Full wwPDB EM Validation Report (i)

Aug 7, 2026 – 03:15 AM JST

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

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

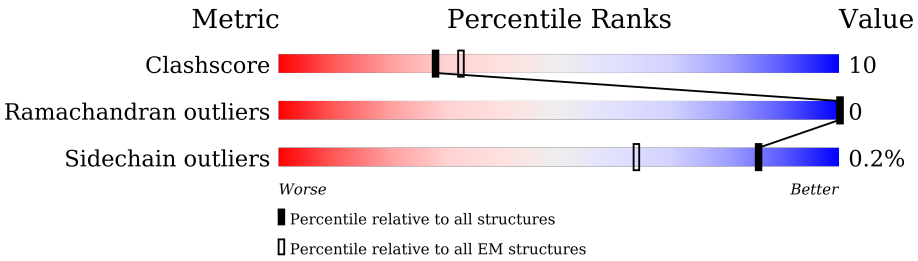
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using 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

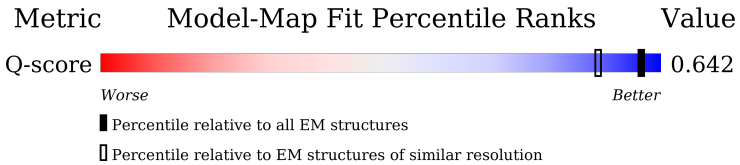
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.49 Å.

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





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

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

Mol	Chain	Length	Quality of chain
1	A	76	76% 21% •
2	1	51	94% 6%
2	3	51	86% 14%
2	5	51	86% 14%

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	n	44	82% 18%
3	p	44	86% 14%
3	r	44	7% 82% 18%
3	t	44	77% 23%
3	v	44	77% 23%
3	x	44	91% 9%
4	C	357	82% 18%
5	H	255	94% 6%
6	L	273	91% 8%
7	M	325	91% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	SPN	1	102	-	X	-	-
10	SPN	1	103	-	X	-	-
10	SPN	1	104	-	X	-	-
10	SPN	1	105	-	X	-	-
10	SPN	3	102	-	X	-	-
10	SPN	5	102	-	X	-	-
10	SPN	5	103	-	X	-	-
10	SPN	7	102	-	X	-	-
10	SPN	7	103	-	X	-	-
10	SPN	9	103	-	X	-	-
10	SPN	a	102	-	X	-	-
10	SPN	a	103	-	X	-	-
10	SPN	c	102	-	X	-	-
10	SPN	c	103	-	X	-	-
10	SPN	e	102	-	X	-	-
10	SPN	h	102	-	X	-	-
10	SPN	h	103	-	X	-	-
10	SPN	i	102	-	X	-	-
10	SPN	j	102	-	X	-	-
10	SPN	k	102	-	X	-	-

Continued on next page...

Continued from previous page...

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

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 28463 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Protein LRC.

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

There are 5 discrepancies between the modelled and reference sequences:

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 3 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

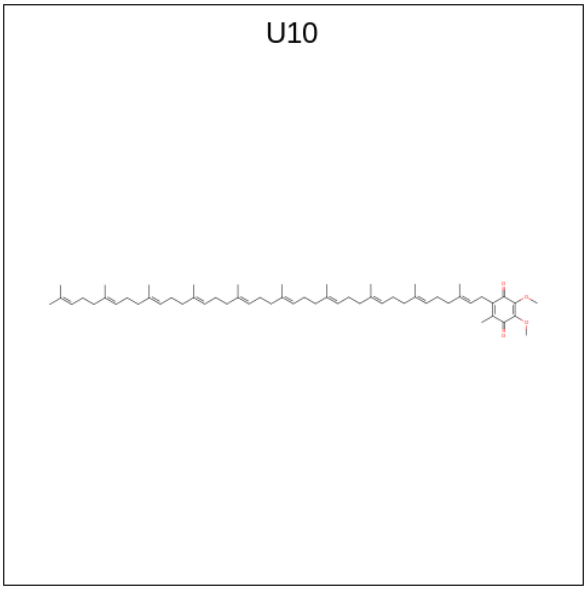
- Molecule 7 is a protein called Reaction center protein M chain.

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

There is a discrepancy between the modelled and reference sequences:

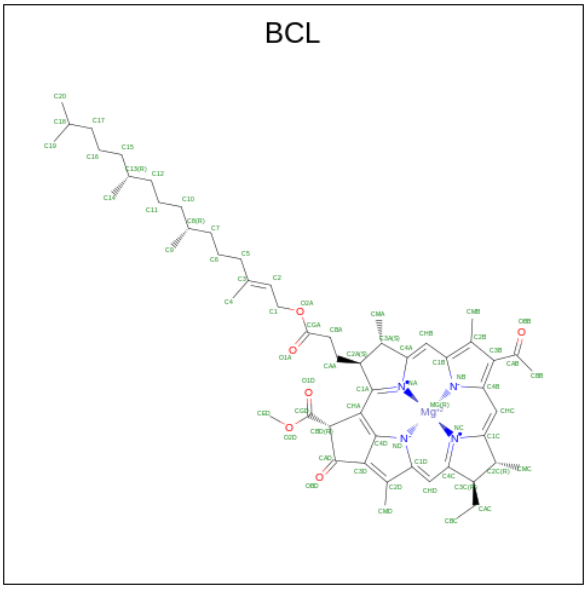
Chain	Residue	Modelled	Actual	Comment	Reference
M	134	THR	SER	conflict	UNP A8LQ17

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



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

- Molecule 9 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
			Total	C	Mg	N	O	
9	1	1	66	55	1	4	6	0
9	2	1	66	55	1	4	6	0
9	5	1	66	55	1	4	6	0
9	6	1	66	55	1	4	6	0
9	3	1	66	55	1	4	6	0
9	4	1	66	55	1	4	6	0
9	w	1	66	55	1	4	6	0
9	x	1	66	55	1	4	6	0
9	u	1	66	55	1	4	6	0
9	v	1	66	55	1	4	6	0
9	s	1	66	55	1	4	6	0
9	t	1	66	55	1	4	6	0

Continued on next page...

Continued from previous page...

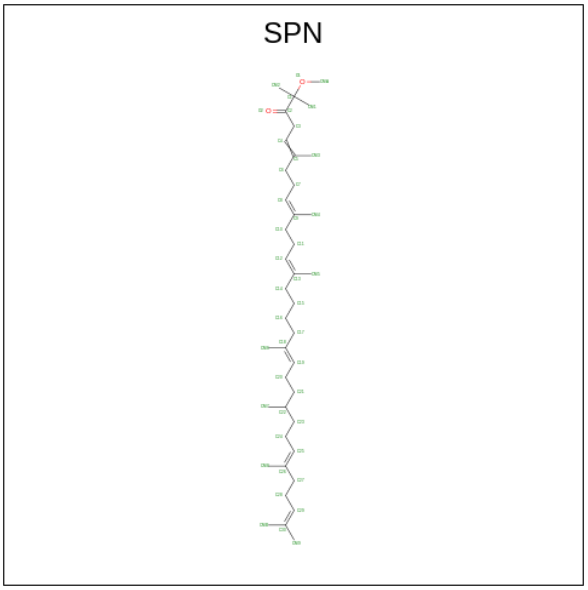
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
9	q	1	66	55	1	4	6	0
9	r	1	66	55	1	4	6	0
9	o	1	66	55	1	4	6	0
9	p	1	66	55	1	4	6	0
9	m	1	66	55	1	4	6	0
9	n	1	66	55	1	4	6	0
9	k	1	66	55	1	4	6	0
9	l	1	66	55	1	4	6	0
9	g	1	66	55	1	4	6	0
9	h	1	66	55	1	4	6	0
9	e	1	66	55	1	4	6	0
9	f	1	66	55	1	4	6	0
9	c	1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

Continued on next page...

Continued from previous page...

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

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



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

Continued on next page...

Continued from previous page...

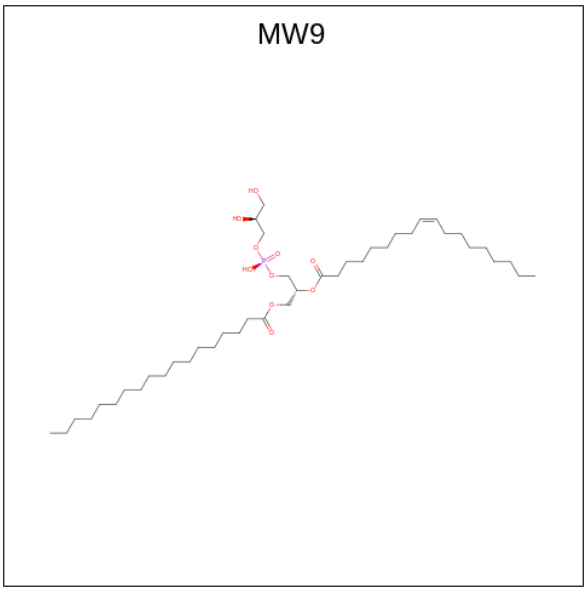
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
10	3	1	43	41	2	0
10	w	1	43	41	2	0
10	u	1	43	41	2	0
10	v	1	43	41	2	0
10	s	1	43	41	2	0
10	t	1	43	41	2	0
10	q	1	43	41	2	0
10	r	1	43	41	2	0
10	p	1	43	41	2	0
10	p	1	43	41	2	0
10	m	1	43	41	2	0
10	n	1	43	41	2	0
10	k	1	43	41	2	0
10	l	1	43	41	2	0
10	h	1	43	41	2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

Continued on next page...

Continued from previous page...

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

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



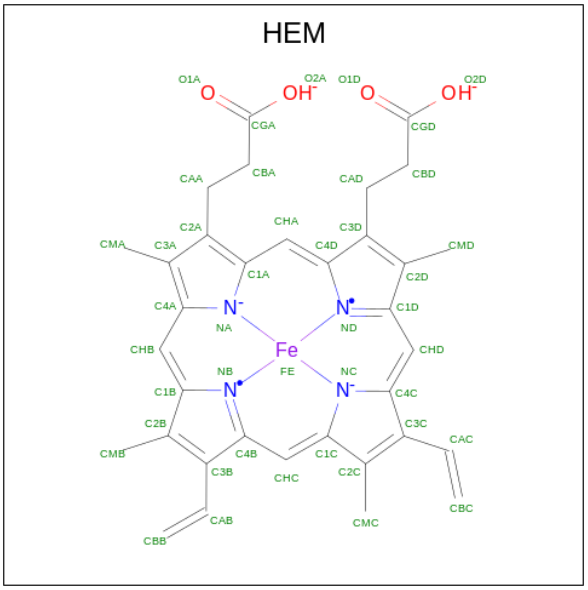
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
11	g	1	53	42	10	1	0
11	g	1	50	39	10	1	0

Continued on next page...

Continued from previous page...

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

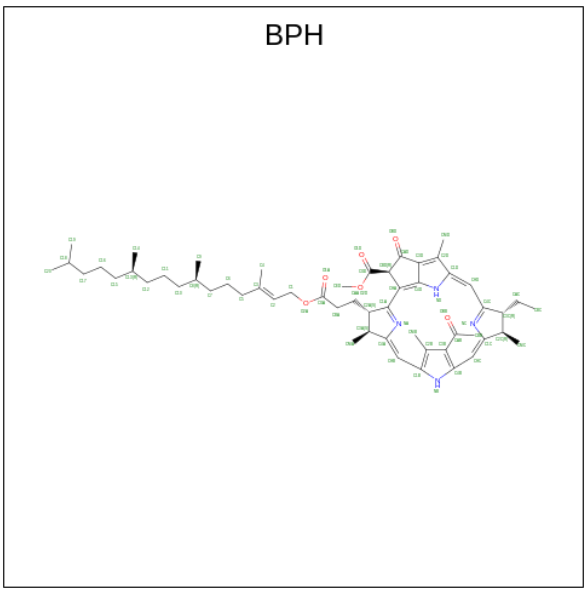
- Molecule 12 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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

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

beled as "Ligand of Interest" by depositor).



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

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

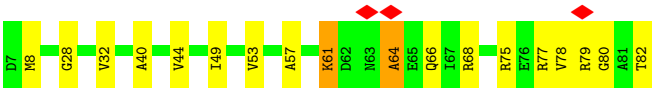
Mol	Chain	Residues	Atoms		AltConf
			Total	Fe	
14	M	1	1	1	0

3 Residue-property plots (i)

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

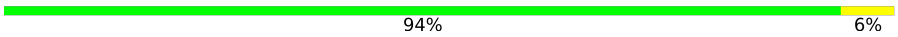
• Molecule 1: Protein LRC

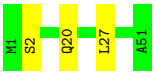
Chain A:



• Molecule 2: Antenna pigment protein alpha chain

Chain 1:



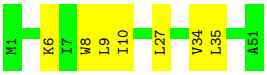


• Molecule 2: Antenna pigment protein alpha chain

Chain 5:

• Molecule 2: Antenna pigment protein alpha chain

Chain 3:

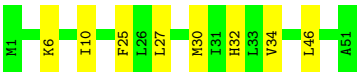


• Molecule 2: Antenna pigment protein alpha chain

Chain w:

• Molecule 2: Antenna pigment protein alpha chain

Chain u: 84% 16%

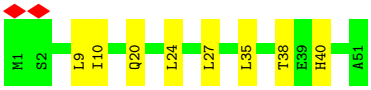


- Molecule 2: Antenna pigment protein alpha chain

Chain s: 82% 18%

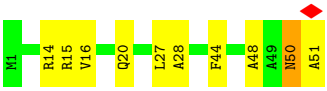
- Molecule 2: Antenna pigment protein alpha chain

Chain q: 84% 16%



- Molecule 2: Antenna pigment protein alpha chain

Chain o: 80% 18%

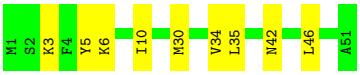


- Molecule 2: Antenna pigment protein alpha chain

Chain m: 94% 6%

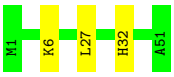
- Molecule 2: Antenna pigment protein alpha chain

Chain k: 82% 18%



- Molecule 2: Antenna pigment protein alpha chain

Chain g: 94% 6%



- Molecule 2: Antenna pigment protein alpha chain

Chain e: 84% 16%

- Molecule 2: Antenna pigment protein alpha chain

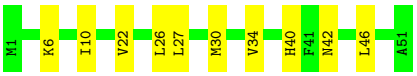
Chain c: 90% 10%

- Molecule 2: Antenna pigment protein alpha chain

Chain a: 92% 8%

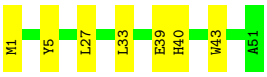
- Molecule 2: Antenna pigment protein alpha chain

Chain i: 80% 20%



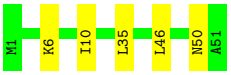
- Molecule 2: Antenna pigment protein alpha chain

Chain 7: 86% 14%



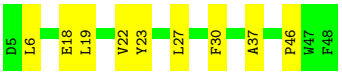
- Molecule 2: Antenna pigment protein alpha chain

Chain 9: 90% 10%



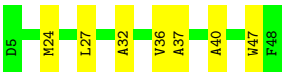
- Molecule 3: Antenna pigment protein beta chain

Chain 2: 80% 20%



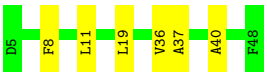
- Molecule 3: Antenna pigment protein beta chain

Chain 6: 84% 16%



- Molecule 3: Antenna pigment protein beta chain

Chain 4: 86% 14%

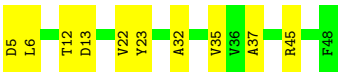


- Molecule 3: Antenna pigment protein beta chain

Chain x: 91% 9%

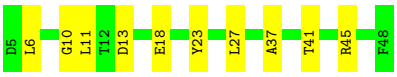
- Molecule 3: Antenna pigment protein beta chain

Chain v: 77% 23%



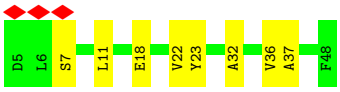
- Molecule 3: Antenna pigment protein beta chain

Chain t: 77% 23%



- Molecule 3: Antenna pigment protein beta chain

Chain r: 7% 82% 18%

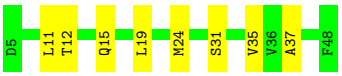


- Molecule 3: Antenna pigment protein beta chain

Chain p: 86% 14%

- Molecule 3: Antenna pigment protein beta chain

Chain n: 82% 18%



- Molecule 3: Antenna pigment protein beta chain

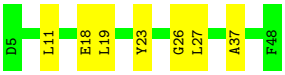
Chain l: 91% 9%

- Molecule 3: Antenna pigment protein beta chain

Chain h: 70% 27%

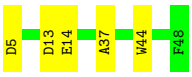
- Molecule 3: Antenna pigment protein beta chain

Chain f: 84% 16%



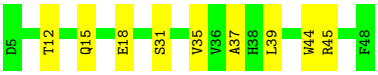
- Molecule 3: Antenna pigment protein beta chain

Chain d: 89% 11%



- Molecule 3: Antenna pigment protein beta chain

Chain b: 80% 20%



- Molecule 3: Antenna pigment protein beta chain

Chain j: 86% 14%

- Molecule 3: Antenna pigment protein beta chain

Chain 8: 82% 18%

D5 D13 Q17 E18 Y23 A34 V35 Y36 A37 W44 F48

• Molecule 3: Antenna pigment protein beta chain

Chain 0: 91% 9%

D5 E18 V22 A37 P46 W47 F48

• Molecule 4: Photosynthetic reaction center cytochrome c subunit

Chain C: 82% 18%

K4 W5 F6 D7 E8 W9 N10 S11 K12 N13 P14 T15 D16 I17 P20 G28 M40 T46 P53 T56 G57 M58 S59 V60 P61 E62 D71 I74 E89 Y98 E99 N100 V101 D102 P103 V104 L116 L117 A118 A119 M120 W123 T124 L129 L130 I142

N143 M144 I145 Q146 M147 T150 C169 C172 P179 D187 S194 G195 W196 L206 Y218 L222 E233 V236 E237 N256 L262 N265 C269 T282 A288 G307 L311 V319 Y320 C331 H332 Q337 P338 L352 V355

D370

• Molecule 5: Reaction center protein H chain

Chain H: 94% 6%

E2 M35 L41 P54 L57 E60 R69 L123 V153 W168 Y178 L181 V199 K207 V208 R209 S210 D234 L256

• Molecule 6: Reaction center protein L chain

Chain L: 91% 8%

A2 D21 D24 V32 V37 L44 L132 V133 V134 F135 R136 P137 M140 L166 H167 F168 H169 L176 L186 N212 S245 A246 V247 C248 I249 I250 I251 S252 G253 P254 P274

• Molecule 7: Reaction center protein M chain

Chain M: 91% 9%

P2 N6 E30 Y53 W56 G65 F69 V80 Q90 L94 P109 L110 D111 I117 S120 W131 T134 Y135 Q136 E139 M140 M143 G162 Y178 F181 P182 H183 V208 F217 T228 W271 V275 Y312 R326

4 Experimental information (i)

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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

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

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

All (7) bond length outliers are listed below:

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

All (55) bond angle outliers are listed below:

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

Continued on next page...

Continued from previous page...

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

There are no chirality outliers.

There are no planarity outliers.

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

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

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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

5.3.3 RNA (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 93 ligands modelled in this entry, 1 is monoatomic - leaving 92 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	U10	L	302	-	38,38,63	0.20	0	46,49,79	0.52	1 (2%)
10	SPN	a	102	-	40,42,42	3.86	19 (47%)	50,52,52	2.48	20 (40%)
13	BPH	M	405	-	59,70,70	1.19	4 (6%)	61,101,101	0.98	3 (4%)
10	SPN	j	102	-	40,42,42	3.91	19 (47%)	50,52,52	2.63	18 (36%)
10	SPN	1	102	-	40,42,42	3.87	19 (47%)	50,52,52	2.45	20 (40%)
10	SPN	7	103	-	40,42,42	3.93	19 (47%)	50,52,52	2.47	19 (38%)
9	BCL	d	101	3	69,74,74	0.83	1 (1%)	83,115,115	1.19	10 (12%)
9	BCL	e	101	2	69,74,74	0.81	2 (2%)	83,115,115	1.20	12 (14%)
9	BCL	L	304	6	69,74,74	0.96	2 (2%)	83,115,115	1.35	14 (16%)
9	BCL	i	101	2	69,74,74	0.91	1 (1%)	83,115,115	1.27	11 (13%)
9	BCL	M	404	7	69,74,74	0.92	2 (2%)	83,115,115	1.23	12 (14%)
9	BCL	k	101	2	69,74,74	0.80	1 (1%)	83,115,115	1.22	11 (13%)
10	SPN	r	102	-	40,42,42	3.91	19 (47%)	50,52,52	2.44	20 (40%)
11	MW9	H	301	-	52,52,52	0.60	1 (1%)	55,58,58	0.61	2 (3%)
12	HEM	C	402	4	50,50,50	0.84	1 (2%)	66,82,82	1.52	5 (7%)
10	SPN	s	102	-	40,42,42	3.90	19 (47%)	50,52,52	2.44	21 (42%)
11	MW9	H	303	-	52,52,52	0.58	1 (1%)	55,58,58	0.61	2 (3%)
11	MW9	M	408	-	52,52,52	0.59	1 (1%)	55,58,58	0.52	2 (3%)
10	SPN	3	102	-	40,42,42	3.86	19 (47%)	50,52,52	2.49	20 (40%)
9	BCL	h	101	3	69,74,74	0.86	3 (4%)	83,115,115	1.17	10 (12%)
10	SPN	f	102	-	40,42,42	3.93	19 (47%)	50,52,52	2.55	17 (34%)
9	BCL	b	101	3	69,74,74	1.75	19 (27%)	83,115,115	2.79	27 (32%)
10	SPN	w	102	-	40,42,42	3.90	19 (47%)	50,52,52	2.45	21 (42%)
9	BCL	7	101	2	69,74,74	0.83	1 (1%)	83,115,115	1.25	11 (13%)
9	BCL	n	101	3	69,74,74	0.82	1 (1%)	83,115,115	1.22	9 (10%)
12	HEM	C	401	4	50,50,50	0.86	2 (4%)	66,82,82	0.77	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
9	BCL	f	101	3	69,74,74	0.84	1 (1%)	83,115,115	1.21	11 (13%)
10	SPN	5	102	-	40,42,42	3.86	19 (47%)	50,52,52	2.50	20 (40%)
11	MW9	M	407	-	52,52,52	0.58	1 (1%)	55,58,58	0.83	3 (5%)
13	BPH	L	303	-	59,70,70	1.14	3 (5%)	61,101,101	1.19	7 (11%)
11	MW9	g	102	-	52,52,52	0.58	1 (1%)	55,58,58	0.64	2 (3%)
10	SPN	0	102	-	40,42,42	3.92	19 (47%)	50,52,52	2.45	18 (36%)
9	BCL	c	101	2	69,74,74	0.82	1 (1%)	83,115,115	1.21	11 (13%)
10	SPN	1	105	-	40,42,42	3.99	19 (47%)	50,52,52	2.43	20 (40%)
9	BCL	q	101	2	69,74,74	0.89	1 (1%)	83,115,115	1.24	9 (10%)
10	SPN	9	103	-	40,42,42	3.89	19 (47%)	50,52,52	2.46	22 (44%)
10	SPN	M	406	-	40,42,42	3.91	19 (47%)	50,52,52	2.74	18 (36%)
9	BCL	p	101	3	69,74,74	0.81	2 (2%)	83,115,115	1.23	10 (12%)
9	BCL	0	101	3	69,74,74	1.76	17 (24%)	83,115,115	2.84	26 (31%)
11	MW9	g	103	-	49,49,52	0.60	1 (2%)	52,55,58	0.66	2 (3%)
10	SPN	n	102	-	40,42,42	3.93	19 (47%)	50,52,52	2.46	20 (40%)
9	BCL	a	101	2	69,74,74	0.82	2 (2%)	83,115,115	1.20	12 (14%)
9	BCL	8	101	3	69,74,74	1.75	18 (26%)	83,115,115	2.88	27 (32%)
10	SPN	p	102	-	40,42,42	3.90	19 (47%)	50,52,52	2.59	19 (38%)
9	BCL	j	101	3	69,74,74	0.80	1 (1%)	83,115,115	1.19	11 (13%)
9	BCL	1	101	2	69,74,74	0.86	1 (1%)	83,115,115	1.30	10 (12%)
9	BCL	6	101	3	69,74,74	1.76	19 (27%)	83,115,115	2.82	26 (31%)
9	BCL	g	101	2	69,74,74	0.82	1 (1%)	83,115,115	1.19	12 (14%)
9	BCL	M	402	7	69,74,74	1.80	17 (24%)	83,115,115	2.78	31 (37%)
10	SPN	c	103	-	40,42,42	3.95	19 (47%)	50,52,52	2.50	20 (40%)
10	SPN	7	102	-	40,42,42	3.90	19 (47%)	50,52,52	2.45	21 (42%)
13	BPH	M	409	-	59,70,70	1.06	4 (6%)	61,101,101	1.05	5 (8%)
10	SPN	m	102	-	40,42,42	3.91	19 (47%)	50,52,52	2.44	21 (42%)
10	SPN	c	102	-	40,42,42	3.91	19 (47%)	50,52,52	2.45	22 (44%)
9	BCL	t	101	3	69,74,74	0.84	1 (1%)	83,115,115	1.19	9 (10%)
10	SPN	h	103	-	40,42,42	3.91	19 (47%)	50,52,52	2.56	18 (36%)
10	SPN	l	102	-	40,42,42	3.92	19 (47%)	50,52,52	2.55	18 (36%)
9	BCL	3	101	2	69,74,74	0.88	2 (2%)	83,115,115	1.23	11 (13%)
10	SPN	q	102	-	40,42,42	3.91	19 (47%)	50,52,52	2.55	20 (40%)
10	SPN	1	104	-	40,42,42	3.92	19 (47%)	50,52,52	2.63	18 (36%)
10	SPN	i	102	-	40,42,42	3.89	19 (47%)	50,52,52	2.45	21 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
10	SPN	k	102	-	40,42,42	3.90	19 (47%)	50,52,52	2.45	21 (42%)
10	SPN	a	103	-	40,42,42	3.91	19 (47%)	50,52,52	2.64	21 (42%)
9	BCL	l	101	3	69,74,74	0.80	1 (1%)	83,115,115	1.23	11 (13%)
9	BCL	m	101	2	69,74,74	0.80	2 (2%)	83,115,115	1.23	9 (10%)
8	U10	L	305	-	38,38,63	1.29	2 (5%)	46,49,79	2.18	12 (26%)
9	BCL	v	101	3	69,74,74	0.77	1 (1%)	83,115,115	1.27	11 (13%)
10	SPN	1	103	-	40,42,42	3.89	19 (47%)	50,52,52	2.79	21 (42%)
10	SPN	t	102	-	40,42,42	3.90	19 (47%)	50,52,52	2.46	21 (42%)
10	SPN	u	102	-	40,42,42	3.91	19 (47%)	50,52,52	2.45	21 (42%)
10	SPN	e	102	-	40,42,42	3.91	19 (47%)	50,52,52	2.45	22 (44%)
9	BCL	o	101	2	69,74,74	0.94	2 (2%)	83,115,115	1.30	12 (14%)
12	HEM	C	403	4	50,50,50	0.79	1 (2%)	66,82,82	0.83	2 (3%)
10	SPN	h	102	-	40,42,42	3.89	19 (47%)	50,52,52	2.45	22 (44%)
9	BCL	x	101	3	69,74,74	0.82	1 (1%)	83,115,115	1.22	10 (12%)
9	BCL	u	101	2	69,74,74	0.81	2 (2%)	83,115,115	1.19	11 (13%)
9	BCL	9	102	2	69,74,74	0.82	2 (2%)	83,115,115	1.19	10 (12%)
9	BCL	L	301	6	69,74,74	0.91	2 (2%)	83,115,115	1.24	12 (14%)
9	BCL	r	101	3	69,74,74	0.82	1 (1%)	83,115,115	1.26	13 (15%)
10	SPN	5	103	-	40,42,42	3.94	19 (47%)	50,52,52	2.48	18 (36%)
8	U10	A	101	-	43,43,63	1.27	2 (4%)	52,55,79	1.87	15 (28%)
9	BCL	2	101	3	69,74,74	1.75	17 (24%)	83,115,115	2.82	26 (31%)
11	MW9	H	302	-	52,52,52	0.59	1 (1%)	55,58,58	0.72	3 (5%)
9	BCL	s	101	2	69,74,74	0.91	3 (4%)	83,115,115	1.30	12 (14%)
8	U10	M	403	-	63,63,63	1.16	2 (3%)	76,79,79	1.57	15 (19%)
9	BCL	w	101	2	69,74,74	0.81	2 (2%)	83,115,115	1.23	10 (12%)
10	SPN	p	103	-	40,42,42	3.91	19 (47%)	50,52,52	2.50	21 (42%)
10	SPN	v	102	-	40,42,42	3.93	19 (47%)	50,52,52	2.58	18 (36%)
11	MW9	9	101	-	52,52,52	0.57	1 (1%)	55,58,58	0.53	2 (3%)
9	BCL	5	101	2	69,74,74	0.87	2 (2%)	83,115,115	1.24	10 (12%)
11	MW9	H	304	-	52,52,52	0.57	1 (1%)	55,58,58	0.55	2 (3%)
9	BCL	4	101	3	69,74,74	1.75	19 (27%)	83,115,115	2.79	28 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	U10	L	302	-	-	6/33/57/87	0/1/1/1
10	SPN	a	102	-	-	23/50/51/51	-
13	BPH	M	405	-	-	11/37/105/105	0/5/6/6
10	SPN	j	102	-	-	23/50/51/51	-
10	SPN	1	102	-	-	24/50/51/51	-
10	SPN	7	103	-	-	21/50/51/51	-
9	BCL	d	101	3	-	20/41/137/137	-
9	BCL	e	101	2	-	20/41/137/137	-
9	BCL	L	304	6	-	28/41/137/137	-
9	BCL	i	101	2	-	12/41/137/137	-
9	BCL	M	404	7	-	13/41/137/137	-
9	BCL	k	101	2	-	17/41/137/137	-
10	SPN	r	102	-	-	19/50/51/51	-
11	MW9	H	301	-	-	38/57/57/57	-
12	HEM	C	402	4	-	4/14/54/54	-
10	SPN	s	102	-	-	18/50/51/51	-
11	MW9	H	303	-	-	34/57/57/57	-
11	MW9	M	408	-	-	26/57/57/57	-
10	SPN	3	102	-	-	25/50/51/51	-
9	BCL	h	101	3	-	20/41/137/137	-
10	SPN	f	102	-	-	20/50/51/51	-
9	BCL	b	101	3	-	22/41/137/137	-
10	SPN	w	102	-	-	18/50/51/51	-
9	BCL	7	101	2	-	20/41/137/137	-
9	BCL	n	101	3	-	20/41/137/137	-
12	HEM	C	401	4	-	6/14/54/54	-
9	BCL	f	101	3	-	16/41/137/137	-
10	SPN	5	102	-	-	24/50/51/51	-
11	MW9	M	407	-	-	20/57/57/57	-
13	BPH	L	303	-	-	13/37/105/105	0/5/6/6
11	MW9	g	102	-	-	21/57/57/57	-
10	SPN	0	102	-	-	20/50/51/51	-
9	BCL	c	101	2	-	22/41/137/137	-
10	SPN	1	105	-	-	22/50/51/51	-
9	BCL	q	101	2	-	18/41/137/137	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	SPN	9	103	-	-	19/50/51/51	-
10	SPN	M	406	-	-	17/50/51/51	-
9	BCL	p	101	3	-	17/41/137/137	-
9	BCL	0	101	3	-	19/41/137/137	-
11	MW9	g	103	-	-	21/54/54/57	-
10	SPN	n	102	-	-	21/50/51/51	-
9	BCL	a	101	2	-	20/41/137/137	-
9	BCL	8	101	3	-	12/41/137/137	-
10	SPN	p	102	-	-	25/50/51/51	-
9	BCL	j	101	3	-	21/41/137/137	-
9	BCL	1	101	2	-	18/41/137/137	-
9	BCL	6	101	3	-	15/41/137/137	-
9	BCL	g	101	2	-	27/41/137/137	-
9	BCL	M	402	7	-	16/41/137/137	-
10	SPN	c	103	-	-	20/50/51/51	-
10	SPN	7	102	-	-	22/50/51/51	-
13	BPH	M	409	-	-	17/37/105/105	0/5/6/6
10	SPN	m	102	-	-	18/50/51/51	-
10	SPN	c	102	-	-	20/50/51/51	-
9	BCL	t	101	3	-	18/41/137/137	-
10	SPN	h	103	-	-	21/50/51/51	-
10	SPN	l	102	-	-	21/50/51/51	-
9	BCL	3	101	2	-	18/41/137/137	-
10	SPN	q	102	-	-	23/50/51/51	-
10	SPN	1	104	-	-	22/50/51/51	-
10	SPN	i	102	-	-	22/50/51/51	-
10	SPN	k	102	-	-	22/50/51/51	-
10	SPN	a	103	-	-	21/50/51/51	-
9	BCL	l	101	3	-	20/41/137/137	-
9	BCL	m	101	2	-	25/41/137/137	-
8	U10	L	305	-	-	11/33/57/87	0/1/1/1
9	BCL	v	101	3	-	15/41/137/137	-
10	SPN	1	103	-	-	18/50/51/51	-
10	SPN	t	102	-	-	18/50/51/51	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	SPN	u	102	-	-	21/50/51/51	-
10	SPN	e	102	-	-	19/50/51/51	-
9	BCL	o	101	2	-	15/41/137/137	-
12	HEM	C	403	4	-	4/14/54/54	-
10	SPN	h	102	-	-	20/50/51/51	-
9	BCL	x	101	3	-	19/41/137/137	-
9	BCL	u	101	2	-	16/41/137/137	-
9	BCL	9	102	2	-	18/41/137/137	-
9	BCL	L	301	6	-	11/41/137/137	-
9	BCL	r	101	3	-	24/41/137/137	-
10	SPN	5	103	-	-	21/50/51/51	-
8	U10	A	101	-	-	7/39/63/87	0/1/1/1
9	BCL	2	101	3	-	18/41/137/137	-
11	MW9	H	302	-	-	21/57/57/57	-
9	BCL	s	101	2	-	22/41/137/137	-
8	U10	M	403	-	-	19/63/87/87	0/1/1/1
9	BCL	w	101	2	-	19/41/137/137	-
10	SPN	p	103	-	-	22/50/51/51	-
10	SPN	v	102	-	-	18/50/51/51	-
11	MW9	9	101	-	-	34/57/57/57	-
9	BCL	5	101	2	-	21/41/137/137	-
11	MW9	H	304	-	-	36/57/57/57	-
9	BCL	4	101	3	-	19/41/137/137	-

All (869) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	a	103	SPN	C3-C4	-12.57	1.32	1.50
10	5	103	SPN	C3-C4	-12.56	1.32	1.50
10	c	103	SPN	C3-C4	-12.54	1.32	1.50
10	7	103	SPN	C3-C4	-12.50	1.32	1.50
10	1	104	SPN	C3-C4	-12.42	1.32	1.50
10	q	102	SPN	C3-C4	-12.40	1.32	1.50
10	1	105	SPN	C3-C4	-12.37	1.32	1.50
10	t	102	SPN	C3-C4	-12.30	1.32	1.50
10	1	103	SPN	C3-C4	-12.30	1.32	1.50
10	f	102	SPN	C3-C4	-12.29	1.32	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	0	102	SPN	C3-C4	-12.27	1.32	1.50
10	v	102	SPN	C3-C4	-12.27	1.32	1.50
10	l	102	SPN	C3-C4	-12.23	1.33	1.50
10	n	102	SPN	C3-C4	-12.21	1.33	1.50
10	h	103	SPN	C3-C4	-12.21	1.33	1.50
10	p	102	SPN	C3-C4	-12.18	1.33	1.50
10	M	406	SPN	C3-C4	-12.15	1.33	1.50
10	p	103	SPN	C3-C4	-12.14	1.33	1.50
10	j	102	SPN	C3-C4	-12.12	1.33	1.50
10	k	102	SPN	C3-C4	-12.04	1.33	1.50
10	c	102	SPN	C3-C4	-12.04	1.33	1.50
10	e	102	SPN	C3-C4	-12.03	1.33	1.50
10	r	102	SPN	C3-C4	-12.03	1.33	1.50
10	u	102	SPN	C3-C4	-12.02	1.33	1.50
10	7	102	SPN	C3-C4	-12.01	1.33	1.50
10	m	102	SPN	C3-C4	-12.00	1.33	1.50
10	s	102	SPN	C3-C4	-12.00	1.33	1.50
10	i	102	SPN	C3-C4	-11.98	1.33	1.50
10	w	102	SPN	C3-C4	-11.97	1.33	1.50
10	h	102	SPN	C3-C4	-11.93	1.33	1.50
10	9	103	SPN	C3-C4	-11.89	1.33	1.50
10	1	102	SPN	C3-C4	-11.83	1.33	1.50
10	5	102	SPN	C3-C4	-11.83	1.33	1.50
10	3	102	SPN	C3-C4	-11.83	1.33	1.50
10	a	102	SPN	C3-C4	-11.81	1.33	1.50
8	M	403	U10	C6-C1	7.98	1.49	1.35
10	p	102	SPN	C17-C18	-7.58	1.35	1.51
10	1	105	SPN	C17-C18	-7.53	1.35	1.51
10	1	105	SPN	C10-C9	-7.50	1.35	1.51
10	M	406	SPN	C14-C13	-7.50	1.35	1.51
10	M	406	SPN	C10-C9	-7.48	1.35	1.51
10	0	102	SPN	C17-C18	-7.46	1.35	1.51
10	1	105	SPN	C14-C13	-7.45	1.35	1.51
10	v	102	SPN	C10-C9	-7.45	1.35	1.51
10	f	102	SPN	C6-C5	-7.44	1.35	1.51
10	c	102	SPN	C6-C5	-7.43	1.35	1.51
10	c	103	SPN	C17-C18	-7.43	1.35	1.51
10	1	105	SPN	C6-C5	-7.43	1.35	1.51
10	M	406	SPN	C6-C5	-7.43	1.35	1.51
10	h	103	SPN	C6-C5	-7.42	1.35	1.51
10	m	102	SPN	C10-C9	-7.42	1.35	1.51
10	w	102	SPN	C14-C13	-7.42	1.35	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	j	102	SPN	C17-C18	-7.42	1.35	1.51
10	p	103	SPN	C6-C5	-7.42	1.35	1.51
10	r	102	SPN	C17-C18	-7.42	1.35	1.51
10	v	102	SPN	C6-C5	-7.41	1.35	1.51
10	1	103	SPN	C6-C5	-7.41	1.35	1.51
10	n	102	SPN	C6-C5	-7.41	1.35	1.51
10	q	102	SPN	C6-C5	-7.41	1.35	1.51
10	s	102	SPN	C10-C9	-7.41	1.35	1.51
10	e	102	SPN	C14-C13	-7.41	1.35	1.51
10	u	102	SPN	C10-C9	-7.41	1.35	1.51
10	n	102	SPN	C17-C18	-7.41	1.35	1.51
10	m	102	SPN	C14-C13	-7.41	1.35	1.51
10	w	102	SPN	C10-C9	-7.40	1.35	1.51
10	m	102	SPN	C17-C18	-7.40	1.35	1.51
10	h	103	SPN	C10-C9	-7.40	1.35	1.51
10	l	102	SPN	C10-C9	-7.40	1.35	1.51
10	v	102	SPN	C14-C13	-7.40	1.35	1.51
10	e	102	SPN	C17-C18	-7.40	1.35	1.51
10	m	102	SPN	C6-C5	-7.40	1.35	1.51
10	7	103	SPN	C17-C18	-7.39	1.35	1.51
10	l	102	SPN	C6-C5	-7.39	1.35	1.51
10	f	102	SPN	C10-C9	-7.39	1.35	1.51
10	c	102	SPN	C10-C9	-7.39	1.35	1.51
10	k	102	SPN	C10-C9	-7.39	1.35	1.51
10	a	102	SPN	C14-C13	-7.39	1.35	1.51
10	c	102	SPN	C14-C13	-7.39	1.35	1.51
10	e	102	SPN	C10-C9	-7.38	1.35	1.51
10	u	102	SPN	C17-C18	-7.38	1.35	1.51
10	9	103	SPN	C14-C13	-7.38	1.35	1.51
10	h	102	SPN	C10-C9	-7.38	1.35	1.51
10	c	103	SPN	C6-C5	-7.38	1.35	1.51
10	9	103	SPN	C6-C5	-7.38	1.35	1.51
10	r	102	SPN	C10-C9	-7.38	1.35	1.51
10	h	102	SPN	C14-C13	-7.38	1.35	1.51
10	h	102	SPN	C6-C5	-7.38	1.35	1.51
10	s	102	SPN	C6-C5	-7.38	1.36	1.51
10	u	102	SPN	C6-C5	-7.38	1.36	1.51
10	p	103	SPN	C10-C9	-7.38	1.36	1.51
10	n	102	SPN	C14-C13	-7.38	1.36	1.51
10	c	103	SPN	C10-C9	-7.38	1.36	1.51
10	p	102	SPN	C10-C9	-7.38	1.36	1.51
10	0	102	SPN	C10-C9	-7.38	1.36	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	u	102	SPN	C14-C13	-7.37	1.36	1.51
10	7	102	SPN	C10-C9	-7.37	1.36	1.51
10	w	102	SPN	C17-C18	-7.37	1.36	1.51
10	5	103	SPN	C17-C18	-7.37	1.36	1.51
10	t	102	SPN	C17-C18	-7.37	1.36	1.51
10	9	103	SPN	C17-C18	-7.37	1.36	1.51
10	r	102	SPN	C14-C13	-7.37	1.36	1.51
10	k	102	SPN	C14-C13	-7.37	1.36	1.51
10	i	102	SPN	C14-C13	-7.37	1.36	1.51
10	c	102	SPN	C17-C18	-7.37	1.36	1.51
10	i	102	SPN	C10-C9	-7.37	1.36	1.51
10	j	102	SPN	C6-C5	-7.37	1.36	1.51
10	w	102	SPN	C6-C5	-7.37	1.36	1.51
10	p	103	SPN	C14-C13	-7.37	1.36	1.51
10	s	102	SPN	C17-C18	-7.37	1.36	1.51
10	p	102	SPN	C14-C13	-7.37	1.36	1.51
10	9	103	SPN	C10-C9	-7.37	1.36	1.51
10	1	104	SPN	C6-C5	-7.37	1.36	1.51
10	n	102	SPN	C10-C9	-7.37	1.36	1.51
10	7	102	SPN	C6-C5	-7.37	1.36	1.51
10	5	103	SPN	C10-C9	-7.37	1.36	1.51
10	k	102	SPN	C17-C18	-7.37	1.36	1.51
10	f	102	SPN	C17-C18	-7.37	1.36	1.51
10	r	102	SPN	C6-C5	-7.36	1.36	1.51
10	M	406	SPN	C17-C18	-7.36	1.36	1.51
10	1	103	SPN	C10-C9	-7.36	1.36	1.51
10	t	102	SPN	C6-C5	-7.36	1.36	1.51
10	j	102	SPN	C10-C9	-7.36	1.36	1.51
10	e	102	SPN	C6-C5	-7.36	1.36	1.51
10	p	102	SPN	C6-C5	-7.35	1.36	1.51
10	1	102	SPN	C14-C13	-7.35	1.36	1.51
10	s	102	SPN	C14-C13	-7.35	1.36	1.51
10	7	102	SPN	C17-C18	-7.35	1.36	1.51
10	7	103	SPN	C10-C9	-7.35	1.36	1.51
10	1	104	SPN	C10-C9	-7.35	1.36	1.51
10	k	102	SPN	C6-C5	-7.35	1.36	1.51
10	7	102	SPN	C14-C13	-7.35	1.36	1.51
10	7	103	SPN	C14-C13	-7.35	1.36	1.51
10	3	102	SPN	C17-C18	-7.35	1.36	1.51
10	l	102	SPN	C14-C13	-7.35	1.36	1.51
10	3	102	SPN	C14-C13	-7.34	1.36	1.51
10	1	102	SPN	C17-C18	-7.34	1.36	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	1	104	SPN	C17-C18	-7.34	1.36	1.51
10	f	102	SPN	C14-C13	-7.34	1.36	1.51
10	0	102	SPN	C14-C13	-7.34	1.36	1.51
10	5	103	SPN	C6-C5	-7.34	1.36	1.51
10	c	103	SPN	C14-C13	-7.34	1.36	1.51
10	h	103	SPN	C17-C18	-7.34	1.36	1.51
10	5	102	SPN	C14-C13	-7.34	1.36	1.51
10	a	102	SPN	C17-C18	-7.33	1.36	1.51
10	1	102	SPN	C10-C9	-7.33	1.36	1.51
10	i	102	SPN	C17-C18	-7.33	1.36	1.51
10	5	103	SPN	C14-C13	-7.33	1.36	1.51
10	l	102	SPN	C17-C18	-7.33	1.36	1.51
10	a	103	SPN	C6-C5	-7.33	1.36	1.51
10	t	102	SPN	C14-C13	-7.33	1.36	1.51
10	7	103	SPN	C6-C5	-7.33	1.36	1.51
10	q	102	SPN	C10-C9	-7.32	1.36	1.51
10	p	103	SPN	C17-C18	-7.32	1.36	1.51
10	h	102	SPN	C17-C18	-7.32	1.36	1.51
10	h	103	SPN	C14-C13	-7.32	1.36	1.51
10	5	102	SPN	C6-C5	-7.32	1.36	1.51
10	a	103	SPN	C17-C18	-7.32	1.36	1.51
10	3	102	SPN	C10-C9	-7.32	1.36	1.51
10	1	102	SPN	C6-C5	-7.31	1.36	1.51
10	i	102	SPN	C6-C5	-7.31	1.36	1.51
10	5	102	SPN	C10-C9	-7.30	1.36	1.51
10	0	102	SPN	C6-C5	-7.30	1.36	1.51
10	q	102	SPN	C17-C18	-7.30	1.36	1.51
10	a	102	SPN	C10-C9	-7.30	1.36	1.51
10	1	104	SPN	C14-C13	-7.29	1.36	1.51
10	3	102	SPN	C6-C5	-7.29	1.36	1.51
10	q	102	SPN	C14-C13	-7.28	1.36	1.51
10	j	102	SPN	C14-C13	-7.28	1.36	1.51
10	1	103	SPN	C14-C13	-7.28	1.36	1.51
10	a	103	SPN	C10-C9	-7.27	1.36	1.51
10	a	102	SPN	C6-C5	-7.27	1.36	1.51
10	t	102	SPN	C10-C9	-7.26	1.36	1.51
10	v	102	SPN	C17-C18	-7.26	1.36	1.51
10	5	102	SPN	C17-C18	-7.26	1.36	1.51
10	a	103	SPN	C14-C13	-7.25	1.36	1.51
10	1	103	SPN	C17-C18	-7.15	1.36	1.51
8	A	101	U10	C6-C1	7.15	1.48	1.35
8	L	305	U10	C6-C1	6.59	1.47	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	404	BCL	C4D-ND	-6.02	1.29	1.37
9	o	101	BCL	C4D-ND	-6.02	1.29	1.37
10	1	103	SPN	C19-C18	5.98	1.47	1.33
9	s	101	BCL	C4D-ND	-5.97	1.29	1.37
13	M	405	BPH	C1D-C2D	5.95	1.46	1.39
10	p	102	SPN	C8-C9	5.93	1.47	1.33
9	L	304	BCL	C4D-ND	-5.91	1.29	1.37
13	L	303	BPH	C1D-C2D	5.79	1.46	1.39
10	j	102	SPN	C19-C18	5.78	1.46	1.33
10	l	102	SPN	C19-C18	5.75	1.46	1.33
10	1	104	SPN	C19-C18	5.74	1.46	1.33
10	a	103	SPN	C19-C18	5.74	1.46	1.33
10	v	102	SPN	C19-C18	5.70	1.46	1.33
10	M	406	SPN	C19-C18	5.63	1.46	1.33
9	i	101	BCL	C4D-ND	-5.61	1.30	1.37
10	3	102	SPN	C12-C13	5.49	1.46	1.33
10	f	102	SPN	C19-C18	5.48	1.46	1.33
10	p	102	SPN	C12-C13	5.48	1.46	1.33
10	p	103	SPN	C19-C18	5.48	1.46	1.33
13	M	409	BPH	C1D-C2D	5.47	1.45	1.39
9	1	101	BCL	C4D-ND	-5.47	1.30	1.37
10	a	102	SPN	C12-C13	5.47	1.46	1.33
10	t	102	SPN	C12-C13	5.46	1.46	1.33
10	h	103	SPN	C19-C18	5.46	1.46	1.33
10	5	102	SPN	C12-C13	5.46	1.46	1.33
10	3	102	SPN	C8-C9	5.45	1.46	1.33
10	a	103	SPN	C12-C13	5.45	1.46	1.33
10	a	102	SPN	C4-C5	5.45	1.46	1.33
9	5	101	BCL	C4D-ND	-5.44	1.30	1.37
10	1	102	SPN	C12-C13	5.44	1.46	1.33
10	5	102	SPN	C8-C9	5.43	1.46	1.33
10	q	102	SPN	C12-C13	5.43	1.46	1.33
10	5	102	SPN	C4-C5	5.42	1.46	1.33
10	c	103	SPN	C8-C9	5.42	1.46	1.33
10	u	102	SPN	C8-C9	5.41	1.46	1.33
10	h	102	SPN	C8-C9	5.41	1.46	1.33
10	t	102	SPN	C8-C9	5.41	1.46	1.33
10	e	102	SPN	C12-C13	5.40	1.45	1.33
10	0	102	SPN	C8-C9	5.40	1.45	1.33
10	n	102	SPN	C8-C9	5.40	1.45	1.33
10	h	102	SPN	C12-C13	5.40	1.45	1.33
10	a	102	SPN	C8-C9	5.40	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	w	102	SPN	C12-C13	5.40	1.45	1.33
10	h	102	SPN	C4-C5	5.40	1.45	1.33
10	5	103	SPN	C8-C9	5.40	1.45	1.33
10	u	102	SPN	C4-C5	5.40	1.45	1.33
10	i	102	SPN	C8-C9	5.40	1.45	1.33
10	j	102	SPN	C12-C13	5.39	1.45	1.33
10	9	103	SPN	C8-C9	5.39	1.45	1.33
10	k	102	SPN	C4-C5	5.39	1.45	1.33
10	c	102	SPN	C12-C13	5.39	1.45	1.33
10	1	102	SPN	C8-C9	5.39	1.45	1.33
10	1	102	SPN	C4-C5	5.39	1.45	1.33
10	7	102	SPN	C8-C9	5.38	1.45	1.33
10	0	102	SPN	C12-C13	5.38	1.45	1.33
10	e	102	SPN	C8-C9	5.38	1.45	1.33
10	M	406	SPN	C4-C5	5.38	1.45	1.33
10	w	102	SPN	C8-C9	5.38	1.45	1.33
10	n	102	SPN	C4-C5	5.38	1.45	1.33
10	i	102	SPN	C12-C13	5.37	1.45	1.33
10	k	102	SPN	C8-C9	5.37	1.45	1.33
10	t	102	SPN	C19-C18	5.37	1.45	1.33
10	1	104	SPN	C12-C13	5.37	1.45	1.33
10	k	102	SPN	C12-C13	5.37	1.45	1.33
10	p	103	SPN	C4-C5	5.37	1.45	1.33
10	h	103	SPN	C8-C9	5.37	1.45	1.33
10	f	102	SPN	C4-C5	5.37	1.45	1.33
10	j	102	SPN	C8-C9	5.37	1.45	1.33
10	7	103	SPN	C8-C9	5.37	1.45	1.33
10	s	102	SPN	C8-C9	5.37	1.45	1.33
10	r	102	SPN	C8-C9	5.37	1.45	1.33
10	f	102	SPN	C8-C9	5.36	1.45	1.33
10	w	102	SPN	C4-C5	5.36	1.45	1.33
10	m	102	SPN	C12-C13	5.36	1.45	1.33
10	j	102	SPN	C4-C5	5.36	1.45	1.33
10	c	102	SPN	C8-C9	5.36	1.45	1.33
10	s	102	SPN	C12-C13	5.36	1.45	1.33
10	r	102	SPN	C12-C13	5.36	1.45	1.33
10	1	104	SPN	C8-C9	5.36	1.45	1.33
10	e	102	SPN	C4-C5	5.36	1.45	1.33
10	1	103	SPN	C8-C9	5.36	1.45	1.33
10	p	103	SPN	C12-C13	5.36	1.45	1.33
10	m	102	SPN	C4-C5	5.36	1.45	1.33
10	a	103	SPN	C8-C9	5.36	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	s	102	SPN	C4-C5	5.36	1.45	1.33
10	h	103	SPN	C4-C5	5.36	1.45	1.33
10	u	102	SPN	C12-C13	5.36	1.45	1.33
10	l	102	SPN	C4-C5	5.35	1.45	1.33
10	M	406	SPN	C8-C9	5.35	1.45	1.33
10	7	102	SPN	C12-C13	5.35	1.45	1.33
10	9	103	SPN	C4-C5	5.35	1.45	1.33
10	3	102	SPN	C4-C5	5.35	1.45	1.33
10	3	102	SPN	C19-C18	5.35	1.45	1.33
10	m	102	SPN	C8-C9	5.35	1.45	1.33
9	L	301	BCL	C4D-ND	-5.35	1.30	1.37
10	m	102	SPN	C19-C18	5.35	1.45	1.33
10	r	102	SPN	C4-C5	5.35	1.45	1.33
10	c	102	SPN	C19-C18	5.34	1.45	1.33
10	i	102	SPN	C19-C18	5.34	1.45	1.33
10	v	102	SPN	C4-C5	5.34	1.45	1.33
10	i	102	SPN	C4-C5	5.34	1.45	1.33
10	q	102	SPN	C8-C9	5.34	1.45	1.33
10	9	103	SPN	C12-C13	5.34	1.45	1.33
9	q	101	BCL	C4D-ND	-5.33	1.30	1.37
10	p	103	SPN	C8-C9	5.33	1.45	1.33
10	e	102	SPN	C19-C18	5.33	1.45	1.33
10	9	103	SPN	C19-C18	5.33	1.45	1.33
10	s	102	SPN	C19-C18	5.33	1.45	1.33
10	l	102	SPN	C12-C13	5.33	1.45	1.33
10	c	102	SPN	C4-C5	5.33	1.45	1.33
10	a	102	SPN	C19-C18	5.33	1.45	1.33
10	7	102	SPN	C4-C5	5.33	1.45	1.33
9	3	101	BCL	C4D-ND	-5.33	1.30	1.37
10	n	102	SPN	C12-C13	5.33	1.45	1.33
10	1	103	SPN	C4-C5	5.33	1.45	1.33
10	h	102	SPN	C19-C18	5.33	1.45	1.33
10	c	103	SPN	C12-C13	5.33	1.45	1.33
10	7	102	SPN	C19-C18	5.33	1.45	1.33
10	l	102	SPN	C8-C9	5.33	1.45	1.33
10	M	406	SPN	C12-C13	5.32	1.45	1.33
10	5	103	SPN	C12-C13	5.32	1.45	1.33
10	w	102	SPN	C19-C18	5.32	1.45	1.33
10	v	102	SPN	C12-C13	5.32	1.45	1.33
10	n	102	SPN	C19-C18	5.32	1.45	1.33
10	u	102	SPN	C19-C18	5.31	1.45	1.33
10	7	103	SPN	C12-C13	5.31	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	r	102	SPN	C19-C18	5.31	1.45	1.33
10	h	103	SPN	C12-C13	5.31	1.45	1.33
10	f	102	SPN	C12-C13	5.31	1.45	1.33
10	p	102	SPN	C19-C18	5.31	1.45	1.33
10	k	102	SPN	C19-C18	5.30	1.45	1.33
10	v	102	SPN	C8-C9	5.30	1.45	1.33
10	q	102	SPN	C19-C18	5.30	1.45	1.33
10	p	102	SPN	C4-C5	5.30	1.45	1.33
10	1	105	SPN	C4-C5	5.29	1.45	1.33
10	7	103	SPN	C19-C18	5.29	1.45	1.33
10	0	102	SPN	C19-C18	5.29	1.45	1.33
10	0	102	SPN	C4-C5	5.28	1.45	1.33
10	5	102	SPN	C19-C18	5.28	1.45	1.33
10	5	103	SPN	C4-C5	5.28	1.45	1.33
10	1	105	SPN	C8-C9	5.27	1.45	1.33
10	t	102	SPN	C4-C5	5.27	1.45	1.33
10	a	103	SPN	C4-C5	5.27	1.45	1.33
10	c	103	SPN	C19-C18	5.26	1.45	1.33
10	5	103	SPN	C19-C18	5.26	1.45	1.33
10	1	104	SPN	C4-C5	5.25	1.45	1.33
10	1	102	SPN	C19-C18	5.24	1.45	1.33
10	1	105	SPN	C12-C13	5.24	1.45	1.33
9	t	101	BCL	C4D-ND	-5.22	1.30	1.37
10	1	105	SPN	C20-C19	-5.22	1.33	1.50
10	q	102	SPN	C4-C5	5.22	1.45	1.33
10	1	103	SPN	C12-C13	5.22	1.45	1.33
10	c	103	SPN	C4-C5	5.20	1.45	1.33
9	f	101	BCL	C4D-ND	-5.20	1.30	1.37
10	7	103	SPN	C4-C5	5.20	1.45	1.33
9	h	101	BCL	C4D-ND	-5.18	1.30	1.37
10	1	105	SPN	C19-C18	5.15	1.45	1.33
9	x	101	BCL	C4D-ND	-5.15	1.30	1.37
9	d	101	BCL	C4D-ND	-5.14	1.30	1.37
10	M	406	SPN	C11-C12	-5.11	1.33	1.50
9	M	402	BCL	C3B-C4B	5.10	1.50	1.41
9	n	101	BCL	C4D-ND	-5.09	1.30	1.37
9	p	101	BCL	C4D-ND	-5.08	1.30	1.37
10	1	105	SPN	C7-C8	-5.04	1.34	1.50
10	5	103	SPN	C20-C19	-5.03	1.34	1.50
10	c	103	SPN	C20-C19	-5.02	1.34	1.50
9	c	101	BCL	C4D-ND	-5.02	1.30	1.37
10	1	105	SPN	C11-C12	-5.01	1.34	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	0	102	SPN	C20-C19	-5.01	1.34	1.50
10	M	406	SPN	C7-C8	-5.00	1.34	1.50
10	r	102	SPN	C7-C8	-4.99	1.34	1.50
10	q	102	SPN	C20-C19	-4.99	1.34	1.50
9	7	101	BCL	C4D-ND	-4.98	1.30	1.37
10	c	103	SPN	C7-C8	-4.97	1.34	1.50
10	p	103	SPN	C7-C8	-4.96	1.34	1.50
10	i	102	SPN	C20-C19	-4.96	1.34	1.50
10	7	103	SPN	C20-C19	-4.96	1.34	1.50
10	c	103	SPN	C11-C12	-4.96	1.34	1.50
10	v	102	SPN	C11-C12	-4.95	1.34	1.50
10	7	103	SPN	C7-C8	-4.95	1.34	1.50
10	v	102	SPN	C7-C8	-4.95	1.34	1.50
10	7	102	SPN	C11-C12	-4.95	1.34	1.50
10	m	102	SPN	C7-C8	-4.95	1.34	1.50
10	n	102	SPN	C7-C8	-4.95	1.34	1.50
9	w	101	BCL	C4D-ND	-4.95	1.30	1.37
10	j	102	SPN	C7-C8	-4.94	1.34	1.50
10	f	102	SPN	C7-C8	-4.94	1.34	1.50
9	l	101	BCL	C4D-ND	-4.94	1.30	1.37
10	n	102	SPN	C20-C19	-4.94	1.34	1.50
10	u	102	SPN	C7-C8	-4.93	1.34	1.50
10	t	102	SPN	C20-C19	-4.93	1.34	1.50
10	7	102	SPN	C7-C8	-4.93	1.34	1.50
10	9	103	SPN	C11-C12	-4.93	1.34	1.50
10	u	102	SPN	C20-C19	-4.93	1.34	1.50
10	m	102	SPN	C11-C12	-4.93	1.34	1.50
10	e	102	SPN	C20-C19	-4.92	1.34	1.50
10	c	102	SPN	C7-C8	-4.92	1.34	1.50
9	r	101	BCL	C4D-ND	-4.92	1.30	1.37
10	r	102	SPN	C20-C19	-4.92	1.34	1.50
10	k	102	SPN	C20-C19	-4.92	1.34	1.50
10	s	102	SPN	C7-C8	-4.92	1.34	1.50
10	n	102	SPN	C11-C12	-4.92	1.34	1.50
10	r	102	SPN	C11-C12	-4.92	1.34	1.50
10	h	103	SPN	C7-C8	-4.92	1.34	1.50
10	1	102	SPN	C11-C12	-4.92	1.34	1.50
10	9	103	SPN	C20-C19	-4.92	1.34	1.50
10	1	102	SPN	C20-C19	-4.91	1.34	1.50
10	l	102	SPN	C7-C8	-4.91	1.34	1.50
10	h	102	SPN	C20-C19	-4.91	1.34	1.50
10	k	102	SPN	C7-C8	-4.91	1.34	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	s	102	SPN	C20-C19	-4.90	1.34	1.50
10	j	102	SPN	C11-C12	-4.90	1.34	1.50
10	u	102	SPN	C11-C12	-4.90	1.34	1.50
10	w	102	SPN	C7-C8	-4.90	1.34	1.50
10	7	102	SPN	C20-C19	-4.89	1.34	1.50
10	k	102	SPN	C11-C12	-4.89	1.34	1.50
10	i	102	SPN	C11-C12	-4.89	1.34	1.50
9	M	402	BCL	C3D-C4D	-4.89	1.33	1.44
10	c	102	SPN	C20-C19	-4.89	1.34	1.50
10	7	103	SPN	C11-C12	-4.89	1.34	1.50
10	c	102	SPN	C11-C12	-4.89	1.34	1.50
10	p	103	SPN	C11-C12	-4.89	1.34	1.50
10	w	102	SPN	C11-C12	-4.89	1.34	1.50
10	1	104	SPN	C7-C8	-4.88	1.34	1.50
10	e	102	SPN	C11-C12	-4.88	1.34	1.50
10	9	103	SPN	C7-C8	-4.88	1.34	1.50
10	h	102	SPN	C7-C8	-4.88	1.34	1.50
10	m	102	SPN	C20-C19	-4.88	1.34	1.50
10	s	102	SPN	C11-C12	-4.88	1.34	1.50
10	1	103	SPN	C7-C8	-4.87	1.34	1.50
10	h	102	SPN	C11-C12	-4.87	1.34	1.50
10	e	102	SPN	C7-C8	-4.87	1.34	1.50
10	f	102	SPN	C11-C12	-4.87	1.34	1.50
9	g	101	BCL	C4D-ND	-4.86	1.31	1.37
10	0	102	SPN	C11-C12	-4.86	1.34	1.50
10	l	102	SPN	C11-C12	-4.86	1.34	1.50
10	p	102	SPN	C11-C12	-4.86	1.34	1.50
10	i	102	SPN	C7-C8	-4.85	1.34	1.50
10	w	102	SPN	C20-C19	-4.85	1.34	1.50
10	a	103	SPN	C7-C8	-4.85	1.34	1.50
10	5	103	SPN	C11-C12	-4.84	1.34	1.50
10	t	102	SPN	C7-C8	-4.83	1.34	1.50
10	a	102	SPN	C7-C8	-4.83	1.34	1.50
10	3	102	SPN	C11-C12	-4.82	1.34	1.50
10	h	103	SPN	C11-C12	-4.82	1.34	1.50
10	q	102	SPN	C7-C8	-4.82	1.34	1.50
9	m	101	BCL	C4D-ND	-4.82	1.31	1.37
10	5	102	SPN	C7-C8	-4.81	1.34	1.50
10	5	102	SPN	C20-C19	-4.81	1.34	1.50
10	3	102	SPN	C7-C8	-4.81	1.34	1.50
10	5	103	SPN	C7-C8	-4.81	1.34	1.50
9	9	102	BCL	C4D-ND	-4.80	1.31	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	1	102	SPN	C7-C8	-4.80	1.34	1.50
10	a	102	SPN	C11-C12	-4.80	1.34	1.50
9	u	101	BCL	C4D-ND	-4.80	1.31	1.37
10	a	102	SPN	C20-C19	-4.79	1.34	1.50
10	0	102	SPN	C7-C8	-4.79	1.34	1.50
10	5	102	SPN	C11-C12	-4.79	1.34	1.50
10	3	102	SPN	C20-C19	-4.79	1.34	1.50
10	q	102	SPN	C11-C12	-4.79	1.34	1.50
9	e	101	BCL	C4D-ND	-4.78	1.31	1.37
10	a	103	SPN	C11-C12	-4.77	1.34	1.50
9	6	101	BCL	C3B-C4B	4.76	1.50	1.41
9	v	101	BCL	C4D-ND	-4.76	1.31	1.37
9	0	101	BCL	C3B-C4B	4.75	1.50	1.41
9	a	101	BCL	C4D-ND	-4.74	1.31	1.37
10	1	104	SPN	C11-C12	-4.73	1.35	1.50
10	p	102	SPN	C20-C19	-4.72	1.35	1.50
10	p	103	SPN	C20-C19	-4.70	1.35	1.50
9	k	101	BCL	C4D-ND	-4.70	1.31	1.37
9	8	101	BCL	C3B-C4B	4.70	1.49	1.41
9	j	101	BCL	C4D-ND	-4.69	1.31	1.37
9	2	101	BCL	C3B-C4B	4.67	1.49	1.41
10	t	102	SPN	C11-C12	-4.66	1.35	1.50
10	h	103	SPN	C20-C19	-4.65	1.35	1.50
10	f	102	SPN	C20-C19	-4.65	1.35	1.50
10	1	103	SPN	C11-C12	-4.62	1.35	1.50
9	b	101	BCL	C3B-C4B	4.61	1.49	1.41
9	4	101	BCL	C3B-C4B	4.55	1.49	1.41
10	v	102	SPN	C20-C19	-4.49	1.35	1.50
9	4	101	BCL	C3D-C4D	-4.45	1.34	1.44
9	0	101	BCL	C3D-C4D	-4.41	1.34	1.44
9	2	101	BCL	C3D-C4D	-4.36	1.34	1.44
10	l	102	SPN	C20-C19	-4.36	1.36	1.50
9	b	101	BCL	C3D-C4D	-4.35	1.34	1.44
9	6	101	BCL	C3D-C4D	-4.33	1.34	1.44
10	1	104	SPN	C20-C19	-4.32	1.36	1.50
9	8	101	BCL	C3D-C4D	-4.31	1.34	1.44
9	2	101	BCL	O2D-CGD	4.26	1.43	1.33
10	j	102	SPN	C20-C19	-4.25	1.36	1.50
10	M	406	SPN	C20-C19	-4.22	1.36	1.50
9	M	402	BCL	O2D-CGD	4.20	1.43	1.33
10	a	103	SPN	C20-C19	-4.20	1.36	1.50
9	6	101	BCL	O2A-CGA	4.18	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	8	101	BCL	O2A-CGA	4.14	1.45	1.33
9	4	101	BCL	O2A-CGA	4.11	1.45	1.33
9	2	101	BCL	O2A-CGA	4.11	1.45	1.33
9	0	101	BCL	O2A-CGA	4.01	1.45	1.33
10	p	102	SPN	C7-C8	-3.98	1.37	1.50
9	b	101	BCL	O2D-CGD	3.98	1.42	1.33
9	b	101	BCL	O2A-CGA	3.97	1.44	1.33
10	1	103	SPN	C20-C19	-3.94	1.37	1.50
13	M	405	BPH	C2C-C3C	3.88	1.58	1.54
9	4	101	BCL	O2D-CGD	3.87	1.42	1.33
9	0	101	BCL	O2D-CGD	3.85	1.42	1.33
12	C	402	HEM	FE-NB	3.83	2.06	1.94
13	L	303	BPH	C2C-C3C	3.78	1.58	1.54
9	0	101	BCL	C1D-ND	-3.70	1.33	1.37
9	8	101	BCL	O2D-CGD	3.69	1.42	1.33
9	6	101	BCL	O2D-CGD	3.68	1.42	1.33
9	b	101	BCL	C1D-ND	-3.62	1.33	1.37
11	H	301	MW9	C9-C8	-3.59	1.31	1.51
11	M	408	MW9	C9-C8	-3.57	1.31	1.51
9	M	402	BCL	CHD-C1D	3.56	1.45	1.38
9	2	101	BCL	CHB-C1B	3.52	1.47	1.39
11	H	302	MW9	C9-C8	-3.51	1.31	1.51
9	M	402	BCL	O2A-CGA	3.50	1.43	1.33
13	M	409	BPH	C3B-C2B	3.50	1.45	1.39
10	1	105	SPN	C21-C22	-3.50	1.34	1.52
11	g	103	MW9	C9-C8	-3.50	1.31	1.51
9	8	101	BCL	CHB-C1B	3.49	1.47	1.39
11	9	101	MW9	C9-C8	-3.48	1.32	1.51
11	M	407	MW9	C9-C8	-3.47	1.32	1.51
10	q	102	SPN	C21-C22	-3.47	1.34	1.52
11	H	304	MW9	C9-C8	-3.46	1.32	1.51
10	n	102	SPN	C21-C22	-3.46	1.34	1.52
11	H	303	MW9	C9-C8	-3.46	1.32	1.51
10	p	102	SPN	C21-C22	-3.45	1.34	1.52
10	5	103	SPN	C21-C22	-3.45	1.34	1.52
10	r	102	SPN	C21-C22	-3.45	1.34	1.52
11	g	102	MW9	C9-C8	-3.45	1.32	1.51
10	u	102	SPN	C21-C22	-3.44	1.34	1.52
10	7	103	SPN	C21-C22	-3.44	1.34	1.52
10	5	102	SPN	C21-C22	-3.44	1.34	1.52
10	1	102	SPN	C21-C22	-3.44	1.34	1.52
10	1	104	SPN	C21-C22	-3.44	1.34	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	7	102	SPN	C21-C22	-3.44	1.34	1.52
10	0	102	SPN	C21-C22	-3.43	1.34	1.52
10	c	103	SPN	C21-C22	-3.43	1.34	1.52
10	m	102	SPN	C21-C22	-3.43	1.34	1.52
10	e	102	SPN	C21-C22	-3.43	1.34	1.52
10	c	102	SPN	C21-C22	-3.43	1.34	1.52
10	w	102	SPN	C21-C22	-3.42	1.34	1.52
10	h	102	SPN	C21-C22	-3.42	1.34	1.52
10	j	102	SPN	C21-C22	-3.42	1.34	1.52
10	1	105	SPN	C21-C20	-3.42	1.41	1.53
10	l	102	SPN	C21-C22	-3.42	1.34	1.52
10	9	103	SPN	C21-C22	-3.41	1.34	1.52
10	f	102	SPN	C21-C22	-3.41	1.34	1.52
10	s	102	SPN	C21-C22	-3.41	1.34	1.52
9	M	402	BCL	CHC-C4B	3.41	1.47	1.39
10	i	102	SPN	C21-C22	-3.41	1.34	1.52
10	k	102	SPN	C21-C22	-3.41	1.34	1.52
10	p	103	SPN	C21-C22	-3.40	1.34	1.52
10	3	102	SPN	C21-C22	-3.40	1.34	1.52
10	M	406	SPN	C21-C22	-3.40	1.34	1.52
9	4	101	BCL	OBD-CAD	3.39	1.28	1.22
10	1	105	SPN	C10-C11	-3.39	1.42	1.53
10	a	102	SPN	C21-C22	-3.37	1.34	1.52
10	h	103	SPN	C21-C22	-3.37	1.34	1.52
9	8	101	BCL	CHD-C1D	3.37	1.44	1.38
10	t	102	SPN	C21-C22	-3.36	1.34	1.52
9	6	101	BCL	CHD-C1D	3.36	1.44	1.38
10	a	103	SPN	C21-C22	-3.35	1.34	1.52
9	4	101	BCL	CHC-C4B	3.35	1.46	1.39
9	8	101	BCL	CHC-C4B	3.34	1.46	1.39
10	v	102	SPN	C21-C22	-3.34	1.35	1.52
9	M	402	BCL	CHB-C1B	3.33	1.46	1.39
13	M	405	BPH	C3B-C2B	3.33	1.45	1.39
9	M	402	BCL	OBD-CAD	3.32	1.28	1.22
9	4	101	BCL	CHB-C1B	3.32	1.46	1.39
9	6	101	BCL	C1D-ND	-3.32	1.33	1.37
9	4	101	BCL	C1D-ND	-3.31	1.33	1.37
9	0	101	BCL	CHD-C1D	3.30	1.44	1.38
8	M	403	U10	C4-C3	3.29	1.49	1.36
9	0	101	BCL	CHC-C4B	3.29	1.46	1.39
8	A	101	U10	C4-C3	3.28	1.49	1.36
10	1	103	SPN	C21-C22	-3.28	1.35	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	305	U10	C4-C3	3.27	1.49	1.36
10	1	103	SPN	C10-C11	-3.26	1.42	1.53
9	6	101	BCL	CHC-C4B	3.26	1.46	1.39
10	5	103	SPN	C21-C20	-3.24	1.42	1.53
9	0	101	BCL	OBD-CAD	3.23	1.28	1.22
9	b	101	BCL	CHB-C1B	3.23	1.46	1.39
9	0	101	BCL	CHB-C1B	3.23	1.46	1.39
10	1	105	SPN	C6-C7	-3.22	1.42	1.53
9	4	101	BCL	CHD-C1D	3.22	1.44	1.38
10	f	102	SPN	C10-C11	-3.22	1.42	1.53
10	v	102	SPN	C10-C11	-3.20	1.42	1.53
10	c	103	SPN	C21-C20	-3.20	1.42	1.53
9	2	101	BCL	CHC-C4B	3.20	1.46	1.39
10	q	102	SPN	C6-C7	-3.20	1.43	1.53
10	l	102	SPN	C10-C11	-3.20	1.43	1.53
10	h	103	SPN	C10-C11	-3.19	1.43	1.53
9	b	101	BCL	CHD-C1D	3.19	1.44	1.38
10	v	102	SPN	C6-C7	-3.19	1.43	1.53
10	n	102	SPN	C6-C7	-3.18	1.43	1.53
9	6	101	BCL	CHB-C1B	3.18	1.46	1.39
9	M	402	BCL	C1D-ND	-3.17	1.33	1.37
10	h	103	SPN	C21-C20	-3.17	1.42	1.53
10	n	102	SPN	C10-C11	-3.17	1.43	1.53
10	c	103	SPN	C6-C7	-3.17	1.43	1.53
10	7	103	SPN	C6-C7	-3.17	1.43	1.53
9	6	101	BCL	OBD-CAD	3.17	1.27	1.22
10	1	104	SPN	C6-C7	-3.16	1.43	1.53
9	8	101	BCL	OBD-CAD	3.16	1.27	1.22
10	1	104	SPN	C21-C20	-3.16	1.42	1.53
10	1	103	SPN	C6-C7	-3.16	1.43	1.53
10	5	103	SPN	C10-C11	-3.16	1.43	1.53
9	2	101	BCL	OBD-CAD	3.16	1.27	1.22
10	p	103	SPN	C10-C11	-3.15	1.43	1.53
9	2	101	BCL	C1D-ND	-3.15	1.33	1.37
10	0	102	SPN	C21-C20	-3.14	1.42	1.53
10	5	103	SPN	C6-C7	-3.14	1.43	1.53
10	c	103	SPN	C10-C11	-3.14	1.43	1.53
10	j	102	SPN	C10-C11	-3.14	1.43	1.53
10	p	102	SPN	C21-C20	-3.13	1.42	1.53
10	j	102	SPN	C6-C7	-3.13	1.43	1.53
10	M	406	SPN	C10-C11	-3.13	1.43	1.53
10	u	102	SPN	C6-C7	-3.13	1.43	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	b	101	BCL	CHC-C4B	3.12	1.46	1.39
10	r	102	SPN	C10-C11	-3.12	1.43	1.53
10	a	103	SPN	C21-C20	-3.12	1.42	1.53
10	f	102	SPN	C6-C7	-3.12	1.43	1.53
9	b	101	BCL	OBD-CAD	3.12	1.27	1.22
9	8	101	BCL	C1D-ND	-3.12	1.34	1.37
10	7	103	SPN	C10-C11	-3.11	1.43	1.53
10	M	406	SPN	C6-C7	-3.11	1.43	1.53
10	u	102	SPN	C10-C11	-3.11	1.43	1.53
10	c	102	SPN	C10-C11	-3.10	1.43	1.53
9	2	101	BCL	CHD-C1D	3.10	1.44	1.38
10	w	102	SPN	C10-C11	-3.10	1.43	1.53
12	C	401	HEM	FE-NB	3.10	2.04	1.94
10	1	102	SPN	C21-C20	-3.09	1.42	1.53
10	l	102	SPN	C6-C7	-3.09	1.43	1.53
10	5	102	SPN	C21-C20	-3.09	1.42	1.53
10	i	102	SPN	C10-C11	-3.09	1.43	1.53
10	e	102	SPN	C21-C20	-3.08	1.42	1.53
10	c	102	SPN	C6-C7	-3.08	1.43	1.53
10	1	104	SPN	C10-C11	-3.08	1.43	1.53
10	9	103	SPN	C10-C11	-3.07	1.43	1.53
10	9	103	SPN	C6-C7	-3.07	1.43	1.53
10	a	103	SPN	C6-C7	-3.07	1.43	1.53
10	s	102	SPN	C6-C7	-3.07	1.43	1.53
10	e	102	SPN	C6-C7	-3.06	1.43	1.53
10	j	102	SPN	C21-C20	-3.06	1.43	1.53
10	f	102	SPN	C21-C20	-3.06	1.43	1.53
9	b	101	BCL	C4B-NB	-3.06	1.34	1.37
10	u	102	SPN	C21-C20	-3.06	1.43	1.53
10	r	102	SPN	C6-C7	-3.05	1.43	1.53
10	p	103	SPN	C6-C7	-3.05	1.43	1.53
10	9	103	SPN	C21-C20	-3.05	1.43	1.53
10	m	102	SPN	C10-C11	-3.05	1.43	1.53
10	k	102	SPN	C6-C7	-3.05	1.43	1.53
10	s	102	SPN	C10-C11	-3.04	1.43	1.53
10	c	102	SPN	C21-C20	-3.04	1.43	1.53
9	M	402	BCL	C3D-C2D	3.04	1.47	1.39
10	m	102	SPN	C6-C7	-3.04	1.43	1.53
10	t	102	SPN	C6-C7	-3.03	1.43	1.53
10	h	103	SPN	C6-C7	-3.03	1.43	1.53
10	7	102	SPN	C10-C11	-3.03	1.43	1.53
10	s	102	SPN	C21-C20	-3.03	1.43	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	w	102	SPN	C6-C7	-3.03	1.43	1.53
10	7	102	SPN	C6-C7	-3.03	1.43	1.53
10	k	102	SPN	C10-C11	-3.02	1.43	1.53
10	i	102	SPN	C21-C20	-3.02	1.43	1.53
10	a	102	SPN	C21-C20	-3.02	1.43	1.53
10	7	102	SPN	C21-C20	-3.01	1.43	1.53
10	n	102	SPN	C21-C20	-3.01	1.43	1.53
10	0	102	SPN	C10-C11	-3.00	1.43	1.53
10	h	102	SPN	C21-C20	-2.99	1.43	1.53
10	k	102	SPN	C21-C20	-2.99	1.43	1.53
10	h	102	SPN	C6-C7	-2.98	1.43	1.53
10	q	102	SPN	C21-C20	-2.98	1.43	1.53
10	h	102	SPN	C10-C11	-2.98	1.43	1.53
10	l	102	SPN	C21-C20	-2.98	1.43	1.53
10	e	102	SPN	C10-C11	-2.98	1.43	1.53
10	m	102	SPN	C21-C20	-2.97	1.43	1.53
10	1	105	SPN	C16-C15	-2.97	1.34	1.51
10	7	103	SPN	C21-C20	-2.97	1.43	1.53
10	i	102	SPN	C6-C7	-2.97	1.43	1.53
10	p	102	SPN	C16-C15	-2.97	1.34	1.51
10	q	102	SPN	C10-C11	-2.97	1.43	1.53
10	p	102	SPN	C10-C11	-2.96	1.43	1.53
10	p	103	SPN	C21-C20	-2.95	1.43	1.53
10	0	102	SPN	C6-C7	-2.95	1.43	1.53
10	w	102	SPN	C21-C20	-2.94	1.43	1.53
10	1	102	SPN	C6-C7	-2.93	1.43	1.53
10	t	102	SPN	C10-C11	-2.93	1.43	1.53
10	r	102	SPN	C21-C20	-2.93	1.43	1.53
10	v	102	SPN	C21-C20	-2.92	1.43	1.53
9	6	101	BCL	C3D-C2D	2.92	1.47	1.39
10	a	102	SPN	C6-C7	-2.92	1.43	1.53
10	1	102	SPN	C10-C11	-2.91	1.43	1.53
9	0	101	BCL	C1B-NB	-2.91	1.34	1.37
10	3	102	SPN	C21-C20	-2.90	1.43	1.53
10	0	102	SPN	C16-C15	-2.90	1.35	1.51
9	6	101	BCL	C1B-NB	-2.89	1.34	1.37
10	3	102	SPN	C10-C11	-2.88	1.44	1.53
9	4	101	BCL	C1B-NB	-2.86	1.34	1.37
10	5	102	SPN	C6-C7	-2.86	1.44	1.53
9	2	101	BCL	C3D-C2D	2.86	1.46	1.39
10	5	102	SPN	C10-C11	-2.86	1.44	1.53
10	a	102	SPN	C10-C11	-2.85	1.44	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	c	102	SPN	C16-C15	-2.84	1.35	1.51
10	e	102	SPN	C16-C15	-2.84	1.35	1.51
10	c	103	SPN	C16-C15	-2.83	1.35	1.51
9	b	101	BCL	C1B-NB	-2.83	1.34	1.37
10	r	102	SPN	C16-C15	-2.83	1.35	1.51
10	1	105	SPN	C15-C14	-2.82	1.41	1.52
10	v	102	SPN	C16-C15	-2.82	1.35	1.51
10	w	102	SPN	C16-C15	-2.82	1.35	1.51
10	h	102	SPN	C16-C15	-2.82	1.35	1.51
10	9	103	SPN	C16-C15	-2.82	1.35	1.51
10	k	102	SPN	C16-C15	-2.82	1.35	1.51
9	8	101	BCL	C3D-C2D	2.82	1.46	1.39
9	b	101	BCL	C3D-C2D	2.82	1.46	1.39
10	l	102	SPN	C16-C15	-2.81	1.35	1.51
10	m	102	SPN	C16-C15	-2.81	1.35	1.51
10	n	102	SPN	C16-C15	-2.81	1.35	1.51
10	7	103	SPN	C16-C15	-2.81	1.35	1.51
10	7	102	SPN	C16-C15	-2.81	1.35	1.51
10	u	102	SPN	C16-C15	-2.81	1.35	1.51
10	i	102	SPN	C16-C15	-2.80	1.35	1.51
10	j	102	SPN	C16-C15	-2.80	1.35	1.51
10	f	102	SPN	C16-C15	-2.80	1.35	1.51
10	a	102	SPN	C16-C15	-2.79	1.35	1.51
9	6	101	BCL	C4B-NB	-2.79	1.34	1.37
10	t	102	SPN	C21-C20	-2.79	1.43	1.53
10	p	103	SPN	C16-C15	-2.78	1.36	1.51
10	s	102	SPN	C16-C15	-2.78	1.36	1.51
10	1	102	SPN	C16-C15	-2.78	1.36	1.51
10	5	102	SPN	C16-C15	-2.77	1.36	1.51
10	t	102	SPN	C16-C15	-2.77	1.36	1.51
10	5	103	SPN	C16-C15	-2.77	1.36	1.51
9	0	101	BCL	C3D-C2D	2.77	1.46	1.39
10	1	105	SPN	C16-C17	-2.77	1.42	1.52
10	3	102	SPN	C6-C7	-2.76	1.44	1.53
10	a	103	SPN	C10-C11	-2.75	1.44	1.53
10	h	103	SPN	C16-C15	-2.75	1.36	1.51
9	M	402	BCL	CHD-C4C	2.75	1.47	1.39
9	8	101	BCL	C4B-NB	-2.72	1.34	1.37
10	1	104	SPN	C16-C15	-2.72	1.36	1.51
10	a	103	SPN	C16-C15	-2.71	1.36	1.51
10	M	406	SPN	C16-C15	-2.71	1.36	1.51
10	3	102	SPN	C16-C15	-2.71	1.36	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	1	103	SPN	C15-C14	-2.70	1.42	1.52
9	0	101	BCL	C4B-NB	-2.70	1.34	1.37
9	8	101	BCL	C1B-NB	-2.69	1.34	1.37
9	4	101	BCL	C3D-C2D	2.68	1.46	1.39
10	v	102	SPN	C15-C14	-2.67	1.42	1.52
9	o	101	BCL	MG-NA	-2.64	2.00	2.06
9	2	101	BCL	C4B-NB	-2.63	1.34	1.37
10	1	103	SPN	C16-C15	-2.63	1.36	1.51
10	j	102	SPN	C15-C14	-2.62	1.42	1.52
10	q	102	SPN	C16-C15	-2.62	1.36	1.51
13	L	303	BPH	C3B-C2B	2.61	1.44	1.39
12	C	401	HEM	FE-NC	2.60	2.03	1.95
9	4	101	BCL	C4B-NB	-2.60	1.34	1.37
9	2	101	BCL	C1B-NB	-2.58	1.34	1.37
10	v	102	SPN	C16-C17	-2.56	1.42	1.52
10	p	102	SPN	C6-C7	-2.56	1.45	1.53
9	M	402	BCL	C1B-NB	-2.54	1.34	1.37
9	M	402	BCL	C4B-NB	-2.54	1.34	1.37
10	M	406	SPN	C15-C14	-2.54	1.42	1.52
10	1	103	SPN	C21-C20	-2.54	1.44	1.53
9	6	101	BCL	CHD-C4C	2.53	1.46	1.39
10	f	102	SPN	C15-C14	-2.52	1.42	1.52
10	f	102	SPN	C16-C17	-2.52	1.42	1.52
9	L	301	BCL	C1D-C2D	-2.51	1.40	1.45
9	M	402	BCL	C1D-C2D	2.51	1.50	1.45
10	h	103	SPN	C16-C17	-2.51	1.43	1.52
10	1	103	SPN	C16-C17	-2.50	1.43	1.52
10	a	103	SPN	C16-C17	-2.50	1.43	1.52
10	l	102	SPN	C15-C14	-2.50	1.43	1.52
10	n	102	SPN	C16-C17	-2.48	1.43	1.52
10	n	102	SPN	C15-C14	-2.48	1.43	1.52
10	e	102	SPN	C16-C17	-2.48	1.43	1.52
10	7	103	SPN	C15-C14	-2.48	1.43	1.52
10	0	102	SPN	C15-C14	-2.48	1.43	1.52
10	0	102	SPN	C16-C17	-2.48	1.43	1.52
10	p	103	SPN	C16-C17	-2.47	1.43	1.52
10	r	102	SPN	C15-C14	-2.47	1.43	1.52
10	c	103	SPN	C16-C17	-2.47	1.43	1.52
9	8	101	BCL	CHD-C4C	2.47	1.46	1.39
10	j	102	SPN	C16-C17	-2.46	1.43	1.52
12	C	403	HEM	FE-NB	2.46	2.02	1.94
10	r	102	SPN	C16-C17	-2.46	1.43	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	e	101	BCL	MG-NC	2.45	2.12	2.06
13	M	405	BPH	CHA-CBD	2.45	1.54	1.51
10	1	104	SPN	C16-C17	-2.45	1.43	1.52
10	m	102	SPN	C15-C14	-2.44	1.43	1.52
10	u	102	SPN	C15-C14	-2.43	1.43	1.52
9	0	101	BCL	CHD-C4C	2.43	1.46	1.39
10	p	103	SPN	C15-C14	-2.43	1.43	1.52
10	l	102	SPN	C16-C17	-2.43	1.43	1.52
10	5	103	SPN	C16-C17	-2.43	1.43	1.52
10	h	103	SPN	C15-C14	-2.43	1.43	1.52
10	c	102	SPN	C15-C14	-2.43	1.43	1.52
10	1	104	SPN	C15-C14	-2.42	1.43	1.52
10	u	102	SPN	C16-C17	-2.42	1.43	1.52
10	s	102	SPN	C15-C14	-2.41	1.43	1.52
9	8	101	BCL	C1B-C2B	2.41	1.48	1.43
10	m	102	SPN	C16-C17	-2.41	1.43	1.52
10	c	103	SPN	C15-C14	-2.41	1.43	1.52
10	7	103	SPN	C16-C17	-2.41	1.43	1.52
10	9	103	SPN	C15-C14	-2.40	1.43	1.52
9	4	101	BCL	CHD-C4C	2.40	1.46	1.39
9	2	101	BCL	CHD-C4C	2.40	1.46	1.39
10	k	102	SPN	C15-C14	-2.39	1.43	1.52
10	7	102	SPN	C16-C17	-2.39	1.43	1.52
10	9	103	SPN	C16-C17	-2.39	1.43	1.52
10	t	102	SPN	C16-C17	-2.39	1.43	1.52
10	3	102	SPN	C15-C14	-2.39	1.43	1.52
10	7	102	SPN	C15-C14	-2.38	1.43	1.52
10	e	102	SPN	C15-C14	-2.38	1.43	1.52
9	2	101	BCL	C1B-C2B	2.38	1.48	1.43
10	w	102	SPN	C16-C17	-2.37	1.43	1.52
10	h	102	SPN	C16-C17	-2.37	1.43	1.52
10	i	102	SPN	C16-C17	-2.37	1.43	1.52
10	5	103	SPN	C15-C14	-2.36	1.43	1.52
9	b	101	BCL	CHC-C1C	-2.36	1.32	1.37
10	i	102	SPN	C15-C14	-2.36	1.43	1.52
10	c	102	SPN	C16-C17	-2.36	1.43	1.52
13	M	409	BPH	C3B-C4B	-2.35	1.37	1.41
10	k	102	SPN	C16-C17	-2.35	1.43	1.52
10	w	102	SPN	C15-C14	-2.34	1.43	1.52
10	s	102	SPN	C16-C17	-2.33	1.43	1.52
10	p	102	SPN	C15-C14	-2.33	1.43	1.52
10	p	102	SPN	C16-C17	-2.33	1.43	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	a	103	SPN	C15-C14	-2.30	1.43	1.52
9	4	101	BCL	MG-NA	-2.30	2.00	2.06
10	h	102	SPN	C15-C14	-2.30	1.43	1.52
10	M	406	SPN	C21-C20	-2.30	1.45	1.53
9	0	101	BCL	MG-NA	-2.30	2.00	2.06
10	a	102	SPN	C15-C14	-2.29	1.43	1.52
9	M	402	BCL	MG-NA	-2.29	2.00	2.06
9	2	101	BCL	MG-NA	-2.27	2.00	2.06
10	1	102	SPN	C15-C14	-2.27	1.43	1.52
10	t	102	SPN	C15-C14	-2.27	1.43	1.52
9	b	101	BCL	CHD-C4C	2.25	1.45	1.39
9	8	101	BCL	C1D-C2D	2.25	1.49	1.45
10	1	102	SPN	C16-C17	-2.25	1.43	1.52
10	a	102	SPN	C16-C17	-2.24	1.44	1.52
9	u	101	BCL	MG-NC	2.24	2.11	2.06
13	M	409	BPH	CHA-CBD	2.23	1.54	1.51
9	6	101	BCL	CHB-C4A	-2.22	1.32	1.37
9	5	101	BCL	C1D-C2D	-2.21	1.41	1.45
9	s	101	BCL	C1D-C2D	-2.20	1.41	1.45
9	2	101	BCL	CHC-C1C	-2.20	1.32	1.37
10	q	102	SPN	C15-C14	-2.20	1.44	1.52
10	3	102	SPN	C16-C17	-2.20	1.44	1.52
10	5	102	SPN	C16-C17	-2.20	1.44	1.52
9	8	101	BCL	CHC-C1C	-2.20	1.32	1.37
9	8	101	BCL	MG-NC	-2.19	2.01	2.06
9	b	101	BCL	MG-NA	-2.18	2.01	2.06
9	M	402	BCL	CHC-C1C	-2.17	1.32	1.37
10	q	102	SPN	C16-C17	-2.17	1.44	1.52
10	5	102	SPN	C15-C14	-2.17	1.44	1.52
9	0	101	BCL	CHB-C4A	-2.16	1.32	1.37
9	8	101	BCL	MG-NA	-2.16	2.01	2.06
9	0	101	BCL	C1D-C2D	2.15	1.49	1.45
9	2	101	BCL	C3C-C4C	-2.15	1.48	1.51
10	M	406	SPN	C16-C17	-2.14	1.44	1.52
9	6	101	BCL	MG-NA	-2.14	2.01	2.06
9	6	101	BCL	CHC-C1C	-2.14	1.32	1.37
9	0	101	BCL	C1B-C2B	2.13	1.48	1.43
9	6	101	BCL	C1B-C2B	2.13	1.48	1.43
9	m	101	BCL	C3C-C4C	2.12	1.54	1.51
9	L	304	BCL	C1D-C2D	-2.12	1.41	1.45
9	4	101	BCL	CHC-C1C	-2.10	1.32	1.37
9	6	101	BCL	C1D-C2D	2.10	1.49	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	402	BCL	CHB-C4A	-2.09	1.32	1.37
9	s	101	BCL	C1B-NB	-2.09	1.35	1.37
9	6	101	BCL	MG-NC	-2.09	2.01	2.06
9	9	102	BCL	MG-NC	2.09	2.11	2.06
9	b	101	BCL	CHB-C4A	-2.08	1.32	1.37
9	b	101	BCL	C3C-C4C	-2.08	1.49	1.51
9	4	101	BCL	MG-NC	-2.07	2.01	2.06
9	a	101	BCL	MG-NC	2.07	2.11	2.06
9	h	101	BCL	C4B-NB	2.07	1.40	1.37
9	b	101	BCL	C1B-C2B	2.06	1.48	1.43
9	p	101	BCL	C3C-C4C	2.06	1.54	1.51
9	4	101	BCL	C1B-C2B	2.05	1.48	1.43
9	4	101	BCL	C1D-C2D	2.05	1.49	1.45
9	b	101	BCL	C1D-C2D	2.04	1.49	1.45
9	w	101	BCL	MG-NC	2.04	2.11	2.06
9	h	101	BCL	MG-NC	2.04	2.11	2.06
9	M	404	BCL	C1B-NB	-2.02	1.35	1.37
9	4	101	BCL	C3C-C4C	-2.01	1.49	1.51
9	3	101	BCL	C4B-NB	2.01	1.40	1.37

All (1313) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	6	101	BCL	C2B-C1B-NB	11.18	117.73	110.23
9	8	101	BCL	O2D-CGD-CBD	10.93	130.70	111.27
9	0	101	BCL	C2B-C1B-NB	10.92	117.56	110.23
9	0	101	BCL	O2D-CGD-CBD	10.91	130.66	111.27
9	4	101	BCL	C2B-C1B-NB	10.69	117.40	110.23
9	b	101	BCL	C2B-C1B-NB	10.59	117.33	110.23
9	b	101	BCL	O2D-CGD-CBD	10.51	129.95	111.27
9	8	101	BCL	C2B-C1B-NB	10.25	117.11	110.23
9	2	101	BCL	O2D-CGD-CBD	10.22	129.44	111.27
9	2	101	BCL	C2B-C1B-NB	10.10	117.00	110.23
9	M	402	BCL	C2B-C1B-NB	10.06	116.98	110.23
9	6	101	BCL	O2D-CGD-CBD	9.54	128.23	111.27
9	4	101	BCL	O2D-CGD-CBD	9.48	128.12	111.27
8	L	305	U10	C7-C6-C5	8.93	129.22	118.48
9	M	402	BCL	CHD-C1D-ND	-8.19	116.92	124.45
9	6	101	BCL	CHD-C1D-ND	-7.79	117.29	124.45
12	C	402	HEM	CAC-C3C-C4C	7.71	143.53	124.90
9	2	101	BCL	CHD-C1D-ND	-7.70	117.38	124.45
10	v	102	SPN	C21-C20-C19	7.70	132.56	112.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	8	101	BCL	CHD-C1D-ND	-7.65	117.42	124.45
9	0	101	BCL	CHD-C1D-ND	-7.61	117.47	124.45
10	a	103	SPN	C21-C20-C19	7.55	132.16	112.23
9	M	402	BCL	CMD-C2D-C1D	7.50	137.93	124.71
10	1	104	SPN	C21-C20-C19	7.50	132.03	112.23
10	j	102	SPN	C21-C20-C19	7.49	132.00	112.23
9	b	101	BCL	CHD-C1D-ND	-7.45	117.61	124.45
9	4	101	BCL	CHD-C1D-ND	-7.43	117.62	124.45
10	1	103	SPN	C21-C20-C19	7.41	131.79	112.23
9	4	101	BCL	CMD-C2D-C1D	7.18	137.37	124.71
10	h	103	SPN	C21-C20-C19	7.05	130.85	112.23
10	f	102	SPN	C21-C20-C19	6.83	130.28	112.23
9	6	101	BCL	CMD-C2D-C1D	6.72	136.56	124.71
9	2	101	BCL	CMD-C2D-C1D	6.70	136.52	124.71
9	M	402	BCL	O2D-CGD-CBD	6.69	123.16	111.27
9	8	101	BCL	CMD-C2D-C1D	6.64	136.41	124.71
9	0	101	BCL	CMD-C2D-C1D	6.63	136.40	124.71
10	l	102	SPN	C21-C20-C19	6.60	129.66	112.23
9	b	101	BCL	CMD-C2D-C1D	6.52	136.21	124.71
9	8	101	BCL	O2D-CGD-O1D	-6.46	111.21	123.84
10	M	406	SPN	C16-C17-C18	6.35	130.11	113.45
10	1	103	SPN	C15-C16-C17	6.26	135.69	113.19
10	M	406	SPN	C15-C14-C13	6.24	129.81	113.45
9	M	402	BCL	CHC-C4B-NB	-6.16	117.74	124.26
9	0	101	BCL	O2D-CGD-O1D	-6.13	111.85	123.84
10	p	103	SPN	C21-C20-C19	6.01	128.11	112.23
10	1	103	SPN	C16-C15-C14	5.90	134.40	113.19
9	M	402	BCL	C1-C2-C3	-5.90	115.84	126.04
10	j	102	SPN	C16-C17-C18	5.89	128.91	113.45
9	2	101	BCL	C2D-C1D-ND	5.89	114.44	110.10
9	b	101	BCL	O2D-CGD-O1D	-5.87	112.36	123.84
10	a	103	SPN	C16-C17-C18	5.86	128.81	113.45
10	h	103	SPN	C16-C17-C18	5.85	128.79	113.45
10	1	104	SPN	C16-C17-C18	5.84	128.78	113.45
10	f	102	SPN	C16-C17-C18	5.76	128.57	113.45
10	M	406	SPN	C21-C20-C19	5.76	127.44	112.23
10	q	102	SPN	C16-C17-C18	5.75	128.53	113.45
10	5	102	SPN	C15-C14-C13	5.74	128.51	113.45
10	3	102	SPN	C15-C14-C13	5.73	128.47	113.45
10	a	102	SPN	C15-C14-C13	5.72	128.45	113.45
12	C	402	HEM	CAC-C3C-C2C	-5.71	109.78	128.60
10	1	102	SPN	C15-C14-C13	5.65	128.28	113.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	l	102	SPN	C16-C17-C18	5.63	128.23	113.45
10	q	102	SPN	C15-C14-C13	5.62	128.20	113.45
10	n	102	SPN	C15-C14-C13	5.60	128.15	113.45
10	c	103	SPN	C15-C14-C13	5.59	128.12	113.45
9	8	101	BCL	C2D-C1D-ND	5.59	114.22	110.10
10	p	103	SPN	C15-C14-C13	5.59	128.10	113.45
9	6	101	BCL	C2D-C1D-ND	5.58	114.22	110.10
10	e	102	SPN	C15-C14-C13	5.57	128.06	113.45
10	5	103	SPN	C15-C14-C13	5.57	128.05	113.45
10	i	102	SPN	C15-C14-C13	5.57	128.05	113.45
10	7	102	SPN	C15-C14-C13	5.56	128.04	113.45
10	p	102	SPN	C6-C7-C8	5.55	130.14	111.88
10	1	105	SPN	C15-C14-C13	5.55	128.00	113.45
10	9	103	SPN	C15-C14-C13	5.54	127.99	113.45
10	h	102	SPN	C15-C14-C13	5.54	127.99	113.45
10	r	102	SPN	C15-C14-C13	5.54	127.98	113.45
10	7	103	SPN	C16-C17-C18	5.53	127.96	113.45
10	0	102	SPN	C15-C14-C13	5.53	127.94	113.45
10	c	102	SPN	C15-C14-C13	5.52	127.94	113.45
10	u	102	SPN	C15-C14-C13	5.52	127.94	113.45
10	w	102	SPN	C15-C14-C13	5.52	127.93	113.45
10	v	102	SPN	C15-C14-C13	5.50	127.87	113.45
10	k	102	SPN	C15-C14-C13	5.50	127.86	113.45
10	a	103	SPN	C15-C14-C13	5.50	127.86	113.45
9	4	101	BCL	C2D-C1D-ND	5.49	114.15	110.10
10	t	102	SPN	C15-C14-C13	5.49	127.85	113.45
10	m	102	SPN	C15-C14-C13	5.49	127.85	113.45
10	p	103	SPN	C16-C17-C18	5.47	127.81	113.45
10	s	102	SPN	C15-C14-C13	5.47	127.81	113.45
10	7	103	SPN	C15-C14-C13	5.47	127.80	113.45
10	t	102	SPN	C16-C17-C18	5.47	127.80	113.45
9	4	101	BCL	O2D-CGD-O1D	-5.46	113.17	123.84
10	v	102	SPN	C16-C17-C18	5.43	127.69	113.45
9	b	101	BCL	C2D-C1D-ND	5.42	114.10	110.10
10	1	104	SPN	C15-C14-C13	5.41	127.64	113.45
10	5	103	SPN	C16-C17-C18	5.41	127.63	113.45
9	0	101	BCL	C2D-C1D-ND	5.40	114.09	110.10
10	c	103	SPN	C16-C17-C18	5.39	127.58	113.45
10	u	102	SPN	C16-C17-C18	5.38	127.56	113.45
10	j	102	SPN	C15-C14-C13	5.38	127.56	113.45
10	i	102	SPN	C16-C17-C18	5.37	127.54	113.45
10	s	102	SPN	C16-C17-C18	5.37	127.53	113.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	f	102	SPN	C15-C14-C13	5.36	127.50	113.45
10	3	102	SPN	C16-C17-C18	5.35	127.50	113.45
10	M	406	SPN	CM5-C13-C14	5.34	124.26	115.27
9	6	101	BCL	O2D-CGD-O1D	-5.34	113.40	123.84
10	l	102	SPN	C15-C14-C13	5.34	127.46	113.45
10	7	102	SPN	C16-C17-C18	5.34	127.45	113.45
10	9	103	SPN	C16-C17-C18	5.33	127.43	113.45
10	w	102	SPN	C16-C17-C18	5.33	127.42	113.45
10	n	102	SPN	C16-C17-C18	5.33	127.42	113.45
10	m	102	SPN	C16-C17-C18	5.32	127.41	113.45
10	1	105	SPN	C16-C17-C18	5.32	127.40	113.45
10	r	102	SPN	C16-C17-C18	5.32	127.40	113.45
10	k	102	SPN	C16-C17-C18	5.31	127.39	113.45
10	c	102	SPN	C16-C17-C18	5.31	127.38	113.45
10	e	102	SPN	C16-C17-C18	5.30	127.34	113.45
10	h	103	SPN	C15-C14-C13	5.28	127.31	113.45
10	h	102	SPN	C16-C17-C18	5.28	127.30	113.45
10	a	102	SPN	C16-C17-C18	5.28	127.29	113.45
10	5	102	SPN	C16-C17-C18	5.27	127.27	113.45
10	p	102	SPN	C15-C14-C13	5.27	127.27	113.45
10	0	102	SPN	C16-C17-C18	5.26	127.25	113.45
10	M	406	SPN	C15-C16-C17	5.25	132.07	113.19
10	1	102	SPN	C16-C17-C18	5.25	127.23	113.45
10	5	103	SPN	CM3-C5-C6	5.20	124.02	115.27
10	p	102	SPN	C16-C17-C18	5.17	127.02	113.45
10	7	103	SPN	CM3-C5-C6	5.17	123.97	115.27
9	1	101	BCL	CAC-C3C-C2C	-5.17	101.35	114.26
9	2	101	BCL	CHC-C4B-NB	-5.16	118.80	124.26
9	0	101	BCL	CHC-C4B-NB	-5.15	118.81	124.26
9	s	101	BCL	CAC-C3C-C2C	-5.15	101.40	114.26
9	6	101	BCL	CHC-C4B-NB	-5.10	118.86	124.26
10	a	103	SPN	CM3-C5-C6	5.10	123.85	115.27
10	0	102	SPN	C21-C20-C19	5.10	125.69	112.23
10	c	103	SPN	CM3-C5-C6	5.09	123.83	115.27
10	0	102	SPN	CM3-C5-C6	5.08	123.82	115.27
9	4	101	BCL	CHC-C4B-NB	-5.07	118.89	124.26
9	7	101	BCL	CAC-C3C-C2C	-5.06	101.63	114.26
10	1	103	SPN	CM3-C5-C6	5.05	123.77	115.27
9	2	101	BCL	O2D-CGD-O1D	-5.05	113.97	123.84
10	1	104	SPN	CM3-C5-C6	5.05	123.76	115.27
10	q	102	SPN	CM3-C5-C6	5.05	123.76	115.27
10	M	406	SPN	CM4-C9-C10	5.03	123.74	115.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	t	102	SPN	CM3-C5-C6	5.03	123.74	115.27
9	8	101	BCL	CHC-C4B-NB	-5.03	118.93	124.26
9	M	402	BCL	O2D-CGD-O1D	-5.02	114.03	123.84
9	M	402	BCL	C3D-C2D-C1D	-5.01	99.00	105.83
10	1	105	SPN	CM3-C5-C6	5.01	123.69	115.27
9	M	402	BCL	C2D-C1D-ND	5.00	113.79	110.10
10	5	103	SPN	C7-C6-C5	5.00	129.41	112.98
9	M	402	BCL	C4-C3-C5	4.94	123.58	115.27
10	f	102	SPN	CM3-C5-C6	4.93	123.56	115.27
10	j	102	SPN	CM3-C5-C6	4.91	123.54	115.27
10	M	406	SPN	CM6-C18-C17	4.90	123.52	115.27
10	M	406	SPN	C11-C10-C9	4.90	129.10	112.98
12	C	402	HEM	CAB-C3B-C2B	-4.90	112.45	128.60
10	7	103	SPN	C7-C6-C5	4.90	129.10	112.98
10	1	103	SPN	C7-C6-C5	4.90	129.09	112.98
10	a	103	SPN	C7-C6-C5	4.90	129.08	112.98
10	0	102	SPN	C7-C6-C5	4.89	129.08	112.98
10	c	103	SPN	C7-C6-C5	4.89	129.05	112.98
9	4	101	BCL	C3D-C2D-C1D	-4.87	99.18	105.83
10	f	102	SPN	CM4-C9-C10	4.87	123.46	115.27
9	b	101	BCL	CHC-C4B-NB	-4.87	119.11	124.26
10	1	104	SPN	CM4-C9-C10	4.86	123.45	115.27
10	p	102	SPN	C10-C11-C12	4.86	127.86	111.88
10	1	104	SPN	C7-C6-C5	4.86	128.97	112.98
10	q	102	SPN	C7-C6-C5	4.86	128.95	112.98
10	q	102	SPN	CM4-C9-C10	4.85	123.44	115.27
10	n	102	SPN	CM4-C9-C10	4.85	123.43	115.27
10	h	103	SPN	CM6-C18-C17	4.85	123.43	115.27
10	n	102	SPN	CM3-C5-C6	4.84	123.42	115.27
10	t	102	SPN	CM4-C9-C10	4.84	123.42	115.27
10	j	102	SPN	CM4-C9-C10	4.84	123.42	115.27
10	q	102	SPN	CM6-C18-C17	4.84	123.41	115.27
10	7	103	SPN	CM4-C9-C10	4.83	123.40	115.27
9	r	101	BCL	CAC-C3C-C2C	-4.83	102.18	114.26
10	l	102	SPN	CM3-C5-C6	4.83	123.40	115.27
10	1	105	SPN	C7-C6-C5	4.83	128.87	112.98
10	j	102	SPN	C7-C6-C5	4.83	128.86	112.98
10	1	103	SPN	CM4-C9-C10	4.83	123.39	115.27
8	A	101	U10	C7-C8-C9	-4.82	118.76	126.79
10	t	102	SPN	C7-C6-C5	4.82	128.84	112.98
10	p	102	SPN	C20-C21-C22	4.82	132.44	115.76
10	h	103	SPN	CM3-C5-C6	4.82	123.38	115.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	p	103	SPN	CM4-C9-C10	4.81	123.37	115.27
9	2	101	BCL	C3C-C4C-CHD	-4.80	113.13	123.39
10	h	103	SPN	CM4-C9-C10	4.79	123.33	115.27
10	5	103	SPN	CM4-C9-C10	4.79	123.33	115.27
9	4	101	BCL	CHD-C4C-NC	4.79	130.39	125.08
10	a	103	SPN	CM4-C9-C10	4.79	123.32	115.27
10	h	103	SPN	C7-C6-C5	4.78	128.71	112.98
9	2	101	BCL	C3D-C2D-C1D	-4.78	99.31	105.83
10	f	102	SPN	C7-C6-C5	4.78	128.69	112.98
9	o	101	BCL	CAC-C3C-C2C	-4.77	102.34	114.26
10	n	102	SPN	C7-C6-C5	4.77	128.67	112.98
10	c	103	SPN	CM4-C9-C10	4.77	123.29	115.27
10	1	105	SPN	CM4-C9-C10	4.77	123.29	115.27
10	j	102	SPN	C11-C10-C9	4.76	128.62	112.98
10	f	102	SPN	CM6-C18-C17	4.75	123.27	115.27
10	1	104	SPN	C11-C10-C9	4.75	128.61	112.98
10	p	103	SPN	CM3-C5-C6	4.75	123.27	115.27
10	l	102	SPN	CM4-C9-C10	4.75	123.27	115.27
10	a	103	SPN	C11-C10-C9	4.75	128.61	112.98
9	2	101	BCL	CHD-C4C-NC	4.75	130.35	125.08
10	7	103	SPN	C11-C10-C9	4.74	128.57	112.98
9	4	101	BCL	C3C-C4C-CHD	-4.74	113.26	123.39
9	c	101	BCL	CAC-C3C-C2C	-4.74	102.42	114.26
9	6	101	BCL	C3D-C2D-C1D	-4.74	99.37	105.83
9	i	101	BCL	CAC-C3C-C2C	-4.74	102.42	114.26
10	n	102	SPN	CM5-C13-C14	4.74	123.24	115.27
10	p	102	SPN	CM7-C22-C21	4.73	128.44	111.29
9	v	101	BCL	CAC-C3C-C2C	-4.73	102.43	114.26
10	v	102	SPN	CM3-C5-C6	4.72	123.22	115.27
10	q	102	SPN	C11-C10-C9	4.72	128.50	112.98
10	M	406	SPN	CM3-C5-C6	4.72	123.21	115.27
10	5	103	SPN	C11-C10-C9	4.72	128.49	112.98
10	1	103	SPN	C11-C10-C9	4.71	128.48	112.98
10	t	102	SPN	C11-C10-C9	4.71	128.47	112.98
10	5	102	SPN	CM5-C13-C14	4.71	123.19	115.27
10	0	102	SPN	CM4-C9-C10	4.71	123.19	115.27
10	l	102	SPN	C7-C6-C5	4.70	128.45	112.98
10	1	104	SPN	CM6-C18-C17	4.70	123.18	115.27
10	1	103	SPN	C15-C14-C13	4.70	125.78	113.45
10	f	102	SPN	C11-C10-C9	4.70	128.44	112.98
9	m	101	BCL	CAC-C3C-C2C	-4.70	102.52	114.26
10	p	103	SPN	C11-C10-C9	4.70	128.42	112.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	1	105	SPN	CM5-C13-C14	4.70	123.17	115.27
9	a	101	BCL	CAC-C3C-C2C	-4.69	102.53	114.26
10	n	102	SPN	C11-C10-C9	4.69	128.40	112.98
10	0	102	SPN	C11-C10-C9	4.68	128.38	112.98
10	c	103	SPN	C11-C10-C9	4.68	128.37	112.98
10	1	105	SPN	C11-C10-C9	4.68	128.37	112.98
10	p	103	SPN	C7-C6-C5	4.68	128.37	112.98
10	j	102	SPN	CM6-C18-C17	4.68	123.14	115.27
10	v	102	SPN	CM5-C13-C14	4.68	123.14	115.27
10	c	103	SPN	CM5-C13-C14	4.68	123.14	115.27
10	v	102	SPN	CM4-C9-C10	4.67	123.13	115.27
9	8	101	BCL	C3D-C2D-C1D	-4.67	99.46	105.83
9	w	101	BCL	CAC-C3C-C2C	-4.67	102.59	114.26
9	e	101	BCL	CAC-C3C-C2C	-4.67	102.59	114.26
9	x	101	BCL	CAC-C3C-C2C	-4.67	102.59	114.26
10	a	103	SPN	CM6-C18-C17	4.67	123.12	115.27
10	q	102	SPN	CM5-C13-C14	4.67	123.12	115.27
10	h	103	SPN	C11-C10-C9	4.66	128.31	112.98
9	g	101	BCL	CAC-C3C-C2C	-4.66	102.62	114.26
10	p	103	SPN	CM5-C13-C14	4.65	123.10	115.27
9	0	101	BCL	C3D-C2D-C1D	-4.65	99.48	105.83
10	1	103	SPN	CM6-C18-C17	4.65	123.09	115.27
10	l	102	SPN	C11-C10-C9	4.65	128.27	112.98
10	0	102	SPN	CM5-C13-C14	4.65	123.09	115.27
10	5	103	SPN	CM5-C13-C14	4.65	123.09	115.27
10	1	103	SPN	C16-C17-C18	4.64	125.63	113.45
10	r	102	SPN	CM5-C13-C14	4.64	123.08	115.27
10	M	406	SPN	C7-C6-C5	4.64	128.24	112.98
10	a	102	SPN	CM5-C13-C14	4.64	123.07	115.27
8	L	305	U10	C1M-C1-C6	-4.63	116.85	124.40
10	1	102	SPN	CM5-C13-C14	4.63	123.05	115.27
10	3	102	SPN	CM5-C13-C14	4.63	123.05	115.27
9	b	101	BCL	C3C-C4C-CHD	-4.62	113.51	123.39
9	k	101	BCL	CAC-C3C-C2C	-4.62	102.70	114.26
9	n	101	BCL	CAC-C3C-C2C	-4.62	102.71	114.26
10	e	102	SPN	CM5-C13-C14	4.62	123.04	115.27
10	u	102	SPN	CM5-C13-C14	4.62	123.04	115.27
10	s	102	SPN	CM4-C9-C10	4.62	123.04	115.27
9	M	404	BCL	CHC-C4B-NB	-4.62	119.37	124.26
10	m	102	SPN	CM5-C13-C14	4.62	123.04	115.27
10	v	102	SPN	C7-C6-C5	4.61	128.16	112.98
10	s	102	SPN	CM5-C13-C14	4.61	123.03	115.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	7	103	SPN	CM6-C18-C17	4.61	123.03	115.27
10	7	103	SPN	CM5-C13-C14	4.61	123.02	115.27
9	5	101	BCL	CAC-C3C-C2C	-4.61	102.75	114.26
10	c	102	SPN	CM4-C9-C10	4.60	123.01	115.27
10	w	102	SPN	CM5-C13-C14	4.60	123.01	115.27
10	h	102	SPN	CM5-C13-C14	4.60	123.01	115.27
10	7	102	SPN	CM5-C13-C14	4.60	123.01	115.27
10	i	102	SPN	CM5-C13-C14	4.60	123.01	115.27
10	a	103	SPN	CM5-C13-C14	4.60	123.00	115.27
10	c	102	SPN	CM5-C13-C14	4.60	123.00	115.27
10	5	102	SPN	CM4-C9-C10	4.60	123.00	115.27
10	j	102	SPN	CM5-C13-C14	4.59	122.99	115.27
9	u	101	BCL	CAC-C3C-C2C	-4.59	102.79	114.26
9	d	101	BCL	CAC-C3C-C2C	-4.59	102.79	114.26
10	k	102	SPN	CM5-C13-C14	4.59	122.99	115.27
10	u	102	SPN	CM4-C9-C10	4.59	122.98	115.27
9	8	101	BCL	CHD-C4C-NC	4.58	130.16	125.08
10	9	103	SPN	CM5-C13-C14	4.58	122.98	115.27
10	3	102	SPN	CM4-C9-C10	4.58	122.97	115.27
10	e	102	SPN	CM3-C5-C6	4.58	122.97	115.27
10	k	102	SPN	CM4-C9-C10	4.58	122.97	115.27
9	f	101	BCL	CAC-C3C-C2C	-4.57	102.83	114.26
10	r	102	SPN	CM4-C9-C10	4.57	122.96	115.27
10	9	103	SPN	CM4-C9-C10	4.57	122.96	115.27
9	p	101	BCL	CAC-C3C-C2C	-4.57	102.84	114.26
10	e	102	SPN	C21-C20-C19	4.57	124.30	112.23
9	9	102	BCL	CAC-C3C-C2C	-4.56	102.85	114.26
10	c	102	SPN	C11-C10-C9	4.56	127.98	112.98
10	5	102	SPN	C11-C10-C9	4.56	127.97	112.98
10	c	103	SPN	CM6-C18-C17	4.56	122.94	115.27
9	b	101	BCL	C3D-C2D-C1D	-4.56	99.61	105.83
10	u	102	SPN	CM3-C5-C6	4.56	122.94	115.27
10	k	102	SPN	CM3-C5-C6	4.56	122.94	115.27
10	1	104	SPN	CM5-C13-C14	4.56	122.94	115.27
10	5	103	SPN	CM6-C18-C17	4.56	122.94	115.27
9	6	101	BCL	CHD-C4C-NC	4.56	130.14	125.08
10	w	102	SPN	CM3-C5-C6	4.55	122.93	115.27
10	9	103	SPN	C11-C10-C9	4.55	127.95	112.98
9	0	101	BCL	C3C-C4C-CHD	-4.55	113.67	123.39
10	i	102	SPN	CM4-C9-C10	4.55	122.92	115.27
10	i	102	SPN	C11-C10-C9	4.55	127.94	112.98
10	9	103	SPN	CM3-C5-C6	4.55	122.92	115.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	s	102	SPN	C11-C10-C9	4.54	127.93	112.98
10	u	102	SPN	C11-C10-C9	4.54	127.92	112.98
10	e	102	SPN	CM4-C9-C10	4.54	122.91	115.27
10	v	102	SPN	C11-C10-C9	4.54	127.91	112.98
10	1	105	SPN	CM6-C18-C17	4.54	122.90	115.27
10	f	102	SPN	CM5-C13-C14	4.54	122.90	115.27
10	h	102	SPN	CM3-C5-C6	4.53	122.90	115.27
10	3	102	SPN	C11-C10-C9	4.53	127.89	112.98
10	w	102	SPN	CM4-C9-C10	4.53	122.89	115.27
10	7	102	SPN	CM4-C9-C10	4.53	122.89	115.27
10	h	102	SPN	CM4-C9-C10	4.53	122.89	115.27
10	l	102	SPN	CM5-C13-C14	4.53	122.89	115.27
10	k	102	SPN	C11-C10-C9	4.53	127.87	112.98
10	m	102	SPN	CM3-C5-C6	4.52	122.88	115.27
10	i	102	SPN	CM6-C18-C17	4.52	122.88	115.27
10	i	102	SPN	CM3-C5-C6	4.52	122.88	115.27
10	w	102	SPN	C11-C10-C9	4.52	127.84	112.98
9	0	101	BCL	CHD-C4C-NC	4.52	130.09	125.08
9	t	101	BCL	CAC-C3C-C2C	-4.52	102.98	114.26
10	a	102	SPN	CM3-C5-C6	4.51	122.87	115.27
10	e	102	SPN	C11-C10-C9	4.51	127.83	112.98
10	a	102	SPN	C7-C6-C5	4.51	127.83	112.98
10	p	102	SPN	C7-C6-C5	4.51	127.81	112.98
10	l	102	SPN	CM6-C18-C17	4.51	122.86	115.27
10	7	102	SPN	C11-C10-C9	4.51	127.81	112.98
10	s	102	SPN	CM6-C18-C17	4.51	122.85	115.27
10	r	102	SPN	CM6-C18-C17	4.51	122.85	115.27
10	r	102	SPN	C11-C10-C9	4.51	127.80	112.98
10	1	102	SPN	CM3-C5-C6	4.50	122.85	115.27
10	1	105	SPN	C21-C20-C19	4.50	124.12	112.23
10	c	102	SPN	CM3-C5-C6	4.50	122.85	115.27
10	a	102	SPN	C11-C10-C9	4.50	127.78	112.98
10	u	102	SPN	CM6-C18-C17	4.50	122.84	115.27
10	s	102	SPN	CM3-C5-C6	4.50	122.84	115.27
10	w	102	SPN	C7-C6-C5	4.50	127.77	112.98
10	t	102	SPN	CM5-C13-C14	4.50	122.83	115.27
10	t	102	SPN	C21-C20-C19	4.50	124.10	112.23
10	v	102	SPN	CM6-C18-C17	4.50	122.83	115.27
10	h	102	SPN	C11-C10-C9	4.49	127.76	112.98
10	7	102	SPN	CM6-C18-C17	4.49	122.83	115.27
10	3	102	SPN	CM3-C5-C6	4.49	122.83	115.27
10	p	102	SPN	CM3-C5-C6	4.49	122.83	115.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	5	102	SPN	CM3-C5-C6	4.49	122.82	115.27
10	h	102	SPN	C7-C6-C5	4.49	127.74	112.98
10	m	102	SPN	CM6-C18-C17	4.48	122.81	115.27
10	c	102	SPN	CM6-C18-C17	4.48	122.81	115.27
10	9	103	SPN	C7-C6-C5	4.48	127.72	112.98
10	3	102	SPN	C7-C6-C5	4.48	127.72	112.98
10	p	103	SPN	CM6-C18-C17	4.48	122.81	115.27
10	1	102	SPN	C21-C20-C19	4.48	124.07	112.23
10	h	102	SPN	C21-C20-C19	4.48	124.07	112.23
10	m	102	SPN	CM4-C9-C10	4.48	122.81	115.27
9	l	101	BCL	CAC-C3C-C2C	-4.48	103.06	114.26
10	i	102	SPN	C7-C6-C5	4.48	127.71	112.98
10	n	102	SPN	CM6-C18-C17	4.48	122.81	115.27
10	a	102	SPN	CM4-C9-C10	4.48	122.81	115.27
10	u	102	SPN	C7-C6-C5	4.48	127.71	112.98
10	m	102	SPN	C11-C10-C9	4.48	127.70	112.98
10	7	102	SPN	CM3-C5-C6	4.48	122.80	115.27
10	c	102	SPN	C7-C6-C5	4.48	127.70	112.98
10	k	102	SPN	C7-C6-C5	4.47	127.69	112.98
9	6	101	BCL	C3C-C4C-CHD	-4.47	113.83	123.39
10	s	102	SPN	C7-C6-C5	4.47	127.69	112.98
10	9	103	SPN	CM6-C18-C17	4.47	122.79	115.27
10	k	102	SPN	CM6-C18-C17	4.47	122.79	115.27
10	h	103	SPN	CM5-C13-C14	4.47	122.79	115.27
10	e	102	SPN	C7-C6-C5	4.47	127.67	112.98
9	h	101	BCL	CAC-C3C-C2C	-4.47	103.10	114.26
10	3	102	SPN	CM6-C18-C17	4.47	122.78	115.27
10	w	102	SPN	CM6-C18-C17	4.47	122.78	115.27
10	1	102	SPN	C7-C6-C5	4.47	127.67	112.98
10	5	102	SPN	C7-C6-C5	4.46	127.65	112.98
10	c	102	SPN	C21-C20-C19	4.46	124.01	112.23
10	t	102	SPN	CM6-C18-C17	4.46	122.77	115.27
10	r	102	SPN	CM3-C5-C6	4.46	122.77	115.27
9	8	101	BCL	C3C-C4C-CHD	-4.46	113.87	123.39
10	a	102	SPN	C21-C20-C19	4.46	124.00	112.23
10	h	102	SPN	CM6-C18-C17	4.45	122.76	115.27
10	k	102	SPN	C21-C20-C19	4.44	123.95	112.23
10	r	102	SPN	C7-C6-C5	4.44	127.57	112.98
10	1	102	SPN	C11-C10-C9	4.44	127.57	112.98
10	5	102	SPN	C21-C20-C19	4.43	123.94	112.23
10	e	102	SPN	CM6-C18-C17	4.43	122.73	115.27
10	7	102	SPN	C7-C6-C5	4.43	127.53	112.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	w	102	SPN	C21-C20-C19	4.42	123.91	112.23
10	m	102	SPN	C7-C6-C5	4.42	127.52	112.98
10	m	102	SPN	C21-C20-C19	4.42	123.90	112.23
9	j	101	BCL	CAC-C3C-C2C	-4.42	103.22	114.26
10	M	406	SPN	C20-C21-C22	4.42	131.05	115.76
10	3	102	SPN	C21-C20-C19	4.41	123.88	112.23
10	1	102	SPN	CM6-C18-C17	4.41	122.69	115.27
10	1	102	SPN	CM4-C9-C10	4.40	122.67	115.27
9	s	101	BCL	CHC-C4B-NB	-4.40	119.60	124.26
9	2	101	BCL	C1D-ND-C4D	-4.39	103.21	106.33
9	8	101	BCL	C1D-ND-C4D	-4.39	103.22	106.33
10	9	103	SPN	C21-C20-C19	4.39	123.83	112.23
10	a	102	SPN	CM6-C18-C17	4.38	122.65	115.27
9	3	101	BCL	CAC-C3C-C2C	-4.38	103.31	114.26
10	5	102	SPN	CM6-C18-C17	4.38	122.64	115.27
8	A	101	U10	C12-C13-C14	-4.38	117.11	127.66
10	7	102	SPN	C21-C20-C19	4.34	123.70	112.23
10	s	102	SPN	C21-C20-C19	4.34	123.70	112.23
9	L	301	BCL	CHC-C4B-NB	-4.34	119.66	124.26
10	0	102	SPN	CM6-C18-C17	4.33	122.56	115.27
10	n	102	SPN	C21-C20-C19	4.33	123.66	112.23
10	p	102	SPN	C11-C10-C9	4.32	127.19	112.98
9	1	101	BCL	CHC-C4B-NB	-4.32	119.69	124.26
10	i	102	SPN	C21-C20-C19	4.31	123.62	112.23
9	b	101	BCL	CHD-C4C-NC	4.30	129.85	125.08
10	7	103	SPN	C21-C20-C19	4.28	123.55	112.23
9	q	101	BCL	CAC-C3C-C2C	-4.27	103.60	114.26
9	i	101	BCL	CHC-C4B-NB	-4.26	119.74	124.26
10	r	102	SPN	C21-C20-C19	4.25	123.46	112.23
10	5	103	SPN	C21-C20-C19	4.25	123.45	112.23
9	7	101	BCL	CHC-C4B-NB	-4.25	119.76	124.26
10	u	102	SPN	C21-C20-C19	4.24	123.44	112.23
9	5	101	BCL	CHC-C4B-NB	-4.24	119.77	124.26
9	q	101	BCL	CHC-C4B-NB	-4.23	119.78	124.26
10	c	103	SPN	C21-C20-C19	4.22	123.39	112.23
9	3	101	BCL	CHC-C4B-NB	-4.22	119.78	124.26
9	m	101	BCL	CHC-C4B-NB	-4.16	119.85	124.26
9	2	101	BCL	C4A-NA-C1A	4.14	108.57	106.71
9	L	304	BCL	CHC-C4B-NB	-4.14	119.88	124.26
9	g	101	BCL	CHC-C4B-NB	-4.09	119.92	124.26
9	u	101	BCL	CHC-C4B-NB	-4.08	119.94	124.26
10	q	102	SPN	C20-C21-C22	4.07	129.86	115.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	a	101	BCL	CHC-C4B-NB	-4.06	119.96	124.26
9	c	101	BCL	CHC-C4B-NB	-4.05	119.97	124.26
9	o	101	BCL	CHC-C4B-NB	-4.03	119.99	124.26
9	9	102	BCL	CHC-C4B-NB	-4.03	119.99	124.26
8	L	305	U10	C6-C1-C2	4.02	122.36	119.18
10	p	102	SPN	CM4-C9-C10	4.01	122.02	115.27
10	1	103	SPN	CM5-C13-C14	4.01	122.01	115.27
9	6	101	BCL	C1D-ND-C4D	-4.00	103.49	106.33
10	p	102	SPN	CM5-C13-C14	4.00	122.01	115.27
9	p	101	BCL	CHC-C4B-NB	-4.00	120.02	124.26
9	b	101	BCL	C1D-ND-C4D	-3.99	103.50	106.33
9	v	101	BCL	CHC-C4B-NB	-3.99	120.04	124.26
9	e	101	BCL	CHC-C4B-NB	-3.98	120.04	124.26
9	M	402	BCL	CHD-C4C-NC	3.97	129.49	125.08
9	w	101	BCL	CHC-C4B-NB	-3.96	120.06	124.26
9	k	101	BCL	CHC-C4B-NB	-3.96	120.06	124.26
10	M	406	SPN	CM7-C22-C21	3.95	125.60	111.29
10	p	102	SPN	CM6-C18-C17	3.95	121.91	115.27
10	j	102	SPN	CM7-C22-C21	3.94	125.56	111.29
8	A	101	U10	C17-C18-C19	-3.93	118.19	127.66
9	4	101	BCL	C1D-ND-C4D	-3.93	103.54	106.33
13	L	303	BPH	C1-C2-C3	3.93	132.84	126.04
9	n	101	BCL	CHC-C4B-NB	-3.91	120.11	124.26
9	l	101	BCL	CHC-C4B-NB	-3.91	120.12	124.26
9	x	101	BCL	CHC-C4B-NB	-3.91	120.12	124.26
10	5	102	SPN	CM7-C22-C21	3.90	125.42	111.29
9	0	101	BCL	C1D-ND-C4D	-3.90	103.56	106.33
13	M	409	BPH	C4D-CHA-CBD	3.88	110.27	108.52
9	2	101	BCL	O1D-CGD-CBD	-3.86	116.58	124.48
9	j	101	BCL	CHC-C4B-NB	-3.85	120.18	124.26
9	f	101	BCL	CHC-C4B-NB	-3.83	120.20	124.26
9	d	101	BCL	CHC-C4B-NB	-3.83	120.20	124.26
10	p	102	SPN	C21-C20-C19	3.80	122.27	112.23
8	A	101	U10	C22-C23-C24	-3.79	118.53	127.66
9	i	101	BCL	CHC-C1C-NC	3.79	129.76	124.51
10	1	104	SPN	CM7-C22-C21	3.79	125.02	111.29
9	h	101	BCL	CHC-C4B-NB	-3.79	120.24	124.26
9	M	402	BCL	C1D-ND-C4D	-3.79	103.64	106.33
9	t	101	BCL	CHC-C4B-NB	-3.79	120.25	124.26
9	r	101	BCL	CHC-C4B-NB	-3.75	120.29	124.26
13	L	303	BPH	C4D-CHA-CBD	3.74	110.21	108.52
10	q	102	SPN	CM7-C22-C21	3.74	124.83	111.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	3	102	SPN	C20-C21-C22	3.70	128.56	115.76
9	o	101	BCL	CHC-C1C-NC	3.69	129.62	124.51
10	q	102	SPN	C21-C20-C19	3.69	121.97	112.23
9	8	101	BCL	CED-O2D-CGD	-3.68	107.62	115.94
9	M	402	BCL	C3C-C4C-CHD	-3.67	115.55	123.39
10	1	102	SPN	C6-C7-C8	3.63	123.82	111.88
9	1	101	BCL	CHC-C1C-NC	3.63	129.53	124.51
10	5	102	SPN	C20-C21-C22	3.62	128.27	115.76
10	7	102	SPN	C6-C7-C8	3.61	123.76	111.88
10	a	102	SPN	C6-C7-C8	3.61	123.74	111.88
10	v	102	SPN	C23-C22-C21	3.60	131.06	112.13
13	L	303	BPH	C2D-C1D-ND	-3.60	107.04	109.53
13	M	405	BPH	C2D-C1D-ND	-3.59	107.05	109.53
10	m	102	SPN	C6-C7-C8	3.58	123.65	111.88
9	L	304	BCL	O2A-C1-C2	3.57	118.03	108.64
10	5	102	SPN	C6-C7-C8	3.57	123.62	111.88
10	1	102	SPN	C10-C11-C12	3.56	123.59	111.88
10	c	103	SPN	CM7-C22-C21	3.56	124.17	111.29
10	a	102	SPN	C20-C21-C22	3.55	128.05	115.76
10	3	102	SPN	C6-C7-C8	3.55	123.54	111.88
10	a	102	SPN	CM7-C22-C21	3.54	124.11	111.29
10	j	102	SPN	C16-C15-C14	3.53	125.90	113.19
10	h	102	SPN	C6-C7-C8	3.53	123.47	111.88
12	C	403	HEM	CAC-C3C-C4C	-3.50	116.44	124.90
9	8	101	BCL	CHB-C1B-NB	-3.50	120.55	124.26
10	c	103	SPN	C20-C21-C22	3.50	127.87	115.76
10	w	102	SPN	C6-C7-C8	3.49	123.36	111.88
10	c	102	SPN	C6-C7-C8	3.49	123.36	111.88
10	r	102	SPN	C6-C7-C8	3.49	123.36	111.88
12	C	402	HEM	CAB-C3B-C4B	3.48	140.71	124.47
10	e	102	SPN	C6-C7-C8	3.48	123.32	111.88
10	a	102	SPN	C10-C11-C12	3.48	123.31	111.88
8	L	305	U10	C10-C9-C11	3.47	121.11	115.27
10	7	103	SPN	C20-C21-C22	3.47	127.77	115.76
8	M	403	U10	C22-C23-C24	-3.47	119.31	127.66
10	9	103	SPN	C6-C7-C8	3.47	123.27	111.88
10	l	102	SPN	CM7-C22-C21	3.45	123.80	111.29
8	M	403	U10	C4M-O4-C4	3.45	128.71	116.47
10	i	102	SPN	C6-C7-C8	3.45	123.23	111.88
9	5	101	BCL	CHC-C1C-NC	3.45	129.28	124.51
10	h	103	SPN	C23-C22-C21	3.45	130.27	112.13
10	k	102	SPN	C6-C7-C8	3.44	123.20	111.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	u	102	SPN	C6-C7-C8	3.43	123.15	111.88
10	5	102	SPN	C15-C16-C17	3.43	125.51	113.19
9	7	101	BCL	CHC-C1C-NC	3.43	129.25	124.51
9	b	101	BCL	CED-O2D-CGD	-3.42	108.19	115.94
9	0	101	BCL	O1D-CGD-CBD	-3.42	117.49	124.48
10	s	102	SPN	C6-C7-C8	3.41	123.09	111.88
10	h	103	SPN	C16-C15-C14	3.41	125.45	113.19
9	8	101	BCL	C4B-C3B-C2B	-3.39	102.90	108.36
10	w	102	SPN	C10-C11-C12	3.38	122.99	111.88
10	3	102	SPN	C10-C11-C12	3.38	122.99	111.88
10	m	102	SPN	C10-C11-C12	3.38	122.98	111.88
9	k	101	BCL	CHC-C1C-NC	3.37	129.18	124.51
9	M	402	BCL	C4B-C3B-C2B	-3.37	102.94	108.36
8	L	305	U10	C22-C23-C24	-3.36	119.58	127.66
10	h	102	SPN	C10-C11-C12	3.36	122.91	111.88
10	f	102	SPN	C23-C22-C21	3.36	129.78	112.13
9	M	402	BCL	C3D-C4D-ND	3.35	115.66	110.24
9	4	101	BCL	C4B-C3B-C2B	-3.35	102.97	108.36
10	1	102	SPN	C15-C16-C17	3.34	125.19	113.19
9	v	101	BCL	CHC-C1C-NC	3.34	129.13	124.51
10	a	102	SPN	C15-C16-C17	3.34	125.18	113.19
9	2	101	BCL	C4B-C3B-C2B	-3.33	102.99	108.36
9	L	304	BCL	CAC-C3C-C2C	-3.33	105.93	114.26
9	M	402	BCL	CAA-C2A-C3A	-3.33	103.66	112.78
9	b	101	BCL	O1D-CGD-CBD	-3.32	117.68	124.48
9	w	101	BCL	CHC-C1C-NC	3.32	129.10	124.51
10	e	102	SPN	C10-C11-C12	3.31	122.75	111.88
9	3	101	BCL	CHC-C1C-NC	3.30	129.07	124.51
10	i	102	SPN	C20-C21-C22	3.30	127.17	115.76
10	7	102	SPN	C10-C11-C12	3.29	122.71	111.88
9	6	101	BCL	CED-O2D-CGD	-3.29	108.50	115.94
10	5	102	SPN	C10-C11-C12	3.29	122.69	111.88
10	7	102	SPN	C20-C21-C22	3.29	127.14	115.76
10	u	102	SPN	C10-C11-C12	3.29	122.68	111.88
9	M	404	BCL	CAC-C3C-C2C	-3.28	106.06	114.26
9	f	101	BCL	CHC-C1C-NC	3.28	129.04	124.51
10	f	102	SPN	C16-C15-C14	3.27	124.96	113.19
10	3	102	SPN	C15-C16-C17	3.27	124.94	113.19
9	s	101	BCL	CHC-C1C-NC	3.27	129.03	124.51
10	c	102	SPN	C10-C11-C12	3.27	122.62	111.88
9	6	101	BCL	C4B-C3B-C2B	-3.26	103.11	108.36
10	k	102	SPN	C10-C11-C12	3.26	122.60	111.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	5	103	SPN	C20-C21-C22	3.26	127.03	115.76
10	i	102	SPN	C10-C11-C12	3.25	122.57	111.88
10	1	104	SPN	C16-C15-C14	3.25	124.88	113.19
10	5	103	SPN	CM7-C22-C21	3.25	123.06	111.29
10	9	103	SPN	C10-C11-C12	3.25	122.56	111.88
9	l	101	BCL	CHC-C1C-NC	3.25	129.00	124.51
10	u	102	SPN	C20-C21-C22	3.24	126.98	115.76
10	r	102	SPN	C10-C11-C12	3.24	122.54	111.88
10	r	102	SPN	C20-C21-C22	3.24	126.97	115.76
9	b	101	BCL	C4B-C3B-C2B	-3.23	103.16	108.36
10	1	103	SPN	C20-C21-C22	3.23	126.93	115.76
9	L	304	BCL	CHC-C1C-NC	3.22	128.97	124.51
10	1	103	SPN	C10-C11-C12	3.22	122.47	111.88
10	0	102	SPN	C23-C22-C21	3.21	129.03	112.13
9	r	101	BCL	CHC-C1C-NC	3.21	128.96	124.51
10	s	102	SPN	C10-C11-C12	3.21	122.44	111.88
10	e	102	SPN	C15-C16-C17	3.21	124.73	113.19
9	q	101	BCL	CHC-C1C-NC	3.20	128.93	124.51
10	7	103	SPN	CM7-C22-C21	3.19	122.86	111.29
9	t	101	BCL	CHC-C1C-NC	3.19	128.92	124.51
10	a	103	SPN	C16-C15-C14	3.19	124.65	113.19
9	8	101	BCL	C3D-C4D-ND	3.19	115.39	110.24
10	v	102	SPN	C10-C11-C12	3.18	122.33	111.88
9	d	101	BCL	CHC-C1C-NC	3.18	128.91	124.51
10	l	102	SPN	C16-C15-C14	3.18	124.61	113.19
9	L	301	BCL	CAC-C3C-C2C	-3.17	106.33	114.26
13	M	409	BPH	C2D-C1D-ND	-3.17	107.34	109.53
9	w	101	BCL	CHB-C1B-NB	-3.17	120.90	124.26
10	s	102	SPN	C20-C21-C22	3.17	126.72	115.76
8	M	403	U10	C17-C18-C19	-3.16	120.05	127.66
10	n	102	SPN	C20-C21-C22	3.16	126.70	115.76
8	M	403	U10	C10-C9-C11	3.16	120.59	115.27
9	h	101	BCL	CHC-C1C-NC	3.16	128.88	124.51
10	h	102	SPN	C15-C16-C17	3.16	124.54	113.19
9	m	101	BCL	CHB-C1B-NB	-3.16	120.92	124.26
8	M	403	U10	C47-C48-C49	-3.15	120.07	127.66
10	n	102	SPN	C15-C16-C17	3.15	124.52	113.19
9	4	101	BCL	CHB-C4A-NA	3.15	128.87	124.51
8	A	101	U10	C4M-O4-C4	3.15	127.63	116.47
10	9	103	SPN	C20-C21-C22	3.15	126.65	115.76
10	i	102	SPN	CM7-C22-C21	3.13	122.64	111.29
10	7	102	SPN	C15-C16-C17	3.13	124.45	113.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	w	102	SPN	C20-C21-C22	3.13	126.59	115.76
9	8	101	BCL	O1D-CGD-CBD	-3.13	118.08	124.48
9	6	101	BCL	C3D-C4D-ND	3.13	115.29	110.24
9	0	101	BCL	C4B-C3B-C2B	-3.13	103.33	108.36
10	l	102	SPN	C10-C11-C12	3.12	122.14	111.88
9	0	101	BCL	CED-O2D-CGD	-3.12	108.88	115.94
9	c	101	BCL	CHB-C1B-NB	-3.12	120.96	124.26
10	5	103	SPN	C15-C16-C17	3.11	124.38	113.19
10	9	103	SPN	C15-C16-C17	3.11	124.38	113.19
10	0	102	SPN	C15-C16-C17	3.11	124.38	113.19
10	k	102	SPN	C20-C21-C22	3.11	126.53	115.76
10	u	102	SPN	CM7-C22-C21	3.11	122.54	111.29
10	w	102	SPN	C15-C16-C17	3.10	124.32	113.19
8	A	101	U10	C15-C14-C16	3.10	120.48	115.27
10	p	102	SPN	C16-C15-C14	3.09	124.31	113.19
9	b	101	BCL	C3D-C4D-ND	3.09	115.24	110.24
9	x	101	BCL	CHC-C1C-NC	3.09	128.79	124.51
10	i	102	SPN	C15-C16-C17	3.08	124.25	113.19
10	3	102	SPN	CM7-C22-C21	3.08	122.43	111.29
10	r	102	SPN	C15-C16-C17	3.07	124.24	113.19
10	k	102	SPN	C15-C16-C17	3.07	124.22	113.19
10	c	102	SPN	C15-C16-C17	3.07	124.22	113.19
9	0	101	BCL	C3D-C4D-ND	3.07	115.20	110.24
9	6	101	BCL	C4-C3-C5	3.07	120.43	115.27
10	n	102	SPN	CM7-C22-C21	3.07	122.40	111.29
13	L	303	BPH	C2B-C1B-NB	-3.07	107.41	109.53
9	p	101	BCL	CHB-C1B-NB	-3.06	121.01	124.26
9	x	101	BCL	CHB-C1B-NB	-3.06	121.01	124.26
9	4	101	BCL	CMB-C2B-C3B	3.06	134.19	125.93
9	l	101	BCL	CHB-C1B-NB	-3.06	121.02	124.26
9	s	101	BCL	CHB-C1B-NB	-3.05	121.02	124.26
10	q	102	SPN	O1-C1-C2	3.05	115.04	108.78
10	m	102	SPN	C15-C16-C17	3.05	124.14	113.19
9	k	101	BCL	CHB-C1B-NB	-3.05	121.03	124.26
9	j	101	BCL	CHC-C1C-NC	3.05	128.72	124.51
10	c	102	SPN	C20-C21-C22	3.04	126.28	115.76
10	7	103	SPN	C16-C15-C14	3.04	124.11	113.19
9	r	101	BCL	CHB-C1B-NB	-3.04	121.04	124.26
10	h	103	SPN	C10-C11-C12	3.04	121.86	111.88
10	t	102	SPN	C16-C15-C14	3.03	124.10	113.19
10	k	102	SPN	CM7-C22-C21	3.03	122.28	111.29
9	g	101	BCL	CHB-C1B-NB	-3.03	121.05	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	s	102	SPN	CM7-C22-C21	3.03	122.27	111.29
9	4	101	BCL	CHB-C1B-NB	-3.03	121.05	124.26
9	9	102	BCL	CHB-C1B-NB	-3.03	121.05	124.26
10	1	105	SPN	C15-C16-C17	3.03	124.07	113.19
9	2	101	BCL	C3D-C4D-ND	3.02	115.13	110.24
10	r	102	SPN	CM7-C22-C21	3.02	122.23	111.29
10	q	102	SPN	C15-C16-C17	3.02	124.05	113.19
9	v	101	BCL	CHB-C1B-NB	-3.02	121.06	124.26
10	c	103	SPN	C15-C16-C17	3.02	124.05	113.19
9	s	101	BCL	CMA-C3A-C4A	-3.02	103.66	111.77
9	n	101	BCL	CHC-C1C-NC	3.02	128.68	124.51
9	a	101	BCL	CHC-C1C-NC	3.01	128.68	124.51
10	m	102	SPN	C20-C21-C22	3.01	126.17	115.76
10	h	102	SPN	C20-C21-C22	3.01	126.17	115.76
9	p	101	BCL	CHC-C1C-NC	3.01	128.67	124.51
10	u	102	SPN	C15-C16-C17	3.00	123.99	113.19
9	6	101	BCL	O1D-CGD-CBD	-3.00	118.34	124.48
9	M	404	BCL	CHC-C1C-NC	3.00	128.66	124.51
9	a	101	BCL	CHB-C1B-NB	-3.00	121.08	124.26
9	e	101	BCL	CHB-C1B-NB	-3.00	121.08	124.26
10	7	102	SPN	CM7-C22-C21	3.00	122.15	111.29
9	o	101	BCL	CHB-C1B-NB	-3.00	121.09	124.26
9	8	101	BCL	CHB-C4A-NA	3.00	128.65	124.51
8	M	403	U10	C20-C19-C21	2.99	120.31	115.27
13	L	303	BPH	O2A-C1-C2	-2.99	100.78	108.64
10	t	102	SPN	C10-C11-C12	2.98	121.66	111.88
9	b	101	BCL	CMB-C2B-C3B	2.97	133.96	125.93
10	9	103	SPN	CM7-C22-C21	2.97	122.06	111.29
9	2	101	BCL	CHB-C1B-NB	-2.97	121.11	124.26
10	s	102	SPN	C15-C16-C17	2.97	123.86	113.19
8	L	305	U10	C17-C18-C19	-2.97	120.51	127.66
10	1	102	SPN	C20-C21-C22	2.97	126.02	115.76
9	m	101	BCL	CHC-C1C-NC	2.96	128.61	124.51
9	u	101	BCL	CHB-C1B-NB	-2.96	121.12	124.26
10	w	102	SPN	CM7-C22-C21	2.96	122.01	111.29
10	c	102	SPN	CM7-C22-C21	2.96	122.00	111.29
8	A	101	U10	C30-C29-C31	2.96	120.24	115.27
9	L	304	BCL	C4D-CHA-C1A	2.95	124.84	121.25
9	e	101	BCL	CHC-C1C-NC	2.94	128.58	124.51
10	1	102	SPN	CM7-C22-C21	2.94	121.94	111.29
10	c	103	SPN	C10-C11-C12	2.93	121.51	111.88
10	t	102	SPN	C20-C21-C22	2.93	125.89	115.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	n	101	BCL	CHB-C1B-NB	-2.92	121.16	124.26
12	C	401	HEM	CAB-C3B-C2B	2.91	138.21	128.60
10	0	102	SPN	C10-C11-C12	2.91	121.46	111.88
9	5	101	BCL	CHB-C1B-NB	-2.91	121.18	124.26
10	p	103	SPN	C15-C16-C17	2.91	123.65	113.19
9	f	101	BCL	CHB-C1B-NB	-2.91	121.18	124.26
10	v	102	SPN	C6-C7-C8	2.91	121.43	111.88
9	L	304	BCL	C2A-C1A-CHA	2.90	128.94	123.86
10	p	102	SPN	C15-C16-C17	2.90	123.63	113.19
9	2	101	BCL	CHB-C4A-NA	2.90	128.53	124.51
10	q	102	SPN	C10-C11-C12	2.90	121.42	111.88
9	8	101	BCL	O2A-CGA-CBA	2.90	121.00	111.91
13	M	409	BPH	C4A-C3A-C2A	-2.90	100.08	102.84
10	5	103	SPN	C10-C11-C12	2.89	121.39	111.88
10	a	103	SPN	C10-C11-C12	2.89	121.38	111.88
9	6	101	BCL	CMB-C2B-C3B	2.89	133.73	125.93
9	i	101	BCL	CHB-C1B-NB	-2.89	121.20	124.26
10	h	102	SPN	CM7-C22-C21	2.89	121.74	111.29
9	2	101	BCL	O2A-CGA-CBA	2.88	120.96	111.91
9	4	101	BCL	C3D-C4D-ND	2.88	114.89	110.24
9	c	101	BCL	CHC-C1C-NC	2.87	128.49	124.51
9	g	101	BCL	CHC-C1C-NC	2.87	128.48	124.51
9	M	404	BCL	CHA-C1A-NA	-2.87	119.83	126.40
10	f	102	SPN	C10-C11-C12	2.86	121.28	111.88
9	L	304	BCL	CHA-C1A-NA	-2.86	119.86	126.40
10	1	105	SPN	CM7-C22-C21	2.85	121.62	111.29
9	M	402	BCL	C11-C12-C13	-2.85	106.71	115.92
10	m	102	SPN	CM7-C22-C21	2.85	121.61	111.29
9	6	101	BCL	C1-C2-C3	-2.85	121.12	126.04
9	0	101	BCL	C4A-NA-C1A	2.84	107.98	106.71
9	0	101	BCL	CHB-C1B-NB	-2.84	121.25	124.26
9	o	101	BCL	C2A-C3A-C4A	-2.84	97.29	101.87
9	2	101	BCL	C1C-NC-C4C	-2.83	105.43	106.71
9	4	101	BCL	O1D-CGD-CBD	-2.82	118.71	124.48
10	1	104	SPN	C10-C11-C12	2.82	121.16	111.88
11	H	301	MW9	C8-C9-C10	2.82	128.75	114.42
9	r	101	BCL	CHA-C1A-NA	-2.81	119.97	126.40
9	p	101	BCL	CHA-C1A-NA	-2.81	119.97	126.40
9	f	101	BCL	CHA-C1A-NA	-2.81	119.97	126.40
9	j	101	BCL	CHB-C1B-NB	-2.80	121.29	124.26
9	6	101	BCL	CHB-C1B-NB	-2.80	121.29	124.26
9	q	101	BCL	CHB-C1B-NB	-2.80	121.29	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	M	403	U10	C15-C14-C16	2.80	119.98	115.27
8	L	305	U10	C20-C19-C21	2.79	119.97	115.27
9	n	101	BCL	CHA-C1A-NA	-2.79	120.01	126.40
10	7	103	SPN	C10-C11-C12	2.79	121.04	111.88
10	p	103	SPN	C10-C11-C12	2.79	121.04	111.88
10	t	102	SPN	C15-C16-C17	2.78	123.19	113.19
10	e	102	SPN	CM7-C22-C21	2.78	121.36	111.29
9	1	101	BCL	CHB-C1B-NB	-2.78	121.31	124.26
9	0	101	BCL	CMB-C2B-C3B	2.78	133.44	125.93
9	b	101	BCL	C1-C2-C3	-2.78	121.24	126.04
9	b	101	BCL	CHB-C4A-NA	2.78	128.35	124.51
9	9	102	BCL	CHC-C1C-NC	2.78	128.35	124.51
9	t	101	BCL	CHB-C1B-NB	-2.78	121.32	124.26
10	e	102	SPN	C20-C21-C22	2.77	125.34	115.76
9	L	301	BCL	C3C-C4C-CHD	-2.77	117.48	123.39
9	2	101	BCL	C1-O2A-CGA	2.77	123.70	116.44
9	6	101	BCL	CHC-C1C-NC	2.76	128.33	124.51
9	L	301	BCL	CHC-C1C-NC	2.75	128.32	124.51
10	c	103	SPN	C16-C15-C14	2.75	123.06	113.19
9	0	101	BCL	CHB-C4A-NA	2.75	128.31	124.51
9	M	402	BCL	C4-C3-C2	-2.74	116.65	123.68
9	7	101	BCL	CHB-C1B-NB	-2.73	121.36	124.26
9	x	101	BCL	CHA-C1A-NA	-2.73	120.15	126.40
9	4	101	BCL	C4A-NA-C1A	2.73	107.93	106.71
9	L	304	BCL	C2A-C3A-C4A	-2.73	97.46	101.87
10	p	103	SPN	C6-C7-C8	2.73	120.84	111.88
9	o	101	BCL	C3C-C4C-CHD	-2.73	117.57	123.39
10	v	102	SPN	C16-C15-C14	2.72	122.98	113.19
10	j	102	SPN	C10-C11-C12	2.72	120.83	111.88
9	b	101	BCL	C4A-NA-C1A	2.72	107.93	106.71
10	q	102	SPN	C16-C15-C14	2.72	122.97	113.19
9	h	101	BCL	CHB-C1B-NB	-2.72	121.38	124.26
8	L	305	U10	C15-C14-C16	2.71	119.83	115.27
9	u	101	BCL	C4D-CHA-C1A	2.71	124.55	121.25
9	b	101	BCL	CHB-C1B-NB	-2.71	121.39	124.26
9	d	101	BCL	CHB-C1B-NB	-2.70	121.39	124.26
8	A	101	U10	C25-C24-C26	2.70	119.82	115.27
10	s	102	SPN	C16-C15-C14	2.70	122.89	113.19
8	L	305	U10	C12-C13-C14	-2.70	121.17	127.66
9	4	101	BCL	CED-O2D-CGD	-2.70	109.84	115.94
10	n	102	SPN	C10-C11-C12	2.69	120.74	111.88
9	8	101	BCL	CMB-C2B-C3B	2.69	133.21	125.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	p	103	SPN	C16-C15-C14	2.69	122.87	113.19
10	v	102	SPN	C15-C16-C17	2.68	122.84	113.19
10	1	103	SPN	C23-C22-C21	2.68	126.24	112.13
9	8	101	BCL	C4A-NA-C1A	2.68	107.91	106.71
10	1	105	SPN	C10-C11-C12	2.68	120.67	111.88
10	t	102	SPN	C23-C22-C21	2.67	126.17	112.13
10	k	102	SPN	C16-C15-C14	2.67	122.77	113.19
10	0	102	SPN	C16-C15-C14	2.66	122.77	113.19
9	v	101	BCL	CHA-C1A-NA	-2.66	120.30	126.40
10	c	102	SPN	C16-C15-C14	2.66	122.76	113.19
9	M	402	BCL	O2A-CGA-CBA	2.66	120.26	111.91
9	L	301	BCL	CHB-C1B-NB	-2.66	121.44	124.26
10	7	103	SPN	C15-C16-C17	2.66	122.74	113.19
10	5	103	SPN	C16-C15-C14	2.65	122.73	113.19
8	A	101	U10	C20-C19-C21	2.65	119.73	115.27
10	l	102	SPN	C6-C7-C8	2.65	120.60	111.88
10	u	102	SPN	C16-C15-C14	2.65	122.72	113.19
9	3	101	BCL	CHB-C1B-NB	-2.65	121.45	124.26
9	L	304	BCL	C1D-ND-C4D	2.65	108.21	106.33
9	m	101	BCL	CMA-C3A-C4A	-2.65	104.66	111.77
9	4	101	BCL	O2A-CGA-CBA	2.64	120.21	111.91
10	M	406	SPN	C6-C7-C8	2.64	120.56	111.88
11	M	407	MW9	C8-C9-C10	2.64	127.83	114.42
9	d	101	BCL	CHA-C1A-NA	-2.64	120.36	126.40
10	m	102	SPN	C16-C15-C14	2.64	122.67	113.19
9	5	101	BCL	CMA-C3A-C4A	-2.64	104.69	111.77
9	j	101	BCL	CHA-C1A-NA	-2.63	120.36	126.40
11	g	102	MW9	C9-C8-C7	2.63	127.79	114.42
10	i	102	SPN	C16-C15-C14	2.63	122.65	113.19
9	L	304	BCL	CHB-C1B-NB	-2.63	121.47	124.26
11	M	407	MW9	C19-O8-C24	2.63	124.26	117.79
9	9	102	BCL	C4D-CHA-C1A	2.62	124.44	121.25
10	9	103	SPN	C16-C15-C14	2.62	122.61	113.19
10	r	102	SPN	C16-C15-C14	2.62	122.60	113.19
11	g	103	MW9	C8-C9-C10	2.62	127.71	114.42
9	s	101	BCL	C4D-CHA-C1A	2.62	124.43	121.25
9	3	101	BCL	CMD-C2D-C1D	2.61	129.32	124.71
9	6	101	BCL	O2A-CGA-CBA	2.61	120.11	111.91
9	9	102	BCL	CMA-C3A-C4A	-2.61	104.75	111.77
10	7	102	SPN	C16-C15-C14	2.61	122.56	113.19
10	w	102	SPN	C16-C15-C14	2.61	122.56	113.19
11	g	103	MW9	C9-C8-C7	2.61	127.65	114.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	101	U10	C12-C11-C9	-2.60	104.41	112.98
9	q	101	BCL	CMA-C3A-C4A	-2.60	104.78	111.77
9	g	101	BCL	C4D-CHA-C1A	2.60	124.42	121.25
9	7	101	BCL	CMA-C3A-C4A	-2.60	104.78	111.77
9	v	101	BCL	C1D-ND-C4D	2.60	108.18	106.33
10	1	103	SPN	O1-C1-C2	2.60	114.12	108.78
9	h	101	BCL	CHA-C1A-NA	-2.60	120.45	126.40
9	M	402	BCL	CHC-C1C-NC	2.59	128.09	124.51
8	M	403	U10	C50-C49-C51	2.58	119.62	115.27
9	2	101	BCL	CMB-C2B-C3B	2.58	132.90	125.93
9	c	101	BCL	C4D-CHA-C1A	2.58	124.39	121.25
11	M	407	MW9	C9-C8-C7	2.58	127.51	114.42
9	e	101	BCL	C4D-CHA-C1A	2.58	124.39	121.25
10	p	103	SPN	C23-C22-C21	2.57	125.67	112.13
10	h	102	SPN	C16-C15-C14	2.57	122.44	113.19
9	6	101	BCL	CHB-C4A-NA	2.57	128.06	124.51
9	l	101	BCL	CHA-C1A-NA	-2.57	120.52	126.40
9	p	101	BCL	C1D-ND-C4D	2.57	108.16	106.33
9	c	101	BCL	CMA-C3A-C4A	-2.56	104.89	111.77
9	t	101	BCL	CHA-C1A-NA	-2.56	120.54	126.40
9	p	101	BCL	CMA-C3A-C4A	-2.55	104.91	111.77
11	H	301	MW9	C9-C8-C7	2.55	127.39	114.42
10	a	103	SPN	C23-C22-C21	2.55	125.54	112.13
10	3	102	SPN	C16-C15-C14	2.55	122.34	113.19
9	u	101	BCL	CMA-C3A-C4A	-2.55	104.93	111.77
9	u	101	BCL	CHC-C1C-NC	2.54	128.03	124.51
9	n	101	BCL	C1D-ND-C4D	2.53	108.13	106.33
9	q	101	BCL	C4D-CHA-C1A	2.53	124.33	121.25
8	L	302	U10	C7-C6-C5	-2.53	115.43	118.48
9	q	101	BCL	CHA-C1A-NA	-2.53	120.60	126.40
9	m	101	BCL	C4D-CHA-C1A	2.53	124.33	121.25
12	C	403	HEM	CAC-C3C-C2C	2.52	136.92	128.60
8	M	403	U10	C42-C43-C44	-2.52	121.59	127.66
10	n	102	SPN	C6-C7-C8	2.52	120.16	111.88
11	H	302	MW9	C8-C9-C10	2.52	127.21	114.42
9	a	101	BCL	CMA-C3A-C4A	-2.51	105.04	111.77
11	H	302	MW9	C9-C8-C7	2.50	127.14	114.42
9	s	101	BCL	CHA-C1A-NA	-2.50	120.67	126.40
9	M	404	BCL	CHB-C1B-NB	-2.50	121.61	124.26
9	l	101	BCL	CMA-C3A-C4A	-2.50	105.07	111.77
10	1	102	SPN	C16-C15-C14	2.49	122.15	113.19
10	h	103	SPN	C6-C7-C8	2.49	120.07	111.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	0	101	BCL	O2A-CGA-CBA	2.48	119.70	111.91
9	2	101	BCL	CAC-C3C-C4C	-2.48	107.07	112.58
10	1	103	SPN	CM5-C13-C12	-2.48	117.31	123.68
11	g	102	MW9	C8-C9-C10	2.48	127.01	114.42
9	t	101	BCL	CMA-C3A-C4A	-2.48	105.11	111.77
10	e	102	SPN	C16-C15-C14	2.48	122.10	113.19
10	j	102	SPN	C6-C7-C8	2.48	120.02	111.88
9	w	101	BCL	C4D-CHA-C1A	2.48	124.26	121.25
9	3	101	BCL	CMA-C3A-C4A	-2.48	105.12	111.77
13	M	409	BPH	C2B-C1B-NB	-2.47	107.82	109.53
9	k	101	BCL	C4D-CHA-C1A	2.47	124.26	121.25
10	a	103	SPN	C20-C21-C22	2.47	124.30	115.76
9	0	101	BCL	CGD-CBD-CAD	2.47	118.72	110.73
10	n	102	SPN	C16-C15-C14	2.46	122.04	113.19
10	l	102	SPN	C15-C16-C17	2.46	122.03	113.19
10	p	102	SPN	CM5-C13-C12	-2.46	117.37	123.68
9	5	101	BCL	C3C-C4C-CHD	-2.46	118.14	123.39
10	l	102	SPN	C20-C21-C22	2.45	124.25	115.76
10	a	102	SPN	C16-C15-C14	2.45	122.00	113.19
9	v	101	BCL	C2A-C1A-CHA	2.45	128.15	123.86
9	L	301	BCL	C2A-C1A-CHA	2.45	128.15	123.86
9	x	101	BCL	CMA-C3A-C4A	-2.45	105.18	111.77
10	1	105	SPN	C16-C15-C14	2.45	122.00	113.19
9	0	101	BCL	CHC-C1C-NC	2.45	127.90	124.51
11	H	304	MW9	C8-C9-C10	2.45	126.85	114.42
9	2	101	BCL	CED-O2D-CGD	-2.45	110.40	115.94
9	1	101	BCL	C4D-CHA-C1A	2.45	124.22	121.25
9	w	101	BCL	CHA-C1A-NA	-2.44	120.80	126.40
9	L	301	BCL	CHA-C1A-NA	-2.44	120.80	126.40
9	i	101	BCL	CHA-C1A-NA	-2.44	120.81	126.40
9	3	101	BCL	C3C-C4C-CHD	-2.44	118.18	123.39
10	t	102	SPN	C6-C7-C8	2.43	119.88	111.88
10	5	102	SPN	C16-C15-C14	2.43	121.94	113.19
9	M	402	BCL	CMB-C2B-C3B	2.43	132.50	125.93
11	H	303	MW9	C8-C9-C10	2.43	126.77	114.42
9	a	101	BCL	C4D-CHA-C1A	2.43	124.21	121.25
9	x	101	BCL	C1D-ND-C4D	2.43	108.06	106.33
9	M	404	BCL	CMD-C2D-C1D	2.43	128.99	124.71
9	1	101	BCL	CHA-C1A-NA	-2.43	120.84	126.40
10	1	102	SPN	CM6-C18-C19	-2.43	117.45	123.68
9	1	101	BCL	C3C-C4C-CHD	-2.42	118.22	123.39
10	f	102	SPN	C6-C7-C8	2.42	119.84	111.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	8	101	BCL	C11-C10-C8	-2.42	108.10	115.92
10	5	102	SPN	CM6-C18-C19	-2.42	117.48	123.68
11	H	303	MW9	C9-C8-C7	2.42	126.69	114.42
8	M	403	U10	C32-C33-C34	-2.42	121.84	127.66
10	3	102	SPN	CM6-C18-C19	-2.42	117.48	123.68
9	h	101	BCL	CMA-C3A-C4A	-2.41	105.29	111.77
10	c	103	SPN	C6-C7-C8	2.41	119.81	111.88
9	4	101	BCL	CHC-C1C-NC	2.41	127.85	124.51
9	q	101	BCL	C3C-C4C-CHD	-2.41	118.25	123.39
9	r	101	BCL	C2A-C3A-C4A	-2.41	97.98	101.87
9	L	301	BCL	C2A-C3A-C4A	-2.40	97.98	101.87
9	c	101	BCL	CHA-C1A-NA	-2.40	120.89	126.40
11	H	304	MW9	C9-C8-C7	2.40	126.62	114.42
10	a	102	SPN	CM6-C18-C19	-2.40	117.51	123.68
10	0	102	SPN	C6-C7-C8	2.40	119.75	111.88
10	q	102	SPN	C6-C7-C8	2.40	119.75	111.88
9	8	101	BCL	CHC-C1C-NC	2.40	127.82	124.51
9	M	404	BCL	C4D-CHA-C1A	2.39	124.16	121.25
10	r	102	SPN	C4-C3-C2	2.39	122.86	111.34
9	k	101	BCL	CMA-C3A-C4A	-2.39	105.36	111.77
10	p	102	SPN	O1-C1-C2	2.39	113.68	108.78
10	a	103	SPN	C15-C16-C17	2.38	121.76	113.19
9	k	101	BCL	CHA-C1A-NA	-2.38	120.94	126.40
9	2	101	BCL	C1D-CHD-C4C	-2.38	120.88	126.62
9	n	101	BCL	CMA-C3A-C4A	-2.37	105.39	111.77
10	M	406	SPN	CM6-C18-C19	-2.37	117.59	123.68
9	7	101	BCL	C3C-C4C-CHD	-2.37	118.32	123.39
9	4	101	BCL	C4-C3-C5	2.37	119.26	115.27
10	5	102	SPN	C4-C3-C2	2.37	122.75	111.34
10	a	103	SPN	C20-C19-C18	2.37	133.36	127.66
10	j	102	SPN	C20-C19-C18	2.37	133.36	127.66
9	e	101	BCL	CHA-C1A-NA	-2.36	120.98	126.40
9	4	101	BCL	C1-C2-C3	-2.36	121.95	126.04
8	M	403	U10	C25-C24-C26	2.36	119.25	115.27
8	M	403	U10	C12-C13-C14	-2.36	121.97	127.66
9	i	101	BCL	C3C-C4C-CHD	-2.36	118.35	123.39
10	p	102	SPN	CM6-C18-C19	-2.36	117.62	123.68
11	9	101	MW9	C9-C8-C7	2.36	126.40	114.42
9	a	101	BCL	CHA-C1A-NA	-2.36	121.00	126.40
9	o	101	BCL	CMD-C2D-C1D	2.36	128.87	124.71
9	m	101	BCL	CHA-C1A-NA	-2.36	121.00	126.40
10	9	103	SPN	C4-C3-C2	2.35	122.66	111.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	v	101	BCL	CMA-C3A-C4A	-2.35	105.46	111.77
9	f	101	BCL	C1D-ND-C4D	2.35	108.00	106.33
9	9	102	BCL	CHA-C1A-NA	-2.35	121.02	126.40
9	j	101	BCL	C1D-ND-C4D	2.35	108.00	106.33
9	e	101	BCL	CMA-C3A-C4A	-2.34	105.47	111.77
9	b	101	BCL	CGD-CBD-CAD	2.34	118.31	110.73
9	0	101	BCL	C1-O2A-CGA	2.34	122.58	116.44
10	0	102	SPN	CM6-C18-C19	-2.34	117.68	123.68
9	w	101	BCL	CMA-C3A-C4A	-2.34	105.50	111.77
9	o	101	BCL	C3D-C2D-C1D	-2.33	102.65	105.83
9	r	101	BCL	CMA-C3A-C4A	-2.33	105.51	111.77
9	M	402	BCL	C11-C10-C8	-2.33	108.39	115.92
9	L	304	BCL	CAA-C2A-C1A	2.33	119.61	111.97
11	9	101	MW9	C8-C9-C10	2.33	126.23	114.42
9	f	101	BCL	CMA-C3A-C4A	-2.33	105.52	111.77
9	5	101	BCL	C4D-CHA-C1A	2.32	124.08	121.25
9	L	301	BCL	C4D-CHA-C1A	2.32	124.08	121.25
9	w	101	BCL	C2B-C1B-NB	-2.32	108.67	110.23
9	9	102	BCL	C2B-C1B-NB	-2.32	108.68	110.23
10	e	102	SPN	CM6-C18-C19	-2.32	117.73	123.68
11	H	302	MW9	O8-C19-C18	-2.32	100.01	108.40
10	p	102	SPN	CM3-C5-C4	-2.32	117.73	123.68
10	1	104	SPN	C6-C7-C8	2.31	119.48	111.88
13	M	409	BPH	CMD-C2D-C3D	2.31	129.00	124.68
8	A	101	U10	C36-C34-C35	2.31	119.70	114.60
9	4	101	BCL	C1D-CHD-C4C	-2.31	121.06	126.62
10	9	103	SPN	CM6-C18-C19	-2.31	117.76	123.68
9	M	402	BCL	CAA-C2A-C1A	2.31	119.53	111.97
10	h	102	SPN	CM6-C18-C19	-2.31	117.76	123.68
10	c	103	SPN	CM6-C18-C19	-2.30	117.77	123.68
9	8	101	BCL	C4-C3-C5	2.30	119.14	115.27
9	d	101	BCL	CMA-C3A-C4A	-2.30	105.59	111.77
10	5	102	SPN	CM3-C5-C4	-2.30	117.78	123.68
9	m	101	BCL	C2B-C1B-NB	-2.30	108.69	110.23
9	b	101	BCL	C1C-NC-C4C	-2.30	105.67	106.71
10	3	102	SPN	CM3-C5-C4	-2.30	117.79	123.68
10	c	102	SPN	CM6-C18-C19	-2.30	117.79	123.68
10	M	406	SPN	O1-C1-C2	2.30	113.50	108.78
9	8	101	BCL	C4D-CHA-C1A	-2.30	118.46	121.25
10	7	103	SPN	CM6-C18-C19	-2.29	117.79	123.68
10	a	103	SPN	CM7-C22-C21	2.29	119.60	111.29
9	3	101	BCL	C3D-C2D-C1D	-2.29	102.70	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	a	102	SPN	CM4-C9-C8	-2.29	117.80	123.68
10	1	105	SPN	CM6-C18-C19	-2.29	117.80	123.68
10	m	102	SPN	CM3-C5-C4	-2.29	117.80	123.68
10	m	102	SPN	CM6-C18-C19	-2.29	117.80	123.68
10	i	102	SPN	CM6-C18-C19	-2.29	117.80	123.68
10	7	102	SPN	CM6-C18-C19	-2.29	117.81	123.68
9	L	301	BCL	O2A-C1-C2	2.29	114.65	108.64
10	w	102	SPN	CM6-C18-C19	-2.29	117.81	123.68
13	M	405	BPH	C2B-C1B-NB	-2.29	107.95	109.53
9	g	101	BCL	CMA-C3A-C4A	-2.29	105.63	111.77
10	9	103	SPN	O1-C1-C2	2.29	113.47	108.78
10	7	102	SPN	C4-C3-C2	2.29	122.34	111.34
10	5	103	SPN	CM6-C18-C19	-2.29	117.82	123.68
10	k	102	SPN	CM6-C18-C19	-2.28	117.82	123.68
10	m	102	SPN	C4-C3-C2	2.28	122.33	111.34
10	9	103	SPN	CM3-C5-C4	-2.28	117.83	123.68
10	a	103	SPN	C6-C7-C8	2.28	119.37	111.88
10	7	102	SPN	CM3-C5-C4	-2.28	117.83	123.68
10	1	104	SPN	C20-C19-C18	2.28	133.15	127.66
10	u	102	SPN	CM6-C18-C19	-2.28	117.83	123.68
9	u	101	BCL	C2B-C1B-NB	-2.28	108.71	110.23
10	r	102	SPN	CM6-C18-C19	-2.28	117.84	123.68
9	l	101	BCL	C3C-C4C-CHD	-2.27	118.53	123.39
9	b	101	BCL	C4-C3-C5	2.27	119.09	115.27
9	b	101	BCL	O2A-CGA-CBA	2.27	119.04	111.91
8	L	305	U10	C11-C9-C8	-2.27	116.52	121.12
10	p	103	SPN	O1-C1-C2	2.27	113.44	108.78
9	i	101	BCL	C4D-CHA-C1A	2.27	124.01	121.25
10	e	102	SPN	CM3-C5-C4	-2.27	117.86	123.68
10	1	105	SPN	C6-C7-C8	2.27	119.33	111.88
10	1	105	SPN	C20-C21-C22	2.27	123.60	115.76
8	M	403	U10	C56-C54-C55	2.27	119.61	114.60
10	1	102	SPN	CM4-C9-C8	-2.27	117.87	123.68
10	n	102	SPN	CM6-C18-C19	-2.27	117.87	123.68
9	p	101	BCL	C2B-C1B-NB	-2.26	108.71	110.23
9	k	101	BCL	C2B-C1B-NB	-2.26	108.71	110.23
10	k	102	SPN	CM3-C5-C4	-2.26	117.87	123.68
10	s	102	SPN	CM6-C18-C19	-2.26	117.87	123.68
10	t	102	SPN	CM6-C18-C19	-2.26	117.88	123.68
10	c	102	SPN	C4-C3-C2	2.26	122.22	111.34
9	x	101	BCL	C2B-C1B-NB	-2.26	108.72	110.23
10	5	102	SPN	CM4-C9-C8	-2.26	117.89	123.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	c	101	BCL	C2B-C1B-NB	-2.26	108.72	110.23
9	a	101	BCL	CMD-C2D-C1D	2.26	128.69	124.71
9	j	101	BCL	CMD-C2D-C1D	2.26	128.69	124.71
10	3	102	SPN	CM4-C9-C8	-2.25	117.90	123.68
9	e	101	BCL	C3D-C4D-ND	-2.25	106.60	110.24
10	c	102	SPN	CM3-C5-C4	-2.25	117.91	123.68
9	8	101	BCL	O2A-CGA-O1A	-2.25	117.92	123.59
10	1	104	SPN	C15-C16-C17	2.25	121.28	113.19
9	n	101	BCL	C2A-C1A-CHA	2.25	127.79	123.86
10	m	102	SPN	CM4-C9-C8	-2.25	117.91	123.68
10	h	102	SPN	CM3-C5-C4	-2.25	117.91	123.68
10	u	102	SPN	CM3-C5-C4	-2.25	117.92	123.68
10	h	103	SPN	CM5-C13-C12	-2.24	117.92	123.68
10	a	102	SPN	CM3-C5-C4	-2.24	117.92	123.68
10	w	102	SPN	CM3-C5-C4	-2.24	117.92	123.68
10	u	102	SPN	CM4-C9-C8	-2.24	117.92	123.68
10	f	102	SPN	C15-C16-C17	2.24	121.26	113.19
9	r	101	BCL	CMD-C2D-C1D	2.24	128.67	124.71
9	u	101	BCL	CHA-C1A-NA	-2.24	121.26	126.40
10	1	103	SPN	C20-C19-C18	2.24	133.06	127.66
10	r	102	SPN	CM3-C5-C4	-2.24	117.93	123.68
10	1	102	SPN	CM3-C5-C4	-2.24	117.93	123.68
10	h	102	SPN	CM4-C9-C8	-2.24	117.93	123.68
10	t	102	SPN	O1-C1-C2	2.24	113.38	108.78
9	a	101	BCL	C2B-C1B-NB	-2.24	108.73	110.23
10	1	103	SPN	C6-C7-C8	2.24	119.23	111.88
10	i	102	SPN	CM3-C5-C4	-2.23	117.95	123.68
10	w	102	SPN	CM4-C9-C8	-2.23	117.95	123.68
9	7	101	BCL	C4D-CHA-C1A	2.23	123.97	121.25
10	l	102	SPN	CM5-C13-C12	-2.23	117.95	123.68
8	A	101	U10	C27-C28-C29	-2.23	122.30	127.66
9	j	101	BCL	CMA-C3A-C4A	-2.23	105.79	111.77
10	1	104	SPN	CM5-C13-C12	-2.23	117.97	123.68
10	9	103	SPN	CM4-C9-C8	-2.23	117.97	123.68
10	f	102	SPN	CM5-C13-C12	-2.23	117.97	123.68
9	g	101	BCL	CHA-C1A-NA	-2.23	121.30	126.40
10	q	102	SPN	CM6-C18-C19	-2.22	117.97	123.68
9	i	101	BCL	CMD-C2D-C1D	2.22	128.63	124.71
10	5	102	SPN	CM5-C13-C12	-2.22	117.97	123.68
10	c	102	SPN	CM4-C9-C8	-2.22	117.98	123.68
10	7	102	SPN	CM4-C9-C8	-2.22	117.98	123.68
10	e	102	SPN	CM4-C9-C8	-2.22	117.98	123.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	d	101	BCL	C3C-C4C-CHD	-2.22	118.64	123.39
10	k	102	SPN	CM4-C9-C8	-2.22	117.99	123.68
10	m	102	SPN	CM5-C13-C12	-2.22	117.99	123.68
9	g	101	BCL	C3D-C4D-ND	-2.22	106.65	110.24
10	v	102	SPN	O1-C1-C2	2.22	113.33	108.78
10	i	102	SPN	CM4-C9-C8	-2.22	117.99	123.68
10	j	102	SPN	CM5-C13-C12	-2.22	117.99	123.68
9	6	101	BCL	CHB-C1B-C2B	-2.22	120.98	127.24
10	r	102	SPN	CM4-C9-C8	-2.22	117.99	123.68
9	o	101	BCL	CMA-C3A-C4A	-2.21	105.82	111.77
10	w	102	SPN	CM5-C13-C12	-2.21	118.00	123.68
9	M	402	BCL	CHB-C1B-NB	-2.21	121.91	124.26
10	e	102	SPN	O1-C1-C2	2.21	113.33	108.78
8	L	305	U10	C31-C29-C30	2.21	119.49	114.60
10	s	102	SPN	CM3-C5-C4	-2.21	118.00	123.68
9	x	101	BCL	C3C-C4C-CHD	-2.21	118.67	123.39
10	k	102	SPN	CM5-C13-C12	-2.21	118.01	123.68
10	w	102	SPN	O1-C1-C2	2.21	113.32	108.78
10	i	102	SPN	CM5-C13-C12	-2.21	118.01	123.68
9	5	101	BCL	CHA-C1A-NA	-2.21	121.34	126.40
9	b	101	BCL	CHC-C1C-NC	2.20	127.56	124.51
10	s	102	SPN	CM4-C9-C8	-2.20	118.02	123.68
10	a	103	SPN	CM5-C13-C12	-2.20	118.02	123.68
9	e	101	BCL	C2B-C1B-NB	-2.20	108.75	110.23
9	M	404	BCL	C3C-C4C-CHD	-2.20	118.69	123.39
9	M	402	BCL	CAA-CBA-CGA	-2.20	106.82	113.25
9	n	101	BCL	C2B-C1B-NB	-2.20	108.76	110.23
10	h	102	SPN	CM5-C13-C12	-2.20	118.03	123.68
10	u	102	SPN	CM5-C13-C12	-2.20	118.03	123.68
10	9	103	SPN	CM5-C13-C12	-2.20	118.03	123.68
9	2	101	BCL	O2A-CGA-O1A	-2.20	118.04	123.59
10	3	102	SPN	C4-C3-C2	2.20	121.94	111.34
10	t	102	SPN	CM5-C13-C12	-2.20	118.03	123.68
10	7	102	SPN	CM5-C13-C12	-2.20	118.03	123.68
10	7	103	SPN	CM5-C13-C12	-2.20	118.04	123.68
9	o	101	BCL	C2B-C1B-NB	-2.20	108.76	110.23
10	7	103	SPN	C6-C7-C8	2.20	119.10	111.88
10	1	102	SPN	CM5-C13-C12	-2.20	118.04	123.68
10	r	102	SPN	CM5-C13-C12	-2.20	118.04	123.68
10	5	103	SPN	CM5-C13-C12	-2.20	118.05	123.68
9	v	101	BCL	C2B-C1B-NB	-2.19	108.76	110.23
10	s	102	SPN	CM5-C13-C12	-2.19	118.05	123.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	v	101	BCL	C2A-C3A-C4A	-2.19	98.33	101.87
9	c	101	BCL	CMD-C2D-C1D	2.19	128.58	124.71
9	1	101	BCL	CMD-C2D-C1D	2.19	128.57	124.71
10	c	103	SPN	CM5-C13-C12	-2.19	118.06	123.68
10	c	102	SPN	CM5-C13-C12	-2.19	118.07	123.68
9	6	101	BCL	C11-C12-C13	-2.19	108.85	115.92
10	3	102	SPN	CM5-C13-C12	-2.19	118.07	123.68
10	0	102	SPN	CM3-C5-C4	-2.19	118.07	123.68
10	v	102	SPN	CM5-C13-C12	-2.18	118.07	123.68
9	h	101	BCL	C3C-C4C-CHD	-2.18	118.72	123.39
11	M	408	MW9	C9-C8-C7	2.18	125.51	114.42
10	j	102	SPN	CM3-C5-C4	-2.18	118.08	123.68
9	M	402	BCL	C6-C5-C3	-2.18	107.73	113.45
10	M	406	SPN	CM3-C5-C4	-2.18	118.08	123.68
13	L	303	BPH	CMD-C2D-C3D	2.18	128.76	124.68
10	e	102	SPN	C4-C3-C2	2.18	121.84	111.34
9	j	101	BCL	C2B-C1B-NB	-2.18	108.77	110.23
10	p	103	SPN	CM3-C5-C4	-2.18	118.08	123.68
9	M	402	BCL	CHB-C1B-C2B	-2.18	121.08	127.24
9	g	101	BCL	C2B-C1B-NB	-2.18	108.77	110.23
9	3	101	BCL	C4D-CHA-C1A	2.18	123.90	121.25
10	p	103	SPN	CM5-C13-C12	-2.18	118.09	123.68
9	l	101	BCL	CMD-C2D-C1D	2.18	128.55	124.71
10	c	103	SPN	CM3-C5-C4	-2.18	118.10	123.68
10	q	102	SPN	CM3-C5-C4	-2.17	118.10	123.68
10	7	103	SPN	CM3-C5-C4	-2.17	118.10	123.68
10	1	104	SPN	CM3-C5-C4	-2.17	118.11	123.68
10	t	102	SPN	CM4-C9-C8	-2.17	118.11	123.68
10	q	102	SPN	CM5-C13-C12	-2.17	118.11	123.68
8	L	305	U10	C25-C24-C26	2.17	118.92	115.27
10	v	102	SPN	CM4-C9-C8	-2.17	118.11	123.68
10	t	102	SPN	CM3-C5-C4	-2.17	118.11	123.68
10	a	102	SPN	CM5-C13-C12	-2.17	118.11	123.68
9	t	101	BCL	C3C-C4C-CHD	-2.17	118.76	123.39
10	h	102	SPN	C4-C3-C2	2.17	121.78	111.34
9	l	101	BCL	C2B-C1B-NB	-2.17	108.78	110.23
9	s	101	BCL	C2B-C1B-NB	-2.17	108.78	110.23
10	0	102	SPN	CM5-C13-C12	-2.17	118.12	123.68
9	e	101	BCL	CMD-C2D-C1D	2.16	128.53	124.71
9	7	101	BCL	C3D-C2D-C1D	-2.16	102.88	105.83
10	e	102	SPN	CM5-C13-C12	-2.16	118.13	123.68
10	a	103	SPN	CM3-C5-C4	-2.16	118.13	123.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	f	101	BCL	C2B-C1B-NB	-2.16	108.78	110.23
10	l	102	SPN	CM3-C5-C4	-2.16	118.13	123.68
9	3	101	BCL	CHA-C1A-NA	-2.16	121.45	126.40
9	l	101	BCL	C1D-ND-C4D	2.16	107.87	106.33
9	M	402	BCL	CHB-C4A-NA	2.16	127.50	124.51
9	r	101	BCL	C1D-ND-C4D	2.16	107.87	106.33
9	2	101	BCL	CHC-C1C-NC	2.16	127.50	124.51
9	r	101	BCL	C3C-C4C-CHD	-2.15	118.79	123.39
10	n	102	SPN	CM5-C13-C12	-2.15	118.15	123.68
9	0	101	BCL	CHB-C1B-C2B	-2.15	121.15	127.24
9	7	101	BCL	CMD-C2D-C1D	2.15	128.50	124.71
10	s	102	SPN	O1-C1-C2	2.15	113.20	108.78
9	q	101	BCL	C2B-C1B-NB	-2.15	108.79	110.23
9	r	101	BCL	C2A-C1A-CHA	2.15	127.62	123.86
13	M	405	BPH	CMD-C2D-C3D	2.15	128.70	124.68
8	A	101	U10	C17-C16-C14	-2.15	105.91	112.98
11	M	408	MW9	C8-C9-C10	2.15	125.33	114.42
10	k	102	SPN	C4-C3-C2	2.15	121.68	111.34
10	i	102	SPN	C4-C3-C2	2.15	121.68	111.34
9	u	101	BCL	C3D-C4D-ND	-2.15	106.77	110.24
10	l	102	SPN	CM4-C9-C8	-2.15	118.17	123.68
9	u	101	BCL	CMD-C2D-C1D	2.15	128.49	124.71
9	t	101	BCL	C2B-C1B-NB	-2.15	108.79	110.23
10	1	105	SPN	CM3-C5-C4	-2.14	118.18	123.68
10	q	102	SPN	CM4-C9-C8	-2.14	118.18	123.68
9	1	101	BCL	CMA-C3A-C4A	-2.14	106.02	111.77
10	5	103	SPN	CM3-C5-C4	-2.14	118.19	123.68
9	a	101	BCL	C3D-C4D-ND	-2.14	106.77	110.24
9	j	101	BCL	C3C-C4C-CHD	-2.14	118.82	123.39
10	f	102	SPN	CM3-C5-C4	-2.14	118.19	123.68
10	e	102	SPN	C23-C22-C21	2.14	123.38	112.13
10	v	102	SPN	CM3-C5-C4	-2.14	118.19	123.68
9	i	101	BCL	C3D-C2D-C1D	-2.14	102.91	105.83
10	c	103	SPN	O1-C1-C2	2.14	113.17	108.78
10	h	102	SPN	O1-C1-C2	2.13	113.16	108.78
8	A	101	U10	C10-C9-C11	2.13	118.86	115.27
12	C	402	HEM	CBC-CAC-C3C	2.13	138.23	127.62
8	M	403	U10	C3M-O3-C3	2.13	124.02	116.47
10	h	103	SPN	CM3-C5-C4	-2.13	118.22	123.68
9	f	101	BCL	C3C-C4C-CHD	-2.13	118.84	123.39
10	c	102	SPN	O1-C1-C2	2.13	113.15	108.78
10	p	103	SPN	CM4-C9-C8	-2.12	118.23	123.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	1	105	SPN	CM5-C13-C12	-2.12	118.23	123.68
9	e	101	BCL	C3C-C4C-CHD	-2.12	118.86	123.39
10	n	102	SPN	CM3-C5-C4	-2.12	118.24	123.68
9	L	301	BCL	C1D-ND-C4D	2.12	107.84	106.33
9	i	101	BCL	CMA-C3A-C4A	-2.12	106.08	111.77
10	c	103	SPN	CM4-C9-C8	-2.12	118.25	123.68
9	b	101	BCL	CHB-C1B-C2B	-2.12	121.26	127.24
10	0	102	SPN	CM4-C9-C8	-2.12	118.25	123.68
9	i	101	BCL	C2B-C1B-NB	-2.12	108.81	110.23
10	h	103	SPN	CM4-C9-C8	-2.11	118.25	123.68
9	s	101	BCL	C3C-C4C-CHD	-2.11	118.88	123.39
9	w	101	BCL	C3C-C4C-CHD	-2.11	118.88	123.39
9	x	101	BCL	C2A-C1A-CHA	2.11	127.56	123.86
9	M	404	BCL	C2A-C1A-CHA	2.11	127.55	123.86
10	f	102	SPN	CM4-C9-C8	-2.11	118.26	123.68
10	n	102	SPN	CM4-C9-C8	-2.11	118.27	123.68
9	M	402	BCL	C14-C13-C12	-2.11	103.65	111.29
9	L	304	BCL	C1C-NC-C4C	2.11	107.65	106.71
9	7	101	BCL	C2B-C1B-NB	-2.11	108.82	110.23
10	h	103	SPN	C15-C16-C17	2.11	120.76	113.19
10	1	103	SPN	CM7-C22-C21	2.11	118.92	111.29
10	t	102	SPN	CM7-C22-C21	2.11	118.92	111.29
9	M	402	BCL	CAB-C3B-C2B	-2.10	125.19	128.34
9	4	101	BCL	C4D-C3D-CAD	2.10	110.57	108.10
9	0	101	BCL	C11-C12-C13	-2.10	109.12	115.92
9	v	101	BCL	C3C-C4C-CHD	-2.10	118.91	123.39
10	k	102	SPN	O1-C1-C2	2.10	113.09	108.78
10	1	103	SPN	CM3-C5-C4	-2.10	118.29	123.68
9	u	101	BCL	C3D-C2D-C1D	-2.10	102.97	105.83
10	m	102	SPN	C23-C22-C21	2.10	123.17	112.13
10	p	103	SPN	CM7-C22-C21	2.10	118.89	111.29
10	a	103	SPN	CM4-C9-C8	-2.10	118.30	123.68
9	a	101	BCL	C3C-C4C-CHD	-2.09	118.92	123.39
9	c	101	BCL	C3D-C2D-C1D	-2.09	102.97	105.83
9	a	101	BCL	C3D-C2D-C1D	-2.09	102.97	105.83
10	u	102	SPN	C4-C3-C2	2.09	121.41	111.34
9	e	101	BCL	C3D-C2D-C1D	-2.09	102.98	105.83
10	1	103	SPN	CM4-C9-C8	-2.09	118.31	123.68
10	a	103	SPN	O1-C1-C2	2.09	113.07	108.78
10	1	105	SPN	C23-C22-C21	2.09	123.10	112.13
9	j	101	BCL	C3D-C2D-C1D	-2.09	102.98	105.83
9	5	101	BCL	C2B-C1B-NB	-2.08	108.83	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	r	101	BCL	C2B-C1B-NB	-2.08	108.83	110.23
9	r	101	BCL	C3D-C2D-C1D	-2.08	102.99	105.83
8	A	101	U10	C32-C33-C34	-2.08	120.63	127.75
9	8	101	BCL	C1D-CHD-C4C	-2.08	121.60	126.62
10	1	104	SPN	CM4-C9-C8	-2.08	118.34	123.68
9	s	101	BCL	C3D-C2D-C1D	-2.08	102.99	105.83
9	6	101	BCL	C1D-CHD-C4C	-2.08	121.61	126.62
10	j	102	SPN	CM4-C9-C8	-2.08	118.34	123.68
10	n	102	SPN	O1-C1-C2	2.08	113.05	108.78
13	L	303	BPH	OBD-CAD-CBD	-2.08	122.78	125.82
9	b	101	BCL	C1D-CHD-C4C	-2.08	121.61	126.62
9	d	101	BCL	C2B-C1B-NB	-2.07	108.84	110.23
10	p	103	SPN	C20-C21-C22	2.07	122.94	115.76
9	M	402	BCL	C1D-CHD-C4C	-2.07	121.62	126.62
9	8	101	BCL	C1-C2-C3	-2.07	122.46	126.04
9	s	101	BCL	C1D-ND-C4D	2.07	107.81	106.33
9	l	101	BCL	C4D-CHA-C1A	2.07	123.77	121.25
10	h	102	SPN	C23-C22-C21	2.07	123.01	112.13
9	h	101	BCL	C2B-C1B-NB	-2.07	108.84	110.23
9	p	101	BCL	C2A-C1A-CHA	2.07	127.48	123.86
9	4	101	BCL	C4D-CHA-C1A	-2.07	118.73	121.25
9	L	301	BCL	C2B-C1B-NB	-2.07	108.85	110.23
10	M	406	SPN	CM4-C9-C8	-2.06	118.39	123.68
10	i	102	SPN	O1-C1-C2	2.06	113.01	108.78
10	1	105	SPN	CM4-C9-C8	-2.06	118.39	123.68
10	s	102	SPN	C4-C3-C2	2.06	121.26	111.34
9	m	101	BCL	CMD-C2D-C1D	2.06	128.34	124.71
9	L	304	BCL	CMD-C2D-C1D	2.06	128.34	124.71
10	7	102	SPN	O1-C1-C2	2.06	113.00	108.78
9	p	101	BCL	CMD-C2D-C1D	2.06	128.34	124.71
9	c	101	BCL	C3C-C4C-CHD	-2.05	119.00	123.39
9	6	101	BCL	CGD-CBD-CAD	2.05	117.38	110.73
9	9	102	BCL	CMD-C2D-C1D	2.05	128.33	124.71
9	g	101	BCL	C3C-C4C-CHD	-2.05	119.01	123.39
9	g	101	BCL	CMD-C2D-C1D	2.05	128.32	124.71
9	h	101	BCL	C1D-ND-C4D	2.05	107.79	106.33
9	M	404	BCL	C2B-C1B-NB	-2.05	108.86	110.23
10	7	103	SPN	CM4-C9-C8	-2.05	118.42	123.68
10	u	102	SPN	O1-C1-C2	2.05	112.98	108.78
10	1	102	SPN	C23-C22-C21	2.04	122.87	112.13
9	d	101	BCL	CMD-C2D-C1D	2.04	128.31	124.71
9	g	101	BCL	C3D-C2D-C1D	-2.04	103.05	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	d	101	BCL	C2A-C3A-C4A	-2.04	98.58	101.87
9	s	101	BCL	CMD-C2D-C1D	2.03	128.30	124.71
10	a	102	SPN	O1-C1-C2	2.03	112.95	108.78
9	0	101	BCL	C1D-CHD-C4C	-2.03	121.73	126.62
10	w	102	SPN	C23-C22-C21	2.03	122.80	112.13
10	j	102	SPN	C15-C16-C17	2.03	120.48	113.19
9	f	101	BCL	C2A-C1A-CHA	2.03	127.41	123.86
10	5	103	SPN	CM4-C9-C8	-2.03	118.48	123.68
9	k	101	BCL	C3C-C4C-CHD	-2.03	119.06	123.39
9	L	304	BCL	C2B-C1B-NB	-2.03	108.87	110.23
9	4	101	BCL	CHB-C1B-C2B	-2.03	121.51	127.24
9	h	101	BCL	CMD-C2D-C1D	2.03	128.28	124.71
9	M	404	BCL	O2A-C1-C2	2.02	113.95	108.64
10	c	102	SPN	C23-C22-C21	2.02	122.77	112.13
9	k	101	BCL	C3D-C4D-ND	-2.02	106.96	110.24
10	p	103	SPN	CM6-C18-C19	-2.02	118.49	123.68
10	M	406	SPN	C14-C13-C12	-2.02	117.03	121.12
8	M	403	U10	C1-C6-C5	-2.02	117.68	119.58
9	3	101	BCL	C2B-C1B-NB	-2.02	108.88	110.23
9	9	102	BCL	C3C-C4C-CHD	-2.02	119.08	123.39
9	4	101	BCL	O2A-CGA-O1A	-2.02	118.50	123.59
10	h	103	SPN	O1-C1-C2	2.02	112.92	108.78
12	C	401	HEM	CAB-C3B-C4B	-2.01	115.09	124.47
9	f	101	BCL	CMD-C2D-C1D	2.01	128.26	124.71
9	1	101	BCL	C2B-C1B-NB	-2.01	108.88	110.23
9	7	101	BCL	CHA-C1A-NA	-2.01	121.80	126.40
9	o	101	BCL	C4D-CHA-C1A	2.01	123.69	121.25
9	t	101	BCL	C2A-C3A-C4A	-2.01	98.62	101.87
10	9	103	SPN	C23-C22-C21	2.01	122.68	112.13
9	o	101	BCL	C1-C2-C3	-2.01	122.57	126.04
9	5	101	BCL	CMD-C2D-C1D	2.01	128.25	124.71
9	w	101	BCL	CMD-C2D-C1D	2.01	128.25	124.71
9	k	101	BCL	CMD-C2D-C1D	2.00	128.25	124.71
9	M	404	BCL	C4B-C3B-C2B	-2.00	105.14	108.36

There are no chirality outliers.

All (1788) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	101	U10	C29-C31-C32-C33
8	L	305	U10	C1-C6-C7-C8
8	L	305	U10	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	L	305	U10	C15-C14-C16-C17
9	1	101	BCL	C2C-C3C-CAC-CBC
9	1	101	BCL	C4C-C3C-CAC-CBC
9	1	101	BCL	C11-C12-C13-C14
9	5	101	BCL	C1A-C2A-CAA-CBA
9	5	101	BCL	C3A-C2A-CAA-CBA
9	5	101	BCL	C2C-C3C-CAC-CBC
9	5	101	BCL	C4C-C3C-CAC-CBC
9	3	101	BCL	C1A-C2A-CAA-CBA
9	3	101	BCL	C3A-C2A-CAA-CBA
9	3	101	BCL	C1-C2-C3-C4
9	3	101	BCL	C1-C2-C3-C5
9	4	101	BCL	C2C-C3C-CAC-CBC
9	4	101	BCL	C4C-C3C-CAC-CBC
9	w	101	BCL	C2C-C3C-CAC-CBC
9	w	101	BCL	C4C-C3C-CAC-CBC
9	w	101	BCL	C1-C2-C3-C4
9	w	101	BCL	C1-C2-C3-C5
9	w	101	BCL	C2-C3-C5-C6
9	w	101	BCL	C4-C3-C5-C6
9	x	101	BCL	C11-C12-C13-C14
9	u	101	BCL	C4C-C3C-CAC-CBC
9	u	101	BCL	C1-C2-C3-C4
9	u	101	BCL	C1-C2-C3-C5
9	v	101	BCL	CBA-CGA-O2A-C1
9	v	101	BCL	O1A-CGA-O2A-C1
9	v	101	BCL	C2C-C3C-CAC-CBC
9	v	101	BCL	CHA-CBD-CGD-O1D
9	v	101	BCL	CHA-CBD-CGD-O2D
9	v	101	BCL	CAD-CBD-CGD-O1D
9	s	101	BCL	C2C-C3C-CAC-CBC
9	s	101	BCL	C1-C2-C3-C4
9	s	101	BCL	C2-C3-C5-C6
9	s	101	BCL	C4-C3-C5-C6
9	t	101	BCL	C1A-C2A-CAA-CBA
9	t	101	BCL	C3A-C2A-CAA-CBA
9	q	101	BCL	C1-C2-C3-C4
9	q	101	BCL	C4-C3-C5-C6
9	q	101	BCL	C11-C12-C13-C14
9	r	101	BCL	C2C-C3C-CAC-CBC
9	r	101	BCL	C4C-C3C-CAC-CBC
9	r	101	BCL	C2-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	r	101	BCL	C4-C3-C5-C6
9	o	101	BCL	C2C-C3C-CAC-CBC
9	o	101	BCL	C4C-C3C-CAC-CBC
9	m	101	BCL	C4C-C3C-CAC-CBC
9	m	101	BCL	C1-C2-C3-C4
9	n	101	BCL	C1A-C2A-CAA-CBA
9	n	101	BCL	C3A-C2A-CAA-CBA
9	n	101	BCL	C2C-C3C-CAC-CBC
9	n	101	BCL	C4C-C3C-CAC-CBC
9	k	101	BCL	C1A-C2A-CAA-CBA
9	k	101	BCL	C3A-C2A-CAA-CBA
9	k	101	BCL	C2C-C3C-CAC-CBC
9	l	101	BCL	C1A-C2A-CAA-CBA
9	l	101	BCL	C3A-C2A-CAA-CBA
9	l	101	BCL	C2C-C3C-CAC-CBC
9	l	101	BCL	C1-C2-C3-C4
9	g	101	BCL	C2C-C3C-CAC-CBC
9	g	101	BCL	C4C-C3C-CAC-CBC
9	g	101	BCL	C1-C2-C3-C4
9	h	101	BCL	C2C-C3C-CAC-CBC
9	h	101	BCL	C1-C2-C3-C4
9	e	101	BCL	C2C-C3C-CAC-CBC
9	e	101	BCL	C4C-C3C-CAC-CBC
9	e	101	BCL	C1-C2-C3-C4
9	e	101	BCL	C14-C13-C15-C16
9	f	101	BCL	C2C-C3C-CAC-CBC
9	f	101	BCL	O2A-C1-C2-C3
9	f	101	BCL	C1-C2-C3-C4
9	f	101	BCL	C1-C2-C3-C5
9	c	101	BCL	C1A-C2A-CAA-CBA
9	c	101	BCL	C3A-C2A-CAA-CBA
9	c	101	BCL	C4C-C3C-CAC-CBC
9	c	101	BCL	C1-C2-C3-C4
9	c	101	BCL	C1-C2-C3-C5
9	d	101	BCL	CBA-CGA-O2A-C1
9	d	101	BCL	O1A-CGA-O2A-C1
9	d	101	BCL	C1-C2-C3-C4
9	d	101	BCL	C1-C2-C3-C5
9	d	101	BCL	C2-C3-C5-C6
9	d	101	BCL	C4-C3-C5-C6
9	a	101	BCL	C1A-C2A-CAA-CBA
9	a	101	BCL	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	a	101	BCL	C4C-C3C-CAC-CBC
9	a	101	BCL	C1-C2-C3-C4
9	a	101	BCL	C11-C12-C13-C14
9	b	101	BCL	C11-C10-C8-C9
9	i	101	BCL	C2C-C3C-CAC-CBC
9	i	101	BCL	C4C-C3C-CAC-CBC
9	j	101	BCL	C1A-C2A-CAA-CBA
9	j	101	BCL	C3A-C2A-CAA-CBA
9	j	101	BCL	C2C-C3C-CAC-CBC
9	7	101	BCL	C1A-C2A-CAA-CBA
9	7	101	BCL	C3A-C2A-CAA-CBA
9	7	101	BCL	C2C-C3C-CAC-CBC
9	7	101	BCL	C4C-C3C-CAC-CBC
9	7	101	BCL	C1-C2-C3-C4
9	8	101	BCL	C1A-C2A-CAA-CBA
9	8	101	BCL	C3A-C2A-CAA-CBA
9	8	101	BCL	C2C-C3C-CAC-CBC
9	8	101	BCL	C4C-C3C-CAC-CBC
9	L	301	BCL	C1-C2-C3-C4
9	L	301	BCL	C1-C2-C3-C5
9	L	304	BCL	C1A-C2A-CAA-CBA
9	L	304	BCL	C3A-C2A-CAA-CBA
9	L	304	BCL	C4C-C3C-CAC-CBC
9	L	304	BCL	O2A-C1-C2-C3
9	L	304	BCL	C1-C2-C3-C4
9	L	304	BCL	C1-C2-C3-C5
9	M	404	BCL	C2-C3-C5-C6
9	M	404	BCL	C4-C3-C5-C6
9	9	102	BCL	C1A-C2A-CAA-CBA
9	9	102	BCL	C3A-C2A-CAA-CBA
9	9	102	BCL	C4C-C3C-CAC-CBC
10	1	102	SPN	CM1-C1-O1-CMA
10	1	102	SPN	C2-C1-O1-CMA
10	1	102	SPN	CM1-C1-C2-O2
10	1	102	SPN	CM1-C1-C2-C3
10	1	102	SPN	C20-C21-C22-CM7
10	1	103	SPN	C12-C13-C14-C15
10	1	103	SPN	C18-C19-C20-C21
10	1	104	SPN	CM2-C1-O1-CMA
10	1	104	SPN	C2-C1-O1-CMA
10	1	104	SPN	O1-C1-C2-O2
10	1	104	SPN	C18-C19-C20-C21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	1	105	SPN	CM1-C1-O1-CMA
10	1	105	SPN	CM2-C1-O1-CMA
10	1	105	SPN	C2-C1-O1-CMA
10	1	105	SPN	O1-C1-C2-O2
10	1	105	SPN	C20-C21-C22-CM7
10	1	105	SPN	C25-C26-C27-C28
10	1	105	SPN	CM8-C26-C27-C28
10	5	102	SPN	CM1-C1-O1-CMA
10	5	102	SPN	C2-C1-O1-CMA
10	5	102	SPN	CM1-C1-C2-O2
10	5	102	SPN	CM1-C1-C2-C3
10	5	102	SPN	CM2-C1-C2-C3
10	5	102	SPN	C20-C21-C22-CM7
10	5	102	SPN	C22-C23-C24-C25
10	5	103	SPN	CM1-C1-O1-CMA
10	5	103	SPN	C2-C1-O1-CMA
10	5	103	SPN	C20-C21-C22-CM7
10	3	102	SPN	C2-C1-O1-CMA
10	3	102	SPN	CM1-C1-C2-O2
10	3	102	SPN	CM1-C1-C2-C3
10	3	102	SPN	CM2-C1-C2-C3
10	3	102	SPN	C20-C21-C22-CM7
10	w	102	SPN	O1-C1-C2-O2
10	w	102	SPN	CM2-C1-C2-C3
10	w	102	SPN	C20-C21-C22-CM7
10	u	102	SPN	CM1-C1-C2-C3
10	u	102	SPN	CM2-C1-C2-O2
10	u	102	SPN	CM2-C1-C2-C3
10	u	102	SPN	C20-C21-C22-CM7
10	u	102	SPN	C26-C27-C28-C29
10	v	102	SPN	O1-C1-C2-O2
10	v	102	SPN	C18-C19-C20-C21
10	s	102	SPN	O1-C1-C2-O2
10	s	102	SPN	CM2-C1-C2-O2
10	s	102	SPN	CM2-C1-C2-C3
10	s	102	SPN	C20-C21-C22-CM7
10	t	102	SPN	O1-C1-C2-O2
10	t	102	SPN	C20-C21-C22-CM7
10	q	102	SPN	O1-C1-C2-O2
10	q	102	SPN	C20-C21-C22-CM7
10	q	102	SPN	C22-C23-C24-C25
10	q	102	SPN	CM8-C26-C27-C28

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	e	102	SPN	O1-C1-C2-O2
10	e	102	SPN	CM2-C1-C2-O2
10	e	102	SPN	CM2-C1-C2-C3
10	e	102	SPN	C20-C21-C22-CM7
10	e	102	SPN	C26-C27-C28-C29
10	f	102	SPN	O1-C1-C2-O2
10	f	102	SPN	C18-C19-C20-C21
10	c	102	SPN	O1-C1-C2-O2
10	c	102	SPN	CM2-C1-C2-O2
10	c	102	SPN	CM2-C1-C2-C3
10	c	102	SPN	C20-C21-C22-CM7
10	c	102	SPN	C26-C27-C28-C29
10	c	103	SPN	O1-C1-C2-O2
10	c	103	SPN	C20-C21-C22-CM7
10	c	103	SPN	C25-C26-C27-C28
10	c	103	SPN	CM8-C26-C27-C28
10	c	103	SPN	C26-C27-C28-C29
10	a	102	SPN	CM1-C1-O1-CMA
10	a	102	SPN	C2-C1-O1-CMA
10	a	102	SPN	O1-C1-C2-O2
10	a	102	SPN	CM2-C1-C2-O2
10	a	102	SPN	CM2-C1-C2-C3
10	a	102	SPN	C20-C21-C22-CM7
10	a	102	SPN	C22-C23-C24-C25
10	a	103	SPN	O1-C1-C2-O2
10	a	103	SPN	C18-C19-C20-C21
10	a	103	SPN	C25-C26-C27-C28
10	a	103	SPN	CM8-C26-C27-C28
10	a	103	SPN	C26-C27-C28-C29
10	i	102	SPN	CM1-C1-C2-C3
10	i	102	SPN	CM2-C1-C2-O2
10	i	102	SPN	CM2-C1-C2-C3
10	i	102	SPN	C20-C21-C22-CM7
10	i	102	SPN	C26-C27-C28-C29
10	j	102	SPN	CM2-C1-O1-CMA
10	j	102	SPN	C2-C1-O1-CMA
10	j	102	SPN	O1-C1-C2-O2
10	j	102	SPN	C18-C19-C20-C21
10	7	102	SPN	CM1-C1-C2-O2
10	7	102	SPN	CM1-C1-C2-C3
10	7	102	SPN	C20-C21-C22-CM7
10	7	102	SPN	C22-C23-C24-C25

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	9	101	MW9	C20-O2-P-O3
11	9	101	MW9	C20-O2-P-O4
11	9	101	MW9	C20-O2-P-O5
11	9	101	MW9	C21-O5-P-O2
11	9	101	MW9	C21-O5-P-O4
13	L	303	BPH	C1-C2-C3-C4
13	L	303	BPH	C1-C2-C3-C5
13	M	405	BPH	C4C-C3C-CAC-CBC
13	M	409	BPH	C1-C2-C3-C4
13	M	409	BPH	C1-C2-C3-C5
9	g	101	BCL	CBD-CGD-O2D-CED
9	2	101	BCL	O1A-CGA-O2A-C1
9	p	101	BCL	O1A-CGA-O2A-C1
9	h	101	BCL	O1A-CGA-O2A-C1
9	0	101	BCL	O1A-CGA-O2A-C1
10	M	406	SPN	C15-C16-C17-C18
9	2	101	BCL	CBA-CGA-O2A-C1
9	p	101	BCL	CBA-CGA-O2A-C1
9	h	101	BCL	CBA-CGA-O2A-C1
9	p	101	BCL	CBD-CGD-O2D-CED
9	x	101	BCL	O1A-CGA-O2A-C1
9	f	101	BCL	O1A-CGA-O2A-C1
9	b	101	BCL	O1A-CGA-O2A-C1
9	j	101	BCL	O1A-CGA-O2A-C1
9	o	101	BCL	CBD-CGD-O2D-CED
9	b	101	BCL	C3-C5-C6-C7
9	0	101	BCL	C3-C5-C6-C7
13	M	409	BPH	C3-C5-C6-C7
9	r	101	BCL	CBA-CGA-O2A-C1
9	f	101	BCL	CBA-CGA-O2A-C1
9	b	101	BCL	CBA-CGA-O2A-C1
9	j	101	BCL	CBA-CGA-O2A-C1
9	0	101	BCL	CBA-CGA-O2A-C1
8	L	305	U10	C20-C19-C21-C22
9	q	101	BCL	C2-C3-C5-C6
10	v	102	SPN	C16-C17-C18-C19
10	q	102	SPN	C25-C26-C27-C28
10	l	102	SPN	C25-C26-C27-C28
9	5	101	BCL	C2A-CAA-CBA-CGA
9	s	101	BCL	C2A-CAA-CBA-CGA
9	m	101	BCL	C2A-CAA-CBA-CGA
9	k	101	BCL	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	g	101	BCL	C2A-CAA-CBA-CGA
9	M	402	BCL	C2A-CAA-CBA-CGA
13	M	409	BPH	C2A-CAA-CBA-CGA
11	H	301	MW9	C7-C8-C9-C10
11	H	303	MW9	C7-C8-C9-C10
11	H	304	MW9	C7-C8-C9-C10
11	M	407	MW9	C7-C8-C9-C10
11	M	408	MW9	C7-C8-C9-C10
11	9	101	MW9	C1-C2-C3-C4
11	9	101	MW9	C7-C8-C9-C10
9	t	101	BCL	C3-C5-C6-C7
9	p	101	BCL	C3-C5-C6-C7
9	f	101	BCL	C3-C5-C6-C7
9	j	101	BCL	C3-C5-C6-C7
9	x	101	BCL	CBA-CGA-O2A-C1
11	H	302	MW9	C7-C8-C9-C10
9	s	101	BCL	C1-C2-C3-C5
9	q	101	BCL	C1-C2-C3-C5
9	m	101	BCL	C1-C2-C3-C5
9	g	101	BCL	C1-C2-C3-C5
9	e	101	BCL	C1-C2-C3-C5
9	7	101	BCL	C1-C2-C3-C5
10	q	102	SPN	C24-C25-C26-CM8
9	r	101	BCL	O1A-CGA-O2A-C1
9	l	101	BCL	O1A-CGA-O2A-C1
11	g	102	MW9	C7-C8-C9-C10
9	g	101	BCL	O1D-CGD-O2D-CED
10	1	103	SPN	C14-C15-C16-C17
9	5	101	BCL	CBD-CGD-O2D-CED
9	e	101	BCL	CBD-CGD-O2D-CED
11	g	103	MW9	O5-C21-C22-O7
9	2	101	BCL	C3-C5-C6-C7
9	M	402	BCL	C3-C5-C6-C7
9	l	101	BCL	CBA-CGA-O2A-C1
11	g	103	MW9	C7-C8-C9-C10
11	M	408	MW9	C13-C14-C15-C16
11	H	304	MW9	C9-C10-C11-C12
9	n	101	BCL	C3-C5-C6-C7
12	C	401	HEM	C3D-CAD-CBD-CGD
9	m	101	BCL	C4-C3-C5-C6
9	g	101	BCL	C4-C3-C5-C6
10	1	102	SPN	CM3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	1	102	SPN	C11-C10-C9-CM4
10	1	102	SPN	CM5-C13-C14-C15
10	1	102	SPN	C16-C17-C18-CM6
10	1	103	SPN	CM3-C5-C6-C7
10	1	103	SPN	C11-C10-C9-CM4
10	1	103	SPN	CM5-C13-C14-C15
10	1	103	SPN	CM8-C26-C27-C28
10	1	104	SPN	CM3-C5-C6-C7
10	1	104	SPN	C11-C10-C9-CM4
10	1	104	SPN	CM5-C13-C14-C15
10	1	104	SPN	C16-C17-C18-CM6
10	1	105	SPN	CM3-C5-C6-C7
10	1	105	SPN	C11-C10-C9-CM4
10	1	105	SPN	CM5-C13-C14-C15
10	1	105	SPN	C16-C17-C18-CM6
10	5	102	SPN	CM3-C5-C6-C7
10	5	102	SPN	C11-C10-C9-CM4
10	5	102	SPN	CM5-C13-C14-C15
10	5	102	SPN	C16-C17-C18-CM6
10	5	103	SPN	CM3-C5-C6-C7
10	5	103	SPN	C11-C10-C9-CM4
10	5	103	SPN	CM5-C13-C14-C15
10	5	103	SPN	C16-C17-C18-CM6
10	5	103	SPN	CM8-C26-C27-C28
10	3	102	SPN	CM3-C5-C6-C7
10	3	102	SPN	C11-C10-C9-CM4
10	3	102	SPN	CM5-C13-C14-C15
10	3	102	SPN	C16-C17-C18-CM6
10	w	102	SPN	CM3-C5-C6-C7
10	w	102	SPN	C11-C10-C9-CM4
10	w	102	SPN	CM5-C13-C14-C15
10	w	102	SPN	C16-C17-C18-CM6
10	u	102	SPN	CM3-C5-C6-C7
10	u	102	SPN	C11-C10-C9-CM4
10	u	102	SPN	CM5-C13-C14-C15
10	u	102	SPN	C16-C17-C18-CM6
10	v	102	SPN	CM3-C5-C6-C7
10	v	102	SPN	C11-C10-C9-CM4
10	v	102	SPN	CM5-C13-C14-C15
10	v	102	SPN	C16-C17-C18-CM6
10	s	102	SPN	CM3-C5-C6-C7
10	s	102	SPN	C11-C10-C9-CM4

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	7	103	SPN	C11-C10-C9-CM4
10	7	103	SPN	CM5-C13-C14-C15
10	7	103	SPN	C16-C17-C18-CM6
10	7	103	SPN	CM8-C26-C27-C28
10	M	406	SPN	CM3-C5-C6-C7
10	M	406	SPN	C11-C10-C9-CM4
10	M	406	SPN	CM5-C13-C14-C15
10	M	406	SPN	C16-C17-C18-CM6
10	9	103	SPN	CM3-C5-C6-C7
10	9	103	SPN	C11-C10-C9-CM4
10	9	103	SPN	CM5-C13-C14-C15
10	9	103	SPN	C16-C17-C18-CM6
10	0	102	SPN	CM3-C5-C6-C7
10	0	102	SPN	C11-C10-C9-CM4
10	0	102	SPN	CM5-C13-C14-C15
10	0	102	SPN	C16-C17-C18-CM6
8	L	305	U10	C13-C14-C16-C17
9	m	101	BCL	C2-C3-C5-C6
9	g	101	BCL	C2-C3-C5-C6
10	1	102	SPN	C4-C5-C6-C7
10	1	102	SPN	C11-C10-C9-C8
10	1	102	SPN	C12-C13-C14-C15
10	1	102	SPN	C16-C17-C18-C19
10	1	103	SPN	C4-C5-C6-C7
10	1	103	SPN	C11-C10-C9-C8
10	1	103	SPN	C25-C26-C27-C28
10	1	104	SPN	C4-C5-C6-C7
10	1	104	SPN	C11-C10-C9-C8
10	1	104	SPN	C12-C13-C14-C15
10	1	104	SPN	C16-C17-C18-C19
10	1	105	SPN	C4-C5-C6-C7
10	1	105	SPN	C11-C10-C9-C8
10	1	105	SPN	C12-C13-C14-C15
10	1	105	SPN	C16-C17-C18-C19
10	5	102	SPN	C4-C5-C6-C7
10	5	102	SPN	C11-C10-C9-C8
10	5	102	SPN	C12-C13-C14-C15
10	5	102	SPN	C16-C17-C18-C19
10	5	103	SPN	C4-C5-C6-C7
10	5	103	SPN	C11-C10-C9-C8
10	5	103	SPN	C12-C13-C14-C15
10	5	103	SPN	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	5	103	SPN	C25-C26-C27-C28
10	3	102	SPN	C4-C5-C6-C7
10	3	102	SPN	C11-C10-C9-C8
10	3	102	SPN	C12-C13-C14-C15
10	3	102	SPN	C16-C17-C18-C19
10	w	102	SPN	C4-C5-C6-C7
10	w	102	SPN	C11-C10-C9-C8
10	w	102	SPN	C12-C13-C14-C15
10	w	102	SPN	C16-C17-C18-C19
10	u	102	SPN	C4-C5-C6-C7
10	u	102	SPN	C11-C10-C9-C8
10	u	102	SPN	C12-C13-C14-C15
10	u	102	SPN	C16-C17-C18-C19
10	v	102	SPN	C4-C5-C6-C7
10	v	102	SPN	C11-C10-C9-C8
10	v	102	SPN	C12-C13-C14-C15
10	s	102	SPN	C4-C5-C6-C7
10	s	102	SPN	C11-C10-C9-C8
10	s	102	SPN	C12-C13-C14-C15
10	s	102	SPN	C16-C17-C18-C19
10	t	102	SPN	C4-C5-C6-C7
10	t	102	SPN	C11-C10-C9-C8
10	t	102	SPN	C12-C13-C14-C15
10	t	102	SPN	C16-C17-C18-C19
10	q	102	SPN	C4-C5-C6-C7
10	q	102	SPN	C11-C10-C9-C8
10	q	102	SPN	C12-C13-C14-C15
10	q	102	SPN	C16-C17-C18-C19
10	r	102	SPN	C4-C5-C6-C7
10	r	102	SPN	C11-C10-C9-C8
10	r	102	SPN	C12-C13-C14-C15
10	r	102	SPN	C16-C17-C18-C19
10	p	102	SPN	C4-C5-C6-C7
10	p	102	SPN	C11-C10-C9-C8
10	p	102	SPN	C12-C13-C14-C15
10	p	102	SPN	C16-C17-C18-C19
10	p	103	SPN	C4-C5-C6-C7
10	p	103	SPN	C11-C10-C9-C8
10	p	103	SPN	C12-C13-C14-C15
10	p	103	SPN	C16-C17-C18-C19
10	m	102	SPN	C4-C5-C6-C7
10	m	102	SPN	C11-C10-C9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	m	102	SPN	C12-C13-C14-C15
10	m	102	SPN	C16-C17-C18-C19
10	n	102	SPN	C4-C5-C6-C7
10	n	102	SPN	C11-C10-C9-C8
10	n	102	SPN	C12-C13-C14-C15
10	n	102	SPN	C16-C17-C18-C19
10	k	102	SPN	C4-C5-C6-C7
10	k	102	SPN	C11-C10-C9-C8
10	k	102	SPN	C12-C13-C14-C15
10	k	102	SPN	C16-C17-C18-C19
10	l	102	SPN	C4-C5-C6-C7
10	l	102	SPN	C11-C10-C9-C8
10	l	102	SPN	C12-C13-C14-C15
10	l	102	SPN	C16-C17-C18-C19
10	h	102	SPN	C4-C5-C6-C7
10	h	102	SPN	C11-C10-C9-C8
10	h	102	SPN	C12-C13-C14-C15
10	h	102	SPN	C16-C17-C18-C19
10	h	103	SPN	C4-C5-C6-C7
10	h	103	SPN	C11-C10-C9-C8
10	h	103	SPN	C12-C13-C14-C15
10	h	103	SPN	C16-C17-C18-C19
10	e	102	SPN	C4-C5-C6-C7
10	e	102	SPN	C11-C10-C9-C8
10	e	102	SPN	C12-C13-C14-C15
10	e	102	SPN	C16-C17-C18-C19
10	f	102	SPN	C4-C5-C6-C7
10	f	102	SPN	C11-C10-C9-C8
10	f	102	SPN	C12-C13-C14-C15
10	f	102	SPN	C16-C17-C18-C19
10	c	102	SPN	C4-C5-C6-C7
10	c	102	SPN	C11-C10-C9-C8
10	c	102	SPN	C12-C13-C14-C15
10	c	102	SPN	C16-C17-C18-C19
10	c	103	SPN	C4-C5-C6-C7
10	c	103	SPN	C11-C10-C9-C8
10	c	103	SPN	C12-C13-C14-C15
10	c	103	SPN	C16-C17-C18-C19
10	a	102	SPN	C4-C5-C6-C7
10	a	102	SPN	C11-C10-C9-C8
10	a	102	SPN	C12-C13-C14-C15
10	a	102	SPN	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	a	103	SPN	C4-C5-C6-C7
10	a	103	SPN	C11-C10-C9-C8
10	a	103	SPN	C12-C13-C14-C15
10	a	103	SPN	C16-C17-C18-C19
10	i	102	SPN	C4-C5-C6-C7
10	i	102	SPN	C11-C10-C9-C8
10	i	102	SPN	C12-C13-C14-C15
10	i	102	SPN	C16-C17-C18-C19
10	j	102	SPN	C4-C5-C6-C7
10	j	102	SPN	C11-C10-C9-C8
10	j	102	SPN	C12-C13-C14-C15
10	j	102	SPN	C16-C17-C18-C19
10	j	102	SPN	C25-C26-C27-C28
10	7	102	SPN	C4-C5-C6-C7
10	7	102	SPN	C11-C10-C9-C8
10	7	102	SPN	C12-C13-C14-C15
10	7	102	SPN	C16-C17-C18-C19
10	7	103	SPN	C4-C5-C6-C7
10	7	103	SPN	C11-C10-C9-C8
10	7	103	SPN	C12-C13-C14-C15
10	7	103	SPN	C16-C17-C18-C19
10	7	103	SPN	C25-C26-C27-C28
10	M	406	SPN	C4-C5-C6-C7
10	M	406	SPN	C11-C10-C9-C8
10	M	406	SPN	C12-C13-C14-C15
10	M	406	SPN	C16-C17-C18-C19
10	9	103	SPN	C4-C5-C6-C7
10	9	103	SPN	C11-C10-C9-C8
10	9	103	SPN	C12-C13-C14-C15
10	9	103	SPN	C16-C17-C18-C19
10	0	102	SPN	C4-C5-C6-C7
10	0	102	SPN	C11-C10-C9-C8
10	0	102	SPN	C12-C13-C14-C15
10	0	102	SPN	C16-C17-C18-C19
9	3	101	BCL	C2A-CAA-CBA-CGA
9	r	101	BCL	C2A-CAA-CBA-CGA
8	A	101	U10	C19-C21-C22-C23
8	L	305	U10	C14-C16-C17-C18
8	L	305	U10	C24-C26-C27-C28
8	M	403	U10	C24-C26-C27-C28
8	M	403	U10	C29-C31-C32-C33
8	M	403	U10	C39-C41-C42-C43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	1	103	SPN	C26-C27-C28-C29
10	5	103	SPN	C26-C27-C28-C29
10	3	102	SPN	C26-C27-C28-C29
10	v	102	SPN	C26-C27-C28-C29
10	s	102	SPN	C26-C27-C28-C29
10	t	102	SPN	C26-C27-C28-C29
10	l	102	SPN	C26-C27-C28-C29
10	h	103	SPN	C26-C27-C28-C29
10	f	102	SPN	C26-C27-C28-C29
10	j	102	SPN	C26-C27-C28-C29
9	l	101	BCL	C1-C2-C3-C5
9	h	101	BCL	C1-C2-C3-C5
9	p	101	BCL	O1D-CGD-O2D-CED
9	h	101	BCL	C10-C11-C12-C13
11	H	304	MW9	O5-C21-C22-C23
10	q	102	SPN	C24-C25-C26-C27
9	4	101	BCL	C3-C5-C6-C7
9	h	101	BCL	C3-C5-C6-C7
9	q	101	BCL	CBA-CGA-O2A-C1
9	i	101	BCL	C15-C16-C17-C18
9	u	101	BCL	CBD-CGD-O2D-CED
11	M	408	MW9	C4-C5-C6-C7
11	9	101	MW9	C35-C36-C37-C38
11	H	304	MW9	C14-C15-C16-C17
11	g	102	MW9	C5-C6-C7-C8
11	H	304	MW9	C12-C13-C14-C15
9	q	101	BCL	C13-C15-C16-C17
9	i	101	BCL	C8-C10-C11-C12
11	H	301	MW9	C4-C5-C6-C7
9	s	101	BCL	C5-C6-C7-C8
9	o	101	BCL	C10-C11-C12-C13
9	h	101	BCL	C5-C6-C7-C8
9	j	101	BCL	C8-C10-C11-C12
9	0	101	BCL	C13-C15-C16-C17
9	0	101	BCL	C15-C16-C17-C18
10	f	102	SPN	CM8-C26-C27-C28
8	L	305	U10	C18-C19-C21-C22
9	5	101	BCL	C11-C12-C13-C14
9	6	101	BCL	C11-C12-C13-C14
9	3	101	BCL	C11-C12-C13-C14
9	4	101	BCL	C11-C12-C13-C14
9	w	101	BCL	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	w	101	BCL	C14-C13-C15-C16
9	v	101	BCL	C11-C10-C8-C9
9	s	101	BCL	C11-C12-C13-C14
9	t	101	BCL	C11-C12-C13-C14
9	r	101	BCL	C6-C7-C8-C9
9	p	101	BCL	C14-C13-C15-C16
9	m	101	BCL	C11-C12-C13-C14
9	k	101	BCL	C11-C12-C13-C14
9	g	101	BCL	C11-C12-C13-C14
9	h	101	BCL	C14-C13-C15-C16
9	e	101	BCL	C11-C12-C13-C14
9	c	101	BCL	C11-C12-C13-C14
9	c	101	BCL	C14-C13-C15-C16
9	d	101	BCL	C11-C12-C13-C14
9	a	101	BCL	C14-C13-C15-C16
9	j	101	BCL	C14-C13-C15-C16
9	7	101	BCL	C11-C12-C13-C14
9	M	402	BCL	C6-C7-C8-C9
9	M	402	BCL	C11-C12-C13-C14
9	9	102	BCL	C11-C12-C13-C14
9	0	101	BCL	C11-C12-C13-C14
10	1	103	SPN	CM7-C22-C23-C24
10	1	104	SPN	CM7-C22-C23-C24
10	v	102	SPN	C20-C21-C22-CM7
10	v	102	SPN	CM7-C22-C23-C24
10	p	102	SPN	CM7-C22-C23-C24
10	p	103	SPN	C20-C21-C22-CM7
10	h	103	SPN	C20-C21-C22-CM7
10	h	103	SPN	CM7-C22-C23-C24
10	f	102	SPN	C20-C21-C22-CM7
10	f	102	SPN	CM7-C22-C23-C24
10	j	102	SPN	CM7-C22-C23-C24
9	c	101	BCL	C2A-CAA-CBA-CGA
9	9	102	BCL	C2A-CAA-CBA-CGA
11	M	407	MW9	C24-C25-C26-C27
11	9	101	MW9	C24-C25-C26-C27
9	n	101	BCL	C8-C10-C11-C12
9	c	101	BCL	C13-C15-C16-C17
13	M	409	BPH	C13-C15-C16-C17
9	w	101	BCL	C3-C5-C6-C7
9	2	101	BCL	C10-C11-C12-C13
9	3	101	BCL	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	v	101	BCL	C10-C11-C12-C13
13	M	409	BPH	C5-C6-C7-C8
13	M	409	BPH	C10-C11-C12-C13
10	i	102	SPN	C22-C23-C24-C25
10	0	102	SPN	C22-C23-C24-C25
9	w	101	BCL	C13-C15-C16-C17
9	s	101	BCL	C8-C10-C11-C12
9	t	101	BCL	C5-C6-C7-C8
9	q	101	BCL	C8-C10-C11-C12
9	m	101	BCL	C10-C11-C12-C13
9	e	101	BCL	C15-C16-C17-C18
9	8	101	BCL	C10-C11-C12-C13
11	H	301	MW9	C24-C25-C26-C27
11	H	303	MW9	C24-C25-C26-C27
11	H	301	MW9	C11-C12-C13-C14
9	1	101	BCL	C10-C11-C12-C13
9	2	101	BCL	C15-C16-C17-C18
9	6	101	BCL	C15-C16-C17-C18
9	3	101	BCL	C15-C16-C17-C18
9	b	101	BCL	C10-C11-C12-C13
9	L	301	BCL	C15-C16-C17-C18
9	k	101	BCL	C10-C11-C12-C13
9	u	101	BCL	C10-C11-C12-C13
9	k	101	BCL	C15-C16-C17-C18
13	L	303	BPH	C15-C16-C17-C18
9	3	101	BCL	C11-C10-C8-C7
9	4	101	BCL	C6-C7-C8-C10
9	p	101	BCL	C11-C10-C8-C7
9	m	101	BCL	C12-C13-C15-C16
9	n	101	BCL	C6-C7-C8-C10
9	n	101	BCL	C11-C12-C13-C15
9	k	101	BCL	C12-C13-C15-C16
9	h	101	BCL	C11-C10-C8-C7
9	j	101	BCL	C11-C10-C8-C7
9	7	101	BCL	C6-C7-C8-C10
9	0	101	BCL	C6-C7-C8-C10
10	1	103	SPN	C20-C21-C22-C23
10	1	104	SPN	C20-C21-C22-C23
10	l	102	SPN	C20-C21-C22-C23
10	a	103	SPN	C20-C21-C22-C23
10	j	102	SPN	C20-C21-C22-C23
10	0	102	SPN	C21-C22-C23-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	M	409	BPH	C6-C7-C8-C10
9	k	101	BCL	C3-C5-C6-C7
9	M	404	BCL	C3-C5-C6-C7
9	a	101	BCL	C2A-CAA-CBA-CGA
9	q	101	BCL	C15-C16-C17-C18
9	f	101	BCL	C13-C15-C16-C17
13	M	409	BPH	C15-C16-C17-C18
9	n	101	BCL	C13-C15-C16-C17
9	b	101	BCL	C13-C15-C16-C17
8	L	305	U10	C19-C21-C22-C23
8	M	403	U10	C14-C16-C17-C18
8	M	403	U10	C34-C36-C37-C38
10	1	102	SPN	C26-C27-C28-C29
10	1	104	SPN	C26-C27-C28-C29
10	1	105	SPN	C26-C27-C28-C29
10	w	102	SPN	C26-C27-C28-C29
10	7	102	SPN	C26-C27-C28-C29
10	9	103	SPN	C26-C27-C28-C29
9	q	101	BCL	C10-C11-C12-C13
9	h	101	BCL	C13-C15-C16-C17
9	7	101	BCL	C10-C11-C12-C13
9	9	102	BCL	C10-C11-C12-C13
9	9	102	BCL	C15-C16-C17-C18
9	q	101	BCL	O1A-CGA-O2A-C1
11	M	408	MW9	C24-C25-C26-C27
9	v	101	BCL	C15-C16-C17-C18
9	r	101	BCL	C10-C11-C12-C13
9	r	101	BCL	C13-C15-C16-C17
9	r	101	BCL	C15-C16-C17-C18
9	l	101	BCL	C15-C16-C17-C18
9	b	101	BCL	C8-C10-C11-C12
9	7	101	BCL	C15-C16-C17-C18
13	M	405	BPH	C8-C10-C11-C12
9	o	101	BCL	O1D-CGD-O2D-CED
9	3	101	BCL	C8-C10-C11-C12
9	x	101	BCL	C5-C6-C7-C8
9	c	101	BCL	C8-C10-C11-C12
9	j	101	BCL	C5-C6-C7-C8
9	M	402	BCL	C5-C6-C7-C8
11	g	102	MW9	C21-O5-P-O2
11	H	302	MW9	C21-O5-P-O2
11	H	304	MW9	C21-O5-P-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	g	102	MW9	C14-C15-C16-C17
9	c	101	BCL	C4-C3-C5-C6
9	r	101	BCL	C5-C6-C7-C8
9	d	101	BCL	C15-C16-C17-C18
9	o	101	BCL	C2A-CAA-CBA-CGA
9	7	101	BCL	C2A-CAA-CBA-CGA
9	p	101	BCL	C16-C17-C18-C20
9	m	101	BCL	C16-C17-C18-C20
9	d	101	BCL	C16-C17-C18-C20
9	n	101	BCL	C15-C16-C17-C18
9	e	101	BCL	C13-C15-C16-C17
9	f	101	BCL	C10-C11-C12-C13
11	g	102	MW9	C33-C34-C35-C36
11	H	301	MW9	C33-C34-C35-C36
11	M	407	MW9	C4-C5-C6-C7
9	g	101	BCL	C16-C17-C18-C20
9	6	101	BCL	CBA-CGA-O2A-C1
11	M	407	MW9	C11-C10-C9-C8
11	M	408	MW9	C28-C29-C30-C31
11	H	303	MW9	C11-C12-C13-C14
11	H	303	MW9	C2-C3-C4-C5
11	H	304	MW9	C26-C27-C28-C29
11	M	408	MW9	C27-C28-C29-C30
13	L	303	BPH	C5-C6-C7-C8
11	H	303	MW9	C35-C36-C37-C38
11	9	101	MW9	C34-C35-C36-C37
11	9	101	MW9	C37-C38-C39-C40
11	M	408	MW9	C14-C15-C16-C17
9	e	101	BCL	O1D-CGD-O2D-CED
10	1	102	SPN	CM2-C1-O1-CMA
10	1	104	SPN	CM1-C1-O1-CMA
10	5	102	SPN	CM2-C1-O1-CMA
10	5	103	SPN	CM2-C1-O1-CMA
10	3	102	SPN	CM1-C1-O1-CMA
10	3	102	SPN	CM2-C1-O1-CMA
10	a	102	SPN	CM2-C1-O1-CMA
10	j	102	SPN	CM1-C1-O1-CMA
10	7	103	SPN	CM1-C1-O1-CMA
10	0	102	SPN	CM1-C1-O1-CMA
11	g	102	MW9	C1-C2-C3-C4
11	g	102	MW9	C28-C29-C30-C31
11	H	303	MW9	C37-C38-C39-C40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	9	102	BCL	C13-C15-C16-C17
9	1	101	BCL	C16-C17-C18-C20
9	L	301	BCL	C11-C10-C8-C9
9	M	402	BCL	C11-C10-C8-C9
13	L	303	BPH	C6-C7-C8-C9
11	H	304	MW9	C35-C36-C37-C38
9	M	402	BCL	C8-C10-C11-C12
9	1	101	BCL	C2A-CAA-CBA-CGA
11	H	301	MW9	C5-C6-C7-C8
11	H	301	MW9	C6-C7-C8-C9
11	M	408	MW9	C11-C10-C9-C8
11	9	101	MW9	C2-C3-C4-C5
11	9	101	MW9	C21-C22-C23-O6
9	q	101	BCL	C5-C6-C7-C8
9	l	101	BCL	C13-C15-C16-C17
11	H	301	MW9	C2-C3-C4-C5
11	H	304	MW9	C3-C4-C5-C6
10	p	103	SPN	C17-C18-C19-C20
9	9	102	BCL	CBD-CGD-O2D-CED
11	g	102	MW9	C35-C36-C37-C38
11	g	103	MW9	C5-C6-C7-C8
11	H	302	MW9	C4-C5-C6-C7
11	H	303	MW9	C27-C28-C29-C30
11	H	304	MW9	C10-C11-C12-C13
11	9	101	MW9	C28-C29-C30-C31
9	d	101	BCL	C16-C17-C18-C19
9	M	404	BCL	C16-C17-C18-C19
9	o	101	BCL	C5-C6-C7-C8
11	H	303	MW9	C34-C35-C36-C37
11	H	302	MW9	C5-C6-C7-C8
11	M	408	MW9	C10-C11-C12-C13
9	5	101	BCL	O1D-CGD-O2D-CED
9	1	101	BCL	C3A-C2A-CAA-CBA
9	6	101	BCL	C3A-C2A-CAA-CBA
9	4	101	BCL	C3A-C2A-CAA-CBA
9	s	101	BCL	C3A-C2A-CAA-CBA
9	m	101	BCL	C3A-C2A-CAA-CBA
9	f	101	BCL	C3A-C2A-CAA-CBA
9	b	101	BCL	C3A-C2A-CAA-CBA
9	L	301	BCL	C3A-C2A-CAA-CBA
13	M	405	BPH	C3A-C2A-CAA-CBA
11	H	302	MW9	C36-C37-C38-C39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	M	408	MW9	C6-C7-C8-C9
11	9	101	MW9	C11-C12-C13-C14
9	M	404	BCL	C16-C17-C18-C20
11	g	103	MW9	C37-C38-C39-C40
11	H	303	MW9	C10-C11-C12-C13
10	3	102	SPN	C22-C23-C24-C25
10	t	102	SPN	C22-C23-C24-C25
10	m	102	SPN	C22-C23-C24-C25
10	a	103	SPN	C22-C23-C24-C25
11	H	304	MW9	C28-C29-C30-C31
9	2	101	BCL	C4-C3-C5-C6
9	x	101	BCL	C4-C3-C5-C6
9	2	101	BCL	C2-C3-C5-C6
9	4	101	BCL	C2-C3-C5-C6
9	M	402	BCL	C2-C3-C5-C6
10	f	102	SPN	C25-C26-C27-C28
11	H	301	MW9	O7-C22-C23-O6
11	H	302	MW9	O7-C22-C23-O6
11	H	304	MW9	O7-C22-C23-O6
11	M	408	MW9	C25-C26-C27-C28
11	9	101	MW9	C27-C28-C29-C30
9	x	101	BCL	C16-C17-C18-C19
9	L	304	BCL	C3-C5-C6-C7
11	H	304	MW9	C37-C38-C39-C40
9	6	101	BCL	O1A-CGA-O2A-C1
11	M	408	MW9	C2-C3-C4-C5
11	H	304	MW9	C25-C26-C27-C28
9	p	101	BCL	C10-C11-C12-C13
11	M	408	MW9	C36-C37-C38-C39
9	m	101	BCL	C16-C17-C18-C19
9	7	101	BCL	C16-C17-C18-C20
11	H	304	MW9	C24-C25-C26-C27
11	H	302	MW9	C12-C13-C14-C15
9	8	101	BCL	CBA-CGA-O2A-C1
9	4	101	BCL	C5-C6-C7-C8
9	v	101	BCL	C5-C6-C7-C8
9	p	101	BCL	C13-C15-C16-C17
9	n	101	BCL	C10-C11-C12-C13
11	g	103	MW9	C10-C11-C12-C13
11	H	302	MW9	C37-C38-C39-C40
9	4	101	BCL	C4-C3-C5-C6
9	n	101	BCL	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	M	403	U10	C28-C29-C31-C32
9	6	101	BCL	C11-C12-C13-C15
9	x	101	BCL	C2-C3-C5-C6
9	x	101	BCL	C6-C7-C8-C10
9	q	101	BCL	C11-C10-C8-C7
9	c	101	BCL	C11-C12-C13-C15
9	b	101	BCL	C6-C7-C8-C10
9	i	101	BCL	C11-C12-C13-C15
9	9	102	BCL	C11-C10-C8-C7
9	0	101	BCL	C12-C13-C15-C16
10	1	102	SPN	C21-C22-C23-C24
10	n	102	SPN	C21-C22-C23-C24
10	c	103	SPN	C21-C22-C23-C24
10	7	103	SPN	C21-C22-C23-C24
13	L	303	BPH	C6-C7-C8-C10
9	b	101	BCL	C15-C16-C17-C18
9	3	101	BCL	C16-C17-C18-C20
9	s	101	BCL	C16-C17-C18-C20
11	H	303	MW9	C29-C30-C31-C32
11	M	407	MW9	C29-C30-C31-C32
11	M	408	MW9	C29-C30-C31-C32
11	9	101	MW9	C33-C34-C35-C36
11	g	103	MW9	C14-C15-C16-C17
9	L	304	BCL	C2A-CAA-CBA-CGA
9	2	101	BCL	C8-C10-C11-C12
9	k	101	BCL	C13-C15-C16-C17
11	H	301	MW9	C12-C13-C14-C15
11	H	301	MW9	C36-C37-C38-C39
11	H	303	MW9	C26-C27-C28-C29
9	v	101	BCL	C3-C5-C6-C7
9	m	101	BCL	C5-C6-C7-C8
9	m	101	BCL	C15-C16-C17-C18
11	g	102	MW9	C3-C4-C5-C6
11	H	301	MW9	C1-C2-C3-C4
11	H	303	MW9	C4-C5-C6-C7
12	C	402	HEM	C4C-C3C-CAC-CBC
9	0	101	BCL	C5-C6-C7-C8
9	8	101	BCL	C3-C5-C6-C7
9	s	101	BCL	C15-C16-C17-C18
11	9	101	MW9	O1-C18-C19-O8
9	1	101	BCL	C16-C17-C18-C19
9	g	101	BCL	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	4	101	BCL	C8-C10-C11-C12
9	l	101	BCL	C5-C6-C7-C8
11	H	304	MW9	C29-C30-C31-C32
8	M	403	U10	C30-C29-C31-C32
9	n	101	BCL	C2-C3-C5-C6
9	c	101	BCL	C2-C3-C5-C6
11	H	301	MW9	C26-C27-C28-C29
9	3	101	BCL	C11-C10-C8-C9
9	x	101	BCL	C6-C7-C8-C9
9	x	101	BCL	C11-C10-C8-C9
9	r	101	BCL	C11-C10-C8-C9
9	p	101	BCL	C11-C10-C8-C9
9	h	101	BCL	C11-C10-C8-C9
9	d	101	BCL	C6-C7-C8-C9
9	7	101	BCL	C6-C7-C8-C9
9	L	304	BCL	C14-C13-C15-C16
9	9	102	BCL	C11-C10-C8-C9
9	0	101	BCL	C6-C7-C8-C9
9	s	101	BCL	C3-C5-C6-C7
13	M	405	BPH	C2A-CAA-CBA-CGA
13	M	405	BPH	C2C-C3C-CAC-CBC
9	5	101	BCL	C15-C16-C17-C18
11	H	304	MW9	C6-C7-C8-C9
9	8	101	BCL	O1A-CGA-O2A-C1
9	1	101	BCL	C1A-C2A-CAA-CBA
9	2	101	BCL	C1A-C2A-CAA-CBA
9	6	101	BCL	C1A-C2A-CAA-CBA
9	4	101	BCL	C1A-C2A-CAA-CBA
9	s	101	BCL	C1A-C2A-CAA-CBA
9	m	101	BCL	C1A-C2A-CAA-CBA
9	f	101	BCL	C1A-C2A-CAA-CBA
9	L	301	BCL	C1A-C2A-CAA-CBA
9	c	101	BCL	C16-C17-C18-C20
9	5	101	BCL	C8-C10-C11-C12
9	5	101	BCL	C10-C11-C12-C13
9	u	101	BCL	C13-C15-C16-C17
9	t	101	BCL	C10-C11-C12-C13
11	H	303	MW9	C21-O5-P-O2
11	H	303	MW9	C36-C37-C38-C39
9	s	101	BCL	C10-C11-C12-C13
9	L	304	BCL	CBA-CGA-O2A-C1
11	H	302	MW9	C18-C19-C20-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	H	303	MW9	C18-C19-C20-O2
11	g	103	MW9	O5-C21-C22-C23
9	M	402	BCL	C4-C3-C5-C6
9	6	101	BCL	C2C-C3C-CAC-CBC
9	x	101	BCL	C2C-C3C-CAC-CBC
9	u	101	BCL	C2C-C3C-CAC-CBC
9	q	101	BCL	C2C-C3C-CAC-CBC
9	m	101	BCL	C2C-C3C-CAC-CBC
9	c	101	BCL	C2C-C3C-CAC-CBC
9	d	101	BCL	C2C-C3C-CAC-CBC
9	a	101	BCL	C2C-C3C-CAC-CBC
9	M	404	BCL	C2C-C3C-CAC-CBC
9	9	102	BCL	C2C-C3C-CAC-CBC
9	l	101	BCL	C8-C10-C11-C12
9	L	304	BCL	C13-C15-C16-C17
10	1	102	SPN	C22-C23-C24-C25
10	n	102	SPN	C22-C23-C24-C25
11	H	303	MW9	O1-C18-C19-C20
9	u	101	BCL	O1D-CGD-O2D-CED
9	g	101	BCL	C10-C11-C12-C13
9	c	101	BCL	C15-C16-C17-C18
10	a	102	SPN	C26-C27-C28-C29
11	g	102	MW9	C11-C12-C13-C14
11	H	304	MW9	C33-C34-C35-C36
11	M	407	MW9	C33-C34-C35-C36
8	L	302	U10	C12-C11-C9-C10
8	L	302	U10	C15-C14-C16-C17
11	M	408	MW9	C38-C39-C40-C41
9	M	404	BCL	CBD-CGD-O2D-CED
9	1	101	BCL	C8-C10-C11-C12
11	M	407	MW9	C-C1-C2-C3
9	j	101	BCL	C10-C11-C12-C13
11	M	408	MW9	C1-C2-C3-C4
11	H	304	MW9	C32-C33-C34-C35
11	H	301	MW9	C28-C29-C30-C31
9	9	102	BCL	C8-C10-C11-C12
9	x	101	BCL	C8-C10-C11-C12
10	t	102	SPN	CM2-C1-O1-CMA
11	9	101	MW9	C13-C14-C15-C16
10	h	103	SPN	CM6-C18-C19-C20
13	L	303	BPH	C10-C11-C12-C13
8	L	302	U10	C12-C11-C9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	L	302	U10	C13-C14-C16-C17
9	2	101	BCL	C11-C10-C8-C7
9	5	101	BCL	C6-C7-C8-C10
9	5	101	BCL	C11-C10-C8-C7
9	5	101	BCL	C11-C12-C13-C15
9	w	101	BCL	C6-C7-C8-C10
9	x	101	BCL	C11-C10-C8-C7
9	x	101	BCL	C12-C13-C15-C16
9	u	101	BCL	C6-C7-C8-C10
9	s	101	BCL	C11-C12-C13-C15
9	t	101	BCL	C12-C13-C15-C16
9	r	101	BCL	C11-C10-C8-C7
9	p	101	BCL	C12-C13-C15-C16
9	k	101	BCL	C11-C10-C8-C7
9	k	101	BCL	C11-C12-C13-C15
9	l	101	BCL	C6-C7-C8-C10
9	l	101	BCL	C11-C10-C8-C7
9	e	101	BCL	C11-C12-C13-C15
9	d	101	BCL	C6-C7-C8-C10
9	d	101	BCL	C11-C10-C8-C7
9	d	101	BCL	C11-C12-C13-C15
9	a	101	BCL	C6-C7-C8-C10
9	a	101	BCL	C12-C13-C15-C16
9	b	101	BCL	C11-C10-C8-C7
9	7	101	BCL	C11-C10-C8-C7
9	L	304	BCL	C12-C13-C15-C16
9	M	402	BCL	C6-C7-C8-C10
9	M	402	BCL	C12-C13-C15-C16
10	5	102	SPN	C21-C22-C23-C24
10	u	102	SPN	C21-C22-C23-C24
10	k	102	SPN	C21-C22-C23-C24
10	l	102	SPN	C21-C22-C23-C24
10	a	102	SPN	C21-C22-C23-C24
13	L	303	BPH	C12-C13-C15-C16
9	5	101	BCL	C11-C10-C8-C9
9	4	101	BCL	C6-C7-C8-C9
9	s	101	BCL	C14-C13-C15-C16
9	t	101	BCL	C14-C13-C15-C16
9	q	101	BCL	C11-C10-C8-C9
9	o	101	BCL	C11-C10-C8-C9
9	m	101	BCL	C14-C13-C15-C16
9	n	101	BCL	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	n	101	BCL	C11-C10-C8-C9
9	n	101	BCL	C11-C12-C13-C14
9	g	101	BCL	C14-C13-C15-C16
9	d	101	BCL	C11-C10-C8-C9
9	a	101	BCL	C6-C7-C8-C9
9	j	101	BCL	C11-C10-C8-C9
9	j	101	BCL	C11-C12-C13-C14
9	7	101	BCL	C11-C10-C8-C9
9	L	304	BCL	C11-C10-C8-C9
9	M	402	BCL	C14-C13-C15-C16
10	t	102	SPN	CM7-C22-C23-C24
13	L	303	BPH	C14-C13-C15-C16
13	M	405	BPH	C11-C12-C13-C14
9	w	101	BCL	CBA-CGA-O2A-C1
9	e	101	BCL	C8-C10-C11-C12
9	d	101	BCL	C10-C11-C12-C13
9	l	101	BCL	C10-C11-C12-C13
9	L	304	BCL	O1A-CGA-O2A-C1
11	g	103	MW9	C11-C12-C13-C14
9	g	101	BCL	C8-C10-C11-C12
9	a	101	BCL	C8-C10-C11-C12
11	g	102	MW9	C18-C19-C20-O2
11	H	304	MW9	C18-C19-C20-O2
11	M	408	MW9	C18-C19-C20-O2
8	L	302	U10	C24-C26-C27-C28
10	5	102	SPN	C26-C27-C28-C29
10	k	102	SPN	C26-C27-C28-C29
9	a	101	BCL	C1-C2-C3-C5
13	L	303	BPH	C3-C5-C6-C7
9	c	101	BCL	C16-C17-C18-C19
9	u	101	BCL	C2A-CAA-CBA-CGA
10	1	102	SPN	CM2-C1-C2-O2
10	1	102	SPN	CM2-C1-C2-C3
10	5	102	SPN	CM2-C1-C2-O2
10	3	102	SPN	CM2-C1-C2-O2
10	w	102	SPN	CM2-C1-C2-O2
10	q	102	SPN	CM2-C1-C2-C3
10	r	102	SPN	CM2-C1-C2-O2
10	p	102	SPN	CM1-C1-C2-O2
10	p	102	SPN	CM1-C1-C2-C3
10	p	103	SPN	CM2-C1-C2-O2
10	m	102	SPN	CM2-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	m	102	SPN	CM2-C1-C2-C3
10	k	102	SPN	CM1-C1-C2-O2
10	k	102	SPN	CM1-C1-C2-C3
10	k	102	SPN	CM2-C1-C2-O2
10	k	102	SPN	CM2-C1-C2-C3
10	7	102	SPN	CM2-C1-C2-O2
10	7	102	SPN	CM2-C1-C2-C3
9	e	101	BCL	CBA-CGA-O2A-C1
9	2	101	BCL	C3A-C2A-CAA-CBA
9	u	101	BCL	C3A-C2A-CAA-CBA
9	h	101	BCL	C3A-C2A-CAA-CBA
11	g	103	MW9	C24-C25-C26-C27
11	M	407	MW9	C9-C10-C11-C12
11	9	101	MW9	C5-C6-C7-C8
9	s	101	BCL	C16-C17-C18-C19
9	t	101	BCL	CBA-CGA-O2A-C1
10	1	104	SPN	C22-C23-C24-C25
10	l	102	SPN	C22-C23-C24-C25
10	e	102	SPN	C22-C23-C24-C25
10	c	103	SPN	C22-C23-C24-C25
11	M	408	MW9	O1-C18-C19-C20
11	H	303	MW9	C13-C14-C15-C16
11	H	303	MW9	C3-C4-C5-C6
10	v	102	SPN	C15-C16-C17-C18
8	M	403	U10	C40-C39-C41-C42
11	g	103	MW9	C35-C36-C37-C38
11	g	103	MW9	C21-O5-P-O2
11	H	302	MW9	O8-C19-C20-O2
10	f	102	SPN	CM6-C18-C19-C20
9	p	101	BCL	C16-C17-C18-C19
9	M	404	BCL	O1D-CGD-O2D-CED
9	9	102	BCL	O1D-CGD-O2D-CED
11	g	103	MW9	O1-C18-C19-O8
11	M	407	MW9	O1-C18-C19-O8
11	M	408	MW9	O1-C18-C19-O8
9	n	101	BCL	C16-C17-C18-C19
11	H	303	MW9	C9-C10-C11-C12
9	3	101	BCL	C2-C1-O2A-CGA
9	1	101	BCL	C14-C13-C15-C16
9	2	101	BCL	C11-C12-C13-C14
9	5	101	BCL	C6-C7-C8-C9
9	6	101	BCL	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	k	101	BCL	C11-C10-C8-C9
9	l	101	BCL	C6-C7-C8-C9
9	g	101	BCL	C6-C7-C8-C9
9	f	101	BCL	C11-C10-C8-C9
9	8	101	BCL	C14-C13-C15-C16
10	1	105	SPN	CM7-C22-C23-C24
11	g	102	MW9	C19-C20-O2-P
9	M	404	BCL	CAA-CBA-CGA-O2A
9	w	101	BCL	O1A-CGA-O2A-C1
9	v	101	BCL	C4C-C3C-CAC-CBC
9	j	101	BCL	C4C-C3C-CAC-CBC
9	x	101	BCL	C16-C17-C18-C20
10	p	102	SPN	C13-C14-C15-C16
9	a	101	BCL	C15-C16-C17-C18
11	H	301	MW9	C18-C19-C20-O2
11	9	101	MW9	C18-C19-C20-O2
9	1	101	BCL	C11-C10-C8-C7
9	6	101	BCL	C6-C7-C8-C10
9	w	101	BCL	C11-C10-C8-C7
9	w	101	BCL	C11-C12-C13-C15
9	w	101	BCL	C12-C13-C15-C16
9	x	101	BCL	C11-C12-C13-C15
9	v	101	BCL	C11-C10-C8-C7
9	s	101	BCL	C11-C10-C8-C7
9	r	101	BCL	C6-C7-C8-C10
9	o	101	BCL	C6-C7-C8-C10
9	m	101	BCL	C11-C10-C8-C7
9	m	101	BCL	C11-C12-C13-C15
9	n	101	BCL	C11-C10-C8-C7
9	g	101	BCL	C11-C12-C13-C15
9	h	101	BCL	C6-C7-C8-C10
9	e	101	BCL	C11-C10-C8-C7
9	e	101	BCL	C12-C13-C15-C16
9	f	101	BCL	C11-C10-C8-C7
9	c	101	BCL	C11-C10-C8-C7
9	a	101	BCL	C11-C10-C8-C7
9	a	101	BCL	C11-C12-C13-C15
9	b	101	BCL	C11-C12-C13-C15
9	j	101	BCL	C11-C12-C13-C15
9	L	301	BCL	C11-C10-C8-C7
9	L	304	BCL	C11-C10-C8-C7
9	M	402	BCL	C11-C12-C13-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	M	404	BCL	C12-C13-C15-C16
9	9	102	BCL	C6-C7-C8-C10
9	0	101	BCL	C11-C10-C8-C7
10	w	102	SPN	C21-C22-C23-C24
10	s	102	SPN	C21-C22-C23-C24
10	r	102	SPN	C21-C22-C23-C24
10	m	102	SPN	C21-C22-C23-C24
10	h	102	SPN	C21-C22-C23-C24
10	e	102	SPN	C21-C22-C23-C24
10	9	103	SPN	C21-C22-C23-C24
9	3	101	BCL	C16-C17-C18-C19
9	7	101	BCL	C16-C17-C18-C19
9	L	301	BCL	C2A-CAA-CBA-CGA
9	t	101	BCL	C13-C15-C16-C17
11	9	101	MW9	C3-C4-C5-C6
9	r	101	BCL	CAD-CBD-CGD-O2D
9	p	101	BCL	CAD-CBD-CGD-O2D
9	l	101	BCL	CAD-CBD-CGD-O2D
9	f	101	BCL	CAD-CBD-CGD-O2D
9	8	101	BCL	CAD-CBD-CGD-O2D
13	M	405	BPH	CAD-CBD-CGD-O2D
11	H	303	MW9	C1-C2-C3-C4
9	m	101	BCL	C13-C15-C16-C17
9	j	101	BCL	C16-C17-C18-C19
9	u	101	BCL	C8-C10-C11-C12
10	5	103	SPN	C22-C23-C24-C25
10	j	102	SPN	C22-C23-C24-C25
11	g	103	MW9	O1-C18-C19-C20
11	H	301	MW9	O1-C18-C19-C20
11	M	407	MW9	O1-C18-C19-C20
11	9	101	MW9	O1-C18-C19-C20
9	m	101	BCL	CBD-CGD-O2D-CED
11	H	303	MW9	O8-C19-C20-O2
11	H	304	MW9	O8-C19-C20-O2
11	M	408	MW9	O8-C19-C20-O2
11	9	101	MW9	O8-C19-C20-O2
12	C	402	HEM	C4B-C3B-CAB-CBB
9	6	101	BCL	C16-C17-C18-C19
9	e	101	BCL	O1A-CGA-O2A-C1
10	t	102	SPN	CM1-C1-O1-CMA
11	H	301	MW9	O1-C18-C19-O8
11	H	303	MW9	O1-C18-C19-O8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	g	101	BCL	C5-C6-C7-C8
9	t	101	BCL	O1A-CGA-O2A-C1
11	M	407	MW9	O7-C22-C23-O6
11	H	301	MW9	C11-C10-C9-C8
8	M	403	U10	C20-C19-C21-C22
9	1	101	BCL	C11-C10-C8-C9
9	4	101	BCL	C11-C10-C8-C9
9	w	101	BCL	C11-C10-C8-C9
9	q	101	BCL	C6-C7-C8-C9
9	o	101	BCL	C6-C7-C8-C9
9	d	101	BCL	C14-C13-C15-C16
9	a	101	BCL	C11-C10-C8-C9
11	H	304	MW9	C27-C28-C29-C30
10	1	102	SPN	O1-C1-C2-O2
10	5	102	SPN	O1-C1-C2-O2
10	3	102	SPN	O1-C1-C2-O2
10	u	102	SPN	O1-C1-C2-O2
10	p	102	SPN	O1-C1-C2-O2
10	k	102	SPN	O1-C1-C2-O2
10	i	102	SPN	O1-C1-C2-O2
10	7	102	SPN	O1-C1-C2-O2
9	u	101	BCL	C1A-C2A-CAA-CBA
9	h	101	BCL	C1A-C2A-CAA-CBA
9	b	101	BCL	C1A-C2A-CAA-CBA
9	M	402	BCL	C1A-C2A-CAA-CBA
9	2	101	BCL	C16-C17-C18-C20
9	i	101	BCL	C16-C17-C18-C19
9	9	102	BCL	C16-C17-C18-C19
9	1	101	BCL	C2-C1-O2A-CGA
9	r	101	BCL	C2-C1-O2A-CGA
11	H	301	MW9	C20-O2-P-O5
11	H	301	MW9	C21-O5-P-O2
11	H	303	MW9	C38-C39-C40-C41
11	H	304	MW9	C13-C14-C15-C16
10	1	104	SPN	CM8-C26-C27-C28
9	g	101	BCL	C15-C16-C17-C18
9	m	101	BCL	C3-C5-C6-C7
11	H	302	MW9	C22-C21-O5-P
8	M	403	U10	C18-C19-C21-C22
11	H	301	MW9	C20-O2-P-O4
11	H	301	MW9	C21-O5-P-O3
11	H	302	MW9	C21-O5-P-O4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	H	303	MW9	C21-O5-P-O3
11	H	304	MW9	C21-O5-P-O3
11	H	304	MW9	C21-O5-P-O4
11	H	304	MW9	C4-C5-C6-C7
11	M	407	MW9	C10-C11-C12-C13
9	6	101	BCL	C8-C10-C11-C12
11	H	302	MW9	C29-C30-C31-C32
11	g	102	MW9	C24-C25-C26-C27
9	L	304	BCL	C16-C17-C18-C19
8	M	403	U10	C25-C24-C26-C27
9	1	101	BCL	C11-C12-C13-C15
9	3	101	BCL	C6-C7-C8-C10
9	4	101	BCL	C11-C10-C8-C7
9	4	101	BCL	C11-C12-C13-C15
9	s	101	BCL	C12-C13-C15-C16
9	t	101	BCL	C2C-C3C-CAC-CBC
9	q	101	BCL	C11-C12-C13-C15
9	p	101	BCL	C6-C7-C8-C10
9	g	101	BCL	C11-C10-C8-C7
9	h	101	BCL	C12-C13-C15-C16
9	f	101	BCL	C6-C7-C8-C10
9	b	101	BCL	C12-C13-C15-C16
9	i	101	BCL	C11-C10-C8-C7
9	j	101	BCL	C6-C7-C8-C10
9	j	101	BCL	C12-C13-C15-C16
9	7	101	BCL	C11-C12-C13-C15
9	M	402	BCL	C3A-C2A-CAA-CBA
9	0	101	BCL	C2C-C3C-CAC-CBC
9	0	101	BCL	C11-C12-C13-C15
10	c	102	SPN	C21-C22-C23-C24
10	i	102	SPN	C21-C22-C23-C24
10	7	102	SPN	C21-C22-C23-C24
11	g	102	MW9	O8-C19-C20-O2
13	M	409	BPH	C11-C10-C8-C7
13	M	409	BPH	C11-C12-C13-C15
9	L	304	BCL	C2B-C3B-CAB-OBB
9	L	304	BCL	C2B-C3B-CAB-CBB
11	H	303	MW9	C5-C6-C7-C8
9	t	101	BCL	C16-C17-C18-C20
11	H	301	MW9	C22-C21-O5-P
11	H	303	MW9	C22-C21-O5-P
9	2	101	BCL	C11-C10-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	5	101	BCL	C14-C13-C15-C16
9	3	101	BCL	C6-C7-C8-C9
9	p	101	BCL	C6-C7-C8-C9
9	m	101	BCL	C11-C10-C8-C9
9	k	101	BCL	C14-C13-C15-C16
9	g	101	BCL	C11-C10-C8-C9
9	h	101	BCL	C6-C7-C8-C9
9	e	101	BCL	C11-C10-C8-C9
9	f	101	BCL	C6-C7-C8-C9
9	c	101	BCL	C11-C10-C8-C9
9	b	101	BCL	C11-C12-C13-C14
9	b	101	BCL	C14-C13-C15-C16
9	j	101	BCL	C6-C7-C8-C9
9	M	404	BCL	C14-C13-C15-C16
9	9	102	BCL	C6-C7-C8-C9
9	0	101	BCL	C11-C10-C8-C9
10	p	103	SPN	CM7-C22-C23-C24
10	c	102	SPN	CM7-C22-C23-C24
10	i	102	SPN	CM7-C22-C23-C24
13	M	409	BPH	C6-C7-C8-C9
11	9	101	MW9	C12-C13-C14-C15
11	H	301	MW9	C13-C14-C15-C16
11	M	408	MW9	C-C1-C2-C3
11	g	102	MW9	C25-C26-C27-C28
9	m	101	BCL	C8-C10-C11-C12
13	M	409	BPH	C8-C10-C11-C12
9	n	101	BCL	C16-C17-C18-C20
9	L	304	BCL	O1D-CGD-O2D-CED
9	o	101	BCL	C2-C1-O2A-CGA
9	h	101	BCL	C2-C1-O2A-CGA
9	a	101	BCL	C2-C1-O2A-CGA
9	b	101	BCL	C2-C1-O2A-CGA
9	9	102	BCL	C2-C1-O2A-CGA
9	r	101	BCL	C16-C17-C18-C19
11	9	101	MW9	C25-C26-C27-C28
9	7	101	BCL	C8-C10-C11-C12
11	9	101	MW9	C38-C39-C40-C41
11	H	301	MW9	C35-C36-C37-C38
11	g	103	MW9	C20-O2-P-O5
11	H	302	MW9	C20-O2-P-O5
11	M	407	MW9	C21-O5-P-O2
11	M	408	MW9	C20-O2-P-O5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	a	101	BCL	C16-C17-C18-C19
9	L	304	BCL	C4B-C3B-CAB-OBB
9	m	101	BCL	O1D-CGD-O2D-CED
8	L	305	U10	C12-C11-C9-C10
11	M	408	MW9	C11-C12-C13-C14
9	6	101	BCL	C5-C6-C7-C8
9	1	101	BCL	C12-C13-C15-C16
9	r	101	BCL	C12-C13-C15-C16
9	o	101	BCL	C11-C10-C8-C7
9	g	101	BCL	C6-C7-C8-C10
9	g	101	BCL	C12-C13-C15-C16
9	c	101	BCL	C12-C13-C15-C16
13	M	405	BPH	C11-C12-C13-C15
9	u	101	BCL	C6-C7-C8-C9
9	s	101	BCL	C11-C10-C8-C9
9	l	101	BCL	C11-C10-C8-C9
9	b	101	BCL	C6-C7-C8-C9
9	i	101	BCL	C11-C12-C13-C14
9	L	304	BCL	C6-C7-C8-C9
10	5	103	SPN	CM7-C22-C23-C24
10	3	102	SPN	CM7-C22-C23-C24
10	q	102	SPN	CM7-C22-C23-C24
9	M	402	BCL	C15-C16-C17-C18
9	u	101	BCL	CBA-CGA-O2A-C1
11	H	304	MW9	C22-C21-O5-P
11	M	407	MW9	C37-C38-C39-C40
11	H	303	MW9	C30-C31-C32-C33
8	M	403	U10	C38-C39-C41-C42
9	4	101	BCL	CBA-CGA-O2A-C1
9	u	101	BCL	O1A-CGA-O2A-C1
12	C	403	HEM	C3D-CAD-CBD-CGD
9	d	101	BCL	C5-C6-C7-C8
9	4	101	BCL	O1A-CGA-O2A-C1
9	g	101	BCL	O1A-CGA-O2A-C1
9	g	101	BCL	CBA-CGA-O2A-C1
11	g	102	MW9	C32-C33-C34-C35
11	g	103	MW9	C28-C29-C30-C31
8	M	403	U10	C19-C21-C22-C23
8	A	101	U10	C25-C24-C26-C27
9	b	101	BCL	C4-C3-C5-C6
9	b	101	BCL	C2-C3-C5-C6
13	M	405	BPH	C2-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	q	102	SPN	CM2-C1-C2-O2
10	n	102	SPN	CM2-C1-C2-O2
10	n	102	SPN	CM2-C1-C2-C3
10	a	103	SPN	CM1-C1-C2-O2
10	i	102	SPN	CM1-C1-C2-O2
11	H	302	MW9	C26-C27-C28-C29
11	H	302	MW9	C27-C28-C29-C30
13	M	409	BPH	C3A-C2A-CAA-CBA
9	t	101	BCL	C4-C3-C5-C6
11	9	101	MW9	O8-C24-C25-C26
9	c	101	BCL	C6-C7-C8-C9
9	8	101	BCL	C11-C12-C13-C14
10	7	102	SPN	CM7-C22-C23-C24
11	H	301	MW9	C37-C38-C39-C40
10	c	102	SPN	C22-C23-C24-C25
9	r	101	BCL	C16-C17-C18-C20
9	2	101	BCL	C13-C15-C16-C17
9	M	404	BCL	C1A-C2A-CAA-CBA
11	M	407	MW9	C12-C13-C14-C15
9	2	101	BCL	C12-C13-C15-C16
9	6	101	BCL	C11-C10-C8-C7
10	p	103	SPN	C21-C22-C23-C24
10	a	103	SPN	C21-C22-C23-C24
12	C	401	HEM	CAD-CBD-CGD-O1D
11	9	101	MW9	C-C1-C2-C3
12	C	401	HEM	CAA-CBA-CGA-O2A
9	1	101	BCL	C3-C5-C6-C7
11	H	301	MW9	C19-C20-O2-P
9	b	101	BCL	C2A-CAA-CBA-CGA
9	1	101	BCL	C13-C15-C16-C17
9	4	101	BCL	C10-C11-C12-C13
8	M	403	U10	C45-C44-C46-C47
12	C	401	HEM	CAA-CBA-CGA-O1A
9	8	101	BCL	C5-C6-C7-C8
9	3	101	BCL	C3-C5-C6-C7
9	x	101	BCL	C3-C5-C6-C7
8	A	101	U10	C5-C4-O4-C4M
10	1	103	SPN	CM2-C1-O1-CMA
11	H	302	MW9	C6-C7-C8-C9
9	e	101	BCL	C2A-CAA-CBA-CGA
10	1	102	SPN	C2-C3-C4-C5
10	1	103	SPN	C2-C3-C4-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	1	104	SPN	C2-C3-C4-C5
10	1	105	SPN	C2-C3-C4-C5
10	5	102	SPN	C2-C3-C4-C5
10	5	103	SPN	C2-C3-C4-C5
10	3	102	SPN	C2-C3-C4-C5
10	w	102	SPN	C2-C3-C4-C5
10	u	102	SPN	C2-C3-C4-C5
10	v	102	SPN	C2-C3-C4-C5
10	s	102	SPN	C2-C3-C4-C5
10	t	102	SPN	C2-C3-C4-C5
10	r	102	SPN	C2-C3-C4-C5
10	p	102	SPN	C2-C3-C4-C5
10	p	103	SPN	C2-C3-C4-C5
10	m	102	SPN	C2-C3-C4-C5
10	n	102	SPN	C2-C3-C4-C5
10	k	102	SPN	C2-C3-C4-C5
10	l	102	SPN	C2-C3-C4-C5
10	h	102	SPN	C2-C3-C4-C5
10	h	103	SPN	C2-C3-C4-C5
10	e	102	SPN	C2-C3-C4-C5
10	f	102	SPN	C2-C3-C4-C5
10	c	102	SPN	C2-C3-C4-C5
10	c	103	SPN	C2-C3-C4-C5
10	a	102	SPN	C2-C3-C4-C5
10	a	103	SPN	C2-C3-C4-C5
10	i	102	SPN	C2-C3-C4-C5
10	j	102	SPN	C2-C3-C4-C5
10	7	102	SPN	C2-C3-C4-C5
10	7	103	SPN	C2-C3-C4-C5
10	M	406	SPN	C2-C3-C4-C5
10	9	103	SPN	C2-C3-C4-C5
10	0	102	SPN	C2-C3-C4-C5
9	o	101	BCL	C4B-C3B-CAB-OBB
9	L	304	BCL	C4B-C3B-CAB-CBB
9	5	101	BCL	C13-C15-C16-C17
11	g	103	MW9	C3-C4-C5-C6
9	s	101	BCL	C2-C1-O2A-CGA
9	k	101	BCL	C2-C1-O2A-CGA
9	L	304	BCL	C2-C1-O2A-CGA
9	t	101	BCL	C2-C3-C5-C6
9	p	101	BCL	C11-C12-C13-C14
11	9	101	MW9	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	L	301	BCL	C13-C15-C16-C17
11	H	304	MW9	O8-C24-C25-C26
11	M	408	MW9	C26-C27-C28-C29
8	A	101	U10	C15-C14-C16-C17
13	M	405	BPH	C4-C3-C5-C6
9	4	101	BCL	C16-C17-C18-C20
9	a	101	BCL	C13-C15-C16-C17
8	L	305	U10	C12-C11-C9-C8
8	M	403	U10	C23-C24-C26-C27
13	L	303	BPH	C13-C15-C16-C17
9	5	101	BCL	C16-C17-C18-C19
9	l	101	BCL	C16-C17-C18-C20
9	L	301	BCL	C3-C5-C6-C7
9	k	101	BCL	C8-C10-C11-C12
8	M	403	U10	C5-C4-O4-C4M
9	l	101	BCL	C3-C5-C6-C7
8	M	403	U10	C35-C34-C36-C37
8	A	101	U10	C23-C24-C26-C27
9	5	101	BCL	C12-C13-C15-C16
9	t	101	BCL	C6-C7-C8-C10
9	q	101	BCL	C6-C7-C8-C10
9	d	101	BCL	C12-C13-C15-C16
9	7	101	BCL	C12-C13-C15-C16
11	9	101	MW9	C32-C33-C34-C35
9	5	101	BCL	C1-C2-C3-C4
9	k	101	BCL	C1-C2-C3-C4
9	i	101	BCL	C1-C2-C3-C4
12	C	402	HEM	CAA-CBA-CGA-O1A
12	C	402	HEM	CAA-CBA-CGA-O2A
10	p	103	SPN	C24-C25-C26-CM8
9	L	304	BCL	C15-C16-C17-C18
9	L	304	BCL	C16-C17-C18-C20
13	M	409	BPH	C16-C17-C18-C20
9	j	101	BCL	O1D-CGD-O2D-CED
11	H	301	MW9	C30-C31-C32-C33
10	p	102	SPN	C15-C16-C17-C18
9	v	101	BCL	C4-C3-C5-C6
12	C	403	HEM	CAD-CBD-CGD-O2D
8	A	101	U10	C13-C14-C16-C17
10	1	104	SPN	C25-C26-C27-C28
9	2	101	BCL	C14-C13-C15-C16
9	6	101	BCL	C11-C10-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	i	101	BCL	C11-C10-C8-C9
9	0	101	BCL	C14-C13-C15-C16
10	a	103	SPN	CM7-C22-C23-C24
13	M	409	BPH	C11-C10-C8-C9
13	M	409	BPH	C11-C12-C13-C14
9	w	101	BCL	C3A-C2A-CAA-CBA
9	e	101	BCL	C3A-C2A-CAA-CBA
9	0	101	BCL	C3A-C2A-CAA-CBA
11	9	101	MW9	C4-C5-C6-C7
9	t	101	BCL	CAA-CBA-CGA-O2A
11	g	102	MW9	C30-C31-C32-C33
11	g	103	MW9	C30-C31-C32-C33
11	M	407	MW9	C32-C33-C34-C35
9	x	101	BCL	CAD-CBD-CGD-O2D
9	g	101	BCL	CAD-CBD-CGD-O2D
9	h	101	BCL	CAD-CBD-CGD-O2D
9	0	101	BCL	CAD-CBD-CGD-O2D
8	M	403	U10	C43-C44-C46-C47
9	v	101	BCL	C2-C3-C5-C6
11	9	101	MW9	C29-C30-C31-C32
9	L	304	BCL	CBD-CGD-O2D-CED
12	C	401	HEM	CAD-CBD-CGD-O2D
11	H	304	MW9	C2-C3-C4-C5
9	2	101	BCL	O2A-C1-C2-C3
12	C	401	HEM	C4C-C3C-CAC-CBC
11	H	301	MW9	C27-C28-C29-C30
11	H	301	MW9	C15-C16-C17-O1
11	g	103	MW9	C32-C33-C34-C35
9	j	101	BCL	CBD-CGD-O2D-CED
9	o	101	BCL	CHA-CBD-CGD-O1D
9	o	101	BCL	CHA-CBD-CGD-O2D
11	H	301	MW9	C14-C15-C16-C17
12	C	403	HEM	CAD-CBD-CGD-O1D
10	f	102	SPN	C2-C1-O1-CMA
11	g	102	MW9	O7-C22-C23-O6
13	L	303	BPH	CHA-CBD-CGD-O1D
9	h	101	BCL	C15-C16-C17-C18
11	M	408	MW9	C37-C38-C39-C40
9	i	101	BCL	C5-C6-C7-C8
11	M	408	MW9	C32-C33-C34-C35
8	L	302	U10	C14-C16-C17-C18
10	1	102	SPN	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	1	102	SPN	C18-C19-C20-C21
10	1	103	SPN	C6-C7-C8-C9
10	1	103	SPN	C23-C24-C25-C26
10	1	104	SPN	C6-C7-C8-C9
10	1	104	SPN	C10-C11-C12-C13
10	1	105	SPN	C6-C7-C8-C9
10	1	105	SPN	C10-C11-C12-C13
10	1	105	SPN	C18-C19-C20-C21
10	5	102	SPN	C6-C7-C8-C9
10	5	102	SPN	C10-C11-C12-C13
10	5	102	SPN	C18-C19-C20-C21
10	5	103	SPN	C6-C7-C8-C9
10	5	103	SPN	C10-C11-C12-C13
10	5	103	SPN	C18-C19-C20-C21
10	3	102	SPN	C6-C7-C8-C9
10	3	102	SPN	C10-C11-C12-C13
10	3	102	SPN	C18-C19-C20-C21
10	w	102	SPN	C6-C7-C8-C9
10	w	102	SPN	C10-C11-C12-C13
10	w	102	SPN	C18-C19-C20-C21
10	u	102	SPN	C6-C7-C8-C9
10	u	102	SPN	C10-C11-C12-C13
10	u	102	SPN	C18-C19-C20-C21
10	v	102	SPN	C6-C7-C8-C9
10	s	102	SPN	C6-C7-C8-C9
10	s	102	SPN	C10-C11-C12-C13
10	s	102	SPN	C18-C19-C20-C21
10	t	102	SPN	C6-C7-C8-C9
10	q	102	SPN	C18-C19-C20-C21
10	r	102	SPN	C6-C7-C8-C9
10	r	102	SPN	C10-C11-C12-C13
10	r	102	SPN	C18-C19-C20-C21
10	p	103	SPN	C6-C7-C8-C9
10	p	103	SPN	C23-C24-C25-C26
10	m	102	SPN	C6-C7-C8-C9
10	m	102	SPN	C10-C11-C12-C13
10	m	102	SPN	C18-C19-C20-C21
10	n	102	SPN	C6-C7-C8-C9
10	n	102	SPN	C10-C11-C12-C13
10	n	102	SPN	C18-C19-C20-C21
10	k	102	SPN	C6-C7-C8-C9
10	k	102	SPN	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	k	102	SPN	C18-C19-C20-C21
10	l	102	SPN	C6-C7-C8-C9
10	l	102	SPN	C10-C11-C12-C13
10	h	102	SPN	C6-C7-C8-C9
10	h	102	SPN	C10-C11-C12-C13
10	h	102	SPN	C18-C19-C20-C21
10	h	103	SPN	C6-C7-C8-C9
10	h	103	SPN	C10-C11-C12-C13
10	e	102	SPN	C6-C7-C8-C9
10	e	102	SPN	C10-C11-C12-C13
10	e	102	SPN	C18-C19-C20-C21
10	f	102	SPN	C6-C7-C8-C9
10	f	102	SPN	C10-C11-C12-C13
10	c	102	SPN	C6-C7-C8-C9
10	c	102	SPN	C10-C11-C12-C13
10	c	102	SPN	C18-C19-C20-C21
10	c	103	SPN	C6-C7-C8-C9
10	c	103	SPN	C10-C11-C12-C13
10	c	103	SPN	C18-C19-C20-C21
10	a	102	SPN	C10-C11-C12-C13
10	a	102	SPN	C18-C19-C20-C21
10	a	103	SPN	C6-C7-C8-C9
10	a	103	SPN	C10-C11-C12-C13
10	i	102	SPN	C6-C7-C8-C9
10	i	102	SPN	C10-C11-C12-C13
10	i	102	SPN	C18-C19-C20-C21
10	j	102	SPN	C6-C7-C8-C9
10	7	102	SPN	C6-C7-C8-C9
10	7	102	SPN	C10-C11-C12-C13
10	7	102	SPN	C18-C19-C20-C21
10	7	103	SPN	C6-C7-C8-C9
10	7	103	SPN	C18-C19-C20-C21
10	M	406	SPN	C6-C7-C8-C9
10	M	406	SPN	C10-C11-C12-C13
10	9	103	SPN	C6-C7-C8-C9
10	9	103	SPN	C10-C11-C12-C13
10	9	103	SPN	C18-C19-C20-C21
10	0	102	SPN	C6-C7-C8-C9
10	q	102	SPN	C2-C3-C4-C5
11	M	407	MW9	C21-C22-C23-O6
9	r	101	BCL	C1A-C2A-CAA-CBA
9	e	101	BCL	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	0	101	BCL	C1A-C2A-CAA-CBA
10	1	102	SPN	C6-C7-C8-C9
10	u	102	SPN	C23-C24-C25-C26
10	v	102	SPN	C10-C11-C12-C13
10	t	102	SPN	C10-C11-C12-C13
10	q	102	SPN	C6-C7-C8-C9
10	q	102	SPN	C10-C11-C12-C13
10	p	102	SPN	C18-C19-C20-C21
10	p	103	SPN	C10-C11-C12-C13
10	a	102	SPN	C6-C7-C8-C9
10	a	102	SPN	C23-C24-C25-C26
10	j	102	SPN	C10-C11-C12-C13
10	7	103	SPN	C10-C11-C12-C13
10	0	102	SPN	C10-C11-C12-C13
9	l	101	BCL	C2-C1-O2A-CGA
9	i	101	BCL	C2-C1-O2A-CGA
11	H	302	MW9	C10-C11-C12-C13
11	H	303	MW9	C-C1-C2-C3
9	b	101	BCL	C5-C6-C7-C8
11	g	103	MW9	C21-O5-P-O3
9	0	101	BCL	C16-C17-C18-C19
10	v	102	SPN	C23-C24-C25-C26
9	M	404	BCL	CAA-CBA-CGA-O1A
11	H	301	MW9	C15-C16-C17-O
9	g	101	BCL	C13-C15-C16-C17
9	t	101	BCL	CAA-CBA-CGA-O1A
11	g	103	MW9	C15-C16-C17-O1
11	M	407	MW9	C35-C36-C37-C38
9	x	101	BCL	C2A-CAA-CBA-CGA
10	1	103	SPN	C10-C11-C12-C13
10	h	102	SPN	C27-C28-C29-C30
10	h	103	SPN	C23-C24-C25-C26
10	0	102	SPN	C18-C19-C20-C21
8	M	403	U10	C33-C34-C36-C37
12	C	403	HEM	CAA-CBA-CGA-O2A
9	n	101	BCL	CAD-CBD-CGD-O1D
10	l	102	SPN	CM7-C22-C23-C24
13	L	303	BPH	C11-C12-C13-C14
10	1	105	SPN	CM1-C1-C2-O2
10	u	102	SPN	CM1-C1-C2-O2
10	l	102	SPN	CM2-C1-C2-O2
10	h	103	SPN	CM2-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	c	103	SPN	CM1-C1-C2-O2
10	j	102	SPN	CM1-C1-C2-O2
10	7	103	SPN	CM1-C1-C2-O2
10	M	406	SPN	CM2-C1-C2-O2
10	0	102	SPN	CM1-C1-C2-O2
9	r	101	BCL	CAA-CBA-CGA-O2A
9	3	101	BCL	C11-C12-C13-C15
9	r	101	BCL	C3A-C2A-CAA-CBA
9	c	101	BCL	C6-C7-C8-C10
9	L	301	BCL	C2C-C3C-CAC-CBC
13	M	405	BPH	C6-C7-C8-C10
9	L	304	BCL	CAA-CBA-CGA-O2A
11	H	301	MW9	O8-C24-C25-C26
9	L	304	BCL	CAA-CBA-CGA-O1A
11	H	301	MW9	O9-C24-C25-C26
11	H	301	MW9	C9-C10-C11-C12
9	w	101	BCL	C15-C16-C17-C18
9	7	101	BCL	C13-C15-C16-C17
11	g	103	MW9	O8-C24-C25-C26
9	r	101	BCL	CAA-CBA-CGA-O1A
10	3	102	SPN	C24-C25-C26-CM8

There are no ring outliers.

83 monomers are involved in 365 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	L	302	U10	1	0
10	a	102	SPN	1	0
10	j	102	SPN	5	0
10	1	102	SPN	2	0
10	7	103	SPN	4	0
9	d	101	BCL	6	0
9	e	101	BCL	3	0
9	L	304	BCL	5	0
9	i	101	BCL	5	0
9	M	404	BCL	3	0
9	k	101	BCL	7	0
10	r	102	SPN	1	0
11	H	301	MW9	2	0
12	C	402	HEM	4	0
10	s	102	SPN	1	0
11	H	303	MW9	1	0

Continued on next page...

Continued from previous page...

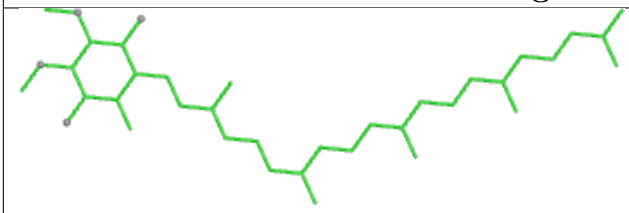
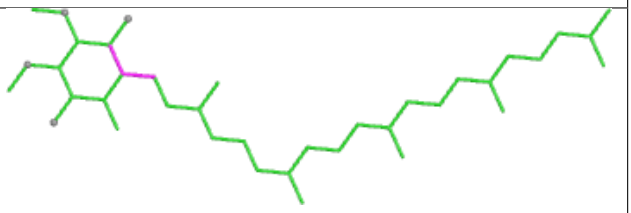
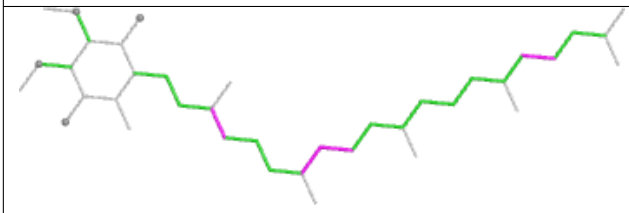
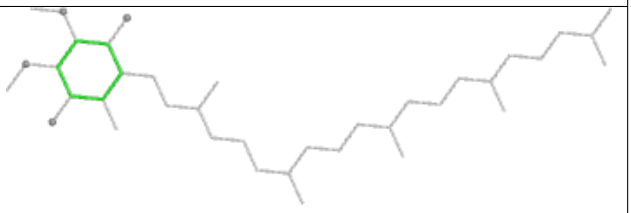
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	3	102	SPN	4	0
9	h	101	BCL	10	0
10	f	102	SPN	8	0
9	b	101	BCL	6	0
10	w	102	SPN	2	0
9	7	101	BCL	5	0
9	n	101	BCL	4	0
12	C	401	HEM	6	0
9	f	101	BCL	7	0
10	5	102	SPN	4	0
11	M	407	MW9	1	0
13	L	303	BPH	2	0
10	0	102	SPN	4	0
9	c	101	BCL	3	0
10	1	105	SPN	3	0
9	q	101	BCL	4	0
10	9	103	SPN	1	0
10	M	406	SPN	11	0
9	p	101	BCL	11	0
9	0	101	BCL	7	0
10	n	102	SPN	4	0
9	a	101	BCL	4	0
9	8	101	BCL	8	0
10	p	102	SPN	13	0
9	j	101	BCL	7	0
9	1	101	BCL	2	0
9	6	101	BCL	4	0
9	g	101	BCL	3	0
9	M	402	BCL	10	0
10	c	103	SPN	1	0
10	7	102	SPN	1	0
13	M	409	BPH	2	0
10	m	102	SPN	1	0
10	c	102	SPN	2	0
9	t	101	BCL	4	0
10	h	103	SPN	9	0
10	l	102	SPN	6	0
9	3	101	BCL	7	0
10	q	102	SPN	8	0
10	1	104	SPN	4	0
10	i	102	SPN	2	0
10	k	102	SPN	2	0

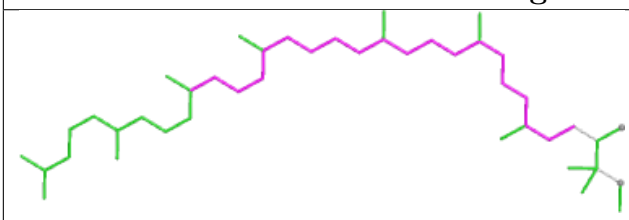
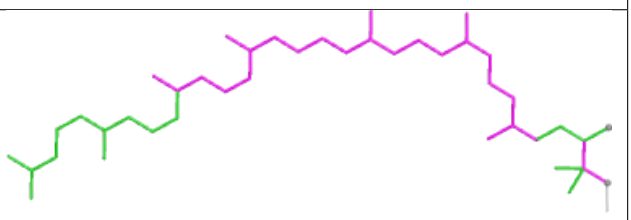
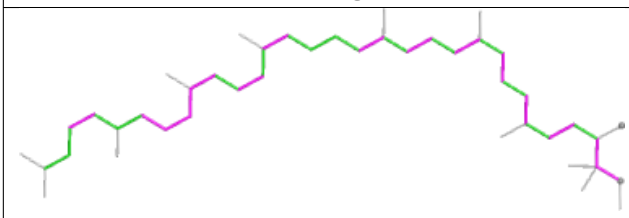
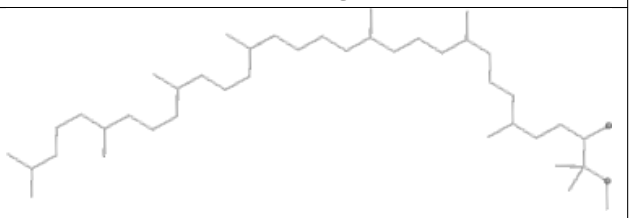
Continued on next page...

Continued from previous page...

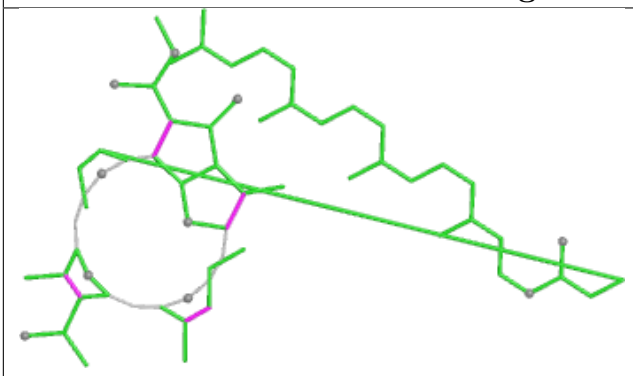
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	a	103	SPN	2	0
9	l	101	BCL	5	0
9	m	101	BCL	6	0
8	L	305	U10	5	0
9	v	101	BCL	7	0
10	1	103	SPN	12	0
10	t	102	SPN	4	0
10	u	102	SPN	3	0
10	e	102	SPN	2	0
9	o	101	BCL	13	0
12	C	403	HEM	5	0
10	h	102	SPN	8	0
9	x	101	BCL	6	0
9	u	101	BCL	5	0
9	9	102	BCL	5	0
9	L	301	BCL	4	0
9	r	101	BCL	7	0
10	5	103	SPN	3	0
9	2	101	BCL	6	0
9	s	101	BCL	7	0
9	w	101	BCL	4	0
10	p	103	SPN	7	0
10	v	102	SPN	14	0
9	5	101	BCL	5	0
9	4	101	BCL	4	0

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

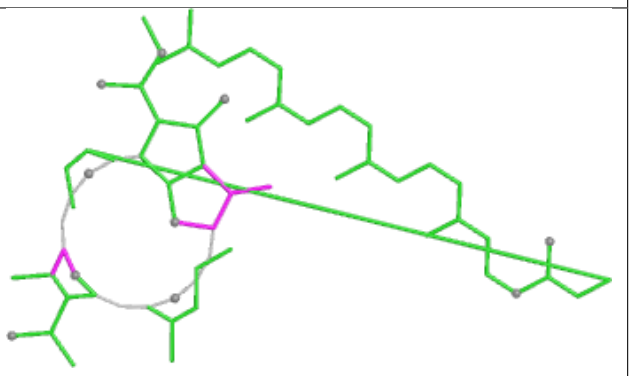
Ligand U10 L 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SPN a 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

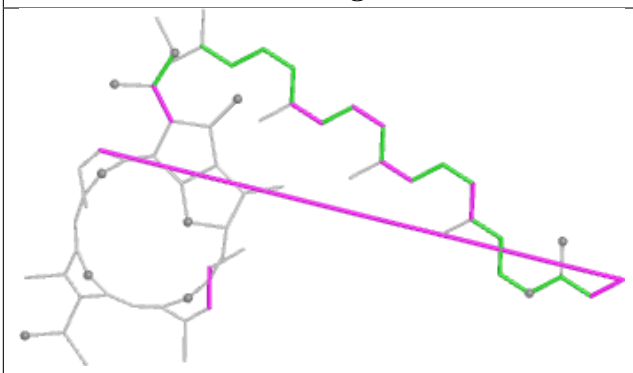
Ligand BPH M 405



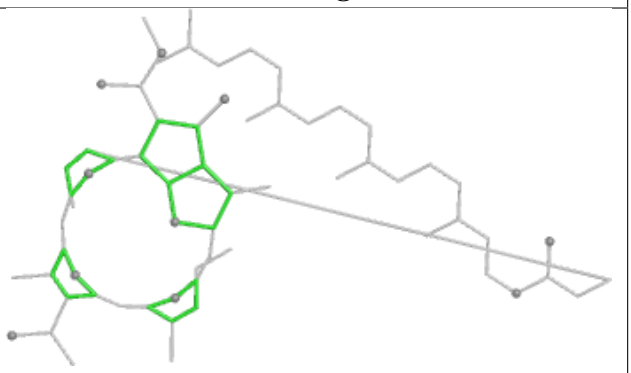
Bond lengths



Bond angles

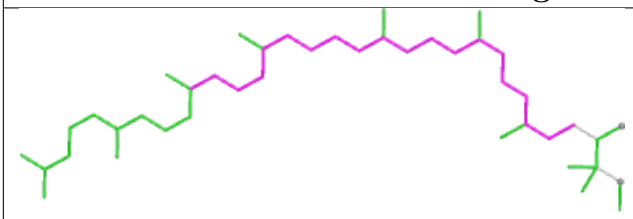


Torsions

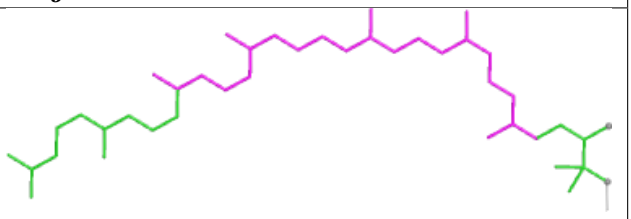


Rings

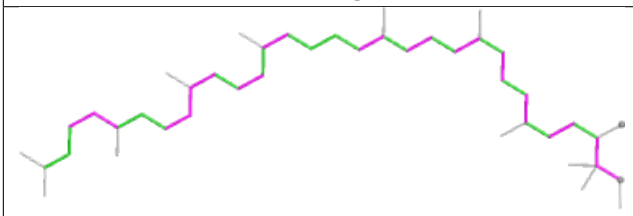
Ligand SPN j 102



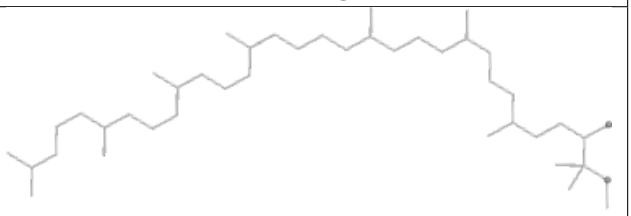
Bond lengths



Bond angles

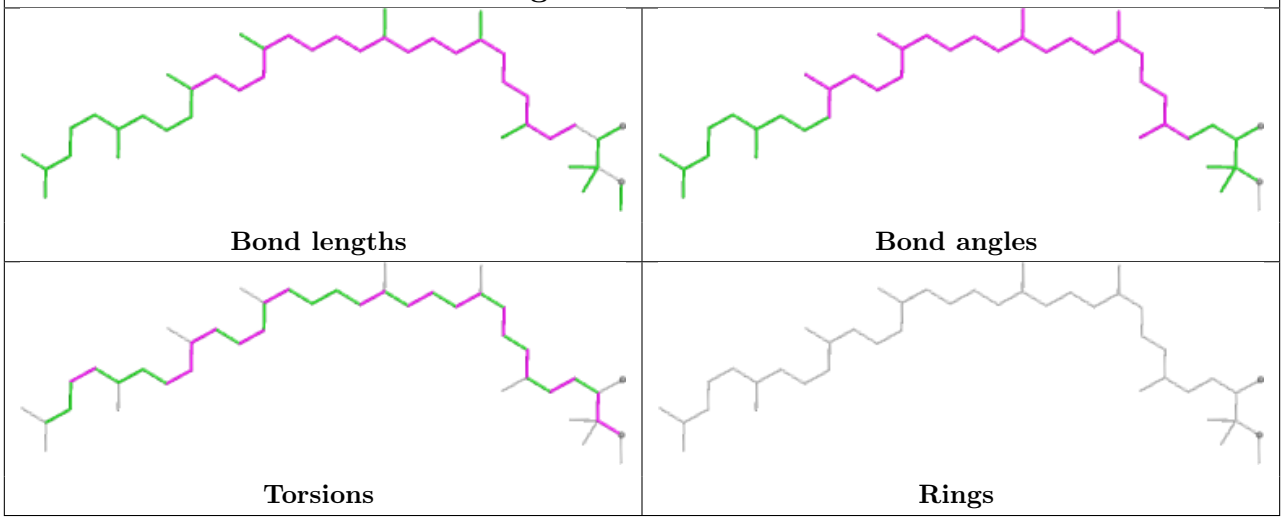


Torsions

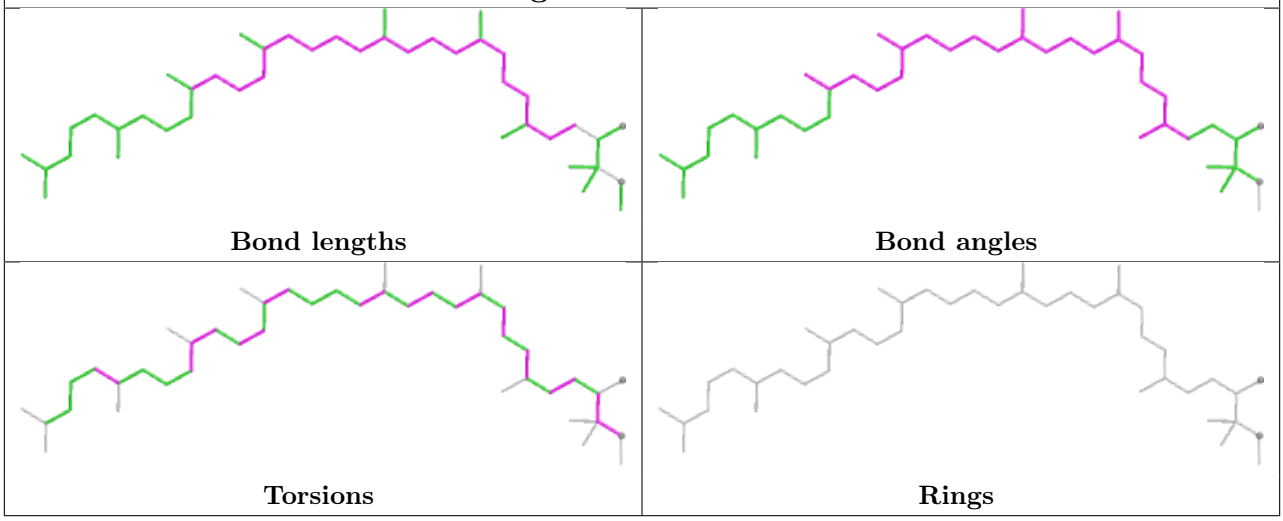


Rings

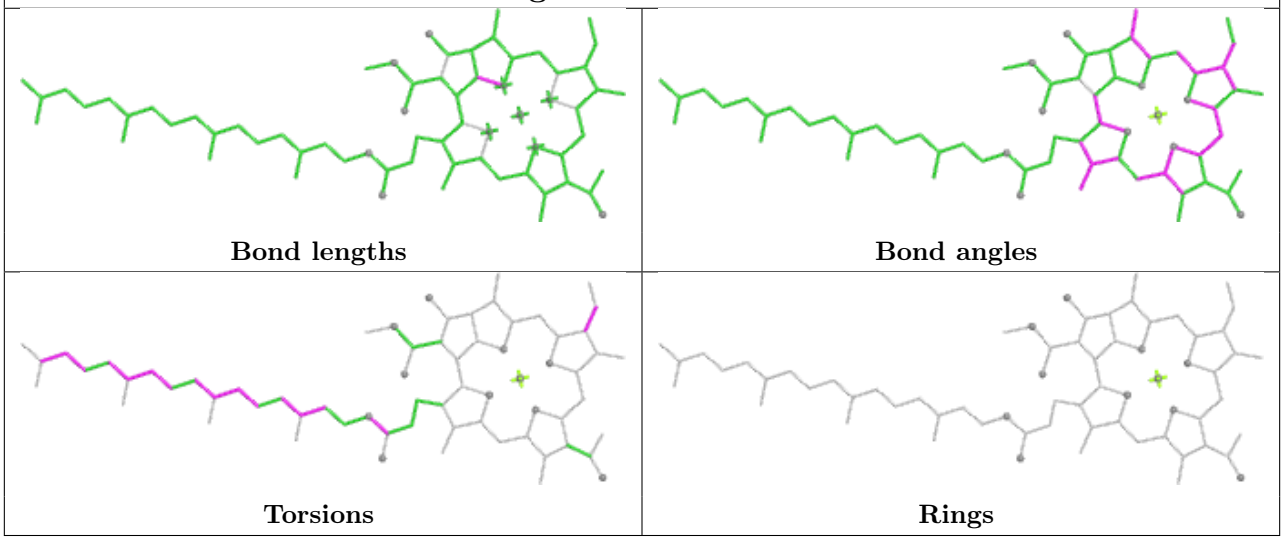
Ligand SPN 1 102



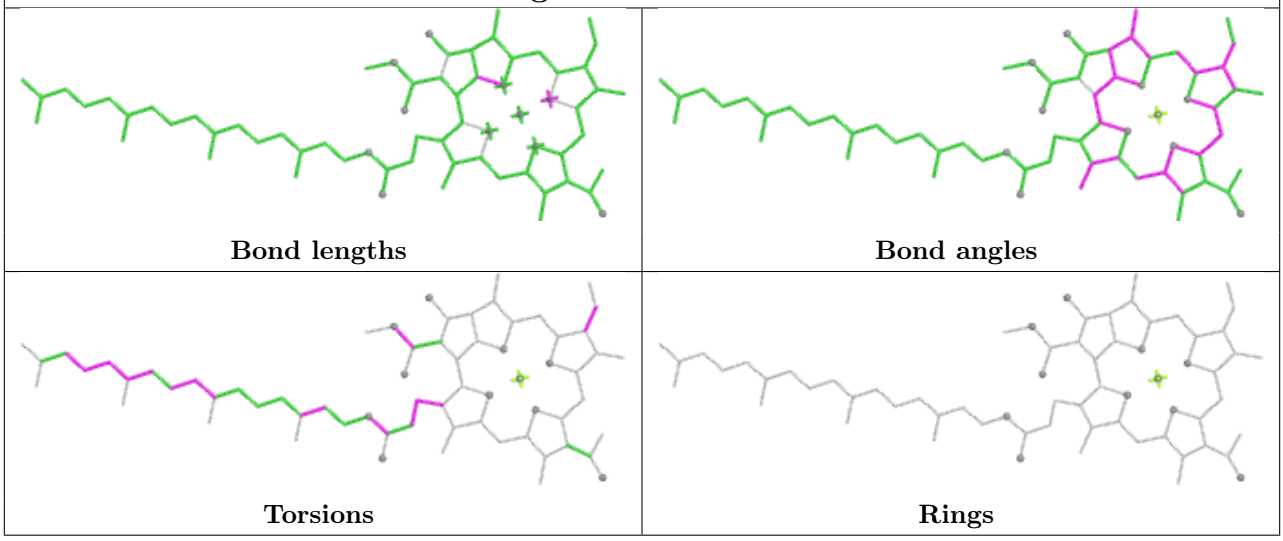
Ligand SPN 7 103



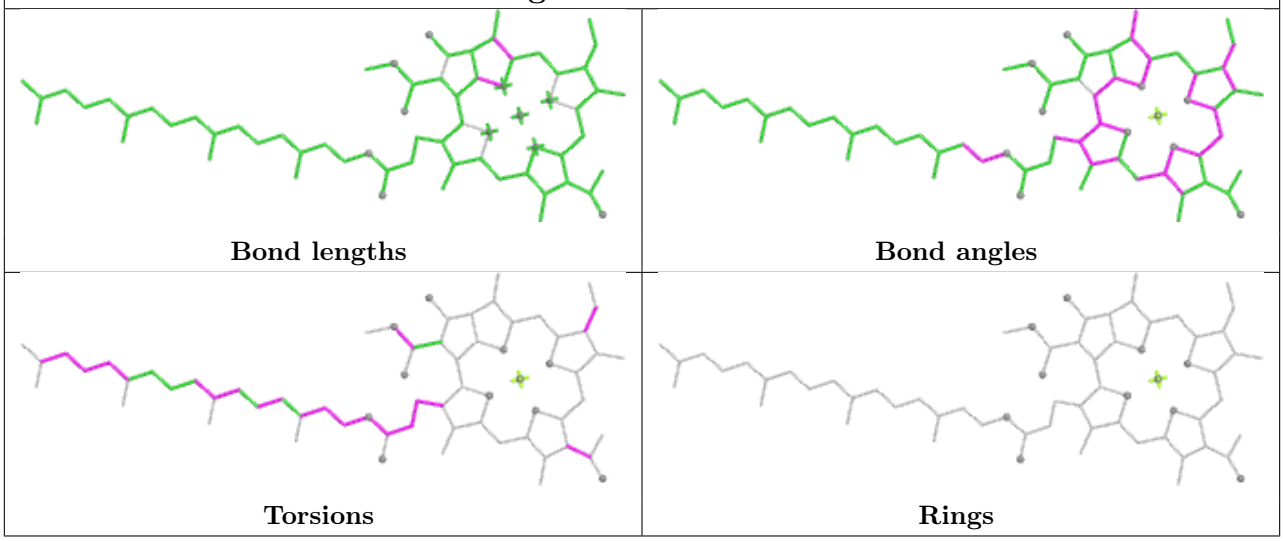
Ligand BCL d 101



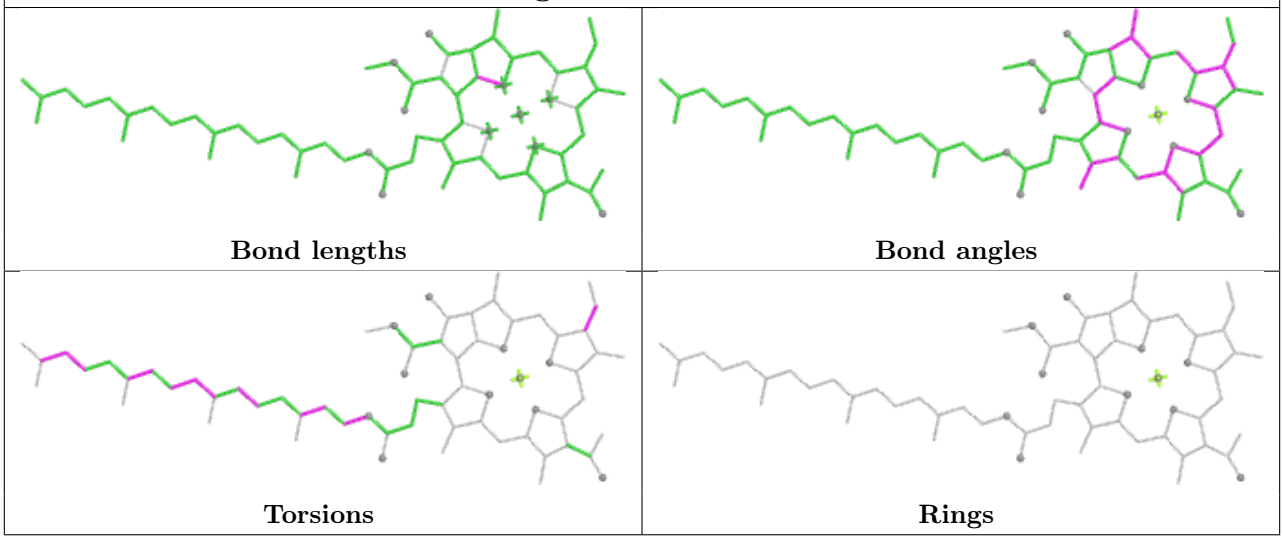
Ligand BCL e 101



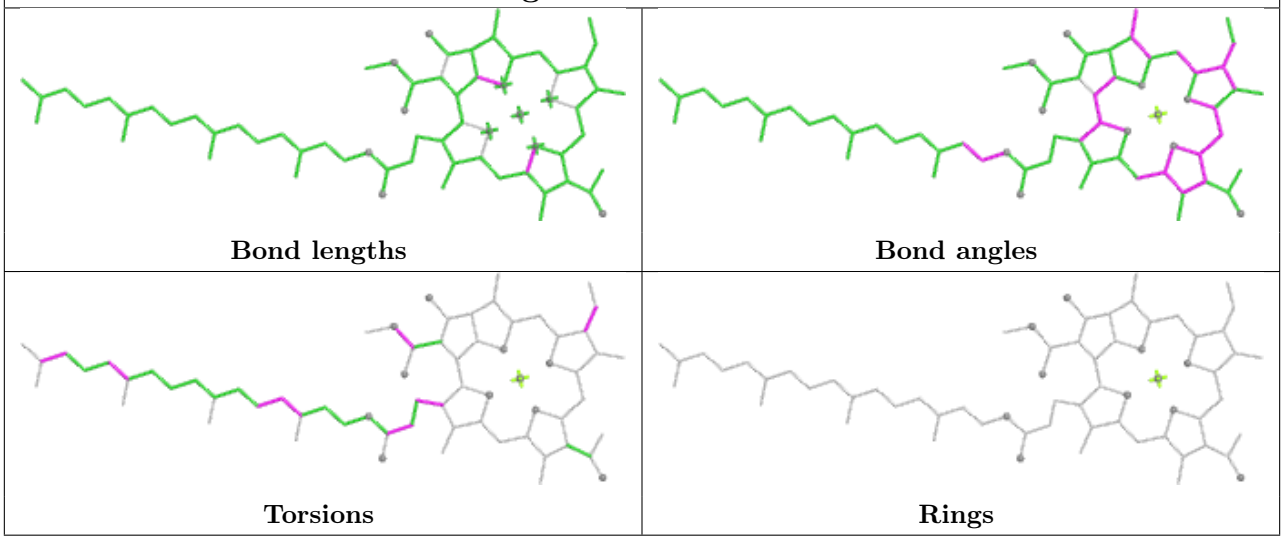
Ligand BCL L 304



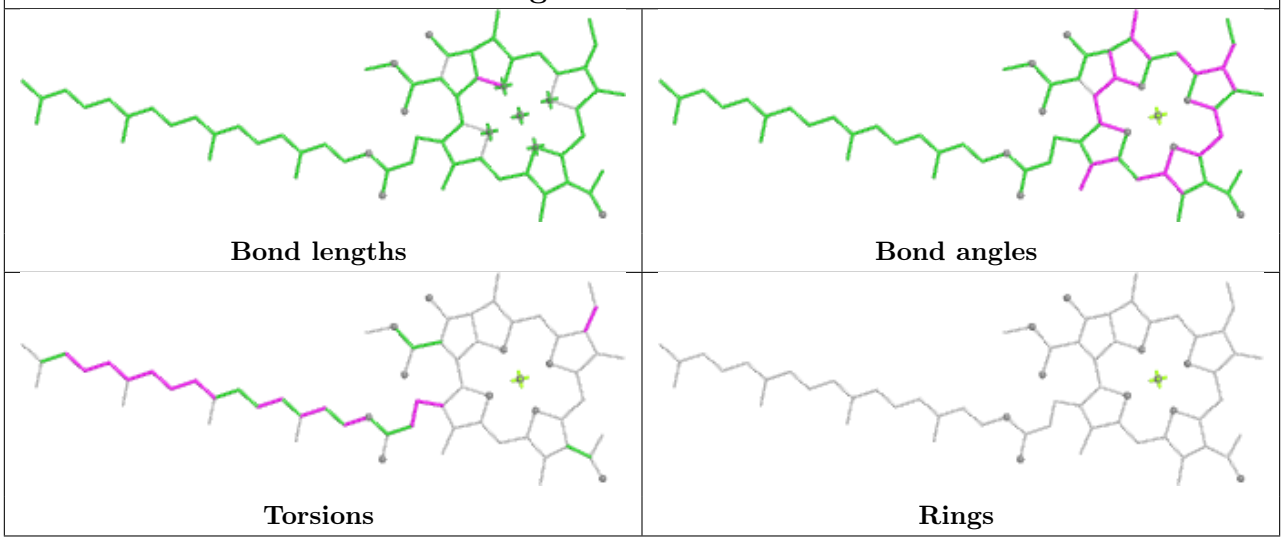
Ligand BCL i 101



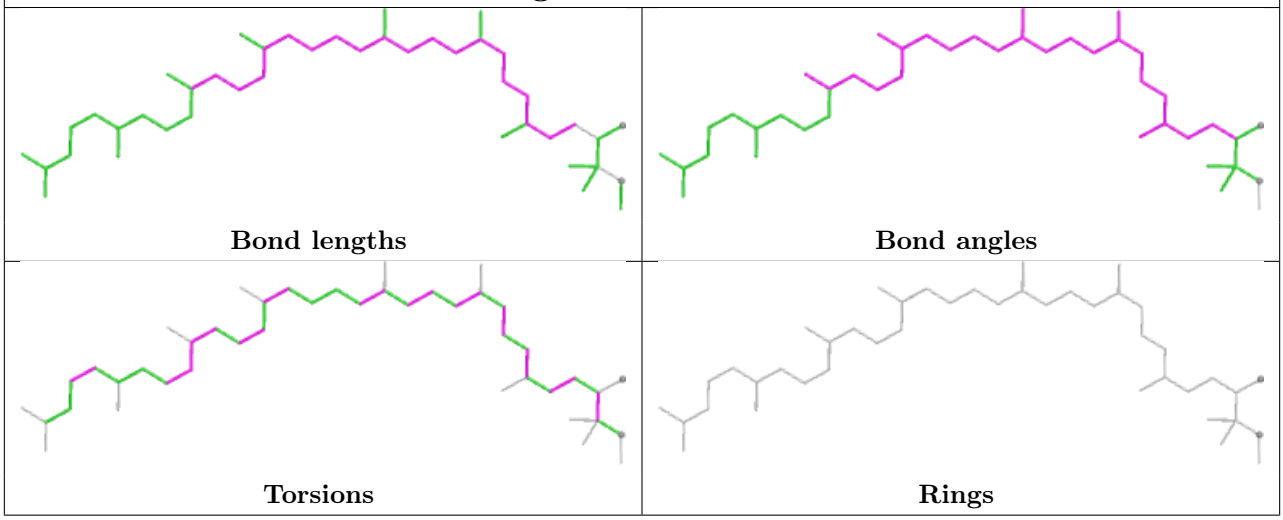
Ligand BCL M 404



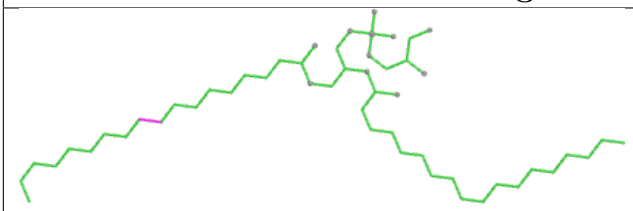
Ligand BCL k 101



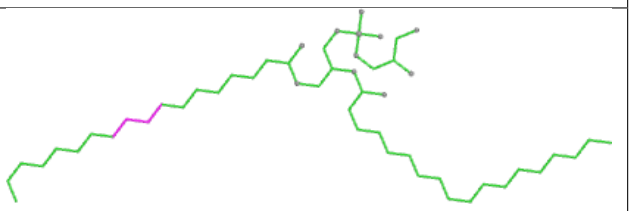
Ligand SPN r 102



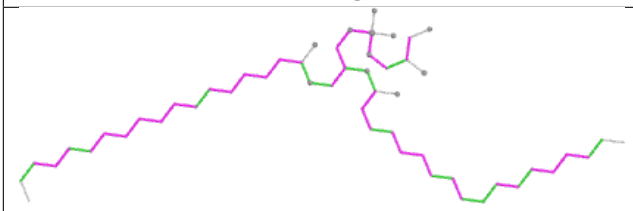
Ligand MW9 H 301



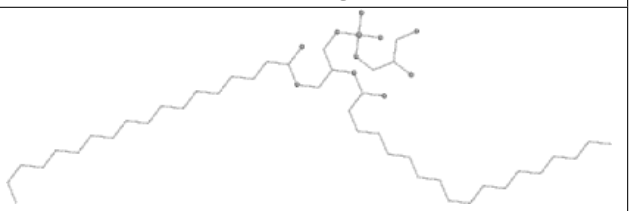
Bond lengths



Bond angles

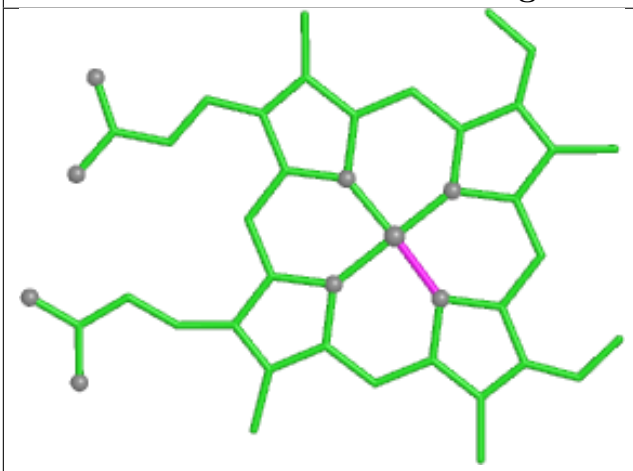


Torsions

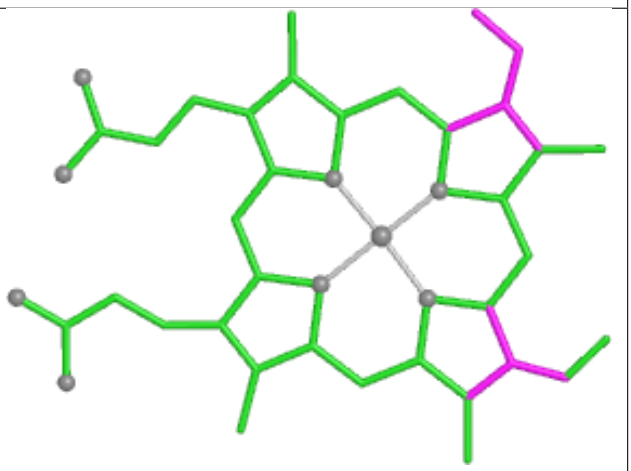


Rings

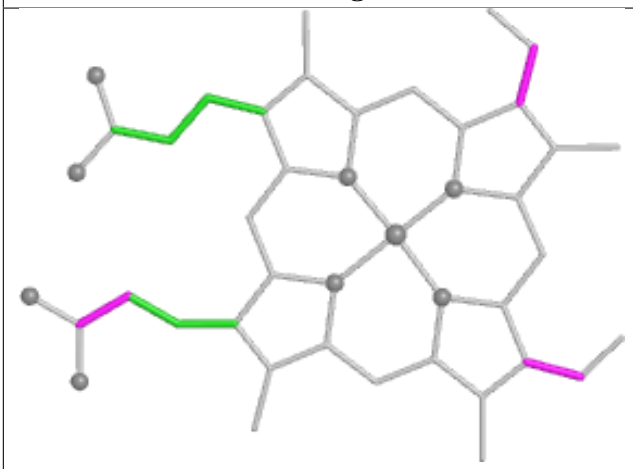
Ligand HEM C 402



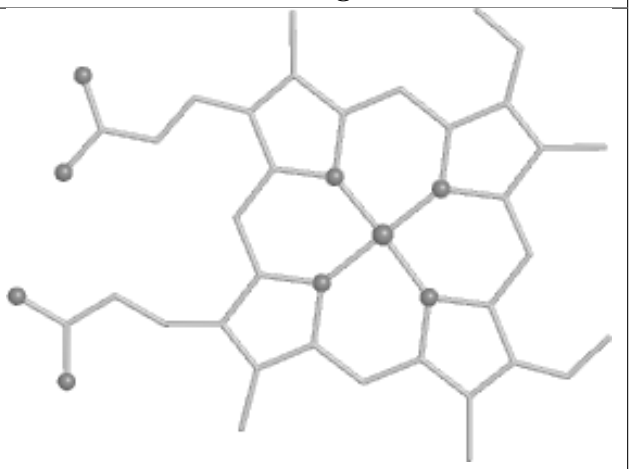
Bond lengths



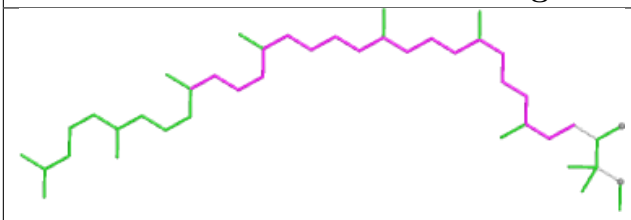
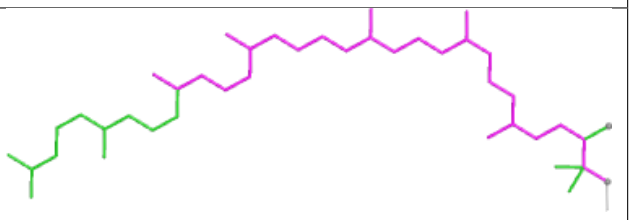
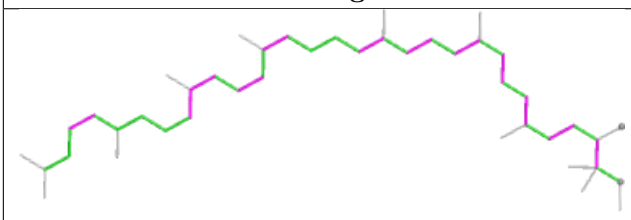
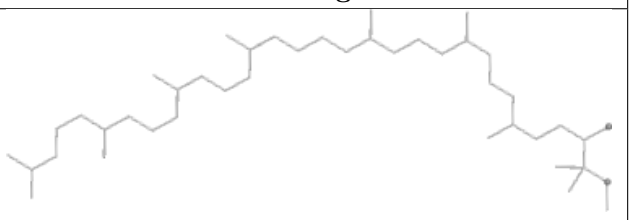
Bond angles

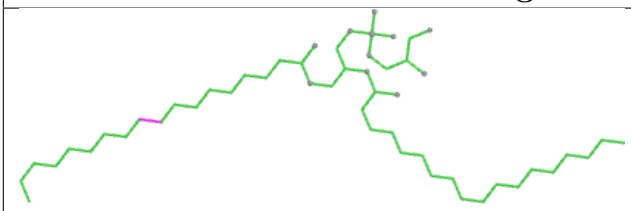
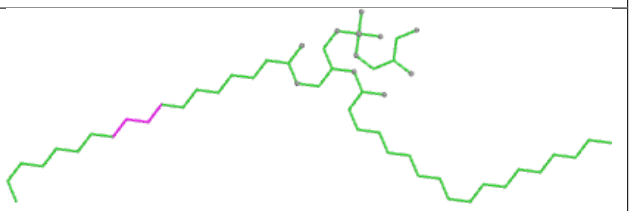
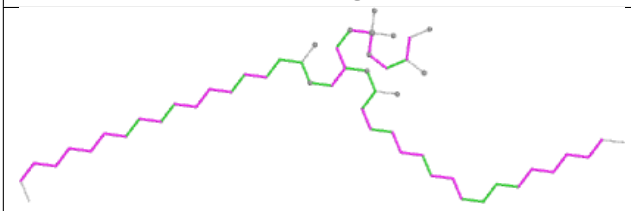
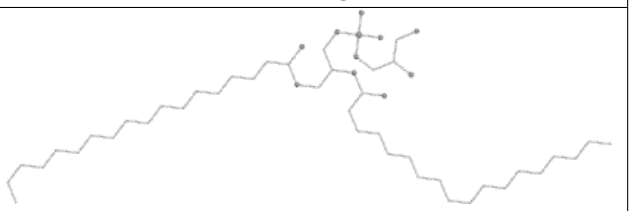


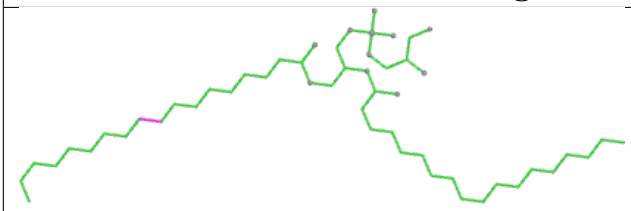
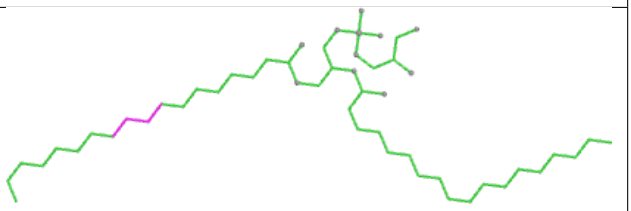
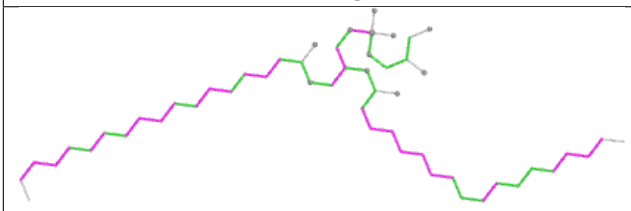
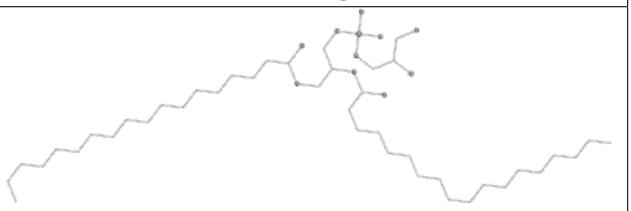
Torsions



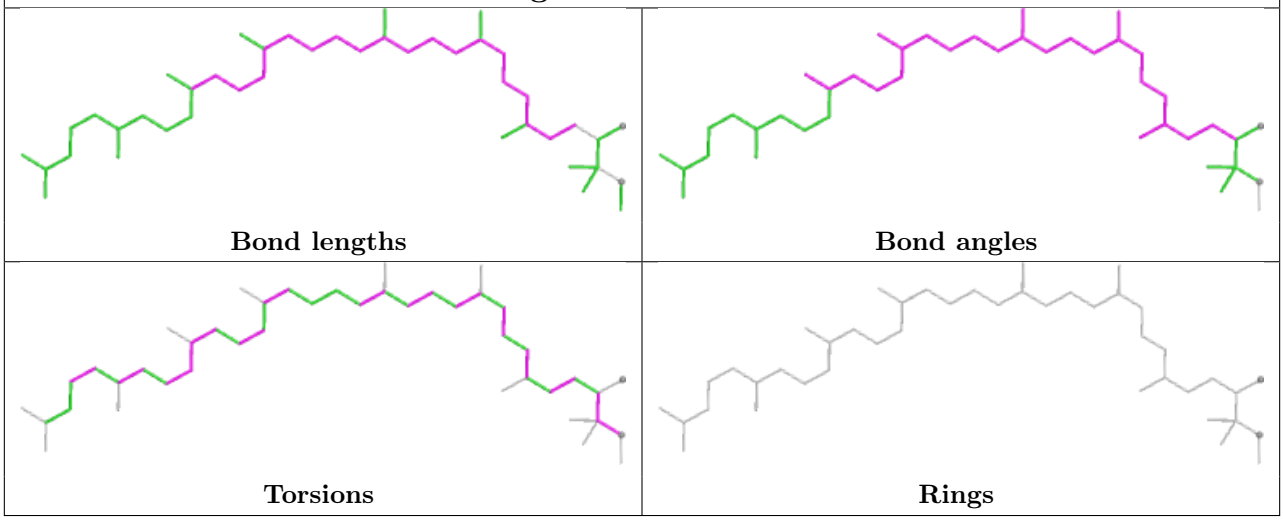
Rings

Ligand SPN s 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

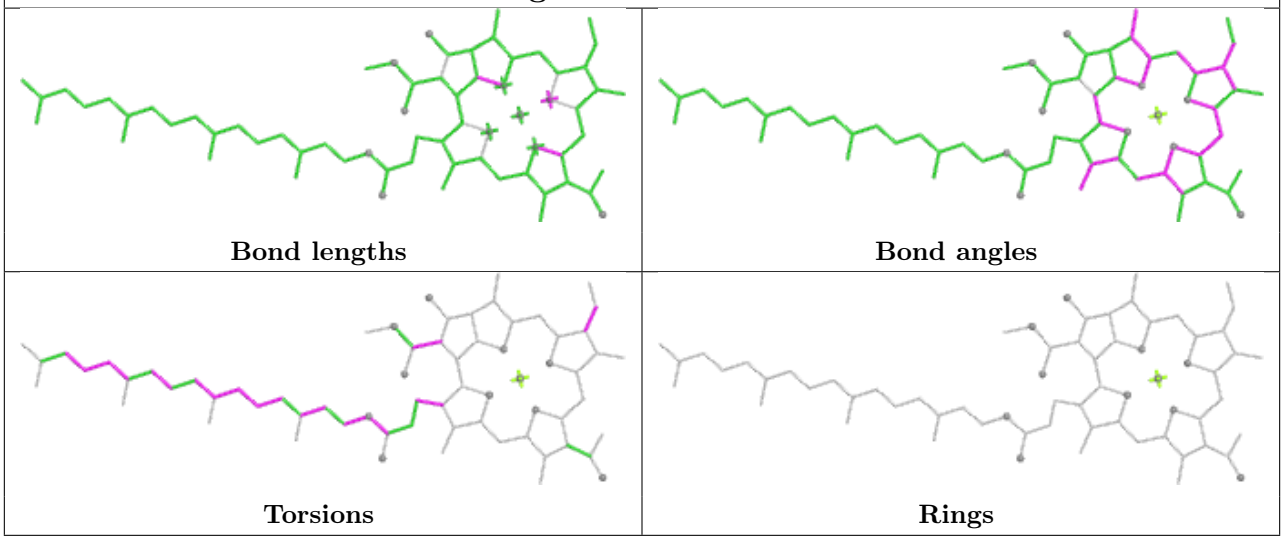
Ligand MW9 H 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand MW9 M 408	
 Bond lengths	 Bond angles
 Torsions	 Rings

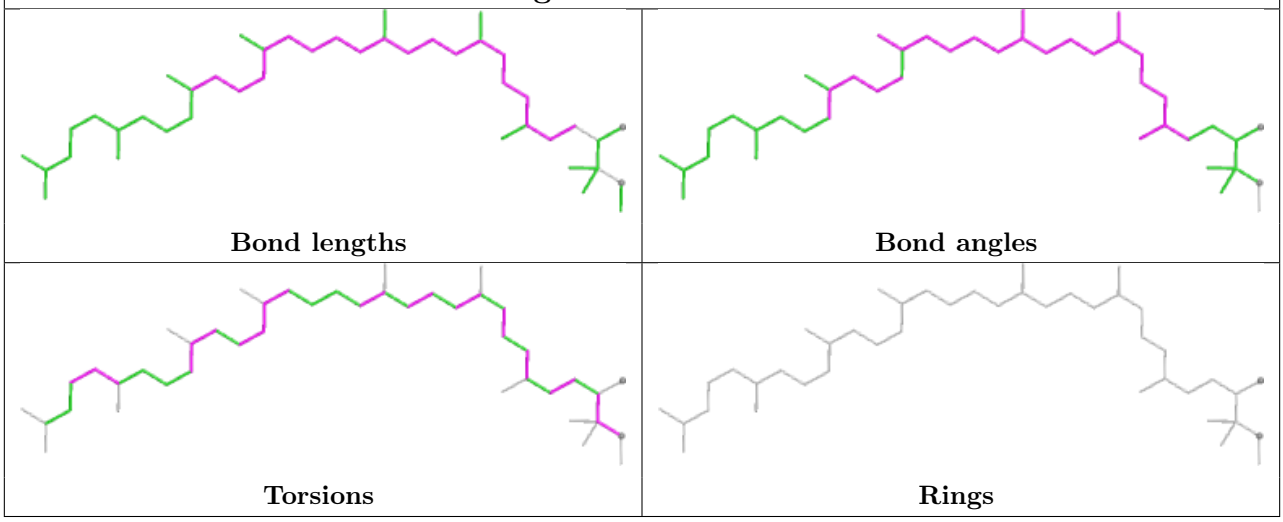
Ligand SPN 3 102



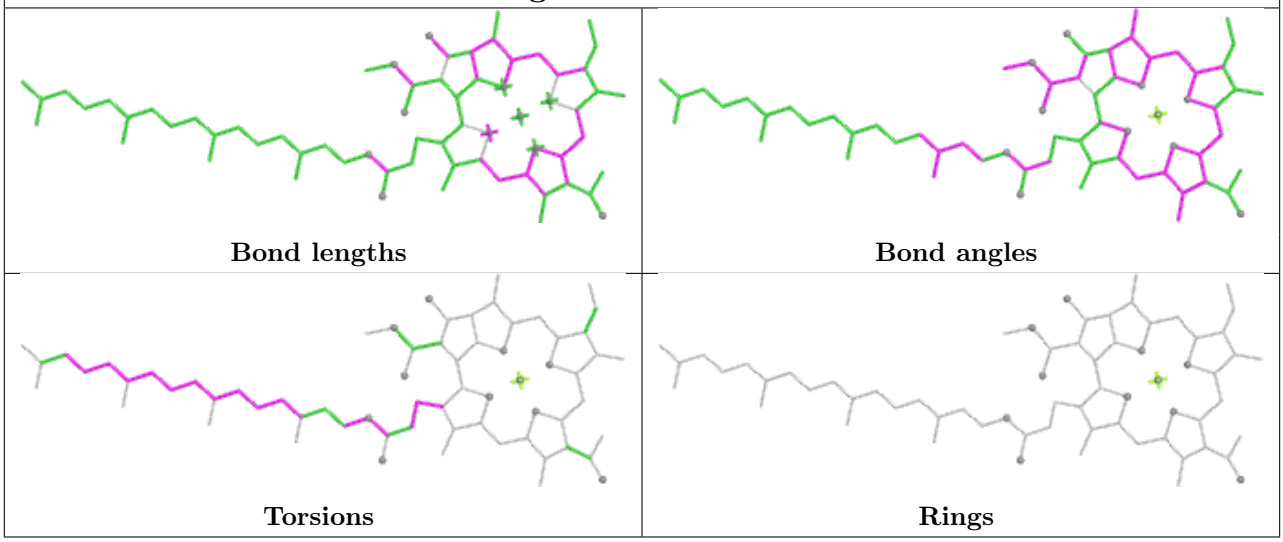
Ligand BCL h 101



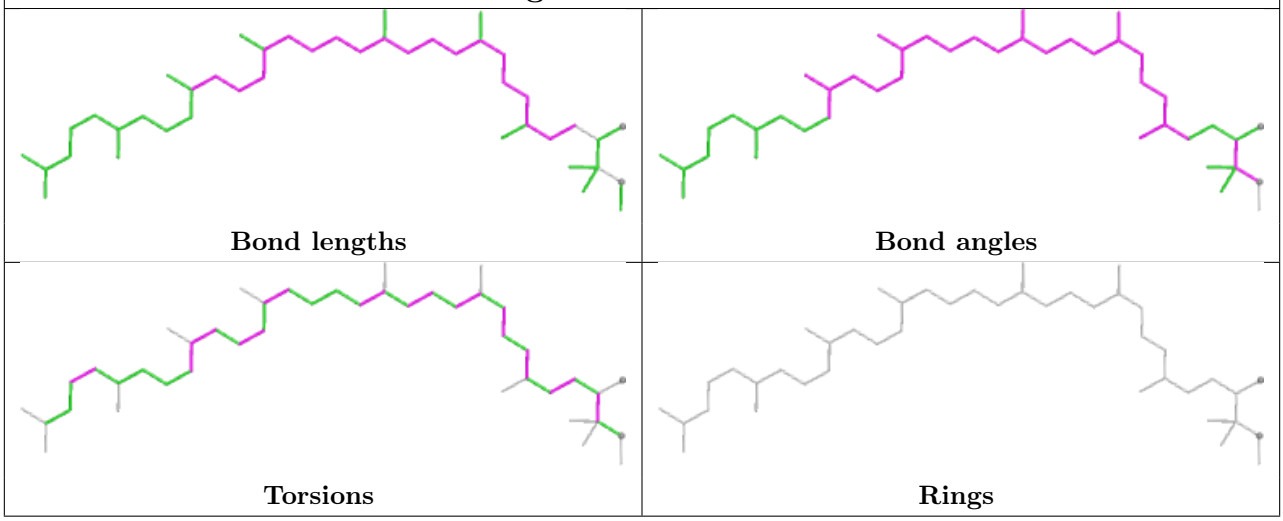
Ligand SPN f 102



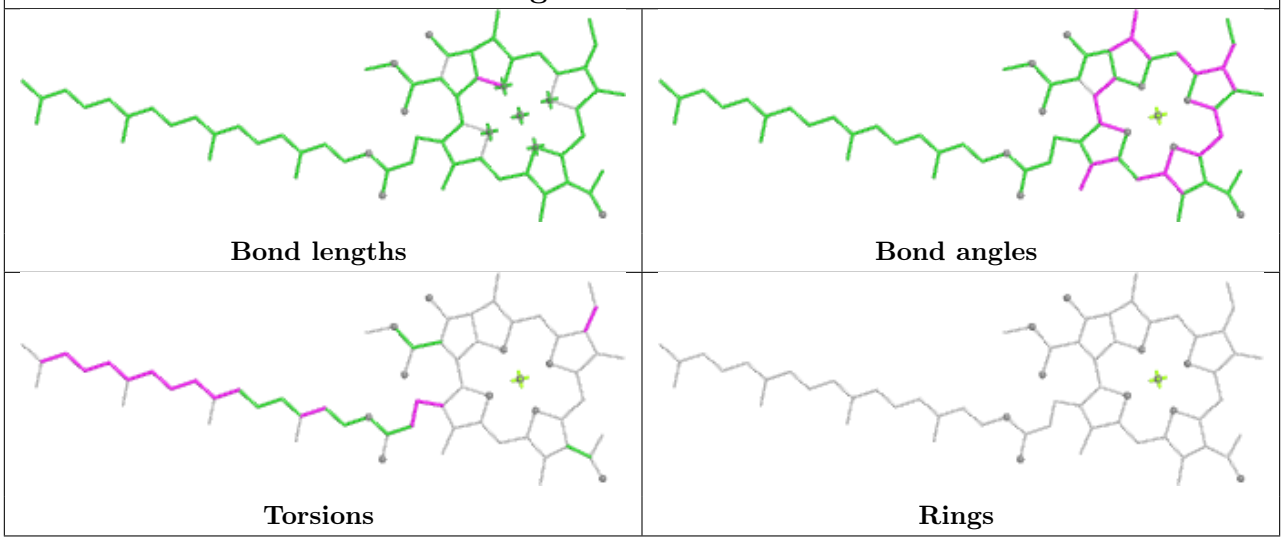
Ligand BCL b 101



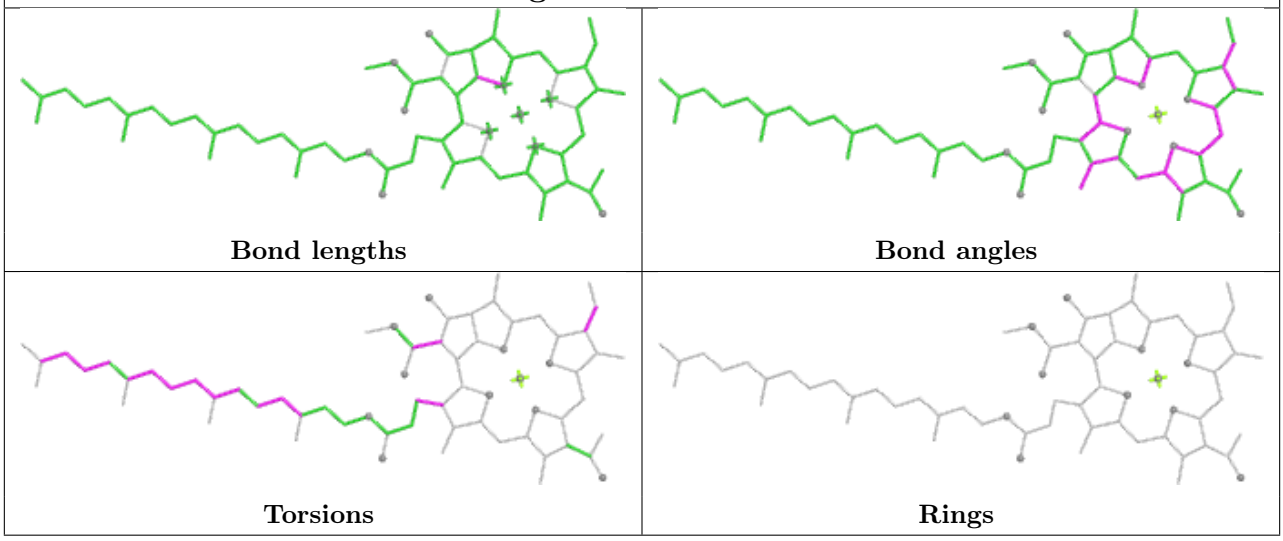
Ligand SPN w 102



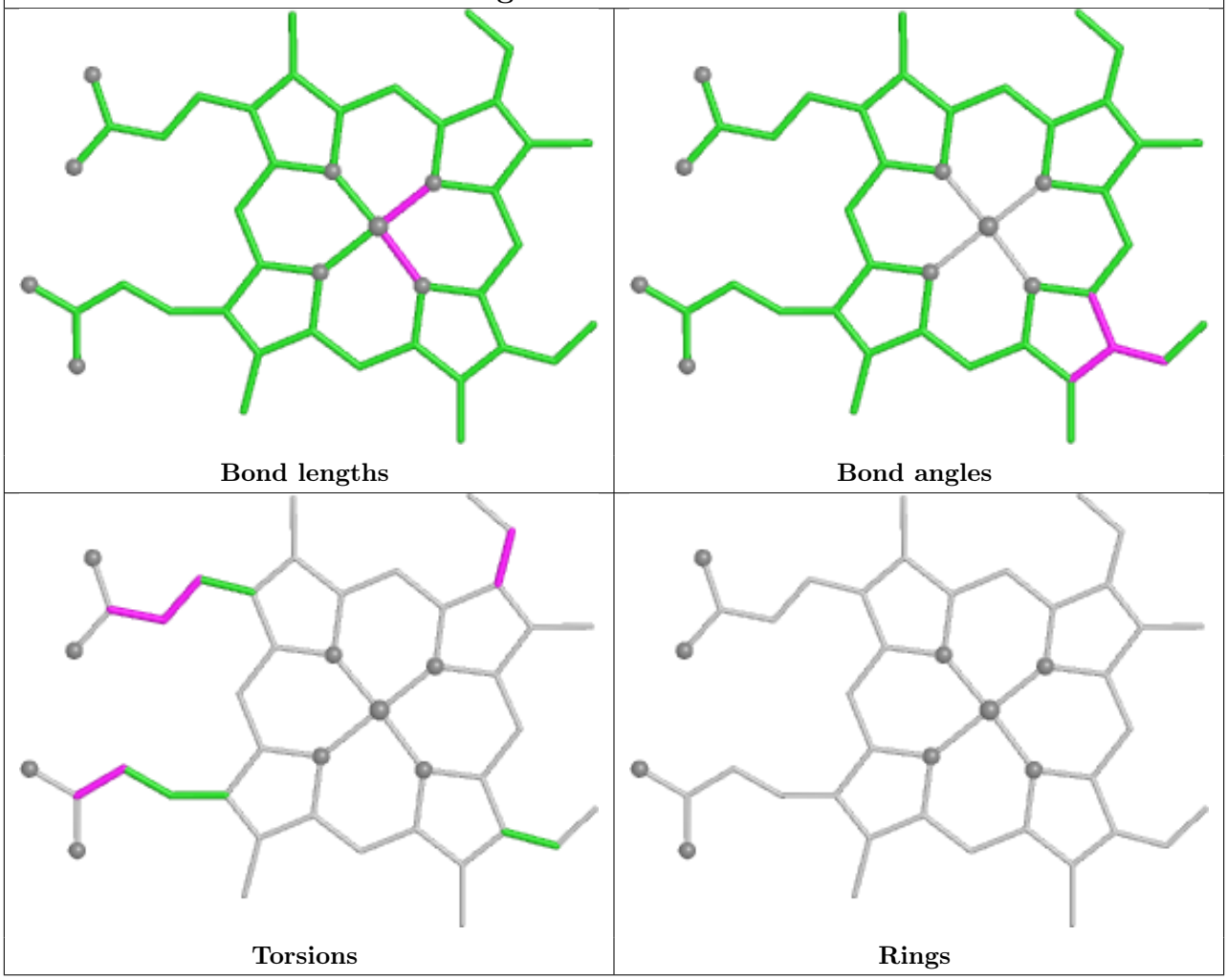
Ligand BCL 7 101



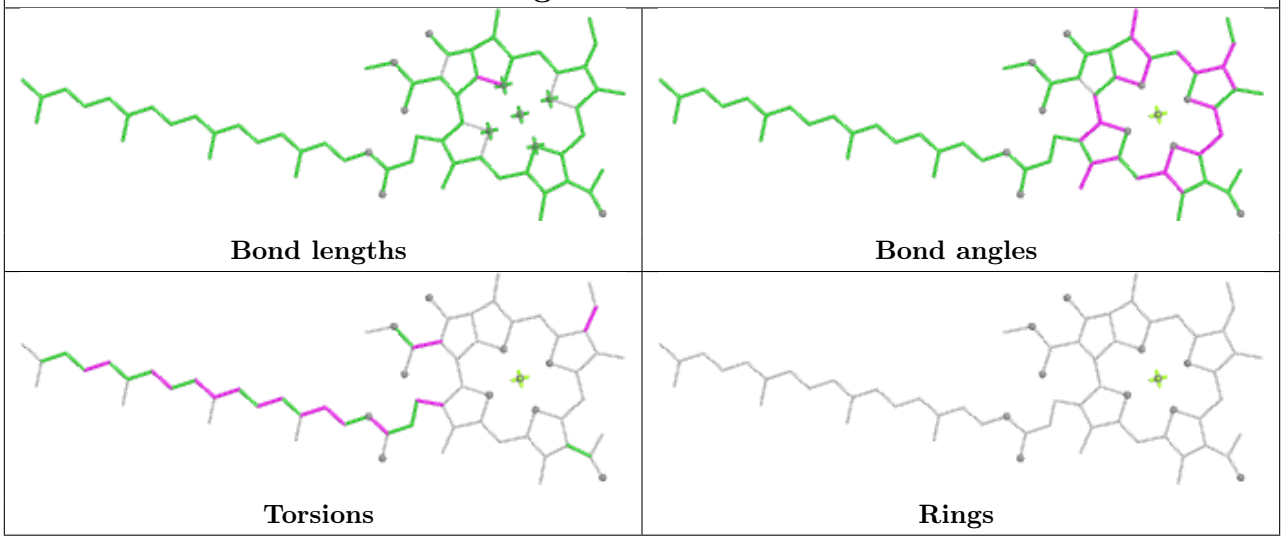
Ligand BCL n 101



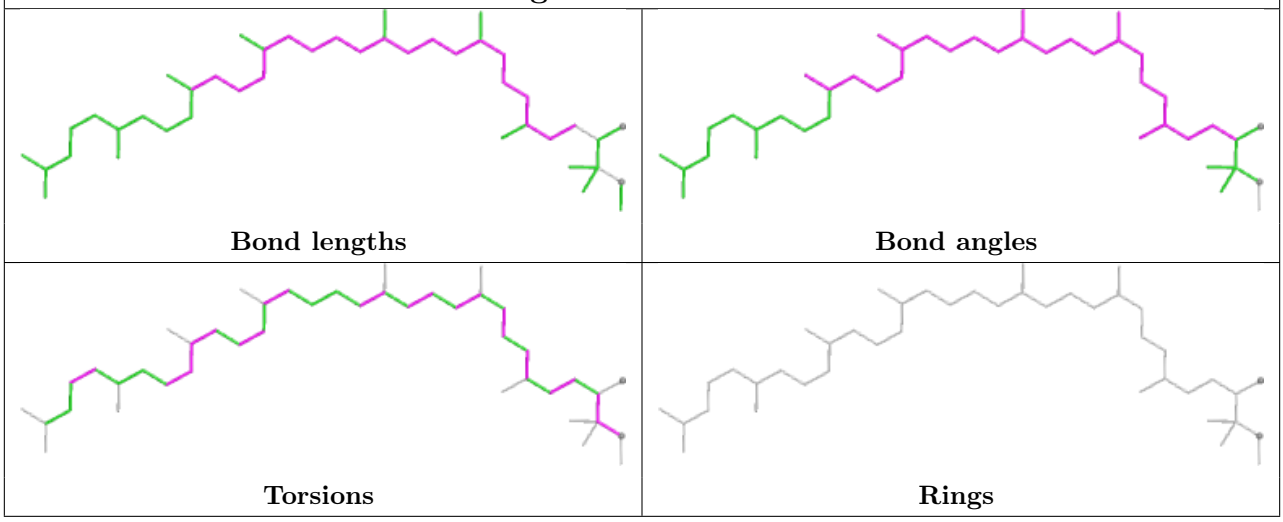
Ligand HEM C 401



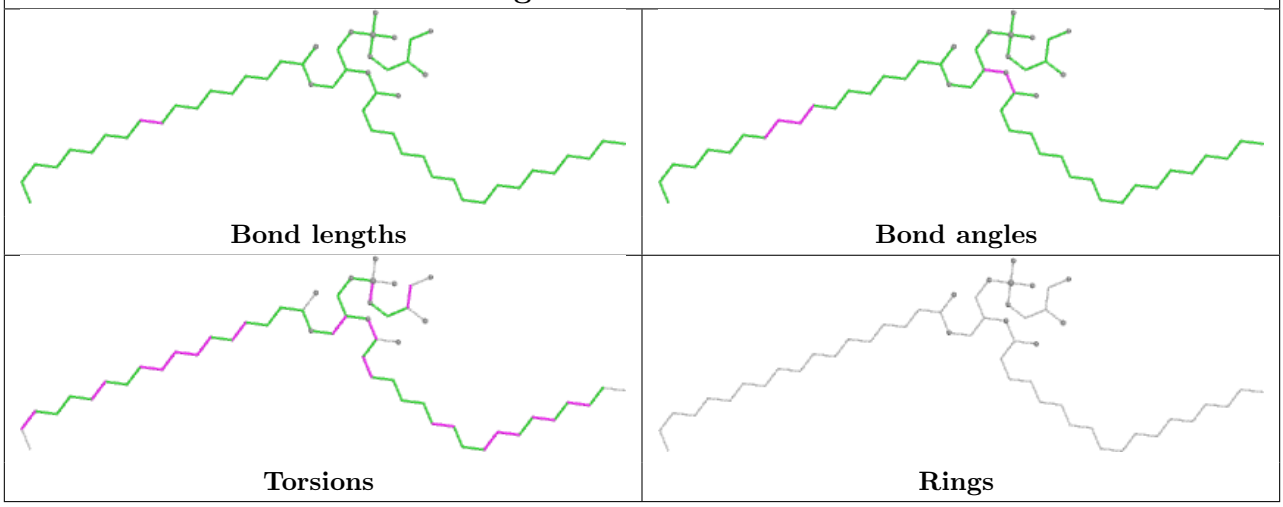
Ligand BCL f 101



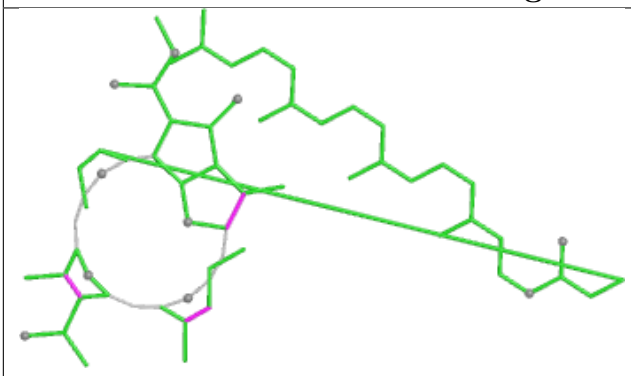
Ligand SPN 5 102



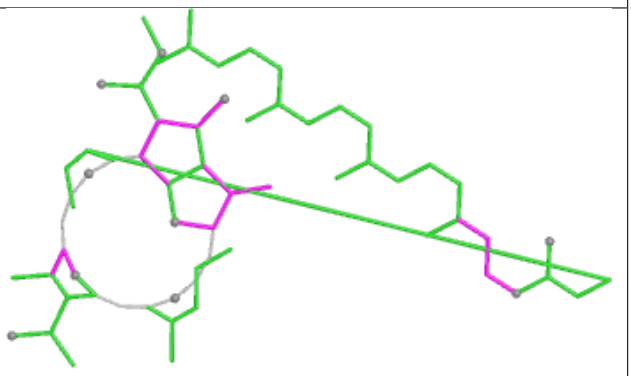
Ligand MW9 M 407



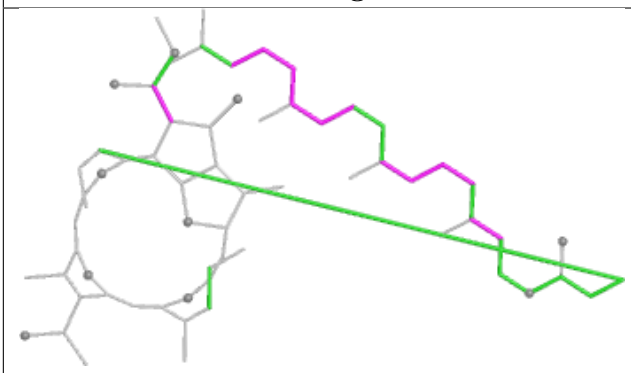
Ligand BPH L 303



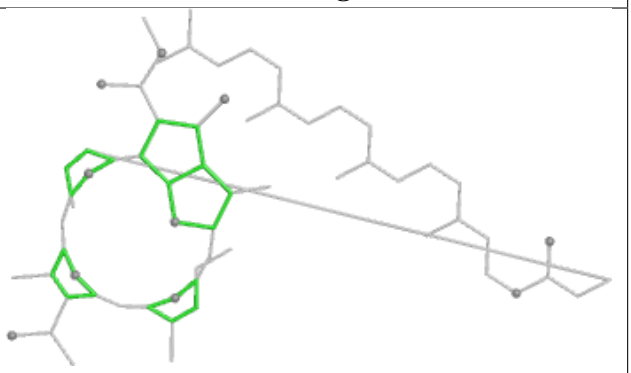
Bond lengths



Bond angles

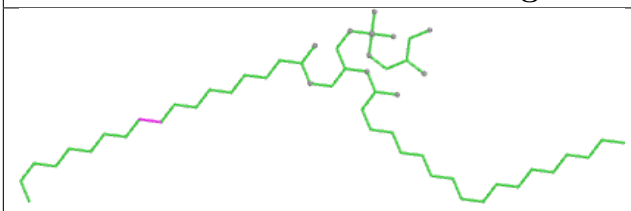


Torsions

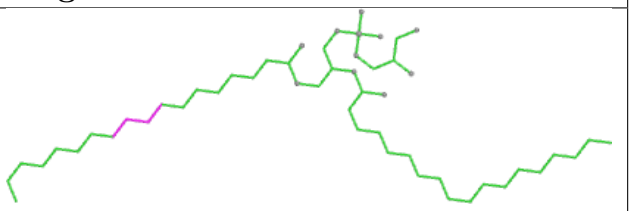


Rings

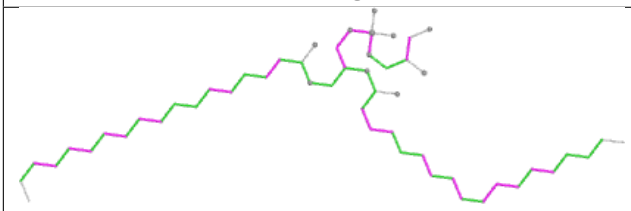
Ligand MW9 g 102



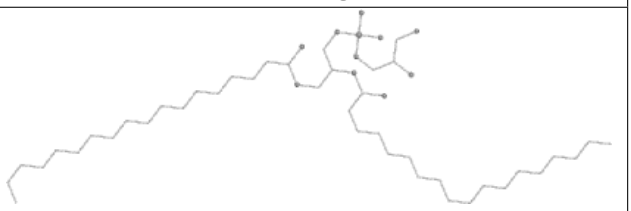
Bond lengths



Bond angles

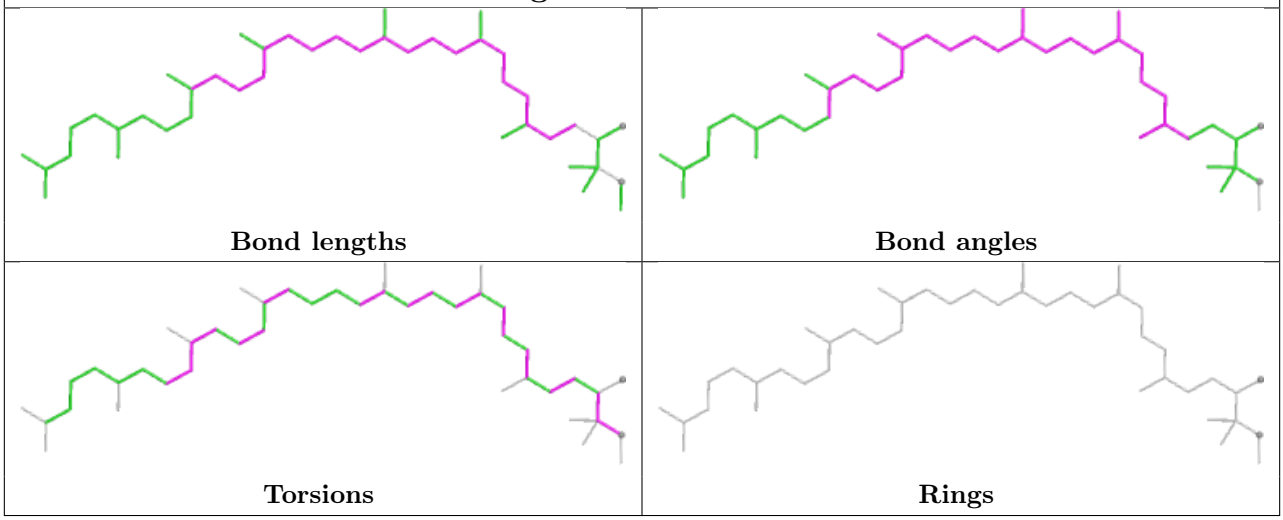


Torsions

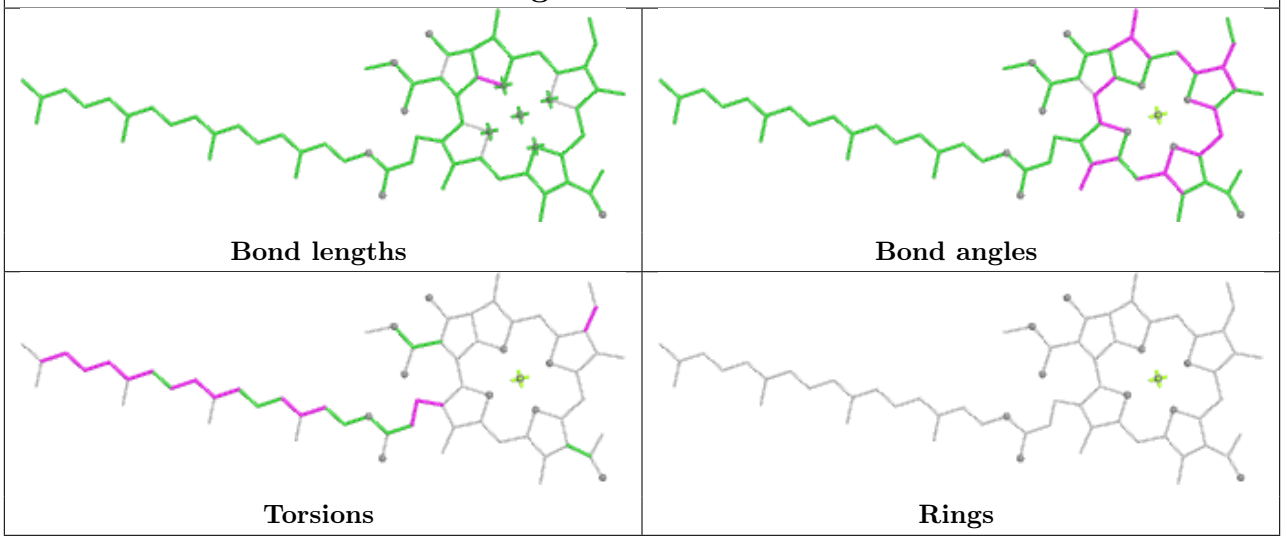


Rings

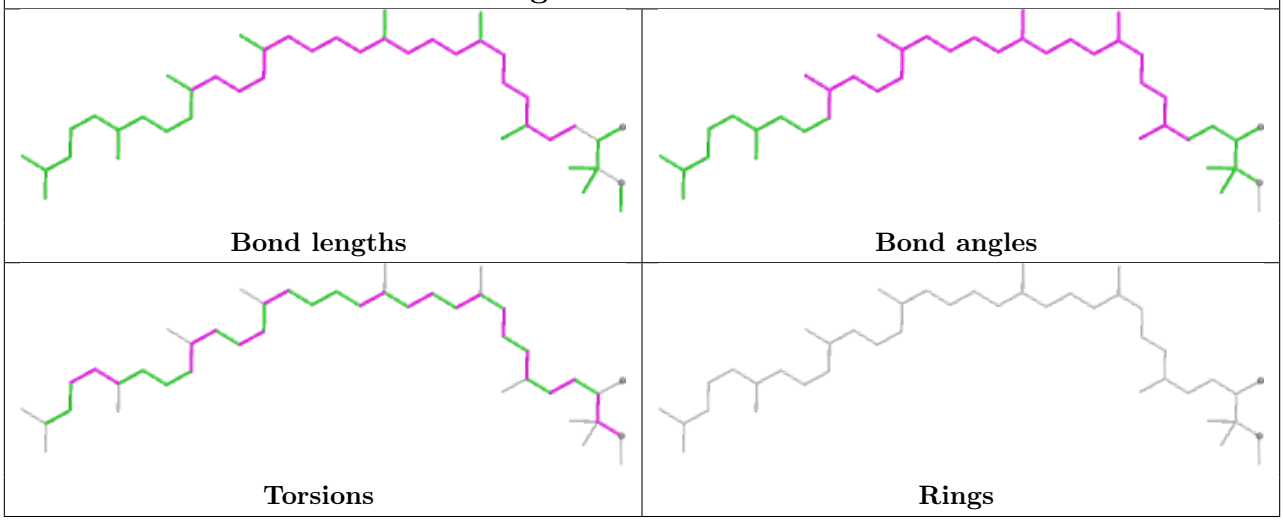
Ligand SPN 0 102



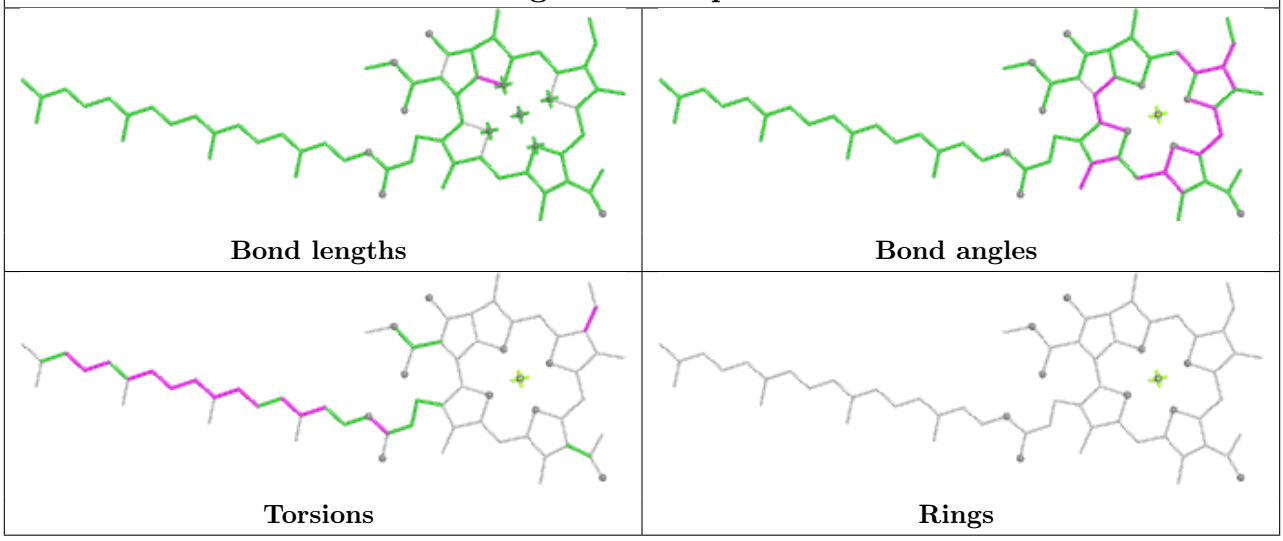
Ligand BCL c 101



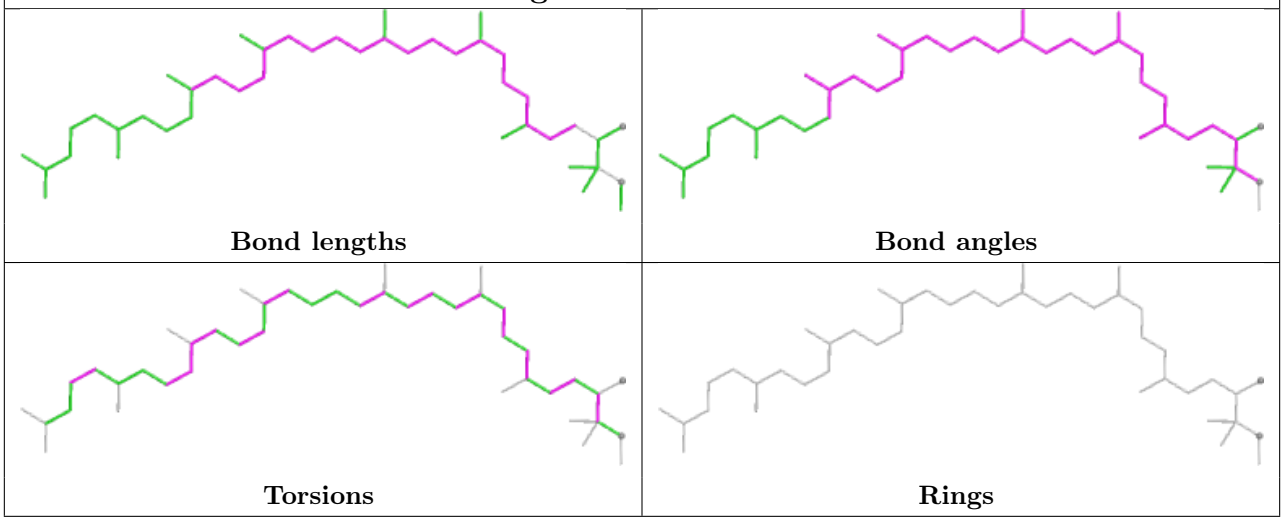
Ligand SPN 1 105



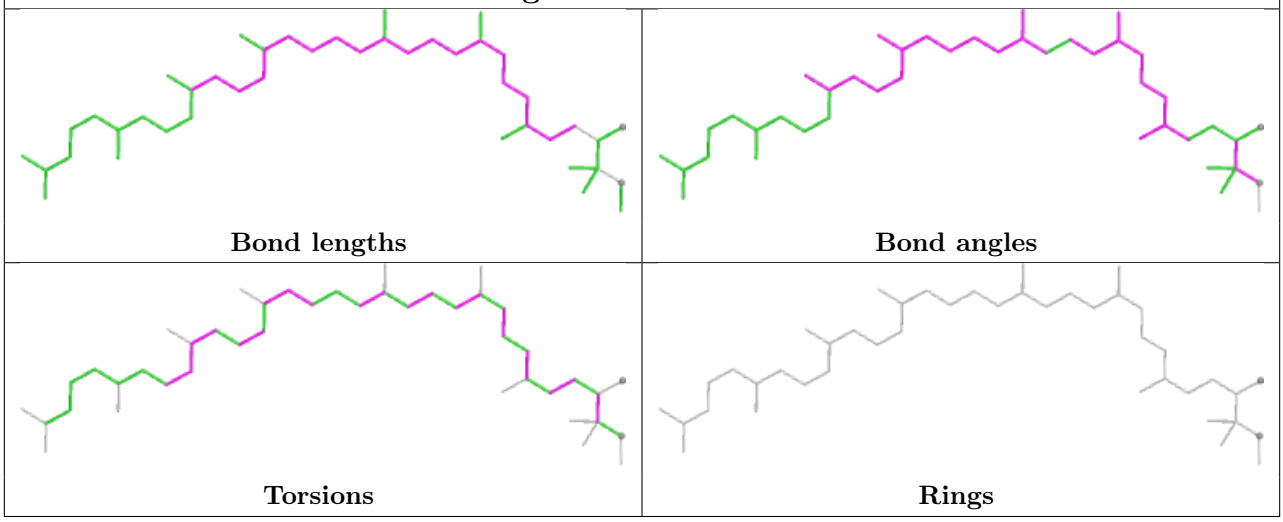
Ligand BCL q 101



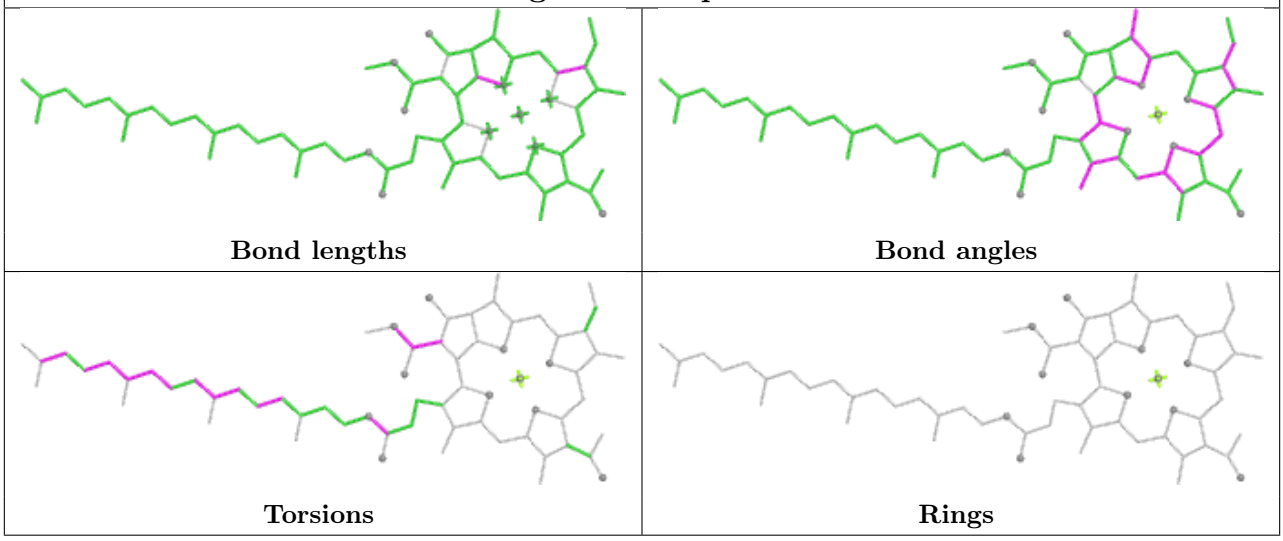
Ligand SPN 9 103



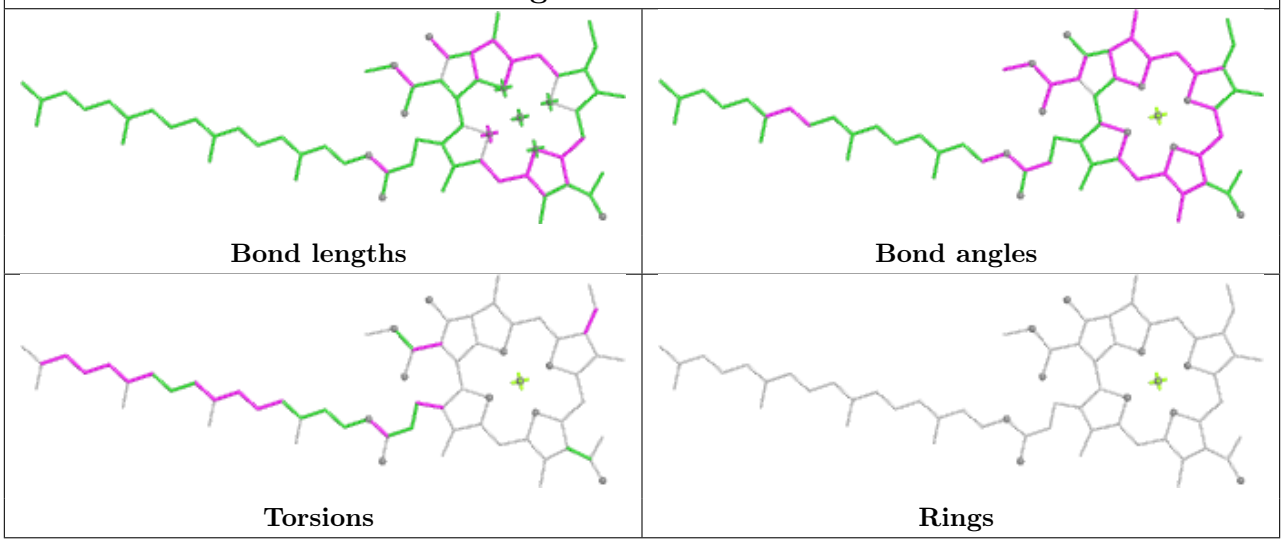
Ligand SPN M 406



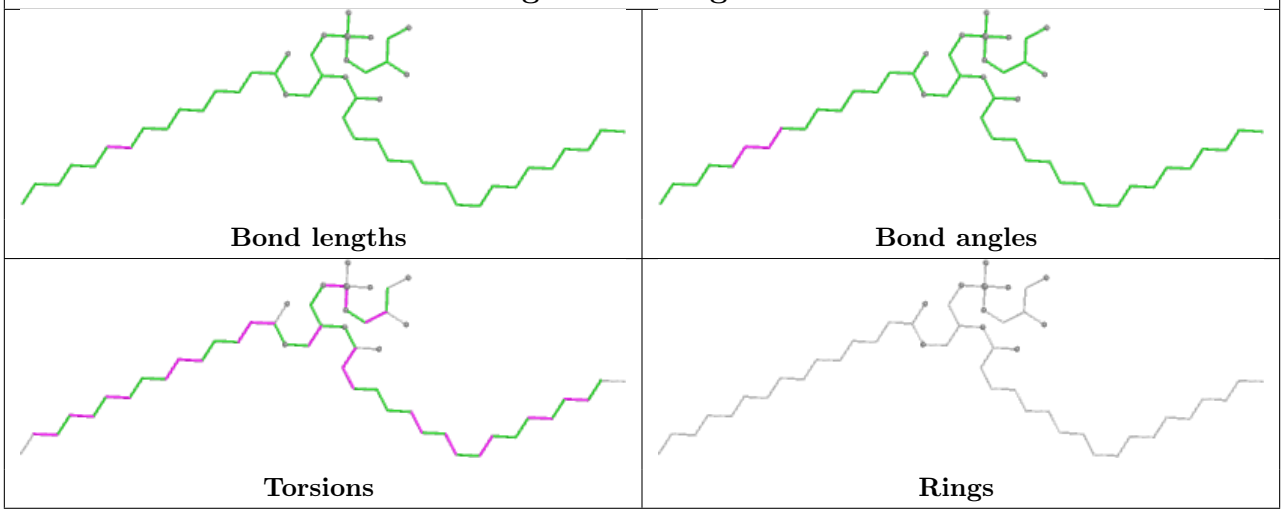
Ligand BCL p 101



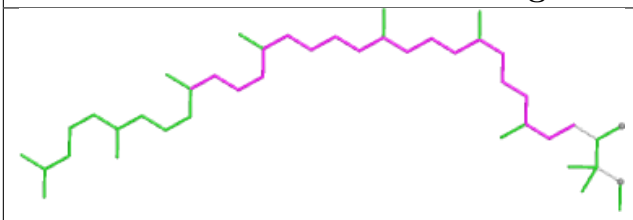
Ligand BCL 0 101



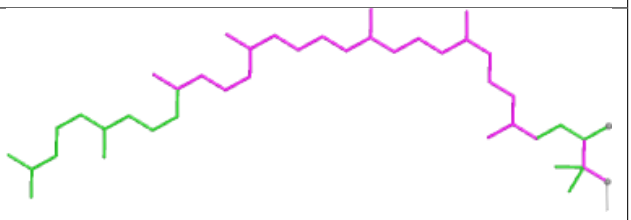
Ligand MW9 g 103



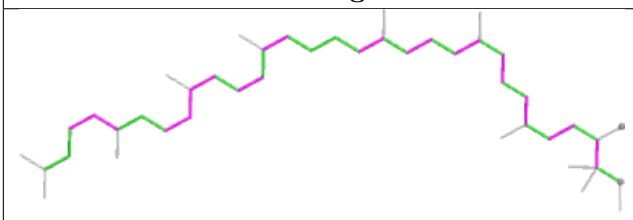
Ligand SPN n 102



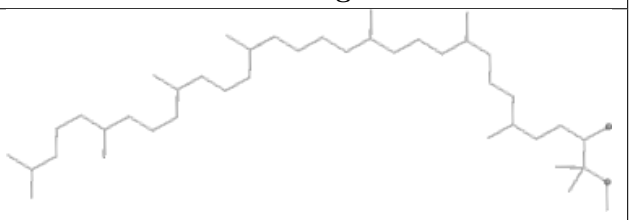
Bond lengths



Bond angles

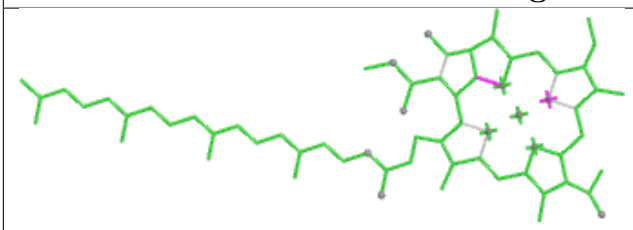


Torsions

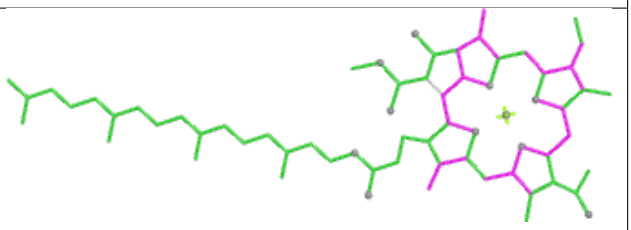


Rings

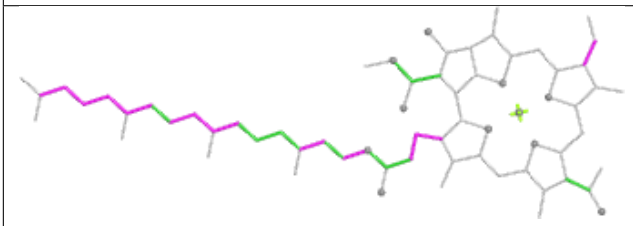
Ligand BCL a 101



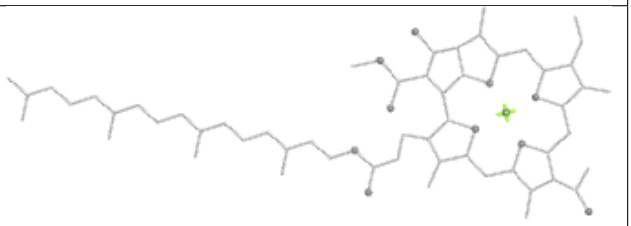
Bond lengths



Bond angles

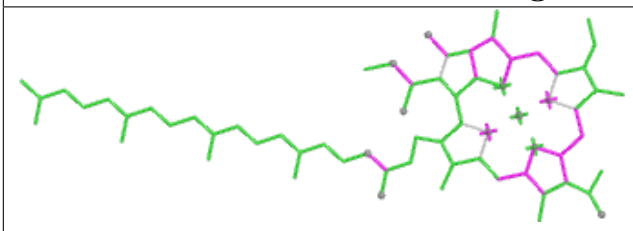


Torsions

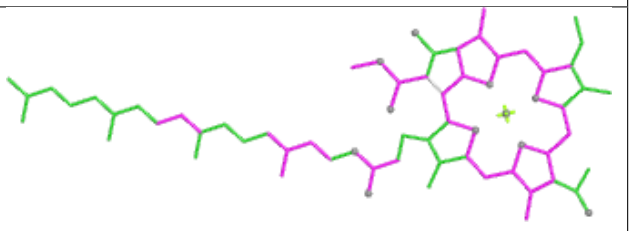


Rings

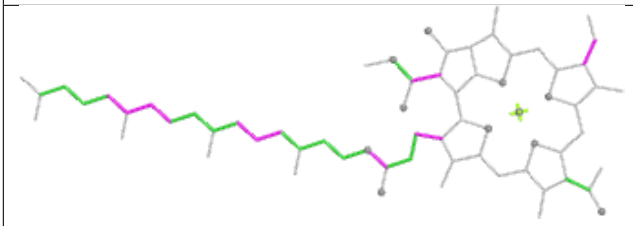
Ligand BCL 8 101



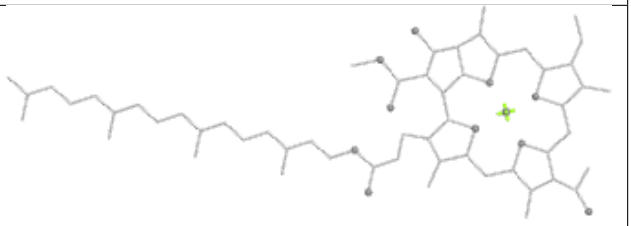
Bond lengths



Bond angles

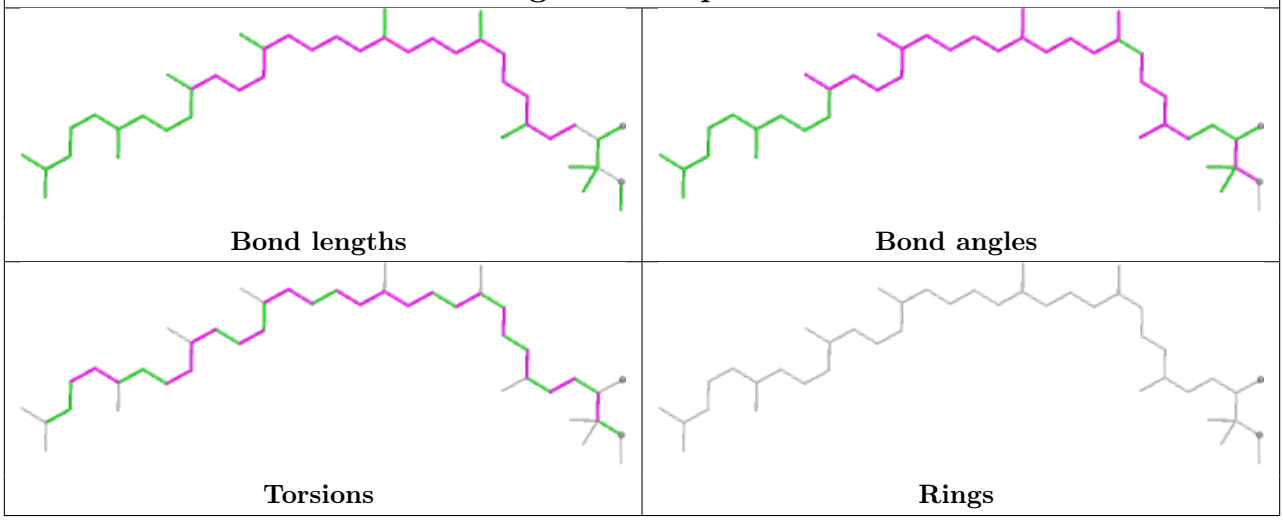


Torsions

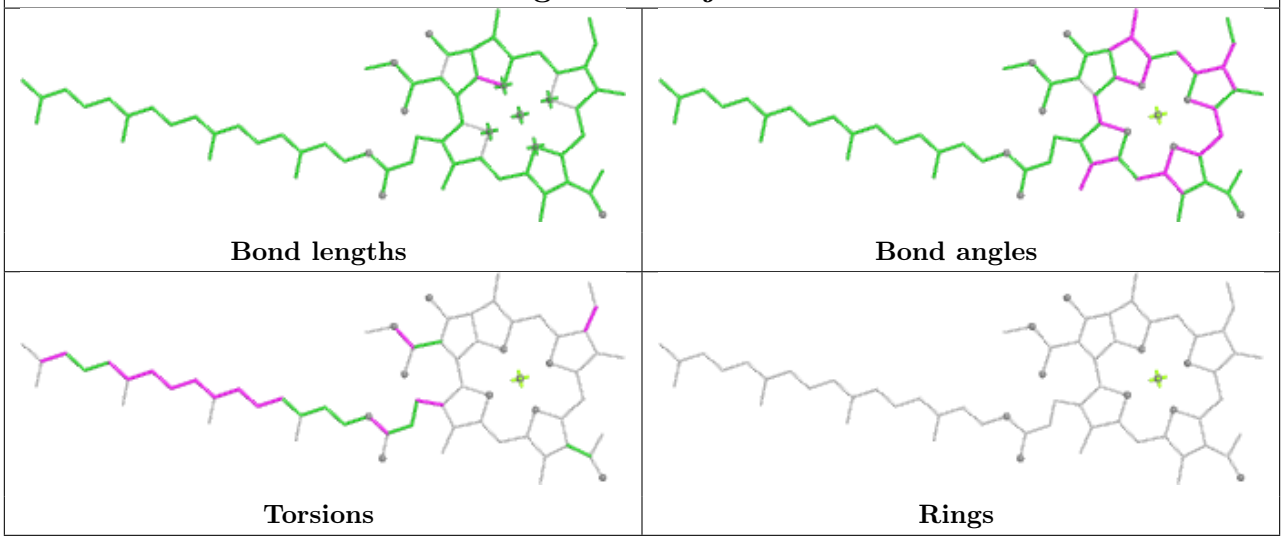


Rings

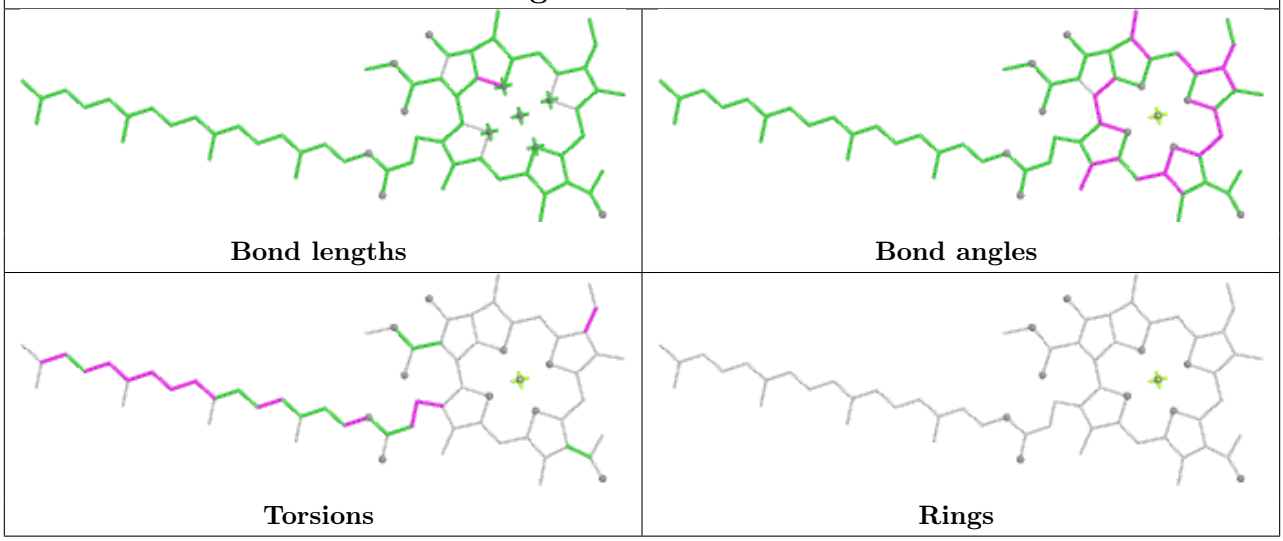
Ligand SPN p 102



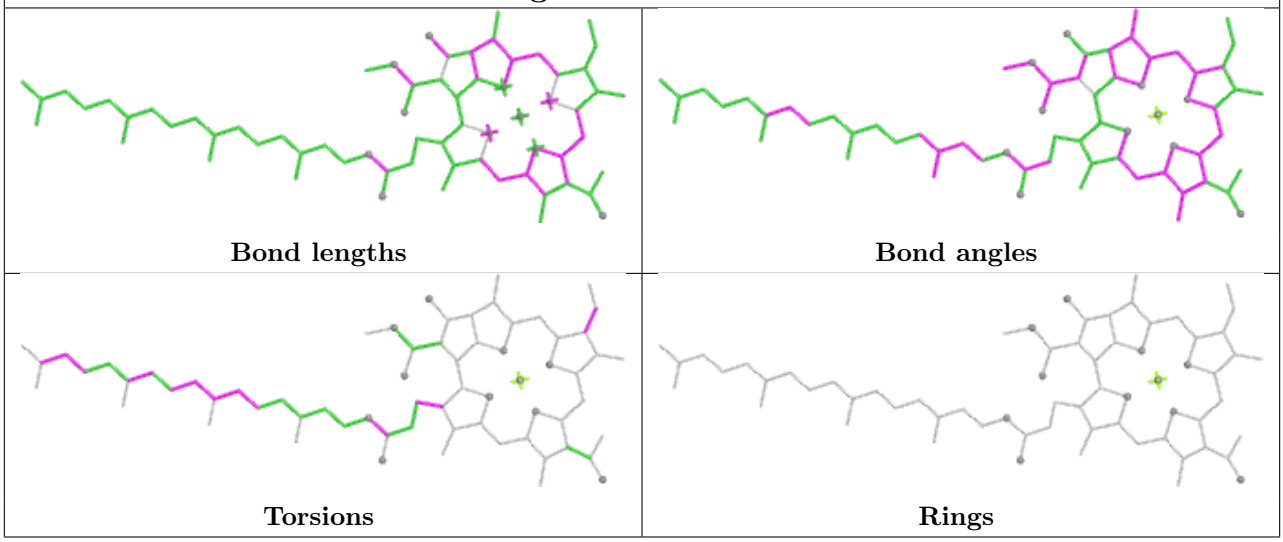
Ligand BCL j 101



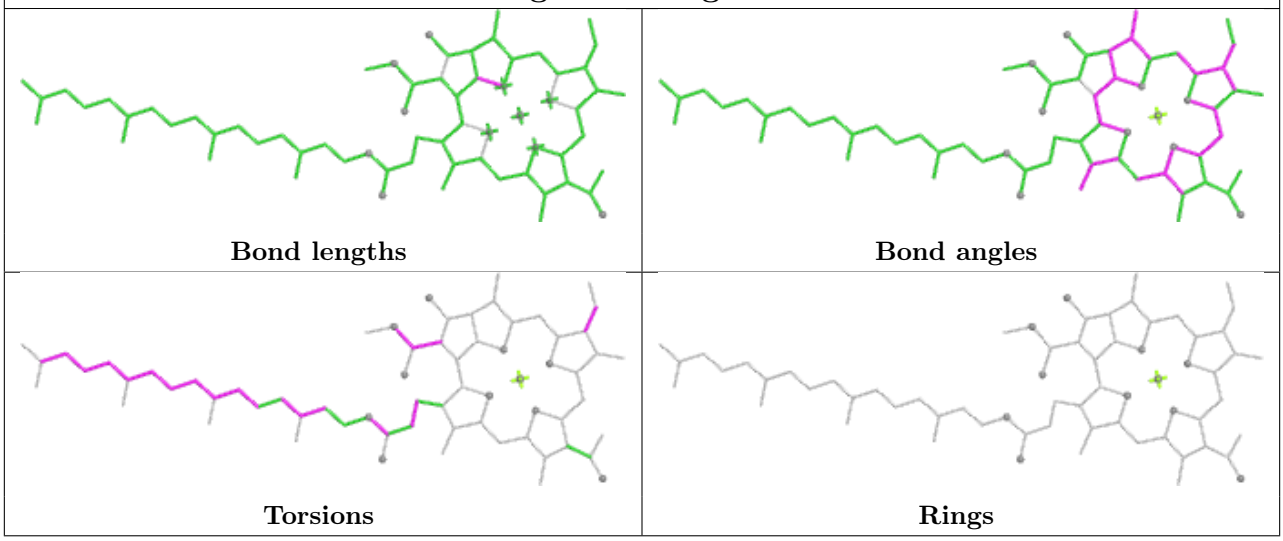
Ligand BCL 1 101



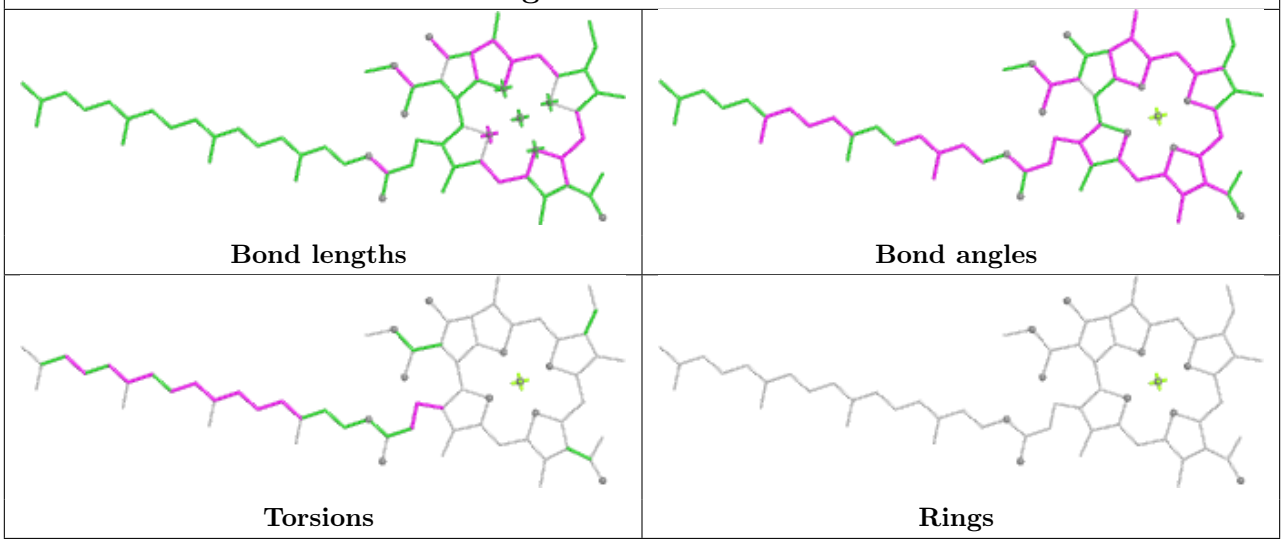
Ligand BCL 6 101

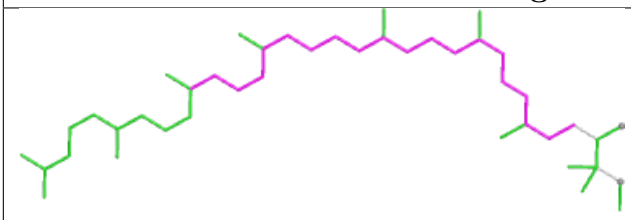
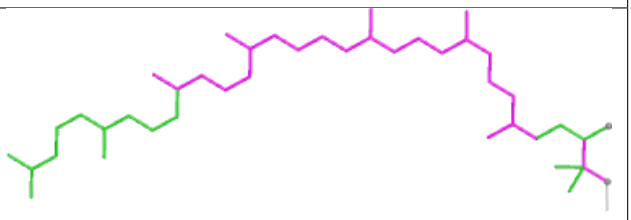
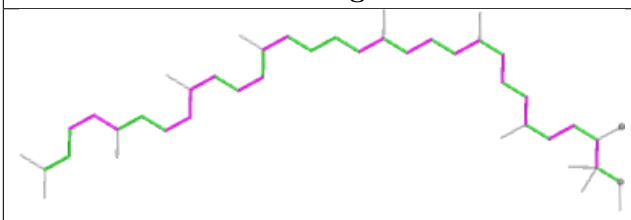
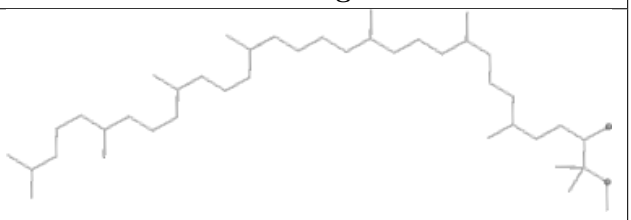


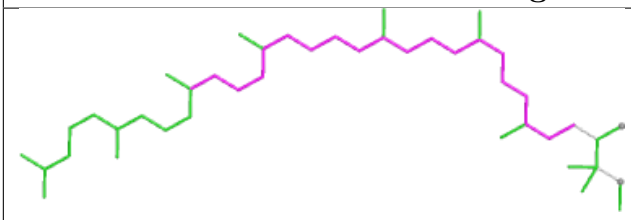
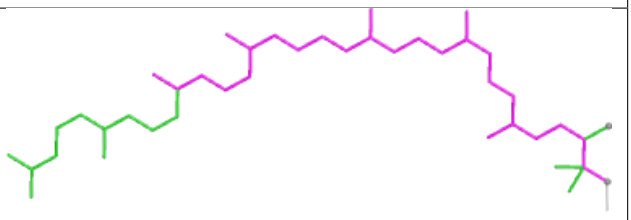
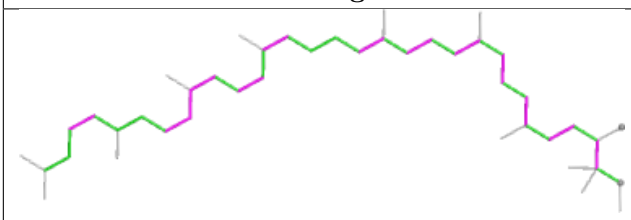
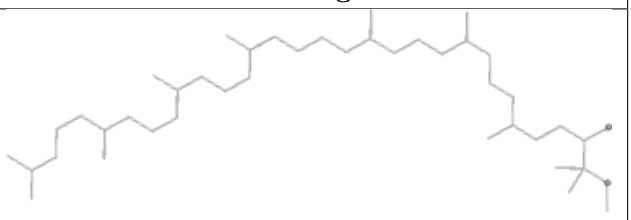
Ligand BCL g 101



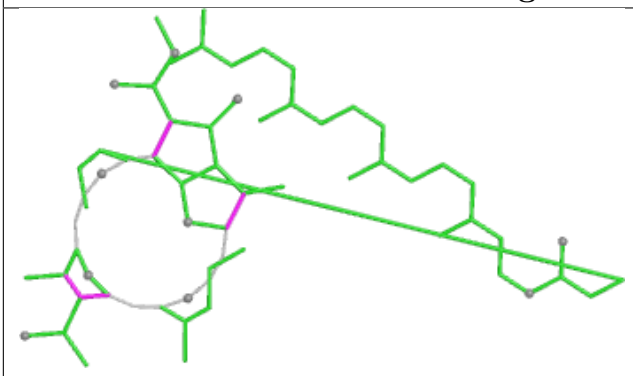
Ligand BCL M 402



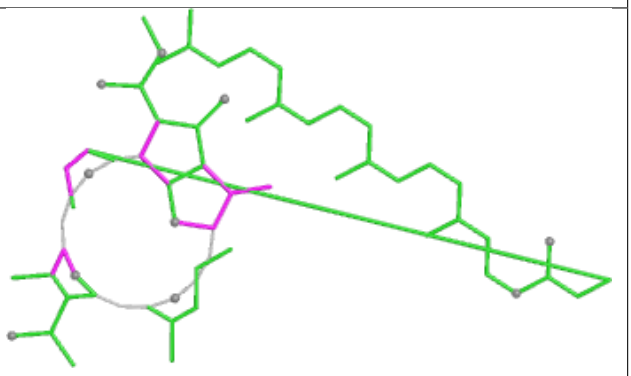
Ligand SPN c 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SPN 7 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

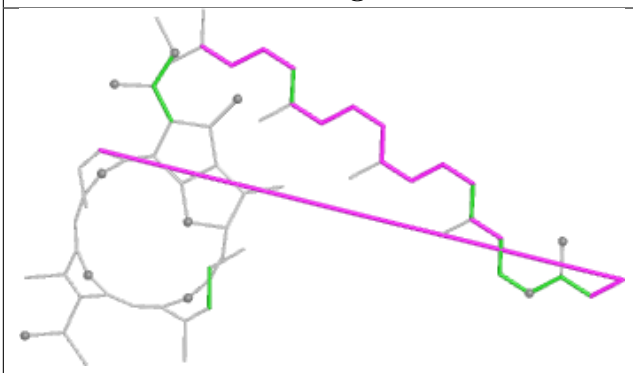
Ligand BPH M 409



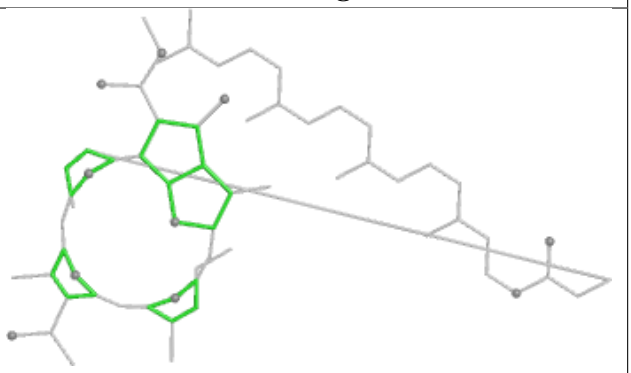
Bond lengths



Bond angles

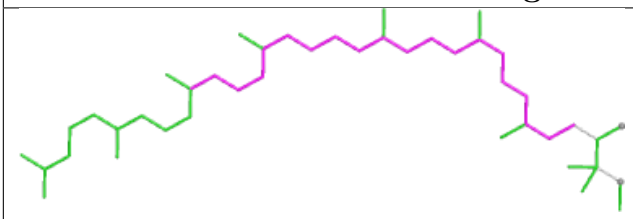


Torsions

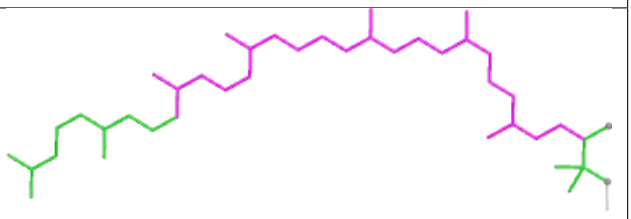


Rings

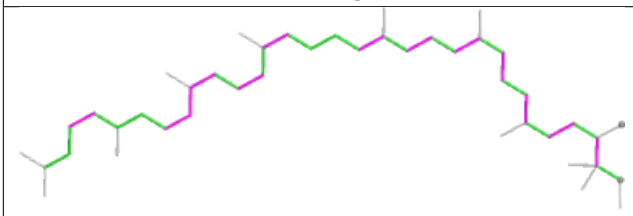
Ligand SPN m 102



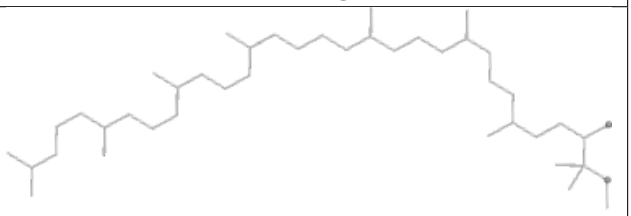
Bond lengths



Bond angles

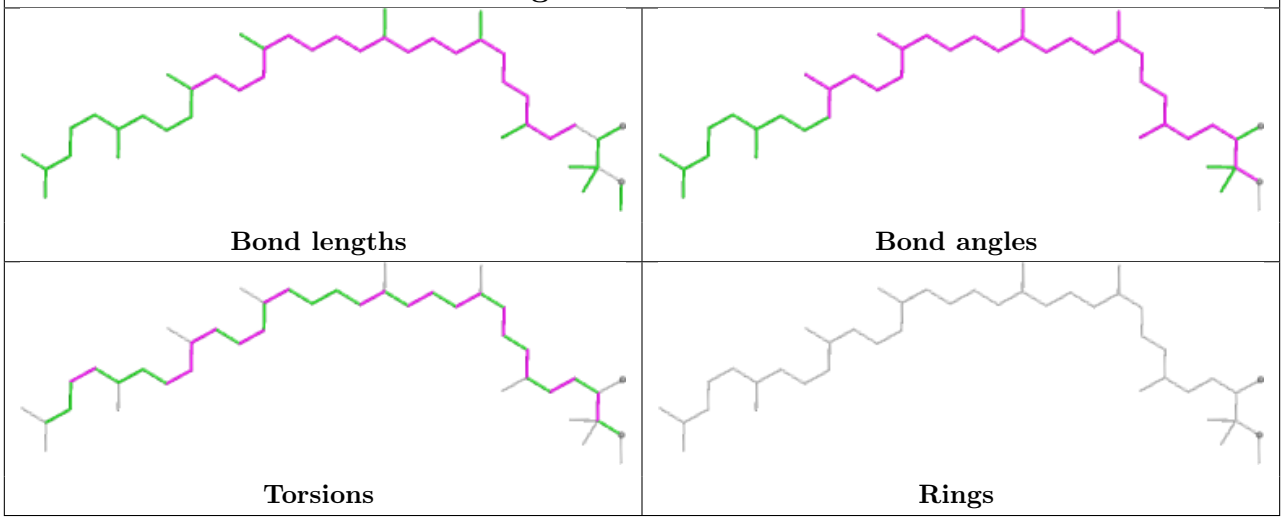


Torsions

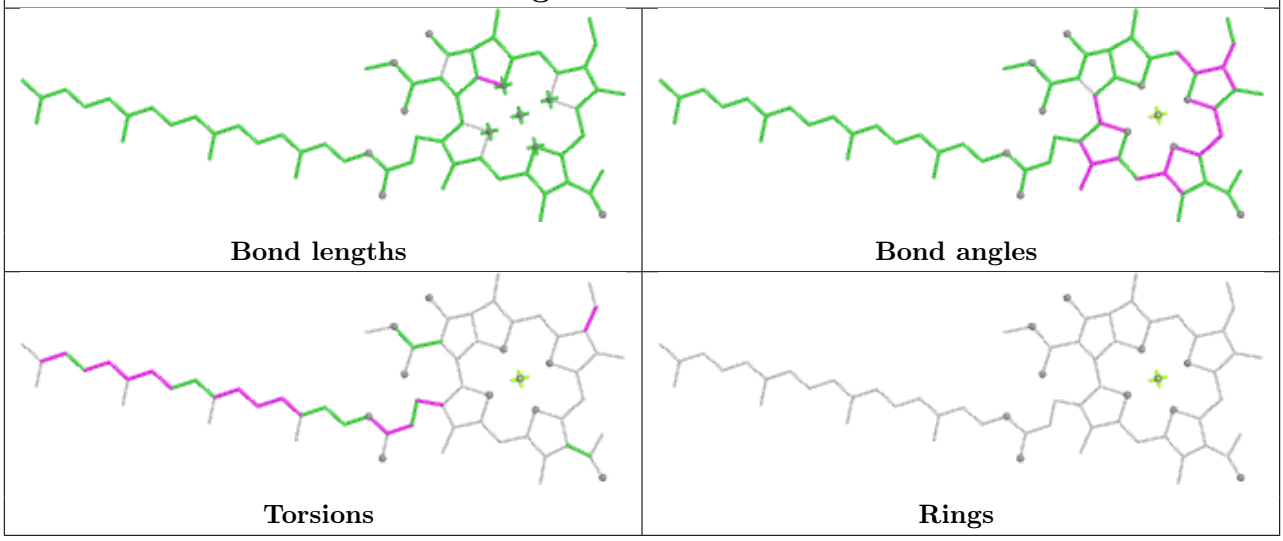


Rings

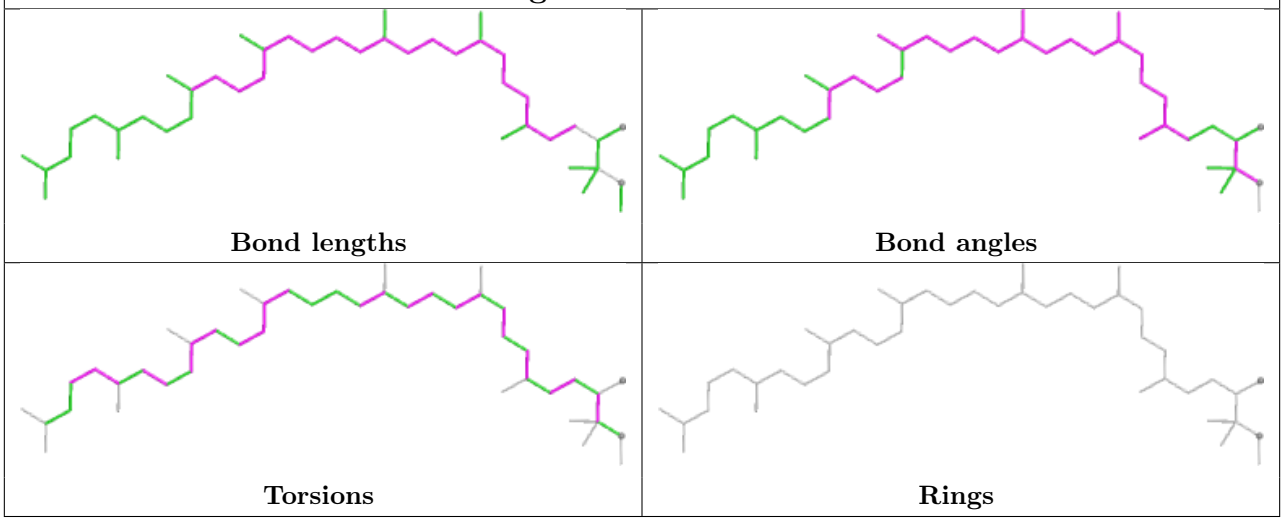
Ligand SPN c 102



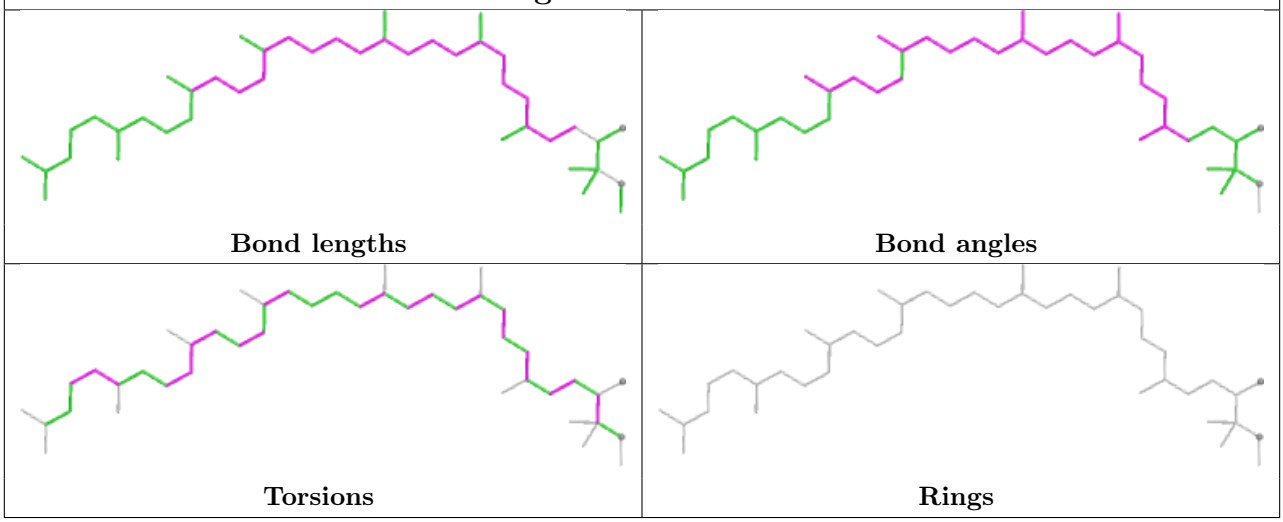
Ligand BCL t 101



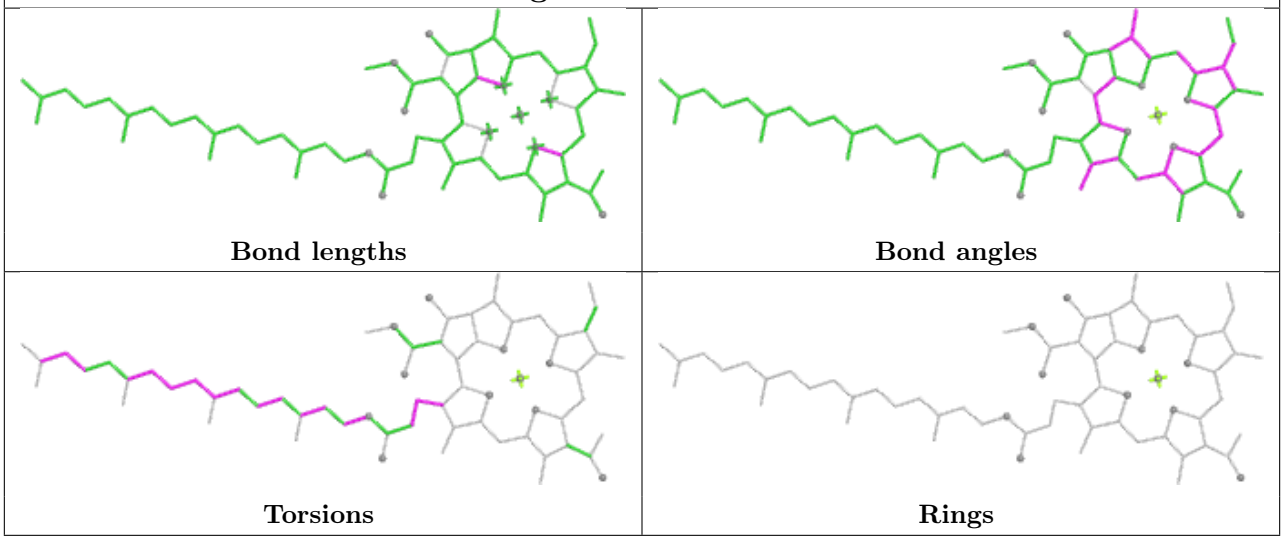
Ligand SPN h 103



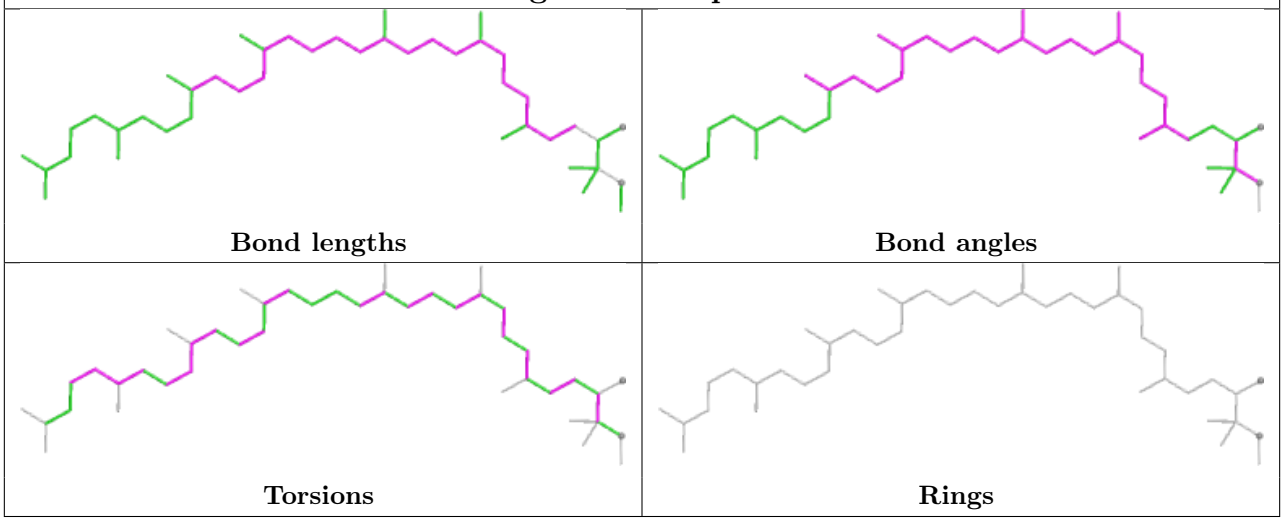
Ligand SPN l 102



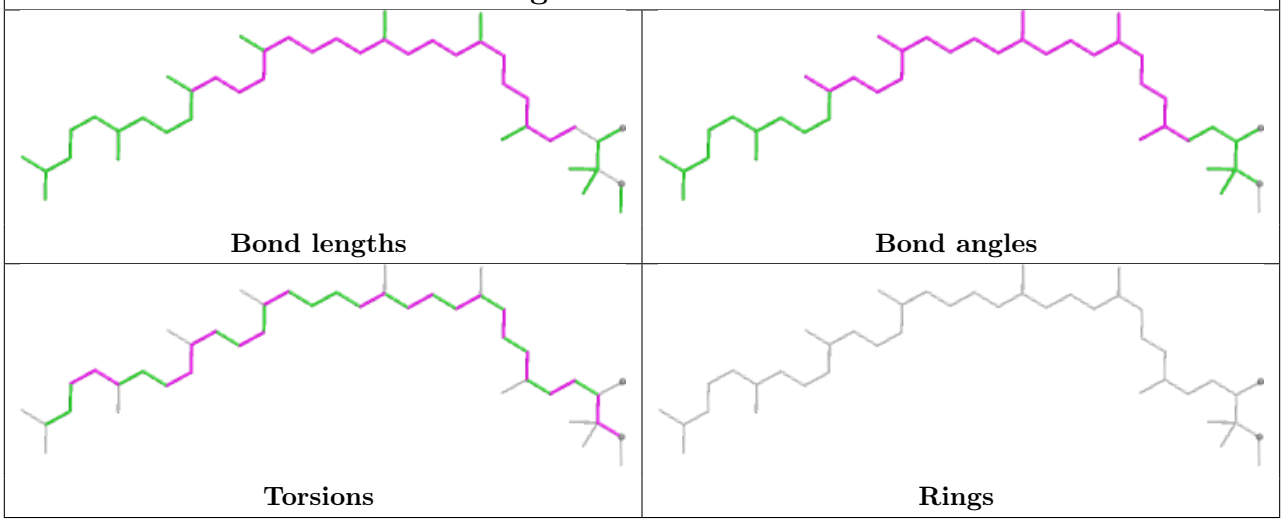
Ligand BCL 3 101



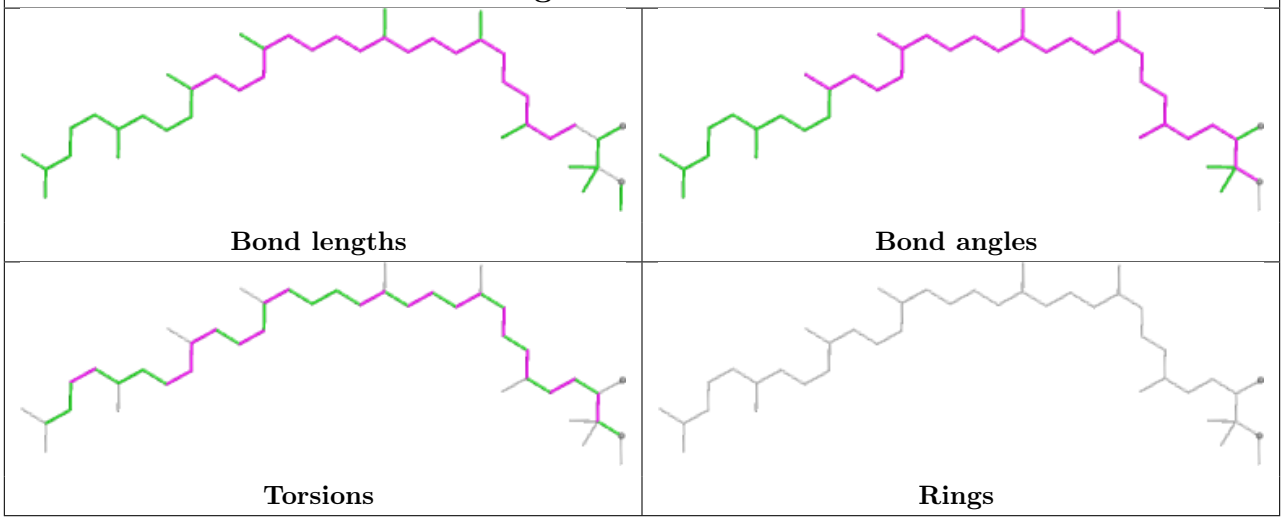
Ligand SPN q 102



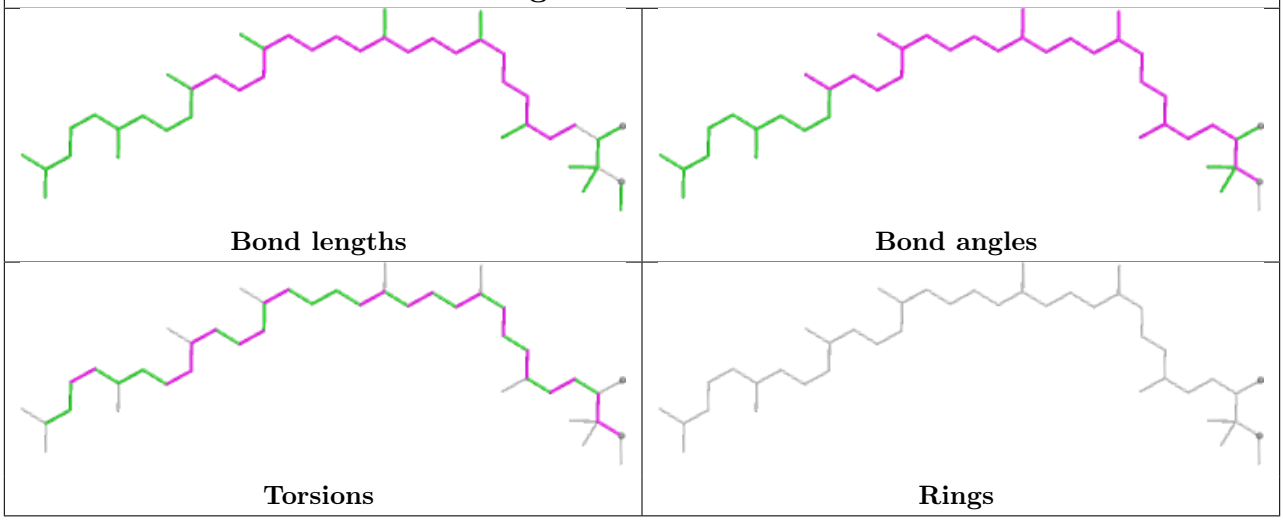
Ligand SPN 1 104



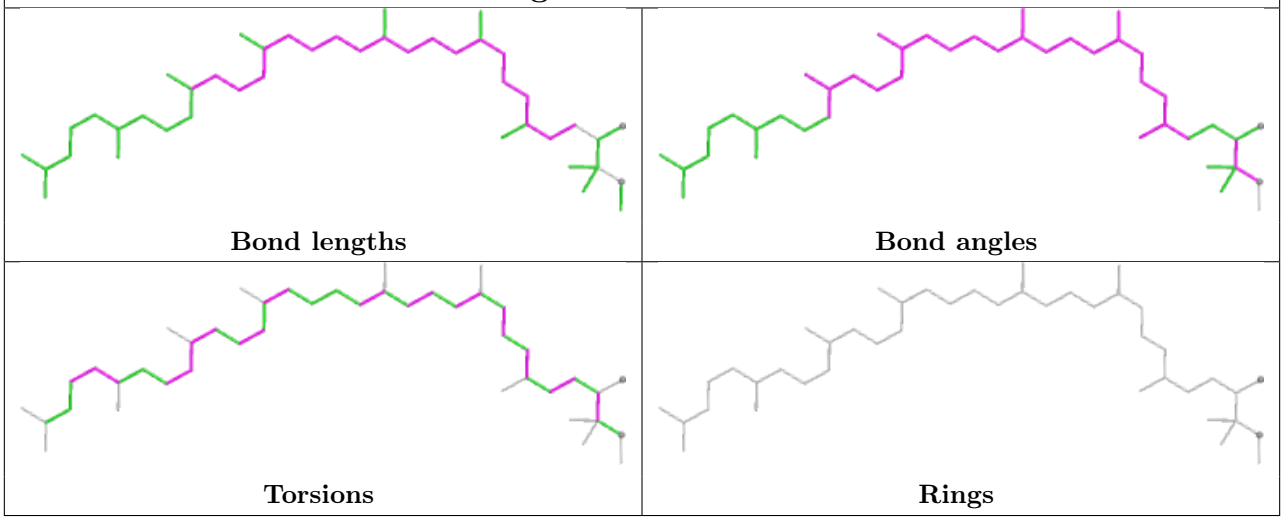
Ligand SPN i 102



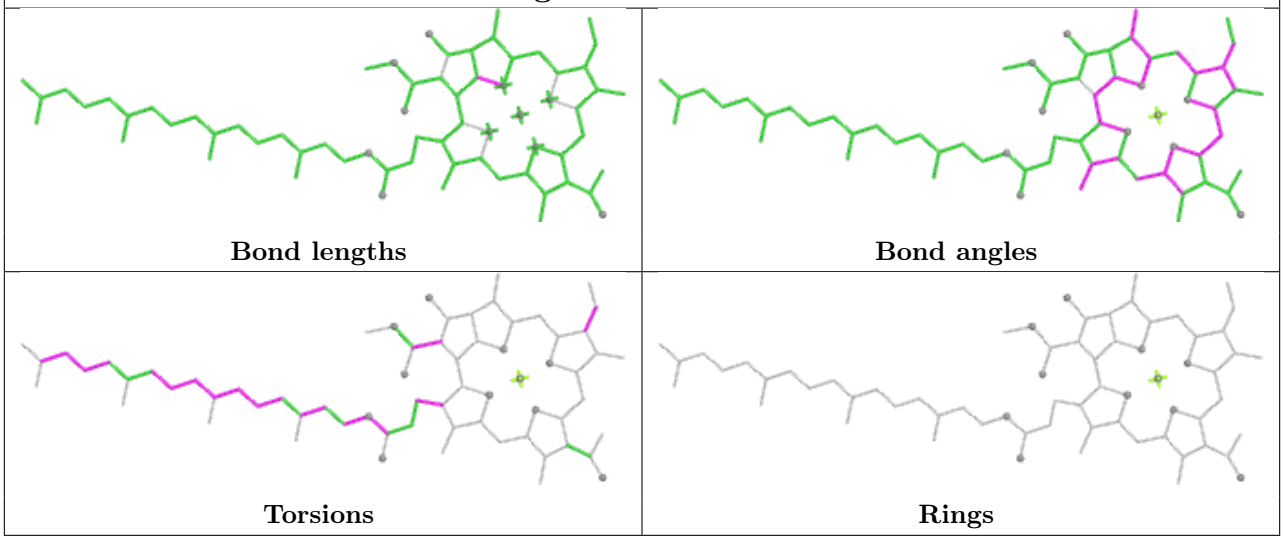
Ligand SPN k 102



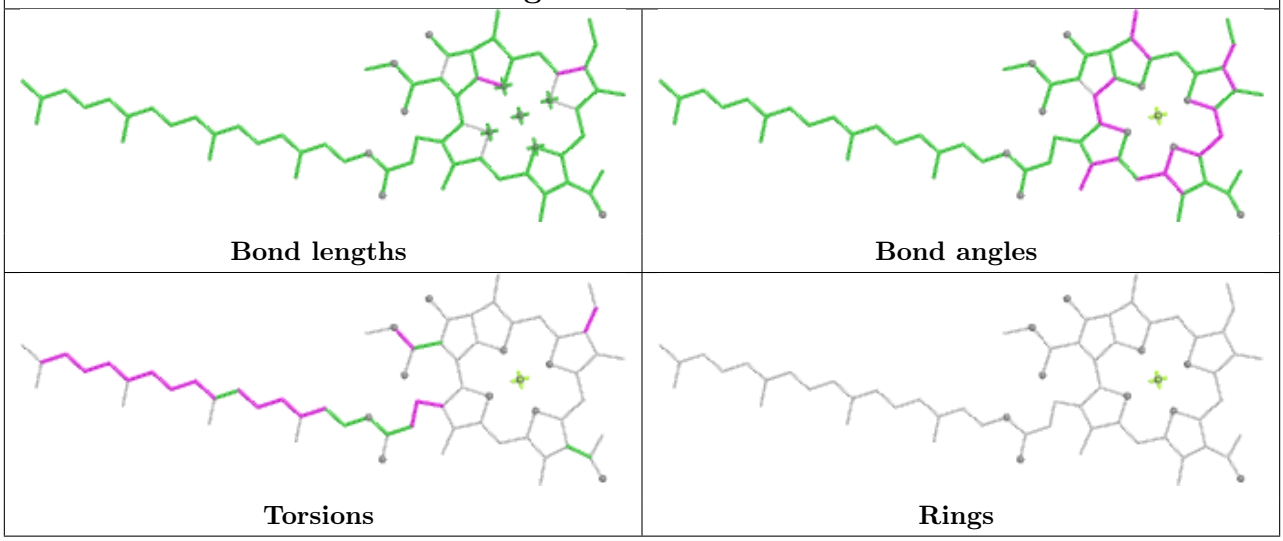
Ligand SPN a 103



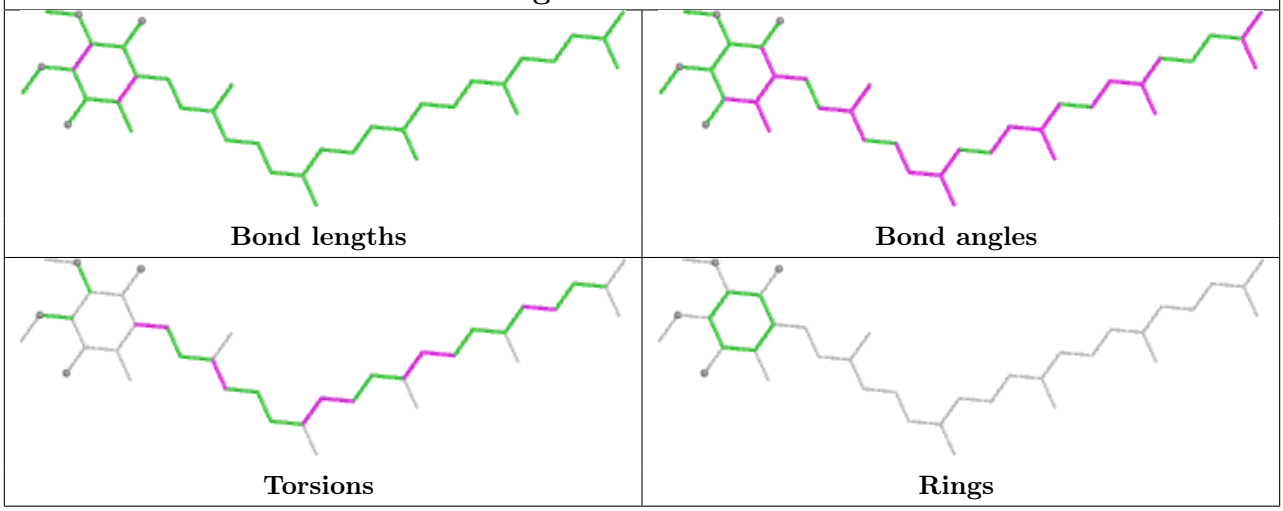
Ligand BCL l 101



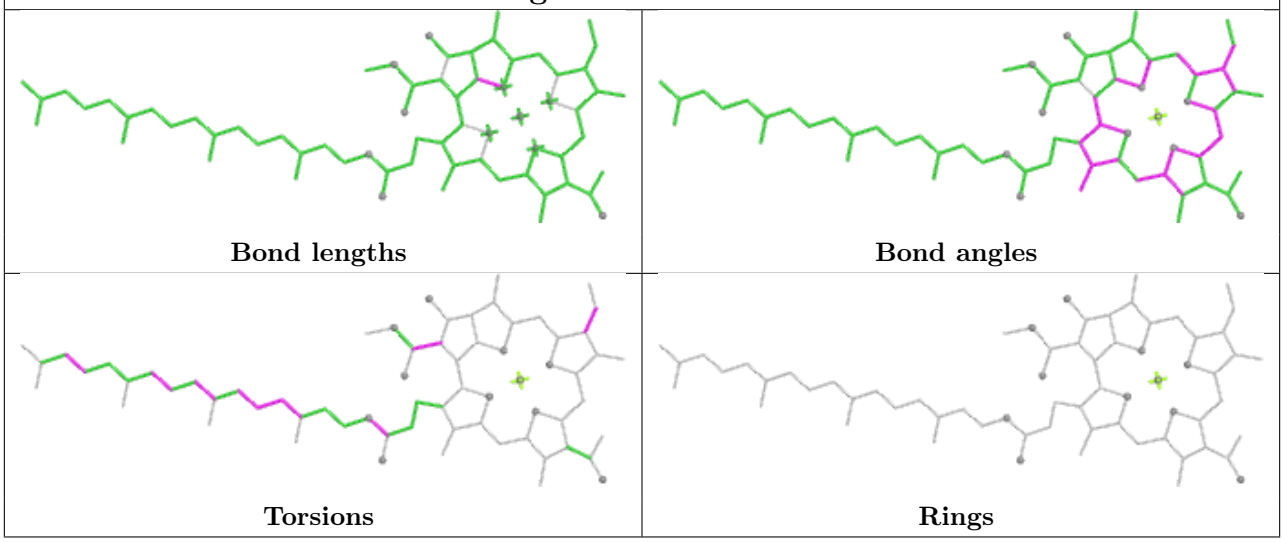
Ligand BCL m 101



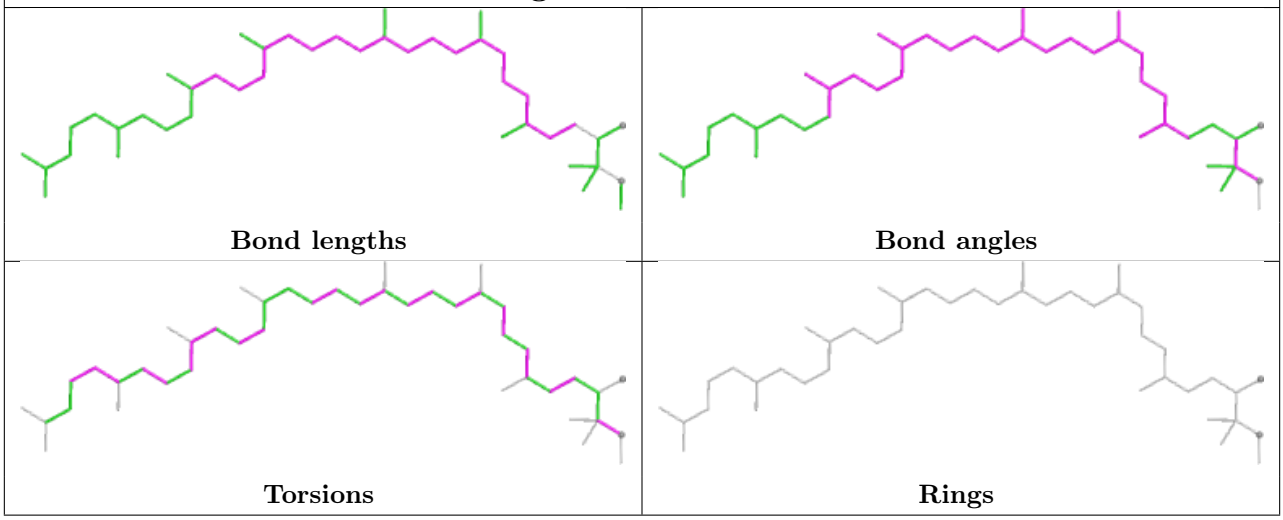
Ligand U10 L 305



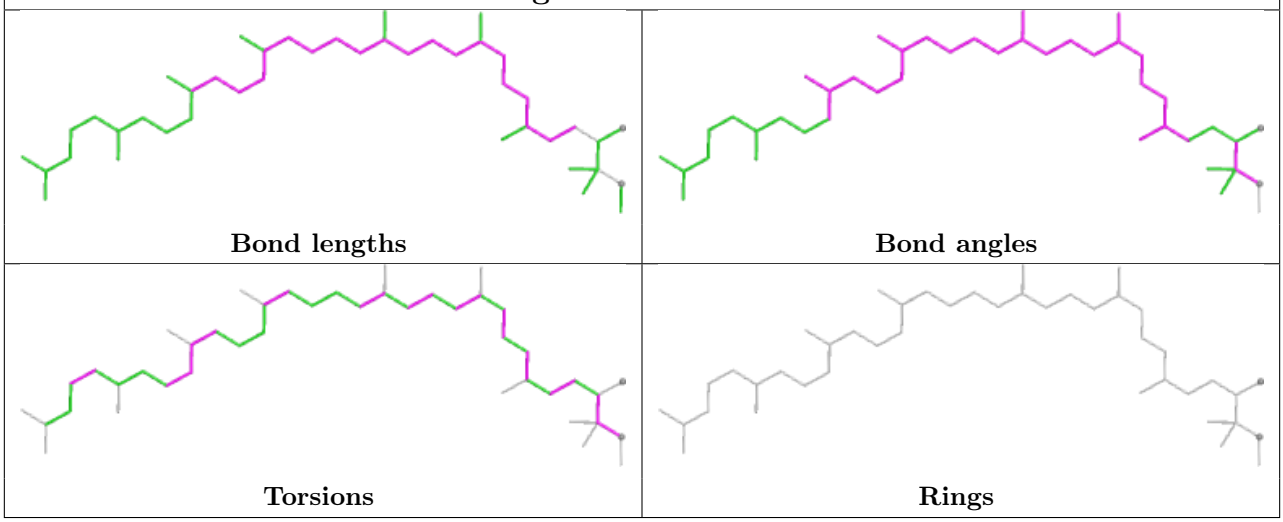
Ligand BCL v 101



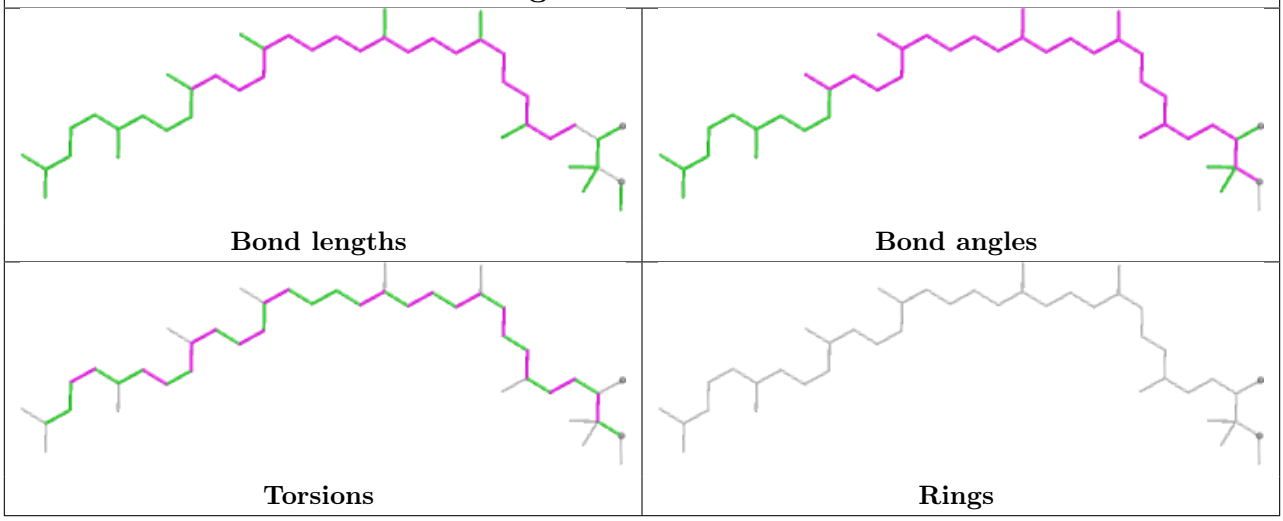
Ligand SPN 1 103



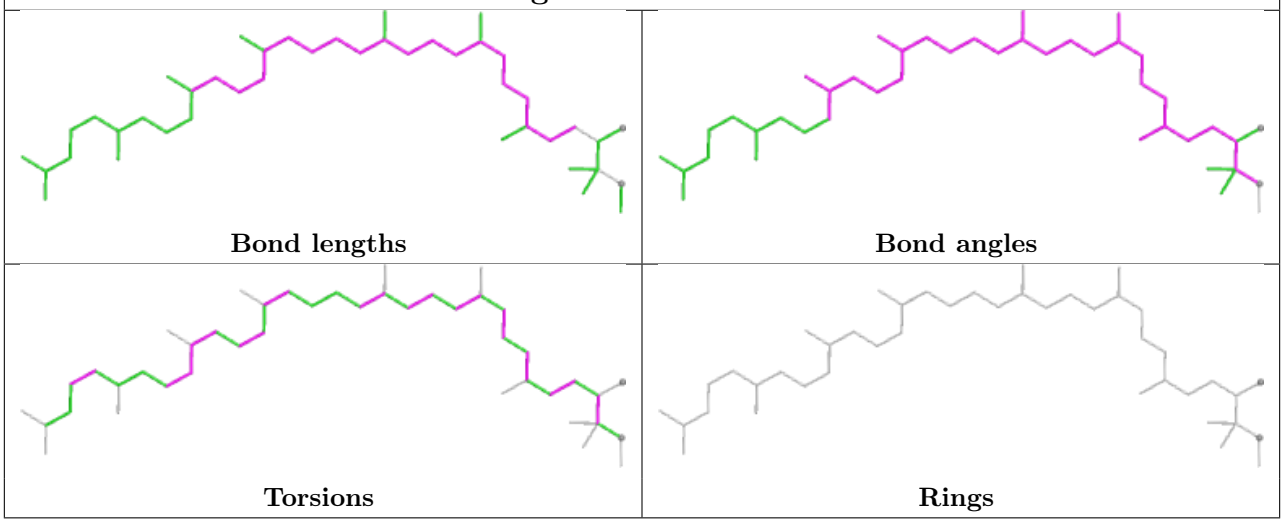
Ligand SPN t 102



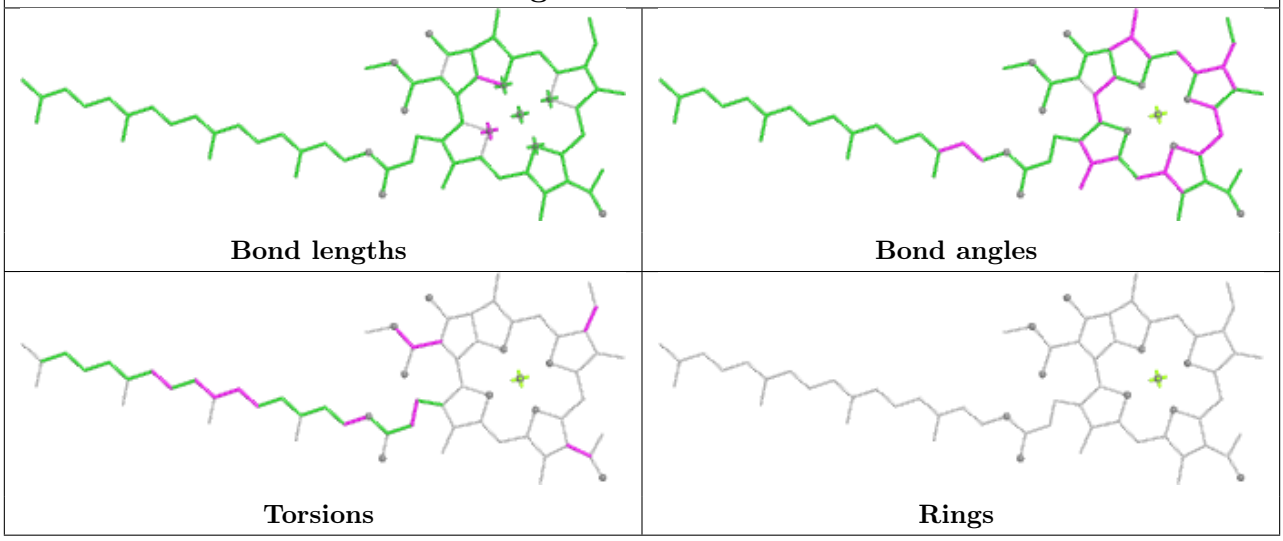
Ligand SPN u 102



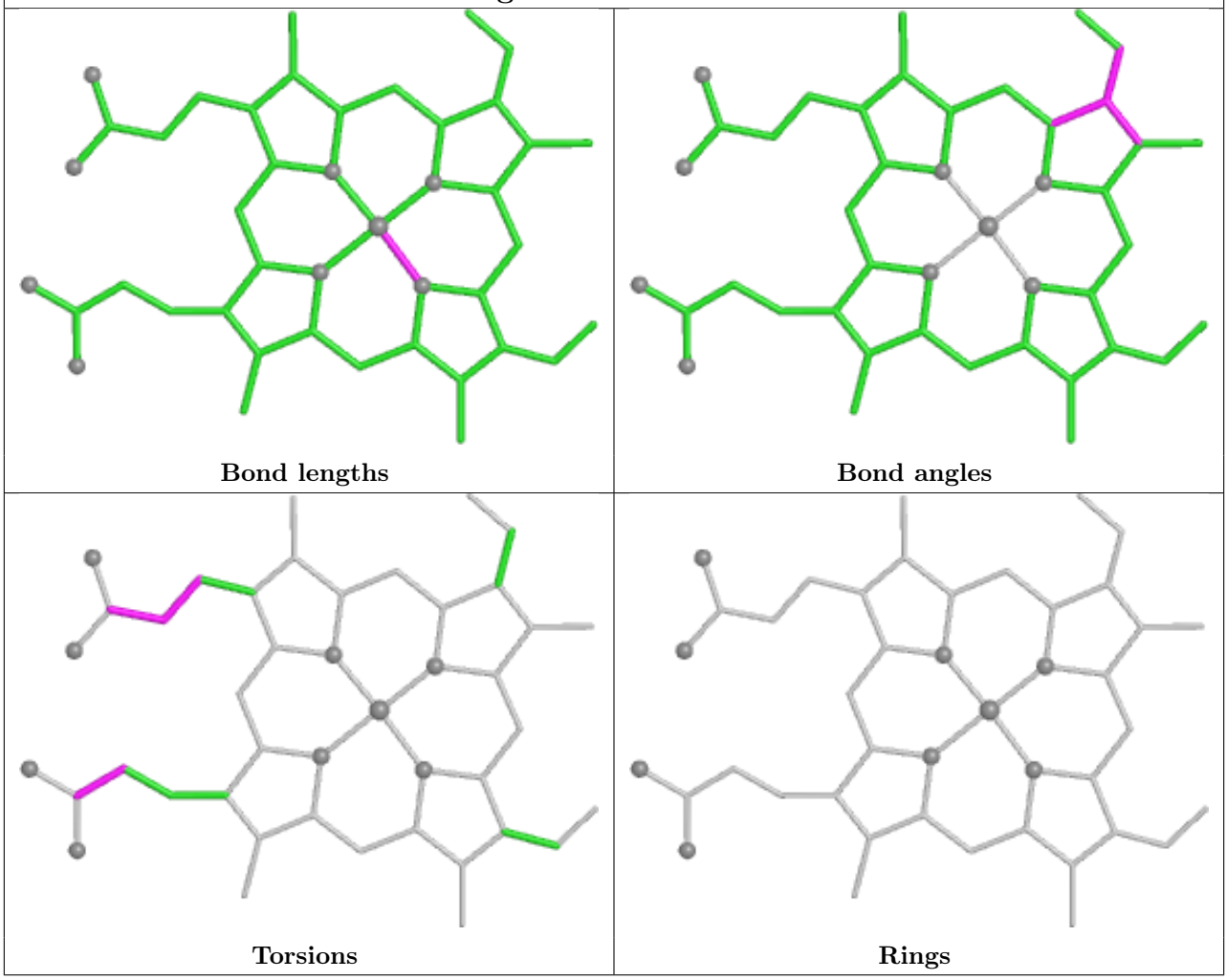
Ligand SPN e 102



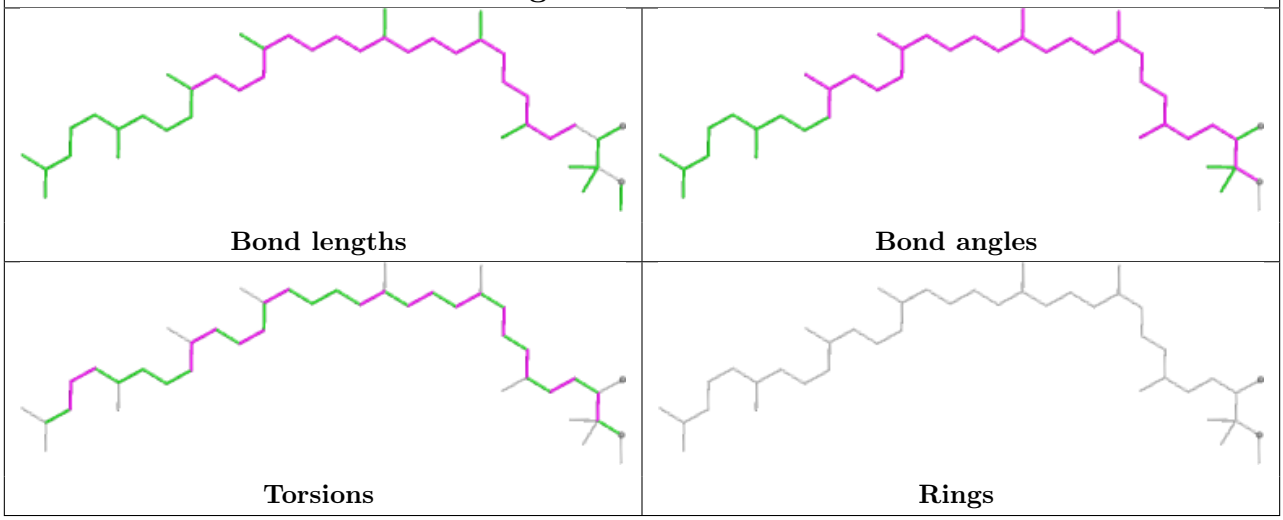
Ligand BCL o 101



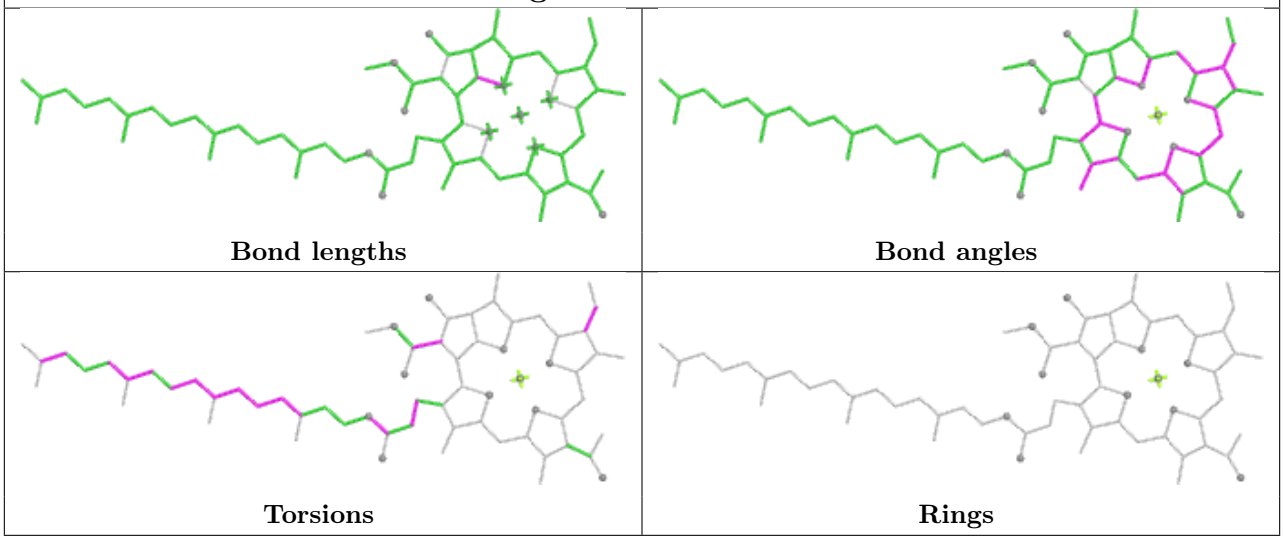
Ligand HEM C 403



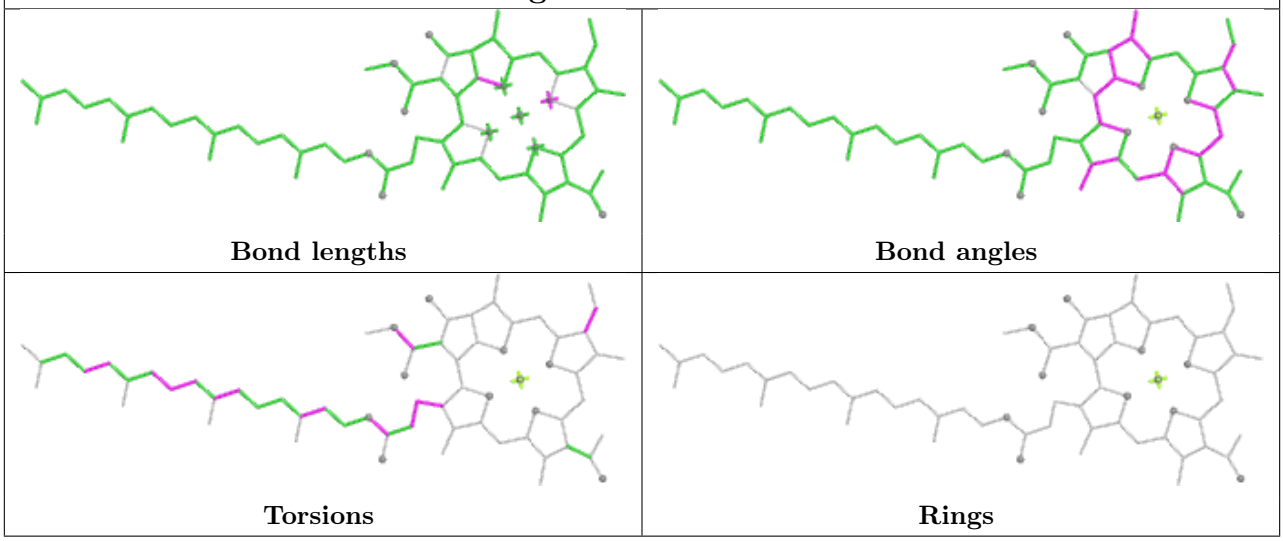
Ligand SPN h 102



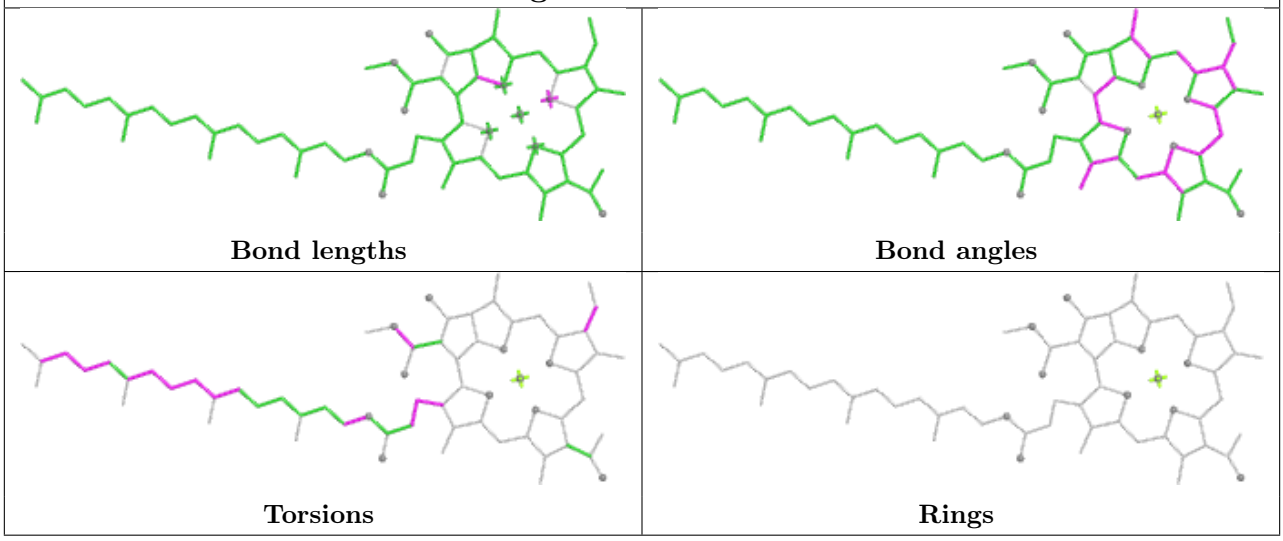
Ligand BCL x 101



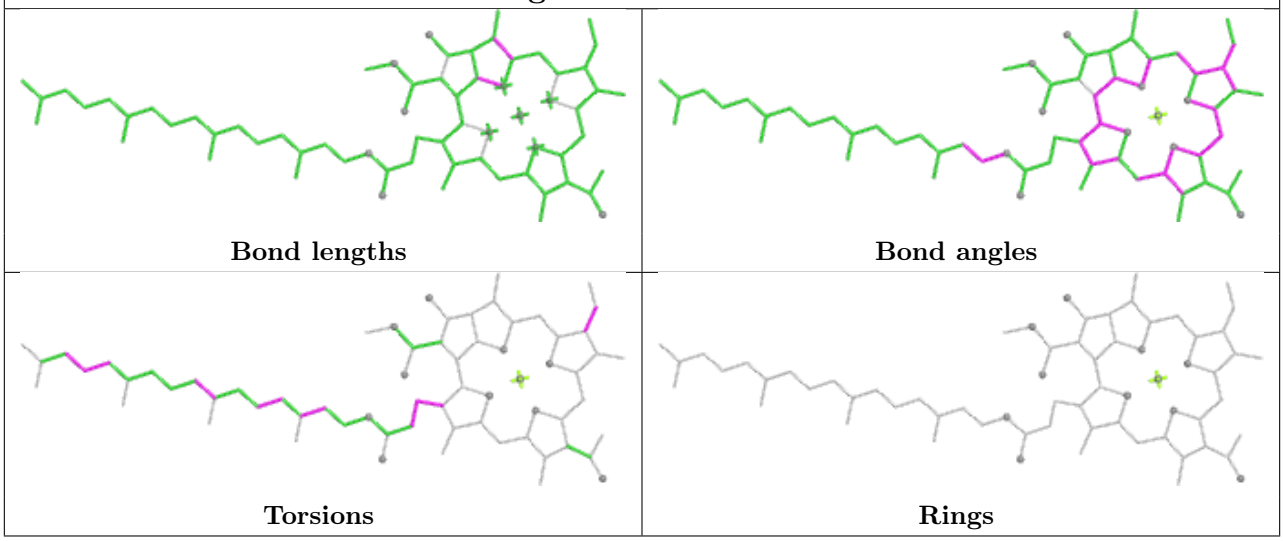
Ligand BCL u 101



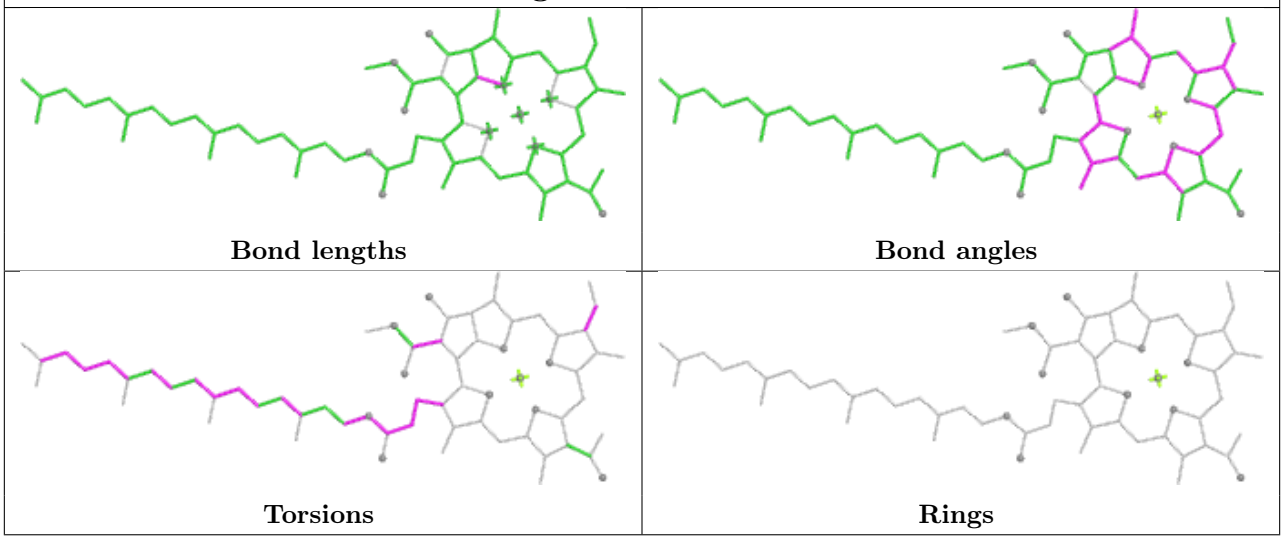
Ligand BCL 9 102



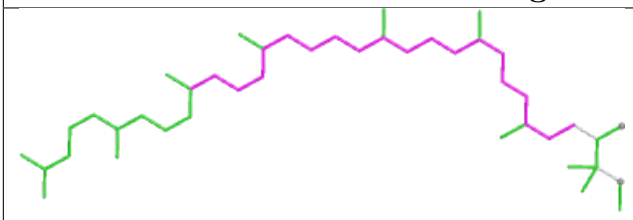
Ligand BCL L 301



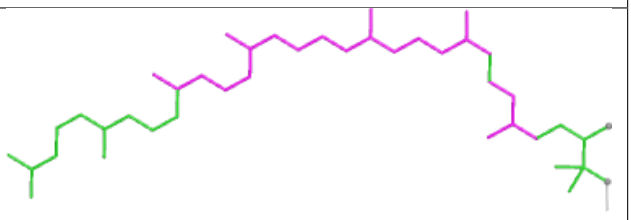
Ligand BCL r 101



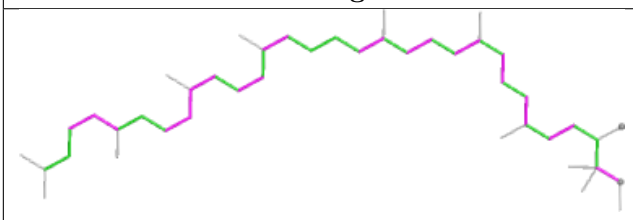
Ligand SPN 5 103



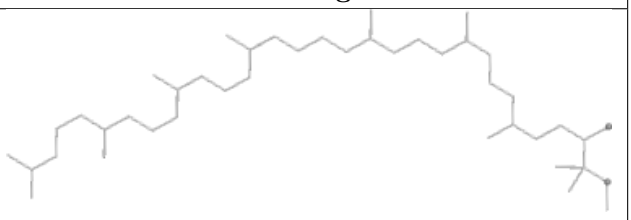
Bond lengths



Bond angles

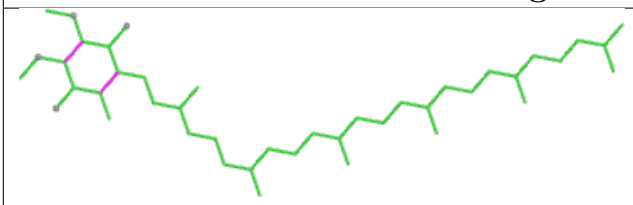


Torsions

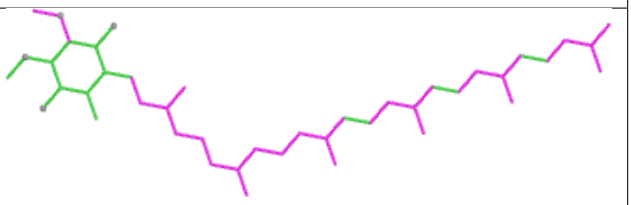


Rings

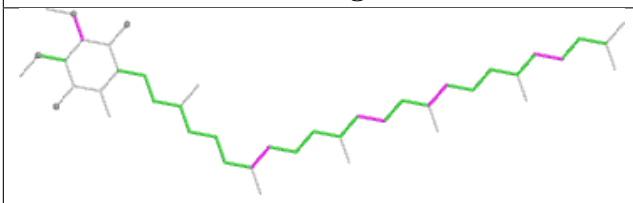
Ligand U10 A 101



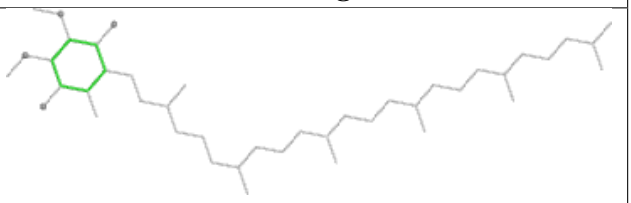
Bond lengths



Bond angles

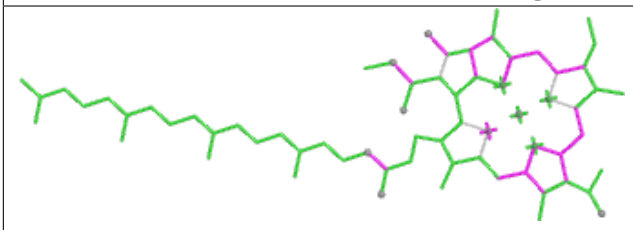


Torsions

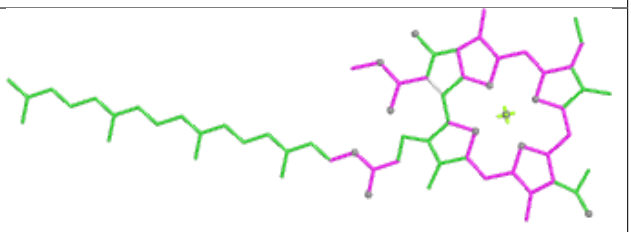


Rings

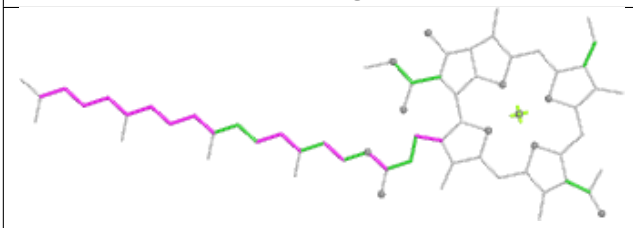
Ligand BCL 2 101



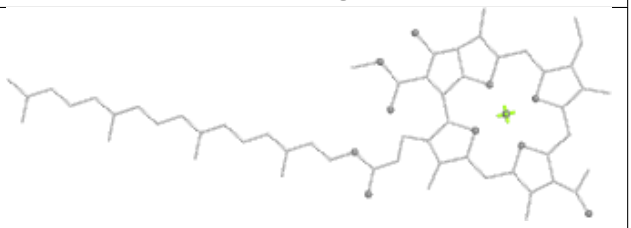
Bond lengths



Bond angles

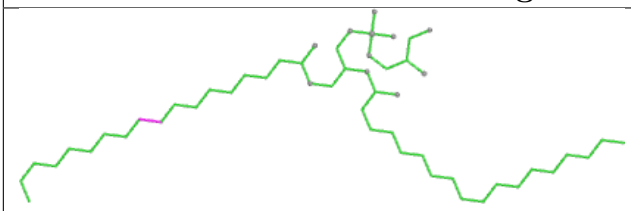


Torsions

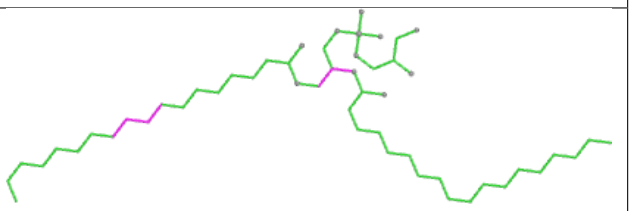


Rings

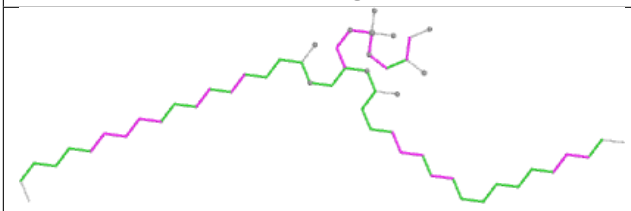
Ligand MW9 H 302



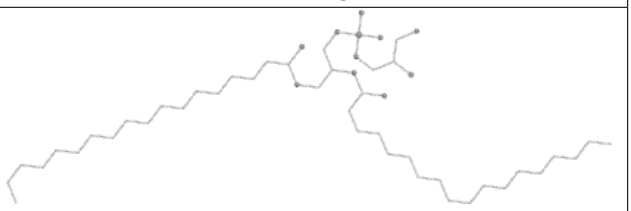
Bond lengths



Bond angles

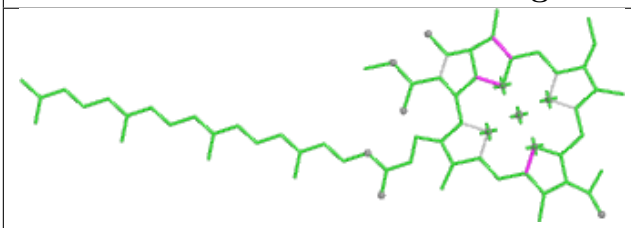


Torsions

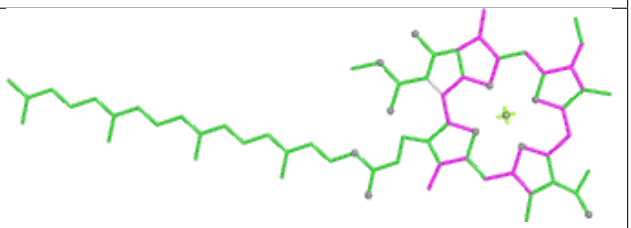


Rings

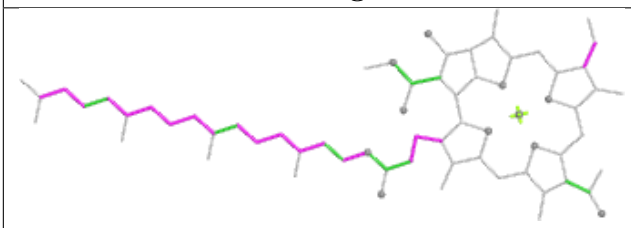
Ligand BCL s 101



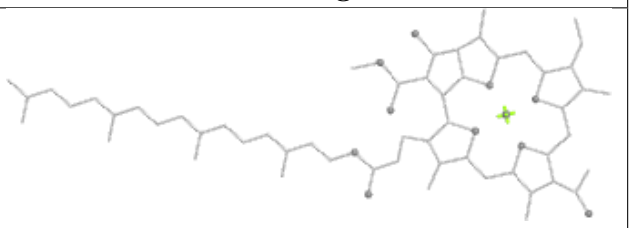
Bond lengths



Bond angles

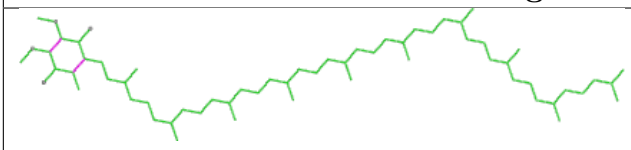


Torsions

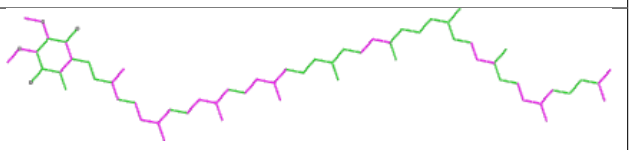


Rings

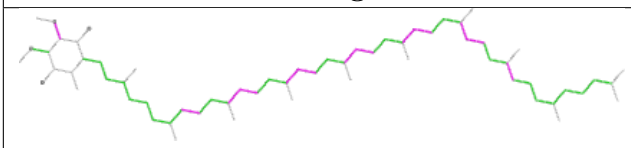
Ligand U10 M 403



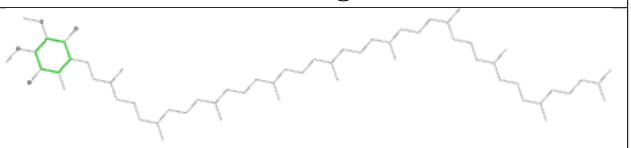
Bond lengths



Bond angles

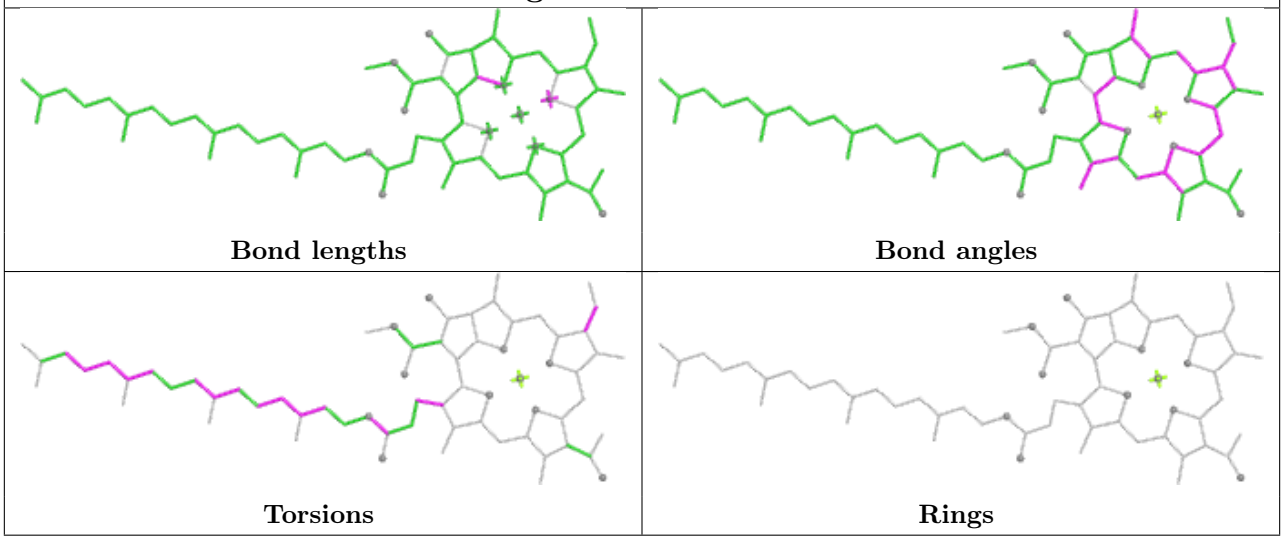


Torsions

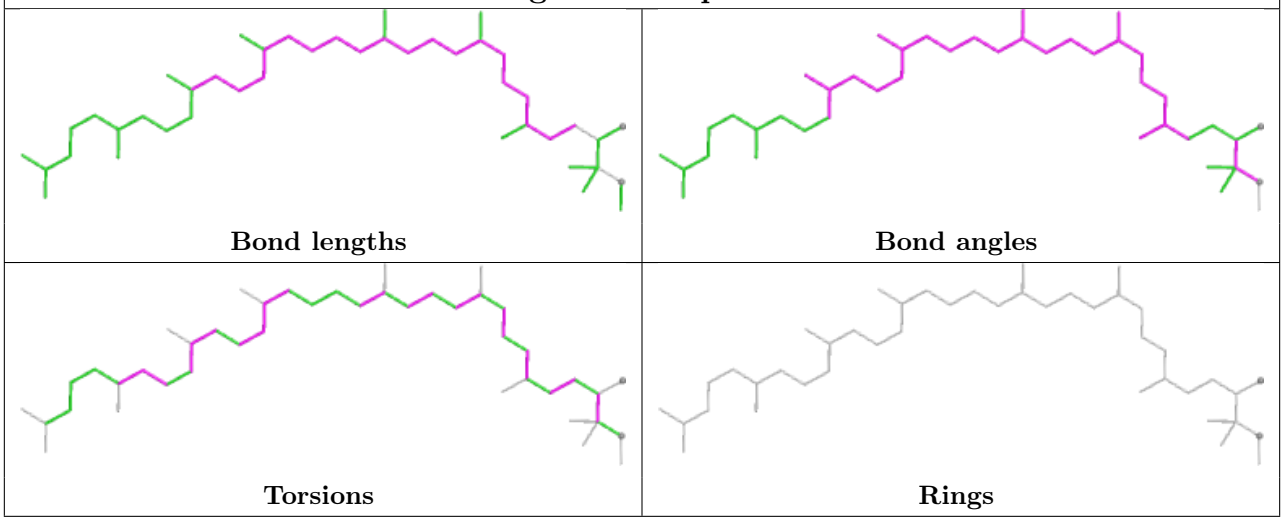


Rings

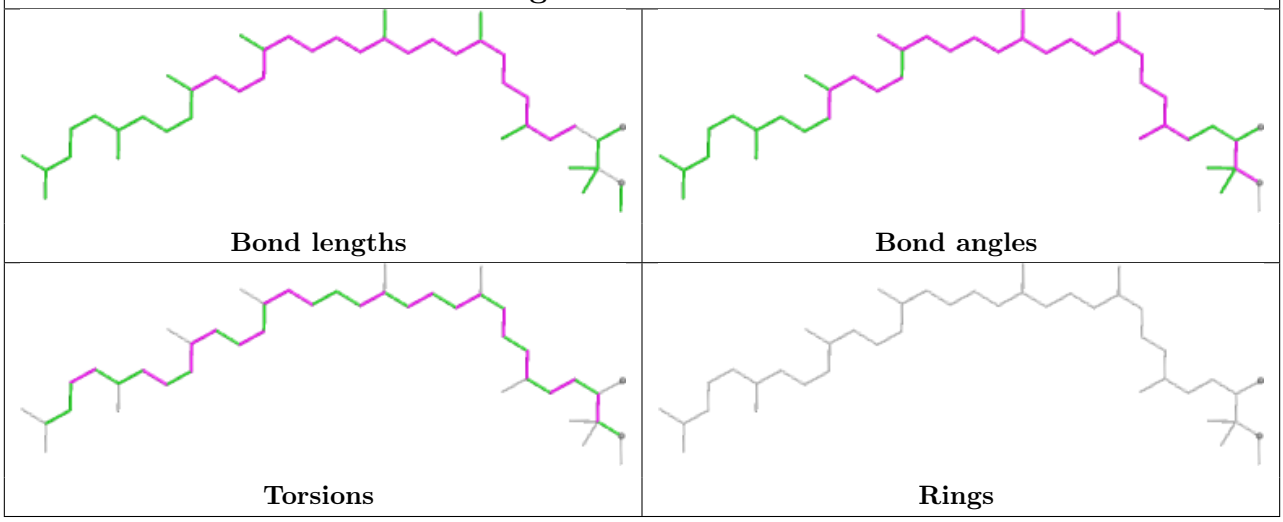
Ligand BCL w 101



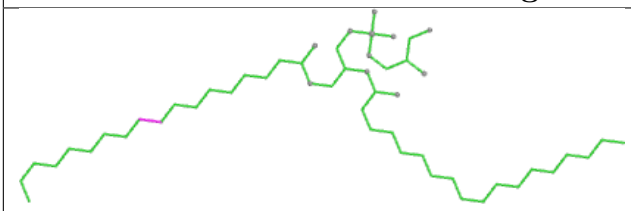
Ligand SPN p 103



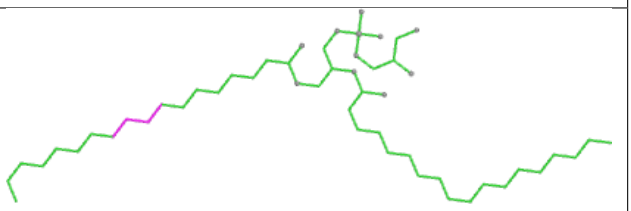
Ligand SPN v 102



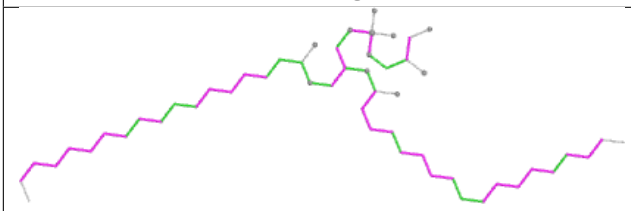
Ligand MW9 9 101



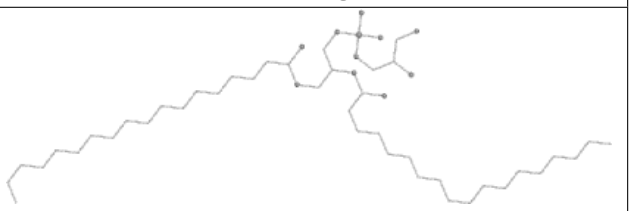
Bond lengths



Bond angles

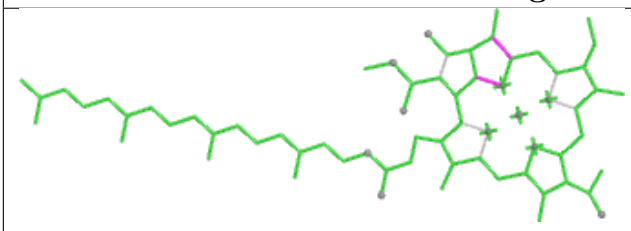


Torsions

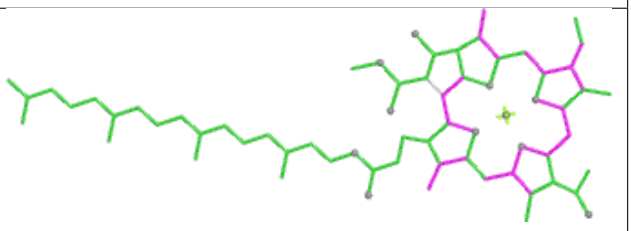


Rings

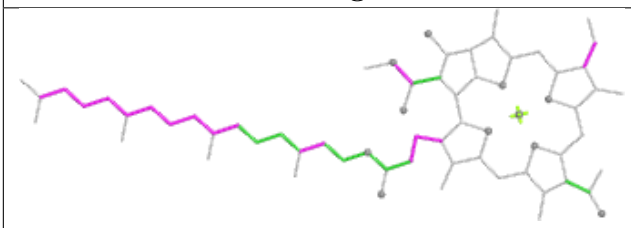
Ligand BCL 5 101



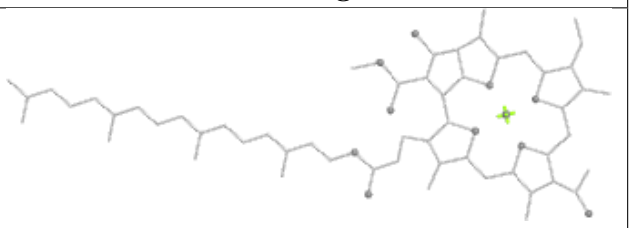
Bond lengths



Bond angles

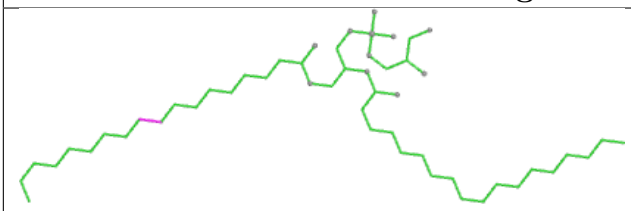


Torsions

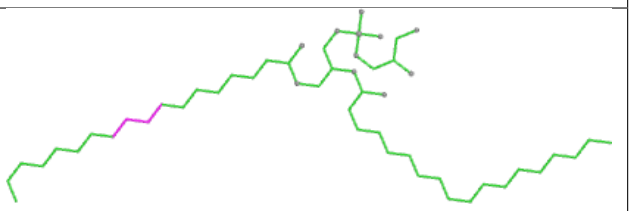


Rings

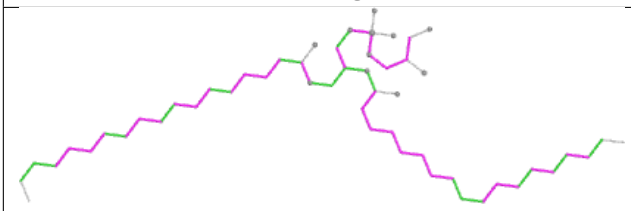
Ligand MW9 H 304



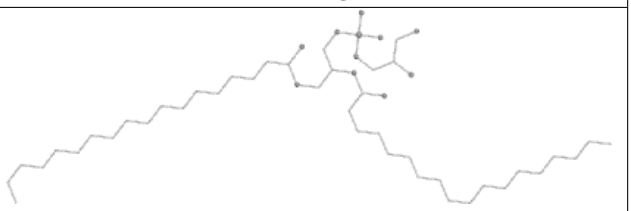
Bond lengths



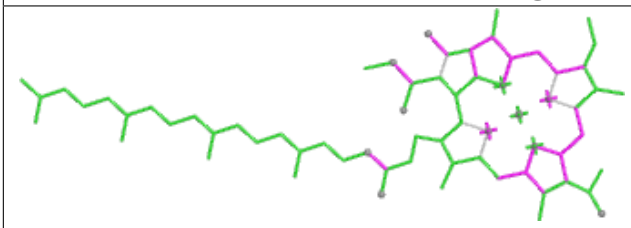
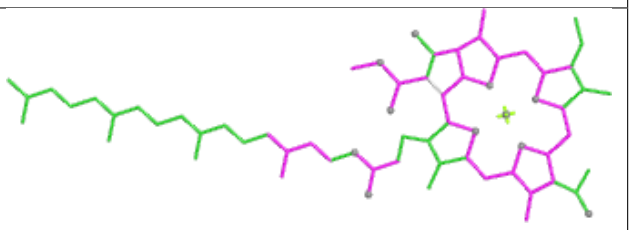
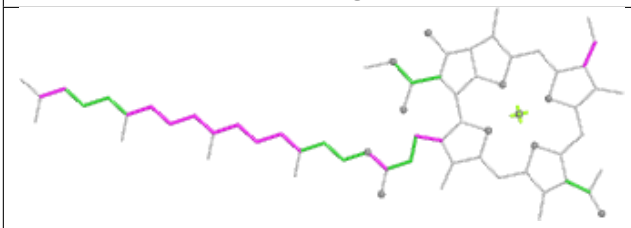
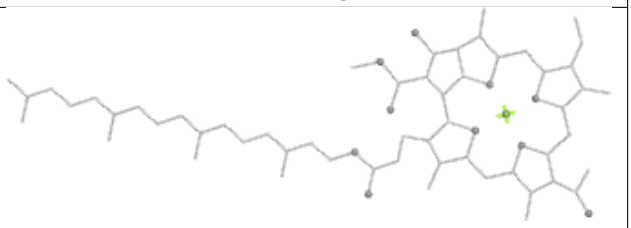
Bond angles



Torsions



Rings

Ligand BCL 4 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

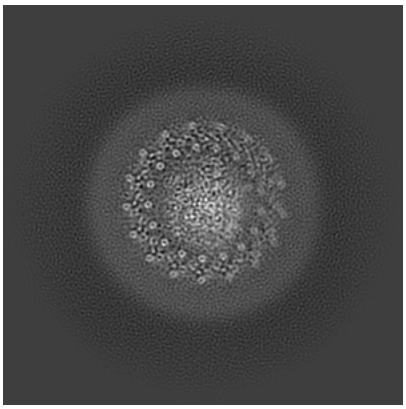
6 Map visualisation (i)

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

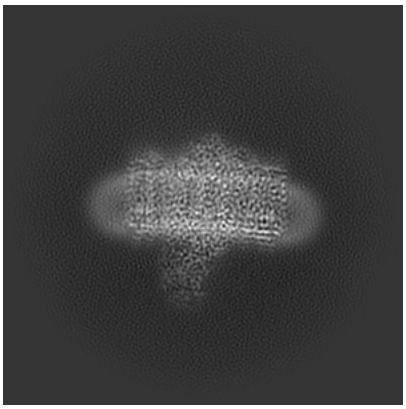
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

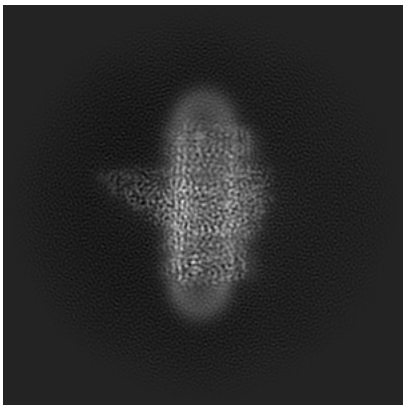
6.1.1 Primary map



X

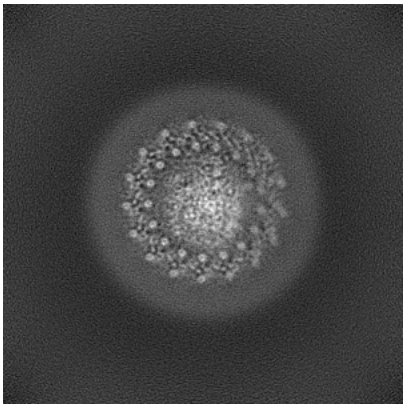


Y

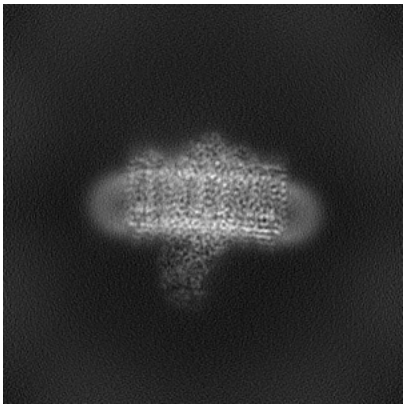


Z

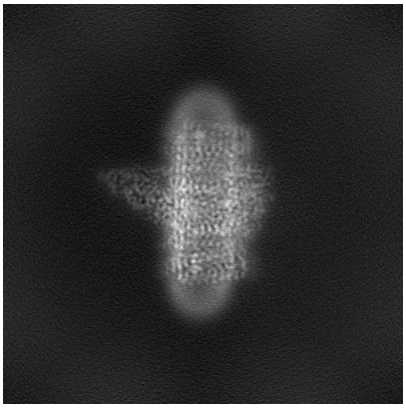
6.1.2 Raw map



X



Y

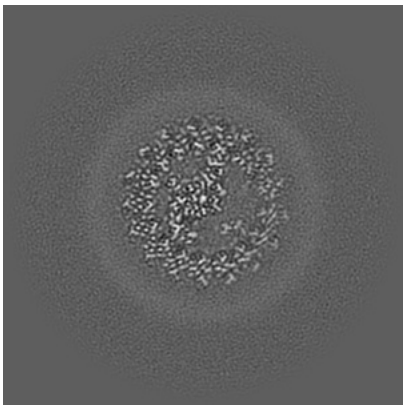


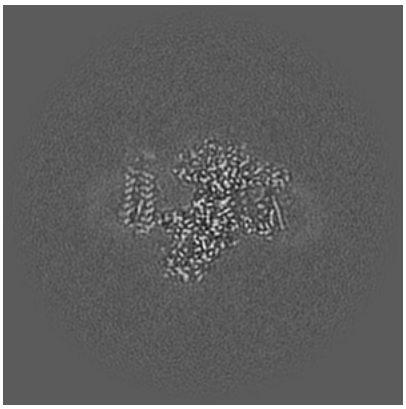
Z

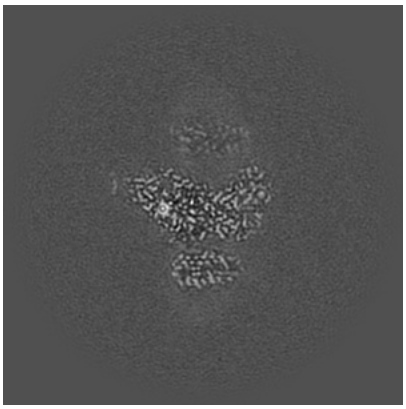
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

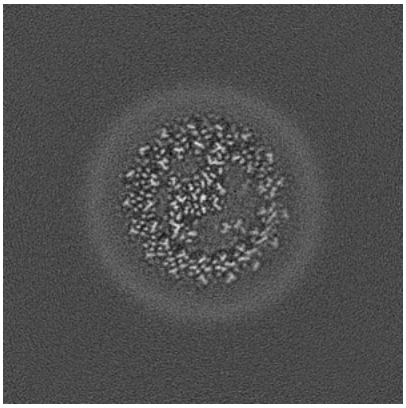
6.2.1 Primary map

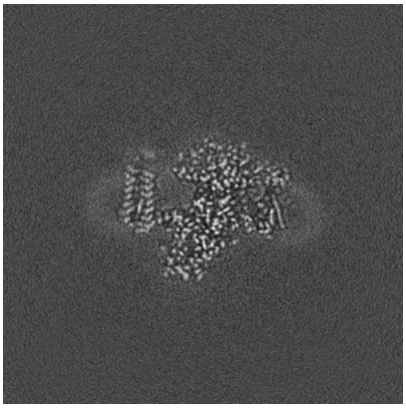

X Index: 150

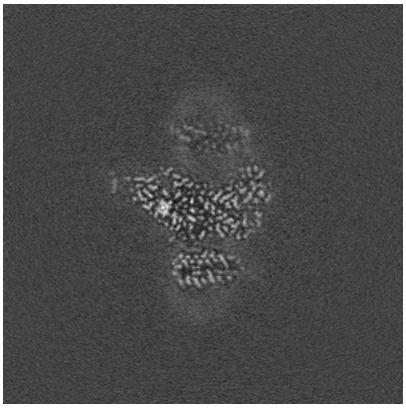

Y Index: 150


Z Index: 150

6.2.2 Raw map


X Index: 150

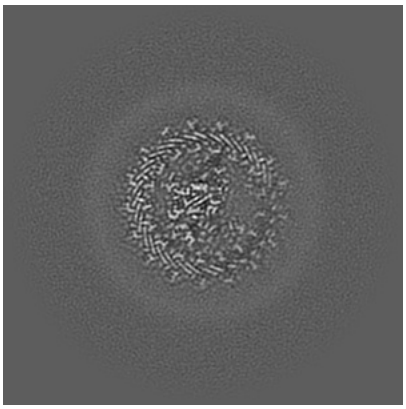

Y Index: 150

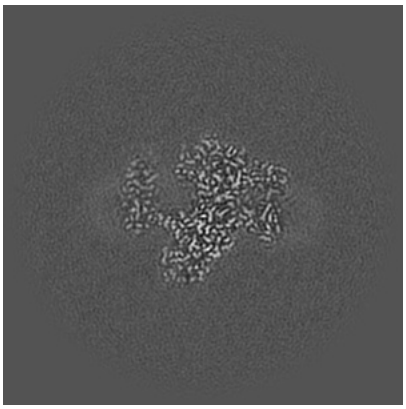

Z Index: 150

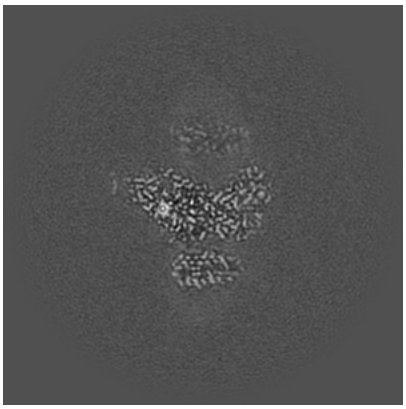
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

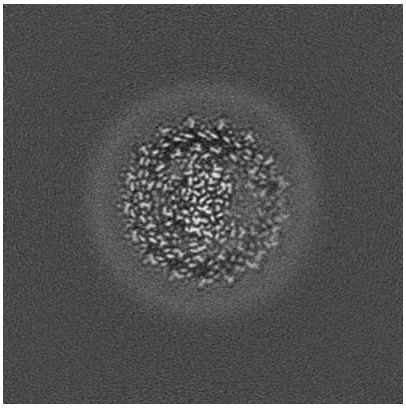
6.3.1 Primary map

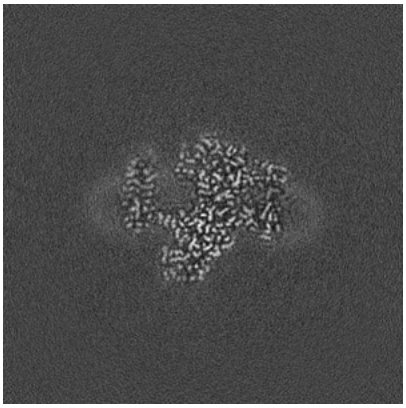

X Index: 143

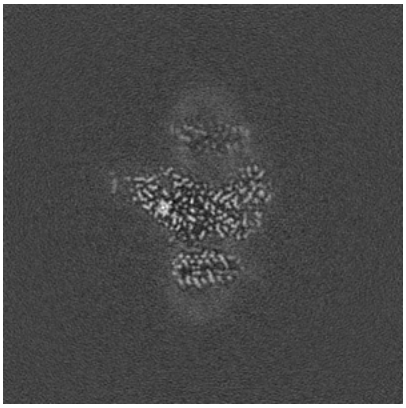

Y Index: 152


Z Index: 150

6.3.2 Raw map


X Index: 137

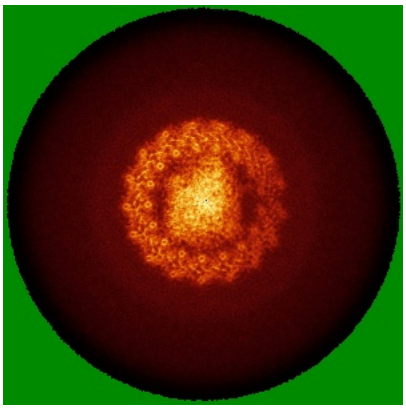

Y Index: 152

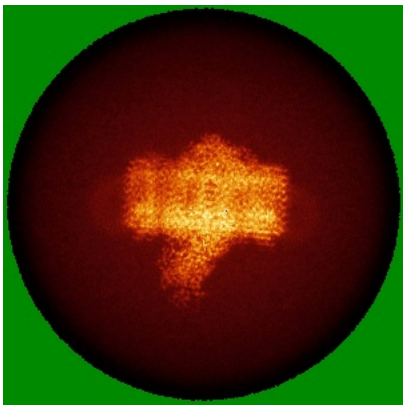

Z Index: 150

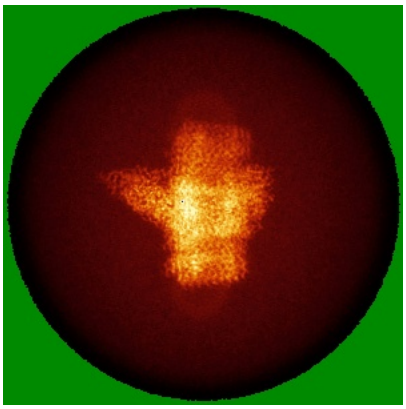
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

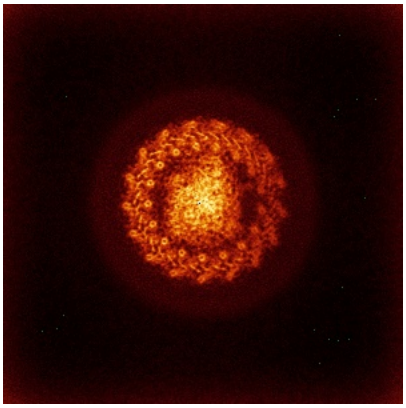
6.4.1 Primary map

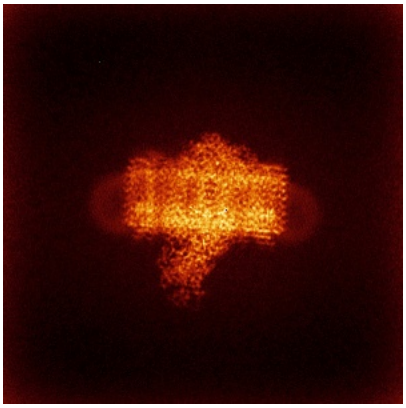

X

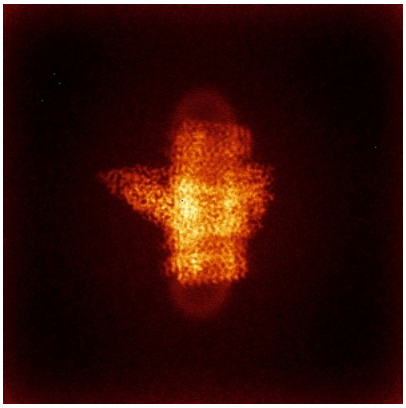

Y


Z

6.4.2 Raw map


X


Y


Z

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

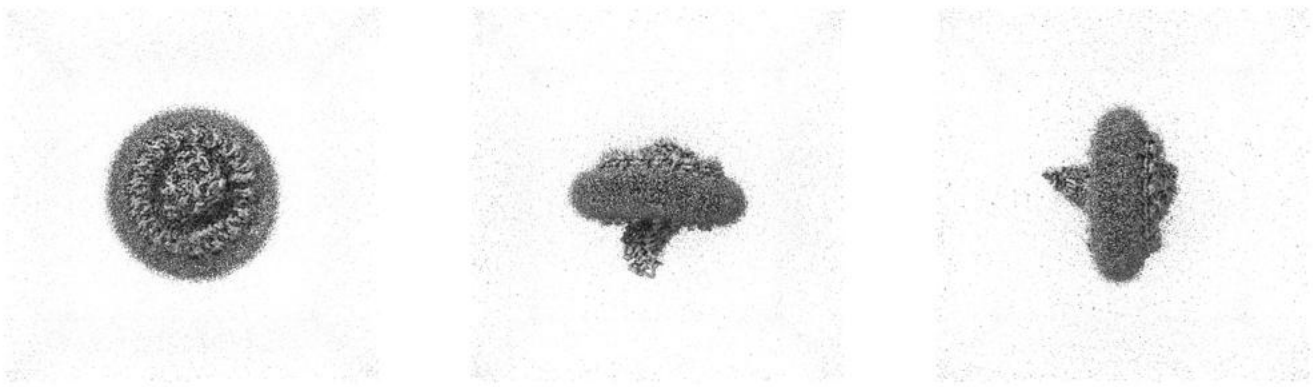
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

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

6.5.2 Raw map



X Y Z

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

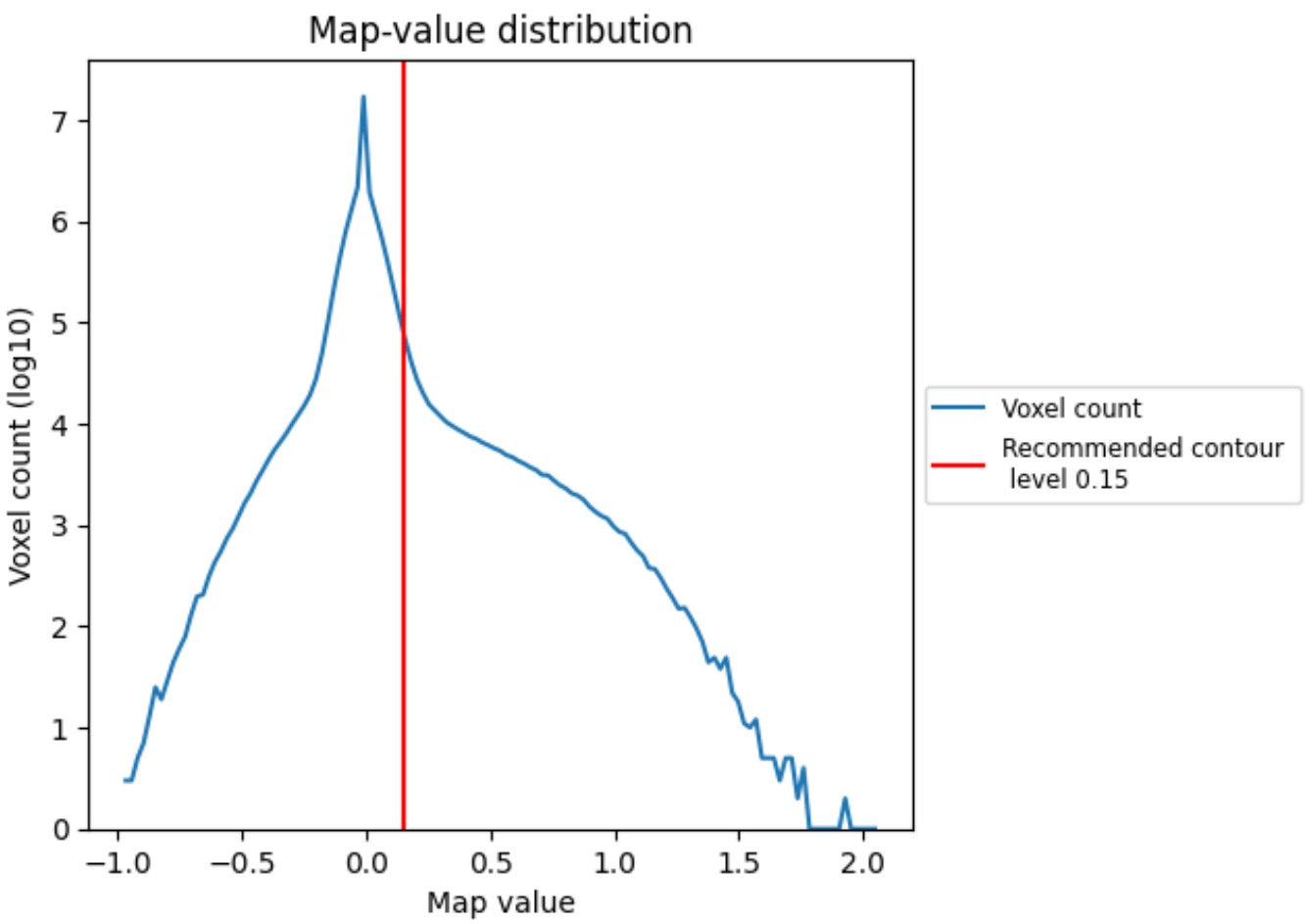
6.6 Mask visualisation (i)

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

7 Map analysis (i)

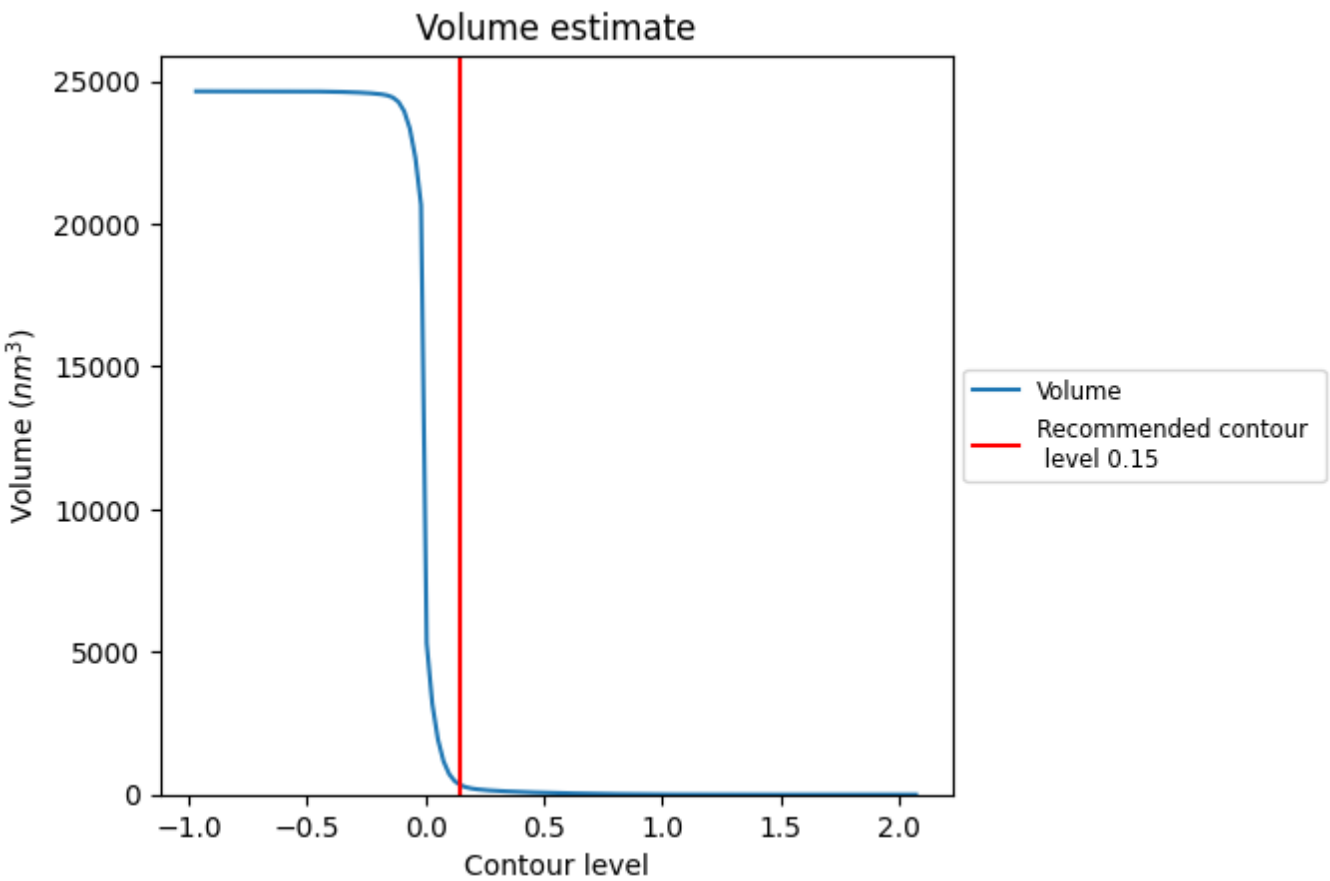
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

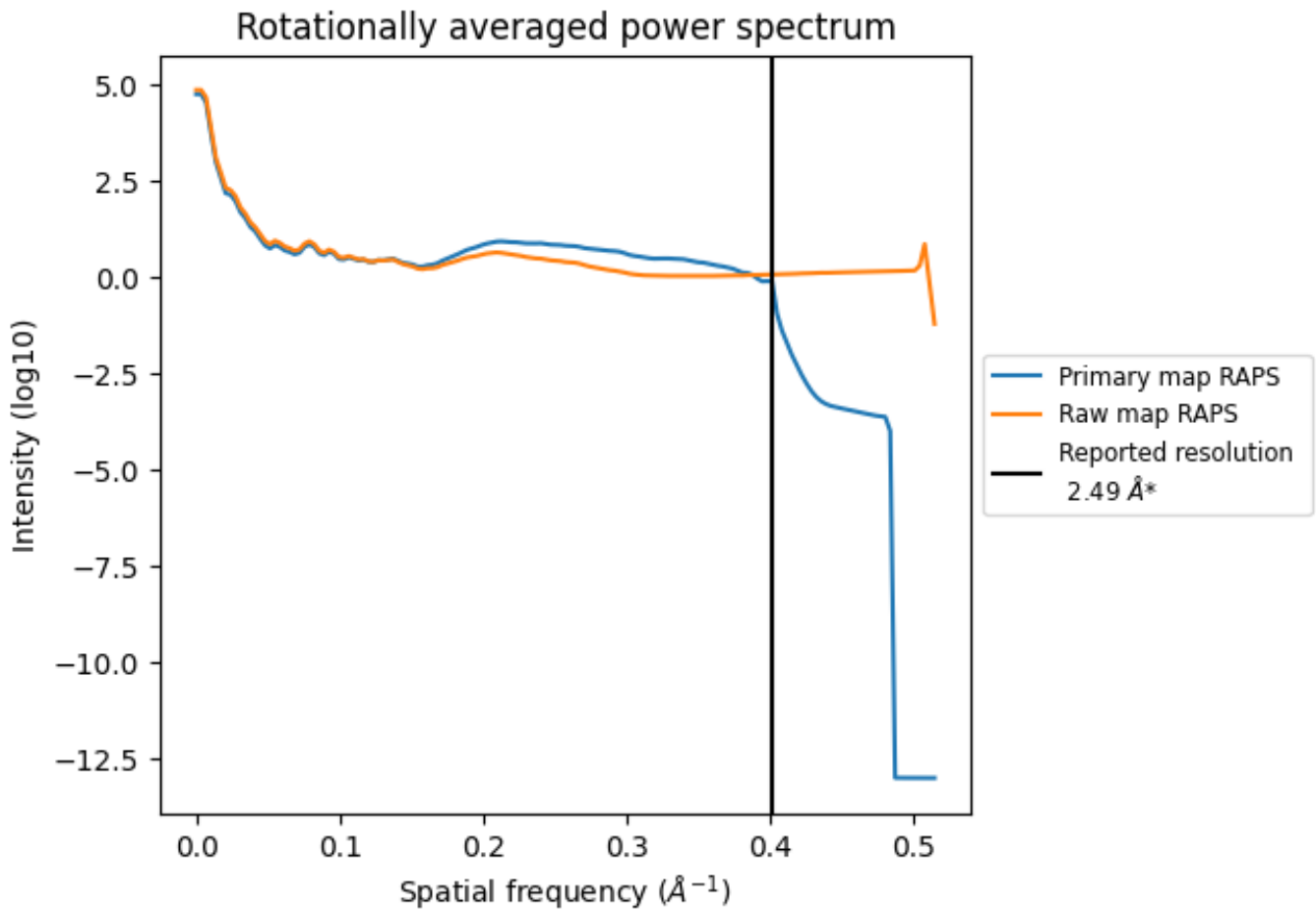
7.2 Volume estimate (i)



The volume at the recommended contour level is 326 nm^3; this corresponds to an approximate mass of 295 kDa.

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

7.3 Rotationally averaged power spectrum (i)

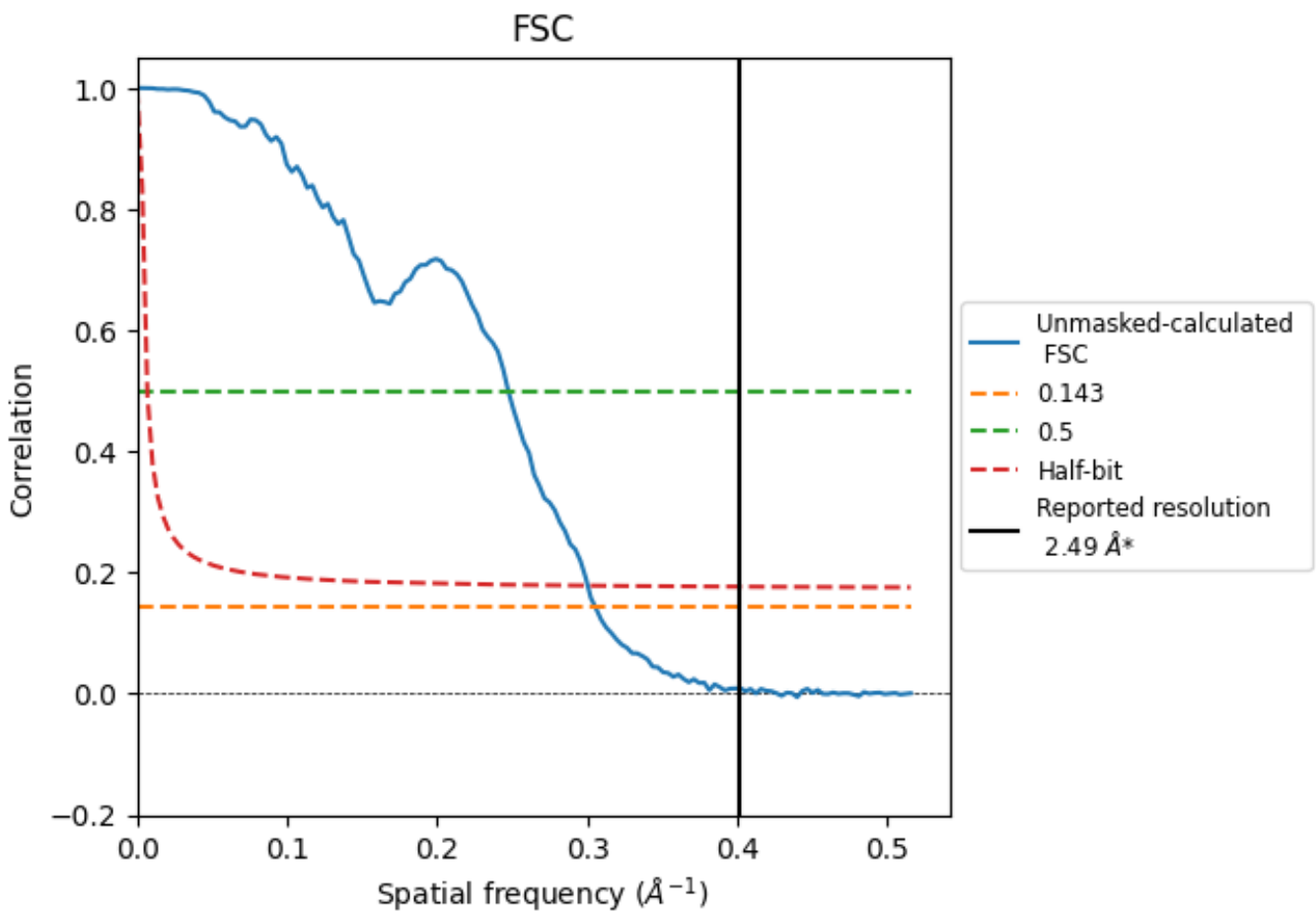


*Reported resolution corresponds to spatial frequency of 0.402 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.402 Å^{-1}

8.2 Resolution estimates (i)

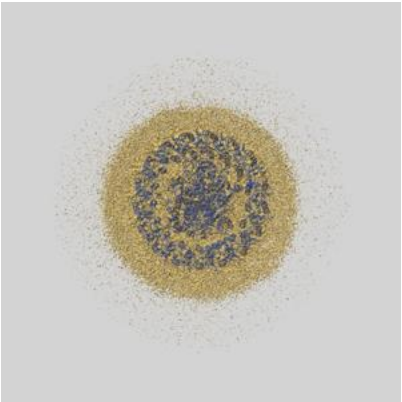
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.27	4.04	3.33

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

9 Map-model fit (i)

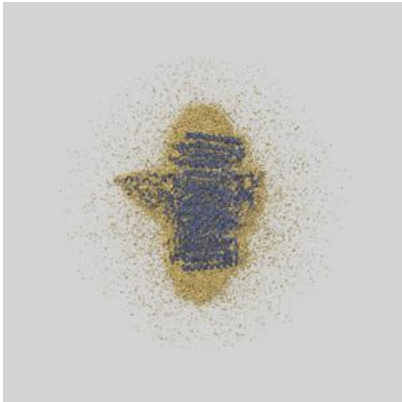
This section contains information regarding the fit between EMDB map EMD-63379 and PDB model 9LTS. Per-residue inclusion information can be found in section 3 on page 17.

9.1 Map-model overlay (i)



X

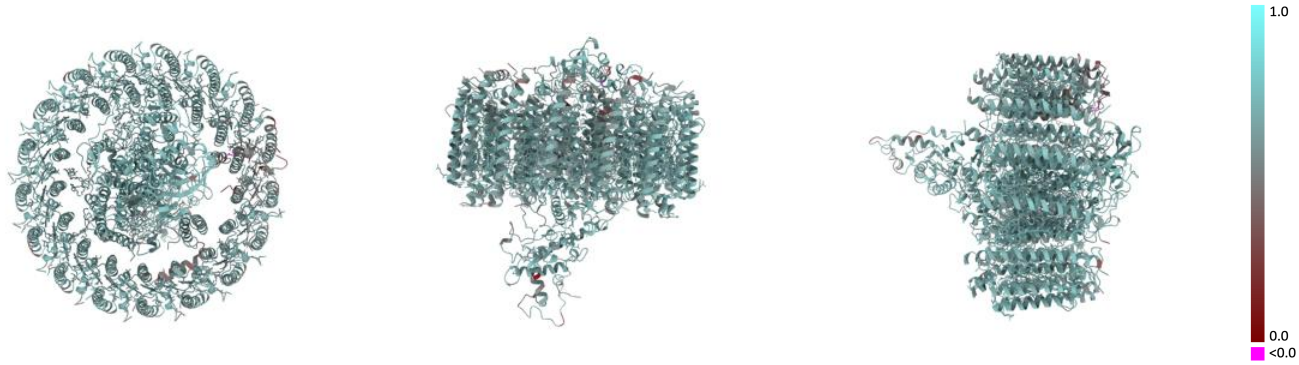
Y



Z

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

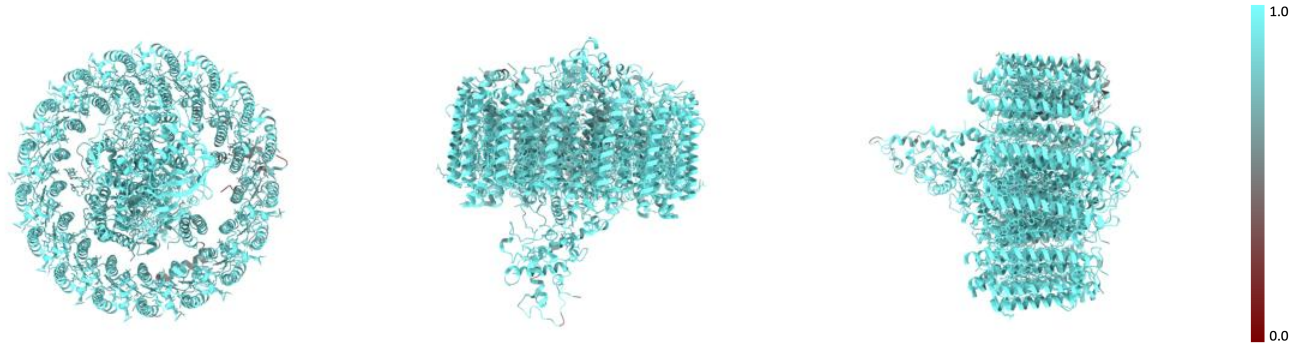
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

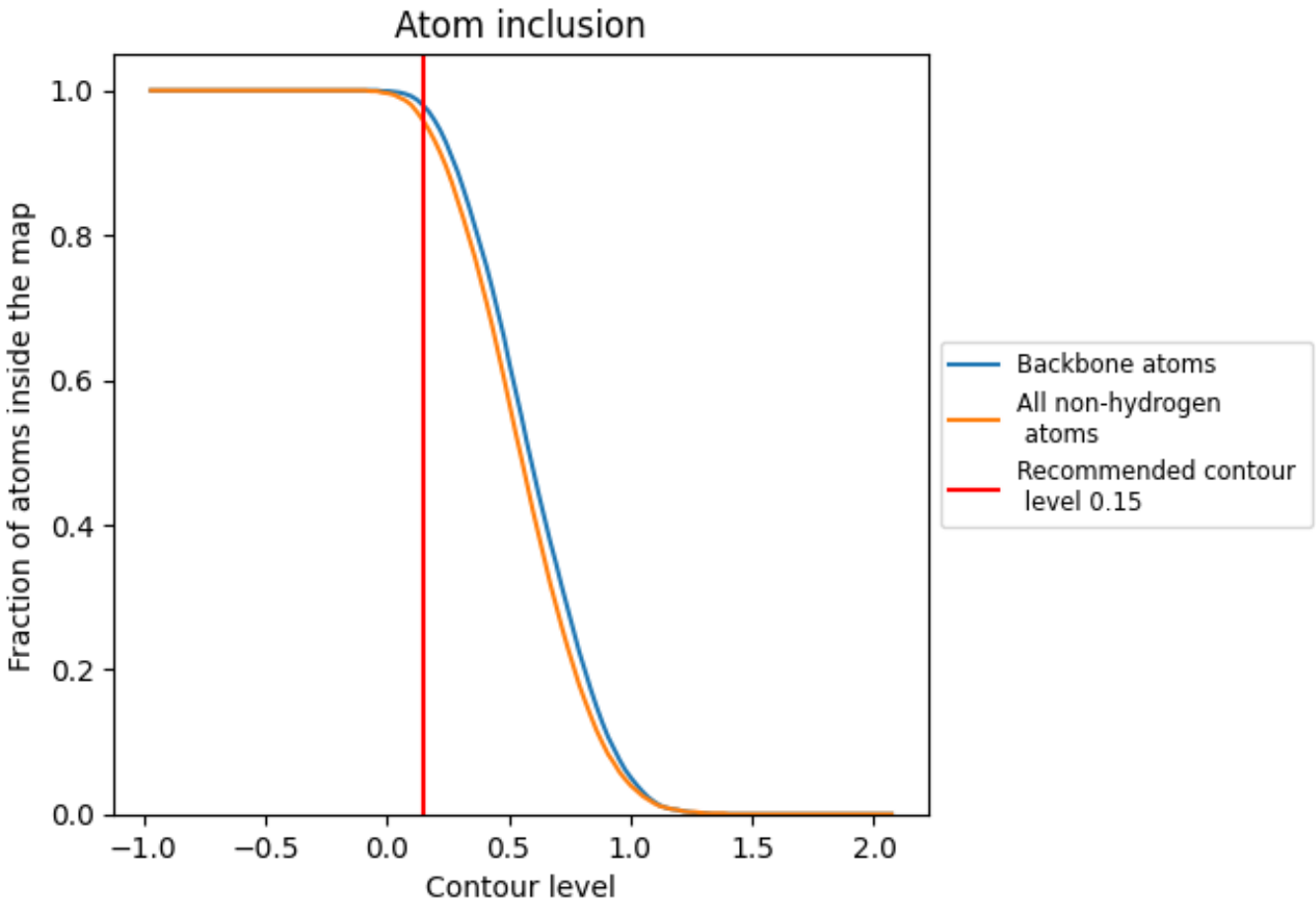
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).

9.4 Atom inclusion (i)



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

9.5 Map-model fit summary (i)

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

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

Continued on next page...

Continued from previous page...

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