBB-CAB	-2.50	1.17	1.23
10	L	308	MW9	O8-C19	-2.49	1.40	1.46
8	K	101	BCL	OBB-CAB	-2.49	1.17	1.23
8	Q	101	BCL	C1D-C2D	-2.49	1.40	1.45
13	M	403	BPH	C3B-C4B	-2.49	1.37	1.41
8	P	101	BCL	OBB-CAB	-2.49	1.17	1.23
8	D	101	BCL	OBB-CAB	-2.49	1.17	1.23
8	I	102	BCL	OBB-CAB	-2.49	1.17	1.23
8	e	101	BCL	OBB-CAB	-2.49	1.17	1.23
8	R	101	BCL	C3B-CAB	2.49	1.54	1.46
8	M	405	BCL	OBB-CAB	-2.49	1.17	1.23
8	k	102	BCL	C3B-CAB	2.49	1.54	1.46
8	A	101	BCL	C3B-CAB	2.48	1.54	1.46
8	E	101	BCL	OBB-CAB	-2.48	1.17	1.23
8	L	304	BCL	C3B-CAB	2.48	1.54	1.46
8	d	101	BCL	C1D-C2D	-2.48	1.40	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	R	103	BCL	OBB-CAB	-2.48	1.17	1.23
10	M	408	MW9	O8-C19	-2.48	1.40	1.46
8	a	102	BCL	C3B-CAB	2.48	1.54	1.46
8	q	102	BCL	C3B-CAB	2.48	1.54	1.46
10	I	103	MW9	C6-C7	-2.48	1.34	1.51
8	s	101	BCL	C3B-CAB	2.48	1.54	1.46
8	r	102	BCL	C3B-CAB	2.48	1.54	1.46
8	s	101	BCL	OBB-CAB	-2.48	1.17	1.23
8	l	101	BCL	C3B-CAB	2.48	1.54	1.46
8	D	101	BCL	C1D-C2D	-2.48	1.40	1.45
8	p	103	BCL	OBB-CAB	-2.48	1.17	1.23
8	l	101	BCL	OBB-CAB	-2.48	1.17	1.23
10	F	103	MW9	C6-C7	-2.48	1.34	1.51
8	F	101	BCL	OBB-CAB	-2.48	1.17	1.23
8	2	101	BCL	OBB-CAB	-2.48	1.17	1.23
8	Q	101	BCL	C3B-CAB	2.47	1.54	1.46
8	N	101	BCL	C3B-CAB	2.47	1.54	1.46
8	2	101	BCL	C3B-CAB	2.47	1.54	1.46
8	G	101	BCL	C1D-C2D	-2.47	1.40	1.45
8	K	101	BCL	C3B-CAB	2.47	1.54	1.46
10	L	307	MW9	O8-C19	-2.47	1.40	1.46
8	p	103	BCL	C3B-CAB	2.47	1.54	1.46
8	J	101	BCL	C3B-CAB	2.47	1.54	1.46
8	M	405	BCL	C1B-C2B	-2.47	1.37	1.43
8	E	101	BCL	C3B-CAB	2.47	1.54	1.46
15	H	304	CDL	OB6-CB4	-2.46	1.40	1.46
8	B	101	BCL	OBB-CAB	-2.46	1.17	1.23
8	D	101	BCL	C3B-CAB	2.46	1.54	1.46
8	s	101	BCL	C1D-C2D	-2.46	1.40	1.45
8	T	101	BCL	C3B-CAB	2.46	1.54	1.46
8	v	101	BCL	OBB-CAB	-2.46	1.17	1.23
8	V	101	BCL	C3B-CAB	2.45	1.54	1.46
8	P	101	BCL	C1D-C2D	-2.45	1.40	1.45
8	K	101	BCL	C1D-C2D	-2.45	1.40	1.45
8	b	101	BCL	OBB-CAB	-2.45	1.17	1.23
11	E	103	LMT	O2'-C2'	-2.45	1.37	1.43
8	j	101	BCL	C3B-CAB	2.45	1.54	1.46
8	f	101	BCL	C3B-CAB	2.45	1.54	1.46
8	l	101	BCL	C1D-C2D	-2.44	1.40	1.45
8	B	101	BCL	C1D-C2D	-2.44	1.40	1.45
8	n	101	BCL	C3B-CAB	2.44	1.54	1.46
8	a	102	BCL	OBB-CAB	-2.44	1.17	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	p	103	BCL	C1B-C2B	-2.44	1.37	1.43
8	j	101	BCL	OBB-CAB	-2.43	1.17	1.23
8	A	101	BCL	OBB-CAB	-2.43	1.17	1.23
8	F	101	BCL	C3B-CAB	2.43	1.54	1.46
8	L	301	BCL	C1D-C2D	-2.43	1.40	1.45
8	k	102	BCL	C1D-C2D	-2.43	1.40	1.45
15	H	304	CDL	OA8-CA7	2.42	1.40	1.33
8	i	102	BCL	C3B-CAB	2.42	1.54	1.46
8	i	102	BCL	C1D-C2D	-2.41	1.40	1.45
8	V	101	BCL	OBB-CAB	-2.41	1.17	1.23
10	F	104	MW9	C35-C34	-2.41	1.34	1.51
10	L	307	MW9	C35-C34	-2.40	1.34	1.51
8	M	405	BCL	C3B-CAB	2.40	1.54	1.46
16	C	403	HEC	CBB-CAB	-2.40	1.40	1.51
8	t	101	BCL	OBB-CAB	-2.40	1.17	1.23
10	F	103	MW9	C35-C34	-2.40	1.34	1.51
8	i	102	BCL	C1B-C2B	-2.40	1.37	1.43
8	G	101	BCL	C3B-CAB	2.39	1.54	1.46
16	C	402	HEC	CBB-CAB	-2.39	1.40	1.51
8	K	101	BCL	C1B-C2B	-2.39	1.37	1.43
15	H	304	CDL	OB8-CB7	2.39	1.40	1.33
16	C	401	HEC	CBB-CAB	-2.39	1.40	1.51
8	R	101	BCL	C1D-C2D	-2.38	1.40	1.45
11	E	103	LMT	O2B-C2B	-2.38	1.37	1.43
8	r	102	BCL	C1B-C2B	-2.38	1.37	1.43
8	A	101	BCL	C1B-C2B	-2.38	1.37	1.43
8	f	101	BCL	C1D-C2D	-2.38	1.40	1.45
8	T	101	BCL	C1D-C2D	-2.38	1.40	1.45
8	b	101	BCL	C3B-CAB	2.37	1.54	1.46
8	J	101	BCL	C1D-C2D	-2.37	1.40	1.45
8	N	101	BCL	C1B-C2B	-2.37	1.37	1.43
8	A	101	BCL	C1D-C2D	-2.37	1.40	1.45
8	e	101	BCL	C3B-CAB	2.36	1.54	1.46
8	I	102	BCL	C1B-C2B	-2.36	1.37	1.43
8	R	103	BCL	C1D-C2D	-2.36	1.40	1.45
8	j	101	BCL	C1B-C2B	-2.36	1.37	1.43
8	r	102	BCL	C1D-C2D	-2.35	1.40	1.45
8	G	102	BCL	C1B-C2B	-2.35	1.37	1.43
8	j	101	BCL	C1D-C2D	-2.35	1.40	1.45
8	2	101	BCL	C1B-C2B	-2.34	1.37	1.43
8	2	101	BCL	C1D-C2D	-2.34	1.40	1.45
8	M	402	BCL	C1D-C2D	-2.34	1.40	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	n	101	BCL	C1D-C2D	-2.34	1.40	1.45
8	L	304	BCL	C1D-C2D	-2.34	1.40	1.45
8	N	101	BCL	C1D-C2D	-2.34	1.40	1.45
8	L	304	BCL	C1B-C2B	-2.34	1.37	1.43
8	b	101	BCL	C1B-C2B	-2.33	1.37	1.43
11	E	103	LMT	O3B-C3B	-2.33	1.37	1.43
8	I	102	BCL	C1D-C2D	-2.33	1.40	1.45
11	H	301	LMT	O2'-C2'	-2.33	1.37	1.43
15	H	303	CDL	OA8-CA7	2.33	1.40	1.33
15	H	303	CDL	OB8-CB7	2.33	1.40	1.33
8	q	102	BCL	C1B-C2B	-2.33	1.37	1.43
8	q	102	BCL	C1D-C2D	-2.32	1.40	1.45
8	a	102	BCL	C1D-C2D	-2.32	1.40	1.45
8	v	101	BCL	C1D-C2D	-2.32	1.40	1.45
8	e	101	BCL	C1D-C2D	-2.32	1.40	1.45
15	H	303	CDL	OA6-CA4	-2.32	1.40	1.46
8	b	101	BCL	C1D-C2D	-2.32	1.40	1.45
8	F	101	BCL	C1B-C2B	-2.31	1.37	1.43
8	V	101	BCL	C1D-C2D	-2.31	1.40	1.45
8	e	101	BCL	C1B-C2B	-2.31	1.37	1.43
8	F	101	BCL	C1D-C2D	-2.31	1.40	1.45
8	J	101	BCL	C1B-C2B	-2.31	1.37	1.43
8	a	102	BCL	C1B-C2B	-2.31	1.37	1.43
8	E	101	BCL	C1D-C2D	-2.31	1.40	1.45
8	n	101	BCL	C1B-C2B	-2.30	1.37	1.43
8	E	101	BCL	C1B-C2B	-2.30	1.37	1.43
16	C	401	HEC	CAB-C3B	2.30	1.57	1.51
8	p	103	BCL	C1D-C2D	-2.30	1.40	1.45
8	T	101	BCL	C1B-C2B	-2.30	1.37	1.43
8	l	101	BCL	C1B-C2B	-2.30	1.37	1.43
8	s	101	BCL	C1B-C2B	-2.29	1.37	1.43
11	C	404	LMT	O2'-C2'	-2.29	1.37	1.43
11	L	306	LMT	O2'-C2'	-2.29	1.37	1.43
10	H	302	MW9	C35-C34	-2.28	1.34	1.49
8	R	101	BCL	C1B-C2B	-2.28	1.37	1.43
8	L	301	BCL	C1B-C2B	-2.28	1.37	1.43
8	G	102	BCL	C1D-C2D	-2.27	1.40	1.45
15	H	304	CDL	OA6-CA4	-2.27	1.40	1.46
15	H	304	CDL	OA6-CA5	2.27	1.40	1.34
8	M	405	BCL	C1D-C2D	-2.27	1.40	1.45
8	F	101	BCL	C3D-C4D	-2.27	1.39	1.44
8	P	101	BCL	C1B-C2B	-2.26	1.37	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	G	101	BCL	C1B-C2B	-2.26	1.37	1.43
8	R	103	BCL	C1B-C2B	-2.26	1.37	1.43
15	H	303	CDL	OB8-CB6	-2.26	1.40	1.45
8	M	402	BCL	C1B-C2B	-2.25	1.37	1.43
16	C	403	HEC	CAB-C3B	2.25	1.56	1.51
8	D	101	BCL	C1B-C2B	-2.25	1.38	1.43
15	H	303	CDL	OA6-CA5	2.25	1.40	1.34
8	d	101	BCL	C3D-C4D	-2.25	1.39	1.44
8	G	101	BCL	C3D-C4D	-2.25	1.39	1.44
8	j	101	BCL	C3D-C4D	-2.24	1.39	1.44
9	b	102	SPN	C17-C18	2.24	1.56	1.51
9	S	101	SPN	C24-C25	2.24	1.57	1.50
8	B	101	BCL	C1B-C2B	-2.24	1.38	1.43
8	n	101	BCL	C3B-C2B	-2.24	1.35	1.42
8	Q	101	BCL	C1B-C2B	-2.24	1.38	1.43
8	f	101	BCL	C1B-C2B	-2.24	1.38	1.43
8	e	101	BCL	C3D-C4D	-2.24	1.39	1.44
8	A	101	BCL	C3B-C2B	-2.23	1.35	1.42
9	i	101	SPN	C1-C2	2.23	1.55	1.53
8	k	102	BCL	C1B-C2B	-2.22	1.38	1.43
8	p	103	BCL	C3B-C2B	-2.22	1.35	1.42
9	q	101	SPN	C24-C25	2.22	1.57	1.50
8	I	102	BCL	C3D-C4D	-2.22	1.39	1.44
8	i	102	BCL	C3D-C4D	-2.22	1.39	1.44
8	r	102	BCL	C3B-C2B	-2.22	1.35	1.42
8	v	101	BCL	C1B-C2B	-2.22	1.38	1.43
9	p	101	SPN	C24-C25	2.21	1.57	1.50
8	t	101	BCL	C3D-C4D	-2.21	1.39	1.44
8	J	101	BCL	C3D-C4D	-2.21	1.39	1.44
8	t	101	BCL	C3B-C2B	-2.21	1.35	1.42
8	2	101	BCL	C3D-C4D	-2.21	1.39	1.44
13	M	403	BPH	C3B-C2B	2.21	1.43	1.39
8	a	102	BCL	C3D-C4D	-2.20	1.39	1.44
8	E	101	BCL	C3D-C4D	-2.20	1.39	1.44
8	l	101	BCL	C3D-C4D	-2.20	1.39	1.44
8	n	101	BCL	C3D-C4D	-2.20	1.39	1.44
8	r	102	BCL	C3D-C4D	-2.20	1.39	1.44
8	M	405	BCL	C3D-C4D	-2.20	1.39	1.44
8	t	101	BCL	C1D-C2D	-2.20	1.41	1.45
8	f	101	BCL	C3D-C4D	-2.19	1.39	1.44
8	G	102	BCL	C3D-C4D	-2.19	1.39	1.44
8	b	101	BCL	C3D-C4D	-2.19	1.39	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	101	BCL	C3D-C4D	-2.18	1.39	1.44
9	V	102	SPN	C24-C25	2.18	1.57	1.50
9	r	101	SPN	C1-C2	2.18	1.55	1.53
8	L	301	BCL	C3D-C2D	-2.17	1.33	1.39
8	R	103	BCL	C3D-C4D	-2.17	1.39	1.44
8	k	102	BCL	C3D-C4D	-2.17	1.39	1.44
15	H	304	CDL	OB6-CB5	2.17	1.40	1.34
8	s	101	BCL	C3D-C4D	-2.17	1.39	1.44
9	v	102	SPN	C24-C25	2.17	1.57	1.50
15	H	303	CDL	OA8-CA6	-2.17	1.40	1.45
9	S	101	SPN	C17-C18	2.17	1.55	1.51
8	p	103	BCL	C3D-C4D	-2.16	1.39	1.44
9	Q	102	SPN	C24-C25	2.16	1.57	1.50
9	F	102	SPN	C17-C18	2.16	1.55	1.51
8	A	101	BCL	C3D-C4D	-2.15	1.39	1.44
9	Q	102	SPN	C1-C2	2.15	1.55	1.53
8	M	402	BCL	C3D-C4D	-2.15	1.39	1.44
9	r	103	SPN	C24-C25	2.15	1.57	1.50
8	N	101	BCL	C3D-C4D	-2.15	1.39	1.44
9	D	102	SPN	C24-C25	2.14	1.57	1.50
9	a	104	SPN	C24-C25	2.14	1.57	1.50
9	p	102	SPN	C24-C25	2.14	1.57	1.50
8	P	101	BCL	C3D-C4D	-2.14	1.39	1.44
9	G	103	SPN	C24-C25	2.14	1.57	1.50
8	Q	101	BCL	C3D-C4D	-2.14	1.39	1.44
9	k	103	SPN	C1-C2	2.14	1.55	1.53
8	q	102	BCL	C3D-C4D	-2.13	1.39	1.44
9	M	404	SPN	C24-C25	2.13	1.57	1.50
8	N	101	BCL	C3D-C2D	-2.13	1.33	1.39
9	2	103	SPN	C24-C25	2.13	1.57	1.50
16	C	403	HEC	CMD-C2D	2.13	1.55	1.50
15	H	304	CDL	OB8-CB6	-2.13	1.40	1.45
8	B	101	BCL	C3D-C4D	-2.13	1.39	1.44
9	t	102	SPN	C24-C25	2.13	1.57	1.50
8	v	101	BCL	C3D-C4D	-2.13	1.39	1.44
9	R	102	SPN	C24-C25	2.13	1.57	1.50
9	r	101	SPN	C24-C25	2.12	1.57	1.50
9	K	102	SPN	C24-C25	2.12	1.57	1.50
8	f	101	BCL	C5-C3	2.12	1.55	1.51
8	R	101	BCL	C3D-C4D	-2.12	1.39	1.44
8	T	101	BCL	C3D-C4D	-2.12	1.39	1.44
8	L	304	BCL	C3D-C4D	-2.12	1.39	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	F	102	SPN	C24-C25	2.12	1.57	1.50
9	2	102	SPN	C24-C25	2.11	1.57	1.50
16	C	401	HEC	CMD-C2D	2.11	1.55	1.50
9	D	103	SPN	C24-C25	2.11	1.57	1.50
9	a	103	SPN	C24-C25	2.11	1.57	1.50
9	j	102	SPN	C15-C14	2.11	1.60	1.52
8	V	101	BCL	C3D-C4D	-2.11	1.39	1.44
9	j	102	SPN	C24-C25	2.11	1.57	1.50
9	v	102	SPN	C1-C2	2.11	1.55	1.53
9	f	102	SPN	C17-C18	2.10	1.55	1.51
9	b	102	SPN	C24-C25	2.10	1.57	1.50
8	K	101	BCL	C3B-C2B	-2.10	1.35	1.42
16	C	402	HEC	CAB-C3B	2.10	1.56	1.51
8	P	101	BCL	C3D-C2D	-2.10	1.33	1.39
8	b	101	BCL	C3B-C2B	-2.10	1.35	1.42
9	I	101	SPN	C24-C25	2.09	1.57	1.50
16	C	401	HEC	CMB-C2B	2.09	1.55	1.50
9	n	102	SPN	C24-C25	2.09	1.57	1.50
15	H	304	CDL	OA8-CA6	-2.09	1.40	1.45
8	L	304	BCL	C3B-C2B	-2.09	1.35	1.42
9	S	102	SPN	C24-C25	2.09	1.57	1.50
8	G	102	BCL	C3D-C2D	-2.09	1.33	1.39
9	a	101	SPN	C15-C14	2.09	1.59	1.52
9	M	404	SPN	C15-C14	2.08	1.59	1.52
8	M	402	BCL	C3B-C2B	-2.08	1.35	1.42
8	Q	101	BCL	C3D-C2D	-2.08	1.33	1.39
9	a	101	SPN	C24-C25	2.08	1.57	1.50
8	L	301	BCL	C3B-C2B	-2.08	1.35	1.42
8	2	101	BCL	C3B-C2B	-2.08	1.35	1.42
8	D	101	BCL	C3D-C2D	-2.08	1.33	1.39
8	L	301	BCL	C3D-C4D	-2.08	1.39	1.44
8	1	101	BCL	C3D-C2D	-2.07	1.33	1.39
9	k	101	SPN	C24-C25	2.07	1.57	1.50
9	k	103	SPN	C24-C25	2.07	1.57	1.50
9	R	102	SPN	C17-C18	2.07	1.55	1.51
11	E	103	LMT	O4'-C4B	-2.07	1.38	1.43
9	f	102	SPN	C24-C25	2.07	1.57	1.50
8	F	101	BCL	C3B-C2B	-2.07	1.35	1.42
8	E	101	BCL	C3B-C2B	-2.07	1.35	1.42
9	S	101	SPN	C1-C2	2.07	1.55	1.53
8	R	103	BCL	C3B-C2B	-2.07	1.35	1.42
9	I	101	SPN	C15-C14	2.07	1.59	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	t	102	SPN	C1-C2	2.07	1.55	1.53
8	a	102	BCL	C3B-C2B	-2.07	1.35	1.42
9	V	102	SPN	C15-C14	2.07	1.59	1.52
9	i	103	SPN	C24-C25	2.07	1.57	1.50
8	F	101	BCL	C3D-C2D	-2.07	1.33	1.39
8	N	101	BCL	C3B-C2B	-2.07	1.35	1.42
8	k	102	BCL	C3B-C2B	-2.06	1.35	1.42
9	S	102	SPN	C17-C18	2.06	1.55	1.51
9	S	102	SPN	C15-C14	2.06	1.59	1.52
9	D	103	SPN	C1-C2	2.06	1.55	1.53
9	E	102	SPN	C24-C25	2.06	1.57	1.50
9	a	103	SPN	C15-C14	2.06	1.59	1.52
9	D	102	SPN	C17-C18	2.06	1.55	1.51
9	D	103	SPN	C15-C14	2.06	1.59	1.52
8	B	101	BCL	C3D-C2D	-2.06	1.33	1.39
9	G	103	SPN	C15-C14	2.06	1.59	1.52
8	P	101	BCL	C3B-C2B	-2.06	1.35	1.42
9	i	101	SPN	C24-C25	2.06	1.57	1.50
8	M	405	BCL	C3B-C2B	-2.06	1.35	1.42
8	R	101	BCL	C3B-C2B	-2.06	1.35	1.42
8	l	101	BCL	C3B-C2B	-2.06	1.35	1.42
9	F	102	SPN	C15-C14	2.06	1.59	1.52
9	a	104	SPN	C15-C14	2.06	1.59	1.52
8	f	101	BCL	C3B-C2B	-2.06	1.35	1.42
9	t	102	SPN	C15-C14	2.05	1.59	1.52
9	k	103	SPN	C15-C14	2.05	1.59	1.52
9	K	102	SPN	C15-C14	2.05	1.59	1.52
16	C	403	HEC	FE-ND	2.05	2.01	1.94
8	I	102	BCL	C3D-C2D	-2.05	1.33	1.39
8	I	102	BCL	C3B-C2B	-2.05	1.35	1.42
8	J	101	BCL	C3B-C2B	-2.05	1.35	1.42
9	e	102	SPN	C24-C25	2.05	1.57	1.50
8	e	101	BCL	C3B-C2B	-2.05	1.35	1.42
9	b	102	SPN	C15-C14	2.05	1.59	1.52
8	Q	101	BCL	C3B-C2B	-2.05	1.35	1.42
9	a	103	SPN	C17-C18	2.05	1.55	1.51
9	n	102	SPN	C15-C14	2.05	1.59	1.52
8	B	101	BCL	C3B-C2B	-2.04	1.36	1.42
8	J	101	BCL	C3D-C2D	-2.04	1.33	1.39
9	p	102	SPN	C15-C14	2.04	1.59	1.52
8	K	101	BCL	C3D-C4D	-2.04	1.39	1.44
9	D	102	SPN	C15-C14	2.04	1.59	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	G	101	BCL	C3B-C2B	-2.04	1.36	1.42
9	e	102	SPN	C1-C2	2.04	1.55	1.53
8	v	101	BCL	C3B-C2B	-2.04	1.36	1.42
9	G	104	SPN	C24-C25	2.04	1.57	1.50
9	G	104	SPN	C1-C2	2.04	1.55	1.53
8	T	101	BCL	C3B-C2B	-2.04	1.36	1.42
15	H	303	CDL	OB6-CB5	2.04	1.40	1.34
9	S	101	SPN	C15-C14	2.03	1.59	1.52
9	k	101	SPN	C15-C14	2.03	1.59	1.52
8	i	102	BCL	C3B-C2B	-2.03	1.36	1.42
9	i	103	SPN	C1-C2	2.03	1.55	1.53
9	r	103	SPN	C15-C14	2.03	1.59	1.52
9	E	102	SPN	C17-C18	2.03	1.55	1.51
9	e	102	SPN	C15-C14	2.03	1.59	1.52
8	2	101	BCL	C3D-C2D	-2.03	1.33	1.39
9	E	102	SPN	C15-C14	2.03	1.59	1.52
8	G	102	BCL	C3B-C2B	-2.03	1.36	1.42
13	M	403	BPH	CHA-CBD	2.03	1.53	1.51
8	j	101	BCL	C3B-C2B	-2.03	1.36	1.42
9	b	102	SPN	C1-C2	2.03	1.55	1.53
8	q	102	BCL	C3B-C2B	-2.03	1.36	1.42
8	s	101	BCL	C3B-C2B	-2.02	1.36	1.42
9	v	102	SPN	C15-C14	2.02	1.59	1.52
9	Q	102	SPN	C15-C14	2.02	1.59	1.52
8	D	101	BCL	C3B-C2B	-2.02	1.36	1.42
9	r	101	SPN	C15-C14	2.02	1.59	1.52
8	K	101	BCL	C3D-C2D	-2.02	1.33	1.39
9	a	103	SPN	C1-C2	2.02	1.55	1.53
9	R	102	SPN	C15-C14	2.01	1.59	1.52
8	v	101	BCL	C3D-C2D	-2.01	1.33	1.39
8	v	101	BCL	C5-C3	2.01	1.55	1.51
9	i	103	SPN	C15-C14	2.01	1.59	1.52
9	n	102	SPN	C1-C2	2.01	1.55	1.53
8	q	102	BCL	C3D-C2D	-2.01	1.33	1.39
9	2	103	SPN	C15-C14	2.01	1.59	1.52
9	p	101	SPN	C15-C14	2.01	1.59	1.52
8	V	101	BCL	C3D-C2D	-2.00	1.33	1.39
9	q	101	SPN	C15-C14	2.00	1.59	1.52
8	R	101	BCL	C3D-C2D	-2.00	1.33	1.39
8	E	101	BCL	C3D-C2D	-2.00	1.33	1.39
9	2	102	SPN	C15-C14	2.00	1.59	1.52
9	i	101	SPN	C15-C14	2.00	1.59	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	r	102	BCL	C3D-C2D	-2.00	1.33	1.39

All (2005) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	K	102	SPN	C3-C4-C5	16.39	154.07	126.79
9	V	102	SPN	C3-C4-C5	16.22	153.80	126.79
9	G	104	SPN	C3-C4-C5	16.13	153.65	126.79
9	i	103	SPN	C3-C4-C5	15.96	153.35	126.79
9	a	101	SPN	C3-C4-C5	15.83	153.15	126.79
9	I	101	SPN	C3-C4-C5	15.79	153.07	126.79
9	a	104	SPN	C3-C4-C5	15.77	153.05	126.79
9	f	102	SPN	C3-C4-C5	15.75	153.01	126.79
9	M	404	SPN	C3-C4-C5	15.70	152.93	126.79
9	e	102	SPN	C3-C4-C5	15.68	152.89	126.79
9	k	103	SPN	C3-C4-C5	15.66	152.85	126.79
9	r	103	SPN	C3-C4-C5	15.61	152.78	126.79
9	p	102	SPN	C3-C4-C5	15.60	152.76	126.79
9	2	102	SPN	C3-C4-C5	15.54	152.66	126.79
9	S	102	SPN	C3-C4-C5	15.53	152.65	126.79
9	D	103	SPN	C3-C4-C5	15.51	152.61	126.79
9	2	103	SPN	C3-C4-C5	15.50	152.59	126.79
9	v	102	SPN	C3-C4-C5	15.45	152.52	126.79
9	Q	102	SPN	C3-C4-C5	15.42	152.46	126.79
9	r	101	SPN	C3-C4-C5	15.41	152.45	126.79
9	t	102	SPN	C3-C4-C5	15.36	152.36	126.79
9	k	101	SPN	C3-C4-C5	15.33	152.31	126.79
9	E	102	SPN	C3-C4-C5	15.32	152.30	126.79
9	i	101	SPN	C3-C4-C5	15.28	152.23	126.79
9	q	101	SPN	C3-C4-C5	15.26	152.20	126.79
9	a	103	SPN	C3-C4-C5	15.20	152.09	126.79
9	b	102	SPN	C3-C4-C5	15.08	151.90	126.79
9	G	103	SPN	C3-C4-C5	15.01	151.78	126.79
9	p	101	SPN	C3-C4-C5	14.93	151.65	126.79
9	S	101	SPN	C3-C4-C5	14.86	151.53	126.79
9	D	102	SPN	C3-C4-C5	14.73	151.31	126.79
9	j	102	SPN	C3-C4-C5	14.57	151.05	126.79
9	R	102	SPN	C3-C4-C5	14.40	150.77	126.79
9	F	102	SPN	C3-C4-C5	14.11	150.29	126.79
9	n	102	SPN	C3-C4-C5	13.80	149.77	126.79
9	R	102	SPN	C15-C16-C17	11.75	155.42	113.19
9	S	101	SPN	C15-C16-C17	11.68	155.16	113.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	b	102	SPN	C15-C16-C17	11.61	154.93	113.19
9	i	101	SPN	C11-C12-C13	11.55	155.46	127.66
9	D	102	SPN	C15-C16-C17	11.43	154.27	113.19
9	S	102	SPN	C15-C16-C17	11.41	154.19	113.19
9	E	102	SPN	C15-C16-C17	11.40	154.16	113.19
9	2	102	SPN	C15-C16-C17	11.31	153.86	113.19
9	t	102	SPN	C15-C16-C17	11.29	153.78	113.19
9	M	404	SPN	C15-C16-C17	11.29	153.78	113.19
9	j	102	SPN	C15-C16-C17	11.25	153.63	113.19
9	F	102	SPN	C15-C16-C17	11.23	153.57	113.19
9	I	101	SPN	C15-C16-C17	11.17	153.35	113.19
9	i	101	SPN	C7-C8-C9	11.17	154.55	127.66
9	f	102	SPN	C15-C16-C17	11.16	153.31	113.19
9	Q	102	SPN	C15-C16-C17	11.12	153.15	113.19
9	K	102	SPN	C15-C16-C17	11.10	153.10	113.19
9	V	102	SPN	C15-C16-C17	11.10	153.08	113.19
9	Q	102	SPN	C7-C8-C9	11.09	154.37	127.66
9	n	102	SPN	C7-C8-C9	11.09	154.37	127.66
9	p	102	SPN	C15-C16-C17	11.08	153.02	113.19
9	r	103	SPN	C15-C16-C17	11.06	152.96	113.19
9	q	101	SPN	C15-C16-C17	11.06	152.94	113.19
9	G	104	SPN	C15-C16-C17	11.05	152.91	113.19
9	k	101	SPN	C15-C16-C17	11.04	152.87	113.19
9	S	102	SPN	C7-C8-C9	11.00	154.15	127.66
9	a	104	SPN	C7-C8-C9	10.99	154.11	127.66
9	a	104	SPN	C15-C16-C17	10.96	152.60	113.19
9	v	102	SPN	C15-C16-C17	10.94	152.51	113.19
9	D	103	SPN	C15-C16-C17	10.92	152.46	113.19
9	i	103	SPN	C15-C16-C17	10.92	152.45	113.19
9	i	101	SPN	C15-C16-C17	10.90	152.38	113.19
9	R	102	SPN	C7-C8-C9	10.90	153.90	127.66
9	p	101	SPN	C15-C16-C17	10.89	152.34	113.19
9	F	102	SPN	C7-C8-C9	10.87	153.83	127.66
9	e	102	SPN	C7-C8-C9	10.85	153.79	127.66
9	S	101	SPN	C7-C8-C9	10.85	153.79	127.66
9	e	102	SPN	C15-C16-C17	10.84	152.16	113.19
9	j	102	SPN	C11-C12-C13	10.80	153.67	127.66
9	S	101	SPN	C11-C12-C13	10.80	153.67	127.66
9	I	101	SPN	C7-C8-C9	10.80	153.67	127.66
9	k	103	SPN	C15-C16-C17	10.80	152.01	113.19
9	j	102	SPN	C7-C8-C9	10.78	153.62	127.66
9	E	102	SPN	C11-C12-C13	10.77	153.59	127.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	102	SPN	C11-C12-C13	10.76	153.58	127.66
9	a	101	SPN	C15-C16-C17	10.76	151.87	113.19
9	G	103	SPN	C15-C16-C17	10.75	151.84	113.19
9	b	102	SPN	C11-C12-C13	10.75	153.53	127.66
9	2	103	SPN	C15-C16-C17	10.69	151.63	113.19
9	b	102	SPN	C7-C8-C9	10.69	153.39	127.66
9	a	103	SPN	C15-C16-C17	10.67	151.55	113.19
9	F	102	SPN	C11-C12-C13	10.65	153.30	127.66
9	G	103	SPN	C7-C8-C9	10.60	153.18	127.66
9	r	101	SPN	C15-C16-C17	10.58	151.23	113.19
9	R	102	SPN	C11-C12-C13	10.57	153.11	127.66
9	G	103	SPN	C11-C12-C13	10.54	153.03	127.66
9	G	104	SPN	C11-C12-C13	10.53	153.02	127.66
9	n	102	SPN	C15-C16-C17	10.53	151.04	113.19
9	V	102	SPN	C11-C12-C13	10.53	153.01	127.66
9	2	103	SPN	C11-C12-C13	10.51	152.96	127.66
9	k	103	SPN	C7-C8-C9	10.51	152.96	127.66
9	S	102	SPN	C11-C12-C13	10.48	152.90	127.66
9	p	102	SPN	C7-C8-C9	10.47	152.88	127.66
9	a	103	SPN	C7-C8-C9	10.47	152.88	127.66
9	t	102	SPN	C11-C12-C13	10.45	152.83	127.66
9	K	102	SPN	C7-C8-C9	10.41	152.71	127.66
9	2	102	SPN	C11-C12-C13	10.40	152.71	127.66
9	I	101	SPN	C11-C12-C13	10.40	152.70	127.66
9	t	102	SPN	C7-C8-C9	10.39	152.68	127.66
9	r	103	SPN	C11-C12-C13	10.39	152.67	127.66
9	2	102	SPN	C7-C8-C9	10.36	152.62	127.66
9	v	102	SPN	C7-C8-C9	10.36	152.61	127.66
9	r	101	SPN	C7-C8-C9	10.33	152.53	127.66
9	a	101	SPN	C7-C8-C9	10.32	152.51	127.66
9	a	104	SPN	C11-C12-C13	10.31	152.49	127.66
9	M	404	SPN	C7-C8-C9	10.31	152.48	127.66
9	Q	102	SPN	C11-C12-C13	10.26	152.37	127.66
9	e	102	SPN	C11-C12-C13	10.25	152.34	127.66
9	a	101	SPN	C11-C12-C13	10.22	152.26	127.66
9	f	102	SPN	C7-C8-C9	10.21	152.25	127.66
9	G	104	SPN	C7-C8-C9	10.21	152.25	127.66
9	v	102	SPN	C11-C12-C13	10.21	152.24	127.66
9	f	102	SPN	C11-C12-C13	10.18	152.17	127.66
9	q	101	SPN	C7-C8-C9	10.18	152.16	127.66
9	k	101	SPN	C7-C8-C9	10.16	152.13	127.66
9	r	103	SPN	C7-C8-C9	10.16	152.12	127.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	q	101	SPN	C11-C12-C13	10.15	152.11	127.66
9	p	101	SPN	C7-C8-C9	10.14	152.07	127.66
9	r	101	SPN	C11-C12-C13	10.12	152.03	127.66
9	p	102	SPN	C11-C12-C13	10.12	152.03	127.66
9	i	103	SPN	C7-C8-C9	10.12	152.02	127.66
9	V	102	SPN	C7-C8-C9	10.11	152.01	127.66
9	p	101	SPN	C11-C12-C13	10.11	151.99	127.66
9	D	103	SPN	C11-C12-C13	10.10	151.99	127.66
9	K	102	SPN	C11-C12-C13	10.09	151.95	127.66
9	i	103	SPN	C11-C12-C13	10.03	151.80	127.66
9	k	103	SPN	C11-C12-C13	10.02	151.79	127.66
9	M	404	SPN	C11-C12-C13	9.97	151.67	127.66
9	a	103	SPN	C11-C12-C13	9.87	151.43	127.66
9	D	103	SPN	C7-C8-C9	9.82	151.31	127.66
9	n	102	SPN	C11-C12-C13	9.76	151.16	127.66
9	k	101	SPN	C11-C12-C13	9.76	151.15	127.66
9	2	103	SPN	C7-C8-C9	9.69	150.98	127.66
9	D	102	SPN	C7-C8-C9	9.62	150.83	127.66
9	E	102	SPN	C7-C8-C9	9.52	150.59	127.66
10	H	302	MW9	C35-C34-C33	8.69	152.50	112.71
10	M	407	MW9	C35-C34-C33	7.07	152.95	112.43
10	M	408	MW9	C35-C34-C33	7.03	152.72	112.43
10	B	102	MW9	C35-C34-C33	7.00	152.53	112.43
10	Q	103	MW9	C35-C34-C33	6.96	152.33	112.43
10	G	105	MW9	C35-C34-C33	6.96	152.30	112.43
9	2	103	SPN	C24-C25-C26	-6.81	111.27	127.66
9	r	101	SPN	C24-C25-C26	-6.65	111.65	127.66
9	j	102	SPN	C24-C25-C26	-6.63	111.69	127.66
9	G	103	SPN	C24-C25-C26	-6.62	111.71	127.66
8	L	301	BCL	C1D-ND-C4D	-6.61	101.64	106.33
9	G	104	SPN	C24-C25-C26	-6.56	111.85	127.66
9	a	101	SPN	C24-C25-C26	-6.56	111.88	127.66
8	2	101	BCL	C1D-ND-C4D	-6.54	101.69	106.33
9	i	101	SPN	C24-C25-C26	-6.54	111.92	127.66
9	S	101	SPN	C24-C25-C26	-6.52	111.97	127.66
9	b	102	SPN	C24-C25-C26	-6.50	112.00	127.66
9	i	103	SPN	C24-C25-C26	-6.48	112.06	127.66
9	K	102	SPN	C17-C18-C19	-6.46	108.04	121.12
8	M	402	BCL	C1D-ND-C4D	-6.45	101.75	106.33
9	S	102	SPN	C24-C25-C26	-6.44	112.15	127.66
9	k	103	SPN	C24-C25-C26	-6.44	112.17	127.66
8	k	102	BCL	C1D-ND-C4D	-6.43	101.77	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	s	101	BCL	C1D-ND-C4D	-6.42	101.77	106.33
9	e	102	SPN	C17-C18-C19	-6.42	108.13	121.12
8	v	101	BCL	C1D-ND-C4D	-6.41	101.78	106.33
8	p	103	BCL	C1D-ND-C4D	-6.40	101.78	106.33
8	i	102	BCL	C1D-ND-C4D	-6.40	101.79	106.33
9	f	102	SPN	C24-C25-C26	-6.39	112.28	127.66
9	e	102	SPN	C24-C25-C26	-6.38	112.29	127.66
9	p	102	SPN	C24-C25-C26	-6.38	112.30	127.66
9	p	101	SPN	C24-C25-C26	-6.38	112.31	127.66
9	2	102	SPN	C24-C25-C26	-6.36	112.34	127.66
9	n	102	SPN	C24-C25-C26	-6.36	112.36	127.66
9	E	102	SPN	C24-C25-C26	-6.34	112.40	127.66
8	n	101	BCL	C1D-ND-C4D	-6.33	101.83	106.33
9	k	101	SPN	C24-C25-C26	-6.30	112.48	127.66
9	a	103	SPN	C24-C25-C26	-6.30	112.49	127.66
9	q	101	SPN	C24-C25-C26	-6.29	112.51	127.66
8	q	102	BCL	C1D-ND-C4D	-6.28	101.87	106.33
9	F	102	SPN	C24-C25-C26	-6.27	112.57	127.66
9	t	102	SPN	C24-C25-C26	-6.25	112.62	127.66
9	S	102	SPN	C27-C26-C25	-6.21	108.55	121.12
9	i	101	SPN	C10-C9-C8	-6.20	108.56	121.12
8	B	101	BCL	C1D-ND-C4D	-6.18	101.94	106.33
9	D	103	SPN	C24-C25-C26	-6.17	112.81	127.66
9	n	102	SPN	C17-C18-C19	-6.16	108.65	121.12
8	E	101	BCL	C1D-ND-C4D	-6.16	101.96	106.33
9	D	102	SPN	C24-C25-C26	-6.15	112.84	127.66
9	k	103	SPN	C10-C9-C8	-6.15	108.68	121.12
8	f	101	BCL	C1D-ND-C4D	-6.15	101.97	106.33
10	F	103	MW9	C35-C34-C33	6.14	152.45	112.55
8	r	102	BCL	C1D-ND-C4D	-6.14	101.97	106.33
8	G	102	BCL	C1D-ND-C4D	-6.13	101.98	106.33
8	a	102	BCL	C1D-ND-C4D	-6.13	101.98	106.33
9	2	103	SPN	CM8-C26-C25	-6.13	107.96	123.68
9	i	101	SPN	C6-C5-C4	-6.13	108.72	121.12
8	N	101	BCL	C1D-ND-C4D	-6.12	101.98	106.33
9	b	102	SPN	CM4-C9-C8	-6.12	107.97	123.68
9	F	102	SPN	CM3-C5-C4	-6.12	107.98	123.68
10	L	307	MW9	C35-C34-C33	6.12	152.27	112.55
9	q	101	SPN	CM6-C18-C19	-6.11	108.01	123.68
8	G	101	BCL	C1D-ND-C4D	-6.11	102.00	106.33
8	Q	101	BCL	C1D-ND-C4D	-6.10	102.00	106.33
8	L	304	BCL	C1D-ND-C4D	-6.10	102.00	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	F	104	MW9	C35-C34-C33	6.10	152.16	112.55
8	A	101	BCL	C1D-ND-C4D	-6.07	102.03	106.33
9	q	101	SPN	C14-C13-C12	-6.07	108.84	121.12
8	1	101	BCL	C1D-ND-C4D	-6.06	102.03	106.33
8	F	101	BCL	C1D-ND-C4D	-6.05	102.03	106.33
8	b	101	BCL	C1D-ND-C4D	-6.05	102.03	106.33
8	P	101	BCL	C1D-ND-C4D	-6.05	102.04	106.33
9	I	101	SPN	CM6-C18-C19	-6.04	108.17	123.68
8	D	101	BCL	C1D-ND-C4D	-6.03	102.05	106.33
9	D	102	SPN	CM3-C5-C4	-6.03	108.20	123.68
9	r	103	SPN	C24-C25-C26	-6.03	113.14	127.66
8	R	101	BCL	C1D-ND-C4D	-6.03	102.05	106.33
9	R	102	SPN	CM3-C5-C4	-6.02	108.22	123.68
8	K	101	BCL	C1D-ND-C4D	-6.01	102.06	106.33
8	V	101	BCL	C1D-ND-C4D	-6.01	102.07	106.33
8	J	101	BCL	C1D-ND-C4D	-6.01	102.07	106.33
8	T	101	BCL	C1D-ND-C4D	-6.00	102.08	106.33
9	f	102	SPN	C6-C5-C4	-5.99	109.00	121.12
9	i	101	SPN	C14-C13-C12	-5.98	109.01	121.12
9	i	103	SPN	C17-C18-C19	-5.97	109.03	121.12
9	p	101	SPN	C14-C13-C12	-5.97	109.04	121.12
9	n	102	SPN	CM3-C5-C4	-5.96	108.39	123.68
9	K	102	SPN	C27-C26-C25	-5.96	109.06	121.12
9	S	102	SPN	CM3-C5-C4	-5.96	108.39	123.68
9	K	102	SPN	C24-C25-C26	-5.95	113.34	127.66
9	k	103	SPN	CM4-C9-C8	-5.94	108.44	123.68
9	r	103	SPN	C27-C26-C25	-5.93	109.11	121.12
9	M	404	SPN	CM5-C13-C12	-5.93	108.46	123.68
9	I	101	SPN	C27-C26-C25	-5.93	109.12	121.12
9	q	101	SPN	CM8-C26-C25	-5.93	108.47	123.68
9	V	102	SPN	C24-C25-C26	-5.93	113.39	127.66
9	a	104	SPN	C27-C26-C25	-5.92	109.15	121.12
8	j	101	BCL	C1D-ND-C4D	-5.92	102.13	106.33
9	G	103	SPN	C17-C18-C19	-5.91	109.15	121.12
9	v	102	SPN	C24-C25-C26	-5.91	113.42	127.66
9	Q	102	SPN	C24-C25-C26	-5.91	113.42	127.66
9	j	102	SPN	CM6-C18-C19	-5.91	108.52	123.68
9	G	104	SPN	C6-C5-C4	-5.91	109.16	121.12
8	t	101	BCL	C2B-C1B-NB	-5.90	106.28	110.23
9	j	102	SPN	CM4-C9-C8	-5.90	108.54	123.68
9	q	101	SPN	C10-C9-C8	-5.90	109.18	121.12
9	K	102	SPN	C14-C13-C12	-5.90	109.18	121.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	Q	102	SPN	C27-C26-C25	-5.89	109.19	121.12
9	K	102	SPN	CM3-C5-C4	-5.89	108.58	123.68
9	v	102	SPN	C27-C26-C25	-5.88	109.21	121.12
9	R	102	SPN	CM6-C18-C19	-5.88	108.59	123.68
9	D	103	SPN	C27-C26-C25	-5.88	109.22	121.12
9	f	102	SPN	C17-C18-C19	-5.87	109.23	121.12
9	n	102	SPN	C27-C26-C25	-5.87	109.23	121.12
8	I	102	BCL	C1D-ND-C4D	-5.87	102.16	106.33
9	I	101	SPN	C24-C25-C26	-5.87	113.52	127.66
9	G	103	SPN	CM3-C5-C4	-5.87	108.62	123.68
9	G	104	SPN	C27-C26-C25	-5.86	109.26	121.12
8	L	301	BCL	C2D-C1D-ND	5.86	114.42	110.10
9	i	103	SPN	CM5-C13-C12	-5.86	108.65	123.68
9	r	101	SPN	C17-C18-C19	-5.85	109.27	121.12
9	M	404	SPN	C17-C18-C19	-5.85	109.27	121.12
9	p	101	SPN	C17-C18-C19	-5.85	109.27	121.12
9	2	102	SPN	C6-C5-C4	-5.85	109.27	121.12
9	2	103	SPN	C14-C13-C12	-5.85	109.27	121.12
9	k	103	SPN	C27-C26-C25	-5.85	109.28	121.12
9	i	101	SPN	C17-C18-C19	-5.85	109.28	121.12
9	i	103	SPN	C27-C26-C25	-5.85	109.29	121.12
9	e	102	SPN	C14-C13-C12	-5.85	109.29	121.12
9	E	102	SPN	CM3-C5-C4	-5.85	108.68	123.68
9	t	102	SPN	C17-C18-C19	-5.84	109.29	121.12
9	f	102	SPN	C27-C26-C25	-5.84	109.29	121.12
9	a	104	SPN	C24-C25-C26	-5.84	113.60	127.66
9	p	102	SPN	CM3-C5-C4	-5.83	108.71	123.68
9	F	102	SPN	CM4-C9-C8	-5.83	108.72	123.68
9	S	102	SPN	CM5-C13-C12	-5.83	108.72	123.68
8	M	405	BCL	C1D-ND-C4D	-5.83	102.19	106.33
8	R	103	BCL	C1D-ND-C4D	-5.83	102.20	106.33
9	v	102	SPN	CM5-C13-C12	-5.83	108.73	123.68
9	E	102	SPN	C27-C26-C25	-5.82	109.34	121.12
9	r	103	SPN	CM4-C9-C8	-5.82	108.75	123.68
9	S	101	SPN	CM5-C13-C12	-5.82	108.76	123.68
9	t	102	SPN	C6-C5-C4	-5.82	109.35	121.12
8	e	101	BCL	C1D-ND-C4D	-5.82	102.20	106.33
9	p	102	SPN	C17-C18-C19	-5.81	109.35	121.12
9	V	102	SPN	C14-C13-C12	-5.81	109.35	121.12
9	I	101	SPN	CM3-C5-C4	-5.79	108.82	123.68
9	S	101	SPN	CM4-C9-C8	-5.79	108.82	123.68
9	f	102	SPN	CM4-C9-C8	-5.79	108.83	123.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	v	102	SPN	C10-C9-C8	-5.79	109.41	121.12
9	k	101	SPN	C6-C5-C4	-5.79	109.41	121.12
9	f	102	SPN	C10-C9-C8	-5.78	109.42	121.12
9	p	102	SPN	C14-C13-C12	-5.78	109.42	121.12
9	a	104	SPN	CM6-C18-C19	-5.78	108.85	123.68
9	M	404	SPN	C24-C25-C26	-5.78	113.75	127.66
9	r	103	SPN	C14-C13-C12	-5.78	109.43	121.12
9	D	102	SPN	CM4-C9-C8	-5.77	108.87	123.68
9	j	102	SPN	CM8-C26-C25	-5.77	108.88	123.68
9	F	102	SPN	CM5-C13-C12	-5.76	108.89	123.68
9	K	102	SPN	CM4-C9-C8	-5.76	108.89	123.68
9	i	103	SPN	CM4-C9-C8	-5.76	108.90	123.68
9	R	102	SPN	C24-C25-C26	-5.76	113.79	127.66
9	j	102	SPN	CM3-C5-C4	-5.76	108.91	123.68
9	G	103	SPN	CM4-C9-C8	-5.75	108.92	123.68
9	n	102	SPN	CM4-C9-C8	-5.75	108.92	123.68
9	R	102	SPN	CM4-C9-C8	-5.75	108.92	123.68
9	a	101	SPN	C6-C5-C4	-5.75	109.48	121.12
9	q	101	SPN	CM3-C5-C4	-5.75	108.94	123.68
9	S	101	SPN	CM3-C5-C4	-5.74	108.94	123.68
9	D	103	SPN	C6-C5-C4	-5.74	109.50	121.12
9	p	102	SPN	CM4-C9-C8	-5.74	108.95	123.68
9	Q	102	SPN	C14-C13-C12	-5.74	109.50	121.12
9	F	102	SPN	CM6-C18-C19	-5.74	108.96	123.68
9	K	102	SPN	CM5-C13-C12	-5.74	108.97	123.68
9	M	404	SPN	CM8-C26-C25	-5.73	108.97	123.68
9	R	102	SPN	C27-C26-C25	-5.73	109.51	121.12
9	E	102	SPN	CM6-C18-C19	-5.73	108.98	123.68
9	v	102	SPN	C17-C18-C19	-5.73	109.52	121.12
9	n	102	SPN	CM8-C26-C25	-5.73	108.98	123.68
9	v	102	SPN	C6-C5-C4	-5.73	109.53	121.12
9	D	102	SPN	CM5-C13-C12	-5.73	108.99	123.68
9	n	102	SPN	CM5-C13-C12	-5.73	108.99	123.68
9	R	102	SPN	CM5-C13-C12	-5.73	108.99	123.68
9	2	103	SPN	CM3-C5-C4	-5.72	108.99	123.68
9	e	102	SPN	C27-C26-C25	-5.72	109.54	121.12
9	j	102	SPN	C17-C18-C19	-5.72	109.54	121.12
9	D	103	SPN	CM8-C26-C25	-5.72	109.00	123.68
9	2	102	SPN	C10-C9-C8	-5.72	109.54	121.12
9	i	103	SPN	C10-C9-C8	-5.72	109.54	121.12
9	I	101	SPN	C10-C9-C8	-5.72	109.54	121.12
9	Q	102	SPN	C10-C9-C8	-5.72	109.55	121.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	G	104	SPN	C17-C18-C19	-5.72	109.55	121.12
9	r	101	SPN	CM8-C26-C25	-5.72	109.01	123.68
9	p	102	SPN	C27-C26-C25	-5.72	109.55	121.12
9	E	102	SPN	CM8-C26-C25	-5.71	109.02	123.68
9	a	104	SPN	CM3-C5-C4	-5.71	109.02	123.68
9	G	103	SPN	CM8-C26-C25	-5.71	109.03	123.68
9	r	103	SPN	C6-C5-C4	-5.71	109.56	121.12
9	G	104	SPN	C10-C9-C8	-5.71	109.56	121.12
9	r	101	SPN	C6-C5-C4	-5.71	109.56	121.12
9	b	102	SPN	CM5-C13-C12	-5.71	109.03	123.68
9	a	104	SPN	C17-C18-C19	-5.71	109.57	121.12
9	i	101	SPN	C27-C26-C25	-5.71	109.57	121.12
9	f	102	SPN	CM6-C18-C19	-5.71	109.04	123.68
9	M	404	SPN	CM3-C5-C4	-5.71	109.04	123.68
9	F	102	SPN	CM8-C26-C25	-5.70	109.05	123.68
9	D	102	SPN	CM6-C18-C19	-5.70	109.05	123.68
9	k	101	SPN	C14-C13-C12	-5.70	109.58	121.12
9	r	101	SPN	CM5-C13-C12	-5.69	109.07	123.68
9	k	103	SPN	CM8-C26-C25	-5.69	109.07	123.68
9	2	102	SPN	CM5-C13-C12	-5.69	109.08	123.68
9	E	102	SPN	CM4-C9-C8	-5.69	109.08	123.68
9	S	101	SPN	CM6-C18-C19	-5.69	109.09	123.68
9	a	101	SPN	C14-C13-C12	-5.69	109.61	121.12
9	t	102	SPN	C27-C26-C25	-5.68	109.61	121.12
9	p	102	SPN	C6-C5-C4	-5.68	109.61	121.12
9	p	101	SPN	CM4-C9-C8	-5.68	109.10	123.68
9	2	103	SPN	C17-C18-C19	-5.68	109.62	121.12
9	G	103	SPN	CM6-C18-C19	-5.68	109.11	123.68
9	q	101	SPN	C6-C5-C4	-5.67	109.64	121.12
9	S	101	SPN	CM8-C26-C25	-5.67	109.13	123.68
9	b	102	SPN	CM8-C26-C25	-5.67	109.13	123.68
9	k	101	SPN	C27-C26-C25	-5.67	109.64	121.12
9	V	102	SPN	CM3-C5-C4	-5.67	109.13	123.68
8	d	101	BCL	C1D-ND-C4D	-5.67	102.31	106.33
9	k	103	SPN	C17-C18-C19	-5.67	109.65	121.12
9	i	103	SPN	CM8-C26-C25	-5.67	109.14	123.68
9	j	102	SPN	CM5-C13-C12	-5.66	109.15	123.68
9	K	102	SPN	C6-C5-C4	-5.66	109.65	121.12
9	2	102	SPN	C14-C13-C12	-5.66	109.66	121.12
9	p	101	SPN	CM3-C5-C4	-5.66	109.15	123.68
9	v	102	SPN	CM4-C9-C8	-5.66	109.15	123.68
9	r	103	SPN	CM6-C18-C19	-5.66	109.15	123.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	G	104	SPN	CM4-C9-C8	-5.66	109.16	123.68
9	a	103	SPN	C27-C26-C25	-5.66	109.67	121.12
9	f	102	SPN	CM8-C26-C25	-5.66	109.17	123.68
9	b	102	SPN	C27-C26-C25	-5.66	109.67	121.12
9	a	101	SPN	CM3-C5-C4	-5.65	109.17	123.68
9	M	404	SPN	CM6-C18-C19	-5.65	109.17	123.68
9	t	102	SPN	C14-C13-C12	-5.65	109.68	121.12
9	D	102	SPN	CM8-C26-C25	-5.65	109.19	123.68
9	i	101	SPN	CM8-C26-C25	-5.65	109.20	123.68
9	M	404	SPN	CM4-C9-C8	-5.64	109.20	123.68
9	a	103	SPN	CM4-C9-C8	-5.64	109.20	123.68
8	2	101	BCL	C2D-C1D-ND	5.64	114.26	110.10
9	k	101	SPN	CM8-C26-C25	-5.64	109.21	123.68
9	I	101	SPN	CM4-C9-C8	-5.64	109.22	123.68
9	a	101	SPN	C27-C26-C25	-5.64	109.71	121.12
9	f	102	SPN	CM5-C13-C12	-5.63	109.23	123.68
9	G	103	SPN	C14-C13-C12	-5.63	109.72	121.12
9	e	102	SPN	CM8-C26-C25	-5.63	109.23	123.68
9	e	102	SPN	C6-C5-C4	-5.63	109.72	121.12
9	p	101	SPN	CM8-C26-C25	-5.63	109.23	123.68
9	V	102	SPN	C6-C5-C4	-5.63	109.72	121.12
9	Q	102	SPN	CM6-C18-C19	-5.63	109.23	123.68
9	k	101	SPN	C17-C18-C19	-5.63	109.72	121.12
9	p	102	SPN	C10-C9-C8	-5.62	109.74	121.12
9	q	101	SPN	CM4-C9-C8	-5.62	109.26	123.68
9	a	103	SPN	C17-C18-C19	-5.62	109.75	121.12
9	p	102	SPN	CM8-C26-C25	-5.62	109.27	123.68
8	l	101	BCL	C1C-NC-C4C	-5.62	104.18	106.71
9	a	101	SPN	CM5-C13-C12	-5.61	109.28	123.68
9	Q	102	SPN	CM8-C26-C25	-5.61	109.28	123.68
9	a	104	SPN	CM4-C9-C8	-5.61	109.28	123.68
9	G	103	SPN	C10-C9-C8	-5.61	109.76	121.12
9	v	102	SPN	CM3-C5-C4	-5.61	109.29	123.68
9	D	103	SPN	C14-C13-C12	-5.61	109.77	121.12
9	S	102	SPN	CM6-C18-C19	-5.61	109.29	123.68
9	e	102	SPN	CM3-C5-C4	-5.61	109.29	123.68
9	E	102	SPN	C14-C13-C12	-5.61	109.77	121.12
9	E	102	SPN	CM5-C13-C12	-5.60	109.30	123.68
9	G	104	SPN	C14-C13-C12	-5.60	109.78	121.12
9	2	103	SPN	CM5-C13-C12	-5.60	109.31	123.68
9	a	103	SPN	CM8-C26-C25	-5.60	109.31	123.68
9	K	102	SPN	CM6-C18-C19	-5.60	109.32	123.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	2	102	SPN	CM4-C9-C8	-5.60	109.32	123.68
9	G	104	SPN	CM5-C13-C12	-5.60	109.32	123.68
9	r	101	SPN	CM3-C5-C4	-5.59	109.33	123.68
8	p	103	BCL	C2D-C1D-ND	5.59	114.23	110.10
9	F	102	SPN	C27-C26-C25	-5.59	109.80	121.12
9	a	104	SPN	C14-C13-C12	-5.59	109.81	121.12
9	Q	102	SPN	CM5-C13-C12	-5.59	109.34	123.68
9	r	101	SPN	C14-C13-C12	-5.59	109.81	121.12
9	V	102	SPN	CM4-C9-C8	-5.59	109.35	123.68
9	S	102	SPN	CM4-C9-C8	-5.58	109.36	123.68
9	k	101	SPN	CM4-C9-C8	-5.58	109.36	123.68
9	a	103	SPN	CM3-C5-C4	-5.58	109.36	123.68
9	e	102	SPN	C10-C9-C8	-5.58	109.82	121.12
9	a	104	SPN	C10-C9-C8	-5.58	109.83	121.12
9	a	101	SPN	CM6-C18-C19	-5.57	109.38	123.68
9	a	101	SPN	CM8-C26-C25	-5.57	109.38	123.68
9	2	103	SPN	CM6-C18-C19	-5.57	109.39	123.68
9	I	101	SPN	C14-C13-C12	-5.57	109.84	121.12
9	D	103	SPN	CM5-C13-C12	-5.57	109.39	123.68
9	G	103	SPN	CM5-C13-C12	-5.57	109.40	123.68
9	n	102	SPN	CM6-C18-C19	-5.56	109.41	123.68
9	D	103	SPN	CM6-C18-C19	-5.55	109.43	123.68
8	k	102	BCL	C2D-C1D-ND	5.55	114.19	110.10
9	k	103	SPN	CM5-C13-C12	-5.55	109.44	123.68
9	k	103	SPN	C6-C5-C4	-5.55	109.89	121.12
8	i	102	BCL	C2D-C1D-ND	5.55	114.19	110.10
8	M	402	BCL	C2D-C1D-ND	5.55	114.19	110.10
9	G	104	SPN	CM8-C26-C25	-5.55	109.45	123.68
9	p	101	SPN	C10-C9-C8	-5.55	109.89	121.12
8	i	102	BCL	O2D-CGD-CBD	5.54	121.12	111.27
8	K	101	BCL	C2D-C1D-ND	5.54	114.19	110.10
9	V	102	SPN	C17-C18-C19	-5.54	109.90	121.12
9	t	102	SPN	CM8-C26-C25	-5.54	109.46	123.68
9	t	102	SPN	CM4-C9-C8	-5.54	109.46	123.68
8	s	101	BCL	C2D-C1D-ND	5.54	114.19	110.10
9	2	102	SPN	CM6-C18-C19	-5.54	109.47	123.68
9	i	103	SPN	C6-C5-C4	-5.54	109.91	121.12
9	2	102	SPN	CM8-C26-C25	-5.53	109.49	123.68
9	j	102	SPN	C14-C13-C12	-5.53	109.93	121.12
9	i	101	SPN	CM4-C9-C8	-5.53	109.50	123.68
8	v	101	BCL	C2D-C1D-ND	5.53	114.18	110.10
9	Q	102	SPN	CM3-C5-C4	-5.52	109.51	123.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	G	104	SPN	CM6-C18-C19	-5.52	109.51	123.68
9	D	103	SPN	CM3-C5-C4	-5.52	109.51	123.68
9	f	102	SPN	CM3-C5-C4	-5.52	109.52	123.68
9	b	102	SPN	CM3-C5-C4	-5.52	109.52	123.68
9	a	104	SPN	CM5-C13-C12	-5.52	109.53	123.68
8	B	101	BCL	C2D-C1D-ND	5.52	114.17	110.10
9	t	102	SPN	CM5-C13-C12	-5.51	109.53	123.68
9	a	104	SPN	C6-C5-C4	-5.51	109.96	121.12
9	2	102	SPN	C27-C26-C25	-5.51	109.97	121.12
9	a	101	SPN	C17-C18-C19	-5.51	109.97	121.12
9	r	101	SPN	C10-C9-C8	-5.51	109.98	121.12
9	G	104	SPN	CM3-C5-C4	-5.50	109.56	123.68
9	2	102	SPN	CM3-C5-C4	-5.50	109.56	123.68
9	D	103	SPN	C17-C18-C19	-5.50	109.99	121.12
9	S	102	SPN	C10-C9-C8	-5.50	109.99	121.12
9	k	101	SPN	CM3-C5-C4	-5.50	109.58	123.68
9	a	101	SPN	CM4-C9-C8	-5.50	109.58	123.68
9	k	101	SPN	CM6-C18-C19	-5.49	109.58	123.68
9	S	102	SPN	CM8-C26-C25	-5.49	109.60	123.68
9	r	103	SPN	CM3-C5-C4	-5.49	109.61	123.68
9	i	103	SPN	CM3-C5-C4	-5.48	109.61	123.68
9	t	102	SPN	CM6-C18-C19	-5.48	109.61	123.68
9	D	102	SPN	C14-C13-C12	-5.48	110.03	121.12
8	I	102	BCL	O2D-CGD-CBD	5.48	121.01	111.27
8	n	101	BCL	C2D-C1D-ND	5.48	114.14	110.10
9	r	101	SPN	C27-C26-C25	-5.48	110.03	121.12
9	v	102	SPN	C14-C13-C12	-5.47	110.04	121.12
9	V	102	SPN	CM5-C13-C12	-5.47	109.65	123.68
9	i	101	SPN	CM6-C18-C19	-5.47	109.65	123.68
8	R	101	BCL	C2D-C1D-ND	5.47	114.13	110.10
9	M	404	SPN	C14-C13-C12	-5.46	110.06	121.12
9	a	101	SPN	C10-C9-C8	-5.46	110.06	121.12
9	k	101	SPN	C10-C9-C8	-5.46	110.07	121.12
9	r	101	SPN	CM4-C9-C8	-5.46	109.67	123.68
9	F	102	SPN	C17-C18-C19	-5.46	110.07	121.12
9	D	103	SPN	CM4-C9-C8	-5.46	109.68	123.68
8	q	102	BCL	C2D-C1D-ND	5.46	114.13	110.10
8	Q	101	BCL	C2D-C1D-ND	5.46	114.12	110.10
9	a	103	SPN	CM5-C13-C12	-5.46	109.68	123.68
9	t	102	SPN	C10-C9-C8	-5.45	110.09	121.12
9	a	103	SPN	CM6-C18-C19	-5.45	109.71	123.68
9	q	101	SPN	CM5-C13-C12	-5.44	109.72	123.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	101	BCL	C2D-C1D-ND	5.44	114.11	110.10
9	I	101	SPN	CM8-C26-C25	-5.44	109.73	123.68
9	2	103	SPN	CM4-C9-C8	-5.43	109.74	123.68
9	I	101	SPN	CM5-C13-C12	-5.43	109.74	123.68
9	V	102	SPN	C27-C26-C25	-5.43	110.13	121.12
9	n	102	SPN	C14-C13-C12	-5.42	110.14	121.12
9	D	102	SPN	C27-C26-C25	-5.42	110.14	121.12
9	r	101	SPN	CM6-C18-C19	-5.42	109.78	123.68
9	p	101	SPN	CM5-C13-C12	-5.42	109.78	123.68
9	2	102	SPN	C17-C18-C19	-5.41	110.16	121.12
9	V	102	SPN	CM6-C18-C19	-5.41	109.80	123.68
9	v	102	SPN	CM8-C26-C25	-5.41	109.80	123.68
9	p	102	SPN	CM6-C18-C19	-5.41	109.80	123.68
9	r	103	SPN	CM8-C26-C25	-5.40	109.81	123.68
9	f	102	SPN	C14-C13-C12	-5.40	110.18	121.12
9	k	103	SPN	CM3-C5-C4	-5.40	109.82	123.68
8	L	304	BCL	C2D-C1D-ND	5.40	114.08	110.10
9	Q	102	SPN	C17-C18-C19	-5.40	110.19	121.12
9	M	404	SPN	C10-C9-C8	-5.40	110.19	121.12
9	R	102	SPN	C10-C9-C8	-5.40	110.20	121.12
8	f	101	BCL	C2D-C1D-ND	5.40	114.08	110.10
9	i	103	SPN	C14-C13-C12	-5.39	110.21	121.12
9	a	103	SPN	C10-C9-C8	-5.39	110.21	121.12
9	k	103	SPN	C14-C13-C12	-5.39	110.21	121.12
9	M	404	SPN	C6-C5-C4	-5.39	110.21	121.12
9	a	103	SPN	C6-C5-C4	-5.39	110.21	121.12
8	A	101	BCL	C2D-C1D-ND	5.39	114.07	110.10
9	k	103	SPN	CM6-C18-C19	-5.39	109.86	123.68
8	2	101	BCL	O2D-CGD-CBD	5.38	120.84	111.27
9	i	103	SPN	CM6-C18-C19	-5.37	109.91	123.68
8	p	103	BCL	O2D-CGD-CBD	5.37	120.81	111.27
8	I	102	BCL	C1C-NC-C4C	-5.36	104.30	106.71
8	a	102	BCL	C2D-C1D-ND	5.36	114.06	110.10
8	d	101	BCL	O2D-CGD-CBD	5.35	120.78	111.27
9	G	103	SPN	C6-C5-C4	-5.35	110.29	121.12
9	e	102	SPN	CM4-C9-C8	-5.35	109.95	123.68
8	E	101	BCL	C2D-C1D-ND	5.35	114.05	110.10
8	T	101	BCL	C2D-C1D-ND	5.35	114.04	110.10
9	e	102	SPN	CM6-C18-C19	-5.34	109.98	123.68
9	n	102	SPN	C10-C9-C8	-5.34	110.31	121.12
9	p	101	SPN	CM6-C18-C19	-5.34	109.98	123.68
8	G	102	BCL	O2D-CGD-CBD	5.34	120.75	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	N	101	BCL	C1C-NC-C4C	-5.33	104.31	106.71
9	r	103	SPN	C10-C9-C8	-5.33	110.33	121.12
8	P	101	BCL	C2D-C1D-ND	5.33	114.03	110.10
8	N	101	BCL	C2D-C1D-ND	5.33	114.03	110.10
8	J	101	BCL	C2D-C1D-ND	5.32	114.02	110.10
9	V	102	SPN	C10-C9-C8	-5.32	110.36	121.12
8	I	102	BCL	C2D-C1D-ND	5.31	114.02	110.10
8	G	101	BCL	C2D-C1D-ND	5.31	114.02	110.10
8	r	102	BCL	C2D-C1D-ND	5.31	114.02	110.10
9	p	102	SPN	CM5-C13-C12	-5.31	110.06	123.68
9	2	103	SPN	C10-C9-C8	-5.31	110.37	121.12
9	V	102	SPN	CM8-C26-C25	-5.31	110.06	123.68
8	l	101	BCL	C2D-C1D-ND	5.29	114.00	110.10
9	I	101	SPN	C17-C18-C19	-5.27	110.44	121.12
9	j	102	SPN	C27-C26-C25	-5.27	110.44	121.12
9	K	102	SPN	CM8-C26-C25	-5.27	110.15	123.68
8	b	101	BCL	C2D-C1D-ND	5.27	113.98	110.10
9	Q	102	SPN	C6-C5-C4	-5.26	110.47	121.12
8	E	101	BCL	O2D-CGD-CBD	5.26	120.62	111.27
9	v	102	SPN	CM6-C18-C19	-5.26	110.19	123.68
9	r	103	SPN	CM5-C13-C12	-5.26	110.19	123.68
9	p	101	SPN	C6-C5-C4	-5.25	110.48	121.12
9	a	104	SPN	CM8-C26-C25	-5.25	110.20	123.68
9	a	103	SPN	C14-C13-C12	-5.25	110.49	121.12
9	t	102	SPN	CM3-C5-C4	-5.24	110.22	123.68
9	R	102	SPN	C14-C13-C12	-5.24	110.51	121.12
9	E	102	SPN	C17-C18-C19	-5.24	110.52	121.12
8	G	102	BCL	C2D-C1D-ND	5.24	113.96	110.10
9	D	102	SPN	C17-C18-C19	-5.24	110.52	121.12
9	2	103	SPN	C27-C26-C25	-5.23	110.53	121.12
8	V	101	BCL	C2D-C1D-ND	5.23	113.96	110.10
9	j	102	SPN	C6-C5-C4	-5.23	110.53	121.12
8	j	101	BCL	C2D-C1D-ND	5.23	113.96	110.10
8	d	101	BCL	C2D-C1D-ND	5.23	113.95	110.10
9	r	103	SPN	C17-C18-C19	-5.21	110.57	121.12
9	G	103	SPN	C27-C26-C25	-5.20	110.59	121.12
9	S	102	SPN	C14-C13-C12	-5.20	110.60	121.12
8	J	101	BCL	O2D-CGD-CBD	5.19	120.50	111.27
8	F	101	BCL	O2D-CGD-CBD	5.19	120.49	111.27
9	q	101	SPN	C27-C26-C25	-5.19	110.61	121.12
8	d	101	BCL	C1C-NC-C4C	-5.19	104.37	106.71
9	M	404	SPN	C27-C26-C25	-5.18	110.64	121.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	Q	102	SPN	CM4-C9-C8	-5.17	110.41	123.68
9	b	102	SPN	C6-C5-C4	-5.17	110.66	121.12
8	R	103	BCL	C2D-C1D-ND	5.17	113.91	110.10
9	j	102	SPN	C10-C9-C8	-5.16	110.67	121.12
9	k	101	SPN	CM5-C13-C12	-5.16	110.44	123.68
9	F	102	SPN	C14-C13-C12	-5.16	110.68	121.12
8	F	101	BCL	C2D-C1D-ND	5.16	113.91	110.10
9	q	101	SPN	C17-C18-C19	-5.15	110.70	121.12
9	e	102	SPN	CM5-C13-C12	-5.14	110.50	123.68
8	K	101	BCL	C1C-NC-C4C	-5.13	104.40	106.71
9	b	102	SPN	C10-C9-C8	-5.13	110.74	121.12
8	G	101	BCL	O2D-CGD-CBD	5.11	120.35	111.27
9	F	102	SPN	C10-C9-C8	-5.11	110.78	121.12
9	b	102	SPN	C14-C13-C12	-5.10	110.80	121.12
8	L	304	BCL	CAC-C3C-C2C	-5.10	101.53	114.26
9	S	102	SPN	C17-C18-C19	-5.09	110.81	121.12
9	p	101	SPN	C27-C26-C25	-5.09	110.81	121.12
8	M	405	BCL	C2D-C1D-ND	5.09	113.86	110.10
8	L	304	BCL	O2D-CGD-CBD	5.09	120.31	111.27
9	D	103	SPN	C10-C9-C8	-5.08	110.83	121.12
9	S	101	SPN	C10-C9-C8	-5.08	110.83	121.12
9	S	101	SPN	C14-C13-C12	-5.07	110.85	121.12
9	K	102	SPN	C10-C9-C8	-5.04	110.91	121.12
8	e	101	BCL	CAC-C3C-C2C	-5.04	101.66	114.26
9	b	102	SPN	C21-C20-C19	5.04	125.53	112.23
8	M	405	BCL	CAC-C3C-C2C	-5.03	101.69	114.26
8	j	101	BCL	O2D-CGD-CBD	5.02	120.19	111.27
9	S	101	SPN	C6-C5-C4	-5.02	110.97	121.12
9	R	102	SPN	CM8-C26-C25	-5.01	110.82	123.68
8	e	101	BCL	C2D-C1D-ND	5.01	113.80	110.10
9	I	101	SPN	C6-C5-C4	-5.01	110.98	121.12
8	D	101	BCL	CAC-C3C-C2C	-4.99	101.79	114.26
8	f	101	BCL	O2D-CGD-CBD	4.96	120.08	111.27
8	k	102	BCL	O2D-CGD-CBD	4.94	120.05	111.27
9	D	102	SPN	C10-C9-C8	-4.94	111.12	121.12
8	q	102	BCL	O2D-CGD-CBD	4.93	120.03	111.27
8	n	101	BCL	O2D-CGD-CBD	4.93	120.03	111.27
8	d	101	BCL	CAC-C3C-C2C	-4.91	101.99	114.26
8	s	101	BCL	O2D-CGD-CBD	4.90	119.98	111.27
9	2	103	SPN	C6-C5-C4	-4.90	111.20	121.12
8	e	101	BCL	O2D-CGD-CBD	4.90	119.97	111.27
9	S	101	SPN	C17-C18-C19	-4.89	111.22	121.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	b	101	BCL	CAC-C3C-C2C	-4.89	102.04	114.26
8	A	101	BCL	O2D-CGD-CBD	4.88	119.95	111.27
8	b	101	BCL	O2D-CGD-CBD	4.88	119.94	111.27
8	G	101	BCL	CAC-C3C-C2C	-4.87	102.10	114.26
9	R	102	SPN	C6-C5-C4	-4.87	111.27	121.12
8	a	102	BCL	CAC-C3C-C2C	-4.86	102.11	114.26
8	Q	101	BCL	O2D-CGD-CBD	4.86	119.90	111.27
8	K	101	BCL	O2D-CGD-CBD	4.85	119.89	111.27
8	a	102	BCL	O2D-CGD-CBD	4.84	119.88	111.27
8	t	101	BCL	C1D-ND-C4D	-4.83	102.90	106.33
8	r	102	BCL	O2D-CGD-CBD	4.83	119.85	111.27
8	f	101	BCL	CAC-C3C-C2C	-4.82	102.22	114.26
9	E	102	SPN	C10-C9-C8	-4.82	111.37	121.12
8	v	101	BCL	O2D-CGD-CBD	4.81	119.82	111.27
8	B	101	BCL	CAC-C3C-C2C	-4.81	102.23	114.26
8	2	101	BCL	CAC-C3C-C2C	-4.80	102.26	114.26
8	V	101	BCL	CAC-C3C-C2C	-4.80	102.27	114.26
8	r	102	BCL	CAC-C3C-C2C	-4.79	102.28	114.26
8	V	101	BCL	O2D-CGD-CBD	4.79	119.78	111.27
8	B	101	BCL	O2D-CGD-CBD	4.79	119.78	111.27
8	i	102	BCL	CAC-C3C-C2C	-4.78	102.30	114.26
8	L	304	BCL	C1C-NC-C4C	-4.78	104.56	106.71
9	S	101	SPN	C28-C29-C30	-4.77	111.43	127.75
8	k	102	BCL	CAC-C3C-C2C	-4.77	102.33	114.26
8	L	301	BCL	CAC-C3C-C2C	-4.76	102.37	114.26
8	P	101	BCL	CAC-C3C-C2C	-4.76	102.37	114.26
8	R	101	BCL	CAC-C3C-C2C	-4.75	102.38	114.26
8	P	101	BCL	O2D-CGD-CBD	4.75	119.71	111.27
8	p	103	BCL	CAC-C3C-C2C	-4.74	102.41	114.26
8	T	101	BCL	C1C-NC-C4C	-4.74	104.57	106.71
8	j	101	BCL	CAC-C3C-C2C	-4.74	102.42	114.26
8	t	101	BCL	O2D-CGD-CBD	4.73	119.68	111.27
9	i	101	SPN	CM3-C5-C4	-4.73	111.54	123.68
8	D	101	BCL	O2D-CGD-CBD	4.73	119.67	111.27
8	n	101	BCL	CAC-C3C-C2C	-4.71	102.48	114.26
8	R	103	BCL	O2D-CGD-CBD	4.71	119.64	111.27
8	v	101	BCL	CAC-C3C-C2C	-4.70	102.51	114.26
8	s	101	BCL	CAC-C3C-C2C	-4.70	102.51	114.26
8	q	102	BCL	CAC-C3C-C2C	-4.70	102.51	114.26
8	l	101	BCL	O2D-CGD-CBD	4.70	119.62	111.27
9	R	102	SPN	C17-C18-C19	-4.70	111.61	121.12
8	Q	101	BCL	CAC-C3C-C2C	-4.70	102.52	114.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	F	102	SPN	C6-C5-C4	-4.70	111.61	121.12
8	N	101	BCL	O2D-CGD-CBD	4.69	119.60	111.27
8	A	101	BCL	CAC-C3C-C2C	-4.68	102.57	114.26
8	M	402	BCL	CAC-C3C-C2C	-4.65	102.64	114.26
8	F	101	BCL	C1C-NC-C4C	-4.65	104.62	106.71
8	R	101	BCL	O2D-CGD-CBD	4.64	119.51	111.27
9	V	102	SPN	C28-C29-C30	-4.63	111.93	127.75
8	t	101	BCL	C1C-NC-C4C	-4.61	104.63	106.71
9	Q	102	SPN	C28-C29-C30	-4.61	112.00	127.75
8	T	101	BCL	O2D-CGD-CBD	4.61	119.45	111.27
9	S	101	SPN	C27-C26-C25	-4.60	111.81	121.12
8	G	102	BCL	C1C-NC-C4C	-4.60	104.64	106.71
8	L	301	BCL	C4A-NA-C1A	-4.60	104.64	106.71
9	e	102	SPN	C28-C29-C30	-4.60	112.05	127.75
9	r	101	SPN	C28-C29-C30	-4.59	112.05	127.75
8	E	101	BCL	C1C-NC-C4C	-4.59	104.64	106.71
9	a	104	SPN	C28-C29-C30	-4.59	112.07	127.75
8	T	101	BCL	CAC-C3C-C2C	-4.58	102.82	114.26
9	i	101	SPN	CM5-C13-C12	-4.56	111.97	123.68
8	R	103	BCL	CAC-C3C-C2C	-4.55	102.89	114.26
8	J	101	BCL	C1C-NC-C4C	-4.55	104.66	106.71
8	M	405	BCL	CMB-C2B-C1B	-4.54	118.45	125.37
8	i	102	BCL	O2D-CGD-O1D	-4.54	114.96	123.84
9	f	102	SPN	C28-C29-C30	-4.54	112.23	127.75
8	j	101	BCL	CMB-C2B-C1B	-4.52	118.49	125.37
8	J	101	BCL	CAC-C3C-C2C	-4.51	102.98	114.26
9	a	101	SPN	C28-C29-C30	-4.51	112.33	127.75
9	k	101	SPN	C28-C29-C30	-4.51	112.35	127.75
9	E	102	SPN	C6-C5-C4	-4.50	112.00	121.12
8	R	103	BCL	C1C-NC-C4C	-4.50	104.68	106.71
8	L	304	BCL	CMB-C2B-C1B	-4.49	118.53	125.37
8	d	101	BCL	CMB-C2B-C1B	-4.49	118.53	125.37
8	M	405	BCL	CHD-C1D-ND	-4.48	120.34	124.45
8	d	101	BCL	O2D-CGD-O1D	-4.48	115.09	123.84
8	e	101	BCL	CMB-C2B-C1B	-4.46	118.57	125.37
9	b	102	SPN	C28-C29-C30	-4.46	112.52	127.75
9	G	104	SPN	C28-C29-C30	-4.46	112.52	127.75
8	N	101	BCL	CAC-C3C-C2C	-4.45	103.13	114.26
9	i	103	SPN	C28-C29-C30	-4.45	112.55	127.75
9	k	103	SPN	C28-C29-C30	-4.44	112.56	127.75
8	i	102	BCL	CMB-C2B-C1B	-4.44	118.61	125.37
8	p	103	BCL	O2D-CGD-O1D	-4.44	115.16	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	K	101	BCL	CMB-C2B-C1B	-4.43	118.61	125.37
9	F	102	SPN	C28-C29-C30	-4.43	112.60	127.75
8	K	101	BCL	CAC-C3C-C2C	-4.43	103.18	114.26
8	t	101	BCL	C2D-C1D-ND	4.43	113.37	110.10
8	G	102	BCL	CAC-C3C-C2C	-4.43	103.19	114.26
9	b	102	SPN	CM6-C18-C19	-4.41	112.36	123.68
9	K	102	SPN	C28-C29-C30	-4.41	112.68	127.75
8	I	102	BCL	CAC-C3C-C2C	-4.40	103.25	114.26
9	2	103	SPN	C28-C29-C30	-4.40	112.70	127.75
9	t	102	SPN	C28-C29-C30	-4.40	112.72	127.75
9	D	102	SPN	C6-C5-C4	-4.40	112.22	121.12
9	R	102	SPN	C28-C29-C30	-4.39	112.73	127.75
8	E	101	BCL	O2D-CGD-O1D	-4.39	115.25	123.84
8	J	101	BCL	CMB-C2B-C1B	-4.39	118.68	125.37
8	F	101	BCL	CAC-C3C-C2C	-4.39	103.29	114.26
8	1	101	BCL	CMB-C2B-C1B	-4.38	118.70	125.37
8	b	101	BCL	CMB-C2B-C1B	-4.37	118.71	125.37
8	t	101	BCL	CAC-C3C-C2C	-4.37	103.33	114.26
8	E	101	BCL	CAC-C3C-C2C	-4.37	103.35	114.26
8	I	102	BCL	O2D-CGD-O1D	-4.37	115.30	123.84
9	b	102	SPN	C17-C18-C19	-4.37	112.28	121.12
8	F	101	BCL	O2D-CGD-O1D	-4.37	115.30	123.84
8	I	102	BCL	CMB-C2B-C1B	-4.36	118.73	125.37
9	S	102	SPN	C6-C5-C4	-4.36	112.30	121.12
8	G	102	BCL	CMB-C2B-C1B	-4.35	118.74	125.37
8	2	101	BCL	O2D-CGD-O1D	-4.35	115.34	123.84
8	M	402	BCL	O2D-CGD-CBD	4.35	118.99	111.27
8	2	101	BCL	CMB-C2B-C1B	-4.34	118.76	125.37
8	q	102	BCL	CMB-C2B-C1B	-4.34	118.76	125.37
8	F	101	BCL	CMB-C2B-C1B	-4.33	118.77	125.37
8	T	101	BCL	CMB-C2B-C1B	-4.33	118.77	125.37
8	f	101	BCL	CMB-C2B-C1B	-4.32	118.79	125.37
8	G	102	BCL	O2D-CGD-O1D	-4.31	115.40	123.84
9	a	103	SPN	C28-C29-C30	-4.31	113.02	127.75
9	j	102	SPN	C28-C29-C30	-4.31	113.03	127.75
8	N	101	BCL	CMB-C2B-C1B	-4.30	118.82	125.37
8	E	101	BCL	CMB-C2B-C1B	-4.30	118.82	125.37
8	P	101	BCL	CMB-C2B-C1B	-4.29	118.83	125.37
8	G	101	BCL	CMB-C2B-C1B	-4.29	118.84	125.37
8	t	101	BCL	CHD-C1D-ND	-4.29	120.51	124.45
8	R	103	BCL	CMB-C2B-C1B	-4.27	118.86	125.37
8	L	301	BCL	O2D-CGD-CBD	4.27	118.86	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	q	101	SPN	CM8-C26-C27	-4.26	108.10	115.27
9	p	102	SPN	C28-C29-C30	-4.26	113.19	127.75
8	R	101	BCL	CMB-C2B-C1B	-4.26	118.88	125.37
8	J	101	BCL	O2D-CGD-O1D	-4.25	115.53	123.84
8	D	101	BCL	CMB-C2B-C1B	-4.25	118.90	125.37
8	s	101	BCL	CMB-C2B-C1B	-4.25	118.90	125.37
8	M	402	BCL	CMB-C2B-C1B	-4.24	118.91	125.37
9	r	103	SPN	C28-C29-C30	-4.24	113.26	127.75
8	G	101	BCL	O2D-CGD-O1D	-4.24	115.55	123.84
8	L	304	BCL	O2D-CGD-O1D	-4.24	115.56	123.84
8	a	102	BCL	CMB-C2B-C1B	-4.23	118.92	125.37
9	p	101	SPN	C28-C29-C30	-4.23	113.30	127.75
8	v	101	BCL	CMB-C2B-C1B	-4.23	118.93	125.37
10	L	307	MW9	O8-C24-C25	4.22	120.60	111.50
9	2	102	SPN	C28-C29-C30	-4.22	113.33	127.75
8	p	103	BCL	CHB-C1B-NB	4.22	128.72	124.26
8	L	301	BCL	CMB-C2B-C1B	-4.22	118.95	125.37
9	i	101	SPN	C28-C29-C30	-4.22	113.34	127.75
8	Q	101	BCL	CMB-C2B-C1B	-4.21	118.96	125.37
9	I	101	SPN	C28-C29-C30	-4.21	113.37	127.75
9	S	102	SPN	C28-C29-C30	-4.20	113.41	127.75
8	B	101	BCL	CMB-C2B-C1B	-4.19	118.99	125.37
10	G	105	MW9	O8-C24-C25	4.19	120.52	111.50
9	E	102	SPN	C28-C29-C30	-4.19	113.45	127.75
8	f	101	BCL	O2D-CGD-O1D	-4.18	115.66	123.84
9	i	103	SPN	CM9-C30-C29	-4.17	110.59	122.65
9	i	101	SPN	CMB-C30-C29	-4.17	110.59	122.65
8	j	101	BCL	O2D-CGD-O1D	-4.17	115.68	123.84
8	d	101	BCL	C2B-C1B-NB	-4.17	107.44	110.23
9	a	101	SPN	CM9-C30-C29	-4.16	110.63	122.65
8	e	101	BCL	O2D-CGD-O1D	-4.16	115.71	123.84
8	q	102	BCL	O2D-CGD-O1D	-4.15	115.72	123.84
9	K	102	SPN	CM4-C9-C10	-4.15	108.29	115.27
9	2	102	SPN	CM9-C30-C29	-4.15	110.66	122.65
9	G	104	SPN	CMB-C30-C29	-4.15	110.66	122.65
9	M	404	SPN	C28-C29-C30	-4.14	113.58	127.75
9	a	101	SPN	CMB-C30-C29	-4.14	110.68	122.65
9	p	102	SPN	CMB-C30-C29	-4.14	110.68	122.65
8	l	101	BCL	CAC-C3C-C2C	-4.14	103.92	114.26
8	k	102	BCL	CMB-C2B-C1B	-4.14	119.07	125.37
8	r	102	BCL	O2D-CGD-O1D	-4.13	115.76	123.84
8	k	102	BCL	O2D-CGD-O1D	-4.13	115.77	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	s	101	BCL	O2D-CGD-O1D	-4.13	115.77	123.84
10	H	302	MW9	O8-C24-C25	4.13	120.39	111.50
10	M	408	MW9	O8-C24-C25	4.12	120.39	111.50
9	f	102	SPN	CM9-C30-C29	-4.12	110.74	122.65
15	H	303	CDL	OB6-CB5-C51	4.12	120.38	111.50
10	M	407	MW9	O8-C24-C25	4.12	120.38	111.50
9	D	103	SPN	C28-C29-C30	-4.12	113.68	127.75
8	n	101	BCL	O2D-CGD-O1D	-4.11	115.80	123.84
9	r	101	SPN	CMB-C30-C29	-4.11	110.76	122.65
8	b	101	BCL	O2D-CGD-O1D	-4.10	115.82	123.84
8	A	101	BCL	O2D-CGD-O1D	-4.10	115.82	123.84
8	B	101	BCL	O2D-CGD-O1D	-4.10	115.83	123.84
8	r	102	BCL	CHB-C1B-NB	4.09	128.59	124.26
9	r	101	SPN	CM9-C30-C29	-4.09	110.83	122.65
9	v	102	SPN	C28-C29-C30	-4.09	113.78	127.75
8	Q	101	BCL	O2D-CGD-O1D	-4.08	115.86	123.84
15	H	304	CDL	OB6-CB5-C51	4.08	120.29	111.50
9	n	102	SPN	C6-C5-C4	-4.08	112.86	121.12
9	a	104	SPN	CM4-C9-C10	-4.08	108.41	115.27
9	q	101	SPN	CMB-C30-C29	-4.08	110.86	122.65
8	K	101	BCL	O2D-CGD-O1D	-4.08	115.87	123.84
10	F	104	MW9	O8-C24-C25	4.07	120.28	111.50
8	P	101	BCL	O2D-CGD-O1D	-4.07	115.88	123.84
9	r	103	SPN	CMB-C30-C29	-4.07	110.88	122.65
8	V	101	BCL	O2D-CGD-O1D	-4.07	115.88	123.84
8	t	101	BCL	O2D-CGD-O1D	-4.07	115.89	123.84
8	t	101	BCL	OB6-CAB-CBB	-4.06	110.73	119.73
9	Q	102	SPN	CM9-C30-C29	-4.06	110.91	122.65
8	a	102	BCL	O2D-CGD-O1D	-4.06	115.90	123.84
9	e	102	SPN	CM9-C30-C29	-4.06	110.92	122.65
9	v	102	SPN	CMB-C30-C29	-4.06	110.92	122.65
8	D	101	BCL	O2D-CGD-O1D	-4.06	115.91	123.84
8	v	101	BCL	O2D-CGD-O1D	-4.05	115.91	123.84
8	M	402	BCL	CHD-C1D-ND	-4.05	120.73	124.45
9	F	102	SPN	CMB-C30-C29	-4.04	110.97	122.65
8	R	103	BCL	O2D-CGD-O1D	-4.04	115.94	123.84
10	B	102	MW9	O8-C24-C25	4.04	120.21	111.50
9	D	103	SPN	CMB-C30-C29	-4.03	110.99	122.65
8	n	101	BCL	CHB-C1B-NB	4.03	128.53	124.26
10	L	308	MW9	O8-C24-C25	4.03	120.19	111.50
9	e	102	SPN	CMB-C30-C29	-4.03	111.00	122.65
8	1	101	BCL	C2C-C3C-C4C	-4.03	95.31	101.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	n	102	SPN	C28-C29-C30	-4.02	114.00	127.75
9	t	102	SPN	CMB-C30-C29	-4.02	111.03	122.65
9	f	102	SPN	CMB-C30-C29	-4.02	111.03	122.65
8	R	101	BCL	O2D-CGD-O1D	-4.02	115.99	123.84
9	Q	102	SPN	CMB-C30-C29	-4.01	111.06	122.65
8	l	101	BCL	O2D-CGD-O1D	-4.01	116.01	123.84
15	H	303	CDL	OA6-CA5-C11	4.00	120.13	111.50
8	T	101	BCL	O2D-CGD-O1D	-3.99	116.03	123.84
8	A	101	BCL	CHB-C1B-NB	3.99	128.48	124.26
9	k	101	SPN	CMB-C30-C29	-3.99	111.11	122.65
9	D	102	SPN	C28-C29-C30	-3.99	114.12	127.75
8	N	101	BCL	O2D-CGD-O1D	-3.99	116.04	123.84
10	I	103	MW9	O8-C24-C25	3.99	120.09	111.50
9	G	103	SPN	CMB-C30-C29	-3.99	111.12	122.65
8	F	101	BCL	CHD-C1D-ND	-3.98	120.79	124.45
9	a	104	SPN	CMB-C30-C29	-3.97	111.17	122.65
9	R	102	SPN	CM9-C30-C29	-3.96	111.19	122.65
10	D	104	MW9	O8-C24-C25	3.96	120.04	111.50
8	M	402	BCL	O2D-CGD-O1D	-3.96	116.10	123.84
9	k	103	SPN	CMB-C30-C29	-3.96	111.21	122.65
8	L	301	BCL	O2D-CGD-O1D	-3.96	116.11	123.84
8	V	101	BCL	CMB-C2B-C1B	-3.95	119.35	125.37
9	i	103	SPN	CMB-C30-C29	-3.95	111.22	122.65
10	Q	103	MW9	O8-C24-C25	3.95	120.02	111.50
8	i	102	BCL	CHB-C1B-NB	3.95	128.44	124.26
9	n	102	SPN	CM5-C13-C14	-3.95	108.63	115.27
9	2	102	SPN	CMB-C30-C29	-3.94	111.25	122.65
9	n	102	SPN	CM4-C9-C10	-3.94	108.64	115.27
9	F	102	SPN	CM5-C13-C14	-3.94	108.65	115.27
9	a	104	SPN	CM9-C30-C29	-3.94	111.27	122.65
9	b	102	SPN	CM9-C30-C29	-3.93	111.28	122.65
8	e	101	BCL	CHB-C1B-NB	3.93	128.41	124.26
8	j	101	BCL	C1C-NC-C4C	-3.92	104.94	106.71
9	M	404	SPN	CMB-C30-C29	-3.92	111.32	122.65
10	F	103	MW9	O8-C24-C25	3.92	119.94	111.50
8	j	101	BCL	CHB-C1B-NB	3.91	128.40	124.26
9	a	103	SPN	CMB-C30-C29	-3.91	111.35	122.65
8	G	102	BCL	CHD-C1D-ND	-3.91	120.86	124.45
9	F	102	SPN	CM9-C30-C29	-3.90	111.38	122.65
9	j	102	SPN	CM4-C9-C10	-3.90	108.72	115.27
9	F	102	SPN	CM3-C5-C6	-3.90	108.72	115.27
9	V	102	SPN	CM6-C18-C17	-3.89	108.72	115.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	404	SPN	CM5-C13-C14	-3.89	108.73	115.27
9	E	102	SPN	CMB-C30-C29	-3.89	111.41	122.65
9	t	102	SPN	CM9-C30-C29	-3.88	111.42	122.65
8	b	101	BCL	CHB-C1B-NB	3.88	128.36	124.26
9	2	103	SPN	CMB-C30-C29	-3.88	111.44	122.65
9	q	101	SPN	C28-C29-C30	-3.88	114.51	127.75
8	L	304	BCL	CHB-C1B-NB	3.87	128.36	124.26
9	G	103	SPN	C28-C29-C30	-3.87	114.51	127.75
15	H	304	CDL	OA6-CA5-C11	3.87	119.85	111.50
9	q	101	SPN	C20-C19-C18	-3.87	118.35	127.66
9	j	102	SPN	CM9-C30-C29	-3.86	111.50	122.65
9	b	102	SPN	CMB-C30-C29	-3.86	111.50	122.65
9	I	101	SPN	CMB-C30-C29	-3.85	111.51	122.65
9	S	102	SPN	CM4-C9-C10	-3.85	108.79	115.27
8	E	101	BCL	CHD-C1D-ND	-3.85	120.92	124.45
9	R	102	SPN	CMB-C30-C29	-3.85	111.53	122.65
9	n	102	SPN	CMB-C30-C29	-3.84	111.54	122.65
9	G	103	SPN	CM4-C9-C10	-3.84	108.81	115.27
9	2	103	SPN	CM9-C30-C29	-3.84	111.56	122.65
8	V	101	BCL	OBB-CAB-CBB	-3.84	111.23	119.73
9	k	103	SPN	CM9-C30-C29	-3.83	111.57	122.65
9	j	102	SPN	CMB-C30-C29	-3.83	111.58	122.65
8	2	101	BCL	CHB-C1B-NB	3.82	128.30	124.26
9	V	102	SPN	CM9-C30-C29	-3.82	111.61	122.65
8	M	402	BCL	C1C-NC-C4C	-3.82	104.99	106.71
9	a	101	SPN	CM4-C9-C10	-3.82	108.85	115.27
9	G	104	SPN	CM9-C30-C29	-3.82	111.62	122.65
9	D	102	SPN	CMB-C30-C29	-3.82	111.62	122.65
9	b	102	SPN	CM4-C9-C10	-3.82	108.85	115.27
9	I	101	SPN	CM6-C18-C17	-3.81	108.85	115.27
9	k	101	SPN	CM9-C30-C29	-3.81	111.64	122.65
8	q	102	BCL	CHB-C1B-NB	3.81	128.29	124.26
8	a	102	BCL	CHB-C1B-NB	3.81	128.29	124.26
9	R	102	SPN	CM4-C9-C10	-3.81	108.87	115.27
9	a	104	SPN	CM8-C26-C27	-3.80	108.87	115.27
9	K	102	SPN	CMB-C30-C29	-3.80	111.66	122.65
9	E	102	SPN	CM9-C30-C29	-3.80	111.68	122.65
8	K	101	BCL	CHB-C1B-NB	3.80	128.28	124.26
9	S	102	SPN	CMB-C30-C29	-3.79	111.68	122.65
8	F	101	BCL	CHB-C1B-NB	3.79	128.27	124.26
9	S	101	SPN	CM5-C13-C14	-3.79	108.89	115.27
8	k	102	BCL	OBB-CAB-CBB	-3.79	111.33	119.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	V	102	SPN	CM8-C26-C27	-3.79	108.90	115.27
9	p	102	SPN	CM6-C18-C17	-3.79	108.90	115.27
8	G	101	BCL	CHB-C1B-NB	3.79	128.26	124.26
9	G	104	SPN	CM6-C18-C17	-3.78	108.91	115.27
9	p	101	SPN	CM8-C26-C27	-3.77	108.92	115.27
8	M	405	BCL	O2D-CGD-O1D	-3.77	116.47	123.84
8	R	101	BCL	CHD-C1D-ND	-3.77	120.99	124.45
9	D	102	SPN	CM3-C5-C6	-3.76	108.94	115.27
8	n	101	BCL	CHD-C1D-ND	-3.76	121.00	124.45
8	v	101	BCL	CHB-C1B-NB	3.76	128.24	124.26
8	G	101	BCL	OBB-CAB-CBB	-3.76	111.41	119.73
8	L	304	BCL	OBB-CAB-CBB	-3.75	111.41	119.73
8	I	102	BCL	CHD-C1D-ND	-3.75	121.00	124.45
8	e	101	BCL	OBB-CAB-CBB	-3.75	111.41	119.73
9	i	101	SPN	CM9-C30-C29	-3.75	111.82	122.65
8	f	101	BCL	OBB-CAB-CBB	-3.74	111.43	119.73
9	S	101	SPN	CM4-C9-C10	-3.74	108.97	115.27
8	T	101	BCL	CHB-C1B-NB	3.74	128.22	124.26
8	L	301	BCL	OBB-CAB-CBB	-3.74	111.43	119.73
9	2	103	SPN	CM8-C26-C27	-3.74	108.97	115.27
8	s	101	BCL	CHB-C1B-NB	3.74	128.22	124.26
8	M	402	BCL	OBB-CAB-CBB	-3.74	111.44	119.73
9	E	102	SPN	CM4-C9-C10	-3.74	108.98	115.27
8	a	102	BCL	OBB-CAB-CBB	-3.74	111.45	119.73
9	t	102	SPN	CM4-C9-C10	-3.73	108.99	115.27
9	a	104	SPN	CM3-C5-C6	-3.73	108.99	115.27
9	p	102	SPN	CM9-C30-C29	-3.73	111.86	122.65
9	D	103	SPN	CM9-C30-C29	-3.73	111.87	122.65
8	D	101	BCL	C1C-NC-C4C	-3.73	105.03	106.71
8	L	301	BCL	CHD-C1D-ND	-3.72	121.03	124.45
8	v	101	BCL	OBB-CAB-CBB	-3.72	111.48	119.73
9	q	101	SPN	CM4-C9-C10	-3.72	109.01	115.27
9	R	102	SPN	CM5-C13-C14	-3.72	109.01	115.27
8	b	101	BCL	OBB-CAB-CBB	-3.72	111.50	119.73
8	s	101	BCL	OBB-CAB-CBB	-3.71	111.50	119.73
8	R	103	BCL	OBB-CAB-CBB	-3.71	111.51	119.73
8	D	101	BCL	CHD-C1D-ND	-3.71	121.04	124.45
9	F	102	SPN	CM8-C26-C27	-3.71	109.03	115.27
9	K	102	SPN	CM9-C30-C29	-3.71	111.93	122.65
9	S	102	SPN	CM3-C5-C6	-3.71	109.04	115.27
8	G	102	BCL	OBB-CAB-CBB	-3.70	111.52	119.73
8	P	101	BCL	OBB-CAB-CBB	-3.70	111.53	119.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	p	103	BCL	CMB-C2B-C1B	-3.70	119.73	125.37
8	M	402	BCL	CHB-C1B-NB	3.70	128.17	124.26
9	t	102	SPN	CM8-C26-C27	-3.70	109.05	115.27
8	B	101	BCL	CHD-C1D-ND	-3.70	121.06	124.45
9	M	404	SPN	CM8-C26-C27	-3.69	109.06	115.27
8	a	102	BCL	CHD-C1D-ND	-3.69	121.06	124.45
9	e	102	SPN	CM4-C9-C10	-3.69	109.06	115.27
9	r	103	SPN	CM9-C30-C29	-3.69	111.99	122.65
8	q	102	BCL	OBB-CAB-CBB	-3.69	111.56	119.73
8	f	101	BCL	CHB-C1B-NB	3.69	128.16	124.26
8	I	102	BCL	OBB-CAB-CBB	-3.68	111.57	119.73
8	L	301	BCL	C1C-NC-C4C	-3.68	105.05	106.71
9	a	103	SPN	CM9-C30-C29	-3.68	112.01	122.65
8	R	101	BCL	OBB-CAB-CBB	-3.68	111.58	119.73
9	j	102	SPN	CM8-C26-C27	-3.68	109.09	115.27
8	B	101	BCL	OBB-CAB-CBB	-3.67	111.59	119.73
9	q	101	SPN	CM6-C18-C17	-3.67	109.09	115.27
8	2	101	BCL	OBB-CAB-CBB	-3.67	111.59	119.73
9	r	101	SPN	CM6-C18-C17	-3.67	109.09	115.27
9	G	104	SPN	CM8-C26-C27	-3.67	109.09	115.27
8	F	101	BCL	OBB-CAB-CBB	-3.67	111.59	119.73
9	V	102	SPN	CMB-C30-C29	-3.67	112.05	122.65
8	M	405	BCL	O2D-CGD-CBD	3.67	117.78	111.27
8	Q	101	BCL	OBB-CAB-CBB	-3.67	111.60	119.73
8	q	102	BCL	CHD-C1D-ND	-3.67	121.08	124.45
9	R	102	SPN	CM3-C5-C6	-3.67	109.10	115.27
9	E	102	SPN	CM5-C13-C14	-3.66	109.11	115.27
8	e	101	BCL	CHD-C1D-ND	-3.66	121.09	124.45
8	n	101	BCL	OBB-CAB-CBB	-3.66	111.61	119.73
9	q	101	SPN	CM9-C30-C29	-3.66	112.06	122.65
8	J	101	BCL	OBB-CAB-CBB	-3.66	111.61	119.73
8	j	101	BCL	OBB-CAB-CBB	-3.66	111.61	119.73
8	N	101	BCL	OBB-CAB-CBB	-3.66	111.62	119.73
9	I	101	SPN	C20-C19-C18	-3.66	118.85	127.66
8	P	101	BCL	CHD-C1D-ND	-3.66	121.09	124.45
8	A	101	BCL	OBB-CAB-CBB	-3.66	111.62	119.73
9	I	101	SPN	CM3-C5-C6	-3.66	109.12	115.27
9	p	101	SPN	CM5-C13-C14	-3.65	109.12	115.27
8	r	102	BCL	OBB-CAB-CBB	-3.65	111.63	119.73
9	r	101	SPN	CM8-C26-C27	-3.65	109.13	115.27
8	l	101	BCL	OBB-CAB-CBB	-3.65	111.64	119.73
8	E	101	BCL	OBB-CAB-CBB	-3.65	111.64	119.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	a	101	SPN	CM8-C26-C27	-3.65	109.14	115.27
8	G	102	BCL	CHB-C1B-NB	3.65	128.12	124.26
9	i	103	SPN	CM6-C18-C17	-3.65	109.14	115.27
8	N	101	BCL	CHD-C1D-ND	-3.65	121.10	124.45
8	T	101	BCL	OBB-CAB-CBB	-3.65	111.65	119.73
9	M	404	SPN	CM4-C9-C10	-3.64	109.14	115.27
8	L	301	BCL	CHB-C1B-NB	3.64	128.11	124.26
9	S	101	SPN	CM8-C26-C27	-3.64	109.15	115.27
9	p	101	SPN	CM4-C9-C10	-3.64	109.15	115.27
9	2	103	SPN	CM4-C9-C10	-3.64	109.15	115.27
9	i	101	SPN	CM8-C26-C27	-3.64	109.15	115.27
9	D	103	SPN	CM6-C18-C17	-3.64	109.15	115.27
8	R	103	BCL	CHB-C1B-NB	3.63	128.10	124.26
9	Q	102	SPN	CM6-C18-C17	-3.63	109.16	115.27
9	2	102	SPN	CM6-C18-C17	-3.63	109.16	115.27
9	2	102	SPN	CM5-C13-C14	-3.63	109.17	115.27
9	a	101	SPN	CM3-C5-C6	-3.63	109.17	115.27
9	a	103	SPN	CM8-C26-C27	-3.63	109.17	115.27
8	I	102	BCL	CHB-C1B-NB	3.63	128.09	124.26
8	2	101	BCL	CHD-C1D-ND	-3.62	121.12	124.45
8	r	102	BCL	CMB-C2B-C1B	-3.62	119.85	125.37
8	p	103	BCL	OBB-CAB-CBB	-3.62	111.70	119.73
8	K	101	BCL	OBB-CAB-CBB	-3.62	111.70	119.73
8	k	102	BCL	CHB-C1B-NB	3.62	128.09	124.26
8	t	101	BCL	CHA-C1A-NA	-3.62	118.11	126.40
8	E	101	BCL	CHB-C1B-NB	3.61	128.08	124.26
9	R	102	SPN	C20-C19-C18	-3.61	118.96	127.66
8	i	102	BCL	OBB-CAB-CBB	-3.61	111.72	119.73
8	b	101	BCL	CHD-C1D-ND	-3.61	121.13	124.45
9	r	103	SPN	CM4-C9-C10	-3.61	109.19	115.27
8	Q	101	BCL	CHD-C1D-ND	-3.61	121.14	124.45
8	J	101	BCL	CHB-C1B-NB	3.61	128.08	124.26
9	a	103	SPN	CM4-C9-C10	-3.61	109.20	115.27
8	L	304	BCL	CHD-C1D-ND	-3.61	121.14	124.45
9	k	103	SPN	CM6-C18-C17	-3.61	109.20	115.27
8	1	101	BCL	CHB-C1B-NB	3.61	128.08	124.26
8	j	101	BCL	CHD-C1D-ND	-3.61	121.14	124.45
8	f	101	BCL	CHD-C1D-ND	-3.61	121.14	124.45
9	V	102	SPN	CM4-C9-C10	-3.60	109.21	115.27
9	F	102	SPN	CM4-C9-C10	-3.60	109.21	115.27
9	v	102	SPN	CM5-C13-C14	-3.60	109.22	115.27
8	J	101	BCL	CHD-C1D-ND	-3.60	121.15	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	K	101	BCL	CHD-C1D-ND	-3.60	121.15	124.45
8	n	101	BCL	C16-C15-C13	-3.60	104.30	115.92
9	p	101	SPN	CMB-C30-C29	-3.59	112.26	122.65
8	D	101	BCL	OBB-CAB-CBB	-3.59	111.78	119.73
9	Q	102	SPN	C20-C19-C18	-3.59	119.02	127.66
8	A	101	BCL	CHD-C1D-ND	-3.59	121.16	124.45
8	i	102	BCL	CHD-C1D-ND	-3.58	121.16	124.45
8	e	101	BCL	C1C-NC-C4C	-3.58	105.09	106.71
9	p	102	SPN	CM3-C5-C6	-3.58	109.25	115.27
8	M	405	BCL	OBB-CAB-CBB	-3.58	111.80	119.73
8	r	102	BCL	CHD-C1D-ND	-3.58	121.17	124.45
9	D	102	SPN	CM8-C26-C27	-3.57	109.26	115.27
8	i	102	BCL	C16-C15-C13	-3.57	104.37	115.92
8	R	101	BCL	CHB-C1B-NB	3.57	128.04	124.26
9	2	103	SPN	CM3-C5-C6	-3.57	109.27	115.27
9	v	102	SPN	CM9-C30-C29	-3.57	112.33	122.65
9	M	404	SPN	CM9-C30-C29	-3.57	112.33	122.65
9	R	102	SPN	CM8-C26-C27	-3.57	109.27	115.27
9	I	101	SPN	CM9-C30-C29	-3.57	112.34	122.65
9	G	103	SPN	CM8-C26-C27	-3.57	109.27	115.27
9	i	103	SPN	CM3-C5-C6	-3.56	109.29	115.27
9	b	102	SPN	CM5-C13-C14	-3.55	109.29	115.27
9	v	102	SPN	CM8-C26-C27	-3.55	109.30	115.27
9	Q	102	SPN	CM5-C13-C14	-3.55	109.30	115.27
9	e	102	SPN	CM8-C26-C27	-3.55	109.30	115.27
8	k	102	BCL	CHD-C1D-ND	-3.55	121.20	124.45
8	p	103	BCL	CHD-C1D-ND	-3.54	121.20	124.45
9	Q	102	SPN	CM8-C26-C27	-3.54	109.32	115.27
8	R	103	BCL	CHD-C1D-ND	-3.54	121.20	124.45
8	1	101	BCL	CHD-C1D-ND	-3.54	121.20	124.45
9	R	102	SPN	CM6-C18-C17	-3.54	109.32	115.27
9	V	102	SPN	CM5-C13-C14	-3.53	109.33	115.27
9	2	103	SPN	C20-C19-C18	-3.53	119.16	127.66
9	i	101	SPN	CM3-C5-C6	-3.53	109.33	115.27
9	k	101	SPN	CM4-C9-C10	-3.53	109.34	115.27
9	V	102	SPN	CM3-C5-C6	-3.53	109.34	115.27
9	S	102	SPN	CM9-C30-C29	-3.52	112.47	122.65
9	r	103	SPN	CM3-C5-C6	-3.52	109.35	115.27
9	Q	102	SPN	CM4-C9-C10	-3.52	109.36	115.27
9	G	104	SPN	CM5-C13-C14	-3.51	109.36	115.27
8	Q	101	BCL	CHB-C1B-NB	3.51	127.98	124.26
9	f	102	SPN	CM8-C26-C27	-3.51	109.36	115.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	103	SPN	CM4-C9-C10	-3.51	109.37	115.27
9	n	102	SPN	CM3-C5-C6	-3.51	109.37	115.27
9	2	103	SPN	CM6-C18-C17	-3.50	109.38	115.27
8	B	101	BCL	CHB-C1B-NB	3.50	127.97	124.26
9	G	103	SPN	CM9-C30-C29	-3.50	112.52	122.65
9	j	102	SPN	CM6-C18-C17	-3.50	109.38	115.27
9	a	104	SPN	CM5-C13-C14	-3.50	109.38	115.27
9	f	102	SPN	CM4-C9-C10	-3.50	109.39	115.27
8	M	405	BCL	CHB-C1B-NB	3.50	127.96	124.26
8	v	101	BCL	CHD-C1D-ND	-3.50	121.24	124.45
9	k	101	SPN	CM8-C26-C27	-3.49	109.39	115.27
9	Q	102	SPN	CM3-C5-C6	-3.49	109.40	115.27
9	t	102	SPN	CM6-C18-C17	-3.49	109.40	115.27
9	k	103	SPN	CM3-C5-C6	-3.49	109.40	115.27
8	N	101	BCL	CHB-C1B-NB	3.49	127.95	124.26
9	D	102	SPN	CM4-C9-C10	-3.49	109.40	115.27
9	r	101	SPN	CM3-C5-C6	-3.49	109.40	115.27
8	P	101	BCL	CHB-C1B-NB	3.49	127.95	124.26
9	D	103	SPN	CM3-C5-C6	-3.49	109.41	115.27
8	A	101	BCL	CMB-C2B-C1B	-3.49	120.06	125.37
9	q	101	SPN	CM5-C13-C14	-3.49	109.41	115.27
11	L	306	LMT	C3'-C4'-C5'	-3.48	105.17	110.30
9	E	102	SPN	CM3-C5-C6	-3.48	109.41	115.27
8	T	101	BCL	C16-C15-C13	-3.48	104.67	115.92
9	r	103	SPN	C20-C19-C18	-3.48	119.28	127.66
9	G	103	SPN	CM5-C13-C14	-3.48	109.42	115.27
9	e	102	SPN	CM5-C13-C14	-3.48	109.42	115.27
9	p	101	SPN	CM9-C30-C29	-3.48	112.59	122.65
8	L	304	BCL	C16-C15-C13	-3.48	104.68	115.92
9	r	103	SPN	CM6-C18-C17	-3.47	109.43	115.27
8	V	101	BCL	C1C-NC-C4C	-3.47	105.14	106.71
9	2	102	SPN	CM8-C26-C27	-3.47	109.43	115.27
9	G	103	SPN	CM6-C18-C17	-3.47	109.44	115.27
8	f	101	BCL	C16-C15-C13	-3.47	104.71	115.92
9	n	102	SPN	CM8-C26-C27	-3.47	109.44	115.27
8	M	405	BCL	C16-C15-C13	-3.47	104.71	115.92
9	S	101	SPN	CM9-C30-C29	-3.46	112.63	122.65
8	s	101	BCL	CHD-C1D-ND	-3.46	121.28	124.45
9	v	102	SPN	CM3-C5-C6	-3.46	109.45	115.27
9	D	102	SPN	CM9-C30-C29	-3.46	112.65	122.65
9	i	101	SPN	CM6-C18-C17	-3.46	109.45	115.27
9	i	101	SPN	CM5-C13-C14	-3.45	109.46	115.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	F	102	SPN	C20-C19-C18	-3.45	119.35	127.66
9	k	101	SPN	CM6-C18-C17	-3.45	109.47	115.27
8	D	101	BCL	CHB-C1B-NB	3.45	127.91	124.26
9	v	102	SPN	CM6-C18-C17	-3.45	109.47	115.27
8	d	101	BCL	OBB-CAB-CBB	-3.45	112.09	119.73
9	S	102	SPN	C20-C19-C18	-3.45	119.36	127.66
9	r	103	SPN	CM8-C26-C27	-3.45	109.47	115.27
9	a	104	SPN	C20-C19-C18	-3.45	119.36	127.66
9	a	104	SPN	CM6-C18-C17	-3.44	109.48	115.27
9	i	103	SPN	CM8-C26-C27	-3.44	109.48	115.27
9	n	102	SPN	CM9-C30-C29	-3.44	112.69	122.65
8	T	101	BCL	CHD-C1D-ND	-3.44	121.29	124.45
8	v	101	BCL	C1C-NC-C4C	-3.44	105.16	106.71
8	a	102	BCL	C16-C15-C13	-3.44	104.81	115.92
9	I	101	SPN	CM8-C26-C27	-3.43	109.49	115.27
9	f	102	SPN	CM3-C5-C6	-3.43	109.50	115.27
8	L	304	BCL	C4A-NA-C1A	-3.43	105.16	106.71
9	I	101	SPN	CM4-C9-C10	-3.43	109.50	115.27
9	p	102	SPN	CM4-C9-C10	-3.43	109.50	115.27
9	Q	102	SPN	C21-C20-C19	3.43	121.28	112.23
8	E	101	BCL	CHA-C1A-NA	-3.42	118.56	126.40
9	K	102	SPN	CM5-C13-C14	-3.42	109.51	115.27
8	G	101	BCL	CHD-C1D-ND	-3.42	121.31	124.45
8	d	101	BCL	CHD-C1D-ND	-3.41	121.32	124.45
9	t	102	SPN	CM5-C13-C14	-3.41	109.53	115.27
9	r	103	SPN	CM5-C13-C14	-3.41	109.53	115.27
9	q	101	SPN	CM3-C5-C6	-3.41	109.53	115.27
9	D	103	SPN	CM8-C26-C27	-3.41	109.53	115.27
8	2	101	BCL	C16-C15-C13	-3.41	104.90	115.92
9	r	103	SPN	C21-C20-C19	3.41	121.23	112.23
9	M	404	SPN	CM6-C18-C17	-3.40	109.55	115.27
9	p	101	SPN	CM6-C18-C17	-3.40	109.55	115.27
8	V	101	BCL	CHD-C1D-ND	-3.40	121.33	124.45
9	i	103	SPN	CM4-C9-C10	-3.40	109.55	115.27
8	P	101	BCL	C16-C15-C13	-3.40	104.94	115.92
8	n	101	BCL	CMB-C2B-C1B	-3.39	120.20	125.37
8	A	101	BCL	C16-C15-C13	-3.39	104.95	115.92
9	n	102	SPN	C20-C19-C18	-3.39	119.49	127.66
9	K	102	SPN	CM8-C26-C27	-3.39	109.57	115.27
8	B	101	BCL	C1C-NC-C4C	-3.39	105.18	106.71
9	M	404	SPN	CM3-C5-C6	-3.39	109.57	115.27
9	e	102	SPN	CM3-C5-C6	-3.39	109.58	115.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	2	102	SPN	CM3-C5-C6	-3.38	109.58	115.27
8	p	103	BCL	C16-C15-C13	-3.38	104.99	115.92
9	E	102	SPN	CM6-C18-C17	-3.38	109.59	115.27
9	G	104	SPN	CM4-C9-C10	-3.37	109.60	115.27
8	r	102	BCL	C16-C15-C13	-3.37	105.02	115.92
9	D	102	SPN	CM6-C18-C17	-3.37	109.60	115.27
8	s	101	BCL	C16-C15-C13	-3.37	105.03	115.92
8	t	101	BCL	C16-C15-C13	-3.37	105.03	115.92
8	q	102	BCL	C16-C15-C13	-3.37	105.03	115.92
9	S	101	SPN	C20-C19-C18	-3.37	119.56	127.66
9	p	101	SPN	C20-C19-C18	-3.36	119.56	127.66
9	r	101	SPN	CM4-C9-C10	-3.36	109.61	115.27
9	D	102	SPN	CM5-C13-C14	-3.36	109.63	115.27
9	p	101	SPN	CM3-C5-C6	-3.35	109.63	115.27
9	k	103	SPN	CM8-C26-C27	-3.35	109.63	115.27
9	E	102	SPN	C20-C19-C18	-3.35	119.59	127.66
8	F	101	BCL	CHA-C1A-NA	-3.35	118.73	126.40
9	2	102	SPN	CM4-C9-C10	-3.35	109.64	115.27
9	i	101	SPN	C20-C19-C18	-3.35	119.60	127.66
9	p	102	SPN	CM5-C13-C14	-3.34	109.66	115.27
13	M	403	BPH	C2D-C1D-ND	-3.33	107.22	109.53
9	k	103	SPN	C20-C19-C18	-3.33	119.64	127.66
8	Q	101	BCL	C16-C15-C13	-3.33	105.16	115.92
8	k	102	BCL	C16-C15-C13	-3.33	105.16	115.92
9	S	101	SPN	CMB-C30-C29	-3.32	113.04	122.65
9	a	101	SPN	C20-C19-C18	-3.32	119.66	127.66
8	M	402	BCL	CHA-C1A-NA	-3.31	118.83	126.40
9	E	102	SPN	CM8-C26-C27	-3.30	109.72	115.27
9	D	102	SPN	C20-C19-C18	-3.30	119.72	127.66
9	I	101	SPN	C21-C20-C19	3.29	120.93	112.23
9	S	101	SPN	C21-C20-C19	3.29	120.92	112.23
9	G	104	SPN	CM3-C5-C6	-3.29	109.74	115.27
9	a	103	SPN	CM6-C18-C17	-3.28	109.75	115.27
9	j	102	SPN	CM5-C13-C14	-3.28	109.75	115.27
8	A	101	BCL	C2B-C1B-NB	-3.28	108.04	110.23
8	M	405	BCL	C4D-CHA-C1A	3.27	125.23	121.25
9	i	101	SPN	CM4-C9-C10	-3.27	109.76	115.27
9	2	102	SPN	C20-C19-C18	-3.27	119.79	127.66
9	D	103	SPN	C20-C19-C18	-3.27	119.80	127.66
8	b	101	BCL	CHA-C1A-NA	-3.26	118.92	126.40
9	S	101	SPN	CM6-C18-C17	-3.26	109.79	115.27
9	v	102	SPN	CM4-C9-C10	-3.26	109.79	115.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	F	102	SPN	C21-C20-C19	3.26	120.84	112.23
9	e	102	SPN	CM6-C18-C17	-3.26	109.79	115.27
8	R	103	BCL	C16-C15-C13	-3.26	105.39	115.92
9	a	101	SPN	CM6-C18-C17	-3.26	109.79	115.27
8	d	101	BCL	CHA-C1A-NA	-3.25	118.95	126.40
9	k	101	SPN	CM5-C13-C14	-3.25	109.80	115.27
9	S	102	SPN	CM5-C13-C14	-3.25	109.81	115.27
9	I	101	SPN	CM5-C13-C14	-3.24	109.82	115.27
8	j	101	BCL	C16-C15-C13	-3.24	105.45	115.92
8	L	301	BCL	C2A-C3A-C4A	-3.24	96.64	101.87
8	R	103	BCL	CHA-C1A-NA	-3.22	119.03	126.40
9	b	102	SPN	CM8-C26-C27	-3.22	109.86	115.27
8	J	101	BCL	CHA-C1A-NA	-3.22	119.03	126.40
8	k	102	BCL	CBB-CAB-C3B	3.22	127.30	120.43
8	I	102	BCL	CHA-C1A-NA	-3.21	119.04	126.40
9	i	103	SPN	CM5-C13-C14	-3.21	109.86	115.27
9	k	101	SPN	CM3-C5-C6	-3.21	109.87	115.27
8	j	101	BCL	CHA-C1A-NA	-3.21	119.04	126.40
8	J	101	BCL	O2A-CGA-O1A	-3.21	115.50	123.59
8	I	102	BCL	C16-C15-C13	-3.20	105.56	115.92
8	M	402	BCL	CBB-CAB-C3B	3.20	127.26	120.43
9	2	103	SPN	CM5-C13-C14	-3.20	109.89	115.27
9	K	102	SPN	CM6-C18-C17	-3.20	109.89	115.27
8	G	101	BCL	C4A-NA-C1A	-3.20	105.27	106.71
8	G	102	BCL	CHA-C1A-NA	-3.19	119.09	126.40
9	q	101	SPN	C21-C20-C19	3.19	120.64	112.23
8	v	101	BCL	C16-C15-C13	-3.18	105.63	115.92
9	a	103	SPN	C20-C19-C18	-3.18	120.00	127.66
8	D	101	BCL	C16-C15-C13	-3.18	105.64	115.92
9	t	102	SPN	CM3-C5-C6	-3.18	109.92	115.27
8	L	301	BCL	CMA-C3A-C4A	-3.18	103.24	111.77
8	R	101	BCL	C16-C15-C13	-3.17	105.67	115.92
8	d	101	BCL	C16-C15-C13	-3.17	105.67	115.92
8	N	101	BCL	C16-C15-C13	-3.17	105.68	115.92
9	p	101	SPN	C21-C20-C19	3.17	120.60	112.23
13	L	302	BPH	C2D-C1D-ND	-3.16	107.35	109.53
8	D	101	BCL	O2A-CGA-O1A	-3.15	115.64	123.59
8	1	101	BCL	CHA-C1A-NA	-3.15	119.19	126.40
8	R	101	BCL	C1C-NC-C4C	-3.15	105.29	106.71
8	G	102	BCL	C7-C6-C5	-3.14	104.82	113.36
8	G	102	BCL	CBB-CAB-C3B	3.14	127.15	120.43
8	B	101	BCL	CBB-CAB-C3B	3.14	127.14	120.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	f	101	BCL	CBB-CAB-C3B	3.14	127.14	120.43
8	a	102	BCL	C11-C10-C8	-3.14	105.78	115.92
8	E	101	BCL	C2C-C3C-C4C	-3.14	96.64	101.34
8	R	103	BCL	CBB-CAB-C3B	3.13	127.12	120.43
8	d	101	BCL	O2A-CGA-O1A	-3.13	115.69	123.59
8	r	102	BCL	C2B-C1B-NB	-3.13	108.13	110.23
8	R	101	BCL	CBB-CAB-C3B	3.13	127.12	120.43
8	I	102	BCL	CBB-CAB-C3B	3.13	127.11	120.43
8	e	101	BCL	CHA-C1A-NA	-3.13	119.23	126.40
9	p	102	SPN	C20-C19-C18	-3.13	120.13	127.66
8	L	301	BCL	C16-C15-C13	-3.13	105.81	115.92
8	L	301	BCL	CBB-CAB-C3B	3.13	127.11	120.43
8	N	101	BCL	C2C-C3C-C4C	-3.13	96.66	101.34
8	N	101	BCL	CHA-C1A-NA	-3.12	119.24	126.40
8	Q	101	BCL	CBB-CAB-C3B	3.12	127.10	120.43
8	L	304	BCL	CBB-CAB-C3B	3.12	127.10	120.43
8	e	101	BCL	C2B-C1B-NB	-3.12	108.14	110.23
8	F	101	BCL	CBB-CAB-C3B	3.12	127.09	120.43
8	E	101	BCL	CBB-CAB-C3B	3.12	127.09	120.43
8	2	101	BCL	CBB-CAB-C3B	3.12	127.09	120.43
8	M	402	BCL	C7-C6-C5	-3.12	104.89	113.36
8	P	101	BCL	CBB-CAB-C3B	3.12	127.09	120.43
9	S	102	SPN	CM6-C18-C17	-3.12	110.03	115.27
8	l	101	BCL	CBB-CAB-C3B	3.11	127.08	120.43
8	B	101	BCL	C11-C10-C8	-3.11	105.86	115.92
8	N	101	BCL	C7-C6-C5	-3.11	104.91	113.36
8	D	101	BCL	C4D-CHA-C1A	3.11	125.03	121.25
8	V	101	BCL	CBB-CAB-C3B	3.11	127.06	120.43
8	s	101	BCL	CHA-C1A-NA	-3.11	119.29	126.40
8	N	101	BCL	CBB-CAB-C3B	3.10	127.06	120.43
9	a	103	SPN	CM3-C5-C6	-3.10	110.05	115.27
8	F	101	BCL	C16-C15-C13	-3.10	105.89	115.92
8	E	101	BCL	C16-C15-C13	-3.10	105.89	115.92
8	J	101	BCL	C16-C15-C13	-3.10	105.89	115.92
8	q	102	BCL	CBB-CAB-C3B	3.10	127.05	120.43
8	a	102	BCL	CHA-C1A-NA	-3.10	119.31	126.40
8	P	101	BCL	C7-C6-C5	-3.10	104.95	113.36
8	P	101	BCL	CHA-C1A-NA	-3.09	119.31	126.40
8	i	102	BCL	C4A-NA-C1A	-3.09	105.31	106.71
8	q	102	BCL	CHA-C1A-NA	-3.09	119.31	126.40
8	v	101	BCL	CBB-CAB-C3B	3.09	127.04	120.43
8	V	101	BCL	C16-C15-C13	-3.09	105.92	115.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	101	BCL	CHA-C1A-NA	-3.09	119.32	126.40
8	n	101	BCL	CHA-C1A-NA	-3.09	119.32	126.40
8	v	101	BCL	CHA-C1A-NA	-3.09	119.33	126.40
9	j	102	SPN	C20-C19-C18	-3.09	120.23	127.66
9	2	103	SPN	C21-C20-C19	3.09	120.38	112.23
8	T	101	BCL	CBB-CAB-C3B	3.08	127.02	120.43
8	p	103	BCL	C2B-C1B-NB	-3.08	108.17	110.23
8	M	402	BCL	C16-C15-C13	-3.08	105.96	115.92
9	p	102	SPN	CM8-C26-C27	-3.08	110.09	115.27
9	k	103	SPN	CM4-C9-C10	-3.08	110.09	115.27
8	K	101	BCL	CBB-CAB-C3B	3.08	127.01	120.43
8	R	101	BCL	C11-C10-C8	-3.08	105.97	115.92
8	J	101	BCL	CBB-CAB-C3B	3.08	127.00	120.43
8	D	101	BCL	CBB-CAB-C3B	3.08	127.00	120.43
8	1	101	BCL	C16-C15-C13	-3.07	105.99	115.92
8	J	101	BCL	C11-C10-C8	-3.07	106.00	115.92
8	M	405	BCL	C1C-NC-C4C	-3.07	105.33	106.71
8	k	102	BCL	CHA-C1A-NA	-3.07	119.38	126.40
8	L	301	BCL	O2A-CGA-O1A	-3.06	115.86	123.59
8	I	102	BCL	C7-C6-C5	-3.06	105.04	113.36
9	v	102	SPN	C21-C20-C19	3.06	120.32	112.23
8	L	301	BCL	C11-C10-C8	-3.06	106.03	115.92
8	s	101	BCL	CBB-CAB-C3B	3.06	126.97	120.43
8	k	102	BCL	C1C-NC-C4C	-3.06	105.33	106.71
8	b	101	BCL	C11-C10-C8	-3.06	106.04	115.92
8	Q	101	BCL	CHA-C1A-NA	-3.05	119.41	126.40
8	E	101	BCL	CMA-C3A-C4A	-3.05	103.57	111.77
8	G	101	BCL	CBB-CAB-C3B	3.05	126.95	120.43
8	B	101	BCL	CHA-C1A-NA	-3.05	119.41	126.40
8	r	102	BCL	C1C-NC-C4C	-3.05	105.33	106.71
9	R	102	SPN	C21-C20-C19	3.05	120.29	112.23
8	T	101	BCL	CHA-C1A-NA	-3.05	119.42	126.40
9	t	102	SPN	C21-C20-C19	3.05	120.28	112.23
8	G	102	BCL	C16-C15-C13	-3.04	106.08	115.92
9	r	101	SPN	CM5-C13-C14	-3.04	110.15	115.27
8	L	304	BCL	C11-C10-C8	-3.04	106.08	115.92
9	D	102	SPN	C21-C20-C19	3.04	120.27	112.23
8	D	101	BCL	CHA-C1A-NA	-3.04	119.43	126.40
8	V	101	BCL	CHA-C1A-NA	-3.04	119.44	126.40
8	p	103	BCL	CHA-C1A-NA	-3.04	119.44	126.40
9	V	102	SPN	C20-C19-C18	-3.04	120.34	127.66
9	t	102	SPN	C20-C19-C18	-3.04	120.34	127.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	n	101	BCL	C2B-C1B-NB	-3.04	108.19	110.23
9	S	102	SPN	C21-C20-C19	3.04	120.25	112.23
8	M	405	BCL	CHA-C1A-NA	-3.04	119.44	126.40
8	T	101	BCL	C4D-CHA-C1A	3.03	124.94	121.25
8	f	101	BCL	C11-C10-C8	-3.03	106.12	115.92
8	V	101	BCL	O2A-CGA-O1A	-3.03	115.94	123.59
9	2	102	SPN	C21-C20-C19	3.03	120.24	112.23
8	M	405	BCL	O2A-CGA-O1A	-3.03	115.95	123.59
8	L	304	BCL	CHA-C1A-NA	-3.03	119.47	126.40
8	l	101	BCL	C7-C6-C5	-3.02	105.15	113.36
9	n	102	SPN	C21-C20-C19	3.02	120.21	112.23
11	L	306	LMT	C1'-O5'-C5'	-3.02	108.47	113.67
8	V	101	BCL	C4A-NA-C1A	-3.02	105.35	106.71
8	i	102	BCL	CHA-C1A-NA	-3.02	119.48	126.40
8	V	101	BCL	C7-C6-C5	-3.02	105.16	113.36
16	C	403	HEC	O1D-CGD-CBD	-3.02	113.38	123.08
9	n	102	SPN	CM6-C18-C17	-3.02	110.19	115.27
9	p	102	SPN	C21-C20-C19	3.02	120.20	112.23
8	p	103	BCL	O2A-CGA-O1A	-3.02	115.98	123.59
8	R	101	BCL	C4D-CHA-C1A	3.02	124.92	121.25
8	M	405	BCL	CBB-CAB-C3B	3.02	126.87	120.43
8	r	102	BCL	CHA-C1A-NA	-3.01	119.50	126.40
8	a	102	BCL	CBB-CAB-C3B	3.01	126.86	120.43
9	i	101	SPN	C21-C20-C19	3.01	120.18	112.23
8	P	101	BCL	C1C-NC-C4C	-3.01	105.35	106.71
9	V	102	SPN	C21-C20-C19	3.01	120.18	112.23
8	B	101	BCL	C16-C15-C13	-3.01	106.20	115.92
8	R	101	BCL	CHA-C1A-NA	-3.01	119.52	126.40
8	P	101	BCL	C4D-CHA-C1A	3.00	124.91	121.25
9	r	101	SPN	C21-C20-C19	3.00	120.16	112.23
8	l	101	BCL	C11-C10-C8	-3.00	106.21	115.92
8	q	102	BCL	C11-C10-C8	-3.00	106.22	115.92
8	a	102	BCL	C4D-CHA-C1A	3.00	124.89	121.25
8	T	101	BCL	C7-C6-C5	-3.00	105.22	113.36
8	K	101	BCL	C7-C6-C5	-2.99	105.23	113.36
8	N	101	BCL	C11-C10-C8	-2.99	106.24	115.92
9	E	102	SPN	C21-C20-C19	2.99	120.14	112.23
8	B	101	BCL	C7-C6-C5	-2.99	105.23	113.36
9	f	102	SPN	CM5-C13-C14	-2.99	110.24	115.27
8	b	101	BCL	CBB-CAB-C3B	2.99	126.82	120.43
8	f	101	BCL	C4D-CHA-C1A	2.99	124.89	121.25
9	a	101	SPN	C21-C20-C19	2.99	120.12	112.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	R	103	BCL	C7-C6-C5	-2.99	105.25	113.36
9	k	103	SPN	C21-C20-C19	2.98	120.11	112.23
8	B	101	BCL	C4D-CHA-C1A	2.98	124.88	121.25
8	t	101	BCL	C2C-C3C-C4C	-2.98	96.88	101.34
8	l	101	BCL	C4D-CHA-C1A	2.98	124.87	121.25
8	f	101	BCL	CHA-C1A-NA	-2.98	119.58	126.40
8	n	101	BCL	C4D-CHA-C1A	2.98	124.87	121.25
8	v	101	BCL	O2A-CGA-O1A	-2.97	116.10	123.59
9	G	104	SPN	C20-C19-C18	-2.96	120.52	127.66
8	2	101	BCL	CHA-C1A-NA	-2.96	119.61	126.40
8	D	101	BCL	C7-C6-C5	-2.96	105.31	113.36
8	M	402	BCL	CMC-C2C-C3C	-2.96	101.88	113.83
9	r	101	SPN	C20-C19-C18	-2.96	120.53	127.66
8	k	102	BCL	CMA-C3A-C4A	-2.96	103.83	111.77
13	M	403	BPH	C2B-C1B-NB	-2.96	107.48	109.53
8	A	101	BCL	C11-C10-C8	-2.95	106.37	115.92
8	I	102	BCL	C3D-C2D-C1D	-2.95	101.80	105.83
9	D	103	SPN	C21-C20-C19	2.95	120.03	112.23
8	J	101	BCL	C7-C6-C5	-2.95	105.35	113.36
9	a	103	SPN	CM5-C13-C14	-2.95	110.32	115.27
8	K	101	BCL	C16-C15-C13	-2.94	106.41	115.92
8	a	102	BCL	C1C-NC-C4C	-2.94	105.38	106.71
8	M	402	BCL	C11-C10-C8	-2.94	106.42	115.92
8	e	101	BCL	CBB-CAB-C3B	2.94	126.70	120.43
9	S	101	SPN	CM3-C5-C6	-2.93	110.34	115.27
8	Q	101	BCL	C4D-CHA-C1A	2.93	124.82	121.25
8	r	102	BCL	O2A-CGA-O1A	-2.93	116.21	123.59
8	j	101	BCL	C7-C6-C5	-2.93	105.41	113.36
8	e	101	BCL	C11-C10-C8	-2.92	106.47	115.92
8	I	102	BCL	C11-C10-C8	-2.92	106.47	115.92
8	A	101	BCL	C4D-CHA-C1A	2.92	124.80	121.25
9	a	103	SPN	C21-C20-C19	2.92	119.94	112.23
9	M	404	SPN	C20-C19-C18	-2.92	120.63	127.66
8	L	301	BCL	C3D-C2D-C1D	-2.92	101.85	105.83
8	Q	101	BCL	C7-C6-C5	-2.91	105.45	113.36
8	G	101	BCL	C2B-C1B-NB	-2.91	108.28	110.23
8	d	101	BCL	CHB-C1B-NB	2.91	127.34	124.26
8	j	101	BCL	C2B-C1B-NB	-2.91	108.28	110.23
8	j	101	BCL	CBB-CAB-C3B	2.91	126.64	120.43
8	j	101	BCL	O2A-CGA-O1A	-2.91	116.26	123.59
8	I	102	BCL	C2C-C3C-C4C	-2.90	96.99	101.34
8	T	101	BCL	C11-C10-C8	-2.90	106.53	115.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	b	101	BCL	C11-C12-C13	-2.90	106.53	115.92
8	A	101	BCL	C1C-NC-C4C	-2.90	105.40	106.71
8	i	102	BCL	CBB-CAB-C3B	2.90	126.62	120.43
8	s	101	BCL	C11-C10-C8	-2.90	106.55	115.92
8	d	101	BCL	C11-C10-C8	-2.90	106.56	115.92
9	j	102	SPN	CM3-C5-C6	-2.89	110.40	115.27
8	N	101	BCL	C4D-CHA-C1A	2.89	124.77	121.25
8	J	101	BCL	C4D-CHA-C1A	2.89	124.77	121.25
8	i	102	BCL	C7-C6-C5	-2.89	105.51	113.36
9	v	102	SPN	C20-C19-C18	-2.89	120.70	127.66
9	a	104	SPN	C21-C20-C19	2.89	119.86	112.23
8	G	102	BCL	O2A-CGA-O1A	-2.89	116.31	123.59
8	G	102	BCL	C11-C10-C8	-2.89	106.59	115.92
8	R	101	BCL	C7-C6-C5	-2.88	105.52	113.36
8	F	101	BCL	C7-C6-C5	-2.88	105.53	113.36
16	C	402	HEC	O1D-CGD-CBD	-2.88	113.82	123.08
8	b	101	BCL	C4D-CHA-C1A	2.88	124.75	121.25
8	r	102	BCL	C11-C10-C8	-2.88	106.62	115.92
8	G	101	BCL	C7-C6-C5	-2.87	105.55	113.36
8	Q	101	BCL	C11-C10-C8	-2.87	106.63	115.92
8	t	101	BCL	C7-C6-C5	-2.87	105.55	113.36
8	f	101	BCL	CMA-C3A-C4A	-2.87	104.06	111.77
8	Q	101	BCL	O2A-CGA-O1A	-2.87	116.35	123.59
8	A	101	BCL	C7-C6-C5	-2.87	105.57	113.36
8	k	102	BCL	C11-C10-C8	-2.87	106.65	115.92
8	2	101	BCL	C3D-C2D-C1D	-2.87	101.92	105.83
8	K	101	BCL	C3D-C2D-C1D	-2.87	101.92	105.83
9	D	103	SPN	CM5-C13-C14	-2.87	110.45	115.27
8	J	101	BCL	C3D-C2D-C1D	-2.87	101.92	105.83
8	L	304	BCL	C7-C6-C5	-2.87	105.58	113.36
8	f	101	BCL	C1C-NC-C4C	-2.86	105.42	106.71
8	T	101	BCL	O2A-CGA-O1A	-2.86	116.37	123.59
8	d	101	BCL	C3D-C2D-C1D	-2.86	101.93	105.83
8	K	101	BCL	CHA-C1A-NA	-2.86	119.85	126.40
9	i	103	SPN	C20-C19-C18	-2.86	120.78	127.66
9	G	103	SPN	C20-C19-C18	-2.85	120.79	127.66
8	p	103	BCL	C3D-C2D-C1D	-2.85	101.94	105.83
8	A	101	BCL	CAB-C3B-C2B	-2.85	124.07	128.34
8	P	101	BCL	C11-C10-C8	-2.85	106.71	115.92
8	a	102	BCL	C2B-C1B-NB	-2.85	108.32	110.23
8	k	102	BCL	C7-C6-C5	-2.85	105.62	113.36
8	n	101	BCL	C7-C6-C5	-2.85	105.63	113.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	f	102	SPN	C20-C19-C18	-2.85	120.81	127.66
8	F	101	BCL	C4D-CHA-C1A	2.84	124.71	121.25
8	n	101	BCL	CAB-C3B-C2B	-2.84	124.08	128.34
8	R	101	BCL	C3D-C2D-C1D	-2.84	101.95	105.83
8	i	102	BCL	O2A-CGA-O1A	-2.84	116.43	123.59
8	D	101	BCL	C3D-C2D-C1D	-2.84	101.96	105.83
8	j	101	BCL	C11-C10-C8	-2.84	106.75	115.92
8	2	101	BCL	O2A-CGA-O1A	-2.83	116.44	123.59
8	G	101	BCL	CHA-C1A-NA	-2.83	119.92	126.40
8	a	102	BCL	O2A-CGA-O1A	-2.83	116.45	123.59
16	C	401	HEC	O1D-CGD-CBD	-2.83	114.00	123.08
8	v	101	BCL	C3D-C2D-C1D	-2.83	101.97	105.83
8	K	101	BCL	C11-C10-C8	-2.82	106.79	115.92
8	B	101	BCL	C3D-C2D-C1D	-2.82	101.98	105.83
8	E	101	BCL	C3D-C2D-C1D	-2.82	101.98	105.83
8	G	101	BCL	C1C-NC-C4C	-2.82	105.44	106.71
8	r	102	BCL	C7-C6-C5	-2.82	105.70	113.36
8	L	301	BCL	CMC-C2C-C3C	-2.82	102.45	113.83
8	n	101	BCL	C3D-C2D-C1D	-2.82	101.98	105.83
8	2	101	BCL	C1C-NC-C4C	-2.82	105.44	106.71
9	f	102	SPN	CM6-C18-C17	-2.82	110.53	115.27
8	F	101	BCL	O2A-CGA-O1A	-2.82	116.48	123.59
8	G	102	BCL	C3D-C2D-C1D	-2.82	101.99	105.83
8	A	101	BCL	O2A-CGA-O1A	-2.82	116.48	123.59
8	2	101	BCL	C11-C10-C8	-2.81	106.82	115.92
8	f	101	BCL	O2A-CGA-O1A	-2.81	116.49	123.59
8	M	402	BCL	C3D-C2D-C1D	-2.81	101.99	105.83
8	V	101	BCL	C4D-CHA-C1A	2.81	124.67	121.25
9	i	103	SPN	C21-C20-C19	2.81	119.65	112.23
8	e	101	BCL	C4D-CHA-C1A	2.81	124.67	121.25
8	i	102	BCL	C3D-C2D-C1D	-2.81	102.00	105.83
8	T	101	BCL	C3D-C2D-C1D	-2.81	102.00	105.83
8	Q	101	BCL	C2B-C1B-NB	-2.80	108.35	110.23
8	F	101	BCL	CMA-C3A-C4A	-2.80	104.24	111.77
8	R	101	BCL	O2A-CGA-O1A	-2.80	116.52	123.59
8	a	102	BCL	C3D-C2D-C1D	-2.80	102.00	105.83
9	G	103	SPN	CM3-C5-C6	-2.80	110.56	115.27
8	G	101	BCL	C11-C10-C8	-2.80	106.86	115.92
8	n	101	BCL	C1C-NC-C4C	-2.80	105.45	106.71
8	R	103	BCL	O2A-CGA-O1A	-2.80	116.53	123.59
8	f	101	BCL	C2B-C1B-NB	-2.80	108.36	110.23
8	f	101	BCL	C3D-C2D-C1D	-2.80	102.01	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	l	101	BCL	O2A-CGA-O1A	-2.80	116.53	123.59
8	M	402	BCL	O2A-CGA-O1A	-2.80	116.53	123.59
9	b	102	SPN	CM3-C5-C6	-2.79	110.57	115.27
9	k	101	SPN	C20-C19-C18	-2.79	120.93	127.66
8	E	101	BCL	C11-C10-C8	-2.79	106.90	115.92
8	R	103	BCL	C11-C10-C8	-2.79	106.91	115.92
8	R	103	BCL	C2C-C3C-C4C	-2.79	97.17	101.34
8	N	101	BCL	C3D-C2D-C1D	-2.78	102.03	105.83
8	E	101	BCL	O2A-CGA-O1A	-2.78	116.57	123.59
8	r	102	BCL	CAB-C3B-C2B	-2.78	124.17	128.34
11	H	301	LMT	C1'-O5'-C5'	-2.78	108.23	113.69
8	q	102	BCL	C3D-C2D-C1D	-2.78	102.03	105.83
9	G	104	SPN	C21-C20-C19	2.78	119.58	112.23
8	L	304	BCL	C3D-C2D-C1D	-2.78	102.04	105.83
8	b	101	BCL	C3D-C2D-C1D	-2.78	102.04	105.83
8	l	101	BCL	C3D-C2D-C1D	-2.78	102.04	105.83
8	j	101	BCL	C3D-C2D-C1D	-2.78	102.04	105.83
8	p	103	BCL	C11-C10-C8	-2.78	106.94	115.92
8	T	101	BCL	CMA-C3A-C4A	-2.78	104.31	111.77
8	G	102	BCL	CMA-C3A-C4A	-2.78	104.31	111.77
8	v	101	BCL	C7-C6-C5	-2.78	105.82	113.36
8	I	102	BCL	C4D-CHA-C1A	2.77	124.63	121.25
8	F	101	BCL	C3D-C2D-C1D	-2.77	102.05	105.83
8	p	103	BCL	CAB-C3B-C2B	-2.77	124.18	128.34
8	L	301	BCL	C7-C6-C5	-2.77	105.83	113.36
8	A	101	BCL	C3D-C2D-C1D	-2.77	102.05	105.83
8	Q	101	BCL	C3D-C2D-C1D	-2.77	102.06	105.83
8	V	101	BCL	CHB-C1B-NB	2.76	127.18	124.26
8	i	102	BCL	C1C-NC-C4C	-2.76	105.46	106.71
8	G	102	BCL	C2C-C3C-C4C	-2.76	97.20	101.34
8	V	101	BCL	C3D-C2D-C1D	-2.76	102.06	105.83
8	I	102	BCL	O2A-CGA-O1A	-2.76	116.62	123.59
8	R	103	BCL	C3D-C2D-C1D	-2.76	102.06	105.83
8	K	101	BCL	C4D-CHA-C1A	2.76	124.61	121.25
8	s	101	BCL	CMC-C2C-C3C	-2.76	102.69	113.83
8	Q	101	BCL	C1C-NC-C4C	-2.76	105.47	106.71
8	N	101	BCL	CMA-C3A-C4A	-2.76	104.36	111.77
8	s	101	BCL	O2A-CGA-O1A	-2.76	116.63	123.59
9	k	103	SPN	CM5-C13-C14	-2.76	110.63	115.27
8	G	102	BCL	C4D-CHA-C1A	2.76	124.61	121.25
8	L	301	BCL	C11-C12-C13	-2.76	107.00	115.92
8	b	101	BCL	C7-C6-C5	-2.76	105.87	113.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	E	103	LMT	C1'-O5'-C5'	-2.76	108.28	113.69
8	R	103	BCL	C2B-C1B-NB	-2.75	108.39	110.23
10	F	103	MW9	O1-C17-C16	2.75	120.55	111.91
8	B	101	BCL	O2A-CGA-O1A	-2.75	116.64	123.59
9	a	101	SPN	CM5-C13-C14	-2.75	110.64	115.27
8	P	101	BCL	O2A-CGA-O1A	-2.75	116.66	123.59
8	V	101	BCL	CMC-C2C-C3C	-2.75	102.75	113.83
8	P	101	BCL	C3D-C2D-C1D	-2.75	102.08	105.83
8	r	102	BCL	C3D-C2D-C1D	-2.75	102.08	105.83
8	k	102	BCL	C3D-C2D-C1D	-2.75	102.08	105.83
9	b	102	SPN	CM6-C18-C17	-2.74	110.65	115.27
8	M	405	BCL	C3D-C2D-C1D	-2.74	102.09	105.83
8	L	301	BCL	CHA-C1A-NA	-2.74	120.11	126.40
9	F	102	SPN	CM6-C18-C17	-2.74	110.66	115.27
8	v	101	BCL	C4D-CHA-C1A	2.74	124.59	121.25
8	K	101	BCL	C2C-C3C-C4C	-2.74	97.23	101.34
8	r	102	BCL	C4D-CHA-C1A	2.74	124.58	121.25
8	q	102	BCL	C1C-NC-C4C	-2.74	105.47	106.71
8	F	101	BCL	C2B-C1B-NB	-2.74	108.40	110.23
8	Q	101	BCL	CMC-C2C-C3C	-2.74	102.79	113.83
8	s	101	BCL	C7-C6-C5	-2.73	105.94	113.36
8	K	101	BCL	O2A-CGA-O1A	-2.73	116.69	123.59
15	H	304	CDL	OB8-CB7-C71	2.73	120.48	111.91
8	n	101	BCL	C11-C12-C13	-2.73	107.09	115.92
8	D	101	BCL	CMC-C2C-C3C	-2.73	102.81	113.83
8	b	101	BCL	C2B-C1B-NB	-2.73	108.40	110.23
8	L	304	BCL	O2A-CGA-O1A	-2.73	116.71	123.59
15	H	304	CDL	OA8-CA7-C31	2.73	120.46	111.91
8	q	102	BCL	CMC-C2C-C3C	-2.72	102.85	113.83
8	B	101	BCL	CMC-C2C-C3C	-2.72	102.85	113.83
8	L	304	BCL	CMA-C3A-C4A	-2.72	104.46	111.77
8	r	102	BCL	C4A-NA-C1A	-2.72	105.48	106.71
8	i	102	BCL	CMC-C2C-C3C	-2.72	102.87	113.83
8	L	304	BCL	C4D-CHA-C1A	2.72	124.56	121.25
8	F	101	BCL	C11-C10-C8	-2.72	107.14	115.92
8	G	101	BCL	O2A-CGA-O1A	-2.72	116.74	123.59
8	n	101	BCL	CMC-C2C-C3C	-2.72	102.87	113.83
9	j	102	SPN	C21-C20-C19	2.72	119.40	112.23
8	N	101	BCL	O2A-CGA-O1A	-2.71	116.74	123.59
9	K	102	SPN	CM3-C5-C6	-2.71	110.71	115.27
8	j	101	BCL	CMC-C2C-C3C	-2.71	102.89	113.83
8	i	102	BCL	C2B-C1B-NB	-2.71	108.41	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	s	101	BCL	C3D-C2D-C1D	-2.71	102.13	105.83
8	e	101	BCL	C3D-C2D-C1D	-2.71	102.13	105.83
8	V	101	BCL	C2B-C1B-NB	-2.71	108.42	110.23
8	P	101	BCL	CMA-C3A-C4A	-2.71	104.49	111.77
8	e	101	BCL	C7-C6-C5	-2.71	106.00	113.36
8	n	101	BCL	O2A-CGA-O1A	-2.71	116.76	123.59
8	G	102	BCL	CMC-C2C-C3C	-2.71	102.91	113.83
10	L	307	MW9	O1-C17-C16	2.71	120.40	111.91
8	V	101	BCL	CMA-C3A-C4A	-2.71	104.50	111.77
8	T	101	BCL	C2C-C3C-C4C	-2.71	97.29	101.34
8	t	101	BCL	O2A-CGA-O1A	-2.71	116.77	123.59
8	q	102	BCL	C7-C6-C5	-2.70	106.02	113.36
8	R	101	BCL	CMC-C2C-C3C	-2.70	102.92	113.83
8	P	101	BCL	CMC-C2C-C3C	-2.70	102.93	113.83
9	G	103	SPN	C21-C20-C19	2.70	119.36	112.23
8	e	101	BCL	O2A-CGA-O1A	-2.70	116.78	123.59
8	k	102	BCL	C4D-CHA-C1A	2.70	124.53	121.25
8	2	101	BCL	CMC-C2C-C3C	-2.70	102.95	113.83
8	I	102	BCL	CMC-C2C-C3C	-2.70	102.95	113.83
8	t	101	BCL	C3D-C2D-C1D	-2.69	102.15	105.83
11	L	305	LMT	C1'-O5'-C5'	-2.69	108.40	113.69
8	v	101	BCL	CMC-C2C-C3C	-2.69	102.97	113.83
8	R	101	BCL	CMA-C3A-C4A	-2.69	104.54	111.77
8	J	101	BCL	CMC-C2C-C3C	-2.69	102.98	113.83
8	j	101	BCL	CMA-C3A-C4A	-2.69	104.55	111.77
8	s	101	BCL	C1C-NC-C4C	-2.69	105.50	106.71
8	b	101	BCL	O2A-CGA-O1A	-2.69	116.81	123.59
8	M	405	BCL	CMC-C2C-C3C	-2.68	103.00	113.83
8	A	101	BCL	CMC-C2C-C3C	-2.68	103.00	113.83
8	r	102	BCL	CMC-C2C-C3C	-2.68	103.01	113.83
8	p	103	BCL	CMC-C2C-C3C	-2.68	103.01	113.83
8	d	101	BCL	C4D-CHA-C1A	2.68	124.51	121.25
8	f	101	BCL	CMC-C2C-C3C	-2.68	103.02	113.83
8	P	101	BCL	C2B-C1B-NB	-2.68	108.44	110.23
8	a	102	BCL	CMA-C3A-C4A	-2.68	104.58	111.77
8	n	101	BCL	CMA-C3A-C4A	-2.68	104.58	111.77
8	T	101	BCL	CMC-C2C-C3C	-2.67	103.04	113.83
8	a	102	BCL	C4A-NA-C1A	-2.67	105.50	106.71
8	T	101	BCL	C2B-C1B-NB	-2.67	108.44	110.23
10	M	408	MW9	O1-C17-C16	2.67	120.29	111.91
8	R	101	BCL	C11-C12-C13	-2.67	107.30	115.92
8	L	304	BCL	C2C-C3C-C4C	-2.67	97.35	101.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	101	BCL	C11-C12-C13	-2.66	107.31	115.92
8	M	405	BCL	C7-C6-C5	-2.66	106.13	113.36
8	d	101	BCL	C2A-C1A-CHA	2.66	128.51	123.86
8	I	102	BCL	C2B-C1B-NB	-2.66	108.45	110.23
8	F	101	BCL	C2C-C3C-C4C	-2.66	97.35	101.34
8	t	101	BCL	CAB-C3B-C2B	-2.66	124.36	128.34
8	G	101	BCL	C3D-C2D-C1D	-2.66	102.20	105.83
8	M	405	BCL	CMA-C3A-C4A	-2.66	104.63	111.77
8	q	102	BCL	O2A-CGA-O1A	-2.65	116.90	123.59
8	j	101	BCL	C4D-CHA-C1A	2.65	124.47	121.25
8	i	102	BCL	C4D-CHA-C1A	2.65	124.47	121.25
8	l	101	BCL	C11-C12-C13	-2.65	107.36	115.92
8	G	102	BCL	C11-C12-C13	-2.65	107.37	115.92
8	E	101	BCL	CMC-C2C-C3C	-2.64	103.16	113.83
8	k	102	BCL	CMC-C2C-C3C	-2.64	103.17	113.83
8	b	101	BCL	C16-C15-C13	-2.64	107.38	115.92
10	H	302	MW9	O1-C17-C16	2.63	120.17	111.91
8	K	101	BCL	CMC-C2C-C3C	-2.63	103.21	113.83
8	L	304	BCL	CMC-C2C-C3C	-2.63	103.21	113.83
8	a	102	BCL	C7-C6-C5	-2.63	106.21	113.36
8	I	102	BCL	CMA-C3A-C4A	-2.63	104.70	111.77
8	i	102	BCL	CMA-C3A-C4A	-2.63	104.71	111.77
8	k	102	BCL	O2A-CGA-O1A	-2.63	116.96	123.59
8	s	101	BCL	CMA-C3A-C4A	-2.63	104.71	111.77
10	M	407	MW9	O1-C17-C16	2.63	120.16	111.91
11	L	305	LMT	C3'-C4'-C5'	-2.63	105.55	110.24
8	R	103	BCL	CMC-C2C-C3C	-2.63	103.23	113.83
8	2	101	BCL	C7-C6-C5	-2.63	106.22	113.36
8	M	402	BCL	C4D-CHA-C1A	2.63	124.45	121.25
8	v	101	BCL	C2B-C1B-NB	-2.63	108.47	110.23
9	K	102	SPN	C20-C19-C18	-2.63	121.33	127.66
8	l	101	BCL	C2B-C1B-NB	-2.63	108.47	110.23
8	J	101	BCL	C2B-C1B-NB	-2.63	108.47	110.23
8	l	101	BCL	CMA-C3A-C4A	-2.62	104.73	111.77
8	D	101	BCL	CMA-C3A-C4A	-2.62	104.73	111.77
15	H	303	CDL	OB8-CB7-C71	2.62	120.13	111.91
8	p	103	BCL	CMA-C3A-C4A	-2.62	104.73	111.77
8	E	101	BCL	C7-C6-C5	-2.62	106.25	113.36
8	P	101	BCL	CGD-CBD-CAD	-2.62	102.26	110.73
8	G	101	BCL	CMC-C2C-C3C	-2.62	103.27	113.83
8	F	101	BCL	CMC-C2C-C3C	-2.62	103.27	113.83
8	2	101	BCL	C4A-NA-C1A	-2.62	105.53	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	b	101	BCL	CMA-C3A-C4A	-2.61	104.75	111.77
8	Q	101	BCL	CMA-C3A-C4A	-2.61	104.76	111.77
8	j	101	BCL	C11-C12-C13	-2.61	107.49	115.92
8	J	101	BCL	C11-C12-C13	-2.61	107.49	115.92
8	2	101	BCL	C4D-CHA-C1A	2.60	124.42	121.25
8	N	101	BCL	CMC-C2C-C3C	-2.60	103.32	113.83
8	p	103	BCL	C4D-CHA-C1A	2.60	124.42	121.25
8	G	102	BCL	C2B-C1B-NB	-2.60	108.49	110.23
8	M	405	BCL	CMB-C2B-C3B	2.60	132.96	125.93
8	q	102	BCL	CMA-C3A-C4A	-2.60	104.78	111.77
8	R	103	BCL	C4D-CHA-C1A	2.60	124.42	121.25
8	a	102	BCL	CMC-C2C-C3C	-2.60	103.34	113.83
8	e	101	BCL	CMC-C2C-C3C	-2.60	103.34	113.83
8	t	101	BCL	CMC-C2C-C3C	-2.60	103.34	113.83
8	D	101	BCL	CGD-CBD-CAD	-2.60	102.32	110.73
10	Q	103	MW9	O1-C17-C16	2.60	120.06	111.91
10	B	102	MW9	O1-C17-C16	2.60	120.06	111.91
16	C	402	HEC	C1D-ND-C4D	2.59	107.75	105.07
8	p	103	BCL	C1C-NC-C4C	-2.59	105.54	106.71
10	G	105	MW9	O1-C17-C16	2.59	120.04	111.91
8	M	402	BCL	C11-C12-C13	-2.59	107.55	115.92
8	K	101	BCL	C11-C12-C13	-2.59	107.56	115.92
8	q	102	BCL	C2B-C1B-NB	-2.58	108.50	110.23
8	t	101	BCL	C4D-CHA-C1A	2.58	124.39	121.25
8	R	103	BCL	CMA-C3A-C4A	-2.58	104.85	111.77
8	I	102	BCL	C11-C12-C13	-2.57	107.60	115.92
8	J	101	BCL	C2C-C3C-C4C	-2.57	97.49	101.34
8	Q	101	BCL	CGD-CBD-CAD	-2.57	102.41	110.73
8	A	101	BCL	CMA-C3A-C4A	-2.57	104.87	111.77
8	b	101	BCL	CMC-C2C-C3C	-2.57	103.47	113.83
9	k	101	SPN	C21-C20-C19	2.57	119.01	112.23
8	s	101	BCL	C11-C12-C13	-2.56	107.63	115.92
8	T	101	BCL	C11-C12-C13	-2.56	107.64	115.92
8	s	101	BCL	C4D-CHA-C1A	2.56	124.36	121.25
8	b	101	BCL	C1C-NC-C4C	-2.56	105.56	106.71
8	N	101	BCL	CMD-C2D-C1D	2.56	129.22	124.71
8	e	101	BCL	CMA-C3A-C4A	-2.56	104.90	111.77
10	F	104	MW9	O1-C17-C16	2.56	119.93	111.91
8	G	102	BCL	CMD-C2D-C1D	2.56	129.22	124.71
8	2	101	BCL	C2B-C1B-NB	-2.56	108.52	110.23
8	e	101	BCL	C2A-C1A-CHA	2.56	128.33	123.86
8	R	103	BCL	CGD-CBD-CAD	-2.56	102.46	110.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	I	103	MW9	O1-C17-C16	2.55	119.92	111.91
8	G	101	BCL	CMA-C3A-C4A	-2.55	104.91	111.77
8	k	102	BCL	C2B-C1B-NB	-2.55	108.52	110.23
8	b	101	BCL	C4A-NA-C1A	-2.55	105.56	106.71
8	E	101	BCL	C2B-C1B-NB	-2.55	108.52	110.23
8	R	101	BCL	C2B-C1B-NB	-2.55	108.52	110.23
10	D	104	MW9	O1-C17-C16	2.55	119.90	111.91
8	t	101	BCL	C11-C12-C13	-2.54	107.69	115.92
11	C	404	LMT	C1'-O5'-C5'	-2.54	108.70	113.69
8	t	101	BCL	C11-C10-C8	-2.54	107.70	115.92
8	i	102	BCL	C11-C10-C8	-2.54	107.71	115.92
8	V	101	BCL	C11-C12-C13	-2.54	107.72	115.92
8	p	103	BCL	C7-C6-C5	-2.53	106.48	113.36
8	D	101	BCL	C11-C10-C8	-2.53	107.73	115.92
9	f	102	SPN	C21-C20-C19	2.53	118.91	112.23
8	F	101	BCL	CMD-C2D-C1D	2.53	129.16	124.71
8	K	101	BCL	CMA-C3A-C4A	-2.53	104.98	111.77
8	B	101	BCL	C11-C12-C13	-2.53	107.75	115.92
10	L	308	MW9	O1-C17-C16	2.53	119.83	111.91
15	H	303	CDL	OA8-CA7-C31	2.52	119.83	111.91
9	M	404	SPN	C21-C20-C19	2.52	118.89	112.23
13	L	302	BPH	C2B-C1B-NB	-2.52	107.78	109.53
8	r	102	BCL	CMA-C3A-C4A	-2.52	104.99	111.77
8	D	101	BCL	C2B-C1B-NB	-2.52	108.54	110.23
8	2	101	BCL	C2A-C1A-CHA	2.52	128.27	123.86
8	N	101	BCL	C11-C12-C13	-2.52	107.77	115.92
8	F	101	BCL	C11-C12-C13	-2.52	107.77	115.92
8	P	101	BCL	C11-C12-C13	-2.52	107.78	115.92
8	2	101	BCL	C11-C12-C13	-2.52	107.78	115.92
8	i	102	BCL	C11-C12-C13	-2.52	107.78	115.92
8	Q	101	BCL	C11-C12-C13	-2.52	107.79	115.92
16	C	403	HEC	O1A-CGA-CBA	-2.52	115.00	123.08
10	I	103	MW9	C31-C32-C33	-2.51	109.77	126.84
8	M	402	BCL	CMA-C3A-C4A	-2.51	105.03	111.77
8	N	101	BCL	CGD-CBD-CAD	-2.51	102.61	110.73
8	E	101	BCL	C4D-CHA-C1A	2.51	124.30	121.25
8	A	101	BCL	C11-C12-C13	-2.51	107.81	115.92
8	1	101	BCL	CGD-CBD-CAD	-2.51	102.62	110.73
8	1	101	BCL	CMC-C2C-C3C	-2.51	103.72	113.83
8	2	101	BCL	CMA-C3A-C4A	-2.50	105.05	111.77
8	q	102	BCL	C4D-CHA-C1A	2.50	124.29	121.25
8	L	301	BCL	CMD-C2D-C1D	2.50	129.11	124.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	R	101	BCL	CGD-CBD-CAD	-2.49	102.66	110.73
8	M	405	BCL	C11-C12-C13	-2.49	107.86	115.92
8	p	103	BCL	C2A-C1A-CHA	2.49	128.21	123.86
8	M	402	BCL	C2B-C1B-NB	-2.49	108.56	110.23
8	f	101	BCL	C7-C6-C5	-2.49	106.61	113.36
8	L	304	BCL	CMB-C2B-C3B	2.48	132.63	125.93
8	G	101	BCL	C4D-CHA-C1A	2.48	124.27	121.25
8	r	102	BCL	C2A-C1A-CHA	2.48	128.19	123.86
16	C	402	HEC	O1A-CGA-CBA	-2.48	115.13	123.08
8	J	101	BCL	CMA-C3A-C4A	-2.47	105.12	111.77
8	s	101	BCL	C2B-C1B-NB	-2.47	108.57	110.23
8	B	101	BCL	CGD-CBD-CAD	-2.47	102.72	110.73
8	I	102	BCL	CMD-C2D-C1D	2.47	129.07	124.71
8	A	101	BCL	C3C-C2C-C1C	2.47	105.86	101.87
8	n	101	BCL	C11-C10-C8	-2.47	107.94	115.92
8	G	101	BCL	C16-C15-C13	-2.47	107.94	115.92
8	B	101	BCL	CMA-C3A-C4A	-2.47	105.14	111.77
8	e	101	BCL	C16-C15-C13	-2.46	107.96	115.92
8	i	102	BCL	C2A-C1A-CHA	2.46	128.16	123.86
8	t	101	BCL	CHB-C4A-NA	-2.46	121.11	124.51
8	j	101	BCL	CMB-C2B-C3B	2.46	132.58	125.93
8	e	101	BCL	CMB-C2B-C3B	2.45	132.56	125.93
8	B	101	BCL	C3C-C2C-C1C	2.45	105.83	101.87
8	v	101	BCL	CGD-CBD-CAD	-2.45	102.80	110.73
8	i	102	BCL	CMB-C2B-C3B	2.45	132.53	125.93
8	B	101	BCL	C2B-C1B-NB	-2.44	108.59	110.23
9	K	102	SPN	C21-C20-C19	2.44	118.68	112.23
8	K	101	BCL	CMB-C2B-C3B	2.44	132.52	125.93
8	V	101	BCL	CMB-C2B-C3B	2.44	132.51	125.93
16	C	402	HEC	CMD-C2D-C1D	-2.44	121.33	125.04
8	d	101	BCL	C7-C6-C5	-2.43	106.76	113.36
8	R	103	BCL	C11-C12-C13	-2.43	108.06	115.92
8	d	101	BCL	CMC-C2C-C3C	-2.43	104.03	113.83
8	l	101	BCL	CMB-C2B-C3B	2.43	132.49	125.93
8	d	101	BCL	CMA-C3A-C4A	-2.43	105.25	111.77
8	a	102	BCL	C11-C12-C13	-2.43	108.08	115.92
8	L	304	BCL	C11-C12-C13	-2.42	108.09	115.92
8	T	101	BCL	CGD-CBD-CAD	-2.42	102.89	110.73
8	p	103	BCL	C4A-NA-C1A	-2.42	105.62	106.71
8	k	102	BCL	C11-C12-C13	-2.42	108.10	115.92
8	J	101	BCL	CMB-C2B-C3B	2.42	132.46	125.93
8	b	101	BCL	CMB-C2B-C3B	2.41	132.45	125.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	C	402	HEC	C3C-C4C-NC	-2.41	107.45	110.15
8	d	101	BCL	CGD-CBD-CAD	-2.41	102.94	110.73
8	G	102	BCL	CMB-C2B-C3B	2.41	132.43	125.93
8	F	101	BCL	CMB-C2B-C3B	2.40	132.42	125.93
8	M	405	BCL	CMD-C2D-C1D	2.40	128.94	124.71
8	M	405	BCL	C11-C10-C8	-2.40	108.17	115.92
8	N	101	BCL	CMB-C2B-C3B	2.39	132.39	125.93
8	G	102	BCL	C2A-C1A-CHA	2.39	128.04	123.86
16	C	401	HEC	O1A-CGA-CBA	-2.39	115.39	123.08
8	I	102	BCL	CMB-C2B-C3B	2.39	132.39	125.93
8	E	101	BCL	CMB-C2B-C3B	2.39	132.39	125.93
8	f	101	BCL	C11-C12-C13	-2.39	108.19	115.92
8	v	101	BCL	CMA-C3A-C4A	-2.39	105.35	111.77
8	r	102	BCL	CBB-CAB-C3B	2.39	125.53	120.43
8	K	101	BCL	C2B-C1B-NB	-2.39	108.63	110.23
8	V	101	BCL	CGD-CBD-CAD	-2.38	103.01	110.73
8	q	102	BCL	CMB-C2B-C3B	2.38	132.37	125.93
8	2	101	BCL	CMB-C2B-C3B	2.38	132.35	125.93
8	D	101	BCL	CMB-C2B-C3B	2.38	132.35	125.93
13	M	403	BPH	C1C-C2C-C3C	-2.38	100.58	102.84
8	s	101	BCL	CMB-C2B-C3B	2.37	132.34	125.93
8	J	101	BCL	CGD-CBD-CAD	-2.37	103.05	110.73
16	C	401	HEC	CBD-CAD-C3D	2.37	119.22	112.63
8	P	101	BCL	C3C-C2C-C1C	2.37	105.70	101.87
8	d	101	BCL	C11-C12-C13	-2.37	108.26	115.92
8	L	304	BCL	C2B-C1B-NB	-2.37	108.64	110.23
8	T	101	BCL	CMB-C2B-C3B	2.37	132.33	125.93
8	2	101	BCL	C3C-C2C-C1C	2.37	105.69	101.87
8	G	102	BCL	CGD-CBD-CAD	-2.36	103.07	110.73
8	N	101	BCL	C2B-C1B-NB	-2.36	108.65	110.23
8	V	101	BCL	C3C-C2C-C1C	2.36	105.69	101.87
8	f	101	BCL	CMB-C2B-C3B	2.36	132.31	125.93
8	G	101	BCL	CMB-C2B-C3B	2.36	132.30	125.93
8	L	301	BCL	C3C-C2C-C1C	2.36	105.67	101.87
8	P	101	BCL	CMD-C2D-C1D	2.36	128.86	124.71
14	M	406	U10	C7-C6-C5	-2.35	115.65	118.48
8	L	304	BCL	CHC-C1C-NC	2.35	127.77	124.51
8	R	101	BCL	CMB-C2B-C3B	2.35	132.28	125.93
8	P	101	BCL	CMB-C2B-C3B	2.35	132.28	125.93
8	R	103	BCL	C2A-C1A-CHA	2.35	127.96	123.86
13	L	302	BPH	C4D-CHA-CBD	2.34	109.58	108.52
16	C	403	HEC	CBD-CAD-C3D	2.34	119.13	112.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	R	103	BCL	CMB-C2B-C3B	2.34	132.24	125.93
8	V	101	BCL	C11-C10-C8	-2.34	108.36	115.92
8	b	101	BCL	C2A-C1A-CHA	2.34	127.94	123.86
8	J	101	BCL	CMD-C2D-C1D	2.34	128.83	124.71
8	i	102	BCL	C3C-C2C-C1C	2.34	105.64	101.87
8	q	102	BCL	CMD-C2D-C1D	2.34	128.83	124.71
8	M	402	BCL	CMB-C2B-C3B	2.34	132.24	125.93
8	D	101	BCL	C3C-C2C-C1C	2.33	105.64	101.87
8	B	101	BCL	CMB-C2B-C3B	2.33	132.23	125.93
8	s	101	BCL	C4A-NA-C1A	-2.33	105.66	106.71
8	L	301	BCL	C2B-C1B-NB	-2.33	108.67	110.23
8	v	101	BCL	CMB-C2B-C3B	2.33	132.23	125.93
8	B	101	BCL	CMD-C2D-C1D	2.33	128.82	124.71
8	I	102	BCL	CGD-CBD-CAD	-2.33	103.19	110.73
8	L	301	BCL	CMB-C2B-C3B	2.33	132.22	125.93
13	M	403	BPH	C4D-CHA-CBD	2.32	109.57	108.52
8	j	101	BCL	CGD-CBD-CAD	-2.32	103.22	110.73
8	M	402	BCL	CMD-C2D-C1D	2.32	128.80	124.71
8	K	101	BCL	CMD-C2D-C1D	2.32	128.80	124.71
8	p	103	BCL	C3C-C2C-C1C	2.32	105.61	101.87
8	p	103	BCL	CBB-CAB-C3B	2.32	125.38	120.43
8	e	101	BCL	CMD-C2D-C1D	2.31	128.79	124.71
8	R	103	BCL	CMD-C2D-C1D	2.31	128.79	124.71
8	f	101	BCL	CMD-C2D-C1D	2.31	128.79	124.71
8	A	101	BCL	CGD-CBD-CAD	-2.31	103.24	110.73
8	n	101	BCL	C3C-C2C-C1C	2.31	105.60	101.87
8	v	101	BCL	C11-C10-C8	-2.31	108.45	115.92
8	q	102	BCL	C11-C12-C13	-2.31	108.45	115.92
8	v	101	BCL	C4A-NA-C1A	-2.31	105.67	106.71
8	a	102	BCL	CMB-C2B-C3B	2.31	132.16	125.93
8	V	101	BCL	CMD-C2D-C1D	2.31	128.78	124.71
8	Q	101	BCL	CMB-C2B-C3B	2.31	132.16	125.93
8	D	101	BCL	CMD-C2D-C1D	2.30	128.78	124.71
8	f	101	BCL	C3C-C2C-C1C	2.30	105.59	101.87
8	E	101	BCL	CMD-C2D-C1D	2.30	128.77	124.71
8	j	101	BCL	C2C-C3C-C4C	-2.30	97.90	101.34
8	L	304	BCL	CMD-C2D-C1D	2.30	128.76	124.71
8	k	102	BCL	CMB-C2B-C3B	2.30	132.13	125.93
14	L	303	U10	C7-C6-C5	-2.29	115.72	118.48
8	n	101	BCL	CBB-CAB-C3B	2.29	125.33	120.43
8	A	101	BCL	CBB-CAB-C3B	2.29	125.33	120.43
8	l	101	BCL	CMD-C2D-C1D	2.29	128.75	124.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	R	101	BCL	C3C-C2C-C1C	2.29	105.56	101.87
8	s	101	BCL	C3C-C2C-C1C	2.29	105.56	101.87
8	k	102	BCL	C3C-C2C-C1C	2.29	105.56	101.87
8	t	101	BCL	CBB-CAB-C3B	2.28	125.31	120.43
8	L	304	BCL	C2A-C3A-C4A	-2.28	98.18	101.87
8	Q	101	BCL	C3C-C2C-C1C	2.28	105.55	101.87
8	a	102	BCL	C2A-C1A-CHA	2.28	127.85	123.86
8	d	101	BCL	CMB-C2B-C3B	2.28	132.09	125.93
16	C	402	HEC	CHC-C4B-NB	2.28	127.19	124.37
8	v	101	BCL	CMD-C2D-C1D	2.28	128.73	124.71
8	b	101	BCL	C3C-C2C-C1C	2.28	105.55	101.87
8	e	101	BCL	C2C-C3C-C4C	-2.28	97.93	101.34
16	C	401	HEC	C1D-ND-C4D	2.27	107.42	105.07
8	L	304	BCL	C12-C11-C10	-2.27	102.81	113.24
8	D	101	BCL	C12-C11-C10	-2.27	102.82	113.24
9	e	102	SPN	C20-C19-C18	-2.26	122.21	127.66
8	k	102	BCL	C4A-NA-C1A	-2.26	105.69	106.71
8	Q	101	BCL	C12-C11-C10	-2.26	102.86	113.24
8	f	101	BCL	CGD-CBD-CAD	-2.26	103.42	110.73
8	M	402	BCL	C12-C11-C10	-2.25	102.88	113.24
8	p	103	BCL	C12-C11-C10	-2.25	102.90	113.24
13	L	302	BPH	CMD-C2D-C3D	2.25	128.88	124.68
8	Q	101	BCL	CMD-C2D-C1D	2.24	128.66	124.71
8	q	102	BCL	C2A-C3A-C4A	-2.24	98.26	101.87
8	R	101	BCL	CMD-C2D-C1D	2.23	128.65	124.71
8	G	101	BCL	C2A-C1A-CHA	2.23	127.77	123.86
8	a	102	BCL	CMD-C2D-C1D	2.23	128.65	124.71
8	N	101	BCL	C12-C11-C10	-2.22	103.02	113.24
8	r	102	BCL	C11-C12-C13	-2.22	108.73	115.92
8	s	101	BCL	CGD-CBD-CAD	-2.22	103.54	110.73
8	P	101	BCL	C12-C11-C10	-2.22	103.03	113.24
8	A	101	BCL	CMD-C2D-C1D	2.22	128.62	124.71
8	G	101	BCL	C12-C11-C10	-2.22	103.05	113.24
8	V	101	BCL	C2A-C1A-CHA	2.22	127.73	123.86
8	D	101	BCL	C11-C12-C13	-2.21	108.76	115.92
8	T	101	BCL	C12-C11-C10	-2.21	103.06	113.24
8	q	102	BCL	CGD-CBD-CAD	-2.21	103.56	110.73
8	T	101	BCL	CMD-C2D-C1D	2.21	128.61	124.71
8	a	102	BCL	C3C-C2C-C1C	2.21	105.44	101.87
8	E	101	BCL	CGD-CBD-CAD	-2.21	103.59	110.73
8	M	405	BCL	CHC-C1C-NC	2.20	127.56	124.51
8	r	102	BCL	CGD-CBD-CAD	-2.20	103.60	110.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	405	BCL	CHB-C4A-NA	-2.20	121.47	124.51
8	e	101	BCL	CGD-CBD-CAD	-2.20	103.61	110.73
8	t	101	BCL	C12-C11-C10	-2.20	103.14	113.24
8	e	101	BCL	C12-C11-C10	-2.20	103.14	113.24
16	C	403	HEC	C1D-ND-C4D	2.20	107.34	105.07
8	V	101	BCL	C12-C11-C10	-2.20	103.14	113.24
8	k	102	BCL	C12-C11-C10	-2.20	103.14	113.24
8	L	301	BCL	CGD-CBD-CAD	-2.20	103.62	110.73
8	n	101	BCL	CMD-C2D-C1D	2.19	128.57	124.71
8	F	101	BCL	C12-C11-C10	-2.19	103.17	113.24
8	L	301	BCL	C2A-C1A-CHA	2.19	127.69	123.86
8	b	101	BCL	CMD-C2D-C1D	2.19	128.57	124.71
8	i	102	BCL	C12-C11-C10	-2.19	103.20	113.24
8	l	101	BCL	C12-C11-C10	-2.18	103.20	113.24
8	r	102	BCL	CMD-C2D-C1D	2.18	128.56	124.71
9	e	102	SPN	C21-C20-C19	2.18	117.99	112.23
8	v	101	BCL	C11-C12-C13	-2.18	108.88	115.92
8	a	102	BCL	CGD-CBD-CAD	-2.18	103.68	110.73
8	j	101	BCL	CMD-C2D-C1D	2.17	128.54	124.71
8	E	101	BCL	C2A-C1A-CHA	2.17	127.66	123.86
8	q	102	BCL	C3C-C2C-C1C	2.17	105.37	101.87
13	M	403	BPH	CMD-C2D-C3D	2.17	128.73	124.68
8	K	101	BCL	C12-C11-C10	-2.17	103.29	113.24
8	M	405	BCL	C4A-NA-C1A	-2.16	105.73	106.71
8	J	101	BCL	C12-C11-C10	-2.15	103.34	113.24
8	G	102	BCL	C12-C11-C10	-2.15	103.36	113.24
8	G	101	BCL	C3C-C2C-C1C	2.15	105.34	101.87
8	p	103	BCL	CMD-C2D-C1D	2.15	128.50	124.71
8	M	405	BCL	C2B-C1B-NB	-2.15	108.79	110.23
8	j	101	BCL	C2A-C1A-CHA	2.14	127.61	123.86
8	F	101	BCL	C2A-C1A-CHA	2.14	127.60	123.86
8	E	101	BCL	CHC-C1C-NC	2.14	127.47	124.51
16	C	402	HEC	CBD-CAD-C3D	2.14	118.57	112.63
8	I	102	BCL	C12-C11-C10	-2.13	103.44	113.24
8	n	101	BCL	C2A-C1A-CHA	2.13	127.58	123.86
8	r	102	BCL	C2A-C3A-C4A	-2.13	98.43	101.87
8	t	101	BCL	CGD-CBD-CAD	-2.13	103.84	110.73
8	q	102	BCL	C12-C11-C10	-2.12	103.48	113.24
8	A	101	BCL	C2A-C3A-C4A	-2.12	98.45	101.87
8	L	301	BCL	CHC-C1C-NC	2.12	127.44	124.51
8	2	101	BCL	CMD-C2D-C1D	2.12	128.44	124.71
8	G	101	BCL	C2A-C3A-C4A	-2.12	98.45	101.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	s	101	BCL	C12-C11-C10	-2.11	103.56	113.24
8	b	101	BCL	C2A-C3A-C4A	-2.10	98.47	101.87
8	n	101	BCL	CGD-CBD-CAD	-2.10	103.93	110.73
8	n	101	BCL	C12-C11-C10	-2.10	103.60	113.24
8	2	101	BCL	C12-C11-C10	-2.10	103.61	113.24
8	r	102	BCL	C3C-C2C-C1C	2.10	105.25	101.87
8	R	101	BCL	C12-C11-C10	-2.09	103.62	113.24
8	I	102	BCL	C2A-C1A-CHA	2.09	127.51	123.86
8	j	101	BCL	C12-C11-C10	-2.09	103.66	113.24
8	F	101	BCL	CGD-CBD-CAD	-2.09	103.98	110.73
8	t	101	BCL	CMD-C2D-C1D	2.08	128.38	124.71
8	q	102	BCL	C4A-NA-C1A	-2.08	105.77	106.71
8	q	102	BCL	C2A-C1A-CHA	2.08	127.49	123.86
8	d	101	BCL	C12-C11-C10	-2.08	103.69	113.24
8	B	101	BCL	C12-C11-C10	-2.08	103.70	113.24
8	E	101	BCL	C12-C11-C10	-2.07	103.71	113.24
8	M	405	BCL	C2A-C1A-CHA	2.06	127.47	123.86
8	A	101	BCL	C12-C11-C10	-2.06	103.80	113.24
8	F	101	BCL	C1-O2A-CGA	2.05	121.83	116.44
8	R	103	BCL	C12-C11-C10	-2.05	103.81	113.24
8	k	102	BCL	C2A-C1A-CHA	2.04	127.42	123.86
10	G	105	MW9	C31-C32-C33	-2.04	109.09	124.73
8	i	102	BCL	CMD-C2D-C1D	2.04	128.30	124.71
8	N	101	BCL	CHC-C1C-NC	2.04	127.33	124.51
8	k	102	BCL	CGD-CBD-CAD	-2.03	104.14	110.73
10	B	102	MW9	C31-C32-C33	-2.03	109.15	124.73
8	d	101	BCL	CMD-C2D-C1D	2.03	128.29	124.71
8	k	102	BCL	CMD-C2D-C1D	2.03	128.28	124.71
8	b	101	BCL	C12-C11-C10	-2.03	103.93	113.24
8	j	101	BCL	C2A-C3A-C4A	-2.02	98.61	101.87
8	J	101	BCL	C2A-C1A-CHA	2.01	127.38	123.86
16	C	403	HEC	CMD-C2D-C1D	-2.01	121.97	125.04
8	s	101	BCL	CMD-C2D-C1D	2.01	128.26	124.71
8	G	101	BCL	C11-C12-C13	-2.01	109.42	115.92
8	l	101	BCL	CHC-C1C-NC	2.01	127.29	124.51
8	v	101	BCL	C12-C11-C10	-2.00	104.05	113.24

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
16	C	401	HEC	NA
16	C	402	HEC	NA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
16	C	403	HEC	NA

All (1977) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	P	101	BCL	C3A-C2A-CAA-CBA
8	P	101	BCL	C2C-C3C-CAC-CBC
8	P	101	BCL	C4C-C3C-CAC-CBC
8	V	101	BCL	C2C-C3C-CAC-CBC
8	V	101	BCL	C4C-C3C-CAC-CBC
8	v	101	BCL	C1A-C2A-CAA-CBA
8	v	101	BCL	C2C-C3C-CAC-CBC
8	v	101	BCL	C4-C3-C5-C6
8	t	101	BCL	C1-C2-C3-C5
8	Q	101	BCL	C1A-C2A-CAA-CBA
8	Q	101	BCL	C3A-C2A-CAA-CBA
8	Q	101	BCL	C1-C2-C3-C5
8	r	102	BCL	C2C-C3C-CAC-CBC
8	r	102	BCL	C4C-C3C-CAC-CBC
8	R	101	BCL	C2C-C3C-CAC-CBC
8	R	101	BCL	C1-C2-C3-C4
8	R	101	BCL	C2-C3-C5-C6
8	R	103	BCL	C1-C2-C3-C4
8	q	102	BCL	C2C-C3C-CAC-CBC
8	q	102	BCL	C4C-C3C-CAC-CBC
8	q	102	BCL	C2-C3-C5-C6
8	p	103	BCL	C1A-C2A-CAA-CBA
8	p	103	BCL	C3A-C2A-CAA-CBA
8	p	103	BCL	CHA-CBD-CGD-O1D
8	p	103	BCL	CAD-CBD-CGD-O1D
8	p	103	BCL	C1-C2-C3-C4
8	2	101	BCL	C1A-C2A-CAA-CBA
8	2	101	BCL	C3A-C2A-CAA-CBA
8	2	101	BCL	C2C-C3C-CAC-CBC
8	1	101	BCL	C1A-C2A-CAA-CBA
8	1	101	BCL	C3A-C2A-CAA-CBA
8	n	101	BCL	C3A-C2A-CAA-CBA
8	N	101	BCL	C1A-C2A-CAA-CBA
8	N	101	BCL	C3A-C2A-CAA-CBA
8	i	102	BCL	C1A-C2A-CAA-CBA
8	i	102	BCL	CHA-CBD-CGD-O1D
8	i	102	BCL	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	i	102	BCL	O2A-C1-C2-C3
8	i	102	BCL	C1-C2-C3-C4
8	i	102	BCL	C1-C2-C3-C5
8	G	101	BCL	C1A-C2A-CAA-CBA
8	G	101	BCL	C3A-C2A-CAA-CBA
8	f	101	BCL	C3A-C2A-CAA-CBA
8	f	101	BCL	C1-C2-C3-C4
8	f	101	BCL	C1-C2-C3-C5
8	F	101	BCL	CBA-CGA-O2A-C1
8	F	101	BCL	O1A-CGA-O2A-C1
8	E	101	BCL	O1A-CGA-O2A-C1
8	d	101	BCL	C1A-C2A-CAA-CBA
8	d	101	BCL	C1-C2-C3-C4
8	d	101	BCL	C1-C2-C3-C5
8	D	101	BCL	C2C-C3C-CAC-CBC
8	D	101	BCL	C4C-C3C-CAC-CBC
8	b	101	BCL	C1A-C2A-CAA-CBA
8	b	101	BCL	C3A-C2A-CAA-CBA
8	B	101	BCL	C1A-C2A-CAA-CBA
8	B	101	BCL	C3A-C2A-CAA-CBA
8	B	101	BCL	C4C-C3C-CAC-CBC
8	B	101	BCL	C1-C2-C3-C4
8	B	101	BCL	C1-C2-C3-C5
8	a	102	BCL	C1-C2-C3-C4
8	a	102	BCL	C1-C2-C3-C5
8	A	101	BCL	C2C-C3C-CAC-CBC
8	A	101	BCL	C4C-C3C-CAC-CBC
8	A	101	BCL	C4-C3-C5-C6
8	M	402	BCL	CHA-CBD-CGD-O1D
8	M	402	BCL	CHA-CBD-CGD-O2D
8	M	402	BCL	C6-C7-C8-C9
8	M	405	BCL	C2C-C3C-CAC-CBC
8	M	405	BCL	C4C-C3C-CAC-CBC
8	M	405	BCL	CHA-CBD-CGD-O1D
8	M	405	BCL	CHA-CBD-CGD-O2D
8	M	405	BCL	C1-C2-C3-C4
8	M	405	BCL	C1-C2-C3-C5
8	L	301	BCL	C1A-C2A-CAA-CBA
8	L	301	BCL	C2C-C3C-CAC-CBC
8	L	301	BCL	C4C-C3C-CAC-CBC
8	L	301	BCL	C2-C3-C5-C6
8	L	301	BCL	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	L	304	BCL	C3A-C2A-CAA-CBA
8	L	304	BCL	C2C-C3C-CAC-CBC
8	L	304	BCL	C4C-C3C-CAC-CBC
8	L	304	BCL	O2A-C1-C2-C3
8	L	304	BCL	C1-C2-C3-C4
8	L	304	BCL	C1-C2-C3-C5
9	V	102	SPN	O1-C1-C2-O2
9	V	102	SPN	C2-C3-C4-C5
9	V	102	SPN	C3-C4-C5-CM3
9	V	102	SPN	C3-C4-C5-C6
9	V	102	SPN	C7-C8-C9-CM4
9	V	102	SPN	C7-C8-C9-C10
9	V	102	SPN	C10-C11-C12-C13
9	V	102	SPN	C11-C12-C13-CM5
9	V	102	SPN	C11-C12-C13-C14
9	V	102	SPN	C17-C18-C19-C20
9	V	102	SPN	C24-C25-C26-C27
9	V	102	SPN	C26-C27-C28-C29
9	v	102	SPN	C3-C4-C5-C6
9	v	102	SPN	C7-C8-C9-CM4
9	v	102	SPN	C9-C10-C11-C12
9	v	102	SPN	C10-C11-C12-C13
9	v	102	SPN	C22-C23-C24-C25
9	v	102	SPN	C24-C25-C26-CM8
9	v	102	SPN	C25-C26-C27-C28
9	v	102	SPN	C26-C27-C28-C29
9	v	102	SPN	C28-C29-C30-CMB
9	S	101	SPN	CM3-C5-C6-C7
9	S	101	SPN	C6-C7-C8-C9
9	S	101	SPN	C7-C8-C9-CM4
9	S	101	SPN	C10-C11-C12-C13
9	S	101	SPN	C11-C12-C13-CM5
9	S	101	SPN	CM6-C18-C19-C20
9	S	101	SPN	C24-C25-C26-CM8
9	S	102	SPN	O1-C1-C2-O2
9	S	102	SPN	C3-C4-C5-CM3
9	S	102	SPN	C3-C4-C5-C6
9	S	102	SPN	C6-C7-C8-C9
9	S	102	SPN	C7-C8-C9-CM4
9	S	102	SPN	C10-C11-C12-C13
9	S	102	SPN	C11-C12-C13-CM5
9	S	102	SPN	CM5-C13-C14-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	S	102	SPN	CM6-C18-C19-C20
9	S	102	SPN	C24-C25-C26-CM8
9	t	102	SPN	C3-C4-C5-CM3
9	t	102	SPN	C5-C6-C7-C8
9	t	102	SPN	C6-C7-C8-C9
9	t	102	SPN	C7-C8-C9-CM4
9	t	102	SPN	C7-C8-C9-C10
9	t	102	SPN	C10-C11-C12-C13
9	t	102	SPN	C11-C12-C13-CM5
9	t	102	SPN	C12-C13-C14-C15
9	t	102	SPN	C17-C18-C19-C20
9	t	102	SPN	C24-C25-C26-CM8
9	t	102	SPN	C26-C27-C28-C29
9	Q	102	SPN	C3-C4-C5-C6
9	Q	102	SPN	C4-C5-C6-C7
9	Q	102	SPN	C6-C7-C8-C9
9	Q	102	SPN	C7-C8-C9-CM4
9	Q	102	SPN	C11-C12-C13-C14
9	Q	102	SPN	CM6-C18-C19-C20
9	Q	102	SPN	C22-C23-C24-C25
9	Q	102	SPN	C24-C25-C26-CM8
9	Q	102	SPN	C24-C25-C26-C27
9	Q	102	SPN	C25-C26-C27-C28
9	Q	102	SPN	C28-C29-C30-CM9
9	Q	102	SPN	C28-C29-C30-CMB
9	r	101	SPN	C2-C1-O1-CMA
9	r	101	SPN	C3-C4-C5-CM3
9	r	101	SPN	C10-C11-C12-C13
9	r	101	SPN	C11-C12-C13-CM5
9	r	101	SPN	CM5-C13-C14-C15
9	r	101	SPN	C22-C23-C24-C25
9	r	101	SPN	C25-C26-C27-C28
9	r	101	SPN	C26-C27-C28-C29
9	r	101	SPN	C28-C29-C30-CMB
9	r	103	SPN	O1-C1-C2-O2
9	r	103	SPN	C3-C4-C5-CM3
9	r	103	SPN	C10-C11-C12-C13
9	r	103	SPN	C11-C12-C13-CM5
9	r	103	SPN	C16-C17-C18-CM6
9	r	103	SPN	C17-C18-C19-C20
9	r	103	SPN	CM6-C18-C19-C20
9	r	103	SPN	C22-C23-C24-C25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	r	103	SPN	C24-C25-C26-CM8
9	r	103	SPN	C26-C27-C28-C29
9	r	103	SPN	C28-C29-C30-CMB
9	R	102	SPN	C3-C4-C5-CM3
9	R	102	SPN	C6-C7-C8-C9
9	R	102	SPN	C7-C8-C9-CM4
9	R	102	SPN	C7-C8-C9-C10
9	R	102	SPN	C10-C11-C12-C13
9	R	102	SPN	C11-C12-C13-CM5
9	R	102	SPN	CM6-C18-C19-C20
9	R	102	SPN	C24-C25-C26-C27
9	R	102	SPN	C26-C27-C28-C29
9	q	101	SPN	O1-C1-C2-O2
9	q	101	SPN	C5-C6-C7-C8
9	q	101	SPN	C7-C8-C9-C10
9	q	101	SPN	C9-C10-C11-C12
9	q	101	SPN	C11-C12-C13-C14
9	q	101	SPN	C19-C20-C21-C22
9	q	101	SPN	C24-C25-C26-CM8
9	q	101	SPN	C25-C26-C27-C28
9	p	101	SPN	CM1-C1-O1-CMA
9	p	101	SPN	C2-C1-O1-CMA
9	p	101	SPN	C3-C4-C5-CM3
9	p	101	SPN	C7-C8-C9-CM4
9	p	101	SPN	C7-C8-C9-C10
9	p	101	SPN	C9-C10-C11-C12
9	p	101	SPN	C11-C12-C13-C14
9	p	101	SPN	C16-C17-C18-CM6
9	p	101	SPN	CM6-C18-C19-C20
9	p	101	SPN	C24-C25-C26-CM8
9	p	102	SPN	C3-C4-C5-CM3
9	p	102	SPN	C7-C8-C9-C10
9	p	102	SPN	C9-C10-C11-C12
9	p	102	SPN	C11-C12-C13-CM5
9	p	102	SPN	C11-C12-C13-C14
9	p	102	SPN	C17-C18-C19-C20
9	p	102	SPN	C22-C23-C24-C25
9	p	102	SPN	C23-C24-C25-C26
9	p	102	SPN	C24-C25-C26-CM8
9	p	102	SPN	C26-C27-C28-C29
9	2	102	SPN	O1-C1-C2-O2
9	2	102	SPN	C3-C4-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	2	102	SPN	C6-C7-C8-C9
9	2	102	SPN	C11-C12-C13-C14
9	2	102	SPN	C24-C25-C26-CM8
9	2	102	SPN	C27-C28-C29-C30
9	2	103	SPN	CM1-C1-O1-CMA
9	2	103	SPN	CM2-C1-O1-CMA
9	2	103	SPN	C2-C1-O1-CMA
9	2	103	SPN	C3-C4-C5-CM3
9	2	103	SPN	C3-C4-C5-C6
9	2	103	SPN	C7-C8-C9-CM4
9	2	103	SPN	C7-C8-C9-C10
9	2	103	SPN	C9-C10-C11-C12
9	2	103	SPN	C10-C11-C12-C13
9	2	103	SPN	C11-C12-C13-CM5
9	2	103	SPN	CM5-C13-C14-C15
9	2	103	SPN	C16-C17-C18-C19
9	2	103	SPN	CM6-C18-C19-C20
9	n	102	SPN	C3-C4-C5-CM3
9	n	102	SPN	C6-C7-C8-C9
9	n	102	SPN	C7-C8-C9-CM4
9	n	102	SPN	C9-C10-C11-C12
9	n	102	SPN	C11-C12-C13-C14
9	n	102	SPN	C16-C17-C18-CM6
9	n	102	SPN	C17-C18-C19-C20
9	n	102	SPN	C25-C26-C27-C28
9	n	102	SPN	C28-C29-C30-CMB
9	k	101	SPN	O1-C1-C2-O2
9	k	101	SPN	CM1-C1-C2-O2
9	k	101	SPN	CM1-C1-C2-C3
9	k	101	SPN	C3-C4-C5-C6
9	k	101	SPN	C6-C7-C8-C9
9	k	101	SPN	C7-C8-C9-CM4
9	k	101	SPN	C11-C12-C13-C14
9	k	101	SPN	C17-C18-C19-C20
9	k	101	SPN	CM6-C18-C19-C20
9	k	101	SPN	C22-C23-C24-C25
9	k	101	SPN	C24-C25-C26-C27
9	k	103	SPN	C1-C2-C3-C4
9	k	103	SPN	C2-C3-C4-C5
9	k	103	SPN	C3-C4-C5-CM3
9	k	103	SPN	C6-C7-C8-C9
9	k	103	SPN	C7-C8-C9-CM4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	k	103	SPN	C11-C10-C9-C8
9	k	103	SPN	C10-C11-C12-C13
9	k	103	SPN	C11-C12-C13-CM5
9	k	103	SPN	C17-C18-C19-C20
9	k	103	SPN	CM6-C18-C19-C20
9	k	103	SPN	C24-C25-C26-C27
9	K	102	SPN	C2-C3-C4-C5
9	K	102	SPN	C3-C4-C5-CM3
9	K	102	SPN	C3-C4-C5-C6
9	K	102	SPN	C6-C7-C8-C9
9	K	102	SPN	C11-C10-C9-CM4
9	K	102	SPN	C11-C12-C13-CM5
9	K	102	SPN	CM6-C18-C19-C20
9	K	102	SPN	C24-C25-C26-CM8
9	K	102	SPN	C26-C27-C28-C29
9	j	102	SPN	O1-C1-C2-O2
9	j	102	SPN	CM1-C1-C2-C3
9	j	102	SPN	CM3-C5-C6-C7
9	j	102	SPN	C6-C7-C8-C9
9	j	102	SPN	C7-C8-C9-CM4
9	j	102	SPN	C10-C11-C12-C13
9	j	102	SPN	C11-C12-C13-CM5
9	j	102	SPN	CM5-C13-C14-C15
9	j	102	SPN	CM6-C18-C19-C20
9	j	102	SPN	C22-C23-C24-C25
9	i	101	SPN	C1-C2-C3-C4
9	i	101	SPN	C3-C4-C5-CM3
9	i	101	SPN	C6-C7-C8-C9
9	i	101	SPN	C7-C8-C9-CM4
9	i	101	SPN	C7-C8-C9-C10
9	i	101	SPN	C9-C10-C11-C12
9	i	101	SPN	C10-C11-C12-C13
9	i	101	SPN	C11-C12-C13-C14
9	i	101	SPN	CM6-C18-C19-C20
9	i	101	SPN	C19-C20-C21-C22
9	i	103	SPN	O1-C1-C2-O2
9	i	103	SPN	C2-C3-C4-C5
9	i	103	SPN	C7-C8-C9-CM4
9	i	103	SPN	C10-C11-C12-C13
9	i	103	SPN	C11-C12-C13-CM5
9	i	103	SPN	C24-C25-C26-CM8
9	i	103	SPN	C25-C26-C27-C28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	I	101	SPN	O1-C1-C2-O2
9	I	101	SPN	CM1-C1-C2-C3
9	I	101	SPN	C3-C4-C5-C6
9	I	101	SPN	C6-C7-C8-C9
9	I	101	SPN	C7-C8-C9-CM4
9	I	101	SPN	C11-C12-C13-CM5
9	I	101	SPN	C11-C12-C13-C14
9	I	101	SPN	CM6-C18-C19-C20
9	I	101	SPN	C24-C25-C26-CM8
9	I	101	SPN	C26-C27-C28-C29
9	G	103	SPN	O1-C1-C2-O2
9	G	103	SPN	C3-C4-C5-C6
9	G	103	SPN	CM3-C5-C6-C7
9	G	103	SPN	C6-C7-C8-C9
9	G	103	SPN	C7-C8-C9-CM4
9	G	103	SPN	C10-C11-C12-C13
9	G	103	SPN	C11-C12-C13-CM5
9	G	103	SPN	C11-C12-C13-C14
9	G	103	SPN	CM6-C18-C19-C20
9	G	103	SPN	C24-C25-C26-CM8
9	G	103	SPN	C25-C26-C27-C28
9	G	104	SPN	O1-C1-C2-O2
9	G	104	SPN	C2-C3-C4-C5
9	G	104	SPN	C3-C4-C5-C6
9	G	104	SPN	C6-C7-C8-C9
9	G	104	SPN	C11-C10-C9-C8
9	G	104	SPN	C9-C10-C11-C12
9	G	104	SPN	C11-C12-C13-C14
9	G	104	SPN	CM6-C18-C19-C20
9	f	102	SPN	O1-C1-C2-O2
9	f	102	SPN	C7-C8-C9-C10
9	f	102	SPN	C9-C10-C11-C12
9	f	102	SPN	C10-C11-C12-C13
9	f	102	SPN	CM6-C18-C19-C20
9	f	102	SPN	CM7-C22-C23-C24
9	f	102	SPN	C22-C23-C24-C25
9	f	102	SPN	C24-C25-C26-CM8
9	F	102	SPN	C3-C4-C5-C6
9	F	102	SPN	C6-C7-C8-C9
9	F	102	SPN	C7-C8-C9-CM4
9	F	102	SPN	C7-C8-C9-C10
9	F	102	SPN	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	F	102	SPN	C11-C12-C13-CM5
9	F	102	SPN	C16-C17-C18-CM6
9	F	102	SPN	CM6-C18-C19-C20
9	F	102	SPN	C22-C23-C24-C25
9	F	102	SPN	C24-C25-C26-CM8
9	F	102	SPN	C24-C25-C26-C27
9	e	102	SPN	CM1-C1-C2-O2
9	e	102	SPN	CM1-C1-C2-C3
9	e	102	SPN	C3-C4-C5-C6
9	e	102	SPN	C6-C7-C8-C9
9	e	102	SPN	C7-C8-C9-CM4
9	e	102	SPN	C10-C11-C12-C13
9	e	102	SPN	C11-C12-C13-CM5
9	e	102	SPN	CM6-C18-C19-C20
9	e	102	SPN	CM7-C22-C23-C24
9	e	102	SPN	C22-C23-C24-C25
9	e	102	SPN	C24-C25-C26-C27
9	e	102	SPN	C26-C27-C28-C29
9	E	102	SPN	CM2-C1-O1-CMA
9	E	102	SPN	C2-C1-O1-CMA
9	E	102	SPN	C3-C4-C5-CM3
9	E	102	SPN	C3-C4-C5-C6
9	E	102	SPN	C7-C8-C9-CM4
9	E	102	SPN	C7-C8-C9-C10
9	E	102	SPN	C10-C11-C12-C13
9	E	102	SPN	C11-C12-C13-CM5
9	E	102	SPN	C11-C12-C13-C14
9	E	102	SPN	CM6-C18-C19-C20
9	E	102	SPN	C24-C25-C26-CM8
9	E	102	SPN	C24-C25-C26-C27
9	E	102	SPN	C26-C27-C28-C29
9	D	102	SPN	C7-C8-C9-CM4
9	D	102	SPN	C7-C8-C9-C10
9	D	102	SPN	C9-C10-C11-C12
9	D	102	SPN	C10-C11-C12-C13
9	D	102	SPN	C11-C12-C13-CM5
9	D	102	SPN	CM6-C18-C19-C20
9	D	102	SPN	C22-C23-C24-C25
9	D	102	SPN	C24-C25-C26-CM8
9	D	103	SPN	CM2-C1-C2-O2
9	D	103	SPN	CM2-C1-C2-C3
9	D	103	SPN	C3-C4-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	D	103	SPN	C6-C7-C8-C9
9	D	103	SPN	C7-C8-C9-CM4
9	D	103	SPN	C10-C11-C12-C13
9	D	103	SPN	CM6-C18-C19-C20
9	D	103	SPN	CM7-C22-C23-C24
9	D	103	SPN	C22-C23-C24-C25
9	D	103	SPN	C24-C25-C26-CM8
9	D	103	SPN	C24-C25-C26-C27
9	b	102	SPN	O1-C1-C2-O2
9	b	102	SPN	C3-C4-C5-CM3
9	b	102	SPN	CM3-C5-C6-C7
9	b	102	SPN	C6-C7-C8-C9
9	b	102	SPN	C7-C8-C9-CM4
9	b	102	SPN	C10-C11-C12-C13
9	b	102	SPN	C11-C12-C13-CM5
9	b	102	SPN	C11-C12-C13-C14
9	b	102	SPN	C17-C18-C19-C20
9	b	102	SPN	C18-C19-C20-C21
9	b	102	SPN	C22-C23-C24-C25
9	b	102	SPN	C25-C26-C27-C28
9	a	101	SPN	C3-C4-C5-C6
9	a	101	SPN	C5-C6-C7-C8
9	a	101	SPN	C7-C8-C9-CM4
9	a	101	SPN	C10-C11-C12-C13
9	a	101	SPN	C11-C12-C13-CM5
9	a	101	SPN	CM5-C13-C14-C15
9	a	101	SPN	CM6-C18-C19-C20
9	a	101	SPN	C26-C27-C28-C29
9	a	103	SPN	O1-C1-C2-O2
9	a	103	SPN	C3-C4-C5-CM3
9	a	103	SPN	C7-C8-C9-CM4
9	a	103	SPN	C7-C8-C9-C10
9	a	103	SPN	C11-C12-C13-CM5
9	a	103	SPN	C11-C12-C13-C14
9	a	103	SPN	CM5-C13-C14-C15
9	a	103	SPN	C17-C18-C19-C20
9	a	103	SPN	CM6-C18-C19-C20
9	a	103	SPN	C22-C23-C24-C25
9	a	103	SPN	C24-C25-C26-CM8
9	a	104	SPN	C3-C4-C5-CM3
9	a	104	SPN	C3-C4-C5-C6
9	a	104	SPN	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	a	104	SPN	C6-C7-C8-C9
9	a	104	SPN	C7-C8-C9-CM4
9	a	104	SPN	C10-C11-C12-C13
9	a	104	SPN	C11-C12-C13-CM5
9	a	104	SPN	CM6-C18-C19-C20
9	a	104	SPN	C24-C25-C26-C27
9	M	404	SPN	O1-C1-C2-O2
9	M	404	SPN	C2-C3-C4-C5
9	M	404	SPN	C3-C4-C5-CM3
9	M	404	SPN	C6-C7-C8-C9
9	M	404	SPN	C11-C12-C13-CM5
9	M	404	SPN	C11-C12-C13-C14
9	M	404	SPN	C12-C13-C14-C15
9	M	404	SPN	C17-C18-C19-C20
9	M	404	SPN	CM7-C22-C23-C24
9	M	404	SPN	C24-C25-C26-C27
9	M	404	SPN	C26-C27-C28-C29
10	Q	103	MW9	C33-C34-C35-C36
10	Q	103	MW9	C20-O2-P-O4
10	Q	103	MW9	C21-O5-P-O2
10	I	103	MW9	O8-C19-C20-O2
10	I	103	MW9	O5-C21-C22-C23
10	I	103	MW9	C21-C22-C23-O6
10	I	103	MW9	O9-C24-O8-C19
10	I	103	MW9	C21-O5-P-O4
10	G	105	MW9	C21-C22-C23-O6
10	G	105	MW9	C25-C24-O8-C19
10	G	105	MW9	O9-C24-O8-C19
10	G	105	MW9	C20-O2-P-O3
10	F	103	MW9	O-C17-O1-C18
10	F	103	MW9	C16-C17-O1-C18
10	F	103	MW9	O5-C21-C22-C23
10	F	103	MW9	C21-C22-C23-O6
10	F	103	MW9	O7-C22-C23-O6
10	F	103	MW9	C25-C24-O8-C19
10	F	104	MW9	O5-C21-C22-C23
10	D	104	MW9	C25-C24-O8-C19
10	B	102	MW9	O5-C21-C22-C23
10	B	102	MW9	C22-C21-O5-P
10	B	102	MW9	C21-C22-C23-O6
10	B	102	MW9	C25-C24-O8-C19
10	B	102	MW9	C33-C34-C35-C36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	B	102	MW9	C20-O2-P-O3
10	B	102	MW9	C20-O2-P-O4
10	B	102	MW9	C21-O5-P-O3
10	M	407	MW9	C33-C34-C35-C36
10	M	407	MW9	C20-O2-P-O3
10	M	407	MW9	C20-O2-P-O4
10	M	407	MW9	C20-O2-P-O5
10	M	408	MW9	O-C17-O1-C18
10	M	408	MW9	C16-C17-O1-C18
10	M	408	MW9	O8-C19-C20-O2
10	M	408	MW9	O5-C21-C22-C23
10	M	408	MW9	C21-C22-C23-O6
10	M	408	MW9	O9-C24-O8-C19
10	M	408	MW9	C21-O5-P-O3
10	M	408	MW9	C21-O5-P-O4
10	L	307	MW9	O5-C21-C22-O7
10	L	307	MW9	C21-C22-C23-O6
10	L	307	MW9	C20-O2-P-O4
10	L	307	MW9	C20-O2-P-O5
10	L	308	MW9	C21-C22-C23-O6
10	H	302	MW9	C20-O2-P-O3
10	H	302	MW9	C20-O2-P-O5
11	L	305	LMT	C2'-C1'-O1'-C1
11	L	305	LMT	O5'-C1'-O1'-C1
11	L	306	LMT	C2'-C1'-O1'-C1
11	L	306	LMT	O5'-C1'-O1'-C1
11	H	301	LMT	C2'-C1'-O1'-C1
11	H	301	LMT	O5'-C1'-O1'-C1
11	H	301	LMT	C2-C1-O1'-C1'
11	C	404	LMT	O5'-C1'-O1'-C1
13	M	403	BPH	C3A-C2A-CAA-CBA
13	M	403	BPH	C1A-C2A-CAA-CBA
14	M	406	U10	C14-C16-C17-C18
14	M	406	U10	C19-C21-C22-C23
14	M	406	U10	C34-C36-C37-C38
14	M	406	U10	C49-C51-C52-C53
14	L	303	U10	C19-C21-C22-C23
15	H	303	CDL	CA2-OA2-PA1-OA3
15	H	303	CDL	CA2-OA2-PA1-OA4
15	H	303	CDL	CB3-OB5-PB2-OB3
15	H	303	CDL	CB3-OB5-PB2-OB4
15	H	303	CDL	C51-CB5-OB6-CB4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	H	304	CDL	CB2-C1-CA2-OA2
15	H	304	CDL	CA3-OA5-PA1-OA2
15	H	304	CDL	CA3-OA5-PA1-OA3
15	H	304	CDL	CA3-OA5-PA1-OA4
15	H	304	CDL	CB3-OB5-PB2-OB4
8	p	103	BCL	O1A-CGA-O2A-C1
8	L	301	BCL	O1A-CGA-O2A-C1
10	Q	103	MW9	O-C17-O1-C18
15	H	304	CDL	OA9-CA7-OA8-CA6
8	E	101	BCL	CBA-CGA-O2A-C1
10	Q	103	MW9	C16-C17-O1-C18
15	H	304	CDL	C31-CA7-OA8-CA6
9	V	102	SPN	C28-C29-C30-CM9
9	R	102	SPN	C28-C29-C30-CMB
9	2	102	SPN	C28-C29-C30-CMB
9	2	103	SPN	C28-C29-C30-CMB
9	F	102	SPN	C28-C29-C30-CMB
9	D	103	SPN	C28-C29-C30-CMB
9	a	101	SPN	C28-C29-C30-CMB
9	a	104	SPN	C28-C29-C30-CMB
9	M	404	SPN	C28-C29-C30-CMB
8	f	101	BCL	O1A-CGA-O2A-C1
10	L	308	MW9	O-C17-O1-C18
15	H	303	CDL	OA9-CA7-OA8-CA6
10	F	103	MW9	O9-C24-O8-C19
10	D	104	MW9	O9-C24-O8-C19
10	B	102	MW9	O9-C24-O8-C19
15	H	303	CDL	OA7-CA5-OA6-CA4
15	H	303	CDL	OB7-CB5-OB6-CB4
8	t	101	BCL	C3-C5-C6-C7
8	R	101	BCL	C3-C5-C6-C7
8	d	101	BCL	C3-C5-C6-C7
8	D	101	BCL	C3-C5-C6-C7
9	v	102	SPN	C13-C14-C15-C16
9	r	103	SPN	C15-C16-C17-C18
9	k	101	SPN	C15-C16-C17-C18
9	k	103	SPN	C13-C14-C15-C16
9	k	103	SPN	C15-C16-C17-C18
9	i	103	SPN	C15-C16-C17-C18
9	G	104	SPN	C13-C14-C15-C16
9	e	102	SPN	C15-C16-C17-C18
9	b	102	SPN	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	p	103	BCL	CBA-CGA-O2A-C1
10	L	308	MW9	C16-C17-O1-C18
15	H	303	CDL	C31-CA7-OA8-CA6
10	I	103	MW9	C25-C24-O8-C19
10	M	408	MW9	C25-C24-O8-C19
15	H	303	CDL	C11-CA5-OA6-CA4
9	G	103	SPN	C28-C29-C30-CMB
9	e	102	SPN	C28-C29-C30-CMB
9	D	102	SPN	C28-C29-C30-CMB
11	E	103	LMT	C3'-C4'-O1B-C1B
11	E	103	LMT	O5'-C5'-C6'-O6'
8	R	101	BCL	C4-C3-C5-C6
9	n	102	SPN	C11-C10-C9-CM4
9	D	102	SPN	CM5-C13-C14-C15
9	S	101	SPN	C25-C26-C27-C28
9	S	102	SPN	C4-C5-C6-C7
9	r	103	SPN	C25-C26-C27-C28
9	K	102	SPN	C25-C26-C27-C28
9	j	102	SPN	C25-C26-C27-C28
9	I	101	SPN	C25-C26-C27-C28
9	E	102	SPN	C25-C26-C27-C28
9	a	103	SPN	C4-C5-C6-C7
9	V	102	SPN	C14-C15-C16-C17
9	S	101	SPN	C14-C15-C16-C17
9	S	102	SPN	C14-C15-C16-C17
9	Q	102	SPN	C14-C15-C16-C17
9	r	103	SPN	C14-C15-C16-C17
9	R	102	SPN	C14-C15-C16-C17
9	2	102	SPN	C14-C15-C16-C17
9	k	101	SPN	C14-C15-C16-C17
9	k	103	SPN	C14-C15-C16-C17
9	i	101	SPN	C14-C15-C16-C17
9	I	101	SPN	C14-C15-C16-C17
9	G	103	SPN	C14-C15-C16-C17
9	G	104	SPN	C14-C15-C16-C17
9	f	102	SPN	C14-C15-C16-C17
9	F	102	SPN	C14-C15-C16-C17
9	e	102	SPN	C14-C15-C16-C17
9	E	102	SPN	C14-C15-C16-C17
9	D	102	SPN	C14-C15-C16-C17
9	b	102	SPN	C14-C15-C16-C17
9	a	101	SPN	C14-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	a	104	SPN	C14-C15-C16-C17
10	G	105	MW9	C5-C6-C7-C8
10	F	104	MW9	C5-C6-C7-C8
8	B	101	BCL	C3-C5-C6-C7
9	S	102	SPN	C15-C16-C17-C18
9	Q	102	SPN	C15-C16-C17-C18
9	p	101	SPN	C15-C16-C17-C18
9	M	404	SPN	C13-C14-C15-C16
8	i	102	BCL	CBA-CGA-O2A-C1
8	f	101	BCL	CBA-CGA-O2A-C1
10	I	103	MW9	C16-C17-O1-C18
10	L	307	MW9	C16-C17-O1-C18
10	F	104	MW9	C31-C32-C33-C34
10	M	407	MW9	C31-C32-C33-C34
9	D	103	SPN	C14-C15-C16-C17
8	s	101	BCL	C1-C2-C3-C5
8	N	101	BCL	C1-C2-C3-C5
8	E	101	BCL	C1-C2-C3-C5
9	f	102	SPN	C28-C29-C30-CMB
9	b	102	SPN	C28-C29-C30-CMB
9	v	102	SPN	C11-C12-C13-CM5
9	S	101	SPN	C3-C4-C5-CM3
9	r	101	SPN	C7-C8-C9-CM4
9	r	101	SPN	C24-C25-C26-CM8
9	q	101	SPN	CM6-C18-C19-C20
9	p	101	SPN	C11-C12-C13-CM5
9	2	102	SPN	C7-C8-C9-CM4
9	2	102	SPN	CM6-C18-C19-C20
9	2	103	SPN	C24-C25-C26-CM8
9	n	102	SPN	C24-C25-C26-CM8
9	k	101	SPN	C11-C12-C13-CM5
9	k	101	SPN	C24-C25-C26-CM8
9	K	102	SPN	C7-C8-C9-CM4
9	j	102	SPN	C3-C4-C5-CM3
9	j	102	SPN	C24-C25-C26-CM8
9	i	101	SPN	C24-C25-C26-CM8
9	i	103	SPN	C3-C4-C5-CM3
9	I	101	SPN	C3-C4-C5-CM3
9	G	104	SPN	C7-C8-C9-CM4
9	G	104	SPN	C24-C25-C26-CM8
9	f	102	SPN	C3-C4-C5-CM3
9	f	102	SPN	C7-C8-C9-CM4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	f	102	SPN	C11-C12-C13-CM5
9	e	102	SPN	C24-C25-C26-CM8
9	D	103	SPN	C11-C12-C13-CM5
9	b	102	SPN	CM6-C18-C19-C20
9	b	102	SPN	C24-C25-C26-CM8
9	a	101	SPN	C3-C4-C5-CM3
9	a	101	SPN	C24-C25-C26-CM8
9	M	404	SPN	C7-C8-C9-CM4
9	M	404	SPN	CM6-C18-C19-C20
15	H	304	CDL	OA7-CA5-OA6-CA4
9	v	102	SPN	C17-C18-C19-C20
9	S	101	SPN	C7-C8-C9-C10
9	S	101	SPN	C11-C12-C13-C14
9	S	102	SPN	C7-C8-C9-C10
9	S	102	SPN	C11-C12-C13-C14
9	S	102	SPN	C24-C25-C26-C27
9	t	102	SPN	C3-C4-C5-C6
9	r	101	SPN	C7-C8-C9-C10
9	r	101	SPN	C17-C18-C19-C20
9	r	103	SPN	C3-C4-C5-C6
9	R	102	SPN	C11-C12-C13-C14
9	q	101	SPN	C3-C4-C5-C6
9	p	101	SPN	C3-C4-C5-C6
9	p	102	SPN	C24-C25-C26-C27
9	2	103	SPN	C17-C18-C19-C20
9	k	103	SPN	C7-C8-C9-C10
9	k	103	SPN	C11-C12-C13-C14
9	j	102	SPN	C7-C8-C9-C10
9	j	102	SPN	C11-C12-C13-C14
9	i	101	SPN	C3-C4-C5-C6
9	i	101	SPN	C17-C18-C19-C20
9	i	103	SPN	C17-C18-C19-C20
9	f	102	SPN	C24-C25-C26-C27
9	D	102	SPN	C3-C4-C5-C6
9	D	102	SPN	C24-C25-C26-C27
9	a	101	SPN	C7-C8-C9-C10
9	a	104	SPN	C11-C12-C13-C14
8	v	101	BCL	O1A-CGA-O2A-C1
8	n	101	BCL	O1A-CGA-O2A-C1
8	i	102	BCL	O1A-CGA-O2A-C1
10	I	103	MW9	O-C17-O1-C18
10	L	307	MW9	O-C17-O1-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	F	103	MW9	O5-C21-C22-O7
10	B	102	MW9	O5-C21-C22-O7
15	H	303	CDL	O1-C1-CB2-OB2
15	H	304	CDL	O1-C1-CA2-OA2
8	2	101	BCL	C3-C5-C6-C7
8	i	102	BCL	C3-C5-C6-C7
9	e	102	SPN	C13-C14-C15-C16
8	v	101	BCL	CBA-CGA-O2A-C1
15	H	304	CDL	C11-CA5-OA6-CA4
9	V	102	SPN	C28-C29-C30-CMB
9	S	102	SPN	C28-C29-C30-CMB
9	q	101	SPN	C28-C29-C30-CM9
9	p	102	SPN	C28-C29-C30-CMB
9	k	101	SPN	C28-C29-C30-CM9
9	i	101	SPN	C28-C29-C30-CMB
9	E	102	SPN	C28-C29-C30-CMB
8	n	101	BCL	CBA-CGA-O2A-C1
8	L	301	BCL	CBA-CGA-O2A-C1
10	Q	103	MW9	C12-C13-C14-C15
9	S	101	SPN	C28-C29-C30-CM9
9	t	102	SPN	C28-C29-C30-CM9
9	p	101	SPN	C28-C29-C30-CMB
9	k	103	SPN	C28-C29-C30-CM9
9	K	102	SPN	C28-C29-C30-CM9
9	j	102	SPN	C28-C29-C30-CMB
9	i	103	SPN	C28-C29-C30-CMB
9	I	101	SPN	C28-C29-C30-CMB
9	G	104	SPN	C28-C29-C30-CM9
9	F	102	SPN	C28-C29-C30-CM9
9	a	103	SPN	C28-C29-C30-CMB
9	S	102	SPN	CM8-C26-C27-C28
9	K	102	SPN	CM3-C5-C6-C7
9	f	102	SPN	C16-C17-C18-CM6
9	D	103	SPN	CM5-C13-C14-C15
8	v	101	BCL	C2-C3-C5-C6
8	A	101	BCL	C2-C3-C5-C6
9	r	103	SPN	C16-C17-C18-C19
9	q	101	SPN	C12-C13-C14-C15
9	q	101	SPN	C16-C17-C18-C19
9	p	101	SPN	C16-C17-C18-C19
9	p	101	SPN	C25-C26-C27-C28
9	2	102	SPN	C11-C10-C9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	2	102	SPN	C16-C17-C18-C19
9	k	101	SPN	C16-C17-C18-C19
9	k	101	SPN	C25-C26-C27-C28
9	k	103	SPN	C25-C26-C27-C28
9	K	102	SPN	C16-C17-C18-C19
9	j	102	SPN	C16-C17-C18-C19
9	f	102	SPN	C25-C26-C27-C28
9	e	102	SPN	C25-C26-C27-C28
9	D	102	SPN	C25-C26-C27-C28
9	D	103	SPN	C25-C26-C27-C28
9	M	404	SPN	C11-C10-C9-C8
9	M	404	SPN	C25-C26-C27-C28
9	v	102	SPN	C5-C6-C7-C8
9	S	101	SPN	C5-C6-C7-C8
9	S	101	SPN	C9-C10-C11-C12
9	S	102	SPN	C9-C10-C11-C12
9	S	102	SPN	C26-C27-C28-C29
9	t	102	SPN	C9-C10-C11-C12
9	r	103	SPN	C9-C10-C11-C12
9	q	101	SPN	C26-C27-C28-C29
9	p	101	SPN	C5-C6-C7-C8
9	2	103	SPN	C5-C6-C7-C8
9	n	102	SPN	C5-C6-C7-C8
9	n	102	SPN	C26-C27-C28-C29
9	k	101	SPN	C9-C10-C11-C12
9	k	101	SPN	C26-C27-C28-C29
9	k	103	SPN	C26-C27-C28-C29
9	j	102	SPN	C5-C6-C7-C8
9	j	102	SPN	C9-C10-C11-C12
9	i	103	SPN	C26-C27-C28-C29
9	I	101	SPN	C5-C6-C7-C8
9	G	103	SPN	C5-C6-C7-C8
9	G	103	SPN	C9-C10-C11-C12
9	G	103	SPN	C26-C27-C28-C29
9	f	102	SPN	C26-C27-C28-C29
9	F	102	SPN	C5-C6-C7-C8
9	F	102	SPN	C9-C10-C11-C12
9	e	102	SPN	C5-C6-C7-C8
9	E	102	SPN	C9-C10-C11-C12
9	D	102	SPN	C26-C27-C28-C29
9	D	103	SPN	C5-C6-C7-C8
9	D	103	SPN	C26-C27-C28-C29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	b	102	SPN	C5-C6-C7-C8
9	b	102	SPN	C26-C27-C28-C29
9	a	103	SPN	C26-C27-C28-C29
9	a	104	SPN	C9-C10-C11-C12
9	a	104	SPN	C26-C27-C28-C29
14	L	303	U10	C9-C11-C12-C13
14	L	303	U10	C34-C36-C37-C38
8	A	101	BCL	C1-C2-C3-C5
9	V	102	SPN	C24-C25-C26-CM8
9	p	102	SPN	C7-C8-C9-CM4
9	n	102	SPN	CM6-C18-C19-C20
9	M	404	SPN	C24-C25-C26-CM8
10	L	307	MW9	O5-C21-C22-C23
15	H	303	CDL	CA2-C1-CB2-OB2
15	H	304	CDL	CA2-C1-CB2-OB2
9	p	101	SPN	C17-C18-C19-C20
9	K	102	SPN	C11-C12-C13-C14
11	E	103	LMT	C4'-C5'-C6'-O6'
8	E	101	BCL	C3-C5-C6-C7
10	D	104	MW9	C16-C17-O1-C18
10	M	408	MW9	C6-C7-C8-C9
8	2	101	BCL	C10-C11-C12-C13
10	M	408	MW9	O5-C21-C22-O7
8	Q	101	BCL	C3-C5-C6-C7
8	q	102	BCL	C4-C3-C5-C6
8	E	101	BCL	C2-C3-C5-C6
9	K	102	SPN	C11-C10-C9-C8
9	E	102	SPN	C4-C5-C6-C7
8	s	101	BCL	C6-C7-C8-C9
8	2	101	BCL	C6-C7-C8-C9
8	k	102	BCL	C6-C7-C8-C9
8	M	405	BCL	C6-C7-C8-C9
8	L	304	BCL	C6-C7-C8-C9
9	S	102	SPN	CM7-C22-C23-C24
9	t	102	SPN	CM7-C22-C23-C24
9	Q	102	SPN	CM7-C22-C23-C24
9	r	101	SPN	CM7-C22-C23-C24
9	p	102	SPN	CM7-C22-C23-C24
9	2	102	SPN	CM7-C22-C23-C24
9	j	102	SPN	CM7-C22-C23-C24
13	M	403	BPH	C14-C13-C15-C16
13	L	302	BPH	C14-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	T	101	BCL	C2A-CAA-CBA-CGA
10	M	407	MW9	C25-C24-O8-C19
15	H	303	CDL	CA7-C31-C32-C33
9	v	102	SPN	C28-C29-C30-CM9
10	D	104	MW9	O-C17-O1-C18
8	k	102	BCL	C5-C6-C7-C8
8	f	101	BCL	C10-C11-C12-C13
10	D	104	MW9	C14-C15-C16-C17
15	H	303	CDL	CA5-C11-C12-C13
15	H	303	CDL	CB7-C71-C72-C73
15	H	304	CDL	CA5-C11-C12-C13
9	S	102	SPN	C22-C23-C24-C25
9	p	101	SPN	C22-C23-C24-C25
9	E	102	SPN	C22-C23-C24-C25
8	r	102	BCL	C13-C15-C16-C17
8	J	101	BCL	C10-C11-C12-C13
8	e	101	BCL	C15-C16-C17-C18
8	D	101	BCL	C5-C6-C7-C8
9	R	102	SPN	C28-C29-C30-CM9
10	B	102	MW9	O7-C22-C23-O6
10	F	104	MW9	C14-C15-C16-C17
10	B	102	MW9	C24-C25-C26-C27
10	M	407	MW9	C24-C25-C26-C27
10	L	308	MW9	C24-C25-C26-C27
15	H	304	CDL	CB7-C71-C72-C73
8	j	101	BCL	C5-C6-C7-C8
8	f	101	BCL	C15-C16-C17-C18
8	I	102	BCL	C8-C10-C11-C12
8	q	102	BCL	C11-C10-C8-C7
8	f	101	BCL	C11-C10-C8-C7
8	E	101	BCL	C11-C12-C13-C15
9	S	102	SPN	C21-C22-C23-C24
9	G	103	SPN	C21-C22-C23-C24
13	L	302	BPH	C11-C12-C13-C15
8	A	101	BCL	C3-C5-C6-C7
13	M	403	BPH	C2A-CAA-CBA-CGA
8	2	101	BCL	C13-C15-C16-C17
8	G	101	BCL	C15-C16-C17-C18
8	d	101	BCL	C15-C16-C17-C18
8	v	101	BCL	C10-C11-C12-C13
9	V	102	SPN	C9-C10-C11-C12
9	Q	102	SPN	C26-C27-C28-C29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	r	101	SPN	C9-C10-C11-C12
9	R	102	SPN	C5-C6-C7-C8
9	R	102	SPN	C9-C10-C11-C12
9	2	102	SPN	C5-C6-C7-C8
9	2	102	SPN	C26-C27-C28-C29
9	k	103	SPN	C5-C6-C7-C8
9	F	102	SPN	C26-C27-C28-C29
9	E	102	SPN	C5-C6-C7-C8
9	D	102	SPN	C5-C6-C7-C8
14	M	406	U10	C29-C31-C32-C33
10	G	105	MW9	C14-C15-C16-C17
9	S	101	SPN	C28-C29-C30-CMB
9	a	103	SPN	C28-C29-C30-CM9
10	I	103	MW9	C5-C6-C7-C8
10	F	103	MW9	C5-C6-C7-C8
10	I	103	MW9	O5-C21-C22-O7
10	F	104	MW9	O5-C21-C22-O7
15	H	304	CDL	O1-C1-CB2-OB2
8	v	101	BCL	C8-C10-C11-C12
8	p	103	BCL	C15-C16-C17-C18
8	s	101	BCL	C5-C6-C7-C8
8	Q	101	BCL	C15-C16-C17-C18
8	B	101	BCL	C10-C11-C12-C13
8	q	102	BCL	C15-C16-C17-C18
8	f	101	BCL	C13-C15-C16-C17
10	Q	103	MW9	C20-O2-P-O5
10	I	103	MW9	C21-O5-P-O2
10	G	105	MW9	C20-O2-P-O5
10	G	105	MW9	C21-O5-P-O2
10	F	104	MW9	C21-O5-P-O2
10	B	102	MW9	C20-O2-P-O5
10	B	102	MW9	C21-O5-P-O2
10	M	408	MW9	C21-O5-P-O2
15	H	303	CDL	CA2-OA2-PA1-OA5
15	H	303	CDL	CB3-OB5-PB2-OB2
15	H	304	CDL	CB3-OB5-PB2-OB2
9	I	101	SPN	C28-C29-C30-CM9
8	i	102	BCL	C10-C11-C12-C13
10	M	407	MW9	O9-C24-O8-C19
8	L	304	BCL	C4-C3-C5-C6
9	E	102	SPN	CM5-C13-C14-C15
14	L	303	U10	C25-C24-C26-C27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	D	102	SPN	C4-C5-C6-C7
8	j	101	BCL	C8-C10-C11-C12
8	I	102	BCL	C10-C11-C12-C13
8	d	101	BCL	C10-C11-C12-C13
9	D	103	SPN	C13-C14-C15-C16
9	p	101	SPN	C28-C29-C30-CM9
8	l	101	BCL	CBA-CGA-O2A-C1
10	B	102	MW9	C6-C7-C8-C9
10	M	408	MW9	C4-C5-C6-C7
9	D	103	SPN	C15-C16-C17-C18
10	I	103	MW9	C13-C14-C15-C16
10	D	104	MW9	C9-C10-C11-C12
10	B	102	MW9	C27-C28-C29-C30
10	M	408	MW9	C13-C14-C15-C16
10	H	302	MW9	C7-C8-C9-C10
15	H	303	CDL	C58-C59-C60-C61
15	H	303	CDL	C76-C77-C78-C79
9	p	102	SPN	C28-C29-C30-CM9
9	i	101	SPN	C28-C29-C30-CM9
10	M	407	MW9	C13-C14-C15-C16
10	M	408	MW9	C10-C11-C12-C13
10	H	302	MW9	C10-C11-C12-C13
11	C	404	LMT	C3-C4-C5-C6
15	H	304	CDL	C11-C12-C13-C14
15	H	304	CDL	C16-C17-C18-C19
10	H	302	MW9	C27-C28-C29-C30
15	H	304	CDL	C52-C53-C54-C55
10	M	408	MW9	C22-C21-O5-P
10	D	104	MW9	C12-C13-C14-C15
10	L	308	MW9	C13-C14-C15-C16
10	I	103	MW9	C30-C31-C32-C33
16	C	401	HEC	C3D-CAD-CBD-CGD
10	F	104	MW9	C4-C5-C6-C7
15	H	304	CDL	C13-C14-C15-C16
9	r	101	SPN	CM1-C1-O1-CMA
9	p	101	SPN	CM2-C1-O1-CMA
9	e	102	SPN	CM1-C1-O1-CMA
9	E	102	SPN	CM1-C1-O1-CMA
8	v	101	BCL	C1-C2-C3-C5
10	F	103	MW9	C13-C14-C15-C16
10	M	408	MW9	C7-C8-C9-C10
15	H	304	CDL	C54-C55-C56-C57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	p	103	BCL	C16-C17-C18-C19
8	p	103	BCL	C16-C17-C18-C20
8	I	102	BCL	C16-C17-C18-C19
8	I	102	BCL	C16-C17-C18-C20
9	Q	102	SPN	C11-C12-C13-CM5
9	r	103	SPN	C7-C8-C9-CM4
9	i	101	SPN	CM3-C5-C6-C7
9	I	101	SPN	CM3-C5-C6-C7
9	a	104	SPN	CM3-C5-C6-C7
10	F	103	MW9	C11-C12-C13-C14
10	L	307	MW9	C26-C27-C28-C29
10	L	308	MW9	C9-C10-C11-C12
8	E	101	BCL	C11-C12-C13-C14
8	M	402	BCL	C11-C10-C8-C9
9	G	103	SPN	CM7-C22-C23-C24
10	L	308	MW9	C14-C15-C16-C17
10	Q	103	MW9	C27-C28-C29-C30
10	I	103	MW9	C26-C27-C28-C29
10	F	104	MW9	C2-C3-C4-C5
10	B	102	MW9	C12-C13-C14-C15
10	M	407	MW9	C9-C10-C11-C12
10	M	407	MW9	C26-C27-C28-C29
10	M	408	MW9	C35-C36-C37-C38
10	H	302	MW9	C13-C14-C15-C16
15	H	303	CDL	C32-C33-C34-C35
8	R	103	BCL	C2A-CAA-CBA-CGA
8	G	102	BCL	C2A-CAA-CBA-CGA
8	1	101	BCL	O1A-CGA-O2A-C1
10	F	103	MW9	C6-C7-C8-C9
10	F	104	MW9	C13-C14-C15-C16
10	Q	103	MW9	C21-C22-C23-O6
10	F	104	MW9	C21-C22-C23-O6
8	N	101	BCL	C3-C5-C6-C7
9	I	101	SPN	C13-C14-C15-C16
10	G	105	MW9	C27-C28-C29-C30
10	F	103	MW9	C10-C11-C12-C13
10	I	103	MW9	C14-C15-C16-C17
10	G	105	MW9	C10-C11-C12-C13
10	G	105	MW9	C13-C14-C15-C16
10	F	104	MW9	C10-C11-C12-C13
10	F	104	MW9	C12-C13-C14-C15
10	F	104	MW9	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	B	102	MW9	C4-C5-C6-C7
10	M	408	MW9	C25-C26-C27-C28
10	L	307	MW9	C13-C14-C15-C16
15	H	303	CDL	C11-C12-C13-C14
11	H	301	LMT	O5'-C5'-C6'-O6'
9	i	101	SPN	C26-C27-C28-C29
14	L	303	U10	C14-C16-C17-C18
15	H	303	CDL	C72-C73-C74-C75
11	E	103	LMT	C2-C3-C4-C5
10	I	103	MW9	C27-C28-C29-C30
10	I	103	MW9	C6-C7-C8-C9
11	L	306	LMT	C7-C8-C9-C10
9	F	102	SPN	C13-C14-C15-C16
10	H	302	MW9	C16-C17-O1-C18
8	v	101	BCL	C3A-C2A-CAA-CBA
8	t	101	BCL	C3A-C2A-CAA-CBA
8	s	101	BCL	C3A-C2A-CAA-CBA
8	r	102	BCL	C3A-C2A-CAA-CBA
8	q	102	BCL	C3A-C2A-CAA-CBA
8	K	101	BCL	C3A-C2A-CAA-CBA
8	i	102	BCL	C3A-C2A-CAA-CBA
8	d	101	BCL	C3A-C2A-CAA-CBA
8	a	102	BCL	C3A-C2A-CAA-CBA
8	A	101	BCL	C3A-C2A-CAA-CBA
8	L	301	BCL	C3A-C2A-CAA-CBA
11	L	305	LMT	C2-C1-O1'-C1'
11	L	306	LMT	C2-C1-O1'-C1'
11	C	404	LMT	C2-C1-O1'-C1'
10	M	408	MW9	C27-C28-C29-C30
8	s	101	BCL	C16-C17-C18-C20
10	Q	103	MW9	C13-C14-C15-C16
10	M	408	MW9	C11-C12-C13-C14
9	q	101	SPN	C22-C23-C24-C25
9	p	101	SPN	C19-C20-C21-C22
9	G	103	SPN	C22-C23-C24-C25
10	Q	103	MW9	C31-C32-C33-C34
10	Q	103	MW9	C11-C12-C13-C14
10	G	105	MW9	C6-C7-C8-C9
10	M	408	MW9	C9-C10-C11-C12
10	L	307	MW9	C12-C13-C14-C15
9	f	102	SPN	C11-C10-C9-CM4
9	a	104	SPN	C11-C10-C9-CM4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	a	102	BCL	C2-C3-C5-C6
9	e	102	SPN	C12-C13-C14-C15
10	Q	103	MW9	C25-C24-O8-C19
10	F	103	MW9	C9-C10-C11-C12
9	G	104	SPN	C28-C29-C30-CMB
10	Q	103	MW9	O7-C22-C23-O6
10	F	104	MW9	O7-C22-C23-O6
10	L	308	MW9	O7-C22-C23-O6
10	F	103	MW9	C12-C13-C14-C15
15	H	304	CDL	C15-C16-C17-C18
8	s	101	BCL	C16-C17-C18-C19
10	Q	103	MW9	C10-C11-C12-C13
10	H	302	MW9	C12-C13-C14-C15
8	D	101	BCL	C13-C15-C16-C17
10	D	104	MW9	C10-C11-C12-C13
10	M	407	MW9	C11-C12-C13-C14
10	Q	103	MW9	O9-C24-O8-C19
9	r	103	SPN	C7-C8-C9-C10
9	i	103	SPN	C28-C29-C30-CM9
10	F	103	MW9	C28-C29-C30-C31
8	G	101	BCL	C10-C11-C12-C13
10	H	302	MW9	O-C17-O1-C18
10	F	104	MW9	C26-C27-C28-C29
15	H	303	CDL	C74-C75-C76-C77
8	Q	101	BCL	C10-C11-C12-C13
8	i	102	BCL	C13-C15-C16-C17
8	G	101	BCL	C5-C6-C7-C8
8	b	101	BCL	C13-C15-C16-C17
10	D	104	MW9	C4-C5-C6-C7
15	H	304	CDL	C55-C56-C57-C58
10	Q	103	MW9	C14-C15-C16-C17
10	H	302	MW9	C24-C25-C26-C27
10	B	102	MW9	C13-C14-C15-C16
9	S	102	SPN	C28-C29-C30-CM9
9	a	101	SPN	C28-C29-C30-CM9
8	e	101	BCL	C10-C11-C12-C13
8	b	101	BCL	C15-C16-C17-C18
8	d	101	BCL	C4-C3-C5-C6
9	r	103	SPN	CM3-C5-C6-C7
9	r	103	SPN	C11-C10-C9-CM4
9	2	103	SPN	CM8-C26-C27-C28
9	F	102	SPN	CM5-C13-C14-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	a	104	SPN	CM5-C13-C14-C15
13	M	403	BPH	C4-C3-C5-C6
8	v	101	BCL	C6-C7-C8-C10
8	t	101	BCL	C11-C12-C13-C15
8	s	101	BCL	C6-C7-C8-C10
8	k	102	BCL	C11-C10-C8-C7
8	G	101	BCL	C11-C10-C8-C7
8	G	102	BCL	C6-C7-C8-C10
8	f	101	BCL	C2-C3-C5-C6
8	F	101	BCL	C6-C7-C8-C10
8	M	402	BCL	C11-C10-C8-C7
9	V	102	SPN	C12-C13-C14-C15
9	t	102	SPN	C11-C10-C9-C8
9	t	102	SPN	C21-C22-C23-C24
9	R	102	SPN	C20-C21-C22-C23
9	p	102	SPN	C21-C22-C23-C24
9	M	404	SPN	C21-C22-C23-C24
13	M	403	BPH	C2-C3-C5-C6
13	M	403	BPH	C12-C13-C15-C16
10	F	103	MW9	C31-C32-C33-C34
8	a	102	BCL	O1A-CGA-O2A-C1
10	G	105	MW9	C12-C13-C14-C15
8	R	101	BCL	C5-C6-C7-C8
8	b	101	BCL	C10-C11-C12-C13
10	Q	103	MW9	C29-C30-C31-C32
10	B	102	MW9	C29-C30-C31-C32
10	H	302	MW9	C29-C30-C31-C32
10	F	103	MW9	C14-C15-C16-C17
8	L	304	BCL	CBA-CGA-O2A-C1
10	M	407	MW9	C16-C17-O1-C18
10	L	308	MW9	C12-C13-C14-C15
15	H	303	CDL	C60-C61-C62-C63
10	G	105	MW9	C26-C27-C28-C29
10	L	308	MW9	C10-C11-C12-C13
15	H	303	CDL	C75-C76-C77-C78
8	n	101	BCL	C10-C11-C12-C13
8	G	101	BCL	C13-C15-C16-C17
8	a	102	BCL	C8-C10-C11-C12
10	F	104	MW9	C3-C4-C5-C6
8	1	101	BCL	C3-C5-C6-C7
9	S	102	SPN	C13-C14-C15-C16
8	D	101	BCL	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	K	101	BCL	CBA-CGA-O2A-C1
8	e	101	BCL	C8-C10-C11-C12
10	F	104	MW9	C25-C24-O8-C19
9	K	102	SPN	C28-C29-C30-CMB
10	F	104	MW9	O9-C24-O8-C19
11	E	103	LMT	C2'-C1'-O1'-C1
8	N	101	BCL	O1A-CGA-O2A-C1
8	r	102	BCL	C16-C17-C18-C20
10	I	103	MW9	C10-C11-C12-C13
10	M	408	MW9	C36-C37-C38-C39
8	l	101	BCL	C8-C10-C11-C12
10	M	408	MW9	C29-C30-C31-C32
9	S	102	SPN	C16-C17-C18-CM6
9	i	101	SPN	CM8-C26-C27-C28
8	2	101	BCL	C2-C3-C5-C6
9	2	102	SPN	C25-C26-C27-C28
14	L	303	U10	C23-C24-C26-C27
8	P	101	BCL	C6-C7-C8-C9
8	t	101	BCL	C11-C12-C13-C14
8	q	102	BCL	C11-C10-C8-C9
8	k	102	BCL	C11-C10-C8-C9
8	I	102	BCL	C6-C7-C8-C9
8	G	101	BCL	C11-C10-C8-C9
8	G	101	BCL	C14-C13-C15-C16
8	f	101	BCL	C11-C10-C8-C9
8	F	101	BCL	C6-C7-C8-C9
8	B	101	BCL	C11-C10-C8-C9
8	L	301	BCL	C6-C7-C8-C9
8	L	301	BCL	C11-C10-C8-C9
9	k	101	SPN	C20-C21-C22-CM7
9	k	103	SPN	C28-C29-C30-CMB
10	B	102	MW9	C7-C8-C9-C10
10	Q	103	MW9	C25-C26-C27-C28
8	d	101	BCL	C5-C6-C7-C8
10	F	104	MW9	C9-C10-C11-C12
10	M	407	MW9	C7-C8-C9-C10
8	J	101	BCL	O1A-CGA-O2A-C1
8	P	101	BCL	C1A-C2A-CAA-CBA
8	t	101	BCL	C1A-C2A-CAA-CBA
8	q	102	BCL	C1A-C2A-CAA-CBA
8	n	101	BCL	C1A-C2A-CAA-CBA
8	f	101	BCL	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	a	102	BCL	C1A-C2A-CAA-CBA
8	A	101	BCL	C1A-C2A-CAA-CBA
8	M	402	BCL	C1A-C2A-CAA-CBA
8	L	304	BCL	C1A-C2A-CAA-CBA
10	L	307	MW9	C30-C31-C32-C33
10	G	105	MW9	C9-C10-C11-C12
9	r	103	SPN	C28-C29-C30-CM9
10	Q	103	MW9	C22-C21-O5-P
8	A	101	BCL	C15-C16-C17-C18
10	I	103	MW9	C18-C19-C20-O2
10	M	408	MW9	C18-C19-C20-O2
9	2	102	SPN	C11-C12-C13-CM5
10	H	302	MW9	C19-C18-O1-C17
10	G	105	MW9	C34-C35-C36-C37
8	N	101	BCL	C15-C16-C17-C18
9	k	101	SPN	C11-C10-C9-CM4
8	s	101	BCL	C2C-C3C-CAC-CBC
8	k	102	BCL	C2C-C3C-CAC-CBC
8	i	102	BCL	C2C-C3C-CAC-CBC
8	f	101	BCL	C2C-C3C-CAC-CBC
8	B	101	BCL	C2C-C3C-CAC-CBC
8	M	402	BCL	C2C-C3C-CAC-CBC
8	A	101	BCL	C5-C6-C7-C8
10	M	407	MW9	O-C17-O1-C18
9	n	102	SPN	C13-C14-C15-C16
10	I	103	MW9	O1-C18-C19-C20
10	M	407	MW9	O1-C18-C19-C20
11	L	305	LMT	C3-C4-C5-C6
15	H	304	CDL	C32-C33-C34-C35
8	a	102	BCL	C3-C5-C6-C7
8	p	103	BCL	C1-C2-C3-C5
8	2	101	BCL	C5-C6-C7-C8
9	k	103	SPN	C9-C10-C11-C12
10	F	104	MW9	C11-C12-C13-C14
10	H	302	MW9	C6-C7-C8-C9
10	G	105	MW9	O7-C22-C23-O6
10	M	408	MW9	O7-C22-C23-O6
10	L	307	MW9	O7-C22-C23-O6
10	I	103	MW9	C29-C30-C31-C32
10	F	103	MW9	C29-C30-C31-C32
10	M	407	MW9	C29-C30-C31-C32
8	f	101	BCL	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	B	101	BCL	C4-C3-C5-C6
9	v	102	SPN	C16-C17-C18-CM6
9	f	102	SPN	CM5-C13-C14-C15
9	D	102	SPN	C11-C10-C9-CM4
9	a	101	SPN	CM8-C26-C27-C28
8	I	102	BCL	C5-C6-C7-C8
9	2	103	SPN	C11-C12-C13-C14
8	b	101	BCL	C3-C5-C6-C7
10	B	102	MW9	C3-C4-C5-C6
8	1	101	BCL	C10-C11-C12-C13
10	L	308	MW9	C22-C21-O5-P
10	H	302	MW9	C20-O2-P-O4
11	E	103	LMT	C5'-C4'-O1B-C1B
15	H	303	CDL	C79-C80-C81-C82
8	R	103	BCL	CBA-CGA-O2A-C1
10	L	307	MW9	O8-C19-C20-O2
8	r	102	BCL	C16-C17-C18-C19
15	H	303	CDL	C13-C14-C15-C16
8	s	101	BCL	C15-C16-C17-C18
10	M	408	MW9	C34-C35-C36-C37
9	V	102	SPN	CM2-C1-O1-CMA
9	t	102	SPN	CM1-C1-O1-CMA
9	r	101	SPN	CM2-C1-O1-CMA
9	R	102	SPN	CM2-C1-O1-CMA
9	e	102	SPN	CM2-C1-O1-CMA
11	C	404	LMT	C2'-C1'-O1'-C1
10	M	408	MW9	O1-C18-C19-O8
10	D	104	MW9	C3-C4-C5-C6
10	G	105	MW9	C4-C5-C6-C7
10	D	104	MW9	C7-C8-C9-C10
8	V	101	BCL	C4-C3-C5-C6
8	2	101	BCL	C4-C3-C5-C6
9	r	101	SPN	C11-C10-C9-CM4
9	2	102	SPN	CM3-C5-C6-C7
9	e	102	SPN	CM3-C5-C6-C7
9	a	104	SPN	C24-C25-C26-CM8
8	e	101	BCL	C13-C15-C16-C17
8	P	101	BCL	C6-C7-C8-C10
8	s	101	BCL	C11-C12-C13-C15
8	r	102	BCL	C6-C7-C8-C10
8	i	102	BCL	C2-C3-C5-C6
8	I	102	BCL	C6-C7-C8-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	d	101	BCL	C2-C3-C5-C6
8	B	101	BCL	C11-C10-C8-C7
8	a	102	BCL	C11-C10-C8-C7
8	L	301	BCL	C11-C10-C8-C7
8	L	304	BCL	C6-C7-C8-C10
8	L	304	BCL	C12-C13-C15-C16
9	Q	102	SPN	C11-C10-C9-C8
9	Q	102	SPN	C21-C22-C23-C24
9	r	101	SPN	C20-C21-C22-C23
9	r	101	SPN	C21-C22-C23-C24
9	2	102	SPN	C21-C22-C23-C24
9	n	102	SPN	C20-C21-C22-C23
9	j	102	SPN	C21-C22-C23-C24
9	i	101	SPN	C11-C10-C9-C8
9	f	102	SPN	C21-C22-C23-C24
9	e	102	SPN	C21-C22-C23-C24
9	a	103	SPN	C21-C22-C23-C24
9	M	404	SPN	C4-C5-C6-C7
8	L	301	BCL	C3-C5-C6-C7
11	H	301	LMT	C7-C8-C9-C10
8	v	101	BCL	C6-C7-C8-C9
8	T	101	BCL	C6-C7-C8-C9
8	s	101	BCL	C11-C12-C13-C14
8	R	103	BCL	C14-C13-C15-C16
8	J	101	BCL	C6-C7-C8-C9
8	f	101	BCL	C14-C13-C15-C16
8	e	101	BCL	C14-C13-C15-C16
8	a	102	BCL	C11-C10-C8-C9
9	r	103	SPN	C20-C21-C22-CM7
9	2	103	SPN	C20-C21-C22-CM7
9	n	102	SPN	C20-C21-C22-CM7
9	a	103	SPN	CM7-C22-C23-C24
9	a	104	SPN	CM7-C22-C23-C24
8	N	101	BCL	CBA-CGA-O2A-C1
8	k	102	BCL	C10-C11-C12-C13
8	G	102	BCL	C5-C6-C7-C8
10	H	302	MW9	C11-C12-C13-C14
8	K	101	BCL	O1A-CGA-O2A-C1
8	V	101	BCL	C16-C17-C18-C20
11	H	301	LMT	C3-C4-C5-C6
15	H	303	CDL	C15-C16-C17-C18
8	j	101	BCL	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	D	102	SPN	C11-C12-C13-C14
8	q	102	BCL	CBA-CGA-O2A-C1
10	H	302	MW9	C31-C32-C33-C34
15	H	304	CDL	CA7-C31-C32-C33
8	I	102	BCL	C15-C16-C17-C18
8	j	101	BCL	C13-C15-C16-C17
9	i	103	SPN	C9-C10-C11-C12
10	H	302	MW9	C9-C10-C11-C12
9	R	102	SPN	CM3-C5-C6-C7
9	2	103	SPN	C16-C17-C18-CM6
9	i	103	SPN	C16-C17-C18-CM6
9	G	104	SPN	CM8-C26-C27-C28
9	E	102	SPN	C16-C17-C18-CM6
9	k	103	SPN	C16-C17-C18-C19
9	i	103	SPN	C12-C13-C14-C15
9	V	102	SPN	CM1-C1-C2-O2
9	V	102	SPN	CM1-C1-C2-C3
9	r	103	SPN	CM2-C1-C2-O2
9	r	103	SPN	CM2-C1-C2-C3
9	k	103	SPN	CM2-C1-C2-O2
9	k	103	SPN	CM2-C1-C2-C3
9	j	102	SPN	CM1-C1-C2-O2
9	I	101	SPN	CM1-C1-C2-O2
9	G	103	SPN	CM1-C1-C2-O2
9	G	103	SPN	CM1-C1-C2-C3
9	D	102	SPN	CM1-C1-C2-O2
9	a	101	SPN	CM2-C1-C2-O2
9	a	104	SPN	CM2-C1-C2-O2
9	M	404	SPN	CM2-C1-C2-O2
8	a	102	BCL	CBA-CGA-O2A-C1
10	F	103	MW9	C22-C21-O5-P
9	D	102	SPN	C28-C29-C30-CM9
10	F	103	MW9	C7-C8-C9-C10
15	H	304	CDL	C56-C57-C58-C59
8	V	101	BCL	O1A-CGA-O2A-C1
9	t	102	SPN	C22-C23-C24-C25
9	R	102	SPN	C22-C23-C24-C25
9	n	102	SPN	C22-C23-C24-C25
9	I	101	SPN	C22-C23-C24-C25
15	H	304	CDL	CB3-CB4-CB6-OB8
9	a	101	SPN	C16-C17-C18-CM6
11	L	306	LMT	C3-C4-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	L	308	MW9	C21-O5-P-O2
10	M	407	MW9	C4-C5-C6-C7
9	r	103	SPN	C13-C14-C15-C16
8	K	101	BCL	C2A-CAA-CBA-CGA
10	I	103	MW9	O7-C22-C23-O6
11	L	306	LMT	C5-C6-C7-C8
15	H	303	CDL	OA5-CA3-CA4-OA6
9	n	102	SPN	C11-C12-C13-CM5
15	H	304	CDL	OB6-CB4-CB6-OB8
9	S	101	SPN	C26-C27-C28-C29
14	L	303	U10	C29-C31-C32-C33
10	L	308	MW9	C29-C30-C31-C32
9	F	102	SPN	CM3-C5-C6-C7
9	a	101	SPN	C11-C10-C9-CM4
8	P	101	BCL	C2-C1-O2A-CGA
8	J	101	BCL	C2-C1-O2A-CGA
8	G	101	BCL	C2-C1-O2A-CGA
8	f	101	BCL	C2-C1-O2A-CGA
8	e	101	BCL	C2-C1-O2A-CGA
8	b	101	BCL	C2-C1-O2A-CGA
8	B	101	BCL	C2-C1-O2A-CGA
8	M	402	BCL	C2-C1-O2A-CGA
9	a	101	SPN	C4-C5-C6-C7
8	s	101	BCL	O1A-CGA-O2A-C1
8	j	101	BCL	C14-C13-C15-C16
8	G	101	BCL	C6-C7-C8-C9
9	S	101	SPN	CM7-C22-C23-C24
9	k	103	SPN	CM7-C22-C23-C24
9	K	102	SPN	C20-C21-C22-CM7
9	G	103	SPN	C20-C21-C22-CM7
13	L	302	BPH	C11-C12-C13-C14
10	M	408	MW9	C12-C13-C14-C15
10	I	103	MW9	C22-C21-O5-P
10	M	408	MW9	C19-C20-O2-P
10	B	102	MW9	C25-C26-C27-C28
15	H	303	CDL	C33-C34-C35-C36
8	j	101	BCL	C15-C16-C17-C18
8	v	101	BCL	C4C-C3C-CAC-CBC
8	j	101	BCL	C4C-C3C-CAC-CBC
8	d	101	BCL	C4C-C3C-CAC-CBC
8	v	101	BCL	C13-C15-C16-C17
8	M	402	BCL	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	a	104	SPN	C13-C14-C15-C16
9	j	102	SPN	C28-C29-C30-CM9
10	H	302	MW9	C32-C33-C34-C35
8	d	101	BCL	C8-C10-C11-C12
8	L	304	BCL	C5-C6-C7-C8
15	H	303	CDL	C54-C55-C56-C57
10	F	104	MW9	C25-C26-C27-C28
15	H	304	CDL	C53-C54-C55-C56
10	F	103	MW9	C18-C19-C20-O2
8	v	101	BCL	C11-C12-C13-C15
8	T	101	BCL	C6-C7-C8-C10
8	Q	101	BCL	C11-C10-C8-C7
8	R	101	BCL	C11-C12-C13-C15
8	N	101	BCL	C11-C10-C8-C7
8	J	101	BCL	C6-C7-C8-C10
8	f	101	BCL	C12-C13-C15-C16
8	a	102	BCL	C12-C13-C15-C16
8	M	402	BCL	C6-C7-C8-C10
9	r	103	SPN	C20-C21-C22-C23
9	p	101	SPN	C21-C22-C23-C24
9	k	101	SPN	C21-C22-C23-C24
9	k	103	SPN	C21-C22-C23-C24
9	D	103	SPN	C21-C22-C23-C24
9	a	101	SPN	C21-C22-C23-C24
9	a	103	SPN	C20-C21-C22-C23
9	a	104	SPN	C21-C22-C23-C24
15	H	304	CDL	C14-C15-C16-C17
9	M	404	SPN	C3-C4-C5-C6
10	L	308	MW9	C26-C27-C28-C29
8	Q	101	BCL	O1A-CGA-O2A-C1
8	I	102	BCL	C2A-CAA-CBA-CGA
8	T	101	BCL	C13-C15-C16-C17
8	J	101	BCL	C5-C6-C7-C8
10	B	102	MW9	C14-C15-C16-C17
8	r	102	BCL	C3-C5-C6-C7
9	S	101	SPN	C13-C14-C15-C16
9	Q	102	SPN	C13-C14-C15-C16
8	M	402	BCL	C16-C17-C18-C20
8	P	101	BCL	C5-C6-C7-C8
15	H	304	CDL	C71-CB7-OB8-CB6
15	H	303	CDL	C73-C74-C75-C76
8	p	103	BCL	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	2	101	BCL	CAD-CBD-CGD-O2D
8	i	102	BCL	CAD-CBD-CGD-O2D
15	H	303	CDL	CA6-CA4-OA6-CA5
15	H	304	CDL	CA6-CA4-OA6-CA5
15	H	303	CDL	C77-C78-C79-C80
11	E	103	LMT	C1-C2-C3-C4
8	J	101	BCL	C4-C3-C5-C6
9	2	103	SPN	C11-C10-C9-CM4
9	i	103	SPN	C11-C10-C9-CM4
8	t	101	BCL	C2-C3-C5-C6
9	K	102	SPN	C22-C23-C24-C25
9	b	102	SPN	C19-C20-C21-C22
10	B	102	MW9	O1-C18-C19-C20
10	M	408	MW9	O1-C18-C19-C20
15	H	303	CDL	C1-CA2-OA2-PA1
15	H	304	CDL	CA4-CA3-OA5-PA1
8	M	402	BCL	O1A-CGA-O2A-C1
10	F	103	MW9	O8-C19-C20-O2
8	p	103	BCL	CHA-CBD-CGD-O2D
8	i	102	BCL	CHA-CBD-CGD-O2D
8	G	101	BCL	CHA-CBD-CGD-O1D
8	G	101	BCL	CHA-CBD-CGD-O2D
8	G	102	BCL	CHA-CBD-CGD-O1D
8	F	101	BCL	CHA-CBD-CGD-O1D
8	L	304	BCL	C3-C5-C6-C7
9	2	102	SPN	C13-C14-C15-C16
8	L	304	BCL	O1A-CGA-O2A-C1
9	V	102	SPN	CM1-C1-O1-CMA
9	v	102	SPN	CM1-C1-O1-CMA
9	t	102	SPN	CM2-C1-O1-CMA
9	r	103	SPN	CM1-C1-O1-CMA
9	r	103	SPN	CM2-C1-O1-CMA
9	R	102	SPN	CM1-C1-O1-CMA
9	p	102	SPN	CM1-C1-O1-CMA
9	p	102	SPN	CM2-C1-O1-CMA
9	2	102	SPN	CM1-C1-O1-CMA
9	2	102	SPN	CM2-C1-O1-CMA
9	j	102	SPN	CM1-C1-O1-CMA
9	j	102	SPN	CM2-C1-O1-CMA
9	a	103	SPN	CM1-C1-O1-CMA
9	a	103	SPN	CM2-C1-O1-CMA
9	e	102	SPN	C2-C1-O1-CMA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	Q	103	MW9	C34-C35-C36-C37
9	E	102	SPN	C15-C16-C17-C18
8	i	102	BCL	C4-C3-C5-C6
9	Q	102	SPN	C11-C10-C9-CM4
9	q	101	SPN	C11-C12-C13-CM5
9	E	102	SPN	C11-C10-C9-CM4
9	D	102	SPN	C16-C17-C18-CM6
10	D	104	MW9	C13-C14-C15-C16
10	L	307	MW9	C14-C15-C16-C17
8	P	101	BCL	C2-C3-C5-C6
8	R	101	BCL	C11-C12-C13-C14
8	a	102	BCL	C14-C13-C15-C16
9	p	101	SPN	CM7-C22-C23-C24
9	k	101	SPN	CM7-C22-C23-C24
9	a	103	SPN	C20-C21-C22-CM7
15	H	303	CDL	C57-C58-C59-C60
8	v	101	BCL	C5-C6-C7-C8
9	k	103	SPN	O1-C1-C2-O2
9	D	102	SPN	O1-C1-C2-O2
8	J	101	BCL	C8-C10-C11-C12
8	s	101	BCL	C1A-C2A-CAA-CBA
8	r	102	BCL	C1A-C2A-CAA-CBA
8	K	101	BCL	C1A-C2A-CAA-CBA
8	I	102	BCL	C1A-C2A-CAA-CBA
8	G	102	BCL	C1A-C2A-CAA-CBA
15	H	304	CDL	CA2-OA2-PA1-OA5
10	L	307	MW9	C24-C25-C26-C27
8	G	102	BCL	C4-C3-C5-C6
9	R	102	SPN	C13-C14-C15-C16
10	I	103	MW9	C19-C20-O2-P
9	e	102	SPN	C16-C17-C18-C19
10	M	408	MW9	C26-C27-C28-C29
15	H	304	CDL	OB9-CB7-OB8-CB6
10	I	103	MW9	C21-O5-P-O3
10	G	105	MW9	C20-O2-P-O4
10	G	105	MW9	C21-O5-P-O3
10	G	105	MW9	C21-O5-P-O4
10	F	104	MW9	C21-O5-P-O4
10	B	102	MW9	C21-O5-P-O4
10	M	408	MW9	C20-O2-P-O4
15	H	304	CDL	CB3-OB5-PB2-OB3
8	t	101	BCL	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	G	102	BCL	C10-C11-C12-C13
8	M	402	BCL	CBA-CGA-O2A-C1
10	B	102	MW9	C18-C19-C20-O2
10	L	307	MW9	C18-C19-C20-O2
10	H	302	MW9	C18-C19-C20-O2
10	M	408	MW9	C3-C4-C5-C6
9	G	103	SPN	C28-C29-C30-CM9
9	b	102	SPN	C13-C14-C15-C16
9	Q	102	SPN	C23-C24-C25-C26
8	F	101	BCL	CAD-CBD-CGD-O1D
8	E	101	BCL	CAD-CBD-CGD-O1D
8	d	101	BCL	CAD-CBD-CGD-O1D
10	M	408	MW9	C14-C15-C16-C17
8	V	101	BCL	C16-C17-C18-C19
8	N	101	BCL	C4-C3-C5-C6
8	Q	101	BCL	C2C-C3C-CAC-CBC
8	R	103	BCL	C12-C13-C15-C16
8	q	102	BCL	C6-C7-C8-C10
8	2	101	BCL	C6-C7-C8-C10
8	1	101	BCL	C2C-C3C-CAC-CBC
8	1	101	BCL	C6-C7-C8-C10
8	n	101	BCL	C6-C7-C8-C10
8	n	101	BCL	C12-C13-C15-C16
8	j	101	BCL	C12-C13-C15-C16
8	I	102	BCL	C11-C12-C13-C15
8	G	102	BCL	C3A-C2A-CAA-CBA
8	d	101	BCL	C6-C7-C8-C10
8	A	101	BCL	C11-C10-C8-C7
8	M	402	BCL	C3A-C2A-CAA-CBA
9	K	102	SPN	C20-C21-C22-C23
9	M	404	SPN	C20-C21-C22-C23
10	B	102	MW9	O8-C19-C20-O2
10	H	302	MW9	O8-C19-C20-O2
13	M	403	BPH	C6-C7-C8-C10
10	L	307	MW9	C27-C28-C29-C30
9	V	102	SPN	CM6-C18-C19-C20
10	F	103	MW9	C27-C28-C29-C30
13	L	302	BPH	C4C-C3C-CAC-CBC
10	I	103	MW9	O1-C18-C19-O8
10	M	407	MW9	O1-C18-C19-O8
9	v	102	SPN	C1-C2-C3-C4
8	G	102	BCL	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	a	102	BCL	C10-C11-C12-C13
8	D	101	BCL	C4-C3-C5-C6
9	f	102	SPN	CM3-C5-C6-C7
9	i	103	SPN	C4-C5-C6-C7
10	I	103	MW9	C12-C13-C14-C15
8	v	101	BCL	C11-C12-C13-C14
8	Q	101	BCL	C11-C10-C8-C9
8	r	102	BCL	C6-C7-C8-C9
8	l	101	BCL	C6-C7-C8-C9
8	n	101	BCL	C14-C13-C15-C16
8	N	101	BCL	C11-C10-C8-C9
8	G	102	BCL	C6-C7-C8-C9
8	A	101	BCL	C11-C10-C8-C9
8	L	304	BCL	C14-C13-C15-C16
9	r	101	SPN	C20-C21-C22-CM7
9	a	101	SPN	CM7-C22-C23-C24
9	t	102	SPN	C28-C29-C30-CMB
9	F	102	SPN	CM8-C26-C27-C28
9	t	102	SPN	C25-C26-C27-C28
10	L	308	MW9	C11-C12-C13-C14
10	M	407	MW9	C10-C11-C12-C13
8	v	101	BCL	C15-C16-C17-C18
8	q	102	BCL	C5-C6-C7-C8
15	H	303	CDL	OA5-CA3-CA4-CA6
8	B	101	BCL	O1A-CGA-O2A-C1
8	V	101	BCL	C2-C1-O2A-CGA
8	l	101	BCL	C2-C1-O2A-CGA
8	L	301	BCL	C2-C1-O2A-CGA
10	F	104	MW9	C19-C20-O2-P
15	H	304	CDL	C1-CB2-OB2-PB2
9	2	102	SPN	CM5-C13-C14-C15
9	K	102	SPN	CM5-C13-C14-C15
9	I	101	SPN	CM5-C13-C14-C15
9	b	102	SPN	C16-C17-C18-CM6
9	V	102	SPN	C16-C17-C18-C19
8	R	103	BCL	O1A-CGA-O2A-C1
8	2	101	BCL	C8-C10-C11-C12
8	Q	101	BCL	C2A-CAA-CBA-CGA
9	k	103	SPN	CM2-C1-O1-CMA
9	G	104	SPN	CM2-C1-O1-CMA
14	M	406	U10	C24-C26-C27-C28
8	j	101	BCL	C1-C2-C3-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	F	103	MW9	C21-O5-P-O2
10	M	407	MW9	C21-O5-P-O2
10	L	307	MW9	C21-O5-P-O2
15	H	304	CDL	CB2-OB2-PB2-OB5
13	L	302	BPH	CHA-CBD-CGD-O2D
15	H	304	CDL	C72-C73-C74-C75
15	H	303	CDL	C80-C81-C82-C83
9	M	404	SPN	C22-C23-C24-C25
8	I	102	BCL	C4-C3-C5-C6
9	t	102	SPN	CM3-C5-C6-C7
9	q	101	SPN	CM3-C5-C6-C7
9	p	102	SPN	C16-C17-C18-CM6
9	a	104	SPN	C16-C17-C18-CM6
10	M	407	MW9	C6-C7-C8-C9
8	k	102	BCL	C6-C7-C8-C10
8	M	405	BCL	C6-C7-C8-C10
8	q	102	BCL	C6-C7-C8-C9
8	n	101	BCL	C6-C7-C8-C9
8	I	102	BCL	C11-C12-C13-C14
8	d	101	BCL	C6-C7-C8-C9
10	G	105	MW9	C7-C8-C9-C10
14	M	406	U10	C5-C4-O4-C4M
10	B	102	MW9	C35-C36-C37-C38
8	Q	101	BCL	CBA-CGA-O2A-C1
15	H	303	CDL	C62-C63-C64-C65
9	2	102	SPN	C28-C29-C30-CM9
9	v	102	SPN	C11-C10-C9-CM4
9	k	103	SPN	CM3-C5-C6-C7
9	I	101	SPN	C16-C17-C18-CM6
9	a	104	SPN	C27-C28-C29-C30
9	t	102	SPN	C11-C12-C13-C14
8	B	101	BCL	C2-C3-C5-C6
13	M	403	BPH	C8-C10-C11-C12
10	D	104	MW9	C24-C25-C26-C27
10	M	407	MW9	C27-C28-C29-C30
10	M	408	MW9	C30-C31-C32-C33
10	M	408	MW9	C32-C33-C34-C35
10	L	307	MW9	C32-C33-C34-C35
9	G	104	SPN	C15-C16-C17-C18
8	N	101	BCL	C8-C10-C11-C12
14	L	303	U10	C15-C14-C16-C17
8	B	101	BCL	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
16	C	402	HEC	CAA-CBA-CGA-O2A
8	D	101	BCL	C2-C1-O2A-CGA
8	G	101	BCL	C8-C10-C11-C12
9	q	101	SPN	CM2-C1-C2-O2
9	q	101	SPN	CM2-C1-C2-C3
9	D	102	SPN	CM1-C1-C2-C3
11	E	103	LMT	O5B-C5B-C6B-O6B
8	M	405	BCL	C3-C5-C6-C7
8	k	102	BCL	C3A-C2A-CAA-CBA
8	j	101	BCL	C3A-C2A-CAA-CBA
8	e	101	BCL	C3A-C2A-CAA-CBA
8	M	402	BCL	C16-C17-C18-C19
10	F	103	MW9	C32-C33-C34-C35
9	V	102	SPN	CM8-C26-C27-C28
9	G	104	SPN	C16-C17-C18-CM6
8	p	103	BCL	C11-C12-C13-C14
8	N	101	BCL	C6-C7-C8-C9
9	M	404	SPN	C20-C21-C22-CM7
8	v	101	BCL	C16-C17-C18-C20
16	C	403	HEC	C3D-CAD-CBD-CGD
10	B	102	MW9	C10-C11-C12-C13
10	G	105	MW9	O1-C18-C19-C20
8	M	402	BCL	C2A-CAA-CBA-CGA
9	G	104	SPN	C3-C4-C5-CM3
13	L	302	BPH	C16-C17-C18-C20
13	L	302	BPH	O2A-C1-C2-C3
10	M	407	MW9	C34-C35-C36-C37
10	M	407	MW9	C25-C26-C27-C28
10	Q	103	MW9	C20-C19-O8-C24
8	e	101	BCL	C5-C6-C7-C8
8	P	101	BCL	C4-C3-C5-C6
9	Q	102	SPN	CM8-C26-C27-C28
9	i	103	SPN	CM5-C13-C14-C15
8	T	101	BCL	C1A-C2A-CAA-CBA
8	R	103	BCL	C1A-C2A-CAA-CBA
8	k	102	BCL	C1A-C2A-CAA-CBA
8	j	101	BCL	C1A-C2A-CAA-CBA
8	e	101	BCL	C1A-C2A-CAA-CBA
8	M	405	BCL	C1A-C2A-CAA-CBA
9	G	104	SPN	C12-C13-C14-C15
13	M	403	BPH	C11-C12-C13-C15
8	Q	101	BCL	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	H	304	CDL	OB5-CB3-CB4-OB6
8	2	101	BCL	CAA-CBA-CGA-O2A
10	G	105	MW9	C18-C19-C20-O2
8	t	101	BCL	C4-C3-C5-C6
9	r	101	SPN	C16-C17-C18-CM6
9	p	101	SPN	CM5-C13-C14-C15
9	I	101	SPN	C11-C10-C9-CM4
9	b	102	SPN	C11-C10-C9-CM4
8	T	101	BCL	C15-C16-C17-C18
9	r	103	SPN	C12-C13-C14-C15
9	e	102	SPN	C4-C5-C6-C7
9	a	103	SPN	C25-C26-C27-C28
11	L	305	LMT	C6-C7-C8-C9
8	d	101	BCL	O1A-CGA-O2A-C1
9	t	102	SPN	C15-C16-C17-C18
9	v	102	SPN	CM2-C1-O1-CMA
10	L	308	MW9	O1-C18-C19-O8
9	v	102	SPN	C2-C3-C4-C5
9	S	101	SPN	C2-C3-C4-C5
9	S	102	SPN	C2-C3-C4-C5
9	t	102	SPN	C2-C3-C4-C5
9	Q	102	SPN	C2-C3-C4-C5
9	r	101	SPN	C2-C3-C4-C5
9	r	103	SPN	C2-C3-C4-C5
9	R	102	SPN	C2-C3-C4-C5
9	q	101	SPN	C2-C3-C4-C5
9	p	101	SPN	C2-C3-C4-C5
9	p	102	SPN	C2-C3-C4-C5
9	2	102	SPN	C2-C3-C4-C5
9	2	103	SPN	C2-C3-C4-C5
9	n	102	SPN	C2-C3-C4-C5
9	k	101	SPN	C2-C3-C4-C5
9	j	102	SPN	C2-C3-C4-C5
9	i	101	SPN	C2-C3-C4-C5
9	I	101	SPN	C2-C3-C4-C5
9	G	103	SPN	C2-C3-C4-C5
9	f	102	SPN	C2-C3-C4-C5
9	F	102	SPN	C2-C3-C4-C5
9	e	102	SPN	C2-C3-C4-C5
9	E	102	SPN	C2-C3-C4-C5
9	D	102	SPN	C2-C3-C4-C5
9	D	103	SPN	C2-C3-C4-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	b	102	SPN	C2-C3-C4-C5
9	a	101	SPN	C2-C3-C4-C5
9	a	103	SPN	C2-C3-C4-C5
9	a	104	SPN	C2-C3-C4-C5
10	F	104	MW9	C29-C30-C31-C32
10	I	103	MW9	C11-C12-C13-C14
16	C	401	HEC	CAA-CBA-CGA-O2A
9	V	102	SPN	C11-C10-C9-CM4
9	v	102	SPN	CM3-C5-C6-C7
9	S	101	SPN	C16-C17-C18-CM6
9	G	103	SPN	C11-C10-C9-CM4
9	D	103	SPN	C16-C17-C18-CM6
8	K	101	BCL	C2-C1-O2A-CGA
8	d	101	BCL	C2-C1-O2A-CGA
8	a	102	BCL	C2-C1-O2A-CGA
8	A	101	BCL	C2-C1-O2A-CGA
13	M	403	BPH	C2-C1-O2A-CGA
8	p	103	BCL	C2C-C3C-CAC-CBC
9	F	102	SPN	C11-C10-C9-C8
14	L	303	U10	C13-C14-C16-C17
8	q	102	BCL	O1A-CGA-O2A-C1
8	e	101	BCL	C11-C12-C13-C14
9	v	102	SPN	CM7-C22-C23-C24
10	L	307	MW9	C11-C12-C13-C14
8	2	101	BCL	C1-C2-C3-C5
10	F	103	MW9	C30-C31-C32-C33
15	H	303	CDL	CA3-CA4-CA6-OA8
8	T	101	BCL	C4-C3-C5-C6
8	K	101	BCL	C4-C3-C5-C6
9	q	101	SPN	C11-C10-C9-CM4
9	p	101	SPN	C11-C10-C9-CM4
9	p	102	SPN	CM5-C13-C14-C15
9	2	103	SPN	CM3-C5-C6-C7
9	G	104	SPN	CM3-C5-C6-C7
9	a	103	SPN	C11-C10-C9-CM4
14	L	303	U10	C20-C19-C21-C22
8	J	101	BCL	C4C-C3C-CAC-CBC
8	V	101	BCL	C2-C3-C5-C6
8	K	101	BCL	C2-C3-C5-C6
8	J	101	BCL	C2-C3-C5-C6
8	D	101	BCL	C2-C3-C5-C6
9	R	102	SPN	C12-C13-C14-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
16	C	403	HEC	CAD-CBD-CGD-O2D
8	p	103	BCL	C5-C6-C7-C8
9	G	104	SPN	C11-C12-C13-CM5
10	H	302	MW9	C30-C31-C32-C33
8	R	101	BCL	C2A-CAA-CBA-CGA
8	s	101	BCL	C10-C11-C12-C13
8	M	405	BCL	C8-C10-C11-C12
10	Q	103	MW9	C26-C27-C28-C29
9	k	101	SPN	CM5-C13-C14-C15
9	r	101	SPN	C5-C6-C7-C8
8	T	101	BCL	C2-C3-C5-C6
8	G	102	BCL	C2-C3-C5-C6
8	b	101	BCL	C2-C3-C5-C6
9	v	102	SPN	C12-C13-C14-C15
9	Q	102	SPN	C16-C17-C18-C19
9	i	101	SPN	C16-C17-C18-C19
10	G	105	MW9	C32-C33-C34-C35
8	P	101	BCL	C1-C2-C3-C4
8	t	101	BCL	C1-C2-C3-C4
8	Q	101	BCL	C1-C2-C3-C4
8	2	101	BCL	C1-C2-C3-C4
8	1	101	BCL	C1-C2-C3-C4
10	H	302	MW9	C26-C27-C28-C29
15	H	303	CDL	OA6-CA4-CA6-OA8
15	H	304	CDL	OA6-CA4-CA6-OA8
15	H	303	CDL	C55-C56-C57-C58
16	C	403	HEC	CAD-CBD-CGD-O1D
10	F	104	MW9	O8-C24-C25-C26
10	B	102	MW9	O8-C24-C25-C26
8	r	102	BCL	O1A-CGA-O2A-C1
8	B	101	BCL	CBA-CGA-O2A-C1
8	F	101	BCL	C4-C3-C5-C6
9	n	102	SPN	CM5-C13-C14-C15
9	i	101	SPN	CM5-C13-C14-C15
9	D	103	SPN	C11-C10-C9-CM4
9	b	102	SPN	CM8-C26-C27-C28
9	a	104	SPN	CM8-C26-C27-C28
8	K	101	BCL	C5-C6-C7-C8
8	M	402	BCL	C5-C6-C7-C8
16	C	401	HEC	CAA-CBA-CGA-O1A
9	S	101	SPN	C12-C13-C14-C15
9	S	102	SPN	C11-C10-C9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	t	102	SPN	C16-C17-C18-C19
9	e	102	SPN	C11-C10-C9-C8
9	b	102	SPN	C12-C13-C14-C15
13	L	302	BPH	C2-C3-C5-C6
8	Q	101	BCL	C5-C6-C7-C8
8	v	101	BCL	CAA-CBA-CGA-O2A
8	j	101	BCL	CAA-CBA-CGA-O2A
9	V	102	SPN	C20-C21-C22-CM7
9	v	102	SPN	C20-C21-C22-CM7
9	r	103	SPN	CM7-C22-C23-C24
9	R	102	SPN	C20-C21-C22-CM7
8	I	102	BCL	C3A-C2A-CAA-CBA
8	s	101	BCL	CAA-CBA-CGA-O2A
8	I	102	BCL	CAD-CBD-CGD-O2D
10	Q	103	MW9	C18-C19-O8-C24
8	M	405	BCL	C15-C16-C17-C18
10	I	103	MW9	O8-C24-C25-C26
8	k	102	BCL	C4-C3-C5-C6
8	G	101	BCL	C4-C3-C5-C6
9	Q	102	SPN	CM5-C13-C14-C15
9	p	101	SPN	CM3-C5-C6-C7
9	p	102	SPN	CM3-C5-C6-C7
9	G	103	SPN	C16-C17-C18-CM6
9	M	404	SPN	C16-C17-C18-CM6
8	G	102	BCL	C16-C17-C18-C20
8	I	102	BCL	C2-C3-C5-C6
9	r	101	SPN	C4-C5-C6-C7
9	k	103	SPN	C12-C13-C14-C15
9	j	102	SPN	C11-C10-C9-C8
9	D	103	SPN	C4-C5-C6-C7
10	M	407	MW9	O8-C24-C25-C26
15	H	304	CDL	C34-C35-C36-C37
9	b	102	SPN	C9-C10-C11-C12
10	G	105	MW9	C29-C30-C31-C32
16	C	402	HEC	CAA-CBA-CGA-O1A
8	A	101	BCL	C2A-CAA-CBA-CGA
8	M	405	BCL	CAA-CBA-CGA-O2A
8	V	101	BCL	CHA-CBD-CGD-O1D
8	V	101	BCL	CHA-CBD-CGD-O2D
8	2	101	BCL	CHA-CBD-CGD-O1D
8	2	101	BCL	CHA-CBD-CGD-O2D
8	j	101	BCL	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	I	102	BCL	CHA-CBD-CGD-O2D
8	F	101	BCL	CHA-CBD-CGD-O2D
8	E	101	BCL	CHA-CBD-CGD-O1D
8	a	102	BCL	CHA-CBD-CGD-O1D
8	a	102	BCL	CHA-CBD-CGD-O2D
8	L	304	BCL	CHA-CBD-CGD-O1D
8	L	304	BCL	CHA-CBD-CGD-O2D
10	Q	103	MW9	O8-C24-C25-C26
9	k	101	SPN	C4-C5-C6-C7
9	G	103	SPN	C12-C13-C14-C15
9	a	103	SPN	C16-C17-C18-C19
9	k	101	SPN	C13-C14-C15-C16
10	Q	103	MW9	C18-C19-C20-O2
9	k	101	SPN	CM1-C1-O1-CMA
9	f	102	SPN	CM2-C1-O1-CMA
9	D	103	SPN	CM2-C1-O1-CMA
11	L	306	LMT	C6-C7-C8-C9
10	Q	103	MW9	C9-C10-C11-C12
10	Q	103	MW9	C32-C33-C34-C35
9	V	102	SPN	C2-C1-O1-CMA
9	v	102	SPN	C2-C1-O1-CMA
9	r	103	SPN	C2-C1-O1-CMA
9	R	102	SPN	C2-C1-O1-CMA
9	p	102	SPN	C2-C1-O1-CMA
9	2	102	SPN	C2-C1-O1-CMA
9	k	101	SPN	C2-C1-O1-CMA
9	k	103	SPN	C2-C1-O1-CMA
9	j	102	SPN	C2-C1-O1-CMA
9	G	104	SPN	C2-C1-O1-CMA
9	f	102	SPN	C2-C1-O1-CMA
9	D	103	SPN	C2-C1-O1-CMA
9	a	103	SPN	C2-C1-O1-CMA
8	T	101	BCL	CBA-CGA-O2A-C1
8	D	101	BCL	CBA-CGA-O2A-C1
9	R	102	SPN	C15-C16-C17-C18
9	R	102	SPN	CM8-C26-C27-C28
14	M	406	U10	C35-C34-C36-C37
9	R	102	SPN	C11-C10-C9-C8
9	q	101	SPN	C20-C21-C22-C23
13	M	403	BPH	C11-C10-C8-C7
8	s	101	BCL	C14-C13-C15-C16
8	D	101	BCL	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	t	102	SPN	C20-C21-C22-CM7
9	q	101	SPN	C20-C21-C22-CM7
13	M	403	BPH	C6-C7-C8-C9
8	F	101	BCL	C16-C17-C18-C19
15	H	303	CDL	C43-C44-C45-C46
8	N	101	BCL	C2A-CAA-CBA-CGA
9	V	102	SPN	C6-C7-C8-C9
9	V	102	SPN	C18-C19-C20-C21
9	v	102	SPN	C6-C7-C8-C9
9	v	102	SPN	C18-C19-C20-C21
9	S	101	SPN	C18-C19-C20-C21
9	S	102	SPN	C18-C19-C20-C21
9	t	102	SPN	C18-C19-C20-C21
9	Q	102	SPN	C10-C11-C12-C13
9	Q	102	SPN	C18-C19-C20-C21
9	r	101	SPN	C6-C7-C8-C9
9	r	101	SPN	C18-C19-C20-C21
9	r	103	SPN	C6-C7-C8-C9
9	r	103	SPN	C18-C19-C20-C21
9	R	102	SPN	C18-C19-C20-C21
9	q	101	SPN	C6-C7-C8-C9
9	q	101	SPN	C10-C11-C12-C13
9	q	101	SPN	C18-C19-C20-C21
9	q	101	SPN	C23-C24-C25-C26
9	p	101	SPN	C6-C7-C8-C9
9	p	101	SPN	C10-C11-C12-C13
9	p	101	SPN	C18-C19-C20-C21
9	p	102	SPN	C6-C7-C8-C9
9	p	102	SPN	C10-C11-C12-C13
9	p	102	SPN	C18-C19-C20-C21
9	2	102	SPN	C10-C11-C12-C13
9	2	102	SPN	C18-C19-C20-C21
9	2	103	SPN	C6-C7-C8-C9
9	2	103	SPN	C18-C19-C20-C21
9	n	102	SPN	C10-C11-C12-C13
9	n	102	SPN	C18-C19-C20-C21
9	k	101	SPN	C10-C11-C12-C13
9	k	101	SPN	C18-C19-C20-C21
9	k	103	SPN	C18-C19-C20-C21
9	K	102	SPN	C10-C11-C12-C13
9	K	102	SPN	C18-C19-C20-C21
9	j	102	SPN	C18-C19-C20-C21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	i	101	SPN	C18-C19-C20-C21
9	i	103	SPN	C6-C7-C8-C9
9	i	103	SPN	C18-C19-C20-C21
9	I	101	SPN	C10-C11-C12-C13
9	I	101	SPN	C18-C19-C20-C21
9	G	103	SPN	C18-C19-C20-C21
9	G	104	SPN	C10-C11-C12-C13
9	G	104	SPN	C18-C19-C20-C21
9	f	102	SPN	C6-C7-C8-C9
9	f	102	SPN	C18-C19-C20-C21
9	F	102	SPN	C18-C19-C20-C21
9	e	102	SPN	C18-C19-C20-C21
9	E	102	SPN	C6-C7-C8-C9
9	E	102	SPN	C18-C19-C20-C21
9	D	102	SPN	C6-C7-C8-C9
9	D	102	SPN	C18-C19-C20-C21
9	D	103	SPN	C18-C19-C20-C21
9	a	101	SPN	C6-C7-C8-C9
9	a	101	SPN	C18-C19-C20-C21
9	a	103	SPN	C6-C7-C8-C9
9	a	103	SPN	C10-C11-C12-C13
9	a	103	SPN	C18-C19-C20-C21
9	a	104	SPN	C18-C19-C20-C21
9	M	404	SPN	C10-C11-C12-C13
9	M	404	SPN	C18-C19-C20-C21
10	F	104	MW9	C32-C33-C34-C35
9	p	102	SPN	C11-C10-C9-CM4
10	B	102	MW9	O9-C24-C25-C26
16	C	402	HEC	C4C-C3C-CAC-CBC
10	L	308	MW9	C27-C28-C29-C30
10	F	104	MW9	O9-C24-C25-C26
10	M	407	MW9	O9-C24-C25-C26
8	s	101	BCL	CBA-CGA-O2A-C1
8	d	101	BCL	CAA-CBA-CGA-O1A
15	H	304	CDL	CA3-CA4-CA6-OA8
10	Q	103	MW9	O9-C24-C25-C26
10	I	103	MW9	O9-C24-C25-C26
9	n	102	SPN	CM3-C5-C6-C7
9	F	102	SPN	C16-C17-C18-C19
10	I	103	MW9	C20-O2-P-O3
15	H	303	CDL	CA3-OA5-PA1-OA3
15	H	304	CDL	CB2-OB2-PB2-OB3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	b	101	BCL	C16-C17-C18-C20
8	q	102	BCL	CAA-CBA-CGA-O1A
8	V	101	BCL	C13-C15-C16-C17
9	R	102	SPN	C16-C17-C18-CM6
13	L	302	BPH	C4-C3-C5-C6
8	q	102	BCL	CAD-CBD-CGD-O1D
8	B	101	BCL	CAD-CBD-CGD-O1D
8	T	101	BCL	C5-C6-C7-C8
8	i	102	BCL	C6-C7-C8-C9
8	G	102	BCL	C11-C12-C13-C14
9	I	101	SPN	C20-C21-C22-CM7
9	a	104	SPN	C20-C21-C22-CM7
13	M	403	BPH	C11-C10-C8-C9
9	i	101	SPN	C13-C14-C15-C16
10	F	103	MW9	O8-C24-C25-C26
10	M	408	MW9	O8-C24-C25-C26
9	G	103	SPN	C3-C4-C5-CM3
9	S	101	SPN	CM2-C1-C2-O2
9	S	102	SPN	CM2-C1-C2-O2
9	Q	102	SPN	CM2-C1-C2-O2
9	2	102	SPN	CM2-C1-C2-O2
9	G	104	SPN	CM2-C1-C2-O2
9	a	101	SPN	CM2-C1-C2-C3
9	a	103	SPN	CM2-C1-C2-O2
8	d	101	BCL	CAA-CBA-CGA-O2A
10	L	307	MW9	O8-C24-C25-C26
10	H	302	MW9	O8-C24-C25-C26
10	F	104	MW9	C7-C8-C9-C10
8	P	101	BCL	C16-C17-C18-C20
10	Q	103	MW9	C37-C38-C39-C40
8	R	103	BCL	C3A-C2A-CAA-CBA
8	G	101	BCL	C2C-C3C-CAC-CBC
8	G	102	BCL	C11-C12-C13-C15
8	D	101	BCL	C6-C7-C8-C10
8	L	301	BCL	C6-C7-C8-C10
9	v	102	SPN	C20-C21-C22-C23
9	t	102	SPN	C20-C21-C22-C23
9	R	102	SPN	C16-C17-C18-C19
9	q	101	SPN	C21-C22-C23-C24
9	F	102	SPN	C21-C22-C23-C24
9	D	103	SPN	C11-C10-C9-C8
10	Q	103	MW9	O8-C19-C20-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	L	302	BPH	C12-C13-C15-C16
10	H	302	MW9	O9-C24-C25-C26
8	k	102	BCL	CAA-CBA-CGA-O2A
10	M	408	MW9	O9-C24-C25-C26
9	r	103	SPN	C5-C6-C7-C8
9	p	101	SPN	C26-C27-C28-C29
8	R	103	BCL	C15-C16-C17-C18
10	F	103	MW9	O9-C24-C25-C26

There are no ring outliers.

84 monomers are involved in 316 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	C	401	HEC	6	0
9	k	103	SPN	2	0
8	R	101	BCL	2	0
8	r	102	BCL	4	0
9	e	102	SPN	4	0
9	S	102	SPN	4	0
8	R	103	BCL	4	0
9	I	101	SPN	9	0
8	M	405	BCL	4	0
9	a	101	SPN	2	0
9	v	102	SPN	6	0
8	s	101	BCL	2	0
9	a	103	SPN	2	0
8	e	101	BCL	7	0
13	M	403	BPH	2	0
8	b	101	BCL	3	0
9	G	104	SPN	3	0
8	G	101	BCL	6	0
16	C	402	HEC	3	0
13	L	302	BPH	2	0
14	L	303	U10	7	0
9	i	101	SPN	5	0
9	2	102	SPN	2	0
9	K	102	SPN	8	0
8	A	101	BCL	6	0
9	r	103	SPN	1	0
8	p	103	BCL	2	0
15	H	303	CDL	4	0
8	K	101	BCL	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	t	102	SPN	3	0
8	N	101	BCL	4	0
9	k	101	SPN	1	0
9	j	102	SPN	4	0
9	Q	102	SPN	3	0
8	d	101	BCL	8	0
9	F	102	SPN	4	0
8	J	101	BCL	7	0
15	H	304	CDL	2	0
8	Q	101	BCL	5	0
9	b	102	SPN	12	0
8	T	101	BCL	5	0
9	R	102	SPN	10	0
8	q	102	BCL	5	0
8	i	102	BCL	6	0
8	L	301	BCL	3	0
16	C	403	HEC	1	0
8	a	102	BCL	3	0
8	E	101	BCL	4	0
8	F	101	BCL	4	0
8	v	101	BCL	5	0
9	a	104	SPN	7	0
9	2	103	SPN	6	0
14	M	406	U10	6	0
8	f	101	BCL	9	0
9	r	101	SPN	4	0
9	G	103	SPN	5	0
9	D	102	SPN	3	0
8	M	402	BCL	4	0
9	V	102	SPN	9	0
8	j	101	BCL	10	0
9	M	404	SPN	3	0
9	D	103	SPN	3	0
9	E	102	SPN	4	0
9	S	101	SPN	6	0
11	L	305	LMT	1	0
9	f	102	SPN	1	0
9	i	103	SPN	3	0
8	2	101	BCL	2	0
8	1	101	BCL	3	0
11	E	103	LMT	4	0
9	p	102	SPN	5	0

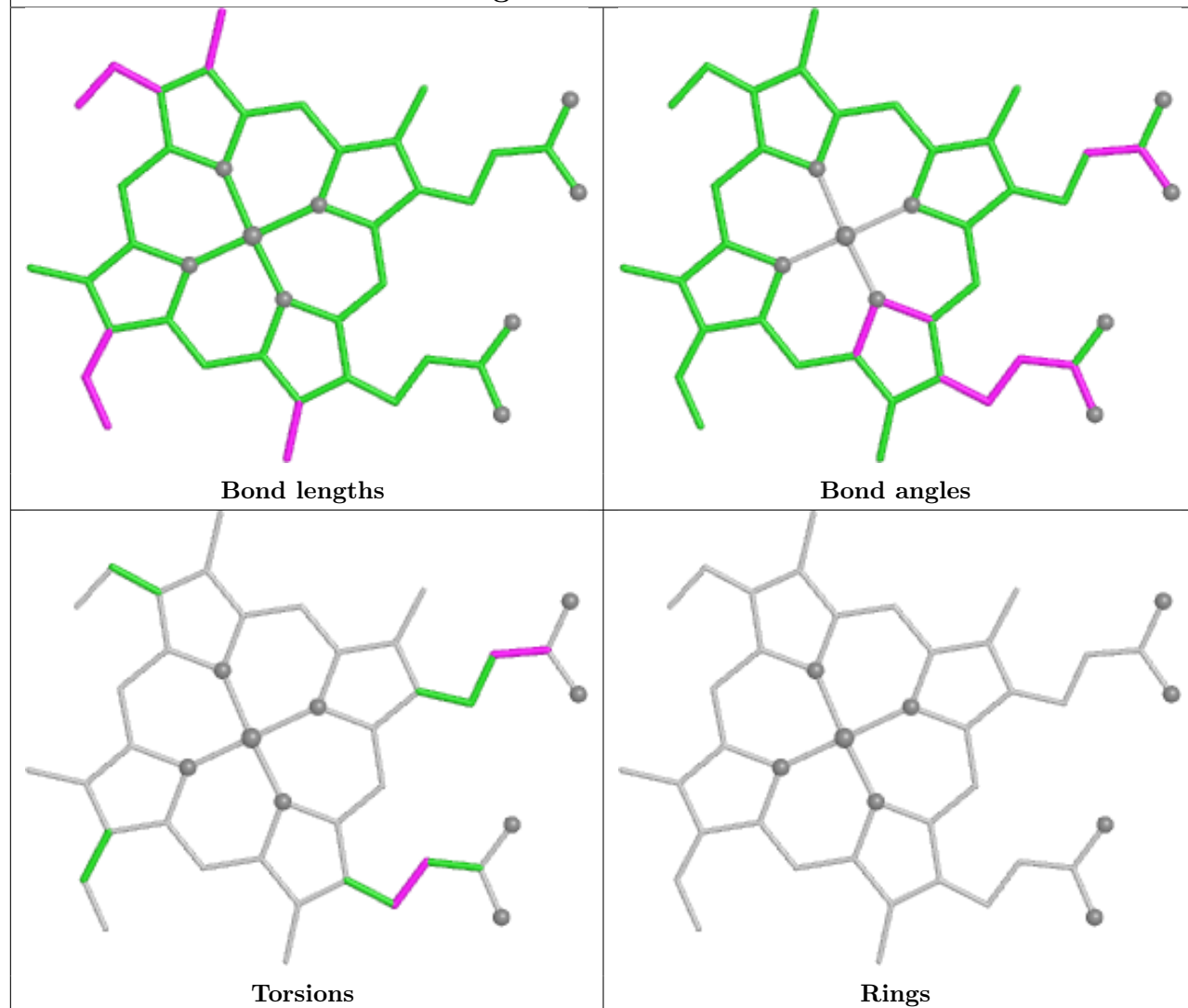
Continued on next page...

Continued from previous page...

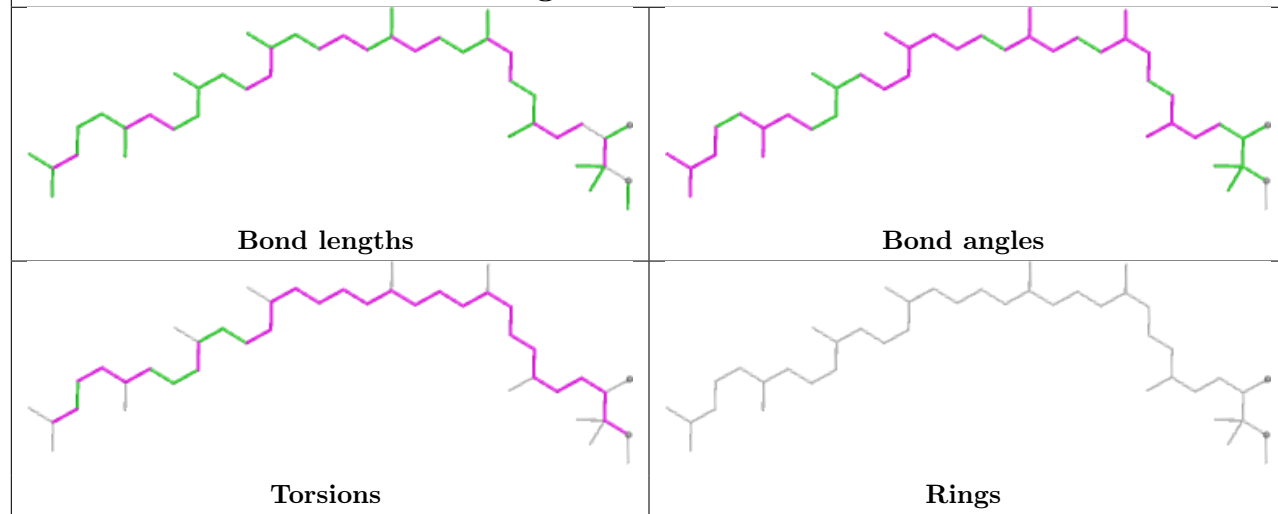
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	V	101	BCL	5	0
8	L	304	BCL	7	0
8	n	101	BCL	3	0
8	B	101	BCL	3	0
8	t	101	BCL	9	0
9	p	101	SPN	10	0
8	I	102	BCL	7	0
9	n	102	SPN	8	0
8	D	101	BCL	2	0
8	P	101	BCL	4	0
8	G	102	BCL	3	0
8	k	102	BCL	4	0
9	q	101	SPN	2	0

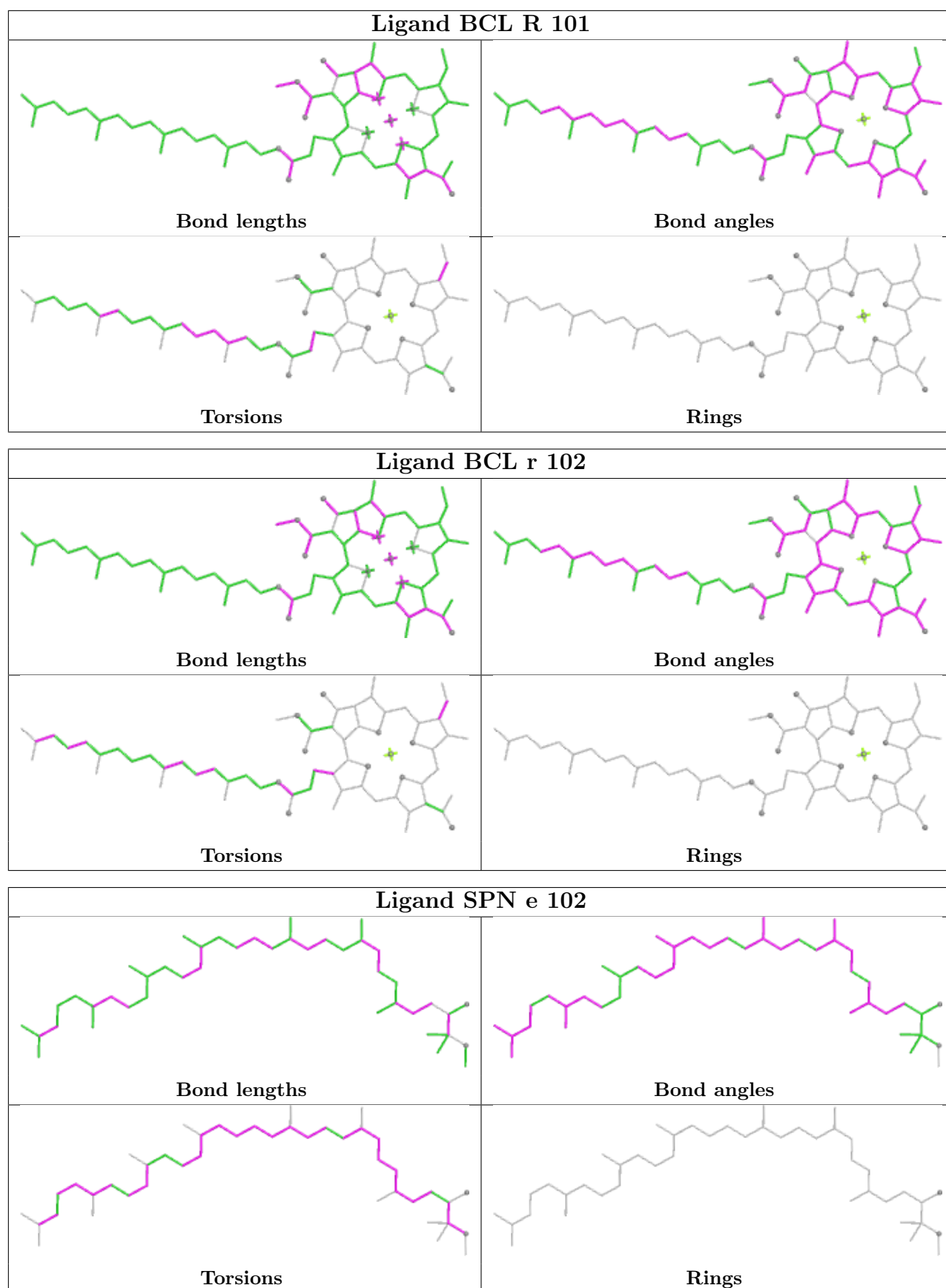
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

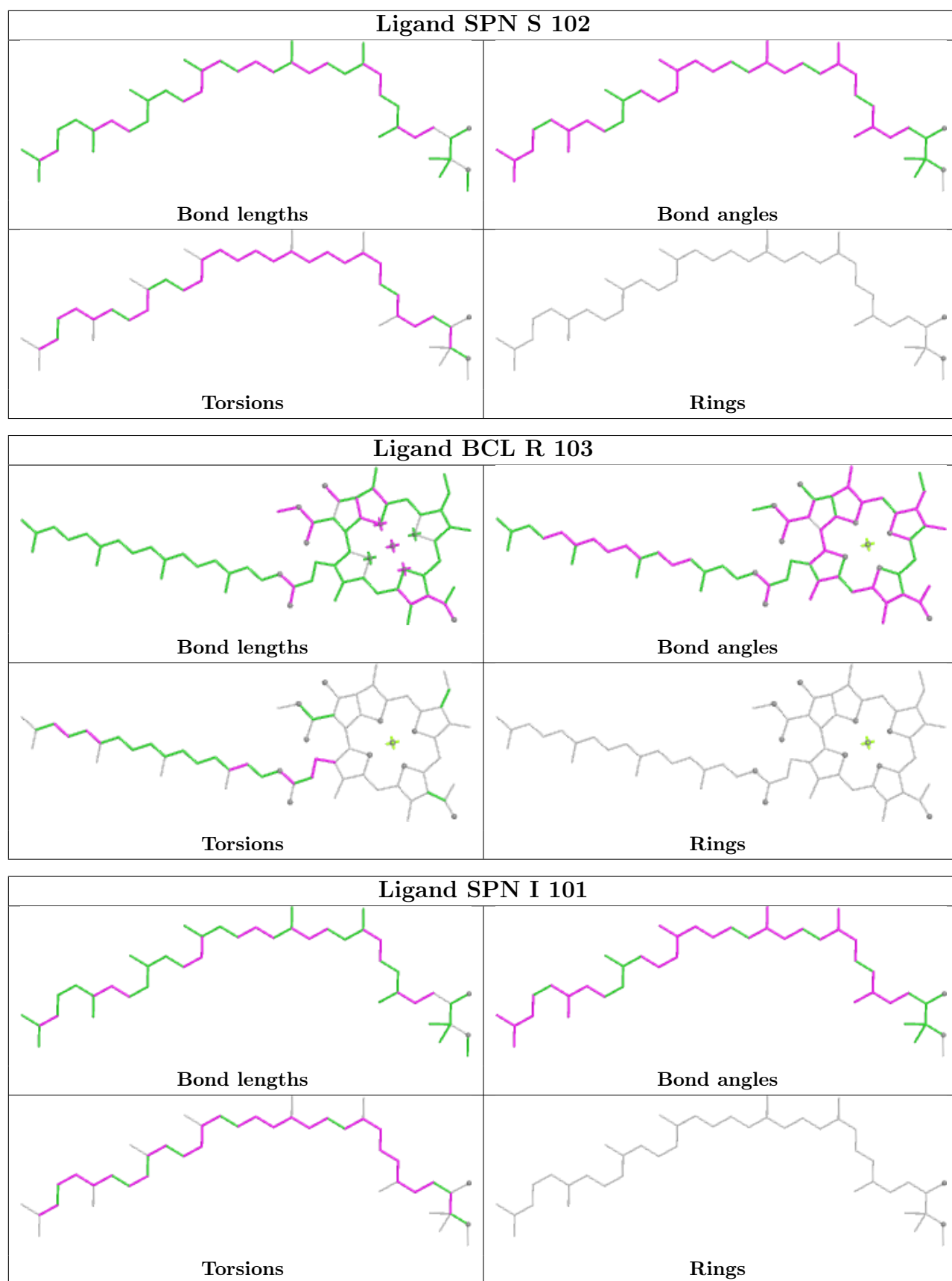
Ligand HEC C 401

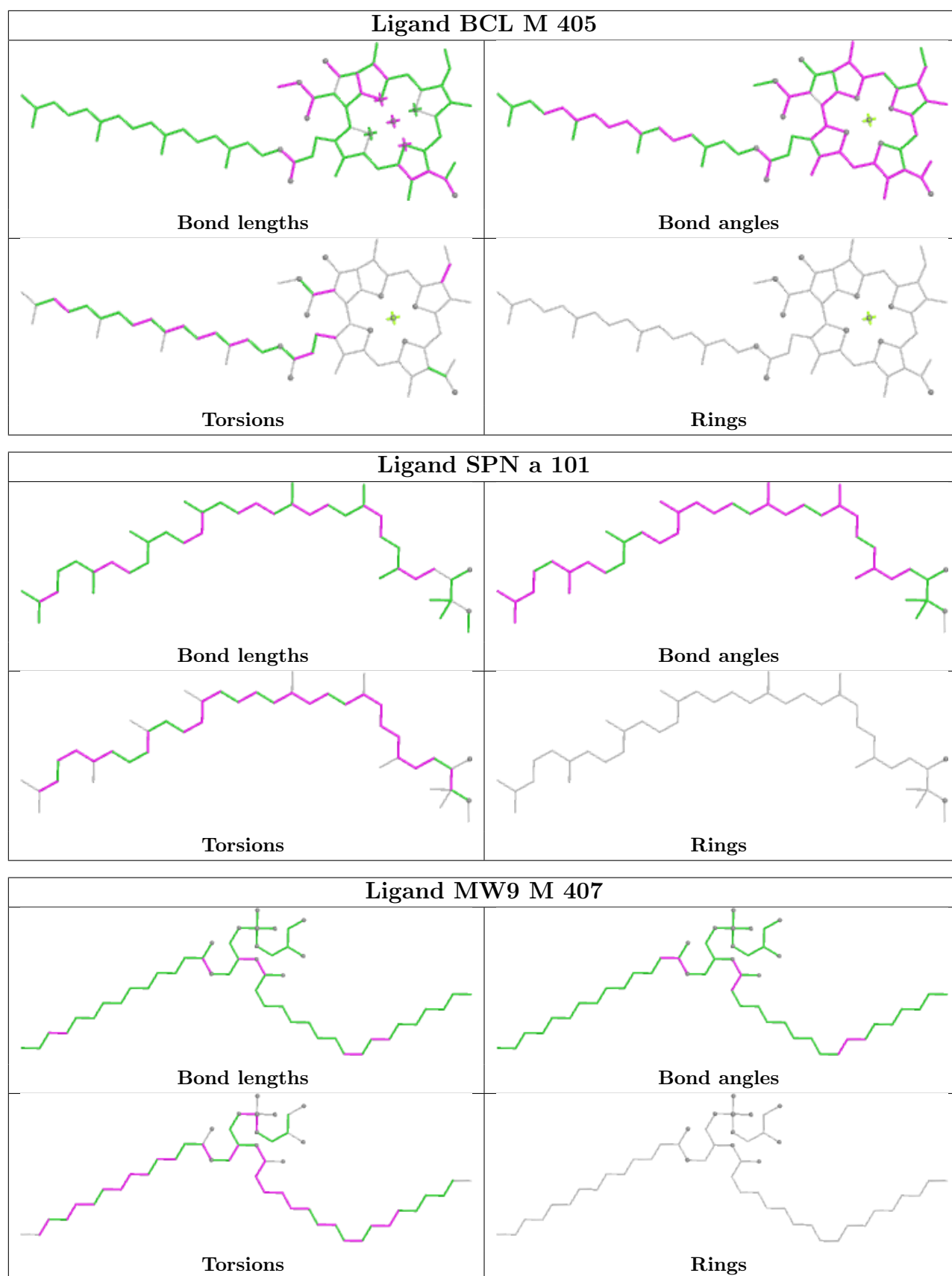


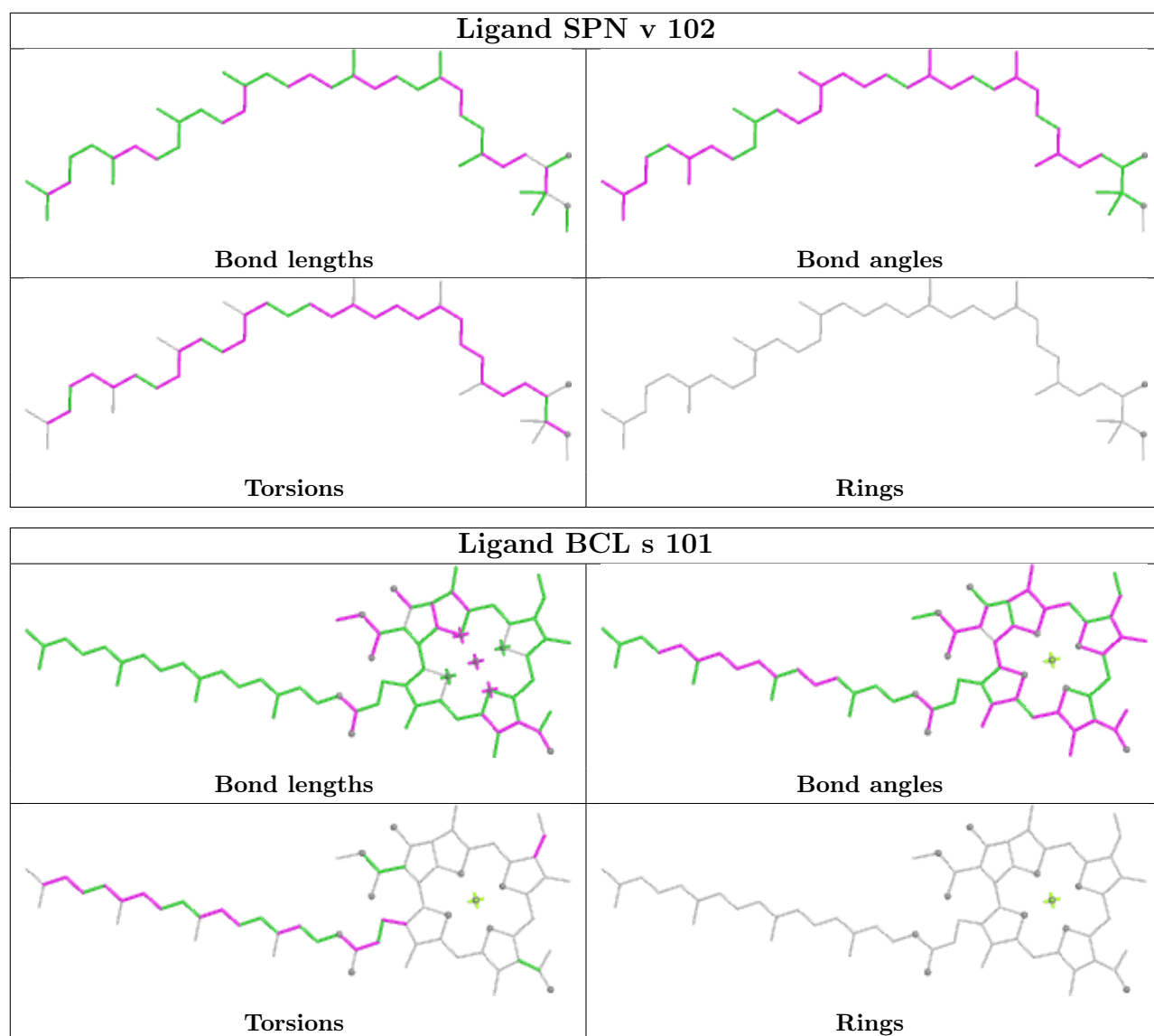
Ligand SPN k 103

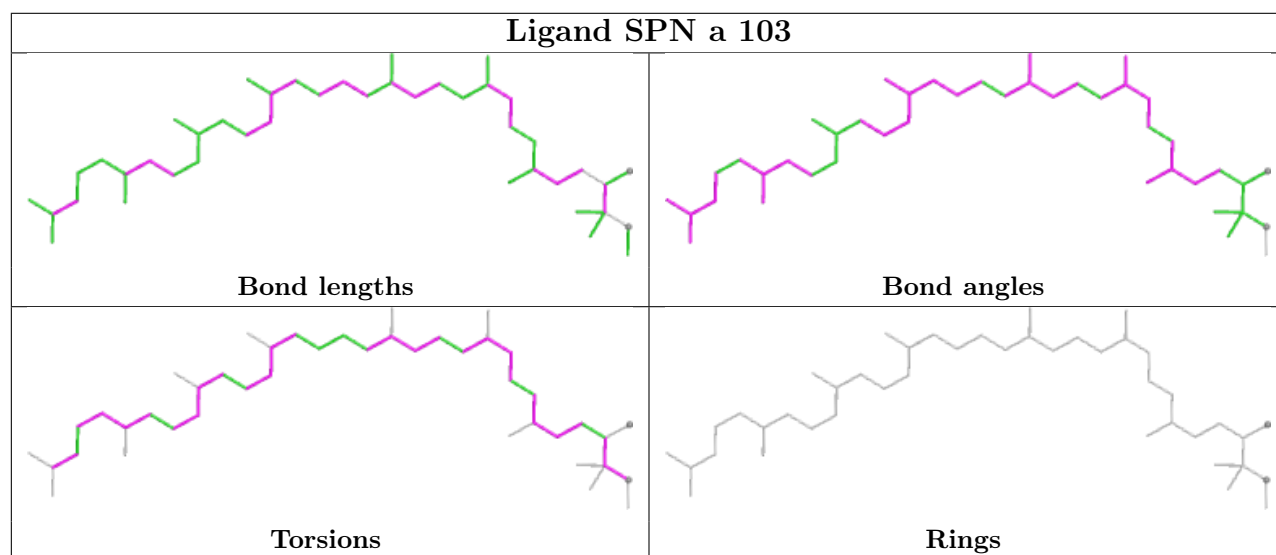
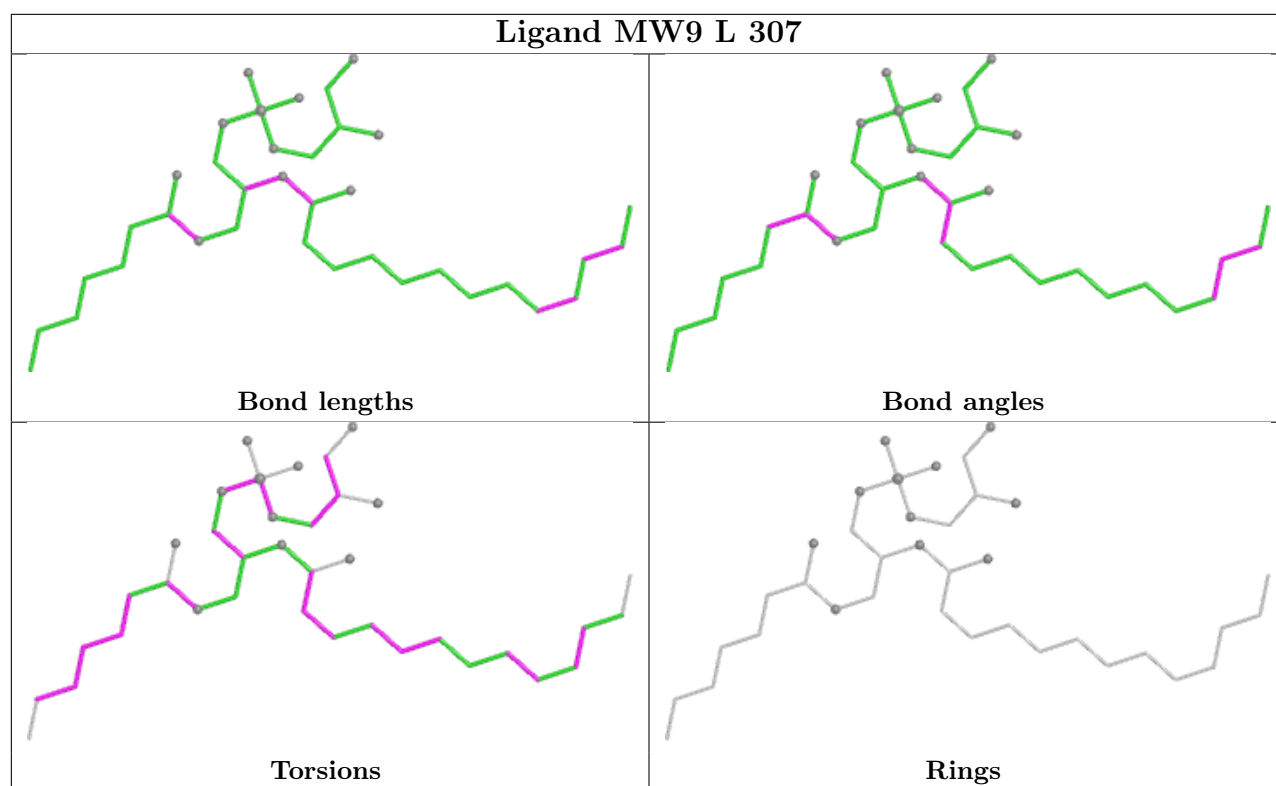


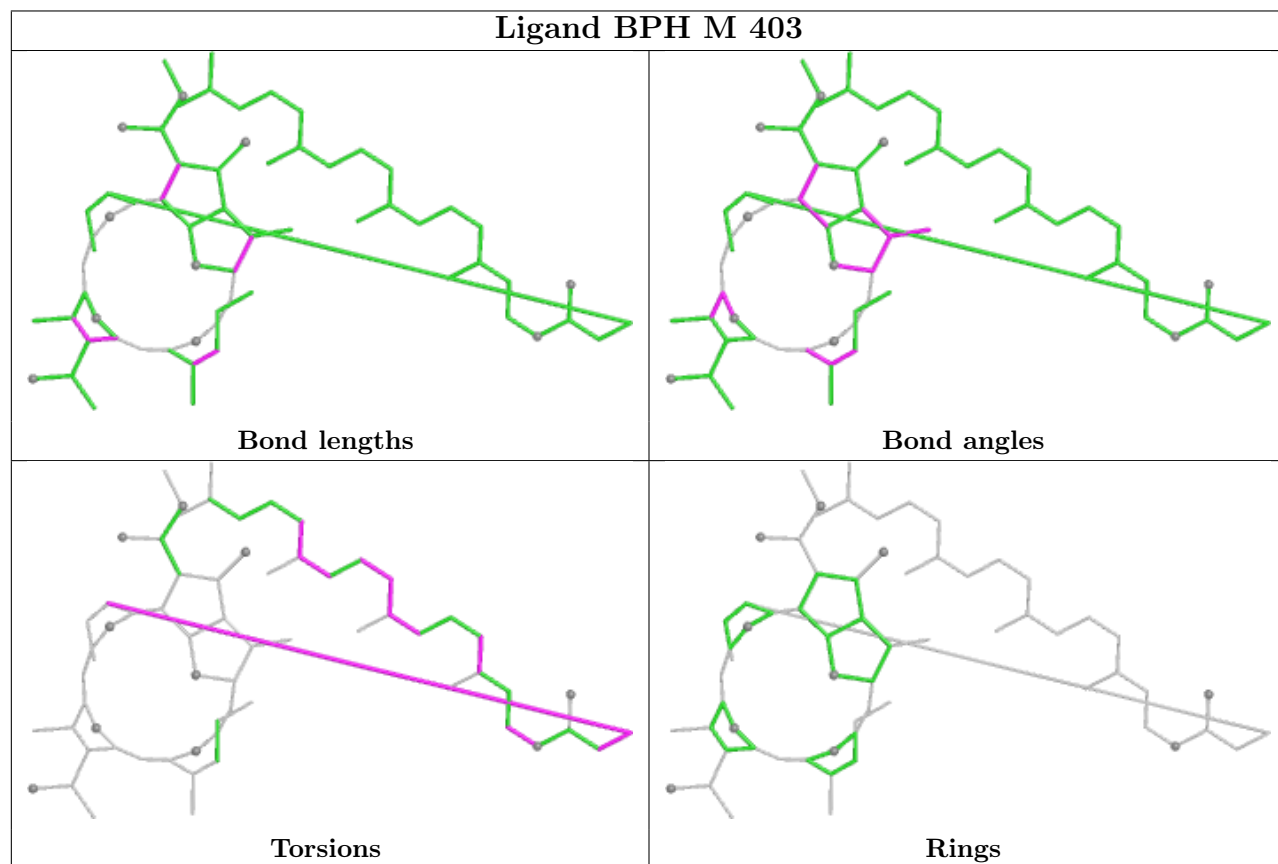
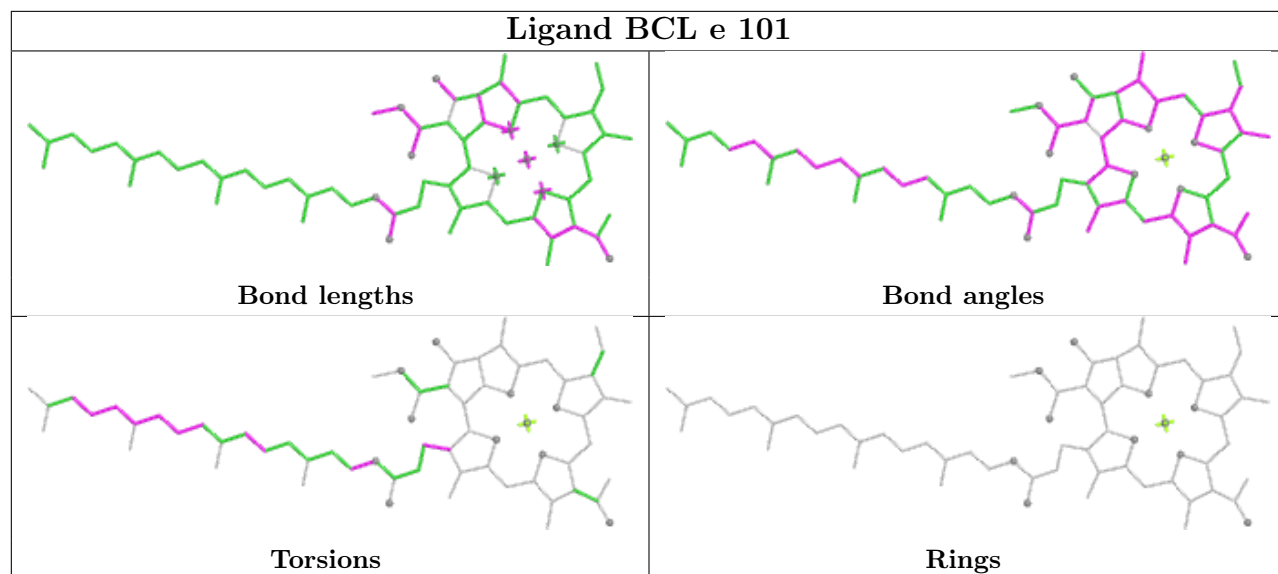


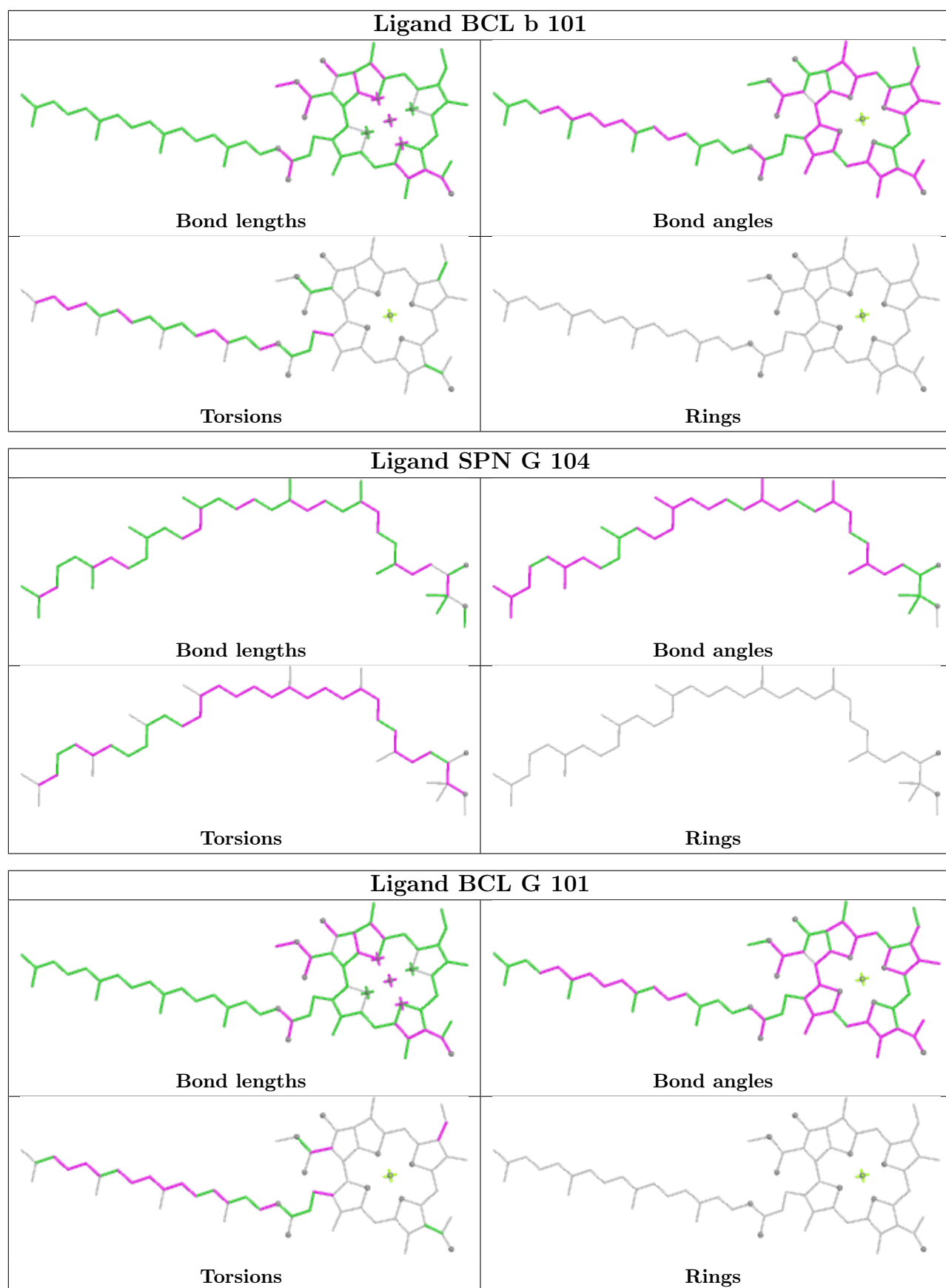


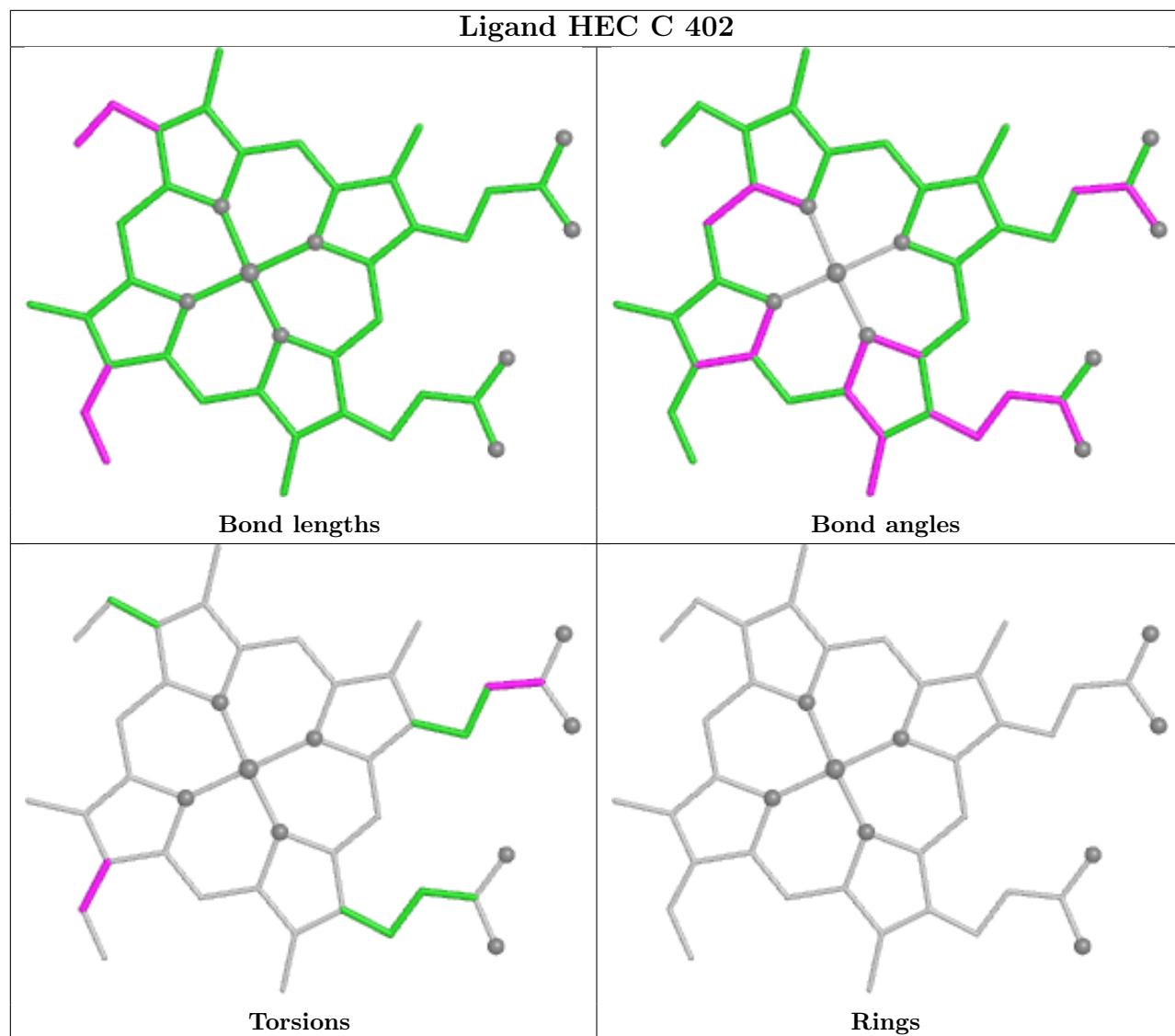




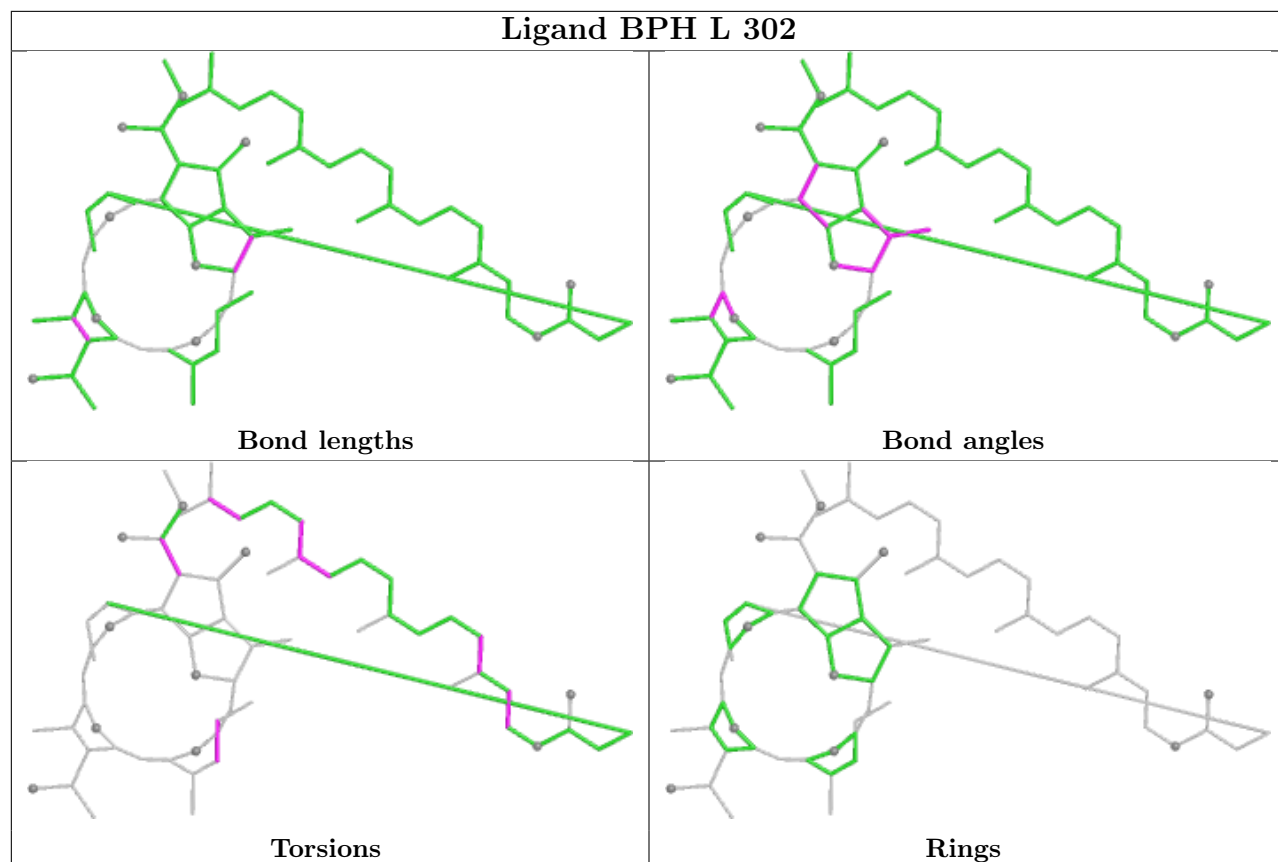




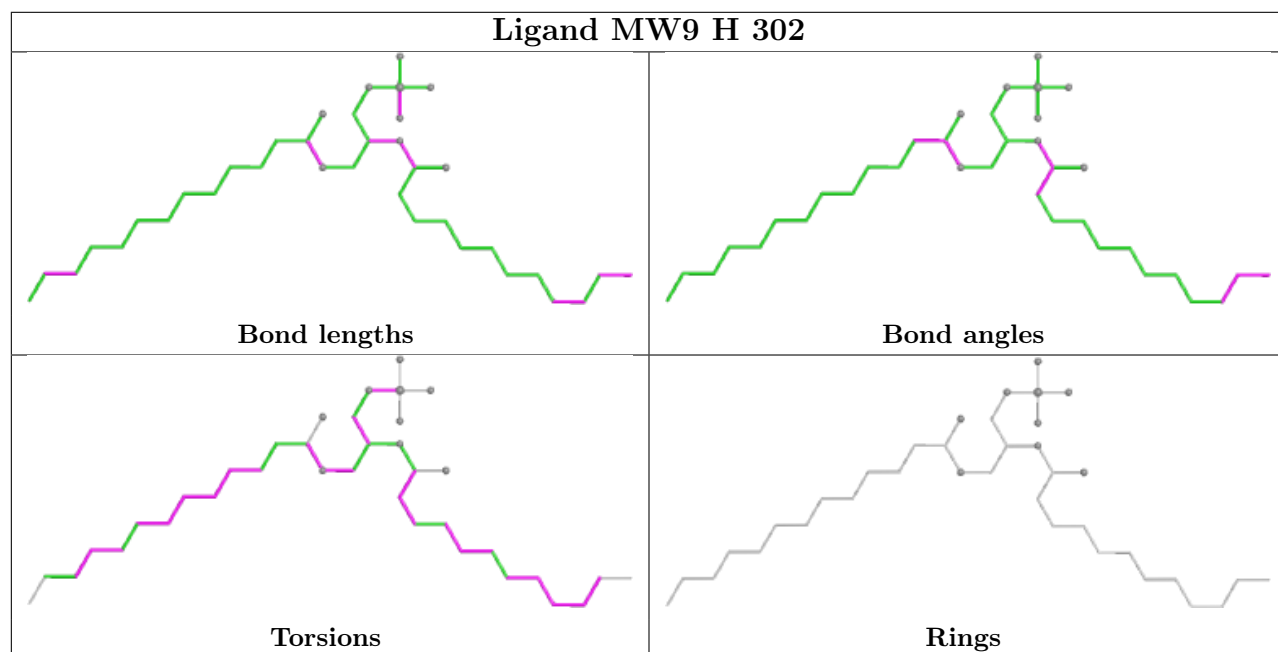


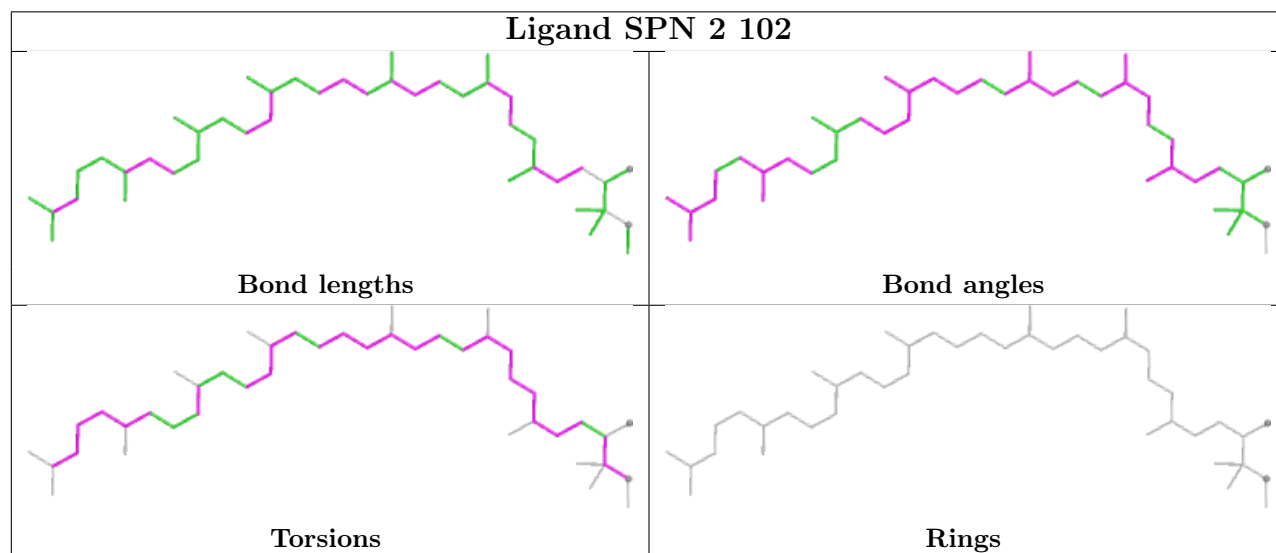
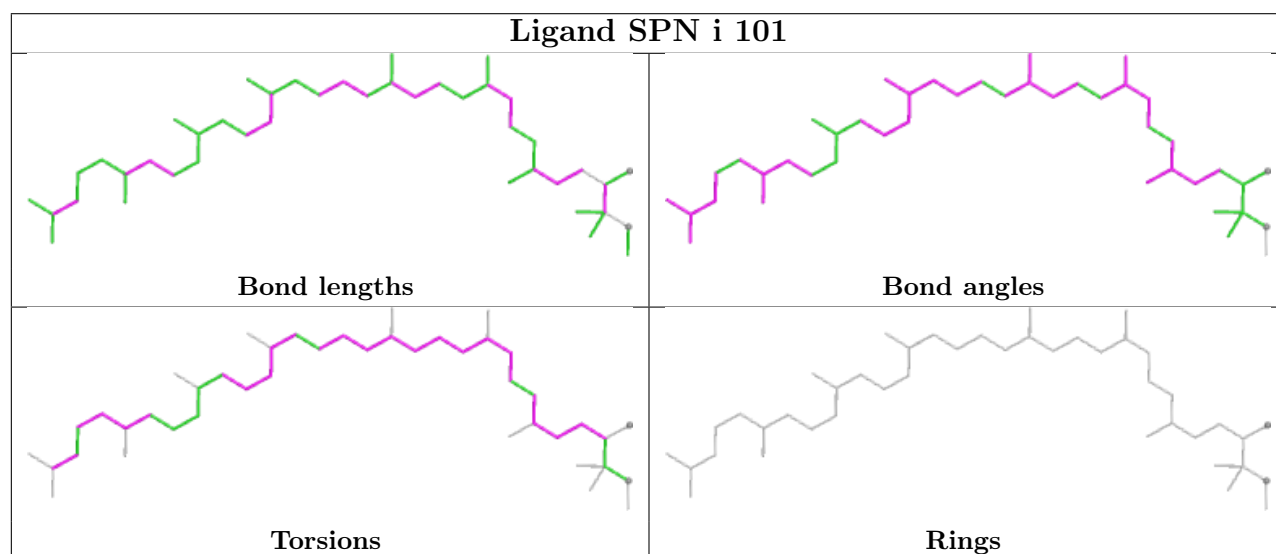
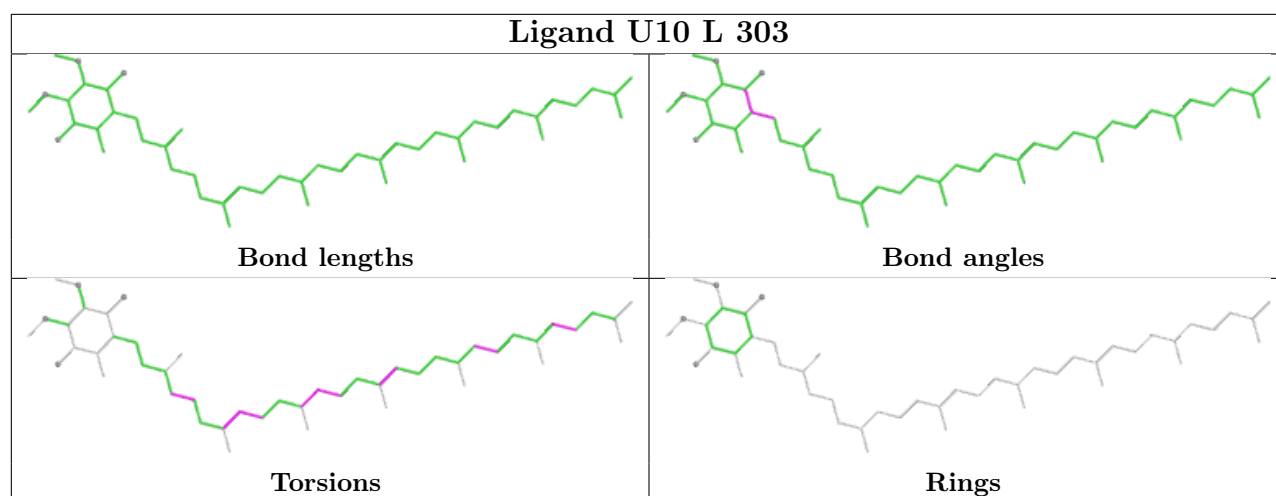


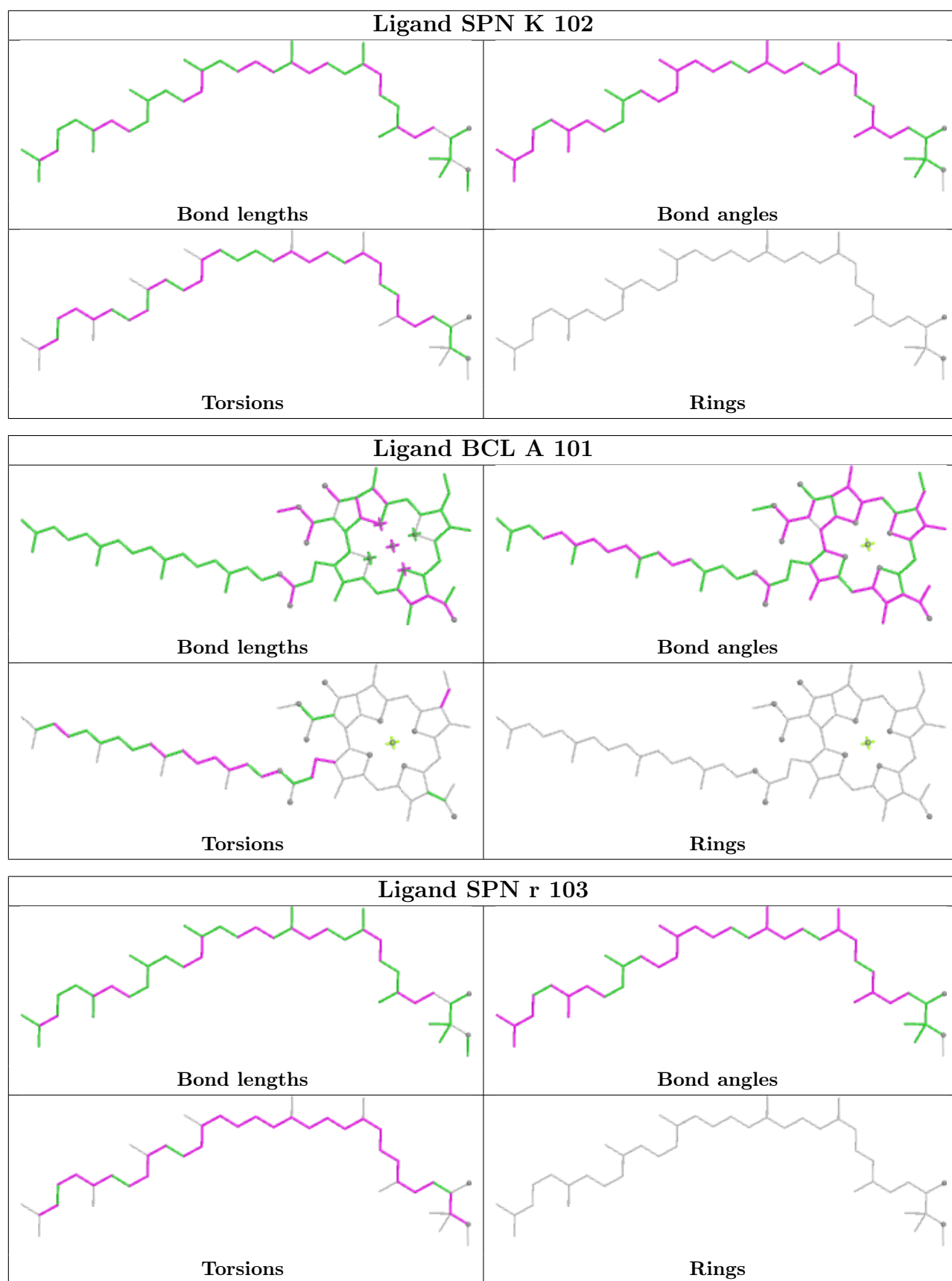
Ligand BPH L 302

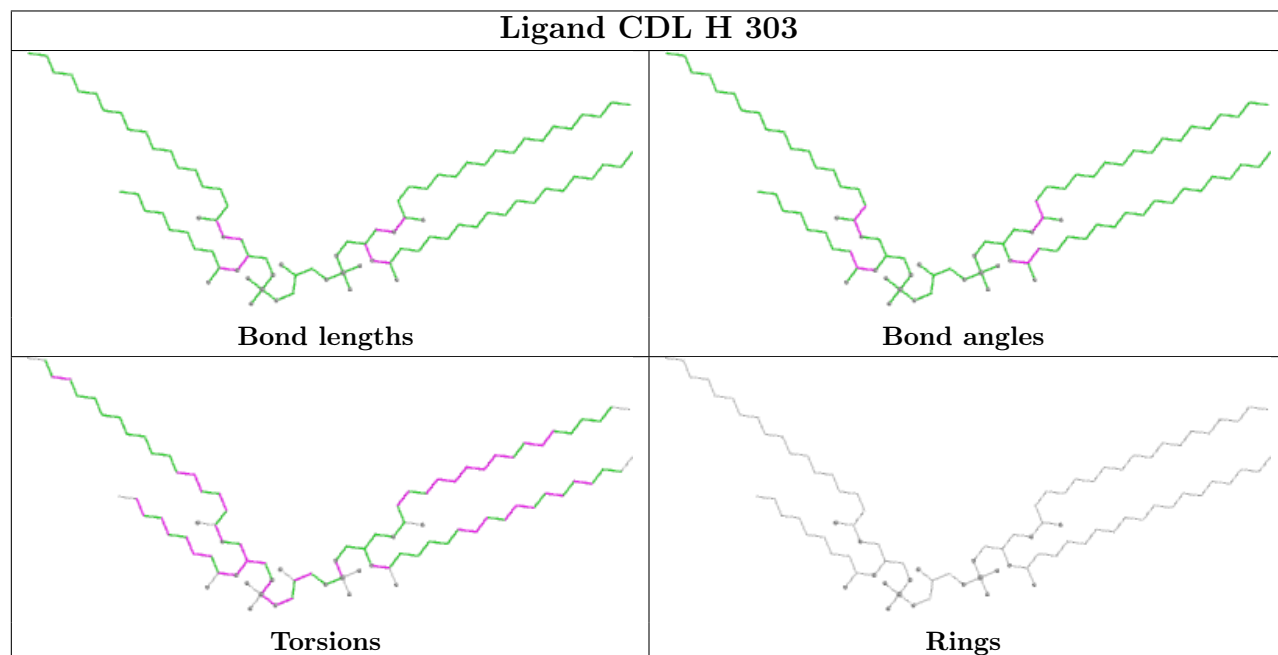
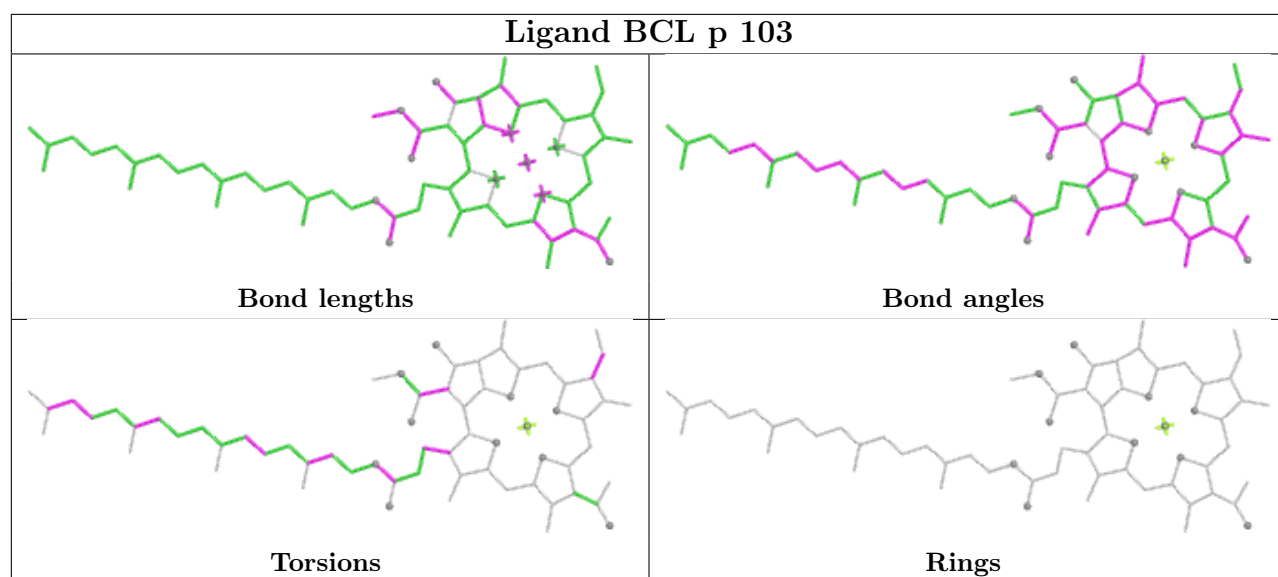


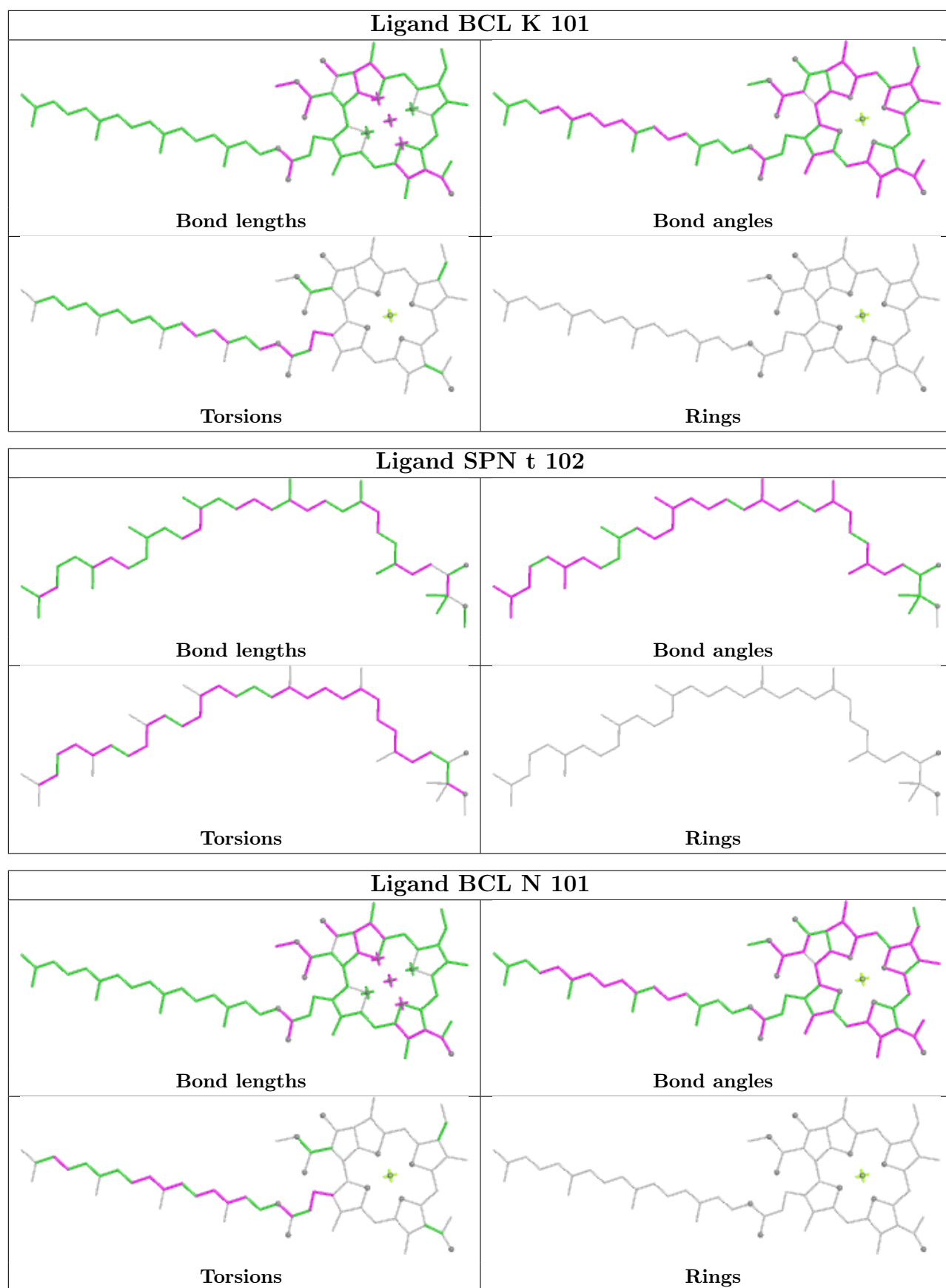
Ligand MW9 H 302

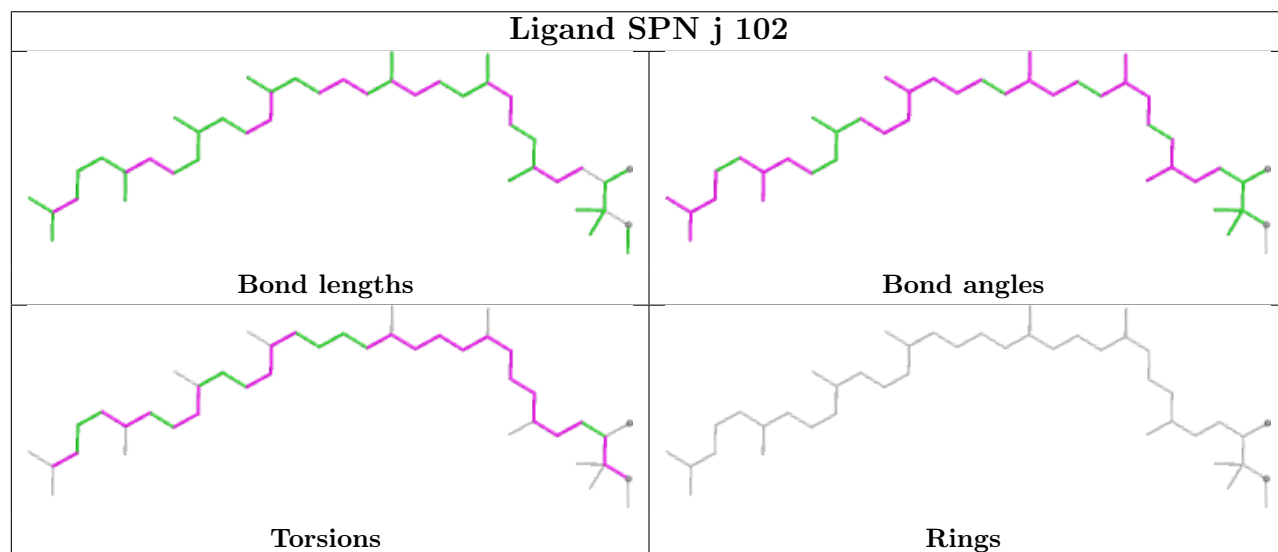
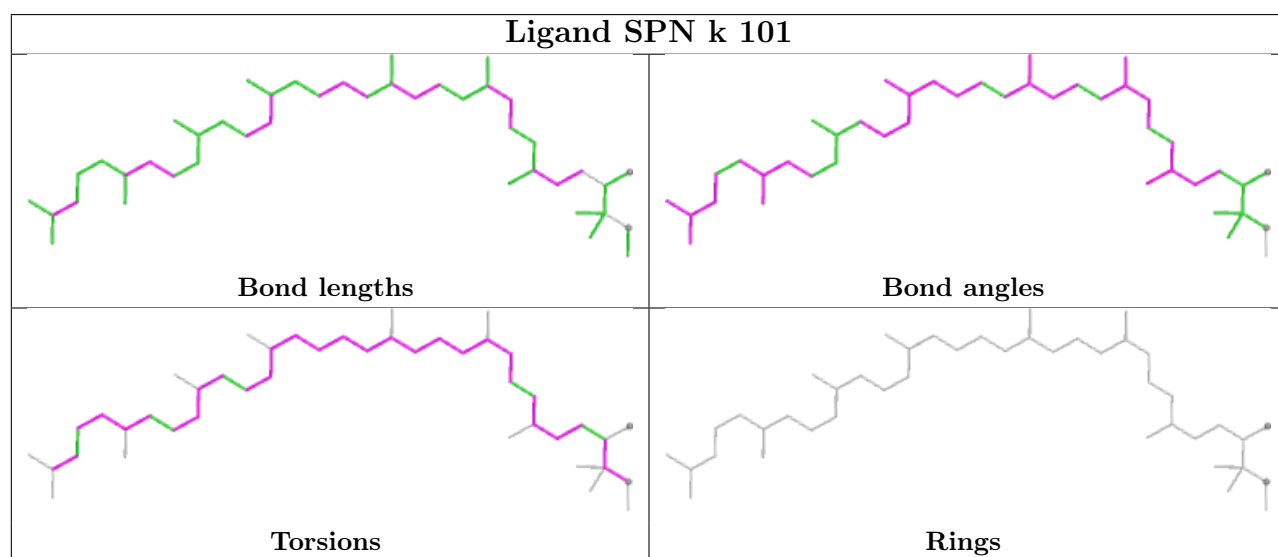
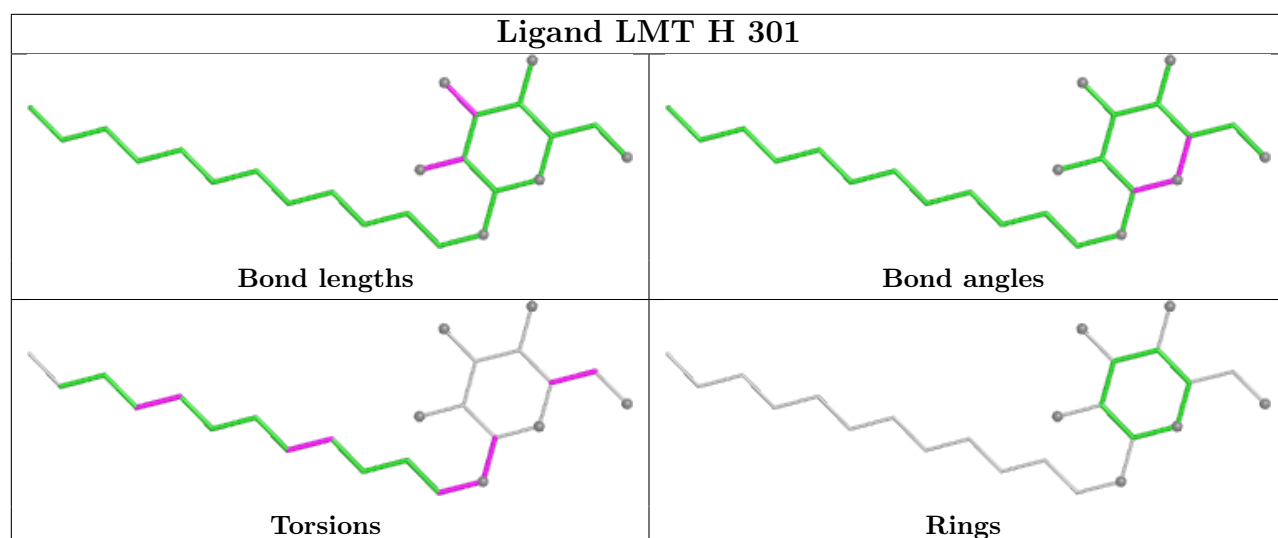


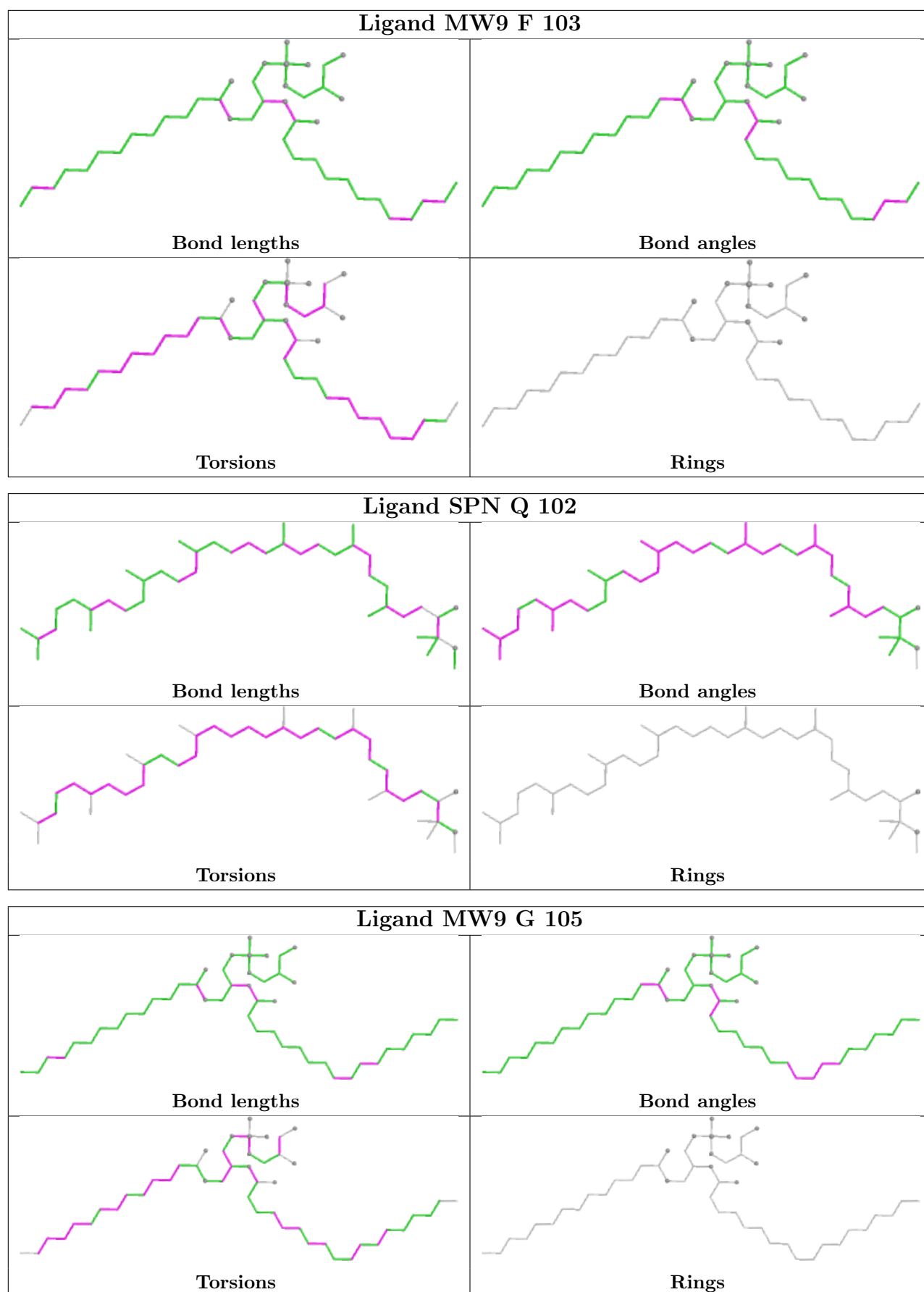


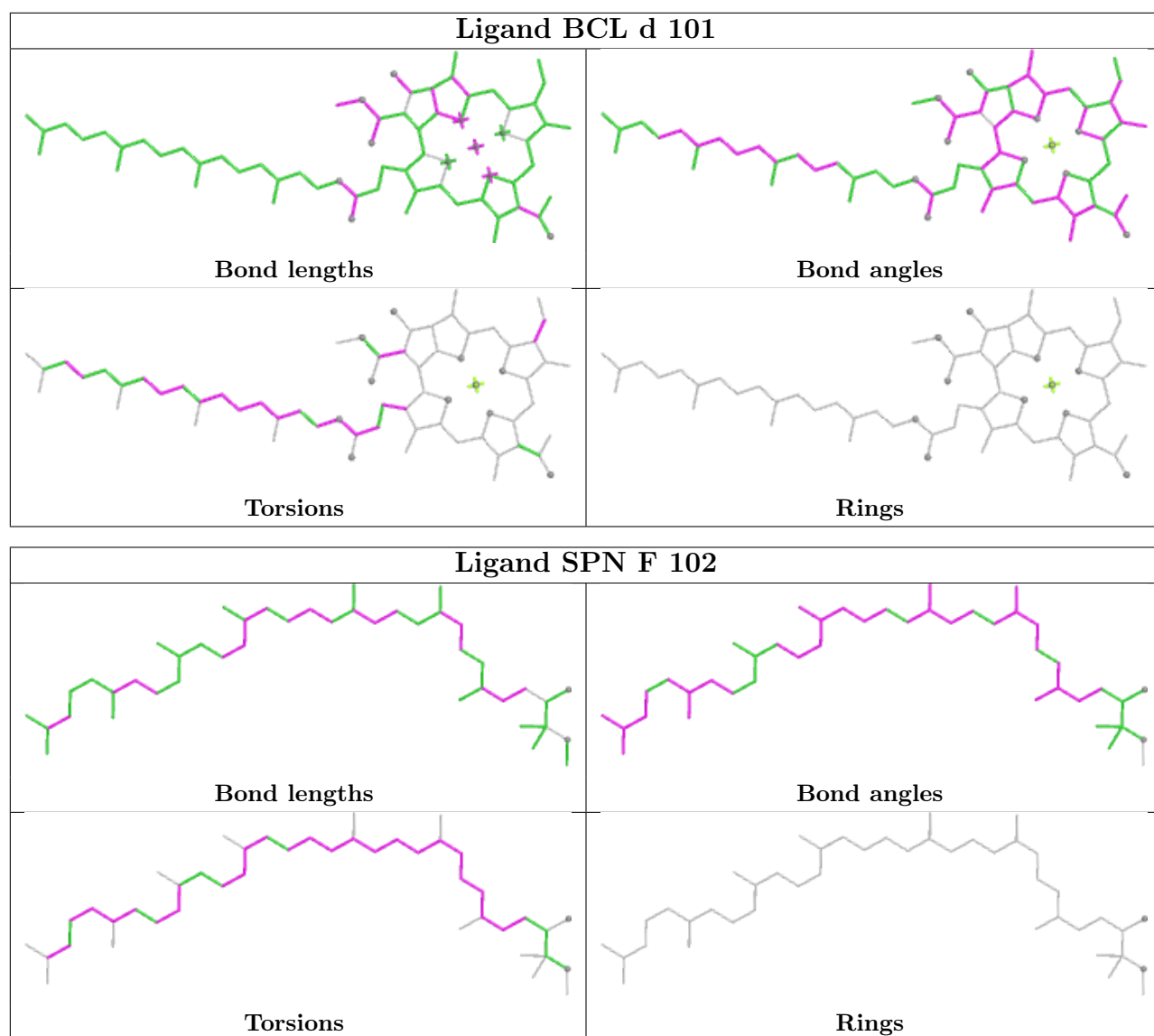


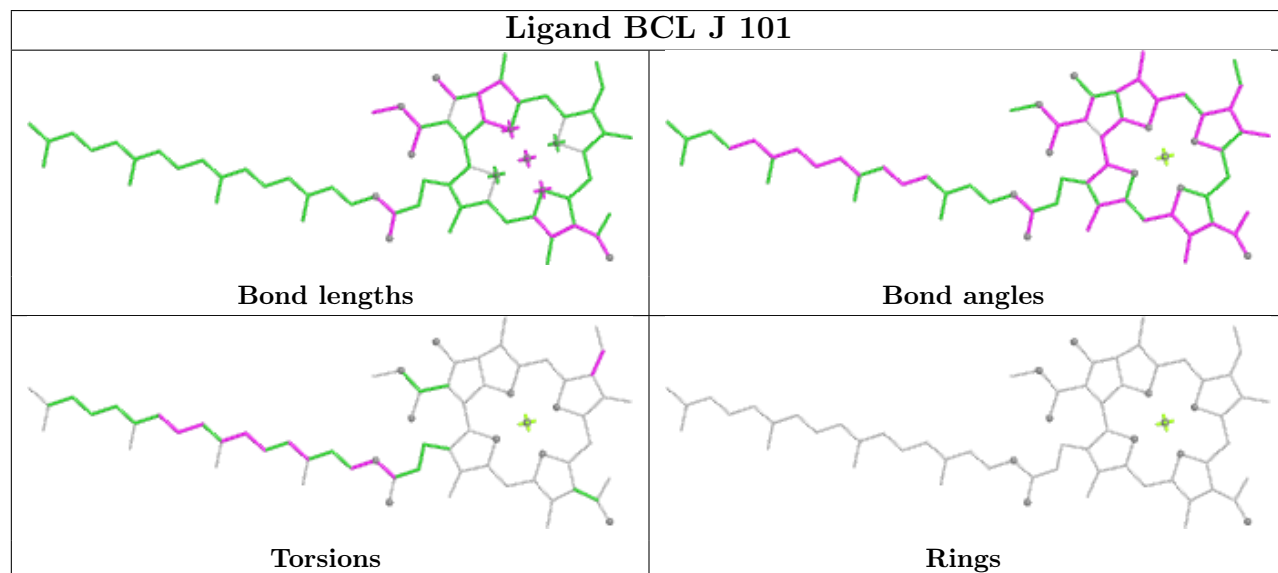
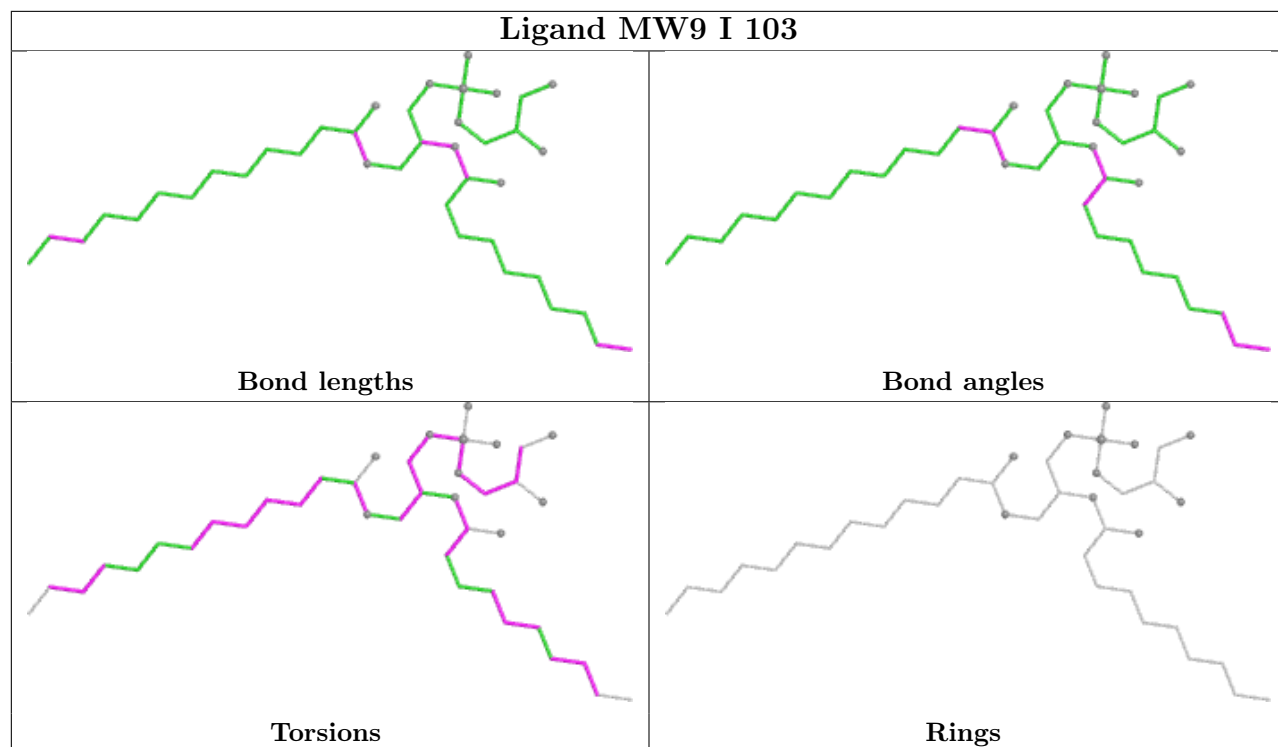


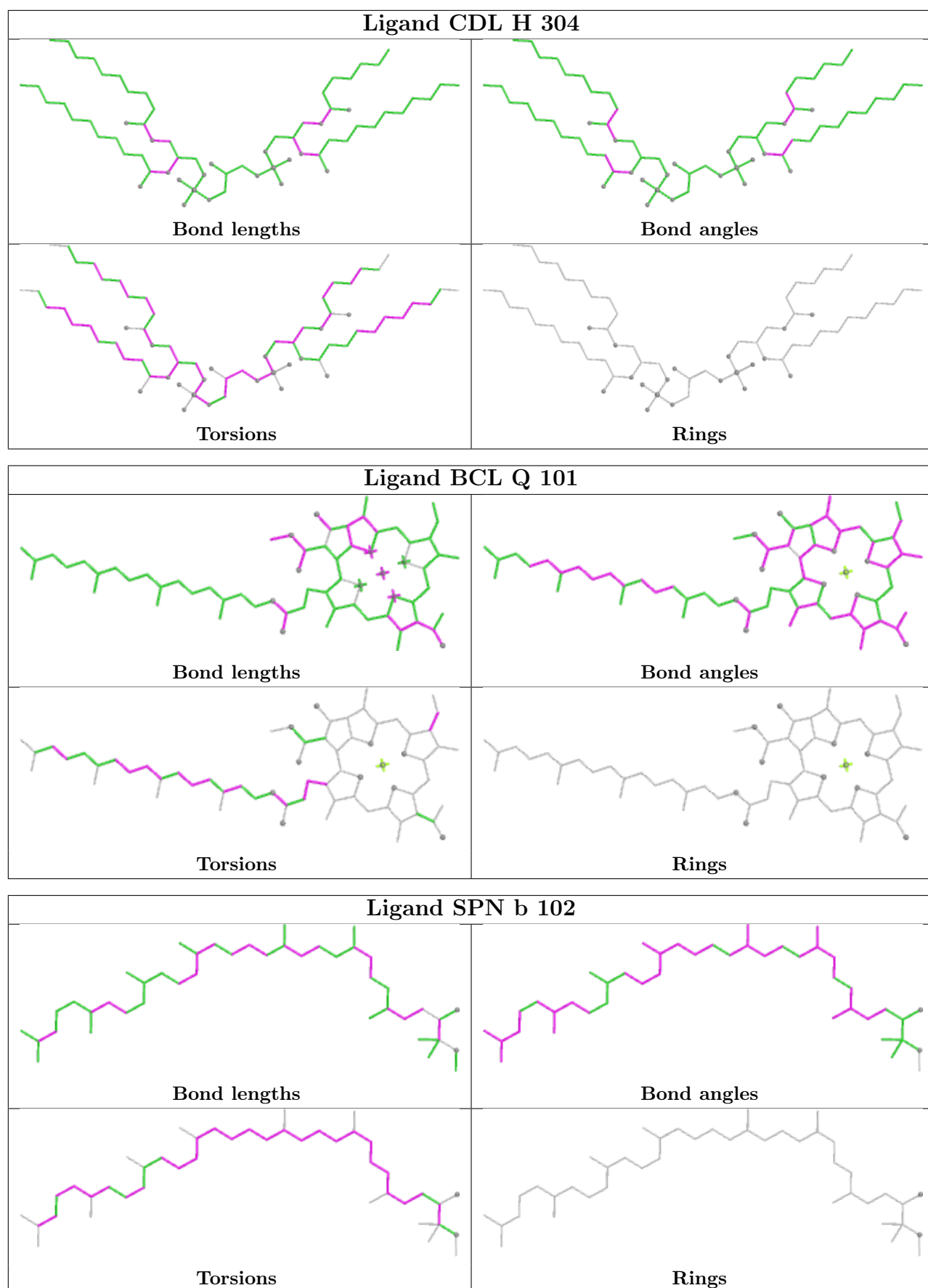


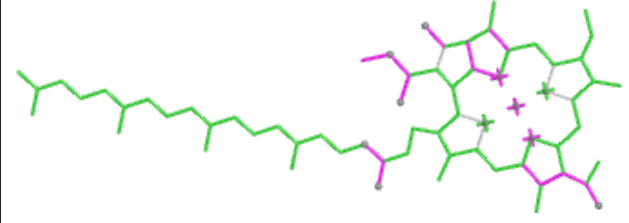
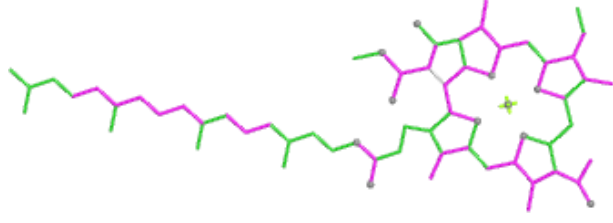
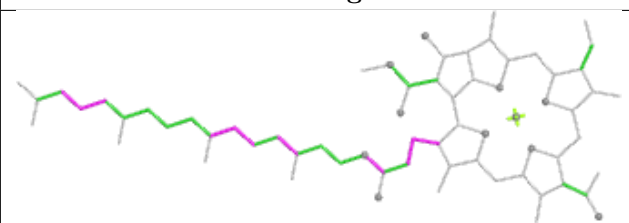
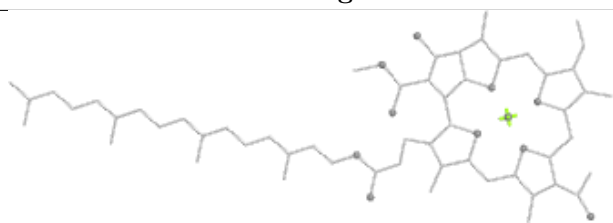
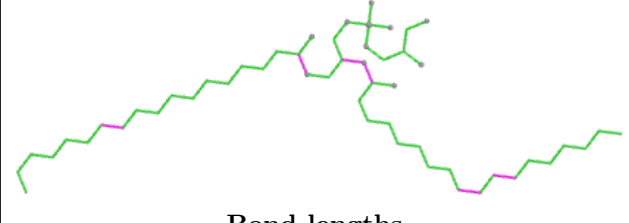
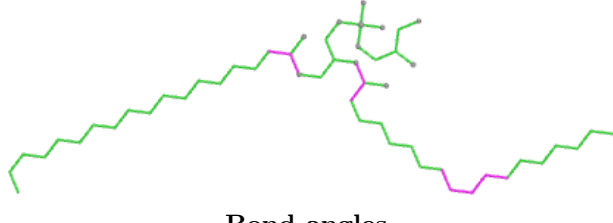
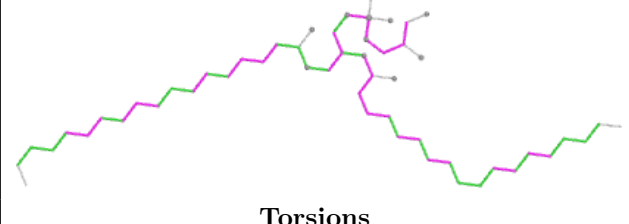
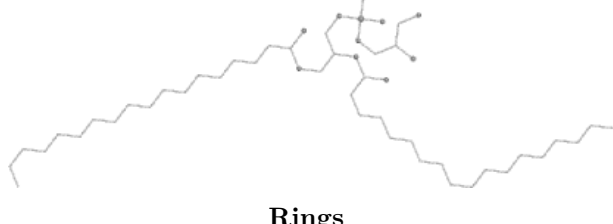
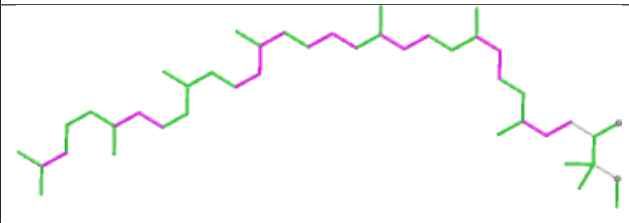
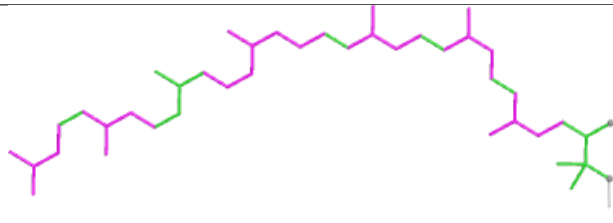
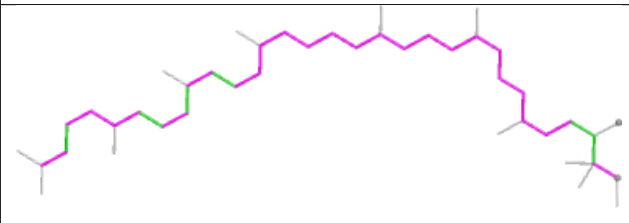
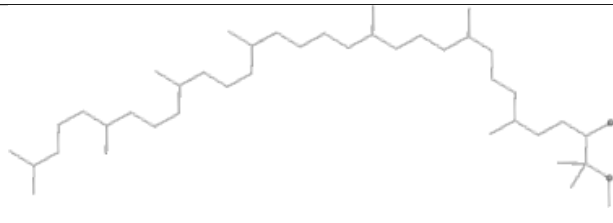


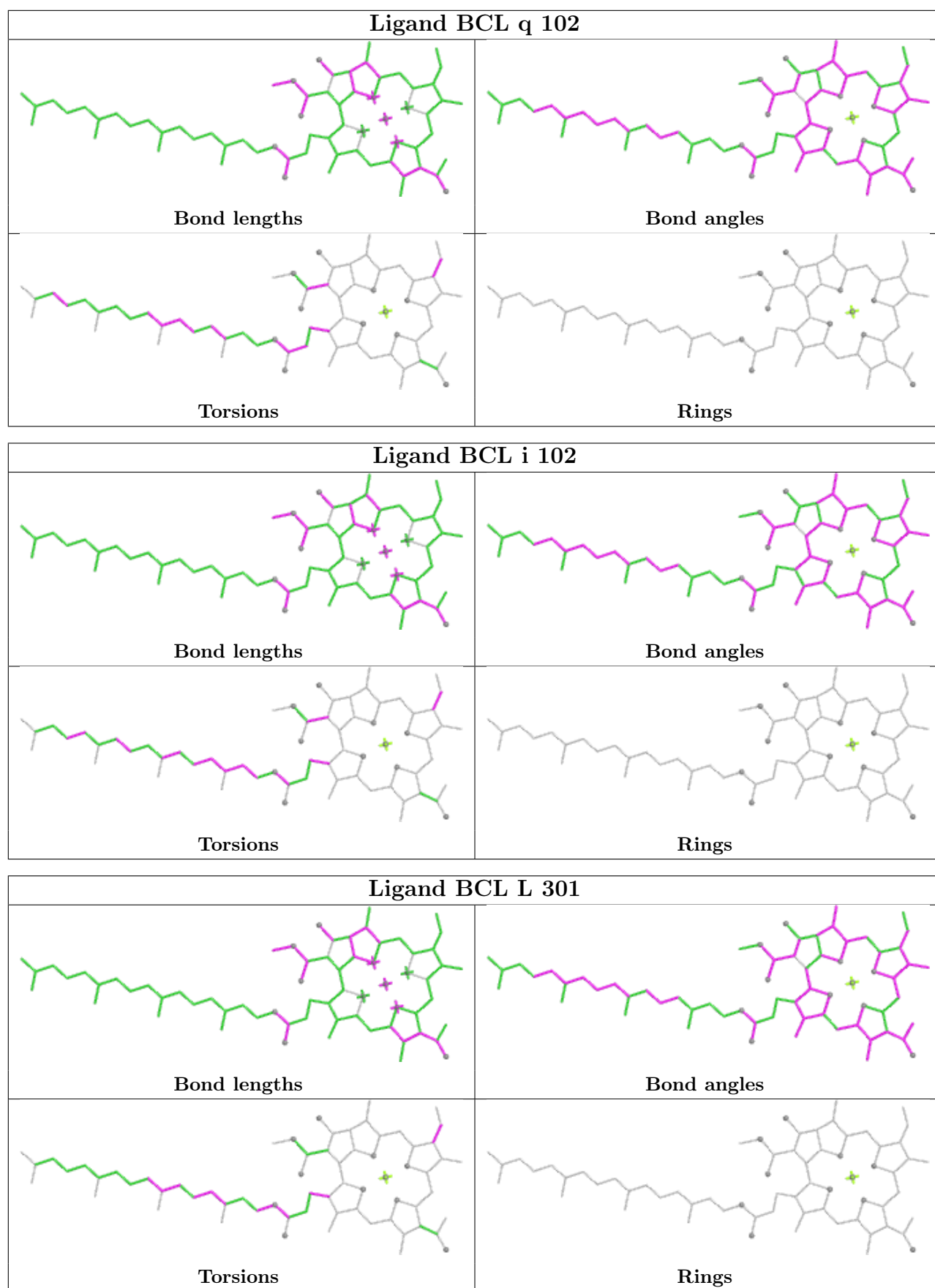




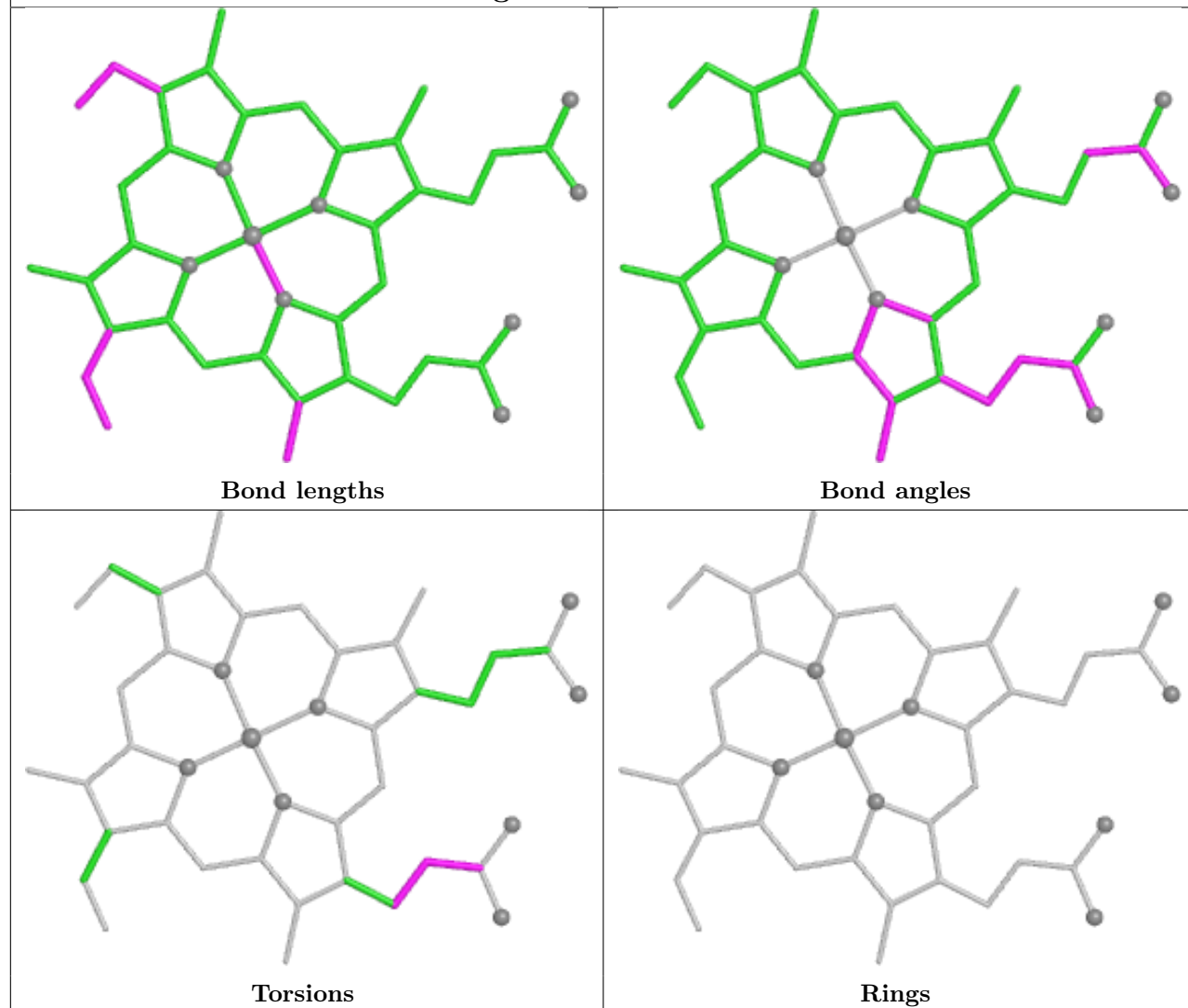




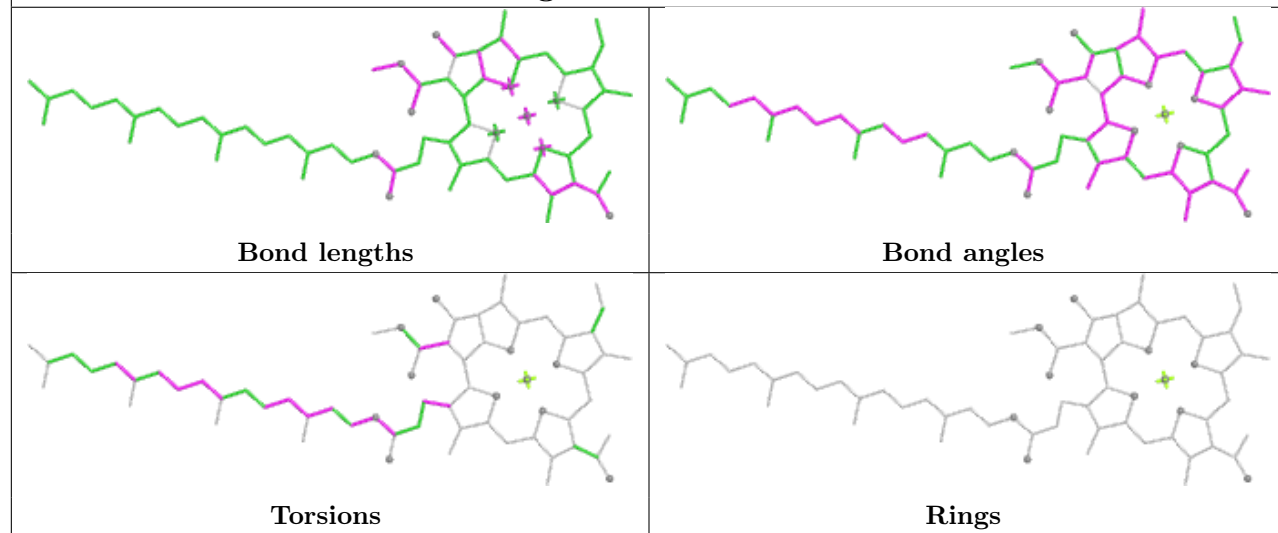
Ligand BCL T 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand MW9 B 102	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand SPN R 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

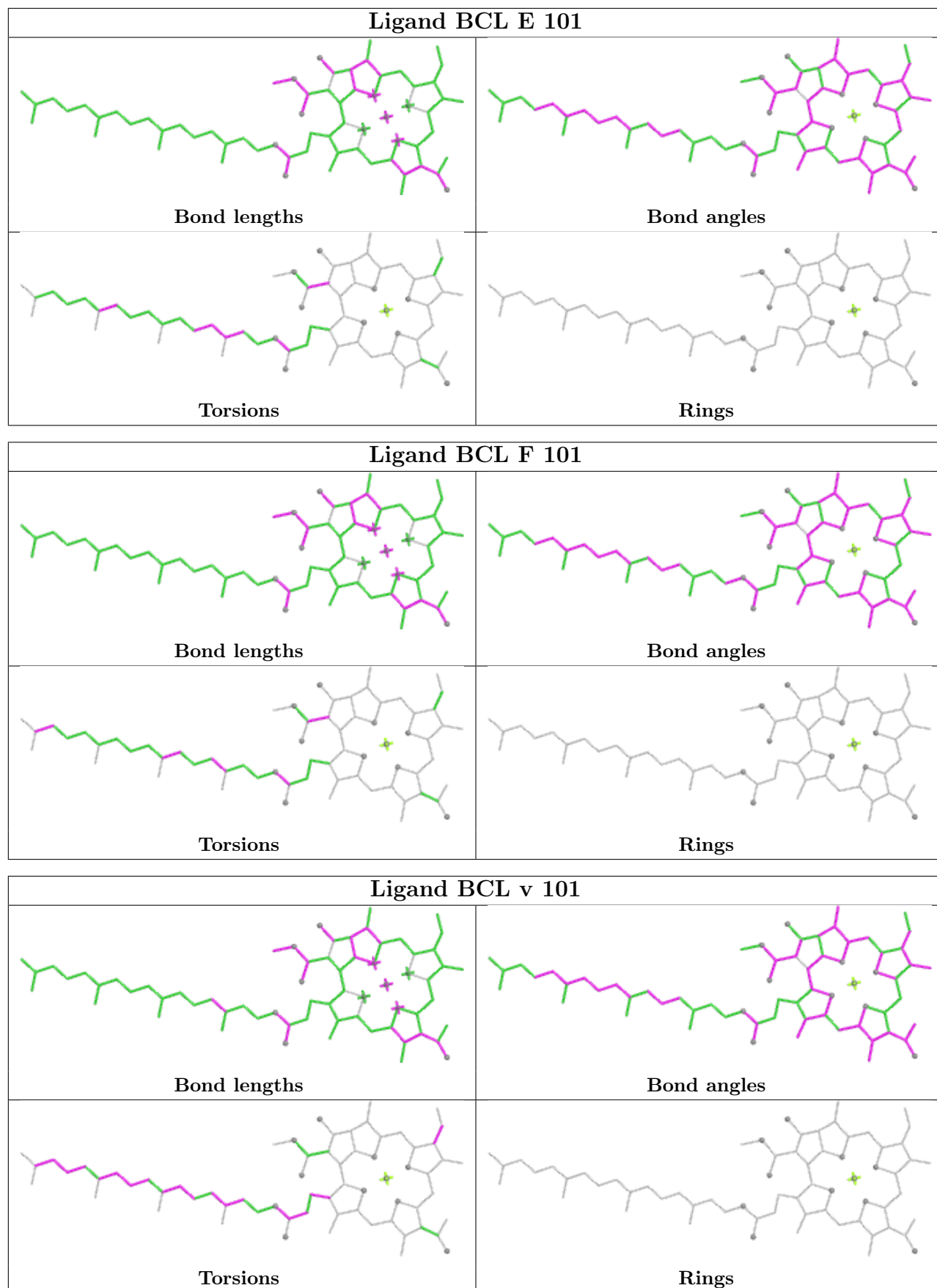


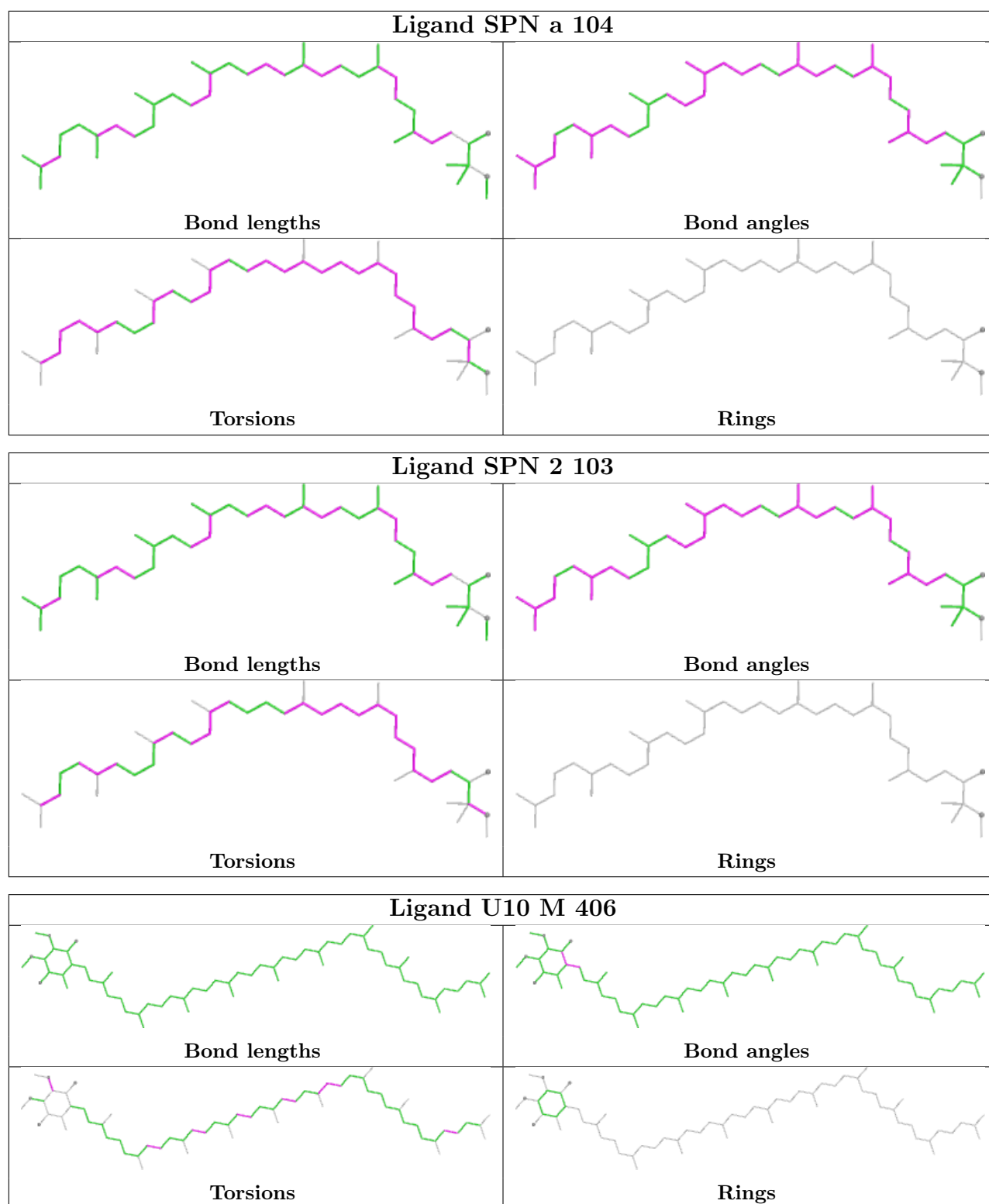
Ligand HEC C 403

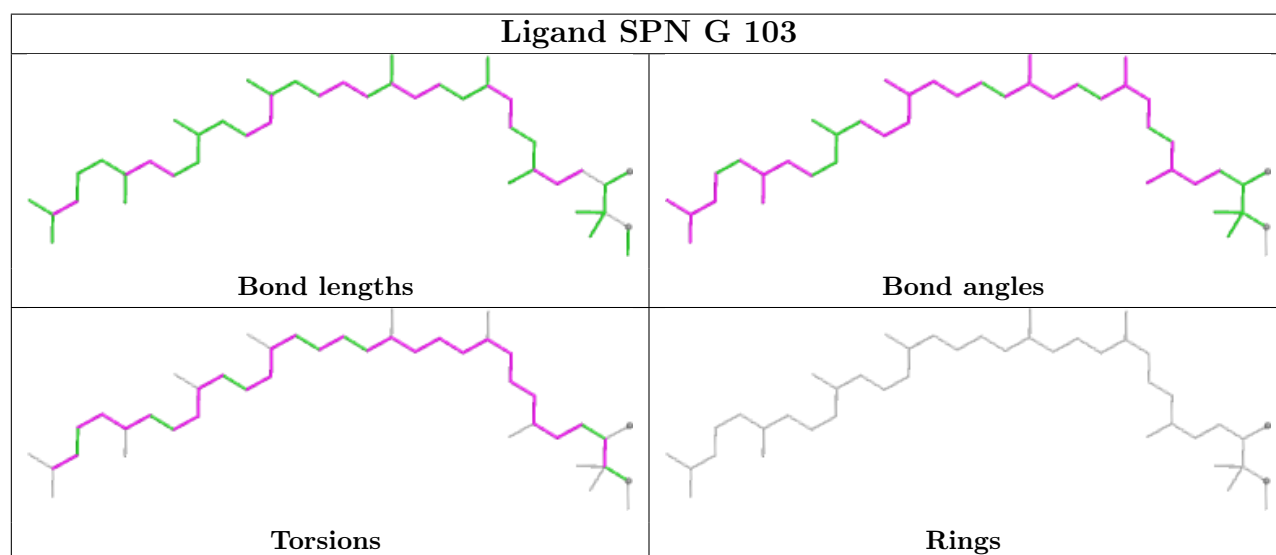
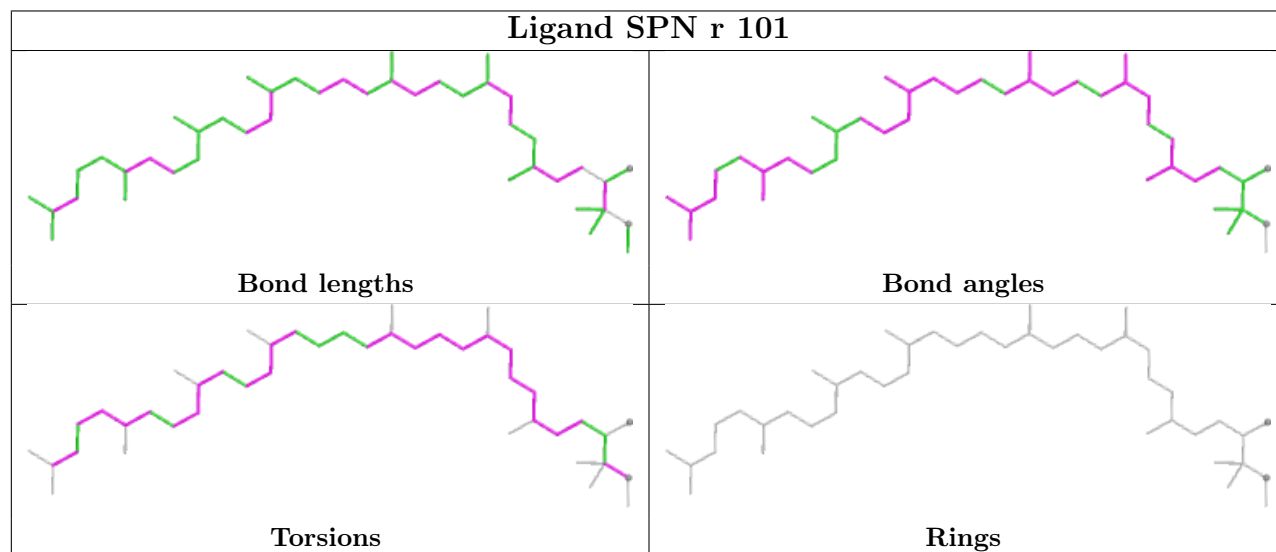
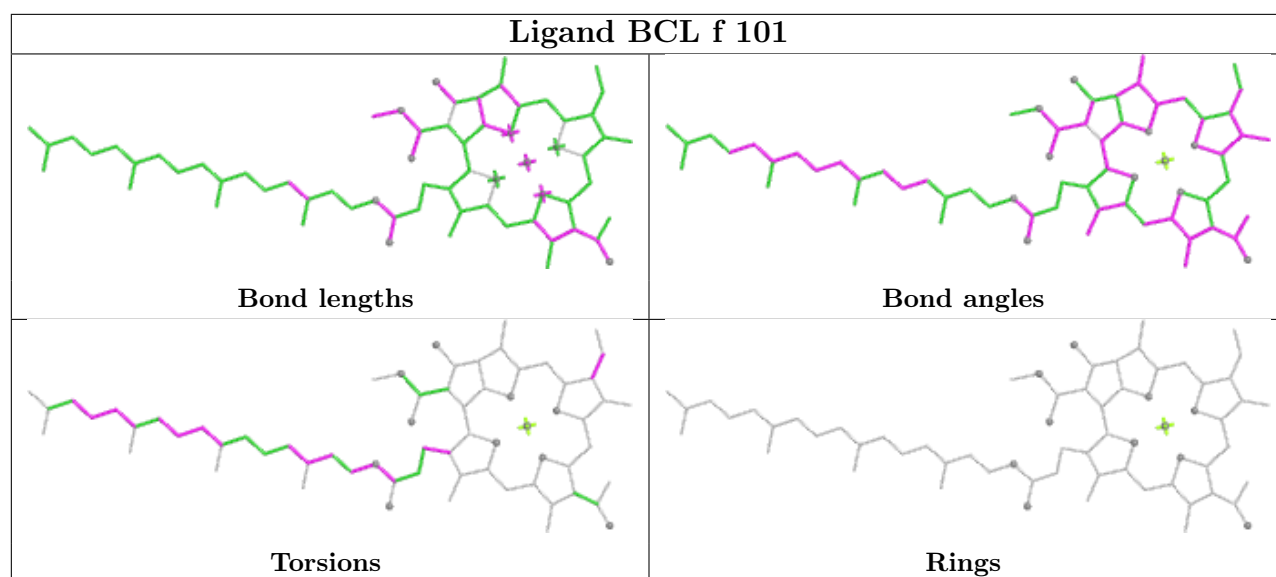


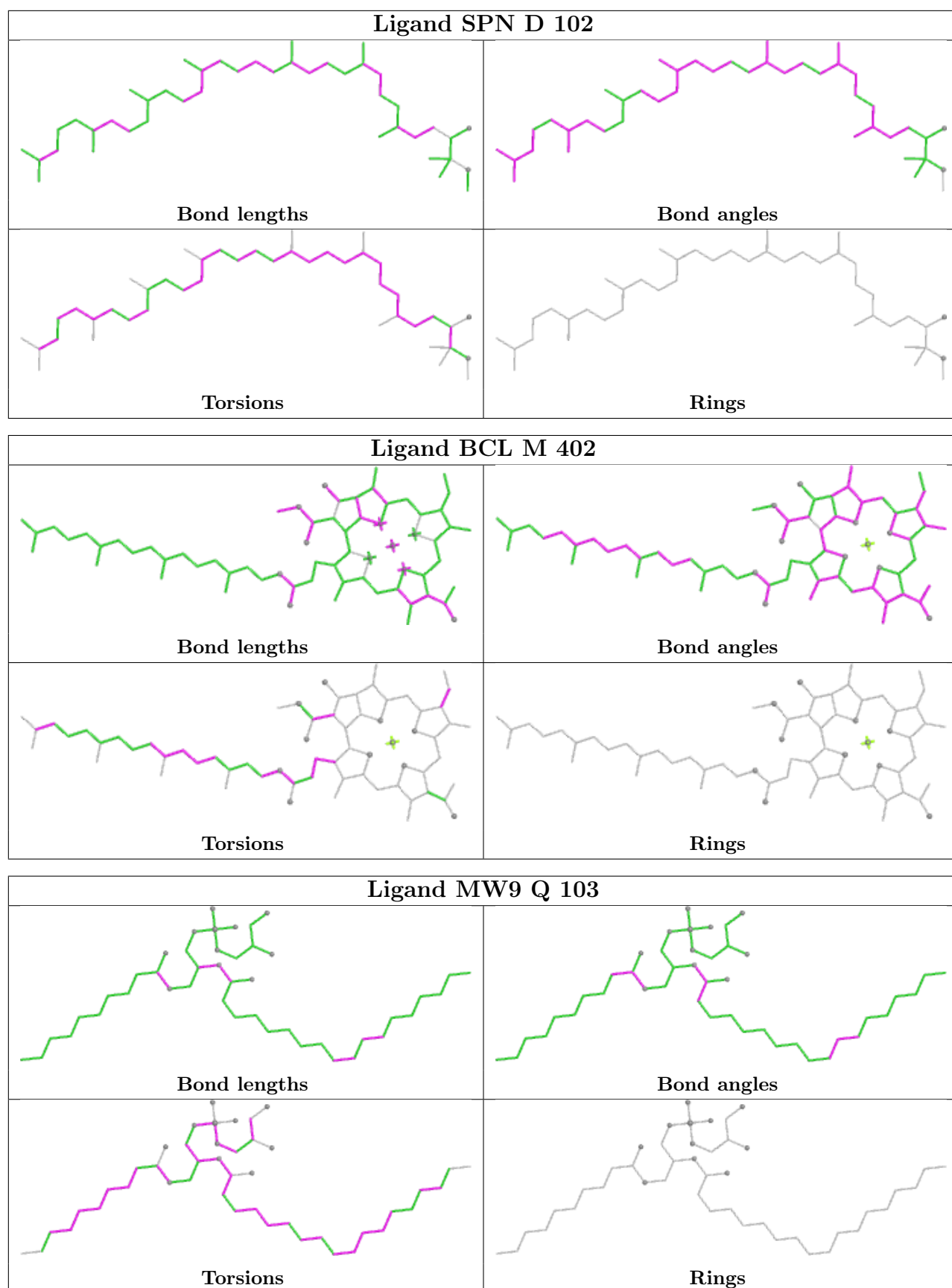
Ligand BCL a 102

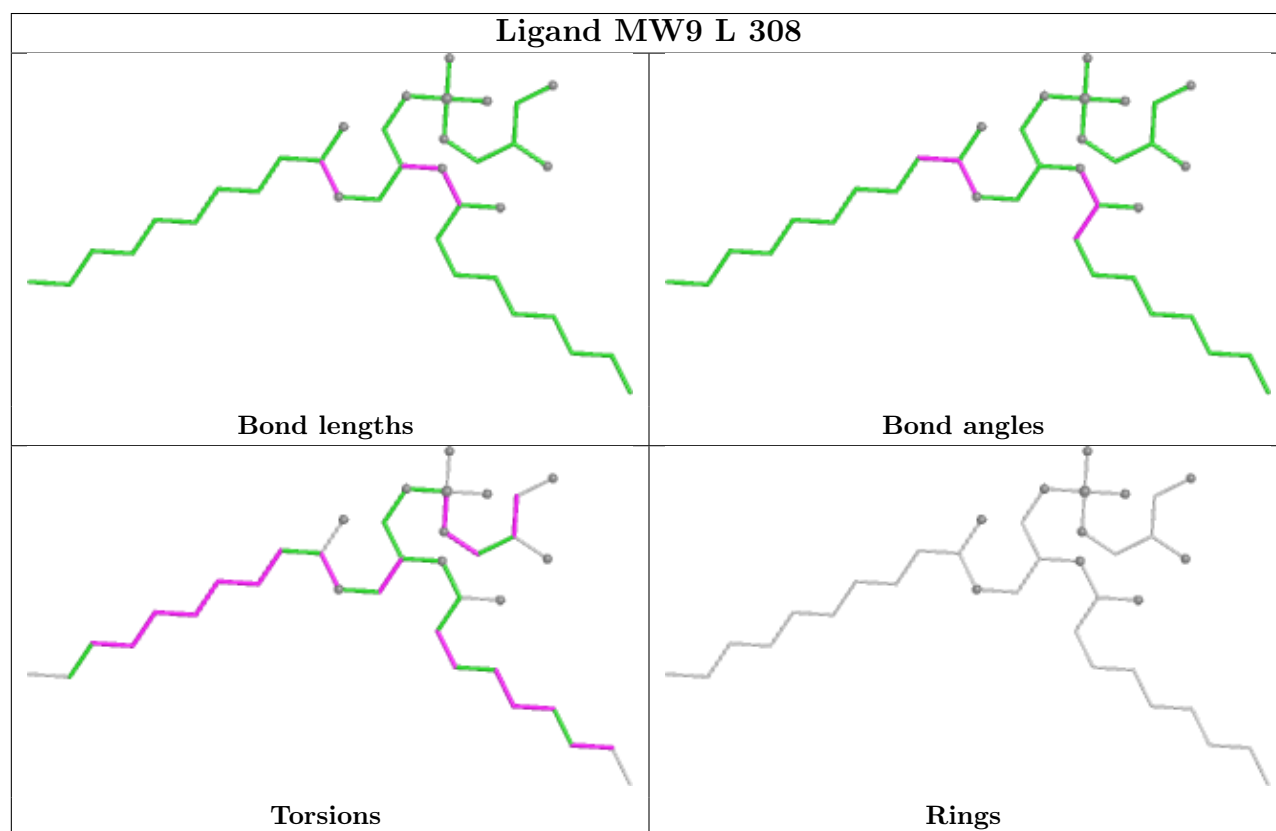
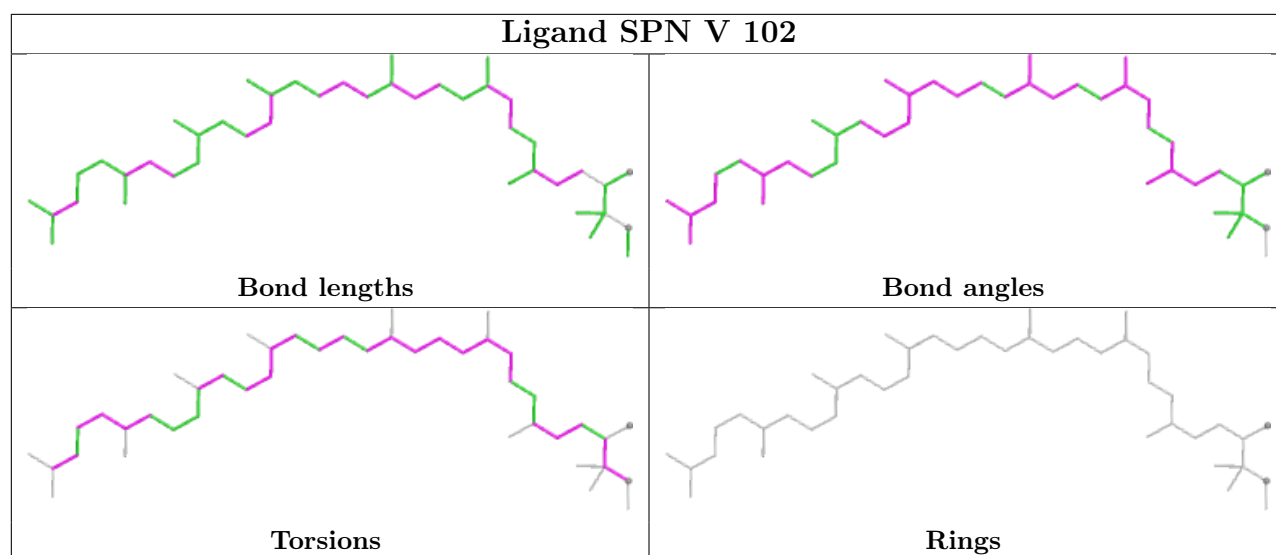


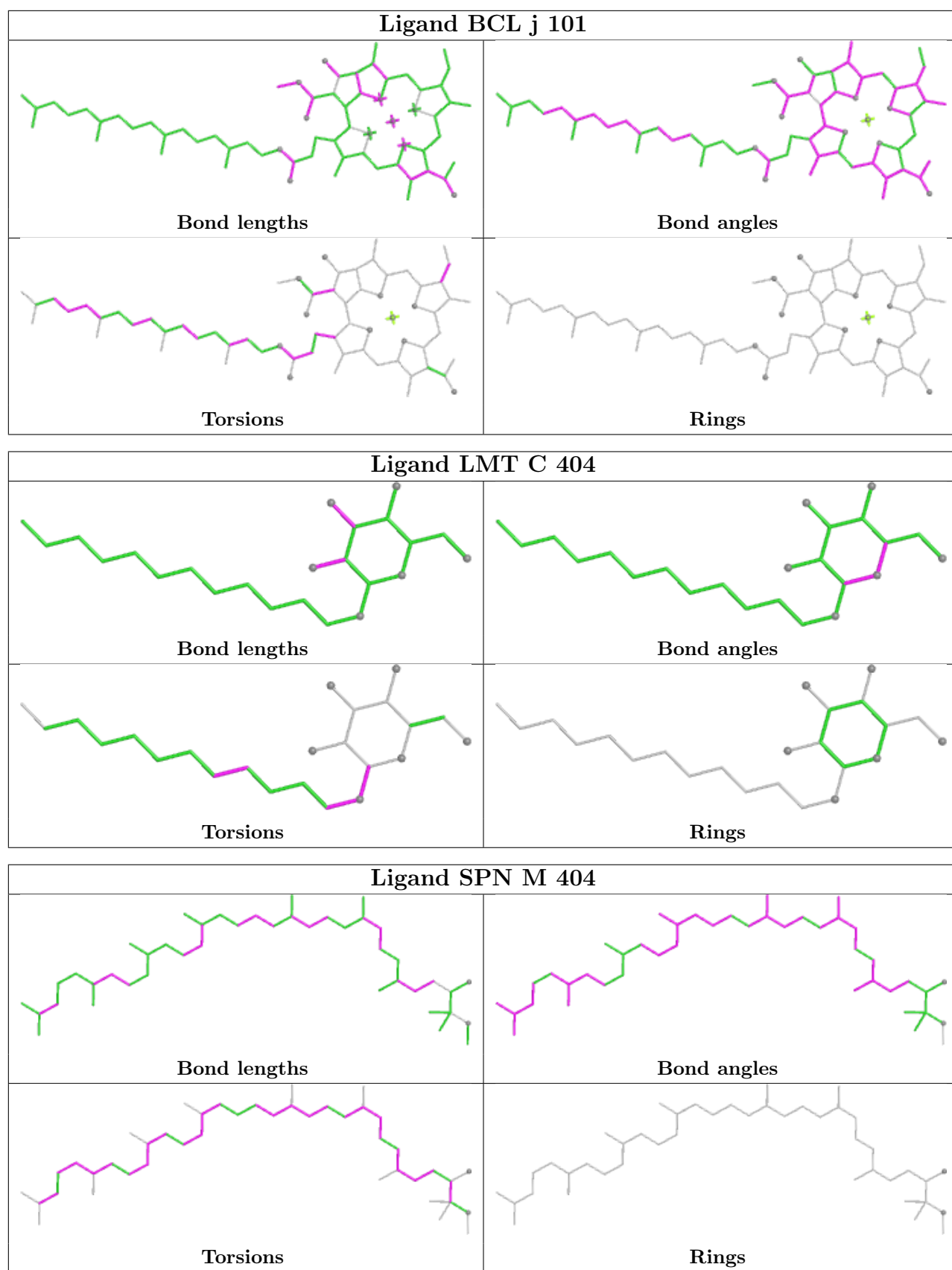


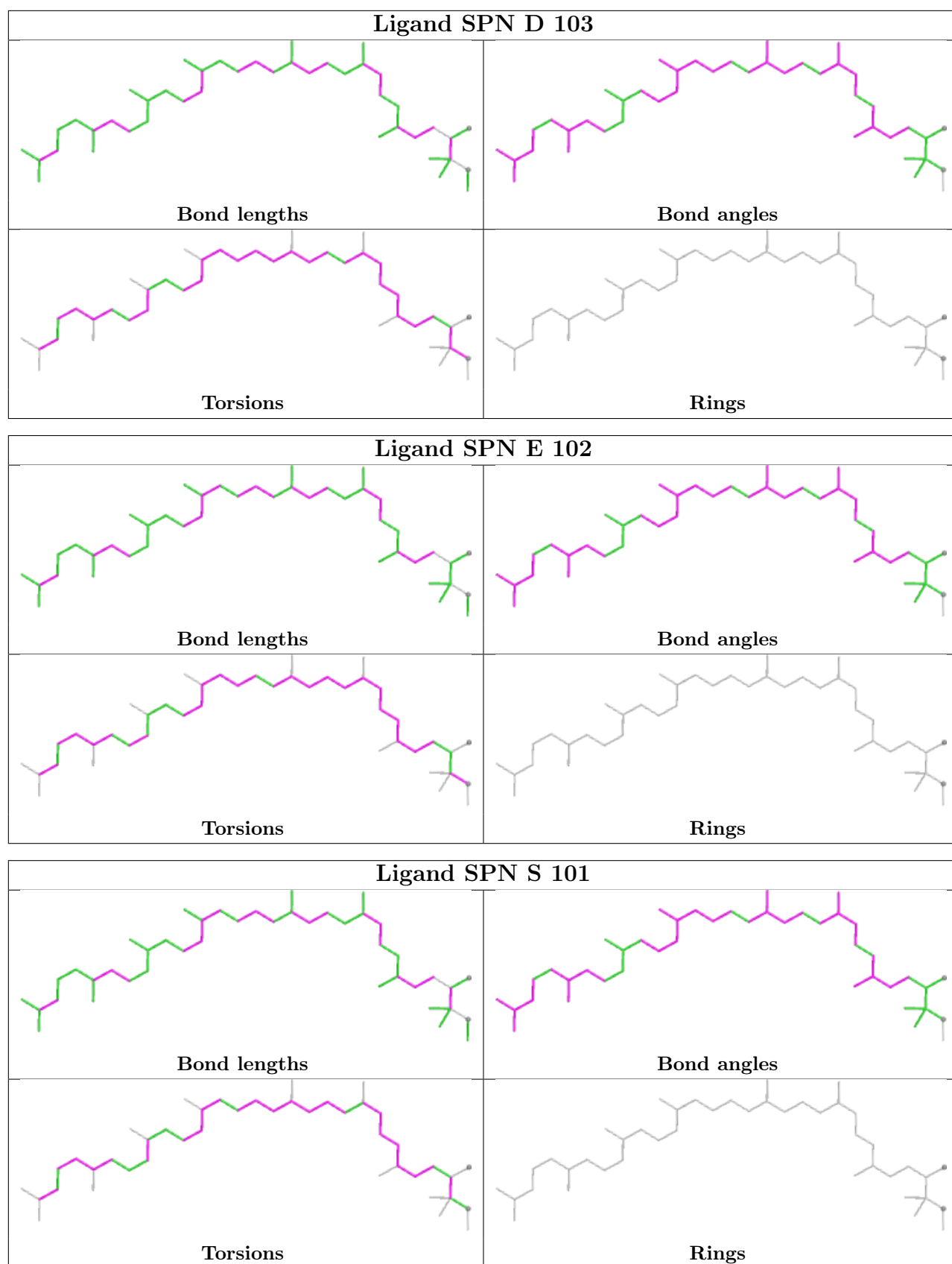


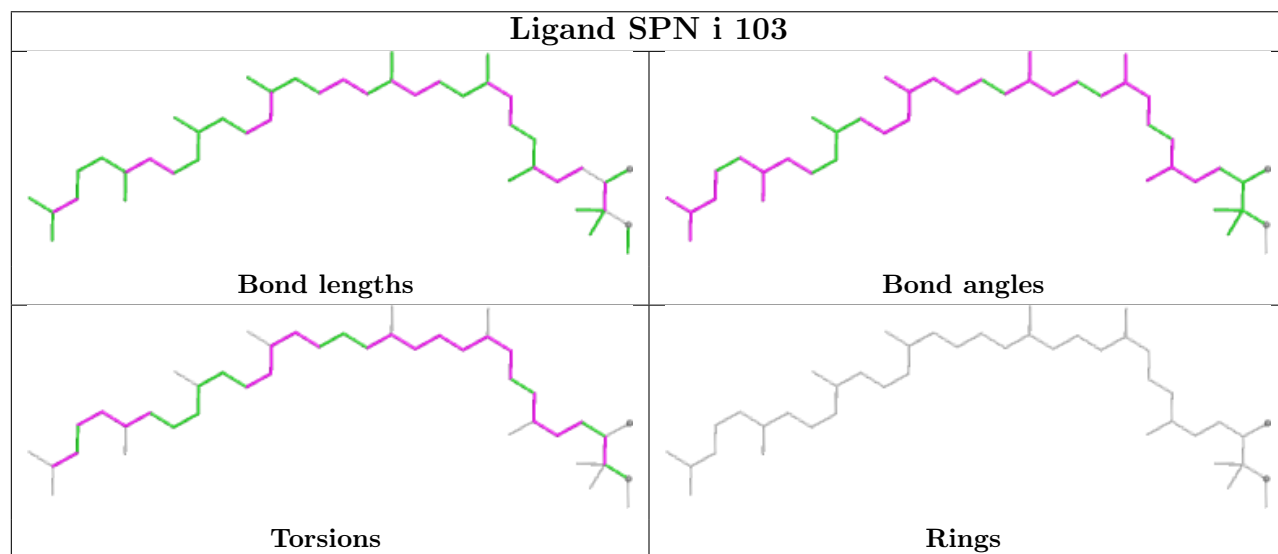
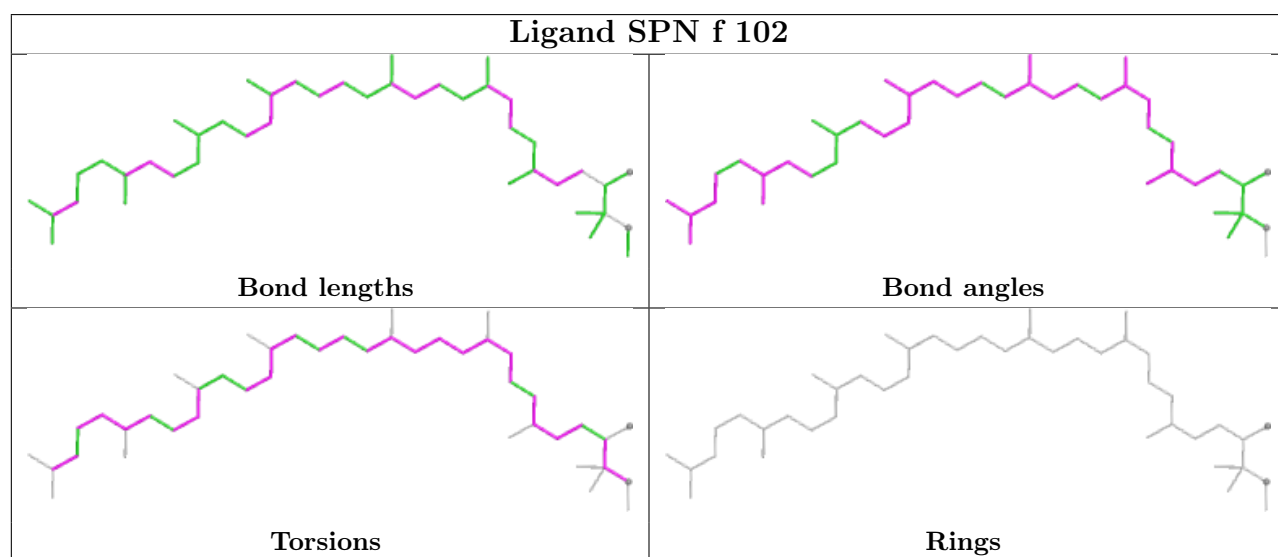
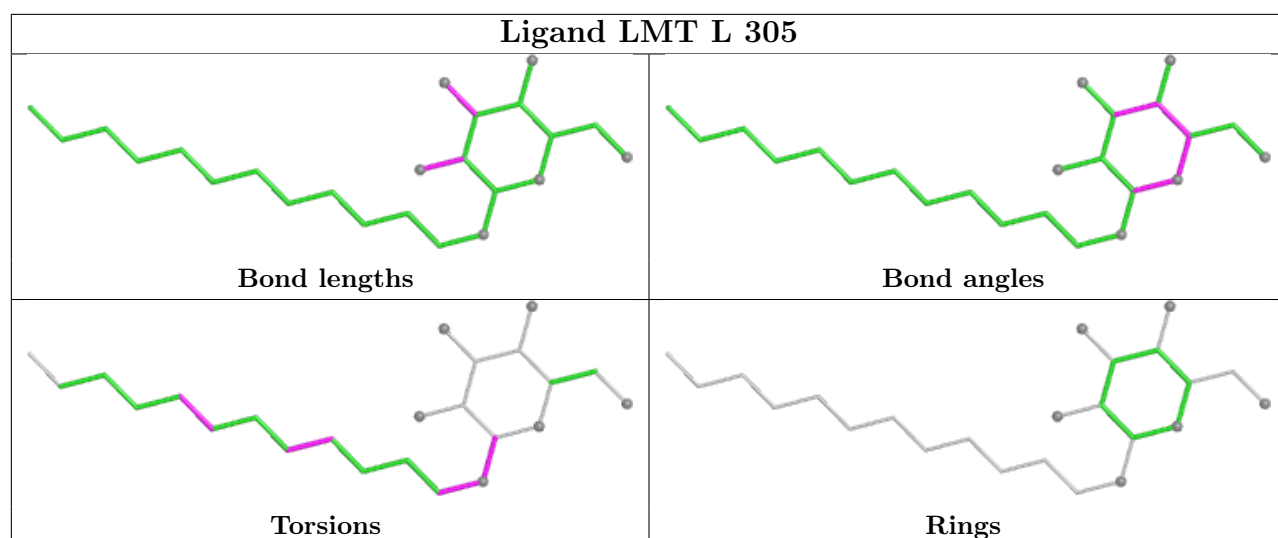


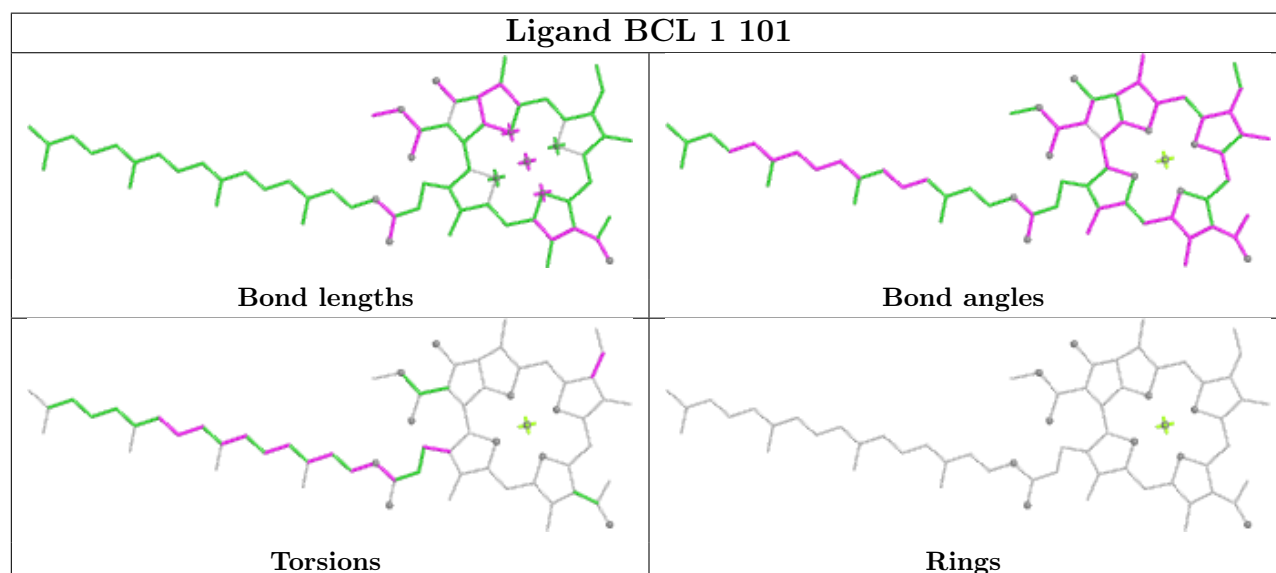
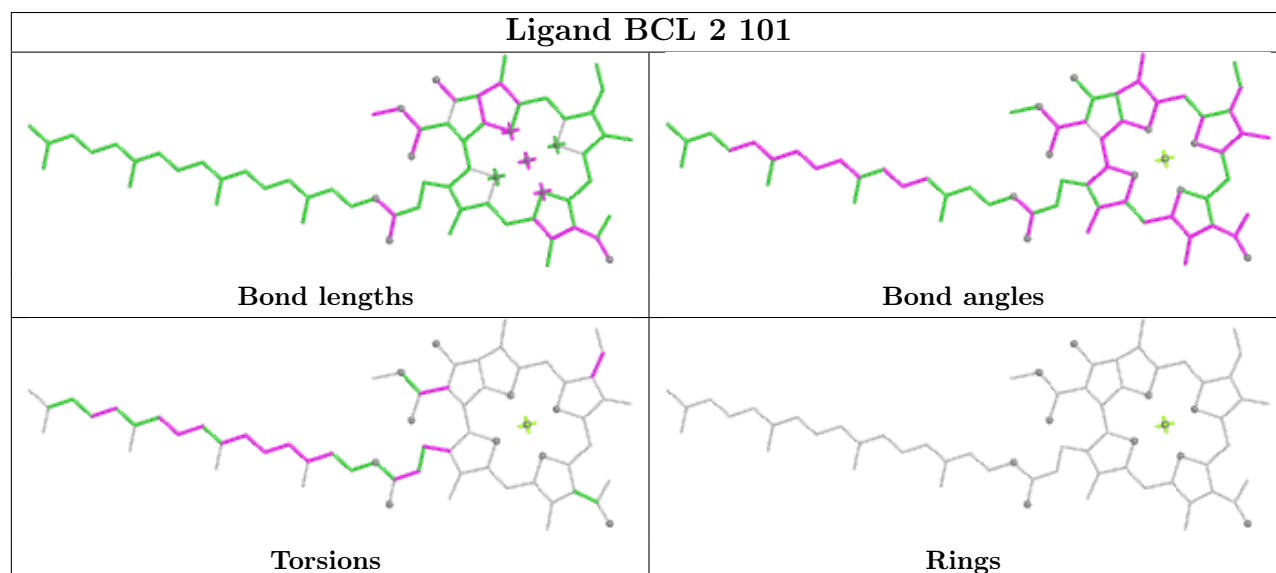
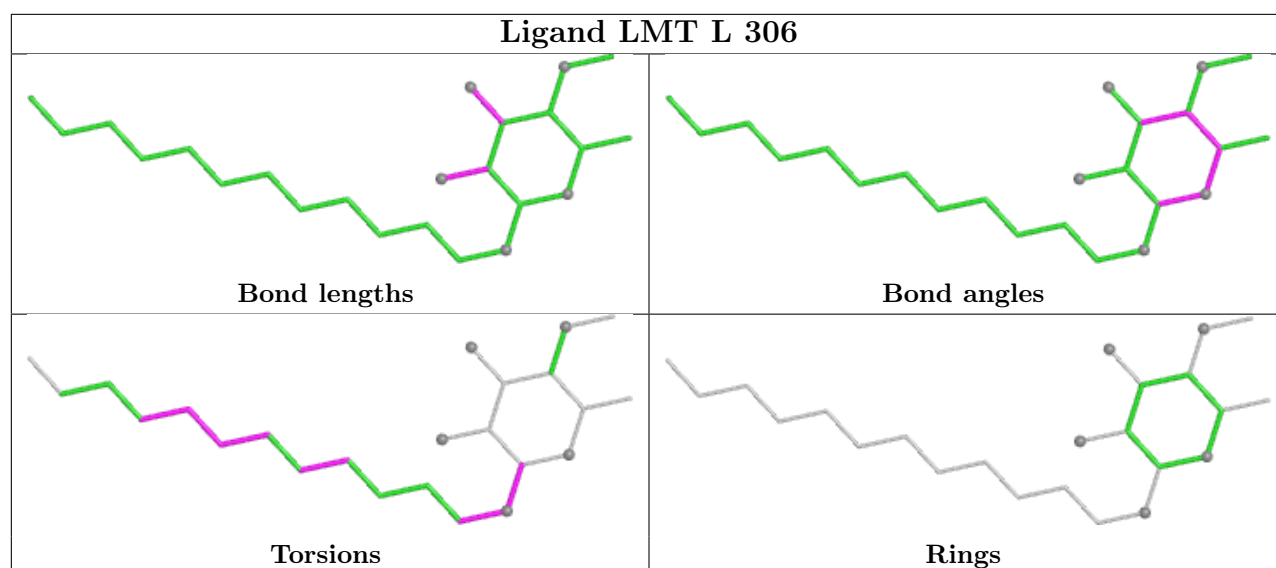


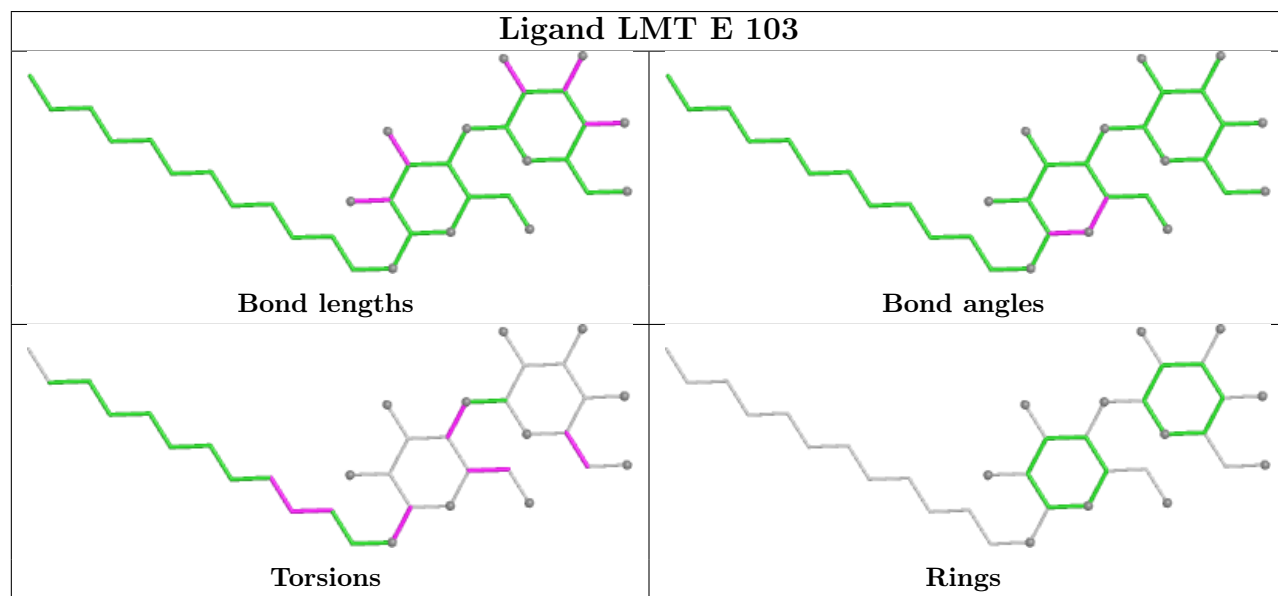
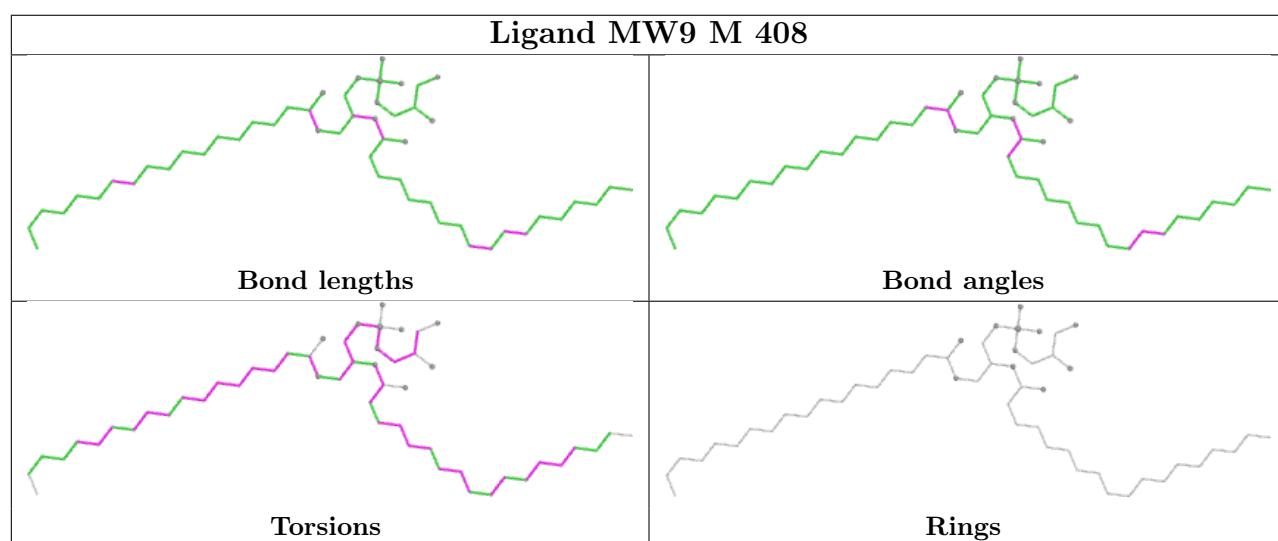
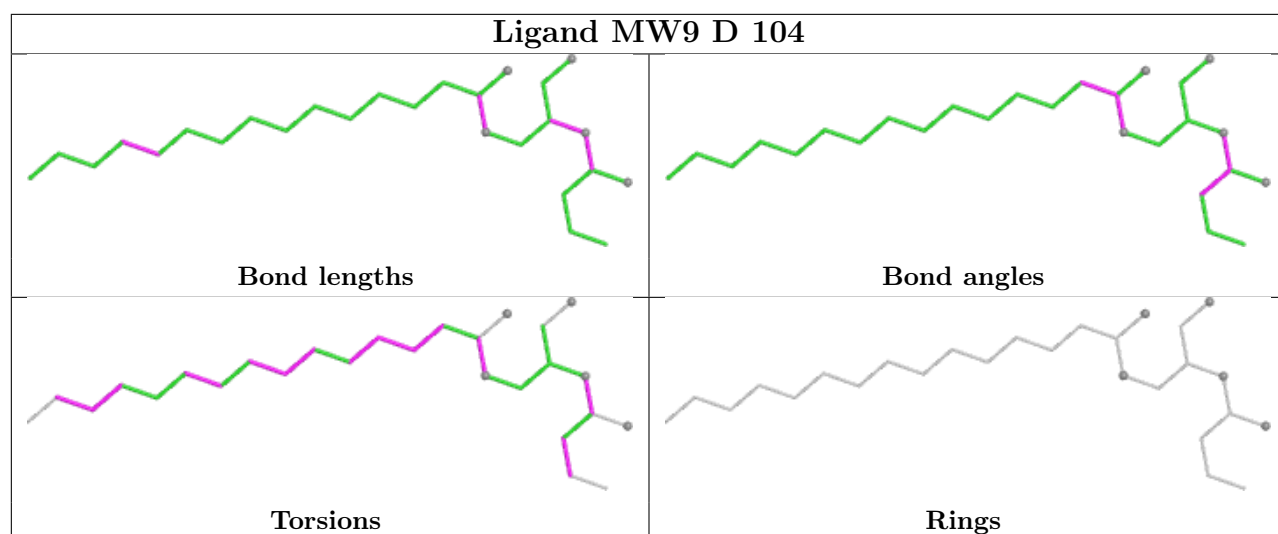


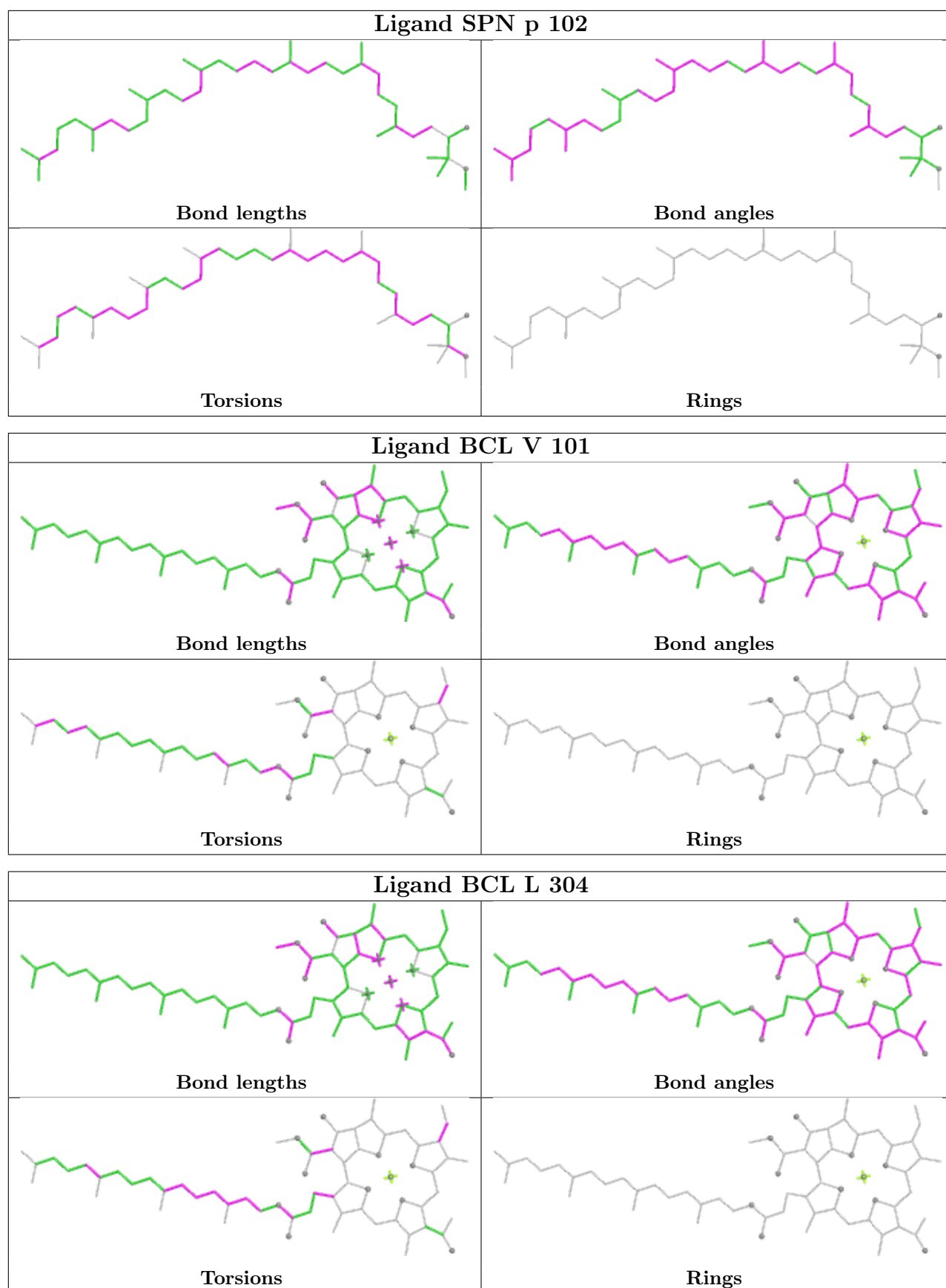


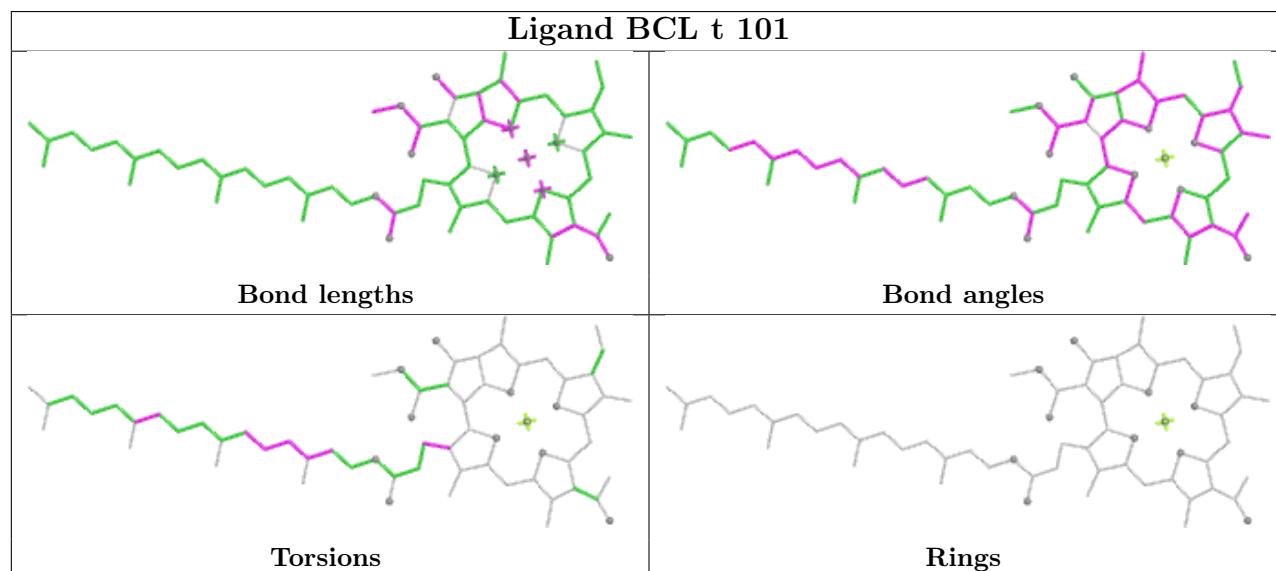
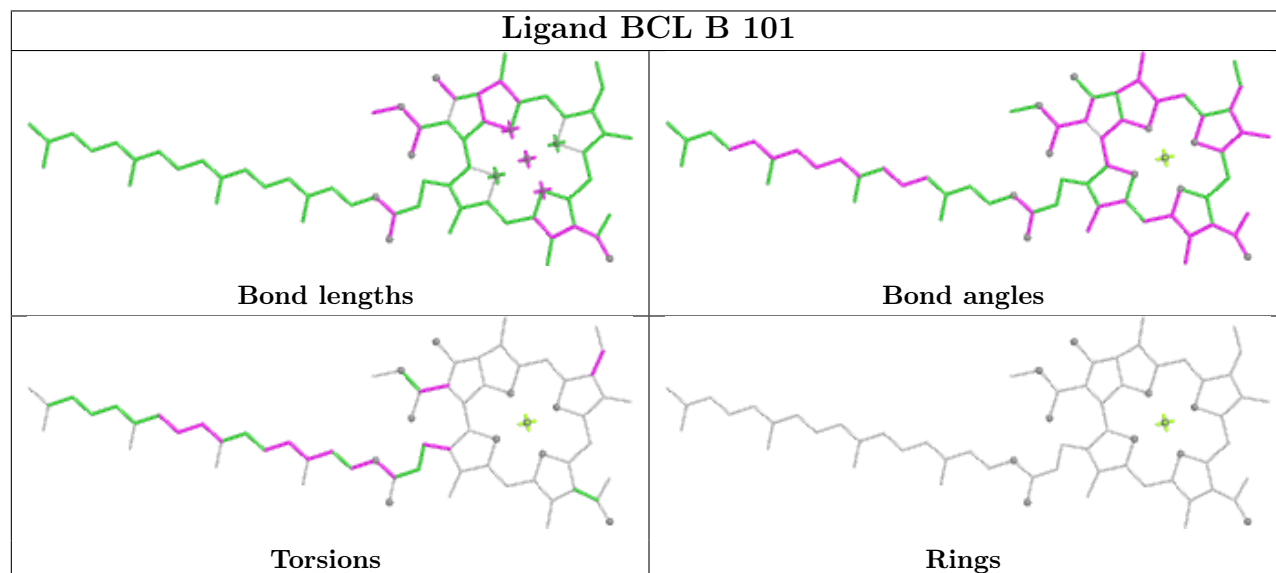
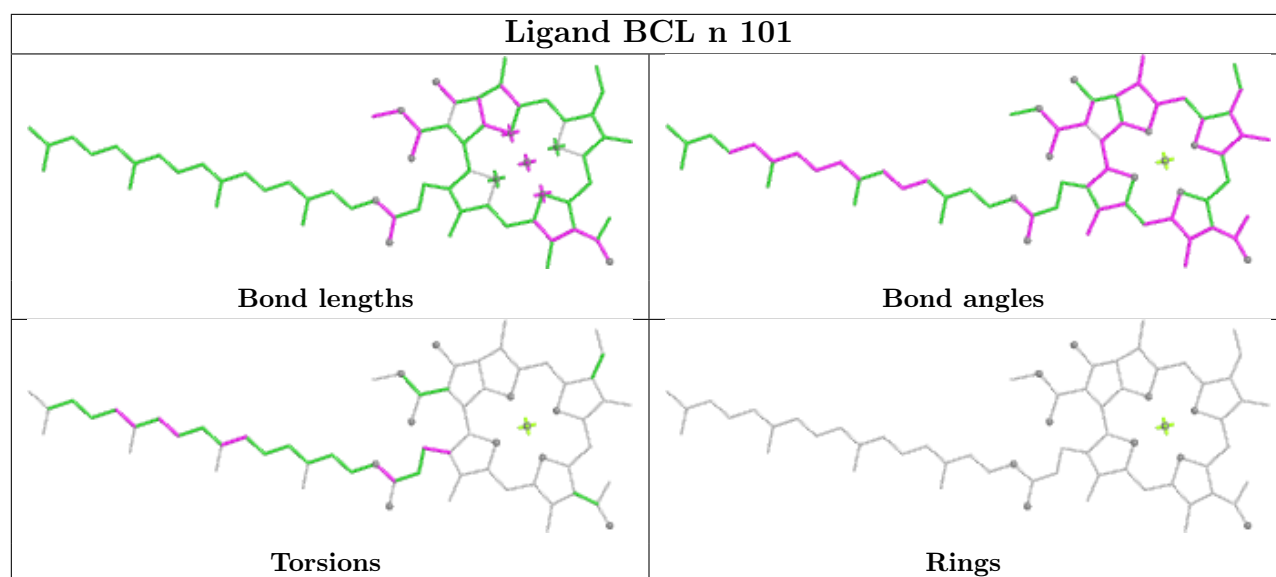


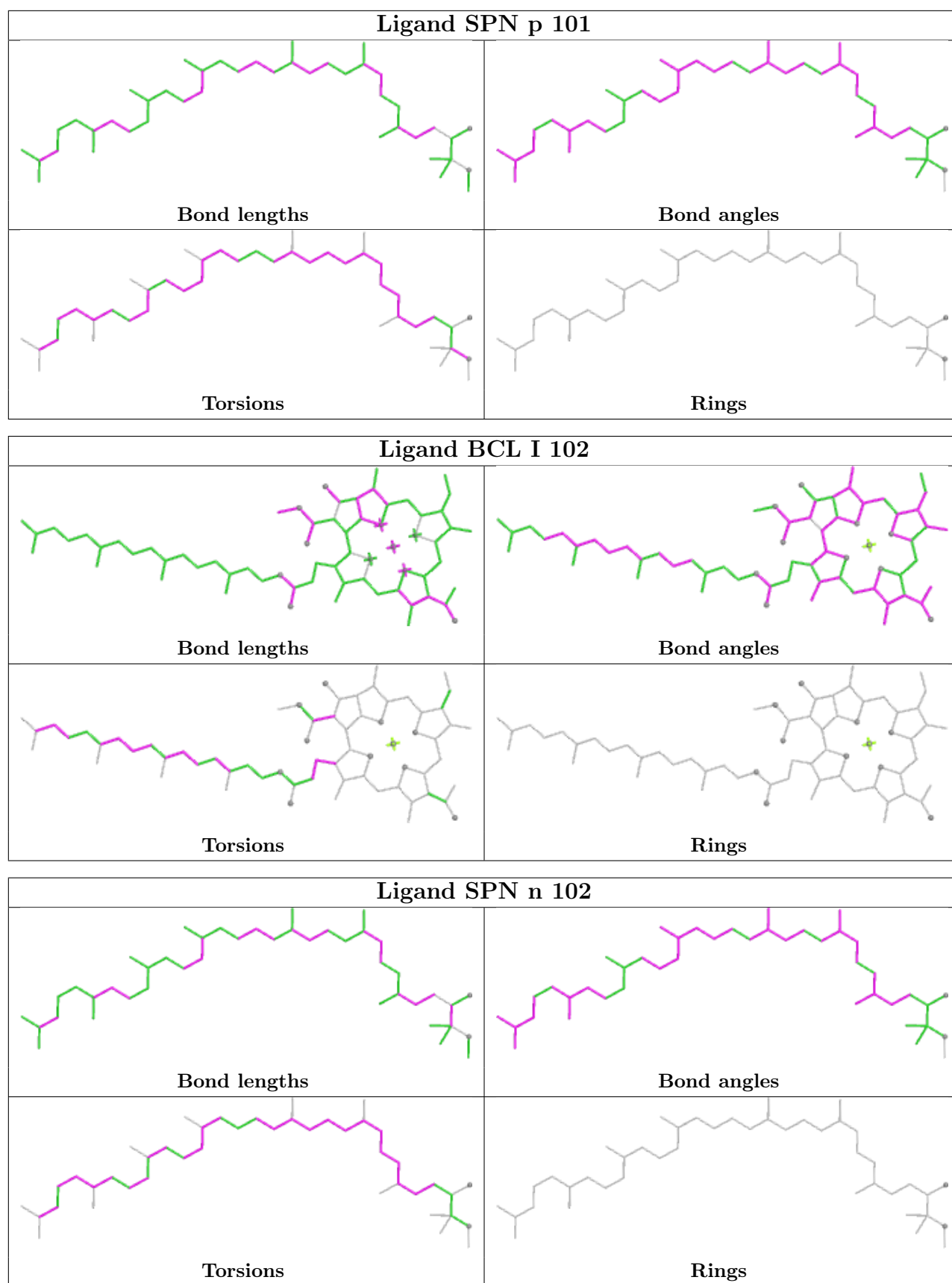


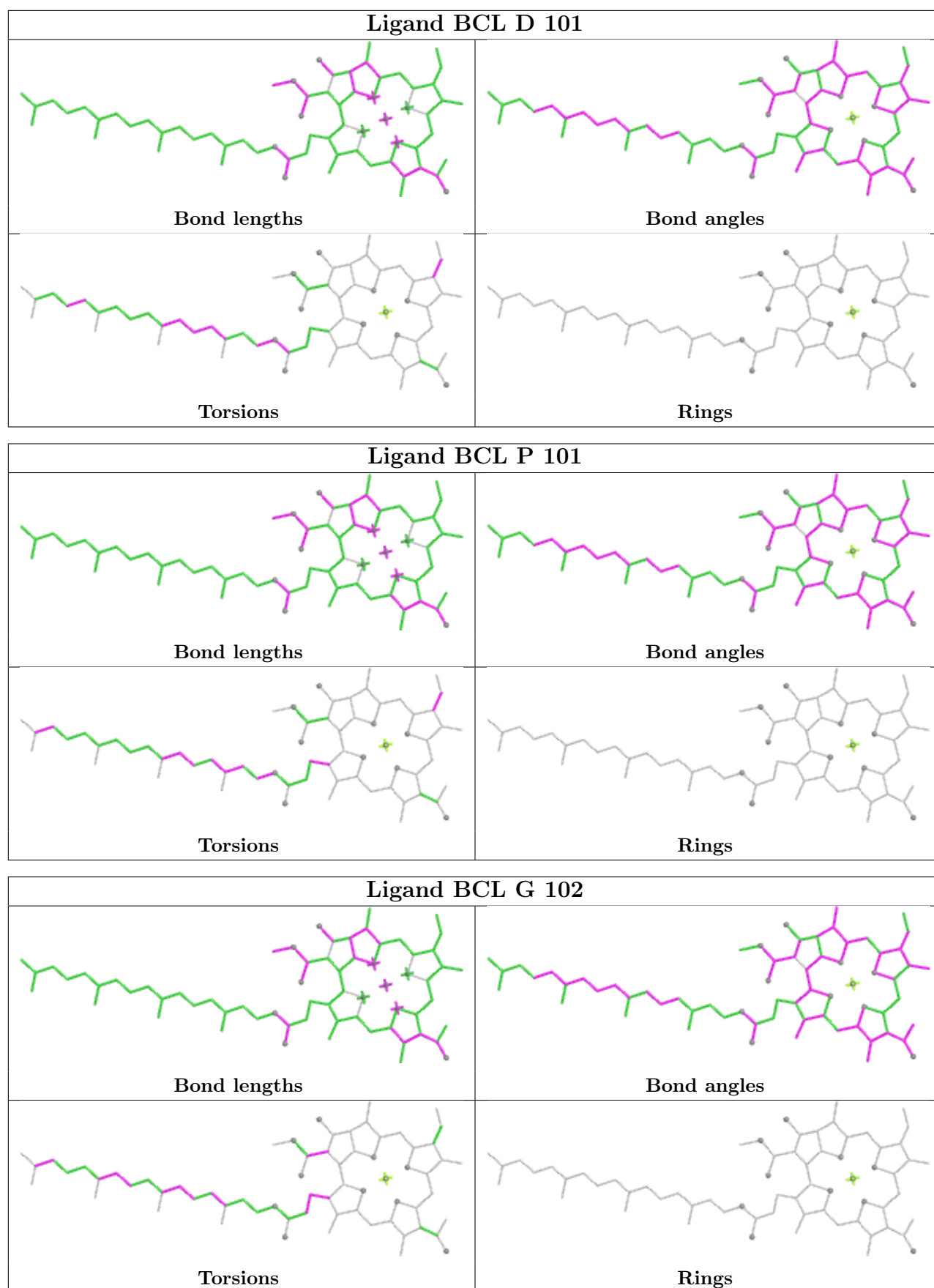


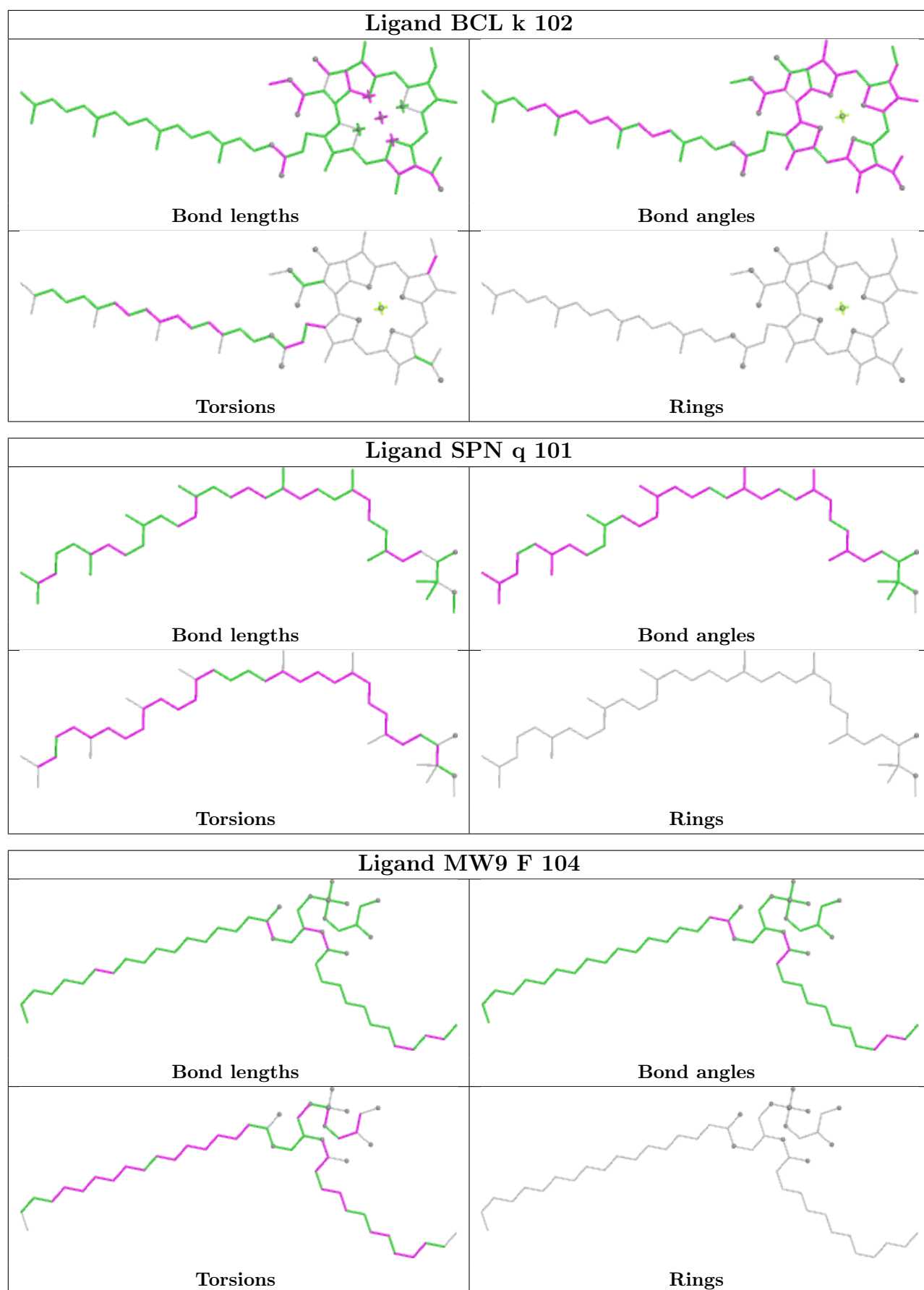












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

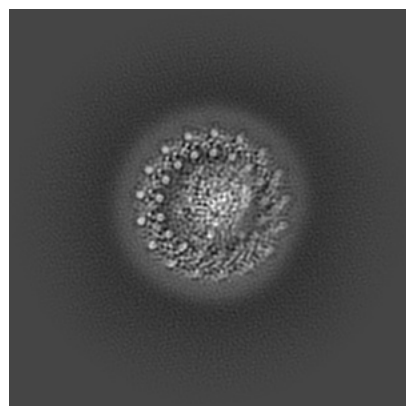
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61695. These allow visual inspection of the internal detail of the map and identification of artifacts.

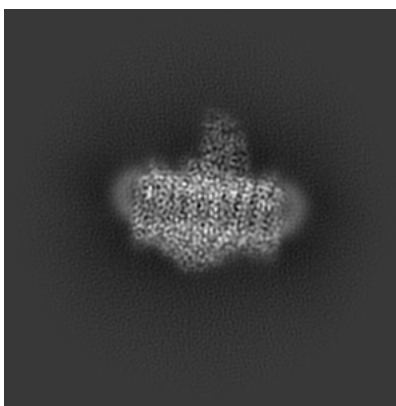
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

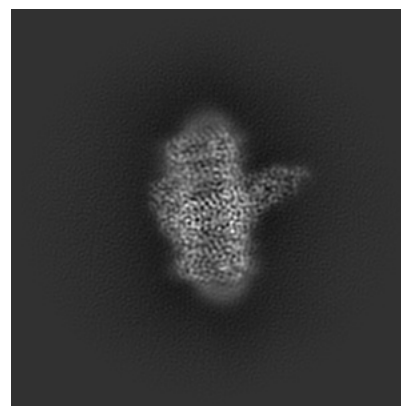
6.1.1 Primary map



X

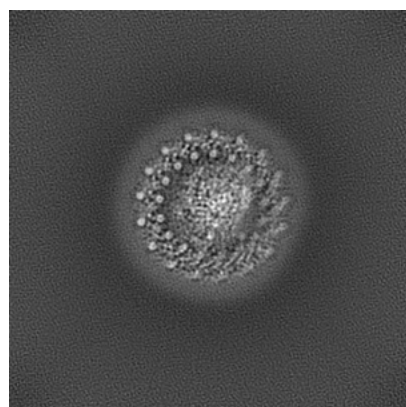


Y

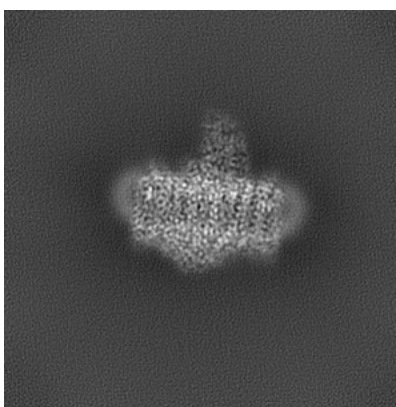


Z

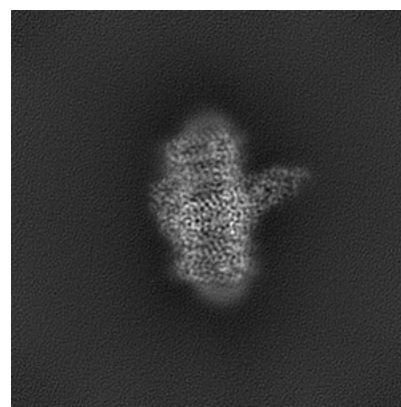
6.1.2 Raw map



X



Y

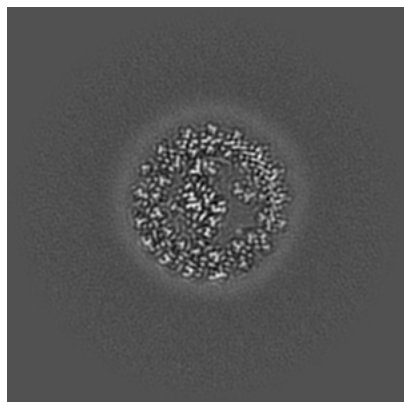


Z

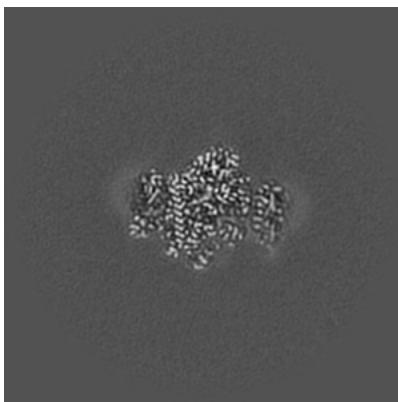
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

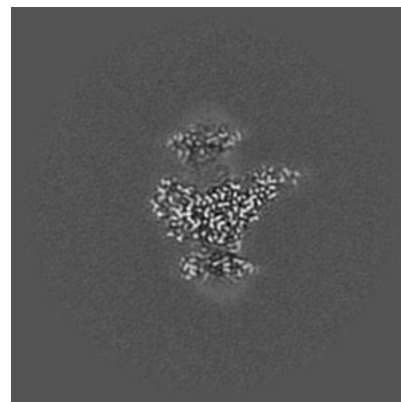
6.2.1 Primary map



X Index: 128

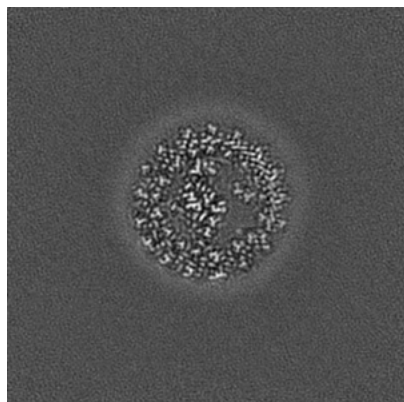


Y Index: 128

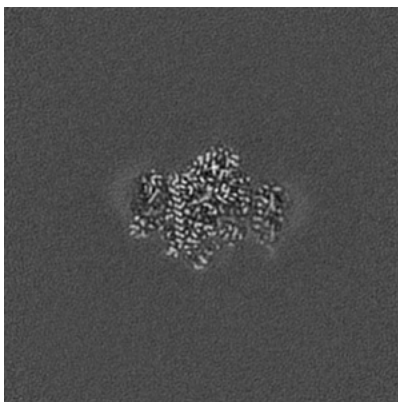


Z Index: 128

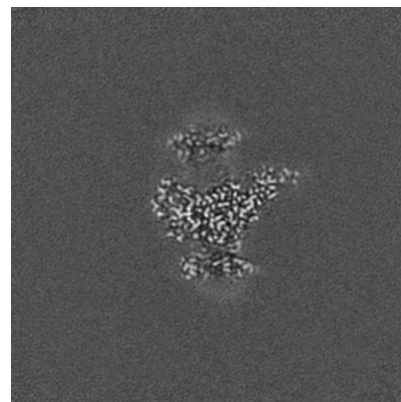
6.2.2 Raw map



X Index: 128



Y Index: 128

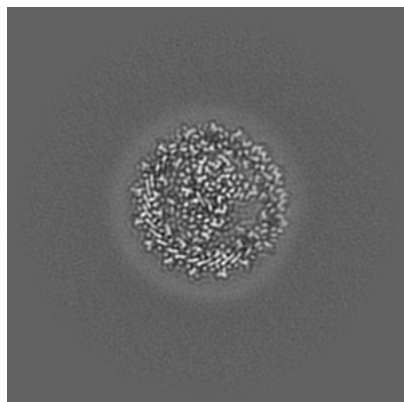


Z Index: 128

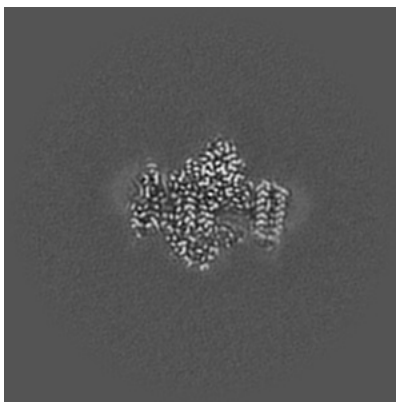
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

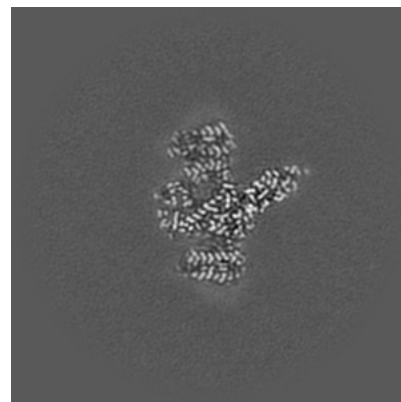
6.3.1 Primary map



X Index: 137

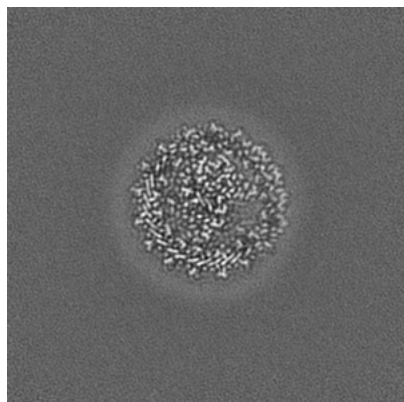


Y Index: 131

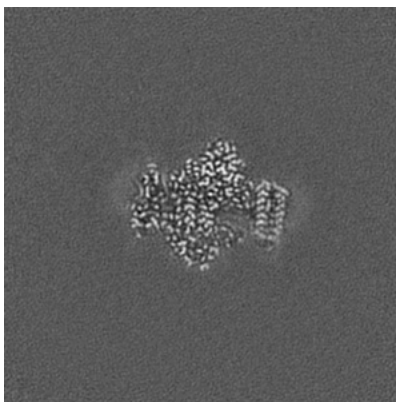


Z Index: 135

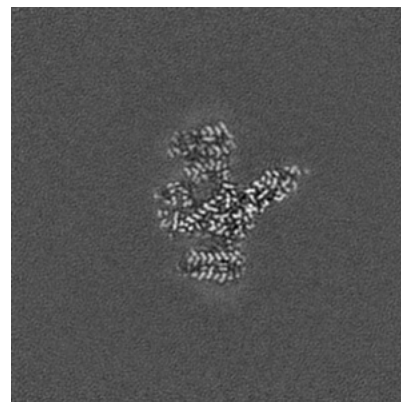
6.3.2 Raw map



X Index: 137



Y Index: 131

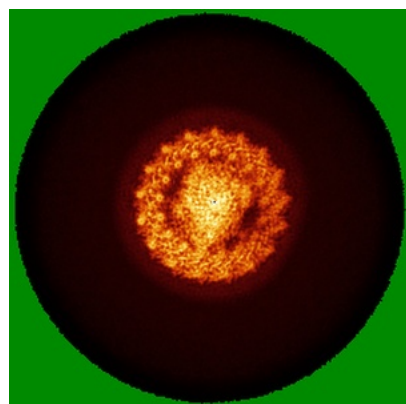


Z Index: 135

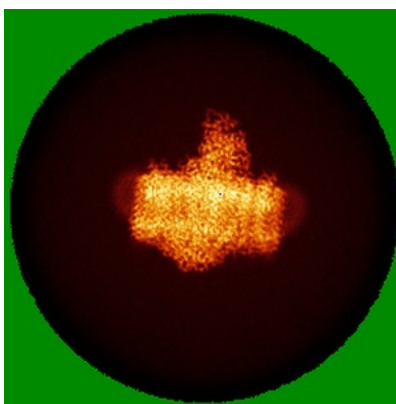
The images above show the largest variance slices of the map in three orthogonal directions.

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

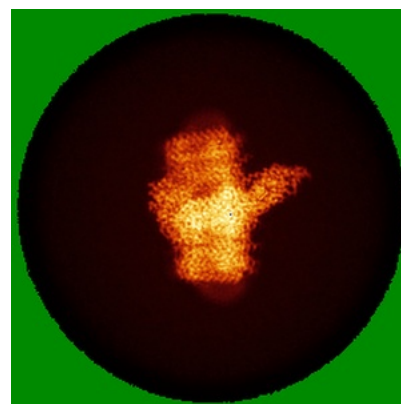
6.4.1 Primary map



X

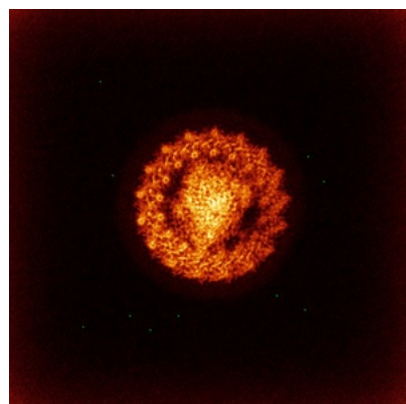


Y

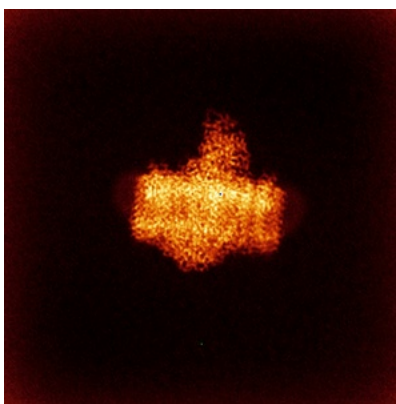


Z

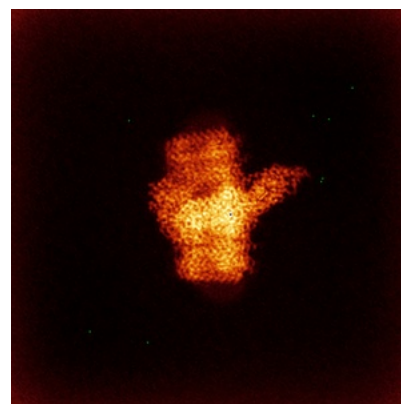
6.4.2 Raw map



X



Y

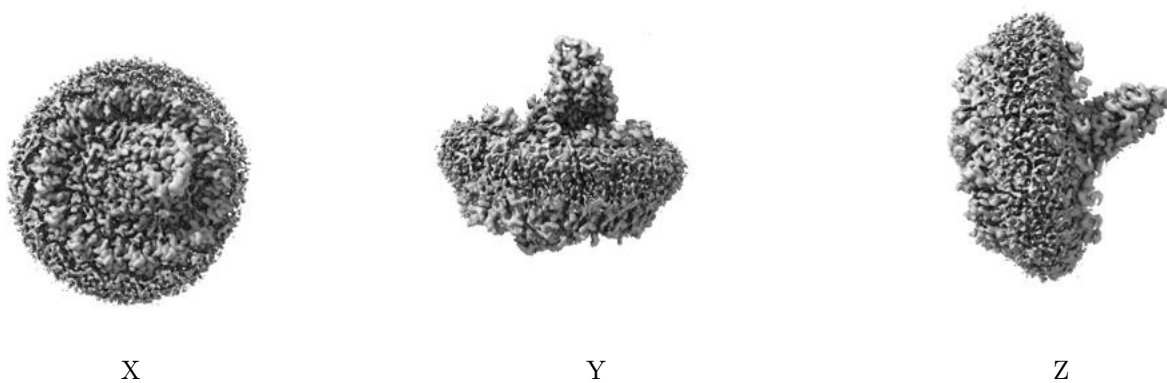


Z

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.

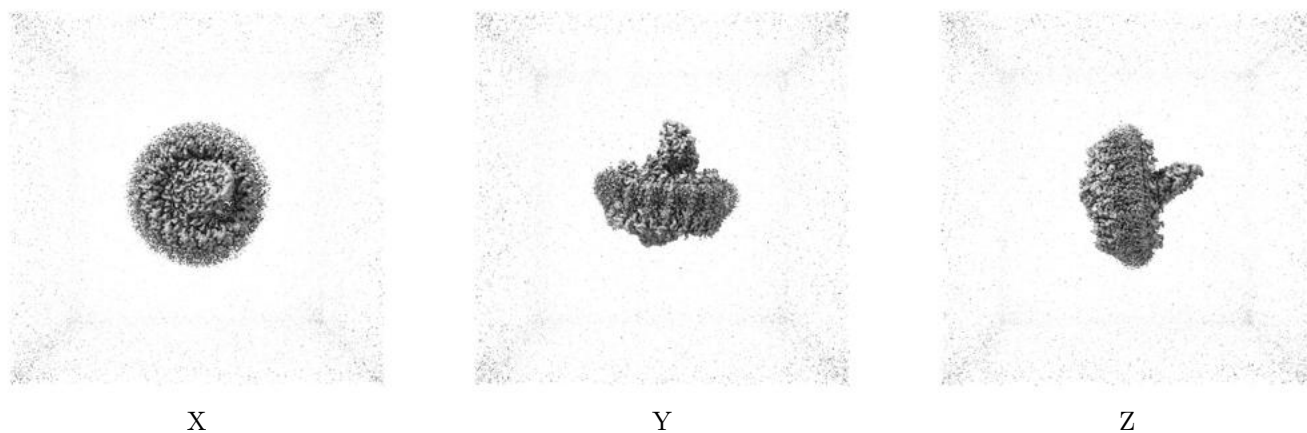
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.103. 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.

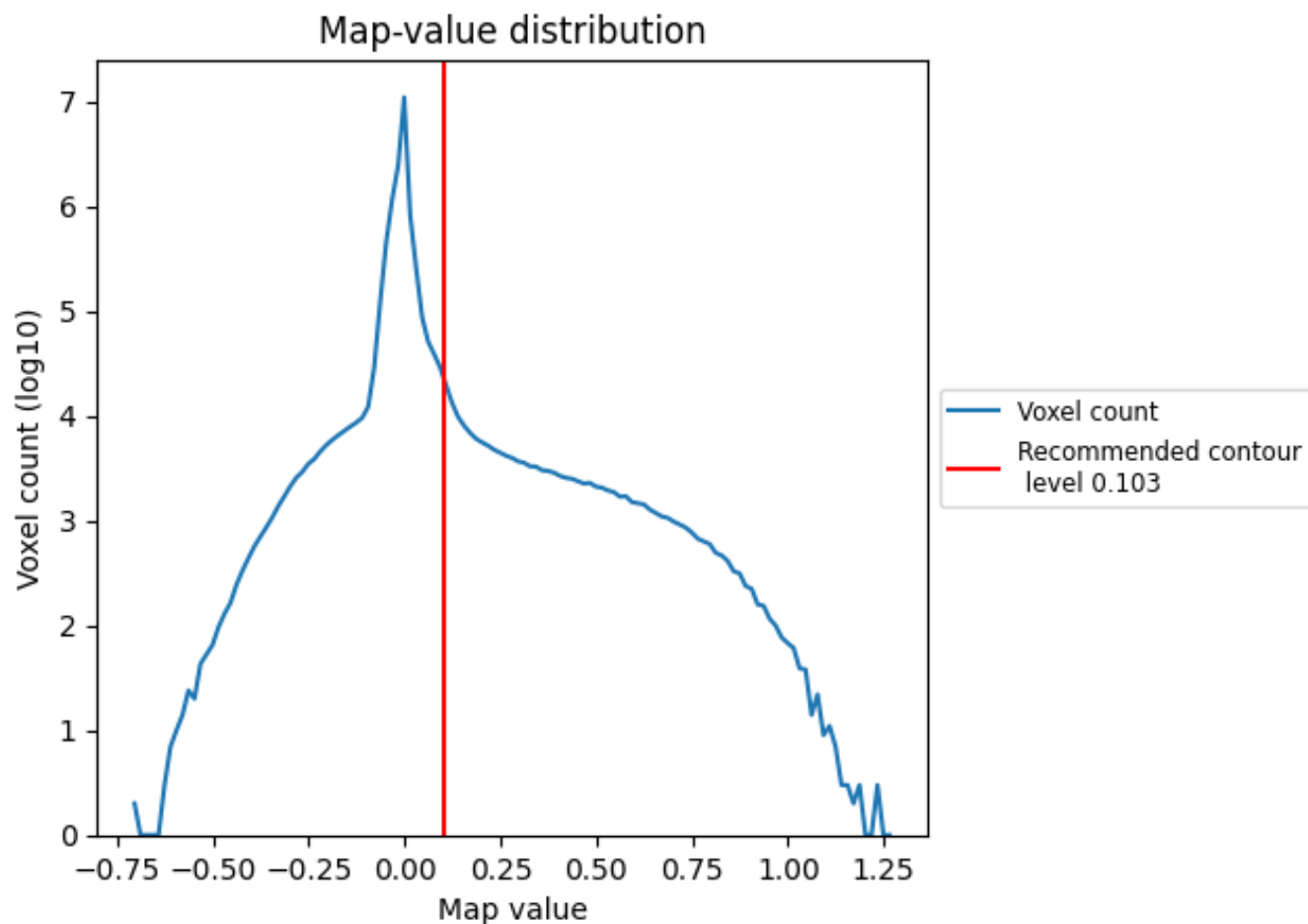
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

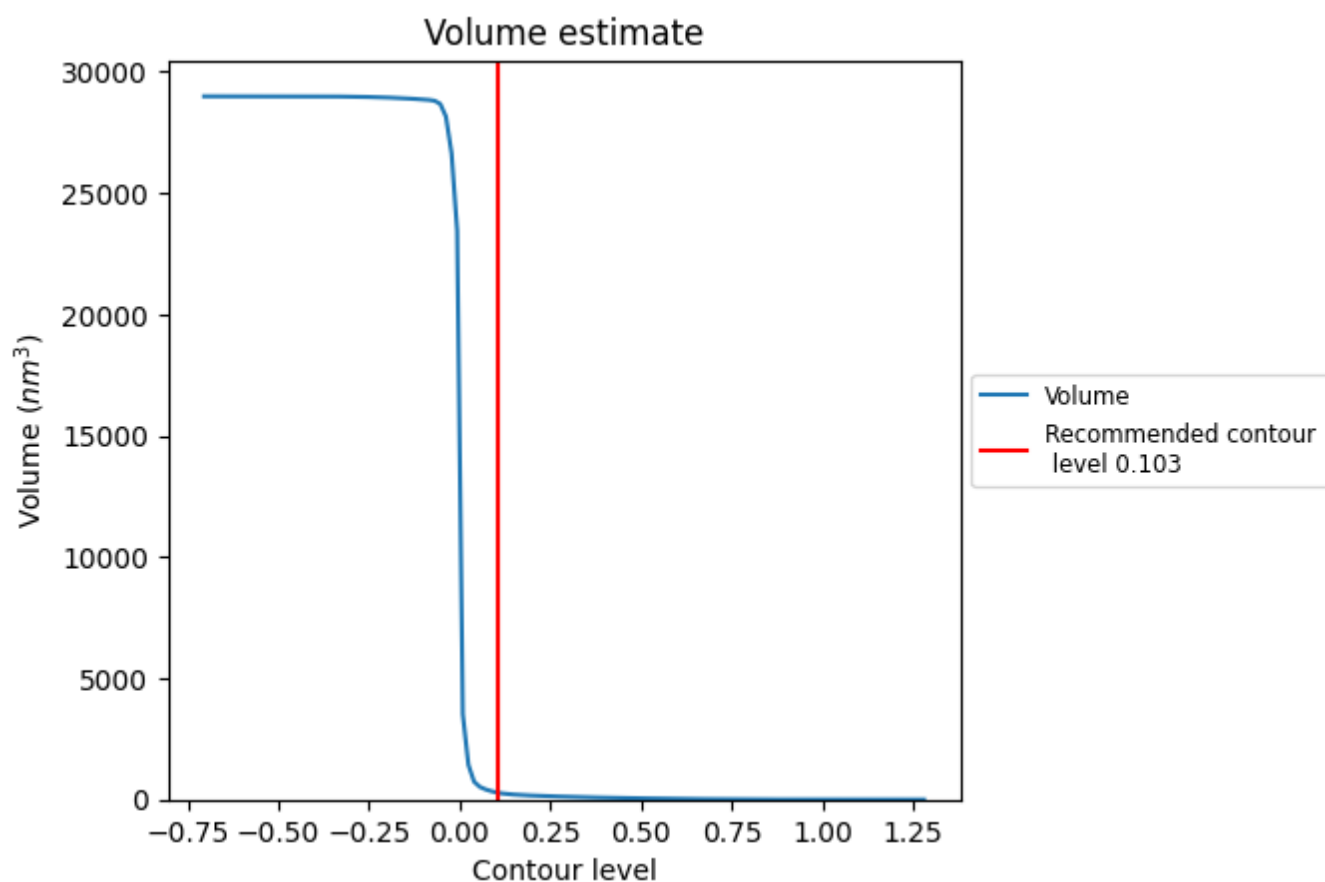
This section contains the results of statistical analysis of the map.

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.

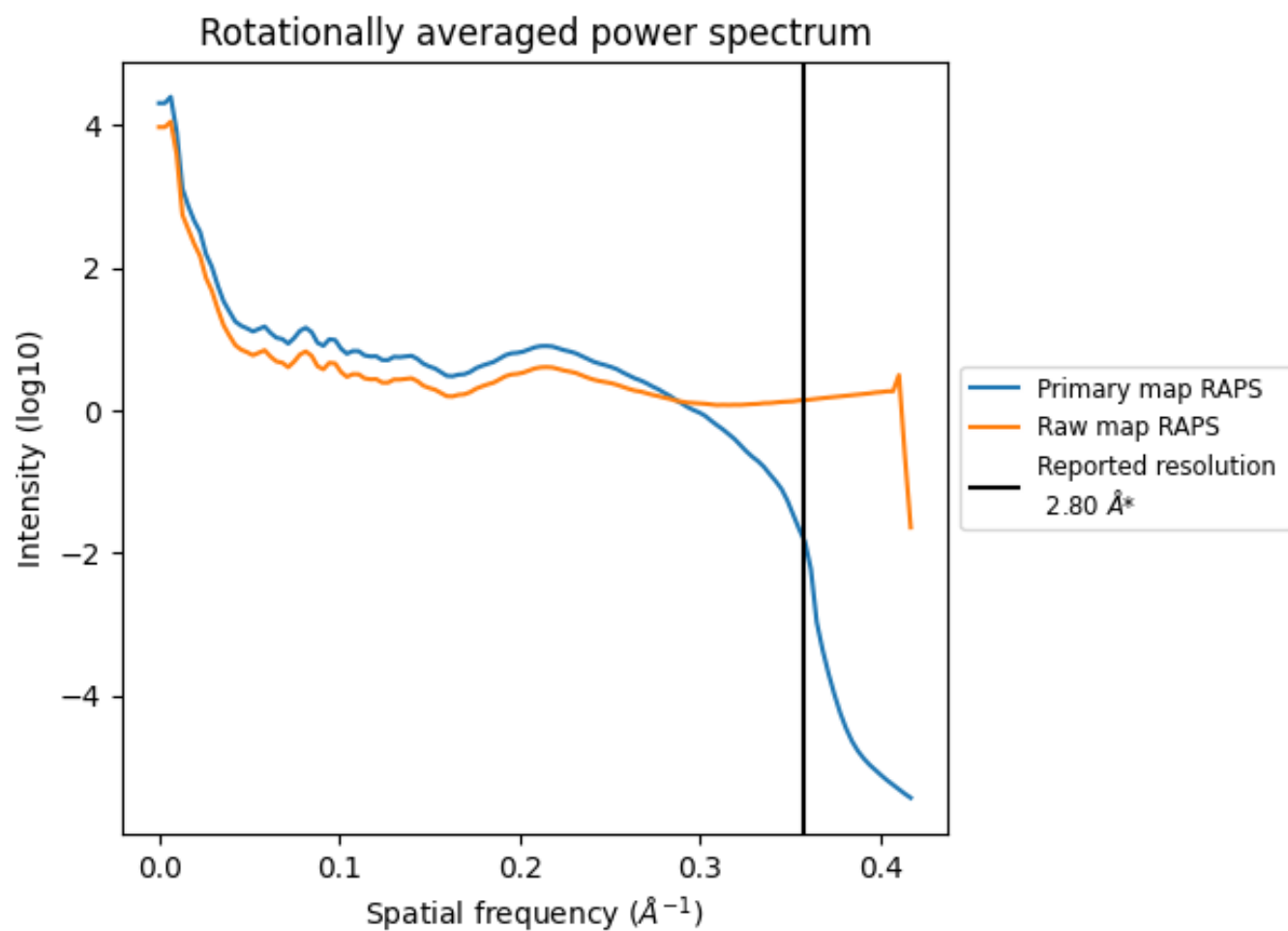
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 290 nm³; this corresponds to an approximate mass of 262 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

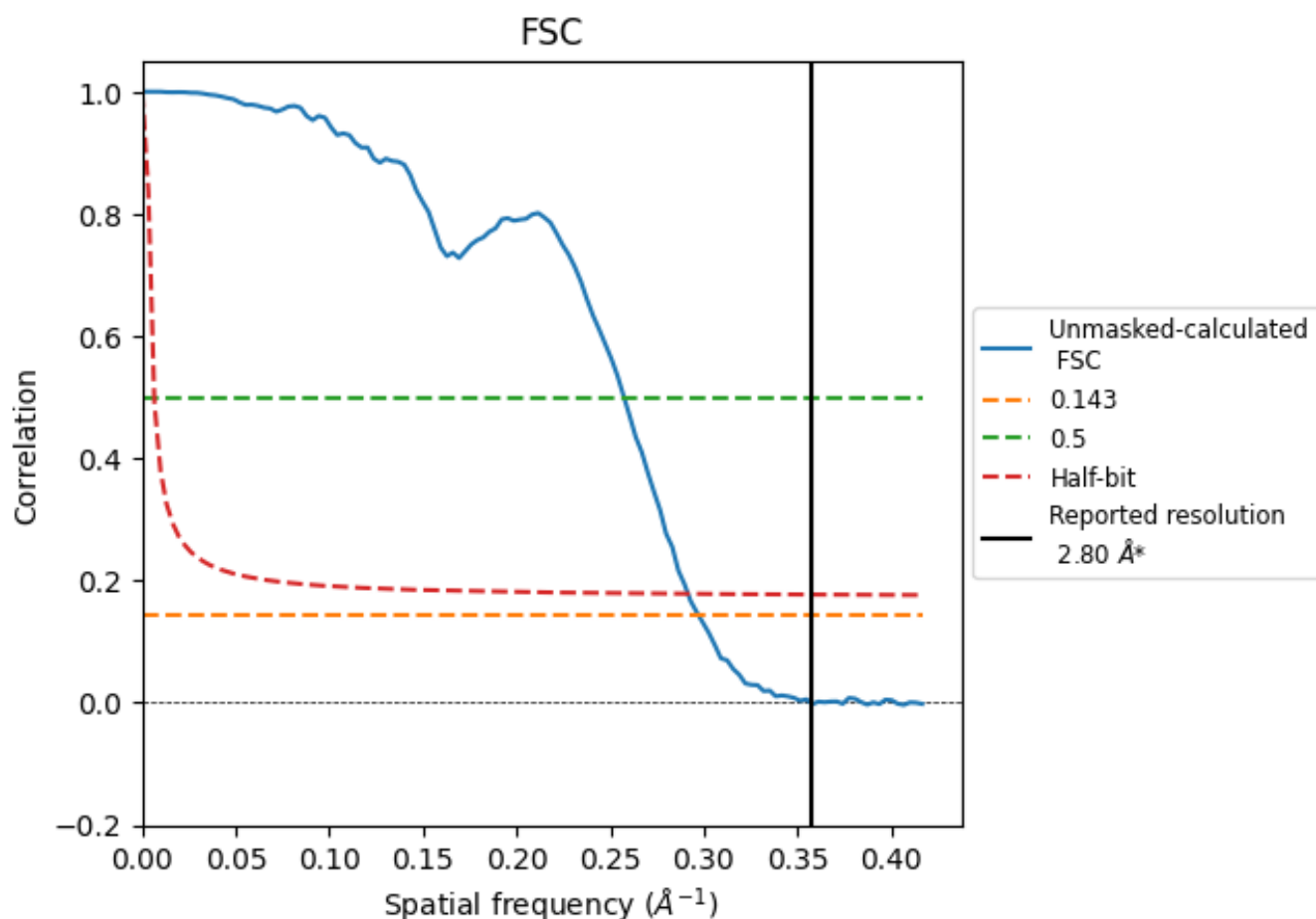


*Reported resolution corresponds to spatial frequency of $0.357 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.357 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

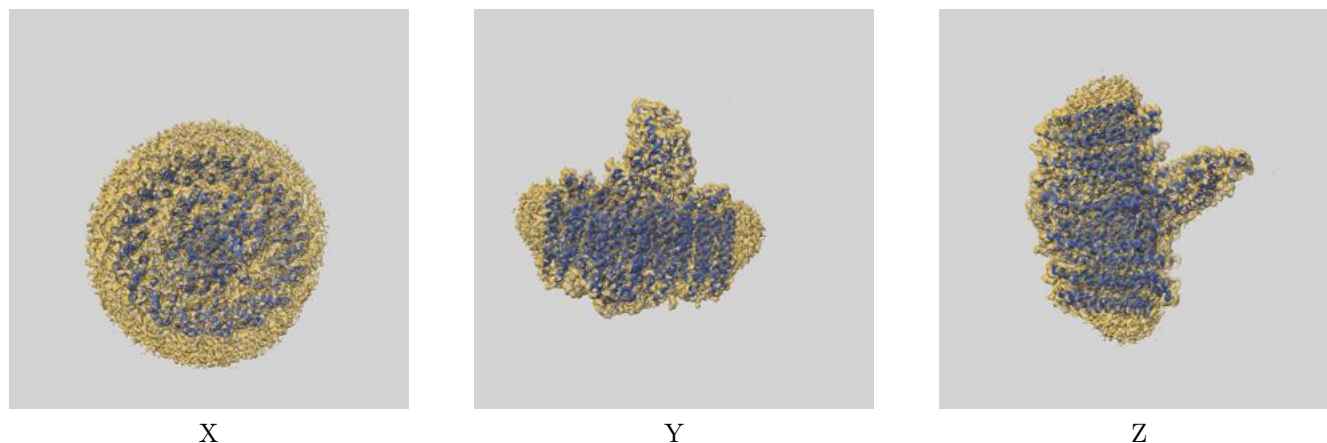
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.36	3.89	3.43

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.36 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

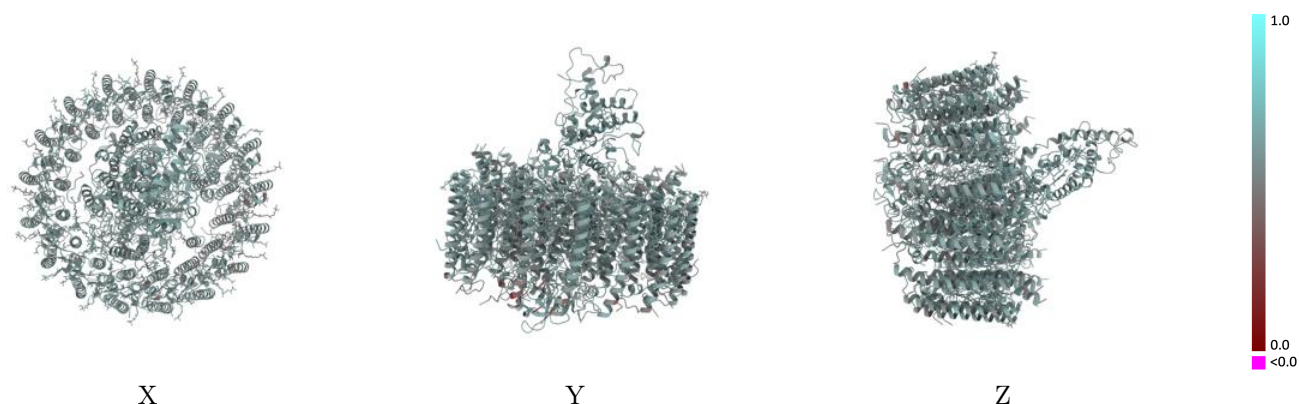
This section contains information regarding the fit between EMDB map EMD-61695 and PDB model 9JPB. Per-residue inclusion information can be found in section [3](#) on page [18](#).

9.1 Map-model overlay [i](#)



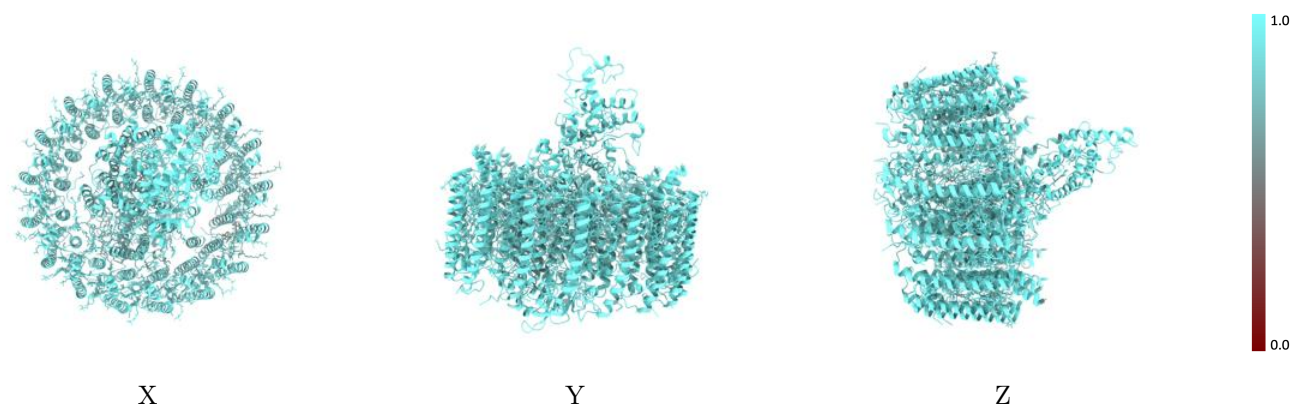
The images above show the 3D surface view of the map at the recommended contour level 0.103 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



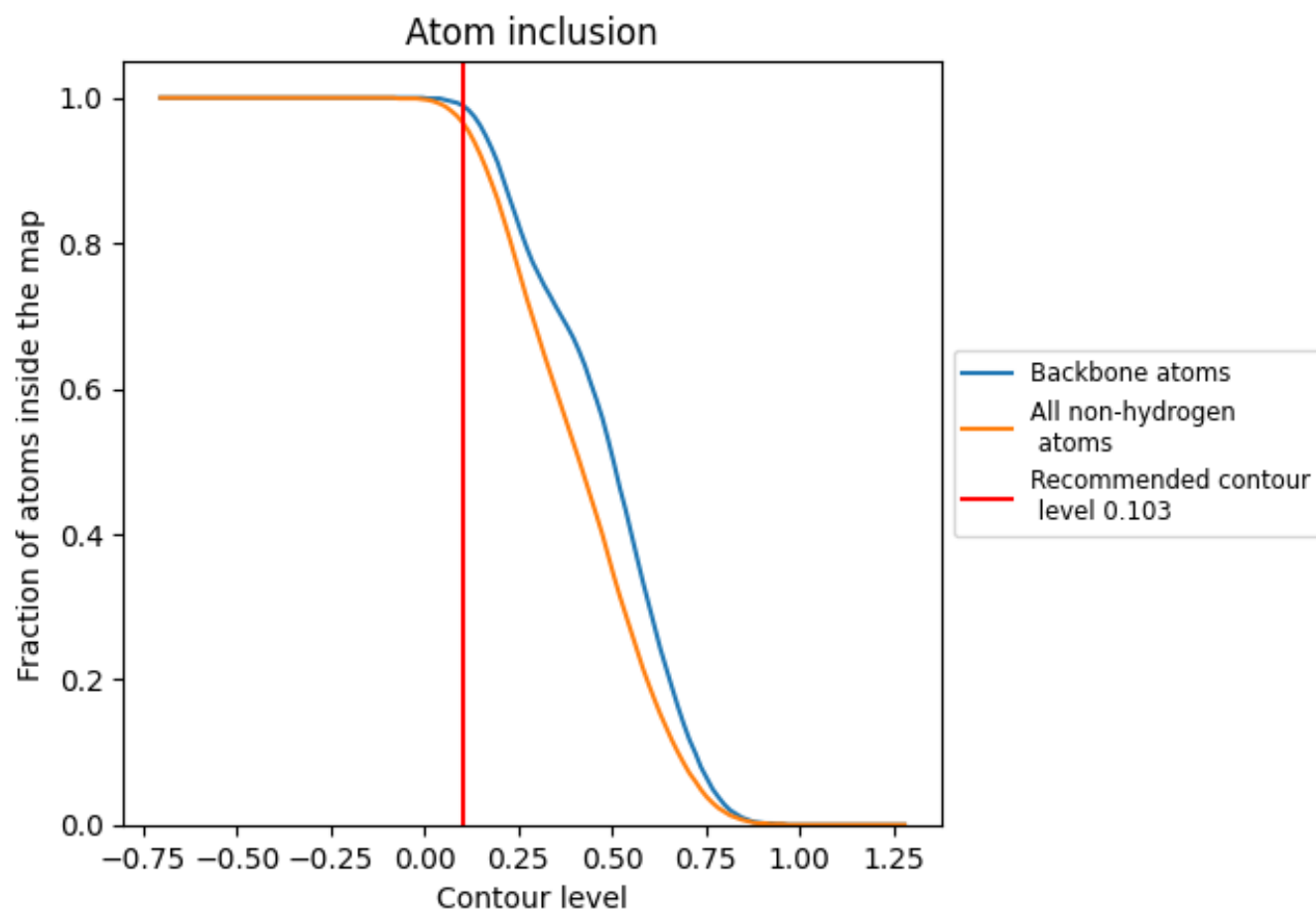
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.103).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.103) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9650	 0.5710
1	 0.9620	 0.5720
2	 0.9620	 0.5640
A	 0.9430	 0.5540
B	 0.9450	 0.5680
C	 0.9730	 0.5730
D	 0.9760	 0.5830
E	 0.9680	 0.5800
F	 0.9790	 0.5910
G	 0.9660	 0.5820
H	 0.9760	 0.5840
I	 0.9820	 0.5840
J	 0.9700	 0.5670
K	 0.9640	 0.5770
L	 0.9790	 0.5930
M	 0.9760	 0.5890
N	 0.9670	 0.5560
O	 0.9650	 0.5620
P	 0.9520	 0.5610
Q	 0.9500	 0.5670
R	 0.9520	 0.5590
S	 0.9300	 0.5580
T	 0.9600	 0.5500
V	 0.8860	 0.5220
a	 0.9450	 0.5430
b	 0.9760	 0.5600
d	 0.9810	 0.5720
e	 0.9820	 0.5830
f	 0.9670	 0.5820
g	 0.9860	 0.5720
i	 0.9550	 0.5620
j	 0.9750	 0.5640
k	 0.9530	 0.5560
n	 0.9600	 0.5620
p	 0.9460	 0.5350



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
q	 0.9690	 0.5640
r	 0.9450	 0.5600
s	 0.9540	 0.5470
t	 0.9240	 0.5260
v	 0.9260	 0.5060