



## Full wwPDB EM Validation Report ⓘ

Mar 24, 2025 – 12:58 PM JST

PDB ID : 8YZ2  
EMDB ID : EMD-39683  
Title : Cryo-EM structure of a tri-heme cytochrome-associated RC-LH1 complex from a marine photoheterotrophic bacterium, purified with magnesium solutions  
Authors : Chen, J.H.; Zheng, Q.; Zhang, X.  
Deposited on : 2024-04-05  
Resolution : 2.68 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

EMDB validation analysis : 0.0.1.dev117  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.41.2

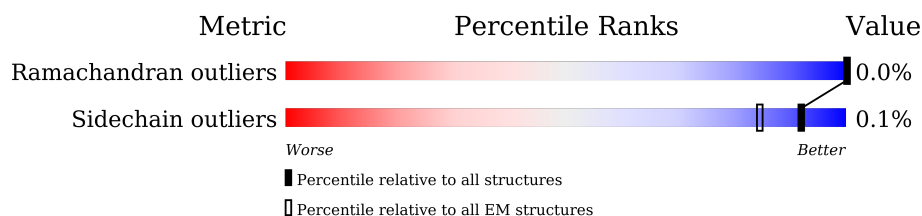
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

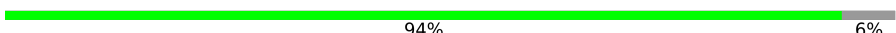
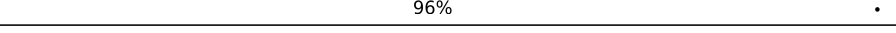
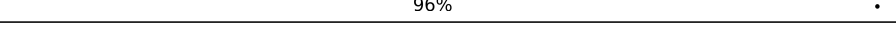
The reported resolution of this entry is 2.68 Å.

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



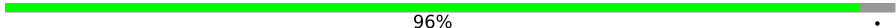
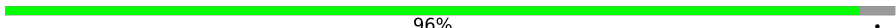
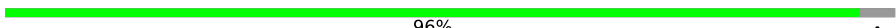
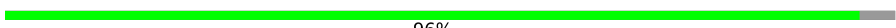
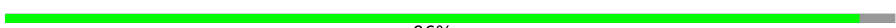








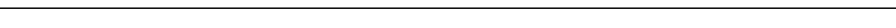











Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	53	 94% 6%
1	A	53	 96% .
1	B	53	 96% .
1	D	53	 96% .
1	E	53	 96% .
1	F	53	 96% .
1	G	53	 96% .
1	I	53	 96% .
1	J	53	 94% 6%


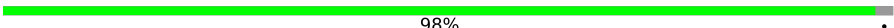
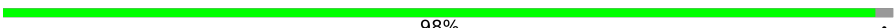
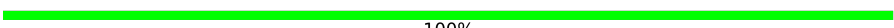
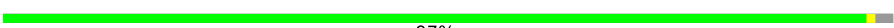
*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	K	53	 96% .
1	N	53	 96% .
1	P	53	 96% .
1	Q	53	 96% .
1	R	53	 96% .
1	S	53	 96% .
1	T	53	 96% .
1	V	53	 96% .
2	O	239	 22% 78%
3	2	49	 90% 10%
3	a	49	 90% 10%
3	b	49	 90% 10%
3	d	49	 90% 10%
3	e	49	 90% 10%
3	f	49	 90% 10%
3	g	49	 90% 10%
3	i	49	 88% 12%
3	j	49	 88% 12%
3	k	49	 88% 12%
3	n	49	 90% 10%
3	p	49	 90% 10%
3	q	49	 90% 10%
3	r	49	 88% 12%
3	s	49	 90% 10%
3	t	49	 88% 12%

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
3	v	49	 82%18%
4	M	330	 98%.
5	L	279	 98%.
6	H	256	 100%
7	C	360	 97%..

## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 28315 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Antenna pigment protein alpha chain.

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	v	40	Total	C	N	O	S	0	0
			325	217	52	55	1		
3	t	43	Total	C	N	O	S	0	0
			350	235	55	59	1		
3	s	44	Total	C	N	O	S	0	0
			358	239	56	62	1		
3	r	43	Total	C	N	O	S	0	0
			350	235	55	59	1		
3	q	44	Total	C	N	O	S	0	0
			358	239	56	62	1		
3	p	44	Total	C	N	O	S	0	0
			358	239	56	62	1		
3	2	44	Total	C	N	O	S	0	0
			358	239	56	62	1		
3	n	44	Total	C	N	O	S	0	0
			358	239	56	62	1		
3	k	43	Total	C	N	O	S	0	0
			350	235	55	59	1		
3	j	43	Total	C	N	O	S	0	0
			350	235	55	59	1		
3	i	43	Total	C	N	O	S	0	0
			350	235	55	59	1		
3	g	44	Total	C	N	O	S	0	0
			358	239	56	62	1		
3	f	44	Total	C	N	O	S	0	0
			358	239	56	62	1		
3	e	44	Total	C	N	O	S	0	0
			358	239	56	62	1		
3	d	44	Total	C	N	O	S	0	0
			358	239	56	62	1		
3	b	44	Total	C	N	O	S	0	0
			358	239	56	62	1		
3	a	44	Total	C	N	O	S	0	0
			358	239	56	62	1		

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

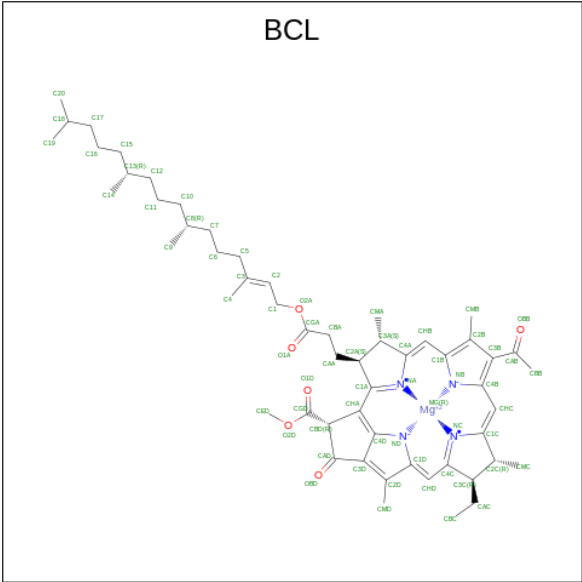
- Molecule 6 is a protein called Reaction center protein H chain.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	352	Total	C	N	O	S	0	0
			2741	1732	455	540	14		

- Molecule 8 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C<sub>55</sub>H<sub>74</sub>MgN<sub>4</sub>O<sub>6</sub>).



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

Continued on next page...



*Continued from previous page...*

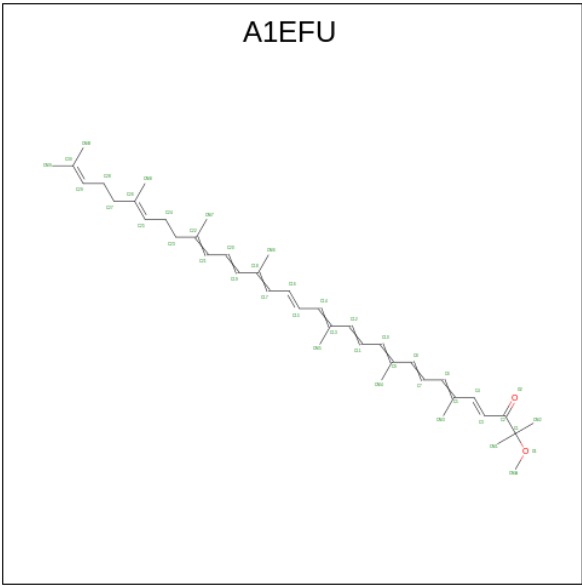
Mol	Chain	Residues	Atoms					AltConf
8	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	k	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	K	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	j	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	J	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	i	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	I	1	Total 66	C 55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

*Continued on next page...*

Continued from previous page...

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

- Molecule 9 is (4 {E},16 {E},26 {E})-2-methoxy-2,6,10,14,19,23,27,31-octamethyl-dotriaconta-4,6,8,10,12,14,16,18,20,22,26,30-dodecaen-3-one (three-letter code: A1EFU) (formula: C<sub>41</sub>H<sub>58</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



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

Continued on next page...

*Continued from previous page...*

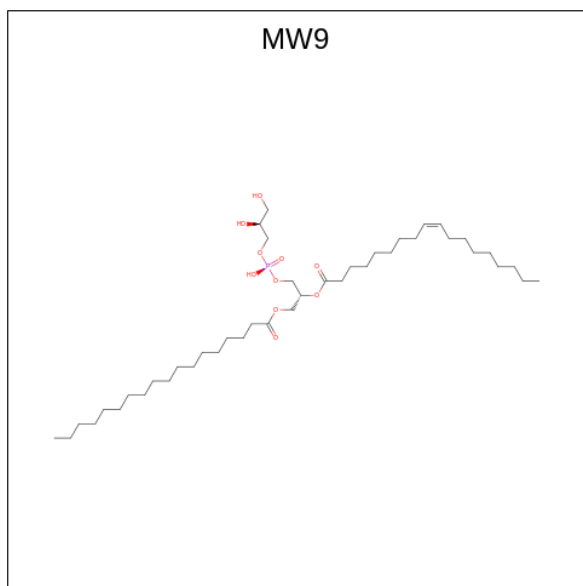
Mol	Chain	Residues	Atoms			AltConf
9	Q	1	Total 43	C 41	O 2	0
9	r	1	Total 43	C 41	O 2	0
9	R	1	Total 43	C 41	O 2	0
9	2	1	Total 43	C 41	O 2	0
9	2	1	Total 43	C 41	O 2	0
9	1	1	Total 43	C 41	O 2	0
9	1	1	Total 43	C 41	O 2	0
9	N	1	Total 43	C 41	O 2	0
9	N	1	Total 43	C 41	O 2	0
9	k	1	Total 43	C 41	O 2	0
9	K	1	Total 43	C 41	O 2	0
9	J	1	Total 43	C 41	O 2	0
9	J	1	Total 43	C 41	O 2	0
9	I	1	Total 43	C 41	O 2	0
9	I	1	Total 43	C 41	O 2	0
9	G	1	Total 43	C 41	O 2	0
9	G	1	Total 43	C 41	O 2	0
9	F	1	Total 43	C 41	O 2	0
9	e	1	Total 43	C 41	O 2	0
9	E	1	Total 43	C 41	O 2	0
9	d	1	Total 43	C 41	O 2	0

*Continued on next page...*

*Continued from previous page...*

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

- Molecule 10 is (21R,24R,27S)-24,27,28-trihydroxy-18,24-dioxo-19,23,25-trioxa-24lambda a 5 -phosphaoctacosan-21-yl (9Z)-octadec-9-enoate (three-letter code: MW9) (formula: C<sub>42</sub>H<sub>81</sub>O<sub>10</sub>P).



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

*Continued on next page...*

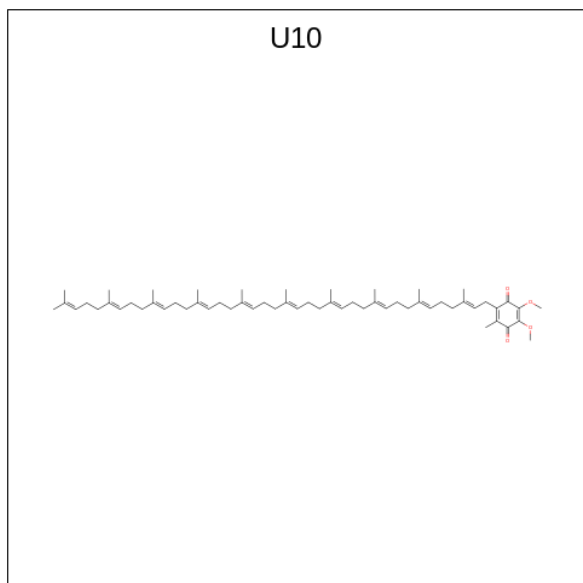
*Continued from previous page...*

Mol	Chain	Residues	Atoms				AltConf
10	F	1	Total	C	O	P	0
			43	32	10	1	
10	F	1	Total	C	O	P	0
			48	37	10	1	
10	D	1	Total	C	O		0
			27	22	5		
10	D	1	Total	C	O	P	0
			53	42	10	1	
10	M	1	Total	C	O	P	0
			49	38	10	1	
10	M	1	Total	C	O	P	0
			53	42	10	1	
10	L	1	Total	C	O	P	0
			37	26	10	1	
10	L	1	Total	C	O	P	0
			36	25	10	1	
10	H	1	Total	C	O	P	0
			37	28	8	1	

- Molecule 11 is FE (III) ION (three-letter code: FE) (formula: Fe).

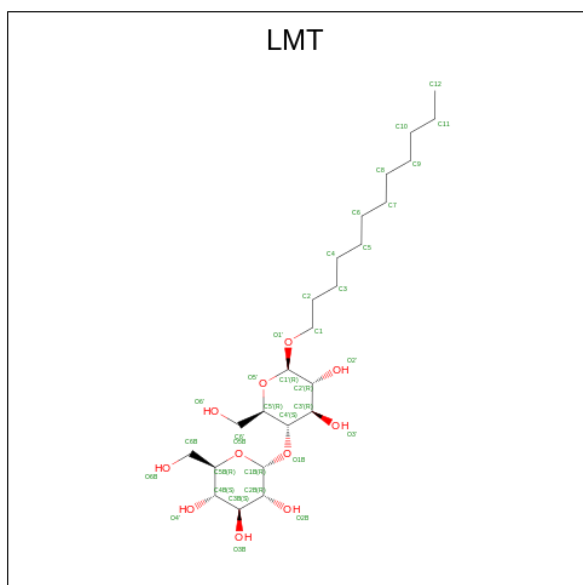
Mol	Chain	Residues	Atoms		AltConf
11	M	1	Total	Fe	0
			1	1	

- Molecule 12 is UBIQUINONE-10 (three-letter code: U10) (formula: C<sub>59</sub>H<sub>90</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



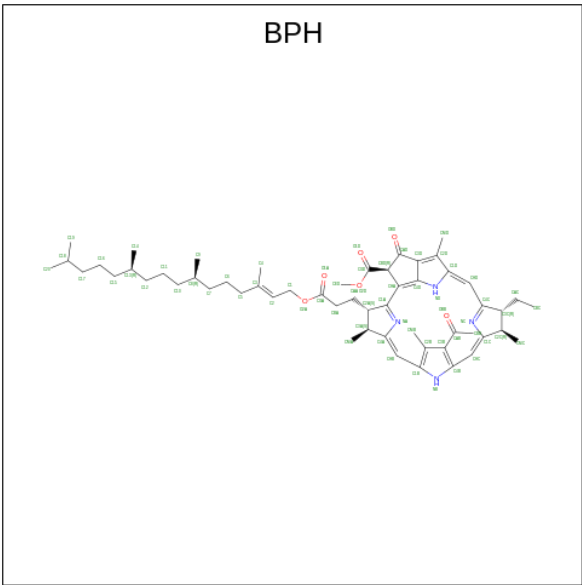
Mol	Chain	Residues	Atoms			AltConf
12	M	1	Total	C	O	0
			63	59	4	
12	L	1	Total	C	O	0
			48	44	4	

- Molecule 13 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



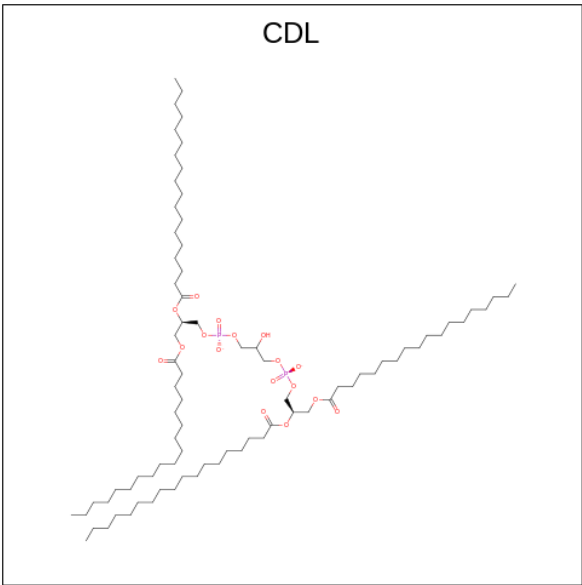
Mol	Chain	Residues	Atoms			AltConf
13	L	1	Total	C	O	0
			35	24	11	
13	L	1	Total	C	O	0
			24	18	6	
13	L	1	Total	C	O	0
			24	19	5	
13	H	1	Total	C	O	0
			24	18	6	
13	C	1	Total	C	O	0
			24	18	6	

- Molecule 14 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula:  $C_{55}H_{76}N_4O_6$ ).



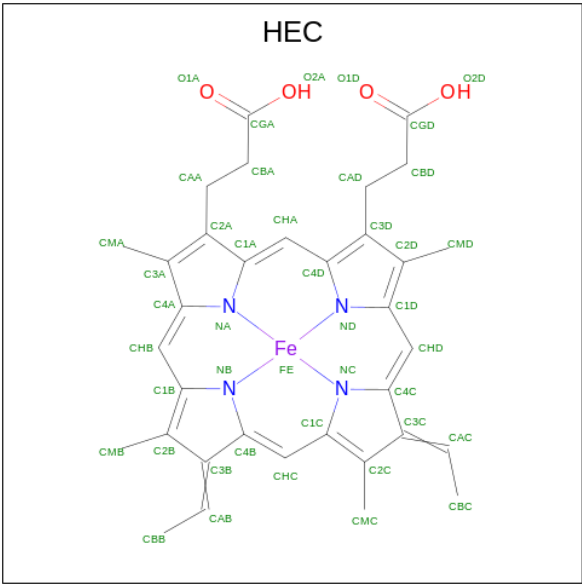
Mol	Chain	Residues	Atoms				AltConf
14	L	1	Total	C	N	O	0
			65	55	4	6	
14	L	1	Total	C	N	O	0
			65	55	4	6	

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



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

- Molecule 16 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ) (labeled as "Ligand of Interest" by depositor).



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

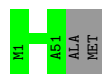


### 3 Residue-property plots [i](#)

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

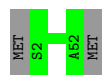
- Molecule 1: Antenna pigment protein alpha chain

Chain P:  96%



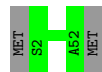
- Molecule 1: Antenna pigment protein alpha chain

Chain V:  96%



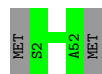
- Molecule 1: Antenna pigment protein alpha chain

Chain S:  96%



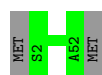
- Molecule 1: Antenna pigment protein alpha chain

Chain T:  96%

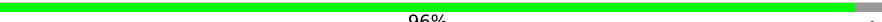


- Molecule 1: Antenna pigment protein alpha chain

Chain Q:  96%



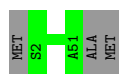
- Molecule 1: Antenna pigment protein alpha chain

Chain R:  96% .



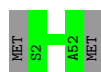
- Molecule 1: Antenna pigment protein alpha chain

Chain 1:  94% 6%



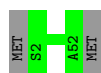
- Molecule 1: Antenna pigment protein alpha chain

Chain N:  96% .



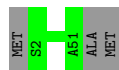
- Molecule 1: Antenna pigment protein alpha chain

Chain K:  96% .



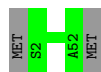
- Molecule 1: Antenna pigment protein alpha chain

Chain J:  94% 6%



- Molecule 1: Antenna pigment protein alpha chain

Chain I:  96% .



- Molecule 1: Antenna pigment protein alpha chain

Chain G:  96% .



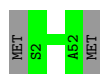
- Molecule 1: Antenna pigment protein alpha chain

Chain F:  96% .



- Molecule 1: Antenna pigment protein alpha chain

Chain E:  96% .



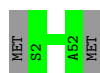
- Molecule 1: Antenna pigment protein alpha chain

Chain D:  96% .



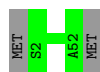
- Molecule 1: Antenna pigment protein alpha chain

Chain B:  96% .



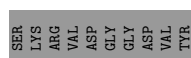
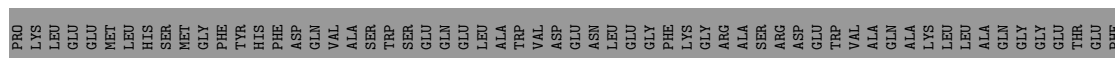
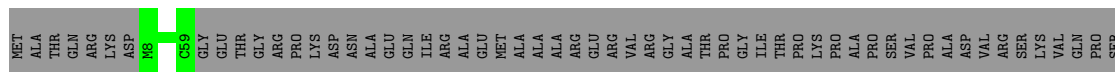
- Molecule 1: Antenna pigment protein alpha chain

Chain A:  96% .




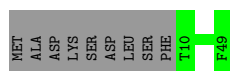
- Molecule 2: Reaction center protein O chain

Chain O:  22%  78%




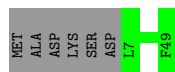
- Molecule 3: Antenna pigment protein beta chain

Chain v:  82% 18%




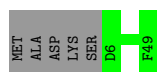
- Molecule 3: Antenna pigment protein beta chain

Chain t:  88% 12%




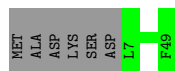
- Molecule 3: Antenna pigment protein beta chain

Chain s:  90% 10%




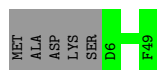
- Molecule 3: Antenna pigment protein beta chain

Chain r:  88% 12%




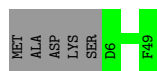
- Molecule 3: Antenna pigment protein beta chain

Chain q:  90% 10%



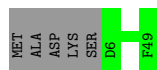
- Molecule 3: Antenna pigment protein beta chain

Chain p:  90% 10%




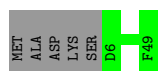
- Molecule 3: Antenna pigment protein beta chain

Chain 2:  90% 10%




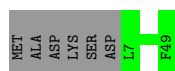
- Molecule 3: Antenna pigment protein beta chain

Chain n:  90% 10%




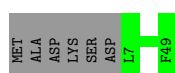
- Molecule 3: Antenna pigment protein beta chain

Chain k:  88% 12%




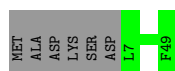
- Molecule 3: Antenna pigment protein beta chain

Chain j:  88% 12%




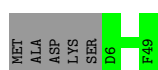
- Molecule 3: Antenna pigment protein beta chain

Chain i:  88% 12%




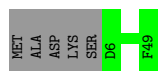
- Molecule 3: Antenna pigment protein beta chain

Chain g:  90% 10%




- Molecule 3: Antenna pigment protein beta chain

Chain f:  90% 10%




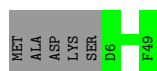
- Molecule 3: Antenna pigment protein beta chain

Chain e:  90% 10%




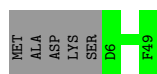
- Molecule 3: Antenna pigment protein beta chain

Chain d:  90% 10%




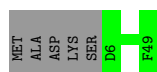
- Molecule 3: Antenna pigment protein beta chain

Chain b:  90% 10%



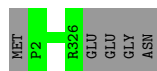
- Molecule 3: Antenna pigment protein beta chain

Chain a:  90% 10%



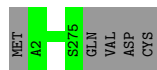
- Molecule 4: Reaction center protein M chain

Chain M:  98% .



- Molecule 5: Reaction center protein L chain

Chain L:  98% .



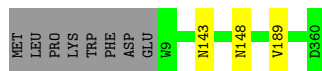
- Molecule 6: Reaction center protein H chain

Chain H:  100%

There are no outlier residues recorded for this chain.

- Molecule 7: Photosynthetic reaction center cytochrome c subunit

Chain C:  97% ..



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	194156	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.698	Depositor
Minimum map value	-0.460	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	238.08, 238.08, 238.08	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.93, 0.93, 0.93	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BPH, MW9, BCL, U10, HEC, LMT, CDL, A1EFU, FE

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	1	0.26	0/431	0.38	0/585
1	A	0.25	0/436	0.40	0/592
1	B	0.25	0/436	0.40	0/592
1	D	0.25	0/436	0.41	0/592
1	E	0.26	0/436	0.40	0/592
1	F	0.26	0/436	0.40	0/592
1	G	0.26	0/436	0.38	0/592
1	I	0.25	0/436	0.38	0/592
1	J	0.25	0/431	0.38	0/585
1	K	0.25	0/436	0.38	0/592
1	N	0.25	0/436	0.40	0/592
1	P	0.25	0/439	0.41	0/595
1	Q	0.25	0/436	0.38	0/592
1	R	0.25	0/436	0.38	0/592
1	S	0.25	0/436	0.39	0/592
1	T	0.24	0/436	0.38	0/592
1	V	0.24	0/436	0.37	0/592
2	O	0.23	0/378	0.38	0/516
3	2	0.24	0/371	0.40	0/508
3	a	0.24	0/371	0.41	0/508
3	b	0.24	0/371	0.39	0/508
3	d	0.25	0/371	0.39	0/508
3	e	0.24	0/371	0.40	0/508
3	f	0.24	0/371	0.39	0/508
3	g	0.23	0/371	0.37	0/508
3	i	0.24	0/363	0.38	0/497
3	j	0.24	0/363	0.39	0/497
3	k	0.24	0/363	0.44	0/497
3	n	0.23	0/371	0.39	0/508
3	p	0.24	0/371	0.42	0/508
3	q	0.24	0/371	0.44	0/508
3	r	0.23	0/363	0.43	0/497



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
3	s	0.24	0/371	0.40	0/508
3	t	0.25	0/363	0.39	0/497
3	v	0.23	0/337	0.36	0/462
4	M	0.26	0/2731	0.45	0/3735
5	L	0.27	0/2267	0.44	0/3105
6	H	0.26	0/2072	0.48	0/2804
7	C	0.25	0/2819	0.45	0/3869
All	All	0.25	0/23905	0.42	0/32617

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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	1	48/53 (91%)	48 (100%)	0	0	100	100
1	A	49/53 (92%)	48 (98%)	1 (2%)	0	100	100
1	B	49/53 (92%)	48 (98%)	1 (2%)	0	100	100
1	D	49/53 (92%)	49 (100%)	0	0	100	100
1	E	49/53 (92%)	48 (98%)	1 (2%)	0	100	100
1	F	49/53 (92%)	49 (100%)	0	0	100	100
1	G	49/53 (92%)	49 (100%)	0	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	49/53 (92%)	49 (100%)	0	0	100	100
1	J	48/53 (91%)	48 (100%)	0	0	100	100
1	K	49/53 (92%)	49 (100%)	0	0	100	100
1	N	49/53 (92%)	49 (100%)	0	0	100	100
1	P	49/53 (92%)	49 (100%)	0	0	100	100
1	Q	49/53 (92%)	49 (100%)	0	0	100	100
1	R	49/53 (92%)	49 (100%)	0	0	100	100
1	S	49/53 (92%)	48 (98%)	1 (2%)	0	100	100
1	T	49/53 (92%)	48 (98%)	1 (2%)	0	100	100
1	V	49/53 (92%)	48 (98%)	1 (2%)	0	100	100
2	O	50/239 (21%)	47 (94%)	3 (6%)	0	100	100
3	2	42/49 (86%)	42 (100%)	0	0	100	100
3	a	42/49 (86%)	41 (98%)	1 (2%)	0	100	100
3	b	42/49 (86%)	42 (100%)	0	0	100	100
3	d	42/49 (86%)	42 (100%)	0	0	100	100
3	e	42/49 (86%)	41 (98%)	1 (2%)	0	100	100
3	f	42/49 (86%)	41 (98%)	1 (2%)	0	100	100
3	g	42/49 (86%)	42 (100%)	0	0	100	100
3	i	41/49 (84%)	41 (100%)	0	0	100	100
3	j	41/49 (84%)	41 (100%)	0	0	100	100
3	k	41/49 (84%)	41 (100%)	0	0	100	100
3	n	42/49 (86%)	41 (98%)	1 (2%)	0	100	100
3	p	42/49 (86%)	41 (98%)	1 (2%)	0	100	100
3	q	42/49 (86%)	40 (95%)	2 (5%)	0	100	100
3	r	41/49 (84%)	41 (100%)	0	0	100	100
3	s	42/49 (86%)	41 (98%)	1 (2%)	0	100	100
3	t	41/49 (84%)	41 (100%)	0	0	100	100
3	v	38/49 (78%)	38 (100%)	0	0	100	100
4	M	323/330 (98%)	314 (97%)	9 (3%)	0	100	100
5	L	272/279 (98%)	264 (97%)	8 (3%)	0	100	100
6	H	254/256 (99%)	249 (98%)	5 (2%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	C	350/360 (97%)	334 (95%)	15 (4%)	1 (0%)	37	59
All	All	2785/3198 (87%)	2730 (98%)	54 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	C	189	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	42/44 (96%)	42 (100%)	0	100	100
1	A	42/44 (96%)	42 (100%)	0	100	100
1	B	42/44 (96%)	42 (100%)	0	100	100
1	D	42/44 (96%)	42 (100%)	0	100	100
1	E	42/44 (96%)	42 (100%)	0	100	100
1	F	42/44 (96%)	42 (100%)	0	100	100
1	G	42/44 (96%)	42 (100%)	0	100	100
1	I	42/44 (96%)	42 (100%)	0	100	100
1	J	42/44 (96%)	42 (100%)	0	100	100
1	K	42/44 (96%)	42 (100%)	0	100	100
1	N	42/44 (96%)	42 (100%)	0	100	100
1	P	43/44 (98%)	43 (100%)	0	100	100
1	Q	42/44 (96%)	42 (100%)	0	100	100
1	R	42/44 (96%)	42 (100%)	0	100	100
1	S	42/44 (96%)	42 (100%)	0	100	100
1	T	42/44 (96%)	42 (100%)	0	100	100
1	V	42/44 (96%)	42 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	O	39/174 (22%)	39 (100%)	0	100	100
3	2	37/41 (90%)	37 (100%)	0	100	100
3	a	37/41 (90%)	37 (100%)	0	100	100
3	b	37/41 (90%)	37 (100%)	0	100	100
3	d	37/41 (90%)	37 (100%)	0	100	100
3	e	37/41 (90%)	37 (100%)	0	100	100
3	f	37/41 (90%)	37 (100%)	0	100	100
3	g	37/41 (90%)	37 (100%)	0	100	100
3	i	36/41 (88%)	36 (100%)	0	100	100
3	j	36/41 (88%)	36 (100%)	0	100	100
3	k	36/41 (88%)	36 (100%)	0	100	100
3	n	37/41 (90%)	37 (100%)	0	100	100
3	p	37/41 (90%)	37 (100%)	0	100	100
3	q	37/41 (90%)	37 (100%)	0	100	100
3	r	36/41 (88%)	36 (100%)	0	100	100
3	s	37/41 (90%)	37 (100%)	0	100	100
3	t	36/41 (88%)	36 (100%)	0	100	100
3	v	33/41 (80%)	33 (100%)	0	100	100
4	M	266/270 (98%)	266 (100%)	0	100	100
5	L	218/223 (98%)	218 (100%)	0	100	100
6	H	214/214 (100%)	214 (100%)	0	100	100
7	C	299/307 (97%)	297 (99%)	2 (1%)	81	92
All	All	2371/2633 (90%)	2369 (100%)	2 (0%)	92	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	C	143	ASN
7	C	148	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	Q	40	HIS
3	q	16	GLN
3	e	16	GLN
5	L	167	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 100 ligands modelled in this entry, 1 is monoatomic - leaving 99 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
8	BCL	t	101	-	64,74,74	1.76	12 (18%)	78,115,115	2.07	24 (30%)
9	A1EFU	N	102	-	40,42,42	1.69	9 (22%)	45,52,52	3.70	20 (44%)
9	A1EFU	2	102	-	40,42,42	1.70	9 (22%)	45,52,52	3.68	21 (46%)
13	LMT	C	404	-	24,24,36	1.02	2 (8%)	29,29,47	1.07	1 (3%)
8	BCL	v	101	-	64,74,74	1.71	11 (17%)	78,115,115	2.30	28 (35%)
8	BCL	L	303	-	64,74,74	1.70	12 (18%)	78,115,115	2.36	29 (37%)
8	BCL	T	102	-	64,74,74	1.73	13 (20%)	78,115,115	2.27	29 (37%)
8	BCL	G	102	-	64,74,74	1.73	11 (17%)	78,115,115	2.29	27 (34%)
8	BCL	k	101	-	64,74,74	1.72	11 (17%)	78,115,115	2.27	28 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	BCL	E	101	-	64,74,74	1.72	11 (17%)	78,115,115	2.31	27 (34%)
14	BPH	L	302	-	51,70,70	0.81	2 (3%)	52,101,101	0.66	1 (1%)
16	HEC	C	401	7	32,50,50	2.00	4 (12%)	24,82,82	2.26	12 (50%)
12	U10	L	305	-	48,48,63	0.17	0	58,61,79	0.46	1 (1%)
8	BCL	V	101	-	64,74,74	1.69	10 (15%)	78,115,115	2.25	29 (37%)
9	A1EFU	I	101	-	40,42,42	1.69	8 (20%)	45,52,52	3.79	19 (42%)
9	A1EFU	a	103	-	40,42,42	1.70	9 (22%)	45,52,52	4.01	20 (44%)
9	A1EFU	t	102	-	40,42,42	1.68	9 (22%)	45,52,52	3.80	19 (42%)
8	BCL	a	102	-	64,74,74	1.72	12 (18%)	78,115,115	2.26	28 (35%)
13	LMT	L	308	-	24,24,36	1.05	2 (8%)	29,29,47	1.17	2 (6%)
8	BCL	L	306	-	64,74,74	1.70	12 (18%)	78,115,115	2.36	29 (37%)
8	BCL	K	101	-	64,74,74	1.72	11 (17%)	78,115,115	2.26	27 (34%)
9	A1EFU	A	102	-	40,42,42	1.69	9 (22%)	45,52,52	3.72	20 (44%)
10	MW9	F	104	-	47,47,52	1.39	6 (12%)	50,53,58	1.44	3 (6%)
9	A1EFU	N	103	-	40,42,42	1.69	9 (22%)	45,52,52	3.81	20 (44%)
8	BCL	i	101	-	64,74,74	1.73	11 (17%)	78,115,115	2.28	26 (33%)
9	A1EFU	l	101	-	40,42,42	1.70	9 (22%)	45,52,52	3.83	20 (44%)
10	MW9	F	103	-	42,42,52	1.43	6 (14%)	45,48,58	1.46	3 (6%)
9	A1EFU	J	103	-	40,42,42	1.69	9 (22%)	45,52,52	3.91	20 (44%)
8	BCL	S	101	-	64,74,74	1.71	10 (15%)	78,115,115	2.24	27 (34%)
8	BCL	Q	101	-	64,74,74	1.72	11 (17%)	78,115,115	2.24	26 (33%)
8	BCL	l	103	-	64,74,74	1.72	11 (17%)	78,115,115	2.28	27 (34%)
10	MW9	D	103	-	52,52,52	1.45	6 (11%)	55,58,58	1.46	4 (7%)
10	MW9	M	406	-	52,52,52	1.45	6 (11%)	55,58,58	1.47	4 (7%)
8	BCL	B	101	-	64,74,74	1.72	13 (20%)	78,115,115	2.25	27 (34%)
8	BCL	d	101	-	64,74,74	1.74	11 (17%)	78,115,115	2.23	22 (28%)
8	BCL	l	102	-	64,74,74	1.70	11 (17%)	78,115,115	2.25	25 (32%)
10	MW9	M	405	-	48,48,52	1.49	6 (12%)	51,54,58	1.50	3 (5%)
8	BCL	q	101	-	64,74,74	1.72	11 (17%)	78,115,115	2.26	26 (33%)
9	A1EFU	T	101	-	40,42,42	1.68	9 (22%)	45,52,52	3.71	20 (44%)
9	A1EFU	Q	103	-	40,42,42	1.70	9 (22%)	45,52,52	3.88	20 (44%)
8	BCL	M	402	-	64,74,74	1.71	11 (17%)	78,115,115	2.22	24 (30%)
9	A1EFU	Q	102	-	40,42,42	1.68	9 (22%)	45,52,52	3.73	21 (46%)
13	LMT	H	301	-	24,24,36	1.04	2 (8%)	29,29,47	1.06	1 (3%)
8	BCL	N	101	-	64,74,74	1.71	11 (17%)	78,115,115	2.28	27 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	BCL	M	403	-	64,74,74	1.71	13 (20%)	78,115,115	2.31	27 (34%)
9	A1EFU	E	102	-	40,42,42	1.69	9 (22%)	45,52,52	3.73	19 (42%)
8	BCL	R	102	-	64,74,74	1.72	12 (18%)	78,115,115	2.27	27 (34%)
9	A1EFU	F	105	-	40,42,42	1.69	7 (17%)	45,52,52	3.80	19 (42%)
8	BCL	j	101	-	64,74,74	1.72	12 (18%)	78,115,115	2.29	29 (37%)
9	A1EFU	e	101	-	40,42,42	1.68	9 (22%)	45,52,52	3.80	19 (42%)
10	MW9	D	102	-	26,26,52	1.42	4 (15%)	28,28,58	1.29	2 (7%)
9	A1EFU	G	104	-	40,42,42	1.69	8 (20%)	45,52,52	3.68	19 (42%)
9	A1EFU	s	102	-	40,42,42	1.69	9 (22%)	45,52,52	3.40	20 (44%)
9	A1EFU	D	105	-	40,42,42	1.68	9 (22%)	45,52,52	3.92	20 (44%)
9	A1EFU	r	102	-	40,42,42	1.68	8 (20%)	45,52,52	3.72	19 (42%)
8	BCL	G	101	-	64,74,74	1.71	11 (17%)	78,115,115	2.25	27 (34%)
10	MW9	L	309	-	36,36,52	1.47	5 (13%)	39,42,58	1.53	3 (7%)
14	BPH	L	304	-	51,70,70	0.62	2 (3%)	52,101,101	0.73	1 (1%)
16	HEC	C	402	7	32,50,50	2.05	4 (12%)	24,82,82	2.23	11 (45%)
8	BCL	F	101	-	64,74,74	1.73	10 (15%)	78,115,115	2.14	23 (29%)
9	A1EFU	M	407	-	40,42,42	1.68	9 (22%)	45,52,52	3.67	19 (42%)
12	U10	M	404	-	63,63,63	0.15	0	76,79,79	0.42	1 (1%)
9	A1EFU	I	103	-	40,42,42	1.68	9 (22%)	45,52,52	3.90	20 (44%)
8	BCL	P	102	-	64,74,74	1.72	12 (18%)	78,115,115	2.19	25 (32%)
9	A1EFU	D	104	-	40,42,42	1.70	9 (22%)	45,52,52	3.72	19 (42%)
9	A1EFU	v	103	-	40,42,42	1.68	9 (22%)	45,52,52	3.87	20 (44%)
9	A1EFU	K	102	-	40,42,42	1.70	9 (22%)	45,52,52	3.66	20 (44%)
10	MW9	Q	104	-	44,44,52	1.48	5 (11%)	47,50,58	1.52	3 (6%)
8	BCL	r	101	-	64,74,74	1.73	12 (18%)	78,115,115	2.22	26 (33%)
8	BCL	P	101	-	64,74,74	1.71	12 (18%)	78,115,115	2.27	26 (33%)
8	BCL	e	102	-	64,74,74	1.72	11 (17%)	78,115,115	2.25	26 (33%)
8	BCL	I	102	-	64,74,74	1.72	11 (17%)	78,115,115	2.31	27 (34%)
8	BCL	s	101	-	64,74,74	1.71	11 (17%)	78,115,115	2.24	27 (34%)
10	MW9	G	103	-	48,48,52	1.49	6 (12%)	51,54,58	1.48	4 (7%)
8	BCL	F	102	-	64,74,74	1.74	10 (15%)	78,115,115	2.27	28 (35%)
9	A1EFU	S	102	-	40,42,42	1.68	9 (22%)	45,52,52	3.84	20 (44%)
8	BCL	D	101	-	64,74,74	1.72	12 (18%)	78,115,115	2.24	28 (35%)
13	LMT	L	301	-	36,36,36	1.16	5 (13%)	47,47,47	0.96	1 (2%)
13	LMT	L	307	-	24,24,36	1.03	2 (8%)	29,29,47	1.11	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	MW9	I	104	-	39,39,52	1.43	5 (12%)	42,45,58	1.17	3 (7%)
8	BCL	n	101	-	64,74,74	1.73	13 (20%)	78,115,115	2.21	27 (34%)
8	BCL	J	101	-	64,74,74	1.72	11 (17%)	78,115,115	2.28	27 (34%)
8	BCL	A	101	-	64,74,74	1.73	12 (18%)	78,115,115	2.19	26 (33%)
9	A1EFU	1	104	-	40,42,42	1.71	9 (22%)	45,52,52	3.61	21 (46%)
10	MW9	H	302	-	36,36,52	1.57	8 (22%)	39,41,58	1.87	3 (7%)
9	A1EFU	d	102	-	40,42,42	1.69	9 (22%)	45,52,52	3.75	20 (44%)
9	A1EFU	R	101	-	40,42,42	1.69	9 (22%)	45,52,52	3.73	20 (44%)
9	A1EFU	2	101	-	40,42,42	1.68	9 (22%)	45,52,52	3.76	20 (44%)
9	A1EFU	J	102	-	40,42,42	1.69	9 (22%)	45,52,52	3.64	20 (44%)
9	A1EFU	v	102	-	40,42,42	1.70	9 (22%)	45,52,52	3.72	20 (44%)
8	BCL	b	101	-	64,74,74	1.72	10 (15%)	78,115,115	2.24	25 (32%)
16	HEC	C	403	7	32,50,50	1.99	4 (12%)	24,82,82	2.32	14 (58%)
9	A1EFU	B	102	-	40,42,42	1.69	9 (22%)	45,52,52	3.75	20 (44%)
9	A1EFU	G	105	-	40,42,42	1.68	9 (22%)	45,52,52	3.96	20 (44%)
15	CDL	H	303	-	90,90,99	0.91	8 (8%)	96,102,111	1.12	4 (4%)
9	A1EFU	k	102	-	40,42,42	1.68	9 (22%)	45,52,52	3.88	19 (42%)
10	MW9	L	310	-	35,35,52	1.25	3 (8%)	38,41,58	1.14	2 (5%)
15	CDL	L	311	-	66,66,99	1.05	8 (12%)	72,78,111	1.16	4 (5%)
9	A1EFU	a	101	-	40,42,42	1.69	9 (22%)	45,52,52	3.76	20 (44%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCL	t	101	-	-	13/37/137/137	-
9	A1EFU	N	102	-	-	23/50/51/51	-
9	A1EFU	2	102	-	-	25/50/51/51	-
13	LMT	C	404	-	-	5/15/35/61	0/1/1/2
8	BCL	v	101	-	-	20/37/137/137	-
8	BCL	L	303	-	-	16/37/137/137	-
8	BCL	T	102	-	-	10/37/137/137	-
8	BCL	G	102	-	-	15/37/137/137	-
8	BCL	k	101	-	-	9/37/137/137	-

Continued on next page...



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCL	E	101	-	-	12/37/137/137	-
14	BPH	L	302	-	-	10/37/105/105	0/5/6/6
16	HEC	C	401	7	-	4/10/54/54	-
12	U10	L	305	-	-	13/45/69/87	0/1/1/1
8	BCL	V	101	-	-	11/37/137/137	-
9	A1EFU	I	101	-	-	18/50/51/51	-
9	A1EFU	a	103	-	-	19/50/51/51	-
9	A1EFU	t	102	-	-	25/50/51/51	-
8	BCL	a	102	-	-	21/37/137/137	-
13	LMT	L	308	-	-	6/15/35/61	0/1/1/2
8	BCL	L	306	-	-	17/37/137/137	-
8	BCL	K	101	-	-	11/37/137/137	-
9	A1EFU	A	102	-	-	17/50/51/51	-
10	MW9	F	104	-	-	29/52/52/57	-
9	A1EFU	N	103	-	-	25/50/51/51	-
8	BCL	i	101	-	-	19/37/137/137	-
9	A1EFU	1	101	-	-	20/50/51/51	-
10	MW9	F	103	-	-	34/47/47/57	-
9	A1EFU	J	103	-	-	22/50/51/51	-
8	BCL	S	101	-	-	13/37/137/137	-
8	BCL	Q	101	-	-	18/37/137/137	-
8	BCL	1	103	-	-	9/37/137/137	-
10	MW9	D	103	-	-	28/57/57/57	-
10	MW9	M	406	-	-	33/57/57/57	-
8	BCL	B	101	-	-	16/37/137/137	-
8	BCL	d	101	-	-	25/37/137/137	-
8	BCL	1	102	-	-	19/37/137/137	-
10	MW9	M	405	-	-	33/53/53/57	-
8	BCL	q	101	-	-	16/37/137/137	-
9	A1EFU	T	101	-	-	25/50/51/51	-
9	A1EFU	Q	103	-	-	19/50/51/51	-
8	BCL	M	402	-	-	11/37/137/137	-
9	A1EFU	Q	102	-	-	18/50/51/51	-
13	LMT	H	301	-	-	6/15/35/61	0/1/1/2

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCL	N	101	-	-	11/37/137/137	-
8	BCL	M	403	-	-	17/37/137/137	-
9	A1EFU	E	102	-	-	19/50/51/51	-
8	BCL	R	102	-	-	14/37/137/137	-
9	A1EFU	F	105	-	-	20/50/51/51	-
8	BCL	j	101	-	-	15/37/137/137	-
9	A1EFU	e	101	-	-	15/50/51/51	-
10	MW9	D	102	-	-	19/28/28/57	-
9	A1EFU	G	104	-	-	24/50/51/51	-
9	A1EFU	s	102	-	-	25/50/51/51	-
9	A1EFU	D	105	-	-	19/50/51/51	-
9	A1EFU	r	102	-	-	22/50/51/51	-
8	BCL	G	101	-	-	14/37/137/137	-
10	MW9	L	309	-	-	19/41/41/57	-
14	BPH	L	304	-	-	8/37/105/105	0/5/6/6
16	HEC	C	402	7	-	3/10/54/54	-
8	BCL	F	101	-	-	10/37/137/137	-
9	A1EFU	M	407	-	-	21/50/51/51	-
12	U10	M	404	-	-	10/63/87/87	0/1/1/1
9	A1EFU	I	103	-	-	20/50/51/51	-
8	BCL	P	102	-	-	13/37/137/137	-
9	A1EFU	D	104	-	-	19/50/51/51	-
9	A1EFU	v	103	-	-	25/50/51/51	-
9	A1EFU	K	102	-	-	25/50/51/51	-
10	MW9	Q	104	-	-	25/49/49/57	-
8	BCL	r	101	-	-	12/37/137/137	-
8	BCL	P	101	-	-	10/37/137/137	-
8	BCL	e	102	-	-	11/37/137/137	-
8	BCL	I	102	-	-	10/37/137/137	-
8	BCL	s	101	-	-	21/37/137/137	-
10	MW9	G	103	-	-	24/53/53/57	-
8	BCL	F	102	-	-	9/37/137/137	-
9	A1EFU	S	102	-	-	18/50/51/51	-
8	BCL	D	101	-	-	15/37/137/137	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	LMT	L	301	-	-	9/21/61/61	0/2/2/2
13	LMT	L	307	-	-	5/15/35/61	0/1/1/2
10	MW9	I	104	-	-	29/44/44/57	-
8	BCL	n	101	-	-	12/37/137/137	-
8	BCL	J	101	-	-	14/37/137/137	-
8	BCL	A	101	-	-	16/37/137/137	-
9	A1EFU	1	104	-	-	21/50/51/51	-
10	MW9	H	302	-	-	22/38/38/57	-
9	A1EFU	d	102	-	-	17/50/51/51	-
9	A1EFU	R	101	-	-	19/50/51/51	-
9	A1EFU	2	101	-	-	18/50/51/51	-
9	A1EFU	J	102	-	-	19/50/51/51	-
9	A1EFU	v	102	-	-	19/50/51/51	-
8	BCL	b	101	-	-	13/37/137/137	-
16	HEC	C	403	7	-	2/10/54/54	-
9	A1EFU	B	102	-	-	15/50/51/51	-
9	A1EFU	G	105	-	-	21/50/51/51	-
15	CDL	H	303	-	-	40/101/101/110	-
9	A1EFU	k	102	-	-	24/50/51/51	-
10	MW9	L	310	-	-	28/40/40/57	-
15	CDL	L	311	-	-	36/77/77/110	-
9	A1EFU	a	101	-	-	15/50/51/51	-

All (853) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	C	402	HEC	C3C-C2C	-6.54	1.33	1.40
16	C	402	HEC	C2B-C3B	-6.36	1.34	1.40
8	t	101	BCL	MG-ND	-6.28	1.93	2.05
16	C	401	HEC	C2B-C3B	-6.27	1.34	1.40
16	C	403	HEC	C3C-C2C	-6.24	1.34	1.40
8	F	102	BCL	MG-ND	-6.13	1.93	2.05
8	d	101	BCL	MG-ND	-6.12	1.93	2.05
16	C	403	HEC	C2B-C3B	-6.01	1.34	1.40
16	C	401	HEC	C3C-C2C	-5.96	1.34	1.40
8	F	101	BCL	MG-ND	-5.94	1.94	2.05
8	I	102	BCL	MG-ND	-5.93	1.94	2.05

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	v	101	BCL	MG-ND	-5.88	1.94	2.05
8	G	102	BCL	MG-ND	-5.88	1.94	2.05
8	E	101	BCL	MG-ND	-5.88	1.94	2.05
8	J	101	BCL	MG-ND	-5.87	1.94	2.05
8	Q	101	BCL	MG-ND	-5.82	1.94	2.05
8	b	101	BCL	MG-ND	-5.80	1.94	2.05
8	D	101	BCL	MG-ND	-5.79	1.94	2.05
8	R	102	BCL	MG-ND	-5.78	1.94	2.05
8	K	101	BCL	MG-ND	-5.78	1.94	2.05
8	l	103	BCL	MG-ND	-5.77	1.94	2.05
8	S	101	BCL	MG-ND	-5.75	1.94	2.05
8	e	102	BCL	MG-ND	-5.75	1.94	2.05
8	N	101	BCL	MG-ND	-5.72	1.94	2.05
9	F	105	A1EFU	C19-C18	-5.72	1.33	1.45
8	A	101	BCL	MG-ND	-5.71	1.94	2.05
8	j	101	BCL	MG-ND	-5.69	1.94	2.05
8	a	102	BCL	MG-ND	-5.69	1.94	2.05
8	B	101	BCL	MG-ND	-5.69	1.94	2.05
8	q	101	BCL	MG-ND	-5.68	1.94	2.05
8	i	101	BCL	MG-ND	-5.68	1.94	2.05
9	B	102	A1EFU	C19-C18	-5.67	1.33	1.45
8	s	101	BCL	MG-ND	-5.67	1.94	2.05
9	R	101	A1EFU	C19-C18	-5.67	1.33	1.45
8	P	101	BCL	MG-ND	-5.66	1.94	2.05
8	G	101	BCL	MG-ND	-5.66	1.94	2.05
8	k	101	BCL	MG-ND	-5.65	1.94	2.05
8	M	403	BCL	MG-ND	-5.65	1.94	2.05
9	l	101	A1EFU	C19-C18	-5.64	1.33	1.45
8	T	102	BCL	MG-ND	-5.64	1.94	2.05
8	M	402	BCL	MG-ND	-5.64	1.94	2.05
8	r	101	BCL	MG-ND	-5.64	1.94	2.05
9	E	102	A1EFU	C19-C18	-5.62	1.33	1.45
9	D	104	A1EFU	C19-C18	-5.61	1.33	1.45
8	L	306	BCL	MG-ND	-5.60	1.94	2.05
8	V	101	BCL	MG-ND	-5.59	1.94	2.05
8	n	101	BCL	MG-ND	-5.58	1.94	2.05
8	P	102	BCL	MG-ND	-5.58	1.94	2.05
9	a	103	A1EFU	C19-C18	-5.58	1.34	1.45
9	r	102	A1EFU	C19-C18	-5.58	1.34	1.45
9	A	102	A1EFU	C19-C18	-5.58	1.34	1.45
9	S	102	A1EFU	C19-C18	-5.58	1.34	1.45
9	a	101	A1EFU	C19-C18	-5.57	1.34	1.45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	1	102	BCL	MG-ND	-5.56	1.94	2.05
9	Q	103	A1EFU	C19-C18	-5.55	1.34	1.45
9	I	101	A1EFU	C19-C18	-5.54	1.34	1.45
9	d	102	A1EFU	C19-C18	-5.54	1.34	1.45
9	D	105	A1EFU	C19-C18	-5.54	1.34	1.45
9	Q	102	A1EFU	C19-C18	-5.54	1.34	1.45
9	G	104	A1EFU	C19-C18	-5.53	1.34	1.45
9	v	103	A1EFU	C19-C18	-5.53	1.34	1.45
9	K	102	A1EFU	C19-C18	-5.52	1.34	1.45
9	G	105	A1EFU	C19-C18	-5.52	1.34	1.45
9	2	101	A1EFU	C19-C18	-5.52	1.34	1.45
9	e	101	A1EFU	C19-C18	-5.52	1.34	1.45
9	N	102	A1EFU	C19-C18	-5.51	1.34	1.45
9	M	407	A1EFU	C19-C18	-5.51	1.34	1.45
9	J	103	A1EFU	C19-C18	-5.51	1.34	1.45
9	T	101	A1EFU	C19-C18	-5.51	1.34	1.45
9	t	102	A1EFU	C19-C18	-5.48	1.34	1.45
9	I	103	A1EFU	C19-C18	-5.48	1.34	1.45
9	1	104	A1EFU	C19-C18	-5.47	1.34	1.45
9	J	102	A1EFU	C19-C18	-5.47	1.34	1.45
9	k	102	A1EFU	C19-C18	-5.47	1.34	1.45
9	N	103	A1EFU	C19-C18	-5.46	1.34	1.45
9	v	102	A1EFU	C19-C18	-5.46	1.34	1.45
8	L	303	BCL	MG-ND	-5.45	1.95	2.05
9	2	102	A1EFU	C19-C18	-5.42	1.34	1.45
9	s	102	A1EFU	C19-C18	-5.42	1.34	1.45
8	F	101	BCL	OBD-CAD	4.85	1.30	1.22
8	F	102	BCL	OBD-CAD	4.78	1.30	1.22
8	t	101	BCL	C4D-ND	-4.74	1.31	1.37
8	v	101	BCL	OBD-CAD	4.74	1.30	1.22
8	r	101	BCL	OBD-CAD	4.73	1.30	1.22
8	F	102	BCL	C4D-ND	-4.72	1.31	1.37
8	A	101	BCL	OBD-CAD	4.71	1.30	1.22
8	1	103	BCL	OBD-CAD	4.71	1.30	1.22
8	k	101	BCL	OBD-CAD	4.70	1.30	1.22
8	V	101	BCL	OBD-CAD	4.70	1.30	1.22
8	q	101	BCL	OBD-CAD	4.70	1.30	1.22
8	T	102	BCL	OBD-CAD	4.70	1.30	1.22
8	B	101	BCL	OBD-CAD	4.69	1.30	1.22
8	L	303	BCL	OBD-CAD	4.69	1.30	1.22
8	R	102	BCL	OBD-CAD	4.69	1.30	1.22
8	G	102	BCL	OBD-CAD	4.69	1.30	1.22

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	n	101	BCL	OBD-CAD	4.68	1.30	1.22
8	b	101	BCL	OBD-CAD	4.68	1.30	1.22
8	a	102	BCL	OBD-CAD	4.68	1.30	1.22
8	M	402	BCL	OBD-CAD	4.68	1.30	1.22
8	N	101	BCL	OBD-CAD	4.67	1.30	1.22
8	D	101	BCL	OBD-CAD	4.67	1.30	1.22
8	j	101	BCL	OBD-CAD	4.66	1.30	1.22
8	t	101	BCL	OBD-CAD	4.66	1.30	1.22
8	K	101	BCL	OBD-CAD	4.66	1.30	1.22
8	i	101	BCL	OBD-CAD	4.66	1.30	1.22
8	e	102	BCL	OBD-CAD	4.66	1.30	1.22
8	P	101	BCL	OBD-CAD	4.65	1.30	1.22
8	s	101	BCL	OBD-CAD	4.65	1.30	1.22
8	d	101	BCL	OBD-CAD	4.65	1.30	1.22
8	Q	101	BCL	OBD-CAD	4.65	1.30	1.22
8	I	102	BCL	OBD-CAD	4.63	1.30	1.22
8	E	101	BCL	OBD-CAD	4.63	1.30	1.22
8	J	101	BCL	OBD-CAD	4.60	1.30	1.22
8	S	101	BCL	OBD-CAD	4.59	1.30	1.22
8	l	102	BCL	OBD-CAD	4.59	1.30	1.22
8	P	102	BCL	OBD-CAD	4.59	1.30	1.22
8	L	306	BCL	OBD-CAD	4.59	1.30	1.22
8	M	403	BCL	OBD-CAD	4.58	1.30	1.22
8	G	101	BCL	OBD-CAD	4.56	1.30	1.22
8	i	101	BCL	C4D-ND	-4.53	1.31	1.37
8	d	101	BCL	C4D-ND	-4.52	1.31	1.37
10	M	406	MW9	C35-C34	-4.50	1.34	1.52
10	G	103	MW9	C35-C34	-4.50	1.34	1.52
10	D	103	MW9	C35-C34	-4.49	1.34	1.52
10	Q	104	MW9	C35-C34	-4.49	1.34	1.52
10	M	405	MW9	C35-C34	-4.48	1.34	1.52
8	M	402	BCL	C4D-ND	-4.38	1.31	1.37
8	b	101	BCL	C4D-ND	-4.37	1.31	1.37
8	v	101	BCL	C4D-ND	-4.36	1.31	1.37
8	s	101	BCL	C4D-ND	-4.34	1.31	1.37
8	K	101	BCL	C4D-ND	-4.34	1.31	1.37
8	G	102	BCL	C4D-ND	-4.34	1.31	1.37
8	q	101	BCL	C4D-ND	-4.34	1.31	1.37
8	E	101	BCL	C4D-ND	-4.33	1.31	1.37
8	j	101	BCL	C4D-ND	-4.33	1.31	1.37
8	e	102	BCL	C4D-ND	-4.32	1.31	1.37
8	n	101	BCL	C4D-ND	-4.32	1.31	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	101	BCL	C4D-ND	-4.31	1.31	1.37
8	r	101	BCL	C4D-ND	-4.30	1.31	1.37
8	k	101	BCL	C4D-ND	-4.29	1.31	1.37
8	D	101	BCL	C4D-ND	-4.28	1.31	1.37
8	I	102	BCL	C4D-ND	-4.27	1.31	1.37
8	T	102	BCL	C4D-ND	-4.27	1.31	1.37
8	a	102	BCL	C4D-ND	-4.27	1.31	1.37
8	B	101	BCL	C4D-ND	-4.26	1.31	1.37
8	l	103	BCL	C4D-ND	-4.26	1.31	1.37
8	P	101	BCL	C4D-ND	-4.26	1.31	1.37
8	N	101	BCL	C4D-ND	-4.24	1.31	1.37
8	A	101	BCL	C4D-ND	-4.24	1.31	1.37
8	V	101	BCL	C4D-ND	-4.24	1.31	1.37
8	S	101	BCL	C4D-ND	-4.24	1.31	1.37
8	R	102	BCL	C4D-ND	-4.23	1.31	1.37
8	Q	101	BCL	C4D-ND	-4.20	1.31	1.37
14	L	302	BPH	C2C-C3C	4.20	1.58	1.54
8	M	403	BCL	C4D-ND	-4.19	1.31	1.37
8	P	102	BCL	C4D-ND	-4.19	1.31	1.37
8	G	101	BCL	C4D-ND	-4.18	1.32	1.37
8	L	306	BCL	C4D-ND	-4.15	1.32	1.37
8	l	102	BCL	C4D-ND	-4.14	1.32	1.37
10	F	103	MW9	C33-C32	4.14	1.55	1.31
10	D	103	MW9	C33-C32	4.13	1.55	1.31
10	Q	104	MW9	C33-C32	4.13	1.55	1.31
10	H	302	MW9	C33-C32	4.12	1.55	1.31
10	F	104	MW9	C33-C32	4.11	1.55	1.31
10	G	103	MW9	C33-C32	4.11	1.55	1.31
10	M	405	MW9	C33-C32	4.11	1.55	1.31
10	L	309	MW9	C33-C32	4.11	1.55	1.31
10	M	406	MW9	C33-C32	4.10	1.55	1.31
8	F	101	BCL	O1D-CGD	-4.08	1.11	1.21
8	L	303	BCL	O1D-CGD	-4.06	1.11	1.21
8	n	101	BCL	O1D-CGD	-4.05	1.11	1.21
8	S	101	BCL	O1D-CGD	-4.04	1.11	1.21
8	B	101	BCL	O1D-CGD	-4.03	1.11	1.21
8	d	101	BCL	O1D-CGD	-4.03	1.11	1.21
8	N	101	BCL	O1D-CGD	-4.03	1.11	1.21
8	r	101	BCL	O1D-CGD	-4.03	1.11	1.21
8	L	306	BCL	O1D-CGD	-4.03	1.11	1.21
8	b	101	BCL	O1D-CGD	-4.03	1.11	1.21
8	j	101	BCL	O1D-CGD	-4.02	1.11	1.21

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	q	101	BCL	O1D-CGD	-4.01	1.11	1.21
8	M	403	BCL	O1D-CGD	-4.01	1.11	1.21
8	l	103	BCL	O1D-CGD	-4.01	1.11	1.21
8	K	101	BCL	O1D-CGD	-4.01	1.11	1.21
10	I	104	MW9	C33-C32	4.01	1.55	1.28
8	P	101	BCL	O1D-CGD	-4.01	1.11	1.21
8	L	303	BCL	C4D-ND	-4.01	1.32	1.37
8	Q	101	BCL	O1D-CGD	-4.00	1.11	1.21
8	V	101	BCL	O1D-CGD	-4.00	1.11	1.21
8	e	102	BCL	O1D-CGD	-4.00	1.11	1.21
8	t	101	BCL	O1D-CGD	-4.00	1.11	1.21
8	G	102	BCL	O1D-CGD	-3.99	1.11	1.21
8	k	101	BCL	O1D-CGD	-3.99	1.11	1.21
8	M	402	BCL	O1D-CGD	-3.98	1.11	1.21
8	T	102	BCL	O1D-CGD	-3.98	1.11	1.21
8	D	101	BCL	O1D-CGD	-3.98	1.11	1.21
8	R	102	BCL	O1D-CGD	-3.98	1.11	1.21
8	a	102	BCL	O1D-CGD	-3.97	1.11	1.21
8	s	101	BCL	O1D-CGD	-3.97	1.11	1.21
8	P	102	BCL	O1D-CGD	-3.97	1.11	1.21
8	A	101	BCL	O1D-CGD	-3.97	1.11	1.21
8	i	101	BCL	O1D-CGD	-3.97	1.11	1.21
8	E	101	BCL	O1D-CGD	-3.97	1.11	1.21
8	l	102	BCL	O1D-CGD	-3.96	1.11	1.21
8	I	102	BCL	O1D-CGD	-3.95	1.11	1.21
8	F	102	BCL	O1D-CGD	-3.95	1.11	1.21
8	J	101	BCL	O1D-CGD	-3.95	1.11	1.21
8	v	101	BCL	O1D-CGD	-3.95	1.11	1.21
8	F	101	BCL	C4D-ND	-3.94	1.32	1.37
8	G	101	BCL	O1D-CGD	-3.92	1.11	1.21
8	F	101	BCL	O2D-CED	3.74	1.54	1.45
9	s	102	A1EFU	C7-C6	3.60	1.54	1.43
9	l	104	A1EFU	C7-C6	3.59	1.54	1.43
8	P	102	BCL	O2D-CED	3.59	1.53	1.45
9	N	102	A1EFU	C7-C6	3.59	1.54	1.43
8	G	101	BCL	O2D-CED	3.58	1.53	1.45
9	l	104	A1EFU	C11-C10	3.58	1.54	1.43
8	l	102	BCL	O2D-CED	3.57	1.53	1.45
9	s	102	A1EFU	C11-C10	3.56	1.54	1.43
9	N	102	A1EFU	C11-C10	3.55	1.54	1.43
9	2	102	A1EFU	C7-C6	3.54	1.54	1.43
9	v	102	A1EFU	C7-C6	3.54	1.54	1.43

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	104	A1EFU	C7-C6	3.54	1.54	1.43
9	2	102	A1EFU	C11-C10	3.53	1.54	1.43
9	G	104	A1EFU	C11-C10	3.53	1.54	1.43
9	v	102	A1EFU	C11-C10	3.53	1.54	1.43
9	J	102	A1EFU	C7-C6	3.53	1.54	1.43
9	E	102	A1EFU	C7-C6	3.53	1.54	1.43
9	Q	102	A1EFU	C7-C6	3.53	1.54	1.43
9	2	101	A1EFU	C7-C6	3.52	1.54	1.43
9	A	102	A1EFU	C7-C6	3.52	1.54	1.43
9	k	102	A1EFU	C7-C6	3.51	1.54	1.43
9	K	102	A1EFU	C7-C6	3.51	1.54	1.43
9	1	104	A1EFU	C16-C17	3.51	1.54	1.43
9	Q	103	A1EFU	C7-C6	3.51	1.54	1.43
9	a	103	A1EFU	C7-C6	3.50	1.54	1.43
9	D	105	A1EFU	C7-C6	3.50	1.54	1.43
9	M	407	A1EFU	C11-C10	3.50	1.54	1.43
9	d	102	A1EFU	C7-C6	3.50	1.54	1.43
9	R	101	A1EFU	C7-C6	3.49	1.54	1.43
9	K	102	A1EFU	C11-C10	3.49	1.54	1.43
9	Q	102	A1EFU	C11-C10	3.49	1.54	1.43
9	N	103	A1EFU	C7-C6	3.49	1.54	1.43
9	1	101	A1EFU	C7-C6	3.48	1.54	1.43
9	a	101	A1EFU	C7-C6	3.48	1.54	1.43
9	R	101	A1EFU	C11-C10	3.48	1.54	1.43
9	I	101	A1EFU	C11-C10	3.48	1.54	1.43
9	v	103	A1EFU	C7-C6	3.47	1.54	1.43
9	G	105	A1EFU	C11-C10	3.47	1.54	1.43
9	t	102	A1EFU	C11-C10	3.47	1.54	1.43
9	J	102	A1EFU	C11-C10	3.47	1.54	1.43
9	t	102	A1EFU	C7-C6	3.47	1.54	1.43
9	T	101	A1EFU	C7-C6	3.47	1.54	1.43
9	r	102	A1EFU	C7-C6	3.47	1.54	1.43
9	e	101	A1EFU	C7-C6	3.47	1.54	1.43
9	S	102	A1EFU	C7-C6	3.47	1.54	1.43
9	G	104	A1EFU	C7-C6	3.47	1.54	1.43
9	T	101	A1EFU	C11-C10	3.47	1.54	1.43
9	N	103	A1EFU	C11-C10	3.46	1.54	1.43
9	1	101	A1EFU	C11-C10	3.46	1.54	1.43
9	B	102	A1EFU	C11-C10	3.46	1.54	1.43
8	A	101	BCL	O2D-CED	3.46	1.53	1.45
9	I	103	A1EFU	C11-C10	3.46	1.54	1.43
9	I	101	A1EFU	C7-C6	3.46	1.54	1.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	Q	103	A1EFU	C11-C10	3.46	1.54	1.43
9	G	105	A1EFU	C7-C6	3.45	1.54	1.43
9	I	103	A1EFU	C7-C6	3.45	1.54	1.43
8	v	101	BCL	O2D-CED	3.45	1.53	1.45
9	v	103	A1EFU	C11-C10	3.45	1.54	1.43
8	Q	101	BCL	O2D-CED	3.45	1.53	1.45
9	E	102	A1EFU	C11-C10	3.45	1.54	1.43
9	D	104	A1EFU	C11-C10	3.45	1.54	1.43
9	B	102	A1EFU	C7-C6	3.44	1.54	1.43
8	V	101	BCL	O2D-CED	3.44	1.53	1.45
9	k	102	A1EFU	C11-C10	3.44	1.54	1.43
8	N	101	BCL	O2D-CED	3.44	1.53	1.45
8	B	101	BCL	O2D-CED	3.44	1.53	1.45
9	2	101	A1EFU	C11-C10	3.44	1.54	1.43
9	J	103	A1EFU	C7-C6	3.44	1.54	1.43
9	M	407	A1EFU	C7-C6	3.44	1.54	1.43
8	t	101	BCL	O2D-CED	3.44	1.53	1.45
8	R	102	BCL	O2D-CED	3.44	1.53	1.45
8	F	102	BCL	O2D-CED	3.44	1.53	1.45
8	E	101	BCL	O2D-CED	3.44	1.53	1.45
9	r	102	A1EFU	C11-C10	3.44	1.54	1.43
8	i	101	BCL	O2D-CED	3.44	1.53	1.45
9	l	104	A1EFU	C15-C14	3.43	1.54	1.43
8	M	402	BCL	O2D-CED	3.43	1.53	1.45
9	J	103	A1EFU	C11-C10	3.43	1.54	1.43
9	F	105	A1EFU	C7-C6	3.43	1.54	1.43
8	s	101	BCL	O2D-CED	3.43	1.53	1.45
8	K	101	BCL	O2D-CED	3.43	1.53	1.45
9	a	103	A1EFU	C11-C10	3.43	1.54	1.43
8	d	101	BCL	O2D-CED	3.43	1.53	1.45
8	I	102	BCL	O2D-CED	3.43	1.53	1.45
9	S	102	A1EFU	C11-C10	3.43	1.54	1.43
8	b	101	BCL	O2D-CED	3.43	1.53	1.45
9	d	102	A1EFU	C11-C10	3.43	1.54	1.43
8	D	101	BCL	O2D-CED	3.43	1.53	1.45
8	a	102	BCL	O2D-CED	3.43	1.53	1.45
8	P	101	BCL	O2D-CED	3.43	1.53	1.45
9	a	101	A1EFU	C11-C10	3.43	1.54	1.43
8	G	102	BCL	O2D-CED	3.42	1.53	1.45
8	j	101	BCL	O2D-CED	3.42	1.53	1.45
8	S	101	BCL	O2D-CED	3.42	1.53	1.45
9	A	102	A1EFU	C11-C10	3.42	1.54	1.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	k	101	BCL	O2D-CED	3.42	1.53	1.45
8	q	101	BCL	O2D-CED	3.42	1.53	1.45
16	C	401	HEC	CBC-CAC	-3.41	1.36	1.49
8	J	101	BCL	O2D-CED	3.41	1.53	1.45
9	F	105	A1EFU	C11-C10	3.41	1.54	1.43
8	n	101	BCL	O2D-CED	3.41	1.53	1.45
9	e	101	A1EFU	C11-C10	3.41	1.54	1.43
8	r	101	BCL	O2D-CED	3.40	1.53	1.45
9	2	102	A1EFU	C16-C17	3.40	1.54	1.43
8	1	103	BCL	O2D-CED	3.40	1.53	1.45
9	2	102	A1EFU	C15-C14	3.40	1.54	1.43
9	D	105	A1EFU	C11-C10	3.39	1.54	1.43
16	C	402	HEC	CBC-CAC	-3.39	1.36	1.49
8	M	403	BCL	O2D-CED	3.39	1.53	1.45
9	s	102	A1EFU	C20-C21	3.38	1.53	1.43
8	e	102	BCL	O2D-CED	3.37	1.53	1.45
9	v	102	A1EFU	C20-C21	3.37	1.53	1.43
9	I	101	A1EFU	C16-C17	3.37	1.53	1.43
9	2	102	A1EFU	C20-C21	3.37	1.53	1.43
9	N	102	A1EFU	C16-C17	3.37	1.53	1.43
9	K	102	A1EFU	C16-C17	3.37	1.53	1.43
8	T	102	BCL	O2D-CED	3.37	1.53	1.45
8	L	306	BCL	O2D-CED	3.36	1.53	1.45
8	L	303	BCL	O2D-CED	3.35	1.53	1.45
9	s	102	A1EFU	C16-C17	3.35	1.53	1.43
9	K	102	A1EFU	C20-C21	3.34	1.53	1.43
16	C	403	HEC	CBC-CAC	-3.34	1.37	1.49
9	N	103	A1EFU	C16-C17	3.33	1.53	1.43
9	J	102	A1EFU	C16-C17	3.33	1.53	1.43
9	v	102	A1EFU	C16-C17	3.32	1.53	1.43
9	1	104	A1EFU	C20-C21	3.32	1.53	1.43
9	s	102	A1EFU	C15-C14	3.31	1.53	1.43
9	Q	103	A1EFU	C15-C14	3.31	1.53	1.43
9	J	102	A1EFU	C20-C21	3.31	1.53	1.43
9	K	102	A1EFU	C15-C14	3.31	1.53	1.43
9	N	103	A1EFU	C15-C14	3.31	1.53	1.43
9	v	102	A1EFU	C15-C14	3.30	1.53	1.43
9	G	104	A1EFU	C20-C21	3.29	1.53	1.43
9	Q	103	A1EFU	C20-C21	3.29	1.53	1.43
9	N	102	A1EFU	C15-C14	3.29	1.53	1.43
9	M	407	A1EFU	C20-C21	3.29	1.53	1.43
9	t	102	A1EFU	C16-C17	3.28	1.53	1.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	103	A1EFU	C20-C21	3.28	1.53	1.43
9	t	102	A1EFU	C20-C21	3.28	1.53	1.43
9	2	101	A1EFU	C15-C14	3.28	1.53	1.43
9	M	407	A1EFU	C15-C14	3.28	1.53	1.43
9	d	102	A1EFU	C20-C21	3.28	1.53	1.43
9	G	104	A1EFU	C16-C17	3.28	1.53	1.43
9	Q	103	A1EFU	C16-C17	3.28	1.53	1.43
9	T	101	A1EFU	C20-C21	3.27	1.53	1.43
9	a	103	A1EFU	C20-C21	3.27	1.53	1.43
9	I	101	A1EFU	C20-C21	3.27	1.53	1.43
9	A	102	A1EFU	C20-C21	3.27	1.53	1.43
9	I	101	A1EFU	C15-C14	3.27	1.53	1.43
9	a	101	A1EFU	C20-C21	3.27	1.53	1.43
9	A	102	A1EFU	C16-C17	3.27	1.53	1.43
9	e	101	A1EFU	C20-C21	3.26	1.53	1.43
9	Q	102	A1EFU	C20-C21	3.26	1.53	1.43
9	T	101	A1EFU	C16-C17	3.26	1.53	1.43
9	D	105	A1EFU	C20-C21	3.26	1.53	1.43
9	G	105	A1EFU	C20-C21	3.26	1.53	1.43
9	D	104	A1EFU	C16-C17	3.26	1.53	1.43
9	a	101	A1EFU	C15-C14	3.26	1.53	1.43
9	2	101	A1EFU	C20-C21	3.26	1.53	1.43
9	1	101	A1EFU	C16-C17	3.26	1.53	1.43
9	D	104	A1EFU	C20-C21	3.26	1.53	1.43
9	Q	102	A1EFU	C15-C14	3.26	1.53	1.43
9	J	102	A1EFU	C15-C14	3.26	1.53	1.43
9	k	102	A1EFU	C20-C21	3.26	1.53	1.43
9	r	102	A1EFU	C20-C21	3.25	1.53	1.43
9	M	407	A1EFU	C16-C17	3.25	1.53	1.43
9	a	103	A1EFU	C16-C17	3.25	1.53	1.43
9	1	101	A1EFU	C20-C21	3.25	1.53	1.43
9	k	102	A1EFU	C15-C14	3.25	1.53	1.43
9	J	103	A1EFU	C20-C21	3.25	1.53	1.43
9	G	104	A1EFU	C15-C14	3.25	1.53	1.43
9	R	101	A1EFU	C16-C17	3.25	1.53	1.43
9	S	102	A1EFU	C20-C21	3.24	1.53	1.43
9	T	101	A1EFU	C15-C14	3.24	1.53	1.43
9	v	103	A1EFU	C20-C21	3.24	1.53	1.43
9	S	102	A1EFU	C15-C14	3.24	1.53	1.43
9	E	102	A1EFU	C16-C17	3.24	1.53	1.43
9	N	102	A1EFU	C20-C21	3.24	1.53	1.43
9	e	101	A1EFU	C16-C17	3.24	1.53	1.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	102	A1EFU	C16-C17	3.23	1.53	1.43
9	R	101	A1EFU	C15-C14	3.23	1.53	1.43
9	I	103	A1EFU	C15-C14	3.23	1.53	1.43
9	d	102	A1EFU	C16-C17	3.23	1.53	1.43
9	t	102	A1EFU	C15-C14	3.23	1.53	1.43
9	D	105	A1EFU	C16-C17	3.23	1.53	1.43
9	N	103	A1EFU	C20-C21	3.23	1.53	1.43
9	J	103	A1EFU	C15-C14	3.23	1.53	1.43
9	R	101	A1EFU	C20-C21	3.22	1.53	1.43
9	l	101	A1EFU	C15-C14	3.22	1.53	1.43
9	A	102	A1EFU	C15-C14	3.22	1.53	1.43
9	B	102	A1EFU	C20-C21	3.22	1.53	1.43
9	r	102	A1EFU	C16-C17	3.22	1.53	1.43
9	S	102	A1EFU	C16-C17	3.22	1.53	1.43
9	Q	102	A1EFU	C16-C17	3.22	1.53	1.43
9	a	101	A1EFU	C16-C17	3.22	1.53	1.43
9	J	103	A1EFU	C16-C17	3.22	1.53	1.43
9	D	105	A1EFU	C15-C14	3.21	1.53	1.43
9	F	105	A1EFU	C20-C21	3.21	1.53	1.43
9	F	105	A1EFU	C16-C17	3.21	1.53	1.43
9	k	102	A1EFU	C16-C17	3.21	1.53	1.43
9	B	102	A1EFU	C15-C14	3.21	1.53	1.43
9	2	101	A1EFU	C16-C17	3.21	1.53	1.43
9	E	102	A1EFU	C20-C21	3.20	1.53	1.43
9	G	105	A1EFU	C16-C17	3.20	1.53	1.43
9	D	104	A1EFU	C15-C14	3.20	1.53	1.43
9	e	101	A1EFU	C15-C14	3.20	1.53	1.43
9	E	102	A1EFU	C15-C14	3.19	1.53	1.43
9	v	103	A1EFU	C16-C17	3.18	1.53	1.43
9	d	102	A1EFU	C15-C14	3.18	1.53	1.43
9	v	103	A1EFU	C15-C14	3.17	1.53	1.43
9	G	105	A1EFU	C15-C14	3.17	1.53	1.43
9	a	103	A1EFU	C15-C14	3.17	1.53	1.43
9	F	105	A1EFU	C15-C14	3.16	1.53	1.43
9	r	102	A1EFU	C15-C14	3.16	1.53	1.43
9	I	103	A1EFU	C16-C17	3.16	1.53	1.43
10	M	406	MW9	C7-C6	-3.14	1.34	1.51
10	M	405	MW9	C7-C6	-3.14	1.34	1.51
10	D	102	MW9	C7-C6	-3.13	1.34	1.51
10	F	104	MW9	C7-C6	-3.13	1.34	1.51
10	L	310	MW9	O1-C17	3.12	1.42	1.33
10	D	103	MW9	C7-C6	-3.11	1.34	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	G	103	MW9	C7-C6	-3.10	1.34	1.51
8	I	103	BCL	O2A-CGA	-3.06	1.24	1.33
8	J	101	BCL	O2A-CGA	-3.06	1.24	1.33
10	M	406	MW9	O1-C17	3.05	1.42	1.33
8	N	101	BCL	O2A-CGA	-3.05	1.24	1.33
8	G	102	BCL	O2A-CGA	-3.05	1.24	1.33
8	P	101	BCL	O2A-CGA	-3.04	1.24	1.33
10	H	302	MW9	P-O5	3.04	1.66	1.54
8	K	101	BCL	O2A-CGA	-3.03	1.24	1.33
10	L	309	MW9	O1-C17	3.02	1.42	1.33
10	G	103	MW9	O1-C17	3.02	1.42	1.33
8	T	102	BCL	O2A-CGA	-3.01	1.24	1.33
8	F	102	BCL	O2A-CGA	-3.01	1.24	1.33
8	D	101	BCL	O2A-CGA	-3.01	1.24	1.33
8	V	101	BCL	O2A-CGA	-3.00	1.24	1.33
8	L	303	BCL	O2A-CGA	-3.00	1.24	1.33
10	D	102	MW9	O1-C17	3.00	1.42	1.33
10	I	104	MW9	O1-C17	3.00	1.42	1.33
10	M	405	MW9	O1-C17	3.00	1.42	1.33
8	I	102	BCL	O2A-CGA	-2.99	1.24	1.33
8	R	102	BCL	O2A-CGA	-2.99	1.24	1.33
8	q	101	BCL	O2A-CGA	-2.99	1.24	1.33
8	B	101	BCL	O2A-CGA	-2.99	1.24	1.33
8	M	403	BCL	O2A-CGA	-2.99	1.24	1.33
8	t	101	BCL	O2A-CGA	-2.99	1.24	1.33
10	D	103	MW9	O1-C17	2.99	1.42	1.33
8	I	102	BCL	O2D-CGD	-2.98	1.25	1.33
8	s	101	BCL	O2A-CGA	-2.98	1.24	1.33
10	H	302	MW9	O1-C17	2.98	1.42	1.33
8	Q	101	BCL	O2A-CGA	-2.98	1.24	1.33
8	i	101	BCL	O2D-CGD	-2.98	1.25	1.33
10	Q	104	MW9	O1-C17	2.97	1.42	1.33
8	j	101	BCL	O2A-CGA	-2.97	1.24	1.33
8	r	101	BCL	O2A-CGA	-2.97	1.24	1.33
8	i	101	BCL	O2A-CGA	-2.97	1.24	1.33
8	L	306	BCL	O2A-CGA	-2.97	1.24	1.33
8	A	101	BCL	O2A-CGA	-2.97	1.24	1.33
8	S	101	BCL	O2A-CGA	-2.97	1.24	1.33
8	v	101	BCL	O2A-CGA	-2.97	1.24	1.33
8	d	101	BCL	O2D-CGD	-2.97	1.26	1.33
8	M	402	BCL	O2A-CGA	-2.97	1.24	1.33
8	G	102	BCL	O2D-CGD	-2.96	1.26	1.33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	101	BCL	O2D-CGD	-2.96	1.26	1.33
10	F	103	MW9	O1-C17	2.96	1.42	1.33
8	e	102	BCL	O2A-CGA	-2.96	1.24	1.33
8	l	102	BCL	O2A-CGA	-2.95	1.24	1.33
8	n	101	BCL	O2A-CGA	-2.95	1.24	1.33
8	E	101	BCL	O2A-CGA	-2.95	1.24	1.33
10	F	104	MW9	O1-C17	2.95	1.42	1.33
8	E	101	BCL	O2D-CGD	-2.94	1.26	1.33
8	k	101	BCL	O2A-CGA	-2.94	1.24	1.33
8	a	102	BCL	O2A-CGA	-2.94	1.24	1.33
8	d	101	BCL	O2A-CGA	-2.94	1.24	1.33
8	F	101	BCL	O2A-CGA	-2.94	1.24	1.33
8	P	102	BCL	O2A-CGA	-2.93	1.24	1.33
8	G	101	BCL	O2A-CGA	-2.93	1.24	1.33
8	b	101	BCL	O2A-CGA	-2.92	1.24	1.33
8	L	303	BCL	O1A-CGA	-2.92	1.13	1.22
8	K	101	BCL	O2D-CGD	-2.90	1.26	1.33
8	L	306	BCL	O2D-CGD	-2.90	1.26	1.33
8	V	101	BCL	O2D-CGD	-2.89	1.26	1.33
8	e	102	BCL	O2D-CGD	-2.89	1.26	1.33
8	T	102	BCL	O2D-CGD	-2.89	1.26	1.33
8	M	403	BCL	O2D-CGD	-2.89	1.26	1.33
8	r	101	BCL	O2D-CGD	-2.88	1.26	1.33
8	B	101	BCL	O2D-CGD	-2.88	1.26	1.33
8	j	101	BCL	O2D-CGD	-2.87	1.26	1.33
8	q	101	BCL	O2D-CGD	-2.87	1.26	1.33
8	a	102	BCL	O2D-CGD	-2.87	1.26	1.33
8	k	101	BCL	O2D-CGD	-2.87	1.26	1.33
8	B	101	BCL	O1A-CGA	-2.86	1.14	1.22
8	A	101	BCL	O2D-CGD	-2.86	1.26	1.33
8	R	102	BCL	O2D-CGD	-2.86	1.26	1.33
8	v	101	BCL	O2D-CGD	-2.86	1.26	1.33
8	s	101	BCL	O2D-CGD	-2.85	1.26	1.33
8	L	303	BCL	O2D-CGD	-2.85	1.26	1.33
8	R	102	BCL	O1A-CGA	-2.85	1.14	1.22
8	P	101	BCL	O2D-CGD	-2.85	1.26	1.33
8	P	101	BCL	O1A-CGA	-2.85	1.14	1.22
8	b	101	BCL	O2D-CGD	-2.85	1.26	1.33
8	K	101	BCL	O1A-CGA	-2.85	1.14	1.22
8	D	101	BCL	O2D-CGD	-2.85	1.26	1.33
8	Q	101	BCL	O1A-CGA	-2.85	1.14	1.22
8	I	102	BCL	O1A-CGA	-2.84	1.14	1.22

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	n	101	BCL	O2D-CGD	-2.84	1.26	1.33
8	L	306	BCL	O1A-CGA	-2.84	1.14	1.22
8	N	101	BCL	O2D-CGD	-2.84	1.26	1.33
8	M	402	BCL	O2D-CGD	-2.84	1.26	1.33
8	S	101	BCL	O2D-CGD	-2.84	1.26	1.33
8	l	103	BCL	O1A-CGA	-2.84	1.14	1.22
8	Q	101	BCL	O2D-CGD	-2.84	1.26	1.33
8	G	102	BCL	O1A-CGA	-2.84	1.14	1.22
14	L	304	BPH	C3B-C2B	2.83	1.44	1.39
8	t	101	BCL	O2D-CGD	-2.83	1.26	1.33
8	l	103	BCL	O2D-CGD	-2.83	1.26	1.33
8	D	101	BCL	O1A-CGA	-2.83	1.14	1.22
8	k	101	BCL	O1A-CGA	-2.82	1.14	1.22
8	d	101	BCL	O1A-CGA	-2.82	1.14	1.22
8	S	101	BCL	O1A-CGA	-2.82	1.14	1.22
8	N	101	BCL	O1A-CGA	-2.81	1.14	1.22
8	M	402	BCL	O1A-CGA	-2.81	1.14	1.22
8	T	102	BCL	O1A-CGA	-2.81	1.14	1.22
8	V	101	BCL	O1A-CGA	-2.81	1.14	1.22
8	M	403	BCL	O1A-CGA	-2.81	1.14	1.22
8	s	101	BCL	O1A-CGA	-2.80	1.14	1.22
8	P	102	BCL	O1A-CGA	-2.80	1.14	1.22
8	j	101	BCL	O1A-CGA	-2.80	1.14	1.22
8	b	101	BCL	O1A-CGA	-2.80	1.14	1.22
8	n	101	BCL	O1A-CGA	-2.80	1.14	1.22
8	i	101	BCL	O1A-CGA	-2.80	1.14	1.22
8	e	102	BCL	O1A-CGA	-2.80	1.14	1.22
8	J	101	BCL	O1A-CGA	-2.79	1.14	1.22
8	F	101	BCL	O1A-CGA	-2.79	1.14	1.22
8	l	102	BCL	O2D-CGD	-2.79	1.26	1.33
8	r	101	BCL	O1A-CGA	-2.79	1.14	1.22
8	G	101	BCL	O1A-CGA	-2.79	1.14	1.22
8	v	101	BCL	O1A-CGA	-2.78	1.14	1.22
8	q	101	BCL	O1A-CGA	-2.78	1.14	1.22
8	a	102	BCL	O1A-CGA	-2.78	1.14	1.22
8	A	101	BCL	O1A-CGA	-2.78	1.14	1.22
8	t	101	BCL	O1A-CGA	-2.77	1.14	1.22
8	l	102	BCL	O1A-CGA	-2.77	1.14	1.22
8	F	102	BCL	O2D-CGD	-2.77	1.26	1.33
10	M	406	MW9	O8-C24	2.76	1.42	1.34
10	D	103	MW9	O8-C24	2.74	1.42	1.34
8	G	101	BCL	O2D-CGD	-2.74	1.26	1.33

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	P	102	BCL	O2D-CGD	-2.72	1.26	1.33
13	L	307	LMT	O3'-C3'	-2.71	1.36	1.43
10	Q	104	MW9	O8-C24	2.69	1.41	1.34
10	L	310	MW9	O8-C24	2.69	1.41	1.34
10	G	103	MW9	O8-C24	2.68	1.41	1.34
10	H	302	MW9	O8-C24	2.67	1.41	1.34
13	L	308	LMT	O3'-C3'	-2.67	1.36	1.43
10	I	104	MW9	O8-C24	2.67	1.41	1.34
10	F	104	MW9	O8-C24	2.66	1.41	1.34
10	D	102	MW9	O8-C24	2.66	1.41	1.34
10	F	103	MW9	O8-C24	2.66	1.41	1.34
13	H	301	LMT	O3'-C3'	-2.66	1.36	1.43
8	n	101	BCL	C4B-NB	2.66	1.37	1.35
13	L	301	LMT	O3'-C3'	-2.64	1.36	1.43
10	L	309	MW9	O8-C24	2.64	1.41	1.34
10	D	102	MW9	O8-C19	-2.64	1.40	1.46
8	E	101	BCL	O1A-CGA	-2.62	1.14	1.22
13	C	404	LMT	O3'-C3'	-2.62	1.36	1.43
10	M	405	MW9	O8-C24	2.62	1.41	1.34
8	r	101	BCL	C4B-NB	2.61	1.37	1.35
8	d	101	BCL	C1D-C2D	-2.60	1.40	1.45
15	H	303	CDL	OB6-CB4	-2.59	1.40	1.46
8	F	102	BCL	O1A-CGA	-2.57	1.14	1.22
8	F	101	BCL	O2D-CGD	-2.57	1.26	1.33
10	F	104	MW9	O8-C19	-2.57	1.40	1.46
10	M	405	MW9	O8-C19	-2.57	1.40	1.46
10	F	103	MW9	O8-C19	-2.56	1.40	1.46
10	I	104	MW9	O8-C19	-2.55	1.40	1.46
10	G	103	MW9	O8-C19	-2.53	1.40	1.46
10	L	309	MW9	O8-C19	-2.51	1.40	1.46
8	Q	101	BCL	C1D-C2D	-2.50	1.40	1.45
10	Q	104	MW9	O8-C19	-2.49	1.40	1.46
10	H	302	MW9	C6-C7	-2.49	1.34	1.51
10	I	104	MW9	C6-C7	-2.49	1.34	1.51
10	M	406	MW9	O8-C19	-2.49	1.40	1.46
10	H	302	MW9	O8-C19	-2.48	1.40	1.46
8	b	101	BCL	C1D-C2D	-2.48	1.40	1.45
10	L	310	MW9	O8-C19	-2.48	1.40	1.46
8	P	102	BCL	C4B-NB	2.48	1.37	1.35
8	F	102	BCL	C3D-C4D	-2.48	1.38	1.44
10	F	103	MW9	C6-C7	-2.47	1.34	1.51
10	D	103	MW9	O8-C19	-2.47	1.40	1.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	S	101	BCL	C1D-C2D	-2.46	1.40	1.45
8	L	303	BCL	C1D-C2D	-2.44	1.40	1.45
15	L	311	CDL	OB6-CB4	-2.44	1.40	1.46
8	1	102	BCL	C1D-C2D	-2.43	1.40	1.45
8	B	101	BCL	C1D-C2D	-2.42	1.40	1.45
15	L	311	CDL	OA8-CA7	2.42	1.40	1.33
8	A	101	BCL	C4B-NB	2.42	1.37	1.35
10	L	309	MW9	C35-C34	-2.41	1.34	1.51
8	G	102	BCL	C1D-C2D	-2.41	1.40	1.45
10	F	104	MW9	C35-C34	-2.41	1.34	1.51
8	D	101	BCL	C1D-C2D	-2.40	1.40	1.45
8	T	102	BCL	C4B-NB	2.40	1.37	1.35
10	F	103	MW9	C35-C34	-2.40	1.34	1.51
8	e	102	BCL	C1D-C2D	-2.40	1.40	1.45
8	F	101	BCL	C1D-C2D	-2.39	1.40	1.45
8	P	102	BCL	C1D-C2D	-2.38	1.40	1.45
8	N	101	BCL	C1D-C2D	-2.38	1.40	1.45
8	E	101	BCL	C1D-C2D	-2.38	1.40	1.45
8	a	102	BCL	C1D-C2D	-2.37	1.40	1.45
15	L	311	CDL	OB8-CB7	2.37	1.40	1.33
8	I	102	BCL	C1D-C2D	-2.37	1.40	1.45
13	L	307	LMT	O2'-C2'	-2.37	1.37	1.43
8	1	103	BCL	C1D-C2D	-2.37	1.40	1.45
8	P	101	BCL	C1D-C2D	-2.36	1.40	1.45
8	R	102	BCL	C1D-C2D	-2.36	1.40	1.45
8	T	102	BCL	C1D-C2D	-2.36	1.40	1.45
13	L	301	LMT	O2'-C2'	-2.35	1.37	1.43
8	d	101	BCL	C3B-CAB	2.35	1.55	1.49
14	L	302	BPH	C3B-C2B	2.35	1.43	1.39
8	q	101	BCL	C1D-C2D	-2.34	1.40	1.45
8	G	101	BCL	C1D-C2D	-2.34	1.40	1.45
8	k	101	BCL	C1D-C2D	-2.34	1.40	1.45
8	s	101	BCL	C1D-C2D	-2.34	1.40	1.45
13	L	301	LMT	O2B-C2B	-2.34	1.37	1.43
15	H	303	CDL	OA8-CA7	2.34	1.40	1.33
8	V	101	BCL	C1D-C2D	-2.33	1.40	1.45
8	L	303	BCL	C4B-NB	2.33	1.37	1.35
8	n	101	BCL	C1D-C2D	-2.33	1.40	1.45
8	A	101	BCL	C1D-C2D	-2.33	1.40	1.45
8	K	101	BCL	C1D-C2D	-2.33	1.40	1.45
8	J	101	BCL	C1D-C2D	-2.33	1.40	1.45
8	L	306	BCL	C1D-C2D	-2.32	1.40	1.45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	L	301	LMT	O3B-C3B	-2.32	1.37	1.43
8	M	403	BCL	C1D-C2D	-2.32	1.40	1.45
13	H	301	LMT	O2'-C2'	-2.32	1.37	1.43
8	n	101	BCL	C3B-C2B	-2.32	1.35	1.39
15	H	303	CDL	OA6-CA4	-2.31	1.40	1.46
8	j	101	BCL	C1D-C2D	-2.30	1.40	1.45
13	C	404	LMT	O2'-C2'	-2.30	1.37	1.43
8	v	101	BCL	C1D-C2D	-2.30	1.40	1.45
16	C	401	HEC	CBB-CAB	-2.30	1.40	1.49
16	C	402	HEC	CBB-CAB	-2.29	1.40	1.49
10	H	302	MW9	C35-C34	-2.29	1.34	1.49
15	H	303	CDL	OB8-CB7	2.29	1.40	1.33
8	r	101	BCL	C1D-C2D	-2.29	1.40	1.45
16	C	403	HEC	CBB-CAB	-2.29	1.40	1.49
9	l	104	A1EFU	C12-C13	2.28	1.50	1.45
13	L	308	LMT	O2'-C2'	-2.28	1.37	1.43
8	i	101	BCL	C1D-C2D	-2.27	1.40	1.45
8	t	101	BCL	C3D-C4D	-2.27	1.39	1.44
15	L	311	CDL	OA6-CA4	-2.27	1.40	1.46
15	H	303	CDL	OA6-CA5	2.26	1.40	1.34
15	L	311	CDL	OA6-CA5	2.26	1.40	1.34
9	s	102	A1EFU	C8-C9	2.25	1.50	1.45
8	P	102	BCL	C3B-C2B	-2.25	1.35	1.39
8	M	402	BCL	C1D-C2D	-2.24	1.40	1.45
8	r	101	BCL	C3B-C2B	-2.24	1.35	1.39
8	A	101	BCL	C3B-C2B	-2.24	1.35	1.39
8	q	101	BCL	C3D-C4D	-2.24	1.39	1.44
8	L	306	BCL	C4B-NB	2.23	1.37	1.35
15	H	303	CDL	OB8-CB6	-2.23	1.40	1.45
9	s	102	A1EFU	C12-C13	2.23	1.50	1.45
8	d	101	BCL	C3D-C4D	-2.23	1.39	1.44
8	R	102	BCL	C4B-NB	2.22	1.37	1.35
8	k	101	BCL	C4B-NB	2.22	1.37	1.35
8	a	102	BCL	C4B-NB	2.21	1.37	1.35
9	v	102	A1EFU	C12-C13	2.20	1.50	1.45
8	G	101	BCL	C3D-C4D	-2.20	1.39	1.44
8	G	102	BCL	C3D-C4D	-2.20	1.39	1.44
9	a	103	A1EFU	C12-C13	2.20	1.50	1.45
8	t	101	BCL	C3B-C2B	-2.19	1.35	1.39
8	e	102	BCL	C3D-C4D	-2.19	1.39	1.44
8	r	101	BCL	C3D-C4D	-2.19	1.39	1.44
8	J	101	BCL	C3D-C4D	-2.19	1.39	1.44

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	L	311	CDL	OB8-CB6	-2.19	1.40	1.45
8	N	101	BCL	C4B-NB	2.19	1.37	1.35
8	E	101	BCL	C3D-C4D	-2.19	1.39	1.44
8	F	102	BCL	C1D-C2D	-2.19	1.41	1.45
8	b	101	BCL	C3D-C4D	-2.19	1.39	1.44
9	l	104	A1EFU	C8-C9	2.18	1.50	1.45
8	I	102	BCL	C3D-C4D	-2.18	1.39	1.44
9	a	103	A1EFU	C8-C9	2.18	1.50	1.45
8	M	403	BCL	C3D-C4D	-2.18	1.39	1.44
8	l	102	BCL	C3D-C4D	-2.18	1.39	1.44
8	S	101	BCL	C3D-C4D	-2.18	1.39	1.44
8	s	101	BCL	C3D-C4D	-2.18	1.39	1.44
8	i	101	BCL	C3D-C4D	-2.17	1.39	1.44
9	k	102	A1EFU	C8-C9	2.17	1.50	1.45
15	L	311	CDL	OB6-CB5	2.16	1.40	1.34
8	j	101	BCL	C3D-C4D	-2.16	1.39	1.44
8	P	102	BCL	C3D-C4D	-2.16	1.39	1.44
8	l	103	BCL	C4B-NB	2.16	1.37	1.35
9	T	101	A1EFU	C12-C13	2.16	1.50	1.45
8	k	101	BCL	C3D-C4D	-2.16	1.39	1.44
8	E	101	BCL	C4B-NB	2.16	1.37	1.35
8	B	101	BCL	C4B-NB	2.15	1.37	1.35
8	R	102	BCL	C3D-C4D	-2.15	1.39	1.44
9	2	102	A1EFU	C12-C13	2.15	1.50	1.45
9	K	102	A1EFU	C12-C13	2.15	1.50	1.45
8	N	101	BCL	C3D-C4D	-2.15	1.39	1.44
9	a	101	A1EFU	C4-C5	2.14	1.50	1.45
8	l	103	BCL	C3D-C4D	-2.14	1.39	1.44
9	l	104	A1EFU	C4-C5	2.14	1.50	1.45
9	G	104	A1EFU	C12-C13	2.14	1.50	1.45
8	l	102	BCL	C4B-NB	2.14	1.37	1.35
9	N	102	A1EFU	C4-C5	2.14	1.50	1.45
15	H	303	CDL	OA8-CA6	-2.14	1.40	1.45
9	v	102	A1EFU	C8-C9	2.14	1.50	1.45
8	K	101	BCL	C3D-C4D	-2.14	1.39	1.44
8	G	102	BCL	C4B-NB	2.14	1.37	1.35
8	L	306	BCL	C3D-C4D	-2.14	1.39	1.44
8	T	102	BCL	C3D-C4D	-2.14	1.39	1.44
8	D	101	BCL	C3D-C4D	-2.13	1.39	1.44
9	Q	102	A1EFU	C12-C13	2.13	1.50	1.45
9	N	102	A1EFU	C8-C9	2.13	1.50	1.45
9	Q	103	A1EFU	C12-C13	2.13	1.50	1.45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	2	101	A1EFU	C8-C9	2.13	1.50	1.45
8	Q	101	BCL	C3D-C4D	-2.13	1.39	1.44
8	T	102	BCL	C1B-NB	2.13	1.37	1.35
15	L	311	CDL	OA8-CA6	-2.13	1.40	1.45
9	I	103	A1EFU	C4-C5	2.13	1.50	1.45
8	q	101	BCL	C4B-NB	2.13	1.37	1.35
9	R	101	A1EFU	C12-C13	2.12	1.50	1.45
9	1	101	A1EFU	C12-C13	2.12	1.50	1.45
9	I	101	A1EFU	C12-C13	2.12	1.50	1.45
9	T	101	A1EFU	C8-C9	2.12	1.50	1.45
9	R	101	A1EFU	C8-C9	2.12	1.50	1.45
8	e	102	BCL	C4B-NB	2.12	1.37	1.35
8	L	303	BCL	C3D-C2D	-2.12	1.33	1.39
8	M	402	BCL	C3D-C4D	-2.12	1.39	1.44
8	n	101	BCL	C3D-C4D	-2.12	1.39	1.44
9	d	102	A1EFU	C4-C5	2.12	1.50	1.45
8	K	101	BCL	C4B-NB	2.12	1.37	1.35
9	Q	103	A1EFU	C4-C5	2.12	1.50	1.45
8	A	101	BCL	C3D-C4D	-2.12	1.39	1.44
9	k	102	A1EFU	C4-C5	2.11	1.50	1.45
8	i	101	BCL	C4B-NB	2.11	1.37	1.35
9	D	104	A1EFU	C12-C13	2.11	1.50	1.45
8	T	102	BCL	C3B-CAB	2.11	1.54	1.49
9	v	102	A1EFU	C4-C5	2.11	1.50	1.45
9	J	103	A1EFU	C4-C5	2.11	1.50	1.45
8	j	101	BCL	C4B-NB	2.11	1.37	1.35
8	v	101	BCL	C3D-C4D	-2.11	1.39	1.44
8	F	101	BCL	C3D-C4D	-2.11	1.39	1.44
9	N	103	A1EFU	C4-C5	2.10	1.50	1.45
8	t	101	BCL	C1D-C2D	-2.10	1.41	1.45
9	S	102	A1EFU	C4-C5	2.10	1.50	1.45
9	2	102	A1EFU	C8-C9	2.10	1.50	1.45
9	a	101	A1EFU	C8-C9	2.10	1.50	1.45
9	v	103	A1EFU	C4-C5	2.10	1.50	1.45
8	V	101	BCL	C3D-C4D	-2.10	1.39	1.44
8	G	101	BCL	C4B-NB	2.10	1.37	1.35
9	D	104	A1EFU	C8-C9	2.09	1.50	1.45
9	A	102	A1EFU	C12-C13	2.09	1.50	1.45
9	2	101	A1EFU	C12-C13	2.09	1.50	1.45
9	s	102	A1EFU	C4-C5	2.09	1.50	1.45
9	1	101	A1EFU	C8-C9	2.09	1.50	1.45
8	P	101	BCL	C3D-C4D	-2.09	1.39	1.44

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	a	103	A1EFU	C4-C5	2.09	1.50	1.45
9	t	102	A1EFU	C4-C5	2.09	1.50	1.45
8	P	101	BCL	C4B-NB	2.09	1.37	1.35
9	2	101	A1EFU	C4-C5	2.09	1.50	1.45
9	T	101	A1EFU	C4-C5	2.09	1.50	1.45
9	2	102	A1EFU	C4-C5	2.09	1.50	1.45
9	e	101	A1EFU	C4-C5	2.08	1.50	1.45
15	H	303	CDL	OB6-CB5	2.08	1.40	1.34
9	t	102	A1EFU	C8-C9	2.08	1.50	1.45
9	K	102	A1EFU	C8-C9	2.08	1.50	1.45
9	D	105	A1EFU	C4-C5	2.08	1.50	1.45
8	a	102	BCL	C3D-C4D	-2.08	1.39	1.44
8	B	101	BCL	C3D-C4D	-2.08	1.39	1.44
9	d	102	A1EFU	C8-C9	2.08	1.50	1.45
9	G	104	A1EFU	C8-C9	2.08	1.50	1.45
9	K	102	A1EFU	C4-C5	2.08	1.50	1.45
9	J	102	A1EFU	C12-C13	2.08	1.50	1.45
9	G	105	A1EFU	C4-C5	2.08	1.50	1.45
8	Q	101	BCL	C3D-C2D	-2.07	1.33	1.39
9	M	407	A1EFU	C12-C13	2.07	1.50	1.45
8	t	101	BCL	C3B-CAB	2.07	1.54	1.49
9	e	101	A1EFU	C8-C9	2.07	1.50	1.45
9	v	103	A1EFU	C8-C9	2.07	1.50	1.45
9	S	102	A1EFU	C8-C9	2.07	1.50	1.45
9	r	102	A1EFU	C4-C5	2.07	1.50	1.45
9	Q	103	A1EFU	C8-C9	2.07	1.50	1.45
9	I	103	A1EFU	C12-C13	2.06	1.50	1.45
9	Q	102	A1EFU	C8-C9	2.06	1.50	1.45
9	J	102	A1EFU	C4-C5	2.06	1.50	1.45
9	J	103	A1EFU	C12-C13	2.06	1.50	1.45
9	D	105	A1EFU	C8-C9	2.06	1.50	1.45
9	B	102	A1EFU	C4-C5	2.06	1.50	1.45
9	S	102	A1EFU	C12-C13	2.06	1.50	1.45
9	N	103	A1EFU	C8-C9	2.06	1.50	1.45
9	I	101	A1EFU	C8-C9	2.06	1.50	1.45
9	A	102	A1EFU	C8-C9	2.06	1.50	1.45
9	J	103	A1EFU	C8-C9	2.05	1.50	1.45
9	N	102	A1EFU	C12-C13	2.05	1.50	1.45
9	G	105	A1EFU	C12-C13	2.05	1.50	1.45
9	E	102	A1EFU	C12-C13	2.05	1.50	1.45
9	v	103	A1EFU	C12-C13	2.05	1.50	1.45
9	M	407	A1EFU	C8-C9	2.05	1.50	1.45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	R	101	A1EFU	C4-C5	2.05	1.50	1.45
9	d	102	A1EFU	C12-C13	2.05	1.50	1.45
9	k	102	A1EFU	C12-C13	2.05	1.50	1.45
9	D	104	A1EFU	C4-C5	2.05	1.50	1.45
9	M	407	A1EFU	C4-C5	2.04	1.50	1.45
9	l	101	A1EFU	C4-C5	2.04	1.50	1.45
9	J	102	A1EFU	C8-C9	2.04	1.50	1.45
9	B	102	A1EFU	C8-C9	2.04	1.50	1.45
8	s	101	BCL	C4B-NB	2.04	1.37	1.35
8	P	101	BCL	C3D-C2D	-2.04	1.33	1.39
9	E	102	A1EFU	C8-C9	2.04	1.50	1.45
9	G	105	A1EFU	C8-C9	2.04	1.50	1.45
9	N	103	A1EFU	C12-C13	2.04	1.50	1.45
9	t	102	A1EFU	C12-C13	2.04	1.50	1.45
8	M	403	BCL	C3D-C2D	-2.04	1.33	1.39
9	a	101	A1EFU	C12-C13	2.04	1.50	1.45
9	Q	102	A1EFU	C4-C5	2.03	1.50	1.45
8	v	101	BCL	C3B-CAB	2.03	1.54	1.49
9	A	102	A1EFU	C4-C5	2.03	1.50	1.45
13	L	301	LMT	O4'-C4B	-2.03	1.38	1.43
8	M	403	BCL	C4B-NB	2.03	1.37	1.35
8	M	403	BCL	C3B-CAB	2.03	1.54	1.49
9	E	102	A1EFU	C4-C5	2.02	1.50	1.45
8	n	101	BCL	C3B-CAB	2.02	1.54	1.49
8	D	101	BCL	C4B-NB	2.02	1.37	1.35
8	R	102	BCL	C3D-C2D	-2.02	1.33	1.39
14	L	304	BPH	C2C-C3C	2.02	1.56	1.54
9	B	102	A1EFU	C12-C13	2.02	1.50	1.45
8	B	101	BCL	C3D-C2D	-2.02	1.33	1.39
8	a	102	BCL	C3B-CAB	2.02	1.54	1.49
9	I	103	A1EFU	C8-C9	2.02	1.50	1.45
8	I	102	BCL	C3D-C2D	-2.01	1.33	1.39
9	e	101	A1EFU	C12-C13	2.01	1.50	1.45
8	B	101	BCL	C3B-CAB	2.01	1.54	1.49
8	J	101	BCL	C3D-C2D	-2.01	1.33	1.39
8	L	306	BCL	C2C-C3C	-2.01	1.48	1.54
9	F	105	A1EFU	C4-C5	2.01	1.50	1.45
10	H	302	MW9	P-O2	2.01	1.66	1.60
8	L	303	BCL	C3D-C4D	-2.01	1.39	1.44
8	j	101	BCL	C2C-C3C	-2.00	1.48	1.54
8	M	402	BCL	C4B-NB	2.00	1.37	1.35
8	D	101	BCL	C3D-C2D	-2.00	1.33	1.39

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	105	A1EFU	C12-C13	2.00	1.50	1.45
9	r	102	A1EFU	C12-C13	2.00	1.50	1.45

All (1799) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	k	102	A1EFU	C11-C10-C9	-10.75	111.97	127.31
9	Q	103	A1EFU	C16-C17-C18	-10.61	112.17	127.31
9	a	103	A1EFU	C15-C14-C13	-10.53	112.29	127.31
9	a	103	A1EFU	C7-C6-C5	-10.43	112.42	127.31
9	Q	102	A1EFU	C16-C17-C18	-10.32	112.58	127.31
9	I	103	A1EFU	C7-C6-C5	-10.20	112.76	127.31
9	J	103	A1EFU	C7-C6-C5	-10.16	112.80	127.31
9	G	105	A1EFU	C7-C6-C5	-10.13	112.85	127.31
9	E	102	A1EFU	C15-C14-C13	-10.10	112.89	127.31
9	F	105	A1EFU	C15-C14-C13	-9.97	113.09	127.31
9	I	103	A1EFU	C11-C10-C9	-9.93	113.14	127.31
9	v	102	A1EFU	C7-C6-C5	-9.92	113.15	127.31
9	M	407	A1EFU	C7-C6-C5	-9.92	113.15	127.31
9	D	105	A1EFU	C11-C10-C9	-9.89	113.20	127.31
9	Q	103	A1EFU	C7-C6-C5	-9.86	113.23	127.31
9	J	103	A1EFU	C11-C10-C9	-9.85	113.26	127.31
9	G	105	A1EFU	C11-C10-C9	-9.79	113.33	127.31
9	a	101	A1EFU	C7-C6-C5	-9.76	113.38	127.31
9	k	102	A1EFU	C7-C6-C5	-9.72	113.44	127.31
9	E	102	A1EFU	C11-C10-C9	-9.70	113.47	127.31
9	B	102	A1EFU	C11-C10-C9	-9.68	113.50	127.31
9	d	102	A1EFU	C7-C6-C5	-9.66	113.52	127.31
9	2	102	A1EFU	C15-C14-C13	-9.62	113.58	127.31
9	S	102	A1EFU	C7-C6-C5	-9.62	113.58	127.31
9	D	105	A1EFU	C15-C14-C13	-9.61	113.59	127.31
9	e	101	A1EFU	C11-C10-C9	-9.60	113.61	127.31
9	N	103	A1EFU	C15-C14-C13	-9.59	113.62	127.31
9	1	101	A1EFU	C15-C14-C13	-9.58	113.63	127.31
9	R	101	A1EFU	C15-C14-C13	-9.58	113.64	127.31
9	t	102	A1EFU	C11-C10-C9	-9.57	113.65	127.31
9	D	105	A1EFU	C7-C6-C5	-9.56	113.66	127.31
9	G	105	A1EFU	C15-C14-C13	-9.54	113.70	127.31
9	A	102	A1EFU	C11-C10-C9	-9.53	113.70	127.31
9	e	101	A1EFU	C7-C6-C5	-9.53	113.71	127.31
9	N	103	A1EFU	C7-C6-C5	-9.49	113.76	127.31
9	S	102	A1EFU	C11-C10-C9	-9.47	113.80	127.31

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	2	101	A1EFU	C11-C10-C9	-9.46	113.81	127.31
9	2	101	A1EFU	C7-C6-C5	-9.45	113.82	127.31
9	J	102	A1EFU	C11-C10-C9	-9.45	113.83	127.31
9	T	101	A1EFU	C15-C14-C13	-9.44	113.84	127.31
9	F	105	A1EFU	C11-C10-C9	-9.44	113.84	127.31
9	r	102	A1EFU	C7-C6-C5	-9.41	113.88	127.31
9	v	103	A1EFU	C7-C6-C5	-9.41	113.88	127.31
9	v	103	A1EFU	C16-C17-C18	-9.40	113.89	127.31
9	t	102	A1EFU	C7-C6-C5	-9.39	113.91	127.31
9	N	102	A1EFU	C11-C10-C9	-9.39	113.91	127.31
9	B	102	A1EFU	C15-C14-C13	-9.37	113.94	127.31
9	N	102	A1EFU	C15-C14-C13	-9.35	113.96	127.31
9	r	102	A1EFU	C15-C14-C13	-9.34	113.98	127.31
9	l	101	A1EFU	C11-C10-C9	-9.33	113.99	127.31
9	D	104	A1EFU	C15-C14-C13	-9.33	113.99	127.31
9	T	101	A1EFU	C7-C6-C5	-9.32	114.01	127.31
9	l	101	A1EFU	C16-C17-C18	-9.32	114.01	127.31
9	M	407	A1EFU	C11-C10-C9	-9.30	114.04	127.31
9	N	103	A1EFU	C11-C10-C9	-9.24	114.12	127.31
9	I	103	A1EFU	C15-C14-C13	-9.24	114.13	127.31
9	K	102	A1EFU	C11-C10-C9	-9.20	114.19	127.31
9	G	105	A1EFU	C16-C17-C18	-9.19	114.20	127.31
9	R	101	A1EFU	C7-C6-C5	-9.16	114.24	127.31
9	I	101	A1EFU	C15-C14-C13	-9.15	114.25	127.31
9	A	102	A1EFU	C15-C14-C13	-9.10	114.32	127.31
9	v	103	A1EFU	C15-C14-C13	-9.10	114.32	127.31
9	Q	103	A1EFU	C11-C10-C9	-9.10	114.32	127.31
9	G	104	A1EFU	C16-C17-C18	-9.10	114.33	127.31
9	J	103	A1EFU	C16-C17-C18	-9.07	114.36	127.31
9	v	102	A1EFU	C11-C10-C9	-9.07	114.37	127.31
9	v	103	A1EFU	C11-C10-C9	-9.05	114.39	127.31
9	d	102	A1EFU	C11-C10-C9	-9.05	114.40	127.31
9	K	102	A1EFU	C15-C14-C13	-9.03	114.42	127.31
9	I	101	A1EFU	C7-C6-C5	-9.03	114.42	127.31
9	I	103	A1EFU	C16-C17-C18	-9.03	114.42	127.31
9	S	102	A1EFU	C16-C17-C18	-9.01	114.45	127.31
9	a	103	A1EFU	C16-C17-C18	-8.98	114.49	127.31
9	D	104	A1EFU	C16-C17-C18	-8.98	114.49	127.31
9	D	105	A1EFU	C16-C17-C18	-8.97	114.51	127.31
9	k	102	A1EFU	C16-C17-C18	-8.97	114.51	127.31
9	J	102	A1EFU	C15-C14-C13	-8.97	114.51	127.31
9	I	101	A1EFU	C11-C10-C9	-8.96	114.53	127.31

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	1	104	A1EFU	C11-C10-C9	-8.96	114.53	127.31
9	R	101	A1EFU	C11-C10-C9	-8.93	114.56	127.31
9	J	103	A1EFU	C15-C14-C13	-8.93	114.56	127.31
9	e	101	A1EFU	C15-C14-C13	-8.93	114.57	127.31
9	t	102	A1EFU	C15-C14-C13	-8.92	114.58	127.31
9	T	101	A1EFU	C11-C10-C9	-8.90	114.60	127.31
9	a	101	A1EFU	C15-C14-C13	-8.90	114.61	127.31
9	I	101	A1EFU	C16-C17-C18	-8.89	114.62	127.31
9	2	101	A1EFU	C15-C14-C13	-8.87	114.66	127.31
9	S	102	A1EFU	C15-C14-C13	-8.85	114.67	127.31
9	G	104	A1EFU	C15-C14-C13	-8.83	114.70	127.31
9	2	101	A1EFU	C16-C17-C18	-8.82	114.72	127.31
9	Q	102	A1EFU	C11-C10-C9	-8.81	114.73	127.31
9	N	102	A1EFU	C7-C6-C5	-8.81	114.73	127.31
9	2	102	A1EFU	C7-C6-C5	-8.78	114.78	127.31
9	a	101	A1EFU	C11-C10-C9	-8.78	114.78	127.31
9	G	104	A1EFU	C7-C6-C5	-8.73	114.84	127.31
10	H	302	MW9	C35-C34-C33	8.72	152.65	112.71
9	K	102	A1EFU	C7-C6-C5	-8.72	114.86	127.31
9	G	104	A1EFU	C11-C10-C9	-8.70	114.89	127.31
9	1	101	A1EFU	C7-C6-C5	-8.64	114.98	127.31
9	2	102	A1EFU	C11-C10-C9	-8.64	114.99	127.31
9	v	102	A1EFU	C15-C14-C13	-8.62	115.00	127.31
9	Q	103	A1EFU	C15-C14-C13	-8.52	115.15	127.31
9	d	102	A1EFU	C15-C14-C13	-8.46	115.24	127.31
9	t	102	A1EFU	C16-C17-C18	-8.45	115.25	127.31
9	D	104	A1EFU	C11-C10-C9	-8.45	115.25	127.31
9	D	104	A1EFU	C7-C6-C5	-8.43	115.29	127.31
9	r	102	A1EFU	C11-C10-C9	-8.42	115.29	127.31
9	a	103	A1EFU	C11-C10-C9	-8.40	115.32	127.31
9	N	103	A1EFU	C16-C17-C18	-8.39	115.33	127.31
9	k	102	A1EFU	C15-C14-C13	-8.38	115.35	127.31
9	B	102	A1EFU	C7-C6-C5	-8.34	115.41	127.31
9	A	102	A1EFU	C7-C6-C5	-8.33	115.42	127.31
9	J	102	A1EFU	C7-C6-C5	-8.30	115.47	127.31
9	A	102	A1EFU	C16-C17-C18	-8.28	115.50	127.31
9	M	407	A1EFU	C15-C14-C13	-8.23	115.56	127.31
9	F	105	A1EFU	C7-C6-C5	-8.23	115.57	127.31
9	1	104	A1EFU	C7-C6-C5	-8.23	115.57	127.31
9	Q	102	A1EFU	C7-C6-C5	-8.22	115.58	127.31
9	d	102	A1EFU	C16-C17-C18	-8.17	115.65	127.31
9	2	102	A1EFU	C16-C17-C18	-8.16	115.66	127.31

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	r	102	A1EFU	C16-C17-C18	-8.15	115.68	127.31
9	J	102	A1EFU	C16-C17-C18	-8.14	115.70	127.31
9	l	104	A1EFU	C15-C14-C13	-8.12	115.73	127.31
9	N	102	A1EFU	C16-C17-C18	-8.10	115.75	127.31
9	v	102	A1EFU	C16-C17-C18	-8.08	115.78	127.31
9	s	102	A1EFU	C15-C14-C13	-8.07	115.80	127.31
9	K	102	A1EFU	C16-C17-C18	-7.99	115.91	127.31
9	a	101	A1EFU	C16-C17-C18	-7.98	115.92	127.31
9	F	105	A1EFU	C16-C17-C18	-7.94	115.98	127.31
9	l	104	A1EFU	C16-C17-C18	-7.91	116.03	127.31
9	s	102	A1EFU	C11-C10-C9	-7.87	116.08	127.31
9	E	102	A1EFU	C16-C17-C18	-7.86	116.09	127.31
9	e	101	A1EFU	C16-C17-C18	-7.84	116.12	127.31
9	M	407	A1EFU	C16-C17-C18	-7.81	116.16	127.31
9	E	102	A1EFU	C7-C6-C5	-7.81	116.17	127.31
9	s	102	A1EFU	C16-C17-C18	-7.78	116.20	127.31
9	B	102	A1EFU	C16-C17-C18	-7.76	116.24	127.31
9	T	101	A1EFU	C16-C17-C18	-7.67	116.37	127.31
9	Q	102	A1EFU	C15-C14-C13	-7.62	116.43	127.31
9	R	101	A1EFU	C16-C17-C18	-7.61	116.45	127.31
9	s	102	A1EFU	C7-C6-C5	-7.27	116.93	127.31
10	M	405	MW9	C35-C34-C33	7.06	152.88	112.43
10	Q	104	MW9	C35-C34-C33	7.03	152.72	112.43
10	M	406	MW9	C35-C34-C33	7.03	152.71	112.43
10	G	103	MW9	C35-C34-C33	6.98	152.44	112.43
10	D	103	MW9	C35-C34-C33	6.98	152.42	112.43
8	L	303	BCL	C1D-ND-C4D	-6.58	101.66	106.33
9	a	103	A1EFU	CM4-C9-C10	-6.50	113.82	122.92
8	d	101	BCL	CMB-C2B-C1B	-6.47	118.53	128.46
8	G	101	BCL	CMB-C2B-C1B	-6.45	118.54	128.46
8	k	101	BCL	CMB-C2B-C1B	-6.40	118.62	128.46
8	n	101	BCL	C1D-ND-C4D	-6.38	101.80	106.33
8	P	102	BCL	C1D-ND-C4D	-6.36	101.81	106.33
8	i	101	BCL	C1D-ND-C4D	-6.36	101.82	106.33
8	v	101	BCL	CMB-C2B-C1B	-6.36	118.69	128.46
8	L	306	BCL	CMB-C2B-C1B	-6.33	118.73	128.46
9	Q	102	A1EFU	C16-C15-C14	-6.33	110.50	123.47
8	l	103	BCL	CMB-C2B-C1B	-6.33	118.74	128.46
8	D	101	BCL	CMB-C2B-C1B	-6.32	118.75	128.46
8	r	101	BCL	C1D-ND-C4D	-6.32	101.85	106.33
8	a	102	BCL	CMB-C2B-C1B	-6.32	118.75	128.46
8	G	102	BCL	CMB-C2B-C1B	-6.31	118.77	128.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	102	BCL	CMB-C2B-C1B	-6.30	118.78	128.46
8	i	101	BCL	CMB-C2B-C1B	-6.30	118.78	128.46
9	Q	103	A1EFU	CM6-C18-C17	-6.30	114.10	122.92
9	Q	102	A1EFU	CM6-C18-C17	-6.29	114.12	122.92
8	q	101	BCL	CMB-C2B-C1B	-6.28	118.81	128.46
8	T	102	BCL	C1D-ND-C4D	-6.27	101.88	106.33
8	N	101	BCL	CMB-C2B-C1B	-6.27	118.83	128.46
8	Q	101	BCL	CMB-C2B-C1B	-6.26	118.83	128.46
8	R	102	BCL	CMB-C2B-C1B	-6.26	118.84	128.46
8	L	303	BCL	CMB-C2B-C1B	-6.26	118.84	128.46
8	e	102	BCL	CMB-C2B-C1B	-6.26	118.84	128.46
8	l	102	BCL	C1D-ND-C4D	-6.26	101.89	106.33
8	P	101	BCL	CMB-C2B-C1B	-6.26	118.84	128.46
8	J	101	BCL	CMB-C2B-C1B	-6.26	118.85	128.46
8	k	101	BCL	C1D-ND-C4D	-6.25	101.89	106.33
8	s	101	BCL	C1D-ND-C4D	-6.24	101.90	106.33
8	q	101	BCL	C1D-ND-C4D	-6.24	101.90	106.33
8	j	101	BCL	CMB-C2B-C1B	-6.24	118.88	128.46
8	F	101	BCL	CMB-C2B-C1B	-6.24	118.88	128.46
8	F	102	BCL	CMB-C2B-C1B	-6.23	118.89	128.46
8	L	306	BCL	C1D-ND-C4D	-6.23	101.91	106.33
8	E	101	BCL	CMB-C2B-C1B	-6.23	118.89	128.46
8	M	402	BCL	CMB-C2B-C1B	-6.22	118.91	128.46
8	b	101	BCL	CMB-C2B-C1B	-6.20	118.93	128.46
8	l	102	BCL	CMB-C2B-C1B	-6.20	118.94	128.46
8	S	101	BCL	CMB-C2B-C1B	-6.19	118.95	128.46
8	M	403	BCL	CMB-C2B-C1B	-6.18	118.96	128.46
8	K	101	BCL	CMB-C2B-C1B	-6.18	118.97	128.46
8	B	101	BCL	CMB-C2B-C1B	-6.17	118.98	128.46
8	a	102	BCL	C1D-ND-C4D	-6.16	101.96	106.33
10	F	103	MW9	C35-C34-C33	6.15	152.47	112.55
8	s	101	BCL	CMB-C2B-C1B	-6.14	119.02	128.46
10	F	104	MW9	C35-C34-C33	6.14	152.44	112.55
9	E	102	A1EFU	C15-C16-C17	-6.14	110.89	123.47
8	j	101	BCL	C1D-ND-C4D	-6.14	101.97	106.33
9	a	103	A1EFU	CM5-C13-C14	-6.14	114.33	122.92
8	N	101	BCL	C1D-ND-C4D	-6.13	101.98	106.33
8	e	102	BCL	C1D-ND-C4D	-6.13	101.98	106.33
9	F	105	A1EFU	C15-C16-C17	-6.12	110.93	123.47
10	L	309	MW9	C35-C34-C33	6.12	152.30	112.55
8	B	101	BCL	C1D-ND-C4D	-6.12	101.99	106.33
8	b	101	BCL	C1D-ND-C4D	-6.11	101.99	106.33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	R	101	A1EFU	C15-C16-C17	-6.08	111.03	123.47
8	G	101	BCL	C1D-ND-C4D	-6.07	102.02	106.33
8	M	403	BCL	C1D-ND-C4D	-6.06	102.03	106.33
8	L	303	BCL	C2D-C1D-ND	6.05	114.56	110.10
8	A	101	BCL	C1D-ND-C4D	-6.01	102.07	106.33
8	M	402	BCL	C1D-ND-C4D	-6.00	102.07	106.33
8	P	101	BCL	C1D-ND-C4D	-5.99	102.08	106.33
8	S	101	BCL	C1D-ND-C4D	-5.97	102.09	106.33
9	e	101	A1EFU	CM3-C5-C6	-5.90	114.65	122.92
9	B	102	A1EFU	C15-C16-C17	-5.90	111.39	123.47
8	D	101	BCL	C1D-ND-C4D	-5.89	102.15	106.33
8	E	101	BCL	C1D-ND-C4D	-5.89	102.15	106.33
9	v	103	A1EFU	CM5-C13-C14	-5.87	114.69	122.92
9	k	102	A1EFU	CM4-C9-C10	-5.86	114.72	122.92
8	R	102	BCL	C1D-ND-C4D	-5.82	102.20	106.33
8	K	101	BCL	C1D-ND-C4D	-5.82	102.20	106.33
8	1	103	BCL	C1D-ND-C4D	-5.81	102.21	106.33
8	V	101	BCL	C1D-ND-C4D	-5.80	102.21	106.33
8	V	101	BCL	CMB-C2B-C1B	-5.80	119.55	128.46
9	D	105	A1EFU	CM3-C5-C6	-5.77	114.83	122.92
8	Q	101	BCL	C1D-ND-C4D	-5.77	102.24	106.33
9	v	103	A1EFU	C16-C15-C14	-5.76	111.67	123.47
9	a	101	A1EFU	C15-C16-C17	-5.76	111.67	123.47
9	r	102	A1EFU	C15-C16-C17	-5.76	111.68	123.47
9	S	102	A1EFU	C16-C15-C14	-5.75	111.69	123.47
9	1	101	A1EFU	CM5-C13-C14	-5.75	114.88	122.92
9	T	101	A1EFU	C15-C16-C17	-5.74	111.72	123.47
9	k	102	A1EFU	C16-C15-C14	-5.72	111.75	123.47
9	G	105	A1EFU	CM6-C18-C17	-5.70	114.93	122.92
9	G	104	A1EFU	CM6-C18-C17	-5.69	114.95	122.92
9	a	103	A1EFU	CM6-C18-C17	-5.69	114.95	122.92
9	J	103	A1EFU	CM6-C18-C17	-5.68	114.97	122.92
9	2	102	A1EFU	CM5-C13-C14	-5.67	114.98	122.92
8	I	102	BCL	C1D-ND-C4D	-5.66	102.31	106.33
9	G	104	A1EFU	CM5-C13-C14	-5.66	114.99	122.92
9	I	103	A1EFU	CM6-C18-C17	-5.66	115.00	122.92
9	J	103	A1EFU	C16-C15-C14	-5.65	111.89	123.47
9	e	101	A1EFU	C15-C16-C17	-5.65	111.91	123.47
9	k	102	A1EFU	CM6-C18-C17	-5.64	115.02	122.92
9	I	101	A1EFU	CM6-C18-C17	-5.64	115.02	122.92
9	I	101	A1EFU	CM5-C13-C14	-5.64	115.03	122.92
9	v	103	A1EFU	CM6-C18-C17	-5.63	115.04	122.92

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	2	101	A1EFU	CM6-C18-C17	-5.62	115.04	122.92
9	a	103	A1EFU	C15-C16-C17	-5.62	111.96	123.47
8	v	101	BCL	C1D-ND-C4D	-5.62	102.35	106.33
9	D	105	A1EFU	CM6-C18-C17	-5.61	115.06	122.92
9	J	103	A1EFU	CM3-C5-C6	-5.61	115.06	122.92
8	J	101	BCL	C1D-ND-C4D	-5.61	102.35	106.33
9	G	105	A1EFU	CM5-C13-C14	-5.60	115.07	122.92
8	T	102	BCL	CMB-C2B-C1B	-5.60	119.86	128.46
8	G	102	BCL	C1D-ND-C4D	-5.60	102.36	106.33
8	E	101	BCL	O2D-CGD-CBD	5.59	121.21	111.27
8	v	101	BCL	C1C-NC-C4C	-5.57	104.20	106.71
9	d	102	A1EFU	C16-C15-C14	-5.57	112.06	123.47
9	v	102	A1EFU	CM3-C5-C6	-5.57	115.12	122.92
9	N	103	A1EFU	CM5-C13-C14	-5.56	115.13	122.92
9	1	101	A1EFU	CM6-C18-C17	-5.56	115.14	122.92
9	Q	103	A1EFU	C16-C15-C14	-5.55	112.10	123.47
9	N	102	A1EFU	C15-C16-C17	-5.55	112.11	123.47
8	n	101	BCL	C2D-C1D-ND	5.54	114.18	110.10
9	Q	103	A1EFU	CM4-C9-C10	-5.53	115.17	122.92
9	I	103	A1EFU	CM3-C5-C6	-5.52	115.19	122.92
8	P	102	BCL	CMB-C2B-C1B	-5.51	120.00	128.46
8	r	101	BCL	CMB-C2B-C1B	-5.49	120.03	128.46
8	B	101	BCL	C2D-C1D-ND	5.49	114.15	110.10
9	G	105	A1EFU	CM3-C5-C6	-5.48	115.24	122.92
9	N	102	A1EFU	CM4-C9-C10	-5.48	115.25	122.92
8	T	102	BCL	C2D-C1D-ND	5.48	114.14	110.10
8	1	102	BCL	C2D-C1D-ND	5.48	114.14	110.10
9	M	407	A1EFU	CM3-C5-C6	-5.47	115.26	122.92
9	r	102	A1EFU	CM3-C5-C6	-5.46	115.27	122.92
8	N	101	BCL	C2D-C1D-ND	5.46	114.13	110.10
8	S	101	BCL	C2D-C1D-ND	5.46	114.13	110.10
9	v	102	A1EFU	C15-C16-C17	-5.46	112.29	123.47
8	i	101	BCL	O2D-CGD-CBD	5.45	120.95	111.27
9	E	102	A1EFU	CM5-C13-C14	-5.45	115.30	122.92
8	A	101	BCL	C2D-C1D-ND	5.44	114.11	110.10
8	k	101	BCL	C2D-C1D-ND	5.44	114.11	110.10
8	b	101	BCL	C2D-C1D-ND	5.43	114.11	110.10
9	F	105	A1EFU	CM5-C13-C14	-5.43	115.31	122.92
9	G	105	A1EFU	C16-C15-C14	-5.43	112.35	123.47
9	D	104	A1EFU	CM5-C13-C14	-5.43	115.32	122.92
8	P	102	BCL	C2D-C1D-ND	5.43	114.11	110.10
8	s	101	BCL	C2D-C1D-ND	5.43	114.10	110.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	S	102	A1EFU	CM3-C5-C6	-5.43	115.32	122.92
9	G	105	A1EFU	CM4-C9-C10	-5.42	115.33	122.92
8	i	101	BCL	C2D-C1D-ND	5.42	114.10	110.10
9	Q	103	A1EFU	CM3-C5-C6	-5.41	115.34	122.92
9	a	101	A1EFU	CM3-C5-C6	-5.41	115.35	122.92
8	n	101	BCL	CMB-C2B-C1B	-5.41	120.15	128.46
8	l	103	BCL	C1C-NC-C4C	-5.41	104.28	106.71
8	q	101	BCL	C2D-C1D-ND	5.40	114.08	110.10
9	l	101	A1EFU	CM3-C5-C6	-5.40	115.36	122.92
8	L	306	BCL	C2D-C1D-ND	5.39	114.08	110.10
9	J	103	A1EFU	CM4-C9-C10	-5.39	115.37	122.92
9	N	103	A1EFU	C15-C16-C17	-5.39	112.43	123.47
9	A	102	A1EFU	C15-C16-C17	-5.39	112.44	123.47
9	B	102	A1EFU	CM5-C13-C14	-5.39	115.38	122.92
9	r	102	A1EFU	CM5-C13-C14	-5.39	115.38	122.92
9	T	101	A1EFU	CM5-C13-C14	-5.39	115.38	122.92
8	P	101	BCL	C2D-C1D-ND	5.38	114.07	110.10
9	R	101	A1EFU	CM5-C13-C14	-5.38	115.39	122.92
8	a	102	BCL	C2D-C1D-ND	5.38	114.07	110.10
9	D	105	A1EFU	C15-C16-C17	-5.38	112.45	123.47
8	r	101	BCL	C2D-C1D-ND	5.38	114.07	110.10
9	I	101	A1EFU	CM3-C5-C6	-5.37	115.39	122.92
9	J	102	A1EFU	CM5-C13-C14	-5.37	115.40	122.92
9	t	102	A1EFU	C16-C15-C14	-5.37	112.47	123.47
9	I	101	A1EFU	CM4-C9-C10	-5.37	115.40	122.92
9	d	102	A1EFU	C15-C16-C17	-5.37	112.48	123.47
9	S	102	A1EFU	CM6-C18-C17	-5.37	115.41	122.92
8	Q	101	BCL	C2D-C1D-ND	5.37	114.06	110.10
9	F	105	A1EFU	CM4-C9-C10	-5.36	115.41	122.92
9	v	103	A1EFU	CM3-C5-C6	-5.36	115.41	122.92
8	A	101	BCL	CMB-C2B-C1B	-5.36	120.23	128.46
9	l	101	A1EFU	CM4-C9-C10	-5.36	115.42	122.92
9	N	103	A1EFU	CM6-C18-C17	-5.35	115.43	122.92
9	s	102	A1EFU	CM6-C18-C17	-5.35	115.43	122.92
9	t	102	A1EFU	CM4-C9-C10	-5.35	115.43	122.92
9	G	105	A1EFU	C15-C16-C17	-5.35	112.52	123.47
9	d	102	A1EFU	CM3-C5-C6	-5.34	115.44	122.92
9	A	102	A1EFU	CM5-C13-C14	-5.34	115.44	122.92
8	d	101	BCL	C1D-ND-C4D	-5.34	102.54	106.33
9	I	103	A1EFU	CM5-C13-C14	-5.34	115.44	122.92
8	I	102	BCL	O2D-CGD-CBD	5.33	120.75	111.27
9	t	102	A1EFU	CM5-C13-C14	-5.33	115.45	122.92

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	102	A1EFU	CM4-C9-C10	-5.33	115.46	122.92
9	S	102	A1EFU	CM5-C13-C14	-5.33	115.46	122.92
9	I	103	A1EFU	CM4-C9-C10	-5.33	115.46	122.92
9	t	102	A1EFU	CM6-C18-C17	-5.33	115.46	122.92
9	K	102	A1EFU	CM4-C9-C10	-5.32	115.47	122.92
9	D	104	A1EFU	CM3-C5-C6	-5.32	115.47	122.92
9	K	102	A1EFU	CM5-C13-C14	-5.31	115.48	122.92
9	A	102	A1EFU	CM4-C9-C10	-5.31	115.48	122.92
9	v	103	A1EFU	C15-C16-C17	-5.31	112.60	123.47
8	e	102	BCL	C2D-C1D-ND	5.31	114.02	110.10
9	S	102	A1EFU	CM4-C9-C10	-5.31	115.49	122.92
8	G	102	BCL	O2D-CGD-CBD	5.30	120.69	111.27
9	t	102	A1EFU	C15-C16-C17	-5.30	112.62	123.47
9	D	105	A1EFU	CM5-C13-C14	-5.30	115.50	122.92
8	j	101	BCL	C2D-C1D-ND	5.30	114.01	110.10
9	2	101	A1EFU	CM4-C9-C10	-5.29	115.51	122.92
9	J	102	A1EFU	C16-C15-C14	-5.29	112.64	123.47
9	A	102	A1EFU	C16-C15-C14	-5.28	112.66	123.47
8	D	101	BCL	C2D-C1D-ND	5.28	113.99	110.10
9	2	102	A1EFU	CM6-C18-C17	-5.28	115.53	122.92
9	t	102	A1EFU	CM3-C5-C6	-5.27	115.54	122.92
8	I	102	BCL	C1C-NC-C4C	-5.27	104.34	106.71
8	v	101	BCL	C2D-C1D-ND	5.27	113.98	110.10
9	J	102	A1EFU	CM4-C9-C10	-5.27	115.55	122.92
9	E	102	A1EFU	CM4-C9-C10	-5.26	115.56	122.92
9	D	104	A1EFU	CM6-C18-C17	-5.25	115.56	122.92
9	T	101	A1EFU	CM3-C5-C6	-5.25	115.57	122.92
9	D	105	A1EFU	CM4-C9-C10	-5.25	115.57	122.92
9	s	102	A1EFU	C16-C15-C14	-5.25	112.72	123.47
9	e	101	A1EFU	C16-C15-C14	-5.24	112.74	123.47
8	K	101	BCL	C2D-C1D-ND	5.24	113.97	110.10
9	r	102	A1EFU	C16-C15-C14	-5.24	112.74	123.47
8	M	402	BCL	C2D-C1D-ND	5.24	113.97	110.10
9	l	104	A1EFU	CM4-C9-C10	-5.24	115.58	122.92
9	e	101	A1EFU	CM4-C9-C10	-5.24	115.59	122.92
9	N	103	A1EFU	CM3-C5-C6	-5.22	115.61	122.92
9	N	102	A1EFU	CM6-C18-C17	-5.21	115.62	122.92
9	I	103	A1EFU	C15-C16-C17	-5.21	112.81	123.47
9	R	101	A1EFU	CM3-C5-C6	-5.20	115.63	122.92
9	a	101	A1EFU	CM6-C18-C17	-5.20	115.64	122.92
9	J	103	A1EFU	CM5-C13-C14	-5.20	115.64	122.92
8	G	101	BCL	C2D-C1D-ND	5.20	113.93	110.10

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	N	102	A1EFU	CM5-C13-C14	-5.20	115.64	122.92
9	d	102	A1EFU	CM5-C13-C14	-5.18	115.67	122.92
9	l	104	A1EFU	CM7-C22-C21	-5.18	109.22	122.59
8	I	102	BCL	C2D-C1D-ND	5.17	113.92	110.10
9	M	407	A1EFU	C15-C16-C17	-5.17	112.88	123.47
9	d	102	A1EFU	CM4-C9-C10	-5.17	115.68	122.92
9	D	104	A1EFU	CM4-C9-C10	-5.16	115.69	122.92
8	M	403	BCL	CAC-C3C-C2C	-5.16	101.36	114.26
9	v	102	A1EFU	CM5-C13-C14	-5.16	115.69	122.92
8	L	306	BCL	CAC-C3C-C2C	-5.16	101.37	114.26
8	d	101	BCL	O2D-CGD-CBD	5.16	120.44	111.27
9	e	101	A1EFU	CM6-C18-C17	-5.16	115.70	122.92
8	V	101	BCL	C2D-C1D-ND	5.16	113.91	110.10
8	M	403	BCL	C2D-C1D-ND	5.16	113.91	110.10
9	v	102	A1EFU	CM6-C18-C17	-5.15	115.70	122.92
9	2	102	A1EFU	C15-C16-C17	-5.15	112.92	123.47
9	M	407	A1EFU	C16-C15-C14	-5.15	112.92	123.47
8	F	102	BCL	C1D-ND-C4D	-5.15	102.67	106.33
9	J	103	A1EFU	C15-C16-C17	-5.15	112.92	123.47
9	l	104	A1EFU	CM5-C13-C14	-5.15	115.71	122.92
8	E	101	BCL	C2D-C1D-ND	5.15	113.90	110.10
8	F	101	BCL	CAC-C3C-C2C	-5.14	101.41	114.26
9	M	407	A1EFU	CM4-C9-C10	-5.14	115.72	122.92
9	e	101	A1EFU	CM5-C13-C14	-5.13	115.73	122.92
9	J	102	A1EFU	CM6-C18-C17	-5.13	115.74	122.92
9	G	104	A1EFU	CM3-C5-C6	-5.12	115.75	122.92
8	R	102	BCL	C2D-C1D-ND	5.12	113.88	110.10
8	l	103	BCL	C2D-C1D-ND	5.12	113.88	110.10
9	N	103	A1EFU	CM4-C9-C10	-5.12	115.75	122.92
8	d	101	BCL	CAC-C3C-C2C	-5.12	101.48	114.26
9	k	102	A1EFU	C15-C16-C17	-5.11	113.01	123.47
9	k	102	A1EFU	CM3-C5-C6	-5.10	115.78	122.92
9	s	102	A1EFU	C15-C16-C17	-5.10	113.02	123.47
9	K	102	A1EFU	C15-C16-C17	-5.10	113.03	123.47
9	a	101	A1EFU	CM4-C9-C10	-5.08	115.81	122.92
9	2	101	A1EFU	CM3-C5-C6	-5.08	115.81	122.92
9	B	102	A1EFU	CM3-C5-C6	-5.08	115.81	122.92
9	K	102	A1EFU	CM6-C18-C17	-5.07	115.82	122.92
9	2	101	A1EFU	C15-C16-C17	-5.07	113.08	123.47
9	d	102	A1EFU	CM6-C18-C17	-5.07	115.82	122.92
9	a	103	A1EFU	CM3-C5-C6	-5.07	115.82	122.92
9	R	101	A1EFU	CM4-C9-C10	-5.07	115.83	122.92

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	101	A1EFU	C16-C15-C14	-5.07	113.09	123.47
9	v	102	A1EFU	C16-C15-C14	-5.06	113.10	123.47
8	G	102	BCL	C1C-NC-C4C	-5.06	104.43	106.71
9	J	102	A1EFU	C15-C16-C17	-5.06	113.12	123.47
9	D	105	A1EFU	C16-C15-C14	-5.05	113.13	123.47
9	a	101	A1EFU	C16-C15-C14	-5.05	113.13	123.47
8	J	101	BCL	C1C-NC-C4C	-5.05	104.44	106.71
9	F	105	A1EFU	CM3-C5-C6	-5.04	115.87	122.92
8	E	101	BCL	C1C-NC-C4C	-5.03	104.44	106.71
9	2	102	A1EFU	CM4-C9-C10	-5.03	115.88	122.92
8	D	101	BCL	CAC-C3C-C2C	-5.03	101.69	114.26
9	S	102	A1EFU	C15-C16-C17	-5.02	113.18	123.47
9	k	102	A1EFU	CM5-C13-C14	-5.01	115.90	122.92
9	Q	102	A1EFU	CM5-C13-C14	-5.01	115.90	122.92
9	s	102	A1EFU	CM5-C13-C14	-5.01	115.91	122.92
8	G	101	BCL	O2D-CGD-CBD	5.01	120.17	111.27
8	J	101	BCL	O2D-CGD-CBD	5.00	120.16	111.27
9	B	102	A1EFU	C16-C15-C14	-5.00	113.23	123.47
8	d	101	BCL	C2D-C1D-ND	5.00	113.79	110.10
9	A	102	A1EFU	CM6-C18-C17	-5.00	115.92	122.92
9	v	103	A1EFU	CM4-C9-C10	-4.99	115.93	122.92
9	a	101	A1EFU	CM5-C13-C14	-4.99	115.93	122.92
9	Q	103	A1EFU	CM5-C13-C14	-4.99	115.94	122.92
8	Q	101	BCL	O2D-CGD-CBD	4.98	120.13	111.27
8	d	101	BCL	C1C-NC-C4C	-4.98	104.47	106.71
9	l	104	A1EFU	CM3-C5-C6	-4.98	115.95	122.92
8	J	101	BCL	C2D-C1D-ND	4.98	113.77	110.10
8	K	101	BCL	O2D-CGD-CBD	4.98	120.11	111.27
8	G	102	BCL	C2D-C1D-ND	4.98	113.77	110.10
9	l	104	A1EFU	CM6-C18-C17	-4.97	115.95	122.92
9	N	102	A1EFU	CM3-C5-C6	-4.97	115.96	122.92
9	a	103	A1EFU	C16-C15-C14	-4.97	113.29	123.47
9	M	407	A1EFU	CM6-C18-C17	-4.97	115.96	122.92
9	T	101	A1EFU	CM4-C9-C10	-4.97	115.96	122.92
9	v	102	A1EFU	CM4-C9-C10	-4.97	115.96	122.92
9	M	407	A1EFU	CM5-C13-C14	-4.96	115.97	122.92
9	K	102	A1EFU	CM3-C5-C6	-4.96	115.98	122.92
9	2	101	A1EFU	C16-C15-C14	-4.96	113.32	123.47
9	D	104	A1EFU	C16-C15-C14	-4.95	113.33	123.47
9	2	101	A1EFU	CM5-C13-C14	-4.95	115.99	122.92
9	T	101	A1EFU	CM6-C18-C17	-4.94	116.00	122.92
9	F	105	A1EFU	CM6-C18-C17	-4.93	116.02	122.92

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	104	A1EFU	C15-C16-C17	-4.93	113.38	123.47
9	E	102	A1EFU	CM6-C18-C17	-4.92	116.03	122.92
9	r	102	A1EFU	CM6-C18-C17	-4.92	116.04	122.92
9	1	104	A1EFU	C16-C15-C14	-4.91	113.41	123.47
9	1	104	A1EFU	C21-C20-C19	-4.91	107.89	123.22
9	B	102	A1EFU	CM6-C18-C17	-4.90	116.06	122.92
9	N	103	A1EFU	C16-C15-C14	-4.90	113.44	123.47
8	r	101	BCL	O2D-CGD-CBD	4.90	119.97	111.27
9	T	101	A1EFU	C16-C15-C14	-4.89	113.45	123.47
8	V	101	BCL	O2D-CGD-CBD	4.88	119.94	111.27
8	1	102	BCL	O2D-CGD-CBD	4.88	119.94	111.27
8	e	102	BCL	CAC-C3C-C2C	-4.88	102.07	114.26
8	F	101	BCL	O2D-CGD-CBD	4.87	119.93	111.27
9	2	102	A1EFU	CM3-C5-C6	-4.87	116.10	122.92
8	V	101	BCL	CAC-C3C-C2C	-4.86	102.12	114.26
9	1	101	A1EFU	C15-C16-C17	-4.86	113.53	123.47
8	P	101	BCL	CAC-C3C-C2C	-4.85	102.13	114.26
8	j	101	BCL	CAC-C3C-C2C	-4.85	102.14	114.26
9	Q	102	A1EFU	CM3-C5-C6	-4.85	116.13	122.92
9	R	101	A1EFU	C16-C15-C14	-4.85	113.54	123.47
9	s	102	A1EFU	CM4-C9-C10	-4.85	116.14	122.92
8	v	101	BCL	O2D-CGD-CBD	4.84	119.88	111.27
8	q	101	BCL	O2D-CGD-CBD	4.84	119.86	111.27
9	I	101	A1EFU	C15-C16-C17	-4.84	113.56	123.47
8	P	102	BCL	CAC-C3C-C2C	-4.83	102.18	114.26
8	B	101	BCL	CAC-C3C-C2C	-4.83	102.18	114.26
8	q	101	BCL	CAC-C3C-C2C	-4.83	102.19	114.26
8	P	102	BCL	O2D-CGD-CBD	4.83	119.85	111.27
8	B	101	BCL	O2D-CGD-CBD	4.83	119.85	111.27
8	r	101	BCL	CAC-C3C-C2C	-4.83	102.20	114.26
8	G	101	BCL	CAC-C3C-C2C	-4.83	102.20	114.26
8	j	101	BCL	C1C-NC-C4C	-4.82	104.54	106.71
8	s	101	BCL	O2D-CGD-CBD	4.82	119.83	111.27
8	j	101	BCL	O2D-CGD-CBD	4.82	119.83	111.27
8	L	306	BCL	O2D-CGD-CBD	4.81	119.82	111.27
9	F	105	A1EFU	C16-C15-C14	-4.81	113.61	123.47
9	A	102	A1EFU	CM3-C5-C6	-4.81	116.19	122.92
9	1	101	A1EFU	C16-C15-C14	-4.81	113.62	123.47
8	a	102	BCL	CAC-C3C-C2C	-4.81	102.25	114.26
8	F	101	BCL	C1D-ND-C4D	-4.81	102.92	106.33
8	b	101	BCL	O2D-CGD-CBD	4.80	119.80	111.27
8	A	101	BCL	O2D-CGD-CBD	4.80	119.80	111.27

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	S	101	BCL	CAC-C3C-C2C	-4.80	102.27	114.26
8	a	102	BCL	O2D-CGD-CBD	4.80	119.79	111.27
8	R	102	BCL	C1C-NC-C4C	-4.80	104.55	106.71
8	R	102	BCL	O2D-CGD-CBD	4.80	119.79	111.27
9	K	102	A1EFU	C16-C15-C14	-4.80	113.65	123.47
8	L	306	BCL	C1C-NC-C4C	-4.79	104.55	106.71
8	Q	101	BCL	CAC-C3C-C2C	-4.79	102.29	114.26
8	k	101	BCL	CAC-C3C-C2C	-4.79	102.30	114.26
8	n	101	BCL	O2D-CGD-CBD	4.78	119.76	111.27
8	s	101	BCL	CAC-C3C-C2C	-4.78	102.33	114.26
8	l	102	BCL	CAC-C3C-C2C	-4.77	102.34	114.26
8	k	101	BCL	O2D-CGD-CBD	4.77	119.74	111.27
8	S	101	BCL	O2D-CGD-CBD	4.77	119.74	111.27
8	b	101	BCL	CAC-C3C-C2C	-4.76	102.37	114.26
8	N	101	BCL	O2D-CGD-CBD	4.75	119.71	111.27
8	M	403	BCL	O2D-CGD-CBD	4.75	119.71	111.27
8	e	102	BCL	O2D-CGD-CBD	4.74	119.70	111.27
8	L	303	BCL	CAC-C3C-C2C	-4.74	102.41	114.26
8	T	102	BCL	O2D-CGD-CBD	4.74	119.70	111.27
8	P	101	BCL	O2D-CGD-CBD	4.74	119.69	111.27
9	R	101	A1EFU	CM6-C18-C17	-4.74	116.28	122.92
9	I	103	A1EFU	C16-C15-C14	-4.74	113.77	123.47
8	t	101	BCL	O2D-CGD-CBD	4.73	119.67	111.27
8	D	101	BCL	O2D-CGD-CBD	4.72	119.65	111.27
8	i	101	BCL	CAC-C3C-C2C	-4.72	102.47	114.26
9	G	104	A1EFU	C16-C15-C14	-4.71	113.83	123.47
9	Q	102	A1EFU	CM4-C9-C10	-4.70	116.34	122.92
9	E	102	A1EFU	C16-C15-C14	-4.69	113.87	123.47
8	M	402	BCL	CAC-C3C-C2C	-4.68	102.56	114.26
8	K	101	BCL	C1C-NC-C4C	-4.68	104.60	106.71
8	T	102	BCL	C1C-NC-C4C	-4.67	104.61	106.71
8	v	101	BCL	CAC-C3C-C2C	-4.67	102.59	114.26
8	t	101	BCL	CHD-C1D-ND	-4.64	120.19	124.45
8	N	101	BCL	C1C-NC-C4C	-4.64	104.62	106.71
8	A	101	BCL	CAC-C3C-C2C	-4.63	102.68	114.26
8	J	101	BCL	CAC-C3C-C2C	-4.63	102.70	114.26
8	n	101	BCL	CAC-C3C-C2C	-4.60	102.76	114.26
9	I	101	A1EFU	CM7-C22-C21	-4.59	110.74	122.59
8	l	103	BCL	O2D-CGD-CBD	4.59	119.43	111.27
8	F	102	BCL	O2D-CGD-CBD	4.59	119.43	111.27
9	a	103	A1EFU	CM5-C13-C12	4.58	125.29	118.08
9	G	104	A1EFU	CM4-C9-C10	-4.56	116.53	122.92

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	Q	103	A1EFU	C15-C16-C17	-4.55	114.15	123.47
8	N	101	BCL	CAC-C3C-C2C	-4.55	102.90	114.26
9	J	102	A1EFU	CM3-C5-C6	-4.53	116.57	122.92
9	a	103	A1EFU	CM4-C9-C8	4.53	125.22	118.08
8	t	101	BCL	C1D-ND-C4D	-4.52	103.12	106.33
8	R	102	BCL	CAC-C3C-C2C	-4.52	102.97	114.26
8	F	102	BCL	CAC-C3C-C2C	-4.52	102.98	114.26
9	G	104	A1EFU	C15-C16-C17	-4.50	114.25	123.47
8	K	101	BCL	CAC-C3C-C2C	-4.50	103.02	114.26
8	F	101	BCL	C2D-C1D-ND	4.50	113.42	110.10
9	N	102	A1EFU	C16-C15-C14	-4.50	114.26	123.47
9	E	102	A1EFU	CM3-C5-C6	-4.48	116.65	122.92
9	l	104	A1EFU	C15-C16-C17	-4.47	114.31	123.47
8	I	102	BCL	CAC-C3C-C2C	-4.47	103.09	114.26
8	F	102	BCL	C2D-C1D-ND	4.46	113.39	110.10
9	r	102	A1EFU	CM7-C22-C21	-4.46	111.08	122.59
8	M	403	BCL	C1C-NC-C4C	-4.44	104.71	106.71
9	e	101	A1EFU	CM7-C22-C21	-4.44	111.14	122.59
9	N	103	A1EFU	CM7-C22-C21	-4.43	111.17	122.59
8	t	101	BCL	CAC-C3C-C2C	-4.42	103.21	114.26
9	J	103	A1EFU	CM3-C5-C4	4.42	125.03	118.08
8	E	101	BCL	O2D-CGD-O1D	-4.42	115.20	123.84
8	M	402	BCL	O2D-CGD-CBD	4.40	119.08	111.27
8	E	101	BCL	CAC-C3C-C2C	-4.40	103.28	114.26
8	T	102	BCL	CAC-C3C-C2C	-4.38	103.33	114.26
9	r	102	A1EFU	CM3-C5-C4	4.37	124.96	118.08
8	i	101	BCL	O2D-CGD-O1D	-4.37	115.29	123.84
8	G	102	BCL	CAC-C3C-C2C	-4.36	103.35	114.26
9	r	102	A1EFU	CM4-C9-C10	-4.36	116.81	122.92
9	I	103	A1EFU	CM3-C5-C4	4.36	124.94	118.08
9	2	101	A1EFU	CM7-C22-C21	-4.36	111.35	122.59
8	d	101	BCL	O2D-CGD-O1D	-4.34	115.34	123.84
9	Q	103	A1EFU	CM7-C22-C21	-4.34	111.40	122.59
9	a	101	A1EFU	CM7-C22-C21	-4.33	111.42	122.59
9	M	407	A1EFU	CM7-C22-C21	-4.33	111.42	122.59
9	a	101	A1EFU	CM3-C5-C4	4.33	124.89	118.08
9	2	102	A1EFU	C16-C15-C14	-4.32	114.63	123.47
16	C	402	HEC	CMD-C2D-C1D	-4.31	121.83	128.46
8	G	102	BCL	O2D-CGD-O1D	-4.31	115.41	123.84
8	L	303	BCL	C4A-NA-C1A	-4.31	104.77	106.71
9	S	102	A1EFU	CM3-C5-C4	4.31	124.86	118.08
9	B	102	A1EFU	CM7-C22-C21	-4.31	111.48	122.59

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	104	A1EFU	CM4-C9-C8	4.31	124.86	118.08
9	M	407	A1EFU	CM3-C5-C4	4.30	124.86	118.08
9	F	105	A1EFU	C6-C7-C8	-4.30	109.79	123.22
9	D	105	A1EFU	CM3-C5-C4	4.30	124.85	118.08
9	I	103	A1EFU	CM7-C22-C21	-4.30	111.50	122.59
9	k	102	A1EFU	CM7-C22-C21	-4.29	111.51	122.59
9	G	105	A1EFU	CM7-C22-C21	-4.29	111.52	122.59
8	K	101	BCL	O2D-CGD-O1D	-4.29	115.44	123.84
9	N	102	A1EFU	C23-C22-C21	-4.29	108.99	121.98
8	L	303	BCL	O2D-CGD-CBD	4.29	118.89	111.27
9	t	102	A1EFU	CM7-C22-C21	-4.29	111.53	122.59
8	v	101	BCL	CHD-C1D-ND	-4.29	120.52	124.45
9	D	105	A1EFU	CM7-C22-C21	-4.28	111.54	122.59
9	Q	102	A1EFU	CM7-C22-C21	-4.28	111.54	122.59
8	I	102	BCL	O2D-CGD-O1D	-4.28	115.47	123.84
9	s	102	A1EFU	CM7-C22-C21	-4.28	111.55	122.59
9	A	102	A1EFU	CM7-C22-C21	-4.27	111.57	122.59
9	F	105	A1EFU	CM3-C5-C4	4.26	124.79	118.08
9	N	102	A1EFU	CM7-C22-C21	-4.26	111.60	122.59
16	C	401	HEC	CMD-C2D-C1D	-4.26	121.92	128.46
9	J	103	A1EFU	CM7-C22-C21	-4.26	111.61	122.59
8	l	103	BCL	CAC-C3C-C2C	-4.26	103.63	114.26
9	k	102	A1EFU	CM4-C9-C8	4.26	124.78	118.08
8	J	101	BCL	O2D-CGD-O1D	-4.25	115.52	123.84
9	e	101	A1EFU	CM3-C5-C4	4.25	124.78	118.08
9	d	102	A1EFU	CM3-C5-C4	4.25	124.78	118.08
9	D	104	A1EFU	C6-C7-C8	-4.25	109.95	123.22
8	G	101	BCL	O2D-CGD-O1D	-4.24	115.54	123.84
9	G	105	A1EFU	CM3-C5-C4	4.24	124.76	118.08
9	t	102	A1EFU	CM3-C5-C4	4.24	124.76	118.08
9	v	103	A1EFU	CM7-C22-C21	-4.24	111.65	122.59
9	F	105	A1EFU	CM4-C9-C8	4.24	124.75	118.08
8	F	102	BCL	CHD-C1D-ND	-4.23	120.57	124.45
9	N	103	A1EFU	C10-C11-C12	-4.23	110.03	123.22
8	t	101	BCL	C2D-C1D-ND	4.22	113.22	110.10
8	G	101	BCL	CMB-C2B-C3B	4.21	132.55	124.68
9	S	102	A1EFU	CM7-C22-C21	-4.20	111.74	122.59
9	d	102	A1EFU	CM7-C22-C21	-4.20	111.75	122.59
9	B	102	A1EFU	CM3-C5-C4	4.20	124.69	118.08
8	F	102	BCL	O2D-CGD-O1D	-4.19	115.64	123.84
9	T	101	A1EFU	CM7-C22-C21	-4.19	111.77	122.59
9	Q	103	A1EFU	CM3-C5-C4	4.19	124.68	118.08

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	r	102	A1EFU	C6-C7-C8	-4.19	110.14	123.22
9	T	101	A1EFU	CM3-C5-C4	4.19	124.68	118.08
9	R	101	A1EFU	CM7-C22-C21	-4.19	111.79	122.59
8	F	101	BCL	O2D-CGD-O1D	-4.18	115.66	123.84
9	l	101	A1EFU	CM7-C22-C21	-4.18	111.80	122.59
9	Q	102	A1EFU	C15-C16-C17	-4.18	114.91	123.47
9	J	102	A1EFU	CM7-C22-C21	-4.18	111.81	122.59
9	a	103	A1EFU	CM7-C22-C21	-4.18	111.81	122.59
10	H	302	MW9	O8-C24-C25	4.17	120.50	111.50
9	G	104	A1EFU	CM7-C22-C21	-4.16	111.85	122.59
9	E	102	A1EFU	CM7-C22-C21	-4.16	111.86	122.59
9	v	102	A1EFU	CM7-C22-C21	-4.16	111.86	122.59
9	v	103	A1EFU	CM3-C5-C4	4.16	124.62	118.08
8	G	102	BCL	CMB-C2B-C3B	4.15	132.44	124.68
9	2	102	A1EFU	C10-C11-C12	-4.15	110.27	123.22
9	G	104	A1EFU	CM3-C5-C4	4.15	124.61	118.08
8	Q	101	BCL	CMB-C2B-C3B	4.15	132.44	124.68
9	R	101	A1EFU	CM3-C5-C4	4.15	124.61	118.08
8	L	306	BCL	CMB-C2B-C3B	4.15	132.44	124.68
9	l	101	A1EFU	CM3-C5-C4	4.14	124.60	118.08
8	k	101	BCL	CMB-C2B-C3B	4.14	132.42	124.68
8	I	102	BCL	CMB-C2B-C3B	4.14	132.42	124.68
8	R	102	BCL	CMB-C2B-C3B	4.13	132.41	124.68
9	v	102	A1EFU	CM3-C5-C4	4.13	124.58	118.08
9	A	102	A1EFU	CM4-C9-C8	4.13	124.58	118.08
9	F	105	A1EFU	CM7-C22-C21	-4.13	111.94	122.59
8	M	403	BCL	CMB-C2B-C3B	4.13	132.40	124.68
10	D	103	MW9	O8-C24-C25	4.13	120.39	111.50
8	D	101	BCL	CMB-C2B-C3B	4.12	132.39	124.68
8	l	103	BCL	CMB-C2B-C3B	4.12	132.39	124.68
10	G	103	MW9	O8-C24-C25	4.12	120.38	111.50
9	A	102	A1EFU	C6-C7-C8	-4.12	110.36	123.22
8	q	101	BCL	CMB-C2B-C3B	4.12	132.39	124.68
9	I	101	A1EFU	CM3-C5-C4	4.12	124.56	118.08
8	t	101	BCL	OBB-CAB-CBB	-4.12	110.91	120.17
8	v	101	BCL	CMB-C2B-C3B	4.12	132.38	124.68
8	l	102	BCL	O2D-CGD-O1D	-4.11	115.79	123.84
8	j	101	BCL	O2D-CGD-O1D	-4.11	115.80	123.84
8	L	306	BCL	O2D-CGD-O1D	-4.11	115.80	123.84
10	L	309	MW9	O8-C24-C25	4.11	120.36	111.50
9	2	102	A1EFU	CM7-C22-C21	-4.11	111.99	122.59
10	L	310	MW9	O8-C24-C25	4.11	120.35	111.50

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	a	101	A1EFU	CM4-C9-C8	4.11	124.55	118.08
9	A	102	A1EFU	CM3-C5-C4	4.11	124.55	118.08
8	v	101	BCL	O2D-CGD-O1D	-4.11	115.81	123.84
9	2	101	A1EFU	C23-C22-C21	-4.10	109.55	121.98
8	M	402	BCL	CMB-C2B-C3B	4.10	132.35	124.68
8	V	101	BCL	C4B-CHC-C1C	-4.10	122.00	130.12
8	r	101	BCL	O2D-CGD-O1D	-4.10	115.82	123.84
8	P	101	BCL	CMB-C2B-C3B	4.10	132.34	124.68
9	d	102	A1EFU	C23-C22-C21	-4.10	109.57	121.98
8	R	102	BCL	O2D-CGD-O1D	-4.10	115.83	123.84
8	i	101	BCL	CMB-C2B-C3B	4.10	132.34	124.68
9	B	102	A1EFU	C6-C7-C8	-4.10	110.44	123.22
8	b	101	BCL	O2D-CGD-O1D	-4.10	115.83	123.84
8	q	101	BCL	O2D-CGD-O1D	-4.09	115.84	123.84
16	C	403	HEC	CMD-C2D-C1D	-4.09	122.17	128.46
8	L	303	BCL	CMB-C2B-C3B	4.09	132.33	124.68
10	F	104	MW9	O8-C24-C25	4.09	120.31	111.50
10	M	406	MW9	O8-C24-C25	4.09	120.31	111.50
8	B	101	BCL	O2D-CGD-O1D	-4.09	115.85	123.84
9	D	104	A1EFU	CM7-C22-C21	-4.09	112.05	122.59
9	G	105	A1EFU	C23-C22-C21	-4.09	109.61	121.98
8	k	101	BCL	O2D-CGD-O1D	-4.08	115.85	123.84
8	P	101	BCL	O2D-CGD-O1D	-4.08	115.85	123.84
8	n	101	BCL	O2D-CGD-O1D	-4.08	115.86	123.84
8	P	102	BCL	O2D-CGD-O1D	-4.08	115.86	123.84
9	D	105	A1EFU	C23-C22-C21	-4.08	109.62	121.98
8	J	101	BCL	CMB-C2B-C3B	4.08	132.31	124.68
8	e	102	BCL	CMB-C2B-C3B	4.08	132.31	124.68
8	s	101	BCL	O2D-CGD-O1D	-4.08	115.86	123.84
8	M	403	BCL	O2D-CGD-O1D	-4.08	115.86	123.84
9	E	102	A1EFU	C6-C7-C8	-4.08	110.49	123.22
8	S	101	BCL	O2D-CGD-O1D	-4.08	115.87	123.84
9	a	103	A1EFU	CM3-C5-C4	4.08	124.50	118.08
15	L	311	CDL	OA6-CA5-C11	4.08	120.29	111.50
9	S	102	A1EFU	CM4-C9-C8	4.08	124.50	118.08
8	N	101	BCL	O2D-CGD-O1D	-4.07	115.87	123.84
8	N	101	BCL	CMB-C2B-C3B	4.07	132.30	124.68
8	D	101	BCL	O2D-CGD-O1D	-4.07	115.87	123.84
8	a	102	BCL	CMB-C2B-C3B	4.07	132.30	124.68
8	Q	101	BCL	O2D-CGD-O1D	-4.07	115.87	123.84
8	b	101	BCL	CMB-C2B-C3B	4.07	132.30	124.68
8	A	101	BCL	O2D-CGD-O1D	-4.07	115.88	123.84

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	e	101	A1EFU	C6-C7-C8	-4.07	110.51	123.22
8	V	101	BCL	CMB-C2B-C3B	4.07	132.29	124.68
8	V	101	BCL	O2D-CGD-O1D	-4.07	115.88	123.84
9	r	102	A1EFU	CM5-C13-C12	4.07	124.49	118.08
9	a	103	A1EFU	CM6-C18-C19	4.07	124.49	118.08
8	e	102	BCL	O2D-CGD-O1D	-4.07	115.88	123.84
9	E	102	A1EFU	CM4-C9-C8	4.06	124.48	118.08
9	D	104	A1EFU	C10-C11-C12	-4.06	110.53	123.22
8	t	101	BCL	O2D-CGD-O1D	-4.06	115.90	123.84
9	G	104	A1EFU	C23-C22-C21	-4.06	109.69	121.98
9	D	105	A1EFU	CM4-C9-C8	4.06	124.47	118.08
8	F	101	BCL	CMB-C2B-C3B	4.06	132.27	124.68
8	j	101	BCL	CMB-C2B-C3B	4.05	132.26	124.68
8	S	101	BCL	CMB-C2B-C3B	4.05	132.26	124.68
9	D	104	A1EFU	CM5-C13-C12	4.05	124.46	118.08
8	M	403	BCL	CHD-C1D-ND	-4.05	120.73	124.45
9	B	102	A1EFU	C23-C22-C21	-4.05	109.73	121.98
8	a	102	BCL	O2D-CGD-O1D	-4.05	115.93	123.84
9	a	101	A1EFU	C10-C11-C12	-4.04	110.59	123.22
9	t	102	A1EFU	CM4-C9-C8	4.04	124.45	118.08
10	Q	104	MW9	O8-C24-C25	4.04	120.21	111.50
9	R	101	A1EFU	C23-C22-C21	-4.04	109.75	121.98
9	1	101	A1EFU	C23-C22-C21	-4.04	109.76	121.98
8	1	103	BCL	O2D-CGD-O1D	-4.03	115.95	123.84
16	C	401	HEC	CMC-C2C-C3C	4.03	130.56	125.82
9	J	102	A1EFU	CM4-C9-C8	4.03	124.43	118.08
8	B	101	BCL	CMB-C2B-C3B	4.03	132.22	124.68
8	T	102	BCL	O2D-CGD-O1D	-4.03	115.96	123.84
9	2	102	A1EFU	C23-C22-C21	-4.03	109.78	121.98
9	Q	102	A1EFU	C6-C7-C8	-4.03	110.65	123.22
8	V	101	BCL	OBB-CAB-CBB	-4.03	111.11	120.17
15	L	311	CDL	OB6-CB5-C51	4.02	120.17	111.50
8	1	102	BCL	CMB-C2B-C3B	4.02	132.20	124.68
10	M	405	MW9	O8-C24-C25	4.02	120.17	111.50
9	D	105	A1EFU	C6-C7-C8	-4.02	110.67	123.22
9	F	105	A1EFU	C23-C22-C21	-4.01	109.83	121.98
8	M	402	BCL	O2D-CGD-O1D	-4.01	116.00	123.84
9	1	101	A1EFU	C6-C7-C8	-4.01	110.71	123.22
8	F	102	BCL	CMB-C2B-C3B	4.01	132.18	124.68
8	E	101	BCL	CMB-C2B-C3B	4.01	132.18	124.68
9	D	104	A1EFU	CM3-C5-C4	4.01	124.39	118.08
15	H	303	CDL	OB6-CB5-C51	4.00	120.12	111.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	Q	102	A1EFU	CM5-C13-C12	4.00	124.37	118.08
15	H	303	CDL	OA6-CA5-C11	4.00	120.11	111.50
9	v	103	A1EFU	CM6-C18-C19	3.99	124.37	118.08
10	I	104	MW9	O8-C24-C25	3.99	120.10	111.50
9	D	105	A1EFU	CM6-C18-C19	3.99	124.36	118.08
9	k	102	A1EFU	CM3-C5-C4	3.98	124.35	118.08
9	N	103	A1EFU	CM3-C5-C4	3.98	124.35	118.08
9	F	105	A1EFU	CM5-C13-C12	3.98	124.35	118.08
10	F	103	MW9	O8-C24-C25	3.98	120.08	111.50
9	A	102	A1EFU	CM5-C13-C12	3.98	124.35	118.08
8	T	102	BCL	OBB-CAB-CBB	-3.98	111.21	120.17
9	I	101	A1EFU	CM4-C9-C8	3.98	124.34	118.08
16	C	402	HEC	CBD-CAD-C3D	3.97	119.40	112.62
9	E	102	A1EFU	C23-C22-C21	-3.97	109.95	121.98
9	G	104	A1EFU	C6-C7-C8	-3.97	110.82	123.22
9	G	105	A1EFU	CM6-C18-C19	3.97	124.33	118.08
9	K	102	A1EFU	CM7-C22-C21	-3.96	112.36	122.59
8	d	101	BCL	CMB-C2B-C3B	3.96	132.09	124.68
9	k	102	A1EFU	C23-C22-C21	-3.96	109.99	121.98
9	l	101	A1EFU	CM4-C9-C8	3.96	124.31	118.08
8	s	101	BCL	CMB-C2B-C3B	3.96	132.08	124.68
9	a	101	A1EFU	CM6-C18-C19	3.95	124.31	118.08
9	B	102	A1EFU	CM4-C9-C8	3.95	124.30	118.08
9	K	102	A1EFU	CM4-C9-C8	3.95	124.30	118.08
9	a	103	A1EFU	C23-C22-C21	-3.95	110.02	121.98
9	e	101	A1EFU	CM4-C9-C8	3.95	124.30	118.08
9	v	103	A1EFU	CM5-C13-C12	3.95	124.30	118.08
9	a	103	A1EFU	C10-C11-C12	-3.95	110.90	123.22
9	d	102	A1EFU	C10-C11-C12	-3.95	110.90	123.22
8	K	101	BCL	CMB-C2B-C3B	3.94	132.06	124.68
9	B	102	A1EFU	CM5-C13-C12	3.94	124.29	118.08
9	v	103	A1EFU	CM4-C9-C8	3.94	124.29	118.08
9	Q	102	A1EFU	CM3-C5-C4	3.94	124.28	118.08
9	v	103	A1EFU	C6-C7-C8	-3.94	110.92	123.22
9	I	101	A1EFU	CM5-C13-C12	3.93	124.27	118.08
9	S	102	A1EFU	CM5-C13-C12	3.93	124.27	118.08
9	R	101	A1EFU	CM5-C13-C12	3.93	124.27	118.08
8	s	101	BCL	OBB-CAB-CBB	-3.93	111.33	120.17
8	M	402	BCL	CHD-C1D-ND	-3.93	120.85	124.45
9	G	105	A1EFU	CM5-C13-C12	3.92	124.26	118.08
9	I	101	A1EFU	C6-C7-C8	-3.92	110.97	123.22
9	e	101	A1EFU	CM6-C18-C19	3.92	124.26	118.08

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	j	101	BCL	OBB-CAB-CBB	-3.92	111.35	120.17
9	l	104	A1EFU	CM3-C5-C4	3.92	124.25	118.08
9	I	103	A1EFU	CM6-C18-C19	3.92	124.25	118.08
9	d	102	A1EFU	CM4-C9-C8	3.92	124.25	118.08
8	e	102	BCL	OBB-CAB-CBB	-3.91	111.36	120.17
9	N	103	A1EFU	C23-C22-C21	-3.90	110.17	121.98
9	S	102	A1EFU	C10-C11-C12	-3.90	111.04	123.22
8	L	303	BCL	O2D-CGD-O1D	-3.90	116.21	123.84
9	l	101	A1EFU	CM5-C13-C12	3.90	124.22	118.08
9	d	102	A1EFU	CM6-C18-C19	3.90	124.22	118.08
8	k	101	BCL	OBB-CAB-CBB	-3.90	111.40	120.17
8	b	101	BCL	OBB-CAB-CBB	-3.89	111.42	120.17
9	d	102	A1EFU	CM5-C13-C12	3.89	124.20	118.08
8	M	402	BCL	OBB-CAB-CBB	-3.88	111.43	120.17
8	q	101	BCL	OBB-CAB-CBB	-3.88	111.43	120.17
9	r	102	A1EFU	C10-C11-C12	-3.88	111.10	123.22
8	a	102	BCL	OBB-CAB-CBB	-3.88	111.44	120.17
9	s	102	A1EFU	CM4-C9-C8	3.88	124.19	118.08
9	E	102	A1EFU	CM5-C13-C12	3.88	124.19	118.08
9	F	105	A1EFU	C10-C11-C12	-3.88	111.12	123.22
9	N	103	A1EFU	CM4-C9-C8	3.87	124.18	118.08
8	L	306	BCL	OBB-CAB-CBB	-3.87	111.46	120.17
9	s	102	A1EFU	C10-C11-C12	-3.87	111.15	123.22
9	I	101	A1EFU	C23-C22-C21	-3.87	110.27	121.98
9	e	101	A1EFU	C23-C22-C21	-3.86	110.28	121.98
9	J	103	A1EFU	C23-C22-C21	-3.86	110.28	121.98
9	J	102	A1EFU	CM5-C13-C12	3.86	124.16	118.08
9	J	102	A1EFU	C6-C7-C8	-3.86	111.17	123.22
9	2	101	A1EFU	CM6-C18-C19	3.86	124.16	118.08
9	2	101	A1EFU	CM3-C5-C4	3.86	124.16	118.08
8	i	101	BCL	OBB-CAB-CBB	-3.86	111.49	120.17
9	A	102	A1EFU	C10-C11-C12	-3.86	111.19	123.22
10	D	102	MW9	O8-C24-C25	3.86	119.81	111.50
8	M	403	BCL	OBB-CAB-CBB	-3.85	111.50	120.17
8	P	101	BCL	C1C-NC-C4C	-3.85	104.97	106.71
8	B	101	BCL	OBB-CAB-CBB	-3.85	111.51	120.17
9	K	102	A1EFU	C6-C7-C8	-3.85	111.21	123.22
8	P	101	BCL	OBB-CAB-CBB	-3.85	111.51	120.17
8	n	101	BCL	OBB-CAB-CBB	-3.85	111.51	120.17
9	t	102	A1EFU	C6-C7-C8	-3.85	111.21	123.22
9	I	103	A1EFU	C23-C22-C21	-3.84	110.34	121.98
9	v	103	A1EFU	C10-C11-C12	-3.84	111.22	123.22

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	K	102	A1EFU	CM3-C5-C4	3.84	124.13	118.08
9	a	101	A1EFU	C6-C7-C8	-3.84	111.23	123.22
8	L	306	BCL	CHD-C1D-ND	-3.84	120.92	124.45
8	J	101	BCL	OBB-CAB-CBB	-3.84	111.53	120.17
8	t	101	BCL	CHA-C1A-NA	-3.84	117.61	126.40
9	S	102	A1EFU	C6-C7-C8	-3.84	111.24	123.22
8	L	303	BCL	OBB-CAB-CBB	-3.84	111.53	120.17
9	I	101	A1EFU	C10-C11-C12	-3.84	111.24	123.22
9	T	101	A1EFU	CM5-C13-C12	3.83	124.12	118.08
8	l	102	BCL	OBB-CAB-CBB	-3.83	111.55	120.17
9	t	102	A1EFU	CM6-C18-C19	3.83	124.11	118.08
8	S	101	BCL	OBB-CAB-CBB	-3.83	111.56	120.17
8	E	101	BCL	OBB-CAB-CBB	-3.83	111.56	120.17
9	s	102	A1EFU	CM5-C13-C12	3.82	124.10	118.08
9	2	102	A1EFU	CM3-C5-C4	3.82	124.09	118.08
8	G	101	BCL	OBB-CAB-CBB	-3.82	111.58	120.17
9	Q	102	A1EFU	CM4-C9-C8	3.81	124.08	118.08
9	J	103	A1EFU	CM5-C13-C12	3.81	124.08	118.08
8	D	101	BCL	OBB-CAB-CBB	-3.81	111.59	120.17
8	F	101	BCL	OBB-CAB-CBB	-3.81	111.59	120.17
9	e	101	A1EFU	C10-C11-C12	-3.81	111.32	123.22
8	l	103	BCL	OBB-CAB-CBB	-3.81	111.59	120.17
8	I	102	BCL	OBB-CAB-CBB	-3.81	111.60	120.17
8	r	101	BCL	OBB-CAB-CBB	-3.81	111.61	120.17
8	N	101	BCL	OBB-CAB-CBB	-3.80	111.61	120.17
8	K	101	BCL	OBB-CAB-CBB	-3.80	111.61	120.17
8	R	102	BCL	OBB-CAB-CBB	-3.80	111.62	120.17
9	K	102	A1EFU	CM5-C13-C12	3.80	124.06	118.08
9	t	102	A1EFU	C10-C11-C12	-3.80	111.37	123.22
9	T	101	A1EFU	CM4-C9-C8	3.79	124.06	118.08
8	F	102	BCL	OBB-CAB-CBB	-3.79	111.63	120.17
8	v	101	BCL	OBB-CAB-CBB	-3.79	111.63	120.17
9	R	101	A1EFU	C21-C20-C19	-3.79	111.38	123.22
9	D	104	A1EFU	C23-C22-C21	-3.79	110.50	121.98
8	F	102	BCL	CGD-CBD-CAD	-3.79	98.46	110.73
9	R	101	A1EFU	CM4-C9-C8	3.79	124.04	118.08
9	R	101	A1EFU	C10-C11-C12	-3.79	111.40	123.22
9	k	102	A1EFU	CM5-C13-C12	3.79	124.04	118.08
8	F	102	BCL	C1C-NC-C4C	-3.78	105.00	106.71
9	2	101	A1EFU	CM4-C9-C8	3.78	124.03	118.08
8	Q	101	BCL	OBB-CAB-CBB	-3.78	111.66	120.17
9	B	102	A1EFU	C10-C11-C12	-3.78	111.42	123.22

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	101	BCL	OBB-CAB-CBB	-3.77	111.68	120.17
8	F	102	BCL	CHA-C1A-NA	-3.77	117.77	126.40
8	L	303	BCL	CHD-C1D-ND	-3.77	120.99	124.45
9	d	102	A1EFU	C6-C7-C8	-3.77	111.46	123.22
9	k	102	A1EFU	CM6-C18-C19	3.76	124.00	118.08
9	F	105	A1EFU	CM6-C18-C19	3.76	124.00	118.08
8	r	101	BCL	CHD-C1D-ND	-3.76	121.00	124.45
9	G	104	A1EFU	CM5-C13-C12	3.76	124.00	118.08
9	E	102	A1EFU	CM3-C5-C4	3.76	124.00	118.08
9	Q	103	A1EFU	C10-C11-C12	-3.76	111.50	123.22
8	K	101	BCL	CHD-C1D-ND	-3.75	121.00	124.45
9	J	103	A1EFU	CM4-C9-C8	3.75	123.99	118.08
9	t	102	A1EFU	CM5-C13-C12	3.75	123.99	118.08
8	G	102	BCL	OBB-CAB-CBB	-3.75	111.72	120.17
9	N	103	A1EFU	C6-C7-C8	-3.75	111.51	123.22
9	v	102	A1EFU	CM4-C9-C8	3.75	123.99	118.08
8	A	101	BCL	CHD-C1D-ND	-3.75	121.01	124.45
9	a	101	A1EFU	C23-C22-C21	-3.74	110.65	121.98
9	t	102	A1EFU	C23-C22-C21	-3.74	110.66	121.98
9	G	105	A1EFU	C10-C11-C12	-3.74	111.55	123.22
9	2	102	A1EFU	C6-C7-C8	-3.74	111.55	123.22
8	P	102	BCL	OBB-CAB-CBB	-3.74	111.76	120.17
9	2	102	A1EFU	CM4-C9-C8	3.73	123.95	118.08
9	R	101	A1EFU	CM6-C18-C19	3.73	123.95	118.08
9	I	103	A1EFU	CM4-C9-C8	3.73	123.95	118.08
9	K	102	A1EFU	C10-C11-C12	-3.72	111.60	123.22
9	B	102	A1EFU	CM6-C18-C19	3.72	123.94	118.08
9	G	105	A1EFU	CM4-C9-C8	3.72	123.93	118.08
9	I	103	A1EFU	CM5-C13-C12	3.72	123.93	118.08
9	J	103	A1EFU	CM6-C18-C19	3.71	123.93	118.08
9	Q	103	A1EFU	CM6-C18-C19	3.71	123.92	118.08
9	Q	103	A1EFU	C6-C7-C8	-3.70	111.66	123.22
9	v	102	A1EFU	C23-C22-C21	-3.70	110.77	121.98
9	v	102	A1EFU	CM5-C13-C12	3.70	123.91	118.08
9	S	102	A1EFU	C23-C22-C21	-3.70	110.79	121.98
9	I	103	A1EFU	C6-C7-C8	-3.70	111.68	123.22
9	K	102	A1EFU	C23-C22-C21	-3.69	110.80	121.98
9	T	101	A1EFU	CM6-C18-C19	3.69	123.89	118.08
9	r	102	A1EFU	CM4-C9-C8	3.69	123.89	118.08
8	N	101	BCL	CHD-C1D-ND	-3.69	121.07	124.45
9	v	103	A1EFU	C23-C22-C21	-3.68	110.83	121.98
9	E	102	A1EFU	CM6-C18-C19	3.68	123.88	118.08

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	105	A1EFU	CM5-C13-C12	3.68	123.88	118.08
9	T	101	A1EFU	C10-C11-C12	-3.67	111.75	123.22
9	J	103	A1EFU	C10-C11-C12	-3.67	111.75	123.22
9	a	101	A1EFU	C21-C20-C19	-3.67	111.76	123.22
8	i	101	BCL	CHD-C1D-ND	-3.67	121.08	124.45
9	Q	103	A1EFU	CM5-C13-C12	3.67	123.86	118.08
9	r	102	A1EFU	CM6-C18-C19	3.67	123.86	118.08
9	D	105	A1EFU	C10-C11-C12	-3.67	111.78	123.22
9	l	104	A1EFU	C6-C7-C8	-3.67	111.78	123.22
9	J	103	A1EFU	C6-C7-C8	-3.66	111.78	123.22
9	S	102	A1EFU	CM6-C18-C19	3.66	123.84	118.08
9	F	105	A1EFU	C21-C20-C19	-3.66	111.80	123.22
8	e	102	BCL	C1C-NC-C4C	-3.66	105.06	106.71
9	T	101	A1EFU	C23-C22-C21	-3.66	110.91	121.98
9	J	102	A1EFU	C10-C11-C12	-3.65	111.81	123.22
9	s	102	A1EFU	CM3-C5-C6	-3.65	117.81	122.92
9	M	407	A1EFU	CM4-C9-C8	3.65	123.83	118.08
8	v	101	BCL	C4A-NA-C1A	-3.65	105.06	106.71
9	G	105	A1EFU	C6-C7-C8	-3.65	111.83	123.22
9	l	101	A1EFU	C10-C11-C12	-3.65	111.84	123.22
8	M	402	BCL	C1C-NC-C4C	-3.64	105.07	106.71
8	J	101	BCL	CHD-C1D-ND	-3.64	121.11	124.45
9	v	102	A1EFU	CM6-C18-C19	3.64	123.81	118.08
8	l	103	BCL	C2C-C3C-C4C	-3.64	95.89	101.34
9	l	104	A1EFU	CM4-C9-C8	3.63	123.80	118.08
9	I	103	A1EFU	C10-C11-C12	-3.63	111.89	123.22
8	q	101	BCL	CHD-C1D-ND	-3.63	121.12	124.45
8	d	101	BCL	OBB-CAB-CBB	-3.62	112.01	120.17
9	s	102	A1EFU	C23-C22-C21	-3.62	111.01	121.98
9	D	105	A1EFU	C21-C20-C19	-3.62	111.92	123.22
9	Q	102	A1EFU	C23-C22-C21	-3.62	111.02	121.98
9	v	102	A1EFU	C6-C7-C8	-3.62	111.92	123.22
8	t	101	BCL	C4B-CHC-C1C	-3.62	122.95	130.12
9	N	102	A1EFU	CM3-C5-C4	3.62	123.78	118.08
9	J	102	A1EFU	CM3-C5-C4	3.62	123.78	118.08
9	e	101	A1EFU	CM5-C13-C12	3.62	123.78	118.08
9	T	101	A1EFU	C6-C7-C8	-3.62	111.93	123.22
9	A	102	A1EFU	C23-C22-C21	-3.62	111.03	121.98
8	j	101	BCL	CHD-C1D-ND	-3.62	121.13	124.45
8	E	101	BCL	CHD-C1D-ND	-3.61	121.13	124.45
9	a	101	A1EFU	CM5-C13-C12	3.61	123.77	118.08
8	k	101	BCL	CHD-C1D-ND	-3.61	121.14	124.45

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	101	BCL	CHD-C1D-ND	-3.61	121.14	124.45
9	N	103	A1EFU	CM6-C18-C19	3.61	123.76	118.08
8	F	101	BCL	CHD-C1D-ND	-3.61	121.14	124.45
9	M	407	A1EFU	CM5-C13-C12	3.61	123.76	118.08
9	s	102	A1EFU	C6-C7-C8	-3.61	111.97	123.22
8	S	101	BCL	CHD-C1D-ND	-3.60	121.14	124.45
9	Q	103	A1EFU	CM4-C9-C8	3.60	123.75	118.08
9	d	102	A1EFU	C21-C20-C19	-3.60	111.99	123.22
8	R	102	BCL	CHD-C1D-ND	-3.60	121.15	124.45
8	I	102	BCL	CHD-C1D-ND	-3.60	121.15	124.45
8	a	102	BCL	CHD-C1D-ND	-3.59	121.15	124.45
8	B	101	BCL	CHD-C1D-ND	-3.59	121.15	124.45
9	G	104	A1EFU	CM6-C18-C19	3.59	123.73	118.08
8	n	101	BCL	CHD-C1D-ND	-3.59	121.16	124.45
9	N	102	A1EFU	CM5-C13-C12	3.58	123.71	118.08
9	r	102	A1EFU	C23-C22-C21	-3.58	111.15	121.98
9	M	407	A1EFU	CM6-C18-C19	3.58	123.71	118.08
9	l	101	A1EFU	CM6-C18-C19	3.57	123.71	118.08
9	B	102	A1EFU	C21-C20-C19	-3.57	112.06	123.22
9	N	103	A1EFU	C21-C20-C19	-3.57	112.08	123.22
8	n	101	BCL	C16-C15-C13	-3.57	104.39	115.92
9	a	103	A1EFU	C21-C20-C19	-3.56	112.09	123.22
9	K	102	A1EFU	C21-C20-C19	-3.56	112.10	123.22
9	2	101	A1EFU	CM5-C13-C12	3.56	123.68	118.08
8	G	102	BCL	CHD-C1D-ND	-3.55	121.19	124.45
9	E	102	A1EFU	C10-C11-C12	-3.55	112.13	123.22
8	s	101	BCL	CHD-C1D-ND	-3.55	121.19	124.45
16	C	403	HEC	CMB-C2B-C3B	3.54	129.99	125.82
9	M	407	A1EFU	C10-C11-C12	-3.54	112.16	123.22
9	k	102	A1EFU	C10-C11-C12	-3.54	112.18	123.22
9	e	101	A1EFU	C21-C20-C19	-3.53	112.20	123.22
9	R	101	A1EFU	C6-C7-C8	-3.53	112.21	123.22
8	Q	101	BCL	CHD-C1D-ND	-3.53	121.21	124.45
9	E	102	A1EFU	C21-C20-C19	-3.52	112.22	123.22
8	T	102	BCL	CHD-C1D-ND	-3.52	121.22	124.45
8	l	102	BCL	C16-C15-C13	-3.52	104.55	115.92
9	G	105	A1EFU	C21-C20-C19	-3.52	112.25	123.22
16	C	403	HEC	CBD-CAD-C3D	3.51	118.61	112.62
9	M	407	A1EFU	C6-C7-C8	-3.51	112.26	123.22
9	2	101	A1EFU	C6-C7-C8	-3.51	112.27	123.22
9	J	103	A1EFU	C21-C20-C19	-3.51	112.28	123.22
9	Q	102	A1EFU	C10-C11-C12	-3.50	112.30	123.22

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	s	102	A1EFU	CM3-C5-C4	3.50	123.59	118.08
8	t	101	BCL	CMB-C2B-C1B	-3.49	123.10	128.46
16	C	401	HEC	CMC-C2C-C1C	-3.49	123.10	128.46
16	C	403	HEC	CMB-C2B-C1B	-3.49	123.10	128.46
8	L	303	BCL	C1C-NC-C4C	-3.48	105.14	106.71
8	L	306	BCL	C16-C15-C13	-3.48	104.66	115.92
8	P	101	BCL	CHD-C1D-ND	-3.48	121.25	124.45
8	b	101	BCL	CHD-C1D-ND	-3.48	121.26	124.45
9	2	101	A1EFU	C10-C11-C12	-3.48	112.36	123.22
9	N	102	A1EFU	C21-C20-C19	-3.48	112.37	123.22
8	D	101	BCL	C1C-NC-C4C	-3.47	105.14	106.71
9	A	102	A1EFU	CM6-C18-C19	3.47	123.54	118.08
8	V	101	BCL	CHD-C1D-ND	-3.46	121.28	124.45
9	s	102	A1EFU	C21-C20-C19	-3.45	112.44	123.22
8	P	102	BCL	C4A-NA-C1A	-3.45	105.16	106.71
9	1	101	A1EFU	C21-C20-C19	-3.45	112.47	123.22
9	1	104	A1EFU	CM5-C13-C12	3.45	123.50	118.08
8	1	103	BCL	CHD-C1D-ND	-3.44	121.29	124.45
8	T	102	BCL	C16-C15-C13	-3.44	104.79	115.92
9	G	104	A1EFU	CM4-C9-C8	3.44	123.50	118.08
8	L	303	BCL	C2A-C3A-C4A	-3.44	96.31	101.87
8	P	101	BCL	C16-C15-C13	-3.43	104.82	115.92
9	t	102	A1EFU	C21-C20-C19	-3.43	112.51	123.22
9	Q	102	A1EFU	CM6-C18-C19	3.43	123.48	118.08
8	G	102	BCL	C2C-C3C-C4C	-3.43	96.21	101.34
8	e	102	BCL	CHD-C1D-ND	-3.43	121.31	124.45
9	2	101	A1EFU	C21-C20-C19	-3.42	112.53	123.22
8	r	101	BCL	C16-C15-C13	-3.42	104.86	115.92
8	A	101	BCL	C1C-NC-C4C	-3.42	105.17	106.71
9	M	407	A1EFU	C23-C22-C21	-3.42	111.64	121.98
16	C	402	HEC	CMC-C2C-C3C	3.41	129.83	125.82
8	a	102	BCL	C16-C15-C13	-3.41	104.91	115.92
9	v	102	A1EFU	C10-C11-C12	-3.40	112.60	123.22
8	T	102	BCL	CMB-C2B-C3B	3.40	131.04	124.68
9	T	101	A1EFU	C21-C20-C19	-3.40	112.60	123.22
8	P	102	BCL	C16-C15-C13	-3.40	104.93	115.92
8	1	102	BCL	CHD-C1D-ND	-3.40	121.33	124.45
9	J	102	A1EFU	C23-C22-C21	-3.39	111.72	121.98
8	M	402	BCL	CHA-C1A-NA	-3.39	118.64	126.40
8	G	101	BCL	CHD-C1D-ND	-3.39	121.34	124.45
9	N	102	A1EFU	C6-C7-C8	-3.38	112.66	123.22
8	d	101	BCL	CHA-C1A-NA	-3.38	118.66	126.40

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	C	403	HEC	CMC-C2C-C1C	-3.38	123.28	128.46
8	M	403	BCL	C16-C15-C13	-3.37	105.03	115.92
8	E	101	BCL	C2C-C3C-C4C	-3.36	96.31	101.34
9	D	104	A1EFU	CM6-C18-C19	3.36	123.36	118.08
16	C	401	HEC	CBD-CAD-C3D	3.35	118.34	112.62
8	k	101	BCL	C16-C15-C13	-3.35	105.08	115.92
8	F	101	BCL	C16-C15-C13	-3.34	105.12	115.92
8	q	101	BCL	C16-C15-C13	-3.34	105.12	115.92
9	N	102	A1EFU	CM4-C9-C8	3.34	123.34	118.08
8	P	102	BCL	CHD-C1D-ND	-3.34	121.39	124.45
9	G	104	A1EFU	C21-C20-C19	-3.31	112.88	123.22
9	l	104	A1EFU	C23-C22-C21	-3.31	111.96	121.98
9	Q	103	A1EFU	C23-C22-C21	-3.31	111.97	121.98
9	G	104	A1EFU	C10-C11-C12	-3.30	112.91	123.22
9	r	102	A1EFU	C21-C20-C19	-3.30	112.92	123.22
8	b	101	BCL	CHA-C1A-NA	-3.30	118.85	126.40
8	S	101	BCL	C16-C15-C13	-3.29	105.28	115.92
9	v	103	A1EFU	C21-C20-C19	-3.29	112.94	123.22
9	l	104	A1EFU	C10-C11-C12	-3.29	112.95	123.22
9	A	102	A1EFU	C21-C20-C19	-3.29	112.95	123.22
8	s	101	BCL	C16-C15-C13	-3.29	105.29	115.92
9	I	103	A1EFU	C21-C20-C19	-3.29	112.96	123.22
8	F	101	BCL	O2A-CGA-O1A	-3.28	115.31	123.59
8	B	101	BCL	C1C-NC-C4C	-3.28	105.23	106.71
8	A	101	BCL	C16-C15-C13	-3.28	105.32	115.92
8	q	101	BCL	CHA-C1A-NA	-3.28	118.90	126.40
9	I	101	A1EFU	C21-C20-C19	-3.27	113.00	123.22
8	e	102	BCL	CHA-C1A-NA	-3.27	118.91	126.40
8	I	102	BCL	C16-C15-C13	-3.26	105.37	115.92
8	Q	101	BCL	C1C-NC-C4C	-3.26	105.24	106.71
8	G	102	BCL	CHA-C1A-NA	-3.26	118.94	126.40
9	N	102	A1EFU	C10-C11-C12	-3.25	113.06	123.22
8	v	101	BCL	C4D-CHA-C1A	3.25	125.21	121.25
9	k	102	A1EFU	C21-C20-C19	-3.25	113.08	123.22
9	N	102	A1EFU	CM6-C18-C19	3.25	123.19	118.08
16	C	403	HEC	CMC-C2C-C3C	3.25	129.64	125.82
8	F	102	BCL	C2A-C1A-CHA	3.24	129.53	123.86
8	L	306	BCL	C4A-NA-C1A	-3.24	105.25	106.71
8	S	101	BCL	C1C-NC-C4C	-3.24	105.25	106.71
9	D	104	A1EFU	C21-C20-C19	-3.23	113.12	123.22
8	t	101	BCL	C16-C15-C13	-3.23	105.47	115.92
8	I	102	BCL	CHA-C1A-NA	-3.23	119.00	126.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	r	101	BCL	CHA-C1A-NA	-3.23	119.00	126.40
8	P	102	BCL	CMB-C2B-C3B	3.23	130.72	124.68
8	M	402	BCL	C4B-CHC-C1C	-3.23	123.72	130.12
8	R	102	BCL	C16-C15-C13	-3.23	105.49	115.92
8	a	102	BCL	CHA-C1A-NA	-3.22	119.03	126.40
13	L	308	LMT	C3'-C4'-C5'	-3.22	105.57	110.30
8	s	101	BCL	CHA-C1A-NA	-3.20	119.06	126.40
8	d	101	BCL	CHD-C1D-ND	-3.20	121.51	124.45
8	d	101	BCL	C11-C10-C8	-3.20	105.57	115.92
8	Q	101	BCL	CGD-CBD-CAD	-3.20	100.38	110.73
9	k	102	A1EFU	C6-C7-C8	-3.20	113.25	123.22
8	t	101	BCL	C1C-NC-C4C	-3.19	105.27	106.71
8	j	101	BCL	CHA-C1A-NA	-3.19	119.09	126.40
9	N	103	A1EFU	CM5-C13-C12	3.19	123.10	118.08
8	N	101	BCL	C16-C15-C13	-3.18	105.63	115.92
9	J	102	A1EFU	CM6-C18-C19	3.18	123.09	118.08
9	a	103	A1EFU	C6-C7-C8	-3.17	113.32	123.22
8	F	101	BCL	C4B-CHC-C1C	-3.17	123.84	130.12
8	V	101	BCL	O2A-CGA-O1A	-3.17	115.59	123.59
9	S	102	A1EFU	C21-C20-C19	-3.17	113.32	123.22
9	2	102	A1EFU	C21-C20-C19	-3.17	113.32	123.22
8	r	101	BCL	CMB-C2B-C3B	3.17	130.61	124.68
8	D	101	BCL	C4B-CHC-C1C	-3.16	123.86	130.12
9	I	101	A1EFU	CM6-C18-C19	3.16	123.05	118.08
8	i	101	BCL	C16-C15-C13	-3.16	105.72	115.92
8	Q	101	BCL	C16-C15-C13	-3.15	105.72	115.92
9	v	102	A1EFU	C21-C20-C19	-3.15	113.40	123.22
8	Q	101	BCL	C4B-CHC-C1C	-3.14	123.89	130.12
8	J	101	BCL	O2A-CGA-O1A	-3.14	115.67	123.59
8	V	101	BCL	C16-C15-C13	-3.14	105.77	115.92
8	i	101	BCL	CHA-C1A-NA	-3.14	119.21	126.40
8	k	101	BCL	C1C-NC-C4C	-3.14	105.30	106.71
8	E	101	BCL	CHA-C1A-NA	-3.13	119.23	126.40
8	D	101	BCL	C7-C6-C5	-3.13	104.86	113.36
9	M	407	A1EFU	C21-C20-C19	-3.13	113.45	123.22
8	J	101	BCL	CHA-C1A-NA	-3.13	119.24	126.40
8	d	101	BCL	O2A-CGA-O1A	-3.12	115.72	123.59
8	R	102	BCL	C2C-C3C-C4C	-3.12	96.67	101.34
16	C	402	HEC	CMB-C2B-C3B	3.11	129.48	125.82
8	Q	101	BCL	CHA-C1A-NA	-3.11	119.27	126.40
8	V	101	BCL	CHA-C1A-NA	-3.11	119.27	126.40
8	K	101	BCL	CHA-C1A-NA	-3.11	119.28	126.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	C	402	HEC	CMB-C2B-C1B	-3.11	123.68	128.46
8	R	102	BCL	CHA-C1A-NA	-3.11	119.28	126.40
8	1	102	BCL	C11-C10-C8	-3.11	105.88	115.92
8	n	101	BCL	CMB-C2B-C3B	3.11	130.49	124.68
8	1	103	BCL	C11-C10-C8	-3.10	105.89	115.92
8	B	101	BCL	C16-C15-C13	-3.10	105.89	115.92
8	K	101	BCL	C4B-CHC-C1C	-3.10	123.97	130.12
8	F	102	BCL	C16-C15-C13	-3.10	105.89	115.92
9	Q	102	A1EFU	C21-C20-C19	-3.10	113.54	123.22
8	F	102	BCL	O2A-CGA-O1A	-3.09	115.79	123.59
8	j	101	BCL	C2C-C3C-C4C	-3.09	96.71	101.34
8	E	101	BCL	C16-C15-C13	-3.09	105.93	115.92
8	G	101	BCL	C4B-CHC-C1C	-3.09	124.00	130.12
8	M	402	BCL	C16-C15-C13	-3.09	105.95	115.92
8	L	306	BCL	C11-C10-C8	-3.08	105.95	115.92
8	I	102	BCL	C4B-CHC-C1C	-3.08	124.01	130.12
8	F	102	BCL	C2C-C3C-C4C	-3.08	96.72	101.34
8	D	101	BCL	C16-C15-C13	-3.08	105.96	115.92
8	k	101	BCL	CHA-C1A-NA	-3.08	119.34	126.40
8	P	101	BCL	C7-C6-C5	-3.08	105.00	113.36
8	T	102	BCL	C7-C6-C5	-3.08	105.00	113.36
13	L	308	LMT	C1'-O5'-C5'	-3.07	108.38	113.67
8	P	101	BCL	C4D-CHA-C1A	3.07	124.99	121.25
8	1	102	BCL	C4B-CHC-C1C	-3.07	124.04	130.12
8	P	101	BCL	CHA-C1A-NA	-3.07	119.38	126.40
8	G	101	BCL	C16-C15-C13	-3.06	106.02	115.92
8	J	101	BCL	C4B-CHC-C1C	-3.06	124.05	130.12
8	F	101	BCL	CHA-C1A-NA	-3.06	119.39	126.40
8	L	303	BCL	C11-C10-C8	-3.06	106.04	115.92
8	I	102	BCL	C4D-CHA-C1A	3.05	124.97	121.25
8	j	101	BCL	C16-C15-C13	-3.05	106.06	115.92
8	M	403	BCL	O2A-CGA-O1A	-3.05	115.89	123.59
8	I	102	BCL	C7-C6-C5	-3.05	105.08	113.36
8	A	101	BCL	C4D-CHA-C1A	3.05	124.96	121.25
8	1	103	BCL	CHA-C1A-NA	-3.05	119.42	126.40
8	A	101	BCL	CMB-C2B-C3B	3.05	130.38	124.68
8	1	103	BCL	C4B-CHC-C1C	-3.05	124.08	130.12
8	V	101	BCL	C4A-NA-C1A	-3.05	105.34	106.71
8	R	102	BCL	C7-C6-C5	-3.04	105.09	113.36
8	P	102	BCL	O2A-CGA-O1A	-3.04	115.91	123.59
8	G	102	BCL	C4B-CHC-C1C	-3.04	124.09	130.12
8	S	101	BCL	CHA-C1A-NA	-3.04	119.43	126.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	J	101	BCL	C11-C10-C8	-3.04	106.08	115.92
8	G	102	BCL	C16-C15-C13	-3.04	106.09	115.92
8	N	101	BCL	CHA-C1A-NA	-3.04	119.44	126.40
8	T	102	BCL	C2C-C3C-C4C	-3.04	96.79	101.34
8	d	101	BCL	C16-C15-C13	-3.04	106.10	115.92
8	V	101	BCL	C7-C6-C5	-3.04	105.11	113.36
9	s	102	A1EFU	CM6-C18-C19	3.03	122.85	118.08
8	B	101	BCL	C11-C10-C8	-3.03	106.13	115.92
8	G	102	BCL	C7-C6-C5	-3.03	105.14	113.36
8	n	101	BCL	CHA-C1A-NA	-3.02	119.47	126.40
8	b	101	BCL	C11-C10-C8	-3.02	106.15	115.92
8	S	101	BCL	C4B-CHC-C1C	-3.02	124.14	130.12
8	D	101	BCL	CHA-C1A-NA	-3.02	119.49	126.40
8	P	101	BCL	C4B-CHC-C1C	-3.02	124.14	130.12
8	1	103	BCL	C16-C15-C13	-3.01	106.18	115.92
8	1	103	BCL	C7-C6-C5	-3.01	105.19	113.36
8	B	101	BCL	CHA-C1A-NA	-3.01	119.52	126.40
8	J	101	BCL	C16-C15-C13	-3.00	106.22	115.92
8	J	101	BCL	C7-C6-C5	-3.00	105.21	113.36
8	T	102	BCL	CHA-C1A-NA	-3.00	119.53	126.40
8	K	101	BCL	C7-C6-C5	-3.00	105.22	113.36
8	L	303	BCL	C3D-C2D-C1D	-3.00	101.74	105.83
8	Q	101	BCL	C7-C6-C5	-2.99	105.24	113.36
8	N	101	BCL	C4B-CHC-C1C	-2.99	124.20	130.12
8	G	102	BCL	C11-C10-C8	-2.99	106.27	115.92
8	D	101	BCL	C4D-CHA-C1A	2.99	124.88	121.25
8	e	102	BCL	C4B-CHC-C1C	-2.98	124.21	130.12
8	L	306	BCL	C2C-C3C-C4C	-2.98	96.87	101.34
8	G	101	BCL	C4A-NA-C1A	-2.98	105.36	106.71
8	k	101	BCL	C4B-CHC-C1C	-2.98	124.21	130.12
8	L	306	BCL	CHA-C1A-NA	-2.98	119.58	126.40
8	M	402	BCL	O2A-CGA-O1A	-2.97	116.09	123.59
8	r	101	BCL	O2A-CGA-O1A	-2.97	116.10	123.59
8	P	102	BCL	C4B-CHC-C1C	-2.97	124.24	130.12
8	A	101	BCL	CHA-C1A-NA	-2.97	119.61	126.40
8	A	101	BCL	C11-C10-C8	-2.97	106.33	115.92
8	a	102	BCL	C11-C10-C8	-2.96	106.34	115.92
8	T	102	BCL	C11-C10-C8	-2.96	106.34	115.92
8	n	101	BCL	C7-C6-C5	-2.96	105.32	113.36
8	F	102	BCL	C4B-CHC-C1C	-2.96	124.26	130.12
8	L	303	BCL	C11-C12-C13	-2.96	106.37	115.92
8	F	101	BCL	C7-C6-C5	-2.95	105.33	113.36

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	101	BCL	C7-C6-C5	-2.95	105.35	113.36
8	F	101	BCL	C11-C10-C8	-2.95	106.40	115.92
8	b	101	BCL	C16-C15-C13	-2.94	106.40	115.92
8	k	101	BCL	C11-C10-C8	-2.94	106.40	115.92
8	J	101	BCL	C4D-CHA-C1A	2.94	124.83	121.25
9	2	102	A1EFU	CM6-C18-C19	2.94	122.71	118.08
8	L	303	BCL	CMC-C2C-C3C	-2.94	101.97	113.83
8	B	101	BCL	C4D-CHA-C1A	2.94	124.83	121.25
8	N	101	BCL	C11-C10-C8	-2.94	106.43	115.92
8	r	101	BCL	C11-C10-C8	-2.94	106.43	115.92
8	l	102	BCL	CHA-C1A-NA	-2.94	119.67	126.40
8	L	303	BCL	CMA-C3A-C4A	-2.94	103.88	111.77
16	C	403	HEC	O1D-CGD-CBD	-2.94	113.65	123.08
8	q	101	BCL	C4B-CHC-C1C	-2.94	124.30	130.12
8	L	303	BCL	C4B-CHC-C1C	-2.93	124.31	130.12
8	S	101	BCL	C4D-CHA-C1A	2.93	124.81	121.25
9	1	104	A1EFU	C19-C18-C17	2.93	123.44	118.94
8	F	102	BCL	C7-C6-C5	-2.93	105.41	113.36
8	R	102	BCL	C4B-CHC-C1C	-2.93	124.32	130.12
8	Q	101	BCL	C4D-CHA-C1A	2.93	124.81	121.25
8	l	103	BCL	O2A-CGA-O1A	-2.93	116.21	123.59
9	K	102	A1EFU	CM6-C18-C19	2.92	122.68	118.08
8	N	101	BCL	C7-C6-C5	-2.92	105.44	113.36
8	E	101	BCL	C4B-CHC-C1C	-2.92	124.34	130.12
8	B	101	BCL	C4B-CHC-C1C	-2.91	124.35	130.12
8	i	101	BCL	O2A-CGA-O1A	-2.91	116.24	123.59
8	i	101	BCL	C4B-CHC-C1C	-2.91	124.35	130.12
8	q	101	BCL	C11-C10-C8	-2.91	106.51	115.92
8	E	101	BCL	C11-C10-C8	-2.91	106.53	115.92
8	n	101	BCL	C4B-CHC-C1C	-2.90	124.38	130.12
8	G	101	BCL	CHA-C1A-NA	-2.89	119.77	126.40
16	C	401	HEC	CMB-C2B-C1B	-2.89	124.02	128.46
8	l	102	BCL	O2A-CGA-O1A	-2.89	116.29	123.59
8	v	101	BCL	C16-C15-C13	-2.89	106.58	115.92
8	a	102	BCL	C4B-CHC-C1C	-2.89	124.40	130.12
8	Q	101	BCL	C11-C10-C8	-2.89	106.58	115.92
8	P	101	BCL	C11-C10-C8	-2.89	106.58	115.92
8	s	101	BCL	C4B-CHC-C1C	-2.88	124.41	130.12
8	Q	101	BCL	CMA-C3A-C4A	-2.88	104.03	111.77
8	P	102	BCL	C11-C10-C8	-2.88	106.62	115.92
8	G	102	BCL	C4D-CHA-C1A	2.88	124.75	121.25
8	v	101	BCL	C7-C6-C5	-2.88	105.55	113.36

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	V	101	BCL	C2A-C1A-CHA	2.87	128.88	123.86
8	b	101	BCL	C7-C6-C5	-2.87	105.56	113.36
8	L	306	BCL	C4B-CHC-C1C	-2.87	124.43	130.12
8	L	303	BCL	O2A-CGA-O1A	-2.87	116.34	123.59
8	v	101	BCL	O2A-CGA-O1A	-2.87	116.35	123.59
8	b	101	BCL	C4B-CHC-C1C	-2.87	124.44	130.12
8	i	101	BCL	C7-C6-C5	-2.87	105.58	113.36
8	M	402	BCL	C11-C10-C8	-2.87	106.66	115.92
8	L	306	BCL	C4D-CHA-C1A	2.86	124.73	121.25
8	l	103	BCL	C4D-CHA-C1A	2.86	124.73	121.25
16	C	403	HEC	C4C-C3C-C2C	2.86	109.44	106.35
8	A	101	BCL	O2A-CGA-O1A	-2.85	116.39	123.59
8	S	101	BCL	C3D-C2D-C1D	-2.85	101.94	105.83
8	A	101	BCL	C3D-C2D-C1D	-2.85	101.94	105.83
8	M	402	BCL	C7-C6-C5	-2.85	105.62	113.36
8	A	101	BCL	C4B-CHC-C1C	-2.85	124.47	130.12
8	v	101	BCL	CHC-C1C-NC	2.85	128.45	124.51
8	F	102	BCL	C11-C10-C8	-2.85	106.72	115.92
8	E	101	BCL	C4D-CHA-C1A	2.84	124.71	121.25
8	r	101	BCL	C4B-CHC-C1C	-2.84	124.48	130.12
8	G	101	BCL	C11-C10-C8	-2.84	106.73	115.92
8	K	101	BCL	C4D-CHA-C1A	2.84	124.71	121.25
8	v	101	BCL	C3D-C2D-C1D	-2.84	101.96	105.83
8	Q	101	BCL	C3D-C2D-C1D	-2.84	101.96	105.83
8	a	102	BCL	C1C-NC-C4C	-2.84	105.43	106.71
8	M	403	BCL	C1B-CHB-C4A	-2.83	124.50	130.12
8	M	403	BCL	C7-C6-C5	-2.83	105.66	113.36
8	P	102	BCL	CHA-C1A-NA	-2.83	119.92	126.40
8	I	102	BCL	C3D-C2D-C1D	-2.83	101.97	105.83
8	B	101	BCL	C7-C6-C5	-2.82	105.69	113.36
8	t	101	BCL	C7-C6-C5	-2.82	105.69	113.36
8	P	101	BCL	C3D-C2D-C1D	-2.82	101.98	105.83
8	K	101	BCL	C16-C15-C13	-2.82	106.80	115.92
8	N	101	BCL	O2A-CGA-O1A	-2.82	116.48	123.59
8	D	101	BCL	O2A-CGA-O1A	-2.82	116.48	123.59
8	B	101	BCL	O2A-CGA-O1A	-2.82	116.48	123.59
8	T	102	BCL	C3D-C2D-C1D	-2.82	101.99	105.83
8	M	403	BCL	C4B-CHC-C1C	-2.82	124.54	130.12
8	e	102	BCL	C7-C6-C5	-2.82	105.71	113.36
13	H	301	LMT	C1'-O5'-C5'	-2.81	108.17	113.69
8	e	102	BCL	C16-C15-C13	-2.81	106.83	115.92
8	P	101	BCL	O2A-CGA-O1A	-2.81	116.49	123.59

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	r	101	BCL	C7-C6-C5	-2.81	105.72	113.36
8	P	102	BCL	CMA-C3A-C4A	-2.81	104.22	111.77
8	P	102	BCL	C4D-CHA-C1A	2.81	124.67	121.25
8	i	101	BCL	C3D-C2D-C1D	-2.81	102.00	105.83
8	K	101	BCL	C11-C10-C8	-2.81	106.84	115.92
8	M	403	BCL	CHA-C1A-NA	-2.81	119.97	126.40
8	k	101	BCL	C7-C6-C5	-2.81	105.73	113.36
8	K	101	BCL	O2A-CGA-O1A	-2.81	116.51	123.59
8	M	403	BCL	C11-C10-C8	-2.81	106.85	115.92
8	K	101	BCL	C3D-C2D-C1D	-2.80	102.00	105.83
8	s	101	BCL	C3D-C2D-C1D	-2.80	102.01	105.83
16	C	401	HEC	O1D-CGD-CBD	-2.80	114.08	123.08
8	B	101	BCL	C3D-C2D-C1D	-2.80	102.01	105.83
9	J	102	A1EFU	C21-C20-C19	-2.80	114.49	123.22
8	N	101	BCL	C4D-CHA-C1A	2.80	124.65	121.25
8	Q	101	BCL	CMC-C2C-C3C	-2.80	102.55	113.83
8	G	102	BCL	O2A-CGA-O1A	-2.80	116.54	123.59
8	d	101	BCL	C4B-CHC-C1C	-2.79	124.58	130.12
8	N	101	BCL	C3D-C2D-C1D	-2.79	102.02	105.83
8	q	101	BCL	C3D-C2D-C1D	-2.79	102.03	105.83
8	k	101	BCL	C3D-C2D-C1D	-2.79	102.03	105.83
8	n	101	BCL	C3D-C2D-C1D	-2.78	102.03	105.83
8	M	402	BCL	CMC-C2C-C3C	-2.78	102.60	113.83
8	M	403	BCL	CMA-C3A-C4A	-2.78	104.30	111.77
8	L	306	BCL	CMA-C3A-C4A	-2.78	104.30	111.77
8	S	101	BCL	C7-C6-C5	-2.78	105.81	113.36
8	j	101	BCL	C7-C6-C5	-2.78	105.82	113.36
8	s	101	BCL	C7-C6-C5	-2.77	105.82	113.36
8	D	101	BCL	C3D-C2D-C1D	-2.77	102.05	105.83
8	R	102	BCL	O2A-CGA-O1A	-2.77	116.59	123.59
10	M	406	MW9	O1-C17-C16	2.77	120.61	111.91
8	F	102	BCL	C3D-C2D-C1D	-2.77	102.05	105.83
8	F	101	BCL	CMA-C3A-C4A	-2.77	104.33	111.77
8	j	101	BCL	C3D-C2D-C1D	-2.77	102.06	105.83
8	n	101	BCL	C4D-CHA-C1A	2.77	124.61	121.25
13	L	307	LMT	C3'-C4'-C5'	-2.76	105.31	110.24
16	C	402	HEC	O1D-CGD-CBD	-2.76	114.20	123.08
8	v	101	BCL	CMC-C2C-C3C	-2.76	102.69	113.83
8	l	102	BCL	C7-C6-C5	-2.76	105.86	113.36
8	q	101	BCL	C7-C6-C5	-2.76	105.86	113.36
8	k	101	BCL	C4D-CHA-C1A	2.76	124.61	121.25
8	M	402	BCL	C3D-C2D-C1D	-2.76	102.07	105.83

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	i	101	BCL	C11-C10-C8	-2.76	107.01	115.92
10	L	310	MW9	O1-C17-C16	2.76	120.56	111.91
15	L	311	CDL	OA8-CA7-C31	2.75	120.55	111.91
8	a	102	BCL	O2A-CGA-O1A	-2.75	116.64	123.59
8	E	101	BCL	C3D-C2D-C1D	-2.75	102.08	105.83
8	L	303	BCL	CHA-C1A-NA	-2.75	120.10	126.40
8	t	101	BCL	CMC-C2C-C3C	-2.75	102.74	113.83
8	L	306	BCL	C7-C6-C5	-2.75	105.90	113.36
8	j	101	BCL	C4B-CHC-C1C	-2.75	124.68	130.12
10	L	309	MW9	O1-C17-C16	2.75	120.53	111.91
8	G	101	BCL	O2A-CGA-O1A	-2.75	116.66	123.59
8	r	101	BCL	C3D-C2D-C1D	-2.75	102.08	105.83
8	J	101	BCL	C3D-C2D-C1D	-2.75	102.08	105.83
8	S	101	BCL	CMC-C2C-C3C	-2.75	102.75	113.83
8	i	101	BCL	C4D-CHA-C1A	2.74	124.59	121.25
8	A	101	BCL	C7-C6-C5	-2.74	105.91	113.36
8	E	101	BCL	C7-C6-C5	-2.74	105.92	113.36
8	d	101	BCL	C4D-CHA-C1A	2.74	124.58	121.25
8	I	102	BCL	C11-C10-C8	-2.74	107.07	115.92
8	L	306	BCL	O2A-CGA-O1A	-2.74	116.69	123.59
8	V	101	BCL	C3D-C2D-C1D	-2.73	102.10	105.83
8	P	102	BCL	CMC-C2C-C3C	-2.73	102.81	113.83
8	L	306	BCL	C3D-C2D-C1D	-2.73	102.11	105.83
8	q	101	BCL	C1C-NC-C4C	-2.73	105.48	106.71
8	b	101	BCL	C4D-CHA-C1A	2.73	124.57	121.25
8	e	102	BCL	C4D-CHA-C1A	2.73	124.57	121.25
8	d	101	BCL	C2A-C1A-CHA	2.73	128.63	123.86
8	e	102	BCL	O2A-CGA-O1A	-2.73	116.71	123.59
9	2	102	A1EFU	CM5-C13-C12	2.73	122.37	118.08
8	b	101	BCL	C3D-C2D-C1D	-2.72	102.11	105.83
8	Q	101	BCL	O2A-CGA-O1A	-2.72	116.72	123.59
8	a	102	BCL	C7-C6-C5	-2.72	105.97	113.36
8	n	101	BCL	C11-C12-C13	-2.72	107.13	115.92
16	C	401	HEC	CMB-C2B-C3B	2.72	129.02	125.82
8	l	103	BCL	C3D-C2D-C1D	-2.72	102.12	105.83
8	j	101	BCL	C11-C10-C8	-2.72	107.13	115.92
8	s	101	BCL	C1C-NC-C4C	-2.72	105.48	106.71
8	T	102	BCL	C11-C12-C13	-2.72	107.14	115.92
8	t	101	BCL	C3D-C2D-C1D	-2.72	102.12	105.83
8	B	101	BCL	CMC-C2C-C3C	-2.71	102.88	113.83
8	t	101	BCL	CHB-C4A-NA	-2.71	120.76	124.51
8	T	102	BCL	O2A-CGA-O1A	-2.71	116.75	123.59

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	R	102	BCL	C11-C12-C13	-2.71	107.15	115.92
8	b	101	BCL	O2A-CGA-O1A	-2.71	116.75	123.59
8	R	102	BCL	C4D-CHA-C1A	2.71	124.55	121.25
8	M	403	BCL	C4D-CHA-C1A	2.71	124.55	121.25
8	l	102	BCL	C4D-CHA-C1A	2.71	124.54	121.25
8	G	101	BCL	C4D-CHA-C1A	2.71	124.54	121.25
8	I	102	BCL	C11-C12-C13	-2.71	107.17	115.92
8	D	101	BCL	CMC-C2C-C3C	-2.71	102.91	113.83
8	P	101	BCL	CMC-C2C-C3C	-2.71	102.91	113.83
8	I	102	BCL	O2A-CGA-O1A	-2.70	116.77	123.59
8	t	101	BCL	O2A-CGA-O1A	-2.70	116.78	123.59
8	G	102	BCL	C3D-C2D-C1D	-2.70	102.14	105.83
8	t	101	BCL	C11-C12-C13	-2.70	107.19	115.92
10	F	104	MW9	O1-C17-C16	2.69	120.36	111.91
8	a	102	BCL	C3D-C2D-C1D	-2.69	102.16	105.83
8	k	101	BCL	O2A-CGA-O1A	-2.69	116.80	123.59
8	s	101	BCL	C4D-CHA-C1A	2.69	124.53	121.25
8	l	102	BCL	CMC-C2C-C3C	-2.69	102.97	113.83
9	l	104	A1EFU	C20-C19-C18	2.69	133.98	126.42
8	R	102	BCL	C3D-C2D-C1D	-2.69	102.16	105.83
8	l	102	BCL	C3D-C2D-C1D	-2.69	102.16	105.83
8	n	101	BCL	C1C-NC-C4C	-2.69	105.50	106.71
8	s	101	BCL	O2A-CGA-O1A	-2.69	116.81	123.59
8	s	101	BCL	C11-C10-C8	-2.69	107.23	115.92
8	T	102	BCL	C4B-CHC-C1C	-2.69	124.79	130.12
8	a	102	BCL	CMC-C2C-C3C	-2.69	102.99	113.83
8	n	101	BCL	O2A-CGA-O1A	-2.69	116.81	123.59
8	P	102	BCL	C3D-C2D-C1D	-2.69	102.17	105.83
8	N	101	BCL	C2C-C3C-C4C	-2.68	97.32	101.34
8	i	101	BCL	CMC-C2C-C3C	-2.68	103.02	113.83
10	M	405	MW9	O1-C17-C16	2.68	120.31	111.91
8	q	101	BCL	CMC-C2C-C3C	-2.68	103.02	113.83
8	M	403	BCL	C3D-C2D-C1D	-2.68	102.18	105.83
8	M	402	BCL	C4D-CHA-C1A	2.68	124.51	121.25
8	L	303	BCL	C7-C6-C5	-2.68	106.09	113.36
8	I	102	BCL	CMC-C2C-C3C	-2.68	103.03	113.83
8	G	101	BCL	C3D-C2D-C1D	-2.68	102.18	105.83
8	e	102	BCL	CMC-C2C-C3C	-2.68	103.04	113.83
8	r	101	BCL	CMC-C2C-C3C	-2.67	103.04	113.83
8	F	102	BCL	CMA-C3A-C4A	-2.67	104.59	111.77
8	e	102	BCL	C3D-C2D-C1D	-2.67	102.19	105.83
8	k	101	BCL	CMC-C2C-C3C	-2.67	103.06	113.83

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	S	101	BCL	O2A-CGA-O1A	-2.67	116.86	123.59
8	d	101	BCL	C3D-C2D-C1D	-2.67	102.19	105.83
8	G	102	BCL	CMA-C3A-C4A	-2.67	104.60	111.77
8	j	101	BCL	O2A-CGA-O1A	-2.67	116.86	123.59
8	G	102	BCL	C11-C12-C13	-2.66	107.31	115.92
8	b	101	BCL	CMC-C2C-C3C	-2.66	103.08	113.83
8	a	102	BCL	C4D-CHA-C1A	2.66	124.49	121.25
8	R	102	BCL	C11-C10-C8	-2.66	107.31	115.92
13	C	404	LMT	C1'-O5'-C5'	-2.66	108.46	113.69
13	L	307	LMT	C1'-O5'-C5'	-2.66	108.46	113.69
8	l	102	BCL	CMA-C3A-C4A	-2.66	104.62	111.77
8	V	101	BCL	CMC-C2C-C3C	-2.65	103.12	113.83
8	j	101	BCL	CMC-C2C-C3C	-2.65	103.14	113.83
8	b	101	BCL	C11-C12-C13	-2.65	107.36	115.92
15	L	311	CDL	OB8-CB7-C71	2.65	120.21	111.91
8	N	101	BCL	CMC-C2C-C3C	-2.65	103.16	113.83
8	q	101	BCL	C4D-CHA-C1A	2.64	124.46	121.25
8	q	101	BCL	O2A-CGA-O1A	-2.64	116.93	123.59
8	s	101	BCL	CMC-C2C-C3C	-2.64	103.18	113.83
8	n	101	BCL	CMC-C2C-C3C	-2.64	103.18	113.83
8	t	101	BCL	C11-C10-C8	-2.64	107.39	115.92
8	e	102	BCL	CMA-C3A-C4A	-2.64	104.68	111.77
8	A	101	BCL	CMC-C2C-C3C	-2.64	103.19	113.83
8	E	101	BCL	C11-C12-C13	-2.64	107.40	115.92
8	E	101	BCL	O2A-CGA-O1A	-2.64	116.94	123.59
8	J	101	BCL	CMC-C2C-C3C	-2.63	103.20	113.83
9	2	102	A1EFU	CM7-C22-C23	-2.63	110.84	115.27
8	b	101	BCL	C1C-NC-C4C	-2.63	105.52	106.71
8	I	102	BCL	CMA-C3A-C4A	-2.63	104.71	111.77
8	r	101	BCL	C4A-NA-C1A	-2.63	105.53	106.71
8	L	306	BCL	CMC-C2C-C3C	-2.63	103.23	113.83
8	l	102	BCL	C4A-NA-C1A	-2.62	105.53	106.71
8	K	101	BCL	CMC-C2C-C3C	-2.62	103.25	113.83
8	E	101	BCL	CMA-C3A-C4A	-2.62	104.73	111.77
8	T	102	BCL	CMC-C2C-C3C	-2.62	103.25	113.83
8	F	102	BCL	C11-C12-C13	-2.62	107.46	115.92
8	R	102	BCL	CMC-C2C-C3C	-2.61	103.29	113.83
13	L	301	LMT	C1'-O5'-C5'	-2.61	108.56	113.69
8	G	101	BCL	CMA-C3A-C4A	-2.61	104.75	111.77
8	J	101	BCL	C11-C12-C13	-2.61	107.47	115.92
8	M	403	BCL	CMC-C2C-C3C	-2.61	103.30	113.83
15	H	303	CDL	OB8-CB7-C71	2.61	120.10	111.91

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	101	BCL	CMA-C3A-C4A	-2.61	104.76	111.77
8	G	101	BCL	C1C-NC-C4C	-2.61	105.53	106.71
10	D	103	MW9	O1-C17-C16	2.60	120.08	111.91
8	I	102	BCL	C2C-C3C-C4C	-2.60	97.44	101.34
8	i	101	BCL	CMA-C3A-C4A	-2.60	104.78	111.77
8	R	102	BCL	CMA-C3A-C4A	-2.60	104.80	111.77
8	N	101	BCL	CMA-C3A-C4A	-2.59	104.80	111.77
10	F	103	MW9	O1-C17-C16	2.59	120.05	111.91
8	G	102	BCL	CMC-C2C-C3C	-2.59	103.37	113.83
8	T	102	BCL	C4D-CHA-C1A	2.59	124.40	121.25
8	n	101	BCL	CMA-C3A-C4A	-2.59	104.81	111.77
8	M	402	BCL	CMA-C3A-C4A	-2.59	104.83	111.77
10	H	302	MW9	O1-C17-C16	2.58	120.02	111.91
8	S	101	BCL	C11-C10-C8	-2.58	107.56	115.92
8	d	101	BCL	C7-C6-C5	-2.58	106.34	113.36
8	v	101	BCL	CHA-C1A-NA	-2.58	120.49	126.40
8	B	101	BCL	C11-C12-C13	-2.58	107.58	115.92
8	F	102	BCL	CMC-C2C-C3C	-2.58	103.42	113.83
8	B	101	BCL	CMA-C3A-C4A	-2.58	104.85	111.77
8	P	101	BCL	C11-C12-C13	-2.57	107.60	115.92
10	G	103	MW9	O1-C17-C16	2.57	119.98	111.91
15	H	303	CDL	OA8-CA7-C31	2.57	119.98	111.91
8	E	101	BCL	CMC-C2C-C3C	-2.57	103.45	113.83
8	l	103	BCL	CMC-C2C-C3C	-2.57	103.47	113.83
16	C	402	HEC	CMC-C2C-C1C	-2.57	124.52	128.46
8	l	103	BCL	C11-C12-C13	-2.57	107.63	115.92
8	G	101	BCL	CMC-C2C-C3C	-2.57	103.48	113.83
10	Q	104	MW9	O1-C17-C16	2.56	119.96	111.91
8	F	101	BCL	CMC-C2C-C3C	-2.56	103.50	113.83
8	M	402	BCL	C11-C12-C13	-2.56	107.65	115.92
8	r	101	BCL	CMA-C3A-C4A	-2.56	104.89	111.77
8	S	101	BCL	CMA-C3A-C4A	-2.56	104.90	111.77
8	a	102	BCL	C11-C12-C13	-2.56	107.65	115.92
8	A	101	BCL	CMA-C3A-C4A	-2.55	104.92	111.77
8	P	102	BCL	C7-C6-C5	-2.54	106.45	113.36
8	v	101	BCL	C4B-CHC-C1C	-2.54	125.08	130.12
10	D	102	MW9	O1-C17-C16	2.54	119.89	111.91
8	K	101	BCL	C11-C12-C13	-2.54	107.70	115.92
10	I	104	MW9	O1-C17-C16	2.54	119.88	111.91
8	N	101	BCL	C11-C12-C13	-2.54	107.71	115.92
8	V	101	BCL	C1C-NC-C4C	-2.54	105.56	106.71
8	V	101	BCL	CMA-C3A-C4A	-2.53	104.96	111.77

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	S	101	BCL	C11-C12-C13	-2.53	107.75	115.92
8	G	102	BCL	C2A-C1A-CHA	2.53	128.28	123.86
10	I	104	MW9	C31-C32-C33	-2.52	109.72	126.84
8	1	103	BCL	CMA-C3A-C4A	-2.52	105.00	111.77
8	J	101	BCL	CMA-C3A-C4A	-2.52	105.01	111.77
8	P	102	BCL	C1C-NC-C4C	-2.52	105.58	106.71
8	V	101	BCL	C11-C10-C8	-2.51	107.81	115.92
8	K	101	BCL	C2C-C3C-C4C	-2.51	97.58	101.34
9	Q	102	A1EFU	CM7-C22-C23	-2.50	111.06	115.27
8	q	101	BCL	CMA-C3A-C4A	-2.50	105.06	111.77
8	L	303	BCL	CMD-C2D-C1D	2.50	129.11	124.71
9	Q	103	A1EFU	CM7-C22-C23	-2.49	111.08	115.27
16	C	401	HEC	CMD-C2D-C3D	2.49	129.63	124.94
8	j	101	BCL	C4D-CHA-C1A	2.49	124.28	121.25
16	C	402	HEC	O1A-CGA-CBA	-2.48	115.10	123.08
8	A	101	BCL	C11-C12-C13	-2.48	107.89	115.92
8	M	403	BCL	CMD-C2D-C1D	2.48	129.09	124.71
8	P	101	BCL	CMA-C3A-C4A	-2.48	105.10	111.77
8	F	101	BCL	C11-C12-C13	-2.48	107.90	115.92
8	J	101	BCL	C2C-C3C-C4C	-2.48	97.63	101.34
8	D	101	BCL	C11-C12-C13	-2.48	107.91	115.92
9	l	104	A1EFU	CM7-C22-C23	-2.47	111.11	115.27
8	a	102	BCL	CMA-C3A-C4A	-2.47	105.13	111.77
8	e	102	BCL	C4A-NA-C1A	-2.47	105.60	106.71
8	F	101	BCL	C3D-C2D-C1D	-2.47	102.46	105.83
8	K	101	BCL	CMA-C3A-C4A	-2.47	105.14	111.77
8	L	303	BCL	C2A-C1A-CHA	2.47	128.17	123.86
8	V	101	BCL	C11-C12-C13	-2.47	107.95	115.92
8	n	101	BCL	C11-C10-C8	-2.47	107.95	115.92
8	J	101	BCL	C2A-C1A-CHA	2.46	128.17	123.86
16	C	402	HEC	CMD-C2D-C3D	2.46	129.58	124.94
8	E	101	BCL	C2A-C1A-CHA	2.46	128.16	123.86
8	S	101	BCL	CGD-CBD-CAD	-2.46	102.78	110.73
8	L	303	BCL	C16-C15-C13	-2.46	107.98	115.92
8	s	101	BCL	CMA-C3A-C4A	-2.45	105.18	111.77
8	b	101	BCL	CMA-C3A-C4A	-2.45	105.18	111.77
8	B	101	BCL	C3C-C2C-C1C	2.45	105.82	101.87
16	C	403	HEC	O1A-CGA-CBA	-2.44	115.25	123.08
8	d	101	BCL	CMC-C2C-C3C	-2.43	104.01	113.83
8	i	101	BCL	C1C-NC-C4C	-2.43	105.61	106.71
8	r	101	BCL	C11-C12-C13	-2.43	108.06	115.92
8	M	403	BCL	C11-C12-C13	-2.43	108.06	115.92

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	403	BCL	CHC-C1C-NC	2.43	127.87	124.51
8	1	102	BCL	C1C-NC-C4C	-2.43	105.61	106.71
8	L	303	BCL	C3C-C2C-C1C	2.42	105.78	101.87
8	k	101	BCL	C11-C12-C13	-2.42	108.09	115.92
8	P	101	BCL	CGD-CBD-CAD	-2.42	102.89	110.73
8	M	402	BCL	CMD-C2D-C1D	2.42	128.98	124.71
9	2	102	A1EFU	C12-C13-C14	2.42	122.65	118.94
8	I	102	BCL	CGD-CBD-CAD	-2.42	102.91	110.73
8	q	101	BCL	C11-C12-C13	-2.42	108.11	115.92
8	L	306	BCL	C11-C12-C13	-2.41	108.12	115.92
16	C	402	HEC	C2B-C3B-C4B	2.41	108.95	106.35
8	r	101	BCL	C2A-C1A-CHA	2.41	128.07	123.86
16	C	401	HEC	O1A-CGA-CBA	-2.40	115.36	123.08
8	r	101	BCL	C1C-NC-C4C	-2.40	105.63	106.71
8	D	101	BCL	C11-C10-C8	-2.40	108.17	115.92
8	T	102	BCL	C2A-C1A-CHA	2.39	128.04	123.86
8	J	101	BCL	CGD-CBD-CAD	-2.39	102.98	110.73
8	s	101	BCL	C11-C12-C13	-2.39	108.19	115.92
8	I	102	BCL	C2A-C1A-CHA	2.39	128.04	123.86
8	D	101	BCL	CGD-CBD-CAD	-2.39	103.00	110.73
9	a	101	A1EFU	CM7-C22-C23	-2.39	111.25	115.27
9	Q	103	A1EFU	C21-C20-C19	-2.39	115.77	123.22
8	1	103	BCL	CGD-CBD-CAD	-2.39	103.01	110.73
8	e	102	BCL	C11-C10-C8	-2.38	108.22	115.92
8	i	101	BCL	C2A-C1A-CHA	2.38	128.02	123.86
8	I	102	BCL	CMD-C2D-C1D	2.37	128.88	124.71
8	T	102	BCL	CGD-CBD-CAD	-2.36	103.08	110.73
8	1	102	BCL	C3C-C2C-C1C	2.36	105.69	101.87
8	T	102	BCL	CBB-CAB-C3B	2.36	127.36	120.34
8	k	101	BCL	CMA-C3A-C4A	-2.36	105.42	111.77
9	K	102	A1EFU	CM7-C22-C23	-2.36	111.31	115.27
12	L	305	U10	C7-C6-C5	-2.36	115.64	118.48
8	P	101	BCL	C3C-C2C-C1C	2.36	105.68	101.87
8	r	101	BCL	C4D-CHA-C1A	2.35	124.11	121.25
8	K	101	BCL	C2A-C1A-CHA	2.35	127.97	123.86
8	1	102	BCL	C11-C12-C13	-2.35	108.32	115.92
8	S	101	BCL	C12-C11-C10	-2.35	102.44	113.24
8	j	101	BCL	CMA-C3A-C4A	-2.34	105.47	111.77
9	B	102	A1EFU	CM7-C22-C23	-2.34	111.33	115.27
8	R	102	BCL	CGD-CBD-CAD	-2.34	103.15	110.73
8	e	102	BCL	C2A-C1A-CHA	2.34	127.95	123.86
8	T	102	BCL	CMA-C3A-C4A	-2.34	105.49	111.77

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	j	101	BCL	C11-C12-C13	-2.34	108.36	115.92
8	T	102	BCL	C1B-CHB-C4A	-2.34	125.49	130.12
8	Q	101	BCL	C11-C12-C13	-2.33	108.38	115.92
8	M	402	BCL	CBB-CAB-C3B	2.33	127.26	120.34
8	L	303	BCL	CGD-CBD-CAD	-2.33	103.19	110.73
9	v	102	A1EFU	CM7-C22-C23	-2.32	111.37	115.27
8	t	101	BCL	C4D-CHA-C1A	2.32	124.07	121.25
9	J	102	A1EFU	CM7-C22-C23	-2.31	111.38	115.27
8	G	101	BCL	C2A-C1A-CHA	2.31	127.90	123.86
8	G	102	BCL	CGD-CBD-CAD	-2.31	103.25	110.73
9	S	102	A1EFU	CM7-C22-C23	-2.31	111.39	115.27
8	r	101	BCL	CMD-C2D-C1D	2.31	128.78	124.71
8	b	101	BCL	C3C-C2C-C1C	2.31	105.59	101.87
16	C	403	HEC	CMD-C2D-C3D	2.31	129.29	124.94
8	P	101	BCL	CMD-C2D-C1D	2.30	128.77	124.71
9	l	101	A1EFU	CM7-C22-C23	-2.30	111.40	115.27
8	v	101	BCL	CMA-C3A-C4A	-2.30	105.59	111.77
8	V	101	BCL	CBB-CAB-C3B	2.30	127.17	120.34
8	K	101	BCL	CBB-CAB-C3B	2.30	127.17	120.34
8	i	101	BCL	C3C-C2C-C1C	2.30	105.58	101.87
8	k	101	BCL	CBB-CAB-C3B	2.30	127.16	120.34
8	v	101	BCL	CMD-C2D-C1D	2.30	128.76	124.71
8	t	101	BCL	CMD-C2D-C1D	2.30	128.76	124.71
8	D	101	BCL	C3C-C2C-C1C	2.30	105.58	101.87
8	L	306	BCL	CHC-C1C-NC	2.30	127.69	124.51
8	l	102	BCL	C2A-C1A-CHA	2.29	127.87	123.86
8	M	403	BCL	CBB-CAB-C3B	2.29	127.15	120.34
8	Q	101	BCL	C12-C11-C10	-2.29	102.71	113.24
8	E	101	BCL	CGD-CBD-CAD	-2.29	103.32	110.73
16	C	402	HEC	C1D-C2D-C3D	2.28	108.58	107.00
8	T	102	BCL	CMD-C2D-C1D	2.28	128.73	124.71
8	j	101	BCL	CMD-C2D-C1D	2.28	128.73	124.71
8	P	102	BCL	C3C-C2C-C1C	2.28	105.55	101.87
8	F	102	BCL	CBB-CAB-C3B	2.28	127.10	120.34
8	L	306	BCL	CBB-CAB-C3B	2.28	127.10	120.34
8	i	101	BCL	C12-C11-C10	-2.28	102.78	113.24
8	D	101	BCL	CMD-C2D-C1D	2.28	128.72	124.71
8	P	101	BCL	CBB-CAB-C3B	2.28	127.10	120.34
8	R	102	BCL	CBB-CAB-C3B	2.28	127.10	120.34
8	t	101	BCL	C2C-C3C-C4C	-2.27	97.93	101.34
8	l	103	BCL	CBB-CAB-C3B	2.27	127.09	120.34
8	D	101	BCL	C12-C11-C10	-2.27	102.80	113.24

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	M	404	U10	C7-C6-C5	-2.27	115.74	118.48
8	G	101	BCL	C12-C11-C10	-2.27	102.80	113.24
8	B	101	BCL	CGD-CBD-CAD	-2.27	103.37	110.73
8	e	102	BCL	CBB-CAB-C3B	2.27	127.08	120.34
8	N	101	BCL	CBB-CAB-C3B	2.27	127.08	120.34
8	R	102	BCL	CMD-C2D-C1D	2.27	128.71	124.71
8	l	102	BCL	CBB-CAB-C3B	2.27	127.07	120.34
8	Q	101	BCL	CBB-CAB-C3B	2.27	127.07	120.34
8	E	101	BCL	CBB-CAB-C3B	2.27	127.06	120.34
8	q	101	BCL	CBB-CAB-C3B	2.26	127.06	120.34
8	s	101	BCL	C3C-C2C-C1C	2.26	105.53	101.87
8	Q	101	BCL	CMD-C2D-C1D	2.26	128.70	124.71
8	i	101	BCL	CBB-CAB-C3B	2.26	127.05	120.34
9	J	103	A1EFU	CM7-C22-C23	-2.26	111.47	115.27
8	F	101	BCL	CBB-CAB-C3B	2.26	127.05	120.34
8	M	402	BCL	C12-C11-C10	-2.26	102.86	113.24
8	v	101	BCL	CBB-CAB-C3B	2.26	127.05	120.34
8	I	102	BCL	CBB-CAB-C3B	2.26	127.04	120.34
8	A	101	BCL	C2A-C1A-CHA	2.26	127.80	123.86
8	J	101	BCL	CBB-CAB-C3B	2.26	127.04	120.34
8	b	101	BCL	CBB-CAB-C3B	2.26	127.04	120.34
9	Q	102	A1EFU	C19-C18-C17	2.25	122.40	118.94
8	q	101	BCL	C3C-C2C-C1C	2.25	105.51	101.87
8	L	306	BCL	CMD-C2D-C1D	2.25	128.68	124.71
8	L	306	BCL	C12-C11-C10	-2.25	102.89	113.24
14	L	304	BPH	CMD-C2D-C3D	2.25	128.89	124.68
8	D	101	BCL	CBB-CAB-C3B	2.25	127.02	120.34
8	V	101	BCL	CMD-C2D-C1D	2.25	128.68	124.71
8	e	102	BCL	C12-C11-C10	-2.25	102.91	113.24
8	K	101	BCL	CMD-C2D-C1D	2.25	128.67	124.71
8	L	306	BCL	C2A-C3A-C4A	-2.25	98.24	101.87
8	i	101	BCL	C11-C12-C13	-2.25	108.66	115.92
8	M	403	BCL	C4A-NA-C1A	-2.24	105.70	106.71
8	L	303	BCL	CBB-CAB-C3B	2.24	127.00	120.34
8	G	102	BCL	CBB-CAB-C3B	2.24	127.00	120.34
8	B	101	BCL	CBB-CAB-C3B	2.24	127.00	120.34
8	s	101	BCL	CBB-CAB-C3B	2.24	127.00	120.34
8	J	101	BCL	CMD-C2D-C1D	2.24	128.66	124.71
8	A	101	BCL	CGD-CBD-CAD	-2.24	103.47	110.73
8	S	101	BCL	C3C-C2C-C1C	2.24	105.49	101.87
8	V	101	BCL	C4B-C3B-CAB	-2.24	122.80	127.13
9	I	103	A1EFU	CM7-C22-C23	-2.24	111.50	115.27

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	F	101	BCL	C1C-NC-C4C	-2.24	105.70	106.71
8	S	101	BCL	CMD-C2D-C1D	2.24	128.66	124.71
8	S	101	BCL	CBB-CAB-C3B	2.24	126.98	120.34
8	i	101	BCL	CMD-C2D-C1D	2.23	128.65	124.71
8	a	102	BCL	CBB-CAB-C3B	2.23	126.96	120.34
8	G	101	BCL	C11-C12-C13	-2.23	108.71	115.92
8	V	101	BCL	C4D-CHA-C1A	2.23	123.96	121.25
8	B	101	BCL	CMD-C2D-C1D	2.23	128.64	124.71
8	F	102	BCL	C2A-C3A-C4A	-2.23	98.27	101.87
8	E	101	BCL	CMD-C2D-C1D	2.23	128.63	124.71
8	l	103	BCL	CMD-C2D-C1D	2.22	128.63	124.71
8	T	102	BCL	C2A-C3A-C4A	-2.22	98.28	101.87
8	d	101	BCL	CGD-CBD-CAD	-2.22	103.53	110.73
8	n	101	BCL	C2A-C1A-CHA	2.22	127.75	123.86
9	D	105	A1EFU	CM7-C22-C23	-2.22	111.53	115.27
8	t	101	BCL	OBB-CAB-C3B	2.22	123.93	119.99
8	r	101	BCL	C3C-C2C-C1C	2.22	105.45	101.87
8	j	101	BCL	CBB-CAB-C3B	2.22	126.92	120.34
8	q	101	BCL	C4A-NA-C1A	-2.22	105.71	106.71
16	C	403	HEC	C1D-C2D-C3D	2.21	108.54	107.00
8	N	101	BCL	CMD-C2D-C1D	2.21	128.61	124.71
8	F	102	BCL	CAA-CBA-CGA	-2.21	106.80	113.25
8	R	102	BCL	C2A-C1A-CHA	2.21	127.72	123.86
9	s	102	A1EFU	CM7-C22-C23	-2.21	111.56	115.27
14	L	302	BPH	CMD-C2D-C3D	2.20	128.80	124.68
8	P	101	BCL	C12-C11-C10	-2.20	103.14	113.24
8	Q	101	BCL	C3C-C2C-C1C	2.20	105.42	101.87
8	V	101	BCL	CGD-CBD-CAD	-2.20	103.62	110.73
8	d	101	BCL	CMA-C3A-C4A	-2.19	105.88	111.77
8	l	103	BCL	C2A-C1A-CHA	2.19	127.69	123.86
9	d	102	A1EFU	CM7-C22-C23	-2.19	111.59	115.27
8	B	101	BCL	C12-C11-C10	-2.19	103.19	113.24
8	G	101	BCL	CBB-CAB-C3B	2.18	126.82	120.34
8	A	101	BCL	CMD-C2D-C1D	2.18	128.56	124.71
16	C	401	HEC	C2B-C3B-C4B	2.18	108.70	106.35
8	V	101	BCL	C12-C11-C10	-2.18	103.23	113.24
8	K	101	BCL	C12-C11-C10	-2.18	103.23	113.24
8	G	102	BCL	CMD-C2D-C1D	2.18	128.55	124.71
8	n	101	BCL	C12-C11-C10	-2.18	103.24	113.24
9	R	101	A1EFU	CM7-C22-C23	-2.17	111.61	115.27
8	r	101	BCL	C2A-C3A-C4A	-2.17	98.36	101.87
8	J	101	BCL	C12-C11-C10	-2.17	103.26	113.24

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	F	102	BCL	C12-C11-C10	-2.17	103.28	113.24
8	A	101	BCL	C3C-C2C-C1C	2.17	105.37	101.87
8	s	101	BCL	CMD-C2D-C1D	2.16	128.53	124.71
8	j	101	BCL	CGD-CBD-CAD	-2.16	103.73	110.73
9	G	105	A1EFU	CM7-C22-C23	-2.16	111.63	115.27
8	L	306	BCL	C1B-CHB-C4A	-2.16	125.84	130.12
8	a	102	BCL	CGD-CBD-CAD	-2.16	103.75	110.73
8	F	101	BCL	C12-C11-C10	-2.15	103.35	113.24
8	q	101	BCL	C12-C11-C10	-2.15	103.36	113.24
8	t	101	BCL	C12-C11-C10	-2.15	103.36	113.24
8	N	101	BCL	C12-C11-C10	-2.15	103.36	113.24
8	v	101	BCL	CGD-CBD-CAD	-2.15	103.78	110.73
8	P	102	BCL	C12-C11-C10	-2.14	103.40	113.24
8	G	102	BCL	C12-C11-C10	-2.14	103.41	113.24
16	C	401	HEC	CMA-C3A-C2A	2.14	128.97	124.94
8	F	102	BCL	CMD-C2D-C1D	2.13	128.47	124.71
8	j	101	BCL	C2A-C1A-CHA	2.13	127.59	123.86
8	L	303	BCL	CHC-C1C-NC	2.13	127.46	124.51
9	a	103	A1EFU	CM7-C22-C23	-2.13	111.69	115.27
8	a	102	BCL	C12-C11-C10	-2.12	103.49	113.24
9	T	101	A1EFU	CM7-C22-C23	-2.12	111.70	115.27
8	n	101	BCL	CGD-CBD-CAD	-2.12	103.88	110.73
8	T	102	BCL	C12-C11-C10	-2.11	103.52	113.24
8	K	101	BCL	CGD-CBD-CAD	-2.11	103.89	110.73
8	b	101	BCL	C2A-C1A-CHA	2.11	127.55	123.86
9	N	103	A1EFU	CM7-C22-C23	-2.11	111.72	115.27
8	v	101	BCL	C11-C10-C8	-2.11	109.11	115.92
8	n	101	BCL	C3C-C2C-C1C	2.11	105.27	101.87
8	k	101	BCL	CMD-C2D-C1D	2.10	128.42	124.71
8	G	101	BCL	C3C-C2C-C1C	2.10	105.26	101.87
8	k	101	BCL	C2A-C1A-CHA	2.10	127.53	123.86
8	s	101	BCL	C12-C11-C10	-2.10	103.60	113.24
8	k	101	BCL	CGD-CBD-CAD	-2.09	103.95	110.73
8	E	101	BCL	C12-C11-C10	-2.09	103.62	113.24
8	k	101	BCL	C3C-C2C-C1C	2.09	105.25	101.87
8	e	102	BCL	C2C-C3C-C4C	-2.09	98.21	101.34
8	G	101	BCL	CMD-C2D-C1D	2.09	128.39	124.71
8	l	103	BCL	C12-C11-C10	-2.09	103.65	113.24
8	F	101	BCL	C2C-C3C-C4C	-2.09	98.22	101.34
8	N	101	BCL	CGD-CBD-CAD	-2.08	103.98	110.73
16	C	401	HEC	C1D-C2D-C3D	2.08	108.45	107.00
8	q	101	BCL	CMD-C2D-C1D	2.08	128.38	124.71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	R	102	BCL	CHC-C1C-NC	2.08	127.39	124.51
8	P	102	BCL	C11-C12-C13	-2.08	109.20	115.92
8	k	101	BCL	C12-C11-C10	-2.08	103.69	113.24
8	k	101	BCL	C4A-NA-C1A	-2.08	105.77	106.71
8	e	102	BCL	C11-C12-C13	-2.07	109.22	115.92
8	a	102	BCL	CHC-C1C-NC	2.07	127.38	124.51
8	n	101	BCL	CMD-C2D-C1D	2.07	128.36	124.71
8	L	303	BCL	C1B-CHB-C4A	-2.07	126.02	130.12
16	C	403	HEC	CMA-C3A-C2A	2.07	128.84	124.94
8	j	101	BCL	C12-C11-C10	-2.07	103.75	113.24
9	N	102	A1EFU	CM7-C22-C23	-2.06	111.80	115.27
8	b	101	BCL	C12-C11-C10	-2.06	103.78	113.24
8	V	101	BCL	C3C-C2C-C1C	2.06	105.19	101.87
8	s	101	BCL	C2A-C1A-CHA	2.05	127.45	123.86
8	D	101	BCL	CHC-C1C-NC	2.05	127.35	124.51
9	v	103	A1EFU	CM7-C22-C23	-2.05	111.82	115.27
8	n	101	BCL	C4A-NA-C1A	-2.05	105.78	106.71
8	a	102	BCL	C2A-C3A-C4A	-2.04	98.57	101.87
8	s	101	BCL	CGD-CBD-CAD	-2.04	104.12	110.73
8	a	102	BCL	C2A-C1A-CHA	2.04	127.43	123.86
8	M	403	BCL	C12-C11-C10	-2.04	103.86	113.24
8	A	101	BCL	C12-C11-C10	-2.04	103.86	113.24
10	M	406	MW9	C34-C33-C32	-2.04	109.07	124.73
8	v	101	BCL	C3C-C4C-CHD	-2.04	119.04	123.39
16	C	403	HEC	O2A-CGA-O1A	2.04	128.38	123.30
8	j	101	BCL	C1B-CHB-C4A	-2.03	126.09	130.12
8	B	101	BCL	C2A-C1A-CHA	2.03	127.41	123.86
8	D	101	BCL	C2A-C1A-CHA	2.03	127.40	123.86
8	N	101	BCL	C2A-C1A-CHA	2.03	127.40	123.86
8	I	102	BCL	C12-C11-C10	-2.02	103.94	113.24
10	G	103	MW9	C31-C32-C33	-2.02	109.21	124.73
8	a	102	BCL	CMD-C2D-C1D	2.02	128.28	124.71
8	S	101	BCL	C2A-C1A-CHA	2.02	127.39	123.86
9	A	102	A1EFU	CM7-C22-C23	-2.02	111.87	115.27
8	j	101	BCL	C2A-C3A-C4A	-2.01	98.62	101.87
10	D	103	MW9	C31-C32-C33	-2.01	109.33	124.73
8	v	101	BCL	C2A-C1A-CHA	2.01	127.37	123.86
16	C	403	HEC	C2B-C3B-C4B	2.01	108.52	106.35
8	v	101	BCL	C11-C12-C13	-2.01	109.44	115.92
8	P	102	BCL	C2A-C1A-CHA	2.00	127.36	123.86
9	2	101	A1EFU	CM7-C22-C23	-2.00	111.90	115.27

There are no chirality outliers.

All (1734) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	P	101	BCL	C1A-C2A-CAA-CBA
8	P	101	BCL	C3A-C2A-CAA-CBA
8	P	101	BCL	C4C-C3C-CAC-CBC
8	P	102	BCL	C1-C2-C3-C4
8	V	101	BCL	C1A-C2A-CAA-CBA
8	V	101	BCL	C3A-C2A-CAA-CBA
8	V	101	BCL	C2C-C3C-CAC-CBC
8	V	101	BCL	C4C-C3C-CAC-CBC
8	v	101	BCL	C1A-C2A-CAA-CBA
8	v	101	BCL	C2C-C3C-CAC-CBC
8	v	101	BCL	C4C-C3C-CAC-CBC
8	t	101	BCL	C1-C2-C3-C4
8	t	101	BCL	C1-C2-C3-C5
8	Q	101	BCL	C3A-C2A-CAA-CBA
8	Q	101	BCL	C2C-C3C-CAC-CBC
8	Q	101	BCL	C4C-C3C-CAC-CBC
8	Q	101	BCL	C1-C2-C3-C4
8	Q	101	BCL	C1-C2-C3-C5
8	r	101	BCL	C1A-C2A-CAA-CBA
8	R	102	BCL	C1A-C2A-CAA-CBA
8	q	101	BCL	C1A-C2A-CAA-CBA
8	q	101	BCL	C2-C3-C5-C6
8	l	102	BCL	C2C-C3C-CAC-CBC
8	n	101	BCL	C3A-C2A-CAA-CBA
8	k	101	BCL	C2C-C3C-CAC-CBC
8	i	101	BCL	C2C-C3C-CAC-CBC
8	i	101	BCL	O2A-C1-C2-C3
8	i	101	BCL	C1-C2-C3-C4
8	i	101	BCL	C1-C2-C3-C5
8	G	101	BCL	C1A-C2A-CAA-CBA
8	G	101	BCL	CHA-CBD-CGD-O2D
8	G	102	BCL	C2A-CAA-CBA-CGA
8	e	102	BCL	C1A-C2A-CAA-CBA
8	E	101	BCL	C1-C2-C3-C4
8	E	101	BCL	C1-C2-C3-C5
8	E	101	BCL	C2-C3-C5-C6
8	d	101	BCL	C1A-C2A-CAA-CBA
8	d	101	BCL	C1-C2-C3-C4
8	d	101	BCL	C1-C2-C3-C5
8	D	101	BCL	C4C-C3C-CAC-CBC
8	B	101	BCL	C1A-C2A-CAA-CBA
8	B	101	BCL	C3A-C2A-CAA-CBA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
8	B	101	BCL	C2A-CAA-CBA-CGA
8	B	101	BCL	C2C-C3C-CAC-CBC
8	B	101	BCL	C4C-C3C-CAC-CBC
8	a	102	BCL	C2C-C3C-CAC-CBC
8	a	102	BCL	C4C-C3C-CAC-CBC
8	a	102	BCL	C1-C2-C3-C4
8	A	101	BCL	C1A-C2A-CAA-CBA
8	A	101	BCL	C4C-C3C-CAC-CBC
8	A	101	BCL	C4-C3-C5-C6
8	M	402	BCL	CHA-CBD-CGD-O1D
8	M	402	BCL	CHA-CBD-CGD-O2D
8	M	403	BCL	C4C-C3C-CAC-CBC
8	M	403	BCL	O2A-C1-C2-C3
8	M	403	BCL	C1-C2-C3-C4
8	M	403	BCL	C1-C2-C3-C5
8	M	403	BCL	C2-C3-C5-C6
8	L	303	BCL	C1A-C2A-CAA-CBA
8	L	303	BCL	C2C-C3C-CAC-CBC
8	L	303	BCL	C4C-C3C-CAC-CBC
8	L	306	BCL	C1A-C2A-CAA-CBA
8	L	306	BCL	C3A-C2A-CAA-CBA
8	L	306	BCL	C4C-C3C-CAC-CBC
8	L	306	BCL	O2A-C1-C2-C3
8	L	306	BCL	C1-C2-C3-C4
8	L	306	BCL	C1-C2-C3-C5
8	L	306	BCL	C4-C3-C5-C6
9	v	102	A1EFU	C2-C3-C4-C5
9	v	102	A1EFU	C4-C5-C6-C7
9	v	102	A1EFU	CM3-C5-C6-C7
9	v	102	A1EFU	C6-C7-C8-C9
9	v	102	A1EFU	C10-C11-C12-C13
9	v	102	A1EFU	C16-C17-C18-C19
9	v	102	A1EFU	C16-C17-C18-CM6
9	v	102	A1EFU	C11-C10-C9-C8
9	v	102	A1EFU	C11-C10-C9-CM4
9	v	102	A1EFU	C12-C13-C14-C15
9	v	102	A1EFU	CM5-C13-C14-C15
9	v	102	A1EFU	C20-C21-C22-C23
9	v	102	A1EFU	C20-C21-C22-CM7
9	v	103	A1EFU	C1-C2-C3-C4
9	v	103	A1EFU	O2-C2-C3-C4
9	v	103	A1EFU	C2-C3-C4-C5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
9	v	103	A1EFU	C4-C5-C6-C7
9	v	103	A1EFU	CM3-C5-C6-C7
9	v	103	A1EFU	C6-C7-C8-C9
9	v	103	A1EFU	C10-C11-C12-C13
9	v	103	A1EFU	C14-C15-C16-C17
9	v	103	A1EFU	C18-C19-C20-C21
9	v	103	A1EFU	C16-C17-C18-C19
9	v	103	A1EFU	C16-C17-C18-CM6
9	v	103	A1EFU	C11-C10-C9-C8
9	v	103	A1EFU	C11-C10-C9-CM4
9	v	103	A1EFU	C12-C13-C14-C15
9	v	103	A1EFU	CM5-C13-C14-C15
9	v	103	A1EFU	C19-C20-C21-C22
9	v	103	A1EFU	C20-C21-C22-C23
9	v	103	A1EFU	C20-C21-C22-CM7
9	S	102	A1EFU	C2-C3-C4-C5
9	S	102	A1EFU	C4-C5-C6-C7
9	S	102	A1EFU	CM3-C5-C6-C7
9	S	102	A1EFU	C6-C7-C8-C9
9	S	102	A1EFU	C10-C11-C12-C13
9	S	102	A1EFU	C16-C17-C18-C19
9	S	102	A1EFU	C16-C17-C18-CM6
9	S	102	A1EFU	C11-C10-C9-C8
9	S	102	A1EFU	C11-C10-C9-CM4
9	S	102	A1EFU	C12-C13-C14-C15
9	S	102	A1EFU	CM5-C13-C14-C15
9	S	102	A1EFU	C20-C21-C22-CM7
9	t	102	A1EFU	C2-C3-C4-C5
9	t	102	A1EFU	C4-C5-C6-C7
9	t	102	A1EFU	CM3-C5-C6-C7
9	t	102	A1EFU	C6-C7-C8-C9
9	t	102	A1EFU	C10-C11-C12-C13
9	t	102	A1EFU	C2-C1-O1-CMA
9	t	102	A1EFU	CM1-C1-O1-CMA
9	t	102	A1EFU	C18-C19-C20-C21
9	t	102	A1EFU	C16-C17-C18-C19
9	t	102	A1EFU	C16-C17-C18-CM6
9	t	102	A1EFU	C11-C10-C9-C8
9	t	102	A1EFU	C11-C10-C9-CM4
9	t	102	A1EFU	C12-C13-C14-C15
9	t	102	A1EFU	CM5-C13-C14-C15
9	t	102	A1EFU	C20-C21-C22-C23

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
9	t	102	A1EFU	C20-C21-C22-CM7
9	t	102	A1EFU	C22-C23-C24-C25
9	t	102	A1EFU	C26-C27-C28-C29
9	T	101	A1EFU	C2-C3-C4-C5
9	T	101	A1EFU	C4-C5-C6-C7
9	T	101	A1EFU	CM3-C5-C6-C7
9	T	101	A1EFU	C6-C7-C8-C9
9	T	101	A1EFU	C10-C11-C12-C13
9	T	101	A1EFU	C2-C1-O1-CMA
9	T	101	A1EFU	CM1-C1-O1-CMA
9	T	101	A1EFU	C16-C17-C18-C19
9	T	101	A1EFU	C16-C17-C18-CM6
9	T	101	A1EFU	C11-C10-C9-C8
9	T	101	A1EFU	C11-C10-C9-CM4
9	T	101	A1EFU	C12-C13-C14-C15
9	T	101	A1EFU	CM5-C13-C14-C15
9	T	101	A1EFU	C20-C21-C22-CM7
9	s	102	A1EFU	C10-C11-C12-C13
9	s	102	A1EFU	C2-C1-O1-CMA
9	s	102	A1EFU	CM1-C1-O1-CMA
9	s	102	A1EFU	C18-C19-C20-C21
9	s	102	A1EFU	C16-C17-C18-CM6
9	s	102	A1EFU	C11-C10-C9-CM4
9	s	102	A1EFU	C12-C13-C14-C15
9	s	102	A1EFU	CM5-C13-C14-C15
9	s	102	A1EFU	C20-C21-C22-C23
9	s	102	A1EFU	C20-C21-C22-CM7
9	s	102	A1EFU	C26-C27-C28-C29
9	Q	102	A1EFU	O1-C1-C2-O2
9	Q	102	A1EFU	C4-C5-C6-C7
9	Q	102	A1EFU	CM3-C5-C6-C7
9	Q	102	A1EFU	C6-C7-C8-C9
9	Q	102	A1EFU	C10-C11-C12-C13
9	Q	102	A1EFU	C16-C17-C18-C19
9	Q	102	A1EFU	C16-C17-C18-CM6
9	Q	102	A1EFU	C11-C10-C9-C8
9	Q	102	A1EFU	C11-C10-C9-CM4
9	Q	102	A1EFU	C12-C13-C14-C15
9	Q	102	A1EFU	CM5-C13-C14-C15
9	Q	102	A1EFU	C20-C21-C22-C23
9	Q	102	A1EFU	C26-C27-C28-C29
9	Q	103	A1EFU	O1-C1-C2-O2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
9	Q	103	A1EFU	C2-C3-C4-C5
9	Q	103	A1EFU	C4-C5-C6-C7
9	Q	103	A1EFU	CM3-C5-C6-C7
9	Q	103	A1EFU	C6-C7-C8-C9
9	Q	103	A1EFU	C10-C11-C12-C13
9	Q	103	A1EFU	C18-C19-C20-C21
9	Q	103	A1EFU	C16-C17-C18-C19
9	Q	103	A1EFU	C16-C17-C18-CM6
9	Q	103	A1EFU	C12-C13-C14-C15
9	Q	103	A1EFU	CM5-C13-C14-C15
9	Q	103	A1EFU	C20-C21-C22-CM7
9	Q	103	A1EFU	C26-C27-C28-C29
9	r	102	A1EFU	C2-C3-C4-C5
9	r	102	A1EFU	C4-C5-C6-C7
9	r	102	A1EFU	CM3-C5-C6-C7
9	r	102	A1EFU	C6-C7-C8-C9
9	r	102	A1EFU	C10-C11-C12-C13
9	r	102	A1EFU	C14-C15-C16-C17
9	r	102	A1EFU	C11-C10-C9-C8
9	r	102	A1EFU	C11-C10-C9-CM4
9	r	102	A1EFU	C12-C13-C14-C15
9	r	102	A1EFU	CM5-C13-C14-C15
9	r	102	A1EFU	C20-C21-C22-CM7
9	r	102	A1EFU	CM7-C22-C23-C24
9	r	102	A1EFU	C26-C27-C28-C29
9	R	101	A1EFU	C2-C3-C4-C5
9	R	101	A1EFU	C4-C5-C6-C7
9	R	101	A1EFU	CM3-C5-C6-C7
9	R	101	A1EFU	C6-C7-C8-C9
9	R	101	A1EFU	C10-C11-C12-C13
9	R	101	A1EFU	C18-C19-C20-C21
9	R	101	A1EFU	C16-C17-C18-C19
9	R	101	A1EFU	C16-C17-C18-CM6
9	R	101	A1EFU	C11-C10-C9-C8
9	R	101	A1EFU	C11-C10-C9-CM4
9	R	101	A1EFU	C12-C13-C14-C15
9	R	101	A1EFU	CM5-C13-C14-C15
9	R	101	A1EFU	C20-C21-C22-CM7
9	2	101	A1EFU	C2-C3-C4-C5
9	2	101	A1EFU	C4-C5-C6-C7
9	2	101	A1EFU	CM3-C5-C6-C7
9	2	101	A1EFU	C6-C7-C8-C9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
9	2	101	A1EFU	C10-C11-C12-C13
9	2	101	A1EFU	C14-C15-C16-C17
9	2	101	A1EFU	C16-C17-C18-C19
9	2	101	A1EFU	C16-C17-C18-CM6
9	2	101	A1EFU	C11-C10-C9-C8
9	2	101	A1EFU	C11-C10-C9-CM4
9	2	101	A1EFU	C12-C13-C14-C15
9	2	101	A1EFU	CM5-C13-C14-C15
9	2	101	A1EFU	C20-C21-C22-CM7
9	2	101	A1EFU	C21-C22-C23-C24
9	2	101	A1EFU	C26-C27-C28-C29
9	2	102	A1EFU	C2-C3-C4-C5
9	2	102	A1EFU	C4-C5-C6-C7
9	2	102	A1EFU	CM3-C5-C6-C7
9	2	102	A1EFU	C6-C7-C8-C9
9	2	102	A1EFU	C14-C15-C16-C17
9	2	102	A1EFU	C13-C14-C15-C16
9	2	102	A1EFU	C17-C18-C19-C20
9	2	102	A1EFU	CM6-C18-C19-C20
9	2	102	A1EFU	C18-C19-C20-C21
9	2	102	A1EFU	C16-C17-C18-C19
9	2	102	A1EFU	C16-C17-C18-CM6
9	2	102	A1EFU	C11-C10-C9-C8
9	2	102	A1EFU	C11-C10-C9-CM4
9	2	102	A1EFU	C12-C13-C14-C15
9	2	102	A1EFU	CM5-C13-C14-C15
9	2	102	A1EFU	C11-C12-C13-C14
9	2	102	A1EFU	C11-C12-C13-CM5
9	2	102	A1EFU	C20-C21-C22-C23
9	2	102	A1EFU	C20-C21-C22-CM7
9	1	101	A1EFU	C4-C5-C6-C7
9	1	101	A1EFU	CM3-C5-C6-C7
9	1	101	A1EFU	C6-C7-C8-C9
9	1	101	A1EFU	C10-C11-C12-C13
9	1	101	A1EFU	C14-C15-C16-C17
9	1	101	A1EFU	C18-C19-C20-C21
9	1	101	A1EFU	C16-C17-C18-C19
9	1	101	A1EFU	C16-C17-C18-CM6
9	1	101	A1EFU	C11-C10-C9-C8
9	1	101	A1EFU	C11-C10-C9-CM4
9	1	101	A1EFU	C12-C13-C14-C15
9	1	101	A1EFU	CM5-C13-C14-C15

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
9	1	101	A1EFU	C20-C21-C22-CM7
9	1	101	A1EFU	C21-C22-C23-C24
9	1	104	A1EFU	C4-C5-C6-C7
9	1	104	A1EFU	CM3-C5-C6-C7
9	1	104	A1EFU	C6-C7-C8-C9
9	1	104	A1EFU	C10-C11-C12-C13
9	1	104	A1EFU	C17-C18-C19-C20
9	1	104	A1EFU	CM6-C18-C19-C20
9	1	104	A1EFU	C11-C10-C9-C8
9	1	104	A1EFU	C11-C10-C9-CM4
9	1	104	A1EFU	C12-C13-C14-C15
9	1	104	A1EFU	CM5-C13-C14-C15
9	1	104	A1EFU	C20-C21-C22-C23
9	1	104	A1EFU	C21-C22-C23-C24
9	N	102	A1EFU	C4-C5-C6-C7
9	N	102	A1EFU	CM3-C5-C6-C7
9	N	102	A1EFU	C6-C7-C8-C9
9	N	102	A1EFU	C17-C18-C19-C20
9	N	102	A1EFU	CM6-C18-C19-C20
9	N	102	A1EFU	C18-C19-C20-C21
9	N	102	A1EFU	C16-C17-C18-C19
9	N	102	A1EFU	C16-C17-C18-CM6
9	N	102	A1EFU	C11-C10-C9-C8
9	N	102	A1EFU	C11-C10-C9-CM4
9	N	102	A1EFU	C12-C13-C14-C15
9	N	102	A1EFU	CM5-C13-C14-C15
9	N	102	A1EFU	C20-C21-C22-C23
9	N	102	A1EFU	C20-C21-C22-CM7
9	N	103	A1EFU	O1-C1-C2-O2
9	N	103	A1EFU	C2-C3-C4-C5
9	N	103	A1EFU	C4-C5-C6-C7
9	N	103	A1EFU	CM3-C5-C6-C7
9	N	103	A1EFU	C6-C7-C8-C9
9	N	103	A1EFU	C10-C11-C12-C13
9	N	103	A1EFU	C14-C15-C16-C17
9	N	103	A1EFU	C13-C14-C15-C16
9	N	103	A1EFU	C17-C18-C19-C20
9	N	103	A1EFU	CM6-C18-C19-C20
9	N	103	A1EFU	C18-C19-C20-C21
9	N	103	A1EFU	C16-C17-C18-C19
9	N	103	A1EFU	C16-C17-C18-CM6
9	N	103	A1EFU	C11-C10-C9-C8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
9	N	103	A1EFU	C11-C10-C9-CM4
9	N	103	A1EFU	C12-C13-C14-C15
9	N	103	A1EFU	CM5-C13-C14-C15
9	N	103	A1EFU	C11-C12-C13-C14
9	N	103	A1EFU	C11-C12-C13-CM5
9	N	103	A1EFU	C20-C21-C22-C23
9	k	102	A1EFU	C1-C2-C3-C4
9	k	102	A1EFU	O2-C2-C3-C4
9	k	102	A1EFU	O1-C1-C2-O2
9	k	102	A1EFU	C2-C3-C4-C5
9	k	102	A1EFU	C4-C5-C6-C7
9	k	102	A1EFU	CM3-C5-C6-C7
9	k	102	A1EFU	C6-C7-C8-C9
9	k	102	A1EFU	C10-C11-C12-C13
9	k	102	A1EFU	C17-C18-C19-C20
9	k	102	A1EFU	CM6-C18-C19-C20
9	k	102	A1EFU	C18-C19-C20-C21
9	k	102	A1EFU	C16-C17-C18-C19
9	k	102	A1EFU	C16-C17-C18-CM6
9	k	102	A1EFU	C11-C10-C9-C8
9	k	102	A1EFU	C11-C10-C9-CM4
9	k	102	A1EFU	C12-C13-C14-C15
9	k	102	A1EFU	CM5-C13-C14-C15
9	k	102	A1EFU	C20-C21-C22-C23
9	k	102	A1EFU	C20-C21-C22-CM7
9	k	102	A1EFU	C21-C22-C23-C24
9	K	102	A1EFU	O1-C1-C2-O2
9	K	102	A1EFU	C4-C5-C6-C7
9	K	102	A1EFU	CM3-C5-C6-C7
9	K	102	A1EFU	C6-C7-C8-C9
9	K	102	A1EFU	C10-C11-C12-C13
9	K	102	A1EFU	C17-C18-C19-C20
9	K	102	A1EFU	CM6-C18-C19-C20
9	K	102	A1EFU	C18-C19-C20-C21
9	K	102	A1EFU	C11-C10-C9-C8
9	K	102	A1EFU	C11-C10-C9-CM4
9	K	102	A1EFU	C12-C13-C14-C15
9	K	102	A1EFU	CM5-C13-C14-C15
9	K	102	A1EFU	C19-C20-C21-C22
9	K	102	A1EFU	C20-C21-C22-C23
9	K	102	A1EFU	C20-C21-C22-CM7
9	K	102	A1EFU	C25-C26-C27-C28

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
9	K	102	A1EFU	CM8-C26-C27-C28
9	J	102	A1EFU	C6-C7-C8-C9
9	J	102	A1EFU	C10-C11-C12-C13
9	J	102	A1EFU	C11-C10-C9-C8
9	J	102	A1EFU	C11-C10-C9-CM4
9	J	102	A1EFU	C12-C13-C14-C15
9	J	102	A1EFU	CM5-C13-C14-C15
9	J	102	A1EFU	C20-C21-C22-CM7
9	J	102	A1EFU	C22-C23-C24-C25
9	J	103	A1EFU	O1-C1-C2-O2
9	J	103	A1EFU	C2-C3-C4-C5
9	J	103	A1EFU	C4-C5-C6-C7
9	J	103	A1EFU	CM3-C5-C6-C7
9	J	103	A1EFU	C6-C7-C8-C9
9	J	103	A1EFU	C10-C11-C12-C13
9	J	103	A1EFU	C17-C18-C19-C20
9	J	103	A1EFU	CM6-C18-C19-C20
9	J	103	A1EFU	C16-C17-C18-C19
9	J	103	A1EFU	C16-C17-C18-CM6
9	J	103	A1EFU	C11-C10-C9-C8
9	J	103	A1EFU	C11-C10-C9-CM4
9	J	103	A1EFU	C12-C13-C14-C15
9	J	103	A1EFU	CM5-C13-C14-C15
9	J	103	A1EFU	C19-C20-C21-C22
9	J	103	A1EFU	C20-C21-C22-C23
9	J	103	A1EFU	C20-C21-C22-CM7
9	I	101	A1EFU	C2-C3-C4-C5
9	I	101	A1EFU	C4-C5-C6-C7
9	I	101	A1EFU	CM3-C5-C6-C7
9	I	101	A1EFU	C6-C7-C8-C9
9	I	101	A1EFU	C10-C11-C12-C13
9	I	101	A1EFU	C14-C15-C16-C17
9	I	101	A1EFU	C18-C19-C20-C21
9	I	101	A1EFU	C16-C17-C18-C19
9	I	101	A1EFU	C16-C17-C18-CM6
9	I	101	A1EFU	C11-C10-C9-C8
9	I	101	A1EFU	C11-C10-C9-CM4
9	I	101	A1EFU	C12-C13-C14-C15
9	I	101	A1EFU	CM5-C13-C14-C15
9	I	101	A1EFU	C20-C21-C22-C23
9	I	101	A1EFU	CM7-C22-C23-C24
9	I	101	A1EFU	C26-C27-C28-C29

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
9	I	103	A1EFU	O1-C1-C2-O2
9	I	103	A1EFU	C2-C3-C4-C5
9	I	103	A1EFU	C4-C5-C6-C7
9	I	103	A1EFU	CM3-C5-C6-C7
9	I	103	A1EFU	C6-C7-C8-C9
9	I	103	A1EFU	C10-C11-C12-C13
9	I	103	A1EFU	C14-C15-C16-C17
9	I	103	A1EFU	C16-C17-C18-C19
9	I	103	A1EFU	C16-C17-C18-CM6
9	I	103	A1EFU	C11-C10-C9-C8
9	I	103	A1EFU	C11-C10-C9-CM4
9	I	103	A1EFU	C12-C13-C14-C15
9	I	103	A1EFU	CM5-C13-C14-C15
9	I	103	A1EFU	C20-C21-C22-CM7
9	I	103	A1EFU	C26-C27-C28-C29
9	G	104	A1EFU	O1-C1-C2-O2
9	G	104	A1EFU	C4-C5-C6-C7
9	G	104	A1EFU	CM3-C5-C6-C7
9	G	104	A1EFU	C6-C7-C8-C9
9	G	104	A1EFU	C10-C11-C12-C13
9	G	104	A1EFU	C14-C15-C16-C17
9	G	104	A1EFU	C13-C14-C15-C16
9	G	104	A1EFU	C18-C19-C20-C21
9	G	104	A1EFU	C16-C17-C18-C19
9	G	104	A1EFU	C16-C17-C18-CM6
9	G	104	A1EFU	C12-C13-C14-C15
9	G	104	A1EFU	CM5-C13-C14-C15
9	G	104	A1EFU	C20-C21-C22-CM7
9	G	104	A1EFU	C21-C22-C23-C24
9	G	104	A1EFU	C26-C27-C28-C29
9	G	105	A1EFU	C2-C3-C4-C5
9	G	105	A1EFU	C5-C6-C7-C8
9	G	105	A1EFU	C4-C5-C6-C7
9	G	105	A1EFU	CM3-C5-C6-C7
9	G	105	A1EFU	C10-C11-C12-C13
9	G	105	A1EFU	C14-C15-C16-C17
9	G	105	A1EFU	C16-C17-C18-C19
9	G	105	A1EFU	C16-C17-C18-CM6
9	G	105	A1EFU	C11-C10-C9-C8
9	G	105	A1EFU	C11-C10-C9-CM4
9	G	105	A1EFU	C12-C13-C14-C15
9	G	105	A1EFU	CM5-C13-C14-C15

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
9	G	105	A1EFU	C20-C21-C22-CM7
9	F	105	A1EFU	C4-C5-C6-C7
9	F	105	A1EFU	CM3-C5-C6-C7
9	F	105	A1EFU	C6-C7-C8-C9
9	F	105	A1EFU	C10-C11-C12-C13
9	F	105	A1EFU	C18-C19-C20-C21
9	F	105	A1EFU	C16-C17-C18-C19
9	F	105	A1EFU	C16-C17-C18-CM6
9	F	105	A1EFU	C11-C10-C9-C8
9	F	105	A1EFU	C11-C10-C9-CM4
9	F	105	A1EFU	C12-C13-C14-C15
9	F	105	A1EFU	CM5-C13-C14-C15
9	F	105	A1EFU	C20-C21-C22-C23
9	F	105	A1EFU	C20-C21-C22-CM7
9	F	105	A1EFU	C22-C23-C24-C25
9	e	101	A1EFU	C2-C3-C4-C5
9	e	101	A1EFU	C4-C5-C6-C7
9	e	101	A1EFU	CM3-C5-C6-C7
9	e	101	A1EFU	C6-C7-C8-C9
9	e	101	A1EFU	C10-C11-C12-C13
9	e	101	A1EFU	C16-C17-C18-C19
9	e	101	A1EFU	C16-C17-C18-CM6
9	e	101	A1EFU	C11-C10-C9-C8
9	e	101	A1EFU	C11-C10-C9-CM4
9	e	101	A1EFU	C12-C13-C14-C15
9	e	101	A1EFU	CM5-C13-C14-C15
9	e	101	A1EFU	C20-C21-C22-CM7
9	e	101	A1EFU	C26-C27-C28-C29
9	E	102	A1EFU	C10-C11-C12-C13
9	E	102	A1EFU	C18-C19-C20-C21
9	E	102	A1EFU	C16-C17-C18-C19
9	E	102	A1EFU	C16-C17-C18-CM6
9	E	102	A1EFU	C11-C10-C9-C8
9	E	102	A1EFU	C11-C10-C9-CM4
9	E	102	A1EFU	C12-C13-C14-C15
9	E	102	A1EFU	CM5-C13-C14-C15
9	E	102	A1EFU	C20-C21-C22-C23
9	E	102	A1EFU	C20-C21-C22-CM7
9	E	102	A1EFU	C22-C23-C24-C25
9	E	102	A1EFU	C25-C26-C27-C28
9	E	102	A1EFU	CM8-C26-C27-C28
9	E	102	A1EFU	C26-C27-C28-C29

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
9	d	102	A1EFU	O1-C1-C2-O2
9	d	102	A1EFU	C2-C3-C4-C5
9	d	102	A1EFU	C4-C5-C6-C7
9	d	102	A1EFU	CM3-C5-C6-C7
9	d	102	A1EFU	C10-C11-C12-C13
9	d	102	A1EFU	C18-C19-C20-C21
9	d	102	A1EFU	C16-C17-C18-C19
9	d	102	A1EFU	C16-C17-C18-CM6
9	d	102	A1EFU	C11-C10-C9-C8
9	d	102	A1EFU	C11-C10-C9-CM4
9	d	102	A1EFU	C12-C13-C14-C15
9	d	102	A1EFU	CM5-C13-C14-C15
9	d	102	A1EFU	C20-C21-C22-CM7
9	d	102	A1EFU	C26-C27-C28-C29
9	D	104	A1EFU	C4-C5-C6-C7
9	D	104	A1EFU	CM3-C5-C6-C7
9	D	104	A1EFU	C6-C7-C8-C9
9	D	104	A1EFU	C10-C11-C12-C13
9	D	104	A1EFU	C14-C15-C16-C17
9	D	104	A1EFU	C18-C19-C20-C21
9	D	104	A1EFU	C16-C17-C18-C19
9	D	104	A1EFU	C16-C17-C18-CM6
9	D	104	A1EFU	C11-C10-C9-C8
9	D	104	A1EFU	C11-C10-C9-CM4
9	D	104	A1EFU	C12-C13-C14-C15
9	D	104	A1EFU	CM5-C13-C14-C15
9	D	104	A1EFU	C20-C21-C22-C23
9	D	104	A1EFU	C20-C21-C22-CM7
9	D	104	A1EFU	C22-C23-C24-C25
9	D	104	A1EFU	C25-C26-C27-C28
9	D	104	A1EFU	CM8-C26-C27-C28
9	D	104	A1EFU	C26-C27-C28-C29
9	D	105	A1EFU	C1-C2-C3-C4
9	D	105	A1EFU	O2-C2-C3-C4
9	D	105	A1EFU	O1-C1-C2-O2
9	D	105	A1EFU	C2-C3-C4-C5
9	D	105	A1EFU	C6-C7-C8-C9
9	D	105	A1EFU	C10-C11-C12-C13
9	D	105	A1EFU	C14-C15-C16-C17
9	D	105	A1EFU	C18-C19-C20-C21
9	D	105	A1EFU	C16-C17-C18-C19
9	D	105	A1EFU	C16-C17-C18-CM6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
9	D	105	A1EFU	C11-C10-C9-C8
9	D	105	A1EFU	C11-C10-C9-CM4
9	D	105	A1EFU	C12-C13-C14-C15
9	D	105	A1EFU	CM5-C13-C14-C15
9	D	105	A1EFU	C20-C21-C22-CM7
9	D	105	A1EFU	C26-C27-C28-C29
9	B	102	A1EFU	O1-C1-C2-O2
9	B	102	A1EFU	C4-C5-C6-C7
9	B	102	A1EFU	CM3-C5-C6-C7
9	B	102	A1EFU	C6-C7-C8-C9
9	B	102	A1EFU	C10-C11-C12-C13
9	B	102	A1EFU	C18-C19-C20-C21
9	B	102	A1EFU	C16-C17-C18-C19
9	B	102	A1EFU	C16-C17-C18-CM6
9	B	102	A1EFU	C11-C10-C9-C8
9	B	102	A1EFU	C11-C10-C9-CM4
9	B	102	A1EFU	C12-C13-C14-C15
9	B	102	A1EFU	CM5-C13-C14-C15
9	B	102	A1EFU	C20-C21-C22-CM7
9	a	101	A1EFU	O1-C1-C2-O2
9	a	101	A1EFU	C2-C3-C4-C5
9	a	101	A1EFU	C4-C5-C6-C7
9	a	101	A1EFU	CM3-C5-C6-C7
9	a	101	A1EFU	C10-C11-C12-C13
9	a	101	A1EFU	C18-C19-C20-C21
9	a	101	A1EFU	C16-C17-C18-C19
9	a	101	A1EFU	C16-C17-C18-CM6
9	a	101	A1EFU	C11-C10-C9-C8
9	a	101	A1EFU	C11-C10-C9-CM4
9	a	101	A1EFU	C12-C13-C14-C15
9	a	101	A1EFU	CM5-C13-C14-C15
9	a	101	A1EFU	C20-C21-C22-CM7
9	a	101	A1EFU	C26-C27-C28-C29
9	a	103	A1EFU	C2-C3-C4-C5
9	a	103	A1EFU	C4-C5-C6-C7
9	a	103	A1EFU	CM3-C5-C6-C7
9	a	103	A1EFU	C6-C7-C8-C9
9	a	103	A1EFU	C10-C11-C12-C13
9	a	103	A1EFU	C18-C19-C20-C21
9	a	103	A1EFU	C16-C17-C18-C19
9	a	103	A1EFU	C16-C17-C18-CM6
9	a	103	A1EFU	C12-C13-C14-C15

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
9	a	103	A1EFU	CM5-C13-C14-C15
9	a	103	A1EFU	C19-C20-C21-C22
9	a	103	A1EFU	C20-C21-C22-CM7
9	A	102	A1EFU	C2-C3-C4-C5
9	A	102	A1EFU	C4-C5-C6-C7
9	A	102	A1EFU	CM3-C5-C6-C7
9	A	102	A1EFU	C6-C7-C8-C9
9	A	102	A1EFU	C10-C11-C12-C13
9	A	102	A1EFU	C18-C19-C20-C21
9	A	102	A1EFU	C16-C17-C18-C19
9	A	102	A1EFU	C16-C17-C18-CM6
9	A	102	A1EFU	C11-C10-C9-C8
9	A	102	A1EFU	C11-C10-C9-CM4
9	A	102	A1EFU	C12-C13-C14-C15
9	A	102	A1EFU	CM5-C13-C14-C15
9	A	102	A1EFU	C20-C21-C22-CM7
9	M	407	A1EFU	C2-C3-C4-C5
9	M	407	A1EFU	C4-C5-C6-C7
9	M	407	A1EFU	CM3-C5-C6-C7
9	M	407	A1EFU	C6-C7-C8-C9
9	M	407	A1EFU	C10-C11-C12-C13
9	M	407	A1EFU	C14-C15-C16-C17
9	M	407	A1EFU	C18-C19-C20-C21
9	M	407	A1EFU	C16-C17-C18-C19
9	M	407	A1EFU	C16-C17-C18-CM6
9	M	407	A1EFU	C11-C10-C9-C8
9	M	407	A1EFU	C11-C10-C9-CM4
9	M	407	A1EFU	C12-C13-C14-C15
9	M	407	A1EFU	CM5-C13-C14-C15
9	M	407	A1EFU	C19-C20-C21-C22
9	M	407	A1EFU	C20-C21-C22-C23
9	M	407	A1EFU	C20-C21-C22-CM7
9	M	407	A1EFU	CM7-C22-C23-C24
10	Q	104	MW9	C33-C34-C35-C36
10	Q	104	MW9	C21-O5-P-O2
10	Q	104	MW9	C21-O5-P-O3
10	Q	104	MW9	C21-O5-P-O4
10	I	104	MW9	C25-C24-O8-C19
10	I	104	MW9	O9-C24-O8-C19
10	I	104	MW9	C20-O2-P-O4
10	I	104	MW9	C21-O5-P-O3
10	I	104	MW9	C21-O5-P-O4

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
10	G	103	MW9	C21-C22-C23-O6
10	G	103	MW9	C25-C24-O8-C19
10	G	103	MW9	O9-C24-O8-C19
10	G	103	MW9	C20-O2-P-O3
10	G	103	MW9	C20-O2-P-O4
10	F	103	MW9	O5-C21-C22-C23
10	F	103	MW9	C25-C24-O8-C19
10	F	103	MW9	O9-C24-O8-C19
10	F	103	MW9	C21-O5-P-O4
10	F	104	MW9	O5-C21-C22-O7
10	F	104	MW9	C21-O5-P-O2
10	F	104	MW9	C21-O5-P-O3
10	D	102	MW9	C18-C19-C20-O2
10	D	102	MW9	O8-C19-C20-O2
10	D	102	MW9	C25-C24-O8-C19
10	D	103	MW9	C21-C22-C23-O6
10	D	103	MW9	O7-C22-C23-O6
10	D	103	MW9	C25-C24-O8-C19
10	D	103	MW9	O9-C24-O8-C19
10	D	103	MW9	C33-C34-C35-C36
10	D	103	MW9	C21-O5-P-O2
10	D	103	MW9	C21-O5-P-O4
10	M	405	MW9	C33-C34-C35-C36
10	M	405	MW9	C20-O2-P-O3
10	M	405	MW9	C20-O2-P-O4
10	M	405	MW9	C21-O5-P-O4
10	M	406	MW9	O-C17-O1-C18
10	M	406	MW9	C16-C17-O1-C18
10	M	406	MW9	O9-C24-O8-C19
10	M	406	MW9	C21-O5-P-O2
10	M	406	MW9	C21-O5-P-O3
10	M	406	MW9	C21-O5-P-O4
10	L	309	MW9	C21-O5-P-O2
10	L	309	MW9	C21-O5-P-O3
10	L	310	MW9	O-C17-O1-C18
10	L	310	MW9	C16-C17-O1-C18
10	L	310	MW9	C22-C21-O5-P
10	H	302	MW9	C20-O2-P-O3
10	H	302	MW9	C20-O2-P-O4
10	H	302	MW9	C20-O2-P-O5
12	M	404	U10	C19-C21-C22-C23
12	M	404	U10	C34-C36-C37-C38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
12	M	404	U10	C49-C51-C52-C53
12	L	305	U10	C14-C16-C17-C18
13	L	301	LMT	C2-C1-O1'-C1'
13	L	307	LMT	O5'-C1'-O1'-C1
13	L	307	LMT	C2-C1-O1'-C1'
13	L	308	LMT	C2'-C1'-O1'-C1
13	L	308	LMT	O5'-C1'-O1'-C1
13	C	404	LMT	O5'-C1'-O1'-C1
14	L	302	BPH	C3A-C2A-CAA-CBA
14	L	302	BPH	C1A-C2A-CAA-CBA
15	L	311	CDL	O1-C1-CB2-OB2
15	L	311	CDL	CA2-OA2-PA1-OA4
15	L	311	CDL	CA3-OA5-PA1-OA2
15	L	311	CDL	CA3-OA5-PA1-OA3
15	L	311	CDL	CA3-OA5-PA1-OA4
15	L	311	CDL	OA9-CA7-OA8-CA6
15	L	311	CDL	C31-CA7-OA8-CA6
15	L	311	CDL	CB3-OB5-PB2-OB3
15	L	311	CDL	CB3-OB5-PB2-OB4
15	H	303	CDL	CA2-OA2-PA1-OA3
15	H	303	CDL	CA2-OA2-PA1-OA4
15	H	303	CDL	OA9-CA7-OA8-CA6
15	H	303	CDL	C51-CB5-OB6-CB4
8	P	102	BCL	O1A-CGA-O2A-C1
8	F	102	BCL	O1A-CGA-O2A-C1
10	Q	104	MW9	O-C17-O1-C18
10	Q	104	MW9	C16-C17-O1-C18
8	E	101	BCL	O1A-CGA-O2A-C1
8	L	303	BCL	O1A-CGA-O2A-C1
10	F	103	MW9	O-C17-O1-C18
10	D	102	MW9	O9-C24-O8-C19
15	L	311	CDL	OA7-CA5-OA6-CA4
15	H	303	CDL	OA7-CA5-OA6-CA4
15	H	303	CDL	OB7-CB5-OB6-CB4
8	1	102	BCL	C3-C5-C6-C7
8	i	101	BCL	C3-C5-C6-C7
8	d	101	BCL	C3-C5-C6-C7
8	a	102	BCL	C3-C5-C6-C7
8	P	102	BCL	CBA-CGA-O2A-C1
8	E	101	BCL	CBA-CGA-O2A-C1
15	H	303	CDL	C31-CA7-OA8-CA6
10	M	405	MW9	C25-C24-O8-C19

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
10	M	406	MW9	C25-C24-O8-C19
15	L	311	CDL	C11-CA5-OA6-CA4
15	H	303	CDL	C11-CA5-OA6-CA4
8	n	101	BCL	O1A-CGA-O2A-C1
9	S	102	A1EFU	CM8-C26-C27-C28
9	K	102	A1EFU	CM7-C22-C23-C24
9	I	103	A1EFU	CM8-C26-C27-C28
9	G	104	A1EFU	CM7-C22-C23-C24
9	F	105	A1EFU	CM7-C22-C23-C24
12	L	305	U10	C35-C34-C36-C37
8	s	101	BCL	C2-C3-C5-C6
8	b	101	BCL	C2-C3-C5-C6
8	L	303	BCL	C2-C3-C5-C6
9	S	102	A1EFU	C25-C26-C27-C28
9	2	102	A1EFU	C21-C22-C23-C24
9	N	102	A1EFU	C21-C22-C23-C24
9	a	103	A1EFU	C21-C22-C23-C24
8	R	102	BCL	C2A-CAA-CBA-CGA
8	N	101	BCL	C2A-CAA-CBA-CGA
8	K	101	BCL	C2A-CAA-CBA-CGA
8	D	101	BCL	C2A-CAA-CBA-CGA
10	G	103	MW9	C5-C6-C7-C8
10	F	104	MW9	C5-C6-C7-C8
13	L	301	LMT	C3'-C4'-O1B-C1B
8	1	103	BCL	CBA-CGA-O2A-C1
8	i	101	BCL	CBA-CGA-O2A-C1
8	F	102	BCL	CBA-CGA-O2A-C1
8	L	303	BCL	CBA-CGA-O2A-C1
10	F	103	MW9	C16-C17-O1-C18
10	L	309	MW9	C16-C17-O1-C18
13	L	301	LMT	O5'-C5'-C6'-O6'
10	M	405	MW9	C31-C32-C33-C34
8	a	102	BCL	C1-C2-C3-C5
10	M	405	MW9	O9-C24-O8-C19
8	v	101	BCL	O1A-CGA-O2A-C1
8	1	103	BCL	O1A-CGA-O2A-C1
8	i	101	BCL	O1A-CGA-O2A-C1
9	s	102	A1EFU	C5-C6-C7-C8
9	r	102	A1EFU	C9-C10-C11-C12
9	2	101	A1EFU	C15-C16-C17-C18
9	2	102	A1EFU	C15-C16-C17-C18
9	1	104	A1EFU	C15-C16-C17-C18

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
9	J	103	A1EFU	C9-C10-C11-C12
9	I	101	A1EFU	C13-C14-C15-C16
9	I	103	A1EFU	C13-C14-C15-C16
9	G	105	A1EFU	C13-C14-C15-C16
10	F	103	MW9	O5-C21-C22-O7
8	t	101	BCL	C3-C5-C6-C7
8	Q	101	BCL	C3-C5-C6-C7
8	b	101	BCL	C3-C5-C6-C7
8	n	101	BCL	CBA-CGA-O2A-C1
10	I	104	MW9	C16-C17-O1-C18
13	H	301	LMT	O5'-C5'-C6'-O6'
10	Q	104	MW9	C12-C13-C14-C15
9	e	101	A1EFU	CM7-C22-C23-C24
8	A	101	BCL	C2-C3-C5-C6
9	Q	103	A1EFU	C21-C22-C23-C24
9	N	103	A1EFU	C21-C22-C23-C24
9	I	103	A1EFU	C21-C22-C23-C24
9	G	105	A1EFU	C21-C22-C23-C24
9	d	102	A1EFU	C21-C22-C23-C24
9	D	105	A1EFU	C21-C22-C23-C24
9	a	101	A1EFU	C21-C22-C23-C24
14	L	302	BPH	C2A-CAA-CBA-CGA
8	J	101	BCL	O1A-CGA-O2A-C1
10	I	104	MW9	O-C17-O1-C18
10	L	309	MW9	O-C17-O1-C18
9	v	102	A1EFU	C22-C23-C24-C25
9	S	102	A1EFU	C22-C23-C24-C25
9	T	101	A1EFU	C26-C27-C28-C29
9	s	102	A1EFU	C22-C23-C24-C25
9	l	101	A1EFU	C22-C23-C24-C25
9	N	102	A1EFU	C22-C23-C24-C25
9	k	102	A1EFU	C26-C27-C28-C29
9	K	102	A1EFU	C26-C27-C28-C29
12	L	305	U10	C9-C11-C12-C13
12	L	305	U10	C19-C21-C22-C23
12	L	305	U10	C24-C26-C27-C28
12	L	305	U10	C34-C36-C37-C38
8	v	101	BCL	CBA-CGA-O2A-C1
8	s	101	BCL	C1-C2-C3-C5
8	e	102	BCL	C1-C2-C3-C5
10	F	104	MW9	O5-C21-C22-C23
15	L	311	CDL	CA2-C1-CB2-OB2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	L	301	LMT	C4'-C5'-C6'-O6'
9	Q	102	A1EFU	C15-C16-C17-C18
9	2	102	A1EFU	C5-C6-C7-C8
9	N	102	A1EFU	C9-C10-C11-C12
9	N	102	A1EFU	C19-C20-C21-C22
10	I	104	MW9	O8-C19-C20-O2
13	L	301	LMT	O5B-C5B-C6B-O6B
8	s	101	BCL	C6-C7-C8-C9
8	j	101	BCL	C6-C7-C8-C9
8	i	101	BCL	C6-C7-C8-C9
8	a	102	BCL	C6-C7-C8-C9
8	M	403	BCL	C6-C7-C8-C9
8	L	306	BCL	C6-C7-C8-C9
14	L	304	BPH	C14-C13-C15-C16
8	F	101	BCL	C10-C11-C12-C13
15	L	311	CDL	CB7-C71-C72-C73
8	V	101	BCL	O1A-CGA-O2A-C1
8	n	101	BCL	C5-C6-C7-C8
8	b	101	BCL	C10-C11-C12-C13
8	v	101	BCL	C8-C10-C11-C12
8	v	101	BCL	C15-C16-C17-C18
8	l	102	BCL	C5-C6-C7-C8
8	J	101	BCL	C10-C11-C12-C13
8	b	101	BCL	C15-C16-C17-C18
8	B	101	BCL	C5-C6-C7-C8
10	Q	104	MW9	C24-C25-C26-C27
10	G	103	MW9	C14-C15-C16-C17
10	D	102	MW9	C14-C15-C16-C17
10	H	302	MW9	C24-C25-C26-C27
15	H	303	CDL	CB7-C71-C72-C73
8	L	303	BCL	C15-C16-C17-C18
8	J	101	BCL	CBA-CGA-O2A-C1
10	M	405	MW9	C16-C17-O1-C18
10	I	104	MW9	C14-C15-C16-C17
10	F	103	MW9	C14-C15-C16-C17
15	H	303	CDL	CA5-C11-C12-C13
10	I	104	MW9	C30-C31-C32-C33
10	M	406	MW9	C6-C7-C8-C9
8	t	101	BCL	C11-C12-C13-C15
8	q	101	BCL	C12-C13-C15-C16
8	F	101	BCL	C11-C10-C8-C7
14	L	304	BPH	C11-C12-C13-C15

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
9	v	102	A1EFU	C19-C20-C21-C22
9	t	102	A1EFU	C5-C6-C7-C8
9	r	102	A1EFU	C15-C16-C17-C18
9	R	101	A1EFU	C5-C6-C7-C8
9	l	101	A1EFU	C13-C14-C15-C16
9	k	102	A1EFU	C19-C20-C21-C22
9	G	104	A1EFU	C15-C16-C17-C18
8	I	102	BCL	C2A-CAA-CBA-CGA
8	r	101	BCL	C13-C15-C16-C17
10	H	302	MW9	C11-C12-C13-C14
9	v	103	A1EFU	C22-C23-C24-C25
9	Q	102	A1EFU	C22-C23-C24-C25
9	Q	103	A1EFU	C22-C23-C24-C25
9	r	102	A1EFU	C22-C23-C24-C25
9	l	101	A1EFU	C26-C27-C28-C29
9	N	102	A1EFU	C26-C27-C28-C29
9	N	103	A1EFU	C22-C23-C24-C25
9	k	102	A1EFU	C22-C23-C24-C25
9	J	102	A1EFU	C26-C27-C28-C29
9	I	103	A1EFU	C22-C23-C24-C25
9	G	104	A1EFU	C22-C23-C24-C25
9	B	102	A1EFU	C26-C27-C28-C29
9	a	103	A1EFU	C22-C23-C24-C25
12	M	404	U10	C24-C26-C27-C28
9	v	102	A1EFU	C18-C19-C20-C21
9	S	102	A1EFU	C18-C19-C20-C21
9	T	101	A1EFU	C18-C19-C20-C21
9	s	102	A1EFU	C6-C7-C8-C9
9	l	104	A1EFU	C18-C19-C20-C21
9	N	102	A1EFU	C10-C11-C12-C13
9	J	103	A1EFU	C18-C19-C20-C21
9	G	105	A1EFU	C6-C7-C8-C9
9	E	102	A1EFU	C6-C7-C8-C9
9	s	102	A1EFU	CM1-C1-C2-C3
9	G	104	A1EFU	CM1-C1-C2-C3
10	I	104	MW9	C5-C6-C7-C8
10	F	103	MW9	C5-C6-C7-C8
10	D	103	MW9	O5-C21-C22-O7
8	A	101	BCL	C3-C5-C6-C7
8	e	102	BCL	C10-C11-C12-C13
8	L	303	BCL	C13-C15-C16-C17
8	K	101	BCL	O1A-CGA-O2A-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
8	j	101	BCL	C5-C6-C7-C8
8	d	101	BCL	C15-C16-C17-C18
10	M	405	MW9	O-C17-O1-C18
8	A	101	BCL	C1-C2-C3-C5
10	I	104	MW9	C21-O5-P-O2
10	G	103	MW9	C20-O2-P-O5
10	F	103	MW9	C21-O5-P-O2
10	M	405	MW9	C20-O2-P-O5
10	L	310	MW9	C20-O2-P-O5
10	L	310	MW9	C21-O5-P-O2
15	L	311	CDL	CA2-OA2-PA1-OA5
15	L	311	CDL	CB3-OB5-PB2-OB2
15	H	303	CDL	CA2-OA2-PA1-OA5
10	M	405	MW9	C24-C25-C26-C27
8	Q	101	BCL	CBA-CGA-O2A-C1
8	a	102	BCL	C10-C11-C12-C13
10	F	104	MW9	C24-C25-C26-C27
10	D	103	MW9	O5-C21-C22-C23
8	I	102	BCL	C16-C17-C18-C20
8	v	101	BCL	C3-C5-C6-C7
13	H	301	LMT	C4'-C5'-C6'-O6'
8	G	101	BCL	C5-C6-C7-C8
9	2	102	A1EFU	C19-C20-C21-C22
9	N	103	A1EFU	C9-C10-C11-C12
15	L	311	CDL	C11-C12-C13-C14
10	F	104	MW9	C25-C24-O8-C19
10	L	310	MW9	C25-C24-O8-C19
8	M	403	BCL	C5-C6-C7-C8
9	Q	103	A1EFU	C11-C10-C9-CM4
9	r	102	A1EFU	C16-C17-C18-CM6
9	1	104	A1EFU	C16-C17-C18-CM6
9	K	102	A1EFU	C16-C17-C18-CM6
9	J	102	A1EFU	CM3-C5-C6-C7
9	J	102	A1EFU	C16-C17-C18-CM6
9	G	104	A1EFU	C11-C10-C9-CM4
9	D	105	A1EFU	CM3-C5-C6-C7
10	I	104	MW9	C13-C14-C15-C16
10	D	102	MW9	C12-C13-C14-C15
10	M	406	MW9	C13-C14-C15-C16
10	L	310	MW9	C9-C10-C11-C12
10	H	302	MW9	C10-C11-C12-C13
15	H	303	CDL	C76-C77-C78-C79

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
8	Q	101	BCL	C16-C17-C18-C19
10	Q	104	MW9	C10-C11-C12-C13
10	G	103	MW9	C12-C13-C14-C15
10	F	104	MW9	C12-C13-C14-C15
10	D	102	MW9	C9-C10-C11-C12
13	L	308	LMT	C5-C6-C7-C8
10	F	104	MW9	O9-C24-O8-C19
10	L	310	MW9	O9-C24-O8-C19
10	L	310	MW9	C24-C25-C26-C27
10	D	102	MW9	C4-C5-C6-C7
10	Q	104	MW9	C11-C12-C13-C14
10	F	104	MW9	C27-C28-C29-C30
10	D	103	MW9	C4-C5-C6-C7
15	L	311	CDL	C52-C53-C54-C55
15	L	311	CDL	C54-C55-C56-C57
10	L	309	MW9	O5-C21-C22-O7
10	G	103	MW9	C10-C11-C12-C13
10	M	406	MW9	C4-C5-C6-C7
15	H	303	CDL	C77-C78-C79-C80
9	t	102	A1EFU	CM2-C1-O1-CMA
9	T	101	A1EFU	CM2-C1-O1-CMA
9	s	102	A1EFU	CM2-C1-O1-CMA
9	s	102	A1EFU	C16-C17-C18-C19
9	s	102	A1EFU	C11-C10-C9-C8
9	Q	103	A1EFU	C11-C10-C9-C8
9	r	102	A1EFU	C16-C17-C18-C19
9	l	104	A1EFU	C16-C17-C18-C19
9	K	102	A1EFU	C16-C17-C18-C19
9	J	102	A1EFU	C4-C5-C6-C7
9	J	102	A1EFU	C16-C17-C18-C19
9	G	104	A1EFU	C11-C10-C9-C8
9	D	105	A1EFU	C4-C5-C6-C7
8	j	101	BCL	C1-C2-C3-C5
10	G	103	MW9	C27-C28-C29-C30
10	F	103	MW9	C6-C7-C8-C9
10	M	405	MW9	C13-C14-C15-C16
10	L	309	MW9	C26-C27-C28-C29
8	s	101	BCL	C5-C6-C7-C8
8	Q	101	BCL	O1A-CGA-O2A-C1
8	R	102	BCL	C16-C17-C18-C19
12	L	305	U10	C30-C29-C31-C32
10	F	104	MW9	C6-C7-C8-C9

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
10	D	102	MW9	C10-C11-C12-C13
10	H	302	MW9	C7-C8-C9-C10
15	L	311	CDL	C16-C17-C18-C19
15	H	303	CDL	C72-C73-C74-C75
9	I	103	A1EFU	C25-C26-C27-C28
12	L	305	U10	C33-C34-C36-C37
8	t	101	BCL	C11-C12-C13-C14
8	T	102	BCL	C6-C7-C8-C9
8	q	101	BCL	C11-C10-C8-C9
8	q	101	BCL	C14-C13-C15-C16
8	F	101	BCL	C11-C10-C8-C9
8	d	101	BCL	C11-C12-C13-C14
8	B	101	BCL	C6-C7-C8-C9
8	a	102	BCL	C14-C13-C15-C16
8	A	101	BCL	C14-C13-C15-C16
10	G	103	MW9	C13-C14-C15-C16
10	F	104	MW9	C4-C5-C6-C7
10	D	102	MW9	C7-C8-C9-C10
10	D	103	MW9	C37-C38-C39-C40
10	M	405	MW9	C9-C10-C11-C12
10	M	406	MW9	C7-C8-C9-C10
10	L	309	MW9	C13-C14-C15-C16
10	H	302	MW9	C12-C13-C14-C15
8	G	101	BCL	C8-C10-C11-C12
8	A	101	BCL	C2A-CAA-CBA-CGA
10	F	104	MW9	C21-C22-C23-O6
10	M	405	MW9	C21-C22-C23-O6
10	L	310	MW9	C21-C22-C23-O6
10	L	310	MW9	C12-C13-C14-C15
15	H	303	CDL	C58-C59-C60-C61
10	F	104	MW9	C29-C30-C31-C32
10	M	406	MW9	C14-C15-C16-C17
10	Q	104	MW9	C13-C14-C15-C16
10	I	104	MW9	C6-C7-C8-C9
10	F	103	MW9	C7-C8-C9-C10
10	D	103	MW9	C6-C7-C8-C9
8	Q	101	BCL	C16-C17-C18-C20
8	I	102	BCL	C16-C17-C18-C19
8	q	101	BCL	C15-C16-C17-C18
10	F	103	MW9	C10-C11-C12-C13
10	F	104	MW9	C2-C3-C4-C5
15	L	311	CDL	C13-C14-C15-C16

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
15	H	303	CDL	C11-C12-C13-C14
15	H	303	CDL	C75-C76-C77-C78
10	F	103	MW9	C13-C14-C15-C16
10	F	104	MW9	C13-C14-C15-C16
8	d	101	BCL	C10-C11-C12-C13
10	F	103	MW9	C9-C10-C11-C12
10	F	104	MW9	C26-C27-C28-C29
10	D	103	MW9	C12-C13-C14-C15
10	I	104	MW9	C27-C28-C29-C30
10	M	406	MW9	C25-C26-C27-C28
8	P	102	BCL	C3A-C2A-CAA-CBA
8	v	101	BCL	C3A-C2A-CAA-CBA
8	t	101	BCL	C3A-C2A-CAA-CBA
8	T	102	BCL	C3A-C2A-CAA-CBA
8	s	101	BCL	C3A-C2A-CAA-CBA
8	r	101	BCL	C3A-C2A-CAA-CBA
8	R	102	BCL	C3A-C2A-CAA-CBA
8	q	101	BCL	C3A-C2A-CAA-CBA
8	l	102	BCL	C3A-C2A-CAA-CBA
8	N	101	BCL	C3A-C2A-CAA-CBA
8	i	101	BCL	C3A-C2A-CAA-CBA
8	G	101	BCL	C3A-C2A-CAA-CBA
8	G	102	BCL	C3A-C2A-CAA-CBA
8	e	102	BCL	C3A-C2A-CAA-CBA
8	d	101	BCL	C3A-C2A-CAA-CBA
8	b	101	BCL	C3A-C2A-CAA-CBA
8	A	101	BCL	C3A-C2A-CAA-CBA
8	L	303	BCL	C3A-C2A-CAA-CBA
16	C	401	HEC	C3D-CAD-CBD-CGD
13	L	308	LMT	C2-C1-O1'-C1'
10	I	104	MW9	C10-C11-C12-C13
15	L	311	CDL	C55-C56-C57-C58
8	S	101	BCL	C16-C17-C18-C20
8	R	102	BCL	C16-C17-C18-C20
10	M	406	MW9	C10-C11-C12-C13
9	d	102	A1EFU	C14-C15-C16-C17
8	M	403	BCL	C3-C5-C6-C7
8	L	306	BCL	C3-C5-C6-C7
8	T	102	BCL	C13-C15-C16-C17
8	d	101	BCL	C4-C3-C5-C6
8	a	102	BCL	C4-C3-C5-C6
14	L	302	BPH	C4-C3-C5-C6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
9	I	101	A1EFU	C21-C22-C23-C24
12	L	305	U10	C18-C19-C21-C22
12	L	305	U10	C28-C29-C31-C32
10	Q	104	MW9	C25-C24-O8-C19
10	M	406	MW9	C27-C28-C29-C30
10	G	103	MW9	O7-C22-C23-O6
10	L	310	MW9	O7-C22-C23-O6
10	D	102	MW9	C6-C7-C8-C9
10	D	102	MW9	C24-C25-C26-C27
8	s	101	BCL	C16-C17-C18-C20
8	i	101	BCL	C10-C11-C12-C13
10	F	103	MW9	C11-C12-C13-C14
8	B	101	BCL	C3-C5-C6-C7
15	H	303	CDL	C60-C61-C62-C63
10	F	103	MW9	C28-C29-C30-C31
10	L	310	MW9	C10-C11-C12-C13
10	L	310	MW9	C11-C12-C13-C14
15	L	311	CDL	C15-C16-C17-C18
8	t	101	BCL	C15-C16-C17-C18
8	Q	101	BCL	C8-C10-C11-C12
8	l	103	BCL	C10-C11-C12-C13
8	F	101	BCL	C5-C6-C7-C8
10	F	104	MW9	C10-C11-C12-C13
10	L	310	MW9	C13-C14-C15-C16
9	G	104	A1EFU	CM1-C1-C2-O2
13	L	307	LMT	C3-C4-C5-C6
8	V	101	BCL	CBA-CGA-O2A-C1
8	K	101	BCL	CBA-CGA-O2A-C1
8	M	403	BCL	CBA-CGA-O2A-C1
8	v	101	BCL	C13-C15-C16-C17
8	G	101	BCL	C10-C11-C12-C13
10	G	103	MW9	C34-C35-C36-C37
10	H	302	MW9	C13-C14-C15-C16
8	e	102	BCL	C15-C16-C17-C18
8	V	101	BCL	C4-C3-C5-C6
9	J	102	A1EFU	CM8-C26-C27-C28
8	T	102	BCL	C6-C7-C8-C10
8	s	101	BCL	C6-C7-C8-C10
8	s	101	BCL	C12-C13-C15-C16
8	q	101	BCL	C11-C10-C8-C7
8	G	101	BCL	C11-C10-C8-C7
8	G	102	BCL	C6-C7-C8-C10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
8	D	101	BCL	C6-C7-C8-C10
8	B	101	BCL	C11-C12-C13-C15
8	a	102	BCL	C12-C13-C15-C16
8	A	101	BCL	C12-C13-C15-C16
9	R	101	A1EFU	C25-C26-C27-C28
10	F	103	MW9	C31-C32-C33-C34
10	F	103	MW9	C25-C26-C27-C28
8	Q	101	BCL	C10-C11-C12-C13
9	T	101	A1EFU	C5-C6-C7-C8
8	S	101	BCL	C16-C17-C18-C19
8	E	101	BCL	C16-C17-C18-C19
8	E	101	BCL	C16-C17-C18-C20
10	Q	104	MW9	O9-C24-O8-C19
10	D	103	MW9	C24-C25-C26-C27
10	D	102	MW9	C16-C17-O1-C18
10	H	302	MW9	C6-C7-C8-C9
8	q	101	BCL	C1-C2-C3-C5
10	H	302	MW9	C14-C15-C16-C17
10	F	104	MW9	C3-C4-C5-C6
8	s	101	BCL	C16-C17-C18-C19
10	G	103	MW9	C26-C27-C28-C29
15	L	311	CDL	C14-C15-C16-C17
9	G	105	A1EFU	C18-C19-C20-C21
10	M	406	MW9	C9-C10-C11-C12
10	G	103	MW9	C6-C7-C8-C9
13	L	307	LMT	C2'-C1'-O1'-C1
13	C	404	LMT	C2'-C1'-O1'-C1
10	D	102	MW9	C13-C14-C15-C16
10	M	406	MW9	C11-C12-C13-C14
15	H	303	CDL	C74-C75-C76-C77
10	G	103	MW9	C7-C8-C9-C10
10	D	103	MW9	C26-C27-C28-C29
10	M	406	MW9	C36-C37-C38-C39
9	R	101	A1EFU	CM8-C26-C27-C28
9	1	104	A1EFU	CM7-C22-C23-C24
12	L	305	U10	C20-C19-C21-C22
14	L	304	BPH	C4-C3-C5-C6
8	S	101	BCL	C2-C3-C5-C6
14	L	302	BPH	C2-C3-C5-C6
10	M	405	MW9	C27-C28-C29-C30
8	s	101	BCL	C14-C13-C15-C16
8	R	102	BCL	C6-C7-C8-C9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
8	N	101	BCL	C6-C7-C8-C9
8	J	101	BCL	C6-C7-C8-C9
8	G	101	BCL	C11-C10-C8-C9
8	G	102	BCL	C6-C7-C8-C9
8	B	101	BCL	C11-C12-C13-C14
8	L	303	BCL	C11-C12-C13-C14
10	D	103	MW9	C27-C28-C29-C30
8	L	303	BCL	C3-C5-C6-C7
8	G	102	BCL	CBA-CGA-O2A-C1
13	L	308	LMT	C4-C5-C6-C7
8	P	102	BCL	C1A-C2A-CAA-CBA
8	t	101	BCL	C1A-C2A-CAA-CBA
8	T	102	BCL	C1A-C2A-CAA-CBA
8	s	101	BCL	C1A-C2A-CAA-CBA
8	Q	101	BCL	C1A-C2A-CAA-CBA
8	l	102	BCL	C1A-C2A-CAA-CBA
8	n	101	BCL	C1A-C2A-CAA-CBA
8	N	101	BCL	C1A-C2A-CAA-CBA
8	i	101	BCL	C1A-C2A-CAA-CBA
8	G	102	BCL	C1A-C2A-CAA-CBA
10	L	309	MW9	C30-C31-C32-C33
9	Q	102	A1EFU	C9-C10-C11-C12
9	l	101	A1EFU	C15-C16-C17-C18
8	L	306	BCL	C5-C6-C7-C8
15	H	303	CDL	CB3-OB5-PB2-OB2
10	D	103	MW9	C10-C11-C12-C13
15	H	303	CDL	C32-C33-C34-C35
8	G	102	BCL	C10-C11-C12-C13
8	A	101	BCL	C5-C6-C7-C8
10	I	104	MW9	C18-C19-C20-O2
10	L	309	MW9	C24-C25-C26-C27
10	M	405	MW9	C29-C30-C31-C32
10	L	309	MW9	O5-C21-C22-C23
8	B	101	BCL	C4-C3-C5-C6
8	P	101	BCL	C2C-C3C-CAC-CBC
8	P	102	BCL	C2C-C3C-CAC-CBC
8	S	101	BCL	C2C-C3C-CAC-CBC
8	r	101	BCL	C2C-C3C-CAC-CBC
8	n	101	BCL	C2C-C3C-CAC-CBC
8	D	101	BCL	C2C-C3C-CAC-CBC
8	A	101	BCL	C2C-C3C-CAC-CBC
8	L	306	BCL	C2C-C3C-CAC-CBC

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
8	G	101	BCL	C15-C16-C17-C18
8	N	101	BCL	O1A-CGA-O2A-C1
10	D	102	MW9	O-C17-O1-C18
10	H	302	MW9	C9-C10-C11-C12
8	M	402	BCL	C3-C5-C6-C7
10	G	103	MW9	C4-C5-C6-C7
10	D	102	MW9	O1-C18-C19-C20
10	D	103	MW9	O1-C18-C19-C20
15	H	303	CDL	C62-C63-C64-C65
8	n	101	BCL	C15-C16-C17-C18
10	M	406	MW9	C12-C13-C14-C15
13	L	301	LMT	C5'-C4'-O1B-C1B
10	M	406	MW9	C35-C36-C37-C38
10	M	405	MW9	O7-C22-C23-O6
10	I	104	MW9	C29-C30-C31-C32
10	H	302	MW9	C29-C30-C31-C32
10	D	103	MW9	C14-C15-C16-C17
8	e	102	BCL	C16-C17-C18-C20
8	s	101	BCL	C15-C16-C17-C18
8	l	102	BCL	C15-C16-C17-C18
13	L	301	LMT	C4B-C5B-C6B-O6B
15	H	303	CDL	CA6-CA4-OA6-CA5
10	G	103	MW9	C9-C10-C11-C12
10	D	102	MW9	C3-C4-C5-C6
8	n	101	BCL	C13-C15-C16-C17
10	M	406	MW9	C22-C21-O5-P
8	L	306	BCL	CBA-CGA-O2A-C1
10	H	302	MW9	C16-C17-O1-C18
10	M	406	MW9	O8-C19-C20-O2
8	k	101	BCL	C10-C11-C12-C13
8	G	102	BCL	C5-C6-C7-C8
8	F	102	BCL	C5-C6-C7-C8
9	l	104	A1EFU	CM1-C1-O1-CMA
13	L	301	LMT	C2'-C1'-O1'-C1
10	Q	104	MW9	O1-C18-C19-O8
8	P	102	BCL	C15-C16-C17-C18
8	K	101	BCL	C5-C6-C7-C8
8	i	101	BCL	C4-C3-C5-C6
9	Q	102	A1EFU	CM8-C26-C27-C28
10	I	104	MW9	C26-C27-C28-C29
8	v	101	BCL	C11-C12-C13-C15
8	t	101	BCL	C2-C3-C5-C6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
8	s	101	BCL	C11-C12-C13-C15
8	R	102	BCL	C6-C7-C8-C10
8	l	102	BCL	C11-C10-C8-C7
8	N	101	BCL	C6-C7-C8-C10
8	j	101	BCL	C6-C7-C8-C10
8	j	101	BCL	C11-C10-C8-C7
8	J	101	BCL	C6-C7-C8-C10
8	F	102	BCL	C6-C7-C8-C10
8	d	101	BCL	C11-C10-C8-C7
8	a	102	BCL	C2-C3-C5-C6
8	a	102	BCL	C11-C10-C8-C7
8	M	402	BCL	C11-C10-C8-C7
8	L	303	BCL	C11-C12-C13-C15
8	L	306	BCL	C6-C7-C8-C10
8	D	101	BCL	C3-C5-C6-C7
8	v	101	BCL	C11-C12-C13-C14
8	s	101	BCL	C11-C12-C13-C14
8	l	102	BCL	C11-C10-C8-C9
8	l	103	BCL	C11-C10-C8-C9
8	n	101	BCL	C14-C13-C15-C16
8	j	101	BCL	C11-C10-C8-C9
8	j	101	BCL	C11-C12-C13-C14
8	G	101	BCL	C6-C7-C8-C9
8	F	102	BCL	C6-C7-C8-C9
8	d	101	BCL	C11-C10-C8-C9
8	D	101	BCL	C6-C7-C8-C9
8	a	102	BCL	C11-C10-C8-C9
9	Q	103	A1EFU	C14-C15-C16-C17
8	D	101	BCL	C10-C11-C12-C13
15	H	303	CDL	C15-C16-C17-C18
15	L	311	CDL	CA7-C31-C32-C33
10	M	405	MW9	C4-C5-C6-C7
8	S	101	BCL	C15-C16-C17-C18
8	d	101	BCL	C5-C6-C7-C8
10	F	104	MW9	C18-C19-C20-O2
9	2	102	A1EFU	C26-C27-C28-C29
9	e	101	A1EFU	C22-C23-C24-C25
9	A	102	A1EFU	C22-C23-C24-C25
12	M	404	U10	C14-C16-C17-C18
12	M	404	U10	C29-C31-C32-C33
9	v	103	A1EFU	CM8-C26-C27-C28
8	d	101	BCL	C2-C3-C5-C6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
8	B	101	BCL	C2-C3-C5-C6
14	L	304	BPH	C2-C3-C5-C6
9	N	102	A1EFU	C2-C3-C4-C5
10	M	405	MW9	C14-C15-C16-C17
8	J	101	BCL	C5-C6-C7-C8
8	B	101	BCL	C10-C11-C12-C13
14	L	302	BPH	C8-C10-C11-C12
15	H	303	CDL	C40-C41-C42-C43
8	r	101	BCL	C3-C5-C6-C7
10	M	405	MW9	C6-C7-C8-C9
15	H	303	CDL	C54-C55-C56-C57
10	I	104	MW9	C22-C21-O5-P
9	a	103	A1EFU	C13-C14-C15-C16
13	C	404	LMT	C2-C1-O1'-C1'
10	Q	104	MW9	C35-C36-C37-C38
10	I	104	MW9	O1-C18-C19-C20
10	M	405	MW9	O1-C18-C19-C20
10	M	405	MW9	C26-C27-C28-C29
10	H	302	MW9	O-C17-O1-C18
8	S	101	BCL	C4-C3-C5-C6
8	P	102	BCL	C16-C17-C18-C20
8	i	101	BCL	C2-C3-C5-C6
8	N	101	BCL	C15-C16-C17-C18
10	M	405	MW9	C21-O5-P-O2
8	P	101	BCL	O1A-CGA-O2A-C1
15	H	303	CDL	C13-C14-C15-C16
10	L	310	MW9	O8-C19-C20-O2
10	D	103	MW9	C13-C14-C15-C16
10	F	104	MW9	C14-C15-C16-C17
10	F	103	MW9	O1-C18-C19-O8
15	L	311	CDL	OA6-CA4-CA6-OA8
10	Q	104	MW9	C31-C32-C33-C34
8	T	102	BCL	C5-C6-C7-C8
8	k	101	BCL	C5-C6-C7-C8
8	j	101	BCL	C10-C11-C12-C13
15	H	303	CDL	CA2-C1-CB2-OB2
8	P	101	BCL	C2-C1-O2A-CGA
8	r	101	BCL	C2-C1-O2A-CGA
8	a	102	BCL	C2-C1-O2A-CGA
8	v	101	BCL	C6-C7-C8-C9
8	l	103	BCL	C6-C7-C8-C9
8	A	101	BCL	C11-C10-C8-C9

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
8	M	402	BCL	C6-C7-C8-C9
8	M	402	BCL	C11-C10-C8-C9
10	D	103	MW9	C7-C8-C9-C10
10	D	103	MW9	C22-C21-O5-P
15	L	311	CDL	C1-CB2-OB2-PB2
8	T	102	BCL	C2A-CAA-CBA-CGA
8	a	102	BCL	C8-C10-C11-C12
9	s	102	A1EFU	CM1-C1-C2-O2
10	M	405	MW9	C7-C8-C9-C10
8	t	101	BCL	C4C-C3C-CAC-CBC
8	N	101	BCL	C5-C6-C7-C8
10	M	405	MW9	C11-C12-C13-C14
10	H	302	MW9	C32-C33-C34-C35
10	L	310	MW9	C29-C30-C31-C32
10	H	302	MW9	C18-C19-C20-O2
10	I	104	MW9	O5-C21-C22-O7
8	V	101	BCL	C2-C3-C5-C6
8	v	101	BCL	C6-C7-C8-C10
8	1	103	BCL	C2-C3-C5-C6
8	1	103	BCL	C6-C7-C8-C10
8	1	103	BCL	C11-C10-C8-C7
8	j	101	BCL	C11-C12-C13-C15
8	i	101	BCL	C6-C7-C8-C10
8	i	101	BCL	C11-C10-C8-C7
8	d	101	BCL	C6-C7-C8-C10
8	A	101	BCL	C11-C10-C8-C7
8	L	306	BCL	C12-C13-C15-C16
9	J	102	A1EFU	C25-C26-C27-C28
14	L	302	BPH	C6-C7-C8-C10
10	M	406	MW9	C32-C33-C34-C35
8	b	101	BCL	C1-C2-C3-C4
9	s	102	A1EFU	C15-C16-C17-C18
10	L	310	MW9	C27-C28-C29-C30
8	S	101	BCL	C2A-CAA-CBA-CGA
10	L	309	MW9	C25-C24-O8-C19
10	H	302	MW9	C25-C26-C27-C28
8	L	306	BCL	CAD-CBD-CGD-O2D
15	L	311	CDL	CA6-CA4-OA6-CA5
13	H	301	LMT	O5'-C1'-O1'-C1
10	G	103	MW9	O1-C18-C19-C20
10	F	104	MW9	C19-C20-O2-P
15	L	311	CDL	CB3-CB4-CB6-OB8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
10	F	104	MW9	O8-C19-C20-O2
10	H	302	MW9	O8-C19-C20-O2
15	H	303	CDL	OA5-CA3-CA4-OA6
8	V	101	BCL	C16-C17-C18-C20
8	d	101	BCL	C16-C17-C18-C20
10	L	309	MW9	O9-C24-O8-C19
8	P	102	BCL	CHA-CBD-CGD-O1D
8	P	102	BCL	CHA-CBD-CGD-O2D
8	1	102	BCL	CHA-CBD-CGD-O1D
8	1	102	BCL	CHA-CBD-CGD-O2D
8	K	101	BCL	CHA-CBD-CGD-O1D
8	K	101	BCL	CHA-CBD-CGD-O2D
8	G	101	BCL	CHA-CBD-CGD-O1D
8	F	101	BCL	CHA-CBD-CGD-O1D
8	F	101	BCL	CHA-CBD-CGD-O2D
8	d	101	BCL	CHA-CBD-CGD-O1D
10	F	103	MW9	C27-C28-C29-C30
15	H	303	CDL	C79-C80-C81-C82
9	S	102	A1EFU	CM2-C1-O1-CMA
9	1	104	A1EFU	CM2-C1-O1-CMA
9	F	105	A1EFU	CM1-C1-O1-CMA
9	E	102	A1EFU	CM1-C1-O1-CMA
9	A	102	A1EFU	CM2-C1-O1-CMA
10	D	103	MW9	O1-C18-C19-O8
10	M	406	MW9	O1-C18-C19-O8
10	L	310	MW9	O1-C18-C19-O8
15	L	311	CDL	OB6-CB4-CB6-OB8
8	b	101	BCL	C13-C15-C16-C17
8	B	101	BCL	O1A-CGA-O2A-C1
10	F	104	MW9	O7-C22-C23-O6
10	F	103	MW9	C12-C13-C14-C15
10	Q	104	MW9	C29-C30-C31-C32
10	F	103	MW9	C29-C30-C31-C32
8	D	101	BCL	C4-C3-C5-C6
9	A	102	A1EFU	CM7-C22-C23-C24
13	C	404	LMT	C5-C6-C7-C8
15	L	311	CDL	C56-C57-C58-C59
8	s	101	BCL	O1A-CGA-O2A-C1
8	1	102	BCL	C2-C3-C5-C6
8	1	102	BCL	C6-C7-C8-C9
8	i	101	BCL	C11-C10-C8-C9
8	d	101	BCL	C6-C7-C8-C9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
8	L	306	BCL	C14-C13-C15-C16
10	Q	104	MW9	C26-C27-C28-C29
9	J	102	A1EFU	O1-C1-C2-O2
10	F	103	MW9	C21-C22-C23-O6
8	L	303	BCL	C8-C10-C11-C12
8	j	101	BCL	C1A-C2A-CAA-CBA
8	I	102	BCL	C1A-C2A-CAA-CBA
8	D	101	BCL	C1A-C2A-CAA-CBA
8	b	101	BCL	C1A-C2A-CAA-CBA
10	L	309	MW9	C20-O2-P-O5
8	S	101	BCL	C3-C5-C6-C7
10	F	103	MW9	C22-C21-O5-P
10	H	302	MW9	C19-C20-O2-P
15	H	303	CDL	C1-CA2-OA2-PA1
10	I	104	MW9	C25-C26-C27-C28
10	G	103	MW9	C21-O5-P-O3
10	F	104	MW9	C21-O5-P-O4
10	D	103	MW9	C20-O2-P-O3
10	L	309	MW9	C21-O5-P-O4
10	L	310	MW9	C20-O2-P-O3
10	L	310	MW9	C20-O2-P-O4
10	L	310	MW9	C21-O5-P-O3
15	H	303	CDL	CB3-OB5-PB2-OB4
8	e	102	BCL	C16-C17-C18-C19
8	R	102	BCL	C5-C6-C7-C8
10	F	103	MW9	C18-C19-C20-O2
10	M	406	MW9	C18-C19-C20-O2
15	H	303	CDL	OA5-CA3-CA4-CA6
8	K	101	BCL	CAD-CBD-CGD-O1D
8	J	101	BCL	CAD-CBD-CGD-O1D
8	i	101	BCL	CAD-CBD-CGD-O1D
8	F	102	BCL	CAD-CBD-CGD-O1D
8	d	101	BCL	CAD-CBD-CGD-O1D
8	s	101	BCL	C8-C10-C11-C12
8	j	101	BCL	C3-C5-C6-C7
8	G	102	BCL	C8-C10-C11-C12
10	G	103	MW9	C29-C30-C31-C32
10	M	406	MW9	C29-C30-C31-C32
10	L	310	MW9	C14-C15-C16-C17
10	H	302	MW9	C19-C18-O1-C17
13	L	308	LMT	C3-C4-C5-C6
10	M	405	MW9	C25-C26-C27-C28

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
10	L	310	MW9	C26-C27-C28-C29
8	L	303	BCL	C16-C17-C18-C20
9	D	104	A1EFU	CM7-C22-C23-C24
9	M	407	A1EFU	CM8-C26-C27-C28
8	P	102	BCL	C12-C13-C15-C16
8	s	101	BCL	C2C-C3C-CAC-CBC
8	Q	101	BCL	C11-C10-C8-C7
8	r	101	BCL	C6-C7-C8-C10
8	q	101	BCL	C2C-C3C-CAC-CBC
8	q	101	BCL	C6-C7-C8-C10
8	n	101	BCL	C12-C13-C15-C16
8	j	101	BCL	C3A-C2A-CAA-CBA
8	G	101	BCL	C2C-C3C-CAC-CBC
8	b	101	BCL	C11-C12-C13-C15
8	a	102	BCL	C6-C7-C8-C10
8	M	403	BCL	C2C-C3C-CAC-CBC
9	T	101	A1EFU	C20-C21-C22-C23
9	R	101	A1EFU	C20-C21-C22-C23
10	Q	104	MW9	O8-C19-C20-O2
10	F	103	MW9	O8-C19-C20-O2
10	M	405	MW9	O8-C19-C20-O2
10	F	103	MW9	C26-C27-C28-C29
9	k	102	A1EFU	C15-C16-C17-C18
8	G	102	BCL	C16-C17-C18-C19
8	a	102	BCL	C15-C16-C17-C18
10	Q	104	MW9	O1-C18-C19-C20
10	M	406	MW9	O1-C18-C19-C20
10	L	310	MW9	O1-C18-C19-C20
10	I	104	MW9	O1-C18-C19-O8
10	D	102	MW9	O1-C18-C19-O8
10	M	405	MW9	O1-C18-C19-O8
14	L	304	BPH	O2A-C1-C2-C3
8	M	402	BCL	O1A-CGA-O2A-C1
8	I	102	BCL	C15-C16-C17-C18
10	D	103	MW9	C3-C4-C5-C6
8	r	101	BCL	C6-C7-C8-C9
8	k	101	BCL	C6-C7-C8-C9
8	b	101	BCL	C11-C12-C13-C14
8	G	102	BCL	O1A-CGA-O2A-C1
10	F	103	MW9	O7-C22-C23-O6
9	G	105	A1EFU	CM2-C1-C2-C3
8	t	101	BCL	C4-C3-C5-C6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
8	F	102	BCL	C2-C3-C5-C6
9	Q	102	A1EFU	C25-C26-C27-C28
10	F	103	MW9	C32-C33-C34-C35
10	F	104	MW9	C32-C33-C34-C35
8	s	101	BCL	C10-C11-C12-C13
8	l	102	BCL	CAA-CBA-CGA-O2A
10	L	310	MW9	C20-C19-O8-C24
10	M	405	MW9	C18-C19-C20-O2
8	k	101	BCL	C2-C1-O2A-CGA
8	G	101	BCL	C2-C1-O2A-CGA
8	A	101	BCL	C2-C1-O2A-CGA
10	M	406	MW9	C19-C20-O2-P
8	D	101	BCL	CBA-CGA-O2A-C1
8	E	101	BCL	C10-C11-C12-C13
9	v	103	A1EFU	C25-C26-C27-C28
9	v	103	A1EFU	CM1-C1-C2-O2
9	r	102	A1EFU	CM1-C1-C2-O2
9	G	105	A1EFU	CM2-C1-C2-O2
8	N	101	BCL	CBA-CGA-O2A-C1
15	H	303	CDL	C73-C74-C75-C76
8	P	102	BCL	C16-C17-C18-C19
9	S	102	A1EFU	C26-C27-C28-C29
12	M	404	U10	C44-C46-C47-C48
15	L	311	CDL	CB2-OB2-PB2-OB5
10	Q	104	MW9	C14-C15-C16-C17
8	l	102	BCL	C16-C17-C18-C19
8	R	102	BCL	C4-C3-C5-C6
8	l	102	BCL	C4-C3-C5-C6
8	N	101	BCL	C2-C3-C5-C6
8	K	101	BCL	C2-C3-C5-C6
8	P	102	BCL	C14-C13-C15-C16
8	Q	101	BCL	C11-C10-C8-C9
8	q	101	BCL	C6-C7-C8-C9
14	L	302	BPH	C6-C7-C8-C9
14	L	304	BPH	C11-C12-C13-C14
8	j	101	BCL	C15-C16-C17-C18
9	l	104	A1EFU	C19-C20-C21-C22
9	N	102	A1EFU	C15-C16-C17-C18
10	G	103	MW9	C36-C37-C38-C39
8	M	402	BCL	C5-C6-C7-C8
10	M	405	MW9	C36-C37-C38-C39
8	j	101	BCL	O1A-CGA-O2A-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
8	a	102	BCL	C5-C6-C7-C8
10	L	309	MW9	C27-C28-C29-C30
8	P	101	BCL	CBA-CGA-O2A-C1
8	s	101	BCL	CBA-CGA-O2A-C1
8	q	101	BCL	CBA-CGA-O2A-C1
8	q	101	BCL	O1A-CGA-O2A-C1
8	d	101	BCL	O1A-CGA-O2A-C1
10	L	309	MW9	C32-C33-C34-C35
8	D	101	BCL	C16-C17-C18-C19
9	Q	103	A1EFU	C19-C20-C21-C22
9	J	103	A1EFU	C13-C14-C15-C16
9	J	103	A1EFU	C15-C16-C17-C18
9	G	104	A1EFU	C9-C10-C11-C12
9	a	103	A1EFU	C5-C6-C7-C8
8	t	101	BCL	C5-C6-C7-C8
15	L	311	CDL	C32-C33-C34-C35
8	s	101	BCL	C3-C5-C6-C7
8	l	103	BCL	C4-C3-C5-C6
9	N	103	A1EFU	CM8-C26-C27-C28
9	v	103	A1EFU	CM1-C1-C2-C3
9	s	102	A1EFU	CM2-C1-C2-C3
9	r	102	A1EFU	CM1-C1-C2-C3
8	A	101	BCL	C15-C16-C17-C18
8	v	101	BCL	C2-C1-O2A-CGA
8	J	101	BCL	C2-C1-O2A-CGA
8	E	101	BCL	C2-C1-O2A-CGA
8	v	101	BCL	C10-C11-C12-C13
8	r	101	BCL	C16-C17-C18-C20
8	K	101	BCL	C16-C17-C18-C19
10	Q	104	MW9	C9-C10-C11-C12
13	H	301	LMT	C2'-C1'-O1'-C1
8	I	102	BCL	C3A-C2A-CAA-CBA
8	d	101	BCL	C16-C17-C18-C19
12	M	404	U10	C5-C4-O4-C4M
9	v	102	A1EFU	C5-C6-C7-C8
9	a	103	A1EFU	C9-C10-C11-C12
9	s	102	A1EFU	CM8-C26-C27-C28
9	v	103	A1EFU	CM2-C1-C2-O2
9	T	101	A1EFU	CM1-C1-C2-O2
9	T	101	A1EFU	CM2-C1-C2-O2
9	r	102	A1EFU	CM2-C1-C2-O2
8	F	101	BCL	C6-C7-C8-C9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
14	L	302	BPH	C14-C13-C15-C16
8	P	101	BCL	C16-C17-C18-C20
8	e	102	BCL	C5-C6-C7-C8
10	I	104	MW9	O5-C21-C22-C23
10	F	103	MW9	C30-C31-C32-C33
8	F	102	BCL	C16-C17-C18-C19
8	R	102	BCL	CBA-CGA-O2A-C1
9	v	102	A1EFU	C26-C27-C28-C29
9	M	407	A1EFU	C22-C23-C24-C25
10	M	405	MW9	C12-C13-C14-C15
10	L	310	MW9	C18-C19-O8-C24
8	v	101	BCL	C5-C6-C7-C8
8	R	102	BCL	C15-C16-C17-C18
8	S	101	BCL	C1A-C2A-CAA-CBA
8	M	402	BCL	C1A-C2A-CAA-CBA
8	S	101	BCL	C11-C12-C13-C15
8	D	101	BCL	C11-C12-C13-C15
14	L	304	BPH	C12-C13-C15-C16
10	D	102	MW9	C11-C10-C9-C8
13	H	301	LMT	C7-C8-C9-C10
8	S	101	BCL	C5-C6-C7-C8
8	1	102	BCL	C2A-CAA-CBA-CGA
8	1	102	BCL	C10-C11-C12-C13
8	V	101	BCL	C16-C17-C18-C19
8	J	101	BCL	C4-C3-C5-C6
12	M	404	U10	C35-C34-C36-C37
16	C	402	HEC	CAA-CBA-CGA-O1A
8	J	101	BCL	C2A-CAA-CBA-CGA
9	N	103	A1EFU	C19-C20-C21-C22
15	H	303	CDL	C42-C43-C44-C45
8	1	102	BCL	C16-C17-C18-C20
9	T	101	A1EFU	C22-C23-C24-C25
9	K	102	A1EFU	C22-C23-C24-C25
8	K	101	BCL	C4-C3-C5-C6
8	G	102	BCL	C4-C3-C5-C6
8	K	101	BCL	C2-C1-O2A-CGA
8	e	102	BCL	C2-C1-O2A-CGA
8	d	101	BCL	C2-C1-O2A-CGA
8	G	102	BCL	C2C-C3C-CAC-CBC
16	C	402	HEC	CAA-CBA-CGA-O2A
10	M	406	MW9	C26-C27-C28-C29
9	v	103	A1EFU	CM2-C1-C2-C3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
9	T	101	A1EFU	CM1-C1-C2-C3
9	T	101	A1EFU	CM2-C1-C2-C3
9	r	102	A1EFU	CM2-C1-C2-C3
9	J	102	A1EFU	CM2-C1-C2-C3
9	G	104	A1EFU	CM2-C1-C2-C3
9	F	105	A1EFU	C27-C28-C29-C30
8	E	101	BCL	C2A-CAA-CBA-CGA
8	J	101	BCL	C16-C17-C18-C19
8	L	306	BCL	O1A-CGA-O2A-C1
9	R	101	A1EFU	CM1-C1-C2-O2
9	J	102	A1EFU	CM2-C1-C2-O2
8	i	101	BCL	C8-C10-C11-C12
9	2	101	A1EFU	C19-C20-C21-C22
8	T	102	BCL	C4-C3-C5-C6
8	N	101	BCL	C4-C3-C5-C6
9	2	101	A1EFU	CM7-C22-C23-C24
8	t	101	BCL	C16-C17-C18-C20
15	L	311	CDL	C53-C54-C55-C56
9	s	102	A1EFU	C14-C15-C16-C17
14	L	304	BPH	C16-C17-C18-C20
8	I	102	BCL	C8-C10-C11-C12
8	I	102	BCL	CBA-CGA-O2A-C1
10	M	406	MW9	C3-C4-C5-C6
8	F	101	BCL	C3-C5-C6-C7
8	G	102	BCL	C16-C17-C18-C20
8	d	101	BCL	C13-C15-C16-C17
13	L	301	LMT	C2-C3-C4-C5
10	Q	104	MW9	C18-C19-C20-O2
8	r	101	BCL	C4-C3-C5-C6
8	G	101	BCL	C4-C3-C5-C6
8	F	102	BCL	C4-C3-C5-C6
9	J	103	A1EFU	CM7-C22-C23-C24
12	L	305	U10	C15-C14-C16-C17
8	J	101	BCL	C2-C3-C5-C6
8	G	102	BCL	C2-C3-C5-C6
8	b	101	BCL	C6-C7-C8-C10
9	B	102	A1EFU	C21-C22-C23-C24
12	M	404	U10	C33-C34-C36-C37
8	S	101	BCL	C1-C2-C3-C4
8	I	102	BCL	C1-C2-C3-C4
8	b	101	BCL	CAA-CBA-CGA-O2A
8	r	101	BCL	O1A-CGA-O2A-C1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
10	I	104	MW9	O8-C24-C25-C26
9	K	102	A1EFU	C2-C3-C4-C5
8	F	101	BCL	C8-C10-C11-C12
15	L	311	CDL	C34-C35-C36-C37
9	a	103	A1EFU	C11-C10-C9-CM4
8	n	101	BCL	C4-C3-C5-C6
8	k	101	BCL	C4-C3-C5-C6
8	M	402	BCL	C4-C3-C5-C6
9	E	102	A1EFU	CM7-C22-C23-C24
8	v	101	BCL	C2-C3-C5-C6
8	D	101	BCL	C2-C3-C5-C6
9	M	407	A1EFU	C25-C26-C27-C28
8	S	101	BCL	C11-C12-C13-C14
8	D	101	BCL	C11-C12-C13-C14
10	M	406	MW9	C31-C32-C33-C34
13	L	307	LMT	C4-C5-C6-C7
8	D	101	BCL	C3A-C2A-CAA-CBA
10	G	103	MW9	C32-C33-C34-C35
8	E	101	BCL	CAD-CBD-CGD-O2D
14	L	302	BPH	CAD-CBD-CGD-O2D
9	K	102	A1EFU	C15-C16-C17-C18
8	L	303	BCL	C2-C1-O2A-CGA
16	C	403	HEC	CAD-CBD-CGD-O2D
15	H	303	CDL	C53-C54-C55-C56
9	2	102	A1EFU	CM7-C22-C23-C24
9	N	102	A1EFU	CM7-C22-C23-C24
16	C	401	HEC	CAA-CBA-CGA-O1A
8	P	101	BCL	C2-C3-C5-C6
10	F	103	MW9	O1-C18-C19-C20
15	L	311	CDL	CA3-CA4-CA6-OA8
8	Q	101	BCL	C15-C16-C17-C18
8	v	101	BCL	CAA-CBA-CGA-O2A
9	t	102	A1EFU	CM2-C1-C2-O2
9	s	102	A1EFU	CM2-C1-C2-O2
9	G	105	A1EFU	CM1-C1-C2-O2
9	F	105	A1EFU	CM2-C1-C2-O2
9	E	102	A1EFU	CM2-C1-C2-O2
16	C	402	HEC	CAD-CBD-CGD-O1D
16	C	403	HEC	CAD-CBD-CGD-O1D
9	t	102	A1EFU	CM1-C1-C2-C3
9	G	105	A1EFU	CM1-C1-C2-C3
10	Q	104	MW9	C32-C33-C34-C35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
15	H	303	CDL	O1-C1-CB2-OB2
8	J	101	BCL	CHA-CBD-CGD-O1D
8	i	101	BCL	CHA-CBD-CGD-O1D
8	E	101	BCL	CHA-CBD-CGD-O1D
8	d	101	BCL	CHA-CBD-CGD-O2D
8	M	403	BCL	CHA-CBD-CGD-O1D
8	M	403	BCL	CHA-CBD-CGD-O2D
12	L	305	U10	C13-C14-C16-C17
10	L	310	MW9	C18-C19-C20-O2
9	a	103	A1EFU	C11-C10-C9-C8
8	B	101	BCL	C8-C10-C11-C12
8	s	101	BCL	CAA-CBA-CGA-O2A
8	M	403	BCL	CAA-CBA-CGA-O2A
9	l	104	A1EFU	C2-C1-O1-CMA
8	T	102	BCL	C2-C3-C5-C6
8	e	102	BCL	C6-C7-C8-C10
8	B	101	BCL	C6-C7-C8-C10
8	M	403	BCL	C6-C7-C8-C10
9	t	102	A1EFU	C21-C22-C23-C24
10	F	103	MW9	O8-C24-C25-C26
8	I	102	BCL	C3-C5-C6-C7
8	n	101	BCL	C6-C7-C8-C9
8	e	102	BCL	C6-C7-C8-C9
8	j	101	BCL	C8-C10-C11-C12
9	M	407	A1EFU	O1-C1-C2-O2
10	D	103	MW9	C30-C31-C32-C33
10	I	104	MW9	O9-C24-C25-C26
8	q	101	BCL	C5-C6-C7-C8
8	M	403	BCL	O1A-CGA-O2A-C1
8	k	101	BCL	C1A-C2A-CAA-CBA
8	a	102	BCL	C1A-C2A-CAA-CBA
8	b	101	BCL	C16-C17-C18-C20
8	l	102	BCL	C2-C1-O2A-CGA
8	J	101	BCL	C8-C10-C11-C12
10	D	103	MW9	C20-O2-P-O5
8	T	102	BCL	C15-C16-C17-C18
10	I	104	MW9	C19-C20-O2-P
8	R	102	BCL	C2-C3-C5-C6
8	R	102	BCL	C10-C11-C12-C13
10	F	104	MW9	C20-O2-P-O4
10	L	309	MW9	C20-O2-P-O4
15	L	311	CDL	CB2-OB2-PB2-OB3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
15	H	303	CDL	CA3-OA5-PA1-OA3
15	H	303	CDL	CB3-OB5-PB2-OB3
8	M	403	BCL	CAA-CBA-CGA-O1A
10	F	103	MW9	O9-C24-C25-C26
8	F	101	BCL	CAA-CBA-CGA-O1A
8	d	101	BCL	CAA-CBA-CGA-O1A
9	t	102	A1EFU	CM1-C1-C2-O2
8	k	101	BCL	CAA-CBA-CGA-O2A
8	R	102	BCL	C8-C10-C11-C12
8	L	303	BCL	C4-C3-C5-C6
9	v	102	A1EFU	C9-C10-C11-C12
10	I	104	MW9	C11-C12-C13-C14
10	H	302	MW9	C28-C29-C30-C31
9	K	102	A1EFU	C27-C28-C29-C30
8	M	403	BCL	C16-C17-C18-C20
16	C	401	HEC	CAA-CBA-CGA-O2A
8	V	101	BCL	CAD-CBD-CGD-O1D
8	a	102	BCL	CAD-CBD-CGD-O1D
9	t	102	A1EFU	CM2-C1-C2-C3
9	R	101	A1EFU	CM1-C1-C2-C3
9	l	101	A1EFU	CM1-C1-C2-C3
9	F	105	A1EFU	CM2-C1-C2-C3
9	E	102	A1EFU	CM2-C1-C2-C3
10	Q	104	MW9	C18-C19-O8-C24
15	H	303	CDL	C38-C39-C40-C41
10	M	405	MW9	O8-C24-C25-C26
10	L	309	MW9	O8-C24-C25-C26
8	k	101	BCL	O1A-CGA-O2A-C1
8	q	101	BCL	C4-C3-C5-C6
8	Q	101	BCL	C2-C3-C5-C6
8	a	102	BCL	C3A-C2A-CAA-CBA
9	s	102	A1EFU	C25-C26-C27-C28
9	J	102	A1EFU	C20-C21-C22-C23
9	A	102	A1EFU	C20-C21-C22-C23
10	F	104	MW9	O8-C24-C25-C26
10	M	406	MW9	O8-C24-C25-C26
9	F	105	A1EFU	C19-C20-C21-C22
9	d	102	A1EFU	C19-C20-C21-C22
13	H	301	LMT	C2-C1-O1'-C1'
8	r	101	BCL	CAA-CBA-CGA-O2A
10	D	103	MW9	C35-C36-C37-C38
13	C	404	LMT	C6-C7-C8-C9

*Continued on next page...*

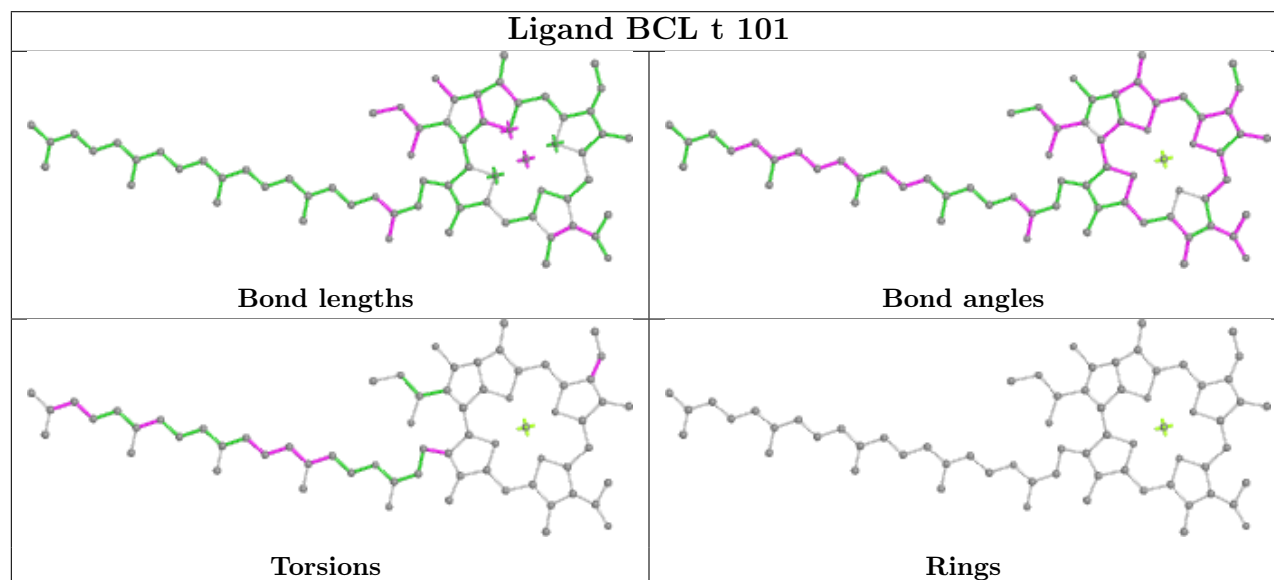
*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
8	v	101	BCL	CAA-CBA-CGA-O1A
10	F	104	MW9	O9-C24-C25-C26
10	M	405	MW9	O9-C24-C25-C26
10	M	406	MW9	O9-C24-C25-C26
8	P	101	BCL	C2A-CAA-CBA-CGA
8	M	402	BCL	C2A-CAA-CBA-CGA
16	C	401	HEC	CAD-CBD-CGD-O1D
8	Q	101	BCL	C5-C6-C7-C8
10	L	309	MW9	O9-C24-C25-C26
9	T	101	A1EFU	CM8-C26-C27-C28
9	1	101	A1EFU	CM8-C26-C27-C28
8	d	101	BCL	CAA-CBA-CGA-O2A

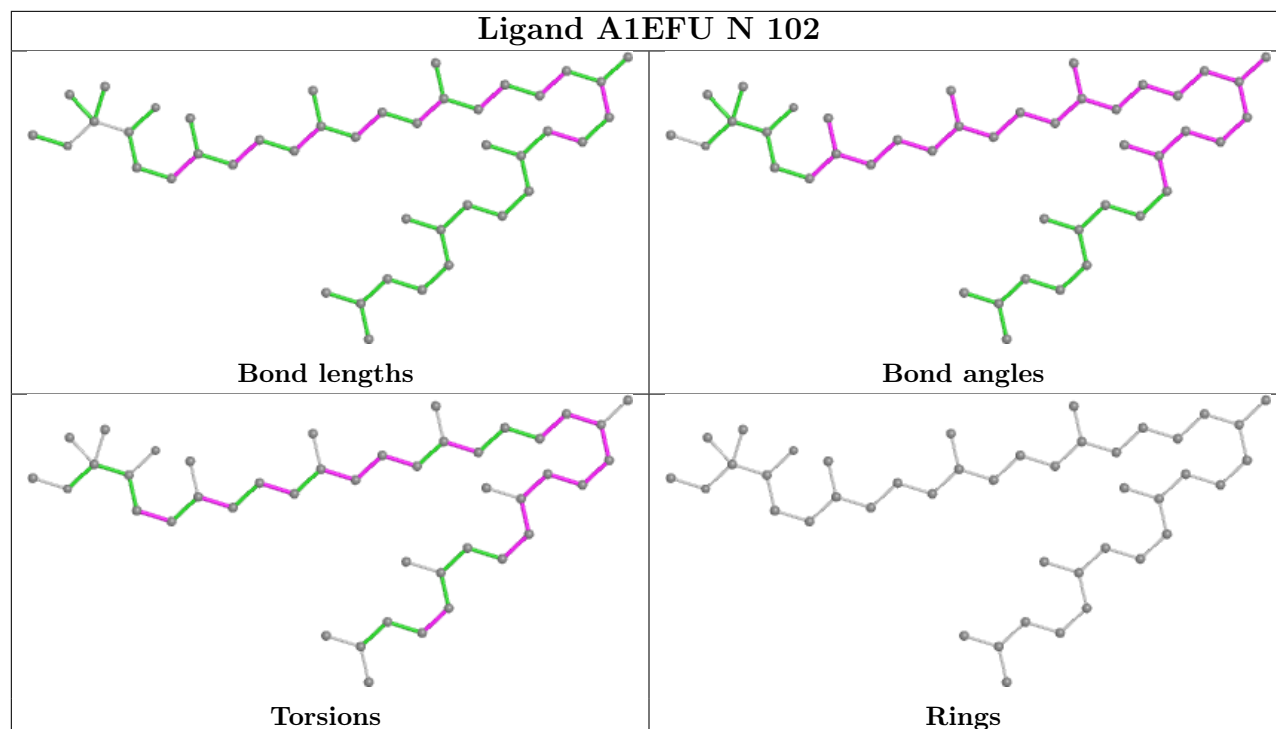
There are no ring outliers.

No monomer is involved in short contacts.

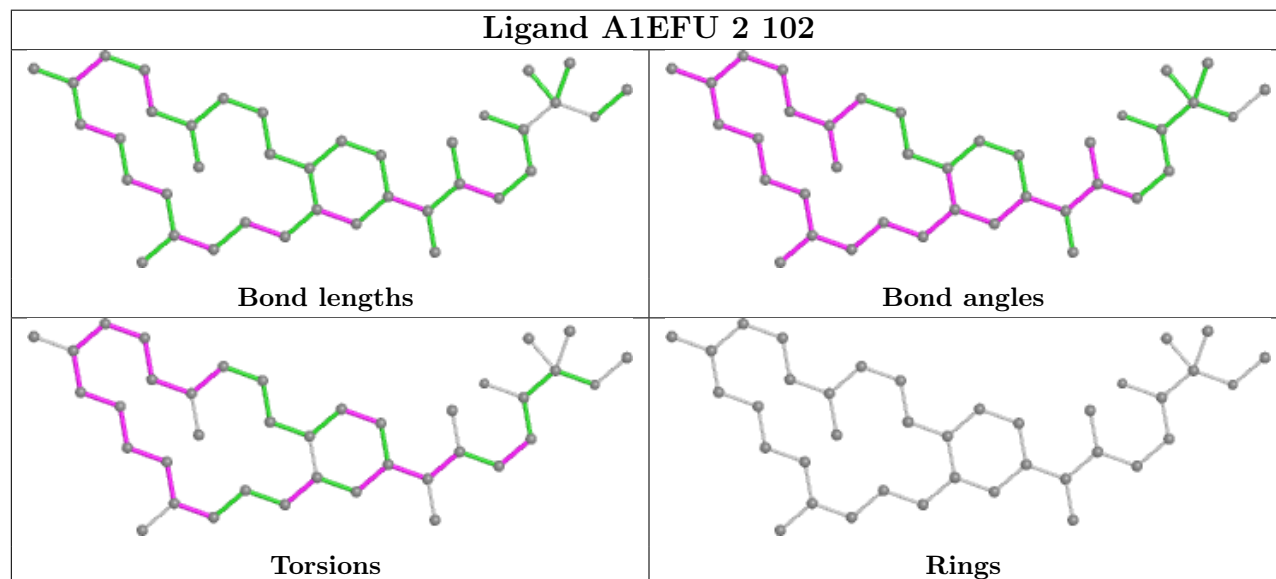
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

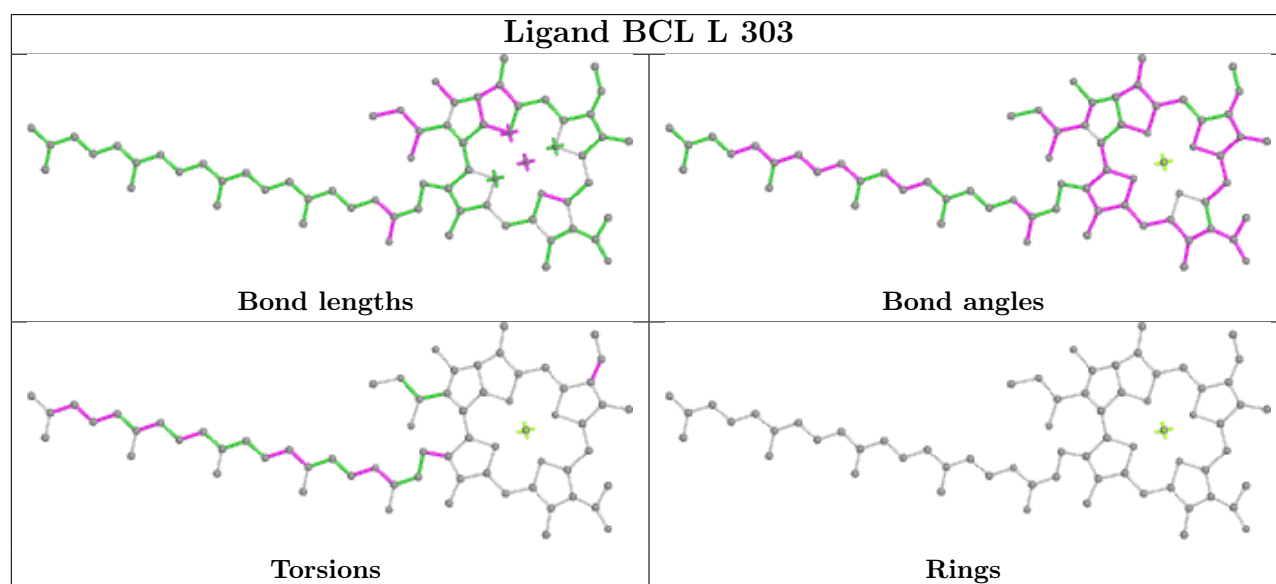
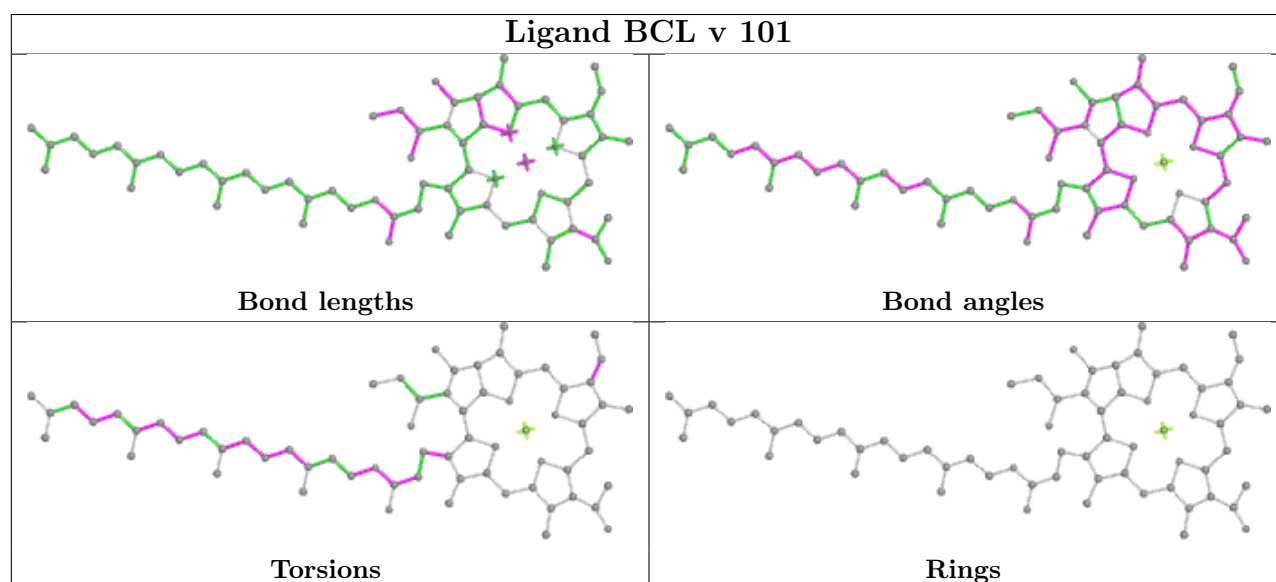
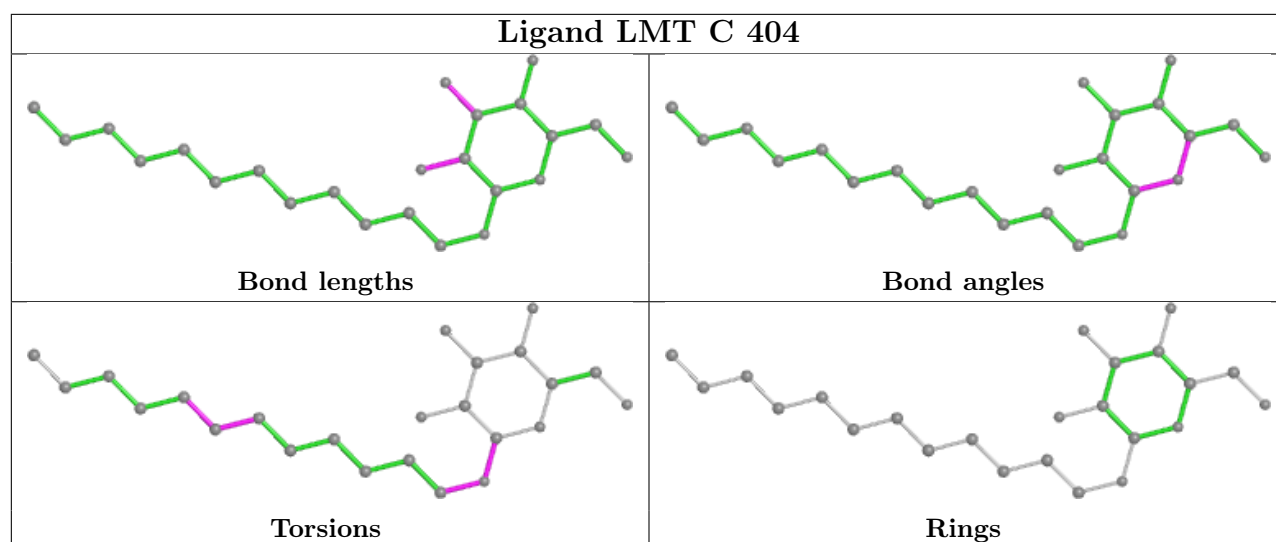


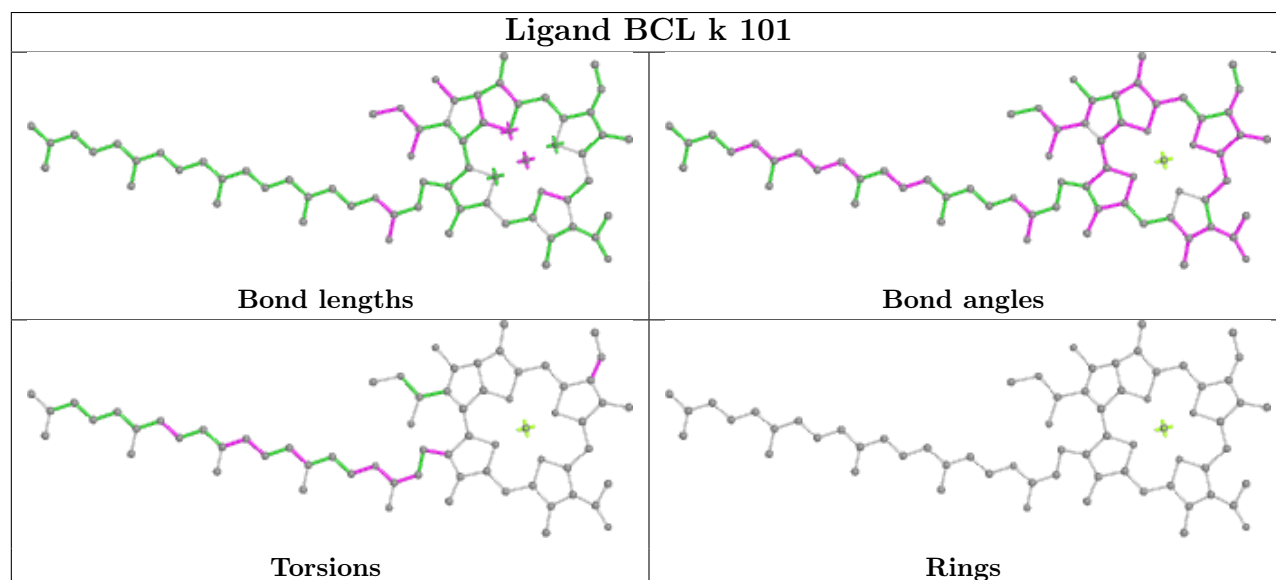
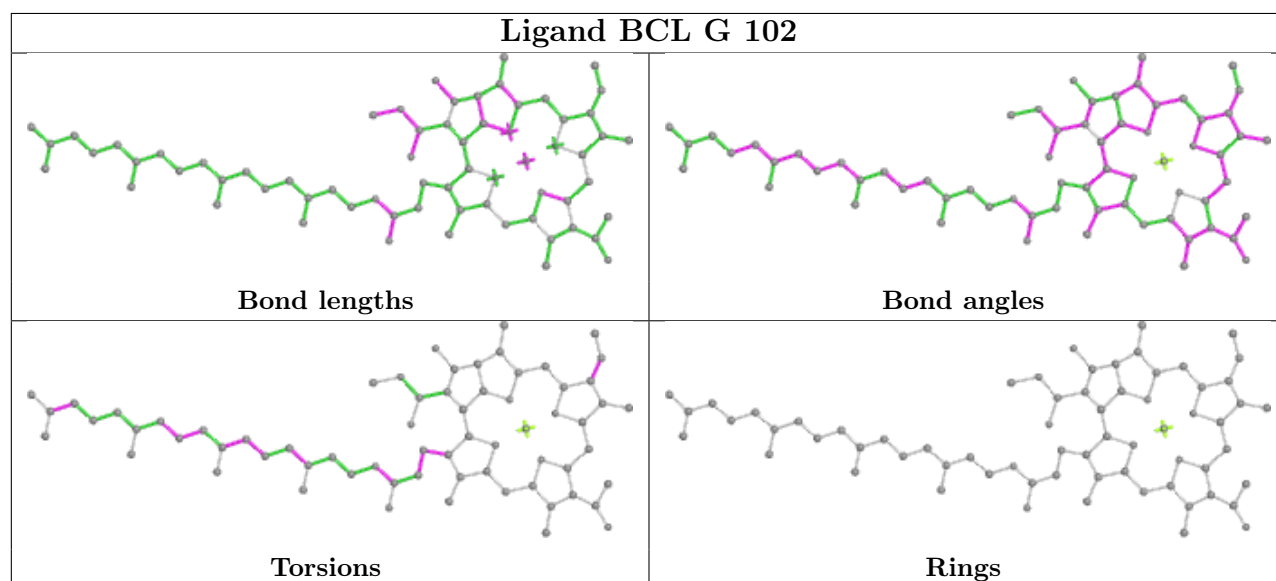
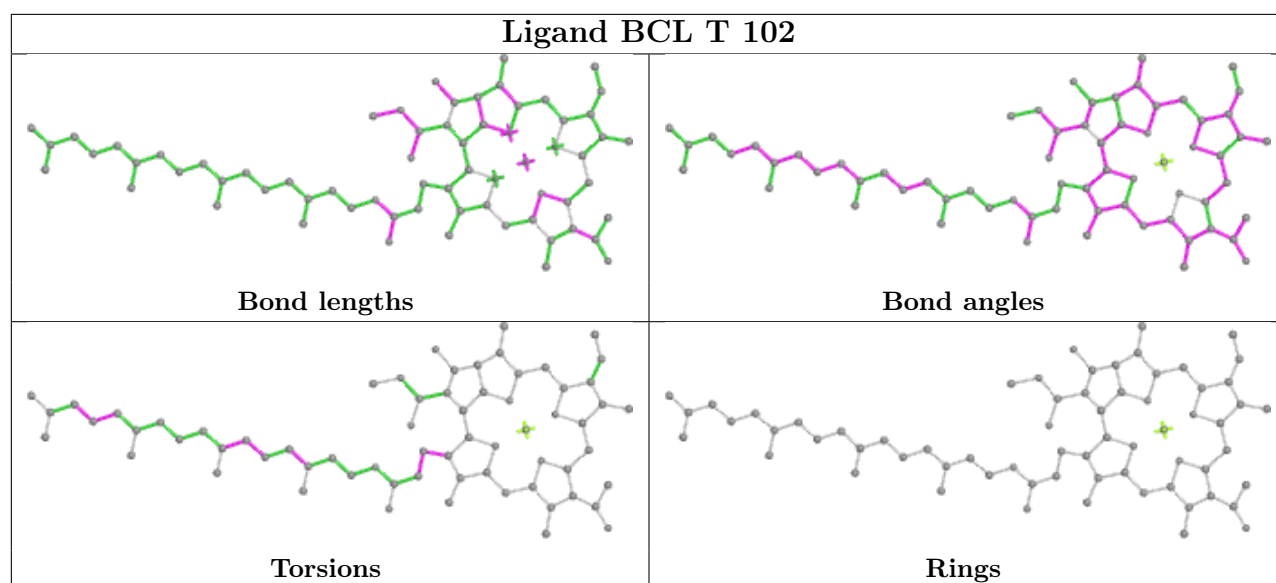
## Ligand A1EFU N 102



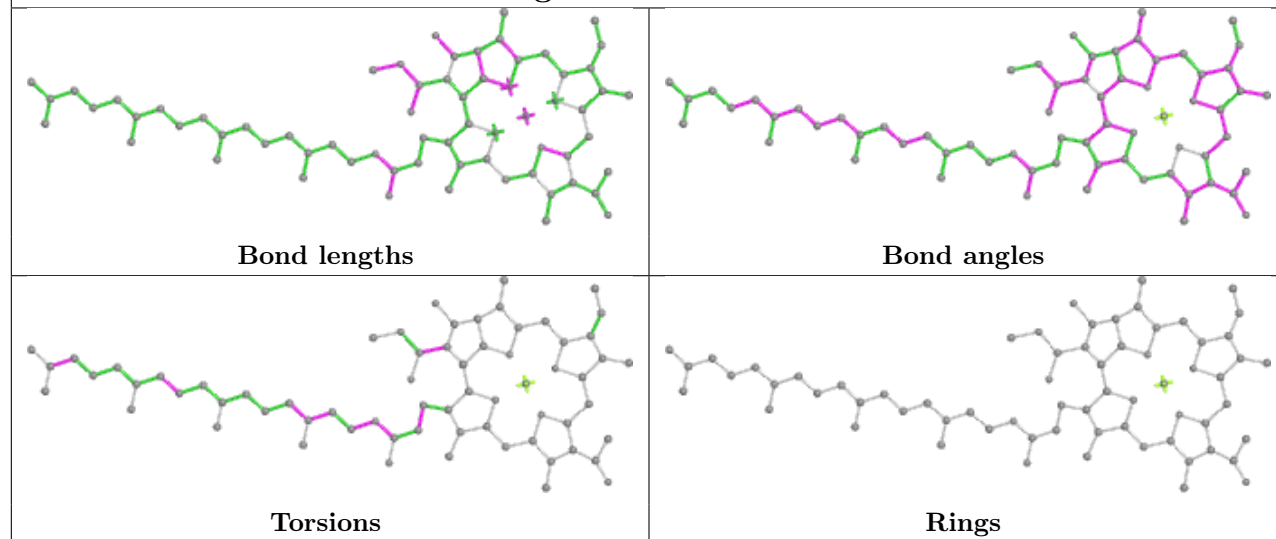
## Ligand A1EFU 2 102



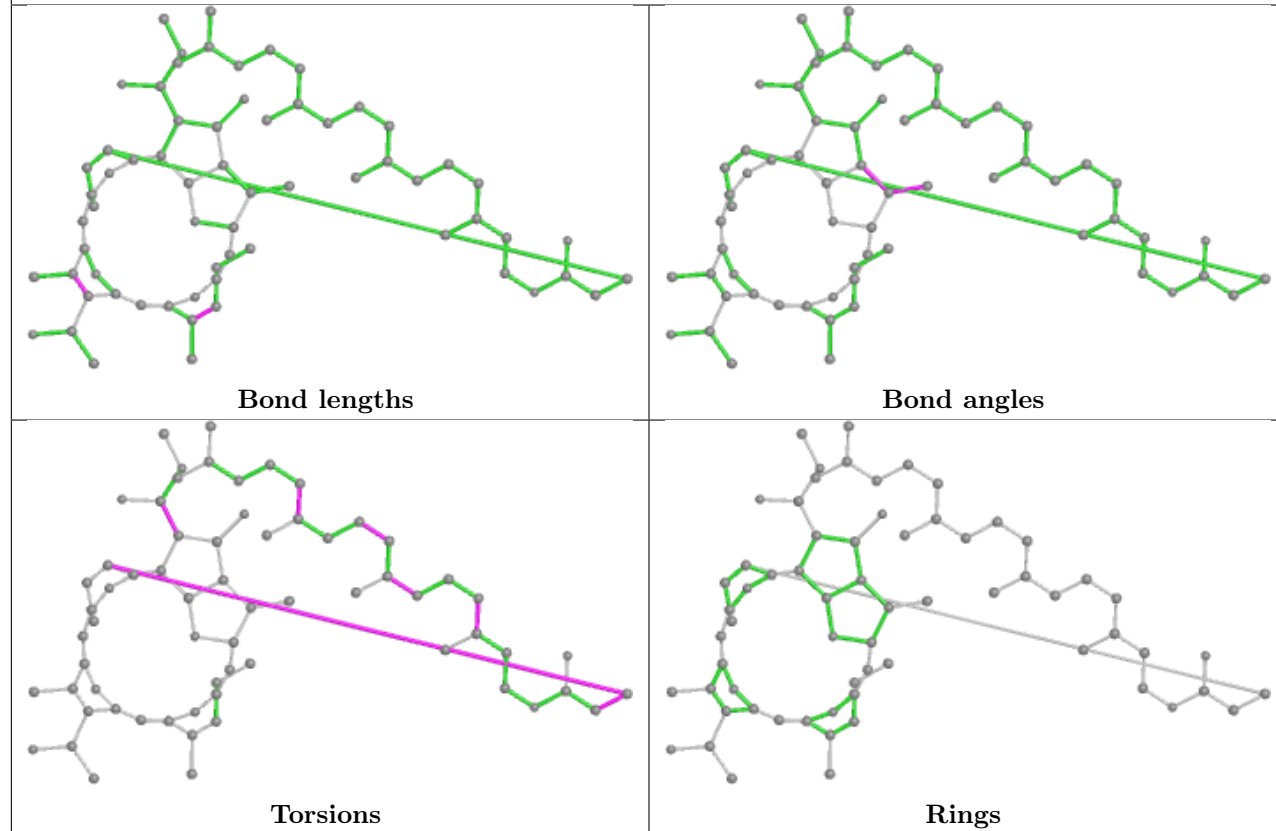




## Ligand BCL E 101

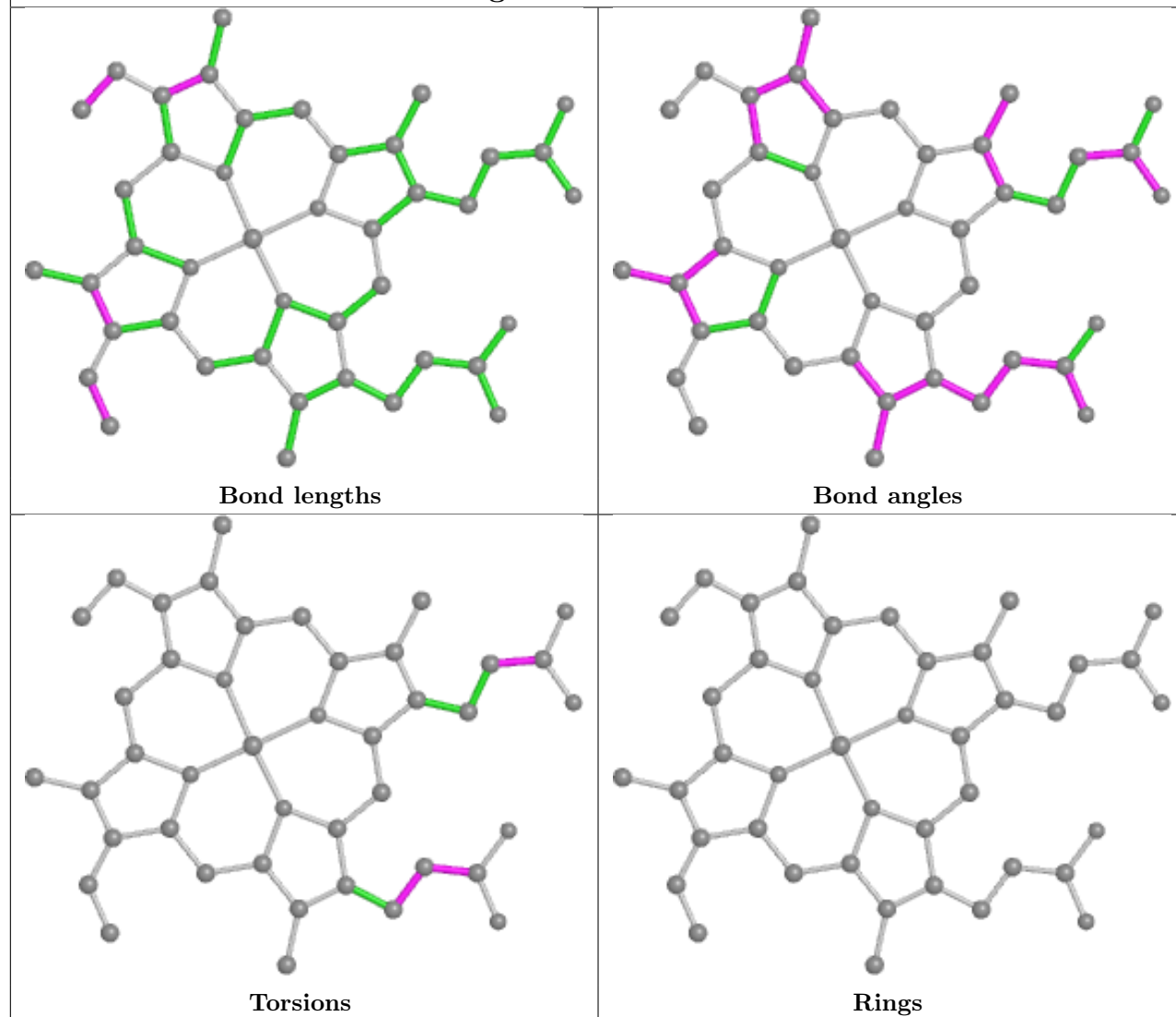


## Ligand BPH L 302

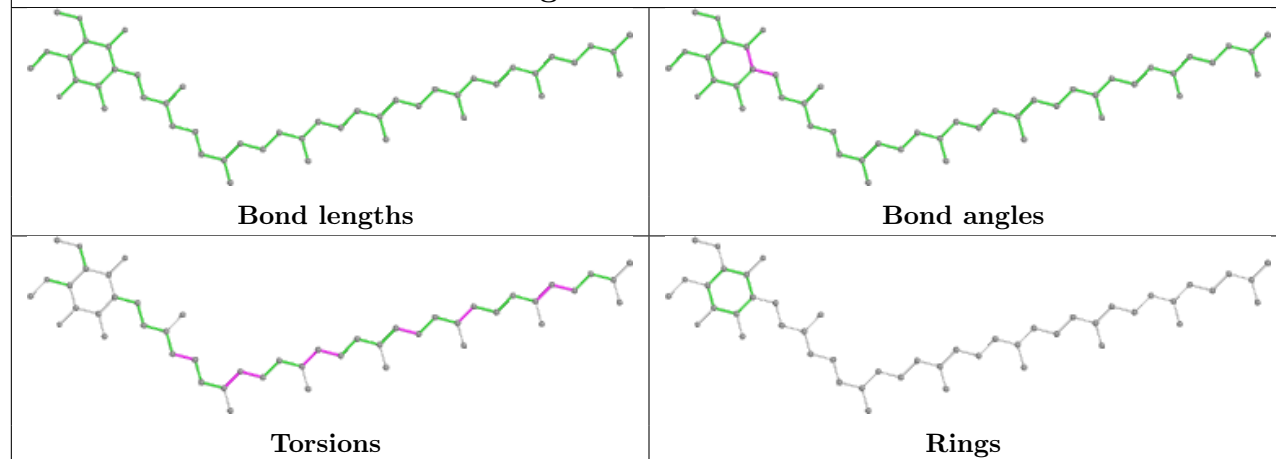


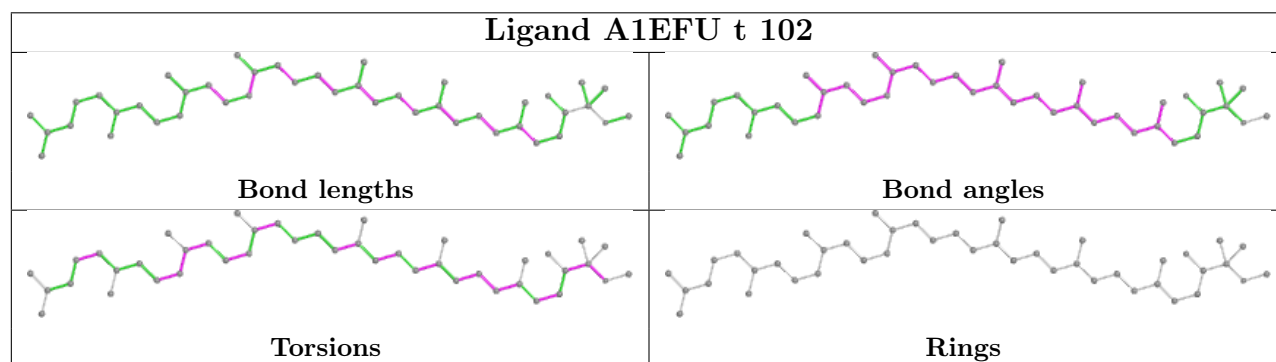
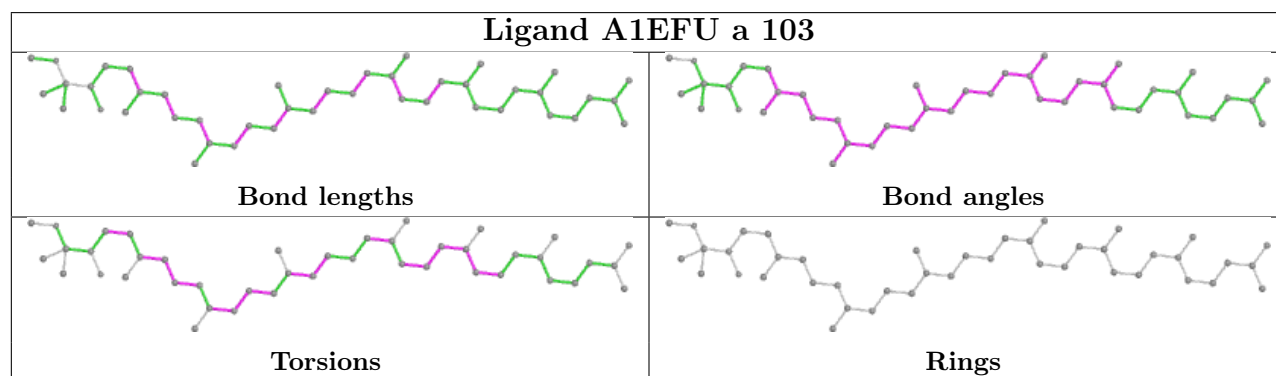
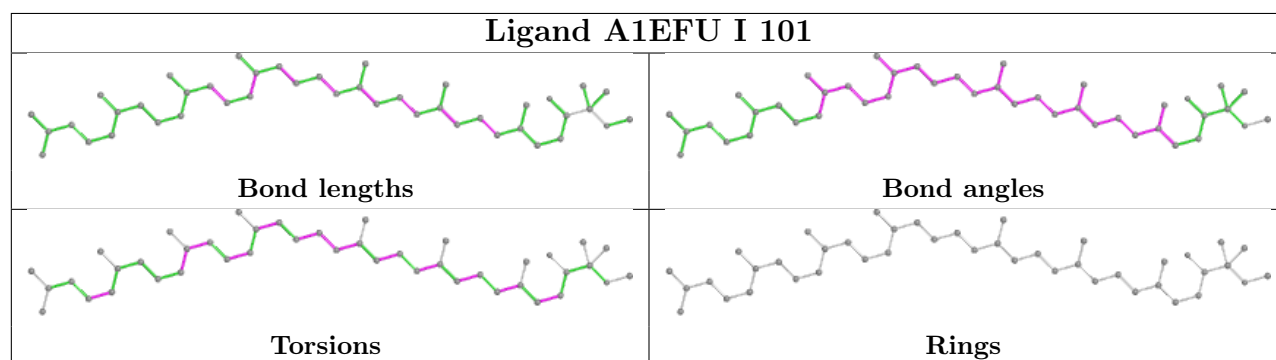
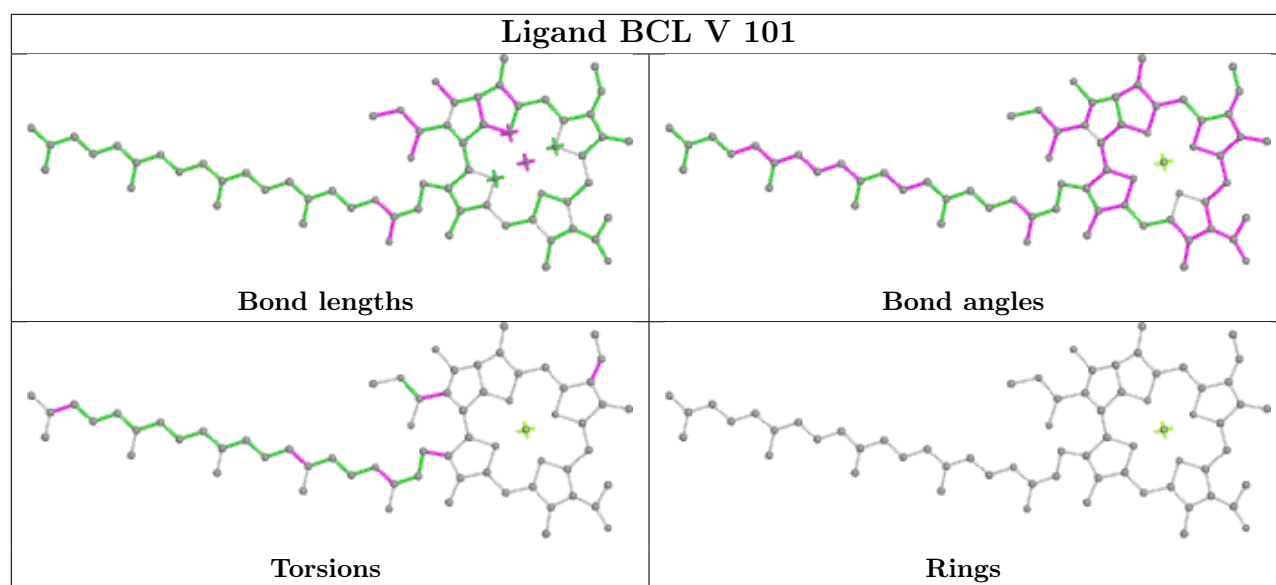


## Ligand HEC C 401

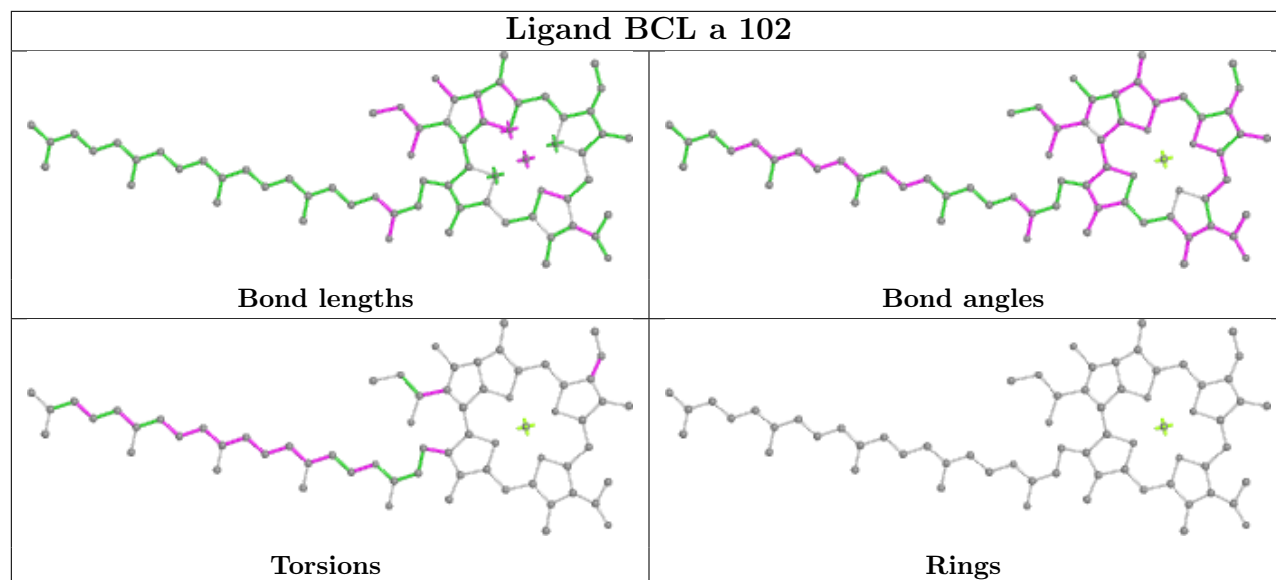


## Ligand U10 L 305

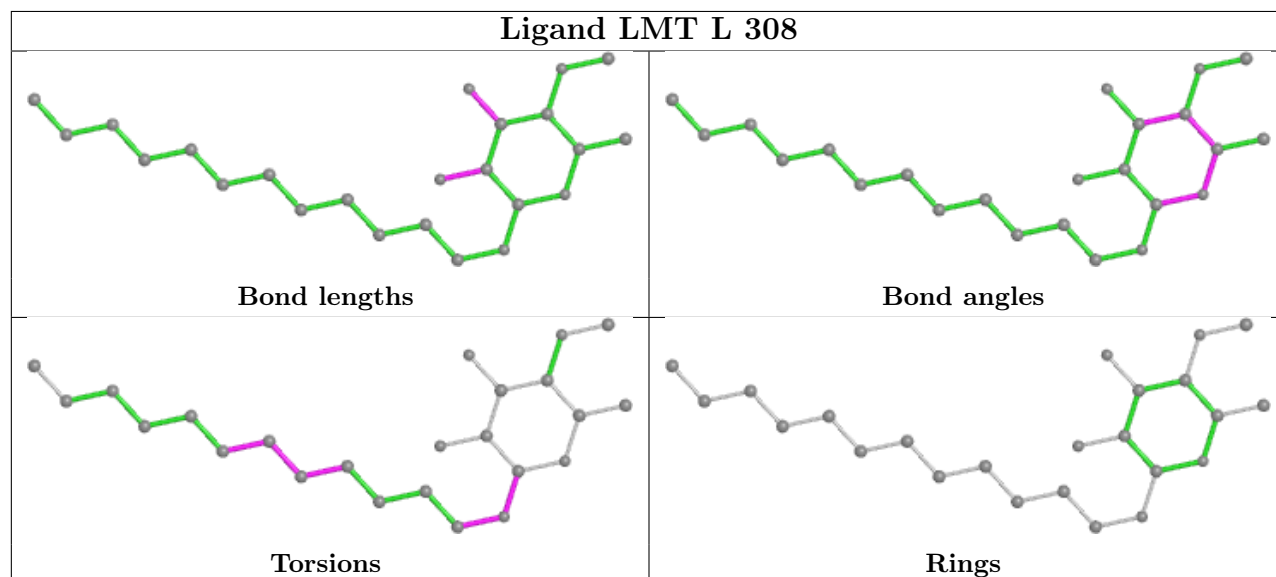




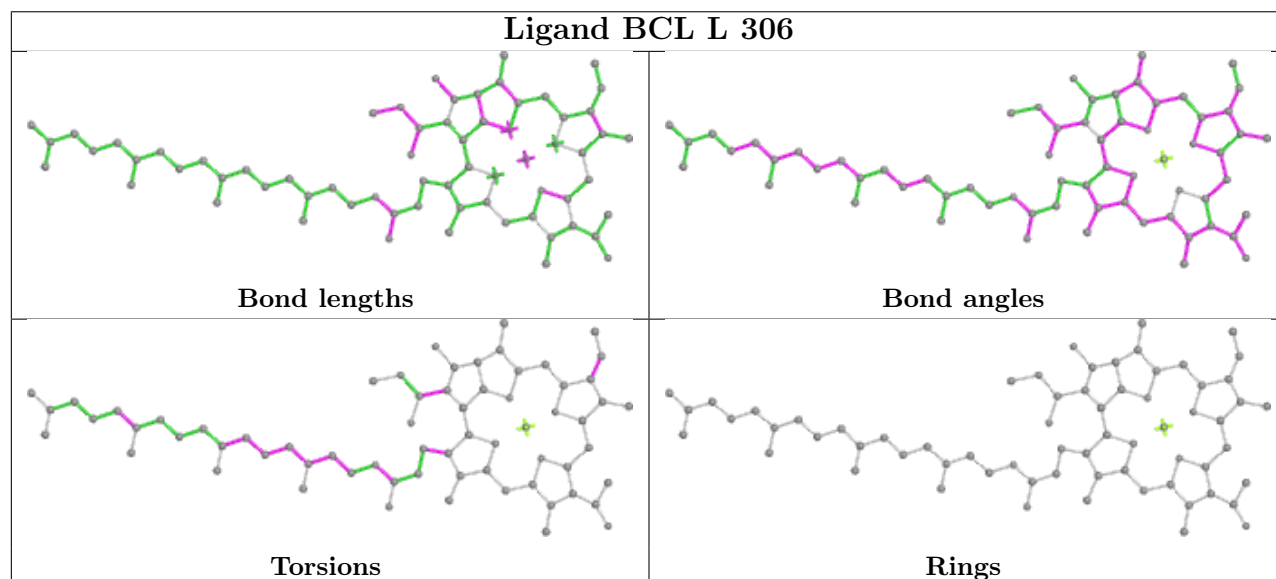
## Ligand BCL a 102

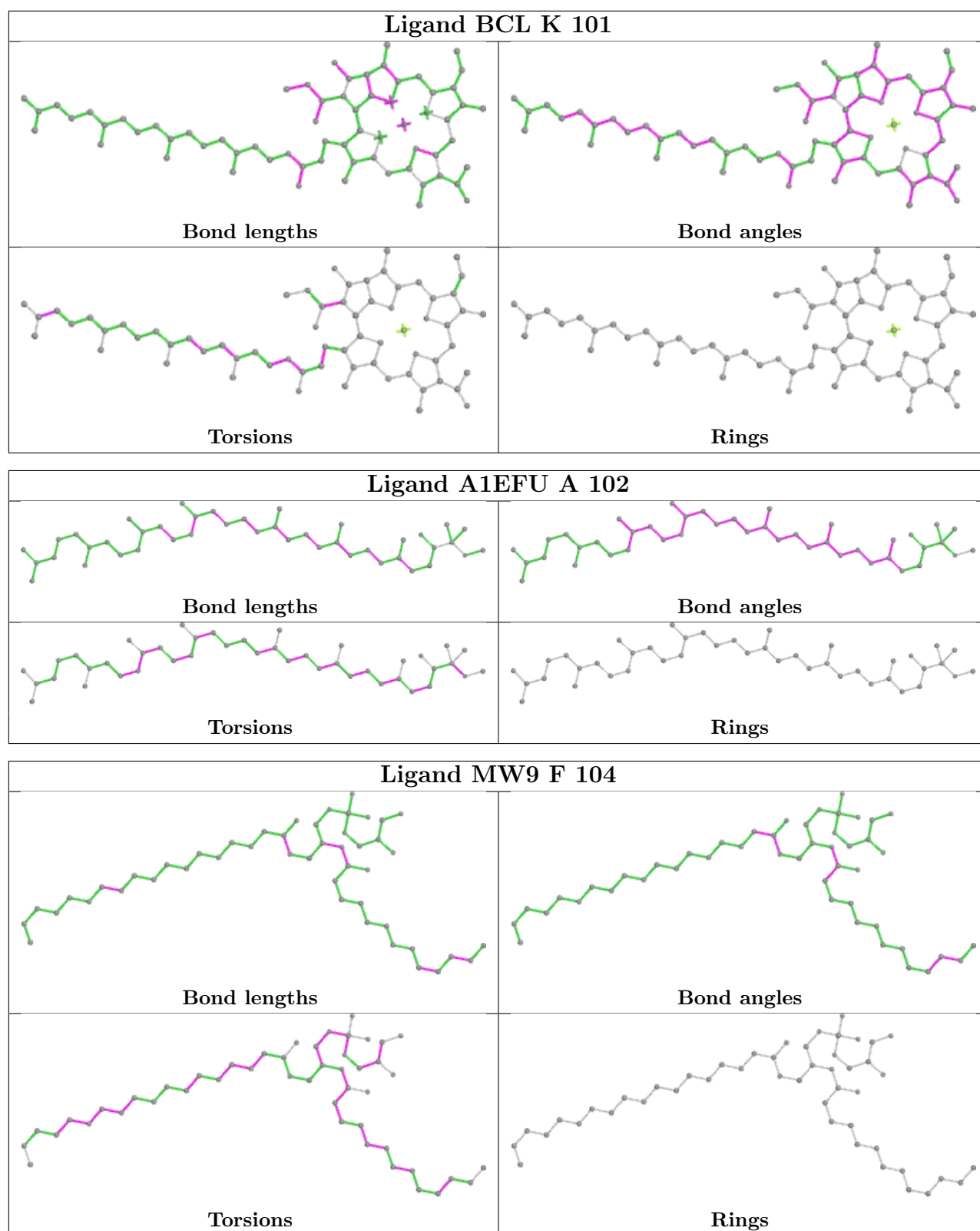


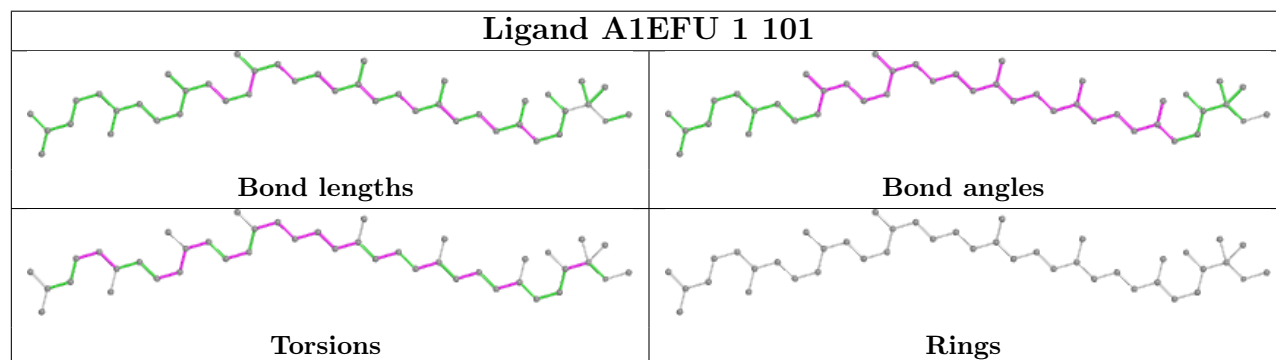
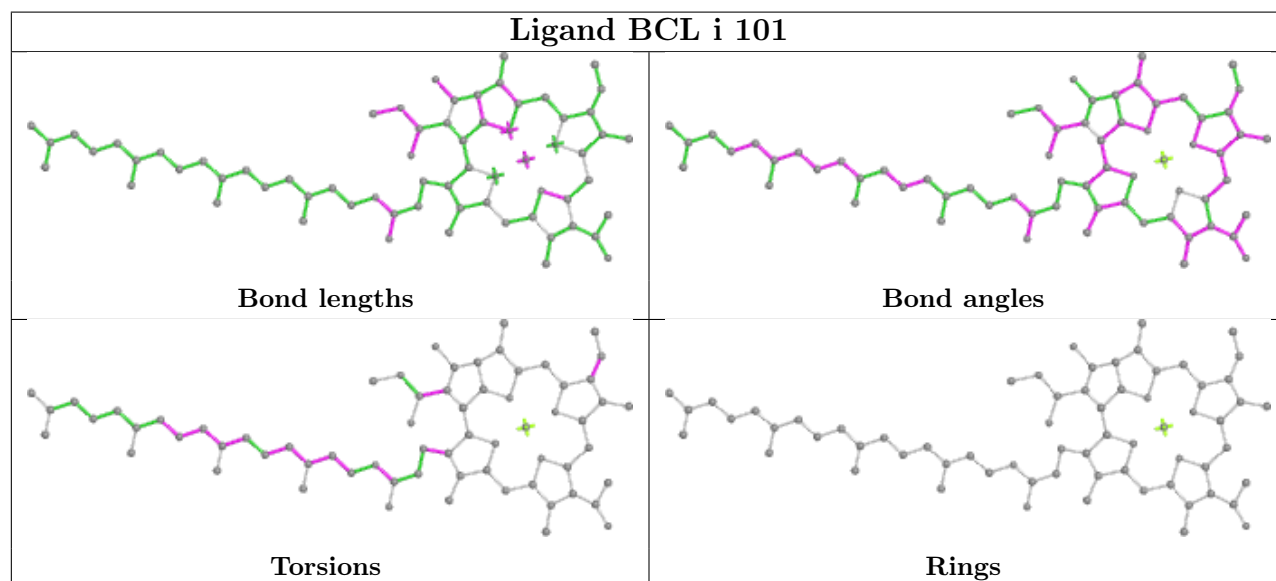
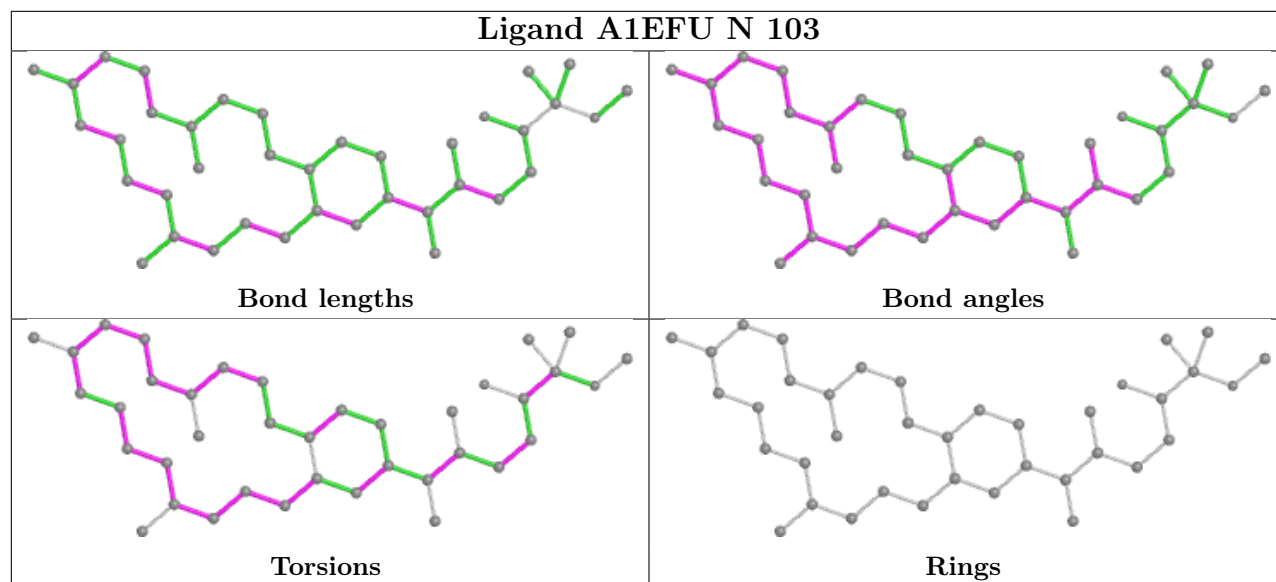
## Ligand LMT L 308

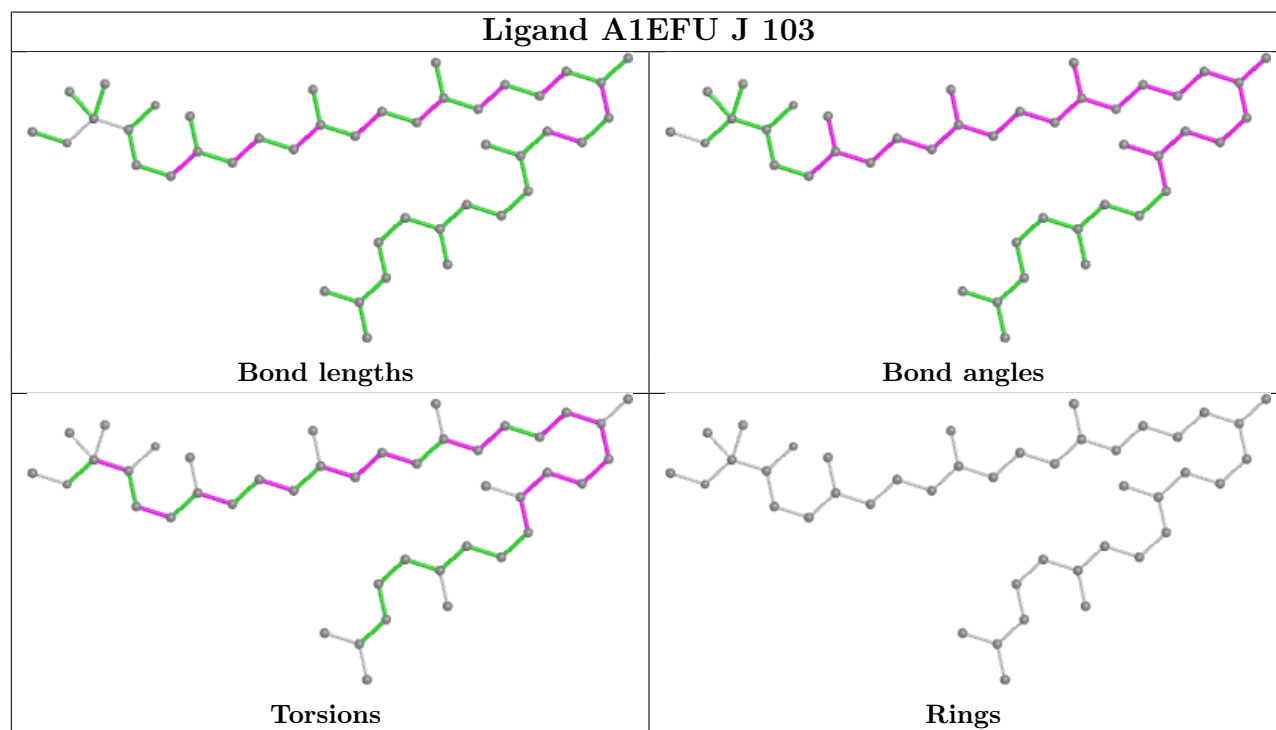
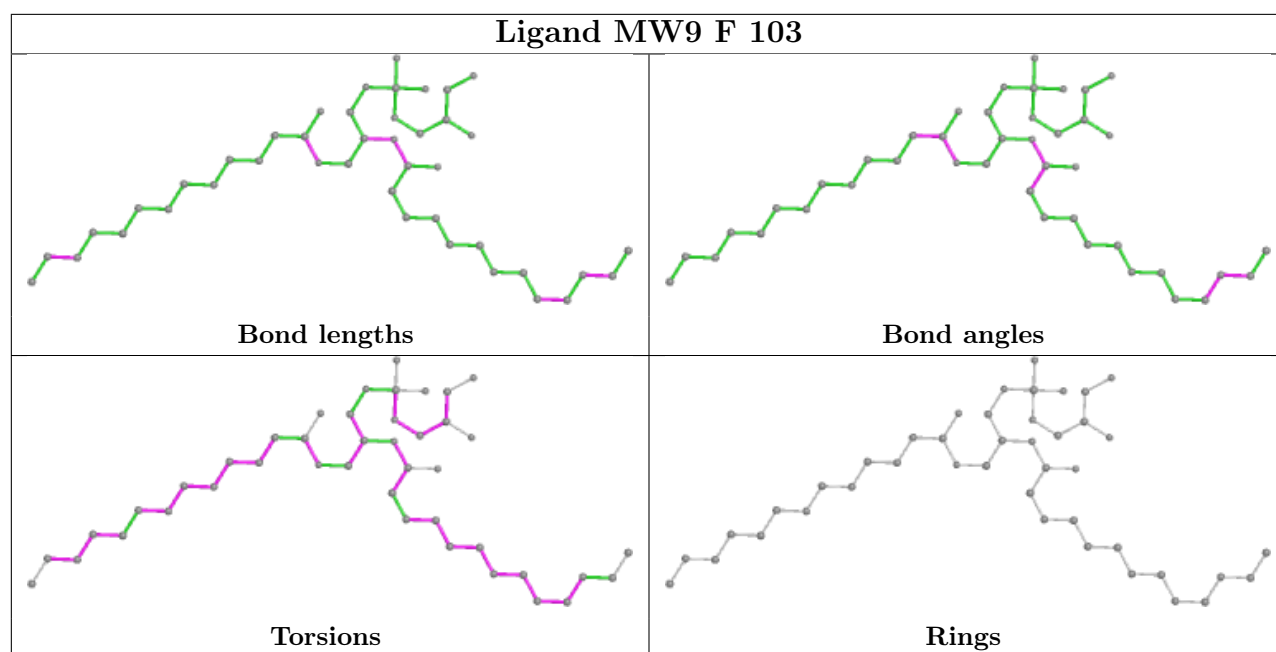


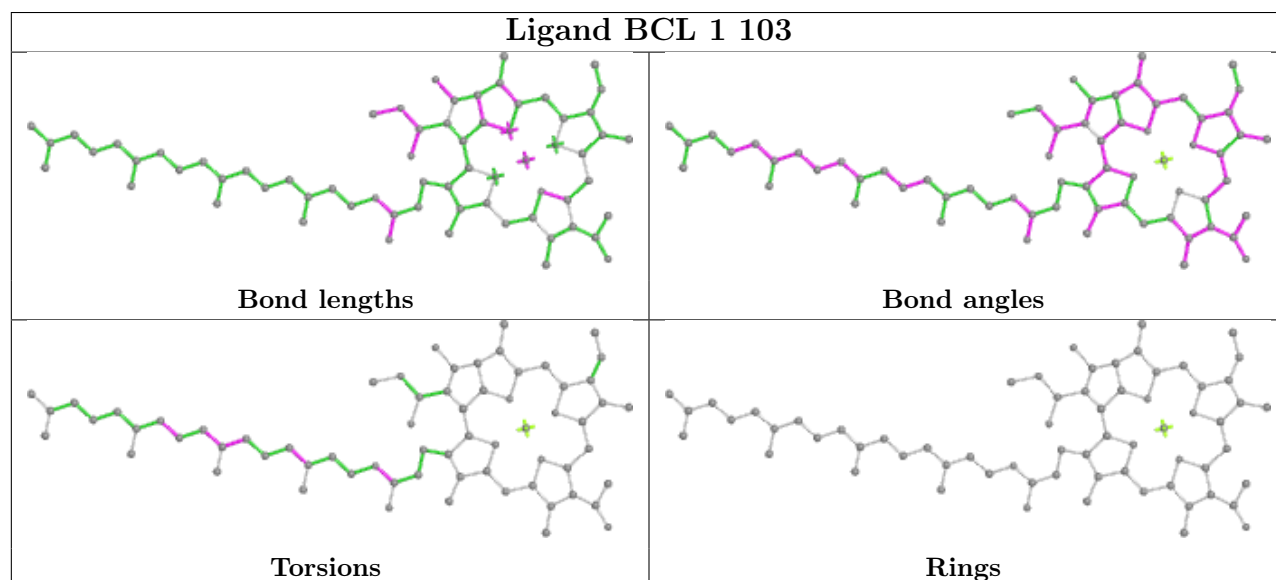
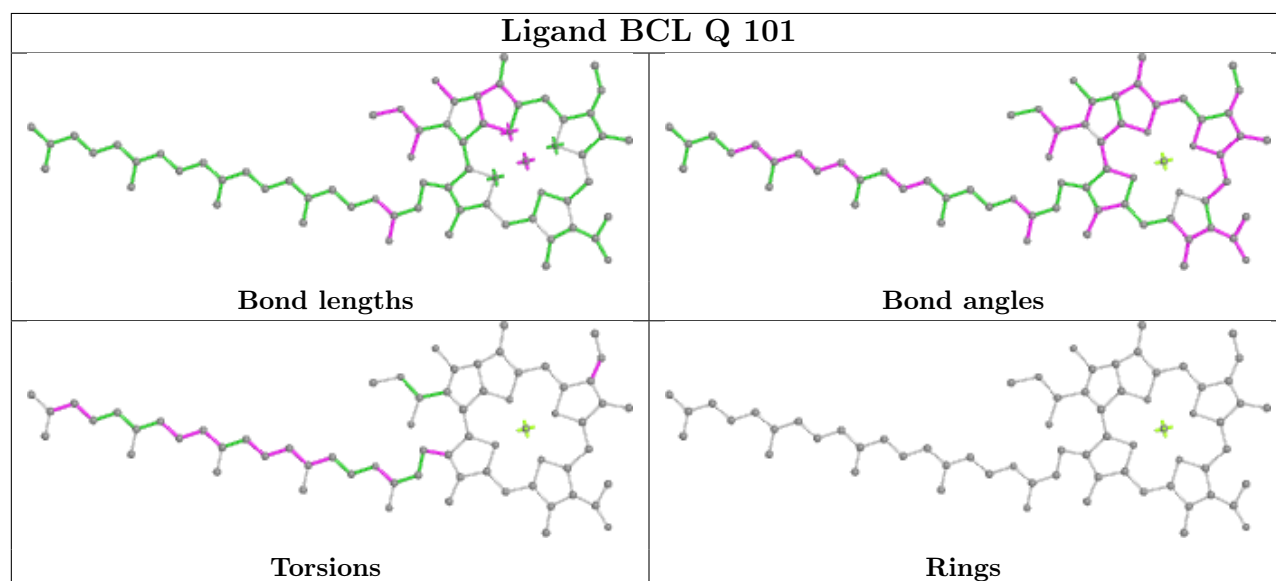
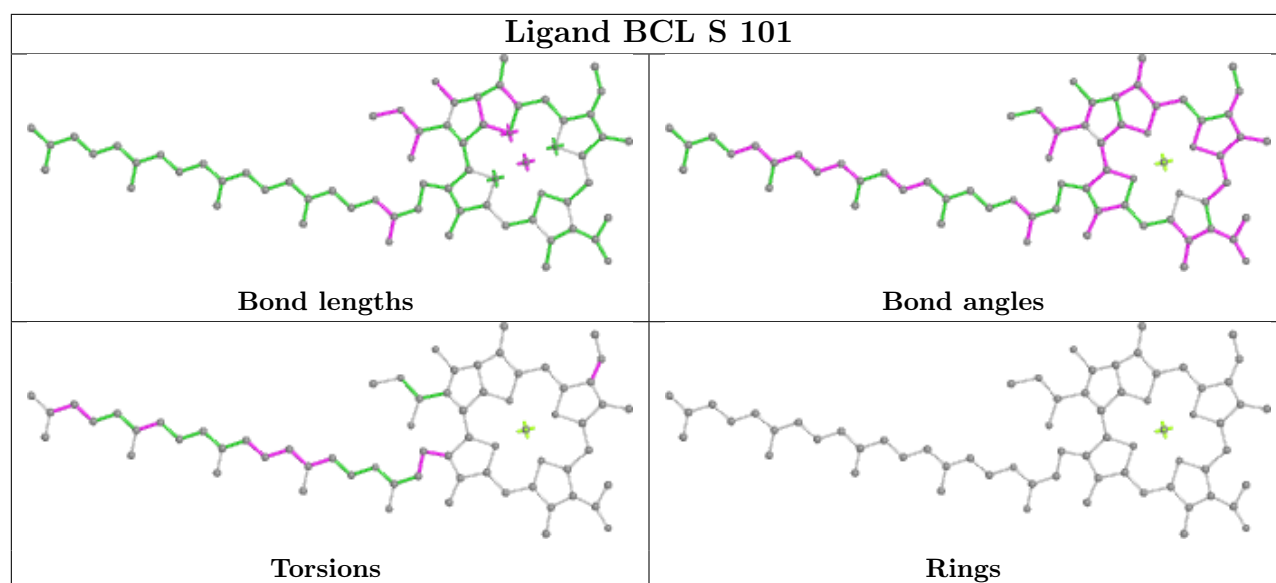
## Ligand BCL L 306

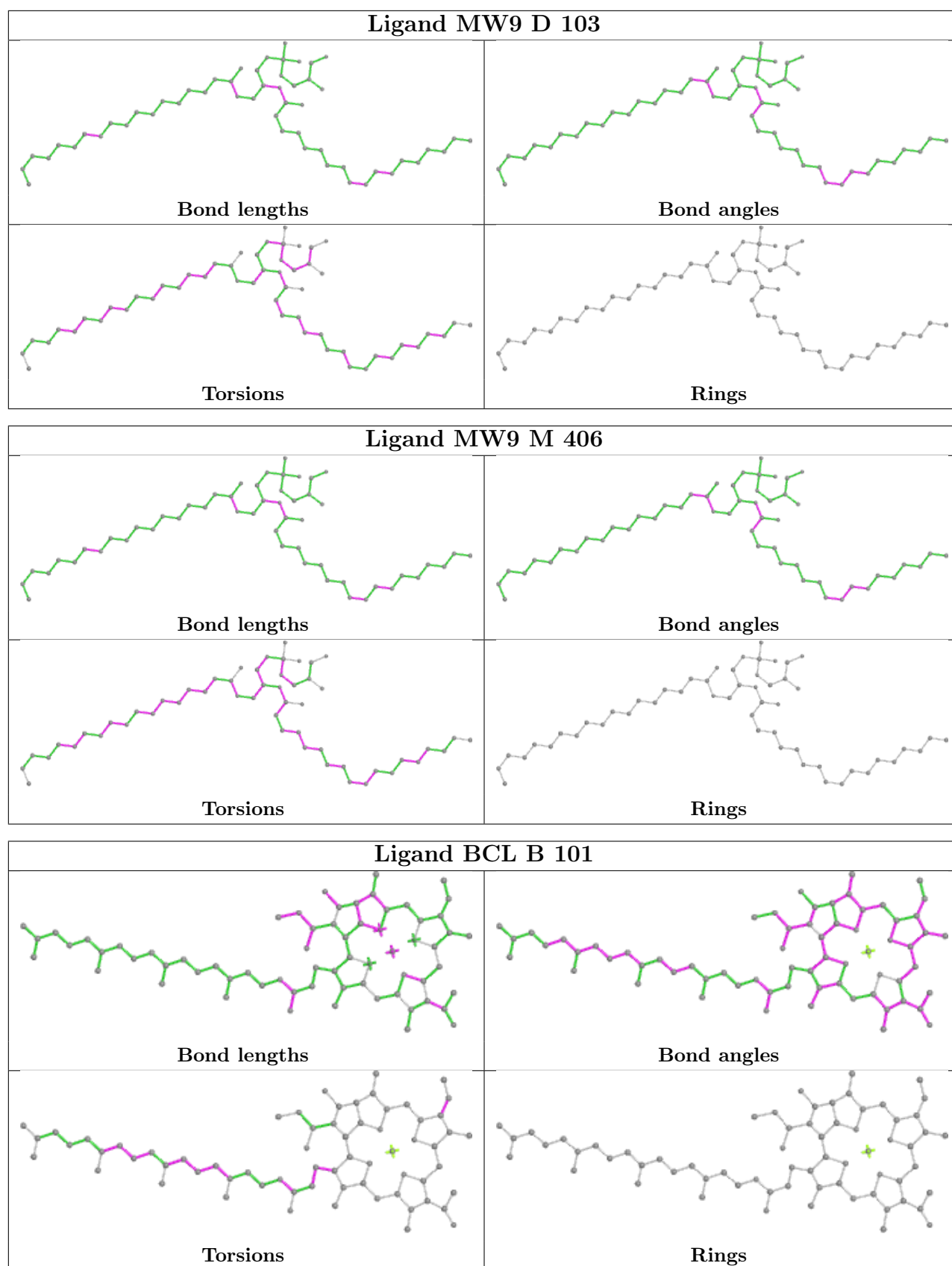




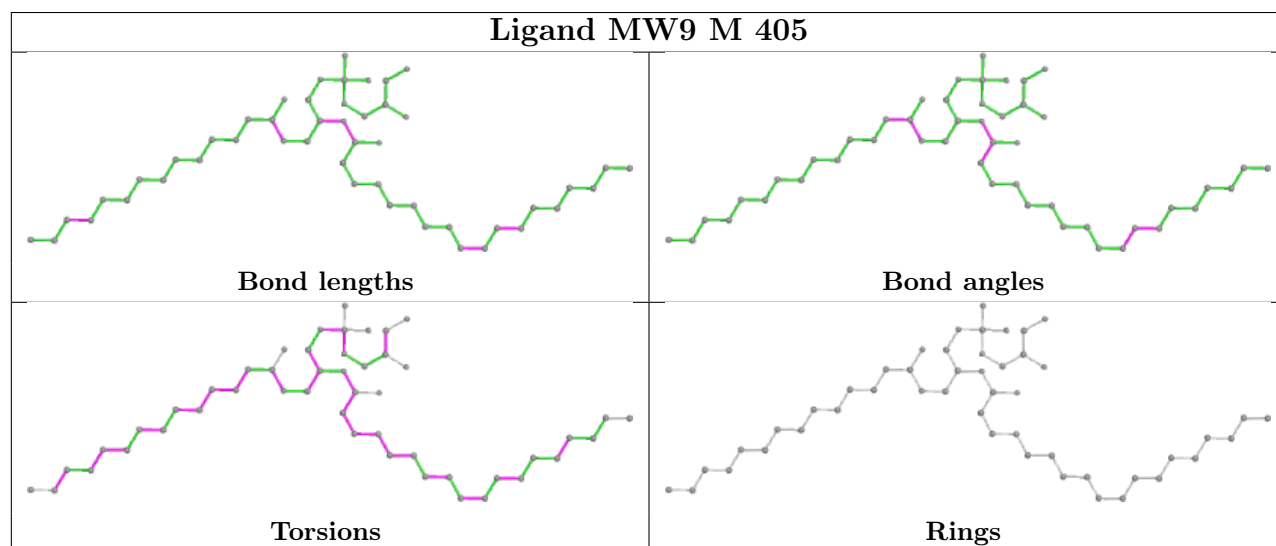
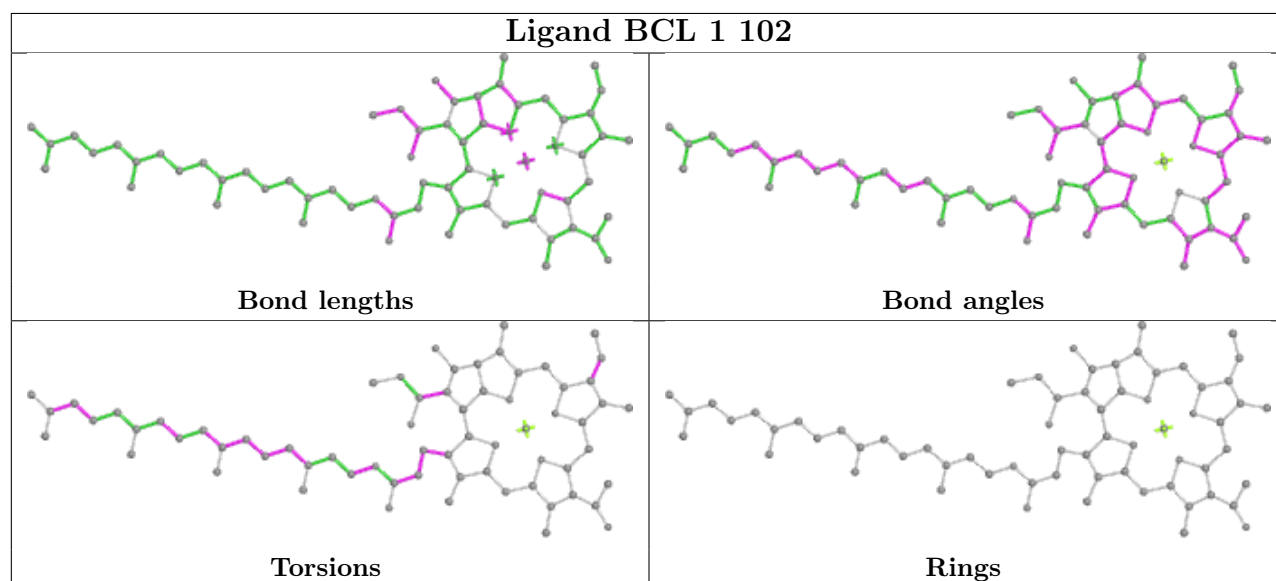
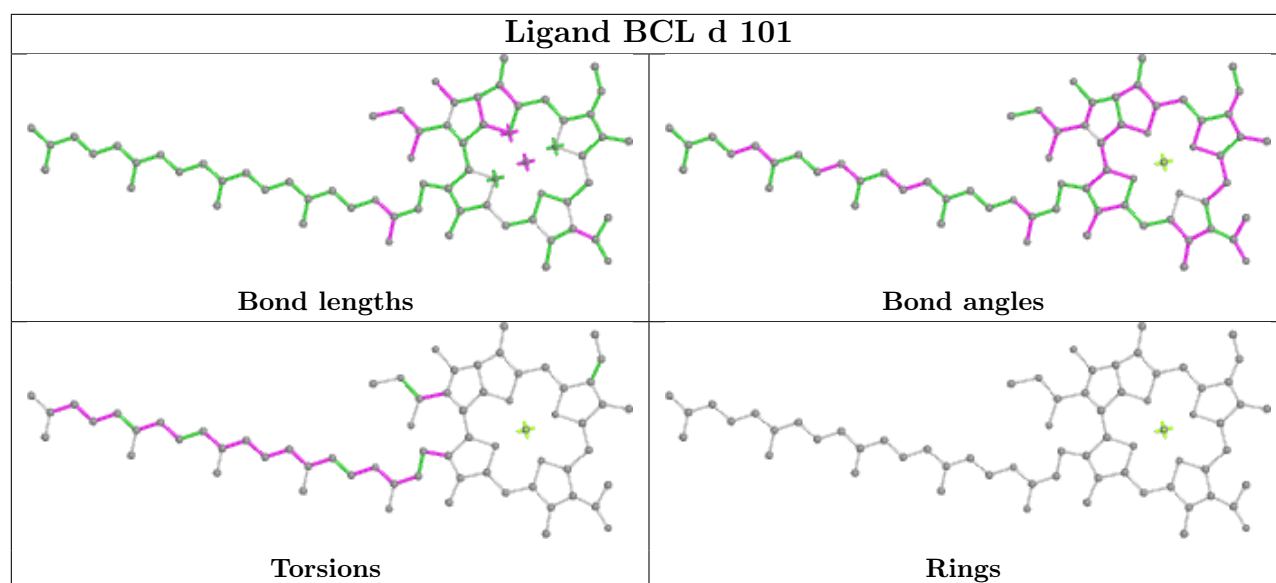


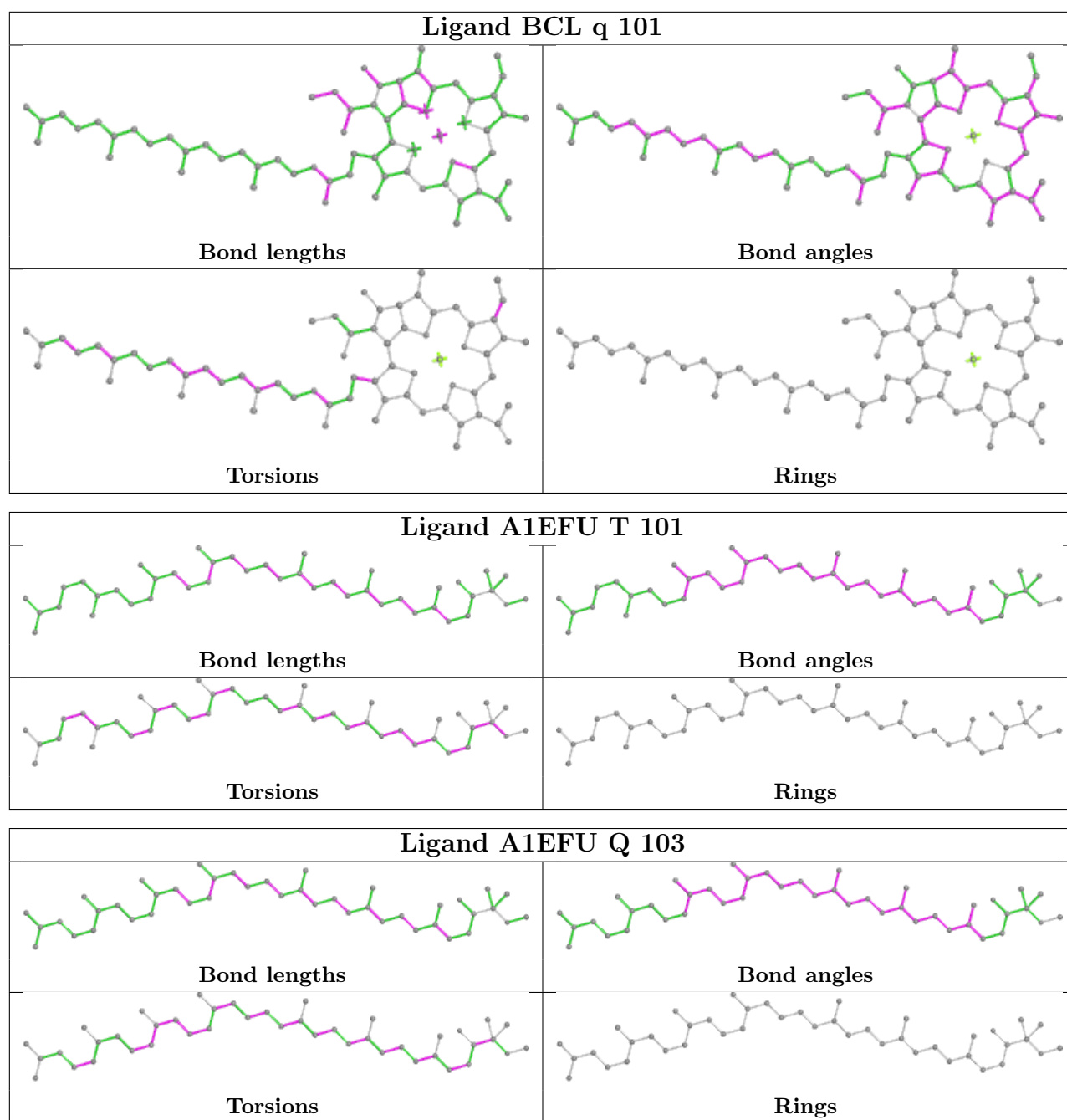


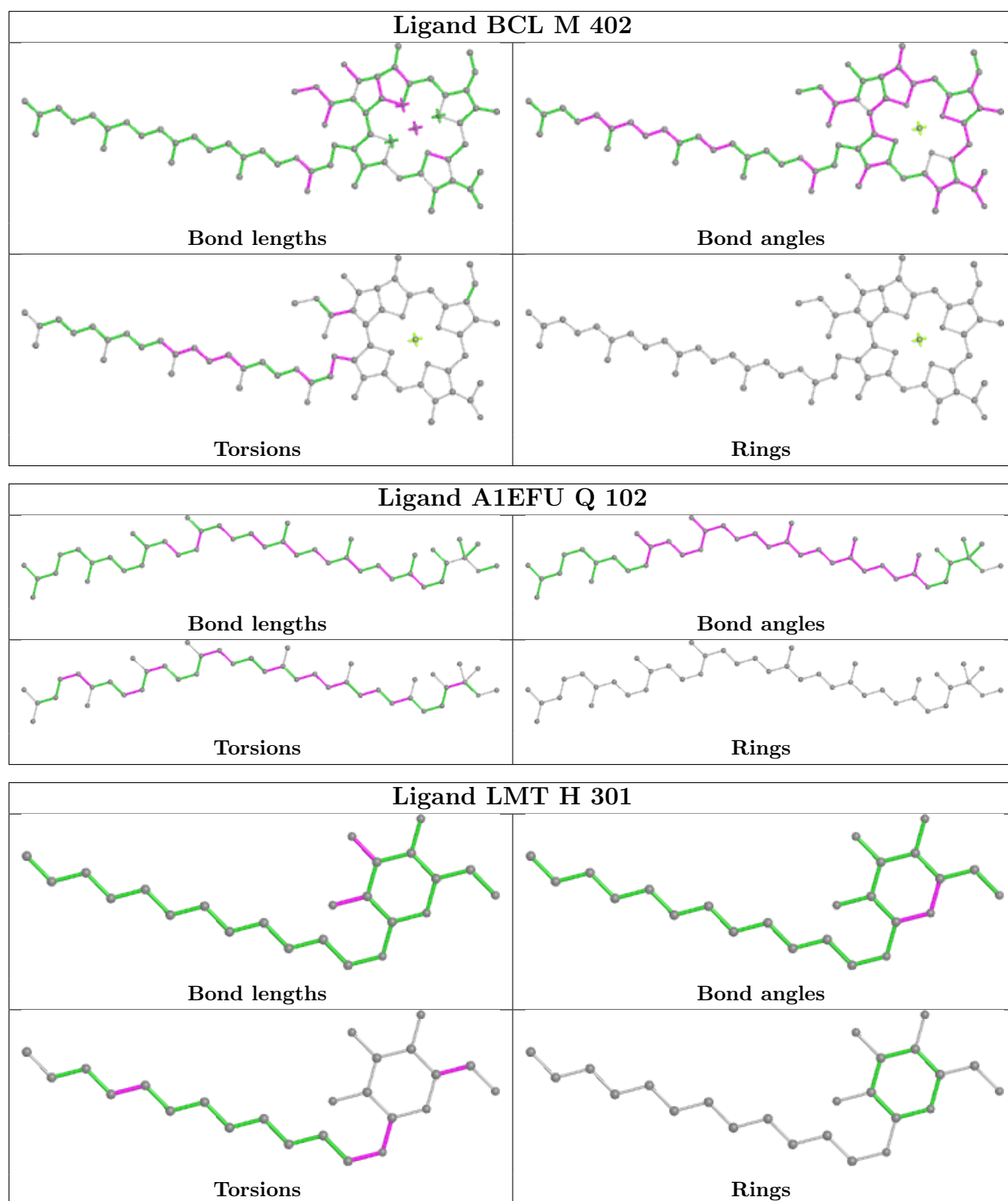


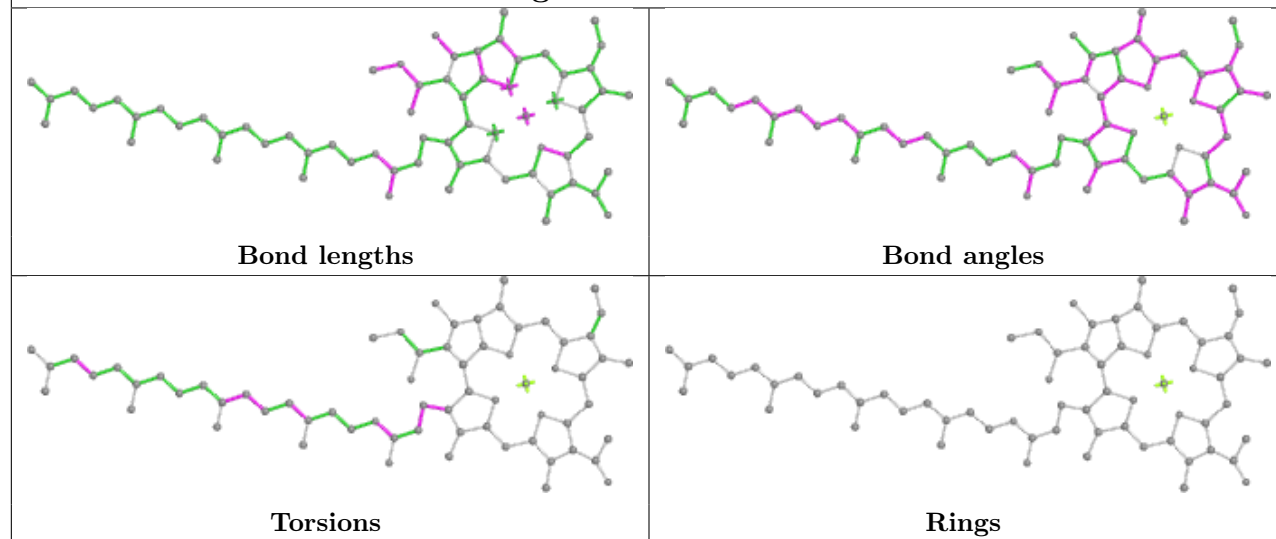
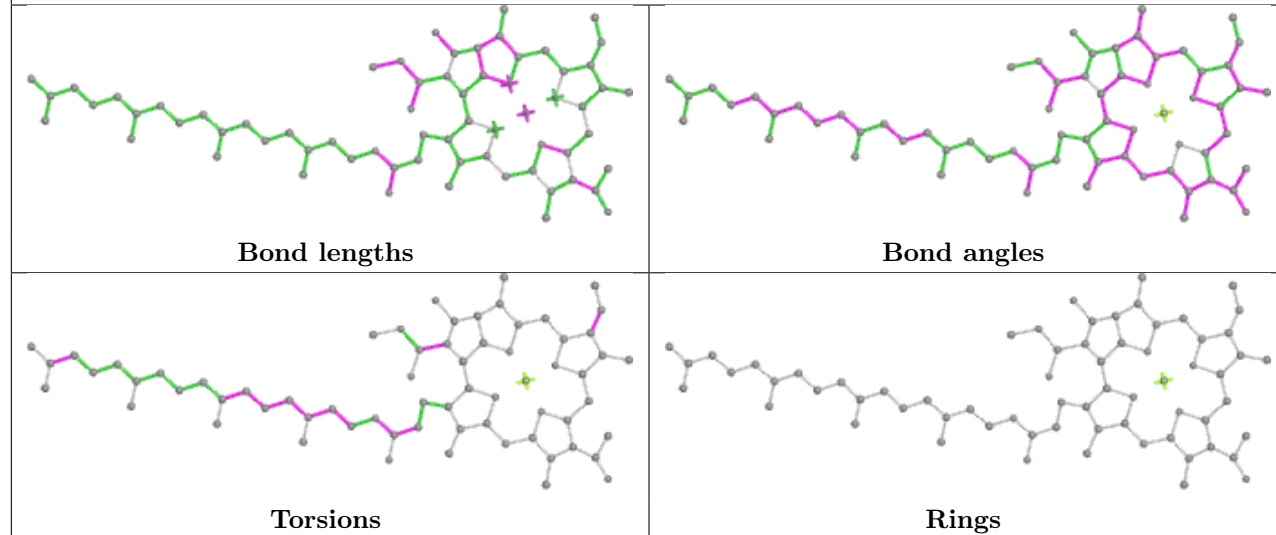
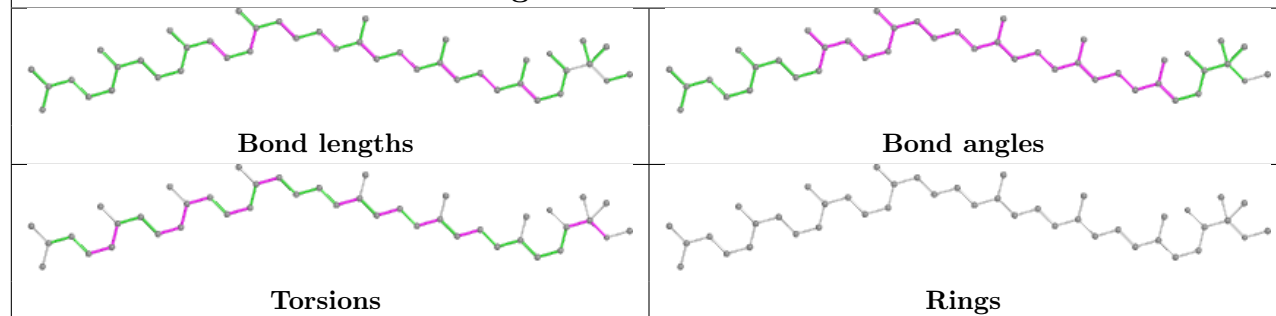


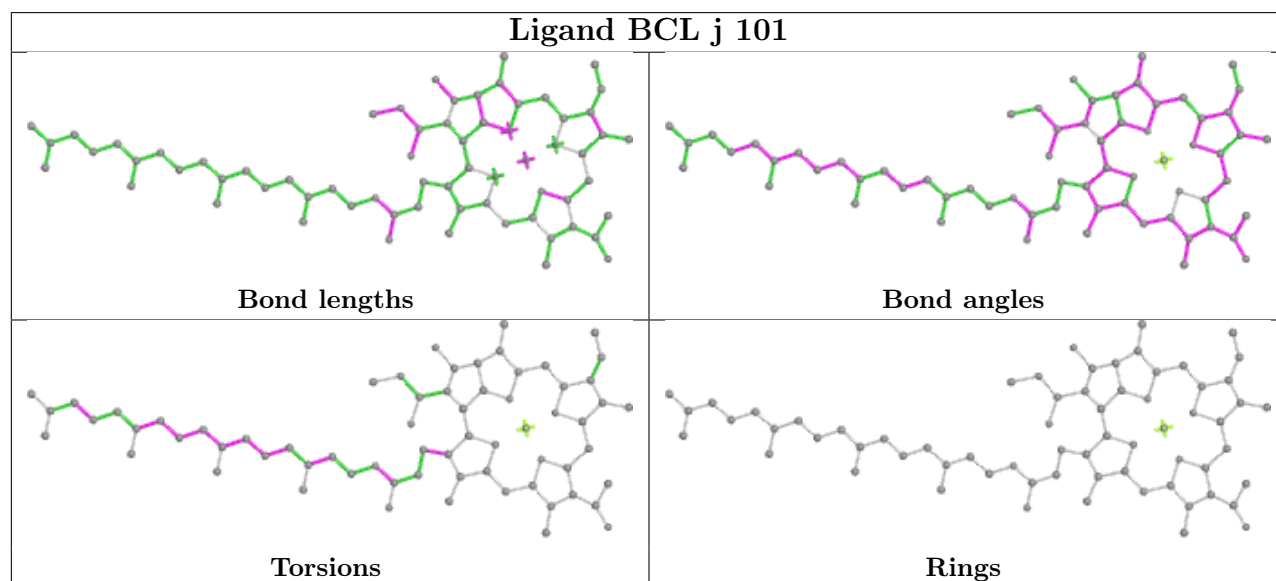
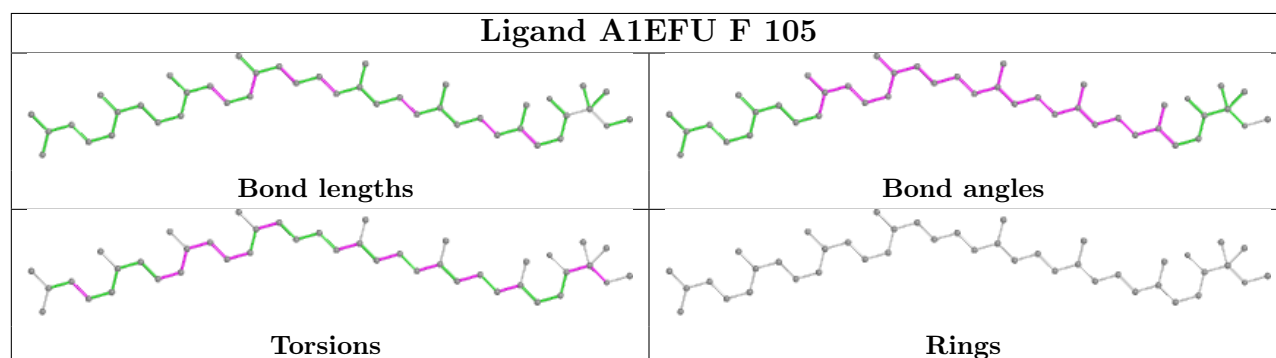
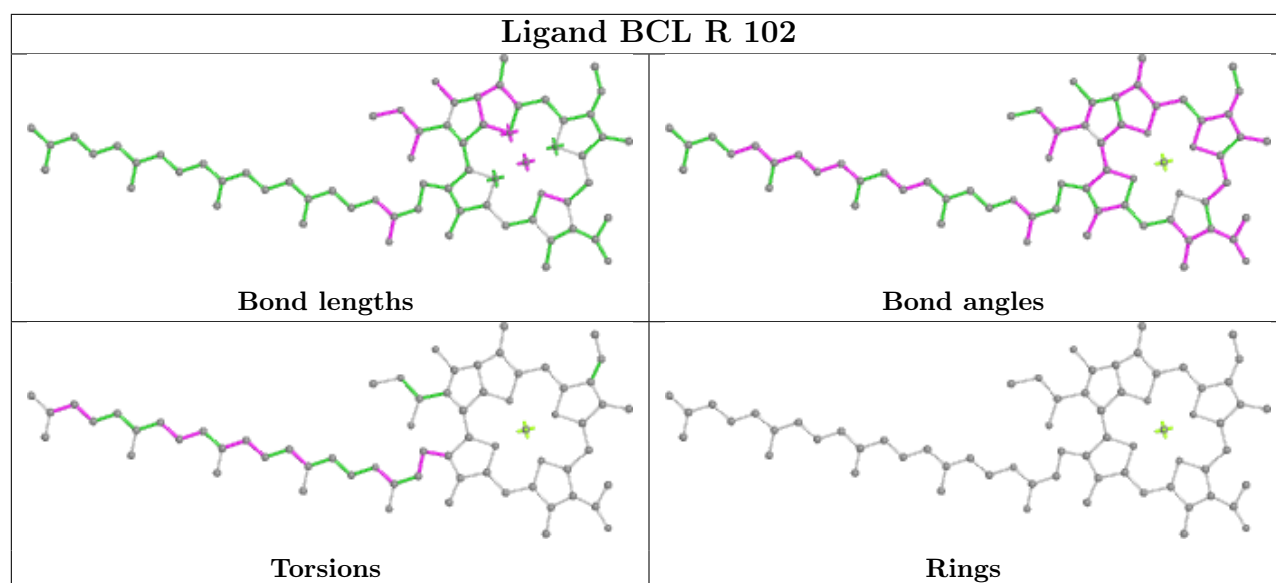


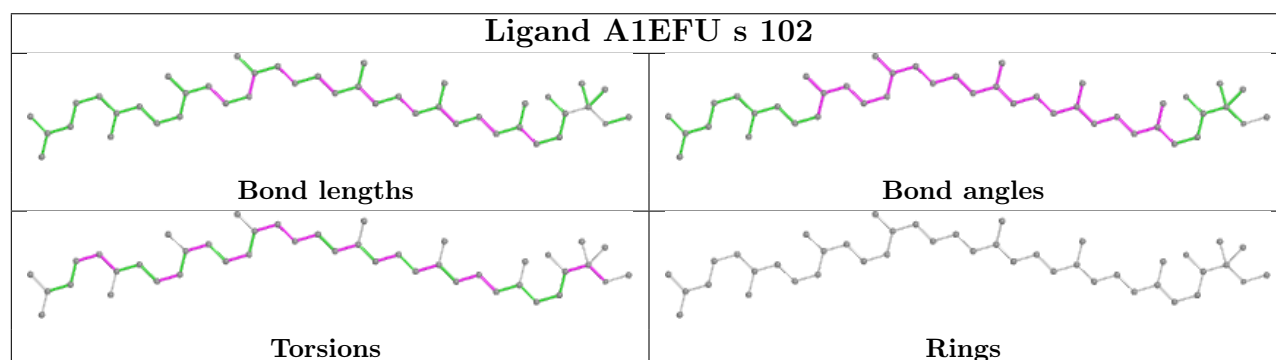
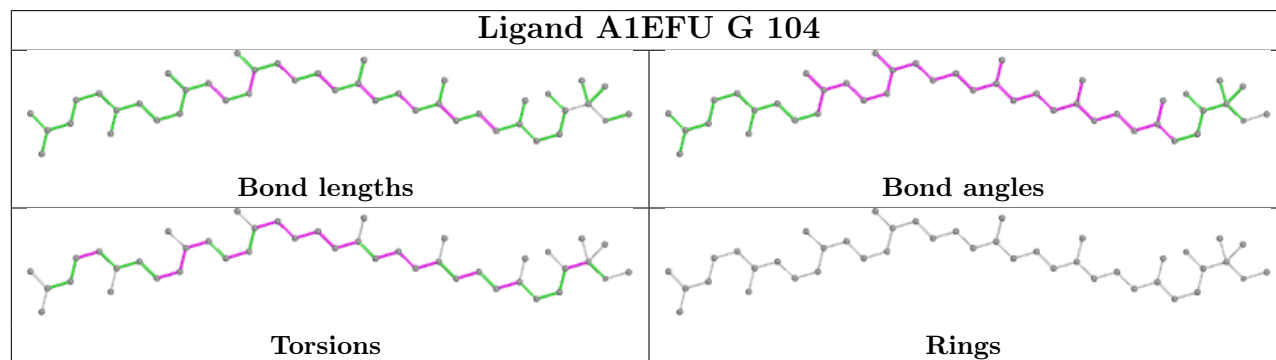
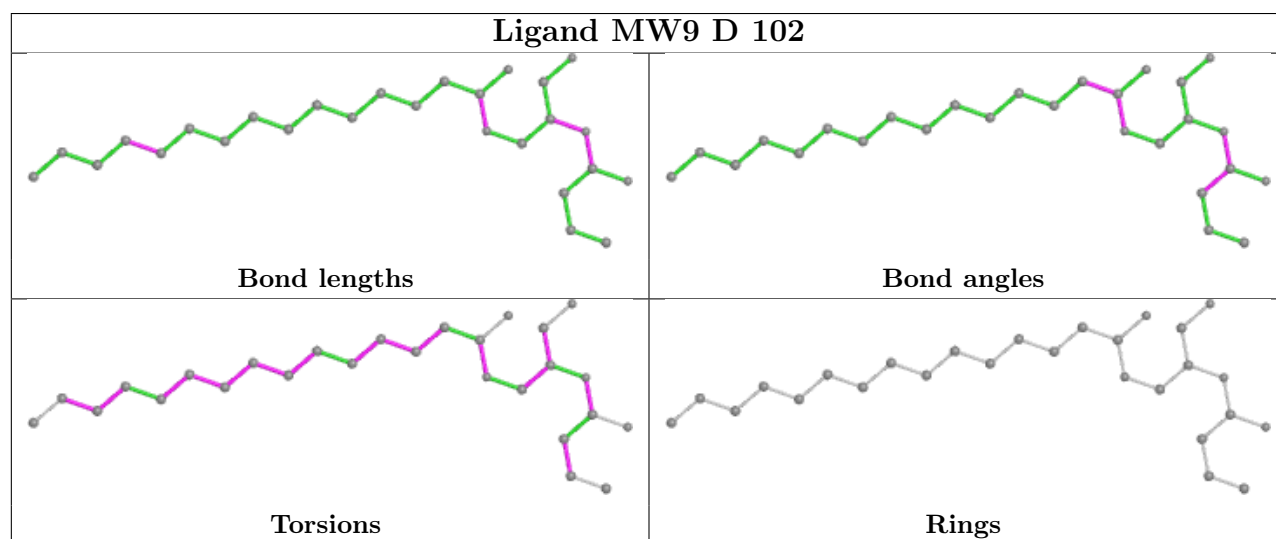
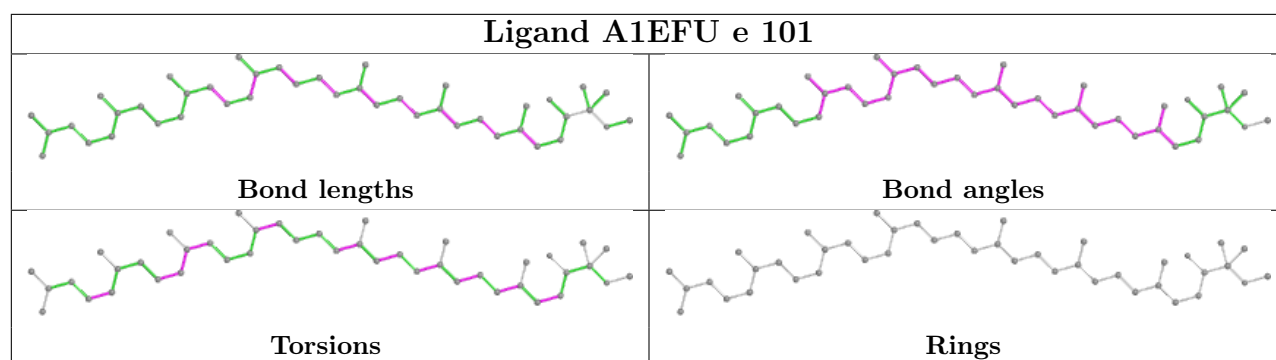


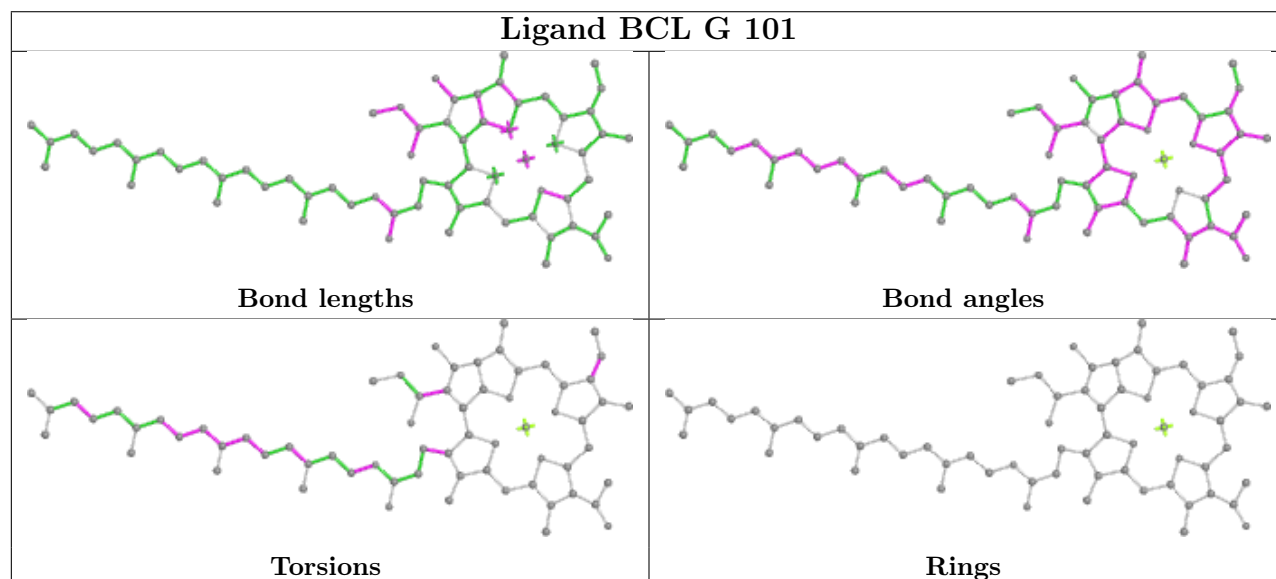
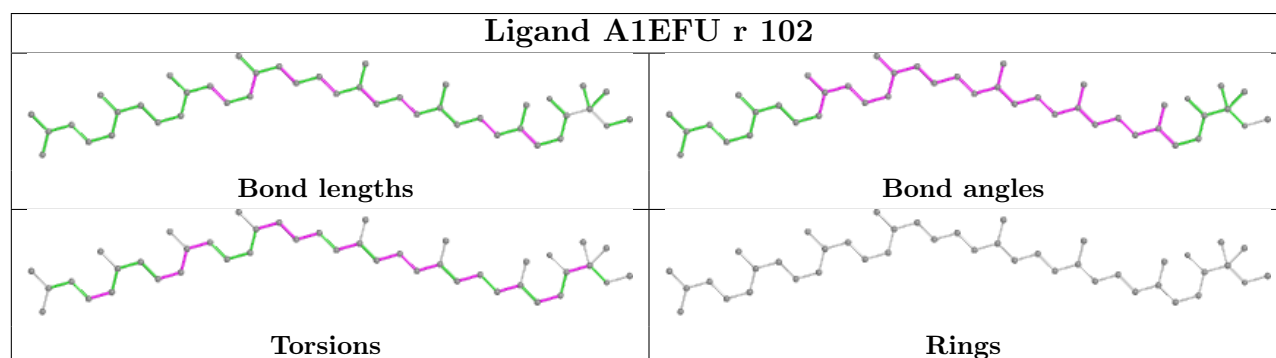
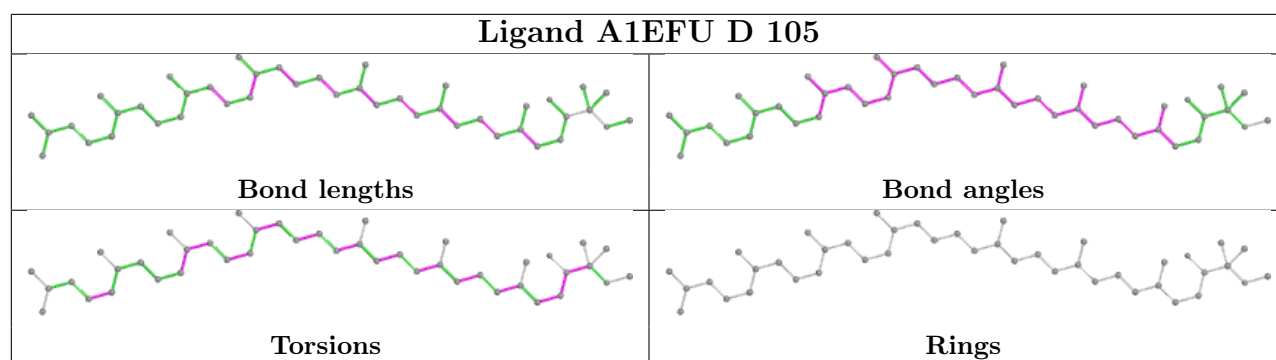


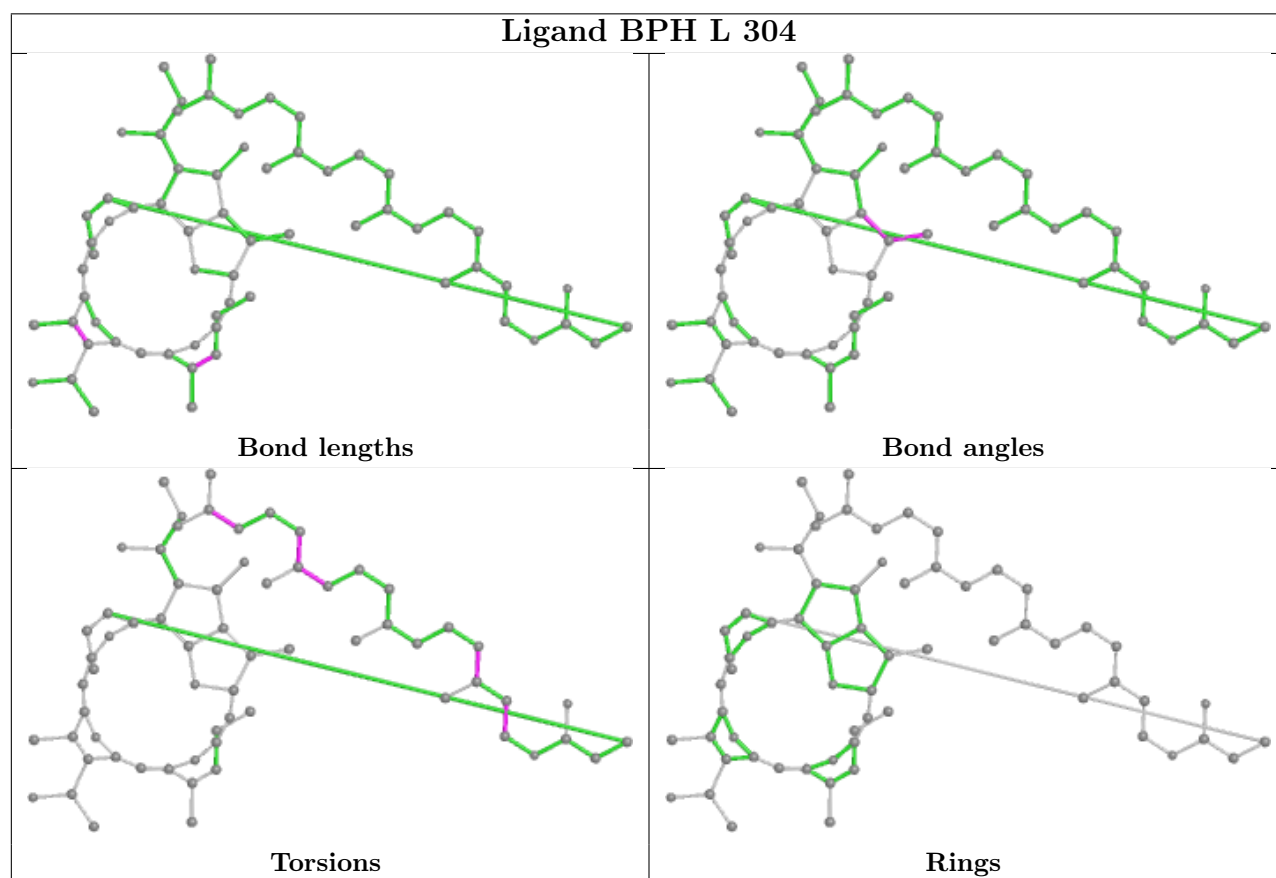
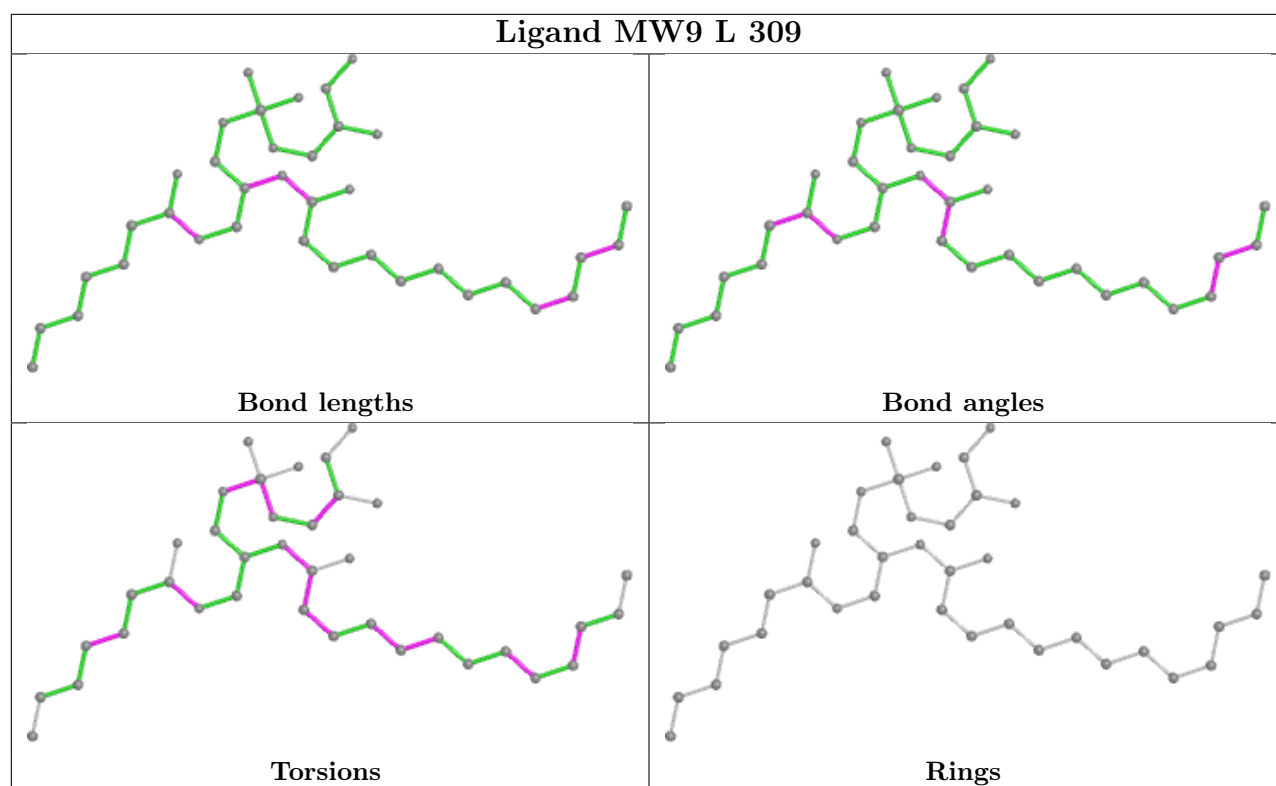


**Ligand BCL N 101****Ligand BCL M 403****Ligand A1EFU E 102**

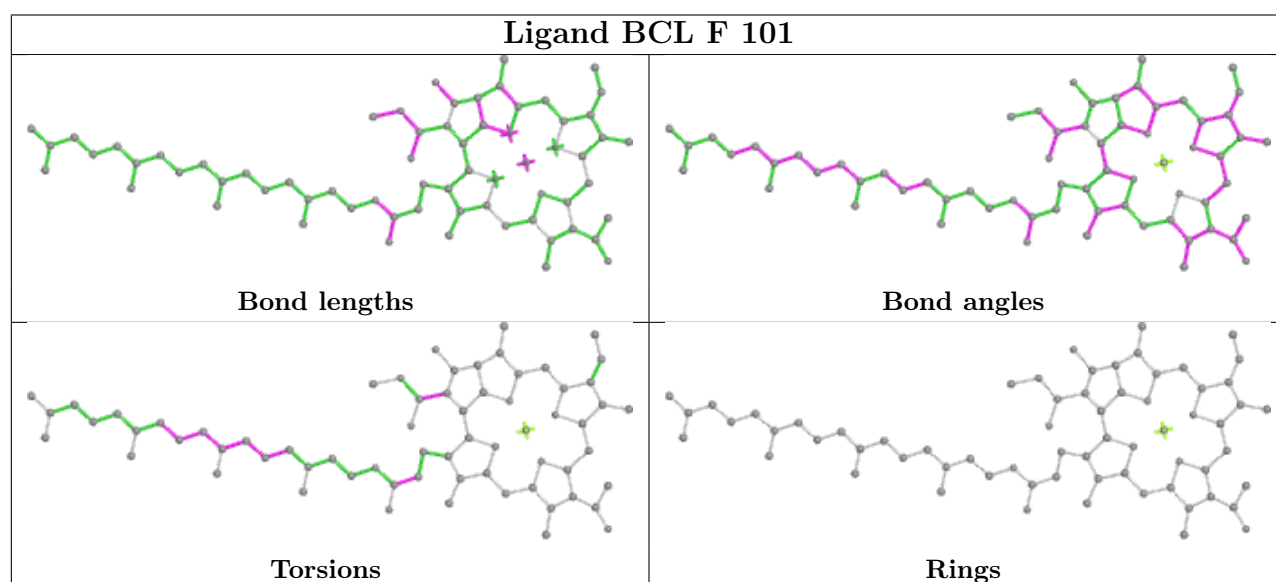
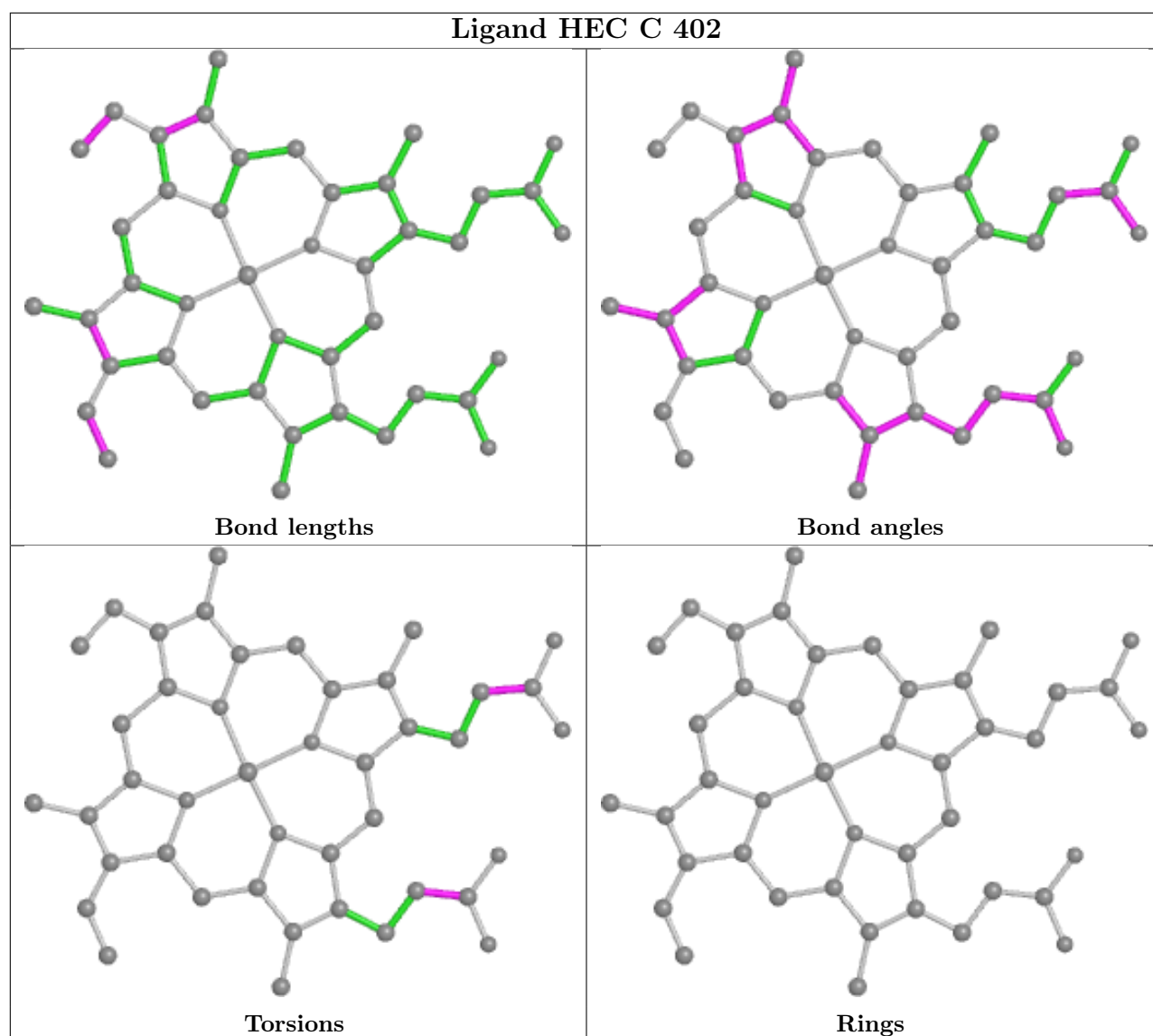


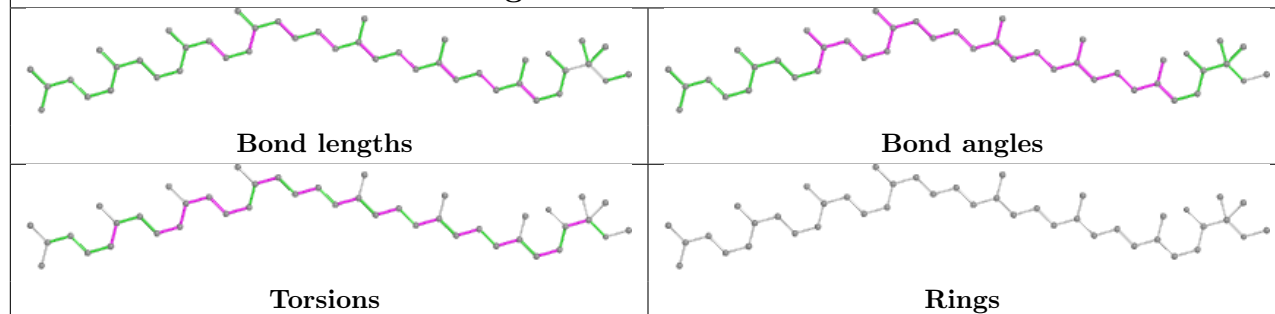
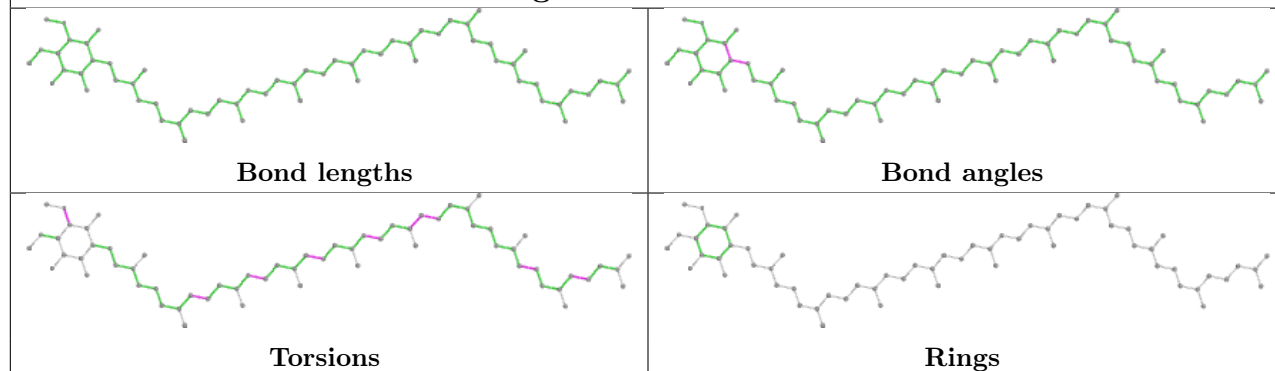
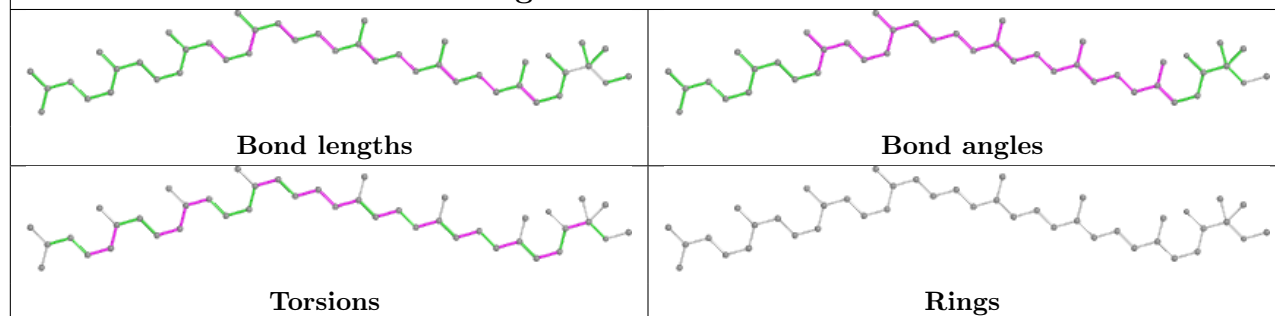
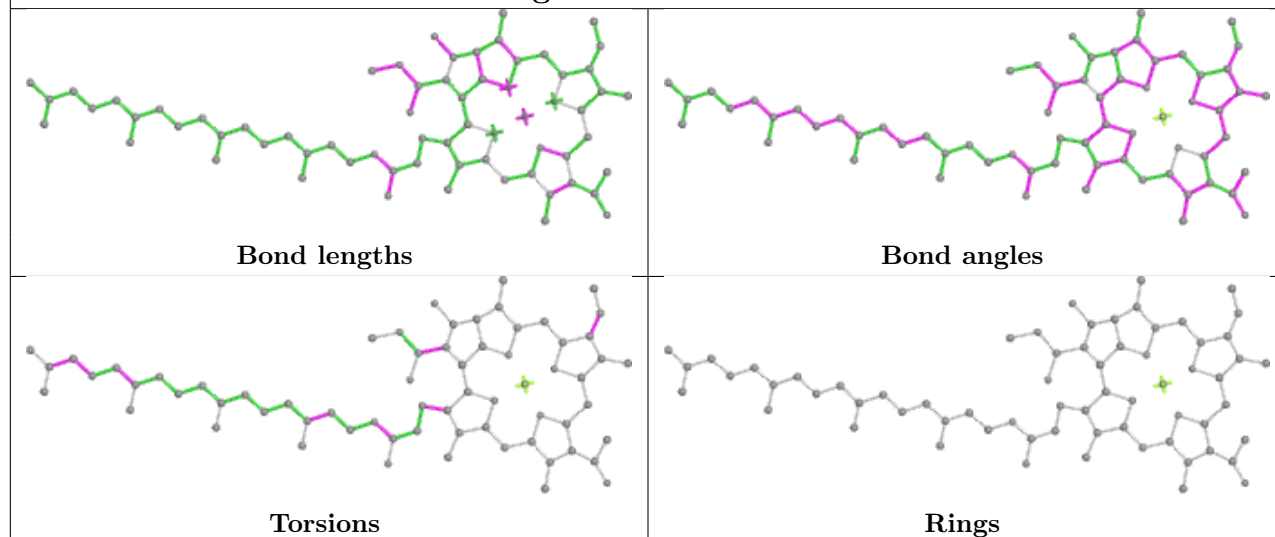


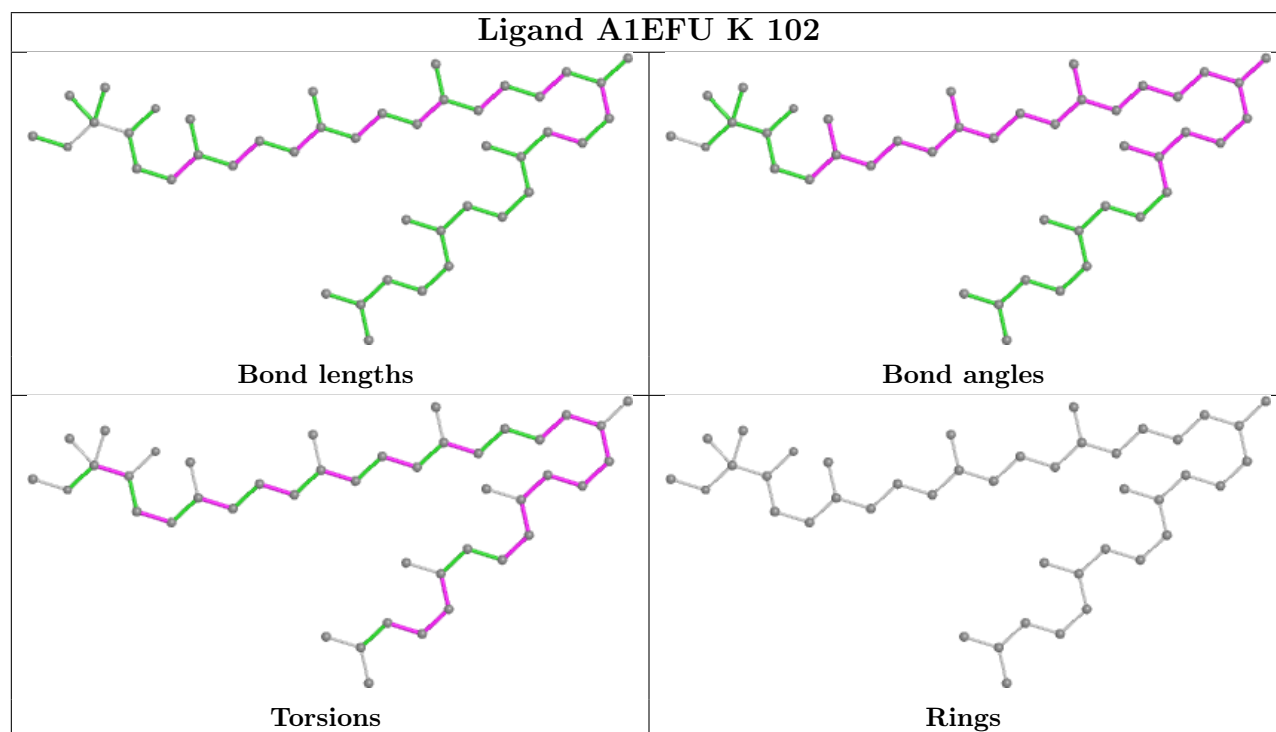
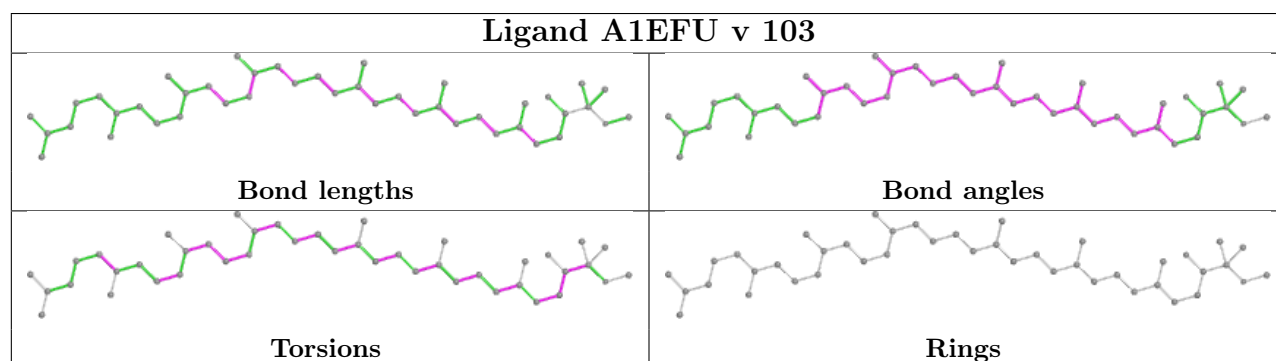
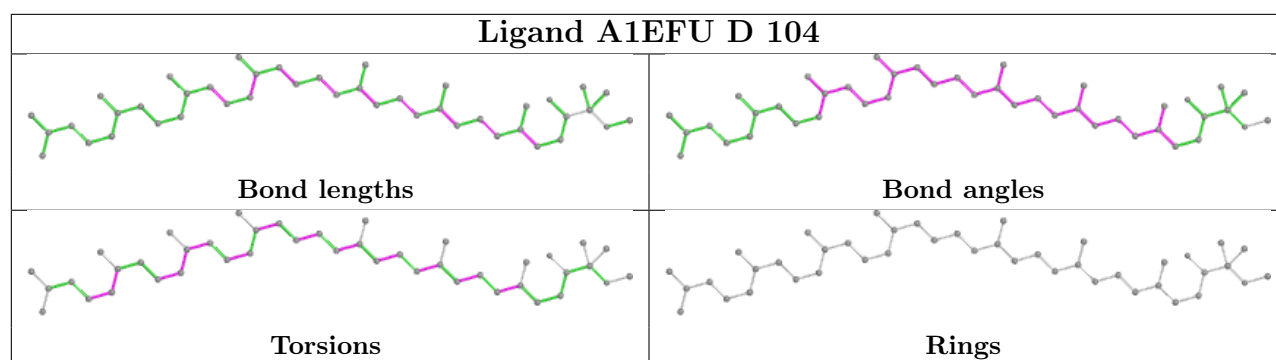


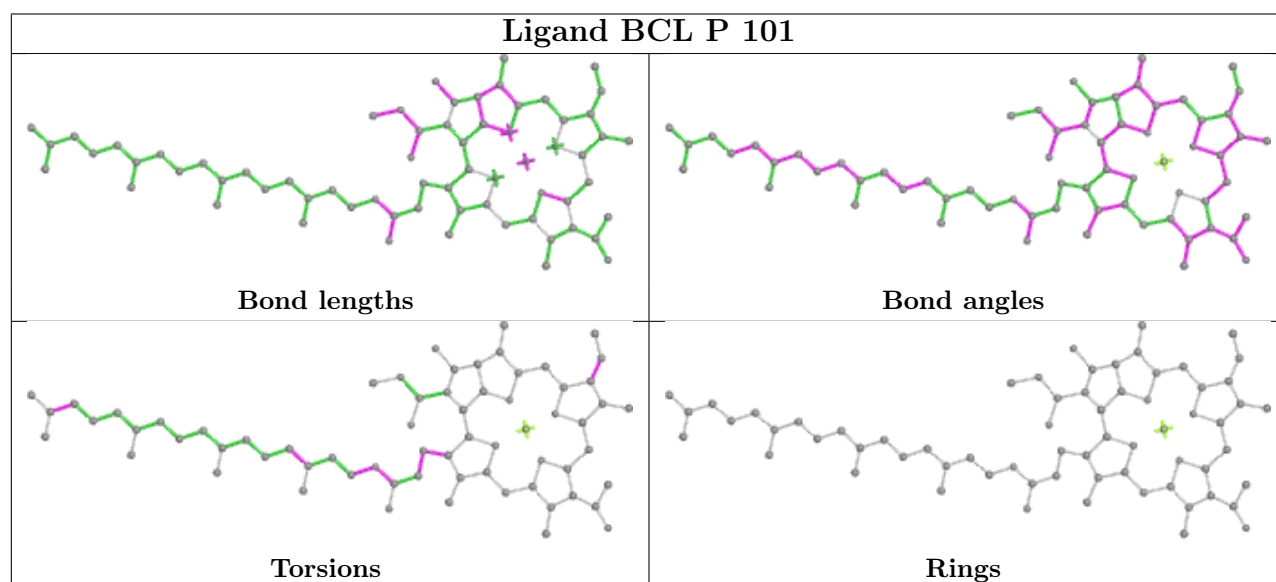
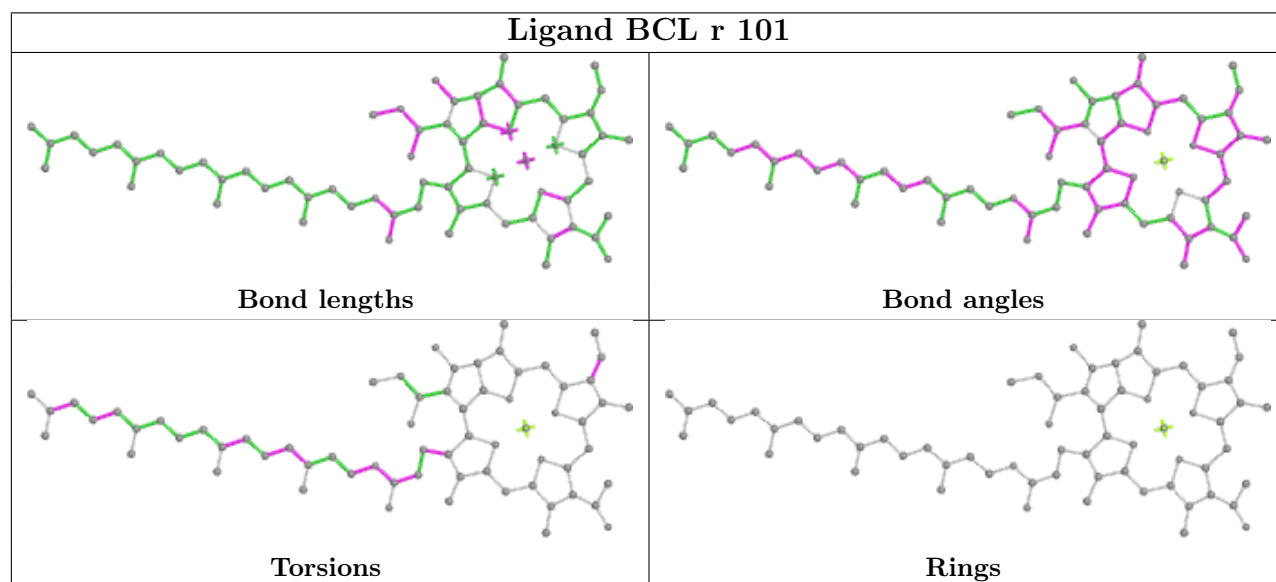
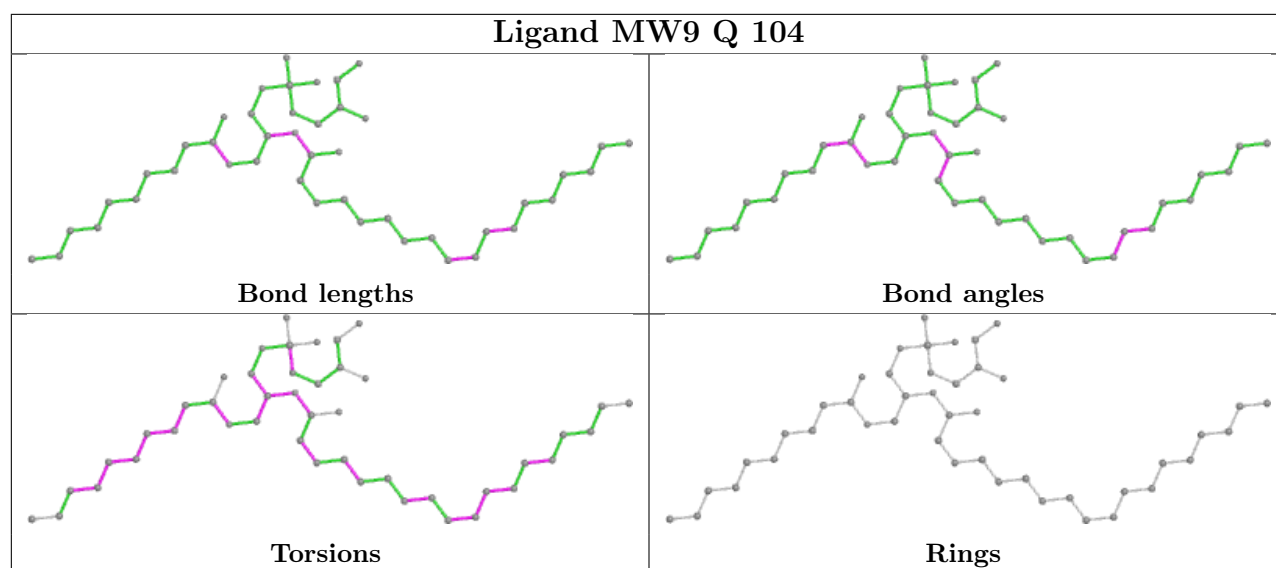


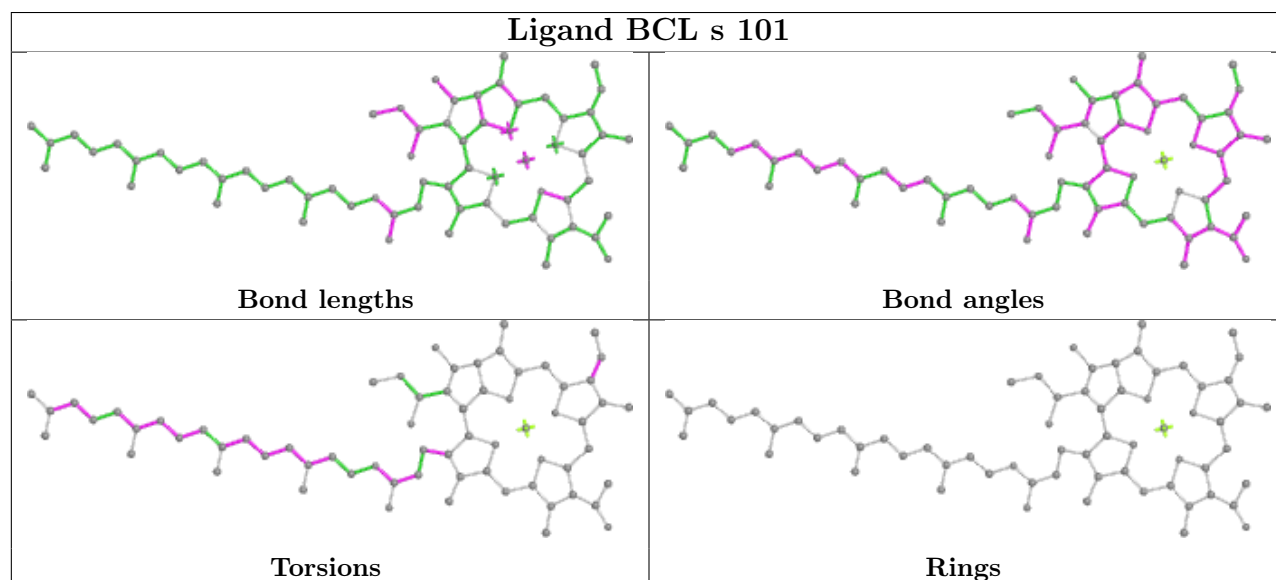
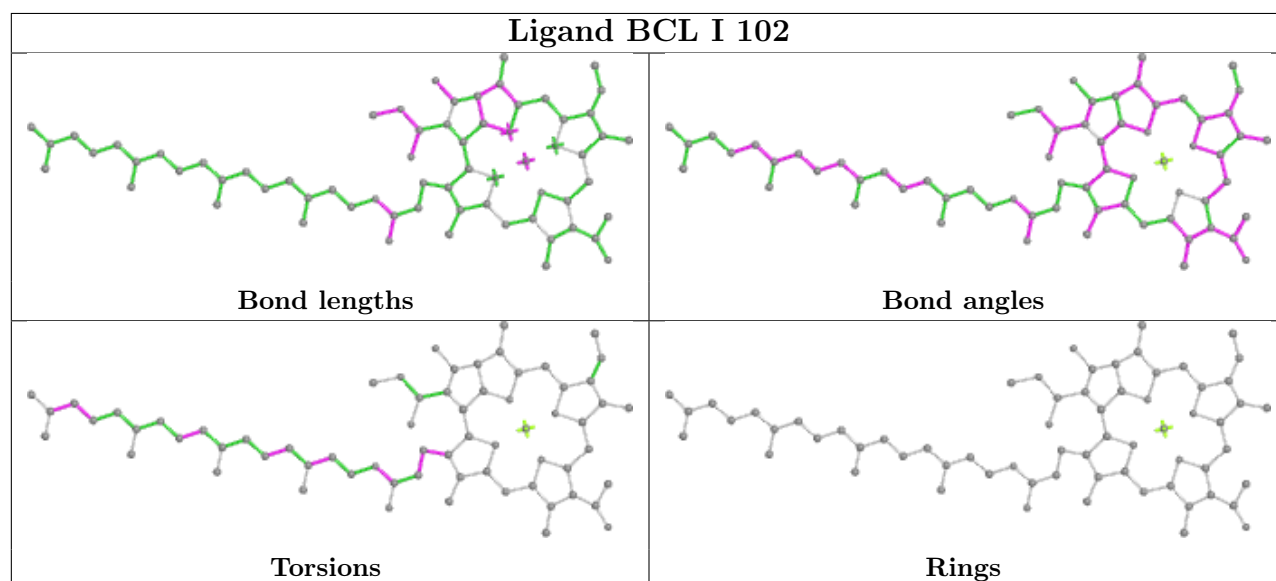
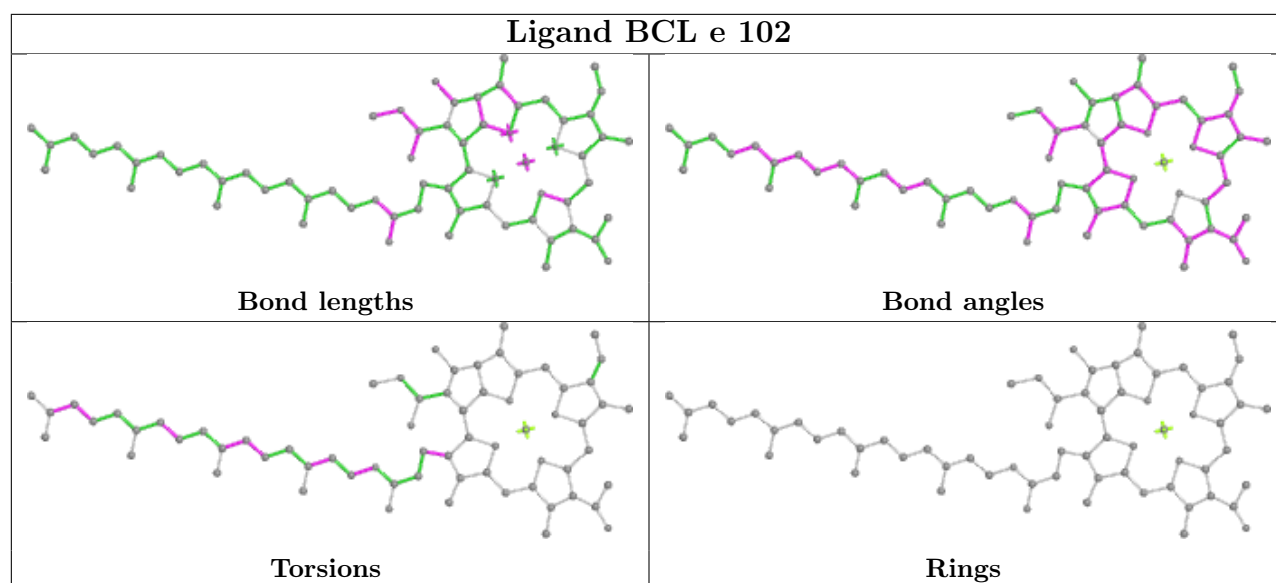


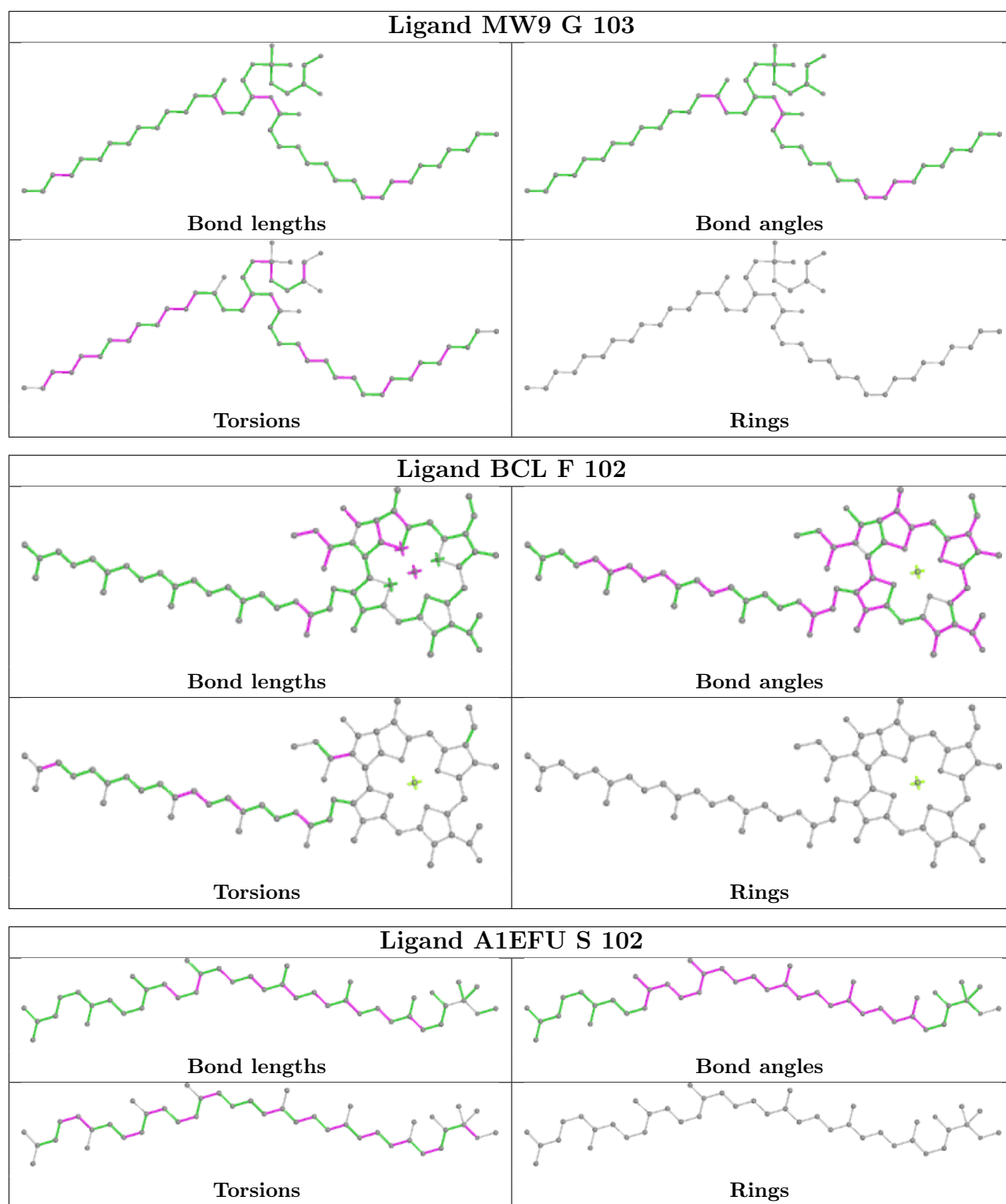


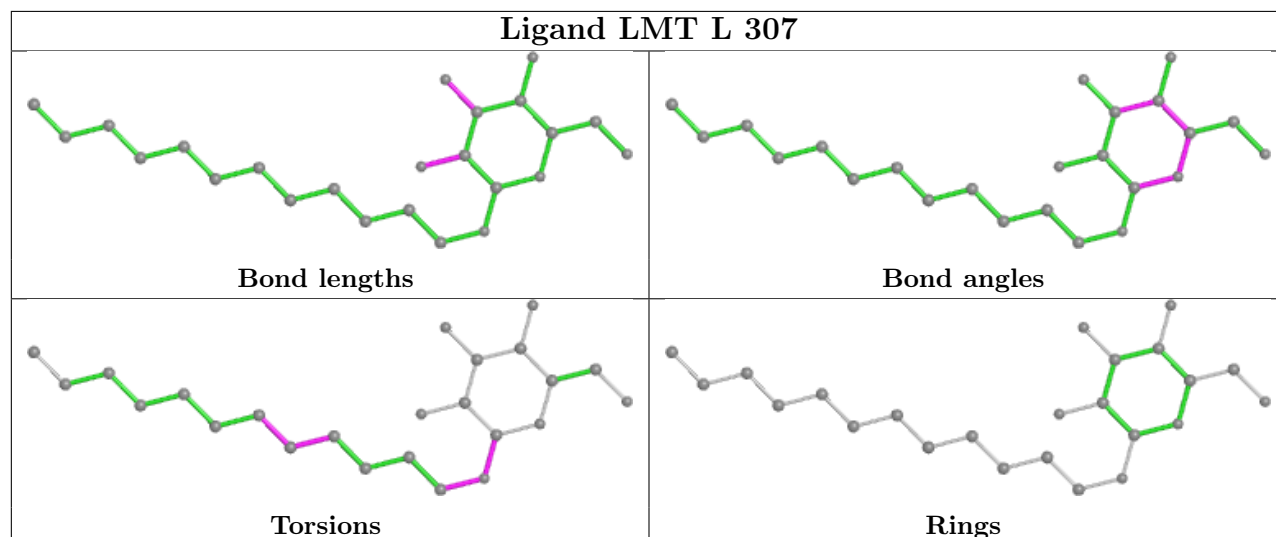
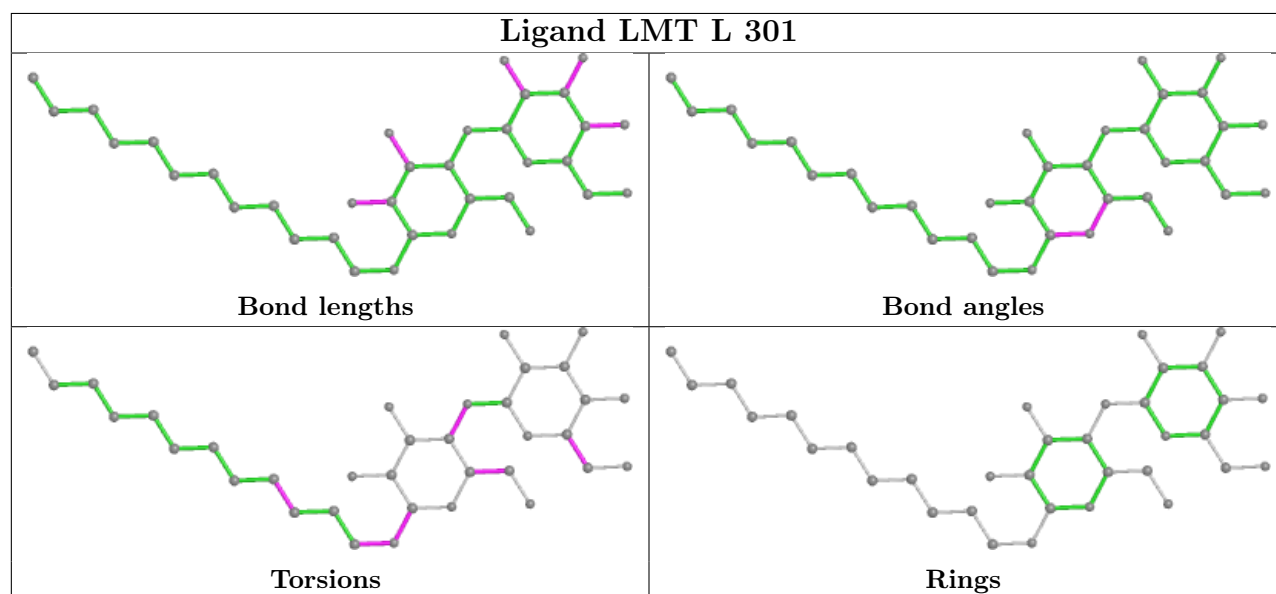
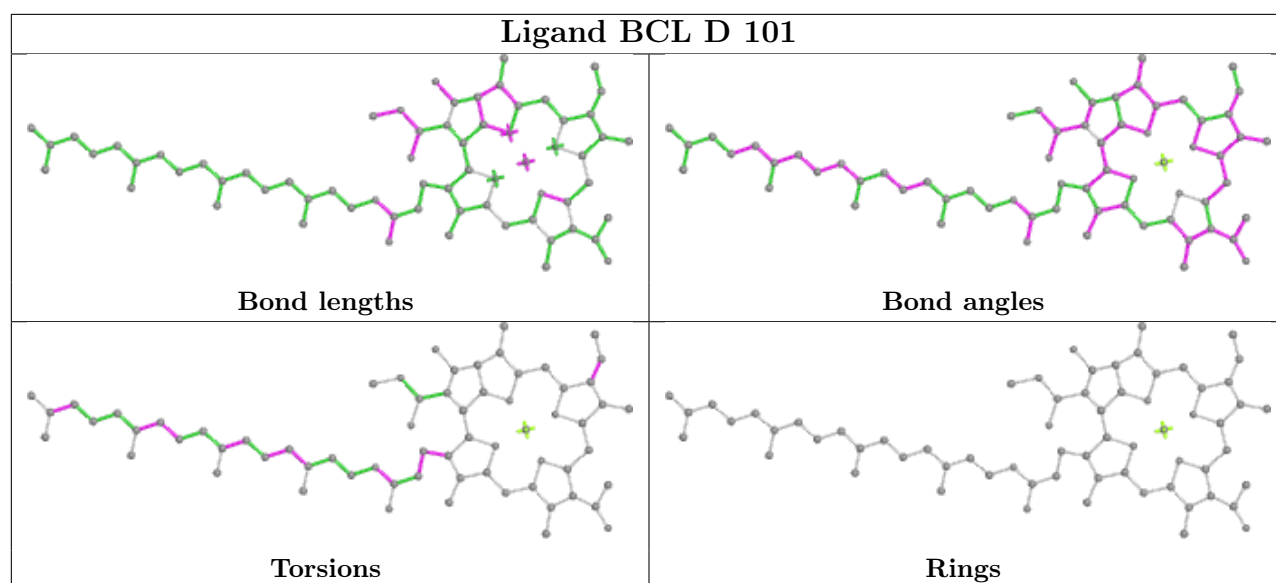
**Ligand A1EFU M 407****Ligand U10 M 404****Ligand A1EFU I 103****Ligand BCL P 102**

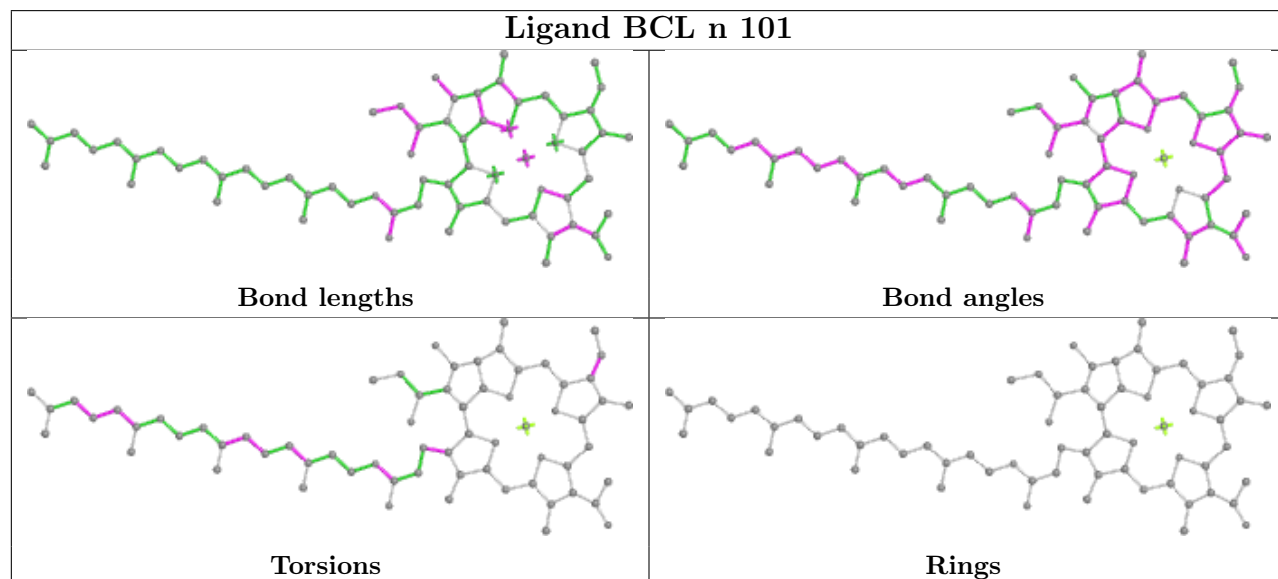
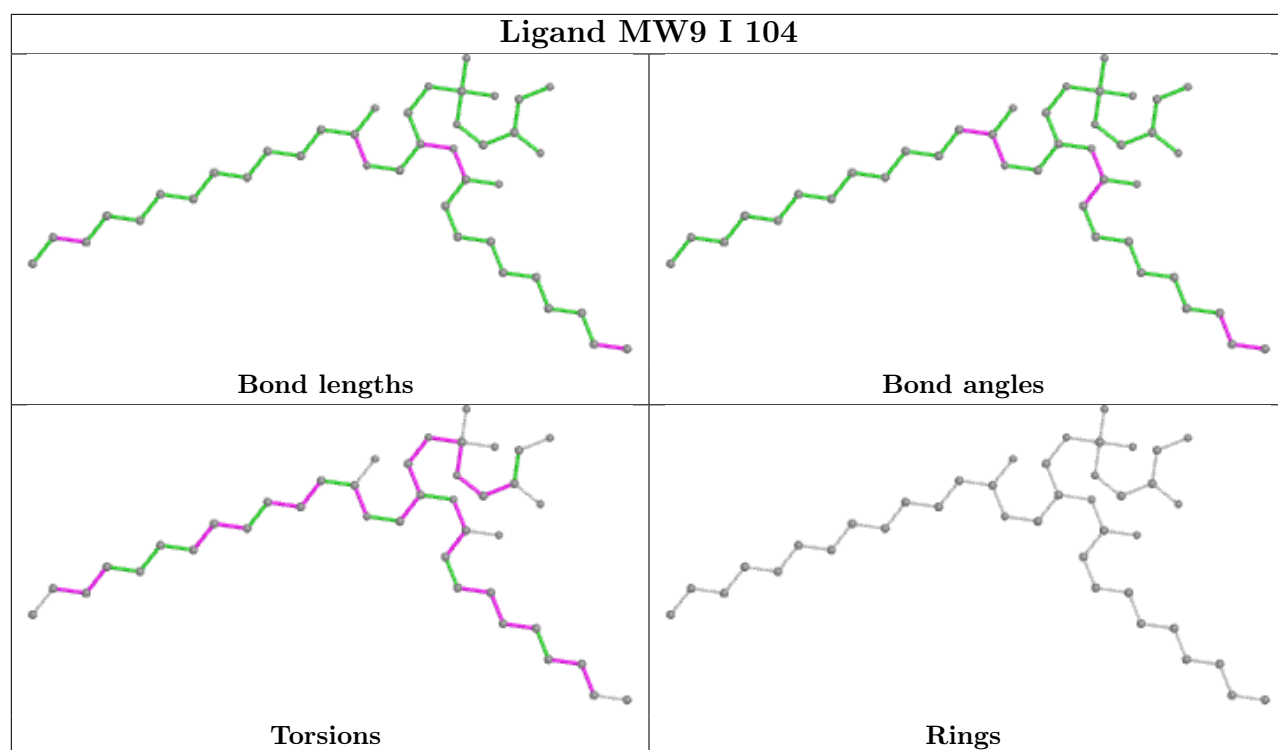




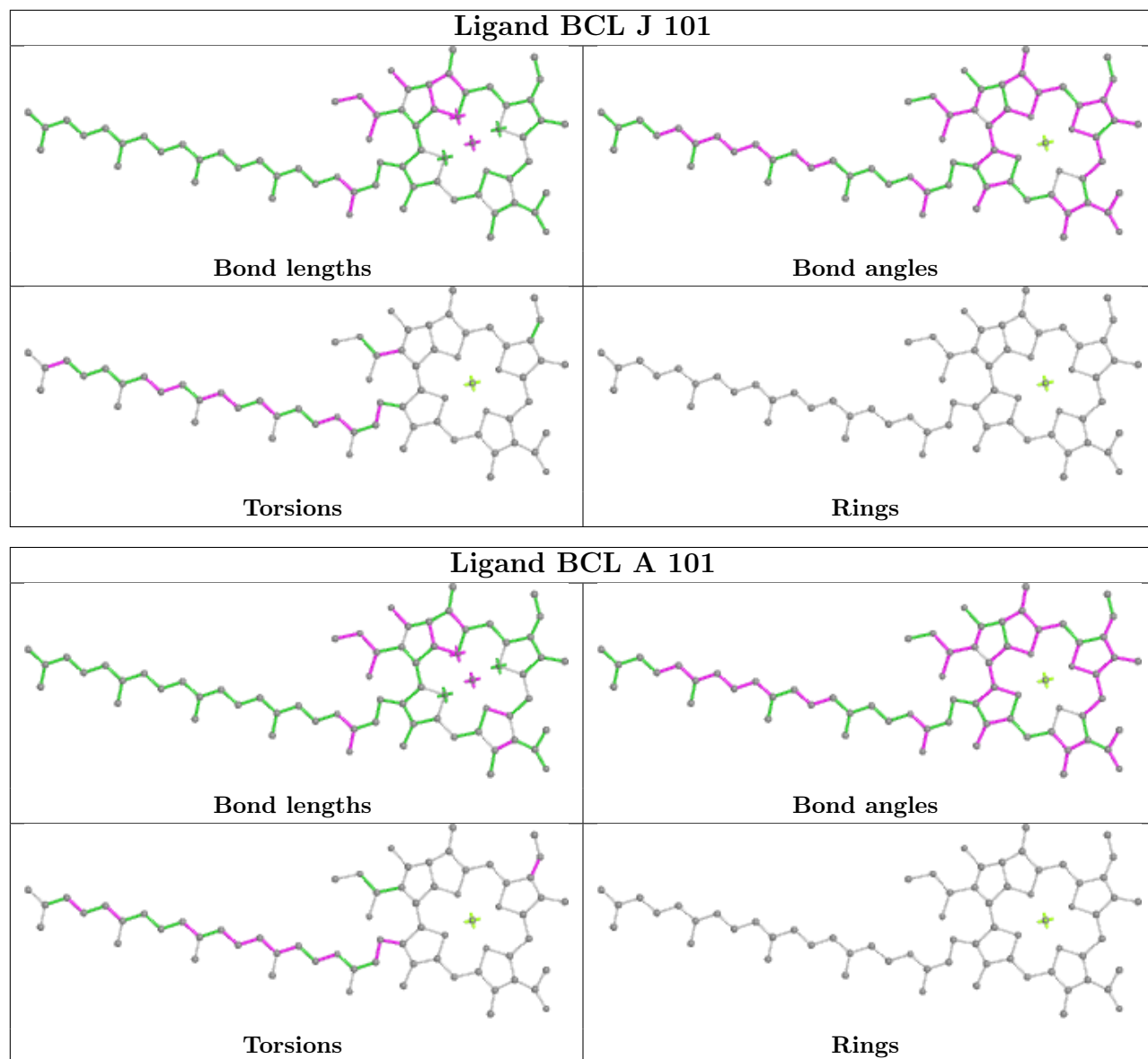


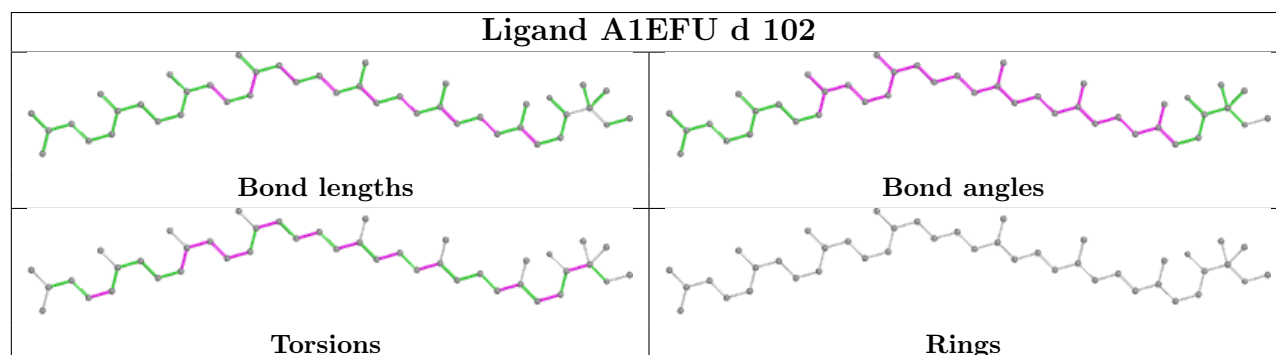
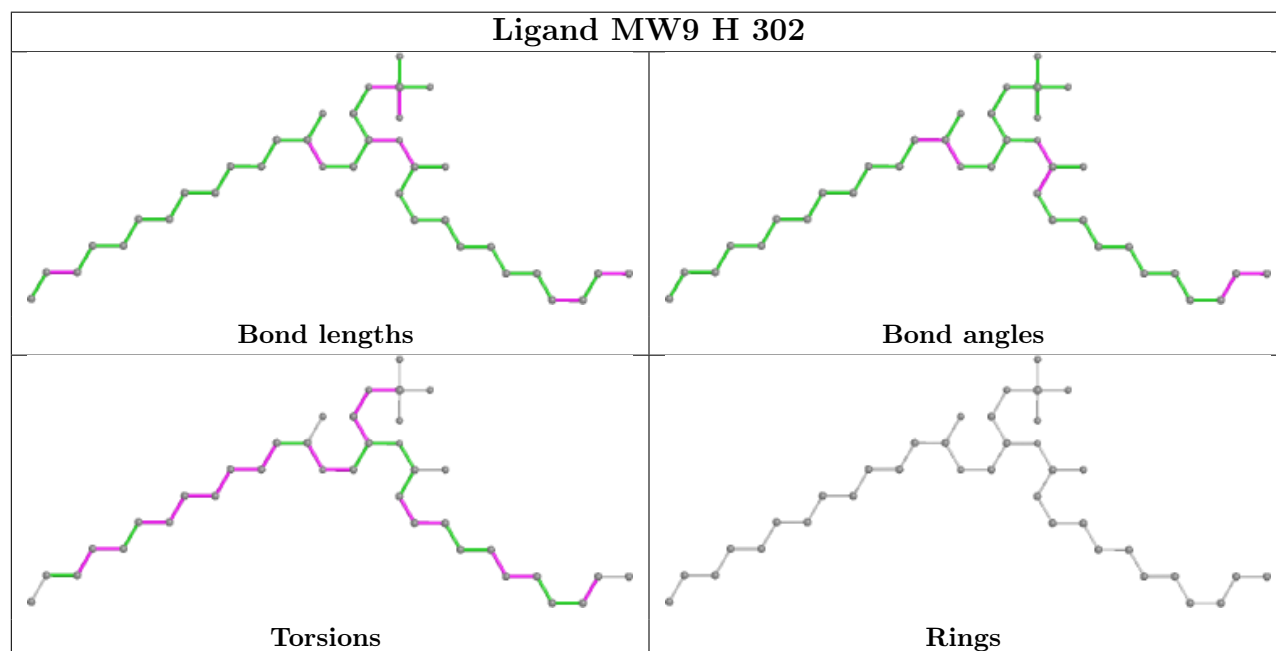
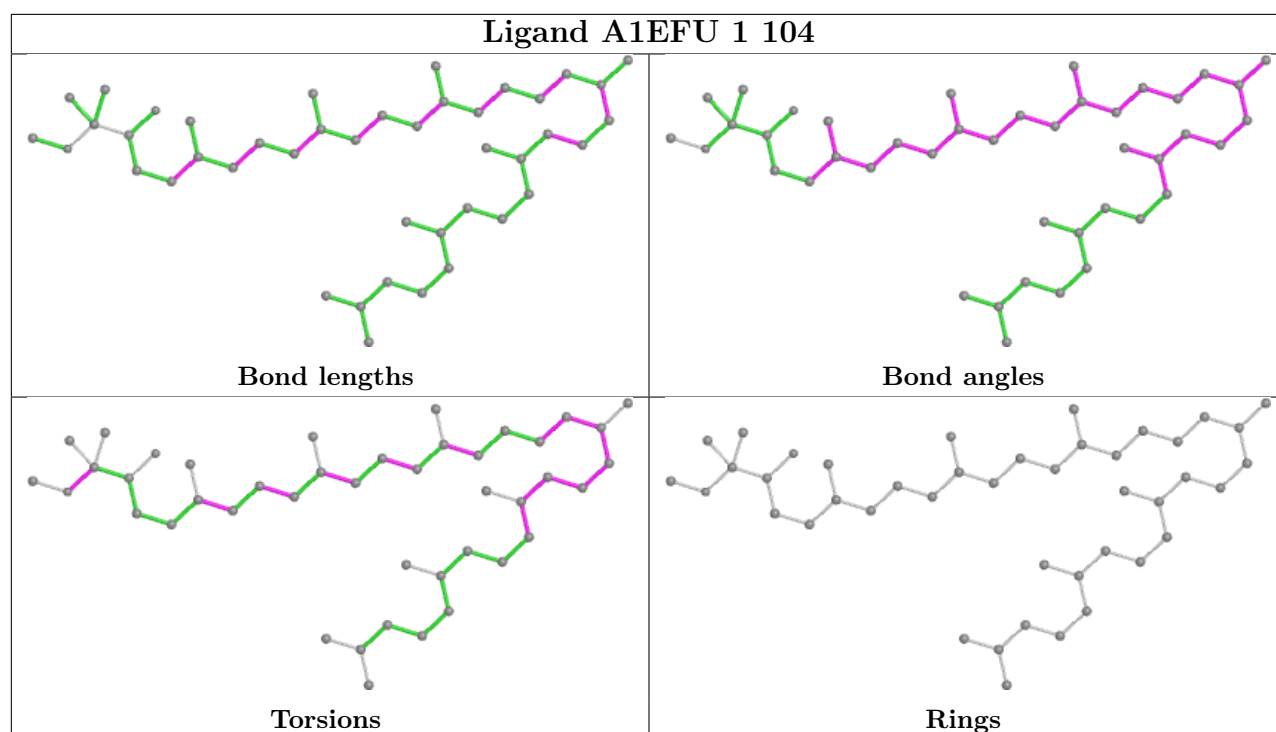


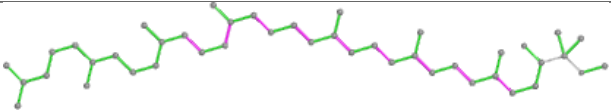
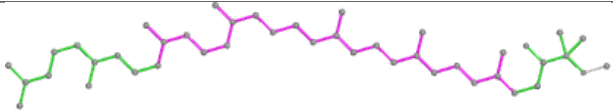
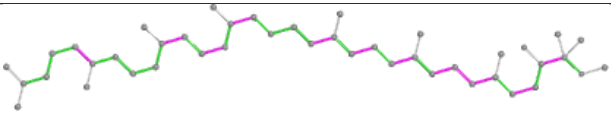
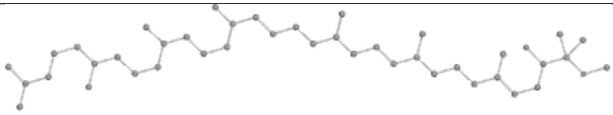
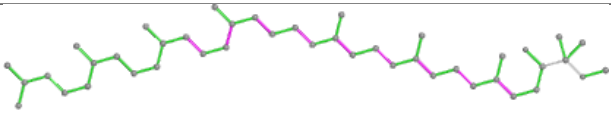
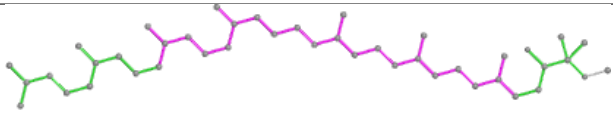
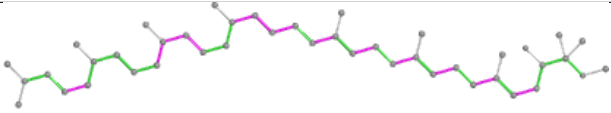
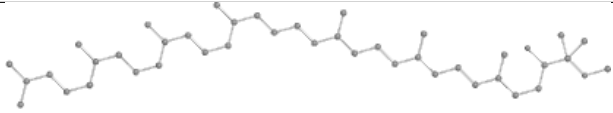
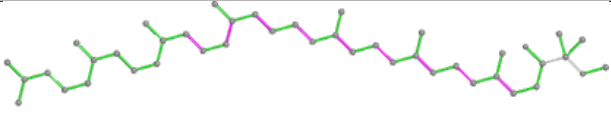
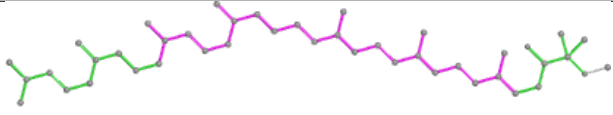
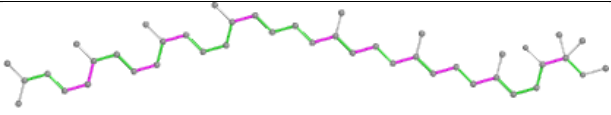
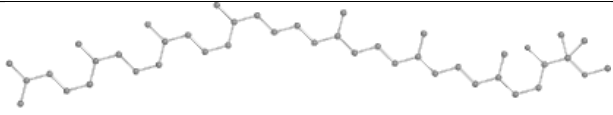
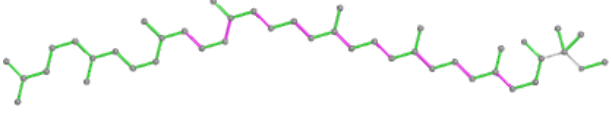
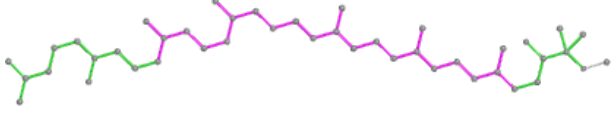
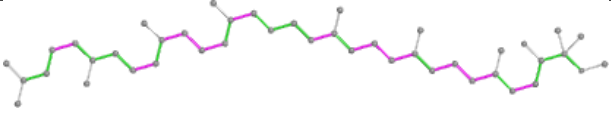
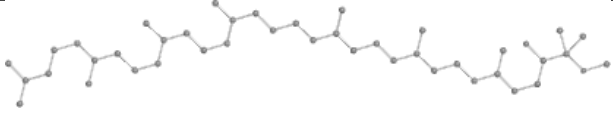


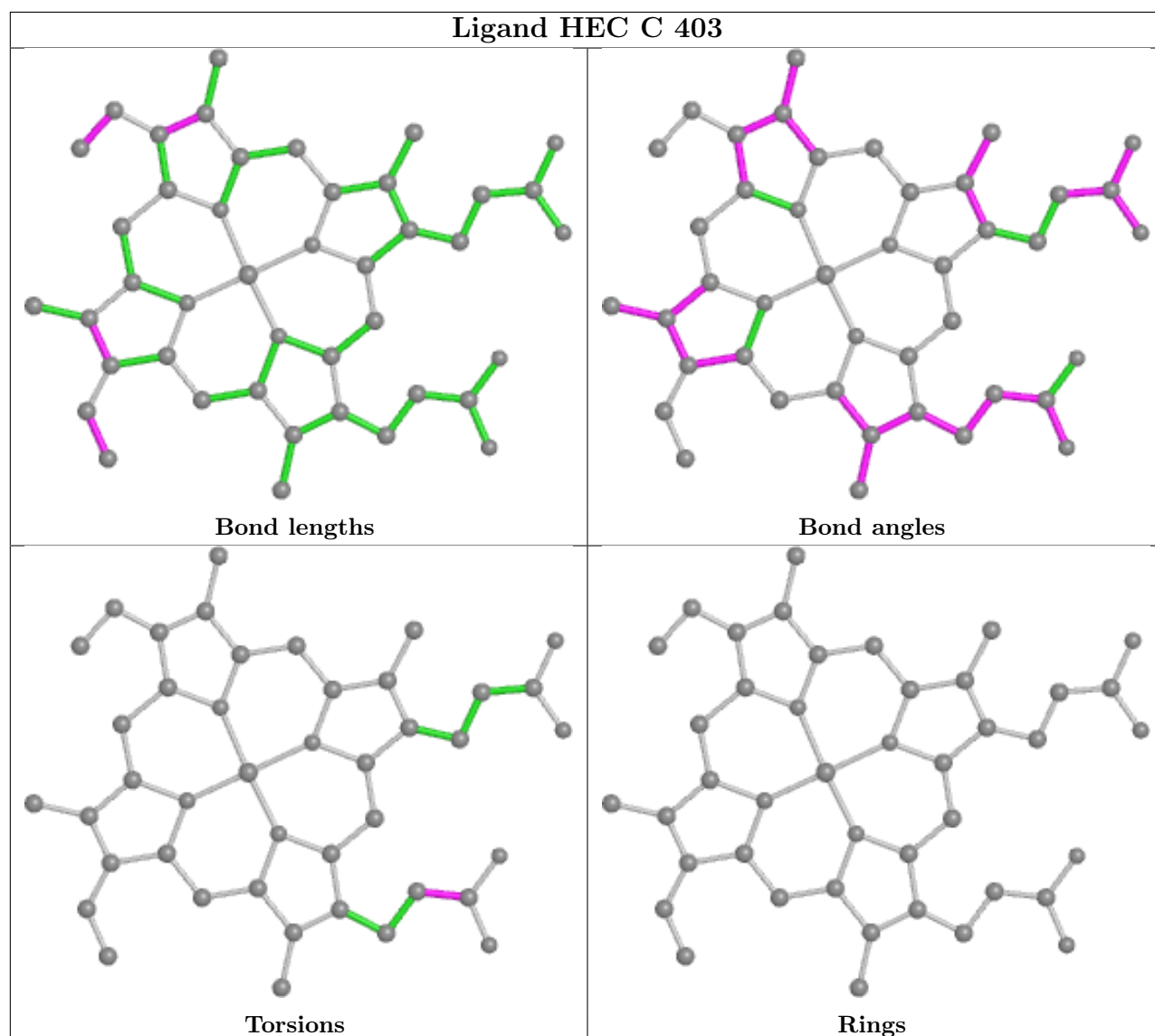
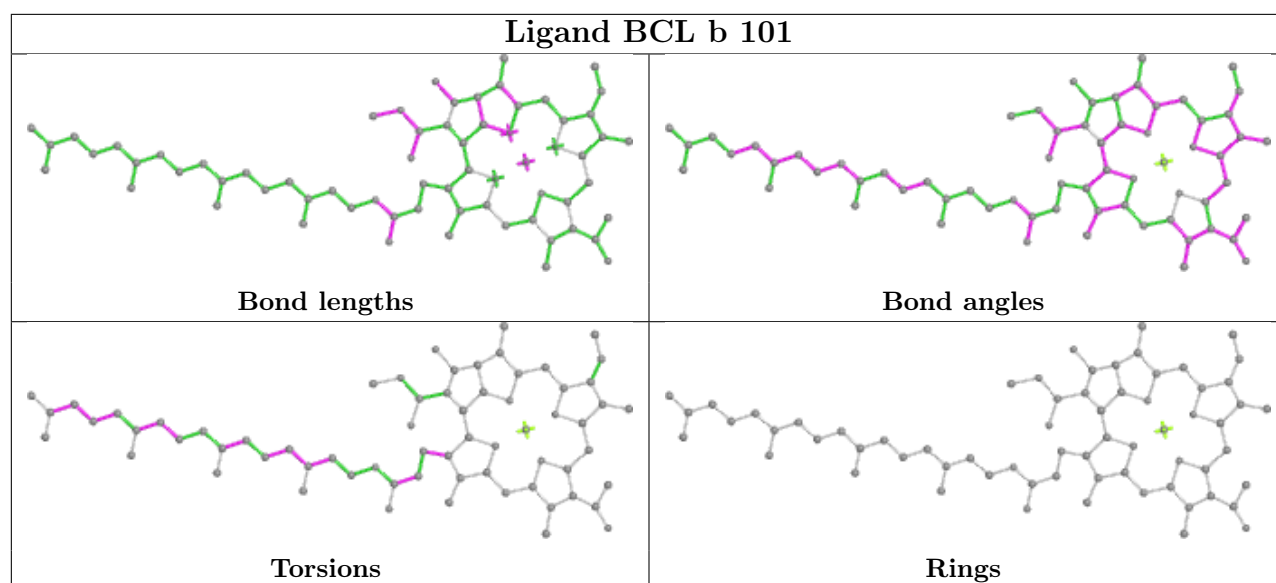


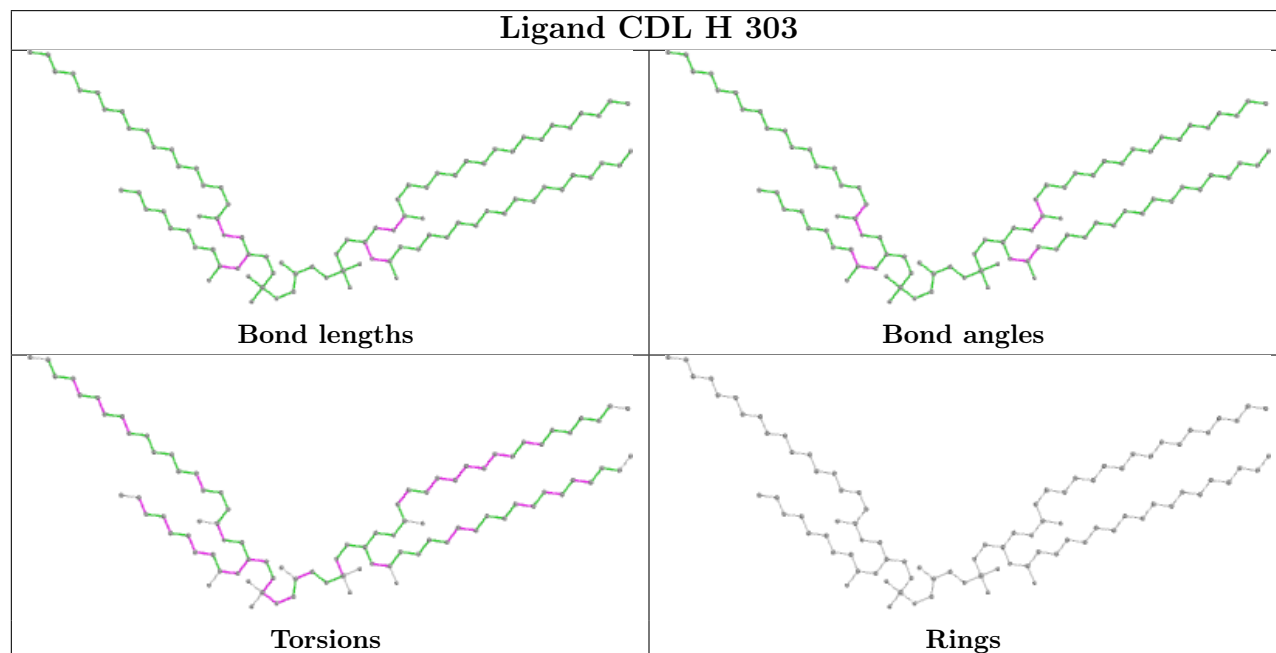
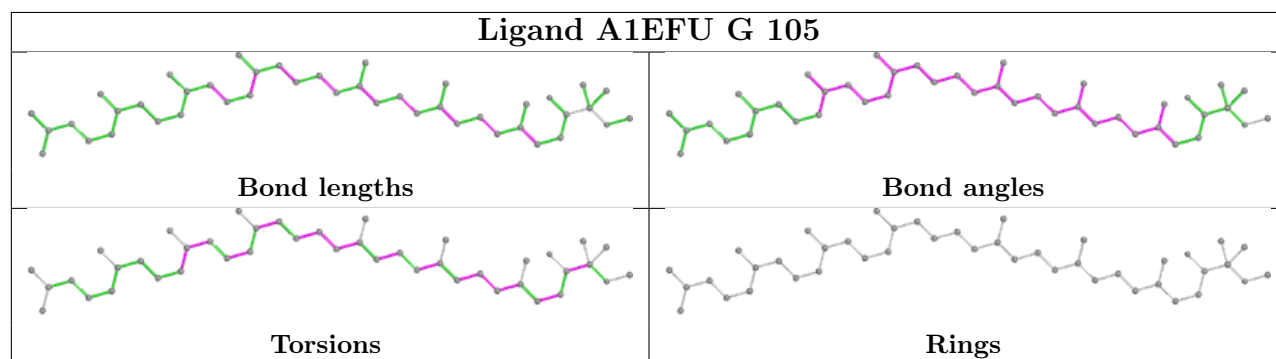
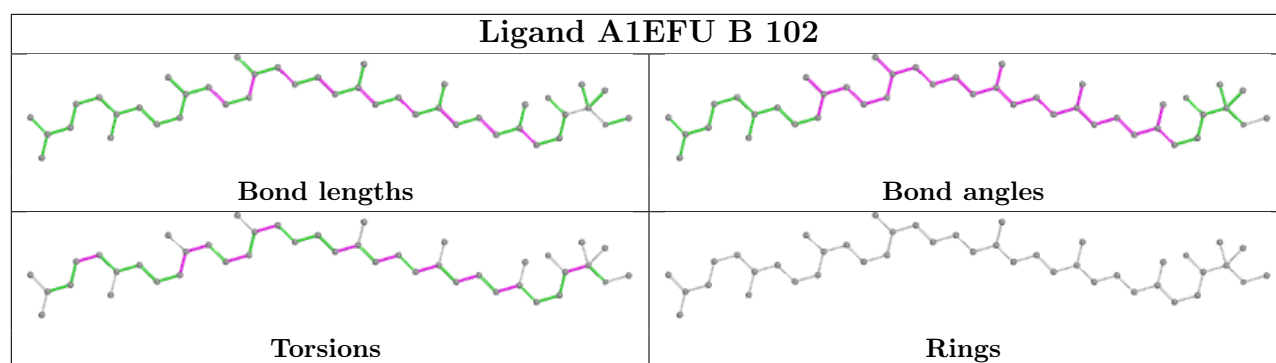


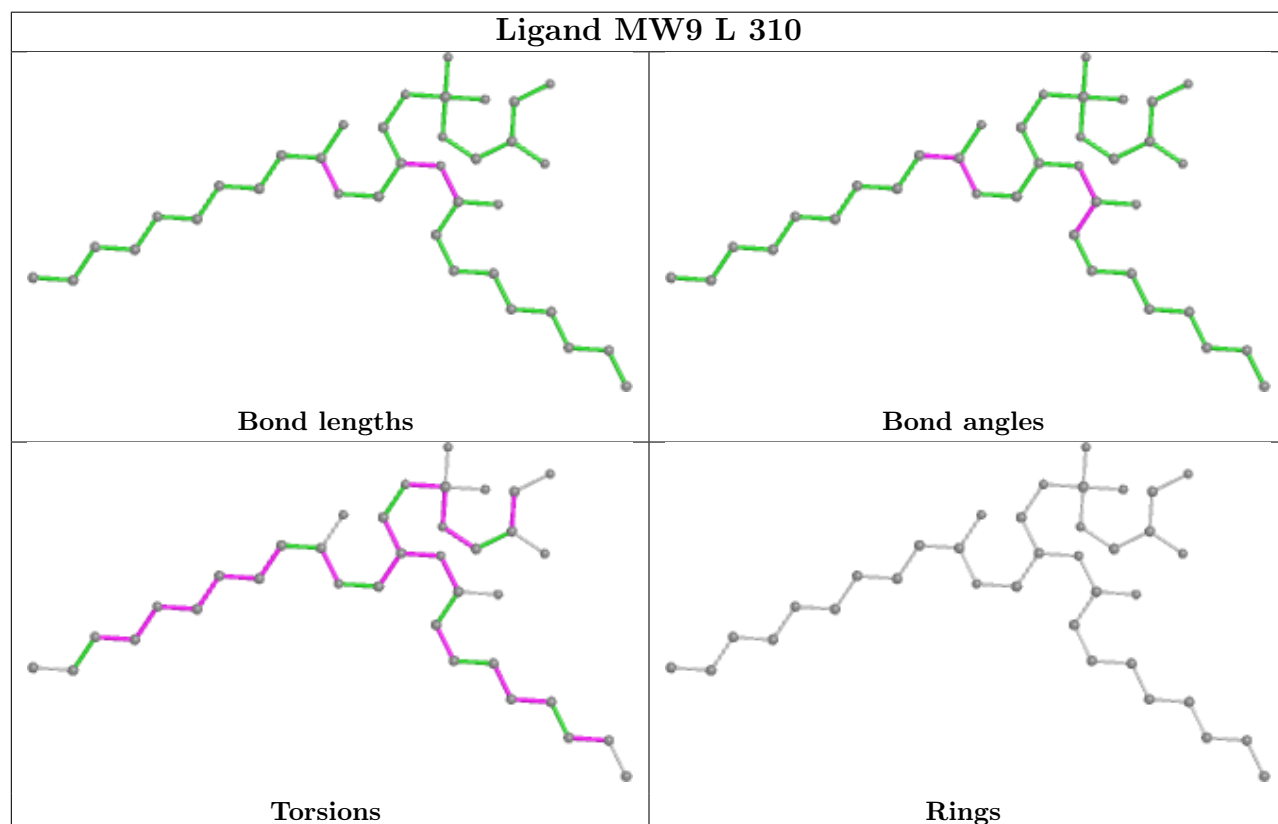
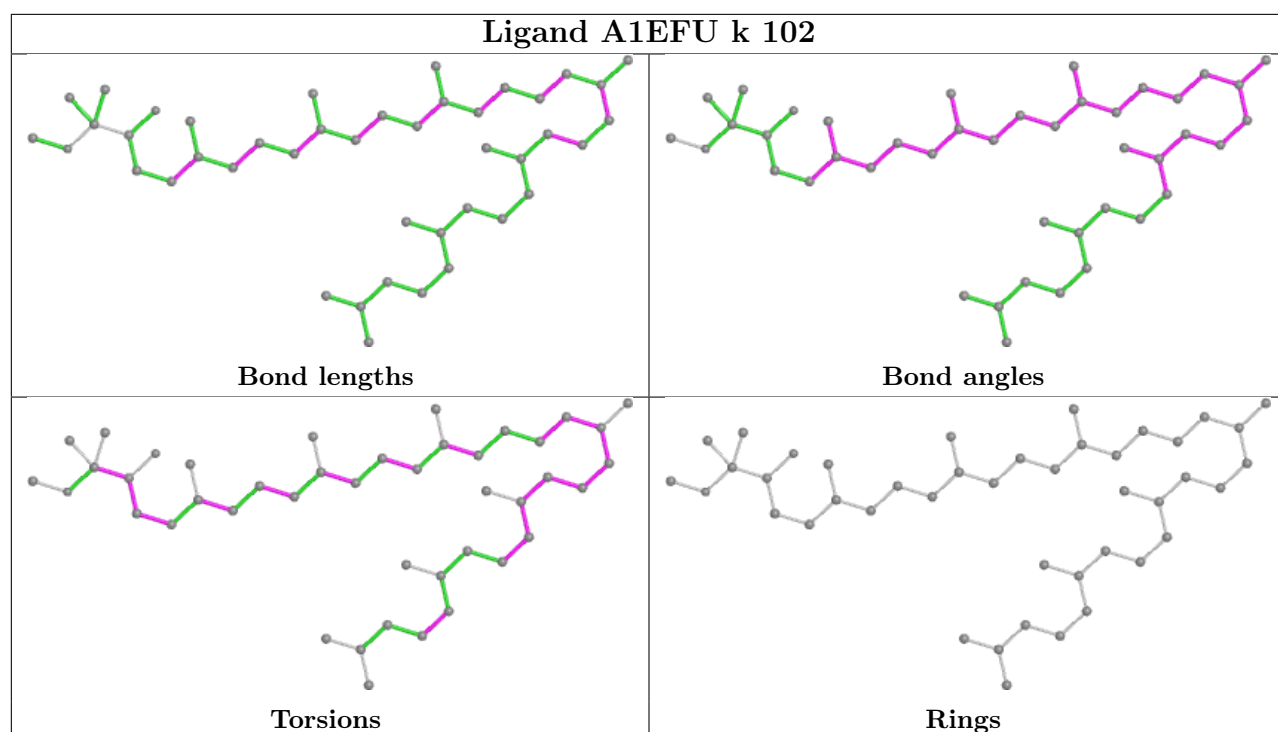


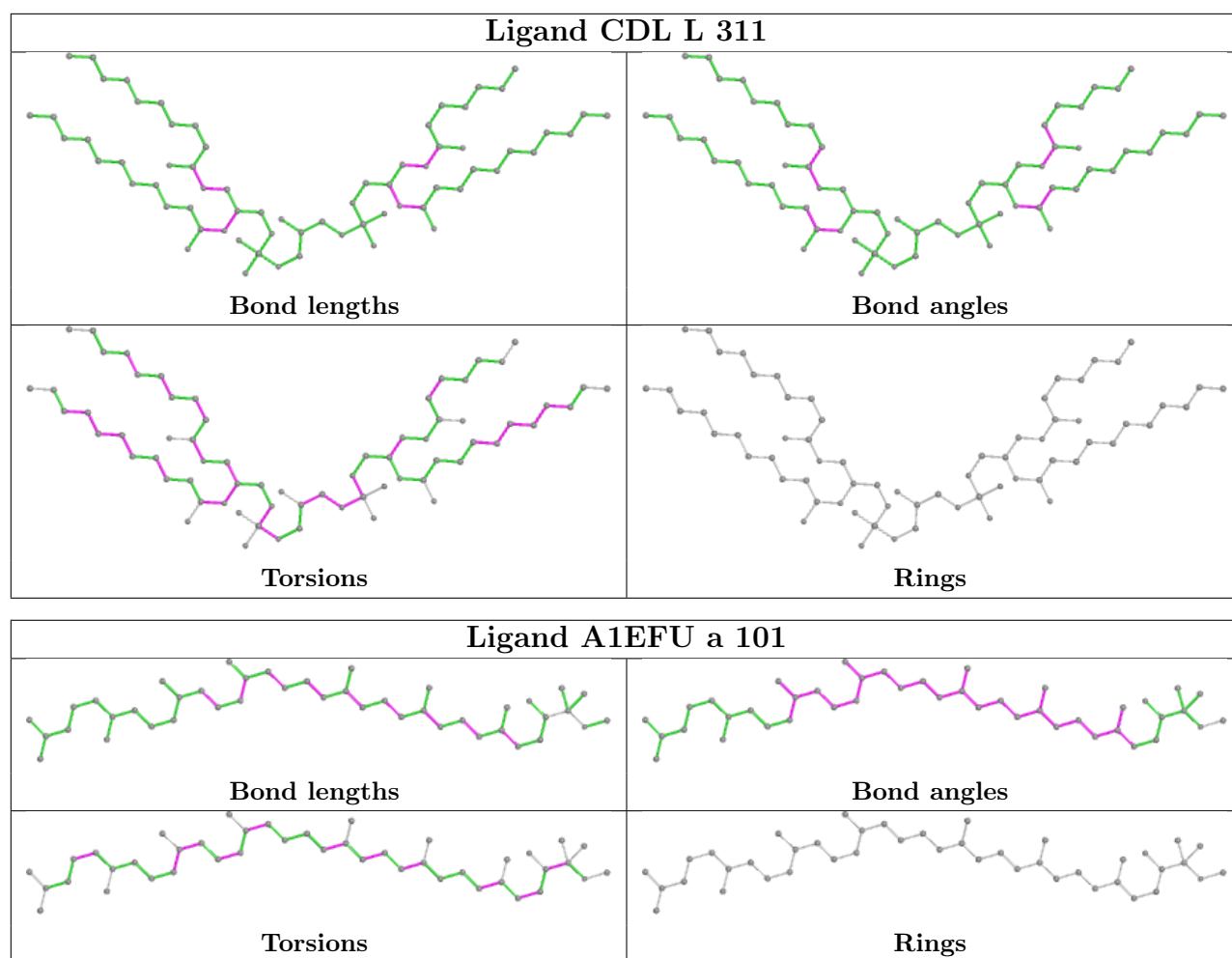


Ligand A1EFU R 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand A1EFU 2 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand A1EFU J 102	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand A1EFU v 102	
 Bond lengths	 Bond angles
 Torsions	 Rings









## 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.

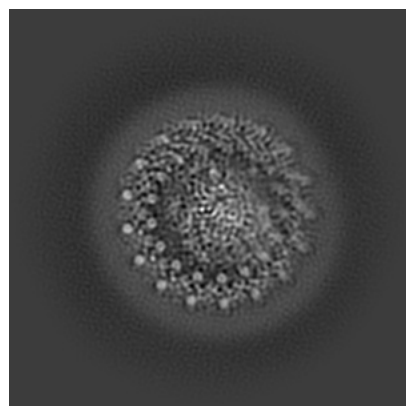
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39683. These allow visual inspection of the internal detail of the map and identification of artifacts.

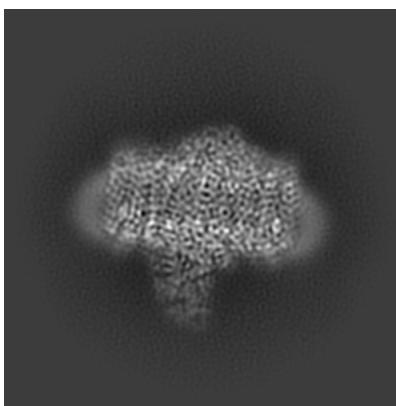
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

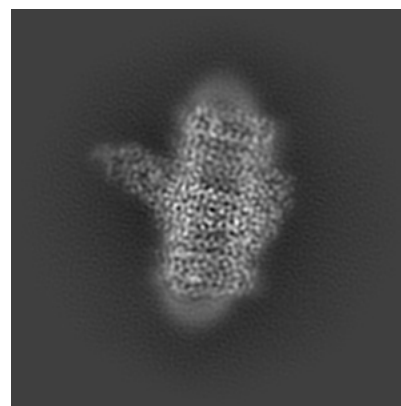
#### 6.1.1 Primary map



X

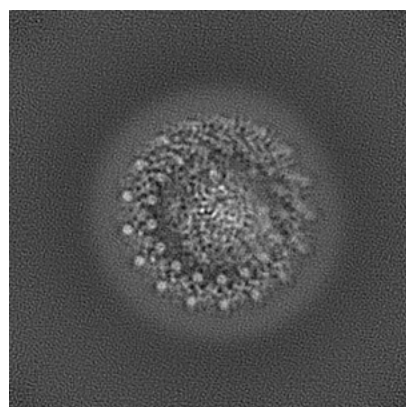


Y

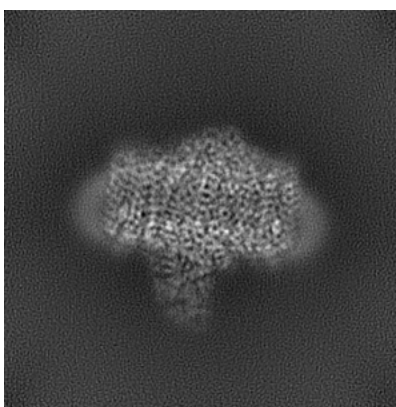


Z

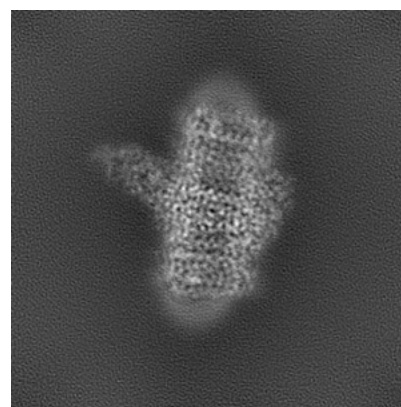
#### 6.1.2 Raw map



X



Y



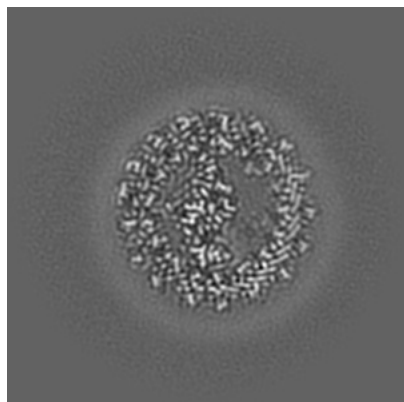
Z

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

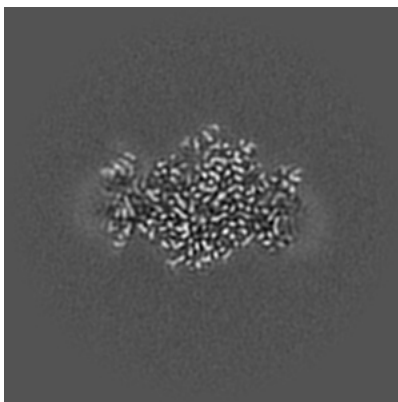


## 6.2 Central slices [i](#)

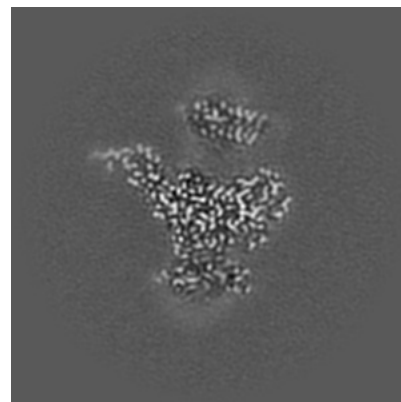
### 6.2.1 Primary map



X Index: 128

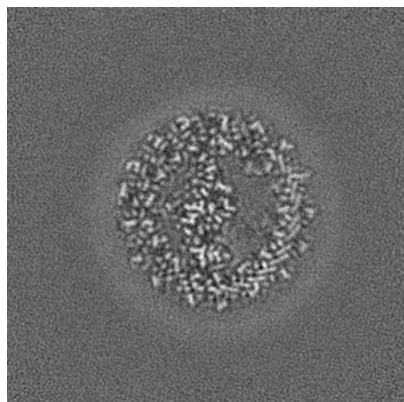


Y Index: 128

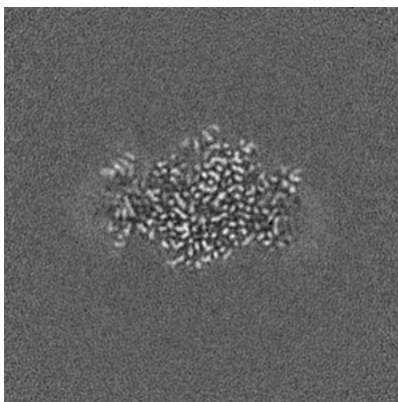


Z Index: 128

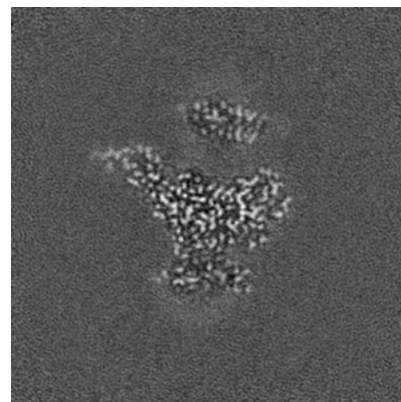
### 6.2.2 Raw map



X Index: 128



Y Index: 128

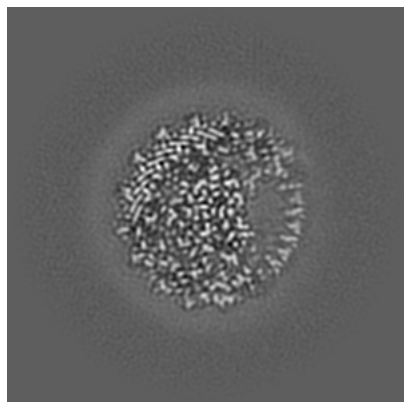


Z Index: 128

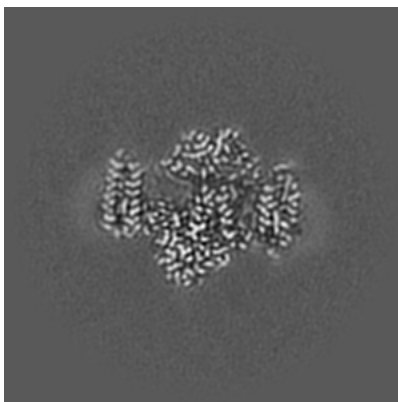
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

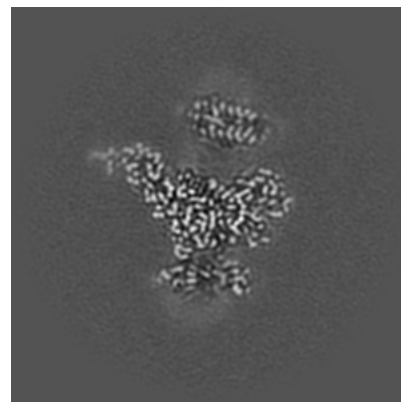
### 6.3.1 Primary map



X Index: 114

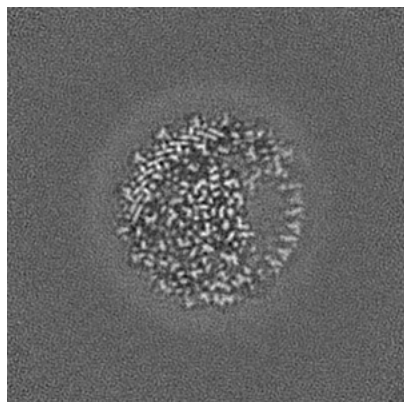


Y Index: 137

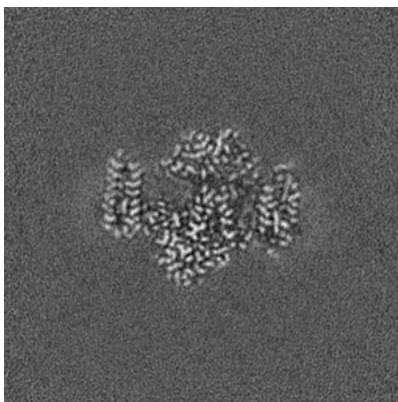


Z Index: 127

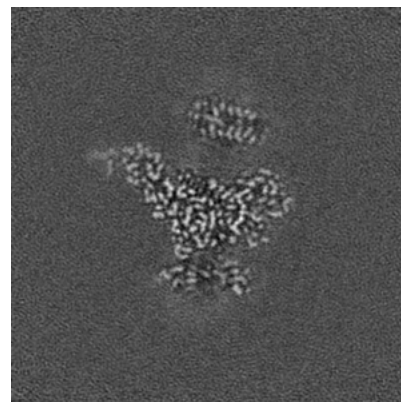
### 6.3.2 Raw map



X Index: 114



Y Index: 137

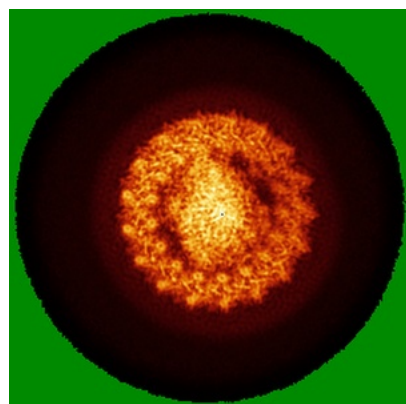


Z Index: 127

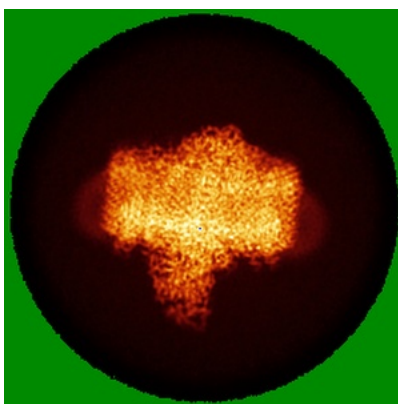
The images above show the largest variance slices of the map in three orthogonal directions.

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

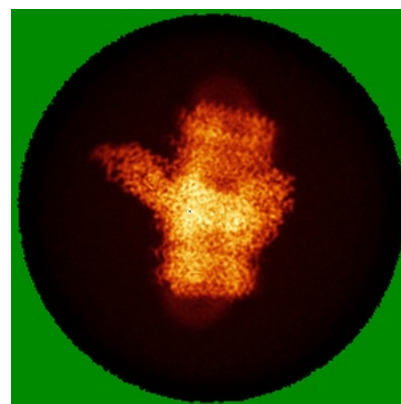
### 6.4.1 Primary map



X

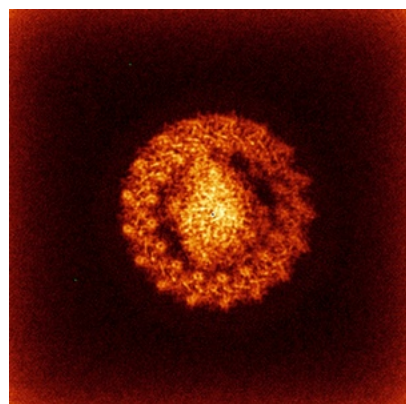


Y

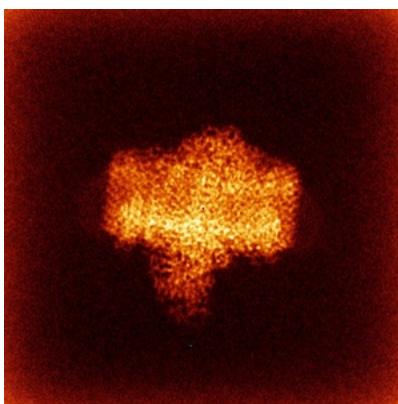


Z

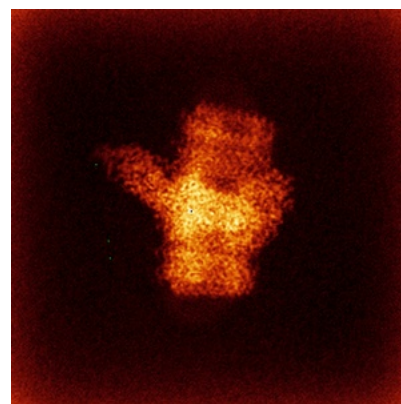
### 6.4.2 Raw map



X



Y

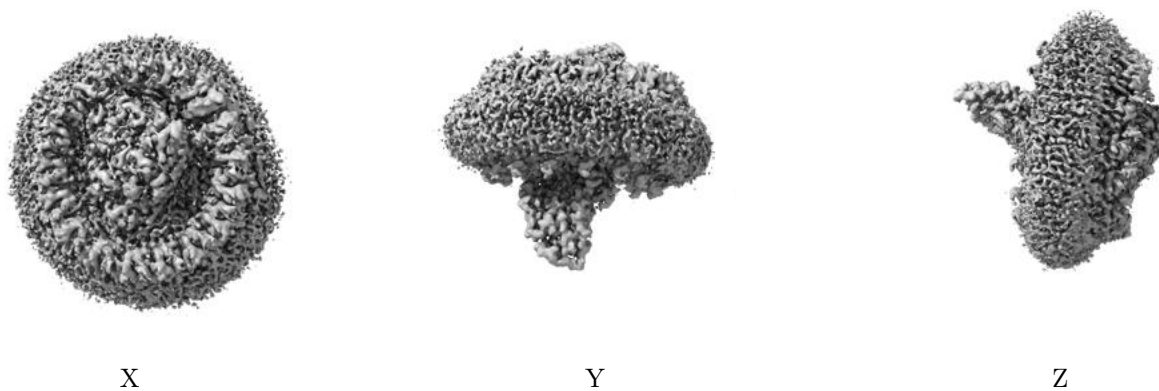


Z

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

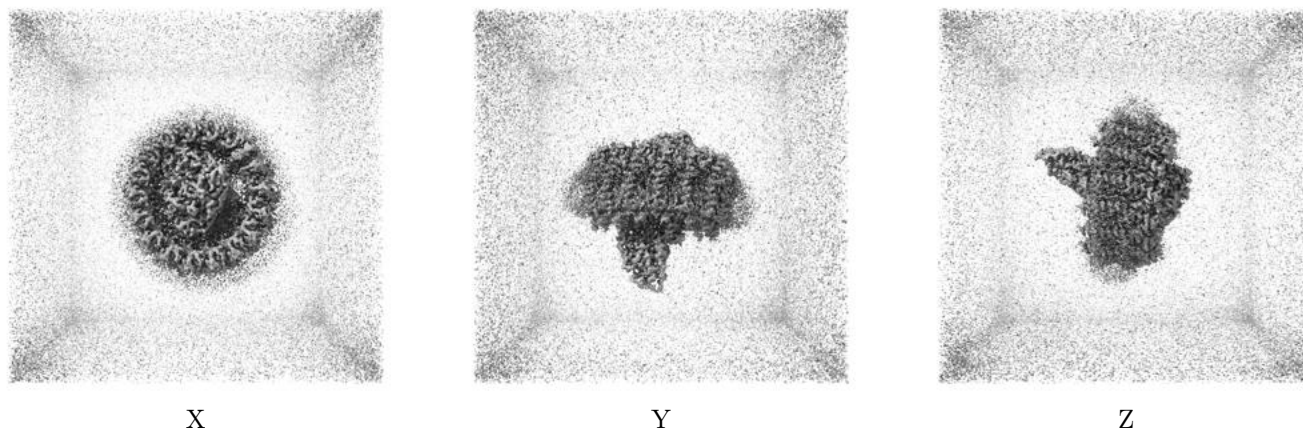
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

## 6.6 Mask visualisation [i](#)

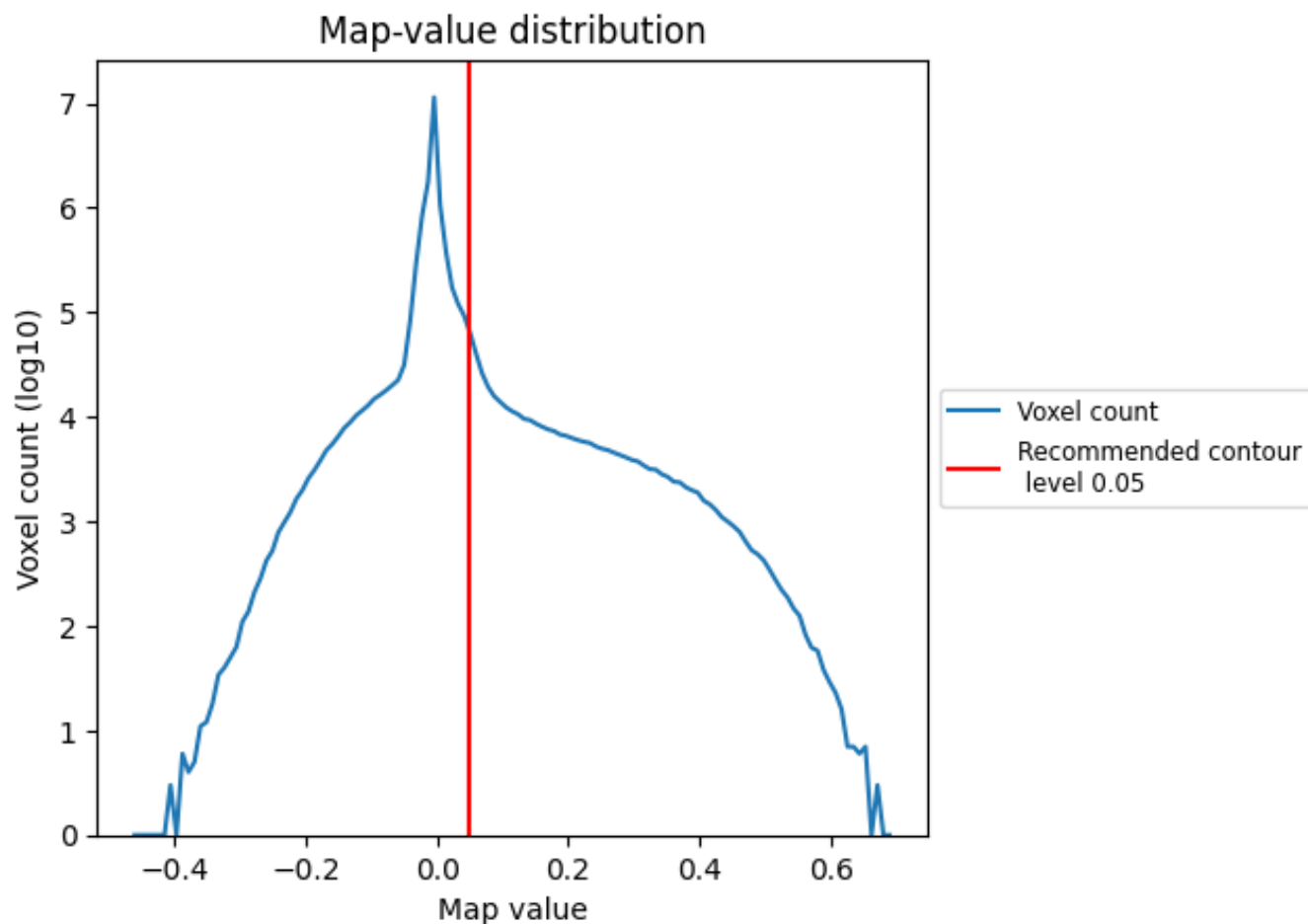
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

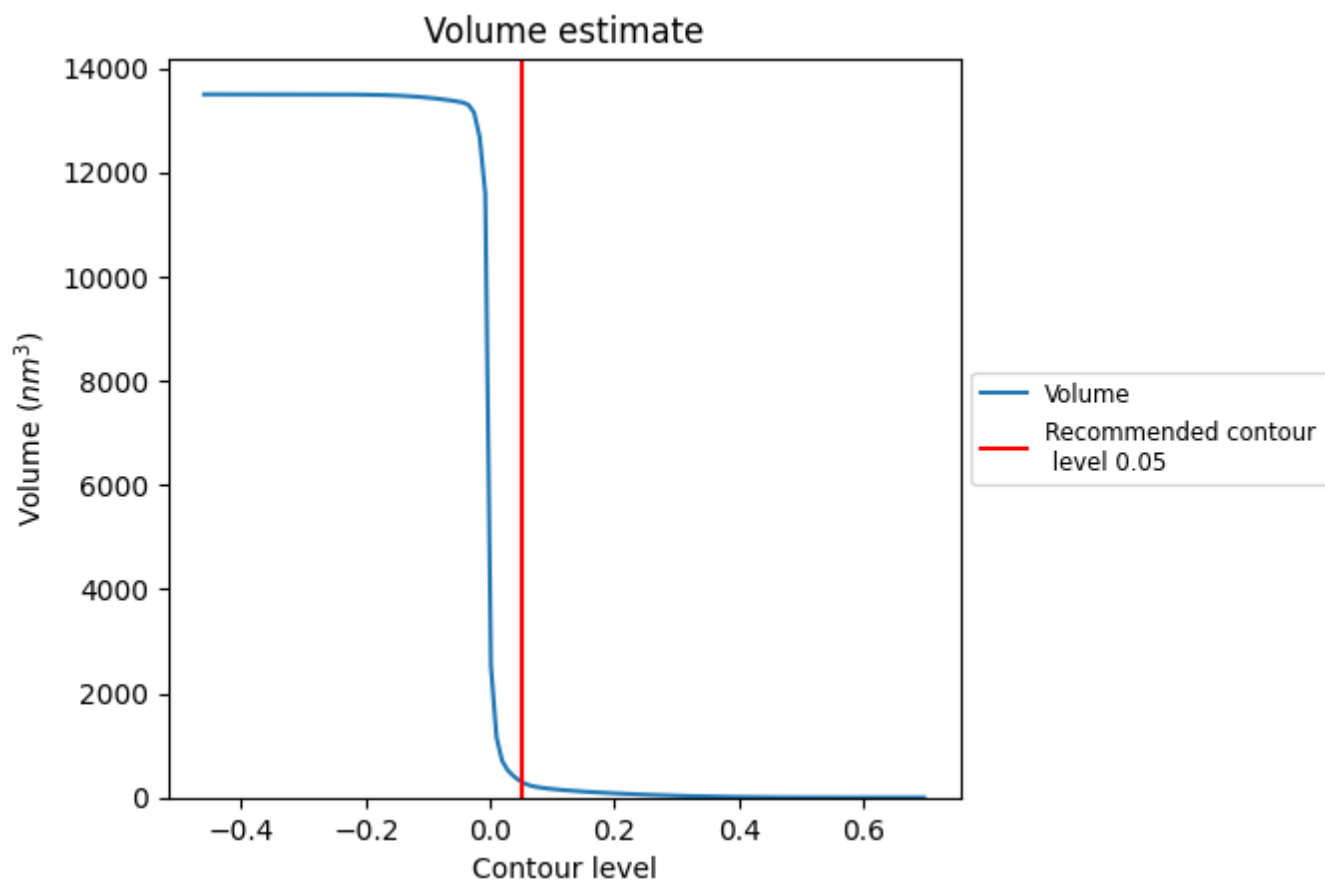
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

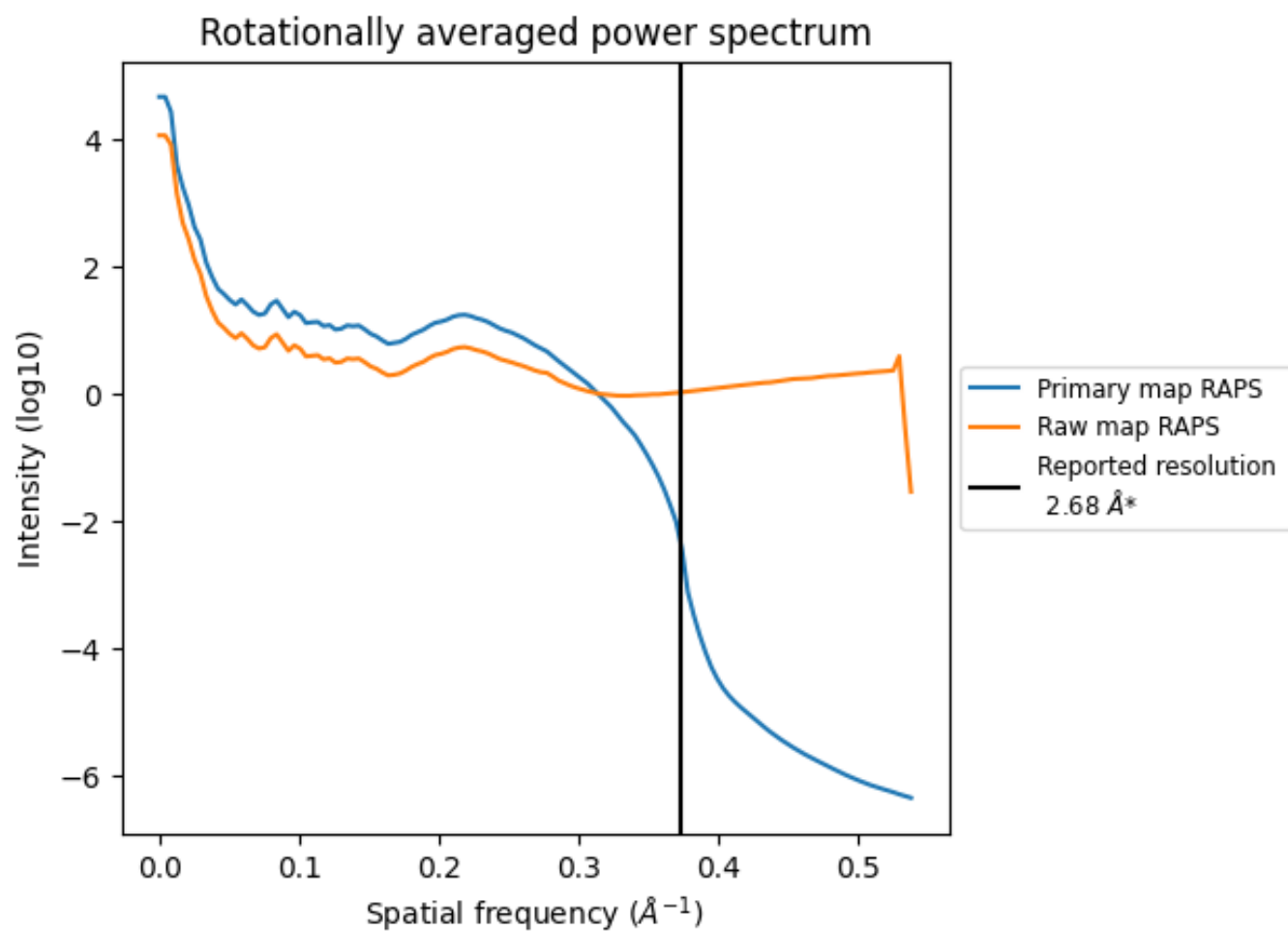
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 307 nm<sup>3</sup>; this corresponds to an approximate mass of 277 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ

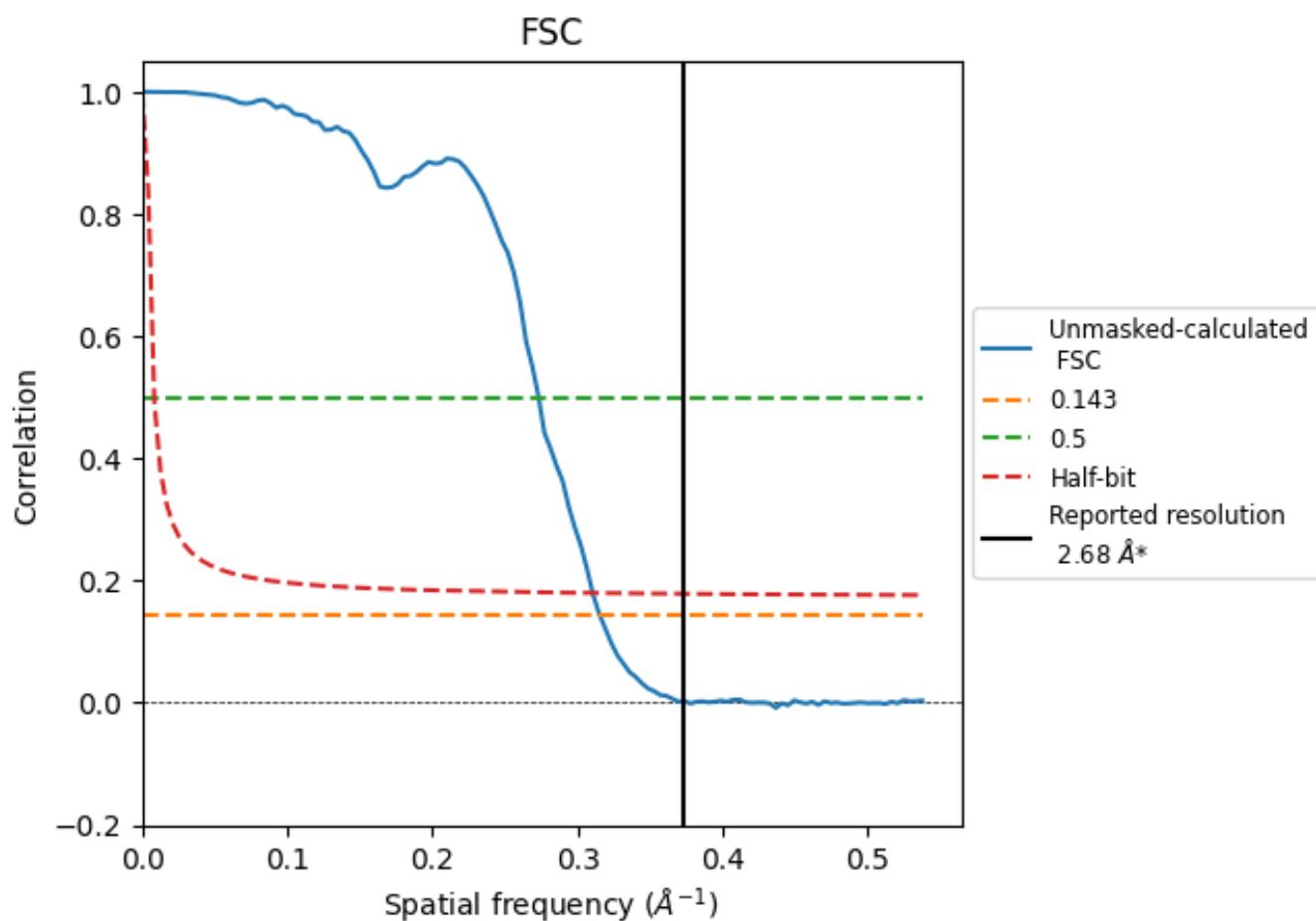


\*Reported resolution corresponds to spatial frequency of 0.373 Å<sup>-1</sup>

## 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 0.373  $\text{\AA}^{-1}$



## 8.2 Resolution estimates [i](#)

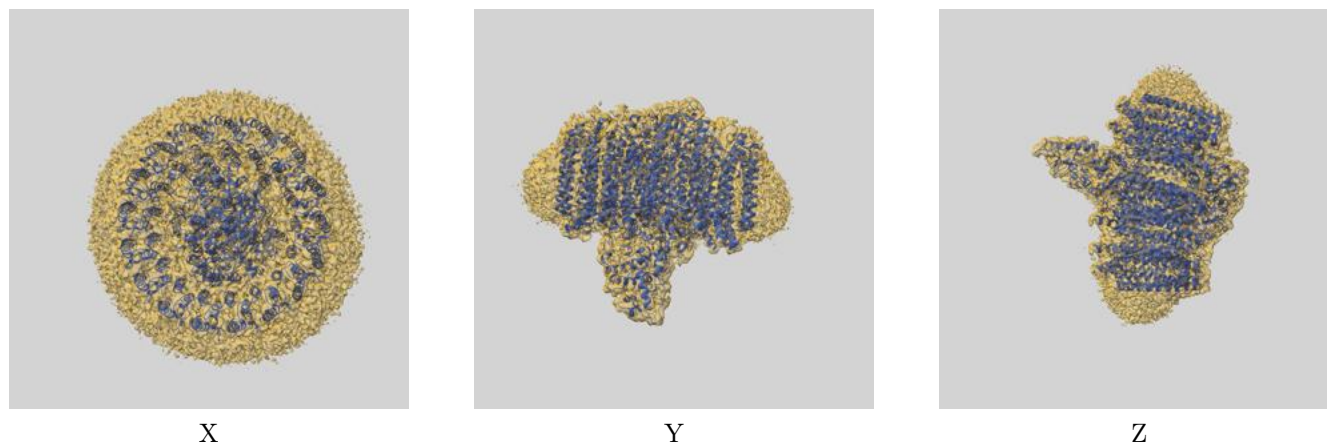
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.68	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.17	3.66	3.22

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.17 differs from the reported value 2.68 by more than 10 %

## 9 Map-model fit [i](#)

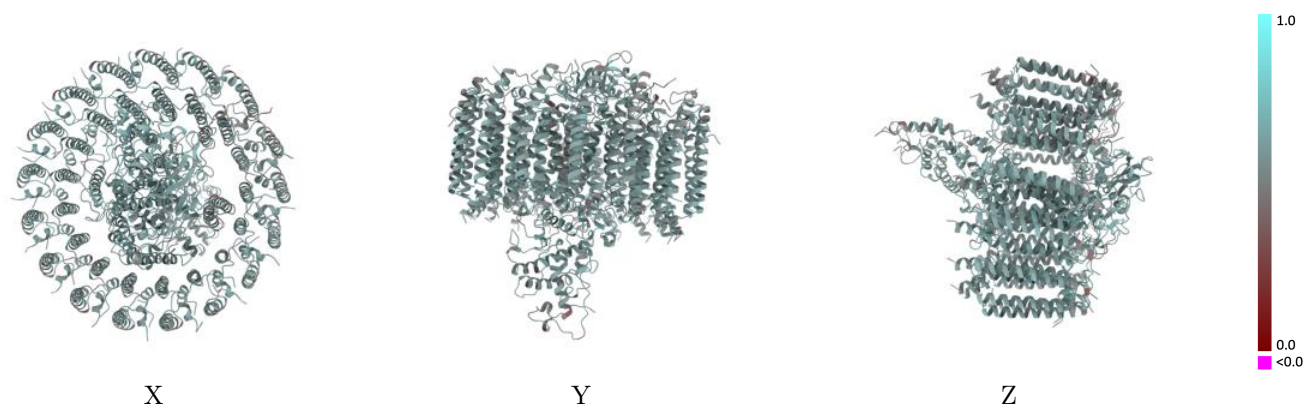
This section contains information regarding the fit between EMDB map EMD-39683 and PDB model 8YZ2. Per-residue inclusion information can be found in section [3](#) on page [17](#).

### 9.1 Map-model overlay [i](#)



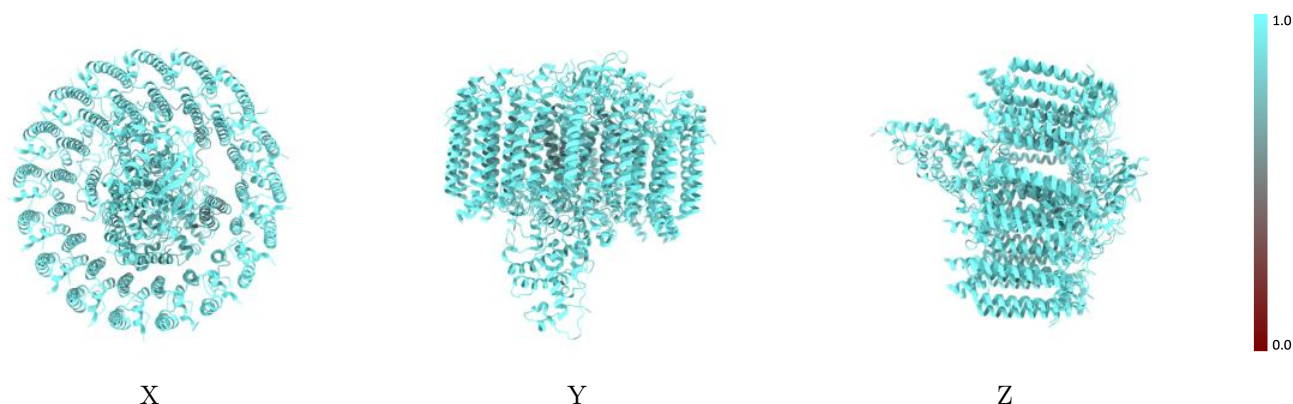
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



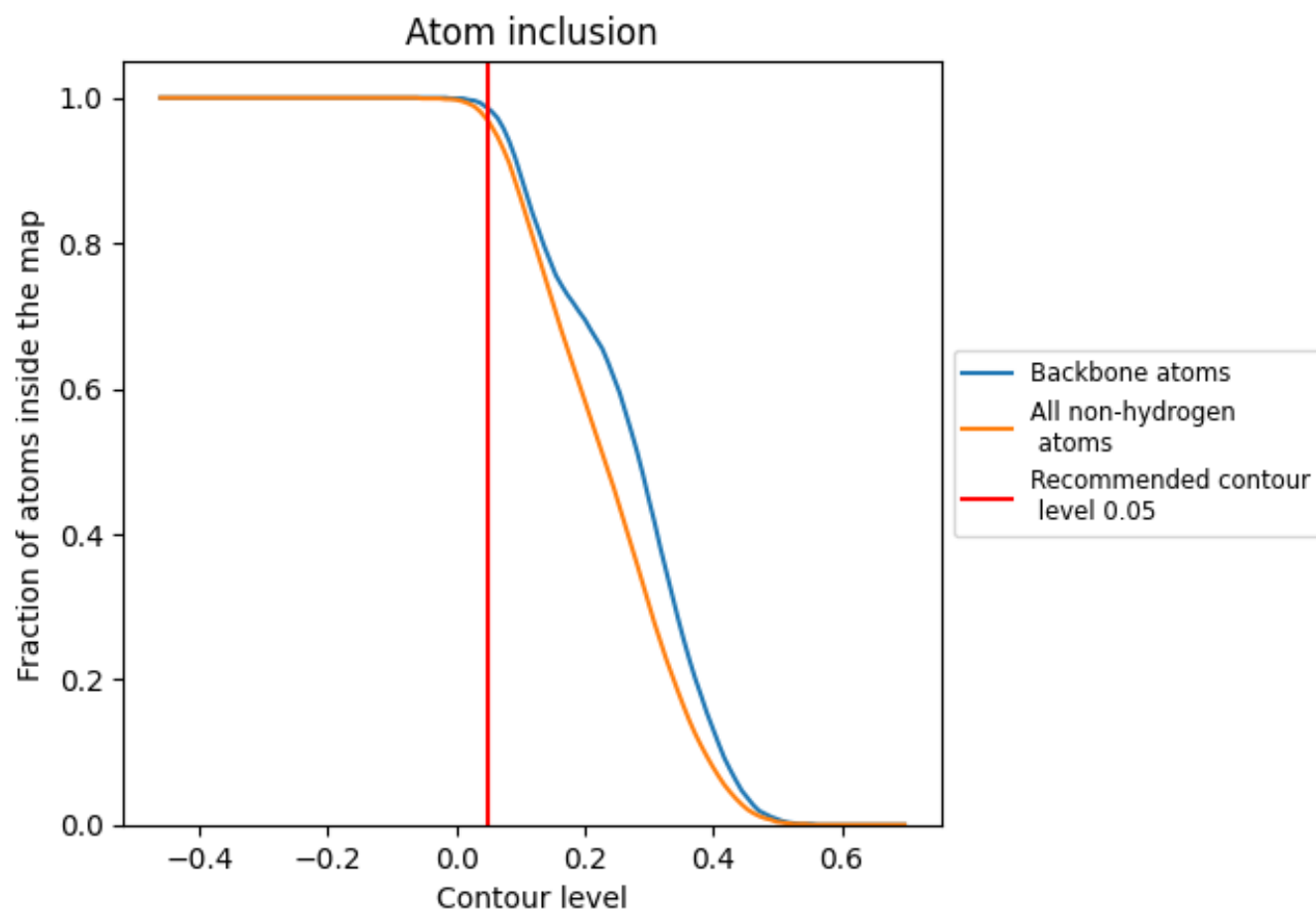
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 97% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ



The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9680	 0.5800
1	 0.9600	 0.5810
2	 0.9520	 0.5530
A	 0.9520	 0.5690
B	 0.9770	 0.5810
C	 0.9760	 0.5720
D	 0.9670	 0.5890
E	 0.9750	 0.5900
F	 0.9750	 0.5920
G	 0.9610	 0.5930
H	 0.9780	 0.5910
I	 0.9770	 0.5850
J	 0.9770	 0.5900
K	 0.9770	 0.5830
L	 0.9730	 0.6040
M	 0.9790	 0.6030
N	 0.9500	 0.5600
O	 0.8260	 0.5340
P	 0.9630	 0.5820
Q	 0.9570	 0.5780
R	 0.9790	 0.5810
S	 0.9650	 0.5760
T	 0.9580	 0.5730
V	 0.9500	 0.5440
a	 0.9520	 0.5520
b	 0.9760	 0.5760
d	 0.9650	 0.5670
e	 0.9800	 0.5820
f	 0.9860	 0.5840
g	 0.9860	 0.5820
i	 0.9750	 0.5830
j	 0.9830	 0.5750
k	 0.9620	 0.5540
n	 0.9610	 0.5570
p	 0.9830	 0.5600



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
q	 0.9690	 0.5700
r	 0.9690	 0.5700
s	 0.9610	 0.5680
t	 0.9560	 0.5480
v	 0.9290	 0.5390