



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 06:12 AM JST

PDB ID : 9KM0 / pdb_00009km0
EMDB ID : EMD-62419
Title : Cryo-EM structure of a tri-heme cytochrome-associated RC-LH1 complex from a marine photoheterotrophic bacterium, purified with EDTA-2Na-containing solutions
Authors : Chen, J.H.
Deposited on : 2024-11-15
Resolution : 2.78 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

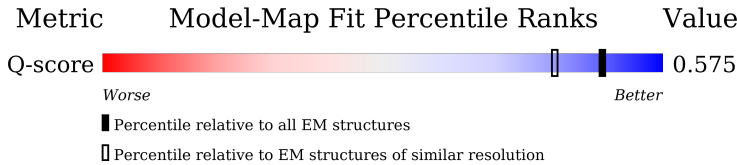
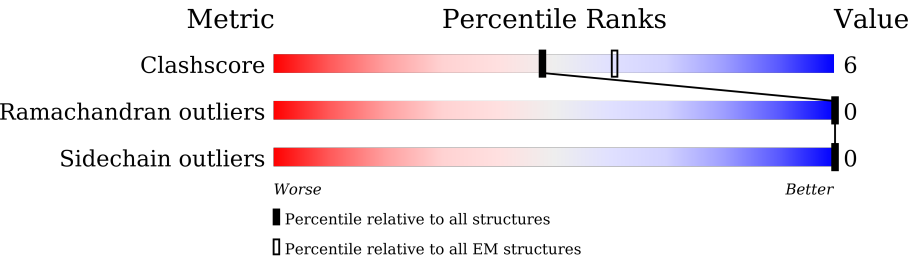
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.78 Å.

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



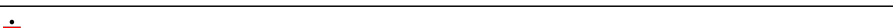
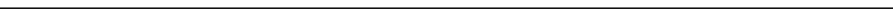
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10754 (2.28 - 3.28)

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

Mol	Chain	Length	Quality of chain
1	1	53	83% 11% 6%
1	A	53	83% 13% .
1	B	53	87% 9% .
1	D	53	89% 8% .

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	HEC	C	401	X	-	-	-
16	HEC	C	402	X	-	-	-
16	HEC	C	403	X	-	-	-
9	A1EFU	2	102	-	X	-	-

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 28252 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 (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆).



Continued on next page...

Continued from previous page...

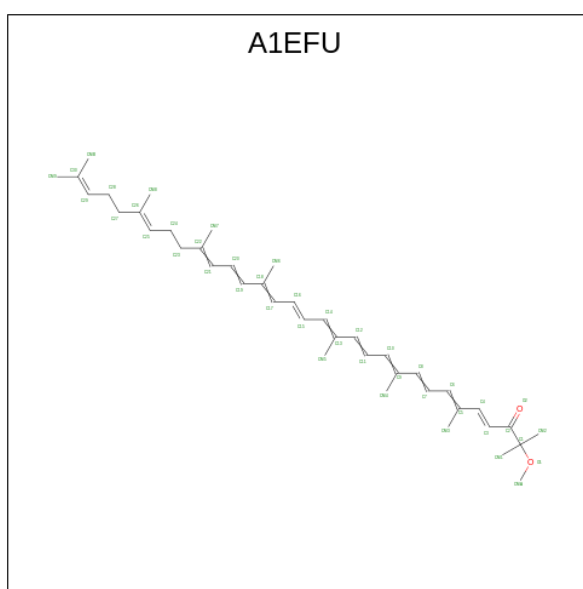
Mol	Chain	Residues	Atoms					AltConf
8	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	k	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	K	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	j	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	J	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	i	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	I	1	Total 66	C 55	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-dotriacont a-4,6,8,10,12,14,16,18,20,22,26,30-dodecaen-3-one (CCD ID: A1EFU) (formula: C₄₁H₅₈O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
9	P	1	Total	C	O	0
			43	41	2	
9	v	1	Total	C	O	0
			43	41	2	
9	v	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	s	1	Total	C	O	0
			43	41	2	
9	s	1	Total	C	O	0
			43	41	2	

Continued on next page...

Continued from previous page...

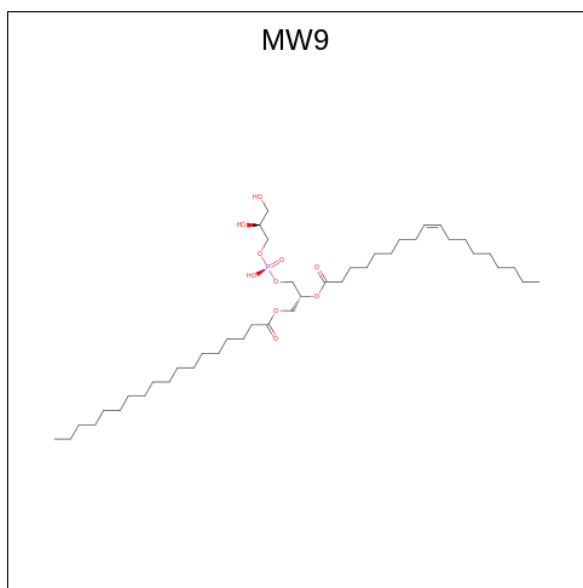
Mol	Chain	Residues	Atoms			AltConf
9	r	1	Total 43	C 41	O 2	0
9	R	1	Total 43	C 41	O 2	0
9	q	1	Total 43	C 41	O 2	0
9	p	1	Total 43	C 41	O 2	0
9	2	1	Total 43	C 41	O 2	0
9	2	1	Total 43	C 41	O 2	0
9	2	1	Total 43	C 41	O 2	0
9	N	1	Total 43	C 41	O 2	0
9	k	1	Total 43	C 41	O 2	0
9	K	1	Total 43	C 41	O 2	0
9	j	1	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	J	1	Total 43	C 41	O 2	0
9	I	1	Total 43	C 41	O 2	0
9	G	1	Total 43	C 41	O 2	0
9	G	1	Total 43	C 41	O 2	0
9	f	1	Total 43	C 41	O 2	0
9	F	1	Total 43	C 41	O 2	0
9	E	1	Total 43	C 41	O 2	0
9	E	1	Total 43	C 41	O 2	0

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	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	M	1	Total	C	O	0
			43	41	2	

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



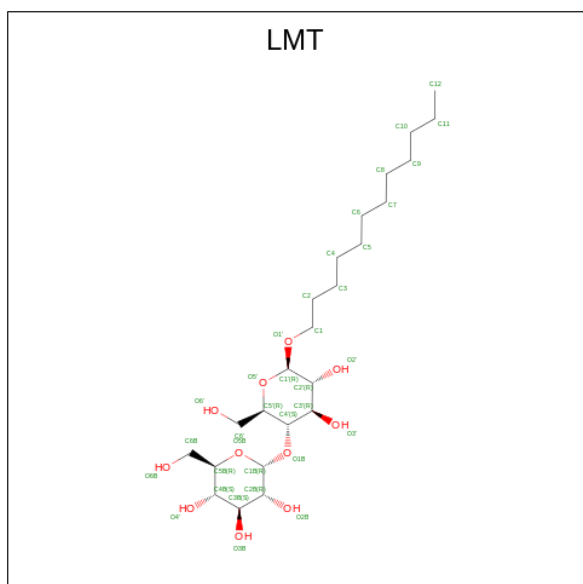
Mol	Chain	Residues	Atoms				AltConf
10	R	1	Total	C	O	P	0
			45	34	10	1	
10	G	1	Total	C	O	P	0
			49	38	10	1	
10	G	1	Total	C	O	P	0
			40	29	10	1	
10	F	1	Total	C	O	P	0
			43	32	10	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
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	H	1	Total	C	O	P	0
			48	37	10	1	
10	H	1	Total	C	O	P	0
			37	28	8	1	

- Molecule 11 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).

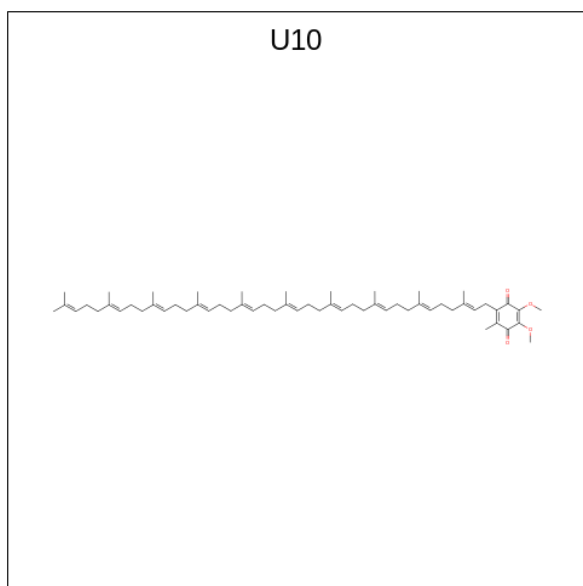


Mol	Chain	Residues	Atoms			AltConf
11	D	1	Total	C	O	0
			35	24	11	
11	L	1	Total	C	O	0
			24	18	6	
11	L	1	Total	C	O	0
			24	19	5	
11	H	1	Total	C	O	0
			24	18	6	
11	C	1	Total	C	O	0
			24	18	6	

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

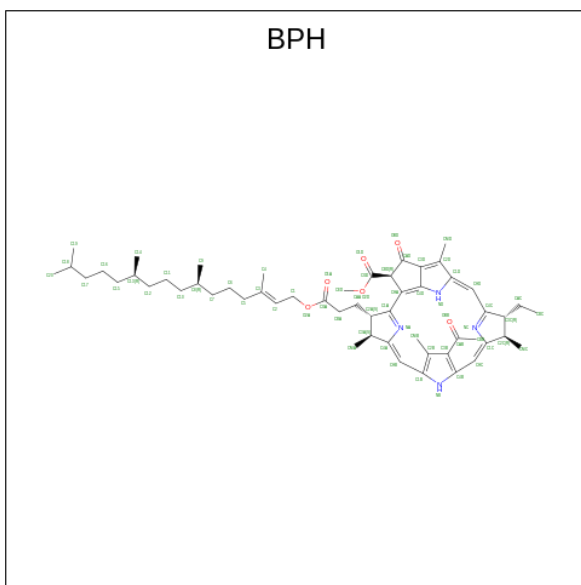
Mol	Chain	Residues	Atoms		AltConf
12	M	1	Total	Fe	0
			1	1	

- Molecule 13 is UBIQUINONE-10 (CCD ID: U10) (formula: C₅₉H₉₀O₄) (labeled as "Ligand of Interest" by depositor).



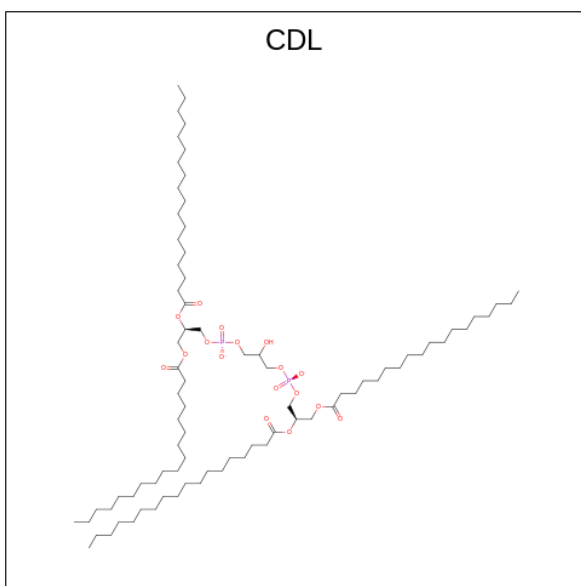
Mol	Chain	Residues	Atoms			AltConf
13	M	1	Total	C	O	0
			63	59	4	
13	L	1	Total	C	O	0
			48	44	4	

- Molecule 14 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: C₅₅H₇₆N₄O₆).



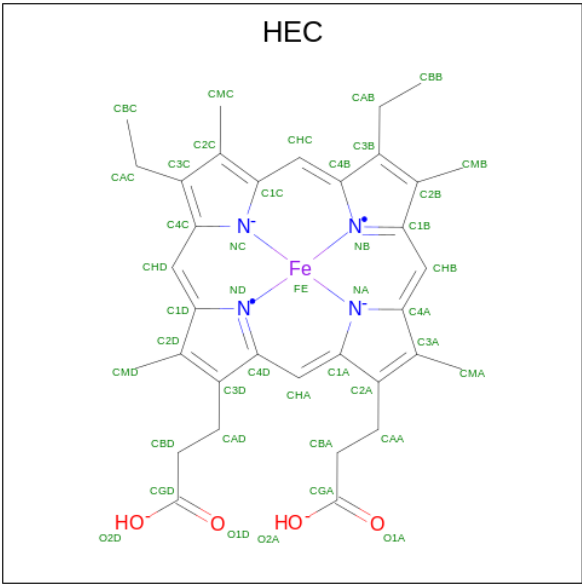
Mol	Chain	Residues	Atoms				AltConf
14	M	1	Total	C	N	O	0
			65	55	4	6	
14	L	1	Total	C	N	O	0
			65	55	4	6	

- Molecule 15 is CARDIOLIPIN (CCD ID: 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 (CCD ID: HEC) (formula: C₃₄H₃₆FeN₄O₄) (labeled as "Ligand of Interest" by depositor).



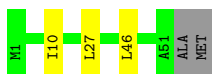
Mol	Chain	Residues	Atoms					AltConf
16	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
16	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
16	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

3 Residue-property plots [i](#)

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

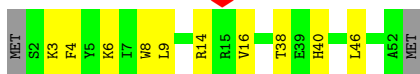
- Molecule 1: Antenna pigment protein alpha chain

Chain P:  91% 6% .



- Molecule 1: Antenna pigment protein alpha chain

Chain V:  77% 19% .



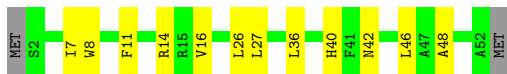
- Molecule 1: Antenna pigment protein alpha chain

Chain S:  85% 11% .



- Molecule 1: Antenna pigment protein alpha chain

Chain T:  74% 23% .



- Molecule 1: Antenna pigment protein alpha chain

Chain Q:  91% 6% .



- Molecule 1: Antenna pigment protein alpha chain

Chain R:  81% 15% .



- Molecule 1: Antenna pigment protein alpha chain

Chain 1:  83% 11% 6%



- Molecule 1: Antenna pigment protein alpha chain

Chain N:  83% 13% .



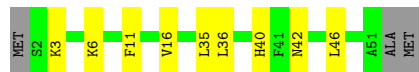
- Molecule 1: Antenna pigment protein alpha chain

Chain K:  89% 8% .



- Molecule 1: Antenna pigment protein alpha chain

Chain J:  77% 17% 6%



- Molecule 1: Antenna pigment protein alpha chain

Chain I:  91% 6% .



- Molecule 1: Antenna pigment protein alpha chain

Chain G:  89% 8% .



- Molecule 1: Antenna pigment protein alpha chain

A diagram of a protein structure with five residues highlighted in different colors: MET (grey), S2 (green), L36 (yellow), A52 (green), and MET (grey). The residues are connected by lines, indicating their sequence in the protein.

-

-

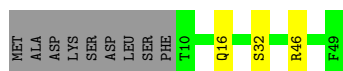
-
- Diagram illustrating the domain structure of a protein, showing a sequence of domains: MET, S2, W8, V16, Q20, H40, A48, A52, and MET. The domains are represented by colored blocks (green for beta-strands, yellow for alpha-helices) connected by lines, indicating the linear arrangement of the protein structure.

-

- | | | | |
|-----|-----|-----|-----|
| GLN | LYS | ARG | MET |
| GLY | LYS | SER | ALA |
| GLY | ILE | LYS | THR |
| GLU | LYS | VAL | GLN |
| THR | GLY | GLN | ARG |
| GLU | VAL | PRO | LYS |
| PHE | VAL | SER | ASP |
| SER | PRO | ALA | M8 |
| LYS | LYS | ALA | T9 |
| ARG | LEU | LEU | C10 |
| VAL | GLU | ALA | T11 |
| ASP | GLU | GLY | |
| GLY | MET | GLU | L20 |
| GLY | LEU | ALA | |
| ASP | HIS | GLU | A55 |
| GLY | SER | LEU | |
| VAL | MET | ALA | C59 |
| TYR | GLY | GLY | GLY |
| | PHE | ARG | GLU |
| | TYR | LYS | THR |
| | HIS | GLY | GLY |
| | PHE | SER | ARG |
| | ASP | TRP | PRO |
| | GLN | SER | LYS |
| | VAL | TYR | ASP |
| | ALA | ASP | ASN |
| | SER | SER | ALA |
| | TRP | GLY | GLU |
| | SER | ALA | GLN |
| | GLU | GLY | ILE |
| | GLN | HIS | ARG |
| | GLU | ALA | ALA |
| | LEU | SER | GLU |
| | ALA | GLY | MET |
| | TRP | ALA | ALA |
| | VAL | GLY | ALA |
| | ASP | HIS | ALA |
| | GLU | ASP | ARG |
| | ASN | ALA | GLU |
| | LEU | GLY | ARG |
| | GLU | THR | VAL |
| | GLY | ASP | ARG |
| | PHE | ALA | GLY |
| | LYS | ALA | ALA |
| | GLY | LYS | THR |
| | ARG | PRO | PRO |
| | ALA | ALA | GLY |
| | SER | THR | ILE |
| | ASP | LEU | THR |
| | GLU | ALA | PRO |
| | TRP | ALA | LYS |
| | VAL | ARG | PRO |
| | ALA | ASP | ALA |
| | GLN | GLY | PRO |
| | ALA | LYS | VAL |
| | LYS | ALA | VAL |
| | LEU | ASP | PRO |
| | LEU | ASP | ALA |
| | ALA | ASP | ASP |

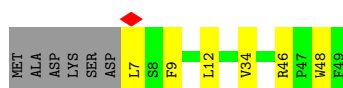
- 
- WORLD WIDE
PDB
PROTEIN DATA BANK

Chain v:  76% 6% 18%



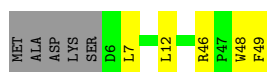
- Molecule 3: Antenna pigment protein beta chain

Chain t:  76% 12% 12%



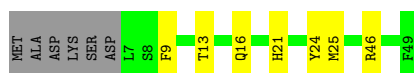
- Molecule 3: Antenna pigment protein beta chain

Chain s:  80% 10% 10%



- Molecule 3: Antenna pigment protein beta chain

Chain r:  73% 14% 12%



- Molecule 3: Antenna pigment protein beta chain

Chain q:  86% 10% 4%



- Molecule 3: Antenna pigment protein beta chain

Chain p:  86% 10% 4%



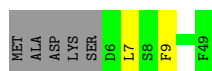
- Molecule 3: Antenna pigment protein beta chain

Chain 2:  82% 8% 10%



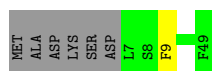
- Molecule 3: Antenna pigment protein beta chain

Chain n:  86% 10%



- Molecule 3: Antenna pigment protein beta chain

Chain k:  86% 12%



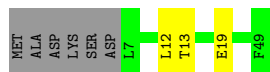
- Molecule 3: Antenna pigment protein beta chain

Chain j:  78% 10% 12%



- Molecule 3: Antenna pigment protein beta chain

Chain i:  82% 6% 12%



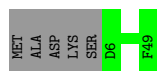
- Molecule 3: Antenna pigment protein beta chain

Chain g:  82% 8% 10%



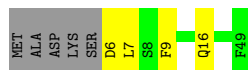
- Molecule 3: Antenna pigment protein beta chain

Chain f:  90% 10%



- Molecule 3: Antenna pigment protein beta chain

Chain e:  82% 8% 10%



- Molecule 3: Antenna pigment protein beta chain

Chain d:  73% 16% 10%

MET
ALA
ASP
LYS
SER
D6
L7
L12
T13
Q16
H21
M25
V48
F49

- Molecule 3: Antenna pigment protein beta chain

Chain b:  86% 10%

MET
ALA
ASP
LYS
SER
D6
F9
R46
F49

- Molecule 3: Antenna pigment protein beta chain

Chain a:  86% 10%

MET
ALA
ASP
LYS
SER
D6
F9
R46
F49

- Molecule 4: Reaction center protein M chain

Chain M:  82% 16%

MET
P2
E3
Y4
Q5
N6
V21
N25
E30
T35
P51
Y53
L54
G55
W56
V72
N75
Q79
A95
L96
P99
M107
P108
P109
L110
G114
R133
M140
I155
F158
L159
V160
F164
P182
F202
V208
L215
L216
F217
T228
R229
F230
R242
G243
T244
A245
S246
E247
R248
W255
T256
G258
F259
A261
W269
A274
V275
P278
I279
T280
V291
V292
D293
N294
W295
F296
L297
R326
GLU
GLY
GLY
ASN

- Molecule 5: Reaction center protein L chain

Chain L:  84% 14%

MET
A2
L3
L4
S5
F6
E7
R8
K9
V12
D21
D24
L44
W52
P69
L76
M82
C109
M114
T131
L132
V133
V134
F135
R136
P137
W143
G144
H154
V158
N171
H174
F180
F181
L188
A189
L190
K208
N212
T215
F216
F217
F220
L221
I221
T225
L228
R232
A241
S275
GLN
VAL
ASP
CYS

- Molecule 6: Reaction center protein H chain

Chain H:  89% 11%

W1
D10
N34
G38
E42
T48
R81
R82
G108
P111
A112
S113
W114
S115
I131
D170
Q174
Y178
D189
G190
E197
R200
V208
I211
Y212
H215
F216
D234
M237
G242
D248
L256

- Molecule 7: Photosynthetic reaction center cytochrome c subunit

Chain C:  83% 15%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	230375	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	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	1.280	Depositor
Minimum map value	-0.705	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.042	Depositor
Recommended contour level	0.15	Depositor
Map size ($\text{\AA}$)	307.2, 307.2, 307.2	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.2, 1.2, 1.2	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.13	0/431	0.23	0/585
1	A	0.11	0/436	0.22	0/592
1	B	0.13	0/436	0.22	0/592
1	D	0.14	0/436	0.23	0/592
1	E	0.16	0/436	0.24	0/592
1	F	0.14	0/436	0.21	0/592
1	G	0.14	0/436	0.24	0/592
1	I	0.14	0/436	0.26	0/592
1	J	0.13	0/431	0.23	0/585
1	K	0.13	0/436	0.32	0/592
1	N	0.14	0/436	0.28	0/592
1	P	0.12	0/439	0.25	0/595
1	Q	0.11	0/436	0.20	0/592
1	R	0.11	0/436	0.21	0/592
1	S	0.12	0/436	0.24	0/592
1	T	0.12	0/436	0.23	0/592
1	V	0.10	0/436	0.21	0/592
2	O	0.11	0/378	0.24	0/516
3	2	0.12	0/371	0.21	0/508
3	a	0.09	0/371	0.18	0/508
3	b	0.12	0/371	0.19	0/508
3	d	0.14	0/371	0.21	0/508
3	e	0.13	0/371	0.16	0/508
3	f	0.13	0/371	0.20	0/508
3	g	0.12	0/371	0.17	0/508
3	i	0.12	0/363	0.24	0/497
3	j	0.12	0/363	0.24	0/497
3	k	0.11	0/363	0.22	0/497
3	n	0.11	0/371	0.18	0/508
3	p	0.11	0/371	0.28	0/508
3	q	0.11	0/371	0.21	0/508
3	r	0.11	0/363	0.21	0/497

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	s	0.12	0/371	0.25	0/508
3	t	0.09	0/363	0.17	0/497
3	v	0.08	0/337	0.15	0/462
4	M	0.16	0/2731	0.27	0/3735
5	L	0.16	0/2267	0.28	0/3105
6	H	0.13	0/2072	0.23	0/2804
7	C	0.15	0/2819	0.31	0/3869
All	All	0.13	0/23905	0.25	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 ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	417	0	419	5	0
1	A	422	0	426	9	0
1	B	422	0	426	4	0
1	D	422	0	426	4	0
1	E	422	0	426	9	0
1	F	422	0	425	2	0
1	G	422	0	426	3	0
1	I	422	0	426	2	0
1	J	417	0	421	7	0
1	K	422	0	426	3	0
1	N	422	0	426	4	0
1	P	425	0	433	3	0
1	Q	422	0	426	2	0
1	R	422	0	426	6	0
1	S	422	0	426	6	0
1	T	422	0	426	9	0
1	V	422	0	426	8	0
2	O	371	0	395	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	2	358	0	338	5	0
3	a	358	0	338	2	0
3	b	358	0	338	2	0
3	d	358	0	338	9	0
3	e	358	0	338	5	0
3	f	358	0	338	0	0
3	g	358	0	338	2	0
3	i	350	0	334	2	0
3	j	350	0	334	5	0
3	k	350	0	334	1	0
3	n	358	0	338	5	0
3	p	358	0	338	2	0
3	q	358	0	338	2	0
3	r	350	0	334	6	0
3	s	358	0	338	4	0
3	t	350	0	334	9	0
3	v	325	0	309	4	0
4	M	2633	0	2524	42	0
5	L	2178	0	2118	36	0
6	H	2022	0	1971	23	0
7	C	2741	0	2584	40	0
8	1	66	0	74	0	0
8	2	66	0	74	4	0
8	A	66	0	74	5	0
8	B	66	0	74	4	0
8	D	66	0	74	2	0
8	E	66	0	74	2	0
8	F	132	0	146	4	0
8	G	132	0	146	4	0
8	I	66	0	74	1	0
8	J	66	0	74	3	0
8	K	66	0	74	2	0
8	L	132	0	143	8	0
8	M	132	0	144	5	0
8	N	66	0	74	2	0
8	P	132	0	146	2	0
8	Q	66	0	74	1	0
8	R	66	0	74	6	0
8	S	66	0	74	0	0
8	V	66	0	72	3	0
8	a	66	0	74	2	0
8	b	66	0	74	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	d	66	0	74	8	0
8	e	66	0	74	4	0
8	i	66	0	74	2	0
8	j	66	0	74	7	0
8	k	66	0	74	1	0
8	n	66	0	74	3	0
8	q	66	0	74	2	0
8	r	66	0	74	4	0
8	s	132	0	147	8	0
8	t	66	0	73	9	0
8	v	66	0	74	5	0
9	2	129	0	0	0	0
9	A	43	0	0	0	0
9	B	86	0	0	0	0
9	D	86	0	0	0	0
9	E	86	0	0	0	0
9	F	43	0	0	0	0
9	G	86	0	0	0	0
9	I	43	0	0	0	0
9	J	86	0	0	0	0
9	K	43	0	0	0	0
9	M	43	0	0	0	0
9	N	43	0	0	0	0
9	P	43	0	0	0	0
9	R	43	0	0	0	0
9	T	43	0	0	0	0
9	a	43	0	0	0	0
9	f	43	0	0	0	0
9	j	86	0	0	0	0
9	k	43	0	0	0	0
9	p	43	0	0	0	0
9	q	43	0	0	0	0
9	r	43	0	0	0	0
9	s	129	0	0	1	0
9	v	86	0	0	0	0
10	D	53	0	0	0	0
10	F	43	0	0	0	0
10	G	89	0	0	0	0
10	H	85	0	0	0	0
10	L	37	0	0	0	0
10	M	102	0	0	0	0
10	R	45	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	C	24	0	34	2	0
11	D	35	0	45	1	0
11	H	24	0	34	0	0
11	L	48	0	65	1	0
12	M	1	0	0	0	0
13	L	48	0	63	5	0
13	M	63	0	90	7	0
14	L	65	0	76	0	0
14	M	65	0	73	2	0
15	H	91	0	135	3	0
15	L	67	0	78	1	0
16	C	129	0	88	5	0
All	All	28252	0	26099	322	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (322) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:144:MET:SD	16:C:401:HEC:NC	2.37	0.98
5:L:131:THR:HA	5:L:135:PHE:HB2	1.63	0.81
7:C:144:MET:SD	16:C:401:HEC:FE	1.73	0.80
7:C:144:MET:SD	16:C:401:HEC:NB	2.58	0.77
3:d:48:TRP:CE2	8:d:101:BCL:HHC	2.22	0.74
4:M:269:TRP:HE1	6:H:34:ASN:HD21	1.35	0.74
7:C:147:MET:HE2	7:C:302:TRP:HB3	1.69	0.74
8:d:101:BCL:H3C	1:D:35:LEU:HD11	1.70	0.73
7:C:330:THR:O	7:C:333:LYS:NZ	2.23	0.70
5:L:190:LEU:HB2	13:L:303:U10:H1M2	1.73	0.69
3:q:13:THR:H	3:q:16:GLN:HE21	1.41	0.68
4:M:21:VAL:HG22	5:L:215:THR:HG21	1.78	0.66
7:C:168:THR:HG23	7:C:170:PHE:H	1.62	0.64
4:M:95:ALA:HB2	4:M:182:PRO:HG2	1.79	0.64
7:C:148:ASN:HD21	7:C:168:THR:HA	1.61	0.64
13:M:404:U10:H103	13:M:404:U10:H171	1.80	0.64
5:L:181:PHE:CE2	8:L:301:BCL:H3A	2.33	0.64
3:j:13:THR:H	3:j:16:GLN:HE21	1.48	0.62
3:e:16:GLN:HE21	3:d:7:LEU:HB2	1.65	0.62
1:A:25:PHE:HB2	8:A:101:BCL:H52	1.82	0.62
1:S:10:ILE:HG23	1:T:14:ARG:HG2	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:35:THR:HG22	4:M:51:PRO:HD3	1.82	0.62
7:C:200:GLN:NE2	7:C:249:GLU:OE2	2.31	0.62
1:G:33:LEU:HD21	11:L:305:LMT:H42	1.82	0.61
3:t:46:ARG:HH21	1:T:46:LEU:HD11	1.64	0.61
8:L:301:BCL:H111	8:L:304:BCL:HBB2	1.82	0.61
6:H:42:GLU:OE2	6:H:81:ARG:NH2	2.33	0.61
7:C:71:ASP:HB3	7:C:74:ILE:HG13	1.83	0.61
1:T:8:TRP:HZ3	1:T:16:VAL:HG11	1.66	0.60
3:t:48:TRP:HE1	8:t:101:BCL:HBB2	1.66	0.60
7:C:212:LEU:HB3	7:C:253:SER:HB2	1.84	0.59
8:e:101:BCL:HAC2	1:E:35:LEU:HD11	1.83	0.59
1:V:6:LYS:HA	1:V:9:LEU:HD23	1.85	0.59
4:M:215:LEU:HD21	13:M:404:U10:H211	1.85	0.59
3:q:13:THR:HB	3:q:16:GLN:HG2	1.84	0.59
5:L:225:ILE:H	13:L:303:U10:H3M3	1.68	0.58
6:H:211:ILE:HG23	6:H:215:HIS:HB2	1.85	0.58
4:M:217:PHE:HB2	5:L:188:LEU:HD13	1.86	0.58
1:A:15:ARG:HB3	7:C:20:PRO:HG2	1.85	0.58
7:C:144:MET:SD	16:C:401:HEC:ND	2.77	0.57
8:v:101:BCL:HAA1	8:v:101:BCL:H52	1.87	0.57
6:H:10:ASP:OD2	7:C:235:ARG:NH1	2.38	0.57
1:S:16:VAL:HG21	8:s:102:BCL:H142	1.84	0.57
13:M:404:U10:H251	15:H:304:CDL:H551	1.87	0.57
7:C:221:LEU:HD13	7:C:295:VAL:HG11	1.87	0.57
4:M:269:TRP:NE1	6:H:34:ASN:HD21	2.03	0.57
4:M:242:ARG:NH1	4:M:247:GLU:OE2	2.38	0.56
4:M:3:GLU:O	4:M:5:GLN:NE2	2.38	0.56
4:M:278:PRO:HD3	14:M:408:BPH:HBC1	1.88	0.56
3:r:46:ARG:HH21	1:R:46:LEU:HD11	1.70	0.56
8:a:101:BCL:H92	8:a:101:BCL:HAA1	1.88	0.56
3:e:9:PHE:HB2	1:E:10:ILE:HA	1.88	0.56
4:M:269:TRP:HE1	6:H:34:ASN:ND2	2.03	0.56
7:C:10:ASN:O	7:C:12:LYS:NZ	2.39	0.55
8:F:101:BCL:HBB2	8:F:101:BCL:H143	1.87	0.55
1:E:6:LYS:HA	1:E:9:LEU:HD13	1.88	0.55
4:M:4:TYR:HA	6:H:200:ARG:HH21	1.72	0.55
1:1:33:LEU:HB3	4:M:107:MET:HE2	1.88	0.55
8:F:101:BCL:H92	8:F:101:BCL:HAA1	1.89	0.55
4:M:208:VAL:HG22	8:L:304:BCL:HAA2	1.89	0.54
7:C:200:GLN:OE1	7:C:201:ASN:ND2	2.40	0.54
8:r:101:BCL:H111	8:r:101:BCL:H2	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:53:PRO:O	7:C:56:THR:OG1	2.26	0.54
7:C:216:ALA:HB1	7:C:254:LEU:HB2	1.88	0.54
2:O:20:LEU:HD13	1:T:26:LEU:HD11	1.89	0.53
3:g:13:THR:HG23	3:g:16:GLN:H	1.74	0.53
1:S:8:TRP:HZ3	1:S:16:VAL:HG11	1.72	0.53
1:V:8:TRP:HZ3	1:V:16:VAL:HG11	1.73	0.53
8:t:101:BCL:HAA1	8:t:101:BCL:H8	1.91	0.53
3:g:45:TRP:CD2	3:g:46:ARG:HG2	2.44	0.53
1:N:3:LYS:HD2	1:N:6:LYS:HD2	1.90	0.52
3:t:12:LEU:HD11	3:s:7:LEU:HD13	1.90	0.52
3:r:46:ARG:NH2	1:R:46:LEU:HD11	2.25	0.52
1:R:2:SER:OG	1:R:3:LYS:N	2.43	0.52
1:J:3:LYS:HG2	1:J:6:LYS:HD2	1.91	0.52
8:d:101:BCL:HAC1	1:D:35:LEU:HD21	1.91	0.52
1:P:10:ILE:HG23	1:Q:14:ARG:HG2	1.91	0.52
5:L:180:PHE:HB3	5:L:241:ALA:HB2	1.92	0.52
8:V:101:BCL:C1B	8:t:101:BCL:HMB2	2.39	0.52
8:L:304:BCL:H143	8:L:304:BCL:HMA1	1.92	0.52
1:J:11:PHE:HB3	1:J:16:VAL:HG21	1.91	0.52
1:1:14:ARG:NH2	3:n:9:PHE:HB3	2.24	0.51
1:R:45:GLU:OE2	10:R:103:MW9:O6	2.27	0.51
3:2:16:GLN:HE22	3:n:7:LEU:HD13	1.75	0.51
4:M:255:TRP:NE1	5:L:7:GLU:OE2	2.29	0.51
3:e:16:GLN:NE2	3:d:7:LEU:HB2	2.25	0.51
5:L:181:PHE:CE1	5:L:241:ALA:HB1	2.45	0.51
8:F:101:BCL:CAD	8:F:102:BCL:HBD	2.40	0.51
5:L:217:PHE:HD1	5:L:221:ILE:HG12	1.76	0.51
4:M:99:PRO:HB3	4:M:108:PRO:HG3	1.93	0.51
5:L:9:LYS:HD2	6:H:113:SER:HB2	1.93	0.51
5:L:225:ILE:HG22	13:L:303:U10:H3M3	1.93	0.51
7:C:41:GLY:HA3	11:C:404:LMT:H6E	1.93	0.51
8:n:101:BCL:HBD	8:N:101:BCL:HBD	1.94	0.50
4:M:6:ASN:OD1	5:L:232:ARG:NH2	2.44	0.50
6:H:212:TYR:OH	6:H:248:ASP:OD1	2.25	0.50
4:M:292:VAL:HG21	4:M:295:TRP:CH2	2.46	0.50
8:d:101:BCL:H91	8:d:101:BCL:HAA1	1.93	0.50
3:j:32:SER:HB3	8:j:102:BCL:H72	1.93	0.49
8:V:101:BCL:HBB3	8:t:101:BCL:NB	2.27	0.49
1:N:36:LEU:O	1:N:42:ASN:ND2	2.45	0.49
8:j:102:BCL:H12	8:j:102:BCL:H102	1.93	0.49
4:M:53:TYR:O	4:M:133:ARG:NH2	2.41	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:TRP:HZ3	1:B:16:VAL:HG11	1.77	0.49
4:M:257:MET:CE	13:M:404:U10:H13	2.41	0.49
1:K:48:ALA:HB2	1:J:40:HIS:HB2	1.94	0.49
7:C:207:SER:O	7:C:210:THR:OG1	2.28	0.49
7:C:251:THR:O	7:C:255:MET:HG2	2.12	0.49
3:i:19:GLU:OE2	1:G:3:LYS:NZ	2.31	0.49
8:B:101:BCL:HBB2	1:A:31:ILE:HD12	1.95	0.49
1:P:46:LEU:HD22	3:p:46:ARG:HH11	1.77	0.49
3:d:49:PHE:HZ	8:d:101:BCL:HBB1	1.78	0.49
5:L:225:ILE:HB	13:L:303:U10:H4M2	1.93	0.49
1:V:38:THR:HG21	1:A:44:PHE:HB3	1.96	0.48
8:F:101:BCL:O2D	8:F:101:BCL:H2A	2.13	0.48
3:t:48:TRP:CZ2	8:t:101:BCL:HHC	2.48	0.48
3:r:21:HIS:CE1	3:r:25:MET:HE3	2.49	0.48
3:n:7:LEU:HD11	3:n:9:PHE:CE1	2.49	0.48
4:M:160:VAL:HA	4:M:164:PHE:HB2	1.96	0.48
1:1:19:ALA:HB2	4:M:56:TRP:CH2	2.48	0.48
8:E:101:BCL:H61	8:E:101:BCL:H41	1.62	0.48
3:s:46:ARG:HG3	3:s:46:ARG:HH11	1.77	0.48
7:C:185:ARG:HE	7:C:187:ASP:HB2	1.78	0.48
1:1:27:LEU:O	1:1:31:ILE:HG13	2.14	0.48
1:R:8:TRP:HZ3	1:R:16:VAL:HG11	1.78	0.48
3:2:16:GLN:NE2	3:n:7:LEU:HD13	2.29	0.48
1:E:37:SER:HB2	5:L:82:MET:HE3	1.94	0.48
6:H:111:PRO:HB2	6:H:242:GLY:HA2	1.96	0.48
3:k:9:PHE:HD1	1:K:10:ILE:HG22	1.78	0.48
4:M:294:ASN:ND2	7:C:231:ASP:O	2.44	0.48
8:t:101:BCL:HED3	1:T:27:LEU:HD23	1.96	0.47
1:R:36:LEU:O	1:R:42:ASN:ND2	2.46	0.47
3:s:12:LEU:HD11	3:r:9:PHE:HZ	1.79	0.47
8:A:101:BCL:H41	8:A:101:BCL:H61	1.44	0.47
4:M:261:ALA:HA	6:H:34:ASN:HB3	1.95	0.47
3:v:16:GLN:HG2	3:t:7:LEU:HD23	1.95	0.47
8:s:102:BCL:H2C	8:s:102:BCL:HBC3	1.58	0.47
1:E:33:LEU:HD21	11:D:102:LMT:H72	1.96	0.47
4:M:30:GLU:HB2	4:M:53:TYR:CE2	2.50	0.47
4:M:228:THR:HG23	6:H:197:GLU:HG2	1.96	0.47
3:2:21:HIS:CE1	3:2:25:MET:HE2	2.50	0.47
4:M:257:MET:HE1	13:M:404:U10:H13	1.97	0.47
1:I:36:LEU:O	1:I:42:ASN:ND2	2.45	0.47
8:e:101:BCL:HBC3	8:e:101:BCL:H2C	1.63	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:44:LEU:HG	15:H:304:CDL:H431	1.97	0.47
2:O:11:THR:HG23	2:O:55:ALA:HB1	1.97	0.47
3:e:7:LEU:O	1:E:9:LEU:HD23	2.15	0.47
14:M:408:BPH:HBA1	14:M:408:BPH:H3A	1.45	0.47
3:d:13:THR:HG23	3:d:16:GLN:H	1.81	0.46
3:d:12:LEU:HD11	3:b:9:PHE:HZ	1.80	0.46
7:C:187:ASP:HB3	7:C:188:PRO:HD3	1.97	0.46
8:Q:101:BCL:HBD	8:q:102:BCL:HBD	1.98	0.46
8:j:102:BCL:H192	8:j:102:BCL:H162	1.76	0.46
8:n:101:BCL:HBC3	1:N:35:LEU:HD11	1.97	0.46
4:M:259:PHE:HE1	13:M:404:U10:H262	1.80	0.46
8:k:102:BCL:HBD	8:K:101:BCL:HBD	1.97	0.46
5:L:76:LEU:O	5:L:143:TRP:NE1	2.49	0.46
3:t:46:ARG:HD3	1:T:40:HIS:CE1	2.50	0.46
8:s:102:BCL:H3A	9:s:104:A1EFU:C7	2.46	0.46
1:I:3:LYS:HE3	1:I:3:LYS:HB2	1.63	0.46
8:j:102:BCL:CAD	8:J:101:BCL:HBD	2.46	0.45
8:L:304:BCL:H61	8:L:304:BCL:H41	1.65	0.45
8:A:101:BCL:H13	8:A:101:BCL:H102	1.73	0.45
3:2:49:PHE:HD2	8:2:103:BCL:H203	1.81	0.45
8:R:102:BCL:H61	8:R:102:BCL:H102	1.82	0.45
3:2:16:GLN:NE2	3:n:7:LEU:HB2	2.32	0.45
3:d:21:HIS:CE1	3:d:25:MET:HE3	2.51	0.45
4:M:275:VAL:O	4:M:278:PRO:HD2	2.17	0.45
8:M:402:BCL:HAA2	8:M:403:BCL:HBC1	1.98	0.45
8:j:102:BCL:HAC2	1:J:35:LEU:HD11	1.99	0.45
8:v:101:BCL:H41	8:v:101:BCL:H62	1.59	0.45
8:A:101:BCL:H161	8:A:101:BCL:H192	1.68	0.45
7:C:220:TYR:O	7:C:296:GLN:NE2	2.43	0.45
4:M:110:LEU:HA	4:M:114:GLY:HA3	1.99	0.45
6:H:170:ASP:O	6:H:174:GLN:N	2.50	0.45
5:L:5:SER:HB3	6:H:38:GLY:HA2	1.98	0.45
5:L:217:PHE:HA	5:L:220:PHE:HB3	1.99	0.45
3:t:34:VAL:HG23	8:s:102:BCL:HED2	1.99	0.44
1:G:12:ASP:OD1	1:G:14:ARG:HG2	2.17	0.44
3:a:9:PHE:HB2	1:A:10:ILE:HA	1.99	0.44
3:r:13:THR:HG23	3:r:16:GLN:H	1.81	0.44
1:J:36:LEU:O	1:J:42:ASN:ND2	2.50	0.44
1:D:32:HIS:HE1	8:D:101:BCL:NA	2.15	0.44
8:B:101:BCL:HBA1	8:B:101:BCL:H3A	1.56	0.44
4:M:274:ALA:HB2	5:L:188:LEU:HD23	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:134:VAL:HA	5:L:143:TRP:HZ3	1.83	0.44
6:H:82:ARG:NH1	6:H:108:GLY:O	2.38	0.44
7:C:115:ARG:NH2	7:C:350:GLU:OE2	2.50	0.44
7:C:199:VAL:O	7:C:213:PRO:HA	2.17	0.44
8:R:102:BCL:H142	8:R:102:BCL:H112	1.77	0.44
8:b:101:BCL:H161	8:b:101:BCL:H143	1.62	0.44
5:L:208:LYS:HB3	5:L:212:ASN:HB2	1.98	0.44
13:L:303:U10:H271	13:L:303:U10:H251	1.86	0.44
1:V:46:LEU:HD11	3:v:46:ARG:NH2	2.33	0.44
8:2:103:BCL:H192	8:2:103:BCL:H161	1.63	0.44
1:F:36:LEU:HD13	5:L:52:TRP:HZ3	1.82	0.44
6:H:189:ASP:OD1	6:H:190:GLY:N	2.51	0.44
7:C:200:GLN:HE21	7:C:249:GLU:CD	2.26	0.44
8:r:101:BCL:HBD	8:R:102:BCL:HBD	2.00	0.44
1:K:2:SER:OG	1:K:3:LYS:N	2.51	0.44
3:a:46:ARG:HD2	1:A:40:HIS:NE2	2.32	0.44
5:L:12:VAL:HG21	6:H:111:PRO:HD3	1.99	0.44
8:L:304:BCL:H91	8:L:304:BCL:H112	1.76	0.44
8:e:101:BCL:H162	8:e:101:BCL:H141	1.60	0.44
4:M:75:ASN:O	4:M:79:GLN:HG3	2.18	0.44
5:L:220:PHE:CD2	5:L:221:ILE:HG23	2.53	0.44
1:N:12:ASP:HB2	1:N:15:ARG:HH21	1.83	0.44
8:e:101:BCL:H112	8:e:101:BCL:H142	1.75	0.43
8:E:101:BCL:HBC3	8:E:101:BCL:H2C	1.75	0.43
4:M:25:ASN:ND2	4:M:140:MET:O	2.46	0.43
2:O:8:MET:C	2:O:10:CYS:H	2.27	0.43
3:p:45:TRP:CD2	3:p:46:ARG:HG2	2.53	0.43
8:i:101:BCL:H141	8:i:101:BCL:H162	1.72	0.43
8:G:102:BCL:H162	8:G:102:BCL:H122	1.76	0.43
4:M:155:ILE:HA	4:M:158:PHE:HB3	1.99	0.43
3:d:48:TRP:CZ2	8:d:101:BCL:HHC	2.52	0.43
1:B:48:ALA:HB2	1:A:40:HIS:HB2	2.01	0.43
8:R:102:BCL:H2C	8:R:102:BCL:HBC3	1.67	0.43
8:M:403:BCL:H91	8:M:403:BCL:H111	1.78	0.43
8:v:101:BCL:H93	8:v:101:BCL:H111	1.53	0.43
8:s:103:BCL:H61	8:s:103:BCL:H41	1.74	0.43
8:M:403:BCL:H152	8:M:403:BCL:H112	1.76	0.43
5:L:4:LEU:HB2	5:L:7:GLU:HB2	2.01	0.43
1:P:27:LEU:HB3	8:P:102:BCL:HED3	1.90	0.43
8:j:102:BCL:H2C	8:j:102:BCL:HBC3	1.78	0.43
3:t:48:TRP:HE1	8:t:101:BCL:CBB	2.30	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:11:PHE:HB3	1:Q:16:VAL:HG21	2.00	0.43
8:B:101:BCL:H92	8:B:101:BCL:H62	1.87	0.43
8:K:101:BCL:HBC3	8:K:101:BCL:H2C	1.82	0.42
8:G:102:BCL:H2C	8:G:102:BCL:HBC3	1.67	0.42
3:v:32:SER:HB2	8:v:101:BCL:H42	2.01	0.42
8:D:101:BCL:H91	1:B:20:GLN:HG3	2.02	0.42
4:M:297:LEU:HG	7:C:276:TYR:OH	2.19	0.42
5:L:109:CYS:HB2	5:L:114:MET:HG3	2.00	0.42
5:L:154:HIS:O	5:L:158:VAL:HG23	2.19	0.42
3:d:49:PHE:CZ	8:d:101:BCL:HBB1	2.53	0.42
5:L:171:ASN:HB3	5:L:174:HIS:HB2	2.01	0.42
1:S:31:ILE:HD11	8:s:102:BCL:HBB2	2.00	0.42
8:2:103:BCL:H162	8:2:103:BCL:H141	1.76	0.42
8:J:101:BCL:HBC3	8:J:101:BCL:H2C	1.80	0.42
8:d:101:BCL:H161	8:d:101:BCL:H141	1.73	0.42
8:a:101:BCL:H142	8:a:101:BCL:H111	1.77	0.42
1:A:27:LEU:O	1:A:31:ILE:HG12	2.20	0.42
4:M:72:VAL:HA	4:M:96:LEU:HD22	2.02	0.42
8:M:402:BCL:HAA2	8:M:402:BCL:HBD	2.01	0.42
5:L:136:ARG:HB3	5:L:137:PRO:HD3	2.02	0.42
1:S:40:HIS:HB2	1:T:48:ALA:HB2	2.01	0.42
8:2:103:BCL:HHH	1:1:35:LEU:HD11	2.01	0.42
1:E:11:PHE:HB3	1:E:16:VAL:HG21	2.02	0.42
3:e:6:ASP:OD1	3:e:6:ASP:N	2.53	0.42
6:H:208:VAL:HG11	6:H:216:PHE:HZ	1.84	0.42
5:L:133:VAL:O	5:L:137:PRO:HG2	2.20	0.42
5:L:190:LEU:HD22	5:L:217:PHE:HZ	1.85	0.42
6:H:178:TYR:OH	6:H:237:MET:HE3	2.19	0.42
7:C:17:ILE:HG23	7:C:18:TYR:CD2	2.54	0.42
8:s:102:BCL:H161	8:s:102:BCL:H192	1.72	0.42
7:C:303:ILE:HG13	7:C:326:LEU:HD23	2.01	0.42
1:V:3:LYS:HG3	1:V:4:PHE:N	2.35	0.42
8:n:101:BCL:H111	8:n:101:BCL:H93	1.66	0.42
1:D:27:LEU:O	1:D:31:ILE:HG13	2.20	0.41
15:L:308:CDL:H311	15:L:308:CDL:HA62	1.94	0.41
6:H:115:SER:N	6:H:234:ASP:OD2	2.45	0.41
1:S:28:ALA:HA	1:S:31:ILE:HG22	2.02	0.41
8:s:102:BCL:HBB1	8:s:103:BCL:HMC3	2.02	0.41
3:b:46:ARG:HH21	1:B:40:HIS:CE1	2.38	0.41
8:M:402:BCL:H143	8:M:402:BCL:H161	1.81	0.41
1:V:3:LYS:HG3	1:V:4:PHE:H	1.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:s:48:TRP:CD1	3:s:49:PHE:HD1	2.39	0.41
1:E:46:LEU:HD23	1:E:46:LEU:HA	1.89	0.41
1:T:7:ILE:HD11	1:T:11:PHE:HE2	1.84	0.41
8:q:102:BCL:H52	8:q:102:BCL:H8	1.87	0.41
6:H:112:ALA:HB2	6:H:242:GLY:HA3	2.01	0.41
8:v:101:BCL:H162	8:v:101:BCL:H141	1.56	0.41
1:T:36:LEU:O	1:T:42:ASN:ND2	2.54	0.41
3:r:24:TYR:HD1	3:r:25:MET:HE2	1.84	0.41
8:J:101:BCL:H162	8:J:101:BCL:H122	1.70	0.41
8:G:101:BCL:H162	8:G:101:BCL:H192	1.82	0.41
8:B:101:BCL:H143	8:B:101:BCL:H161	1.76	0.41
4:M:291:VAL:O	7:C:235:ARG:HG2	2.21	0.41
6:H:42:GLU:HA	6:H:48:THR:HA	2.03	0.41
7:C:144:MET:SD	16:C:401:HEC:NA	2.94	0.41
8:V:101:BCL:H111	8:V:101:BCL:H93	1.76	0.41
8:R:102:BCL:H91	8:R:102:BCL:H111	1.87	0.41
8:b:101:BCL:H41	8:b:101:BCL:H61	1.76	0.41
3:j:28:LEU:HD21	8:j:102:BCL:H42	2.01	0.41
4:M:230:PHE:HB2	4:M:245:ALA:HB2	2.03	0.41
4:M:244:THR:O	4:M:248:ARG:HG3	2.21	0.41
8:L:301:BCL:H143	8:L:301:BCL:H161	1.82	0.41
7:C:185:ARG:NH2	7:C:187:ASP:OD2	2.43	0.41
8:t:101:BCL:H202	8:t:101:BCL:H162	1.84	0.41
8:I:101:BCL:H2C	8:I:101:BCL:HBC3	1.76	0.41
4:M:202:PHE:HD1	4:M:280:THR:HG23	1.86	0.41
7:C:37:LEU:HD13	11:C:404:LMT:H51	2.02	0.41
1:V:40:HIS:NE2	3:v:46:ARG:HD2	2.36	0.41
8:r:101:BCL:H13	8:r:101:BCL:H102	1.81	0.41
1:F:36:LEU:HD13	5:L:52:TRP:CZ3	2.56	0.41
4:M:30:GLU:HB3	4:M:54:LEU:O	2.20	0.41
4:M:292:VAL:HG12	4:M:294:ASN:H	1.86	0.41
13:M:404:U10:H421	15:H:304:CDL:H471	2.02	0.41
5:L:21:ASP:HA	5:L:24:ASP:HB3	2.03	0.41
5:L:69:PRO:HB2	5:L:144:GLY:HA2	2.02	0.41
8:L:304:BCL:H172	8:L:304:BCL:H13	1.88	0.41
6:H:131:ILE:HD13	6:H:178:TYR:HE2	1.86	0.41
7:C:186:ILE:O	7:C:186:ILE:HG13	2.21	0.41
8:R:102:BCL:H192	8:R:102:BCL:H161	1.71	0.41
7:C:261:SER:HA	7:C:329:LYS:HG3	2.03	0.41
8:G:101:BCL:H162	8:G:101:BCL:H141	1.70	0.40
1:A:25:PHE:HB2	8:A:101:BCL:H71	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:12:LYS:HB2	7:C:12:LYS:HE2	1.87	0.40
8:r:101:BCL:H2	8:r:101:BCL:H142	2.03	0.40
3:i:12:LEU:HD23	3:i:13:THR:O	2.21	0.40
8:t:101:BCL:CAB	8:t:101:BCL:H143	2.52	0.40
3:j:46:ARG:HH21	1:J:40:HIS:CD2	2.38	0.40
3:j:46:ARG:NH1	1:J:46:LEU:HD11	2.36	0.40
7:C:258:PHE:O	7:C:262:LEU:HD23	2.21	0.40
8:P:102:BCL:H62	8:P:102:BCL:H102	1.83	0.40
8:N:101:BCL:H162	8:N:101:BCL:H141	1.79	0.40
8:i:101:BCL:H162	8:i:101:BCL:H192	1.78	0.40
5:L:228:LEU:HD21	5:L:232:ARG:NH2	2.37	0.40
7:C:117:LEU:HD21	7:C:121:ARG:CZ	2.51	0.40
1:V:14:ARG:HE	3:t:9:PHE:HD1	1.69	0.40
1:E:24:LEU:HD23	1:E:24:LEU:HA	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	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
1	I	49/53 (92%)	49 (100%)	0	0	100	100
1	J	48/53 (91%)	48 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	49/53 (92%)	48 (98%)	1 (2%)	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%)	49 (100%)	0	0	100	100
1	T	49/53 (92%)	48 (98%)	1 (2%)	0	100	100
1	V	49/53 (92%)	49 (100%)	0	0	100	100
2	O	50/239 (21%)	46 (92%)	4 (8%)	0	100	100
3	2	42/49 (86%)	41 (98%)	1 (2%)	0	100	100
3	a	42/49 (86%)	42 (100%)	0	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%)	42 (100%)	0	0	100	100
3	g	42/49 (86%)	41 (98%)	1 (2%)	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%)	42 (100%)	0	0	100	100
3	p	42/49 (86%)	41 (98%)	1 (2%)	0	100	100
3	q	42/49 (86%)	42 (100%)	0	0	100	100
3	r	41/49 (84%)	41 (100%)	0	0	100	100
3	s	42/49 (86%)	40 (95%)	2 (5%)	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%)	312 (97%)	11 (3%)	0	100	100
5	L	272/279 (98%)	266 (98%)	6 (2%)	0	100	100
6	H	254/256 (99%)	250 (98%)	4 (2%)	0	100	100
7	C	350/360 (97%)	330 (94%)	20 (6%)	0	100	100
All	All	2785/3198 (87%)	2729 (98%)	56 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	299 (100%)	0	100	100
All	All	2371/2633 (90%)	2371 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	V	20	GLN
1	S	42	ASN
3	s	16	GLN
3	q	16	GLN
3	2	16	GLN
1	1	40	HIS
3	k	16	GLN
3	j	16	GLN
1	I	40	HIS
3	f	16	GLN
1	B	42	ASN
4	M	70	ASN
4	M	260	ASN
5	L	212	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	H	34	ASN
6	H	67	HIS
6	H	174	GLN
7	C	42	GLN
7	C	201	ASN
7	C	300	ASN
7	C	321	ASN

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 98 ligands modelled in this entry, 1 is monoatomic - leaving 97 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	I	101	1	69,74,74	1.81	16 (23%)	83,115,115	2.21	27 (32%)
10	MW9	H	303	-	36,36,52	1.56	7 (19%)	39,41,58	1.88	3 (7%)
8	BCL	P	101	1	69,74,74	1.79	16 (23%)	83,115,115	2.11	27 (32%)
9	A1EFU	J	102	1	40,42,42	1.70	9 (22%)	45,52,52	3.56	20 (44%)
8	BCL	M	402	4,14	69,74,74	1.78	15 (21%)	83,115,115	2.12	25 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	BCL	Q	101	1	69,74,74	1.80	16 (23%)	83,115,115	2.13	27 (32%)
9	A1EFU	D	105	-	40,42,42	1.68	8 (20%)	45,52,52	3.91	20 (44%)
9	A1EFU	J	103	-	40,42,42	1.68	9 (22%)	45,52,52	3.93	20 (44%)
9	A1EFU	j	103	3,1	40,42,42	1.69	8 (20%)	45,52,52	3.79	20 (44%)
8	BCL	A	101	1	69,74,74	1.79	16 (23%)	83,115,115	2.12	28 (33%)
8	BCL	s	103	3	69,74,74	1.79	15 (21%)	83,115,115	2.13	27 (32%)
9	A1EFU	s	101	-	40,42,42	1.68	7 (17%)	45,52,52	3.88	20 (44%)
9	A1EFU	F	104	-	40,42,42	1.68	7 (17%)	45,52,52	3.74	19 (42%)
8	BCL	n	101	3	69,74,74	1.78	16 (23%)	83,115,115	2.18	29 (34%)
9	A1EFU	A	102	-	40,42,42	1.70	9 (22%)	45,52,52	3.77	19 (42%)
8	BCL	l	101	1	69,74,74	1.80	16 (23%)	83,115,115	2.18	28 (33%)
9	A1EFU	q	101	-	40,42,42	1.69	9 (22%)	45,52,52	3.70	21 (46%)
11	LMT	H	302	-	24,24,36	1.04	2 (8%)	29,29,47	1.07	2 (6%)
14	BPH	L	302	-	59,70,70	1.04	2 (3%)	61,101,101	0.91	4 (6%)
10	MW9	G	104	-	39,39,52	1.42	5 (12%)	42,45,58	1.18	3 (7%)
13	U10	L	303	-	48,48,63	0.17	0	58,61,79	0.44	1 (1%)
9	A1EFU	p	101	-	40,42,42	1.69	9 (22%)	45,52,52	3.91	20 (44%)
9	A1EFU	T	101	-	40,42,42	1.69	9 (22%)	45,52,52	3.72	20 (44%)
8	BCL	G	101	3,1	69,74,74	1.78	15 (21%)	83,115,115	2.15	28 (33%)
9	A1EFU	j	101	-	40,42,42	1.68	9 (22%)	45,52,52	3.99	20 (44%)
9	A1EFU	B	102	1	40,42,42	1.69	9 (22%)	45,52,52	3.69	20 (44%)
8	BCL	M	403	4	69,74,74	1.79	16 (23%)	83,115,115	2.16	28 (33%)
8	BCL	a	101	3	69,74,74	1.78	16 (23%)	83,115,115	2.17	29 (34%)
8	BCL	B	101	1	69,74,74	1.78	16 (23%)	83,115,115	2.16	27 (32%)
8	BCL	t	101	8,3	69,74,74	1.82	14 (20%)	83,115,115	2.10	26 (31%)
8	BCL	b	101	3	69,74,74	1.79	16 (23%)	83,115,115	2.14	29 (34%)
8	BCL	E	101	1	69,74,74	1.80	16 (23%)	83,115,115	2.19	30 (36%)
8	BCL	G	102	1	69,74,74	1.81	16 (23%)	83,115,115	2.19	28 (33%)
8	BCL	s	102	9,1	69,74,74	1.77	15 (21%)	83,115,115	2.25	27 (32%)
8	BCL	j	102	3	69,74,74	1.80	16 (23%)	83,115,115	2.17	28 (33%)
11	LMT	D	102	-	36,36,36	1.17	5 (13%)	47,47,47	0.96	2 (4%)
8	BCL	L	304	8,5	69,74,74	1.78	16 (23%)	83,115,115	2.24	29 (34%)
8	BCL	D	101	1	69,74,74	1.79	16 (23%)	83,115,115	2.13	28 (33%)
13	U10	M	404	-	63,63,63	0.17	0	76,79,79	0.41	1 (1%)
8	BCL	k	102	3	69,74,74	1.79	15 (21%)	83,115,115	2.15	27 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	A1EFU	R	101	-	40,42,42	1.68	8 (20%)	45,52,52	3.67	20 (44%)
8	BCL	q	102	3	69,74,74	1.79	16 (23%)	83,115,115	2.14	30 (36%)
8	BCL	F	102	1	69,74,74	1.81	16 (23%)	83,115,115	2.18	29 (34%)
9	A1EFU	E	103	-	40,42,42	1.68	7 (17%)	45,52,52	3.82	20 (44%)
9	A1EFU	I	102	-	40,42,42	1.68	7 (17%)	45,52,52	3.98	20 (44%)
10	MW9	H	301	-	47,47,52	1.39	6 (12%)	50,53,58	1.45	4 (8%)
9	A1EFU	K	102	1	40,42,42	1.70	9 (22%)	45,52,52	3.65	20 (44%)
8	BCL	K	101	1	69,74,74	1.80	16 (23%)	83,115,115	2.19	28 (33%)
9	A1EFU	2	102	-	40,42,42	1.69	9 (22%)	45,52,52	3.66	20 (44%)
9	A1EFU	k	101	-	40,42,42	1.69	9 (22%)	45,52,52	3.98	20 (44%)
8	BCL	J	101	1	69,74,74	1.81	16 (23%)	83,115,115	2.18	28 (33%)
9	A1EFU	s	104	9,3,8	40,42,42	1.69	9 (22%)	45,52,52	3.26	20 (44%)
11	LMT	L	306	-	24,24,36	1.04	2 (8%)	29,29,47	1.18	2 (6%)
10	MW9	M	406	-	52,52,52	1.45	6 (11%)	55,58,58	1.47	3 (5%)
9	A1EFU	a	102	3	40,42,42	1.70	9 (22%)	45,52,52	4.01	20 (44%)
9	A1EFU	D	104	-	40,42,42	1.69	9 (22%)	45,52,52	3.63	20 (44%)
11	LMT	L	305	-	24,24,36	1.05	2 (8%)	29,29,47	1.10	2 (6%)
8	BCL	d	101	3	69,74,74	1.82	12 (17%)	83,115,115	2.15	24 (28%)
9	A1EFU	N	102	-	40,42,42	1.69	9 (22%)	45,52,52	3.69	20 (44%)
15	CDL	H	304	-	90,90,99	0.91	8 (8%)	96,102,111	1.14	4 (4%)
9	A1EFU	G	105	-	40,42,42	1.69	8 (20%)	45,52,52	3.57	19 (42%)
9	A1EFU	G	106	-	40,42,42	1.67	7 (17%)	45,52,52	4.00	19 (42%)
8	BCL	V	101	8,1	69,74,74	1.78	14 (20%)	83,115,115	2.10	29 (34%)
8	BCL	N	101	1	69,74,74	1.79	16 (23%)	83,115,115	2.18	27 (32%)
8	BCL	2	103	3	69,74,74	1.78	16 (23%)	83,115,115	2.19	29 (34%)
8	BCL	P	102	3,1	69,74,74	1.78	15 (21%)	83,115,115	2.14	26 (31%)
16	HEC	C	402	7	50,50,50	1.33	6 (12%)	68,82,82	1.22	6 (8%)
10	MW9	D	103	1	52,52,52	1.45	6 (11%)	55,58,58	1.46	3 (5%)
8	BCL	R	102	1	69,74,74	1.80	16 (23%)	83,115,115	2.13	28 (33%)
8	BCL	r	101	3	69,74,74	1.78	15 (21%)	83,115,115	2.18	28 (33%)
9	A1EFU	P	103	-	40,42,42	1.69	9 (22%)	45,52,52	3.73	20 (44%)
8	BCL	i	101	3	69,74,74	1.80	15 (21%)	83,115,115	2.20	28 (33%)
8	BCL	v	101	3	69,74,74	1.78	15 (21%)	83,115,115	2.13	27 (32%)
9	A1EFU	M	407	-	40,42,42	1.68	8 (20%)	45,52,52	3.56	20 (44%)
8	BCL	e	101	3	69,74,74	1.79	16 (23%)	83,115,115	2.15	28 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	A1EFU	v	103	3	40,42,42	1.67	8 (20%)	45,52,52	3.69	19 (42%)
15	CDL	L	308	-	66,66,99	1.05	8 (12%)	72,78,111	1.16	4 (5%)
9	A1EFU	r	102	3	40,42,42	1.70	9 (22%)	45,52,52	3.78	19 (42%)
16	HEC	C	403	7	50,50,50	1.32	5 (10%)	68,82,82	1.19	6 (8%)
8	BCL	L	301	8,5	69,74,74	1.76	16 (23%)	83,115,115	2.27	29 (34%)
9	A1EFU	s	105	9	40,42,42	1.68	9 (22%)	45,52,52	3.80	20 (44%)
9	A1EFU	2	104	3,1	40,42,42	1.69	9 (22%)	45,52,52	3.48	21 (46%)
10	MW9	R	103	-	44,44,52	1.47	5 (11%)	47,50,58	1.52	3 (6%)
9	A1EFU	E	102	-	40,42,42	1.69	7 (17%)	45,52,52	3.67	19 (42%)
16	HEC	C	401	7	50,50,50	1.32	5 (10%)	68,82,82	1.25	7 (10%)
9	A1EFU	2	101	-	40,42,42	1.68	9 (22%)	45,52,52	3.77	20 (44%)
14	BPH	M	408	8,5	59,70,70	1.25	5 (8%)	61,101,101	0.90	4 (6%)
9	A1EFU	f	101	-	40,42,42	1.68	8 (20%)	45,52,52	3.79	19 (42%)
9	A1EFU	v	102	3	40,42,42	1.69	9 (22%)	45,52,52	3.73	20 (44%)
10	MW9	F	103	1	42,42,52	1.43	6 (14%)	45,48,58	1.46	3 (6%)
8	BCL	S	101	1	69,74,74	1.78	16 (23%)	83,115,115	2.13	27 (32%)
10	MW9	M	405	-	48,48,52	1.48	6 (12%)	51,54,58	1.51	3 (5%)
9	A1EFU	B	103	-	40,42,42	1.68	8 (20%)	45,52,52	3.68	20 (44%)
10	MW9	G	103	-	48,48,52	1.49	6 (12%)	51,54,58	1.48	4 (7%)
11	LMT	C	404	-	24,24,36	1.05	2 (8%)	29,29,47	1.06	1 (3%)
8	BCL	F	101	3,1	69,74,74	1.79	15 (21%)	83,115,115	2.12	30 (36%)
10	MW9	L	307	-	36,36,52	1.47	5 (13%)	39,42,58	1.54	3 (7%)

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	I	101	1	-	11/41/137/137	-
10	MW9	H	303	-	-	22/38/38/57	-
8	BCL	P	101	1	-	14/41/137/137	-
9	A1EFU	J	102	1	-	14/50/51/51	-
8	BCL	M	402	4,14	-	14/41/137/137	-
8	BCL	Q	101	1	-	21/41/137/137	-
9	A1EFU	D	105	-	-	19/50/51/51	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	A1EFU	J	103	-	-	20/50/51/51	-
9	A1EFU	j	103	3,1	-	19/50/51/51	-
8	BCL	A	101	1	-	14/41/137/137	-
8	BCL	s	103	3	-	19/41/137/137	-
9	A1EFU	s	101	-	-	20/50/51/51	-
9	A1EFU	F	104	-	-	21/50/51/51	-
8	BCL	n	101	3	-	11/41/137/137	-
9	A1EFU	A	102	-	-	19/50/51/51	-
8	BCL	l	101	1	-	13/41/137/137	-
9	A1EFU	q	101	-	-	24/50/51/51	-
11	LMT	H	302	-	-	6/15/35/61	0/1/1/2
14	BPH	L	302	-	-	8/37/105/105	0/5/6/6
10	MW9	G	104	-	-	27/44/44/57	-
13	U10	L	303	-	-	13/45/69/87	0/1/1/1
9	A1EFU	p	101	-	-	19/50/51/51	-
9	A1EFU	T	101	-	-	21/50/51/51	-
8	BCL	G	101	3,1	-	13/41/137/137	-
9	A1EFU	j	101	-	-	25/50/51/51	-
9	A1EFU	B	102	1	-	16/50/51/51	-
8	BCL	M	403	4	-	20/41/137/137	-
8	BCL	a	101	3	-	19/41/137/137	-
8	BCL	B	101	1	-	15/41/137/137	-
8	BCL	t	101	8,3	-	12/41/137/137	-
8	BCL	b	101	3	-	11/41/137/137	-
8	BCL	E	101	1	-	10/41/137/137	-
8	BCL	G	102	1	-	15/41/137/137	-
8	BCL	s	102	9,1	-	10/41/137/137	-
8	BCL	j	102	3	-	14/41/137/137	-
11	LMT	D	102	-	-	7/21/61/61	0/2/2/2
8	BCL	L	304	8,5	-	17/41/137/137	-
8	BCL	D	101	1	-	9/41/137/137	-
13	U10	M	404	-	-	10/63/87/87	0/1/1/1
8	BCL	k	102	3	-	10/41/137/137	-
9	A1EFU	R	101	-	-	19/50/51/51	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCL	q	102	3	-	14/41/137/137	-
8	BCL	F	102	1	-	10/41/137/137	-
9	A1EFU	E	103	-	-	19/50/51/51	-
9	A1EFU	I	102	-	-	20/50/51/51	-
10	MW9	H	301	-	-	27/52/52/57	-
9	A1EFU	K	102	1	-	21/50/51/51	-
8	BCL	K	101	1	-	10/41/137/137	-
9	A1EFU	2	102	-	-	29/50/51/51	-
9	A1EFU	k	101	-	-	25/50/51/51	-
8	BCL	J	101	1	-	12/41/137/137	-
9	A1EFU	s	104	9,3,8	-	22/50/51/51	-
11	LMT	L	306	-	-	8/15/35/61	0/1/1/2
10	MW9	M	406	-	-	34/57/57/57	-
9	A1EFU	a	102	3	-	18/50/51/51	-
9	A1EFU	D	104	-	-	17/50/51/51	-
11	LMT	L	305	-	-	5/15/35/61	0/1/1/2
8	BCL	d	101	3	-	25/41/137/137	-
9	A1EFU	N	102	-	-	23/50/51/51	-
15	CDL	H	304	-	-	46/101/101/110	-
9	A1EFU	G	105	-	-	25/50/51/51	-
9	A1EFU	G	106	-	-	24/50/51/51	-
8	BCL	V	101	8,1	-	7/41/137/137	-
8	BCL	N	101	1	-	10/41/137/137	-
8	BCL	2	103	3	-	20/41/137/137	-
8	BCL	P	102	3,1	-	16/41/137/137	-
16	HEC	C	402	7	1/1/3/7	5/14/54/54	-
10	MW9	D	103	1	-	29/57/57/57	-
8	BCL	R	102	1	-	9/41/137/137	-
8	BCL	r	101	3	-	11/41/137/137	-
9	A1EFU	P	103	-	-	22/50/51/51	-
8	BCL	i	101	3	-	21/41/137/137	-
8	BCL	v	101	3	-	19/41/137/137	-
9	A1EFU	M	407	-	-	17/50/51/51	-
8	BCL	e	101	3	-	11/41/137/137	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	A1EFU	v	103	3	-	24/50/51/51	-
15	CDL	L	308	-	-	41/77/77/110	-
9	A1EFU	r	102	3	-	21/50/51/51	-
16	HEC	C	403	7	1/1/3/7	2/14/54/54	-
8	BCL	L	301	8,5	-	17/41/137/137	-
9	A1EFU	s	105	9	-	24/50/51/51	-
9	A1EFU	2	104	3,1	-	22/50/51/51	-
10	MW9	R	103	-	-	34/49/49/57	-
9	A1EFU	E	102	-	-	18/50/51/51	-
16	HEC	C	401	7	1/1/3/7	4/14/54/54	-
9	A1EFU	2	101	-	-	20/50/51/51	-
14	BPH	M	408	8,5	-	10/37/105/105	0/5/6/6
9	A1EFU	f	101	-	-	18/50/51/51	-
9	A1EFU	v	102	3	-	23/50/51/51	-
10	MW9	F	103	1	-	33/47/47/57	-
8	BCL	S	101	1	-	13/41/137/137	-
10	MW9	M	405	-	-	30/53/53/57	-
9	A1EFU	B	103	-	-	19/50/51/51	-
10	MW9	G	103	-	-	27/53/53/57	-
11	LMT	C	404	-	-	5/15/35/61	0/1/1/2
8	BCL	F	101	3,1	-	16/41/137/137	-
10	MW9	L	307	-	-	15/41/41/57	-

All (995) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	M	408	BPH	C1D-C2D	6.20	1.46	1.39
14	L	302	BPH	C1D-C2D	6.19	1.46	1.39
8	t	101	BCL	MG-ND	-6.07	1.93	2.05
8	d	101	BCL	MG-ND	-5.99	1.93	2.05
8	I	101	BCL	MG-ND	-5.90	1.94	2.05
8	J	101	BCL	MG-ND	-5.89	1.94	2.05
8	1	101	BCL	MG-ND	-5.87	1.94	2.05
8	F	102	BCL	MG-ND	-5.86	1.94	2.05
8	E	101	BCL	MG-ND	-5.85	1.94	2.05
8	Q	101	BCL	MG-ND	-5.84	1.94	2.05
8	G	102	BCL	MG-ND	-5.84	1.94	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	K	101	BCL	MG-ND	-5.83	1.94	2.05
8	P	101	BCL	MG-ND	-5.80	1.94	2.05
8	R	102	BCL	MG-ND	-5.79	1.94	2.05
8	j	102	BCL	MG-ND	-5.79	1.94	2.05
8	e	101	BCL	MG-ND	-5.77	1.94	2.05
8	N	101	BCL	MG-ND	-5.75	1.94	2.05
8	D	101	BCL	MG-ND	-5.74	1.94	2.05
8	S	101	BCL	MG-ND	-5.74	1.94	2.05
8	F	101	BCL	MG-ND	-5.72	1.94	2.05
8	k	102	BCL	MG-ND	-5.72	1.94	2.05
8	A	101	BCL	MG-ND	-5.72	1.94	2.05
8	i	101	BCL	MG-ND	-5.71	1.94	2.05
8	s	103	BCL	MG-ND	-5.71	1.94	2.05
8	q	102	BCL	MG-ND	-5.70	1.94	2.05
8	M	403	BCL	MG-ND	-5.70	1.94	2.05
9	E	102	A1EFU	C19-C18	-5.69	1.33	1.45
8	b	101	BCL	MG-ND	-5.67	1.94	2.05
9	D	104	A1EFU	C19-C18	-5.67	1.33	1.45
8	a	101	BCL	MG-ND	-5.65	1.94	2.05
9	B	102	A1EFU	C19-C18	-5.65	1.33	1.45
8	V	101	BCL	MG-ND	-5.65	1.94	2.05
8	G	101	BCL	MG-ND	-5.64	1.94	2.05
9	F	104	A1EFU	C19-C18	-5.64	1.33	1.45
8	L	304	BCL	MG-ND	-5.64	1.94	2.05
8	M	402	BCL	MG-ND	-5.63	1.94	2.05
9	P	103	A1EFU	C19-C18	-5.63	1.33	1.45
8	v	101	BCL	MG-ND	-5.62	1.94	2.05
8	n	101	BCL	MG-ND	-5.62	1.94	2.05
9	r	102	A1EFU	C19-C18	-5.62	1.33	1.45
8	r	101	BCL	MG-ND	-5.61	1.94	2.05
9	R	101	A1EFU	C19-C18	-5.61	1.33	1.45
8	P	102	BCL	MG-ND	-5.61	1.94	2.05
9	q	101	A1EFU	C19-C18	-5.60	1.33	1.45
9	I	102	A1EFU	C19-C18	-5.59	1.33	1.45
9	2	101	A1EFU	C19-C18	-5.59	1.33	1.45
8	B	101	BCL	MG-ND	-5.58	1.94	2.05
9	T	101	A1EFU	C19-C18	-5.58	1.34	1.45
9	G	106	A1EFU	C19-C18	-5.57	1.34	1.45
9	s	101	A1EFU	C19-C18	-5.57	1.34	1.45
9	B	103	A1EFU	C19-C18	-5.57	1.34	1.45
9	j	103	A1EFU	C19-C18	-5.56	1.34	1.45
8	2	103	BCL	MG-ND	-5.56	1.94	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	s	102	BCL	MG-ND	-5.55	1.94	2.05
9	k	101	A1EFU	C19-C18	-5.55	1.34	1.45
9	A	102	A1EFU	C19-C18	-5.55	1.34	1.45
9	E	103	A1EFU	C19-C18	-5.55	1.34	1.45
9	G	105	A1EFU	C19-C18	-5.53	1.34	1.45
9	p	101	A1EFU	C19-C18	-5.52	1.34	1.45
9	v	103	A1EFU	C19-C18	-5.52	1.34	1.45
9	s	105	A1EFU	C19-C18	-5.52	1.34	1.45
9	j	101	A1EFU	C19-C18	-5.51	1.34	1.45
9	N	102	A1EFU	C19-C18	-5.50	1.34	1.45
9	v	102	A1EFU	C19-C18	-5.50	1.34	1.45
9	K	102	A1EFU	C19-C18	-5.50	1.34	1.45
9	D	105	A1EFU	C19-C18	-5.49	1.34	1.45
9	a	102	A1EFU	C19-C18	-5.49	1.34	1.45
9	M	407	A1EFU	C19-C18	-5.49	1.34	1.45
8	L	301	BCL	MG-ND	-5.49	1.94	2.05
9	J	102	A1EFU	C19-C18	-5.48	1.34	1.45
9	J	103	A1EFU	C19-C18	-5.47	1.34	1.45
9	f	101	A1EFU	C19-C18	-5.46	1.34	1.45
9	2	102	A1EFU	C19-C18	-5.43	1.34	1.45
9	2	104	A1EFU	C19-C18	-5.42	1.34	1.45
9	s	104	A1EFU	C19-C18	-5.41	1.34	1.45
8	d	101	BCL	MG-NB	-4.98	1.95	2.05
8	t	101	BCL	MG-NB	-4.93	1.96	2.05
8	I	101	BCL	MG-NB	-4.89	1.96	2.05
8	F	102	BCL	MG-NB	-4.87	1.96	2.05
8	V	101	BCL	MG-NB	-4.87	1.96	2.05
8	e	101	BCL	MG-NB	-4.84	1.96	2.05
8	E	101	BCL	MG-NB	-4.84	1.96	2.05
8	R	102	BCL	MG-NB	-4.82	1.96	2.05
8	D	101	BCL	MG-NB	-4.82	1.96	2.05
8	Q	101	BCL	MG-NB	-4.82	1.96	2.05
8	K	101	BCL	MG-NB	-4.81	1.96	2.05
8	j	102	BCL	MG-NB	-4.79	1.96	2.05
8	J	101	BCL	MG-NB	-4.78	1.96	2.05
8	G	102	BCL	MG-NB	-4.77	1.96	2.05
8	P	101	BCL	MG-NB	-4.77	1.96	2.05
8	F	101	BCL	MG-NB	-4.76	1.96	2.05
8	q	102	BCL	MG-NB	-4.76	1.96	2.05
8	l	101	BCL	MG-NB	-4.76	1.96	2.05
8	N	101	BCL	MG-NB	-4.75	1.96	2.05
8	A	101	BCL	MG-NB	-4.73	1.96	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	s	103	BCL	MG-NB	-4.72	1.96	2.05
8	k	102	BCL	MG-NB	-4.71	1.96	2.05
8	i	101	BCL	MG-NB	-4.70	1.96	2.05
8	B	101	BCL	MG-NB	-4.70	1.96	2.05
8	t	101	BCL	OBD-CAD	4.70	1.30	1.22
8	t	101	BCL	C4D-ND	-4.69	1.31	1.37
8	b	101	BCL	MG-NB	-4.69	1.96	2.05
8	s	102	BCL	OBD-CAD	4.68	1.30	1.22
8	s	103	BCL	OBD-CAD	4.68	1.30	1.22
8	M	403	BCL	MG-NB	-4.68	1.96	2.05
8	v	101	BCL	OBD-CAD	4.67	1.30	1.22
8	S	101	BCL	MG-NB	-4.67	1.96	2.05
8	V	101	BCL	OBD-CAD	4.67	1.30	1.22
8	a	101	BCL	MG-NB	-4.66	1.96	2.05
8	n	101	BCL	OBD-CAD	4.66	1.30	1.22
8	F	102	BCL	OBD-CAD	4.66	1.30	1.22
8	2	103	BCL	OBD-CAD	4.65	1.30	1.22
8	L	301	BCL	OBD-CAD	4.65	1.30	1.22
8	2	103	BCL	MG-NB	-4.65	1.96	2.05
8	J	101	BCL	OBD-CAD	4.65	1.30	1.22
8	Q	101	BCL	OBD-CAD	4.64	1.30	1.22
8	F	101	BCL	OBD-CAD	4.64	1.30	1.22
8	j	102	BCL	OBD-CAD	4.64	1.30	1.22
8	G	102	BCL	OBD-CAD	4.64	1.30	1.22
8	N	101	BCL	OBD-CAD	4.64	1.30	1.22
8	k	102	BCL	OBD-CAD	4.64	1.30	1.22
8	a	101	BCL	OBD-CAD	4.63	1.30	1.22
8	r	101	BCL	OBD-CAD	4.63	1.30	1.22
8	i	101	BCL	OBD-CAD	4.63	1.30	1.22
8	K	101	BCL	OBD-CAD	4.62	1.30	1.22
8	e	101	BCL	OBD-CAD	4.62	1.30	1.22
8	R	102	BCL	OBD-CAD	4.62	1.30	1.22
8	A	101	BCL	OBD-CAD	4.62	1.30	1.22
8	P	102	BCL	MG-NB	-4.62	1.96	2.05
8	q	102	BCL	OBD-CAD	4.62	1.30	1.22
8	P	101	BCL	OBD-CAD	4.62	1.30	1.22
8	G	101	BCL	MG-NB	-4.62	1.96	2.05
8	D	101	BCL	OBD-CAD	4.62	1.30	1.22
8	I	101	BCL	OBD-CAD	4.61	1.30	1.22
8	d	101	BCL	OBD-CAD	4.61	1.30	1.22
8	P	102	BCL	OBD-CAD	4.61	1.30	1.22
8	1	101	BCL	OBD-CAD	4.61	1.30	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	v	101	BCL	MG-NB	-4.61	1.96	2.05
8	S	101	BCL	OBD-CAD	4.61	1.30	1.22
8	E	101	BCL	OBD-CAD	4.59	1.30	1.22
8	G	101	BCL	OBD-CAD	4.59	1.30	1.22
8	L	304	BCL	MG-NB	-4.58	1.96	2.05
8	B	101	BCL	OBD-CAD	4.58	1.30	1.22
8	d	101	BCL	C4D-ND	-4.58	1.31	1.37
8	b	101	BCL	OBD-CAD	4.58	1.30	1.22
8	M	402	BCL	MG-NB	-4.57	1.96	2.05
8	r	101	BCL	MG-NB	-4.57	1.96	2.05
8	s	102	BCL	MG-NB	-4.57	1.96	2.05
8	M	402	BCL	OBD-CAD	4.55	1.30	1.22
8	L	304	BCL	OBD-CAD	4.55	1.30	1.22
8	n	101	BCL	MG-NB	-4.54	1.96	2.05
8	E	101	BCL	C4D-ND	-4.54	1.31	1.37
8	L	301	BCL	MG-NB	-4.53	1.96	2.05
8	M	403	BCL	OBD-CAD	4.52	1.30	1.22
10	G	103	MW9	C35-C34	-4.51	1.34	1.52
8	F	102	BCL	C4D-ND	-4.51	1.31	1.37
14	M	408	BPH	C2C-C3C	4.50	1.58	1.54
8	K	101	BCL	C4D-ND	-4.50	1.31	1.37
10	M	405	MW9	C35-C34	-4.50	1.34	1.52
8	M	402	BCL	C4D-ND	-4.49	1.31	1.37
10	M	406	MW9	C35-C34	-4.48	1.34	1.52
10	D	103	MW9	C35-C34	-4.47	1.34	1.52
8	i	101	BCL	C4D-ND	-4.45	1.31	1.37
8	G	102	BCL	C4D-ND	-4.44	1.31	1.37
8	b	101	BCL	C4D-ND	-4.43	1.31	1.37
8	J	101	BCL	C4D-ND	-4.43	1.31	1.37
10	R	103	MW9	C35-C34	-4.42	1.34	1.52
8	j	102	BCL	C4D-ND	-4.40	1.31	1.37
8	M	403	BCL	C4D-ND	-4.38	1.31	1.37
8	R	102	BCL	C4D-ND	-4.37	1.31	1.37
8	n	101	BCL	C4D-ND	-4.37	1.31	1.37
8	e	101	BCL	C4D-ND	-4.36	1.31	1.37
8	k	102	BCL	C4D-ND	-4.36	1.31	1.37
8	q	102	BCL	C4D-ND	-4.36	1.31	1.37
8	s	103	BCL	C4D-ND	-4.36	1.31	1.37
8	v	101	BCL	C4D-ND	-4.36	1.31	1.37
8	I	101	BCL	C4D-ND	-4.35	1.31	1.37
8	2	103	BCL	C4D-ND	-4.34	1.31	1.37
8	s	102	BCL	C4D-ND	-4.34	1.31	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	101	BCL	C4D-ND	-4.32	1.31	1.37
8	A	101	BCL	C4D-ND	-4.32	1.31	1.37
8	a	101	BCL	C4D-ND	-4.32	1.31	1.37
8	N	101	BCL	C4D-ND	-4.30	1.31	1.37
8	B	101	BCL	C4D-ND	-4.29	1.31	1.37
8	S	101	BCL	C4D-ND	-4.28	1.31	1.37
8	r	101	BCL	C4D-ND	-4.28	1.31	1.37
8	Q	101	BCL	C4D-ND	-4.23	1.31	1.37
8	l	101	BCL	C4D-ND	-4.22	1.31	1.37
8	V	101	BCL	C4D-ND	-4.21	1.31	1.37
8	P	102	BCL	C4D-ND	-4.20	1.31	1.37
8	P	101	BCL	C4D-ND	-4.19	1.31	1.37
8	L	304	BCL	C4D-ND	-4.18	1.32	1.37
10	F	103	MW9	C33-C32	4.13	1.55	1.31
10	R	103	MW9	C33-C32	4.12	1.55	1.31
10	L	307	MW9	C33-C32	4.12	1.55	1.31
8	F	101	BCL	O1D-CGD	-4.12	1.10	1.21
10	D	103	MW9	C33-C32	4.12	1.55	1.31
10	M	406	MW9	C33-C32	4.11	1.55	1.31
10	H	301	MW9	C33-C32	4.11	1.55	1.31
8	L	304	BCL	O1D-CGD	-4.11	1.10	1.21
10	M	405	MW9	C33-C32	4.10	1.55	1.31
8	F	101	BCL	C4D-ND	-4.10	1.32	1.37
10	G	103	MW9	C33-C32	4.10	1.55	1.31
8	d	101	BCL	O1D-CGD	-4.10	1.10	1.21
8	l	101	BCL	O1D-CGD	-4.09	1.11	1.21
10	H	303	MW9	C33-C32	4.09	1.55	1.31
8	G	101	BCL	C4D-ND	-4.08	1.32	1.37
8	b	101	BCL	O1D-CGD	-4.07	1.11	1.21
8	M	403	BCL	O1D-CGD	-4.07	1.11	1.21
8	j	102	BCL	O1D-CGD	-4.07	1.11	1.21
8	a	101	BCL	O1D-CGD	-4.07	1.11	1.21
8	R	102	BCL	O1D-CGD	-4.07	1.11	1.21
8	q	102	BCL	O1D-CGD	-4.06	1.11	1.21
8	N	101	BCL	O1D-CGD	-4.06	1.11	1.21
8	e	101	BCL	O1D-CGD	-4.06	1.11	1.21
8	2	103	BCL	O1D-CGD	-4.05	1.11	1.21
8	S	101	BCL	O1D-CGD	-4.05	1.11	1.21
8	k	102	BCL	O1D-CGD	-4.05	1.11	1.21
8	M	402	BCL	O1D-CGD	-4.05	1.11	1.21
8	n	101	BCL	O1D-CGD	-4.05	1.11	1.21
8	Q	101	BCL	O1D-CGD	-4.05	1.11	1.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	301	BCL	O1D-CGD	-4.05	1.11	1.21
8	B	101	BCL	O1D-CGD	-4.04	1.11	1.21
8	L	301	BCL	C4D-ND	-4.03	1.32	1.37
8	G	102	BCL	O1D-CGD	-4.03	1.11	1.21
8	E	101	BCL	O1D-CGD	-4.03	1.11	1.21
8	D	101	BCL	O1D-CGD	-4.03	1.11	1.21
8	P	101	BCL	O1D-CGD	-4.03	1.11	1.21
8	t	101	BCL	O1D-CGD	-4.02	1.11	1.21
8	F	102	BCL	O1D-CGD	-4.02	1.11	1.21
8	J	101	BCL	O1D-CGD	-4.02	1.11	1.21
8	s	103	BCL	O1D-CGD	-4.01	1.11	1.21
8	i	101	BCL	O1D-CGD	-4.01	1.11	1.21
8	s	102	BCL	O1D-CGD	-4.01	1.11	1.21
8	I	101	BCL	O1D-CGD	-4.01	1.11	1.21
8	v	101	BCL	O1D-CGD	-4.01	1.11	1.21
8	V	101	BCL	O1D-CGD	-4.01	1.11	1.21
10	G	104	MW9	C33-C32	4.01	1.55	1.28
8	r	101	BCL	O1D-CGD	-4.00	1.11	1.21
8	A	101	BCL	O1D-CGD	-4.00	1.11	1.21
8	K	101	BCL	O1D-CGD	-3.98	1.11	1.21
8	P	102	BCL	O1D-CGD	-3.97	1.11	1.21
8	G	101	BCL	O1D-CGD	-3.97	1.11	1.21
8	G	101	BCL	O2D-CED	3.67	1.53	1.45
8	P	102	BCL	O2D-CED	3.66	1.53	1.45
8	F	101	BCL	O2D-CED	3.65	1.53	1.45
9	N	102	A1EFU	C11-C10	3.62	1.54	1.43
9	s	104	A1EFU	C11-C10	3.62	1.54	1.43
9	s	104	A1EFU	C7-C6	3.61	1.54	1.43
9	N	102	A1EFU	C7-C6	3.56	1.54	1.43
9	2	104	A1EFU	C7-C6	3.56	1.54	1.43
9	2	104	A1EFU	C11-C10	3.55	1.54	1.43
9	2	102	A1EFU	C7-C6	3.55	1.54	1.43
9	K	102	A1EFU	C11-C10	3.54	1.54	1.43
9	T	101	A1EFU	C7-C6	3.54	1.54	1.43
9	K	102	A1EFU	C7-C6	3.54	1.54	1.43
9	a	102	A1EFU	C7-C6	3.53	1.54	1.43
9	P	103	A1EFU	C11-C10	3.53	1.54	1.43
9	J	102	A1EFU	C7-C6	3.53	1.54	1.43
9	G	105	A1EFU	C11-C10	3.53	1.54	1.43
9	2	101	A1EFU	C7-C6	3.52	1.54	1.43
9	G	105	A1EFU	C7-C6	3.52	1.54	1.43
9	A	102	A1EFU	C7-C6	3.52	1.54	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	q	101	A1EFU	C11-C10	3.52	1.54	1.43
9	P	103	A1EFU	C7-C6	3.51	1.54	1.43
9	r	102	A1EFU	C7-C6	3.51	1.54	1.43
9	2	102	A1EFU	C11-C10	3.51	1.54	1.43
9	v	102	A1EFU	C11-C10	3.50	1.54	1.43
9	B	103	A1EFU	C7-C6	3.50	1.54	1.43
9	v	103	A1EFU	C11-C10	3.50	1.54	1.43
9	s	105	A1EFU	C7-C6	3.50	1.54	1.43
9	R	101	A1EFU	C11-C10	3.49	1.54	1.43
9	E	102	A1EFU	C7-C6	3.49	1.54	1.43
9	j	103	A1EFU	C7-C6	3.49	1.54	1.43
9	p	101	A1EFU	C7-C6	3.48	1.54	1.43
9	v	102	A1EFU	C7-C6	3.48	1.54	1.43
8	v	101	BCL	O2D-CED	3.48	1.53	1.45
9	B	102	A1EFU	C7-C6	3.48	1.54	1.43
9	T	101	A1EFU	C11-C10	3.48	1.54	1.43
9	D	104	A1EFU	C7-C6	3.48	1.54	1.43
9	A	102	A1EFU	C11-C10	3.48	1.54	1.43
9	J	102	A1EFU	C11-C10	3.48	1.54	1.43
9	f	101	A1EFU	C7-C6	3.47	1.54	1.43
9	v	103	A1EFU	C7-C6	3.47	1.54	1.43
9	R	101	A1EFU	C7-C6	3.47	1.54	1.43
9	M	407	A1EFU	C11-C10	3.47	1.54	1.43
8	s	103	BCL	O2D-CED	3.46	1.53	1.45
9	D	105	A1EFU	C7-C6	3.46	1.54	1.43
9	s	105	A1EFU	C11-C10	3.46	1.54	1.43
9	q	101	A1EFU	C7-C6	3.46	1.54	1.43
9	r	102	A1EFU	C11-C10	3.45	1.54	1.43
9	j	103	A1EFU	C11-C10	3.45	1.54	1.43
9	M	407	A1EFU	C7-C6	3.45	1.54	1.43
9	2	104	A1EFU	C16-C17	3.45	1.54	1.43
9	E	102	A1EFU	C11-C10	3.45	1.54	1.43
8	A	101	BCL	O2D-CED	3.45	1.53	1.45
8	G	102	BCL	O2D-CED	3.44	1.53	1.45
9	a	102	A1EFU	C11-C10	3.44	1.54	1.43
9	B	103	A1EFU	C11-C10	3.44	1.54	1.43
9	D	104	A1EFU	C11-C10	3.44	1.54	1.43
8	V	101	BCL	O2D-CED	3.44	1.53	1.45
8	d	101	BCL	O2D-CED	3.44	1.53	1.45
9	B	102	A1EFU	C11-C10	3.44	1.54	1.43
8	J	101	BCL	O2D-CED	3.44	1.53	1.45
8	E	101	BCL	O2D-CED	3.44	1.53	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	E	103	A1EFU	C7-C6	3.44	1.54	1.43
9	J	103	A1EFU	C11-C10	3.43	1.54	1.43
8	q	102	BCL	O2D-CED	3.43	1.53	1.45
9	I	102	A1EFU	C7-C6	3.43	1.54	1.43
9	j	101	A1EFU	C7-C6	3.43	1.54	1.43
8	j	102	BCL	O2D-CED	3.43	1.53	1.45
9	s	101	A1EFU	C7-C6	3.43	1.54	1.43
8	2	103	BCL	O2D-CED	3.43	1.53	1.45
9	F	104	A1EFU	C7-C6	3.43	1.54	1.43
9	D	105	A1EFU	C11-C10	3.42	1.54	1.43
8	1	101	BCL	O2D-CED	3.42	1.53	1.45
8	R	102	BCL	O2D-CED	3.42	1.53	1.45
8	M	402	BCL	O2D-CED	3.42	1.53	1.45
8	i	101	BCL	O2D-CED	3.42	1.53	1.45
8	a	101	BCL	O2D-CED	3.42	1.53	1.45
9	p	101	A1EFU	C11-C10	3.41	1.54	1.43
9	I	102	A1EFU	C11-C10	3.41	1.54	1.43
8	I	101	BCL	O2D-CED	3.41	1.53	1.45
9	2	101	A1EFU	C11-C10	3.41	1.54	1.43
9	G	106	A1EFU	C7-C6	3.41	1.54	1.43
9	f	101	A1EFU	C11-C10	3.40	1.54	1.43
9	s	104	A1EFU	C16-C17	3.40	1.54	1.43
9	F	104	A1EFU	C11-C10	3.40	1.54	1.43
9	E	103	A1EFU	C11-C10	3.40	1.54	1.43
9	k	101	A1EFU	C7-C6	3.40	1.54	1.43
9	2	104	A1EFU	C15-C14	3.40	1.54	1.43
8	F	102	BCL	O2D-CED	3.40	1.53	1.45
8	t	101	BCL	O2D-CED	3.40	1.53	1.45
8	Q	101	BCL	O2D-CED	3.40	1.53	1.45
8	r	101	BCL	O2D-CED	3.40	1.53	1.45
9	G	106	A1EFU	C11-C10	3.40	1.54	1.43
9	J	103	A1EFU	C7-C6	3.39	1.54	1.43
8	k	102	BCL	O2D-CED	3.39	1.53	1.45
9	K	102	A1EFU	C16-C17	3.39	1.53	1.43
8	S	101	BCL	O2D-CED	3.39	1.53	1.45
9	k	101	A1EFU	C11-C10	3.39	1.53	1.43
9	j	101	A1EFU	C11-C10	3.38	1.53	1.43
8	b	101	BCL	O2D-CED	3.38	1.53	1.45
9	J	102	A1EFU	C16-C17	3.38	1.53	1.43
9	s	101	A1EFU	C11-C10	3.38	1.53	1.43
8	N	101	BCL	O2D-CED	3.38	1.53	1.45
9	N	102	A1EFU	C16-C17	3.37	1.53	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	n	101	BCL	O2D-CED	3.37	1.53	1.45
8	L	304	BCL	O2D-CED	3.37	1.53	1.45
9	v	102	A1EFU	C20-C21	3.37	1.53	1.43
9	K	102	A1EFU	C15-C14	3.37	1.53	1.43
8	P	101	BCL	O2D-CED	3.36	1.53	1.45
9	v	102	A1EFU	C15-C14	3.35	1.53	1.43
8	s	102	BCL	O2D-CED	3.35	1.53	1.45
9	2	102	A1EFU	C16-C17	3.35	1.53	1.43
9	s	104	A1EFU	C15-C14	3.35	1.53	1.43
9	p	101	A1EFU	C20-C21	3.35	1.53	1.43
8	K	101	BCL	O2D-CED	3.34	1.53	1.45
8	B	101	BCL	O2D-CED	3.34	1.53	1.45
9	s	104	A1EFU	C20-C21	3.34	1.53	1.43
8	D	101	BCL	O2D-CED	3.34	1.53	1.45
9	K	102	A1EFU	C20-C21	3.34	1.53	1.43
8	L	301	BCL	O2D-CED	3.34	1.53	1.45
8	e	101	BCL	O2D-CED	3.34	1.53	1.45
9	j	103	A1EFU	C16-C17	3.34	1.53	1.43
9	p	101	A1EFU	C16-C17	3.33	1.53	1.43
9	N	102	A1EFU	C15-C14	3.33	1.53	1.43
9	G	105	A1EFU	C20-C21	3.33	1.53	1.43
9	2	104	A1EFU	C20-C21	3.33	1.53	1.43
9	2	102	A1EFU	C15-C14	3.33	1.53	1.43
16	C	401	HEC	CBC-CAC	-3.32	1.36	1.51
9	M	407	A1EFU	C20-C21	3.32	1.53	1.43
9	2	102	A1EFU	C20-C21	3.32	1.53	1.43
9	J	102	A1EFU	C15-C14	3.32	1.53	1.43
9	p	101	A1EFU	C15-C14	3.31	1.53	1.43
9	J	102	A1EFU	C20-C21	3.31	1.53	1.43
9	M	407	A1EFU	C16-C17	3.31	1.53	1.43
9	v	102	A1EFU	C16-C17	3.31	1.53	1.43
16	C	403	HEC	CBC-CAC	-3.31	1.36	1.51
9	R	101	A1EFU	C16-C17	3.31	1.53	1.43
9	2	101	A1EFU	C15-C14	3.30	1.53	1.43
9	A	102	A1EFU	C20-C21	3.30	1.53	1.43
9	q	101	A1EFU	C16-C17	3.30	1.53	1.43
16	C	402	HEC	CBC-CAC	-3.30	1.36	1.51
9	f	101	A1EFU	C15-C14	3.29	1.53	1.43
9	A	102	A1EFU	C16-C17	3.29	1.53	1.43
9	k	101	A1EFU	C16-C17	3.29	1.53	1.43
9	R	101	A1EFU	C20-C21	3.28	1.53	1.43
9	G	105	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	v	103	A1EFU	C20-C21	3.28	1.53	1.43
9	f	101	A1EFU	C16-C17	3.28	1.53	1.43
9	G	105	A1EFU	C15-C14	3.28	1.53	1.43
9	B	103	A1EFU	C20-C21	3.28	1.53	1.43
9	D	104	A1EFU	C15-C14	3.28	1.53	1.43
9	D	105	A1EFU	C20-C21	3.27	1.53	1.43
9	T	101	A1EFU	C20-C21	3.27	1.53	1.43
9	a	102	A1EFU	C16-C17	3.27	1.53	1.43
9	P	103	A1EFU	C20-C21	3.27	1.53	1.43
9	k	101	A1EFU	C15-C14	3.27	1.53	1.43
9	M	407	A1EFU	C15-C14	3.26	1.53	1.43
9	f	101	A1EFU	C20-C21	3.26	1.53	1.43
9	T	101	A1EFU	C15-C14	3.26	1.53	1.43
9	j	101	A1EFU	C20-C21	3.26	1.53	1.43
9	q	101	A1EFU	C20-C21	3.25	1.53	1.43
9	T	101	A1EFU	C16-C17	3.25	1.53	1.43
9	B	102	A1EFU	C16-C17	3.25	1.53	1.43
9	N	102	A1EFU	C20-C21	3.25	1.53	1.43
9	I	102	A1EFU	C20-C21	3.25	1.53	1.43
9	B	103	A1EFU	C16-C17	3.25	1.53	1.43
9	s	101	A1EFU	C20-C21	3.25	1.53	1.43
9	E	103	A1EFU	C20-C21	3.25	1.53	1.43
9	2	101	A1EFU	C20-C21	3.25	1.53	1.43
9	q	101	A1EFU	C15-C14	3.25	1.53	1.43
9	P	103	A1EFU	C15-C14	3.24	1.53	1.43
9	s	105	A1EFU	C16-C17	3.24	1.53	1.43
9	s	105	A1EFU	C20-C21	3.24	1.53	1.43
8	M	403	BCL	O2D-CED	3.24	1.52	1.45
9	k	101	A1EFU	C20-C21	3.24	1.53	1.43
9	j	103	A1EFU	C15-C14	3.24	1.53	1.43
9	A	102	A1EFU	C15-C14	3.24	1.53	1.43
9	j	103	A1EFU	C20-C21	3.24	1.53	1.43
9	F	104	A1EFU	C16-C17	3.24	1.53	1.43
9	B	102	A1EFU	C20-C21	3.24	1.53	1.43
9	J	103	A1EFU	C20-C21	3.24	1.53	1.43
9	B	103	A1EFU	C15-C14	3.24	1.53	1.43
9	a	102	A1EFU	C20-C21	3.24	1.53	1.43
9	P	103	A1EFU	C16-C17	3.24	1.53	1.43
9	s	105	A1EFU	C15-C14	3.23	1.53	1.43
9	r	102	A1EFU	C20-C21	3.23	1.53	1.43
9	E	103	A1EFU	C16-C17	3.23	1.53	1.43
9	D	104	A1EFU	C16-C17	3.23	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	C15-C14	3.23	1.53	1.43
9	v	103	A1EFU	C16-C17	3.22	1.53	1.43
9	G	106	A1EFU	C20-C21	3.22	1.53	1.43
9	F	104	A1EFU	C20-C21	3.22	1.53	1.43
9	j	101	A1EFU	C16-C17	3.22	1.53	1.43
9	R	101	A1EFU	C15-C14	3.22	1.53	1.43
9	j	101	A1EFU	C15-C14	3.22	1.53	1.43
9	D	105	A1EFU	C15-C14	3.21	1.53	1.43
9	D	104	A1EFU	C20-C21	3.21	1.53	1.43
9	s	101	A1EFU	C16-C17	3.21	1.53	1.43
9	J	103	A1EFU	C15-C14	3.21	1.53	1.43
9	r	102	A1EFU	C16-C17	3.21	1.53	1.43
9	D	105	A1EFU	C16-C17	3.21	1.53	1.43
9	E	102	A1EFU	C16-C17	3.20	1.53	1.43
9	r	102	A1EFU	C15-C14	3.20	1.53	1.43
9	J	103	A1EFU	C16-C17	3.20	1.53	1.43
9	a	102	A1EFU	C15-C14	3.19	1.53	1.43
9	E	103	A1EFU	C15-C14	3.19	1.53	1.43
9	I	102	A1EFU	C16-C17	3.19	1.53	1.43
9	E	102	A1EFU	C20-C21	3.19	1.53	1.43
9	E	102	A1EFU	C15-C14	3.19	1.53	1.43
9	s	101	A1EFU	C15-C14	3.19	1.53	1.43
9	I	102	A1EFU	C15-C14	3.19	1.53	1.43
9	2	101	A1EFU	C16-C17	3.17	1.53	1.43
9	v	103	A1EFU	C15-C14	3.17	1.53	1.43
9	F	104	A1EFU	C15-C14	3.17	1.53	1.43
9	G	106	A1EFU	C15-C14	3.16	1.53	1.43
10	H	301	MW9	C7-C6	-3.15	1.33	1.51
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	103	MW9	C7-C6	-3.11	1.34	1.51
9	G	106	A1EFU	C16-C17	3.10	1.53	1.43
8	K	101	BCL	O2A-CGA	-3.08	1.24	1.33
10	G	103	MW9	C7-C6	-3.08	1.34	1.51
8	1	101	BCL	O2A-CGA	-3.08	1.24	1.33
8	K	101	BCL	O2D-CGD	-3.07	1.25	1.33
8	I	101	BCL	O2A-CGA	-3.07	1.24	1.33
8	M	402	BCL	O2A-CGA	-3.06	1.24	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	i	101	BCL	O2D-CGD	-3.04	1.25	1.33
10	L	307	MW9	O1-C17	3.04	1.42	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	101	BCL	O2A-CGA	-3.04	1.24	1.33
8	I	101	BCL	O2D-CGD	-3.04	1.25	1.33
10	M	406	MW9	O1-C17	3.03	1.42	1.33
8	M	403	BCL	O2A-CGA	-3.03	1.24	1.33
8	L	304	BCL	O2A-CGA	-3.03	1.24	1.33
8	E	101	BCL	O2D-CGD	-3.03	1.25	1.33
8	D	101	BCL	O2A-CGA	-3.02	1.24	1.33
8	R	102	BCL	O2A-CGA	-3.02	1.24	1.33
8	B	101	BCL	O2A-CGA	-3.02	1.24	1.33
8	M	403	BCL	O2D-CGD	-3.02	1.25	1.33
8	F	102	BCL	O2D-CGD	-3.02	1.25	1.33
10	G	103	MW9	O1-C17	3.02	1.42	1.33
10	G	104	MW9	O1-C17	3.01	1.42	1.33
8	s	103	BCL	O2A-CGA	-3.01	1.24	1.33
8	2	103	BCL	O2D-CGD	-3.01	1.25	1.33
10	D	103	MW9	O1-C17	3.01	1.42	1.33
10	H	303	MW9	P-O5	3.01	1.66	1.54
8	J	101	BCL	O2D-CGD	-3.01	1.25	1.33
8	r	101	BCL	O2A-CGA	-3.00	1.24	1.33
8	d	101	BCL	O2D-CGD	-3.00	1.25	1.33
8	G	102	BCL	O2D-CGD	-3.00	1.25	1.33
8	Q	101	BCL	O2A-CGA	-3.00	1.24	1.33
8	2	103	BCL	O2A-CGA	-3.00	1.24	1.33
8	E	101	BCL	O2A-CGA	-3.00	1.24	1.33
8	b	101	BCL	O2A-CGA	-3.00	1.24	1.33
10	R	103	MW9	O1-C17	3.00	1.42	1.33
8	a	101	BCL	O2A-CGA	-3.00	1.24	1.33
8	s	102	BCL	O2A-CGA	-3.00	1.24	1.33
8	P	101	BCL	O2A-CGA	-2.99	1.24	1.33
8	F	101	BCL	O2A-CGA	-2.99	1.24	1.33
8	V	101	BCL	O2A-CGA	-2.99	1.24	1.33
8	L	304	BCL	O2D-CGD	-2.98	1.25	1.33
10	M	405	MW9	O1-C17	2.98	1.42	1.33
8	n	101	BCL	O2A-CGA	-2.98	1.24	1.33
8	d	101	BCL	O2A-CGA	-2.98	1.24	1.33
8	t	101	BCL	O2A-CGA	-2.98	1.24	1.33
8	q	102	BCL	O2A-CGA	-2.98	1.24	1.33
8	G	101	BCL	O2A-CGA	-2.98	1.24	1.33
8	S	101	BCL	O2A-CGA	-2.98	1.24	1.33
8	F	102	BCL	O2A-CGA	-2.98	1.24	1.33
8	L	301	BCL	O2A-CGA	-2.97	1.24	1.33
10	F	103	MW9	O1-C17	2.97	1.42	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	i	101	BCL	O2A-CGA	-2.97	1.24	1.33
8	j	102	BCL	O2A-CGA	-2.96	1.24	1.33
8	s	102	BCL	O2D-CGD	-2.96	1.26	1.33
8	e	101	BCL	O2D-CGD	-2.95	1.26	1.33
8	k	102	BCL	O2A-CGA	-2.95	1.24	1.33
10	H	303	MW9	O1-C17	2.95	1.41	1.33
8	v	101	BCL	O2A-CGA	-2.95	1.24	1.33
8	A	101	BCL	O2A-CGA	-2.94	1.24	1.33
8	L	301	BCL	O2D-CGD	-2.94	1.26	1.33
8	l	101	BCL	O2D-CGD	-2.94	1.26	1.33
8	b	101	BCL	O2D-CGD	-2.94	1.26	1.33
8	n	101	BCL	O2D-CGD	-2.93	1.26	1.33
8	e	101	BCL	O2A-CGA	-2.93	1.24	1.33
8	k	102	BCL	O2D-CGD	-2.91	1.26	1.33
8	D	101	BCL	O2D-CGD	-2.91	1.26	1.33
8	B	101	BCL	O2D-CGD	-2.91	1.26	1.33
8	P	102	BCL	O2A-CGA	-2.91	1.24	1.33
8	q	102	BCL	O2D-CGD	-2.90	1.26	1.33
8	A	101	BCL	O2D-CGD	-2.90	1.26	1.33
8	Q	101	BCL	O2D-CGD	-2.90	1.26	1.33
8	V	101	BCL	O2D-CGD	-2.90	1.26	1.33
8	S	101	BCL	O1A-CGA	-2.90	1.13	1.22
8	M	402	BCL	O2D-CGD	-2.90	1.26	1.33
8	J	101	BCL	O1A-CGA	-2.90	1.13	1.22
8	P	101	BCL	O2D-CGD	-2.89	1.26	1.33
8	I	101	BCL	O1A-CGA	-2.89	1.14	1.22
8	N	101	BCL	O2D-CGD	-2.89	1.26	1.33
8	S	101	BCL	O2D-CGD	-2.89	1.26	1.33
8	R	102	BCL	O2D-CGD	-2.88	1.26	1.33
8	j	102	BCL	O2D-CGD	-2.88	1.26	1.33
8	a	101	BCL	O2D-CGD	-2.88	1.26	1.33
8	R	102	BCL	O1A-CGA	-2.88	1.14	1.22
8	n	101	BCL	O1A-CGA	-2.88	1.14	1.22
10	H	301	MW9	O1-C17	2.88	1.41	1.33
8	G	102	BCL	O1A-CGA	-2.87	1.14	1.22
8	L	301	BCL	O1A-CGA	-2.87	1.14	1.22
8	B	101	BCL	O1A-CGA	-2.86	1.14	1.22
8	L	304	BCL	O1A-CGA	-2.85	1.14	1.22
8	V	101	BCL	O1A-CGA	-2.85	1.14	1.22
8	s	103	BCL	O2D-CGD	-2.85	1.26	1.33
8	r	101	BCL	O2D-CGD	-2.85	1.26	1.33
8	K	101	BCL	O1A-CGA	-2.85	1.14	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	l	101	BCL	O1A-CGA	-2.85	1.14	1.22
8	D	101	BCL	O1A-CGA	-2.85	1.14	1.22
8	P	101	BCL	O1A-CGA	-2.84	1.14	1.22
8	d	101	BCL	O1A-CGA	-2.84	1.14	1.22
8	Q	101	BCL	O1A-CGA	-2.84	1.14	1.22
8	s	102	BCL	O1A-CGA	-2.84	1.14	1.22
8	M	402	BCL	O1A-CGA	-2.84	1.14	1.22
8	v	101	BCL	O2D-CGD	-2.84	1.26	1.33
8	t	101	BCL	O2D-CGD	-2.84	1.26	1.33
8	b	101	BCL	O1A-CGA	-2.83	1.14	1.22
8	M	403	BCL	O1A-CGA	-2.83	1.14	1.22
16	C	401	HEC	CAC-C3C	2.83	1.58	1.51
8	F	101	BCL	O2D-CGD	-2.82	1.26	1.33
8	k	102	BCL	O1A-CGA	-2.82	1.14	1.22
8	F	101	BCL	O1A-CGA	-2.82	1.14	1.22
8	N	101	BCL	O1A-CGA	-2.82	1.14	1.22
8	e	101	BCL	O1A-CGA	-2.82	1.14	1.22
8	j	102	BCL	O1A-CGA	-2.82	1.14	1.22
8	i	101	BCL	O1A-CGA	-2.82	1.14	1.22
11	L	305	LMT	O3'-C3'	-2.81	1.36	1.43
8	q	102	BCL	O1A-CGA	-2.81	1.14	1.22
8	v	101	BCL	O1A-CGA	-2.81	1.14	1.22
8	r	101	BCL	O1A-CGA	-2.81	1.14	1.22
8	A	101	BCL	O1A-CGA	-2.81	1.14	1.22
8	a	101	BCL	O1A-CGA	-2.80	1.14	1.22
8	s	103	BCL	O1A-CGA	-2.80	1.14	1.22
14	M	408	BPH	C3B-C4B	-2.80	1.36	1.41
8	2	103	BCL	O1A-CGA	-2.80	1.14	1.22
8	t	101	BCL	O1A-CGA	-2.79	1.14	1.22
8	d	101	BCL	C3B-CAB	2.79	1.55	1.46
8	P	102	BCL	O1A-CGA	-2.79	1.14	1.22
8	G	101	BCL	O1A-CGA	-2.79	1.14	1.22
8	G	101	BCL	O2D-CGD	-2.77	1.26	1.33
10	M	406	MW9	O8-C24	2.75	1.42	1.34
16	C	402	HEC	CAC-C3C	2.75	1.58	1.51
16	C	403	HEC	CAC-C3C	2.74	1.58	1.51
10	D	103	MW9	O8-C24	2.74	1.42	1.34
8	P	102	BCL	O2D-CGD	-2.72	1.26	1.33
11	D	102	LMT	O3'-C3'	-2.70	1.36	1.43
11	H	302	LMT	O3'-C3'	-2.70	1.36	1.43
10	L	307	MW9	O8-C24	2.68	1.41	1.34
10	G	103	MW9	O8-C24	2.67	1.41	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	R	103	MW9	O8-C24	2.67	1.41	1.34
11	C	404	LMT	O3'-C3'	-2.66	1.36	1.43
15	H	304	CDL	OB6-CB4	-2.66	1.39	1.46
10	H	303	MW9	O8-C24	2.66	1.41	1.34
10	F	103	MW9	O8-C24	2.63	1.41	1.34
11	L	306	LMT	O3'-C3'	-2.63	1.36	1.43
8	t	101	BCL	C3B-CAB	2.63	1.54	1.46
10	G	104	MW9	O8-C24	2.62	1.41	1.34
8	F	102	BCL	O1A-CGA	-2.61	1.14	1.22
10	H	301	MW9	O8-C19	-2.60	1.40	1.46
10	F	103	MW9	O8-C19	-2.60	1.40	1.46
10	H	301	MW9	O8-C24	2.59	1.41	1.34
10	M	405	MW9	O8-C24	2.58	1.41	1.34
10	M	405	MW9	O8-C19	-2.57	1.40	1.46
8	L	304	BCL	OBB-CAB	-2.56	1.17	1.23
8	F	102	BCL	OBB-CAB	-2.56	1.17	1.23
10	G	103	MW9	O8-C19	-2.55	1.40	1.46
8	M	403	BCL	OBB-CAB	-2.55	1.17	1.23
10	H	303	MW9	O8-C19	-2.54	1.40	1.46
8	r	101	BCL	OBB-CAB	-2.54	1.17	1.23
10	G	104	MW9	O8-C19	-2.54	1.40	1.46
8	v	101	BCL	C3B-CAB	2.53	1.54	1.46
8	E	101	BCL	O1A-CGA	-2.53	1.15	1.22
10	R	103	MW9	O8-C19	-2.53	1.40	1.46
8	s	102	BCL	C3B-CAB	2.52	1.54	1.46
8	i	101	BCL	OBB-CAB	-2.52	1.17	1.23
8	k	102	BCL	OBB-CAB	-2.52	1.17	1.23
8	D	101	BCL	C1D-C2D	-2.52	1.40	1.45
8	2	103	BCL	OBB-CAB	-2.51	1.17	1.23
8	1	101	BCL	OBB-CAB	-2.51	1.17	1.23
8	N	101	BCL	OBB-CAB	-2.51	1.17	1.23
8	L	301	BCL	OBB-CAB	-2.51	1.17	1.23
8	P	101	BCL	OBB-CAB	-2.51	1.17	1.23
8	J	101	BCL	OBB-CAB	-2.51	1.17	1.23
8	G	102	BCL	OBB-CAB	-2.51	1.17	1.23
8	F	101	BCL	OBB-CAB	-2.51	1.17	1.23
8	P	102	BCL	C3B-CAB	2.50	1.54	1.46
8	I	101	BCL	OBB-CAB	-2.50	1.17	1.23
10	M	406	MW9	O8-C19	-2.50	1.40	1.46
8	A	101	BCL	OBB-CAB	-2.50	1.17	1.23
8	G	101	BCL	OBB-CAB	-2.50	1.17	1.23
8	E	101	BCL	OBB-CAB	-2.50	1.17	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	103	MW9	O8-C19	-2.50	1.40	1.46
8	Q	101	BCL	C1D-C2D	-2.50	1.40	1.45
8	q	102	BCL	OBB-CAB	-2.50	1.17	1.23
8	j	102	BCL	OBB-CAB	-2.50	1.17	1.23
8	j	102	BCL	C3B-CAB	2.50	1.54	1.46
8	R	102	BCL	OBB-CAB	-2.50	1.17	1.23
8	i	101	BCL	C3B-CAB	2.50	1.54	1.46
8	b	101	BCL	OBB-CAB	-2.50	1.17	1.23
11	L	305	LMT	O2'-C2'	-2.49	1.37	1.43
8	I	101	BCL	C1D-C2D	-2.49	1.40	1.45
8	n	101	BCL	OBB-CAB	-2.49	1.17	1.23
8	L	301	BCL	C3B-CAB	2.49	1.54	1.46
10	H	303	MW9	C6-C7	-2.49	1.34	1.51
8	e	101	BCL	OBB-CAB	-2.49	1.17	1.23
8	K	101	BCL	OBB-CAB	-2.49	1.17	1.23
8	V	101	BCL	OBB-CAB	-2.49	1.17	1.23
8	B	101	BCL	C3B-CAB	2.49	1.54	1.46
10	F	103	MW9	C6-C7	-2.48	1.34	1.51
8	d	101	BCL	C1D-C2D	-2.48	1.40	1.45
8	M	402	BCL	OBB-CAB	-2.48	1.17	1.23
8	k	102	BCL	C1D-C2D	-2.48	1.40	1.45
8	A	101	BCL	C3B-CAB	2.48	1.54	1.46
10	G	104	MW9	C6-C7	-2.48	1.34	1.51
8	G	102	BCL	C3B-CAB	2.48	1.54	1.46
8	s	103	BCL	C3B-CAB	2.48	1.54	1.46
8	I	101	BCL	C3B-CAB	2.48	1.54	1.46
8	B	101	BCL	OBB-CAB	-2.48	1.17	1.23
8	l	101	BCL	C1D-C2D	-2.48	1.40	1.45
8	P	102	BCL	OBB-CAB	-2.48	1.17	1.23
8	L	304	BCL	C3B-CAB	2.48	1.54	1.46
8	S	101	BCL	OBB-CAB	-2.48	1.17	1.23
8	R	102	BCL	C3B-CAB	2.47	1.54	1.46
8	r	101	BCL	C3B-CAB	2.47	1.54	1.46
8	s	103	BCL	C1D-C2D	-2.47	1.40	1.45
8	M	402	BCL	C3B-CAB	2.47	1.54	1.46
8	D	101	BCL	OBB-CAB	-2.47	1.17	1.23
8	N	101	BCL	C3B-CAB	2.46	1.54	1.46
8	P	101	BCL	C1D-C2D	-2.46	1.40	1.45
8	J	101	BCL	C3B-CAB	2.46	1.54	1.46
8	v	101	BCL	OBB-CAB	-2.46	1.17	1.23
8	S	101	BCL	C3B-CAB	2.46	1.54	1.46
8	D	101	BCL	C3B-CAB	2.46	1.54	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	a	101	BCL	C3B-CAB	2.46	1.54	1.46
10	L	307	MW9	O8-C19	-2.46	1.40	1.46
15	L	308	CDL	OB6-CB4	-2.45	1.40	1.46
8	V	101	BCL	C3B-CAB	2.45	1.54	1.46
8	P	101	BCL	C3B-CAB	2.45	1.54	1.46
8	a	101	BCL	OBB-CAB	-2.45	1.17	1.23
8	k	102	BCL	C3B-CAB	2.45	1.54	1.46
8	F	102	BCL	C3B-CAB	2.45	1.54	1.46
8	Q	101	BCL	OBB-CAB	-2.45	1.17	1.23
8	M	403	BCL	C1B-C2B	-2.45	1.37	1.43
8	q	102	BCL	C3B-CAB	2.45	1.54	1.46
8	F	101	BCL	C1D-C2D	-2.45	1.40	1.45
8	E	101	BCL	C3B-CAB	2.44	1.54	1.46
8	s	102	BCL	C1D-C2D	-2.44	1.40	1.45
8	G	101	BCL	C3B-CAB	2.44	1.54	1.46
8	2	103	BCL	C3B-CAB	2.44	1.54	1.46
8	K	101	BCL	C1D-C2D	-2.43	1.40	1.45
8	Q	101	BCL	C3B-CAB	2.43	1.54	1.46
8	s	102	BCL	OBB-CAB	-2.43	1.17	1.23
8	s	103	BCL	OBB-CAB	-2.43	1.17	1.23
8	K	101	BCL	C3B-CAB	2.43	1.54	1.46
11	D	102	LMT	O2'-C2'	-2.43	1.37	1.43
8	n	101	BCL	C3B-CAB	2.43	1.54	1.46
8	n	101	BCL	C1D-C2D	-2.43	1.40	1.45
8	1	101	BCL	C3B-CAB	2.42	1.54	1.46
8	G	101	BCL	C1D-C2D	-2.42	1.40	1.45
8	A	101	BCL	C1D-C2D	-2.42	1.40	1.45
8	J	101	BCL	C1D-C2D	-2.42	1.40	1.45
8	M	403	BCL	C3B-CAB	2.41	1.54	1.46
10	H	301	MW9	C35-C34	-2.41	1.34	1.51
8	L	301	BCL	C1D-C2D	-2.41	1.40	1.45
8	B	101	BCL	C1D-C2D	-2.41	1.40	1.45
10	L	307	MW9	C35-C34	-2.41	1.34	1.51
8	j	102	BCL	C1D-C2D	-2.41	1.40	1.45
8	P	102	BCL	C1B-C2B	-2.41	1.37	1.43
14	L	302	BPH	C3B-C2B	2.40	1.43	1.39
8	P	102	BCL	C1D-C2D	-2.40	1.40	1.45
8	t	101	BCL	OBB-CAB	-2.40	1.17	1.23
10	F	103	MW9	C35-C34	-2.40	1.34	1.51
15	L	308	CDL	OB8-CB7	2.40	1.40	1.33
8	F	101	BCL	C3B-CAB	2.40	1.54	1.46
16	C	401	HEC	CBB-CAB	-2.39	1.40	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	C	402	HEC	CBB-CAB	-2.39	1.40	1.51
8	i	101	BCL	C1D-C2D	-2.39	1.40	1.45
8	b	101	BCL	C1D-C2D	-2.39	1.40	1.45
8	q	102	BCL	C1D-C2D	-2.39	1.40	1.45
8	N	101	BCL	C1D-C2D	-2.39	1.40	1.45
8	S	101	BCL	C1D-C2D	-2.39	1.40	1.45
8	2	103	BCL	C1B-C2B	-2.39	1.37	1.43
8	e	101	BCL	C3B-CAB	2.39	1.54	1.46
16	C	403	HEC	CBB-CAB	-2.38	1.40	1.51
8	b	101	BCL	C3B-CAB	2.38	1.54	1.46
15	L	308	CDL	OA8-CA7	2.38	1.40	1.33
11	H	302	LMT	O2'-C2'	-2.38	1.37	1.43
8	L	304	BCL	C1D-C2D	-2.38	1.40	1.45
8	V	101	BCL	C1D-C2D	-2.37	1.40	1.45
11	D	102	LMT	O2B-C2B	-2.36	1.37	1.43
8	r	101	BCL	C1D-C2D	-2.36	1.40	1.45
8	F	102	BCL	C1B-C2B	-2.36	1.37	1.43
8	n	101	BCL	C1B-C2B	-2.36	1.37	1.43
8	L	304	BCL	C1B-C2B	-2.36	1.37	1.43
11	D	102	LMT	O3B-C3B	-2.35	1.37	1.43
15	H	304	CDL	OA6-CA4	-2.35	1.40	1.46
8	v	101	BCL	C1D-C2D	-2.35	1.40	1.45
8	F	102	BCL	C1D-C2D	-2.35	1.40	1.45
8	M	403	BCL	C1D-C2D	-2.35	1.40	1.45
8	E	101	BCL	C1D-C2D	-2.34	1.40	1.45
8	r	101	BCL	C1B-C2B	-2.34	1.37	1.43
8	N	101	BCL	C1B-C2B	-2.34	1.37	1.43
8	A	101	BCL	C1B-C2B	-2.32	1.37	1.43
8	G	102	BCL	C1D-C2D	-2.32	1.40	1.45
8	2	103	BCL	C1D-C2D	-2.32	1.40	1.45
8	e	101	BCL	C1D-C2D	-2.32	1.40	1.45
8	k	102	BCL	C1B-C2B	-2.31	1.37	1.43
8	a	101	BCL	C1B-C2B	-2.31	1.37	1.43
8	R	102	BCL	C1B-C2B	-2.31	1.37	1.43
8	I	101	BCL	C1B-C2B	-2.31	1.37	1.43
15	H	304	CDL	OB8-CB6	-2.31	1.39	1.45
8	i	101	BCL	C1B-C2B	-2.31	1.37	1.43
8	F	102	BCL	C3D-C4D	-2.30	1.39	1.44
8	G	102	BCL	C1B-C2B	-2.30	1.37	1.43
10	H	303	MW9	C35-C34	-2.30	1.34	1.49
15	H	304	CDL	OA8-CA7	2.30	1.40	1.33
8	F	101	BCL	C1B-C2B	-2.30	1.37	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	b	101	BCL	C1B-C2B	-2.30	1.37	1.43
11	C	404	LMT	O2'-C2'	-2.30	1.37	1.43
8	L	301	BCL	C1B-C2B	-2.30	1.37	1.43
15	H	304	CDL	OB8-CB7	2.29	1.40	1.33
8	P	101	BCL	C1B-C2B	-2.29	1.37	1.43
8	D	101	BCL	C1B-C2B	-2.29	1.37	1.43
8	E	101	BCL	C1B-C2B	-2.28	1.37	1.43
9	s	104	A1EFU	C8-C9	2.28	1.50	1.45
8	e	101	BCL	C3D-C4D	-2.28	1.39	1.44
8	1	101	BCL	C1B-C2B	-2.28	1.37	1.43
8	M	402	BCL	C1D-C2D	-2.28	1.40	1.45
9	2	104	A1EFU	C12-C13	2.28	1.50	1.45
15	L	308	CDL	OA6-CA4	-2.28	1.40	1.46
8	J	101	BCL	C1B-C2B	-2.28	1.37	1.43
8	d	101	BCL	C3D-C4D	-2.28	1.39	1.44
8	a	101	BCL	C1D-C2D	-2.28	1.40	1.45
8	G	101	BCL	C1B-C2B	-2.27	1.37	1.43
8	K	101	BCL	C1B-C2B	-2.27	1.37	1.43
8	B	101	BCL	C1B-C2B	-2.27	1.37	1.43
15	L	308	CDL	OA6-CA5	2.27	1.40	1.34
8	q	102	BCL	C1B-C2B	-2.27	1.37	1.43
9	a	102	A1EFU	C12-C13	2.27	1.50	1.45
11	L	306	LMT	O2'-C2'	-2.26	1.37	1.43
8	R	102	BCL	C1D-C2D	-2.26	1.40	1.45
8	e	101	BCL	C1B-C2B	-2.26	1.37	1.43
8	r	101	BCL	C3B-C2B	-2.26	1.35	1.42
8	j	102	BCL	C1B-C2B	-2.26	1.37	1.43
14	M	408	BPH	C3B-C2B	2.26	1.43	1.39
8	I	101	BCL	C3D-C4D	-2.25	1.39	1.44
8	n	101	BCL	C3B-C2B	-2.25	1.35	1.42
8	s	103	BCL	C1B-C2B	-2.25	1.38	1.43
8	v	101	BCL	C1B-C2B	-2.24	1.38	1.43
9	v	102	A1EFU	C12-C13	2.24	1.50	1.45
8	E	101	BCL	C3D-C4D	-2.24	1.39	1.44
8	Q	101	BCL	C1B-C2B	-2.24	1.38	1.43
8	M	402	BCL	C1B-C2B	-2.24	1.38	1.43
8	i	101	BCL	C3D-C4D	-2.23	1.39	1.44
8	t	101	BCL	C3B-C2B	-2.23	1.35	1.42
8	M	403	BCL	C3D-C4D	-2.23	1.39	1.44
9	K	102	A1EFU	C12-C13	2.23	1.50	1.45
8	S	101	BCL	C1B-C2B	-2.23	1.38	1.43
15	H	304	CDL	OA6-CA5	2.23	1.40	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	C	401	HEC	CAB-C3B	2.23	1.56	1.51
8	b	101	BCL	C3D-C4D	-2.23	1.39	1.44
8	A	101	BCL	C3B-C2B	-2.23	1.35	1.42
8	P	102	BCL	C3B-C2B	-2.22	1.35	1.42
8	a	101	BCL	C3D-C4D	-2.22	1.39	1.44
8	t	101	BCL	C3D-C4D	-2.22	1.39	1.44
9	s	104	A1EFU	C12-C13	2.22	1.50	1.45
8	G	102	BCL	C3D-C4D	-2.22	1.39	1.44
8	R	102	BCL	C3D-C4D	-2.21	1.39	1.44
8	J	101	BCL	C3D-C4D	-2.21	1.39	1.44
8	P	102	BCL	C3D-C4D	-2.21	1.39	1.44
8	j	102	BCL	C3D-C4D	-2.21	1.39	1.44
8	l	101	BCL	C3D-C4D	-2.21	1.39	1.44
8	n	101	BCL	C3D-C4D	-2.21	1.39	1.44
8	t	101	BCL	C1D-C2D	-2.20	1.41	1.45
8	F	101	BCL	C3D-C4D	-2.20	1.39	1.44
9	a	102	A1EFU	C8-C9	2.20	1.50	1.45
16	C	403	HEC	CAB-C3B	2.20	1.56	1.51
8	Q	101	BCL	C3D-C4D	-2.19	1.39	1.44
8	s	103	BCL	C3D-C4D	-2.19	1.39	1.44
8	D	101	BCL	C3D-C4D	-2.19	1.39	1.44
8	K	101	BCL	C3D-C4D	-2.19	1.39	1.44
8	G	101	BCL	C3D-C4D	-2.19	1.39	1.44
8	v	101	BCL	C3D-C4D	-2.18	1.39	1.44
8	N	101	BCL	C3D-C4D	-2.18	1.39	1.44
9	N	102	A1EFU	C8-C9	2.18	1.50	1.45
15	L	308	CDL	OB6-CB5	2.18	1.40	1.34
9	P	103	A1EFU	C12-C13	2.17	1.50	1.45
16	C	402	HEC	CAB-C3B	2.17	1.56	1.51
8	k	102	BCL	C3D-C4D	-2.17	1.39	1.44
9	2	104	A1EFU	C8-C9	2.17	1.50	1.45
9	K	102	A1EFU	C8-C9	2.17	1.50	1.45
8	r	101	BCL	C3D-C4D	-2.17	1.39	1.44
15	H	304	CDL	OA8-CA6	-2.16	1.40	1.45
8	L	304	BCL	C3D-C4D	-2.16	1.39	1.44
8	M	402	BCL	C3D-C4D	-2.16	1.39	1.44
8	s	102	BCL	C3D-C4D	-2.15	1.39	1.44
8	q	102	BCL	C3D-C4D	-2.15	1.39	1.44
8	A	101	BCL	C3D-C4D	-2.15	1.39	1.44
8	2	103	BCL	C3D-C4D	-2.15	1.39	1.44
8	L	301	BCL	C3D-C2D	-2.15	1.33	1.39
8	S	101	BCL	C3D-C4D	-2.15	1.39	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	407	A1EFU	C12-C13	2.14	1.50	1.45
8	B	101	BCL	C3D-C4D	-2.14	1.39	1.44
9	J	102	A1EFU	C12-C13	2.14	1.50	1.45
8	P	101	BCL	C3D-C4D	-2.14	1.39	1.44
8	V	101	BCL	C3D-C4D	-2.13	1.39	1.44
9	G	105	A1EFU	C12-C13	2.13	1.50	1.45
9	j	103	A1EFU	C8-C9	2.12	1.50	1.45
9	q	101	A1EFU	C12-C13	2.12	1.50	1.45
9	a	102	A1EFU	C4-C5	2.12	1.50	1.45
15	L	308	CDL	OB8-CB6	-2.12	1.40	1.45
16	C	402	HEC	FE-ND	2.12	2.01	1.94
9	j	101	A1EFU	C8-C9	2.11	1.50	1.45
9	K	102	A1EFU	C4-C5	2.11	1.50	1.45
9	j	103	A1EFU	C12-C13	2.11	1.50	1.45
9	r	102	A1EFU	C4-C5	2.11	1.50	1.45
16	C	401	HEC	CMD-C2D	2.11	1.55	1.50
9	T	101	A1EFU	C12-C13	2.11	1.50	1.45
9	E	103	A1EFU	C4-C5	2.11	1.50	1.45
9	P	103	A1EFU	C8-C9	2.11	1.50	1.45
9	B	103	A1EFU	C4-C5	2.10	1.50	1.45
8	Q	101	BCL	C3D-C2D	-2.10	1.33	1.39
9	D	105	A1EFU	C4-C5	2.10	1.50	1.45
8	L	301	BCL	C3D-C4D	-2.10	1.39	1.44
8	B	101	BCL	C3D-C2D	-2.09	1.33	1.39
9	A	102	A1EFU	C12-C13	2.09	1.50	1.45
16	C	403	HEC	CMD-C2D	2.09	1.55	1.50
9	T	101	A1EFU	C8-C9	2.09	1.50	1.45
9	f	101	A1EFU	C4-C5	2.09	1.50	1.45
15	L	308	CDL	OA8-CA6	-2.09	1.40	1.45
11	D	102	LMT	O4'-C4B	-2.09	1.38	1.43
9	s	101	A1EFU	C4-C5	2.09	1.50	1.45
9	2	104	A1EFU	C4-C5	2.08	1.50	1.45
8	F	102	BCL	C3B-C2B	-2.08	1.35	1.42
8	M	403	BCL	C3B-C2B	-2.08	1.35	1.42
8	2	103	BCL	C3B-C2B	-2.08	1.35	1.42
9	q	101	A1EFU	C8-C9	2.08	1.50	1.45
9	D	104	A1EFU	C12-C13	2.08	1.50	1.45
9	J	103	A1EFU	C4-C5	2.08	1.50	1.45
9	p	101	A1EFU	C12-C13	2.08	1.50	1.45
9	G	106	A1EFU	C4-C5	2.08	1.50	1.45
8	M	402	BCL	C3B-C2B	-2.08	1.35	1.42
9	2	101	A1EFU	C12-C13	2.08	1.50	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	102	A1EFU	C4-C5	2.08	1.50	1.45
9	A	102	A1EFU	C4-C5	2.08	1.50	1.45
8	P	101	BCL	C3D-C2D	-2.07	1.33	1.39
9	s	105	A1EFU	C4-C5	2.07	1.50	1.45
8	a	101	BCL	C3B-C2B	-2.07	1.35	1.42
8	L	304	BCL	C3B-C2B	-2.07	1.35	1.42
8	I	101	BCL	C3D-C2D	-2.07	1.33	1.39
8	I	101	BCL	C3B-C2B	-2.07	1.35	1.42
8	B	101	BCL	C3B-C2B	-2.07	1.35	1.42
8	N	101	BCL	C3B-C2B	-2.07	1.35	1.42
9	T	101	A1EFU	C4-C5	2.07	1.50	1.45
8	k	102	BCL	C3B-C2B	-2.07	1.35	1.42
9	r	102	A1EFU	C8-C9	2.07	1.50	1.45
9	2	102	A1EFU	C8-C9	2.07	1.50	1.45
8	P	101	BCL	C3B-C2B	-2.06	1.35	1.42
8	S	101	BCL	C3B-C2B	-2.06	1.35	1.42
8	b	101	BCL	C3B-C2B	-2.06	1.35	1.42
9	J	102	A1EFU	C4-C5	2.06	1.50	1.45
9	J	103	A1EFU	C8-C9	2.06	1.50	1.45
8	E	101	BCL	C3B-C2B	-2.06	1.35	1.42
8	L	301	BCL	C3B-C2B	-2.06	1.35	1.42
9	B	102	A1EFU	C4-C5	2.06	1.50	1.45
9	v	103	A1EFU	C4-C5	2.06	1.50	1.45
9	s	104	A1EFU	C4-C5	2.06	1.50	1.45
9	R	101	A1EFU	C8-C9	2.06	1.50	1.45
8	D	101	BCL	C3D-C2D	-2.06	1.33	1.39
9	D	104	A1EFU	C8-C9	2.06	1.50	1.45
9	G	105	A1EFU	C8-C9	2.06	1.50	1.45
9	A	102	A1EFU	C8-C9	2.06	1.50	1.45
9	v	102	A1EFU	C8-C9	2.05	1.50	1.45
9	R	101	A1EFU	C12-C13	2.05	1.50	1.45
8	G	101	BCL	C3B-C2B	-2.05	1.35	1.42
9	v	103	A1EFU	C8-C9	2.05	1.50	1.45
9	B	102	A1EFU	C12-C13	2.05	1.50	1.45
9	N	102	A1EFU	C12-C13	2.05	1.50	1.45
8	R	102	BCL	C3B-C2B	-2.05	1.35	1.42
8	G	102	BCL	C3D-C2D	-2.05	1.33	1.39
8	D	101	BCL	C3B-C2B	-2.05	1.35	1.42
9	N	102	A1EFU	C4-C5	2.05	1.50	1.45
8	Q	101	BCL	C3B-C2B	-2.05	1.35	1.42
9	E	102	A1EFU	C12-C13	2.05	1.50	1.45
15	H	304	CDL	OB6-CB5	2.05	1.40	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	103	A1EFU	C8-C9	2.05	1.50	1.45
9	D	105	A1EFU	C8-C9	2.05	1.50	1.45
9	2	102	A1EFU	C12-C13	2.05	1.50	1.45
14	M	408	BPH	CHA-CBD	2.05	1.54	1.51
8	v	101	BCL	C3B-C2B	-2.05	1.35	1.42
8	s	102	BCL	C3D-C2D	-2.04	1.33	1.39
9	v	102	A1EFU	C4-C5	2.04	1.50	1.45
8	K	101	BCL	C3B-C2B	-2.04	1.36	1.42
8	L	304	BCL	C2C-C3C	-2.04	1.48	1.54
8	s	103	BCL	C3B-C2B	-2.04	1.36	1.42
9	j	101	A1EFU	C4-C5	2.04	1.50	1.45
9	s	105	A1EFU	C12-C13	2.04	1.50	1.45
8	G	102	BCL	C3B-C2B	-2.04	1.36	1.42
8	F	101	BCL	C3B-C2B	-2.04	1.36	1.42
8	1	101	BCL	C3D-C2D	-2.04	1.33	1.39
9	B	102	A1EFU	C8-C9	2.04	1.50	1.45
9	2	101	A1EFU	C4-C5	2.04	1.50	1.45
8	J	101	BCL	C3B-C2B	-2.04	1.36	1.42
9	k	101	A1EFU	C12-C13	2.03	1.50	1.45
8	A	101	BCL	C3D-C2D	-2.03	1.33	1.39
16	C	402	HEC	CMD-C2D	2.03	1.55	1.50
8	i	101	BCL	C3B-C2B	-2.03	1.36	1.42
9	F	104	A1EFU	C12-C13	2.03	1.50	1.45
9	p	101	A1EFU	C4-C5	2.03	1.50	1.45
8	s	102	BCL	C3B-C2B	-2.03	1.36	1.42
8	F	102	BCL	C3D-C2D	-2.03	1.33	1.39
8	j	102	BCL	C3B-C2B	-2.03	1.36	1.42
8	e	101	BCL	C3B-C2B	-2.03	1.36	1.42
8	q	102	BCL	C3B-C2B	-2.03	1.36	1.42
9	M	407	A1EFU	C8-C9	2.03	1.50	1.45
9	k	101	A1EFU	C8-C9	2.03	1.50	1.45
8	1	101	BCL	C3B-C2B	-2.03	1.36	1.42
8	2	103	BCL	C3D-C2D	-2.02	1.33	1.39
8	J	101	BCL	C3D-C2D	-2.02	1.33	1.39
8	q	102	BCL	C3D-C2D	-2.02	1.33	1.39
9	P	103	A1EFU	C4-C5	2.02	1.50	1.45
8	n	101	BCL	C3D-C2D	-2.02	1.33	1.39
9	2	102	A1EFU	C4-C5	2.02	1.50	1.45
9	j	101	A1EFU	C12-C13	2.02	1.50	1.45
8	a	101	BCL	C5-C3	2.02	1.55	1.51
9	D	104	A1EFU	C4-C5	2.02	1.50	1.45
9	s	105	A1EFU	C8-C9	2.02	1.50	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	403	BCL	C3D-C2D	-2.02	1.33	1.39
8	N	101	BCL	C3D-C2D	-2.01	1.33	1.39
8	E	101	BCL	C3D-C2D	-2.01	1.33	1.39
9	q	101	A1EFU	C4-C5	2.01	1.50	1.45
9	r	102	A1EFU	C12-C13	2.01	1.50	1.45
9	p	101	A1EFU	C8-C9	2.01	1.50	1.45
9	f	101	A1EFU	C12-C13	2.01	1.50	1.45
8	V	101	BCL	C3D-C2D	-2.01	1.33	1.39
8	R	102	BCL	C3D-C2D	-2.01	1.33	1.39
8	K	101	BCL	C3D-C2D	-2.01	1.33	1.39
8	S	101	BCL	C3D-C2D	-2.00	1.33	1.39
9	k	101	A1EFU	C4-C5	2.00	1.50	1.45
8	b	101	BCL	C3D-C2D	-2.00	1.33	1.39
9	J	102	A1EFU	C8-C9	2.00	1.50	1.45
8	e	101	BCL	C3D-C2D	-2.00	1.33	1.39
9	2	101	A1EFU	C8-C9	2.00	1.50	1.45
9	J	103	A1EFU	C12-C13	2.00	1.50	1.45
8	j	102	BCL	C2C-C3C	-2.00	1.48	1.54

All (1829) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	j	101	A1EFU	C11-C10-C9	-11.21	111.31	127.31
9	k	101	A1EFU	C7-C6-C5	-10.60	112.18	127.31
9	a	102	A1EFU	C7-C6-C5	-10.56	112.24	127.31
9	a	102	A1EFU	C15-C14-C13	-10.54	112.27	127.31
9	I	102	A1EFU	C7-C6-C5	-10.35	112.53	127.31
9	E	103	A1EFU	C7-C6-C5	-10.35	112.54	127.31
9	G	106	A1EFU	C7-C6-C5	-10.30	112.62	127.31
9	p	101	A1EFU	C7-C6-C5	-10.21	112.74	127.31
9	J	103	A1EFU	C7-C6-C5	-10.16	112.81	127.31
9	k	101	A1EFU	C15-C14-C13	-10.14	112.84	127.31
9	I	102	A1EFU	C11-C10-C9	-10.10	112.90	127.31
9	p	101	A1EFU	C16-C17-C18	-10.07	112.93	127.31
9	B	103	A1EFU	C7-C6-C5	-10.07	112.93	127.31
9	I	102	A1EFU	C15-C14-C13	-10.06	112.96	127.31
9	2	101	A1EFU	C11-C10-C9	-10.03	113.00	127.31
9	f	101	A1EFU	C11-C10-C9	-10.01	113.02	127.31
9	G	106	A1EFU	C11-C10-C9	-10.01	113.03	127.31
9	D	105	A1EFU	C7-C6-C5	-9.96	113.10	127.31
9	s	101	A1EFU	C7-C6-C5	-9.91	113.17	127.31
9	s	105	A1EFU	C11-C10-C9	-9.90	113.18	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	J	103	A1EFU	C11-C10-C9	-9.86	113.24	127.31
9	v	102	A1EFU	C7-C6-C5	-9.81	113.31	127.31
9	M	407	A1EFU	C7-C6-C5	-9.68	113.50	127.31
9	2	102	A1EFU	C15-C14-C13	-9.68	113.50	127.31
9	G	106	A1EFU	C15-C14-C13	-9.64	113.56	127.31
9	D	105	A1EFU	C11-C10-C9	-9.63	113.57	127.31
9	s	101	A1EFU	C11-C10-C9	-9.58	113.64	127.31
9	r	102	A1EFU	C7-C6-C5	-9.57	113.64	127.31
9	r	102	A1EFU	C15-C14-C13	-9.57	113.64	127.31
9	j	103	A1EFU	C16-C17-C18	-9.56	113.66	127.31
9	R	101	A1EFU	C7-C6-C5	-9.55	113.69	127.31
9	k	101	A1EFU	C11-C10-C9	-9.52	113.73	127.31
9	A	102	A1EFU	C11-C10-C9	-9.51	113.74	127.31
9	T	101	A1EFU	C15-C14-C13	-9.50	113.75	127.31
9	j	101	A1EFU	C16-C17-C18	-9.50	113.76	127.31
9	G	106	A1EFU	C16-C17-C18	-9.50	113.76	127.31
9	q	101	A1EFU	C16-C17-C18	-9.48	113.78	127.31
9	A	102	A1EFU	C15-C14-C13	-9.46	113.81	127.31
9	j	101	A1EFU	C7-C6-C5	-9.44	113.84	127.31
9	N	102	A1EFU	C11-C10-C9	-9.41	113.88	127.31
9	D	105	A1EFU	C15-C14-C13	-9.40	113.90	127.31
9	2	101	A1EFU	C7-C6-C5	-9.40	113.90	127.31
9	T	101	A1EFU	C11-C10-C9	-9.39	113.91	127.31
9	F	104	A1EFU	C15-C14-C13	-9.39	113.91	127.31
9	E	102	A1EFU	C15-C14-C13	-9.33	114.00	127.31
9	v	103	A1EFU	C7-C6-C5	-9.32	114.01	127.31
9	B	102	A1EFU	C15-C14-C13	-9.31	114.03	127.31
9	K	102	A1EFU	C11-C10-C9	-9.26	114.09	127.31
9	E	103	A1EFU	C11-C10-C9	-9.25	114.11	127.31
9	E	102	A1EFU	C11-C10-C9	-9.24	114.12	127.31
9	M	407	A1EFU	C11-C10-C9	-9.21	114.16	127.31
9	B	102	A1EFU	C11-C10-C9	-9.21	114.17	127.31
9	s	105	A1EFU	C7-C6-C5	-9.18	114.20	127.31
9	J	103	A1EFU	C15-C14-C13	-9.17	114.22	127.31
9	J	102	A1EFU	C11-C10-C9	-9.17	114.23	127.31
9	F	104	A1EFU	C11-C10-C9	-9.16	114.24	127.31
9	P	103	A1EFU	C15-C14-C13	-9.16	114.24	127.31
9	v	102	A1EFU	C11-C10-C9	-9.16	114.24	127.31
9	J	103	A1EFU	C16-C17-C18	-9.15	114.25	127.31
9	p	101	A1EFU	C11-C10-C9	-9.13	114.28	127.31
9	f	101	A1EFU	C7-C6-C5	-9.12	114.29	127.31
9	p	101	A1EFU	C15-C14-C13	-9.06	114.38	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	k	101	A1EFU	C16-C17-C18	-9.05	114.40	127.31
9	j	101	A1EFU	C15-C14-C13	-9.04	114.41	127.31
9	J	102	A1EFU	C15-C14-C13	-8.99	114.48	127.31
9	G	105	A1EFU	C16-C17-C18	-8.96	114.53	127.31
9	F	104	A1EFU	C7-C6-C5	-8.95	114.54	127.31
9	j	103	A1EFU	C15-C14-C13	-8.94	114.54	127.31
9	s	101	A1EFU	C16-C17-C18	-8.94	114.55	127.31
9	A	102	A1EFU	C7-C6-C5	-8.93	114.57	127.31
9	a	102	A1EFU	C16-C17-C18	-8.93	114.57	127.31
9	N	102	A1EFU	C15-C14-C13	-8.92	114.58	127.31
9	s	101	A1EFU	C15-C14-C13	-8.91	114.60	127.31
9	R	101	A1EFU	C11-C10-C9	-8.88	114.64	127.31
9	q	101	A1EFU	C7-C6-C5	-8.88	114.64	127.31
9	D	105	A1EFU	C16-C17-C18	-8.87	114.65	127.31
9	v	103	A1EFU	C15-C14-C13	-8.86	114.67	127.31
9	D	104	A1EFU	C11-C10-C9	-8.83	114.71	127.31
9	R	101	A1EFU	C15-C14-C13	-8.81	114.73	127.31
9	j	103	A1EFU	C7-C6-C5	-8.81	114.73	127.31
9	D	104	A1EFU	C16-C17-C18	-8.79	114.76	127.31
9	P	103	A1EFU	C7-C6-C5	-8.79	114.77	127.31
9	N	102	A1EFU	C7-C6-C5	-8.77	114.80	127.31
10	H	303	MW9	C35-C34-C33	8.75	152.75	112.71
9	v	103	A1EFU	C16-C17-C18	-8.71	114.87	127.31
9	f	101	A1EFU	C15-C14-C13	-8.71	114.88	127.31
9	P	103	A1EFU	C11-C10-C9	-8.70	114.89	127.31
9	2	102	A1EFU	C7-C6-C5	-8.68	114.92	127.31
9	s	105	A1EFU	C15-C14-C13	-8.67	114.94	127.31
9	G	105	A1EFU	C15-C14-C13	-8.64	114.98	127.31
9	2	101	A1EFU	C16-C17-C18	-8.62	115.01	127.31
9	I	102	A1EFU	C16-C17-C18	-8.61	115.02	127.31
9	J	102	A1EFU	C7-C6-C5	-8.60	115.03	127.31
9	j	103	A1EFU	C11-C10-C9	-8.59	115.05	127.31
9	2	104	A1EFU	C11-C10-C9	-8.59	115.05	127.31
9	P	103	A1EFU	C16-C17-C18	-8.58	115.06	127.31
9	D	104	A1EFU	C7-C6-C5	-8.57	115.08	127.31
9	T	101	A1EFU	C7-C6-C5	-8.55	115.10	127.31
9	f	101	A1EFU	C16-C17-C18	-8.55	115.11	127.31
9	2	101	A1EFU	C15-C14-C13	-8.53	115.14	127.31
9	K	102	A1EFU	C7-C6-C5	-8.52	115.15	127.31
9	B	102	A1EFU	C7-C6-C5	-8.50	115.17	127.31
9	E	103	A1EFU	C15-C14-C13	-8.50	115.18	127.31
9	B	103	A1EFU	C11-C10-C9	-8.48	115.21	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	v	102	A1EFU	C16-C17-C18	-8.47	115.22	127.31
9	2	102	A1EFU	C11-C10-C9	-8.44	115.27	127.31
9	r	102	A1EFU	C11-C10-C9	-8.41	115.30	127.31
9	K	102	A1EFU	C15-C14-C13	-8.40	115.32	127.31
9	K	102	A1EFU	C16-C17-C18	-8.36	115.37	127.31
9	v	102	A1EFU	C15-C14-C13	-8.34	115.40	127.31
9	E	103	A1EFU	C16-C17-C18	-8.34	115.41	127.31
9	2	102	A1EFU	C16-C17-C18	-8.32	115.43	127.31
9	B	103	A1EFU	C15-C14-C13	-8.29	115.48	127.31
9	r	102	A1EFU	C16-C17-C18	-8.28	115.50	127.31
9	N	102	A1EFU	C16-C17-C18	-8.23	115.56	127.31
9	s	105	A1EFU	C16-C17-C18	-8.20	115.61	127.31
9	q	101	A1EFU	C15-C14-C13	-8.13	115.71	127.31
9	M	407	A1EFU	C15-C14-C13	-8.13	115.71	127.31
9	G	105	A1EFU	C7-C6-C5	-8.12	115.72	127.31
9	a	102	A1EFU	C11-C10-C9	-8.10	115.76	127.31
9	v	103	A1EFU	C11-C10-C9	-8.09	115.77	127.31
9	A	102	A1EFU	C16-C17-C18	-8.06	115.80	127.31
9	2	104	A1EFU	C7-C6-C5	-8.01	115.88	127.31
9	G	105	A1EFU	C11-C10-C9	-7.93	116.00	127.31
9	q	101	A1EFU	C11-C10-C9	-7.86	116.09	127.31
9	B	103	A1EFU	C16-C17-C18	-7.82	116.15	127.31
9	E	102	A1EFU	C7-C6-C5	-7.76	116.24	127.31
9	F	104	A1EFU	C16-C17-C18	-7.67	116.36	127.31
9	B	102	A1EFU	C16-C17-C18	-7.65	116.39	127.31
9	T	101	A1EFU	C16-C17-C18	-7.65	116.40	127.31
9	s	104	A1EFU	C16-C17-C18	-7.62	116.43	127.31
9	2	104	A1EFU	C15-C14-C13	-7.59	116.47	127.31
9	2	104	A1EFU	C16-C17-C18	-7.54	116.55	127.31
9	R	101	A1EFU	C16-C17-C18	-7.53	116.57	127.31
9	E	102	A1EFU	C16-C17-C18	-7.48	116.63	127.31
9	s	104	A1EFU	C15-C14-C13	-7.43	116.71	127.31
9	J	102	A1EFU	C16-C17-C18	-7.40	116.74	127.31
9	s	104	A1EFU	C11-C10-C9	-7.39	116.77	127.31
9	s	104	A1EFU	C7-C6-C5	-7.29	116.91	127.31
9	D	104	A1EFU	C15-C14-C13	-7.28	116.92	127.31
10	M	405	MW9	C35-C34-C33	7.06	152.91	112.43
10	M	406	MW9	C35-C34-C33	7.06	152.89	112.43
10	R	103	MW9	C35-C34-C33	7.02	152.65	112.43
9	M	407	A1EFU	C16-C17-C18	-6.99	117.33	127.31
10	D	103	MW9	C35-C34-C33	6.98	152.42	112.43
10	G	103	MW9	C35-C34-C33	6.96	152.32	112.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	n	101	BCL	C1D-ND-C4D	-6.60	101.65	106.33
9	a	102	A1EFU	CM4-C9-C10	-6.55	113.75	122.92
8	s	102	BCL	C1D-ND-C4D	-6.51	101.71	106.33
8	2	103	BCL	C1D-ND-C4D	-6.49	101.72	106.33
8	P	102	BCL	C1D-ND-C4D	-6.42	101.77	106.33
8	G	101	BCL	C1D-ND-C4D	-6.36	101.81	106.33
8	r	101	BCL	C1D-ND-C4D	-6.36	101.82	106.33
9	a	102	A1EFU	CM5-C13-C14	-6.36	114.02	122.92
8	L	301	BCL	C1D-ND-C4D	-6.33	101.84	106.33
8	i	101	BCL	C1D-ND-C4D	-6.32	101.84	106.33
8	B	101	BCL	C1D-ND-C4D	-6.29	101.86	106.33
8	v	101	BCL	C1D-ND-C4D	-6.24	101.90	106.33
8	s	103	BCL	C1D-ND-C4D	-6.22	101.91	106.33
8	M	402	BCL	C1D-ND-C4D	-6.19	101.94	106.33
10	H	301	MW9	C35-C34-C33	6.19	152.74	112.55
9	p	101	A1EFU	CM6-C18-C17	-6.19	114.25	122.92
8	b	101	BCL	C1D-ND-C4D	-6.17	101.95	106.33
8	a	101	BCL	C1D-ND-C4D	-6.16	101.96	106.33
8	k	102	BCL	C1D-ND-C4D	-6.15	101.96	106.33
10	F	103	MW9	C35-C34-C33	6.15	152.48	112.55
8	q	102	BCL	C1D-ND-C4D	-6.14	101.98	106.33
9	D	104	A1EFU	C16-C15-C14	-6.13	110.93	123.47
8	s	102	BCL	C1C-NC-C4C	-6.12	103.95	106.71
10	L	307	MW9	C35-C34-C33	6.12	152.28	112.55
8	S	101	BCL	C1D-ND-C4D	-6.09	102.01	106.33
9	E	102	A1EFU	C15-C16-C17	-6.09	111.00	123.47
9	j	101	A1EFU	CM4-C9-C10	-6.07	114.42	122.92
8	K	101	BCL	C1D-ND-C4D	-6.06	102.03	106.33
8	L	304	BCL	C1D-ND-C4D	-6.05	102.04	106.33
8	A	101	BCL	C1D-ND-C4D	-6.05	102.04	106.33
9	v	103	A1EFU	CM5-C13-C14	-6.04	114.46	122.92
8	N	101	BCL	C1D-ND-C4D	-6.01	102.07	106.33
8	E	101	BCL	C1D-ND-C4D	-6.00	102.07	106.33
8	e	101	BCL	C1D-ND-C4D	-5.96	102.10	106.33
8	j	102	BCL	C1D-ND-C4D	-5.95	102.11	106.33
8	G	102	BCL	C1D-ND-C4D	-5.95	102.11	106.33
9	s	105	A1EFU	CM3-C5-C6	-5.93	114.61	122.92
9	T	101	A1EFU	C15-C16-C17	-5.93	111.33	123.47
9	j	103	A1EFU	CM6-C18-C17	-5.92	114.62	122.92
8	M	403	BCL	C1D-ND-C4D	-5.91	102.14	106.33
8	D	101	BCL	C1D-ND-C4D	-5.90	102.14	106.33
8	V	101	BCL	C1D-ND-C4D	-5.90	102.15	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	k	101	A1EFU	CM5-C13-C14	-5.89	114.67	122.92
9	f	101	A1EFU	CM3-C5-C6	-5.89	114.67	122.92
9	F	104	A1EFU	C15-C16-C17	-5.89	111.41	123.47
9	j	101	A1EFU	CM6-C18-C17	-5.87	114.69	122.92
9	G	105	A1EFU	CM6-C18-C17	-5.87	114.69	122.92
9	q	101	A1EFU	C16-C15-C14	-5.86	111.46	123.47
9	G	106	A1EFU	CM6-C18-C17	-5.86	114.72	122.92
8	F	102	BCL	C1D-ND-C4D	-5.85	102.18	106.33
8	t	101	BCL	C2B-C1B-NB	-5.85	106.31	110.23
9	B	102	A1EFU	C15-C16-C17	-5.85	111.49	123.47
8	P	101	BCL	C1D-ND-C4D	-5.83	102.19	106.33
9	r	102	A1EFU	C15-C16-C17	-5.81	111.57	123.47
9	P	103	A1EFU	CM5-C13-C14	-5.81	114.79	122.92
8	l	101	BCL	C1D-ND-C4D	-5.78	102.23	106.33
9	q	101	A1EFU	CM6-C18-C17	-5.77	114.84	122.92
9	J	103	A1EFU	CM6-C18-C17	-5.76	114.86	122.92
8	L	301	BCL	C2D-C1D-ND	5.76	114.35	110.10
9	j	103	A1EFU	CM5-C13-C14	-5.76	114.86	122.92
8	I	101	BCL	C1D-ND-C4D	-5.74	102.26	106.33
9	N	102	A1EFU	CM4-C9-C10	-5.74	114.89	122.92
8	J	101	BCL	C1D-ND-C4D	-5.73	102.26	106.33
9	A	102	A1EFU	C15-C16-C17	-5.73	111.74	123.47
8	R	102	BCL	C1D-ND-C4D	-5.73	102.27	106.33
9	D	105	A1EFU	CM3-C5-C6	-5.72	114.91	122.92
8	Q	101	BCL	C1D-ND-C4D	-5.70	102.29	106.33
9	a	102	A1EFU	C15-C16-C17	-5.68	111.84	123.47
9	G	105	A1EFU	CM5-C13-C14	-5.67	114.97	122.92
9	s	101	A1EFU	C16-C15-C14	-5.67	111.85	123.47
8	F	101	BCL	C1D-ND-C4D	-5.67	102.31	106.33
9	R	101	A1EFU	C15-C16-C17	-5.65	111.91	123.47
9	2	101	A1EFU	CM6-C18-C17	-5.64	115.02	122.92
8	s	102	BCL	C2D-C1D-ND	5.64	114.26	110.10
8	2	103	BCL	C2D-C1D-ND	5.64	114.26	110.10
8	n	101	BCL	C2D-C1D-ND	5.64	114.26	110.10
9	J	103	A1EFU	C16-C15-C14	-5.63	111.95	123.47
9	r	102	A1EFU	CM3-C5-C6	-5.63	115.04	122.92
9	a	102	A1EFU	CM6-C18-C17	-5.62	115.05	122.92
9	E	103	A1EFU	C16-C15-C14	-5.62	111.96	123.47
8	B	101	BCL	C2D-C1D-ND	5.59	114.22	110.10
9	I	102	A1EFU	C15-C16-C17	-5.59	112.03	123.47
8	S	101	BCL	C2D-C1D-ND	5.58	114.22	110.10
8	F	101	BCL	O2D-CGD-CBD	5.57	121.17	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	p	101	A1EFU	CM4-C9-C10	-5.57	115.12	122.92
9	J	103	A1EFU	CM3-C5-C6	-5.57	115.12	122.92
9	P	103	A1EFU	CM6-C18-C17	-5.56	115.13	122.92
9	v	102	A1EFU	CM3-C5-C6	-5.56	115.13	122.92
9	G	106	A1EFU	CM3-C5-C6	-5.56	115.14	122.92
9	q	101	A1EFU	CM5-C13-C14	-5.56	115.14	122.92
9	2	102	A1EFU	CM5-C13-C14	-5.55	115.14	122.92
9	D	105	A1EFU	CM6-C18-C17	-5.55	115.15	122.92
9	B	103	A1EFU	CM3-C5-C6	-5.55	115.15	122.92
9	k	101	A1EFU	CM6-C18-C17	-5.55	115.16	122.92
9	E	103	A1EFU	CM3-C5-C6	-5.54	115.16	122.92
9	s	101	A1EFU	CM3-C5-C6	-5.54	115.16	122.92
9	I	102	A1EFU	CM3-C5-C6	-5.53	115.17	122.92
9	I	102	A1EFU	CM5-C13-C14	-5.53	115.18	122.92
9	p	101	A1EFU	CM3-C5-C6	-5.53	115.18	122.92
9	k	101	A1EFU	CM3-C5-C6	-5.52	115.19	122.92
8	i	101	BCL	O2D-CGD-CBD	5.52	121.07	111.27
8	N	101	BCL	C1C-NC-C4C	-5.52	104.23	106.71
8	i	101	BCL	C2D-C1D-ND	5.51	114.17	110.10
8	d	101	BCL	C1D-ND-C4D	-5.50	102.43	106.33
9	2	101	A1EFU	CM4-C9-C10	-5.50	115.22	122.92
9	j	101	A1EFU	C16-C15-C14	-5.50	112.21	123.47
9	v	103	A1EFU	C16-C15-C14	-5.50	112.21	123.47
8	r	101	BCL	C2D-C1D-ND	5.50	114.15	110.10
9	T	101	A1EFU	CM5-C13-C14	-5.48	115.25	122.92
9	r	102	A1EFU	CM5-C13-C14	-5.47	115.26	122.92
8	k	102	BCL	C2D-C1D-ND	5.47	114.14	110.10
8	P	102	BCL	C2D-C1D-ND	5.47	114.14	110.10
9	J	103	A1EFU	CM5-C13-C14	-5.46	115.27	122.92
8	d	101	BCL	O2D-CGD-CBD	5.46	120.97	111.27
8	I	101	BCL	C1C-NC-C4C	-5.46	104.25	106.71
9	f	101	A1EFU	C16-C15-C14	-5.46	112.30	123.47
8	v	101	BCL	C2D-C1D-ND	5.45	114.12	110.10
9	p	101	A1EFU	C16-C15-C14	-5.44	112.33	123.47
9	s	105	A1EFU	C16-C15-C14	-5.44	112.33	123.47
9	j	103	A1EFU	CM3-C5-C6	-5.43	115.32	122.92
9	s	101	A1EFU	CM6-C18-C17	-5.43	115.32	122.92
8	1	101	BCL	C1C-NC-C4C	-5.42	104.27	106.71
9	D	105	A1EFU	CM5-C13-C14	-5.42	115.33	122.92
9	B	103	A1EFU	C16-C15-C14	-5.41	112.38	123.47
8	s	103	BCL	C2D-C1D-ND	5.41	114.09	110.10
9	E	102	A1EFU	CM5-C13-C14	-5.41	115.35	122.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	K	102	A1EFU	CM4-C9-C10	-5.40	115.36	122.92
8	D	101	BCL	C2D-C1D-ND	5.38	114.07	110.10
9	2	102	A1EFU	C15-C16-C17	-5.38	112.45	123.47
8	K	101	BCL	C2D-C1D-ND	5.38	114.07	110.10
9	E	103	A1EFU	CM5-C13-C14	-5.38	115.39	122.92
9	E	102	A1EFU	CM4-C9-C10	-5.37	115.39	122.92
9	I	102	A1EFU	CM6-C18-C17	-5.37	115.40	122.92
9	k	101	A1EFU	C15-C16-C17	-5.37	112.48	123.47
9	f	101	A1EFU	CM6-C18-C17	-5.36	115.41	122.92
9	A	102	A1EFU	CM5-C13-C14	-5.36	115.41	122.92
9	G	106	A1EFU	CM5-C13-C14	-5.36	115.42	122.92
8	L	304	BCL	C2D-C1D-ND	5.36	114.05	110.10
9	J	102	A1EFU	CM5-C13-C14	-5.35	115.42	122.92
9	J	103	A1EFU	CM4-C9-C10	-5.35	115.43	122.92
8	G	101	BCL	C2D-C1D-ND	5.35	114.05	110.10
9	T	101	A1EFU	CM4-C9-C10	-5.35	115.43	122.92
8	A	101	BCL	C2D-C1D-ND	5.35	114.04	110.10
9	j	103	A1EFU	CM4-C9-C10	-5.35	115.43	122.92
9	P	103	A1EFU	CM4-C9-C10	-5.34	115.45	122.92
9	F	104	A1EFU	CM5-C13-C14	-5.33	115.45	122.92
9	s	104	A1EFU	C16-C15-C14	-5.33	112.56	123.47
9	B	102	A1EFU	CM5-C13-C14	-5.33	115.46	122.92
9	s	101	A1EFU	CM5-C13-C14	-5.33	115.46	122.92
9	v	102	A1EFU	CM6-C18-C17	-5.33	115.46	122.92
8	2	103	BCL	O2D-CGD-CBD	5.33	120.73	111.27
9	s	105	A1EFU	CM4-C9-C10	-5.32	115.47	122.92
8	N	101	BCL	C2D-C1D-ND	5.32	114.02	110.10
8	I	101	BCL	C2D-C1D-ND	5.32	114.02	110.10
9	v	103	A1EFU	CM6-C18-C17	-5.32	115.48	122.92
9	v	102	A1EFU	C15-C16-C17	-5.32	112.58	123.47
8	d	101	BCL	CAC-C3C-C2C	-5.31	100.99	114.26
9	G	106	A1EFU	C15-C16-C17	-5.31	112.60	123.47
8	G	102	BCL	O2D-CGD-CBD	5.31	120.70	111.27
8	Q	101	BCL	C2D-C1D-ND	5.31	114.02	110.10
8	M	402	BCL	C2D-C1D-ND	5.31	114.02	110.10
9	M	407	A1EFU	CM3-C5-C6	-5.31	115.49	122.92
9	D	104	A1EFU	CM4-C9-C10	-5.30	115.50	122.92
8	q	102	BCL	C2D-C1D-ND	5.30	114.01	110.10
9	2	102	A1EFU	CM6-C18-C17	-5.29	115.51	122.92
9	v	103	A1EFU	C15-C16-C17	-5.29	112.63	123.47
9	v	103	A1EFU	CM3-C5-C6	-5.29	115.51	122.92
8	I	101	BCL	O2D-CGD-CBD	5.29	120.67	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	K	102	A1EFU	CM5-C13-C14	-5.28	115.52	122.92
9	G	106	A1EFU	CM4-C9-C10	-5.28	115.53	122.92
9	A	102	A1EFU	CM3-C5-C6	-5.27	115.53	122.92
9	N	102	A1EFU	C15-C16-C17	-5.27	112.68	123.47
8	j	102	BCL	C2D-C1D-ND	5.27	113.99	110.10
9	r	102	A1EFU	CM6-C18-C17	-5.27	115.55	122.92
9	B	102	A1EFU	CM4-C9-C10	-5.26	115.56	122.92
8	P	101	BCL	C2D-C1D-ND	5.25	113.98	110.10
8	b	101	BCL	C2D-C1D-ND	5.25	113.97	110.10
9	A	102	A1EFU	CM6-C18-C17	-5.25	115.57	122.92
8	a	101	BCL	C2D-C1D-ND	5.25	113.97	110.10
9	K	102	A1EFU	CM6-C18-C17	-5.24	115.58	122.92
9	F	104	A1EFU	CM3-C5-C6	-5.24	115.58	122.92
9	s	101	A1EFU	C15-C16-C17	-5.24	112.74	123.47
9	F	104	A1EFU	CM4-C9-C10	-5.24	115.59	122.92
8	E	101	BCL	C2D-C1D-ND	5.24	113.96	110.10
9	P	103	A1EFU	CM3-C5-C6	-5.23	115.59	122.92
9	B	103	A1EFU	C15-C16-C17	-5.23	112.77	123.47
9	K	102	A1EFU	CM3-C5-C6	-5.22	115.61	122.92
9	s	101	A1EFU	CM4-C9-C10	-5.22	115.61	122.92
9	I	102	A1EFU	CM4-C9-C10	-5.22	115.61	122.92
9	E	103	A1EFU	C15-C16-C17	-5.22	112.78	123.47
9	r	102	A1EFU	C16-C15-C14	-5.22	112.79	123.47
8	J	101	BCL	C2D-C1D-ND	5.21	113.95	110.10
9	A	102	A1EFU	CM4-C9-C10	-5.21	115.62	122.92
9	E	103	A1EFU	CM6-C18-C17	-5.21	115.62	122.92
9	s	105	A1EFU	C15-C16-C17	-5.21	112.81	123.47
8	F	102	BCL	O2D-CGD-CBD	5.20	120.52	111.27
8	L	304	BCL	CAC-C3C-C2C	-5.20	101.26	114.26
9	p	101	A1EFU	CM5-C13-C14	-5.20	115.64	122.92
9	s	105	A1EFU	CM5-C13-C14	-5.20	115.64	122.92
9	j	101	A1EFU	CM5-C13-C14	-5.19	115.65	122.92
9	f	101	A1EFU	CM5-C13-C14	-5.19	115.65	122.92
9	D	105	A1EFU	C15-C16-C17	-5.19	112.84	123.47
9	2	101	A1EFU	C15-C16-C17	-5.19	112.85	123.47
9	R	101	A1EFU	CM3-C5-C6	-5.19	115.66	122.92
9	R	101	A1EFU	CM5-C13-C14	-5.18	115.66	122.92
9	J	102	A1EFU	C15-C16-C17	-5.18	112.86	123.47
9	f	101	A1EFU	C15-C16-C17	-5.18	112.87	123.47
9	j	101	A1EFU	CM3-C5-C6	-5.17	115.68	122.92
9	k	101	A1EFU	CM4-C9-C10	-5.17	115.68	122.92
8	E	101	BCL	O2D-CGD-CBD	5.17	120.45	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	K	102	A1EFU	C16-C15-C14	-5.17	112.89	123.47
8	G	102	BCL	C2D-C1D-ND	5.16	113.91	110.10
8	1	101	BCL	C2D-C1D-ND	5.16	113.91	110.10
9	M	407	A1EFU	CM4-C9-C10	-5.16	115.70	122.92
9	R	101	A1EFU	CM4-C9-C10	-5.16	115.70	122.92
9	N	102	A1EFU	CM6-C18-C17	-5.16	115.70	122.92
8	V	101	BCL	C2D-C1D-ND	5.15	113.90	110.10
9	2	104	A1EFU	CM4-C9-C10	-5.15	115.71	122.92
9	j	103	A1EFU	C16-C15-C14	-5.14	112.94	123.47
9	N	102	A1EFU	CM3-C5-C6	-5.13	115.73	122.92
9	D	104	A1EFU	CM3-C5-C6	-5.13	115.74	122.92
9	f	101	A1EFU	CM4-C9-C10	-5.13	115.74	122.92
9	D	105	A1EFU	CM4-C9-C10	-5.12	115.75	122.92
9	J	103	A1EFU	C15-C16-C17	-5.12	112.99	123.47
8	M	403	BCL	C2D-C1D-ND	5.12	113.88	110.10
9	a	102	A1EFU	CM3-C5-C6	-5.12	115.76	122.92
9	j	101	A1EFU	C15-C16-C17	-5.11	113.00	123.47
9	E	103	A1EFU	CM4-C9-C10	-5.11	115.76	122.92
8	D	101	BCL	CAC-C3C-C2C	-5.11	101.49	114.26
9	s	105	A1EFU	CM6-C18-C17	-5.11	115.77	122.92
9	D	105	A1EFU	C16-C15-C14	-5.11	113.02	123.47
9	2	101	A1EFU	CM3-C5-C6	-5.10	115.77	122.92
8	K	101	BCL	O2D-CGD-CBD	5.10	120.34	111.27
9	v	102	A1EFU	CM5-C13-C14	-5.09	115.80	122.92
8	J	101	BCL	O2D-CGD-CBD	5.08	120.30	111.27
9	D	104	A1EFU	CM6-C18-C17	-5.08	115.81	122.92
9	v	102	A1EFU	C16-C15-C14	-5.08	113.07	123.47
8	d	101	BCL	C2D-C1D-ND	5.08	113.84	110.10
9	T	101	A1EFU	CM6-C18-C17	-5.07	115.82	122.92
8	K	101	BCL	C1C-NC-C4C	-5.06	104.43	106.71
9	G	106	A1EFU	C16-C15-C14	-5.06	113.10	123.47
8	Q	101	BCL	O2D-CGD-CBD	5.06	120.27	111.27
8	e	101	BCL	C2D-C1D-ND	5.06	113.83	110.10
8	e	101	BCL	CAC-C3C-C2C	-5.06	101.62	114.26
9	N	102	A1EFU	CM5-C13-C14	-5.06	115.84	122.92
9	B	102	A1EFU	CM3-C5-C6	-5.04	115.86	122.92
8	F	101	BCL	C2D-C1D-ND	5.04	113.82	110.10
9	v	102	A1EFU	CM4-C9-C10	-5.04	115.87	122.92
8	j	102	BCL	O2D-CGD-CBD	5.01	120.17	111.27
8	G	101	BCL	O2D-CGD-CBD	5.01	120.17	111.27
9	R	101	A1EFU	C16-C15-C14	-5.01	113.22	123.47
8	F	102	BCL	C2D-C1D-ND	5.00	113.79	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	R	102	BCL	C2D-C1D-ND	4.99	113.78	110.10
8	L	301	BCL	C4A-NA-C1A	-4.98	104.47	106.71
8	q	102	BCL	O2D-CGD-CBD	4.98	120.12	111.27
9	T	101	A1EFU	CM3-C5-C6	-4.98	115.95	122.92
9	M	407	A1EFU	C15-C16-C17	-4.98	113.28	123.47
9	I	102	A1EFU	C16-C15-C14	-4.97	113.29	123.47
9	s	104	A1EFU	CM6-C18-C17	-4.97	115.96	122.92
9	J	102	A1EFU	CM4-C9-C10	-4.97	115.96	122.92
8	k	102	BCL	O2D-CGD-CBD	4.96	120.08	111.27
8	L	304	BCL	O2D-CGD-CBD	4.96	120.08	111.27
8	M	403	BCL	CAC-C3C-C2C	-4.96	101.88	114.26
8	n	101	BCL	O2D-CGD-CBD	4.95	120.06	111.27
8	s	103	BCL	O2D-CGD-CBD	4.94	120.04	111.27
9	q	101	A1EFU	CM3-C5-C6	-4.93	116.02	122.92
9	2	104	A1EFU	CM7-C22-C21	-4.92	109.88	122.59
8	e	101	BCL	O2D-CGD-CBD	4.92	120.02	111.27
9	F	104	A1EFU	C16-C15-C14	-4.92	113.39	123.47
9	k	101	A1EFU	C16-C15-C14	-4.92	113.40	123.47
8	t	101	BCL	O2D-CGD-CBD	4.91	120.00	111.27
8	P	101	BCL	CAC-C3C-C2C	-4.91	101.99	114.26
9	M	407	A1EFU	CM5-C13-C14	-4.91	116.05	122.92
8	S	101	BCL	CAC-C3C-C2C	-4.90	102.01	114.26
9	J	102	A1EFU	C16-C15-C14	-4.89	113.46	123.47
8	b	101	BCL	O2D-CGD-CBD	4.89	119.95	111.27
9	M	407	A1EFU	C16-C15-C14	-4.89	113.46	123.47
9	2	104	A1EFU	CM3-C5-C6	-4.89	116.08	122.92
8	N	101	BCL	O2D-CGD-CBD	4.89	119.95	111.27
8	a	101	BCL	CAC-C3C-C2C	-4.89	102.05	114.26
9	B	102	A1EFU	CM6-C18-C17	-4.88	116.08	122.92
8	V	101	BCL	CAC-C3C-C2C	-4.87	102.08	114.26
9	2	104	A1EFU	CM5-C13-C14	-4.87	116.10	122.92
8	Q	101	BCL	CAC-C3C-C2C	-4.87	102.09	114.26
8	V	101	BCL	O2D-CGD-CBD	4.87	119.92	111.27
9	2	101	A1EFU	CM5-C13-C14	-4.87	116.11	122.92
8	B	101	BCL	CAC-C3C-C2C	-4.86	102.10	114.26
9	B	103	A1EFU	CM4-C9-C10	-4.86	116.11	122.92
8	2	103	BCL	CAC-C3C-C2C	-4.86	102.12	114.26
9	A	102	A1EFU	C16-C15-C14	-4.85	113.54	123.47
8	F	101	BCL	CAC-C3C-C2C	-4.85	102.14	114.26
8	r	101	BCL	O2D-CGD-CBD	4.85	119.89	111.27
8	G	101	BCL	CAC-C3C-C2C	-4.85	102.15	114.26
9	E	102	A1EFU	C16-C15-C14	-4.84	113.56	123.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	G	105	A1EFU	CM4-C9-C10	-4.84	116.14	122.92
9	F	104	A1EFU	CM6-C18-C17	-4.84	116.14	122.92
8	a	101	BCL	O2D-CGD-CBD	4.84	119.86	111.27
9	2	104	A1EFU	C16-C15-C14	-4.83	113.57	123.47
8	b	101	BCL	CAC-C3C-C2C	-4.83	102.20	114.26
9	K	102	A1EFU	C15-C16-C17	-4.82	113.60	123.47
8	B	101	BCL	O2D-CGD-CBD	4.82	119.83	111.27
8	A	101	BCL	O2D-CGD-CBD	4.82	119.83	111.27
8	r	101	BCL	CAC-C3C-C2C	-4.82	102.23	114.26
9	q	101	A1EFU	CM4-C9-C10	-4.82	116.18	122.92
9	s	104	A1EFU	C15-C16-C17	-4.81	113.62	123.47
9	J	102	A1EFU	CM3-C5-C6	-4.81	116.18	122.92
8	i	101	BCL	CAC-C3C-C2C	-4.81	102.24	114.26
8	P	102	BCL	O2D-CGD-CBD	4.81	119.81	111.27
9	a	102	A1EFU	C16-C15-C14	-4.80	113.63	123.47
9	2	104	A1EFU	CM6-C18-C17	-4.80	116.19	122.92
8	v	101	BCL	O2D-CGD-CBD	4.80	119.80	111.27
9	B	102	A1EFU	C16-C15-C14	-4.80	113.64	123.47
8	P	102	BCL	CAC-C3C-C2C	-4.80	102.28	114.26
8	d	101	BCL	C1C-NC-C4C	-4.78	104.56	106.71
9	N	102	A1EFU	C16-C15-C14	-4.78	113.68	123.47
8	k	102	BCL	CAC-C3C-C2C	-4.78	102.33	114.26
8	L	304	BCL	C1C-NC-C4C	-4.78	104.56	106.71
8	t	101	BCL	C1D-ND-C4D	-4.77	102.94	106.33
8	A	101	BCL	CAC-C3C-C2C	-4.77	102.33	114.26
9	E	102	A1EFU	CM6-C18-C17	-4.77	116.24	122.92
8	D	101	BCL	O2D-CGD-CBD	4.75	119.70	111.27
8	G	102	BCL	C1C-NC-C4C	-4.74	104.57	106.71
9	R	101	A1EFU	CM6-C18-C17	-4.74	116.28	122.92
9	B	103	A1EFU	CM6-C18-C17	-4.73	116.29	122.92
8	R	102	BCL	O2D-CGD-CBD	4.73	119.67	111.27
9	2	101	A1EFU	C16-C15-C14	-4.73	113.79	123.47
9	2	102	A1EFU	CM3-C5-C6	-4.72	116.31	122.92
9	D	104	A1EFU	CM5-C13-C14	-4.72	116.31	122.92
9	P	103	A1EFU	C16-C15-C14	-4.71	113.82	123.47
8	v	101	BCL	CAC-C3C-C2C	-4.71	102.48	114.26
9	2	102	A1EFU	CM4-C9-C10	-4.71	116.32	122.92
8	q	102	BCL	CAC-C3C-C2C	-4.71	102.49	114.26
8	s	103	BCL	CAC-C3C-C2C	-4.71	102.49	114.26
9	T	101	A1EFU	C16-C15-C14	-4.71	113.83	123.47
8	M	402	BCL	CAC-C3C-C2C	-4.71	102.50	114.26
9	J	102	A1EFU	CM6-C18-C17	-4.70	116.34	122.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	j	102	BCL	CAC-C3C-C2C	-4.70	102.53	114.26
9	B	103	A1EFU	CM5-C13-C14	-4.69	116.35	122.92
8	F	102	BCL	C1C-NC-C4C	-4.68	104.60	106.71
9	s	104	A1EFU	CM4-C9-C10	-4.68	116.36	122.92
9	G	105	A1EFU	CM3-C5-C6	-4.67	116.39	122.92
9	P	103	A1EFU	C15-C16-C17	-4.66	113.92	123.47
9	s	104	A1EFU	CM5-C13-C14	-4.66	116.39	122.92
8	d	101	BCL	O2D-CGD-O1D	-4.66	114.73	123.84
8	l	101	BCL	O2D-CGD-CBD	4.65	119.53	111.27
8	n	101	BCL	CAC-C3C-C2C	-4.65	102.64	114.26
8	L	301	BCL	CAC-C3C-C2C	-4.64	102.67	114.26
8	P	101	BCL	O2D-CGD-CBD	4.63	119.50	111.27
9	p	101	A1EFU	C15-C16-C17	-4.63	113.98	123.47
8	S	101	BCL	O2D-CGD-CBD	4.63	119.49	111.27
8	J	101	BCL	C1C-NC-C4C	-4.62	104.63	106.71
9	a	102	A1EFU	CM5-C13-C12	4.62	125.35	118.08
9	q	101	A1EFU	C15-C16-C17	-4.61	114.04	123.47
9	2	104	A1EFU	C15-C16-C17	-4.60	114.04	123.47
8	s	102	BCL	O2D-CGD-CBD	4.60	119.44	111.27
9	G	105	A1EFU	C16-C15-C14	-4.58	114.08	123.47
8	R	102	BCL	CAC-C3C-C2C	-4.58	102.81	114.26
9	a	102	A1EFU	CM4-C9-C8	4.57	125.28	118.08
9	E	102	A1EFU	CM3-C5-C6	-4.57	116.53	122.92
8	J	101	BCL	CAC-C3C-C2C	-4.55	102.88	114.26
8	E	101	BCL	C1C-NC-C4C	-4.54	104.67	106.71
9	s	101	A1EFU	CM3-C5-C4	4.54	125.22	118.08
8	R	102	BCL	C1C-NC-C4C	-4.53	104.67	106.71
9	2	102	A1EFU	C16-C15-C14	-4.53	114.20	123.47
9	p	101	A1EFU	CM7-C22-C21	-4.53	110.92	122.59
8	i	101	BCL	O2D-CGD-O1D	-4.52	115.00	123.84
8	s	102	BCL	CAC-C3C-C2C	-4.50	103.00	114.26
9	r	102	A1EFU	CM4-C9-C10	-4.50	116.62	122.92
9	j	103	A1EFU	C15-C16-C17	-4.48	114.29	123.47
9	r	102	A1EFU	CM7-C22-C21	-4.48	111.04	122.59
9	j	103	A1EFU	CM7-C22-C21	-4.47	111.06	122.59
9	D	104	A1EFU	C15-C16-C17	-4.46	114.33	123.47
8	M	403	BCL	CMB-C2B-C1B	-4.45	118.59	125.37
8	K	101	BCL	CAC-C3C-C2C	-4.45	103.14	114.26
8	d	101	BCL	CMB-C2B-C1B	-4.44	118.60	125.37
9	2	101	A1EFU	CM7-C22-C21	-4.43	111.15	122.59
9	I	102	A1EFU	CM3-C5-C4	4.43	125.06	118.08
8	F	101	BCL	O2D-CGD-O1D	-4.42	115.19	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	304	BCL	CMB-C2B-C1B	-4.42	118.64	125.37
9	G	106	A1EFU	CM7-C22-C21	-4.42	111.20	122.59
8	G	102	BCL	CAC-C3C-C2C	-4.41	103.24	114.26
8	I	101	BCL	CAC-C3C-C2C	-4.41	103.25	114.26
8	F	102	BCL	CAC-C3C-C2C	-4.41	103.25	114.26
9	2	102	A1EFU	CM7-C22-C21	-4.40	111.24	122.59
9	D	105	A1EFU	CM3-C5-C4	4.40	125.01	118.08
9	M	407	A1EFU	CM7-C22-C21	-4.39	111.26	122.59
9	j	101	A1EFU	CM7-C22-C21	-4.39	111.28	122.59
8	i	101	BCL	CMB-C2B-C1B	-4.38	118.69	125.37
9	M	407	A1EFU	CM6-C18-C17	-4.38	116.79	122.92
8	t	101	BCL	C2D-C1D-ND	4.37	113.33	110.10
9	f	101	A1EFU	CM7-C22-C21	-4.37	111.32	122.59
8	t	101	BCL	CAC-C3C-C2C	-4.37	103.34	114.26
8	F	102	BCL	O2D-CGD-O1D	-4.37	115.30	123.84
9	j	101	A1EFU	CM4-C9-C8	4.37	124.96	118.08
9	N	102	A1EFU	C23-C22-C21	-4.37	108.76	121.98
9	r	102	A1EFU	CM3-C5-C4	4.37	124.95	118.08
9	s	104	A1EFU	CM7-C22-C21	-4.36	111.33	122.59
9	D	105	A1EFU	CM7-C22-C21	-4.36	111.34	122.59
8	I	101	BCL	O2D-CGD-O1D	-4.36	115.31	123.84
8	2	103	BCL	O2D-CGD-O1D	-4.35	115.33	123.84
8	j	102	BCL	CMB-C2B-C1B	-4.35	118.74	125.37
8	I	101	BCL	CMB-C2B-C1B	-4.35	118.74	125.37
8	E	101	BCL	O2D-CGD-O1D	-4.35	115.34	123.84
9	G	106	A1EFU	CM3-C5-C4	4.35	124.92	118.08
9	s	105	A1EFU	CM7-C22-C21	-4.34	111.38	122.59
9	a	102	A1EFU	CM7-C22-C21	-4.34	111.39	122.59
8	G	102	BCL	O2D-CGD-O1D	-4.33	115.36	123.84
9	E	103	A1EFU	CM3-C5-C4	4.33	124.89	118.08
8	M	403	BCL	CHD-C1D-ND	-4.32	120.48	124.45
8	2	103	BCL	CMB-C2B-C1B	-4.32	118.79	125.37
8	q	102	BCL	CMB-C2B-C1B	-4.32	118.79	125.37
8	J	101	BCL	CMB-C2B-C1B	-4.32	118.80	125.37
8	E	101	BCL	CAC-C3C-C2C	-4.31	103.48	114.26
8	G	102	BCL	CMB-C2B-C1B	-4.31	118.81	125.37
8	k	102	BCL	CMB-C2B-C1B	-4.31	118.81	125.37
8	a	101	BCL	CMB-C2B-C1B	-4.30	118.81	125.37
8	e	101	BCL	CMB-C2B-C1B	-4.29	118.83	125.37
9	G	105	A1EFU	C15-C16-C17	-4.29	114.68	123.47
8	F	101	BCL	CMB-C2B-C1B	-4.29	118.83	125.37
8	N	101	BCL	CAC-C3C-C2C	-4.29	103.53	114.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	301	BCL	CMB-C2B-C1B	-4.29	118.83	125.37
9	G	106	A1EFU	C23-C22-C21	-4.29	108.99	121.98
8	l	101	BCL	CMB-C2B-C1B	-4.29	118.84	125.37
8	N	101	BCL	CMB-C2B-C1B	-4.29	118.84	125.37
8	M	402	BCL	O2D-CGD-CBD	4.28	118.88	111.27
9	f	101	A1EFU	C6-C7-C8	-4.28	109.85	123.22
9	I	102	A1EFU	CM7-C22-C21	-4.28	111.55	122.59
8	K	101	BCL	O2D-CGD-O1D	-4.28	115.47	123.84
8	E	101	BCL	CMB-C2B-C1B	-4.28	118.86	125.37
9	f	101	A1EFU	CM3-C5-C4	4.27	124.81	118.08
9	k	101	A1EFU	CM7-C22-C21	-4.27	111.57	122.59
9	N	102	A1EFU	CM7-C22-C21	-4.27	111.58	122.59
8	v	101	BCL	CMB-C2B-C1B	-4.27	118.87	125.37
8	t	101	BCL	CHD-C1D-ND	-4.26	120.53	124.45
9	s	101	A1EFU	CM7-C22-C21	-4.26	111.59	122.59
8	G	101	BCL	CMB-C2B-C1B	-4.26	118.88	125.37
9	q	101	A1EFU	CM7-C22-C21	-4.26	111.61	122.59
8	J	101	BCL	O2D-CGD-O1D	-4.26	115.51	123.84
9	B	103	A1EFU	CM3-C5-C4	4.25	124.78	118.08
9	J	103	A1EFU	CM7-C22-C21	-4.25	111.62	122.59
8	M	402	BCL	CMB-C2B-C1B	-4.25	118.89	125.37
8	s	103	BCL	CMB-C2B-C1B	-4.25	118.89	125.37
9	T	101	A1EFU	CM7-C22-C21	-4.25	111.63	122.59
8	Q	101	BCL	CMB-C2B-C1B	-4.25	118.90	125.37
8	R	102	BCL	CMB-C2B-C1B	-4.25	118.90	125.37
8	G	101	BCL	O2D-CGD-O1D	-4.24	115.55	123.84
8	F	102	BCL	CMB-C2B-C1B	-4.24	118.91	125.37
9	j	101	A1EFU	CM3-C5-C4	4.24	124.75	118.08
8	L	301	BCL	O2D-CGD-CBD	4.24	118.80	111.27
8	D	101	BCL	CMB-C2B-C1B	-4.23	118.92	125.37
9	v	103	A1EFU	CM4-C9-C10	-4.23	117.00	122.92
9	J	103	A1EFU	CM3-C5-C4	4.23	124.74	118.08
9	A	102	A1EFU	CM7-C22-C21	-4.23	111.68	122.59
9	B	103	A1EFU	CM7-C22-C21	-4.22	111.69	122.59
9	v	103	A1EFU	CM7-C22-C21	-4.22	111.69	122.59
9	s	105	A1EFU	CM4-C9-C8	4.22	124.72	118.08
8	B	101	BCL	CMB-C2B-C1B	-4.22	118.95	125.37
9	B	102	A1EFU	CM7-C22-C21	-4.21	111.72	122.59
9	D	104	A1EFU	CM4-C9-C8	4.21	124.72	118.08
9	E	103	A1EFU	CM7-C22-C21	-4.21	111.73	122.59
9	B	103	A1EFU	C10-C11-C12	-4.21	110.08	123.22
9	s	105	A1EFU	C6-C7-C8	-4.20	110.11	123.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	102	A1EFU	CM4-C9-C8	4.20	124.69	118.08
8	L	304	BCL	O2D-CGD-O1D	-4.20	115.63	123.84
9	P	103	A1EFU	CM7-C22-C21	-4.20	111.76	122.59
8	e	101	BCL	O2D-CGD-O1D	-4.20	115.63	123.84
8	S	101	BCL	CMB-C2B-C1B	-4.20	118.98	125.37
8	b	101	BCL	CMB-C2B-C1B	-4.19	118.98	125.37
9	E	102	A1EFU	CM7-C22-C21	-4.19	111.78	122.59
9	q	101	A1EFU	CM5-C13-C12	4.19	124.67	118.08
10	D	103	MW9	O8-C24-C25	4.18	120.52	111.50
8	K	101	BCL	CMB-C2B-C1B	-4.18	119.00	125.37
9	v	102	A1EFU	CM3-C5-C4	4.18	124.67	118.08
9	s	105	A1EFU	CM3-C5-C4	4.18	124.67	118.08
8	t	101	BCL	O2D-CGD-O1D	-4.18	115.67	123.84
9	E	102	A1EFU	C6-C7-C8	-4.18	110.18	123.22
8	j	102	BCL	O2D-CGD-O1D	-4.18	115.67	123.84
8	q	102	BCL	O2D-CGD-O1D	-4.17	115.69	123.84
8	r	101	BCL	O2D-CGD-O1D	-4.16	115.70	123.84
8	P	101	BCL	CMB-C2B-C1B	-4.16	119.03	125.37
9	E	103	A1EFU	C23-C22-C21	-4.16	109.38	121.98
9	J	102	A1EFU	CM7-C22-C21	-4.16	111.86	122.59
9	q	101	A1EFU	C10-C11-C12	-4.16	110.24	123.22
10	L	307	MW9	O8-C24-C25	4.16	120.46	111.50
9	T	101	A1EFU	CM3-C5-C4	4.16	124.63	118.08
9	2	101	A1EFU	C23-C22-C21	-4.16	109.39	121.98
9	F	104	A1EFU	CM3-C5-C4	4.16	124.63	118.08
10	H	303	MW9	O8-C24-C25	4.16	120.46	111.50
10	G	103	MW9	O8-C24-C25	4.15	120.45	111.50
9	p	101	A1EFU	CM3-C5-C4	4.15	124.62	118.08
8	t	101	BCL	C1C-NC-C4C	-4.15	104.84	106.71
8	l	101	BCL	CAC-C3C-C2C	-4.15	103.89	114.26
8	d	101	BCL	C2B-C1B-NB	-4.15	107.45	110.23
9	s	101	A1EFU	CM4-C9-C8	4.15	124.61	118.08
8	s	103	BCL	O2D-CGD-O1D	-4.15	115.73	123.84
9	I	102	A1EFU	C23-C22-C21	-4.14	109.44	121.98
8	M	403	BCL	O2D-CGD-CBD	4.14	118.62	111.27
10	H	301	MW9	O8-C24-C25	4.14	120.42	111.50
8	t	101	BCL	OBB-CAB-CBB	-4.14	110.56	119.73
9	B	102	A1EFU	C6-C7-C8	-4.14	110.31	123.22
8	b	101	BCL	O2D-CGD-O1D	-4.13	115.75	123.84
9	2	102	A1EFU	C23-C22-C21	-4.13	109.46	121.98
8	Q	101	BCL	O2D-CGD-O1D	-4.13	115.76	123.84
8	j	102	BCL	C1C-NC-C4C	-4.13	104.85	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	105	A1EFU	C23-C22-C21	-4.12	109.50	121.98
9	v	102	A1EFU	CM7-C22-C21	-4.12	111.96	122.59
8	n	101	BCL	O2D-CGD-O1D	-4.12	115.78	123.84
9	v	103	A1EFU	CM3-C5-C4	4.12	124.57	118.08
15	L	308	CDL	OB6-CB5-C51	4.12	120.37	111.50
10	M	405	MW9	O8-C24-C25	4.11	120.37	111.50
9	R	101	A1EFU	CM7-C22-C21	-4.11	111.98	122.59
15	H	304	CDL	OB6-CB5-C51	4.11	120.36	111.50
8	P	102	BCL	CHB-C1B-NB	4.10	128.60	124.26
8	v	101	BCL	O2D-CGD-O1D	-4.10	115.82	123.84
8	V	101	BCL	O2D-CGD-O1D	-4.10	115.83	123.84
9	k	101	A1EFU	CM3-C5-C4	4.10	124.53	118.08
10	M	406	MW9	O8-C24-C25	4.10	120.33	111.50
9	F	104	A1EFU	CM7-C22-C21	-4.10	112.02	122.59
9	A	102	A1EFU	CM3-C5-C4	4.09	124.53	118.08
8	N	101	BCL	O2D-CGD-O1D	-4.09	115.85	123.84
8	k	102	BCL	O2D-CGD-O1D	-4.09	115.85	123.84
8	A	101	BCL	O2D-CGD-O1D	-4.09	115.85	123.84
8	P	102	BCL	O2D-CGD-O1D	-4.08	115.85	123.84
8	B	101	BCL	O2D-CGD-O1D	-4.08	115.86	123.84
8	n	101	BCL	CHB-C1B-NB	4.08	128.58	124.26
9	j	103	A1EFU	C6-C7-C8	-4.08	110.48	123.22
9	D	104	A1EFU	CM5-C13-C12	4.08	124.50	118.08
10	R	103	MW9	O8-C24-C25	4.08	120.29	111.50
8	a	101	BCL	O2D-CGD-O1D	-4.08	115.86	123.84
9	j	103	A1EFU	CM4-C9-C8	4.08	124.50	118.08
9	G	106	A1EFU	CM6-C18-C19	4.07	124.50	118.08
9	a	102	A1EFU	CM3-C5-C4	4.07	124.49	118.08
9	k	101	A1EFU	C10-C11-C12	-4.07	110.52	123.22
9	B	102	A1EFU	CM4-C9-C8	4.07	124.49	118.08
9	F	104	A1EFU	CM4-C9-C8	4.07	124.48	118.08
8	P	101	BCL	O2D-CGD-O1D	-4.07	115.89	123.84
8	R	102	BCL	O2D-CGD-O1D	-4.06	115.89	123.84
9	j	103	A1EFU	CM3-C5-C4	4.06	124.47	118.08
9	F	104	A1EFU	C6-C7-C8	-4.06	110.56	123.22
9	K	102	A1EFU	CM7-C22-C21	-4.06	112.13	122.59
9	I	102	A1EFU	CM6-C18-C19	4.05	124.46	118.08
8	D	101	BCL	O2D-CGD-O1D	-4.05	115.92	123.84
9	a	102	A1EFU	C23-C22-C21	-4.04	109.74	121.98
9	s	101	A1EFU	C6-C7-C8	-4.04	110.61	123.22
8	S	101	BCL	O2D-CGD-O1D	-4.03	115.95	123.84
9	K	102	A1EFU	CM3-C5-C4	4.03	124.43	118.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	P	103	A1EFU	C23-C22-C21	-4.03	109.78	121.98
9	B	102	A1EFU	CM3-C5-C4	4.03	124.42	118.08
9	q	101	A1EFU	CM3-C5-C4	4.03	124.42	118.08
8	s	102	BCL	OBB-CAB-CBB	-4.02	110.81	119.73
9	2	104	A1EFU	C21-C20-C19	-4.02	110.67	123.22
9	2	102	A1EFU	C10-C11-C12	-4.02	110.68	123.22
9	D	104	A1EFU	CM7-C22-C21	-4.02	112.22	122.59
9	T	101	A1EFU	CM4-C9-C8	4.02	124.41	118.08
9	G	105	A1EFU	CM7-C22-C21	-4.02	112.23	122.59
8	M	403	BCL	C1C-NC-C4C	-4.01	104.90	106.71
8	r	101	BCL	CHB-C1B-NB	4.01	128.50	124.26
15	H	304	CDL	OA6-CA5-C11	4.01	120.13	111.50
9	D	104	A1EFU	C10-C11-C12	-4.00	110.72	123.22
9	2	104	A1EFU	CM3-C5-C4	4.00	124.39	118.08
9	A	102	A1EFU	CM4-C9-C8	4.00	124.39	118.08
9	k	101	A1EFU	C23-C22-C21	-4.00	109.86	121.98
15	L	308	CDL	OA6-CA5-C11	4.00	120.13	111.50
9	s	101	A1EFU	C10-C11-C12	-4.00	110.73	123.22
9	A	102	A1EFU	C6-C7-C8	-4.00	110.73	123.22
9	R	101	A1EFU	CM3-C5-C4	4.00	124.38	118.08
9	E	102	A1EFU	C23-C22-C21	-4.00	109.87	121.98
9	2	101	A1EFU	CM6-C18-C19	3.99	124.37	118.08
9	M	407	A1EFU	CM3-C5-C4	3.99	124.36	118.08
9	D	104	A1EFU	C6-C7-C8	-3.99	110.77	123.22
9	B	103	A1EFU	CM4-C9-C8	3.99	124.36	118.08
8	L	301	BCL	O2D-CGD-O1D	-3.98	116.05	123.84
9	a	102	A1EFU	CM6-C18-C19	3.98	124.35	118.08
9	D	105	A1EFU	CM6-C18-C19	3.98	124.34	118.08
9	r	102	A1EFU	CM5-C13-C12	3.98	124.34	118.08
9	F	104	A1EFU	C10-C11-C12	-3.97	110.82	123.22
9	P	103	A1EFU	CM4-C9-C8	3.97	124.33	118.08
9	D	104	A1EFU	CM3-C5-C4	3.97	124.33	118.08
9	J	103	A1EFU	CM5-C13-C12	3.97	124.33	118.08
8	1	101	BCL	O2D-CGD-O1D	-3.97	116.08	123.84
10	G	104	MW9	O8-C24-C25	3.96	120.03	111.50
8	F	102	BCL	CHD-C1D-ND	-3.96	120.82	124.45
8	s	102	BCL	O2D-CGD-O1D	-3.96	116.10	123.84
9	r	102	A1EFU	C6-C7-C8	-3.95	110.88	123.22
8	S	101	BCL	CHD-C1D-ND	-3.95	120.82	124.45
9	D	104	A1EFU	C23-C22-C21	-3.95	110.01	121.98
9	T	101	A1EFU	C6-C7-C8	-3.95	110.89	123.22
9	F	104	A1EFU	CM5-C13-C12	3.95	124.29	118.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	402	BCL	O2D-CGD-O1D	-3.94	116.13	123.84
9	P	103	A1EFU	CM3-C5-C4	3.94	124.29	118.08
8	A	101	BCL	CHB-C1B-NB	3.94	128.43	124.26
9	G	105	A1EFU	CM3-C5-C4	3.94	124.28	118.08
10	F	103	MW9	O8-C24-C25	3.94	119.98	111.50
9	r	102	A1EFU	CM4-C9-C8	3.93	124.27	118.08
9	2	101	A1EFU	CM3-C5-C4	3.93	124.27	118.08
9	E	102	A1EFU	CM3-C5-C4	3.93	124.27	118.08
9	E	103	A1EFU	C10-C11-C12	-3.93	110.96	123.22
9	j	101	A1EFU	C23-C22-C21	-3.93	110.09	121.98
9	D	105	A1EFU	C6-C7-C8	-3.92	110.99	123.22
9	P	103	A1EFU	C6-C7-C8	-3.92	111.00	123.22
9	G	105	A1EFU	C10-C11-C12	-3.91	111.01	123.22
8	M	403	BCL	O2D-CGD-O1D	-3.91	116.19	123.84
9	j	103	A1EFU	C23-C22-C21	-3.91	110.15	121.98
9	r	102	A1EFU	C10-C11-C12	-3.91	111.02	123.22
9	j	103	A1EFU	C10-C11-C12	-3.90	111.06	123.22
9	F	104	A1EFU	C23-C22-C21	-3.89	110.19	121.98
9	B	102	A1EFU	C23-C22-C21	-3.88	110.23	121.98
9	v	103	A1EFU	C6-C7-C8	-3.88	111.11	123.22
9	R	101	A1EFU	CM5-C13-C12	3.88	124.19	118.08
9	J	103	A1EFU	C23-C22-C21	-3.88	110.24	121.98
9	E	102	A1EFU	CM5-C13-C12	3.88	124.19	118.08
9	q	101	A1EFU	CM4-C9-C8	3.87	124.18	118.08
8	V	101	BCL	CMB-C2B-C1B	-3.87	119.47	125.37
8	V	101	BCL	OBB-CAB-CBB	-3.87	111.15	119.73
9	j	103	A1EFU	CM5-C13-C12	3.87	124.18	118.08
8	G	102	BCL	CHD-C1D-ND	-3.87	120.90	124.45
8	M	402	BCL	CHD-C1D-ND	-3.87	120.90	124.45
8	2	103	BCL	CHB-C1B-NB	3.87	128.35	124.26
9	E	103	A1EFU	CM4-C9-C8	3.86	124.17	118.08
9	2	104	A1EFU	C6-C7-C8	-3.86	111.16	123.22
8	1	101	BCL	C2C-C3C-C4C	-3.86	95.55	101.34
8	i	101	BCL	CHB-C1B-NB	3.86	128.34	124.26
9	P	103	A1EFU	CM5-C13-C12	3.85	124.15	118.08
9	s	104	A1EFU	C10-C11-C12	-3.85	111.20	123.22
9	G	105	A1EFU	C6-C7-C8	-3.85	111.20	123.22
9	R	101	A1EFU	C10-C11-C12	-3.85	111.21	123.22
8	E	101	BCL	CHD-C1D-ND	-3.84	120.92	124.45
9	I	102	A1EFU	C21-C20-C19	-3.84	111.23	123.22
9	R	101	A1EFU	C23-C22-C21	-3.84	110.36	121.98
9	r	102	A1EFU	CM6-C18-C19	3.83	124.11	118.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	102	A1EFU	CM6-C18-C19	3.82	124.10	118.08
9	G	105	A1EFU	CM4-C9-C8	3.82	124.09	118.08
8	L	301	BCL	CHD-C1D-ND	-3.82	120.95	124.45
9	A	102	A1EFU	CM5-C13-C12	3.82	124.09	118.08
8	s	103	BCL	CHB-C1B-NB	3.81	128.29	124.26
9	E	102	A1EFU	C10-C11-C12	-3.81	111.32	123.22
9	T	101	A1EFU	CM5-C13-C12	3.81	124.08	118.08
9	E	103	A1EFU	CM6-C18-C19	3.81	124.08	118.08
9	s	105	A1EFU	C23-C22-C21	-3.81	110.44	121.98
9	D	105	A1EFU	CM4-C9-C8	3.81	124.08	118.08
9	B	102	A1EFU	CM5-C13-C12	3.81	124.08	118.08
9	k	101	A1EFU	C21-C20-C19	-3.81	111.34	123.22
8	e	101	BCL	OBB-CAB-CBB	-3.81	111.30	119.73
8	v	101	BCL	CHB-C1B-NB	3.81	128.29	124.26
9	G	106	A1EFU	C6-C7-C8	-3.80	111.34	123.22
9	s	104	A1EFU	CM5-C13-C12	3.80	124.07	118.08
9	E	102	A1EFU	CM6-C18-C19	3.80	124.07	118.08
8	n	101	BCL	CHD-C1D-ND	-3.80	120.96	124.45
8	k	102	BCL	CHB-C1B-NB	3.80	128.28	124.26
8	L	301	BCL	CHB-C1B-NB	3.79	128.27	124.26
9	v	102	A1EFU	CM4-C9-C8	3.79	124.05	118.08
8	L	304	BCL	CHD-C1D-ND	-3.79	120.97	124.45
9	s	101	A1EFU	CM6-C18-C19	3.79	124.05	118.08
9	J	102	A1EFU	C6-C7-C8	-3.79	111.40	123.22
8	a	101	BCL	CHB-C1B-NB	3.79	128.27	124.26
8	D	101	BCL	CHD-C1D-ND	-3.78	120.98	124.45
8	L	301	BCL	C2A-C3A-C4A	-3.78	95.76	101.87
9	I	102	A1EFU	C6-C7-C8	-3.78	111.42	123.22
8	L	301	BCL	OBB-CAB-CBB	-3.78	111.36	119.73
8	s	102	BCL	C2B-C1B-NB	-3.78	107.70	110.23
9	q	101	A1EFU	C6-C7-C8	-3.77	111.45	123.22
9	B	103	A1EFU	C23-C22-C21	-3.77	110.57	121.98
8	j	102	BCL	OBB-CAB-CBB	-3.77	111.38	119.73
9	E	103	A1EFU	CM5-C13-C12	3.77	124.01	118.08
9	B	102	A1EFU	C10-C11-C12	-3.76	111.48	123.22
8	a	101	BCL	OBB-CAB-CBB	-3.76	111.40	119.73
9	R	101	A1EFU	CM4-C9-C8	3.76	124.00	118.08
9	2	101	A1EFU	CM4-C9-C8	3.76	124.00	118.08
8	b	101	BCL	CHB-C1B-NB	3.76	128.23	124.26
8	F	101	BCL	CHB-C1B-NB	3.76	128.23	124.26
8	F	101	BCL	OBB-CAB-CBB	-3.76	111.41	119.73
9	G	106	A1EFU	C10-C11-C12	-3.76	111.50	123.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	q	102	BCL	OBB-CAB-CBB	-3.75	111.41	119.73
8	G	101	BCL	OBB-CAB-CBB	-3.75	111.41	119.73
9	I	102	A1EFU	CM4-C9-C8	3.75	123.99	118.08
9	E	103	A1EFU	C6-C7-C8	-3.75	111.50	123.22
8	b	101	BCL	OBB-CAB-CBB	-3.75	111.42	119.73
8	L	304	BCL	OBB-CAB-CBB	-3.75	111.42	119.73
8	I	101	BCL	OBB-CAB-CBB	-3.75	111.43	119.73
8	M	402	BCL	OBB-CAB-CBB	-3.74	111.43	119.73
9	f	101	A1EFU	CM4-C9-C8	3.74	123.97	118.08
9	s	101	A1EFU	CM5-C13-C12	3.74	123.97	118.08
9	B	103	A1EFU	C6-C7-C8	-3.74	111.55	123.22
8	s	103	BCL	OBB-CAB-CBB	-3.73	111.45	119.73
9	a	102	A1EFU	C10-C11-C12	-3.73	111.56	123.22
9	G	106	A1EFU	CM5-C13-C12	3.73	123.96	118.08
8	M	402	BCL	C1C-NC-C4C	-3.73	105.03	106.71
8	k	102	BCL	OBB-CAB-CBB	-3.73	111.46	119.73
9	v	102	A1EFU	C23-C22-C21	-3.73	110.68	121.98
8	e	101	BCL	CHB-C1B-NB	3.73	128.21	124.26
9	j	101	A1EFU	CM5-C13-C12	3.73	123.95	118.08
8	P	101	BCL	OBB-CAB-CBB	-3.73	111.47	119.73
9	2	102	A1EFU	CM3-C5-C4	3.73	123.95	118.08
9	p	101	A1EFU	CM6-C18-C19	3.73	123.95	118.08
9	P	103	A1EFU	C10-C11-C12	-3.72	111.59	123.22
8	K	101	BCL	CHD-C1D-ND	-3.72	121.03	124.45
9	v	103	A1EFU	CM5-C13-C12	3.72	123.94	118.08
8	j	102	BCL	CHB-C1B-NB	3.72	128.19	124.26
8	G	101	BCL	CHB-C1B-NB	3.72	128.19	124.26
9	v	102	A1EFU	C6-C7-C8	-3.72	111.61	123.22
9	k	101	A1EFU	CM4-C9-C8	3.72	123.94	118.08
9	I	102	A1EFU	CM5-C13-C12	3.72	123.94	118.08
8	v	101	BCL	OBB-CAB-CBB	-3.72	111.49	119.73
8	D	101	BCL	C1C-NC-C4C	-3.71	105.04	106.71
8	N	101	BCL	OBB-CAB-CBB	-3.71	111.50	119.73
9	r	102	A1EFU	C23-C22-C21	-3.71	110.74	121.98
8	R	102	BCL	OBB-CAB-CBB	-3.71	111.51	119.73
9	B	103	A1EFU	CM5-C13-C12	3.70	123.91	118.08
8	n	101	BCL	C16-C15-C13	-3.70	103.95	115.92
9	v	102	A1EFU	CM6-C18-C19	3.70	123.91	118.08
9	E	102	A1EFU	C21-C20-C19	-3.70	111.66	123.22
9	K	102	A1EFU	CM4-C9-C8	3.70	123.91	118.08
8	l	101	BCL	OBB-CAB-CBB	-3.70	111.53	119.73
8	B	101	BCL	CHD-C1D-ND	-3.70	121.06	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	q	102	BCL	CHB-C1B-NB	3.70	128.17	124.26
9	D	105	A1EFU	C21-C20-C19	-3.69	111.69	123.22
8	G	102	BCL	OBB-CAB-CBB	-3.69	111.54	119.73
9	p	101	A1EFU	C10-C11-C12	-3.69	111.69	123.22
9	v	103	A1EFU	CM6-C18-C19	3.69	123.89	118.08
8	i	101	BCL	OBB-CAB-CBB	-3.69	111.55	119.73
9	J	102	A1EFU	CM4-C9-C8	3.68	123.88	118.08
8	r	101	BCL	OBB-CAB-CBB	-3.68	111.57	119.73
8	S	101	BCL	OBB-CAB-CBB	-3.68	111.58	119.73
9	K	102	A1EFU	CM5-C13-C12	3.68	123.87	118.08
8	J	101	BCL	OBB-CAB-CBB	-3.68	111.58	119.73
8	2	103	BCL	CHD-C1D-ND	-3.67	121.08	124.45
9	K	102	A1EFU	C6-C7-C8	-3.67	111.76	123.22
9	s	105	A1EFU	CM6-C18-C19	3.67	123.86	118.08
9	J	103	A1EFU	CM4-C9-C8	3.67	123.86	118.08
8	n	101	BCL	OBB-CAB-CBB	-3.67	111.60	119.73
9	T	101	A1EFU	CM6-C18-C19	3.67	123.86	118.08
8	R	102	BCL	CHD-C1D-ND	-3.67	121.08	124.45
8	K	101	BCL	OBB-CAB-CBB	-3.67	111.60	119.73
8	L	304	BCL	CHB-C1B-NB	3.67	128.14	124.26
9	K	102	A1EFU	C23-C22-C21	-3.67	110.88	121.98
9	2	101	A1EFU	C21-C20-C19	-3.67	111.78	123.22
8	Q	101	BCL	OBB-CAB-CBB	-3.67	111.61	119.73
8	E	101	BCL	OBB-CAB-CBB	-3.66	111.62	119.73
9	v	103	A1EFU	C10-C11-C12	-3.66	111.80	123.22
9	J	103	A1EFU	CM6-C18-C19	3.66	123.84	118.08
8	2	103	BCL	OBB-CAB-CBB	-3.66	111.62	119.73
8	M	402	BCL	CHB-C1B-NB	3.66	128.13	124.26
8	F	102	BCL	OBB-CAB-CBB	-3.66	111.63	119.73
8	B	101	BCL	OBB-CAB-CBB	-3.66	111.63	119.73
8	e	101	BCL	CHD-C1D-ND	-3.65	121.10	124.45
8	t	101	BCL	CHA-C1A-NA	-3.65	118.03	126.40
9	2	102	A1EFU	C6-C7-C8	-3.65	111.83	123.22
9	s	104	A1EFU	CM4-C9-C8	3.65	123.82	118.08
8	I	101	BCL	CHB-C1B-NB	3.64	128.12	124.26
9	D	105	A1EFU	C10-C11-C12	-3.64	111.87	123.22
9	f	101	A1EFU	CM6-C18-C19	3.64	123.81	118.08
8	B	101	BCL	C1C-NC-C4C	-3.63	105.07	106.71
8	a	101	BCL	CHD-C1D-ND	-3.63	121.11	124.45
9	p	101	A1EFU	C6-C7-C8	-3.63	111.88	123.22
9	v	102	A1EFU	CM5-C13-C12	3.63	123.80	118.08
8	J	101	BCL	CHB-C1B-NB	3.63	128.10	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	P	102	BCL	OBB-CAB-CBB	-3.63	111.69	119.73
8	M	403	BCL	OBB-CAB-CBB	-3.63	111.69	119.73
9	T	101	A1EFU	C23-C22-C21	-3.63	110.99	121.98
9	J	102	A1EFU	CM3-C5-C4	3.63	123.79	118.08
8	F	102	BCL	CHB-C1B-NB	3.63	128.10	124.26
9	q	101	A1EFU	C23-C22-C21	-3.63	111.00	121.98
8	A	101	BCL	OBB-CAB-CBB	-3.63	111.69	119.73
9	2	104	A1EFU	CM4-C9-C8	3.63	123.79	118.08
9	p	101	A1EFU	CM4-C9-C8	3.63	123.79	118.08
9	G	106	A1EFU	C21-C20-C19	-3.63	111.90	123.22
9	s	105	A1EFU	CM5-C13-C12	3.62	123.79	118.08
8	E	101	BCL	CHB-C1B-NB	3.62	128.09	124.26
9	s	101	A1EFU	C23-C22-C21	-3.62	111.01	121.98
9	2	101	A1EFU	C6-C7-C8	-3.62	111.91	123.22
9	T	101	A1EFU	C10-C11-C12	-3.62	111.92	123.22
9	p	101	A1EFU	CM5-C13-C12	3.61	123.77	118.08
9	a	102	A1EFU	C21-C20-C19	-3.61	111.94	123.22
8	r	101	BCL	CHD-C1D-ND	-3.61	121.14	124.45
8	Q	101	BCL	CHD-C1D-ND	-3.61	121.14	124.45
9	s	105	A1EFU	C10-C11-C12	-3.61	111.97	123.22
9	G	106	A1EFU	CM4-C9-C8	3.60	123.75	118.08
9	M	407	A1EFU	CM4-C9-C8	3.60	123.75	118.08
9	M	407	A1EFU	C10-C11-C12	-3.60	111.98	123.22
9	M	407	A1EFU	CM5-C13-C12	3.60	123.74	118.08
8	D	101	BCL	OBB-CAB-CBB	-3.60	111.76	119.73
9	A	102	A1EFU	C10-C11-C12	-3.60	112.00	123.22
8	K	101	BCL	CHB-C1B-NB	3.60	128.06	124.26
8	q	102	BCL	CHD-C1D-ND	-3.59	121.15	124.45
9	J	102	A1EFU	CM5-C13-C12	3.59	123.74	118.08
9	G	105	A1EFU	CM5-C13-C12	3.59	123.74	118.08
9	A	102	A1EFU	C23-C22-C21	-3.59	111.11	121.98
9	B	103	A1EFU	CM6-C18-C19	3.59	123.73	118.08
8	j	102	BCL	CHD-C1D-ND	-3.59	121.15	124.45
9	I	102	A1EFU	C10-C11-C12	-3.58	112.04	123.22
8	I	101	BCL	CHD-C1D-ND	-3.58	121.17	124.45
8	S	101	BCL	CHB-C1B-NB	3.58	128.04	124.26
9	F	104	A1EFU	CM6-C18-C19	3.58	123.71	118.08
8	R	102	BCL	CHB-C1B-NB	3.58	128.04	124.26
8	P	102	BCL	CMB-C2B-C1B	-3.57	119.93	125.37
8	d	101	BCL	CHD-C1D-ND	-3.57	121.17	124.45
8	2	103	BCL	C16-C15-C13	-3.57	104.38	115.92
9	J	103	A1EFU	C10-C11-C12	-3.57	112.09	123.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	J	101	BCL	CHD-C1D-ND	-3.57	121.18	124.45
8	i	101	BCL	CHD-C1D-ND	-3.56	121.18	124.45
8	P	101	BCL	CHD-C1D-ND	-3.56	121.19	124.45
9	D	105	A1EFU	CM5-C13-C12	3.55	123.68	118.08
9	f	101	A1EFU	C23-C22-C21	-3.55	111.23	121.98
9	M	407	A1EFU	C6-C7-C8	-3.55	112.14	123.22
8	e	101	BCL	C1C-NC-C4C	-3.55	105.11	106.71
9	v	103	A1EFU	C23-C22-C21	-3.55	111.24	121.98
8	G	102	BCL	CHB-C1B-NB	3.54	128.01	124.26
8	s	102	BCL	C16-C15-C13	-3.54	104.47	115.92
8	A	101	BCL	CHD-C1D-ND	-3.54	121.20	124.45
9	R	101	A1EFU	CM6-C18-C19	3.54	123.65	118.08
9	P	103	A1EFU	C21-C20-C19	-3.53	112.19	123.22
9	F	104	A1EFU	C21-C20-C19	-3.53	112.19	123.22
8	r	101	BCL	CMB-C2B-C1B	-3.53	119.99	125.37
8	N	101	BCL	CHD-C1D-ND	-3.53	121.21	124.45
9	J	103	A1EFU	C6-C7-C8	-3.53	112.22	123.22
8	G	101	BCL	CHD-C1D-ND	-3.52	121.22	124.45
8	M	403	BCL	CHB-C1B-NB	3.52	127.98	124.26
9	k	101	A1EFU	CM6-C18-C19	3.52	123.62	118.08
9	N	102	A1EFU	CM3-C5-C4	3.52	123.62	118.08
9	R	101	A1EFU	C6-C7-C8	-3.52	112.25	123.22
9	j	101	A1EFU	CM6-C18-C19	3.51	123.61	118.08
8	l	101	BCL	CHB-C1B-NB	3.51	127.98	124.26
9	s	104	A1EFU	CM3-C5-C6	-3.51	118.00	122.92
9	R	101	A1EFU	C21-C20-C19	-3.51	112.25	123.22
9	N	102	A1EFU	C21-C20-C19	-3.51	112.27	123.22
8	b	101	BCL	CHD-C1D-ND	-3.50	121.23	124.45
8	v	101	BCL	CHD-C1D-ND	-3.50	121.24	124.45
9	N	102	A1EFU	CM5-C13-C12	3.50	123.59	118.08
9	G	105	A1EFU	C23-C22-C21	-3.50	111.39	121.98
9	E	103	A1EFU	C21-C20-C19	-3.49	112.31	123.22
9	K	102	A1EFU	C21-C20-C19	-3.49	112.32	123.22
9	M	407	A1EFU	C23-C22-C21	-3.49	111.42	121.98
8	k	102	BCL	CHD-C1D-ND	-3.49	121.25	124.45
9	s	105	A1EFU	C21-C20-C19	-3.49	112.33	123.22
8	a	101	BCL	C16-C15-C13	-3.49	104.65	115.92
8	D	101	BCL	CHB-C1B-NB	3.49	127.95	124.26
9	p	101	A1EFU	C23-C22-C21	-3.49	111.42	121.98
8	L	304	BCL	C16-C15-C13	-3.49	104.65	115.92
9	J	102	A1EFU	C23-C22-C21	-3.48	111.44	121.98
9	v	103	A1EFU	CM4-C9-C8	3.48	123.56	118.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	P	102	BCL	CHD-C1D-ND	-3.48	121.26	124.45
9	B	102	A1EFU	CM6-C18-C19	3.47	123.55	118.08
9	2	104	A1EFU	C10-C11-C12	-3.47	112.40	123.22
9	s	104	A1EFU	CM3-C5-C4	3.46	123.54	118.08
9	G	105	A1EFU	CM6-C18-C19	3.46	123.53	118.08
9	B	103	A1EFU	C21-C20-C19	-3.46	112.42	123.22
9	2	102	A1EFU	CM4-C9-C8	3.46	123.53	118.08
9	B	102	A1EFU	C21-C20-C19	-3.46	112.43	123.22
9	2	104	A1EFU	CM5-C13-C12	3.46	123.52	118.08
8	L	301	BCL	C1C-NC-C4C	-3.46	105.15	106.71
9	f	101	A1EFU	C10-C11-C12	-3.45	112.44	123.22
8	N	101	BCL	C2C-C3C-C4C	-3.45	96.17	101.34
8	N	101	BCL	CHB-C1B-NB	3.44	127.90	124.26
8	B	101	BCL	CHB-C1B-NB	3.44	127.89	124.26
9	k	101	A1EFU	C6-C7-C8	-3.43	112.50	123.22
8	s	102	BCL	CMB-C2B-C1B	-3.43	120.15	125.37
8	A	101	BCL	CMB-C2B-C1B	-3.42	120.15	125.37
9	k	101	A1EFU	CM5-C13-C12	3.42	123.47	118.08
8	s	102	BCL	CHD-C1D-ND	-3.42	121.31	124.45
8	E	101	BCL	CHA-C1A-NA	-3.41	118.58	126.40
8	l	101	BCL	CHD-C1D-ND	-3.41	121.32	124.45
8	n	101	BCL	CMB-C2B-C1B	-3.41	120.17	125.37
8	s	103	BCL	CHD-C1D-ND	-3.41	121.32	124.45
8	M	403	BCL	C16-C15-C13	-3.40	104.92	115.92
8	F	101	BCL	CHD-C1D-ND	-3.40	121.33	124.45
9	v	102	A1EFU	C10-C11-C12	-3.40	112.61	123.22
8	d	101	BCL	OBB-CAB-CBB	-3.40	112.20	119.73
9	s	104	A1EFU	C23-C22-C21	-3.40	111.69	121.98
8	r	101	BCL	C4A-NA-C1A	-3.40	105.18	106.71
8	r	101	BCL	C16-C15-C13	-3.40	104.94	115.92
8	k	102	BCL	C16-C15-C13	-3.39	104.95	115.92
9	2	104	A1EFU	C23-C22-C21	-3.39	111.71	121.98
8	P	101	BCL	CHB-C1B-NB	3.39	127.85	124.26
8	Q	101	BCL	C16-C15-C13	-3.39	104.97	115.92
9	P	103	A1EFU	CM6-C18-C19	3.39	123.41	118.08
8	Q	101	BCL	CHB-C1B-NB	3.38	127.84	124.26
9	A	102	A1EFU	C21-C20-C19	-3.38	112.67	123.22
9	f	101	A1EFU	CM5-C13-C12	3.38	123.40	118.08
8	A	101	BCL	C16-C15-C13	-3.37	105.03	115.92
8	q	102	BCL	C16-C15-C13	-3.36	105.05	115.92
9	j	101	A1EFU	C21-C20-C19	-3.36	112.72	123.22
9	J	103	A1EFU	C21-C20-C19	-3.36	112.73	123.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	Q	101	BCL	C1C-NC-C4C	-3.36	105.20	106.71
9	J	102	A1EFU	C10-C11-C12	-3.35	112.76	123.22
8	t	101	BCL	C16-C15-C13	-3.35	105.10	115.92
8	d	101	BCL	CHA-C1A-NA	-3.34	118.74	126.40
9	K	102	A1EFU	C10-C11-C12	-3.34	112.79	123.22
8	V	101	BCL	CHD-C1D-ND	-3.34	121.39	124.45
9	j	101	A1EFU	C6-C7-C8	-3.34	112.81	123.22
8	I	101	BCL	C16-C15-C13	-3.33	105.15	115.92
9	q	101	A1EFU	C21-C20-C19	-3.32	112.84	123.22
9	D	104	A1EFU	C21-C20-C19	-3.32	112.84	123.22
9	N	102	A1EFU	CM4-C9-C8	3.31	123.29	118.08
8	s	102	BCL	CBB-CAB-C3B	3.31	127.49	120.43
8	s	103	BCL	C16-C15-C13	-3.30	105.24	115.92
11	L	306	LMT	C3'-C4'-C5'	-3.30	105.44	110.30
8	P	101	BCL	C16-C15-C13	-3.30	105.25	115.92
8	G	101	BCL	C4A-NA-C1A	-3.30	105.22	106.71
9	T	101	A1EFU	C21-C20-C19	-3.29	112.94	123.22
8	i	101	BCL	C16-C15-C13	-3.29	105.28	115.92
8	v	101	BCL	C1C-NC-C4C	-3.29	105.23	106.71
8	R	102	BCL	C16-C15-C13	-3.29	105.29	115.92
8	F	102	BCL	CHA-C1A-NA	-3.27	118.90	126.40
9	r	102	A1EFU	C21-C20-C19	-3.27	113.01	123.22
9	D	104	A1EFU	CM6-C18-C19	3.27	123.22	118.08
8	k	102	BCL	CHA-C1A-NA	-3.27	118.92	126.40
8	s	102	BCL	C2C-C3C-C4C	-3.27	96.45	101.34
9	j	101	A1EFU	C10-C11-C12	-3.26	113.05	123.22
8	M	402	BCL	CHA-C1A-NA	-3.25	118.96	126.40
9	2	102	A1EFU	C21-C20-C19	-3.25	113.08	123.22
8	P	101	BCL	CHA-C1A-NA	-3.25	118.96	126.40
9	2	101	A1EFU	C10-C11-C12	-3.25	113.09	123.22
8	P	101	BCL	C1C-NC-C4C	-3.25	105.25	106.71
8	E	101	BCL	C2C-C3C-C4C	-3.24	96.48	101.34
8	S	101	BCL	C16-C15-C13	-3.24	105.46	115.92
8	1	101	BCL	CHA-C1A-NA	-3.23	119.00	126.40
8	b	101	BCL	CHA-C1A-NA	-3.23	119.00	126.40
8	d	101	BCL	O2A-CGA-O1A	-3.23	115.45	123.59
9	N	102	A1EFU	C6-C7-C8	-3.22	113.16	123.22
8	J	101	BCL	CHA-C1A-NA	-3.22	119.02	126.40
14	M	408	BPH	C2D-C1D-ND	-3.22	107.31	109.53
8	I	101	BCL	CBB-CAB-C3B	3.21	127.30	120.43
8	M	403	BCL	C4D-CHA-C1A	3.21	125.16	121.25
8	j	102	BCL	CHA-C1A-NA	-3.20	119.06	126.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	F	101	BCL	C16-C15-C13	-3.20	105.57	115.92
8	s	102	BCL	CHB-C1B-NB	3.20	127.65	124.26
8	G	101	BCL	C16-C15-C13	-3.20	105.57	115.92
8	M	402	BCL	CBB-CAB-C3B	3.19	127.25	120.43
8	N	101	BCL	CHA-C1A-NA	-3.19	119.08	126.40
8	G	102	BCL	CHA-C1A-NA	-3.19	119.09	126.40
8	Q	101	BCL	CGD-CBD-CAD	-3.19	100.41	110.73
9	q	101	A1EFU	CM6-C18-C19	3.19	123.10	118.08
9	s	104	A1EFU	C6-C7-C8	-3.19	113.28	123.22
8	M	402	BCL	C7-C6-C5	-3.18	104.72	113.36
8	V	101	BCL	C1C-NC-C4C	-3.18	105.28	106.71
8	I	101	BCL	CHA-C1A-NA	-3.18	119.12	126.40
8	G	102	BCL	CBB-CAB-C3B	3.18	127.22	120.43
8	A	101	BCL	C2B-C1B-NB	-3.17	108.11	110.23
8	L	301	BCL	CBB-CAB-C3B	3.17	127.21	120.43
9	2	101	A1EFU	CM5-C13-C12	3.17	123.06	118.08
9	v	103	A1EFU	C21-C20-C19	-3.16	113.34	123.22
8	s	103	BCL	CHA-C1A-NA	-3.16	119.15	126.40
8	K	101	BCL	CBB-CAB-C3B	3.16	127.19	120.43
9	v	102	A1EFU	C21-C20-C19	-3.16	113.35	123.22
8	q	102	BCL	CBB-CAB-C3B	3.16	127.17	120.43
9	f	101	A1EFU	C21-C20-C19	-3.16	113.36	123.22
8	R	102	BCL	CHA-C1A-NA	-3.16	119.17	126.40
8	a	101	BCL	CHA-C1A-NA	-3.15	119.18	126.40
8	F	102	BCL	CBB-CAB-C3B	3.15	127.16	120.43
9	J	102	A1EFU	CM6-C18-C19	3.15	123.04	118.08
8	Q	101	BCL	CBB-CAB-C3B	3.15	127.15	120.43
8	k	102	BCL	CBB-CAB-C3B	3.14	127.15	120.43
8	F	102	BCL	O2A-CGA-O1A	-3.14	115.66	123.59
8	M	403	BCL	O2A-CGA-O1A	-3.14	115.67	123.59
8	B	101	BCL	CBB-CAB-C3B	3.14	127.14	120.43
8	e	101	BCL	CHA-C1A-NA	-3.14	119.22	126.40
8	N	101	BCL	CBB-CAB-C3B	3.13	127.12	120.43
8	K	101	BCL	CHA-C1A-NA	-3.13	119.22	126.40
8	1	101	BCL	CBB-CAB-C3B	3.13	127.12	120.43
8	G	102	BCL	C7-C6-C5	-3.13	104.85	113.36
9	2	102	A1EFU	CM6-C18-C19	3.13	123.01	118.08
8	D	101	BCL	C16-C15-C13	-3.13	105.80	115.92
8	S	101	BCL	CBB-CAB-C3B	3.13	127.11	120.43
8	P	102	BCL	C16-C15-C13	-3.13	105.81	115.92
8	V	101	BCL	C16-C15-C13	-3.13	105.81	115.92
14	L	302	BPH	C2D-C1D-ND	-3.12	107.37	109.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	P	101	BCL	C4D-CHA-C1A	3.12	125.05	121.25
8	R	102	BCL	CBB-CAB-C3B	3.12	127.10	120.43
8	1	101	BCL	C7-C6-C5	-3.12	104.89	113.36
8	J	101	BCL	CBB-CAB-C3B	3.12	127.08	120.43
8	V	101	BCL	CBB-CAB-C3B	3.11	127.08	120.43
8	v	101	BCL	CHA-C1A-NA	-3.11	119.28	126.40
8	G	101	BCL	CBB-CAB-C3B	3.11	127.07	120.43
8	J	101	BCL	C16-C15-C13	-3.11	105.87	115.92
8	A	101	BCL	CHA-C1A-NA	-3.11	119.28	126.40
8	F	101	BCL	CBB-CAB-C3B	3.11	127.07	120.43
8	E	101	BCL	CBB-CAB-C3B	3.11	127.07	120.43
8	s	103	BCL	CBB-CAB-C3B	3.11	127.07	120.43
8	i	101	BCL	CBB-CAB-C3B	3.10	127.06	120.43
8	S	101	BCL	C4D-CHA-C1A	3.10	125.02	121.25
8	V	101	BCL	CHA-C1A-NA	-3.10	119.30	126.40
8	Q	101	BCL	CHA-C1A-NA	-3.10	119.30	126.40
8	E	101	BCL	C16-C15-C13	-3.10	105.90	115.92
8	a	101	BCL	C11-C10-C8	-3.10	105.91	115.92
8	e	101	BCL	CBB-CAB-C3B	3.10	127.04	120.43
9	M	407	A1EFU	CM6-C18-C19	3.09	122.95	118.08
8	n	101	BCL	CHA-C1A-NA	-3.09	119.31	126.40
8	D	101	BCL	C4D-CHA-C1A	3.09	125.01	121.25
8	v	101	BCL	O2A-CGA-O1A	-3.09	115.79	123.59
8	v	101	BCL	CBB-CAB-C3B	3.09	127.03	120.43
8	M	403	BCL	CBB-CAB-C3B	3.09	127.03	120.43
8	P	102	BCL	C2B-C1B-NB	-3.09	108.16	110.23
9	M	407	A1EFU	C21-C20-C19	-3.09	113.58	123.22
8	j	102	BCL	C2B-C1B-NB	-3.09	108.16	110.23
8	D	101	BCL	CBB-CAB-C3B	3.08	127.02	120.43
8	L	304	BCL	CBB-CAB-C3B	3.08	127.02	120.43
8	P	101	BCL	C7-C6-C5	-3.08	104.98	113.36
8	J	101	BCL	C11-C10-C8	-3.08	105.95	115.92
8	1	101	BCL	C11-C10-C8	-3.08	105.96	115.92
8	L	304	BCL	C4A-NA-C1A	-3.08	105.32	106.71
8	2	103	BCL	CBB-CAB-C3B	3.08	127.00	120.43
8	V	101	BCL	C7-C6-C5	-3.07	105.01	113.36
8	a	101	BCL	C1C-NC-C4C	-3.07	105.32	106.71
8	1	101	BCL	C4D-CHA-C1A	3.07	124.99	121.25
16	C	403	HEC	O1D-CGD-CBD	-3.07	113.21	123.08
9	s	101	A1EFU	C21-C20-C19	-3.07	113.64	123.22
8	N	101	BCL	C7-C6-C5	-3.07	105.02	113.36
11	L	306	LMT	C1'-O5'-C5'	-3.07	108.39	113.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	P	101	BCL	CBB-CAB-C3B	3.07	126.98	120.43
8	B	101	BCL	C16-C15-C13	-3.07	106.00	115.92
8	e	101	BCL	C2B-C1B-NB	-3.07	108.18	110.23
8	b	101	BCL	CBB-CAB-C3B	3.06	126.96	120.43
8	M	402	BCL	C16-C15-C13	-3.05	106.05	115.92
8	d	101	BCL	C11-C10-C8	-3.05	106.05	115.92
9	j	103	A1EFU	C21-C20-C19	-3.05	113.69	123.22
8	B	101	BCL	C11-C10-C8	-3.05	106.06	115.92
8	a	101	BCL	CBB-CAB-C3B	3.05	126.94	120.43
8	q	102	BCL	CHA-C1A-NA	-3.05	119.42	126.40
8	L	304	BCL	C11-C10-C8	-3.05	106.06	115.92
8	P	102	BCL	C4A-NA-C1A	-3.05	105.34	106.71
8	F	102	BCL	C16-C15-C13	-3.05	106.07	115.92
8	j	102	BCL	CBB-CAB-C3B	3.04	126.93	120.43
8	P	102	BCL	O2A-CGA-O1A	-3.04	115.91	123.59
8	V	101	BCL	O2A-CGA-O1A	-3.04	115.92	123.59
9	N	102	A1EFU	C10-C11-C12	-3.04	113.73	123.22
8	L	301	BCL	O2A-CGA-O1A	-3.04	115.93	123.59
8	K	101	BCL	C7-C6-C5	-3.04	105.11	113.36
8	G	102	BCL	C16-C15-C13	-3.03	106.12	115.92
8	l	101	BCL	C16-C15-C13	-3.03	106.12	115.92
8	a	101	BCL	C4D-CHA-C1A	3.03	124.94	121.25
8	j	102	BCL	C16-C15-C13	-3.03	106.13	115.92
9	j	103	A1EFU	CM6-C18-C19	3.03	122.85	118.08
8	R	102	BCL	C7-C6-C5	-3.02	105.14	113.36
8	D	101	BCL	C7-C6-C5	-3.02	105.15	113.36
8	r	101	BCL	C1C-NC-C4C	-3.02	105.35	106.71
14	M	408	BPH	C2B-C1B-NB	-3.01	107.45	109.53
8	A	101	BCL	C11-C10-C8	-3.01	106.19	115.92
8	D	101	BCL	CHA-C1A-NA	-3.01	119.51	126.40
8	i	101	BCL	CHA-C1A-NA	-3.01	119.52	126.40
8	2	103	BCL	CHA-C1A-NA	-3.00	119.53	126.40
8	L	304	BCL	CHA-C1A-NA	-3.00	119.53	126.40
8	b	101	BCL	C11-C10-C8	-3.00	106.23	115.92
8	I	101	BCL	C7-C6-C5	-2.99	105.23	113.36
8	s	102	BCL	C7-C6-C5	-2.99	105.23	113.36
9	N	102	A1EFU	CM6-C18-C19	2.99	122.79	118.08
8	v	101	BCL	C16-C15-C13	-2.98	106.27	115.92
8	d	101	BCL	C16-C15-C13	-2.98	106.27	115.92
8	q	102	BCL	C11-C10-C8	-2.98	106.28	115.92
8	P	102	BCL	C11-C10-C8	-2.98	106.29	115.92
8	V	101	BCL	C4A-NA-C1A	-2.98	105.37	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	K	101	BCL	C4D-CHA-C1A	2.98	124.87	121.25
8	n	101	BCL	C7-C6-C5	-2.97	105.28	113.36
8	B	101	BCL	CHA-C1A-NA	-2.97	119.59	126.40
8	S	101	BCL	CHA-C1A-NA	-2.97	119.60	126.40
8	r	101	BCL	CHA-C1A-NA	-2.97	119.60	126.40
8	B	101	BCL	C7-C6-C5	-2.97	105.30	113.36
9	s	104	A1EFU	C21-C20-C19	-2.97	113.96	123.22
8	r	101	BCL	C2B-C1B-NB	-2.97	108.24	110.23
8	N	101	BCL	C16-C15-C13	-2.96	106.34	115.92
8	L	301	BCL	C16-C15-C13	-2.96	106.36	115.92
8	k	102	BCL	C1C-NC-C4C	-2.96	105.38	106.71
8	2	103	BCL	C11-C10-C8	-2.96	106.37	115.92
8	E	101	BCL	C2B-C1B-NB	-2.95	108.25	110.23
8	r	101	BCL	O2A-CGA-O1A	-2.95	116.14	123.59
8	i	101	BCL	C4A-NA-C1A	-2.95	105.38	106.71
8	L	301	BCL	C11-C10-C8	-2.95	106.39	115.92
8	P	102	BCL	C1C-NC-C4C	-2.95	105.38	106.71
9	J	102	A1EFU	C21-C20-C19	-2.95	114.02	123.22
8	J	101	BCL	O2A-CGA-O1A	-2.95	116.16	123.59
8	L	301	BCL	C3D-C2D-C1D	-2.94	101.81	105.83
8	M	402	BCL	CMC-C2C-C3C	-2.94	101.96	113.83
8	L	304	BCL	C4D-CHA-C1A	2.94	124.83	121.25
8	J	101	BCL	C7-C6-C5	-2.94	105.39	113.36
8	F	102	BCL	C7-C6-C5	-2.93	105.39	113.36
9	G	105	A1EFU	C21-C20-C19	-2.93	114.07	123.22
8	I	101	BCL	C2B-C1B-NB	-2.92	108.28	110.23
8	I	101	BCL	C3D-C2D-C1D	-2.92	101.85	105.83
8	K	101	BCL	C16-C15-C13	-2.92	106.49	115.92
8	a	101	BCL	C4A-NA-C1A	-2.92	105.39	106.71
8	v	101	BCL	C7-C6-C5	-2.92	105.44	113.36
8	G	101	BCL	C7-C6-C5	-2.91	105.44	113.36
8	B	101	BCL	O2A-CGA-O1A	-2.91	116.24	123.59
8	n	101	BCL	C4D-CHA-C1A	2.91	124.79	121.25
8	S	101	BCL	C1C-NC-C4C	-2.91	105.40	106.71
8	S	101	BCL	C3D-C2D-C1D	-2.91	101.86	105.83
8	s	102	BCL	CHA-C1A-NA	-2.91	119.74	126.40
8	F	101	BCL	C11-C10-C8	-2.90	106.54	115.92
8	v	101	BCL	C4D-CHA-C1A	2.90	124.78	121.25
8	Q	101	BCL	C7-C6-C5	-2.90	105.48	113.36
8	N	101	BCL	C11-C10-C8	-2.90	106.55	115.92
8	b	101	BCL	C11-C12-C13	-2.90	106.55	115.92
8	s	102	BCL	C11-C10-C8	-2.90	106.56	115.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	2	103	BCL	O2A-CGA-O1A	-2.89	116.29	123.59
8	q	102	BCL	C1C-NC-C4C	-2.89	105.41	106.71
8	M	402	BCL	C11-C10-C8	-2.89	106.57	115.92
8	S	101	BCL	O2A-CGA-O1A	-2.89	116.30	123.59
8	P	101	BCL	C11-C10-C8	-2.89	106.59	115.92
8	n	101	BCL	C2B-C1B-NB	-2.89	108.30	110.23
8	K	101	BCL	C2B-C1B-NB	-2.89	108.30	110.23
8	j	102	BCL	O2A-CGA-O1A	-2.88	116.31	123.59
8	j	102	BCL	C11-C10-C8	-2.88	106.61	115.92
8	k	102	BCL	C7-C6-C5	-2.88	105.53	113.36
8	L	304	BCL	C2C-C3C-C4C	-2.88	97.03	101.34
9	K	102	A1EFU	CM6-C18-C19	2.88	122.61	118.08
8	F	101	BCL	C2B-C1B-NB	-2.88	108.30	110.23
8	n	101	BCL	CAB-C3B-C2B	-2.87	124.03	128.34
8	2	103	BCL	C3D-C2D-C1D	-2.87	101.91	105.83
8	a	101	BCL	O2A-CGA-O1A	-2.87	116.34	123.59
8	Q	101	BCL	C3D-C2D-C1D	-2.87	101.91	105.83
8	A	101	BCL	O2A-CGA-O1A	-2.87	116.34	123.59
8	L	301	BCL	CMC-C2C-C3C	-2.87	102.25	113.83
8	F	102	BCL	C4D-CHA-C1A	2.87	124.74	121.25
16	C	401	HEC	O1D-CGD-CBD	-2.87	113.87	123.08
8	J	101	BCL	C3D-C2D-C1D	-2.87	101.92	105.83
8	B	101	BCL	C3D-C2D-C1D	-2.87	101.92	105.83
8	e	101	BCL	C16-C15-C13	-2.86	106.66	115.92
8	N	101	BCL	O2A-CGA-O1A	-2.86	116.36	123.59
8	s	103	BCL	C2B-C1B-NB	-2.86	108.31	110.23
8	D	101	BCL	O2A-CGA-O1A	-2.86	116.37	123.59
8	d	101	BCL	C3D-C2D-C1D	-2.86	101.92	105.83
8	M	403	BCL	CHA-C1A-NA	-2.86	119.85	126.40
8	d	101	BCL	CHB-C1B-NB	2.86	127.28	124.26
8	E	101	BCL	C11-C10-C8	-2.86	106.68	115.92
16	C	402	HEC	O1D-CGD-CBD	-2.86	113.90	123.08
8	I	101	BCL	C2C-C3C-C4C	-2.86	97.06	101.34
8	R	102	BCL	O2A-CGA-O1A	-2.85	116.39	123.59
8	s	102	BCL	C3D-C2D-C1D	-2.85	101.94	105.83
8	q	102	BCL	C2B-C1B-NB	-2.85	108.32	110.23
8	G	102	BCL	C11-C10-C8	-2.85	106.72	115.92
8	r	101	BCL	C11-C10-C8	-2.85	106.72	115.92
9	2	102	A1EFU	CM5-C13-C12	2.85	122.56	118.08
8	r	101	BCL	CAB-C3B-C2B	-2.84	124.08	128.34
8	G	102	BCL	O2A-CGA-O1A	-2.84	116.42	123.59
8	A	101	BCL	C7-C6-C5	-2.84	105.64	113.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	301	BCL	CMA-C3A-C4A	-2.84	104.15	111.77
8	N	101	BCL	C4D-CHA-C1A	2.84	124.70	121.25
8	A	101	BCL	C1C-NC-C4C	-2.84	105.43	106.71
8	i	101	BCL	C2B-C1B-NB	-2.84	108.33	110.23
8	J	101	BCL	C4D-CHA-C1A	2.83	124.70	121.25
8	M	403	BCL	C7-C6-C5	-2.83	105.67	113.36
8	e	101	BCL	C4D-CHA-C1A	2.83	124.69	121.25
8	s	103	BCL	O2A-CGA-O1A	-2.83	116.45	123.59
8	P	102	BCL	CHA-C1A-NA	-2.83	119.93	126.40
8	k	102	BCL	C11-C10-C8	-2.83	106.79	115.92
8	K	101	BCL	C11-C10-C8	-2.83	106.79	115.92
8	K	101	BCL	C3D-C2D-C1D	-2.82	101.98	105.83
10	L	307	MW9	O1-C17-C16	2.82	120.75	111.91
8	I	101	BCL	C11-C12-C13	-2.82	106.81	115.92
8	i	101	BCL	C3D-C2D-C1D	-2.82	101.99	105.83
8	E	101	BCL	O2A-CGA-O1A	-2.82	116.48	123.59
8	M	403	BCL	C11-C10-C8	-2.82	106.82	115.92
8	l	101	BCL	O2A-CGA-O1A	-2.81	116.49	123.59
8	n	101	BCL	C11-C12-C13	-2.81	106.82	115.92
8	Q	101	BCL	C4D-CHA-C1A	2.81	124.67	121.25
8	A	101	BCL	C4D-CHA-C1A	2.81	124.67	121.25
8	A	101	BCL	CAB-C3B-C2B	-2.81	124.13	128.34
8	L	301	BCL	C11-C12-C13	-2.81	106.83	115.92
8	L	301	BCL	CHA-C1A-NA	-2.81	119.96	126.40
8	t	101	BCL	C2C-C3C-C4C	-2.81	97.13	101.34
8	t	101	BCL	CAB-C3B-C2B	-2.81	124.13	128.34
8	v	101	BCL	C3D-C2D-C1D	-2.81	102.00	105.83
8	F	101	BCL	CHA-C1A-NA	-2.81	119.97	126.40
8	F	101	BCL	O2A-CGA-O1A	-2.81	116.51	123.59
8	F	102	BCL	CMA-C3A-C4A	-2.80	104.23	111.77
8	i	101	BCL	C7-C6-C5	-2.80	105.74	113.36
8	D	101	BCL	CMA-C3A-C4A	-2.80	104.24	111.77
8	M	402	BCL	O2A-CGA-O1A	-2.80	116.52	123.59
8	R	102	BCL	C11-C10-C8	-2.80	106.87	115.92
8	D	101	BCL	C3D-C2D-C1D	-2.80	102.01	105.83
8	Q	101	BCL	C11-C10-C8	-2.80	106.88	115.92
8	s	103	BCL	C7-C6-C5	-2.80	105.77	113.36
8	L	304	BCL	C7-C6-C5	-2.80	105.77	113.36
11	H	302	LMT	C1'-O5'-C5'	-2.80	108.20	113.69
8	j	102	BCL	C7-C6-C5	-2.80	105.77	113.36
8	i	101	BCL	O2A-CGA-O1A	-2.79	116.54	123.59
8	b	101	BCL	C4D-CHA-C1A	2.79	124.65	121.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	s	102	BCL	O2A-CGA-O1A	-2.79	116.54	123.59
8	j	102	BCL	C3D-C2D-C1D	-2.79	102.02	105.83
8	v	101	BCL	C2B-C1B-NB	-2.79	108.36	110.23
8	r	101	BCL	C7-C6-C5	-2.79	105.78	113.36
8	J	101	BCL	C2B-C1B-NB	-2.79	108.36	110.23
11	C	404	LMT	C1'-O5'-C5'	-2.79	108.21	113.69
8	F	102	BCL	C2B-C1B-NB	-2.79	108.36	110.23
8	P	102	BCL	CMA-C3A-C4A	-2.79	104.28	111.77
8	E	101	BCL	C3D-C2D-C1D	-2.79	102.03	105.83
8	Q	101	BCL	C2B-C1B-NB	-2.79	108.36	110.23
8	n	101	BCL	C3D-C2D-C1D	-2.79	102.03	105.83
8	b	101	BCL	C7-C6-C5	-2.79	105.79	113.36
8	P	102	BCL	C4D-CHA-C1A	2.79	124.64	121.25
8	t	101	BCL	O2A-CGA-O1A	-2.79	116.56	123.59
8	Q	101	BCL	O2A-CGA-O1A	-2.79	116.56	123.59
8	P	101	BCL	O2A-CGA-O1A	-2.78	116.56	123.59
8	B	101	BCL	C4D-CHA-C1A	2.78	124.64	121.25
8	I	101	BCL	C4D-CHA-C1A	2.78	124.64	121.25
8	i	101	BCL	C1C-NC-C4C	-2.78	105.45	106.71
9	a	102	A1EFU	C6-C7-C8	-2.78	114.54	123.22
8	r	101	BCL	C3D-C2D-C1D	-2.78	102.04	105.83
8	G	101	BCL	C11-C10-C8	-2.78	106.93	115.92
8	G	102	BCL	C3D-C2D-C1D	-2.78	102.04	105.83
8	Q	101	BCL	CMA-C3A-C4A	-2.78	104.31	111.77
8	L	304	BCL	CMA-C3A-C4A	-2.78	104.31	111.77
8	M	403	BCL	CMC-C2C-C3C	-2.78	102.63	113.83
8	P	102	BCL	CAB-C3B-C2B	-2.78	124.18	128.34
8	F	101	BCL	C7-C6-C5	-2.77	105.83	113.36
8	R	102	BCL	C2B-C1B-NB	-2.77	108.38	110.23
8	Q	101	BCL	CMC-C2C-C3C	-2.77	102.66	113.83
8	F	102	BCL	C2C-C3C-C4C	-2.77	97.19	101.34
8	q	102	BCL	C7-C6-C5	-2.77	105.84	113.36
8	s	103	BCL	CMC-C2C-C3C	-2.77	102.66	113.83
8	a	101	BCL	C3D-C2D-C1D	-2.77	102.06	105.83
8	e	101	BCL	C11-C10-C8	-2.76	106.99	115.92
8	L	304	BCL	C3D-C2D-C1D	-2.76	102.06	105.83
8	G	102	BCL	C4D-CHA-C1A	2.76	124.61	121.25
8	t	101	BCL	C7-C6-C5	-2.76	105.86	113.36
8	A	101	BCL	C3D-C2D-C1D	-2.76	102.07	105.83
8	S	101	BCL	C7-C6-C5	-2.76	105.87	113.36
8	M	402	BCL	C3D-C2D-C1D	-2.76	102.07	105.83
8	F	102	BCL	C11-C10-C8	-2.76	107.01	115.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	N	101	BCL	C3D-C2D-C1D	-2.75	102.07	105.83
8	R	102	BCL	C3D-C2D-C1D	-2.75	102.07	105.83
8	n	101	BCL	CMC-C2C-C3C	-2.75	102.72	113.83
8	M	402	BCL	C2B-C1B-NB	-2.75	108.39	110.23
8	V	101	BCL	CMC-C2C-C3C	-2.75	102.73	113.83
8	L	304	BCL	O2A-CGA-O1A	-2.75	116.65	123.59
8	K	101	BCL	O2A-CGA-O1A	-2.75	116.65	123.59
8	I	101	BCL	CMC-C2C-C3C	-2.75	102.74	113.83
8	n	101	BCL	CMA-C3A-C4A	-2.75	104.39	111.77
8	i	101	BCL	C11-C10-C8	-2.75	107.03	115.92
15	L	308	CDL	OB8-CB7-C71	2.75	120.53	111.91
8	i	101	BCL	CMC-C2C-C3C	-2.75	102.75	113.83
8	M	403	BCL	C3D-C2D-C1D	-2.74	102.09	105.83
8	l	101	BCL	C3D-C2D-C1D	-2.74	102.09	105.83
8	G	101	BCL	CHA-C1A-NA	-2.74	120.12	126.40
8	F	102	BCL	C3D-C2D-C1D	-2.74	102.09	105.83
8	G	101	BCL	O2A-CGA-O1A	-2.74	116.68	123.59
8	P	101	BCL	C3D-C2D-C1D	-2.74	102.09	105.83
8	S	101	BCL	CMC-C2C-C3C	-2.74	102.78	113.83
8	R	102	BCL	C2C-C3C-C4C	-2.74	97.24	101.34
8	r	101	BCL	C4D-CHA-C1A	2.74	124.58	121.25
8	k	102	BCL	C3D-C2D-C1D	-2.73	102.10	105.83
8	e	101	BCL	C3D-C2D-C1D	-2.73	102.10	105.83
8	B	101	BCL	CMC-C2C-C3C	-2.73	102.80	113.83
8	G	102	BCL	C2B-C1B-NB	-2.73	108.40	110.23
15	L	308	CDL	OA8-CA7-C31	2.73	120.48	111.91
8	I	101	BCL	C11-C10-C8	-2.73	107.09	115.92
8	E	101	BCL	C11-C12-C13	-2.73	107.10	115.92
8	a	101	BCL	C2B-C1B-NB	-2.73	108.40	110.23
8	q	102	BCL	C3D-C2D-C1D	-2.73	102.11	105.83
8	D	101	BCL	CMC-C2C-C3C	-2.73	102.83	113.83
8	G	102	BCL	CMC-C2C-C3C	-2.72	102.84	113.83
8	n	101	BCL	O2A-CGA-O1A	-2.72	116.72	123.59
8	k	102	BCL	C2B-C1B-NB	-2.72	108.41	110.23
8	e	101	BCL	C7-C6-C5	-2.72	105.96	113.36
16	C	402	HEC	CBD-CAD-C3D	2.72	120.19	112.63
8	V	101	BCL	C3D-C2D-C1D	-2.72	102.12	105.83
8	l	101	BCL	C2B-C1B-NB	-2.71	108.41	110.23
8	i	101	BCL	C4D-CHA-C1A	2.71	124.55	121.25
8	L	301	BCL	C7-C6-C5	-2.71	106.00	113.36
8	s	103	BCL	C3D-C2D-C1D	-2.71	102.13	105.83
8	J	101	BCL	CMC-C2C-C3C	-2.71	102.89	113.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	s	103	BCL	C11-C10-C8	-2.71	107.16	115.92
9	s	104	A1EFU	CM6-C18-C19	2.71	122.34	118.08
11	L	305	LMT	C3'-C4'-C5'	-2.70	105.42	110.24
8	q	102	BCL	CMC-C2C-C3C	-2.70	102.93	113.83
8	b	101	BCL	C3D-C2D-C1D	-2.70	102.14	105.83
8	j	102	BCL	CMC-C2C-C3C	-2.70	102.94	113.83
8	j	102	BCL	CMA-C3A-C4A	-2.70	104.52	111.77
8	G	102	BCL	CMA-C3A-C4A	-2.70	104.52	111.77
8	s	102	BCL	C4D-CHA-C1A	2.70	124.53	121.25
8	P	102	BCL	C3D-C2D-C1D	-2.70	102.15	105.83
8	e	101	BCL	O2A-CGA-O1A	-2.70	116.78	123.59
8	M	403	BCL	CMA-C3A-C4A	-2.70	104.52	111.77
8	d	101	BCL	C4D-CHA-C1A	2.69	124.53	121.25
8	2	103	BCL	CMC-C2C-C3C	-2.69	102.97	113.83
8	2	103	BCL	C4A-NA-C1A	-2.69	105.50	106.71
8	k	102	BCL	C4D-CHA-C1A	2.69	124.52	121.25
8	S	101	BCL	C2B-C1B-NB	-2.69	108.43	110.23
8	G	102	BCL	C2C-C3C-C4C	-2.69	97.31	101.34
8	r	101	BCL	CMC-C2C-C3C	-2.68	103.00	113.83
8	v	101	BCL	CMC-C2C-C3C	-2.68	103.01	113.83
8	V	101	BCL	C2B-C1B-NB	-2.68	108.44	110.23
8	b	101	BCL	CMA-C3A-C4A	-2.68	104.58	111.77
8	I	101	BCL	O2A-CGA-O1A	-2.68	116.84	123.59
10	F	103	MW9	O1-C17-C16	2.68	120.31	111.91
8	P	101	BCL	CGD-CBD-CAD	-2.67	102.07	110.73
8	l	101	BCL	C11-C12-C13	-2.67	107.27	115.92
8	A	101	BCL	CMC-C2C-C3C	-2.67	103.04	113.83
8	J	101	BCL	CGD-CBD-CAD	-2.67	102.08	110.73
8	G	101	BCL	C2B-C1B-NB	-2.67	108.44	110.23
8	t	101	BCL	C4D-CHA-C1A	2.67	124.50	121.25
8	k	102	BCL	O2A-CGA-O1A	-2.67	116.87	123.59
8	b	101	BCL	C1C-NC-C4C	-2.66	105.51	106.71
8	t	101	BCL	CMC-C2C-C3C	-2.66	103.08	113.83
8	P	101	BCL	CMC-C2C-C3C	-2.66	103.08	113.83
8	G	101	BCL	CMC-C2C-C3C	-2.66	103.08	113.83
8	K	101	BCL	CMC-C2C-C3C	-2.66	103.09	113.83
8	k	102	BCL	CMC-C2C-C3C	-2.66	103.09	113.83
8	t	101	BCL	C3D-C2D-C1D	-2.66	102.20	105.83
8	b	101	BCL	O2A-CGA-O1A	-2.66	116.88	123.59
8	P	102	BCL	CMC-C2C-C3C	-2.66	103.10	113.83
8	q	102	BCL	O2A-CGA-O1A	-2.66	116.89	123.59
8	P	101	BCL	CMA-C3A-C4A	-2.65	104.64	111.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	103	MW9	O1-C17-C16	2.65	120.23	111.91
8	L	301	BCL	C2A-C1A-CHA	2.65	128.50	123.86
8	E	101	BCL	CMC-C2C-C3C	-2.65	103.14	113.83
10	M	405	MW9	O1-C17-C16	2.65	120.22	111.91
8	I	101	BCL	CMA-C3A-C4A	-2.65	104.66	111.77
8	F	101	BCL	CMA-C3A-C4A	-2.65	104.66	111.77
8	S	101	BCL	CMA-C3A-C4A	-2.65	104.66	111.77
10	H	303	MW9	O1-C17-C16	2.64	120.21	111.91
8	d	101	BCL	C2A-C1A-CHA	2.64	128.48	123.86
8	R	102	BCL	CMC-C2C-C3C	-2.64	103.17	113.83
10	M	406	MW9	O1-C17-C16	2.64	120.19	111.91
8	j	102	BCL	C11-C12-C13	-2.64	107.40	115.92
8	B	101	BCL	CMA-C3A-C4A	-2.64	104.69	111.77
8	I	101	BCL	CGD-CBD-CAD	-2.63	102.22	110.73
8	L	304	BCL	CMC-C2C-C3C	-2.63	103.22	113.83
8	P	101	BCL	C2B-C1B-NB	-2.63	108.47	110.23
8	q	102	BCL	CMA-C3A-C4A	-2.63	104.71	111.77
8	J	101	BCL	C11-C12-C13	-2.63	107.43	115.92
8	e	101	BCL	CMC-C2C-C3C	-2.63	103.23	113.83
8	B	101	BCL	C11-C12-C13	-2.63	107.43	115.92
8	K	101	BCL	C11-C12-C13	-2.62	107.44	115.92
8	b	101	BCL	C16-C15-C13	-2.62	107.45	115.92
8	G	102	BCL	C11-C12-C13	-2.62	107.46	115.92
8	N	101	BCL	CMA-C3A-C4A	-2.62	104.74	111.77
8	G	101	BCL	C3D-C2D-C1D	-2.62	102.26	105.83
10	R	103	MW9	O1-C17-C16	2.61	120.11	111.91
8	V	101	BCL	CHB-C1B-NB	2.61	127.03	124.26
15	H	304	CDL	OB8-CB7-C71	2.61	120.11	111.91
8	k	102	BCL	CMA-C3A-C4A	-2.61	104.75	111.77
11	L	305	LMT	C1'-O5'-C5'	-2.61	108.56	113.69
8	F	101	BCL	C3D-C2D-C1D	-2.61	102.27	105.83
8	E	101	BCL	C4D-CHA-C1A	2.61	124.42	121.25
14	L	302	BPH	C2B-C1B-NB	-2.61	107.72	109.53
8	s	103	BCL	CMA-C3A-C4A	-2.61	104.76	111.77
8	E	101	BCL	CMA-C3A-C4A	-2.61	104.77	111.77
8	V	101	BCL	C4D-CHA-C1A	2.60	124.42	121.25
8	2	103	BCL	C2A-C1A-CHA	2.60	128.41	123.86
11	D	102	LMT	C1'-O5'-C5'	-2.60	108.58	113.69
8	s	102	BCL	C11-C12-C13	-2.60	107.51	115.92
8	v	101	BCL	C4A-NA-C1A	-2.60	105.54	106.71
8	Q	101	BCL	C11-C12-C13	-2.60	107.52	115.92
8	N	101	BCL	CMC-C2C-C3C	-2.60	103.34	113.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	i	101	BCL	CMA-C3A-C4A	-2.60	104.80	111.77
8	2	103	BCL	C4D-CHA-C1A	2.60	124.41	121.25
8	s	102	BCL	CMC-C2C-C3C	-2.60	103.36	113.83
8	A	101	BCL	CMA-C3A-C4A	-2.59	104.80	111.77
8	b	101	BCL	CMC-C2C-C3C	-2.59	103.37	113.83
8	a	101	BCL	CMC-C2C-C3C	-2.59	103.37	113.83
8	F	101	BCL	CMC-C2C-C3C	-2.59	103.37	113.83
8	V	101	BCL	CMA-C3A-C4A	-2.59	104.81	111.77
8	b	101	BCL	C2B-C1B-NB	-2.59	108.50	110.23
8	S	101	BCL	C11-C10-C8	-2.59	107.55	115.92
10	G	103	MW9	O1-C17-C16	2.59	120.03	111.91
8	L	301	BCL	C2B-C1B-NB	-2.59	108.50	110.23
8	R	102	BCL	C4D-CHA-C1A	2.59	124.40	121.25
8	J	101	BCL	CMA-C3A-C4A	-2.58	104.83	111.77
8	E	101	BCL	C7-C6-C5	-2.58	106.35	113.36
8	G	101	BCL	CMA-C3A-C4A	-2.58	104.84	111.77
8	F	102	BCL	CMC-C2C-C3C	-2.58	103.42	113.83
8	F	102	BCL	C11-C12-C13	-2.58	107.58	115.92
8	e	101	BCL	CMA-C3A-C4A	-2.58	104.84	111.77
8	2	103	BCL	C7-C6-C5	-2.58	106.36	113.36
8	a	101	BCL	C7-C6-C5	-2.58	106.36	113.36
9	q	101	A1EFU	CM7-C22-C23	-2.57	110.94	115.27
16	C	401	HEC	O1A-CGA-CBA	-2.57	114.81	123.08
10	G	104	MW9	O1-C17-C16	2.57	119.98	111.91
8	j	102	BCL	C4D-CHA-C1A	2.57	124.38	121.25
8	S	101	BCL	CGD-CBD-CAD	-2.57	102.41	110.73
8	a	101	BCL	CMA-C3A-C4A	-2.57	104.88	111.77
8	B	101	BCL	CGD-CBD-CAD	-2.56	102.43	110.73
8	R	102	BCL	CMA-C3A-C4A	-2.56	104.88	111.77
8	n	101	BCL	C1C-NC-C4C	-2.56	105.55	106.71
8	P	101	BCL	C11-C12-C13	-2.56	107.64	115.92
8	l	101	BCL	CMA-C3A-C4A	-2.56	104.90	111.77
9	p	101	A1EFU	CM7-C22-C23	-2.55	110.97	115.27
8	N	101	BCL	C2B-C1B-NB	-2.55	108.52	110.23
8	j	102	BCL	C2C-C3C-C4C	-2.55	97.52	101.34
8	2	103	BCL	C1C-NC-C4C	-2.55	105.56	106.71
8	b	101	BCL	C4A-NA-C1A	-2.55	105.56	106.71
8	K	101	BCL	C2C-C3C-C4C	-2.55	97.53	101.34
8	V	101	BCL	C11-C12-C13	-2.54	107.70	115.92
16	C	403	HEC	O1A-CGA-CBA	-2.54	114.92	123.08
8	q	102	BCL	C4D-CHA-C1A	2.54	124.34	121.25
8	M	403	BCL	CMB-C2B-C3B	2.54	132.78	125.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	1	101	BCL	CMC-C2C-C3C	-2.54	103.60	113.83
8	G	101	BCL	C1C-NC-C4C	-2.53	105.57	106.71
8	1	101	BCL	CGD-CBD-CAD	-2.53	102.53	110.73
10	H	301	MW9	O1-C17-C16	2.53	119.85	111.91
8	2	103	BCL	CMA-C3A-C4A	-2.53	104.97	111.77
15	H	304	CDL	OA8-CA7-C31	2.53	119.84	111.91
8	n	101	BCL	C4A-NA-C1A	-2.53	105.57	106.71
8	a	101	BCL	C11-C12-C13	-2.52	107.76	115.92
8	P	102	BCL	C7-C6-C5	-2.52	106.50	113.36
8	M	403	BCL	C11-C12-C13	-2.52	107.78	115.92
8	n	101	BCL	C11-C10-C8	-2.52	107.78	115.92
8	e	101	BCL	C2A-C1A-CHA	2.52	128.26	123.86
8	M	402	BCL	C11-C12-C13	-2.51	107.79	115.92
8	L	304	BCL	C2B-C1B-NB	-2.51	108.55	110.23
10	G	104	MW9	C31-C32-C33	-2.51	109.79	126.84
8	t	101	BCL	C11-C12-C13	-2.51	107.81	115.92
8	D	101	BCL	CGD-CBD-CAD	-2.50	102.63	110.73
8	L	301	BCL	CMD-C2D-C1D	2.50	129.12	124.71
8	S	101	BCL	C11-C12-C13	-2.50	107.85	115.92
16	C	402	HEC	O1A-CGA-CBA	-2.49	115.07	123.08
8	D	101	BCL	C2B-C1B-NB	-2.49	108.56	110.23
8	G	102	BCL	C2A-C1A-CHA	2.49	128.21	123.86
8	s	102	BCL	CGD-CBD-CAD	-2.48	102.69	110.73
8	G	101	BCL	C4D-CHA-C1A	2.48	124.27	121.25
8	J	101	BCL	C2C-C3C-C4C	-2.48	97.62	101.34
8	M	403	BCL	CMD-C2D-C1D	2.48	129.08	124.71
8	F	101	BCL	C1C-NC-C4C	-2.48	105.59	106.71
8	2	103	BCL	C2B-C1B-NB	-2.48	108.57	110.23
8	B	101	BCL	CMD-C2D-C1D	2.48	129.08	124.71
8	r	101	BCL	CMA-C3A-C4A	-2.47	105.13	111.77
8	R	102	BCL	CGD-CBD-CAD	-2.47	102.74	110.73
8	d	101	BCL	C7-C6-C5	-2.47	106.66	113.36
8	s	103	BCL	C11-C12-C13	-2.46	107.96	115.92
16	C	401	HEC	C1D-ND-C4D	2.46	107.62	105.07
8	L	301	BCL	C3C-C2C-C1C	2.46	105.84	101.87
8	v	101	BCL	CMA-C3A-C4A	-2.46	105.16	111.77
8	A	101	BCL	C11-C12-C13	-2.46	107.97	115.92
9	2	104	A1EFU	CM7-C22-C23	-2.46	111.14	115.27
8	F	102	BCL	C2A-C1A-CHA	2.46	128.16	123.86
8	R	102	BCL	C11-C12-C13	-2.46	107.98	115.92
8	K	101	BCL	CMA-C3A-C4A	-2.46	105.17	111.77
14	L	302	BPH	C4D-CHA-CBD	2.45	109.63	108.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	t	101	BCL	CHB-C4A-NA	-2.45	121.12	124.51
9	B	103	A1EFU	CM7-C22-C23	-2.45	111.15	115.27
8	t	101	BCL	C11-C10-C8	-2.45	108.00	115.92
8	E	101	BCL	C2A-C1A-CHA	2.45	128.14	123.86
8	k	102	BCL	C11-C12-C13	-2.44	108.02	115.92
8	J	101	BCL	C2A-C1A-CHA	2.44	128.13	123.86
8	L	304	BCL	CMB-C2B-C3B	2.44	132.53	125.93
8	S	101	BCL	C3C-C2C-C1C	2.44	105.81	101.87
8	2	103	BCL	C3C-C2C-C1C	2.44	105.81	101.87
8	M	402	BCL	CMA-C3A-C4A	-2.44	105.22	111.77
8	V	101	BCL	CMB-C2B-C3B	2.43	132.50	125.93
8	i	101	BCL	C2A-C1A-CHA	2.43	128.11	123.86
8	K	101	BCL	C2A-C1A-CHA	2.43	128.11	123.86
8	I	101	BCL	C2A-C1A-CHA	2.43	128.11	123.86
9	J	102	A1EFU	CM7-C22-C23	-2.42	111.20	115.27
8	G	102	BCL	CMD-C2D-C1D	2.42	128.97	124.71
8	L	304	BCL	C11-C12-C13	-2.42	108.11	115.92
8	B	101	BCL	C3C-C2C-C1C	2.42	105.77	101.87
8	D	101	BCL	C11-C12-C13	-2.41	108.12	115.92
8	D	101	BCL	C3C-C2C-C1C	2.41	105.76	101.87
8	N	101	BCL	C11-C12-C13	-2.41	108.14	115.92
8	j	102	BCL	CGD-CBD-CAD	-2.40	102.95	110.73
16	C	401	HEC	CAC-C3C-C4C	-2.40	121.58	124.92
16	C	402	HEC	C1D-ND-C4D	2.40	107.55	105.07
8	r	101	BCL	C2A-C1A-CHA	2.40	128.05	123.86
8	d	101	BCL	CMA-C3A-C4A	-2.40	105.33	111.77
8	i	101	BCL	CMB-C2B-C3B	2.39	132.40	125.93
8	L	301	BCL	CGD-CBD-CAD	-2.39	102.98	110.73
8	R	102	BCL	C2A-C1A-CHA	2.39	128.04	123.86
8	2	103	BCL	CMB-C2B-C3B	2.39	132.39	125.93
8	N	101	BCL	CMB-C2B-C3B	2.39	132.39	125.93
8	d	101	BCL	CMC-C2C-C3C	-2.39	104.19	113.83
8	s	103	BCL	C3C-C2C-C1C	2.39	105.73	101.87
8	A	101	BCL	C3C-C2C-C1C	2.39	105.72	101.87
8	V	101	BCL	C11-C10-C8	-2.39	108.21	115.92
8	S	101	BCL	C12-C11-C10	-2.39	102.28	113.24
8	q	102	BCL	CMB-C2B-C3B	2.38	132.37	125.93
8	s	102	BCL	CMA-C3A-C4A	-2.38	105.37	111.77
8	J	101	BCL	CMB-C2B-C3B	2.38	132.36	125.93
8	D	101	BCL	CMB-C2B-C3B	2.38	132.36	125.93
8	s	103	BCL	C4D-CHA-C1A	2.38	124.14	121.25
8	F	102	BCL	CMD-C2D-C1D	2.38	128.90	124.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	i	101	BCL	C3C-C2C-C1C	2.37	105.70	101.87
8	B	101	BCL	CMB-C2B-C3B	2.37	132.34	125.93
8	G	102	BCL	CMB-C2B-C3B	2.37	132.33	125.93
8	I	101	BCL	CMB-C2B-C3B	2.37	132.32	125.93
8	n	101	BCL	C3C-C2C-C1C	2.37	105.69	101.87
8	F	101	BCL	CMB-C2B-C3B	2.36	132.31	125.93
8	e	101	BCL	CMB-C2B-C3B	2.36	132.31	125.93
8	L	301	BCL	CMB-C2B-C3B	2.36	132.31	125.93
8	s	103	BCL	C1C-NC-C4C	-2.36	105.64	106.71
8	l	101	BCL	CMB-C2B-C3B	2.36	132.31	125.93
9	B	102	A1EFU	CM7-C22-C23	-2.36	111.30	115.27
8	V	101	BCL	CGD-CBD-CAD	-2.36	103.09	110.73
8	b	101	BCL	CMB-C2B-C3B	2.36	132.31	125.93
8	A	101	BCL	CGD-CBD-CAD	-2.36	103.09	110.73
8	R	102	BCL	CMD-C2D-C1D	2.36	128.87	124.71
8	j	102	BCL	CMB-C2B-C3B	2.36	132.29	125.93
8	Q	101	BCL	CMB-C2B-C3B	2.35	132.29	125.93
14	M	408	BPH	C4D-CHA-CBD	2.35	109.58	108.52
8	Q	101	BCL	CMD-C2D-C1D	2.35	128.86	124.71
8	a	101	BCL	CMB-C2B-C3B	2.35	132.27	125.93
8	G	101	BCL	CMB-C2B-C3B	2.35	132.27	125.93
8	b	101	BCL	C2A-C1A-CHA	2.35	127.96	123.86
8	k	102	BCL	CMB-C2B-C3B	2.35	132.26	125.93
8	E	101	BCL	CMB-C2B-C3B	2.34	132.26	125.93
13	M	404	U10	C7-C6-C5	-2.34	115.66	118.48
8	B	101	BCL	C2B-C1B-NB	-2.34	108.66	110.23
8	r	101	BCL	CBB-CAB-C3B	2.34	125.43	120.43
9	v	102	A1EFU	CM7-C22-C23	-2.34	111.33	115.27
9	I	102	A1EFU	CM7-C22-C23	-2.34	111.33	115.27
8	N	101	BCL	CGD-CBD-CAD	-2.34	103.16	110.73
8	F	102	BCL	CMB-C2B-C3B	2.34	132.24	125.93
9	j	103	A1EFU	C19-C18-C17	2.33	122.52	118.94
8	q	102	BCL	CGD-CBD-CAD	-2.33	103.18	110.73
8	v	101	BCL	CMB-C2B-C3B	2.33	132.23	125.93
8	s	103	BCL	CMB-C2B-C3B	2.33	132.23	125.93
8	P	102	BCL	C3C-C2C-C1C	2.33	105.64	101.87
8	J	101	BCL	CMD-C2D-C1D	2.33	128.82	124.71
8	e	101	BCL	CMD-C2D-C1D	2.33	128.82	124.71
8	q	102	BCL	C11-C12-C13	-2.33	108.40	115.92
8	M	402	BCL	CMB-C2B-C3B	2.32	132.20	125.93
8	D	101	BCL	C12-C11-C10	-2.32	102.57	113.24
8	P	102	BCL	C11-C12-C13	-2.32	108.43	115.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	R	102	BCL	CMB-C2B-C3B	2.32	132.18	125.93
8	i	101	BCL	C11-C12-C13	-2.32	108.44	115.92
8	S	101	BCL	CMB-C2B-C3B	2.31	132.18	125.93
9	k	101	A1EFU	CM7-C22-C23	-2.31	111.38	115.27
8	K	101	BCL	CMB-C2B-C3B	2.31	132.17	125.93
8	P	102	BCL	CBB-CAB-C3B	2.31	125.36	120.43
9	s	105	A1EFU	CM7-C22-C23	-2.31	111.39	115.27
8	Q	101	BCL	C12-C11-C10	-2.31	102.64	113.24
8	s	103	BCL	CGD-CBD-CAD	-2.31	103.26	110.73
8	q	102	BCL	C3C-C2C-C1C	2.31	105.59	101.87
8	I	101	BCL	CMD-C2D-C1D	2.30	128.78	124.71
8	F	101	BCL	C2A-C1A-CHA	2.30	127.89	123.86
8	F	101	BCL	C11-C12-C13	-2.30	108.47	115.92
8	P	101	BCL	CMB-C2B-C3B	2.30	132.15	125.93
8	e	101	BCL	C2C-C3C-C4C	-2.30	97.89	101.34
8	G	101	BCL	C11-C12-C13	-2.30	108.49	115.92
8	G	101	BCL	C2A-C1A-CHA	2.30	127.87	123.86
8	S	101	BCL	CMD-C2D-C1D	2.29	128.76	124.71
9	s	101	A1EFU	CM7-C22-C23	-2.29	111.41	115.27
8	v	101	BCL	C11-C12-C13	-2.29	108.53	115.92
9	J	103	A1EFU	CM7-C22-C23	-2.28	111.43	115.27
8	L	304	BCL	C12-C11-C10	-2.28	102.77	113.24
8	L	304	BCL	CHC-C1C-NC	2.28	127.66	124.51
13	L	303	U10	C7-C6-C5	-2.28	115.74	118.48
8	2	103	BCL	C11-C12-C13	-2.27	108.57	115.92
8	F	101	BCL	C3C-C2C-C1C	2.27	105.54	101.87
8	M	402	BCL	CMD-C2D-C1D	2.27	128.72	124.71
8	i	101	BCL	C12-C11-C10	-2.27	102.80	113.24
16	C	403	HEC	C1D-ND-C4D	2.27	107.42	105.07
8	K	101	BCL	CGD-CBD-CAD	-2.27	103.39	110.73
8	P	101	BCL	C3C-C2C-C1C	2.27	105.53	101.87
9	N	102	A1EFU	CM7-C22-C23	-2.27	111.46	115.27
8	V	101	BCL	C3C-C2C-C1C	2.27	105.53	101.87
8	k	102	BCL	C3C-C2C-C1C	2.27	105.53	101.87
8	D	101	BCL	CMD-C2D-C1D	2.26	128.70	124.71
8	M	402	BCL	C12-C11-C10	-2.26	102.84	113.24
8	s	102	BCL	CMD-C2D-C1D	2.26	128.70	124.71
8	d	101	BCL	CMB-C2B-C3B	2.26	132.04	125.93
8	M	403	BCL	C2B-C1B-NB	-2.26	108.72	110.23
8	V	101	BCL	C2A-C1A-CHA	2.26	127.81	123.86
8	n	101	BCL	CBB-CAB-C3B	2.26	125.25	120.43
8	P	101	BCL	CMD-C2D-C1D	2.26	128.69	124.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	101	BCL	CBB-CAB-C3B	2.26	125.25	120.43
9	P	103	A1EFU	CM7-C22-C23	-2.26	111.47	115.27
8	V	101	BCL	CMD-C2D-C1D	2.26	128.69	124.71
8	e	101	BCL	CGD-CBD-CAD	-2.25	103.43	110.73
8	l	101	BCL	CMD-C2D-C1D	2.25	128.68	124.71
9	D	105	A1EFU	CM7-C22-C23	-2.25	111.48	115.27
8	r	101	BCL	C11-C12-C13	-2.25	108.64	115.92
8	Q	101	BCL	C3C-C2C-C1C	2.25	105.50	101.87
8	t	101	BCL	CBB-CAB-C3B	2.24	125.22	120.43
8	q	102	BCL	CMD-C2D-C1D	2.24	128.66	124.71
14	L	302	BPH	CMD-C2D-C3D	2.23	128.85	124.68
8	L	304	BCL	C2A-C3A-C4A	-2.23	98.27	101.87
8	N	101	BCL	CMD-C2D-C1D	2.22	128.63	124.71
8	b	101	BCL	C3C-C2C-C1C	2.22	105.46	101.87
16	C	403	HEC	CBD-CAD-C3D	2.22	118.80	112.63
8	s	102	BCL	C12-C11-C10	-2.22	103.05	113.24
8	r	101	BCL	CMD-C2D-C1D	2.22	128.62	124.71
8	D	101	BCL	C11-C10-C8	-2.22	108.75	115.92
8	M	402	BCL	C4D-CHA-C1A	2.22	123.95	121.25
8	t	101	BCL	C12-C11-C10	-2.21	103.06	113.24
8	r	101	BCL	CGD-CBD-CAD	-2.21	103.56	110.73
8	t	101	BCL	CGD-CBD-CAD	-2.21	103.57	110.73
9	K	102	A1EFU	CM7-C22-C23	-2.21	111.55	115.27
8	N	101	BCL	C12-C11-C10	-2.21	103.10	113.24
9	2	104	A1EFU	C19-C18-C17	2.21	122.33	118.94
8	P	101	BCL	C12-C11-C10	-2.21	103.10	113.24
9	D	104	A1EFU	CM7-C22-C23	-2.21	111.56	115.27
8	j	102	BCL	C12-C11-C10	-2.20	103.11	113.24
9	p	101	A1EFU	C21-C20-C19	-2.20	116.34	123.22
8	G	102	BCL	CGD-CBD-CAD	-2.20	103.61	110.73
14	M	408	BPH	CMD-C2D-C3D	2.20	128.79	124.68
8	k	102	BCL	C12-C11-C10	-2.20	103.15	113.24
8	F	101	BCL	CGD-CBD-CAD	-2.19	103.63	110.73
9	s	104	A1EFU	CM7-C22-C23	-2.19	111.58	115.27
8	L	304	BCL	CMD-C2D-C1D	2.19	128.57	124.71
8	G	101	BCL	C12-C11-C10	-2.19	103.18	113.24
16	C	401	HEC	CMC-C2C-C3C	2.19	130.34	125.61
8	F	101	BCL	C4A-NA-C1A	-2.19	105.72	106.71
9	2	102	A1EFU	C12-C13-C14	2.19	122.30	118.94
8	v	101	BCL	C11-C10-C8	-2.19	108.86	115.92
8	F	102	BCL	C12-C11-C10	-2.19	103.20	113.24
8	a	101	BCL	CGD-CBD-CAD	-2.18	103.66	110.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	R	101	A1EFU	CM7-C22-C23	-2.18	111.60	115.27
8	G	101	BCL	C3C-C2C-C1C	2.18	105.39	101.87
8	a	101	BCL	C2A-C1A-CHA	2.18	127.67	123.86
8	e	101	BCL	C12-C11-C10	-2.17	103.27	113.24
8	j	102	BCL	CMD-C2D-C1D	2.17	128.53	124.71
8	V	101	BCL	C12-C11-C10	-2.17	103.28	113.24
8	K	101	BCL	C12-C11-C10	-2.17	103.28	113.24
9	T	101	A1EFU	CM7-C22-C23	-2.17	111.63	115.27
8	B	101	BCL	C12-C11-C10	-2.16	103.32	113.24
8	v	101	BCL	C12-C11-C10	-2.16	103.33	113.24
9	2	104	A1EFU	CM6-C18-C19	2.16	121.47	118.08
8	G	102	BCL	C12-C11-C10	-2.15	103.34	113.24
8	J	101	BCL	C12-C11-C10	-2.15	103.35	113.24
8	2	103	BCL	CMD-C2D-C1D	2.15	128.50	124.71
8	a	101	BCL	CMD-C2D-C1D	2.15	128.50	124.71
8	A	101	BCL	CMD-C2D-C1D	2.15	128.50	124.71
8	E	101	BCL	CGD-CBD-CAD	-2.15	103.78	110.73
8	r	101	BCL	C3C-C2C-C1C	2.14	105.33	101.87
8	K	101	BCL	CMD-C2D-C1D	2.14	128.48	124.71
9	a	102	A1EFU	CM7-C22-C23	-2.14	111.68	115.27
8	d	101	BCL	CMD-C2D-C1D	2.14	128.48	124.71
8	E	101	BCL	CMD-C2D-C1D	2.13	128.47	124.71
8	b	101	BCL	C2A-C3A-C4A	-2.13	98.43	101.87
8	e	101	BCL	C11-C12-C13	-2.13	109.04	115.92
8	D	101	BCL	C2A-C1A-CHA	2.13	127.58	123.86
8	l	101	BCL	C12-C11-C10	-2.12	103.47	113.24
16	C	401	HEC	CHC-C4B-NB	2.12	126.99	124.37
8	M	403	BCL	CHC-C1C-NC	2.12	127.44	124.51
8	n	101	BCL	CMD-C2D-C1D	2.12	128.45	124.71
8	q	102	BCL	C12-C11-C10	-2.12	103.51	113.24
8	s	103	BCL	C2A-C1A-CHA	2.12	127.56	123.86
8	s	102	BCL	C2A-C1A-CHA	2.12	127.56	123.86
8	l	101	BCL	C2A-C1A-CHA	2.11	127.55	123.86
8	q	102	BCL	C2A-C1A-CHA	2.11	127.55	123.86
8	A	101	BCL	C2A-C1A-CHA	2.11	127.55	123.86
8	n	101	BCL	CGD-CBD-CAD	-2.11	103.90	110.73
8	j	102	BCL	C2A-C1A-CHA	2.11	127.54	123.86
8	F	101	BCL	C2A-C3A-C4A	-2.11	98.47	101.87
8	s	103	BCL	C12-C11-C10	-2.11	103.56	113.24
9	j	101	A1EFU	CM7-C22-C23	-2.10	111.74	115.27
8	v	101	BCL	CMD-C2D-C1D	2.09	128.40	124.71
8	L	301	BCL	CHC-C1C-NC	2.09	127.40	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	C	402	HEC	CMC-C2C-C3C	2.09	130.13	125.61
9	M	407	A1EFU	CM7-C22-C23	-2.08	111.77	115.27
8	n	101	BCL	C12-C11-C10	-2.08	103.70	113.24
8	b	101	BCL	C12-C11-C10	-2.07	103.71	113.24
8	b	101	BCL	CMD-C2D-C1D	2.07	128.37	124.71
16	C	402	HEC	CMD-C2D-C1D	-2.07	121.88	125.04
8	t	101	BCL	CMD-C2D-C1D	2.07	128.36	124.71
8	a	101	BCL	CHC-C1C-NC	2.07	127.37	124.51
8	F	102	BCL	CGD-CBD-CAD	-2.07	104.03	110.73
8	d	101	BCL	CGD-CBD-CAD	-2.07	104.04	110.73
8	n	101	BCL	C2A-C1A-CHA	2.07	127.47	123.86
8	2	103	BCL	C2A-C3A-C4A	-2.06	98.53	101.87
8	F	101	BCL	C4D-CHA-C1A	2.06	123.76	121.25
8	M	403	BCL	CHB-C4A-NA	-2.06	121.66	124.51
8	M	403	BCL	C4A-NA-C1A	-2.06	105.78	106.71
8	F	102	BCL	C1-O2A-CGA	2.06	121.85	116.44
8	t	101	BCL	OBB-CAB-C3B	2.06	124.21	120.41
8	F	101	BCL	CMD-C2D-C1D	2.06	128.34	124.71
8	R	102	BCL	C12-C11-C10	-2.05	103.80	113.24
8	G	101	BCL	C2A-C3A-C4A	-2.05	98.55	101.87
8	i	101	BCL	CMD-C2D-C1D	2.05	128.33	124.71
8	E	101	BCL	C2A-C3A-C4A	-2.05	98.56	101.87
8	k	102	BCL	CGD-CBD-CAD	-2.05	104.10	110.73
8	q	102	BCL	C4A-NA-C1A	-2.05	105.78	106.71
8	M	403	BCL	C12-C11-C10	-2.05	103.84	113.24
8	a	101	BCL	C12-C11-C10	-2.04	103.85	113.24
11	D	102	LMT	C3'-C4'-C5'	-2.04	106.24	110.93
8	E	101	BCL	CHC-C1C-NC	2.04	127.33	124.51
11	H	302	LMT	C3'-C4'-C5'	-2.04	106.60	110.24
9	q	101	A1EFU	C19-C18-C17	2.04	122.07	118.94
16	C	403	HEC	CHC-C4B-NB	2.04	126.88	124.37
10	G	103	MW9	C31-C32-C33	-2.03	109.15	124.73
8	k	102	BCL	C4A-NA-C1A	-2.03	105.79	106.71
8	A	101	BCL	C12-C11-C10	-2.03	103.92	113.24
8	F	101	BCL	C12-C11-C10	-2.03	103.93	113.24
8	E	101	BCL	C12-C11-C10	-2.02	103.94	113.24
8	P	102	BCL	CMD-C2D-C1D	2.02	128.28	124.71
8	q	102	BCL	C2A-C3A-C4A	-2.02	98.61	101.87
16	C	401	HEC	CMD-C2D-C1D	-2.02	121.97	125.04
8	2	103	BCL	C12-C11-C10	-2.02	103.98	113.24
16	C	403	HEC	C3D-C4D-ND	-2.01	108.40	110.36
9	E	103	A1EFU	CM7-C22-C23	-2.01	111.90	115.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	2	101	A1EFU	CM7-C22-C23	-2.00	111.90	115.27
10	H	301	MW9	C34-C33-C32	-2.00	109.35	124.73
8	v	101	BCL	CGD-CBD-CAD	-2.00	104.25	110.73

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
16	C	401	HEC	NA
16	C	402	HEC	NA
16	C	403	HEC	NA

All (1708) 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	O1A-CGA-O2A-C1
8	P	102	BCL	C1-C2-C3-C4
8	V	101	BCL	C4C-C3C-CAC-CBC
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	C2-C3-C5-C6
8	S	101	BCL	C2C-C3C-CAC-CBC
8	S	101	BCL	C4C-C3C-CAC-CBC
8	S	101	BCL	C1-C2-C3-C4
8	S	101	BCL	C2-C3-C5-C6
8	t	101	BCL	C1-C2-C3-C5
8	s	102	BCL	C2C-C3C-CAC-CBC
8	Q	101	BCL	C1A-C2A-CAA-CBA
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-C5
8	r	101	BCL	C2C-C3C-CAC-CBC
8	R	102	BCL	C2A-CAA-CBA-CGA
8	q	102	BCL	C1A-C2A-CAA-CBA
8	q	102	BCL	C2-C3-C5-C6
8	2	103	BCL	C1A-C2A-CAA-CBA
8	2	103	BCL	C3A-C2A-CAA-CBA
8	2	103	BCL	C2C-C3C-CAC-CBC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	l	101	BCL	C1A-C2A-CAA-CBA
8	l	101	BCL	C3A-C2A-CAA-CBA
8	n	101	BCL	C1A-C2A-CAA-CBA
8	n	101	BCL	C3A-C2A-CAA-CBA
8	N	101	BCL	C3A-C2A-CAA-CBA
8	k	102	BCL	C2C-C3C-CAC-CBC
8	i	101	BCL	C1A-C2A-CAA-CBA
8	i	101	BCL	C3A-C2A-CAA-CBA
8	i	101	BCL	C2C-C3C-CAC-CBC
8	i	101	BCL	CAD-CBD-CGD-O1D
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	102	BCL	C1A-C2A-CAA-CBA
8	e	101	BCL	C1-C2-C3-C4
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	CHA-CBD-CGD-O1D
8	d	101	BCL	CHA-CBD-CGD-O2D
8	d	101	BCL	CAD-CBD-CGD-O1D
8	d	101	BCL	CAD-CBD-CGD-O2D
8	d	101	BCL	C1-C2-C3-C4
8	d	101	BCL	C1-C2-C3-C5
8	D	101	BCL	C2A-CAA-CBA-CGA
8	D	101	BCL	C4C-C3C-CAC-CBC
8	b	101	BCL	C1A-C2A-CAA-CBA
8	b	101	BCL	C3A-C2A-CAA-CBA
8	b	101	BCL	C2-C3-C5-C6
8	B	101	BCL	C3A-C2A-CAA-CBA
8	B	101	BCL	C4C-C3C-CAC-CBC
8	a	101	BCL	C2C-C3C-CAC-CBC
8	a	101	BCL	C1-C2-C3-C4
8	a	101	BCL	C1-C2-C3-C5
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	C1A-C2A-CAA-CBA
8	M	402	BCL	CHA-CBD-CGD-O1D
8	M	402	BCL	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	M	403	BCL	C4C-C3C-CAC-CBC
8	M	403	BCL	CHA-CBD-CGD-O1D
8	M	403	BCL	CHA-CBD-CGD-O2D
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	301	BCL	C1A-C2A-CAA-CBA
8	L	301	BCL	C2C-C3C-CAC-CBC
8	L	301	BCL	C4C-C3C-CAC-CBC
8	L	301	BCL	C2-C3-C5-C6
8	L	304	BCL	C3A-C2A-CAA-CBA
8	L	304	BCL	C4C-C3C-CAC-CBC
8	L	304	BCL	O2A-C1-C2-C3
8	L	304	BCL	C1-C2-C3-C4
8	L	304	BCL	C1-C2-C3-C5
9	P	103	A1EFU	C4-C5-C6-C7
9	P	103	A1EFU	CM3-C5-C6-C7
9	P	103	A1EFU	C6-C7-C8-C9
9	P	103	A1EFU	C10-C11-C12-C13
9	P	103	A1EFU	C14-C15-C16-C17
9	P	103	A1EFU	C18-C19-C20-C21
9	P	103	A1EFU	C16-C17-C18-C19
9	P	103	A1EFU	C16-C17-C18-CM6
9	P	103	A1EFU	C11-C10-C9-C8
9	P	103	A1EFU	C11-C10-C9-CM4
9	P	103	A1EFU	C15-C16-C17-C18
9	P	103	A1EFU	C12-C13-C14-C15
9	P	103	A1EFU	CM5-C13-C14-C15
9	P	103	A1EFU	C20-C21-C22-CM7
9	P	103	A1EFU	C21-C22-C23-C24
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	C18-C19-C20-C21
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
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
9	v	103	A1EFU	C4-C5-C6-C7
9	v	103	A1EFU	CM3-C5-C6-C7
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	C20-C21-C22-C23
9	v	103	A1EFU	C20-C21-C22-CM7
9	v	103	A1EFU	C25-C26-C27-C28
9	v	103	A1EFU	CM8-C26-C27-C28
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	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-C23
9	T	101	A1EFU	C20-C21-C22-CM7
9	T	101	A1EFU	C26-C27-C28-C29
9	s	101	A1EFU	C2-C3-C4-C5
9	s	101	A1EFU	C4-C5-C6-C7
9	s	101	A1EFU	CM3-C5-C6-C7
9	s	101	A1EFU	C6-C7-C8-C9
9	s	101	A1EFU	C10-C11-C12-C13
9	s	101	A1EFU	C16-C17-C18-C19
9	s	101	A1EFU	C16-C17-C18-CM6
9	s	101	A1EFU	C11-C10-C9-C8
9	s	101	A1EFU	C11-C10-C9-CM4
9	s	101	A1EFU	C12-C13-C14-C15
9	s	101	A1EFU	CM5-C13-C14-C15
9	s	101	A1EFU	C20-C21-C22-CM7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	s	104	A1EFU	C2-C3-C4-C5
9	s	104	A1EFU	C6-C7-C8-C9
9	s	104	A1EFU	C2-C1-O1-CMA
9	s	104	A1EFU	CM1-C1-O1-CMA
9	s	104	A1EFU	C18-C19-C20-C21
9	s	104	A1EFU	C20-C21-C22-CM7
9	s	104	A1EFU	C26-C27-C28-C29
9	s	105	A1EFU	C2-C3-C4-C5
9	s	105	A1EFU	C6-C7-C8-C9
9	s	105	A1EFU	C10-C11-C12-C13
9	s	105	A1EFU	C2-C1-O1-CMA
9	s	105	A1EFU	CM1-C1-O1-CMA
9	s	105	A1EFU	CM2-C1-O1-CMA
9	s	105	A1EFU	C18-C19-C20-C21
9	s	105	A1EFU	C16-C17-C18-C19
9	s	105	A1EFU	C16-C17-C18-CM6
9	s	105	A1EFU	C11-C10-C9-C8
9	s	105	A1EFU	C11-C10-C9-CM4
9	s	105	A1EFU	C12-C13-C14-C15
9	s	105	A1EFU	CM5-C13-C14-C15
9	s	105	A1EFU	C20-C21-C22-C23
9	s	105	A1EFU	C20-C21-C22-CM7
9	s	105	A1EFU	C22-C23-C24-C25
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	C14-C15-C16-C17
9	r	102	A1EFU	C16-C17-C18-C19
9	r	102	A1EFU	C16-C17-C18-CM6
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	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
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-C23
9	R	101	A1EFU	C20-C21-C22-CM7
9	q	101	A1EFU	O1-C1-C2-O2
9	q	101	A1EFU	C4-C5-C6-C7
9	q	101	A1EFU	CM3-C5-C6-C7
9	q	101	A1EFU	C6-C7-C8-C9
9	q	101	A1EFU	C10-C11-C12-C13
9	q	101	A1EFU	C16-C17-C18-C19
9	q	101	A1EFU	C16-C17-C18-CM6
9	q	101	A1EFU	C11-C10-C9-C8
9	q	101	A1EFU	C11-C10-C9-CM4
9	q	101	A1EFU	C12-C13-C14-C15
9	q	101	A1EFU	CM5-C13-C14-C15
9	q	101	A1EFU	C20-C21-C22-C23
9	q	101	A1EFU	C21-C22-C23-C24
9	p	101	A1EFU	O1-C1-C2-O2
9	p	101	A1EFU	C2-C3-C4-C5
9	p	101	A1EFU	C4-C5-C6-C7
9	p	101	A1EFU	CM3-C5-C6-C7
9	p	101	A1EFU	C6-C7-C8-C9
9	p	101	A1EFU	C10-C11-C12-C13
9	p	101	A1EFU	C18-C19-C20-C21
9	p	101	A1EFU	C16-C17-C18-C19
9	p	101	A1EFU	C16-C17-C18-CM6
9	p	101	A1EFU	C12-C13-C14-C15
9	p	101	A1EFU	CM5-C13-C14-C15
9	p	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
9	2	101	A1EFU	C10-C11-C12-C13
9	2	101	A1EFU	C14-C15-C16-C17
9	2	101	A1EFU	C13-C14-C15-C16
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
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	C1-C2-C3-C4
9	2	102	A1EFU	O2-C2-C3-C4
9	2	102	A1EFU	C2-C3-C4-C5
9	2	102	A1EFU	C6-C7-C8-C9
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	C15-C16-C17-C18
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	2	102	A1EFU	C21-C22-C23-C24
9	2	104	A1EFU	C4-C5-C6-C7
9	2	104	A1EFU	CM3-C5-C6-C7
9	2	104	A1EFU	C6-C7-C8-C9
9	2	104	A1EFU	C10-C11-C12-C13
9	2	104	A1EFU	C17-C18-C19-C20
9	2	104	A1EFU	CM6-C18-C19-C20
9	2	104	A1EFU	C18-C19-C20-C21
9	2	104	A1EFU	C16-C17-C18-CM6
9	2	104	A1EFU	C11-C10-C9-C8
9	2	104	A1EFU	C11-C10-C9-CM4
9	2	104	A1EFU	C19-C20-C21-C22
9	2	104	A1EFU	C20-C21-C22-C23
9	2	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	C10-C11-C12-C13
9	N	102	A1EFU	C17-C18-C19-C20
9	N	102	A1EFU	CM6-C18-C19-C20

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	G	105	A1EFU	C11-C10-C9-C8
9	G	105	A1EFU	C11-C10-C9-CM4
9	G	105	A1EFU	C15-C16-C17-C18
9	G	105	A1EFU	C12-C13-C14-C15
9	G	105	A1EFU	CM5-C13-C14-C15
9	G	105	A1EFU	C20-C21-C22-C23
9	G	105	A1EFU	C20-C21-C22-CM7
9	G	105	A1EFU	CM7-C22-C23-C24
9	G	105	A1EFU	C26-C27-C28-C29
9	G	106	A1EFU	C2-C3-C4-C5
9	G	106	A1EFU	C4-C5-C6-C7
9	G	106	A1EFU	CM3-C5-C6-C7
9	G	106	A1EFU	C6-C7-C8-C9
9	G	106	A1EFU	C10-C11-C12-C13
9	G	106	A1EFU	C14-C15-C16-C17
9	G	106	A1EFU	C16-C17-C18-C19
9	G	106	A1EFU	C16-C17-C18-CM6
9	G	106	A1EFU	C11-C10-C9-C8
9	G	106	A1EFU	C11-C10-C9-CM4
9	G	106	A1EFU	C12-C13-C14-C15
9	G	106	A1EFU	CM5-C13-C14-C15
9	G	106	A1EFU	C20-C21-C22-CM7
9	G	106	A1EFU	C21-C22-C23-C24
9	f	101	A1EFU	C2-C3-C4-C5
9	f	101	A1EFU	C6-C7-C8-C9
9	f	101	A1EFU	C10-C11-C12-C13
9	f	101	A1EFU	C16-C17-C18-C19
9	f	101	A1EFU	C16-C17-C18-CM6
9	f	101	A1EFU	C11-C10-C9-C8
9	f	101	A1EFU	C11-C10-C9-CM4
9	f	101	A1EFU	C12-C13-C14-C15
9	f	101	A1EFU	CM5-C13-C14-C15
9	f	101	A1EFU	C20-C21-C22-CM7
9	f	101	A1EFU	CM7-C22-C23-C24
9	f	101	A1EFU	C26-C27-C28-C29
9	F	104	A1EFU	C4-C5-C6-C7
9	F	104	A1EFU	CM3-C5-C6-C7
9	F	104	A1EFU	C6-C7-C8-C9
9	F	104	A1EFU	C10-C11-C12-C13
9	F	104	A1EFU	C18-C19-C20-C21
9	F	104	A1EFU	C16-C17-C18-C19
9	F	104	A1EFU	C16-C17-C18-CM6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	F	104	A1EFU	C11-C10-C9-C8
9	F	104	A1EFU	C11-C10-C9-CM4
9	F	104	A1EFU	C12-C13-C14-C15
9	F	104	A1EFU	CM5-C13-C14-C15
9	F	104	A1EFU	C20-C21-C22-C23
9	F	104	A1EFU	C20-C21-C22-CM7
9	F	104	A1EFU	C22-C23-C24-C25
9	E	102	A1EFU	C6-C7-C8-C9
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
9	E	103	A1EFU	O1-C1-C2-O2
9	E	103	A1EFU	C2-C3-C4-C5
9	E	103	A1EFU	C4-C5-C6-C7
9	E	103	A1EFU	CM3-C5-C6-C7
9	E	103	A1EFU	C6-C7-C8-C9
9	E	103	A1EFU	C10-C11-C12-C13
9	E	103	A1EFU	C16-C17-C18-C19
9	E	103	A1EFU	C16-C17-C18-CM6
9	E	103	A1EFU	C11-C10-C9-C8
9	E	103	A1EFU	C11-C10-C9-CM4
9	E	103	A1EFU	C12-C13-C14-C15
9	E	103	A1EFU	CM5-C13-C14-C15
9	E	103	A1EFU	C20-C21-C22-CM7
9	E	103	A1EFU	C21-C22-C23-C24
9	E	103	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	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
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	CM5-C13-C14-C15
9	D	104	A1EFU	C20-C21-C22-CM7
9	D	104	A1EFU	C22-C23-C24-C25
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	C4-C5-C6-C7
9	D	105	A1EFU	CM3-C5-C6-C7
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	C16-C17-C18-C19
9	D	105	A1EFU	C16-C17-C18-CM6
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	B	103	A1EFU	O1-C1-C2-O2
9	B	103	A1EFU	C2-C3-C4-C5
9	B	103	A1EFU	C4-C5-C6-C7
9	B	103	A1EFU	CM3-C5-C6-C7
9	B	103	A1EFU	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	B	103	A1EFU	C10-C11-C12-C13
9	B	103	A1EFU	C14-C15-C16-C17
9	B	103	A1EFU	C11-C10-C9-C8
9	B	103	A1EFU	C11-C10-C9-CM4
9	B	103	A1EFU	C12-C13-C14-C15
9	B	103	A1EFU	CM5-C13-C14-C15
9	B	103	A1EFU	C20-C21-C22-CM7
9	B	103	A1EFU	C26-C27-C28-C29
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	C16-C17-C18-C19
9	a	102	A1EFU	C16-C17-C18-CM6
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	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	C2-C1-O1-CMA
9	A	102	A1EFU	CM1-C1-O1-CMA
9	A	102	A1EFU	CM2-C1-O1-CMA
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	C11-C10-C9-C8
9	M	407	A1EFU	C11-C10-C9-CM4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	M	407	A1EFU	C12-C13-C14-C15
9	M	407	A1EFU	CM5-C13-C14-C15
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	R	103	MW9	C33-C34-C35-C36
10	R	103	MW9	C20-O2-P-O3
10	R	103	MW9	C21-O5-P-O2
10	R	103	MW9	C21-O5-P-O3
10	R	103	MW9	C21-O5-P-O4
10	G	103	MW9	C21-C22-C23-O6
10	G	103	MW9	O7-C22-C23-O6
10	G	103	MW9	O9-C24-O8-C19
10	G	104	MW9	C25-C24-O8-C19
10	G	104	MW9	C21-O5-P-O3
10	G	104	MW9	C21-O5-P-O4
10	F	103	MW9	O5-C21-C22-C23
10	F	103	MW9	C25-C24-O8-C19
10	F	103	MW9	C21-O5-P-O4
10	D	103	MW9	O9-C24-O8-C19
10	D	103	MW9	C33-C34-C35-C36
10	D	103	MW9	C20-O2-P-O3
10	D	103	MW9	C20-O2-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	C20-O2-P-O5
10	M	406	MW9	C16-C17-O1-C18
10	M	406	MW9	O5-C21-C22-C23
10	M	406	MW9	C25-C24-O8-C19
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	L	307	MW9	O5-C21-C22-C23
10	L	307	MW9	O5-C21-C22-O7
10	L	307	MW9	C21-C22-C23-O6
10	H	303	MW9	C20-O2-P-O3
10	H	303	MW9	C20-O2-P-O5
11	D	102	LMT	C2-C1-O1'-C1'
11	L	305	LMT	O5'-C1'-O1'-C1
11	L	305	LMT	C2-C1-O1'-C1'
11	L	306	LMT	C2'-C1'-O1'-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	L	306	LMT	O5'-C1'-O1'-C1
11	L	306	LMT	C2-C1-O1'-C1'
11	H	302	LMT	C2'-C1'-O1'-C1
11	H	302	LMT	O5'-C1'-O1'-C1
11	C	404	LMT	O5'-C1'-O1'-C1
13	M	404	U10	C14-C16-C17-C18
13	M	404	U10	C19-C21-C22-C23
13	M	404	U10	C34-C36-C37-C38
13	M	404	U10	C49-C51-C52-C53
13	L	303	U10	C25-C24-C26-C27
14	M	408	BPH	C3A-C2A-CAA-CBA
14	M	408	BPH	C1A-C2A-CAA-CBA
14	M	408	BPH	C2A-CAA-CBA-CGA
15	L	308	CDL	CB2-C1-CA2-OA2
15	L	308	CDL	CA2-OA2-PA1-OA5
15	L	308	CDL	CA3-OA5-PA1-OA2
15	L	308	CDL	CA3-OA5-PA1-OA3
15	L	308	CDL	CA3-OA5-PA1-OA4
15	L	308	CDL	C31-CA7-OA8-CA6
15	L	308	CDL	CB3-OB5-PB2-OB3
15	L	308	CDL	CB3-OB5-PB2-OB4
15	H	304	CDL	CA2-OA2-PA1-OA3
15	H	304	CDL	CA2-OA2-PA1-OA4
15	H	304	CDL	CB3-OB5-PB2-OB3
15	H	304	CDL	CB3-OB5-PB2-OB4
15	H	304	CDL	C51-CB5-OB6-CB4
8	F	102	BCL	O1A-CGA-O2A-C1
8	E	101	BCL	O1A-CGA-O2A-C1
10	R	103	MW9	O-C17-O1-C18
10	F	103	MW9	O-C17-O1-C18
10	M	406	MW9	O-C17-O1-C18
15	L	308	CDL	OA9-CA7-OA8-CA6
8	F	102	BCL	CBA-CGA-O2A-C1
10	R	103	MW9	C16-C17-O1-C18
10	F	103	MW9	C16-C17-O1-C18
15	H	304	CDL	OA9-CA7-OA8-CA6
16	C	401	HEC	C4C-C3C-CAC-CBC
10	G	104	MW9	O9-C24-O8-C19
10	F	103	MW9	O9-C24-O8-C19
15	L	308	CDL	OA7-CA5-OA6-CA4
15	H	304	CDL	OA7-CA5-OA6-CA4
15	H	304	CDL	OB7-CB5-OB6-CB4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	d	101	BCL	C3-C5-C6-C7
8	P	102	BCL	CBA-CGA-O2A-C1
8	E	101	BCL	CBA-CGA-O2A-C1
15	H	304	CDL	C31-CA7-OA8-CA6
10	G	103	MW9	C25-C24-O8-C19
10	D	103	MW9	C25-C24-O8-C19
15	L	308	CDL	C11-CA5-OA6-CA4
15	H	304	CDL	C11-CA5-OA6-CA4
11	D	102	LMT	O5'-C5'-C6'-O6'
8	L	301	BCL	C4-C3-C5-C6
8	L	304	BCL	C4-C3-C5-C6
9	T	101	A1EFU	CM8-C26-C27-C28
9	s	101	A1EFU	CM8-C26-C27-C28
9	2	102	A1EFU	CM7-C22-C23-C24
9	K	102	A1EFU	CM7-C22-C23-C24
9	F	104	A1EFU	CM7-C22-C23-C24
9	E	103	A1EFU	CM7-C22-C23-C24
9	A	102	A1EFU	CM7-C22-C23-C24
8	s	103	BCL	C2-C3-C5-C6
9	T	101	A1EFU	C25-C26-C27-C28
13	L	303	U10	C23-C24-C26-C27
8	G	102	BCL	C2A-CAA-CBA-CGA
10	G	103	MW9	C5-C6-C7-C8
10	H	301	MW9	C5-C6-C7-C8
11	D	102	LMT	C3'-C4'-O1B-C1B
8	n	101	BCL	CBA-CGA-O2A-C1
10	G	104	MW9	C16-C17-O1-C18
10	L	307	MW9	C16-C17-O1-C18
10	M	405	MW9	C31-C32-C33-C34
8	s	103	BCL	C1-C2-C3-C5
8	n	101	BCL	O1A-CGA-O2A-C1
8	L	301	BCL	O1A-CGA-O2A-C1
10	G	104	MW9	O-C17-O1-C18
10	L	307	MW9	O-C17-O1-C18
9	P	103	A1EFU	C13-C14-C15-C16
9	s	104	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	C5-C6-C7-C8
9	2	104	A1EFU	C15-C16-C17-C18
9	N	102	A1EFU	C19-C20-C21-C22
9	j	101	A1EFU	C19-C20-C21-C22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	G	105	A1EFU	C13-C14-C15-C16
9	G	106	A1EFU	C13-C14-C15-C16
10	F	103	MW9	O5-C21-C22-O7
10	M	406	MW9	O5-C21-C22-O7
15	L	308	CDL	O1-C1-CA2-OA2
8	S	101	BCL	C3-C5-C6-C7
8	t	101	BCL	C3-C5-C6-C7
8	2	103	BCL	C3-C5-C6-C7
8	i	101	BCL	CBA-CGA-O2A-C1
9	2	102	A1EFU	C14-C15-C16-C17
8	b	101	BCL	C3-C5-C6-C7
8	B	101	BCL	C3-C5-C6-C7
8	M	403	BCL	C3-C5-C6-C7
8	i	101	BCL	O1A-CGA-O2A-C1
9	s	104	A1EFU	CM8-C26-C27-C28
9	r	102	A1EFU	CM7-C22-C23-C24
9	q	101	A1EFU	CM8-C26-C27-C28
11	D	102	LMT	C4'-C5'-C6'-O6'
8	A	101	BCL	C2-C3-C5-C6
9	q	101	A1EFU	C25-C26-C27-C28
9	p	101	A1EFU	C21-C22-C23-C24
9	N	102	A1EFU	C21-C22-C23-C24
9	k	101	A1EFU	C21-C22-C23-C24
9	D	105	A1EFU	C21-C22-C23-C24
9	B	103	A1EFU	C21-C22-C23-C24
9	a	102	A1EFU	C21-C22-C23-C24
8	I	101	BCL	C2A-CAA-CBA-CGA
8	v	101	BCL	O1A-CGA-O2A-C1
9	v	102	A1EFU	C22-C23-C24-C25
9	s	101	A1EFU	C22-C23-C24-C25
9	s	104	A1EFU	C22-C23-C24-C25
9	s	105	A1EFU	C26-C27-C28-C29
9	q	101	A1EFU	C22-C23-C24-C25
9	p	101	A1EFU	C26-C27-C28-C29
9	k	101	A1EFU	C22-C23-C24-C25
9	j	101	A1EFU	C26-C27-C28-C29
13	L	303	U10	C9-C11-C12-C13
13	L	303	U10	C19-C21-C22-C23
13	L	303	U10	C29-C31-C32-C33
8	v	101	BCL	CBA-CGA-O2A-C1
8	L	301	BCL	CBA-CGA-O2A-C1
10	D	103	MW9	O5-C21-C22-C23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	H	301	MW9	O5-C21-C22-C23
15	L	308	CDL	CA2-C1-CB2-OB2
8	M	403	BCL	CBA-CGA-O2A-C1
9	N	102	A1EFU	C9-C10-C11-C12
10	R	103	MW9	C12-C13-C14-C15
10	G	104	MW9	O8-C19-C20-O2
10	D	103	MW9	O5-C21-C22-O7
9	s	101	A1EFU	C25-C26-C27-C28
8	s	103	BCL	C6-C7-C8-C9
8	2	103	BCL	C6-C7-C8-C9
8	j	102	BCL	C6-C7-C8-C9
8	i	101	BCL	C6-C7-C8-C9
8	M	402	BCL	C6-C7-C8-C9
8	M	403	BCL	C6-C7-C8-C9
8	L	304	BCL	C6-C7-C8-C9
14	L	302	BPH	C14-C13-C15-C16
8	P	102	BCL	C8-C10-C11-C12
10	M	405	MW9	C25-C24-O8-C19
10	M	406	MW9	C6-C7-C8-C9
15	L	308	CDL	CB7-C71-C72-C73
15	H	304	CDL	CA7-C31-C32-C33
8	d	101	BCL	C15-C16-C17-C18
8	i	101	BCL	C3-C5-C6-C7
8	A	101	BCL	C3-C5-C6-C7
8	k	102	BCL	C10-C11-C12-C13
8	J	101	BCL	C10-C11-C12-C13
8	e	101	BCL	C8-C10-C11-C12
10	M	405	MW9	C24-C25-C26-C27
8	v	101	BCL	C15-C16-C17-C18
8	F	101	BCL	C5-C6-C7-C8
10	H	301	MW9	C14-C15-C16-C17
15	H	304	CDL	CA5-C11-C12-C13
15	H	304	CDL	CB7-C71-C72-C73
8	l	101	BCL	C10-C11-C12-C13
8	n	101	BCL	C5-C6-C7-C8
8	G	101	BCL	C5-C6-C7-C8
8	F	101	BCL	C10-C11-C12-C13
8	k	102	BCL	C5-C6-C7-C8
8	B	101	BCL	C10-C11-C12-C13
10	G	104	MW9	C30-C31-C32-C33
9	G	105	A1EFU	CM1-C1-C2-O2
8	2	103	BCL	C11-C10-C8-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	j	102	BCL	C6-C7-C8-C10
8	E	101	BCL	C11-C12-C13-C15
14	L	302	BPH	C11-C12-C13-C15
9	j	101	A1EFU	C15-C16-C17-C18
9	I	102	A1EFU	C13-C14-C15-C16
9	M	407	A1EFU	C19-C20-C21-C22
10	H	303	MW9	C24-C25-C26-C27
8	B	101	BCL	C2A-CAA-CBA-CGA
9	v	103	A1EFU	C22-C23-C24-C25
9	N	102	A1EFU	C26-C27-C28-C29
9	J	102	A1EFU	C26-C27-C28-C29
9	I	102	A1EFU	C22-C23-C24-C25
9	f	101	A1EFU	C22-C23-C24-C25
9	B	102	A1EFU	C26-C27-C28-C29
9	a	102	A1EFU	C22-C23-C24-C25
13	M	404	U10	C29-C31-C32-C33
13	L	303	U10	C14-C16-C17-C18
9	v	103	A1EFU	C6-C7-C8-C9
9	T	101	A1EFU	C18-C19-C20-C21
9	s	101	A1EFU	C18-C19-C20-C21
9	s	104	A1EFU	C10-C11-C12-C13
9	r	102	A1EFU	C10-C11-C12-C13
9	r	102	A1EFU	C18-C19-C20-C21
9	2	101	A1EFU	C18-C19-C20-C21
9	k	101	A1EFU	C6-C7-C8-C9
9	I	102	A1EFU	C6-C7-C8-C9
9	G	105	A1EFU	C6-C7-C8-C9
9	G	105	A1EFU	C10-C11-C12-C13
9	G	105	A1EFU	C18-C19-C20-C21
9	E	103	A1EFU	C18-C19-C20-C21
9	D	105	A1EFU	C18-C19-C20-C21
9	a	102	A1EFU	C18-C19-C20-C21
9	v	102	A1EFU	CM1-C1-C2-C3
10	G	104	MW9	C5-C6-C7-C8
10	F	103	MW9	C5-C6-C7-C8
10	G	103	MW9	O5-C21-C22-O7
10	H	301	MW9	O5-C21-C22-O7
15	L	308	CDL	O1-C1-CB2-OB2
10	M	405	MW9	O9-C24-O8-C19
8	P	102	BCL	C15-C16-C17-C18
8	r	101	BCL	C13-C15-C16-C17
8	e	101	BCL	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	G	103	MW9	C14-C15-C16-C17
8	q	102	BCL	C15-C16-C17-C18
8	2	103	BCL	C15-C16-C17-C18
8	a	101	BCL	C10-C11-C12-C13
8	2	103	BCL	C10-C11-C12-C13
8	j	102	BCL	C5-C6-C7-C8
10	G	103	MW9	C20-O2-P-O5
10	G	104	MW9	C21-O5-P-O2
10	D	103	MW9	C20-O2-P-O5
10	D	103	MW9	C21-O5-P-O2
10	H	301	MW9	C21-O5-P-O2
15	L	308	CDL	CB3-OB5-PB2-OB2
15	H	304	CDL	CA2-OA2-PA1-OA5
15	H	304	CDL	CB3-OB5-PB2-OB2
10	M	406	MW9	C14-C15-C16-C17
10	G	103	MW9	O5-C21-C22-C23
9	J	102	A1EFU	CM8-C26-C27-C28
14	M	408	BPH	C4-C3-C5-C6
9	j	103	A1EFU	C21-C22-C23-C24
8	F	101	BCL	C13-C15-C16-C17
8	I	101	BCL	C16-C17-C18-C20
8	Q	101	BCL	C3-C5-C6-C7
8	G	101	BCL	C10-C11-C12-C13
8	b	101	BCL	C13-C15-C16-C17
9	v	102	A1EFU	C19-C20-C21-C22
9	R	101	A1EFU	C5-C6-C7-C8
9	2	102	A1EFU	C19-C20-C21-C22
10	G	104	MW9	C14-C15-C16-C17
8	s	103	BCL	C5-C6-C7-C8
8	j	102	BCL	C15-C16-C17-C18
9	s	104	A1EFU	CM5-C13-C14-C15
9	s	105	A1EFU	CM3-C5-C6-C7
9	R	101	A1EFU	C16-C17-C18-CM6
9	p	101	A1EFU	C11-C10-C9-CM4
9	2	102	A1EFU	CM3-C5-C6-C7
9	2	104	A1EFU	CM5-C13-C14-C15
9	N	102	A1EFU	C16-C17-C18-CM6
9	J	102	A1EFU	CM3-C5-C6-C7
9	E	102	A1EFU	CM3-C5-C6-C7
9	B	103	A1EFU	C16-C17-C18-CM6
9	a	102	A1EFU	C11-C10-C9-CM4
10	G	104	MW9	C13-C14-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	D	103	MW9	C6-C7-C8-C9
10	M	405	MW9	C13-C14-C15-C16
10	M	406	MW9	C13-C14-C15-C16
15	L	308	CDL	C54-C55-C56-C57
8	Q	101	BCL	C16-C17-C18-C19
10	F	103	MW9	C13-C14-C15-C16
10	H	303	MW9	C10-C11-C12-C13
10	H	303	MW9	C7-C8-C9-C10
11	D	102	LMT	C2-C3-C4-C5
10	F	103	MW9	C11-C12-C13-C14
10	F	103	MW9	C28-C29-C30-C31
15	L	308	CDL	C11-C12-C13-C14
15	L	308	CDL	C55-C56-C57-C58
10	H	301	MW9	C4-C5-C6-C7
15	H	304	CDL	C58-C59-C60-C61
15	H	304	CDL	C76-C77-C78-C79
10	G	104	MW9	O5-C21-C22-O7
10	M	406	MW9	C4-C5-C6-C7
8	L	301	BCL	C3-C5-C6-C7
9	s	104	A1EFU	CM2-C1-O1-CMA
9	s	104	A1EFU	C12-C13-C14-C15
9	s	105	A1EFU	C4-C5-C6-C7
9	R	101	A1EFU	C16-C17-C18-C19
9	p	101	A1EFU	C11-C10-C9-C8
9	2	102	A1EFU	C4-C5-C6-C7
9	2	104	A1EFU	C16-C17-C18-C19
9	2	104	A1EFU	C12-C13-C14-C15
9	N	102	A1EFU	C16-C17-C18-C19
9	K	102	A1EFU	C16-C17-C18-C19
9	J	102	A1EFU	C4-C5-C6-C7
9	E	102	A1EFU	C4-C5-C6-C7
9	D	104	A1EFU	C12-C13-C14-C15
9	B	103	A1EFU	C16-C17-C18-C19
9	a	102	A1EFU	C11-C10-C9-C8
11	L	305	LMT	C2'-C1'-O1'-C1
8	A	101	BCL	C1-C2-C3-C5
10	M	406	MW9	C27-C28-C29-C30
10	H	303	MW9	C13-C14-C15-C16
11	C	404	LMT	C2-C3-C4-C5
10	G	103	MW9	C10-C11-C12-C13
10	F	103	MW9	C9-C10-C11-C12
10	M	405	MW9	C9-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	M	406	MW9	C7-C8-C9-C10
10	H	301	MW9	C12-C13-C14-C15
10	H	301	MW9	C13-C14-C15-C16
8	a	101	BCL	C2-C3-C5-C6
14	M	408	BPH	C2-C3-C5-C6
8	q	102	BCL	C11-C10-C8-C9
8	N	101	BCL	C6-C7-C8-C9
8	F	102	BCL	C6-C7-C8-C9
8	E	101	BCL	C11-C12-C13-C14
8	M	402	BCL	C11-C10-C8-C9
10	F	103	MW9	C6-C7-C8-C9
10	M	406	MW9	C35-C36-C37-C38
15	H	304	CDL	C32-C33-C34-C35
10	M	405	MW9	C26-C27-C28-C29
10	H	301	MW9	C2-C3-C4-C5
15	L	308	CDL	C52-C53-C54-C55
10	R	103	MW9	C21-C22-C23-O6
10	F	103	MW9	C21-C22-C23-O6
10	M	405	MW9	C21-C22-C23-O6
10	H	301	MW9	C21-C22-C23-O6
10	H	301	MW9	C25-C24-O8-C19
10	G	103	MW9	C27-C28-C29-C30
10	H	301	MW9	C6-C7-C8-C9
15	L	308	CDL	C14-C15-C16-C17
15	L	308	CDL	C16-C17-C18-C19
10	H	301	MW9	C29-C30-C31-C32
10	R	103	MW9	C27-C28-C29-C30
10	G	103	MW9	C13-C14-C15-C16
15	H	304	CDL	C11-C12-C13-C14
16	C	402	HEC	C4C-C3C-CAC-CBC
8	Q	101	BCL	C16-C17-C18-C20
8	I	101	BCL	C16-C17-C18-C19
9	T	101	A1EFU	C22-C23-C24-C25
9	2	102	A1EFU	C26-C27-C28-C29
10	D	103	MW9	C12-C13-C14-C15
10	D	103	MW9	C4-C5-C6-C7
10	M	406	MW9	C10-C11-C12-C13
10	L	307	MW9	C13-C14-C15-C16
10	H	301	MW9	C27-C28-C29-C30
15	H	304	CDL	C72-C73-C74-C75
10	G	103	MW9	C7-C8-C9-C10
10	M	406	MW9	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	E	102	A1EFU	C2-C3-C4-C5
8	i	101	BCL	C10-C11-C12-C13
8	G	101	BCL	C8-C10-C11-C12
10	G	104	MW9	C26-C27-C28-C29
10	L	307	MW9	C26-C27-C28-C29
8	t	101	BCL	C3A-C2A-CAA-CBA
8	s	102	BCL	C3A-C2A-CAA-CBA
8	s	103	BCL	C3A-C2A-CAA-CBA
8	r	101	BCL	C3A-C2A-CAA-CBA
8	R	102	BCL	C3A-C2A-CAA-CBA
8	q	102	BCL	C3A-C2A-CAA-CBA
8	K	101	BCL	C3A-C2A-CAA-CBA
8	j	102	BCL	C3A-C2A-CAA-CBA
8	G	101	BCL	C3A-C2A-CAA-CBA
8	G	102	BCL	C3A-C2A-CAA-CBA
8	F	101	BCL	C3A-C2A-CAA-CBA
8	d	101	BCL	C3A-C2A-CAA-CBA
8	a	101	BCL	C3A-C2A-CAA-CBA
8	A	101	BCL	C3A-C2A-CAA-CBA
8	M	402	BCL	C3A-C2A-CAA-CBA
8	d	101	BCL	C10-C11-C12-C13
11	H	302	LMT	C2-C1-O1'-C1'
10	R	103	MW9	C11-C12-C13-C14
10	G	103	MW9	C26-C27-C28-C29
10	F	103	MW9	C10-C11-C12-C13
15	H	304	CDL	C74-C75-C76-C77
8	e	101	BCL	C16-C17-C18-C20
10	R	103	MW9	C13-C14-C15-C16
10	R	103	MW9	C25-C26-C27-C28
10	H	301	MW9	C10-C11-C12-C13
10	D	103	MW9	C24-C25-C26-C27
8	d	101	BCL	C4-C3-C5-C6
9	D	104	A1EFU	CM8-C26-C27-C28
8	2	103	BCL	C2-C3-C5-C6
9	s	104	A1EFU	C25-C26-C27-C28
10	M	406	MW9	C9-C10-C11-C12
10	M	405	MW9	O7-C22-C23-O6
10	L	307	MW9	O7-C22-C23-O6
8	s	103	BCL	C15-C16-C17-C18
10	G	103	MW9	C6-C7-C8-C9
10	M	406	MW9	C25-C26-C27-C28
11	C	404	LMT	C3-C4-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	D	103	MW9	C27-C28-C29-C30
10	R	103	MW9	C10-C11-C12-C13
10	G	104	MW9	C27-C28-C29-C30
10	M	405	MW9	C11-C12-C13-C14
10	H	301	MW9	O9-C24-O8-C19
10	H	303	MW9	C12-C13-C14-C15
11	L	306	LMT	C5-C6-C7-C8
15	L	308	CDL	C15-C16-C17-C18
8	L	304	BCL	O1A-CGA-O2A-C1
8	G	102	BCL	CBA-CGA-O2A-C1
10	G	104	MW9	C10-C11-C12-C13
9	P	103	A1EFU	CM8-C26-C27-C28
9	s	101	A1EFU	CM7-C22-C23-C24
8	P	101	BCL	C6-C7-C8-C10
8	s	103	BCL	C6-C7-C8-C10
8	q	102	BCL	C11-C10-C8-C7
8	N	101	BCL	C6-C7-C8-C10
8	j	102	BCL	C11-C10-C8-C7
8	F	102	BCL	C6-C7-C8-C10
8	B	101	BCL	C11-C10-C8-C7
8	M	402	BCL	C6-C7-C8-C10
8	M	402	BCL	C11-C10-C8-C7
8	M	403	BCL	C6-C7-C8-C10
8	L	304	BCL	C6-C7-C8-C10
10	R	103	MW9	C31-C32-C33-C34
8	a	101	BCL	O1A-CGA-O2A-C1
9	v	103	A1EFU	C5-C6-C7-C8
8	s	103	BCL	C16-C17-C18-C20
8	L	301	BCL	C16-C17-C18-C19
10	R	103	MW9	C29-C30-C31-C32
10	R	103	MW9	O9-C24-O8-C19
8	L	304	BCL	CBA-CGA-O2A-C1
10	M	405	MW9	C16-C17-O1-C18
10	H	303	MW9	C16-C17-O1-C18
8	v	101	BCL	C8-C10-C11-C12
15	H	304	CDL	C60-C61-C62-C63
15	H	304	CDL	C75-C76-C77-C78
10	G	103	MW9	C9-C10-C11-C12
15	L	308	CDL	C13-C14-C15-C16
10	R	103	MW9	C35-C36-C37-C38
10	G	104	MW9	C6-C7-C8-C9
8	1	101	BCL	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	K	101	BCL	CBA-CGA-O2A-C1
8	e	101	BCL	C16-C17-C18-C19
10	D	103	MW9	C14-C15-C16-C17
10	R	103	MW9	C25-C24-O8-C19
9	J	103	A1EFU	C18-C19-C20-C21
10	F	103	MW9	C12-C13-C14-C15
9	j	101	A1EFU	C14-C15-C16-C17
8	A	101	BCL	C15-C16-C17-C18
8	s	103	BCL	O1A-CGA-O2A-C1
8	P	102	BCL	C10-C11-C12-C13
8	s	102	BCL	C13-C15-C16-C17
10	M	406	MW9	C29-C30-C31-C32
8	v	101	BCL	C4-C3-C5-C6
8	S	101	BCL	C4-C3-C5-C6
9	I	102	A1EFU	CM8-C26-C27-C28
9	M	407	A1EFU	CM8-C26-C27-C28
9	J	102	A1EFU	C25-C26-C27-C28
8	t	101	BCL	C11-C12-C13-C14
8	s	102	BCL	C6-C7-C8-C9
8	2	103	BCL	C11-C10-C8-C9
8	j	102	BCL	C11-C10-C8-C9
8	G	102	BCL	C6-C7-C8-C9
8	B	101	BCL	C11-C10-C8-C9
8	L	301	BCL	C11-C10-C8-C9
8	N	101	BCL	C2A-CAA-CBA-CGA
8	A	101	BCL	C2A-CAA-CBA-CGA
10	H	301	MW9	C3-C4-C5-C6
8	K	101	BCL	O1A-CGA-O2A-C1
8	t	101	BCL	C1A-C2A-CAA-CBA
8	s	103	BCL	C1A-C2A-CAA-CBA
8	R	102	BCL	C1A-C2A-CAA-CBA
8	N	101	BCL	C1A-C2A-CAA-CBA
8	B	101	BCL	C1A-C2A-CAA-CBA
8	a	101	BCL	C1A-C2A-CAA-CBA
8	L	304	BCL	C1A-C2A-CAA-CBA
8	P	102	BCL	C16-C17-C18-C20
8	S	101	BCL	C16-C17-C18-C20
10	G	103	MW9	C34-C35-C36-C37
10	D	103	MW9	C13-C14-C15-C16
10	D	103	MW9	C34-C35-C36-C37
10	L	307	MW9	C30-C31-C32-C33
9	a	102	A1EFU	C13-C14-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	v	101	BCL	C10-C11-C12-C13
10	R	103	MW9	C20-O2-P-O5
11	D	102	LMT	C5'-C4'-O1B-C1B
14	M	408	BPH	C8-C10-C11-C12
10	R	103	MW9	C18-C19-C20-O2
10	G	104	MW9	C18-C19-C20-O2
10	H	303	MW9	C29-C30-C31-C32
8	P	101	BCL	C2C-C3C-CAC-CBC
8	V	101	BCL	C2C-C3C-CAC-CBC
8	q	102	BCL	C2C-C3C-CAC-CBC
8	G	101	BCL	C2C-C3C-CAC-CBC
8	D	101	BCL	C2C-C3C-CAC-CBC
8	B	101	BCL	C2C-C3C-CAC-CBC
8	A	101	BCL	C2C-C3C-CAC-CBC
8	L	304	BCL	C2C-C3C-CAC-CBC
8	N	101	BCL	C15-C16-C17-C18
8	e	101	BCL	C15-C16-C17-C18
8	d	101	BCL	O1A-CGA-O2A-C1
10	M	405	MW9	O-C17-O1-C18
8	s	103	BCL	C16-C17-C18-C19
15	H	304	CDL	C33-C34-C35-C36
10	D	103	MW9	C26-C27-C28-C29
10	H	303	MW9	O-C17-O1-C18
10	M	405	MW9	C7-C8-C9-C10
9	q	101	A1EFU	C26-C27-C28-C29
10	H	301	MW9	O7-C22-C23-O6
10	G	104	MW9	C29-C30-C31-C32
10	F	103	MW9	C29-C30-C31-C32
10	M	405	MW9	C29-C30-C31-C32
8	S	101	BCL	C15-C16-C17-C18
10	H	301	MW9	C11-C12-C13-C14
10	H	301	MW9	C9-C10-C11-C12
8	L	301	BCL	C15-C16-C17-C18
9	2	102	A1EFU	C11-C10-C9-CM4
9	f	101	A1EFU	CM3-C5-C6-C7
8	2	103	BCL	C4-C3-C5-C6
11	H	302	LMT	C7-C8-C9-C10
10	R	103	MW9	C14-C15-C16-C17
8	S	101	BCL	C16-C17-C18-C19
11	H	302	LMT	O5'-C5'-C6'-O6'
10	D	103	MW9	C10-C11-C12-C13
8	G	102	BCL	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	L	304	BCL	C5-C6-C7-C8
10	H	303	MW9	C20-O2-P-O4
10	H	303	MW9	C27-C28-C29-C30
15	H	304	CDL	C54-C55-C56-C57
10	H	303	MW9	C19-C18-O1-C17
10	M	406	MW9	O8-C19-C20-O2
15	H	304	CDL	OA5-CA3-CA4-OA6
8	P	102	BCL	C16-C17-C18-C19
10	F	103	MW9	C14-C15-C16-C17
8	F	101	BCL	O1A-CGA-O2A-C1
10	M	406	MW9	C34-C35-C36-C37
8	2	103	BCL	C5-C6-C7-C8
8	a	101	BCL	C8-C10-C11-C12
8	L	301	BCL	C13-C15-C16-C17
9	T	101	A1EFU	CM1-C1-O1-CMA
9	T	101	A1EFU	CM2-C1-O1-CMA
9	F	104	A1EFU	CM1-C1-O1-CMA
9	F	104	A1EFU	CM2-C1-O1-CMA
9	M	407	A1EFU	CM2-C1-O1-CMA
11	D	102	LMT	C2'-C1'-O1'-C1
11	C	404	LMT	C2'-C1'-O1'-C1
10	R	103	MW9	O1-C18-C19-O8
15	L	308	CDL	OA6-CA4-CA6-OA8
8	2	103	BCL	C1-C2-C3-C5
10	H	303	MW9	C25-C26-C27-C28
8	v	101	BCL	C6-C7-C8-C10
8	t	101	BCL	C11-C12-C13-C15
8	s	102	BCL	C6-C7-C8-C10
8	s	103	BCL	C11-C12-C13-C15
8	s	103	BCL	C12-C13-C15-C16
8	R	102	BCL	C12-C13-C15-C16
8	G	102	BCL	C6-C7-C8-C10
8	d	101	BCL	C11-C10-C8-C7
8	a	101	BCL	C11-C10-C8-C7
8	L	301	BCL	C11-C10-C8-C7
8	L	304	BCL	C12-C13-C15-C16
9	D	104	A1EFU	C25-C26-C27-C28
8	R	102	BCL	C3-C5-C6-C7
10	G	103	MW9	C4-C5-C6-C7
8	P	101	BCL	C6-C7-C8-C9
8	v	101	BCL	C6-C7-C8-C9
8	s	103	BCL	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	s	103	BCL	C14-C13-C15-C16
8	R	102	BCL	C14-C13-C15-C16
8	d	101	BCL	C11-C10-C8-C9
8	d	101	BCL	C11-C12-C13-C14
8	a	101	BCL	C11-C10-C8-C9
8	L	301	BCL	C6-C7-C8-C9
14	M	408	BPH	C6-C7-C8-C9
8	G	102	BCL	C16-C17-C18-C19
11	L	305	LMT	C3-C4-C5-C6
10	G	104	MW9	O5-C21-C22-C23
15	H	304	CDL	C15-C16-C17-C18
8	R	102	BCL	CBA-CGA-O2A-C1
10	H	303	MW9	C11-C12-C13-C14
8	d	101	BCL	C5-C6-C7-C8
10	D	103	MW9	C3-C4-C5-C6
10	G	103	MW9	C18-C19-C20-O2
10	F	103	MW9	C18-C19-C20-O2
9	v	102	A1EFU	C26-C27-C28-C29
9	r	102	A1EFU	C22-C23-C24-C25
9	j	101	A1EFU	C22-C23-C24-C25
13	M	404	U10	C9-C11-C12-C13
10	M	406	MW9	C36-C37-C38-C39
8	G	102	BCL	C10-C11-C12-C13
8	q	102	BCL	C4-C3-C5-C6
9	2	104	A1EFU	CM7-C22-C23-C24
8	d	101	BCL	C2-C3-C5-C6
9	v	103	A1EFU	CM1-C1-C2-C3
9	T	101	A1EFU	C2-C3-C4-C5
9	s	105	A1EFU	CM1-C1-C2-C3
9	G	105	A1EFU	CM1-C1-C2-C3
10	H	303	MW9	C6-C7-C8-C9
10	R	103	MW9	O5-C21-C22-O7
15	H	304	CDL	C13-C14-C15-C16
10	H	303	MW9	C9-C10-C11-C12
8	q	102	BCL	CBA-CGA-O2A-C1
10	G	104	MW9	C22-C21-O5-P
10	M	406	MW9	C22-C21-O5-P
15	H	304	CDL	C1-CA2-OA2-PA1
8	P	102	BCL	C3A-C2A-CAA-CBA
8	L	301	BCL	C3A-C2A-CAA-CBA
9	r	102	A1EFU	C15-C16-C17-C18
9	q	101	A1EFU	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	C	404	LMT	C2-C1-O1'-C1'
16	C	401	HEC	C3D-CAD-CBD-CGD
8	b	101	BCL	C10-C11-C12-C13
10	D	103	MW9	O1-C18-C19-C20
10	M	405	MW9	O1-C18-C19-C20
10	M	406	MW9	C12-C13-C14-C15
8	r	101	BCL	C3-C5-C6-C7
15	H	304	CDL	C79-C80-C81-C82
8	M	403	BCL	O1A-CGA-O2A-C1
8	j	102	BCL	O1A-CGA-O2A-C1
8	a	101	BCL	C3-C5-C6-C7
8	Q	101	BCL	C15-C16-C17-C18
10	R	103	MW9	O8-C19-C20-O2
10	F	103	MW9	O8-C19-C20-O2
8	M	402	BCL	CBA-CGA-O2A-C1
10	D	103	MW9	C7-C8-C9-C10
8	I	101	BCL	C15-C16-C17-C18
9	s	101	A1EFU	C26-C27-C28-C29
10	R	103	MW9	O5-C21-C22-C23
13	L	303	U10	C34-C36-C37-C38
15	H	304	CDL	CA2-C1-CB2-OB2
10	F	103	MW9	C7-C8-C9-C10
11	L	306	LMT	C3-C4-C5-C6
8	D	101	BCL	C4-C3-C5-C6
8	P	101	BCL	C2-C1-O2A-CGA
8	V	101	BCL	C2-C1-O2A-CGA
8	1	101	BCL	C2-C1-O2A-CGA
8	K	101	BCL	C2-C1-O2A-CGA
8	G	101	BCL	C2-C1-O2A-CGA
8	A	101	BCL	C2-C1-O2A-CGA
8	M	402	BCL	C2-C1-O2A-CGA
10	M	405	MW9	C4-C5-C6-C7
8	v	101	BCL	C11-C12-C13-C14
8	Q	101	BCL	C11-C10-C8-C9
8	k	102	BCL	C6-C7-C8-C9
8	J	101	BCL	C6-C7-C8-C9
8	B	101	BCL	C6-C7-C8-C9
14	M	408	BPH	C14-C13-C15-C16
8	P	102	BCL	C13-C15-C16-C17
8	1	101	BCL	C8-C10-C11-C12
8	b	101	BCL	C15-C16-C17-C18
10	D	103	MW9	C19-C20-O2-P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	L	304	BCL	C3-C5-C6-C7
8	F	101	BCL	C8-C10-C11-C12
8	s	103	BCL	CBA-CGA-O2A-C1
8	r	101	BCL	C4C-C3C-CAC-CBC
10	H	303	MW9	C25-C24-O8-C19
8	L	301	BCL	C16-C17-C18-C20
10	H	303	MW9	C32-C33-C34-C35
15	L	308	CDL	C32-C33-C34-C35
8	J	101	BCL	C5-C6-C7-C8
8	v	101	BCL	C11-C12-C13-C15
8	Q	101	BCL	C11-C10-C8-C7
8	l	101	BCL	C6-C7-C8-C10
8	J	101	BCL	C6-C7-C8-C10
8	i	101	BCL	C6-C7-C8-C10
8	i	101	BCL	C11-C10-C8-C7
8	d	101	BCL	C6-C7-C8-C10
14	M	408	BPH	C6-C7-C8-C10
8	M	402	BCL	O1A-CGA-O2A-C1
8	Q	101	BCL	C1-C2-C3-C4
9	N	102	A1EFU	C15-C16-C17-C18
9	G	106	A1EFU	C5-C6-C7-C8
9	f	101	A1EFU	C13-C14-C15-C16
9	f	101	A1EFU	C19-C20-C21-C22
8	J	101	BCL	C8-C10-C11-C12
8	M	403	BCL	C5-C6-C7-C8
8	s	102	BCL	C2A-CAA-CBA-CGA
8	K	101	BCL	C2A-CAA-CBA-CGA
9	s	104	A1EFU	C11-C10-C9-CM4
8	a	101	BCL	CBA-CGA-O2A-C1
10	H	301	MW9	C26-C27-C28-C29
8	G	102	BCL	CAD-CBD-CGD-O2D
8	F	101	BCL	CAD-CBD-CGD-O2D
15	L	308	CDL	CA6-CA4-OA6-CA5
15	H	304	CDL	CA6-CA4-OA6-CA5
8	V	101	BCL	C4-C3-C5-C6
8	J	101	BCL	C4-C3-C5-C6
8	i	101	BCL	C4-C3-C5-C6
9	2	101	A1EFU	CM7-C22-C23-C24
10	R	103	MW9	O1-C18-C19-C20
10	G	104	MW9	O1-C18-C19-C20
15	L	308	CDL	C1-CB2-OB2-PB2
15	L	308	CDL	CB3-CB4-CB6-OB8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	G	103	MW9	O8-C19-C20-O2
8	P	101	BCL	C5-C6-C7-C8
9	p	101	A1EFU	C14-C15-C16-C17
9	s	104	A1EFU	CM1-C1-C2-C3
9	q	101	A1EFU	CM2-C1-C2-C3
10	H	303	MW9	O9-C24-O8-C19
8	P	102	BCL	CHA-CBD-CGD-O1D
8	P	102	BCL	CHA-CBD-CGD-O2D
8	i	101	BCL	CHA-CBD-CGD-O1D
8	i	101	BCL	CHA-CBD-CGD-O2D
8	G	101	BCL	CHA-CBD-CGD-O1D
8	G	101	BCL	CHA-CBD-CGD-O2D
8	F	101	BCL	CHA-CBD-CGD-O1D
8	F	102	BCL	CHA-CBD-CGD-O1D
8	F	102	BCL	CHA-CBD-CGD-O2D
8	E	101	BCL	CHA-CBD-CGD-O1D
10	L	307	MW9	C27-C28-C29-C30
9	2	102	A1EFU	C11-C10-C9-C8
9	f	101	A1EFU	C4-C5-C6-C7
15	L	308	CDL	OB6-CB4-CB6-OB8
8	R	102	BCL	C15-C16-C17-C18
8	V	101	BCL	O1A-CGA-O2A-C1
10	F	103	MW9	O7-C22-C23-O6
8	M	402	BCL	C3-C5-C6-C7
8	B	101	BCL	C4-C3-C5-C6
8	N	101	BCL	O1A-CGA-O2A-C1
8	G	102	BCL	O1A-CGA-O2A-C1
8	B	101	BCL	C2-C3-C5-C6
8	G	101	BCL	C11-C10-C8-C9
8	d	101	BCL	C6-C7-C8-C9
9	J	102	A1EFU	O1-C1-C2-O2
9	A	102	A1EFU	O1-C1-C2-O2
15	H	304	CDL	C77-C78-C79-C80
8	s	102	BCL	C1A-C2A-CAA-CBA
8	r	101	BCL	C1A-C2A-CAA-CBA
8	K	101	BCL	C1A-C2A-CAA-CBA
8	j	102	BCL	C1A-C2A-CAA-CBA
8	J	101	BCL	C1A-C2A-CAA-CBA
8	I	101	BCL	C1A-C2A-CAA-CBA
8	F	101	BCL	C1A-C2A-CAA-CBA
8	2	103	BCL	C16-C17-C18-C19
9	D	104	A1EFU	C19-C20-C21-C22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	F	103	MW9	C21-O5-P-O2
15	H	304	CDL	CA3-OA5-PA1-OA2
8	1	101	BCL	C4-C3-C5-C6
13	L	303	U10	C15-C14-C16-C17
10	G	104	MW9	C19-C20-O2-P
10	F	103	MW9	C22-C21-O5-P
9	P	103	A1EFU	C25-C26-C27-C28
8	1	101	BCL	O1A-CGA-O2A-C1
10	R	103	MW9	C20-O2-P-O4
10	G	103	MW9	C20-O2-P-O4
10	D	103	MW9	C21-O5-P-O4
10	M	406	MW9	C21-O5-P-O4
10	H	301	MW9	C21-O5-P-O4
15	L	308	CDL	CA2-OA2-PA1-OA4
15	H	304	CDL	CA3-OA5-PA1-OA3
8	r	101	BCL	C16-C17-C18-C20
10	M	406	MW9	C18-C19-C20-O2
9	G	106	A1EFU	C26-C27-C28-C29
9	v	102	A1EFU	CM1-C1-C2-O2
9	v	103	A1EFU	CM1-C1-C2-O2
9	s	105	A1EFU	CM1-C1-C2-O2
8	F	102	BCL	CAD-CBD-CGD-O1D
8	E	101	BCL	CAD-CBD-CGD-O1D
9	N	102	A1EFU	C2-C3-C4-C5
9	G	105	A1EFU	C2-C3-C4-C5
15	L	308	CDL	CA5-C11-C12-C13
8	2	103	BCL	C16-C17-C18-C20
8	P	102	BCL	C11-C10-C8-C7
8	r	101	BCL	C6-C7-C8-C10
8	q	102	BCL	C6-C7-C8-C10
8	2	103	BCL	C6-C7-C8-C10
8	n	101	BCL	C6-C7-C8-C10
8	n	101	BCL	C12-C13-C15-C16
8	G	101	BCL	C11-C10-C8-C7
8	D	101	BCL	C11-C12-C13-C15
8	b	101	BCL	C2C-C3C-CAC-CBC
8	A	101	BCL	C11-C10-C8-C7
8	M	403	BCL	C2C-C3C-CAC-CBC
9	s	104	A1EFU	C20-C21-C22-C23
9	M	407	A1EFU	C25-C26-C27-C28
15	H	304	CDL	O1-C1-CB2-OB2
8	G	102	BCL	C16-C17-C18-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	D	103	MW9	C37-C38-C39-C40
10	G	103	MW9	O1-C18-C19-C20
10	D	103	MW9	C2-C3-C4-C5
15	L	308	CDL	CA3-CA4-CA6-OA8
15	H	304	CDL	CA3-CA4-CA6-OA8
10	G	104	MW9	O1-C18-C19-O8
10	D	103	MW9	O1-C18-C19-O8
10	M	405	MW9	O1-C18-C19-O8
15	H	304	CDL	OA6-CA4-CA6-OA8
10	F	103	MW9	C31-C32-C33-C34
8	v	101	BCL	C13-C15-C16-C17
8	j	102	BCL	C8-C10-C11-C12
9	v	103	A1EFU	CM7-C22-C23-C24
8	P	101	BCL	C2-C3-C5-C6
8	s	103	BCL	C10-C11-C12-C13
8	r	101	BCL	C6-C7-C8-C9
8	l	101	BCL	C6-C7-C8-C9
8	i	101	BCL	C11-C10-C8-C9
8	F	101	BCL	C11-C10-C8-C9
8	L	304	BCL	C14-C13-C15-C16
15	H	304	CDL	C62-C63-C64-C65
8	j	102	BCL	C1-C2-C3-C5
10	R	103	MW9	O7-C22-C23-O6
15	L	308	CDL	C56-C57-C58-C59
9	v	102	A1EFU	C5-C6-C7-C8
9	s	104	A1EFU	C15-C16-C17-C18
9	2	104	A1EFU	CM2-C1-C2-C3
8	q	102	BCL	O1A-CGA-O2A-C1
13	L	303	U10	C20-C19-C21-C22
9	I	102	A1EFU	C25-C26-C27-C28
15	L	308	CDL	C72-C73-C74-C75
8	2	103	BCL	CAA-CBA-CGA-O2A
15	H	304	CDL	C80-C81-C82-C83
8	b	101	BCL	C2-C1-O2A-CGA
15	H	304	CDL	C73-C74-C75-C76
10	D	103	MW9	C30-C31-C32-C33
9	f	101	A1EFU	C9-C10-C11-C12
8	S	101	BCL	O1A-CGA-O2A-C1
10	G	104	MW9	C12-C13-C14-C15
14	L	302	BPH	C16-C17-C18-C20
9	s	104	A1EFU	CM1-C1-C2-O2
9	q	101	A1EFU	CM2-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	G	106	A1EFU	CM2-C1-C2-O2
8	V	101	BCL	C16-C17-C18-C20
8	J	101	BCL	C2A-CAA-CBA-CGA
9	R	101	A1EFU	C26-C27-C28-C29
8	P	101	BCL	CBA-CGA-O2A-C1
10	L	307	MW9	C20-O2-P-O5
10	L	307	MW9	C21-O5-P-O2
15	L	308	CDL	CB2-OB2-PB2-OB5
14	L	302	BPH	CHA-CBD-CGD-O2D
10	F	103	MW9	C27-C28-C29-C30
8	F	101	BCL	C11-C10-C8-C7
8	a	101	BCL	C12-C13-C15-C16
13	L	303	U10	C13-C14-C16-C17
8	P	102	BCL	C11-C10-C8-C9
8	q	102	BCL	C6-C7-C8-C9
8	n	101	BCL	C6-C7-C8-C9
8	n	101	BCL	C14-C13-C15-C16
8	A	101	BCL	C11-C10-C8-C9
9	J	103	A1EFU	C13-C14-C15-C16
10	G	103	MW9	C11-C12-C13-C14
8	Q	101	BCL	CBA-CGA-O2A-C1
10	H	301	MW9	C19-C20-O2-P
10	F	103	MW9	C32-C33-C34-C35
10	M	406	MW9	C32-C33-C34-C35
8	D	101	BCL	C10-C11-C12-C13
13	L	303	U10	C30-C29-C31-C32
8	Q	101	BCL	C2-C3-C5-C6
8	F	101	BCL	CBA-CGA-O2A-C1
10	L	307	MW9	C32-C33-C34-C35
9	R	101	A1EFU	C19-C20-C21-C22
9	q	101	A1EFU	C5-C6-C7-C8
9	2	101	A1EFU	C9-C10-C11-C12
9	K	102	A1EFU	C15-C16-C17-C18
9	j	101	A1EFU	C9-C10-C11-C12
9	G	105	A1EFU	C5-C6-C7-C8
9	B	103	A1EFU	C5-C6-C7-C8
9	a	102	A1EFU	C5-C6-C7-C8
15	H	304	CDL	OA5-CA3-CA4-CA6
9	p	101	A1EFU	C22-C23-C24-C25
9	N	102	A1EFU	C22-C23-C24-C25
9	B	103	A1EFU	C18-C19-C20-C21
8	t	101	BCL	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	P	103	A1EFU	CM1-C1-C2-C3
9	v	102	A1EFU	CM2-C1-C2-C3
9	q	101	A1EFU	C2-C3-C4-C5
9	G	106	A1EFU	CM2-C1-C2-C3
10	M	406	MW9	C30-C31-C32-C33
8	N	101	BCL	C5-C6-C7-C8
8	A	101	BCL	C5-C6-C7-C8
10	H	301	MW9	C25-C26-C27-C28
8	e	101	BCL	C2-C1-O2A-CGA
8	L	301	BCL	C2-C1-O2A-CGA
10	M	406	MW9	C19-C20-O2-P
8	M	403	BCL	C3A-C2A-CAA-CBA
16	C	402	HEC	CAA-CBA-CGA-O2A
10	H	301	MW9	C32-C33-C34-C35
8	G	102	BCL	C4-C3-C5-C6
8	D	101	BCL	C2-C3-C5-C6
11	H	302	LMT	C3-C4-C5-C6
8	v	101	BCL	C11-C10-C8-C9
8	D	101	BCL	C11-C12-C13-C14
8	v	101	BCL	C16-C17-C18-C20
11	L	306	LMT	C7-C8-C9-C10
8	B	101	BCL	C15-C16-C17-C18
8	q	102	BCL	C5-C6-C7-C8
9	v	103	A1EFU	CM5-C13-C14-C15
10	F	103	MW9	C30-C31-C32-C33
8	M	402	BCL	C2A-CAA-CBA-CGA
10	R	103	MW9	C34-C35-C36-C37
14	L	302	BPH	O2A-C1-C2-C3
15	L	308	CDL	CA7-C31-C32-C33
13	M	404	U10	C44-C46-C47-C48
8	K	101	BCL	C5-C6-C7-C8
8	P	102	BCL	C1A-C2A-CAA-CBA
8	S	101	BCL	C1A-C2A-CAA-CBA
8	k	102	BCL	C1A-C2A-CAA-CBA
8	e	101	BCL	C1A-C2A-CAA-CBA
8	M	403	BCL	C1A-C2A-CAA-CBA
8	S	101	BCL	C11-C12-C13-C15
8	Q	101	BCL	C11-C12-C13-C15
8	l	101	BCL	C11-C10-C8-C7
9	G	106	A1EFU	C15-C16-C17-C18
9	E	103	A1EFU	C5-C6-C7-C8
8	s	102	BCL	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	L	308	CDL	C53-C54-C55-C56
8	B	101	BCL	C8-C10-C11-C12
8	I	101	BCL	C3-C5-C6-C7
8	d	101	BCL	C2A-CAA-CBA-CGA
8	I	101	BCL	C8-C10-C11-C12
10	H	303	MW9	O8-C19-C20-O2
15	L	308	CDL	OA5-CA3-CA4-CA6
8	P	101	BCL	C4-C3-C5-C6
8	K	101	BCL	C4-C3-C5-C6
8	B	101	BCL	C5-C6-C7-C8
9	R	101	A1EFU	C25-C26-C27-C28
10	M	405	MW9	C25-C26-C27-C28
13	M	404	U10	C5-C4-O4-C4M
9	v	103	A1EFU	C12-C13-C14-C15
15	H	304	CDL	C43-C44-C45-C46
10	M	405	MW9	C10-C11-C12-C13
10	M	405	MW9	C27-C28-C29-C30
8	F	102	BCL	C4-C3-C5-C6
8	d	101	BCL	C2-C1-O2A-CGA
8	a	101	BCL	C2-C1-O2A-CGA
8	t	101	BCL	C2-C3-C5-C6
8	K	101	BCL	C2-C3-C5-C6
8	i	101	BCL	C2-C3-C5-C6
13	L	303	U10	C28-C29-C31-C32
8	Q	101	BCL	O1A-CGA-O2A-C1
14	L	302	BPH	C11-C12-C13-C14
10	M	406	MW9	C3-C4-C5-C6
9	P	103	A1EFU	CM2-C1-C2-C3
9	2	102	A1EFU	CM1-C1-C2-C3
9	2	104	A1EFU	CM2-C1-C2-O2
15	L	308	CDL	C34-C35-C36-C37
9	B	103	A1EFU	C13-C14-C15-C16
8	N	101	BCL	C4-C3-C5-C6
8	G	101	BCL	C4-C3-C5-C6
9	R	101	A1EFU	CM8-C26-C27-C28
8	t	101	BCL	C4C-C3C-CAC-CBC
8	K	101	BCL	C4C-C3C-CAC-CBC
8	j	102	BCL	C4C-C3C-CAC-CBC
8	M	402	BCL	C16-C17-C18-C20
8	J	101	BCL	C2-C3-C5-C6
13	L	303	U10	C18-C19-C21-C22
9	s	101	A1EFU	C14-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	G	103	MW9	C12-C13-C14-C15
10	R	103	MW9	C32-C33-C34-C35
8	Q	101	BCL	C2A-CAA-CBA-CGA
16	C	403	HEC	CAD-CBD-CGD-O1D
8	e	101	BCL	C5-C6-C7-C8
8	I	101	BCL	O1A-CGA-O2A-C1
8	F	101	BCL	C4-C3-C5-C6
9	G	106	A1EFU	CM7-C22-C23-C24
9	K	102	A1EFU	C22-C23-C24-C25
13	M	404	U10	C24-C26-C27-C28
8	N	101	BCL	C2-C3-C5-C6
8	F	102	BCL	C2-C3-C5-C6
8	b	101	BCL	C6-C7-C8-C10
9	s	105	A1EFU	C21-C22-C23-C24
14	M	408	BPH	C12-C13-C15-C16
8	s	102	BCL	C5-C6-C7-C8
8	M	403	BCL	C8-C10-C11-C12
10	M	405	MW9	C32-C33-C34-C35
8	P	101	BCL	C1-C2-C3-C4
8	t	101	BCL	C1-C2-C3-C4
8	2	103	BCL	C1-C2-C3-C4
8	k	102	BCL	C1-C2-C3-C4
9	q	101	A1EFU	C19-C20-C21-C22
9	E	103	A1EFU	C19-C20-C21-C22
10	M	405	MW9	C36-C37-C38-C39
8	a	101	BCL	C5-C6-C7-C8
8	r	101	BCL	C16-C17-C18-C19
8	I	101	BCL	CBA-CGA-O2A-C1
8	j	102	BCL	CAA-CBA-CGA-O2A
8	t	101	BCL	C4-C3-C5-C6
8	s	102	BCL	C4-C3-C5-C6
8	r	101	BCL	C4-C3-C5-C6
8	n	101	BCL	C4-C3-C5-C6
8	e	101	BCL	C4-C3-C5-C6
8	l	101	BCL	C2-C3-C5-C6
9	v	102	A1EFU	C21-C22-C23-C24
11	L	305	LMT	C1-C2-C3-C4
8	S	101	BCL	C11-C12-C13-C14
8	Q	101	BCL	C11-C12-C13-C14
8	l	101	BCL	C11-C10-C8-C9
8	k	102	BCL	C3A-C2A-CAA-CBA
8	J	101	BCL	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	I	101	BCL	C3A-C2A-CAA-CBA
8	e	101	BCL	C3A-C2A-CAA-CBA
8	P	101	BCL	O1A-CGA-O2A-C1
8	J	101	BCL	CAD-CBD-CGD-O2D
8	i	101	BCL	CAD-CBD-CGD-O2D
8	I	101	BCL	CAD-CBD-CGD-O2D
9	q	101	A1EFU	C20-C21-C22-CM7
8	i	101	BCL	C8-C10-C11-C12
8	a	101	BCL	C13-C15-C16-C17
8	j	102	BCL	C10-C11-C12-C13
16	C	402	HEC	CAA-CBA-CGA-O1A
8	G	102	BCL	C8-C10-C11-C12
8	k	102	BCL	C4-C3-C5-C6
8	k	102	BCL	C8-C10-C11-C12
8	V	101	BCL	C2-C3-C5-C6
8	G	102	BCL	C2-C3-C5-C6
10	R	103	MW9	C36-C37-C38-C39
10	G	103	MW9	C32-C33-C34-C35
10	M	405	MW9	C6-C7-C8-C9
16	C	402	HEC	CAD-CBD-CGD-O1D
10	M	405	MW9	O8-C24-C25-C26
8	G	101	BCL	O2A-C1-C2-C3
10	M	405	MW9	C34-C35-C36-C37
9	P	103	A1EFU	CM1-C1-C2-O2
9	v	102	A1EFU	CM2-C1-C2-O2
9	v	103	A1EFU	CM2-C1-C2-O2
9	s	104	A1EFU	CM2-C1-C2-O2
9	s	105	A1EFU	CM2-C1-C2-O2
9	2	102	A1EFU	CM1-C1-C2-O2
9	G	105	A1EFU	CM2-C1-C2-O2
9	G	106	A1EFU	CM1-C1-C2-O2
9	F	104	A1EFU	CM2-C1-C2-O2
16	C	403	HEC	CAD-CBD-CGD-O2D
9	2	104	A1EFU	CM1-C1-C2-C3
9	G	105	A1EFU	CM2-C1-C2-C3
9	G	106	A1EFU	CM1-C1-C2-C3
10	D	103	MW9	C32-C33-C34-C35
8	Q	101	BCL	CHA-CBD-CGD-O1D
8	Q	101	BCL	CHA-CBD-CGD-O2D
8	2	103	BCL	CHA-CBD-CGD-O1D
8	2	103	BCL	CHA-CBD-CGD-O2D
8	F	101	BCL	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	E	101	BCL	CHA-CBD-CGD-O2D
8	L	304	BCL	CHA-CBD-CGD-O1D
9	j	103	A1EFU	C15-C16-C17-C18
10	L	307	MW9	C11-C12-C13-C14
11	L	306	LMT	C6-C7-C8-C9
10	H	303	MW9	C18-C19-C20-O2
16	C	401	HEC	CAA-CBA-CGA-O1A
8	F	101	BCL	CAA-CBA-CGA-O2A
15	H	304	CDL	C57-C58-C59-C60
8	v	101	BCL	CAA-CBA-CGA-O2A
8	s	103	BCL	CAA-CBA-CGA-O2A
9	F	104	A1EFU	C2-C1-O1-CMA
15	H	304	CDL	C71-CB7-OB8-CB6
10	G	104	MW9	O8-C24-C25-C26
9	T	101	A1EFU	C21-C22-C23-C24
14	L	302	BPH	C2-C3-C5-C6
8	s	103	BCL	C8-C10-C11-C12
8	k	102	BCL	CAA-CBA-CGA-O2A
8	a	101	BCL	C14-C13-C15-C16
9	a	102	A1EFU	C9-C10-C11-C12
9	s	101	A1EFU	O1-C1-C2-O2
15	H	304	CDL	OB9-CB7-OB8-CB6
9	D	104	A1EFU	C27-C28-C29-C30
8	F	101	BCL	CAA-CBA-CGA-O1A
10	M	406	MW9	C21-C22-C23-O6
8	d	101	BCL	CAA-CBA-CGA-O1A
10	M	406	MW9	C2-C3-C4-C5
8	D	101	BCL	C1A-C2A-CAA-CBA
8	v	101	BCL	CAA-CBA-CGA-O1A
11	L	306	LMT	C4-C5-C6-C7
8	M	403	BCL	CAA-CBA-CGA-O1A
10	F	103	MW9	O8-C24-C25-C26
8	a	101	BCL	C4-C3-C5-C6
10	H	301	MW9	O8-C24-C25-C26
8	F	102	BCL	C5-C6-C7-C8
10	F	103	MW9	C26-C27-C28-C29
10	G	103	MW9	C21-O5-P-O4
10	L	307	MW9	C20-O2-P-O4
13	M	404	U10	C6-C7-C8-C9
15	L	308	CDL	CB2-OB2-PB2-OB3
8	P	101	BCL	C16-C17-C18-C20
8	M	403	BCL	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	K	102	A1EFU	C26-C27-C28-C29
8	M	403	BCL	C15-C16-C17-C18
9	2	104	A1EFU	CM1-C1-C2-O2
8	Q	101	BCL	C5-C6-C7-C8
10	M	405	MW9	O9-C24-C25-C26
16	C	402	HEC	CAD-CBD-CGD-O2D
8	P	102	BCL	C5-C6-C7-C8
9	r	102	A1EFU	CM8-C26-C27-C28
9	B	102	A1EFU	C21-C22-C23-C24
8	t	101	BCL	CAD-CBD-CGD-O1D
9	v	103	A1EFU	CM2-C1-C2-C3
9	s	104	A1EFU	CM2-C1-C2-C3
9	s	105	A1EFU	CM2-C1-C2-C3
9	F	104	A1EFU	CM2-C1-C2-C3
8	J	101	BCL	C11-C10-C8-C9
10	F	103	MW9	C15-C16-C17-O1
10	G	103	MW9	C29-C30-C31-C32
9	k	101	A1EFU	C23-C24-C25-C26
9	F	104	A1EFU	C27-C28-C29-C30
8	R	102	BCL	C8-C10-C11-C12
8	d	101	BCL	C13-C15-C16-C17
14	L	302	BPH	C4-C3-C5-C6
8	n	101	BCL	C2C-C3C-CAC-CBC
9	r	102	A1EFU	C20-C21-C22-C23
9	B	102	A1EFU	C20-C21-C22-C23
9	A	102	A1EFU	C20-C21-C22-C23
10	R	103	MW9	O8-C24-C25-C26
10	M	406	MW9	O8-C24-C25-C26
8	q	102	BCL	CAA-CBA-CGA-O1A
10	F	103	MW9	O9-C24-C25-C26
16	C	401	HEC	CAD-CBD-CGD-O1D
9	P	103	A1EFU	C19-C20-C21-C22
9	p	101	A1EFU	C19-C20-C21-C22
9	N	102	A1EFU	C5-C6-C7-C8
9	k	101	A1EFU	C9-C10-C11-C12
9	G	106	A1EFU	C9-C10-C11-C12
8	b	101	BCL	C16-C17-C18-C20
10	R	103	MW9	O9-C24-C25-C26
10	G	104	MW9	O9-C24-C25-C26
10	F	103	MW9	C15-C16-C17-O
10	H	301	MW9	O9-C24-C25-C26
8	d	101	BCL	CAA-CBA-CGA-O2A

There are no ring outliers.

46 monomers are involved in 134 short contacts:

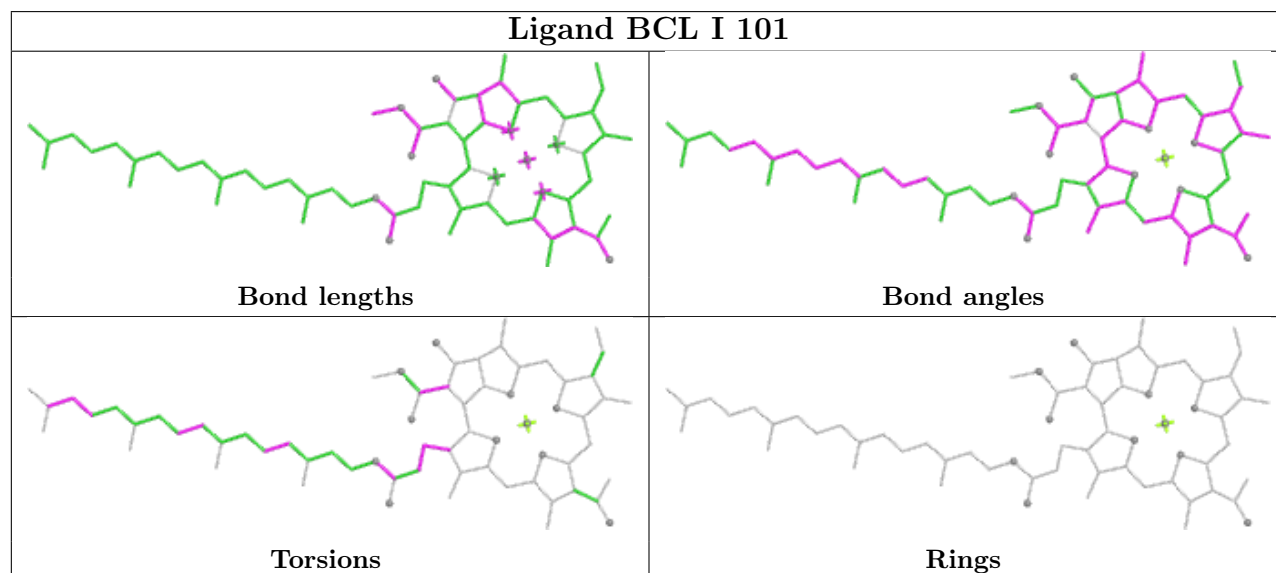
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	I	101	BCL	1	0
8	M	402	BCL	3	0
8	Q	101	BCL	1	0
8	A	101	BCL	5	0
8	s	103	BCL	2	0
8	n	101	BCL	3	0
13	L	303	U10	5	0
8	G	101	BCL	2	0
8	M	403	BCL	3	0
8	a	101	BCL	2	0
8	B	101	BCL	4	0
8	t	101	BCL	9	0
8	b	101	BCL	2	0
8	E	101	BCL	2	0
8	G	102	BCL	2	0
8	s	102	BCL	7	0
8	j	102	BCL	7	0
11	D	102	LMT	1	0
8	L	304	BCL	6	0
8	D	101	BCL	2	0
13	M	404	U10	7	0
8	k	102	BCL	1	0
8	q	102	BCL	2	0
8	F	102	BCL	1	0
8	K	101	BCL	2	0
8	J	101	BCL	3	0
9	s	104	A1EFU	1	0
11	L	305	LMT	1	0
8	d	101	BCL	8	0
15	H	304	CDL	3	0
8	V	101	BCL	3	0
8	N	101	BCL	2	0
8	2	103	BCL	4	0
8	P	102	BCL	2	0
8	R	102	BCL	6	0
8	r	101	BCL	4	0
8	i	101	BCL	2	0
8	v	101	BCL	5	0
8	e	101	BCL	4	0
15	L	308	CDL	1	0

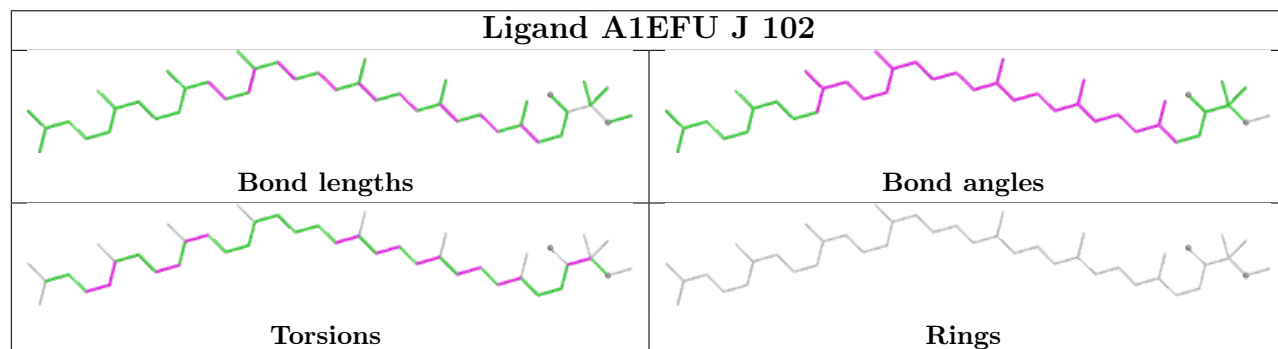
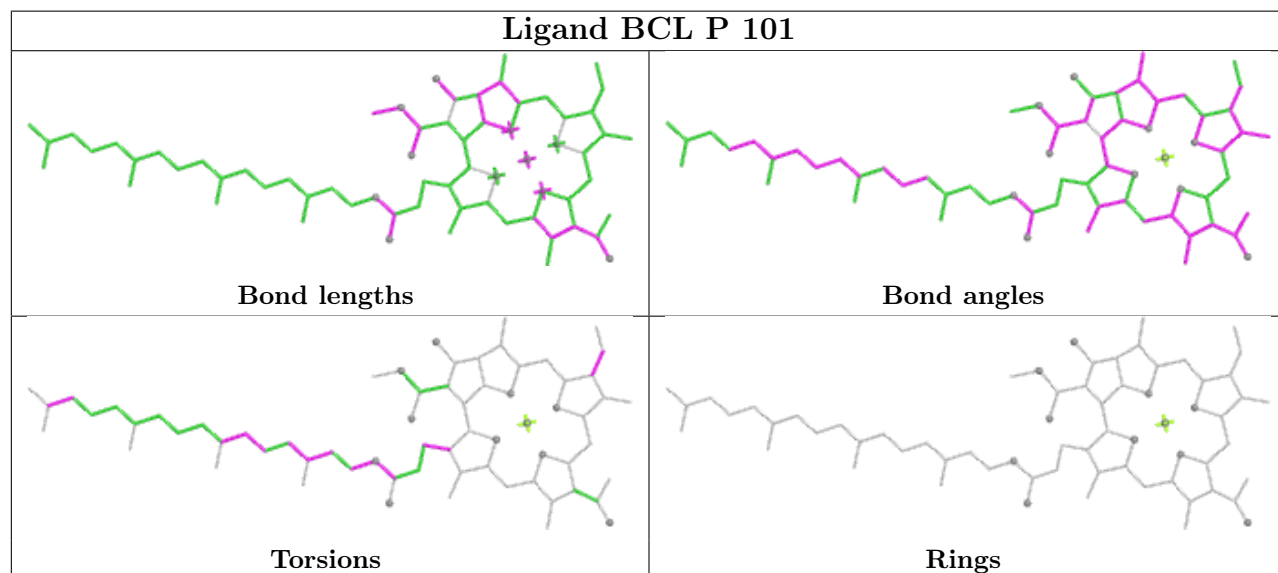
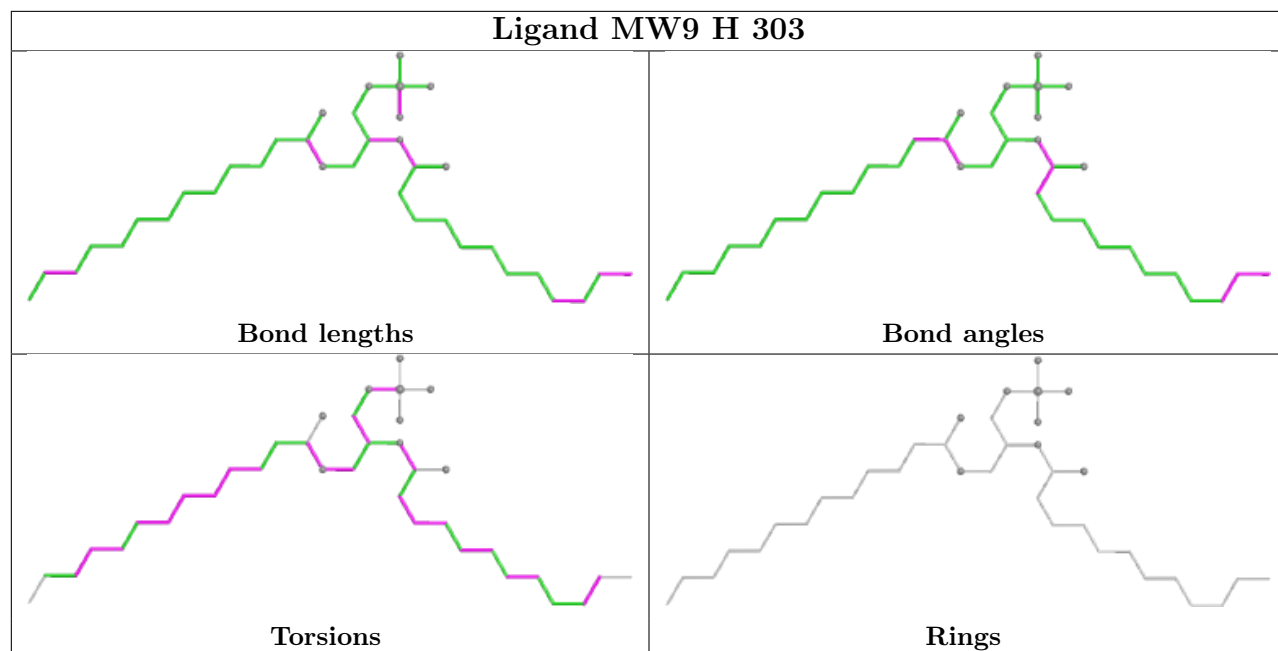
Continued on next page...

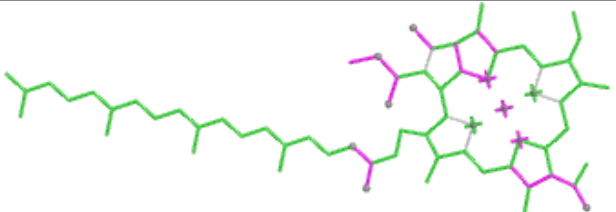
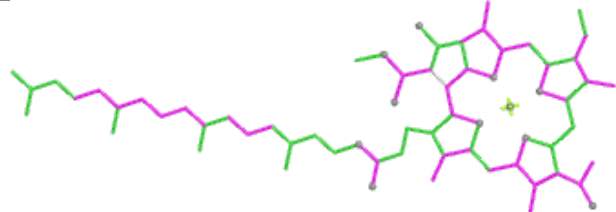
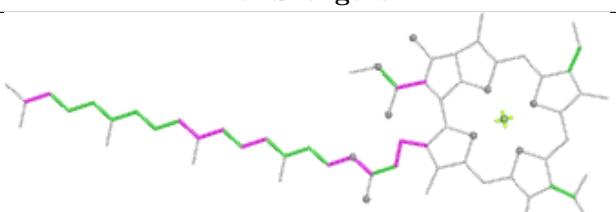
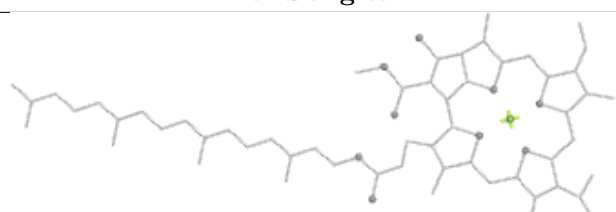
Continued from previous page...

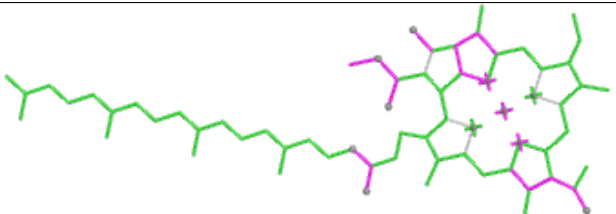
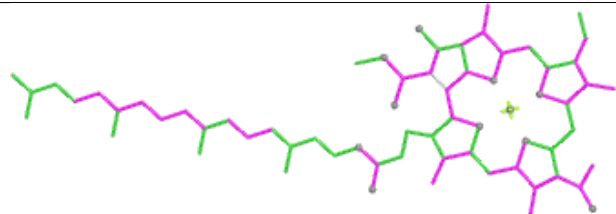
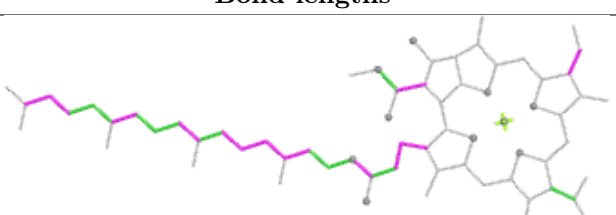
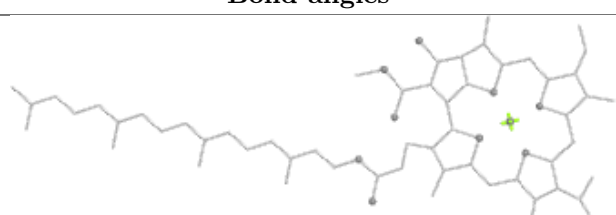
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	L	301	BCL	3	0
10	R	103	MW9	1	0
16	C	401	HEC	5	0
14	M	408	BPH	2	0
11	C	404	LMT	2	0
8	F	101	BCL	4	0

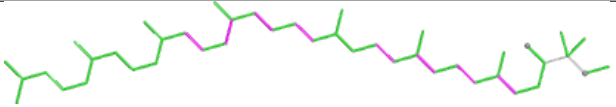
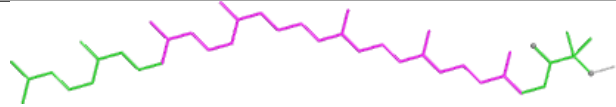
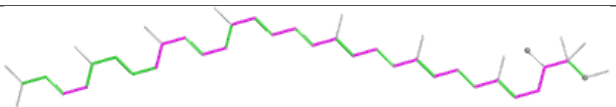
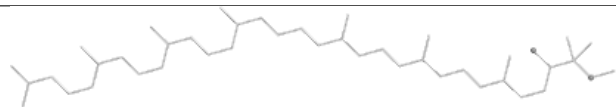
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

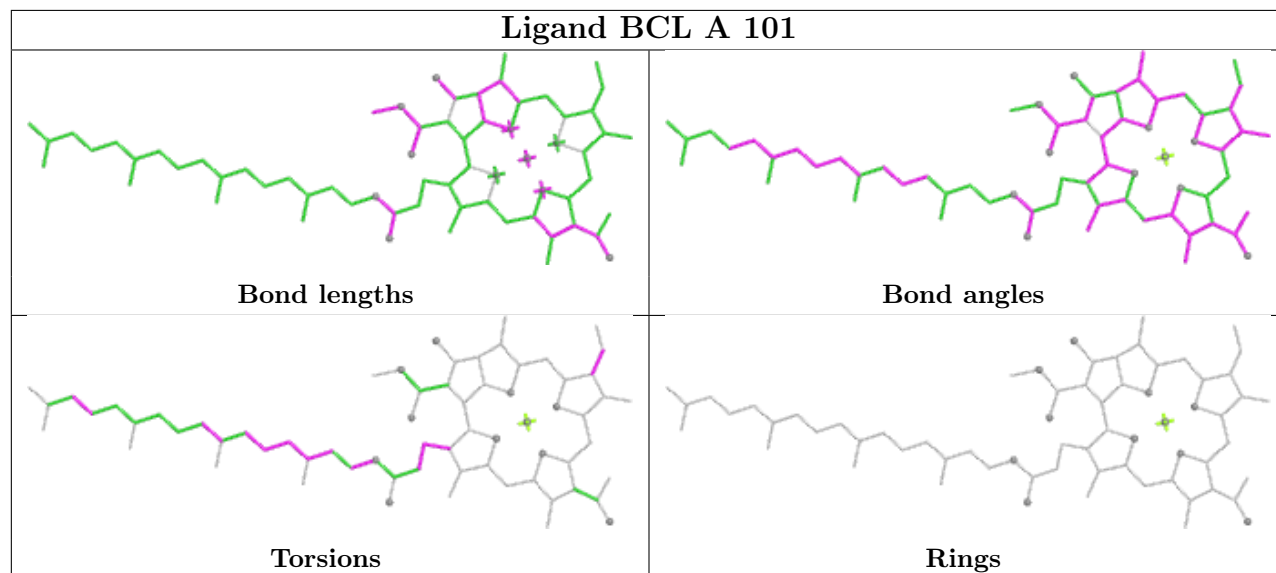
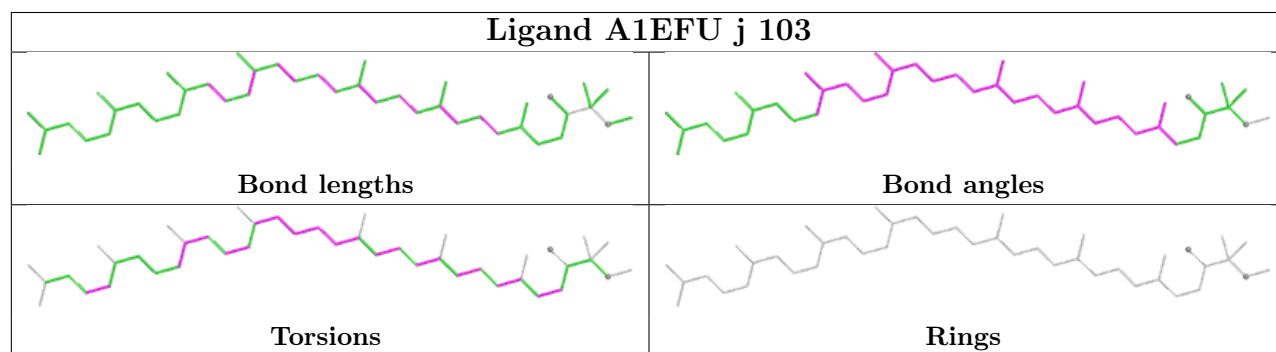
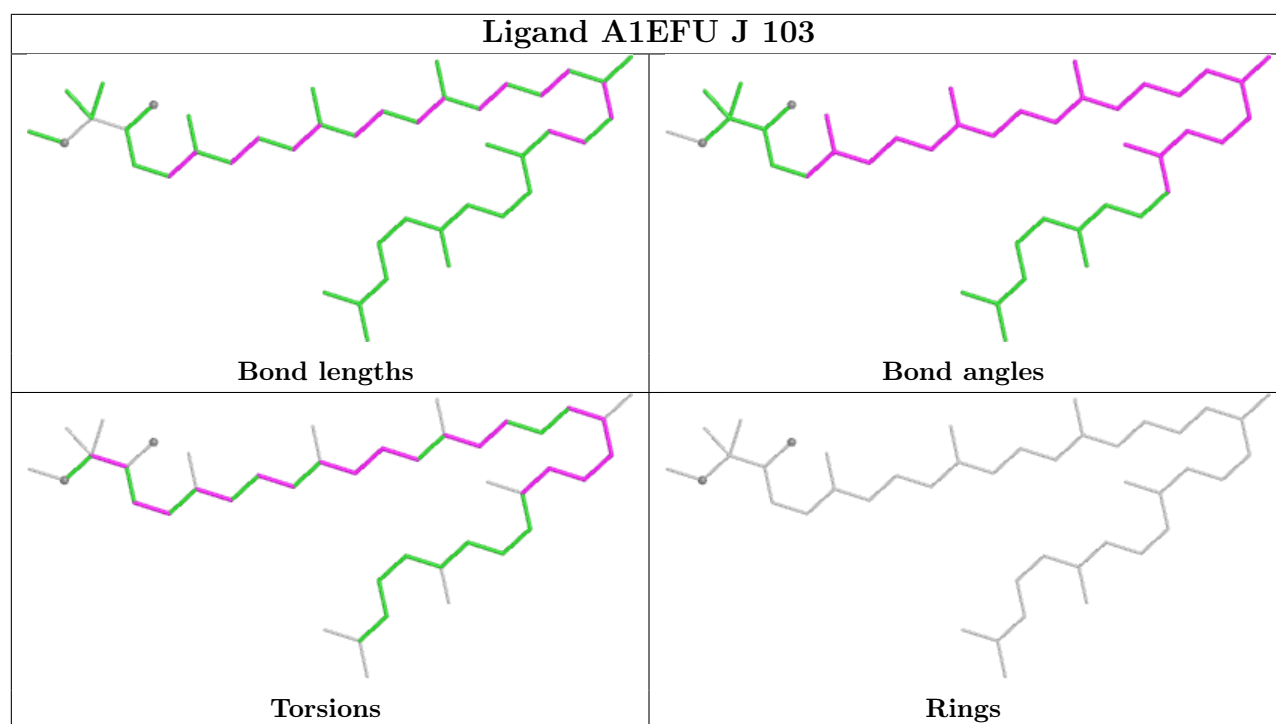


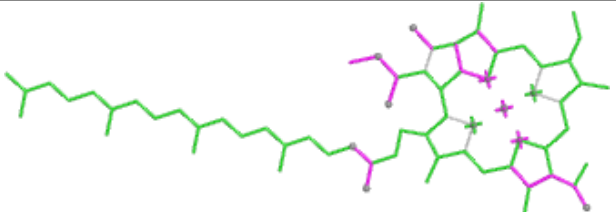
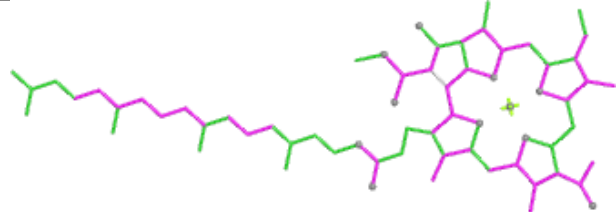
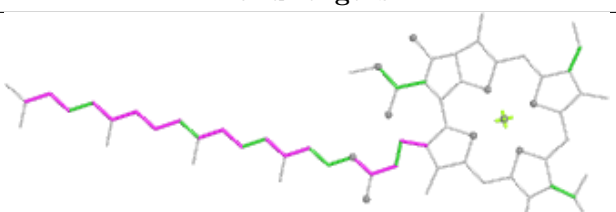
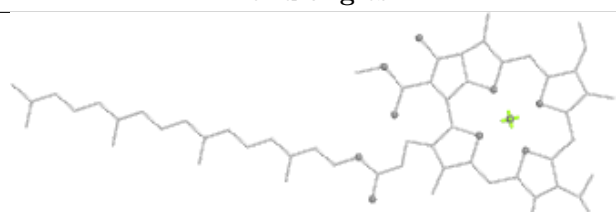
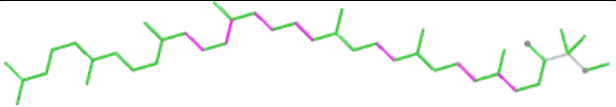
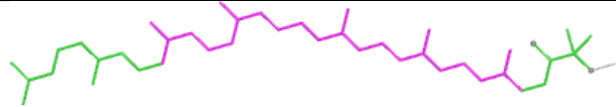
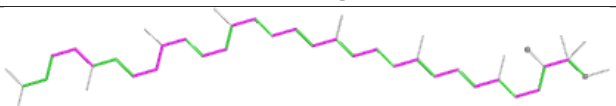
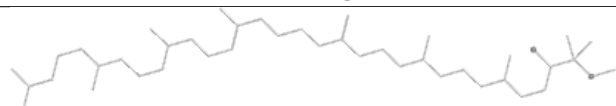
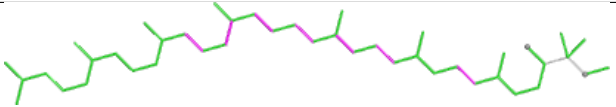
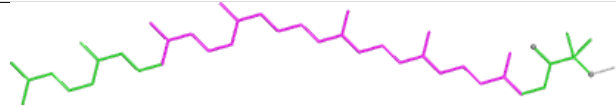
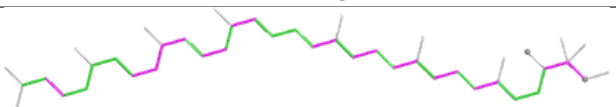
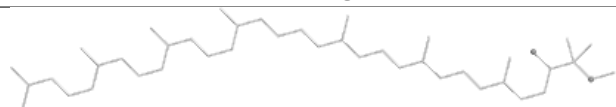


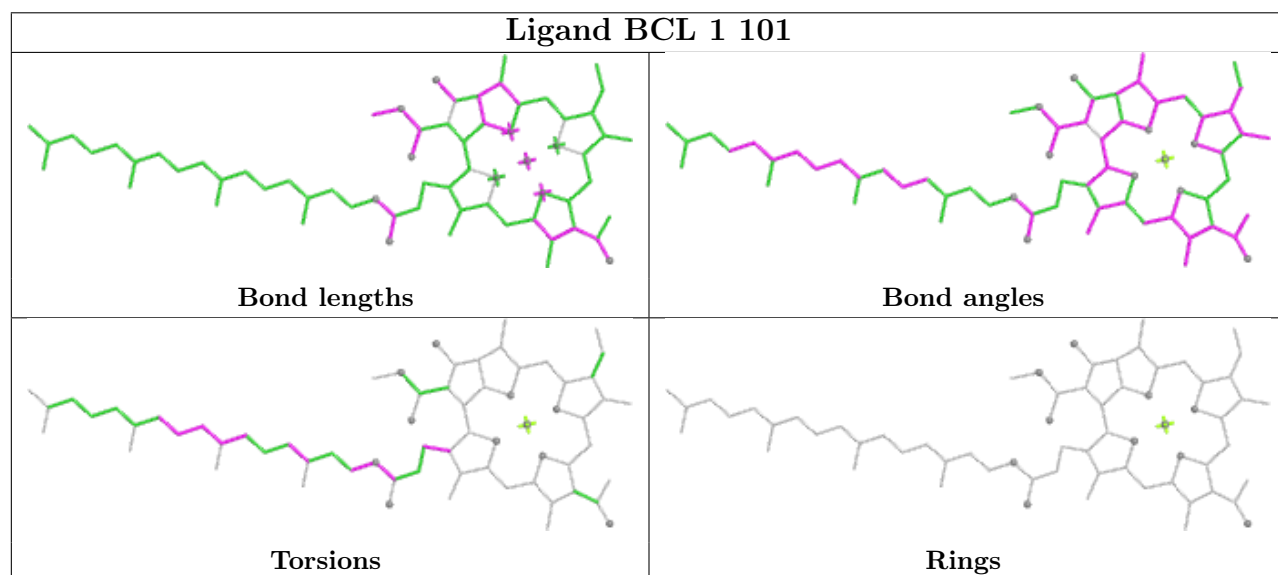
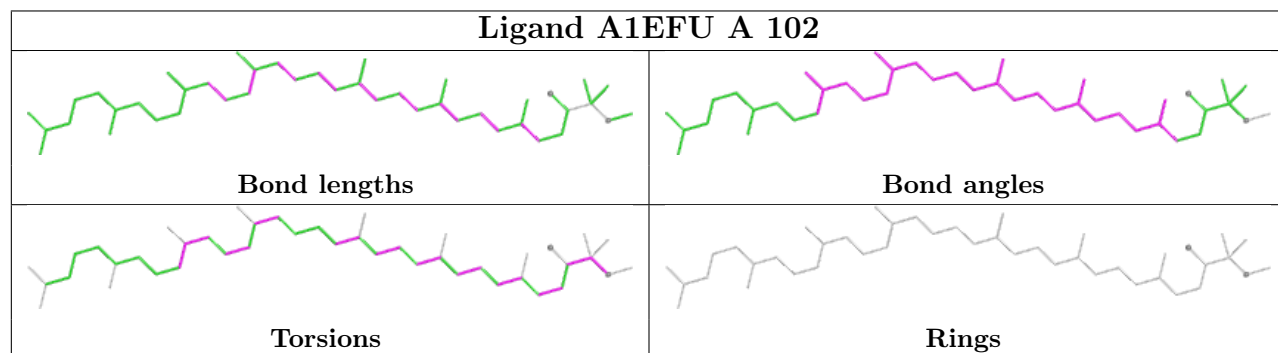
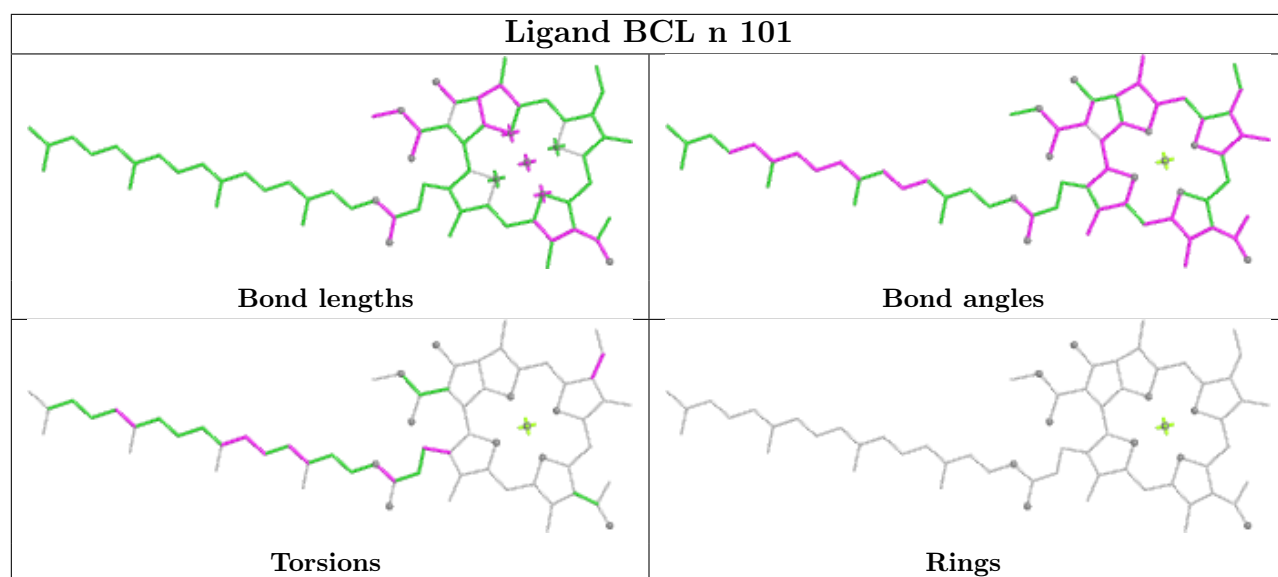
Ligand BCL M 402	
	
Bond lengths	Bond angles
	
Torsions	Rings

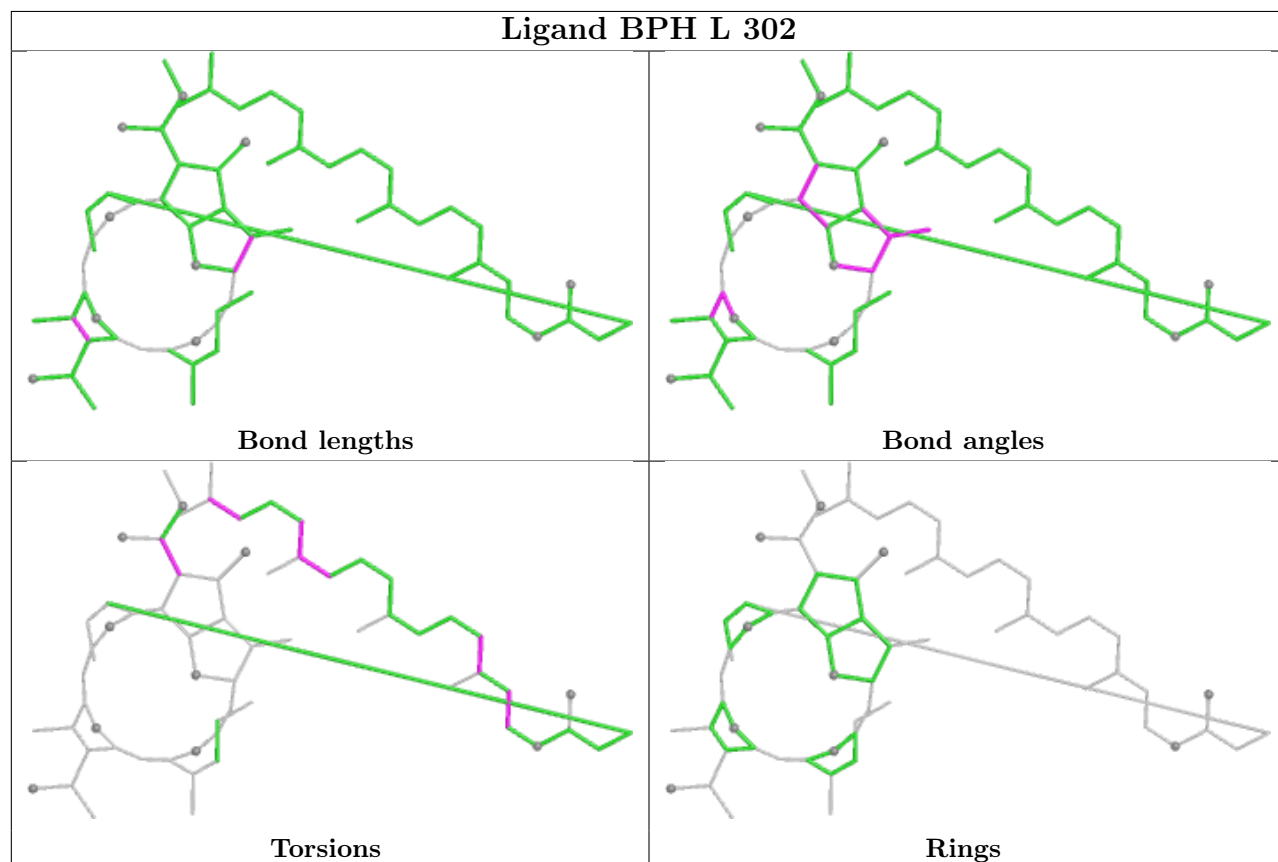
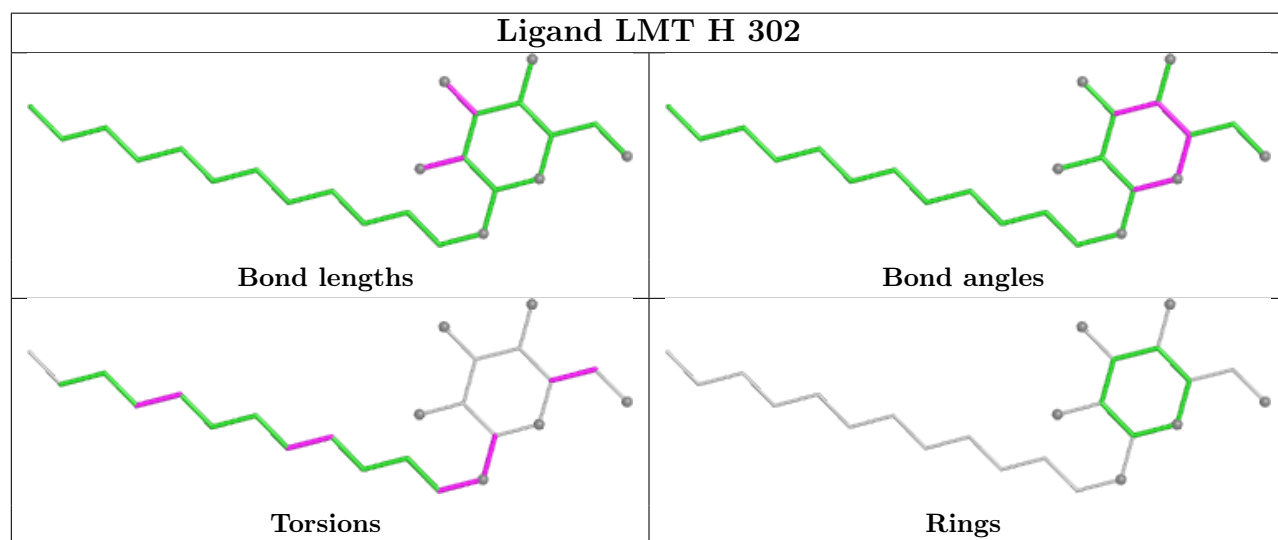
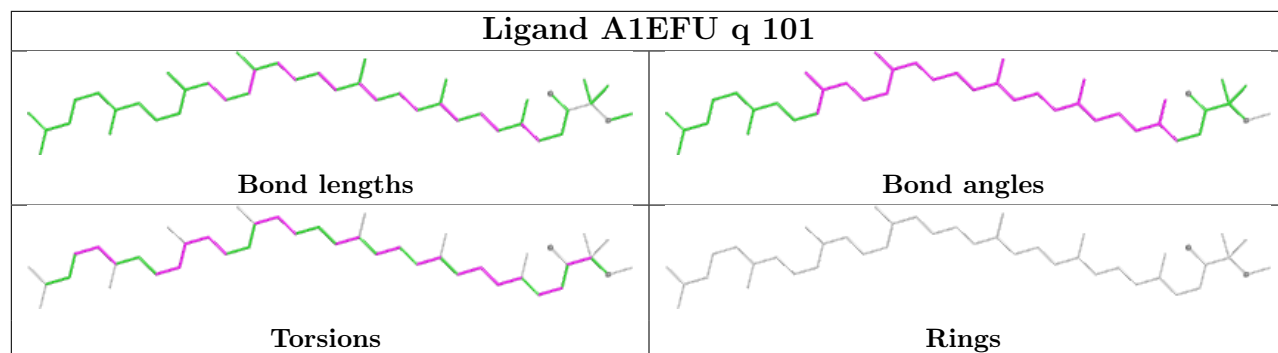
Ligand BCL Q 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

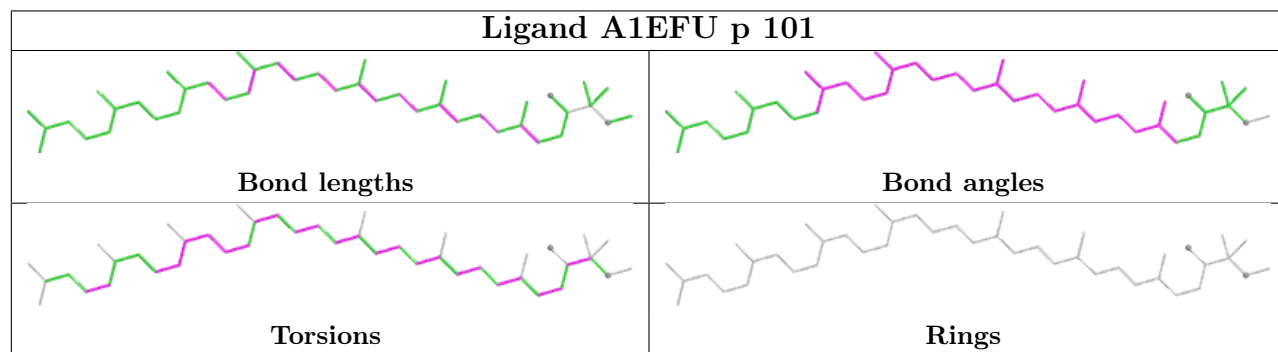
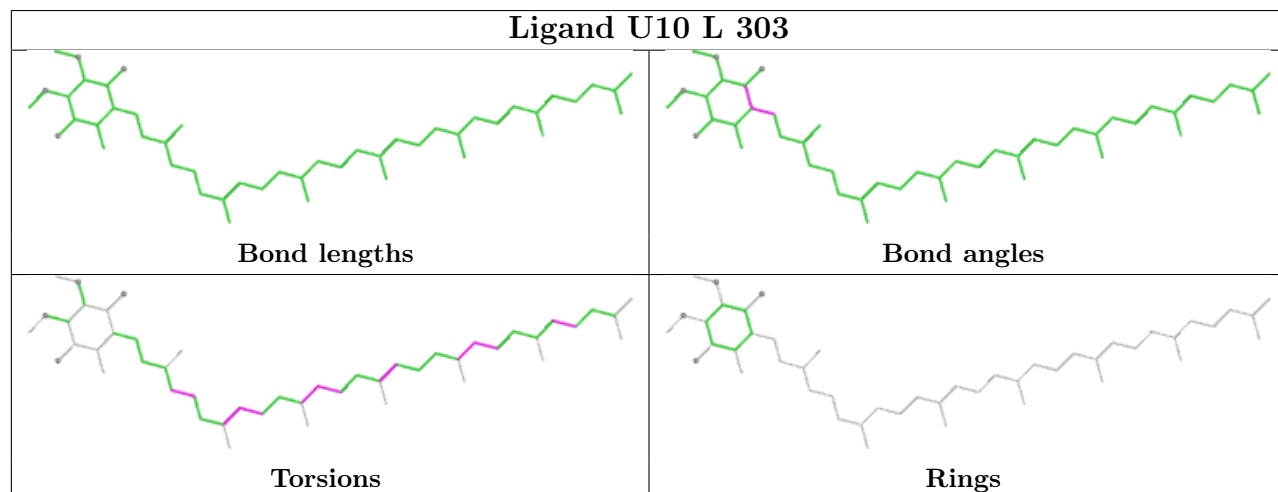
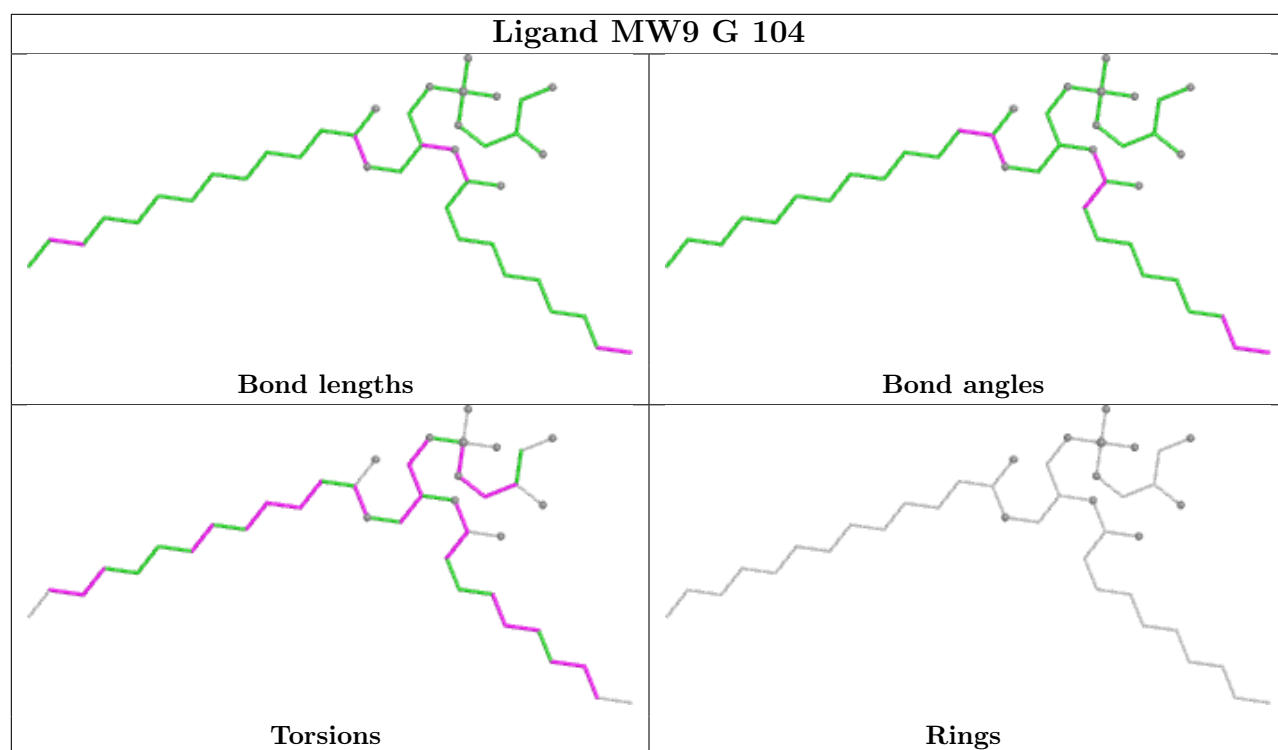
Ligand A1EFU D 105	
	
Bond lengths	Bond angles
	
Torsions	Rings

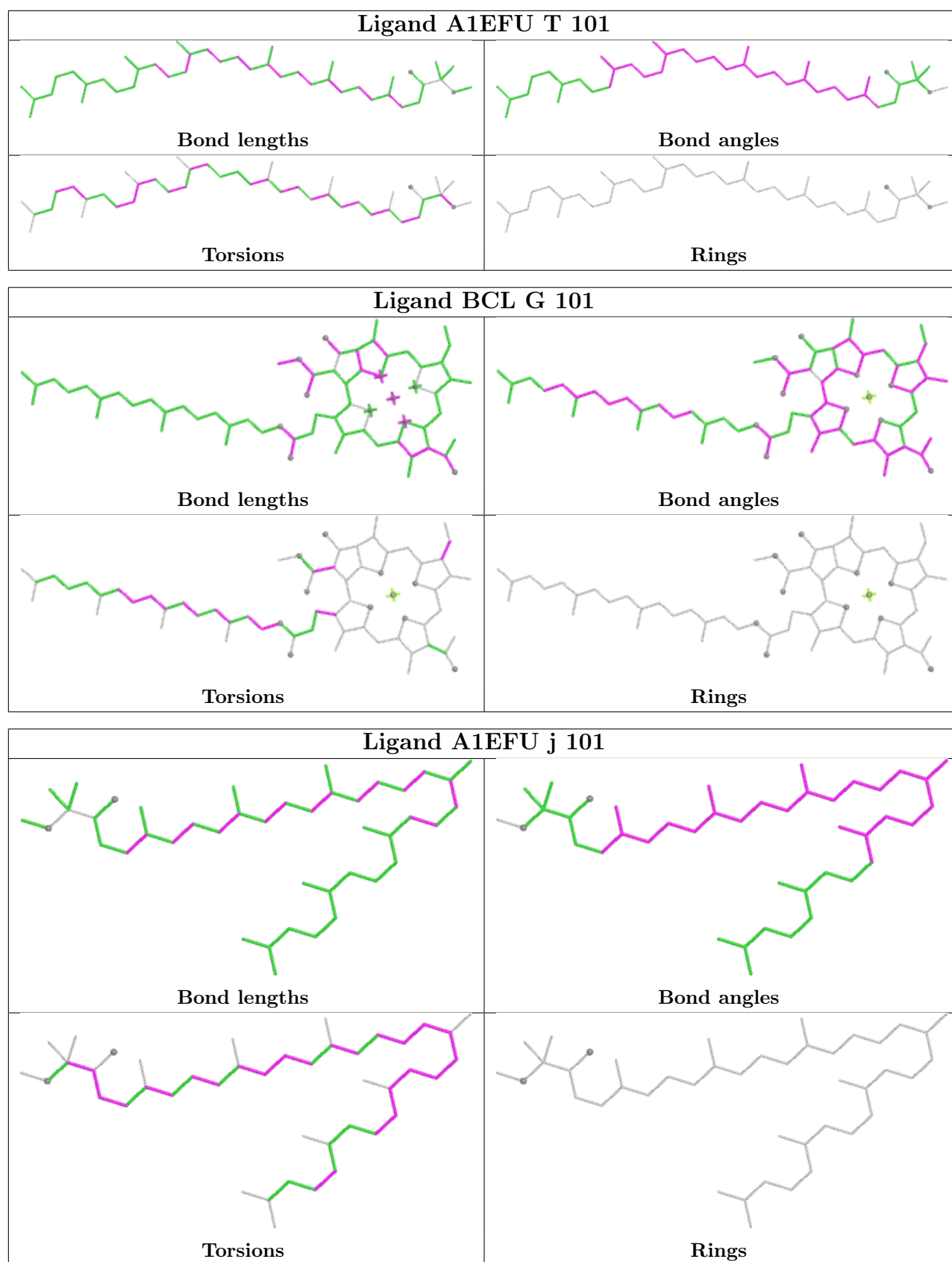


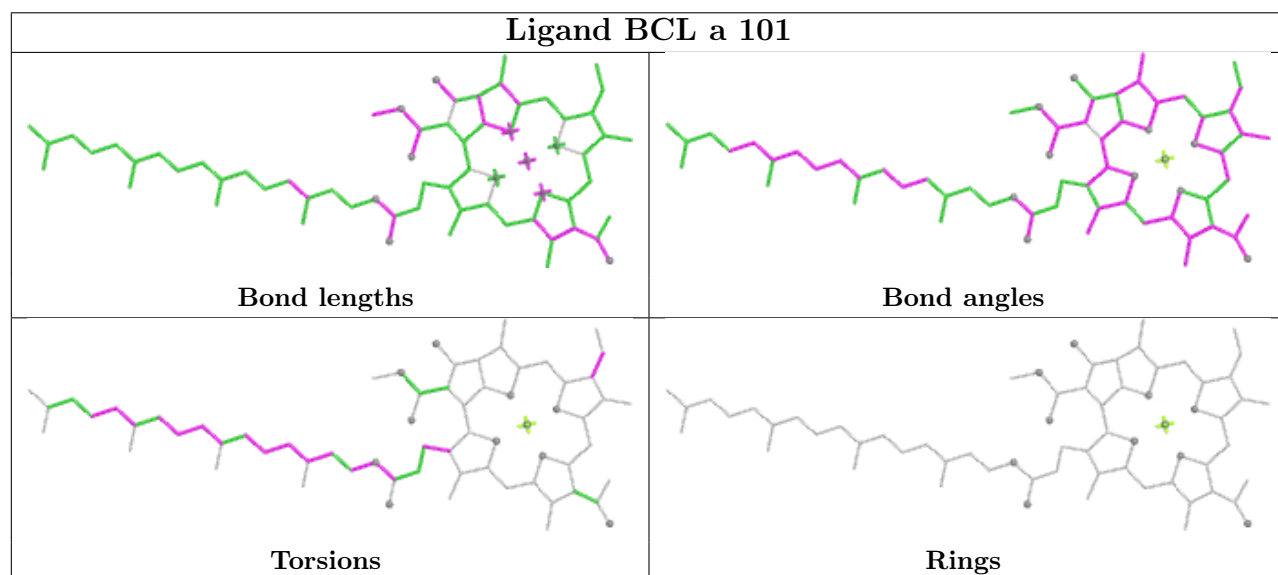
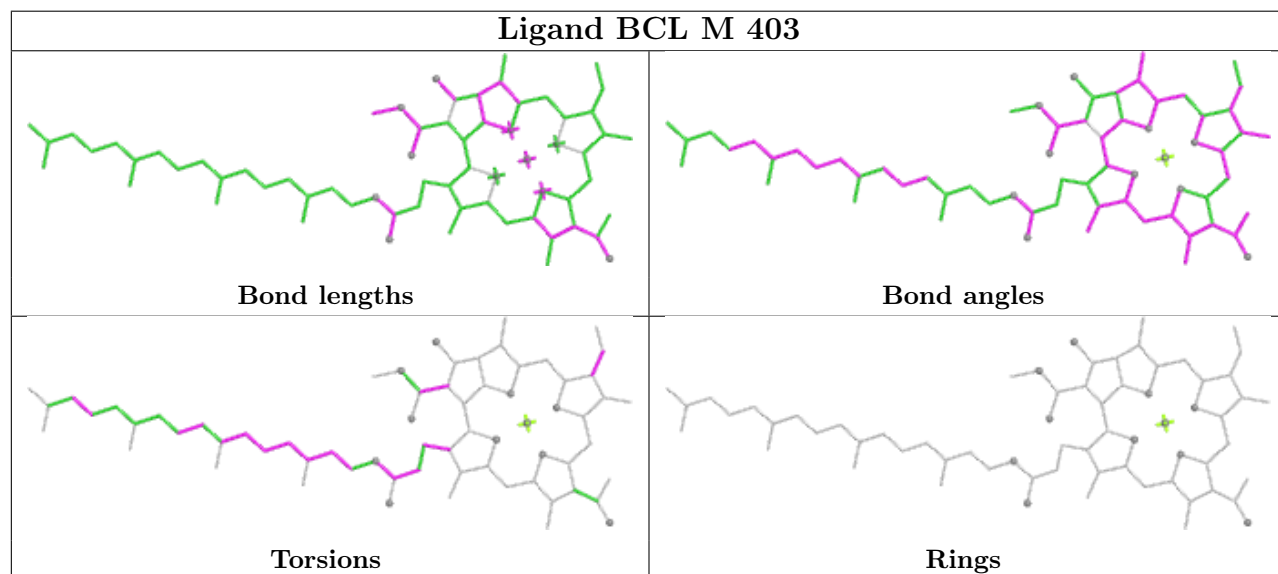
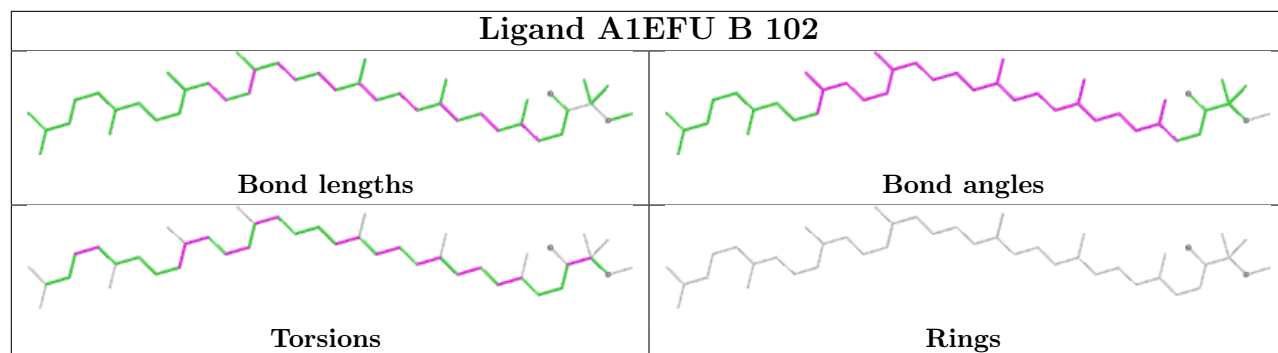
Ligand BCL s 103	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand A1EFU s 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand A1EFU F 104	
 Bond lengths	 Bond angles
 Torsions	 Rings

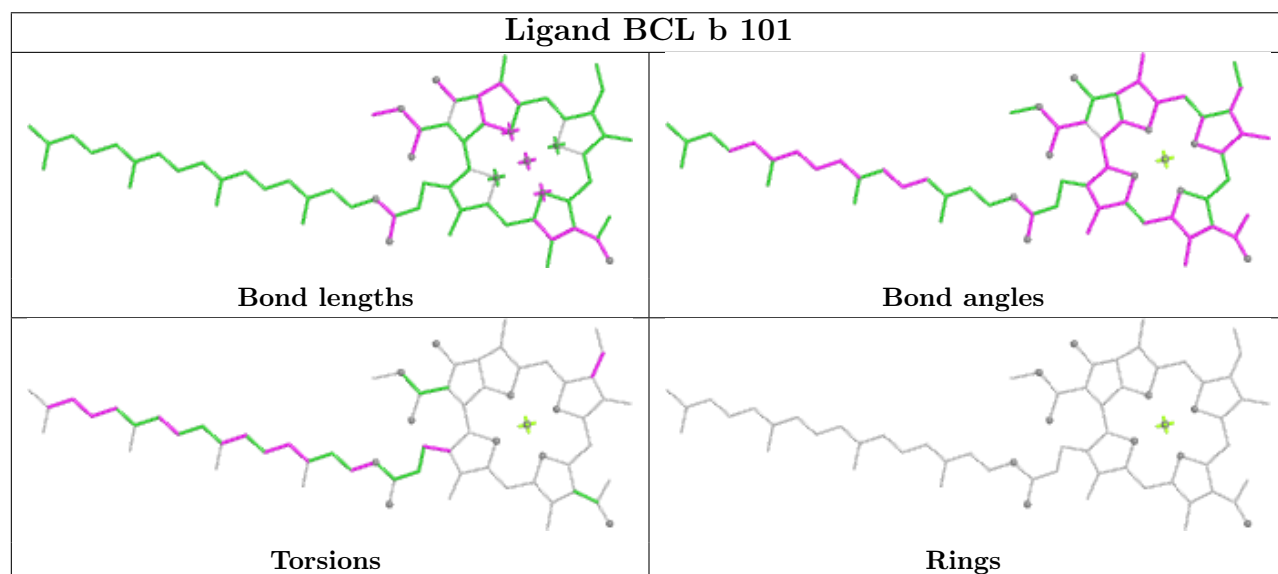
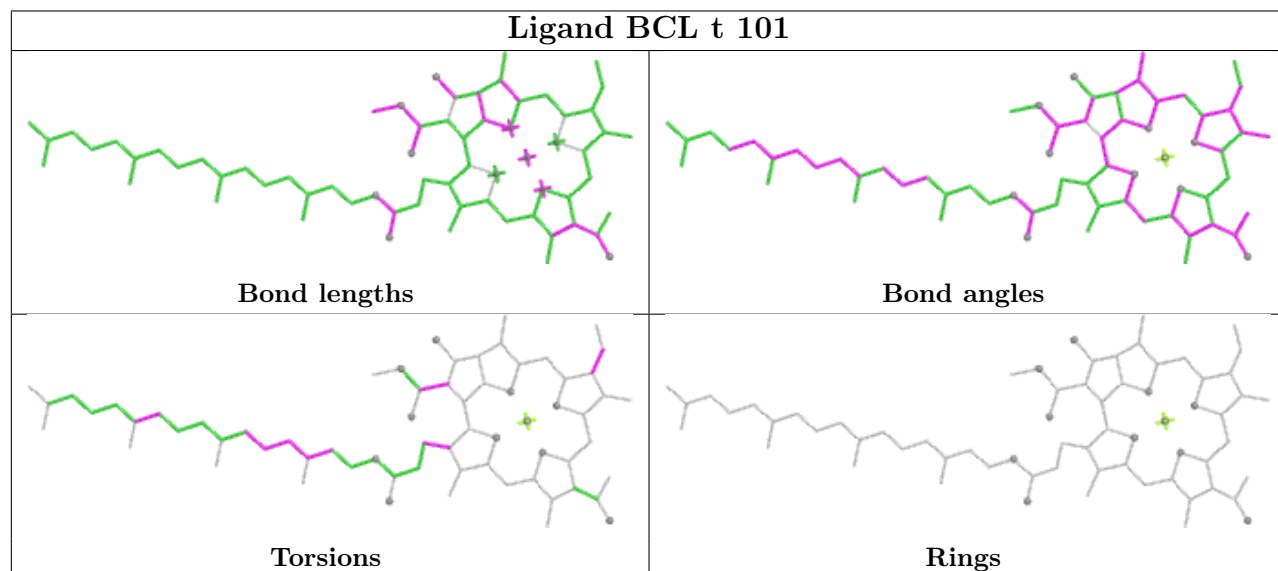
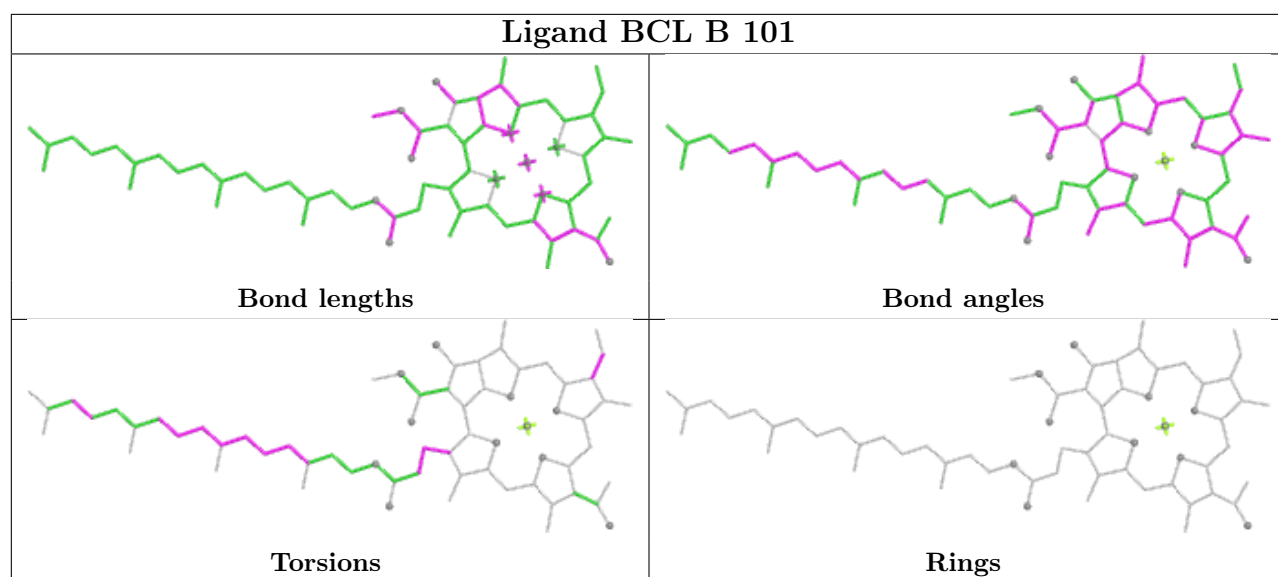


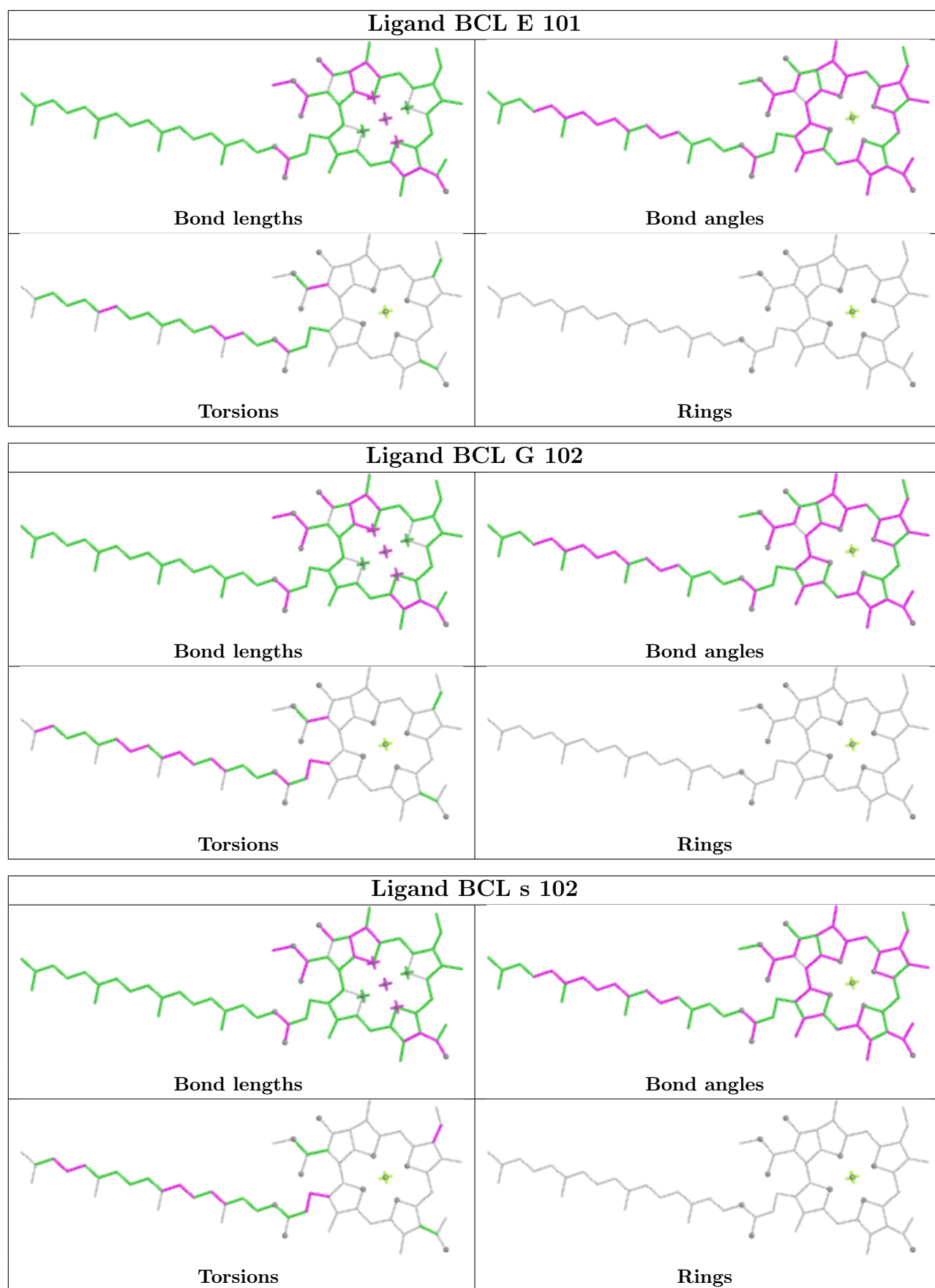


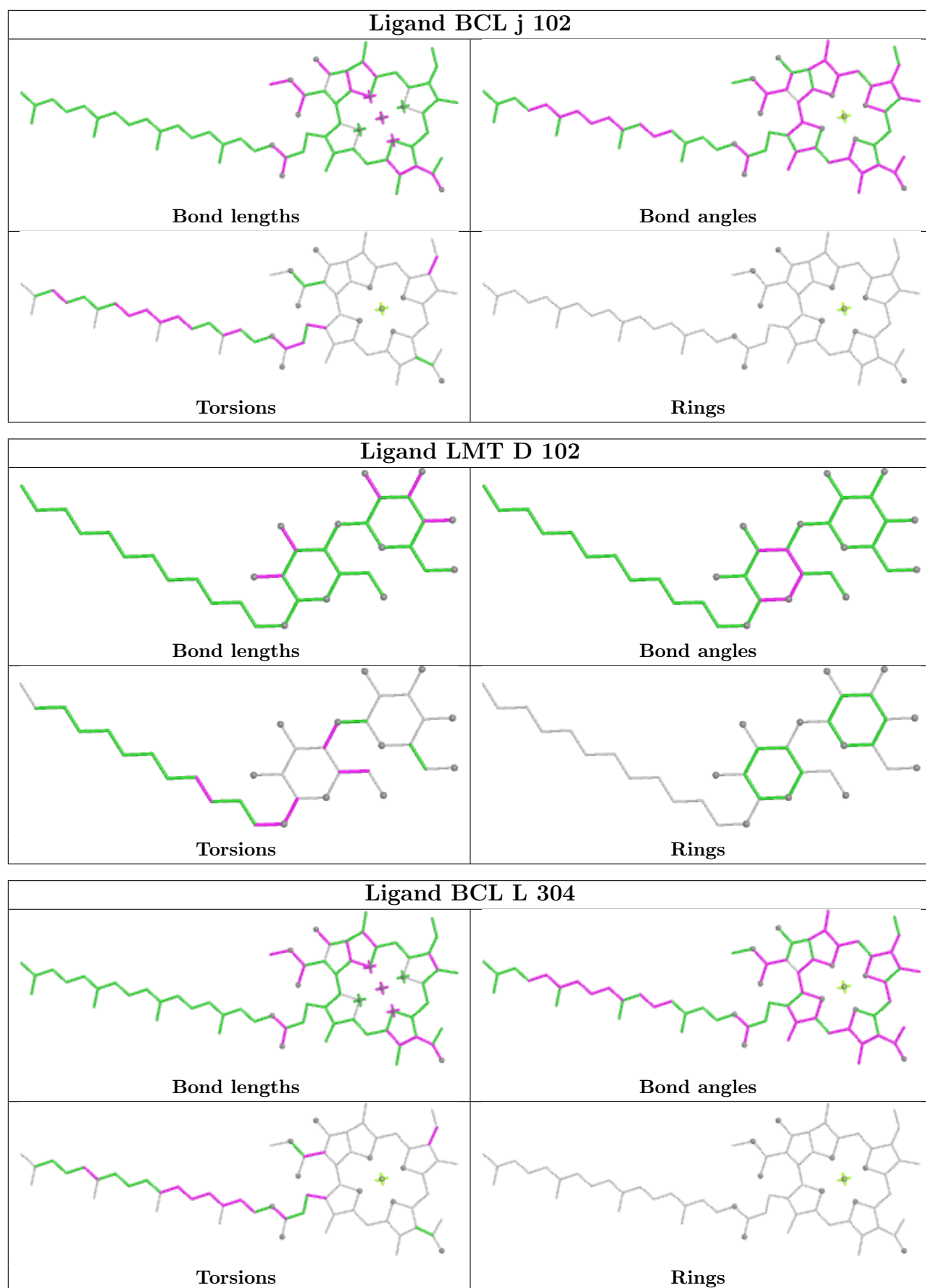


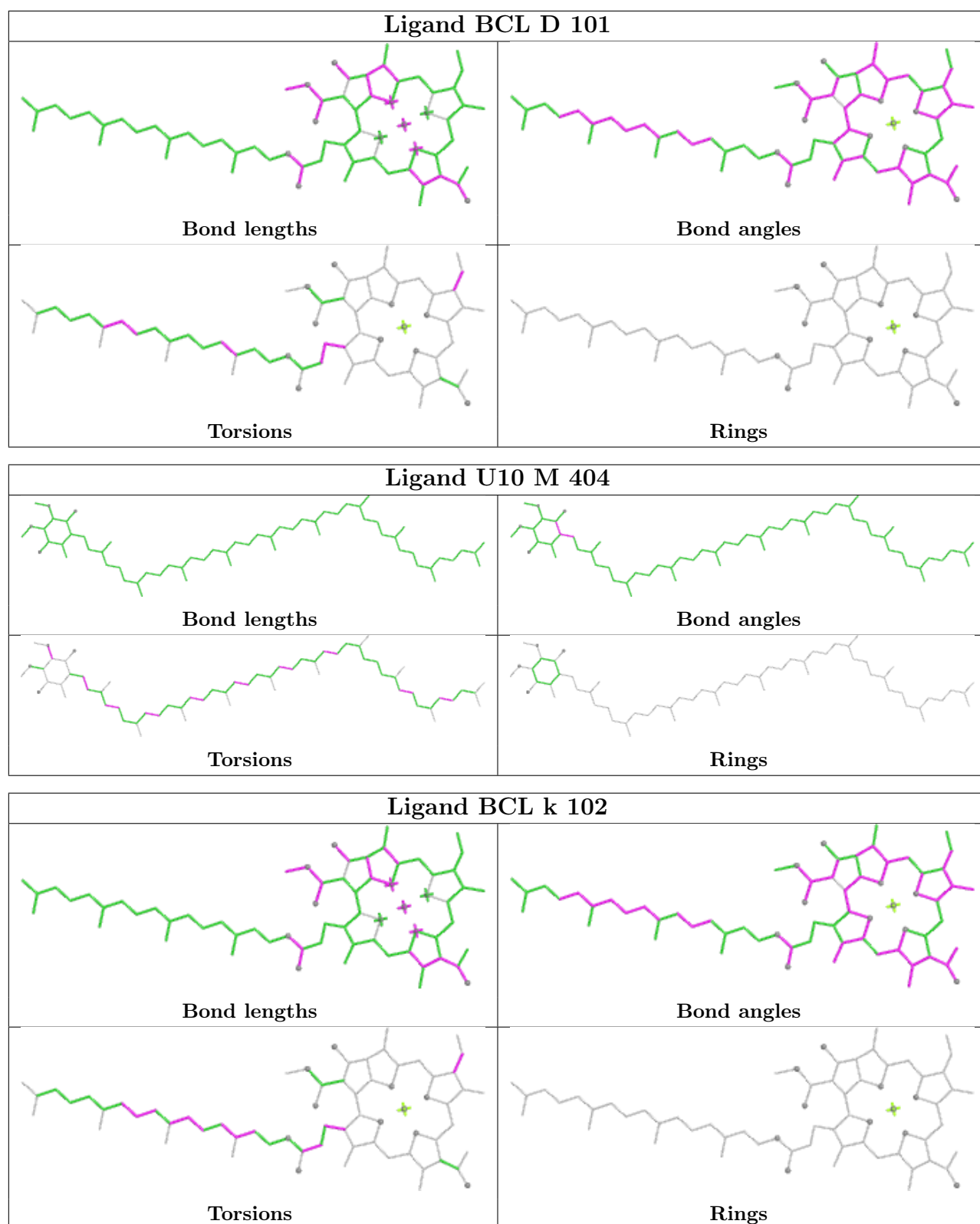


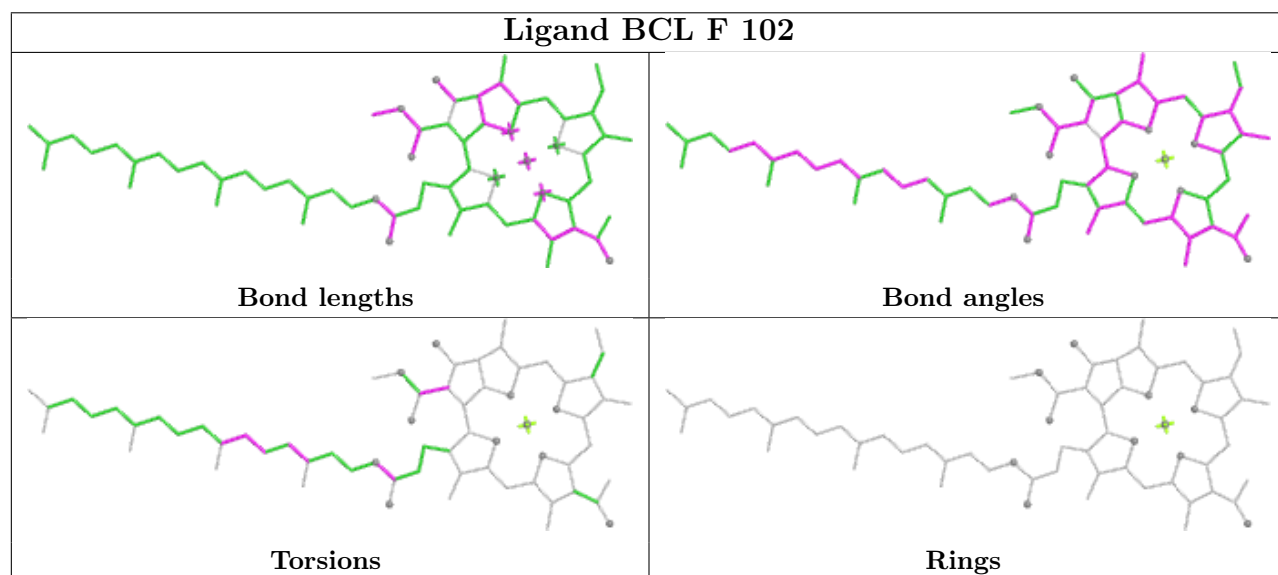
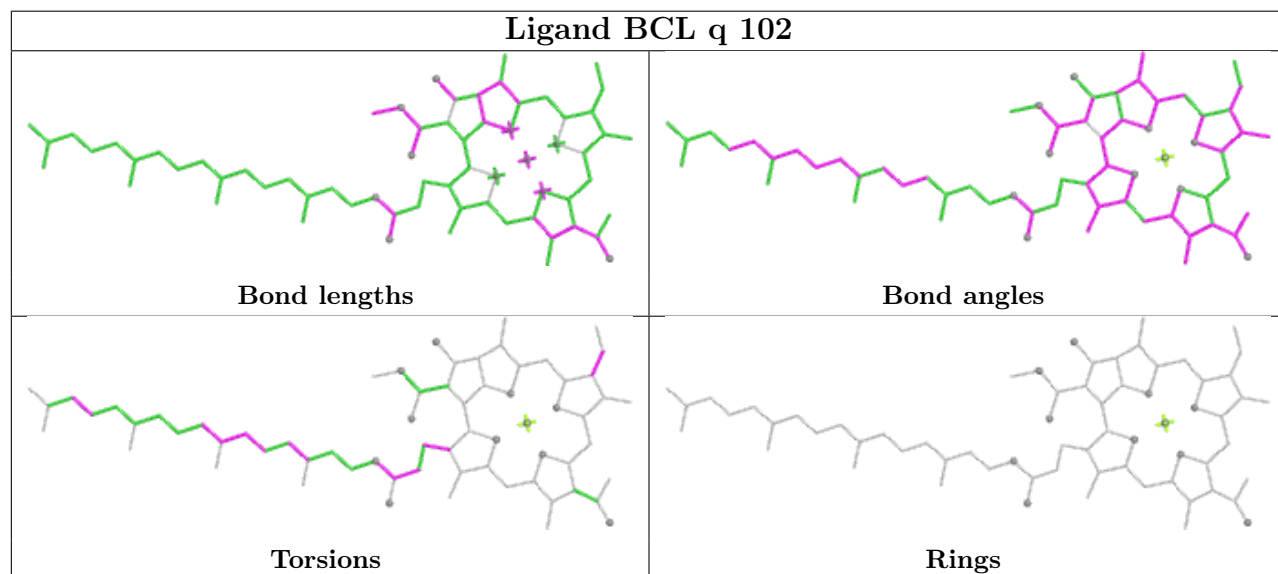
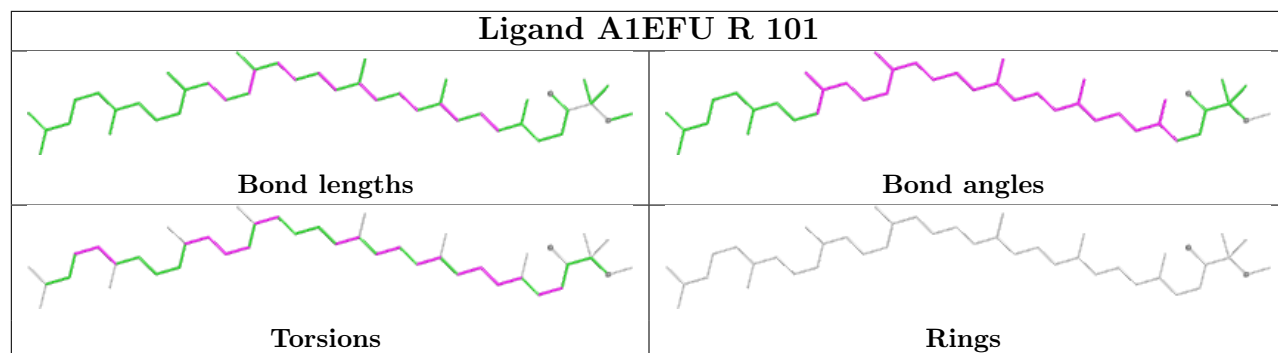


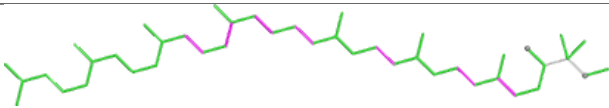
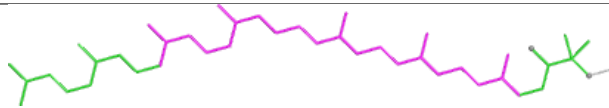
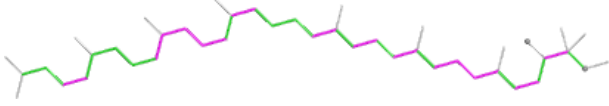
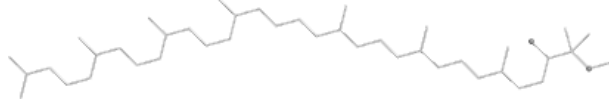


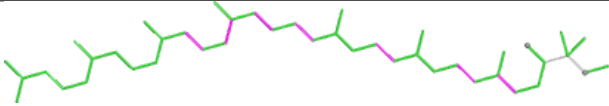
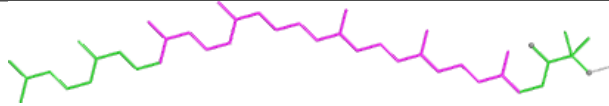
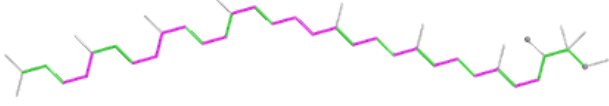
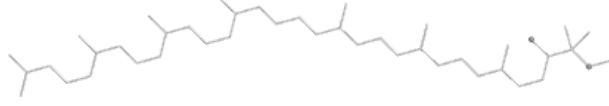


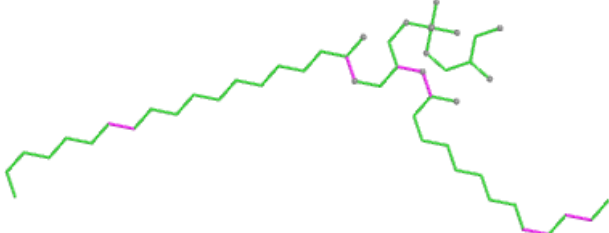
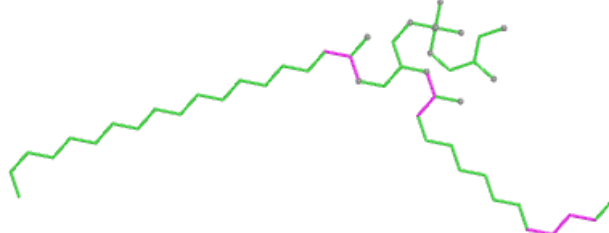
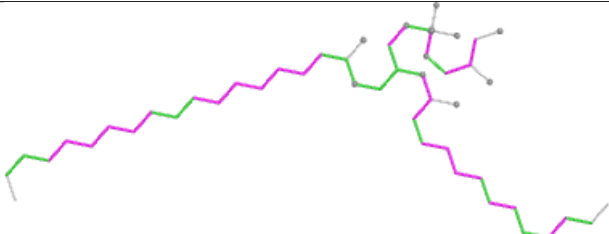
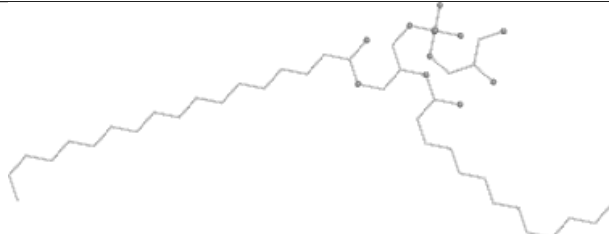


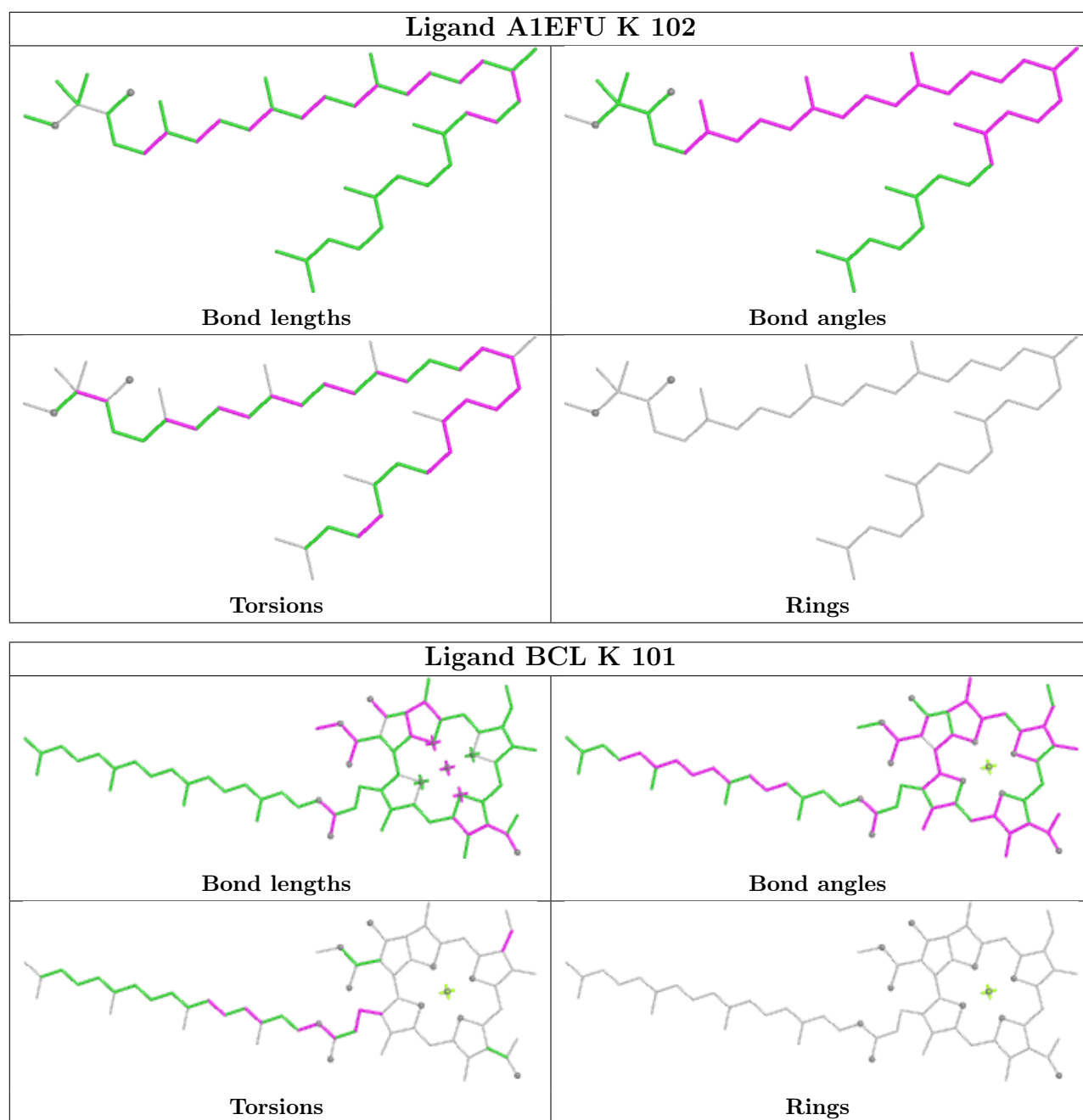


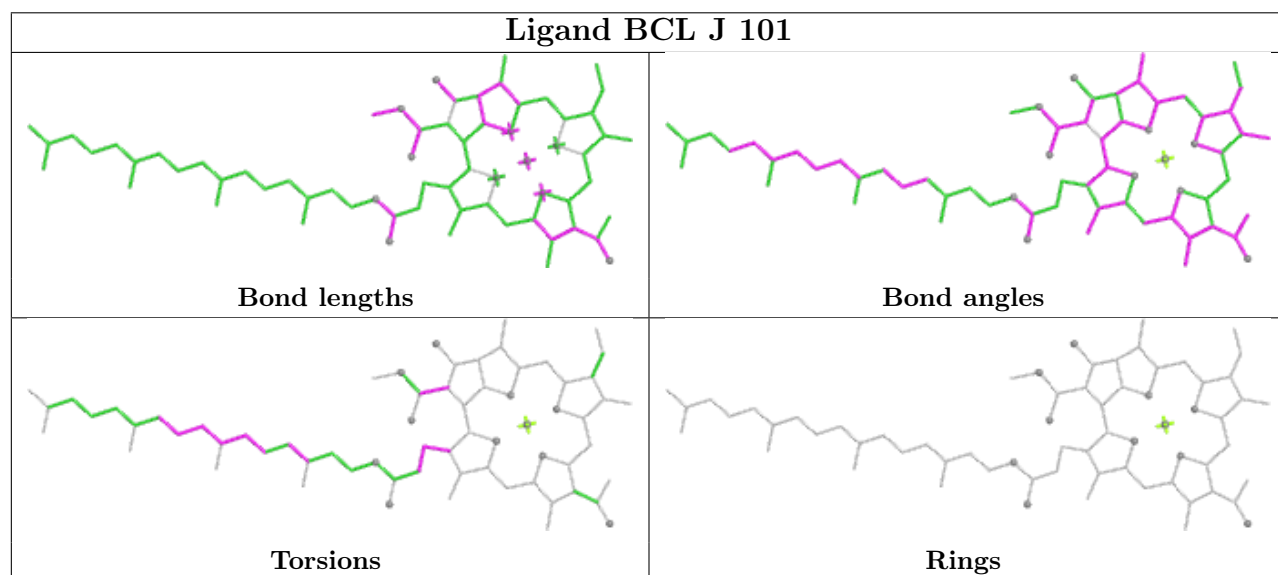
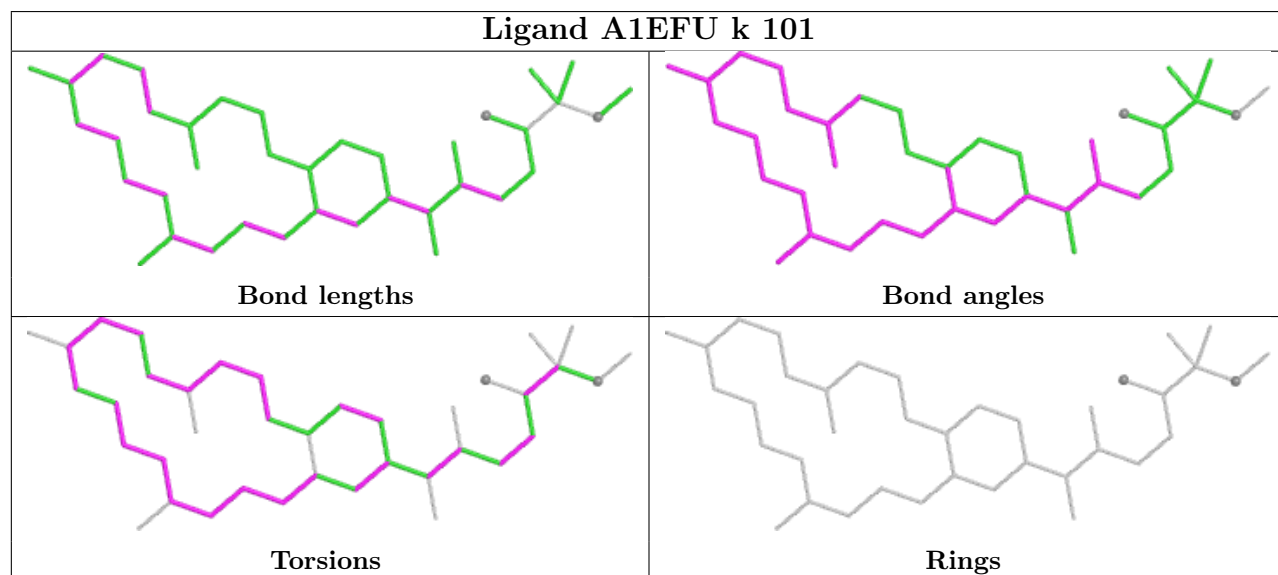
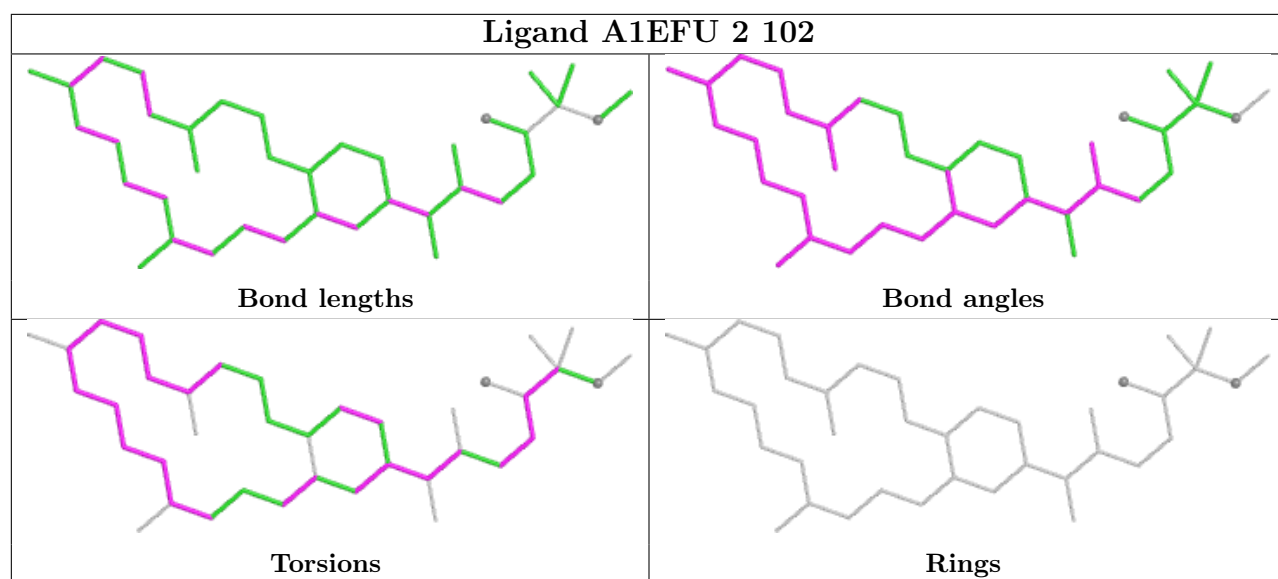


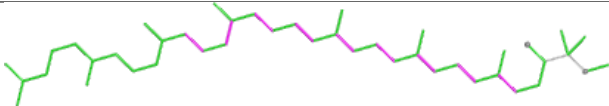
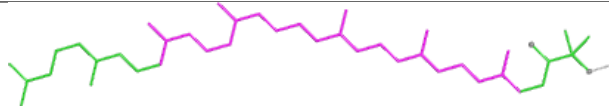
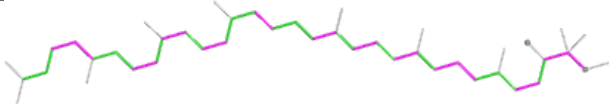
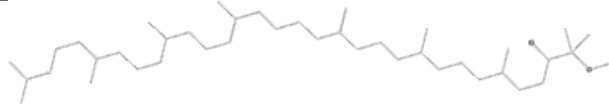
Ligand A1EFU E 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

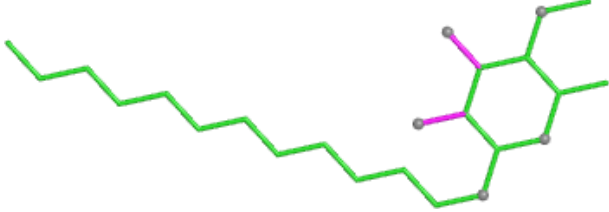
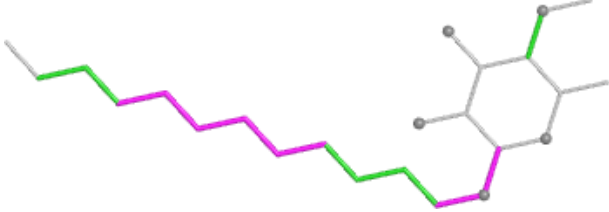
Ligand A1EFU I 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

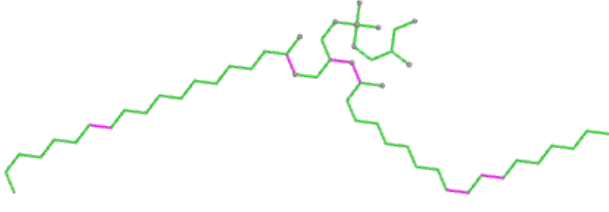
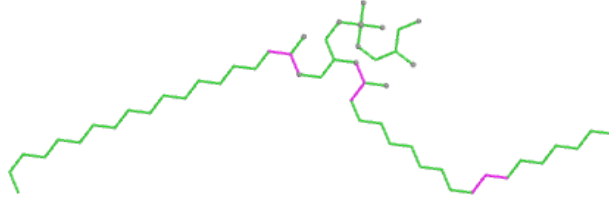
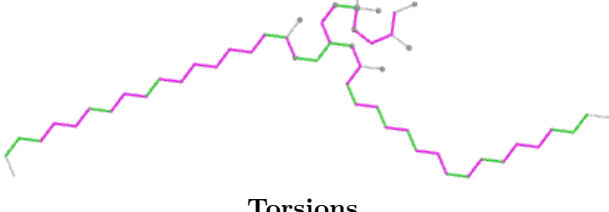
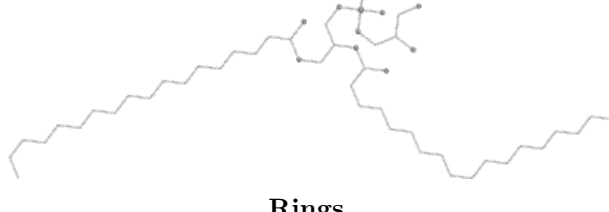
Ligand MW9 H 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

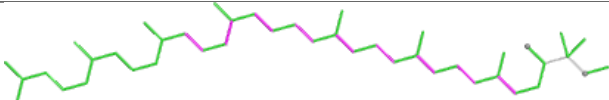
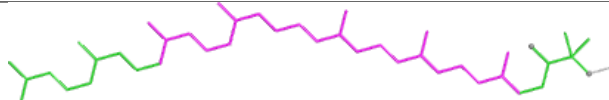
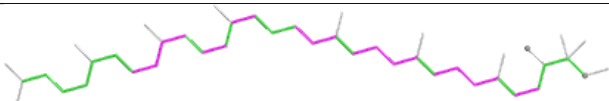
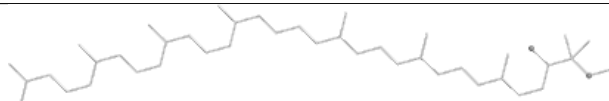


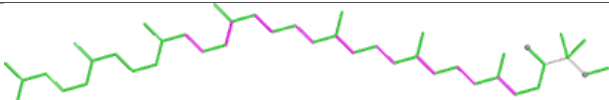
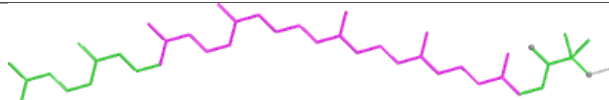
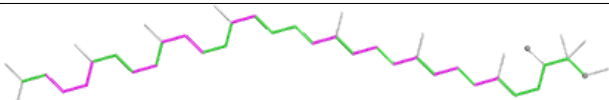
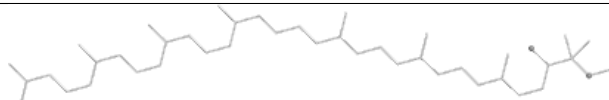


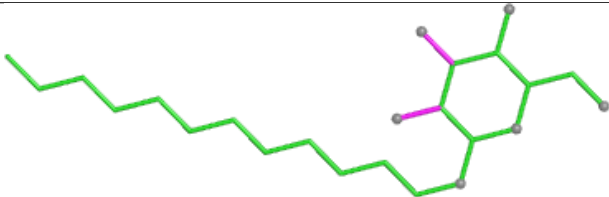
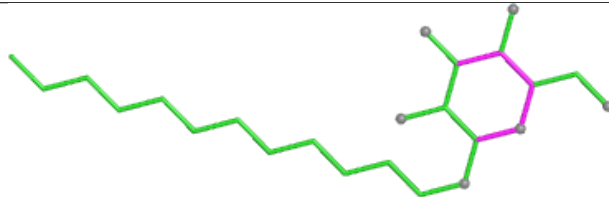
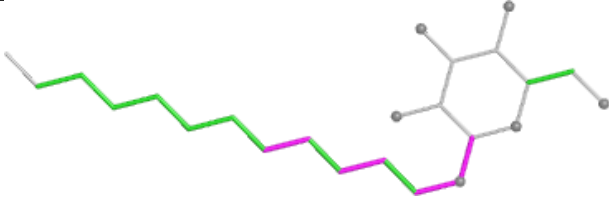
Ligand A1EFU s 104	
	
Bond lengths	Bond angles
	
Torsions	Rings

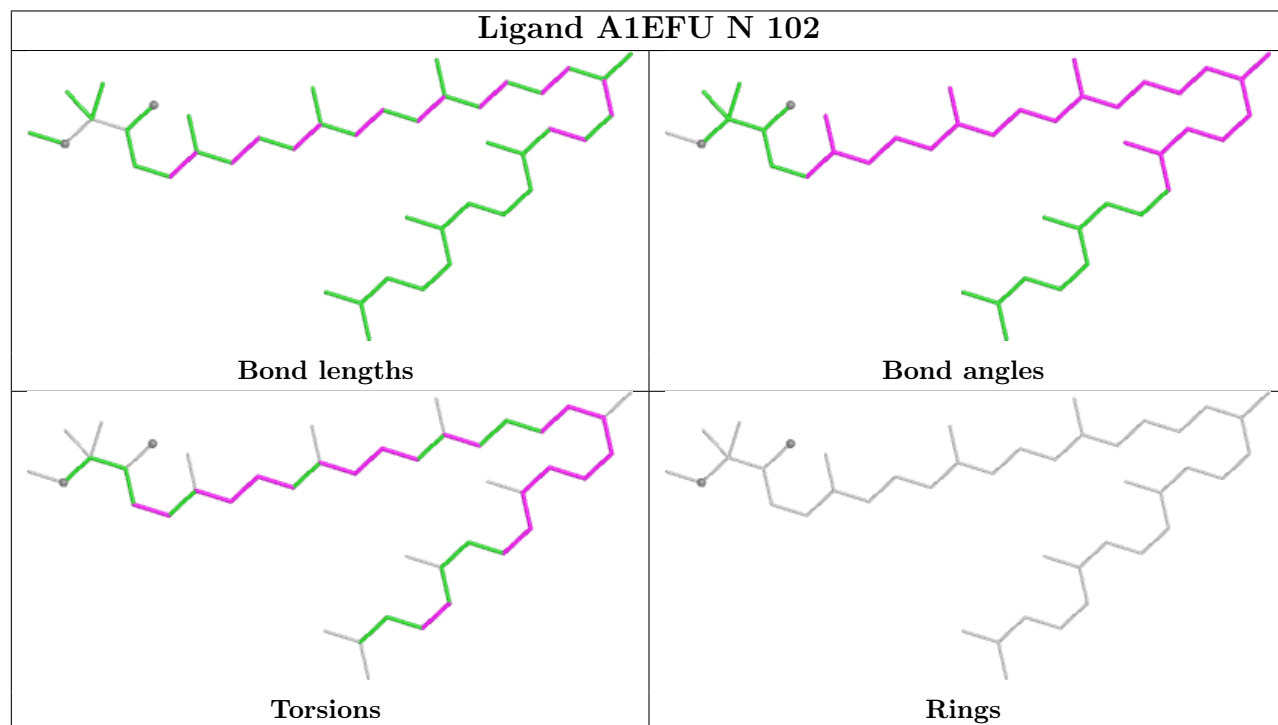
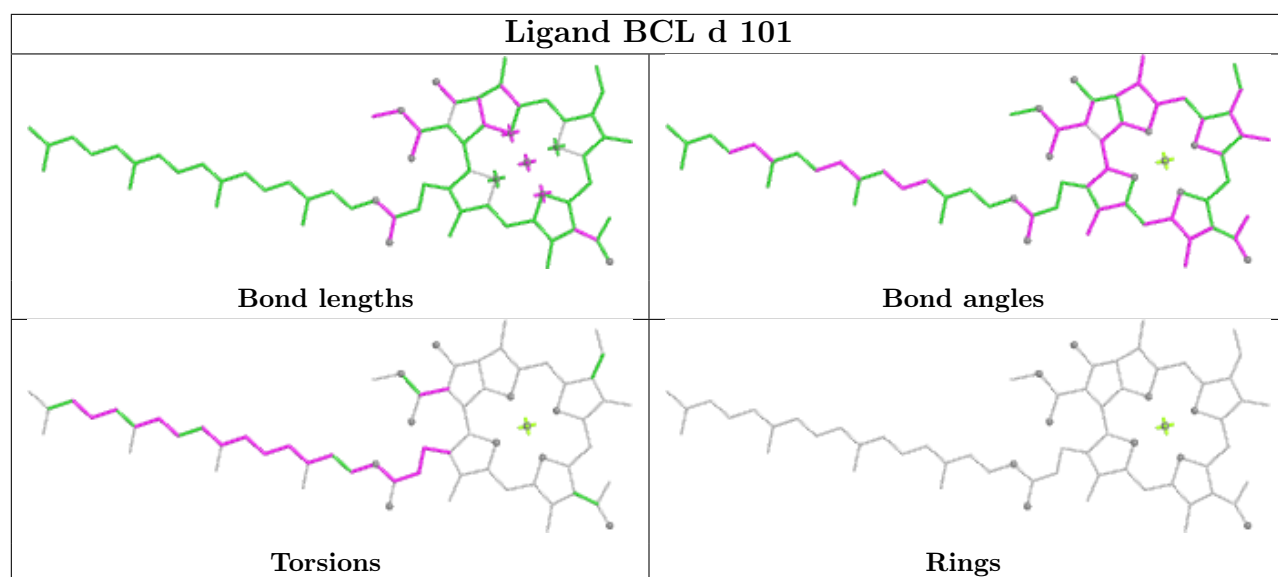
Ligand LMT L 306	
	
Bond lengths	Bond angles
	
Torsions	Rings

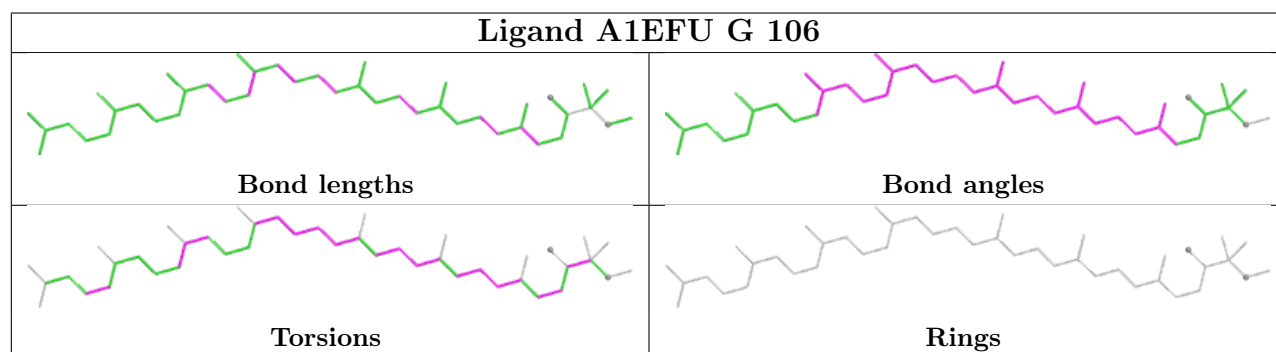
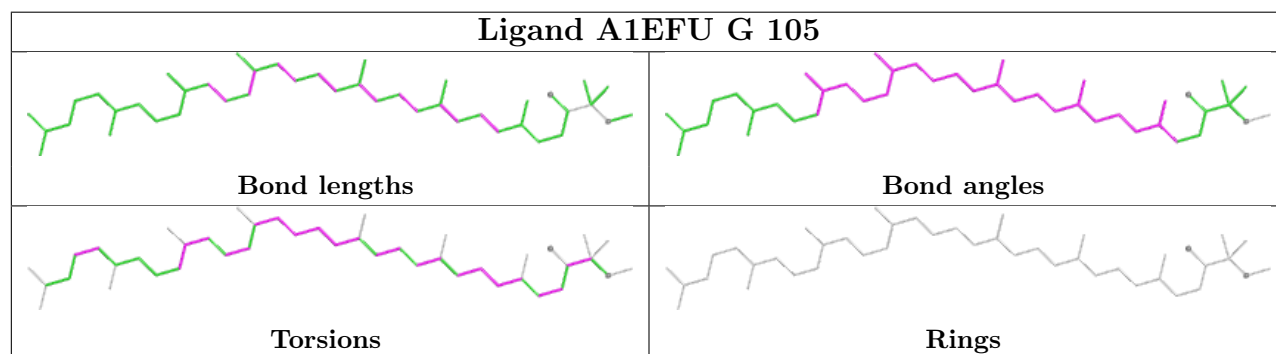
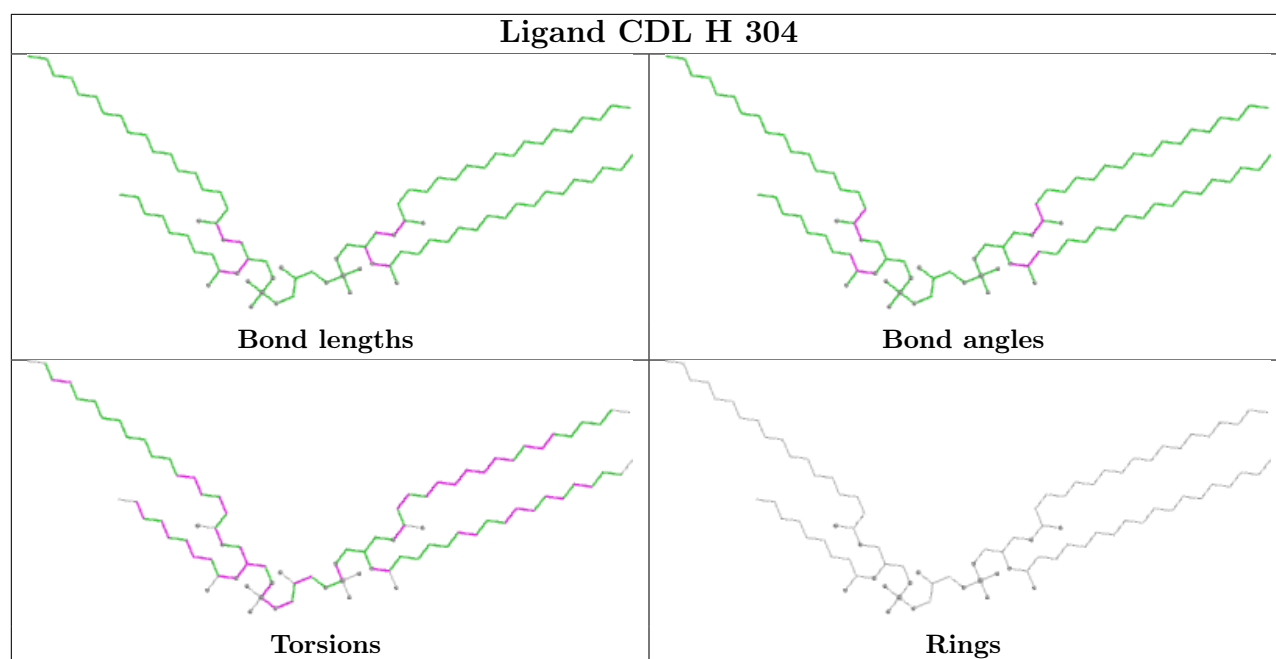
Ligand MW9 M 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

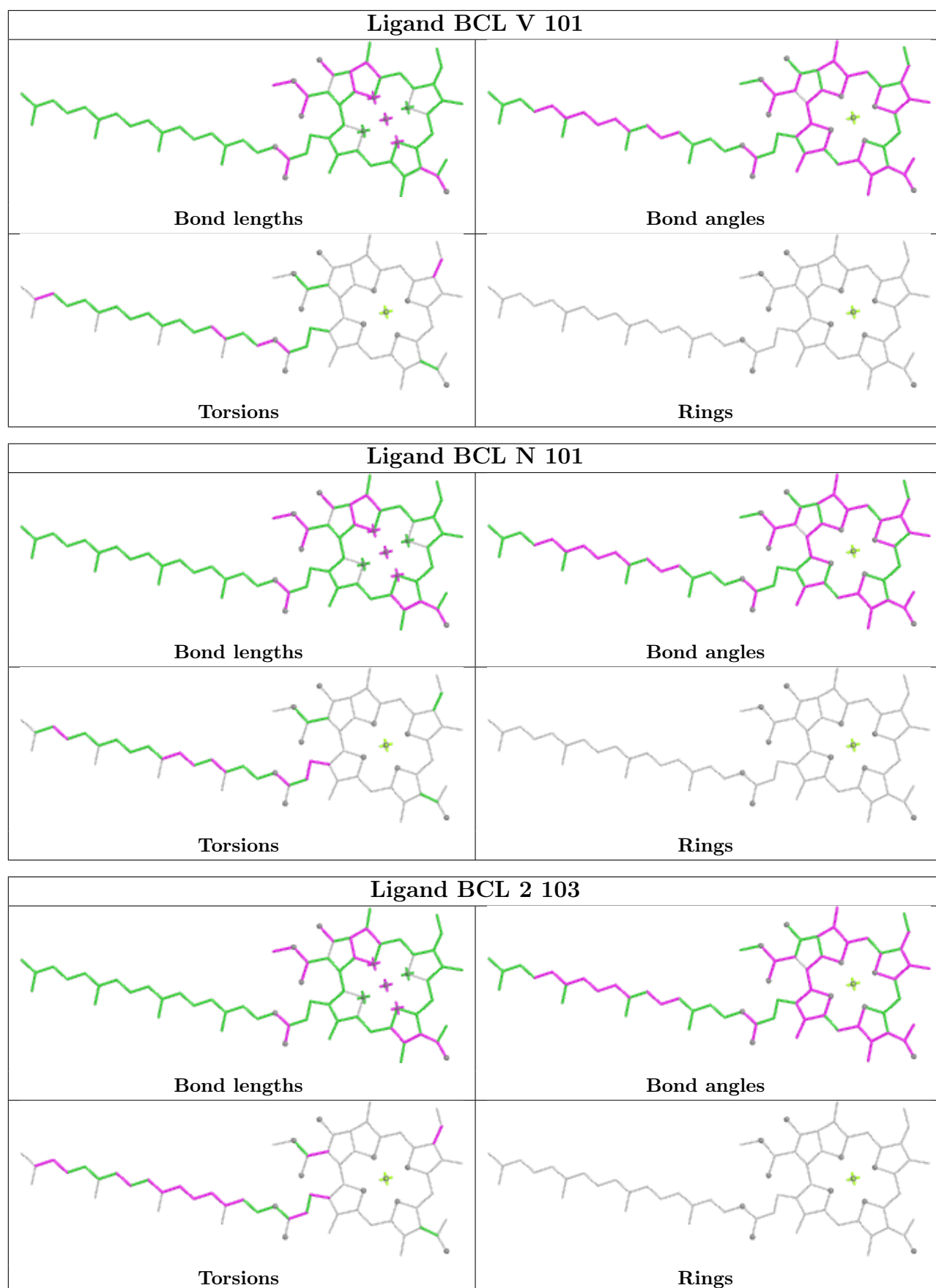
Ligand A1EFU a 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand A1EFU D 104	
 Bond lengths	 Bond angles
 Torsions	 Rings

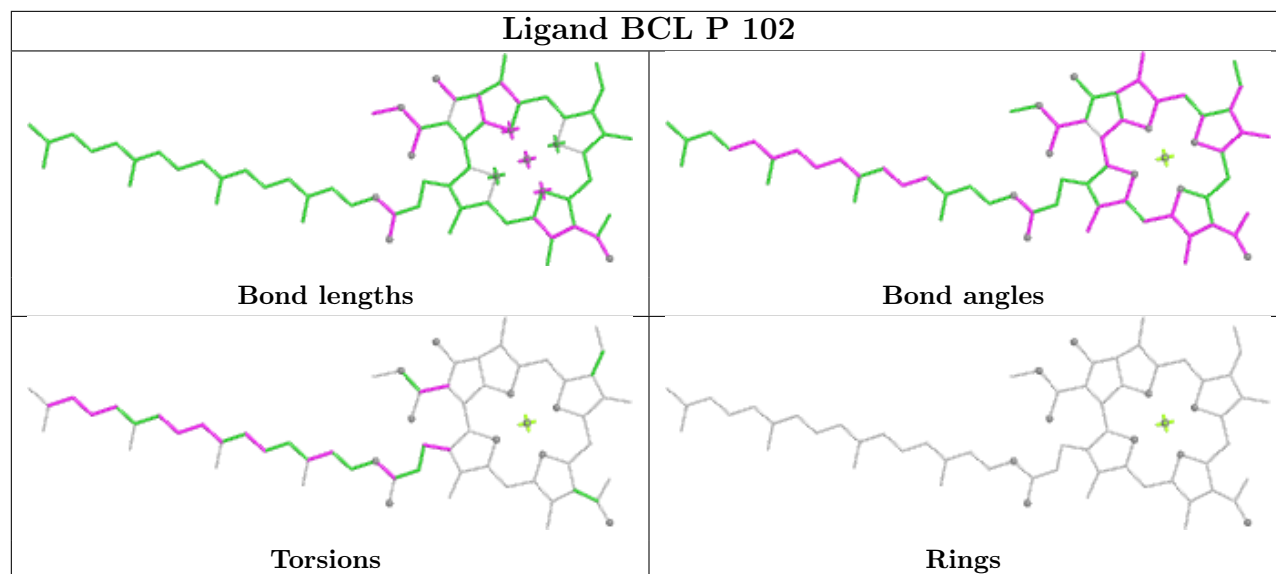
Ligand LMT L 305	
 Bond lengths	 Bond angles
 Torsions	 Rings



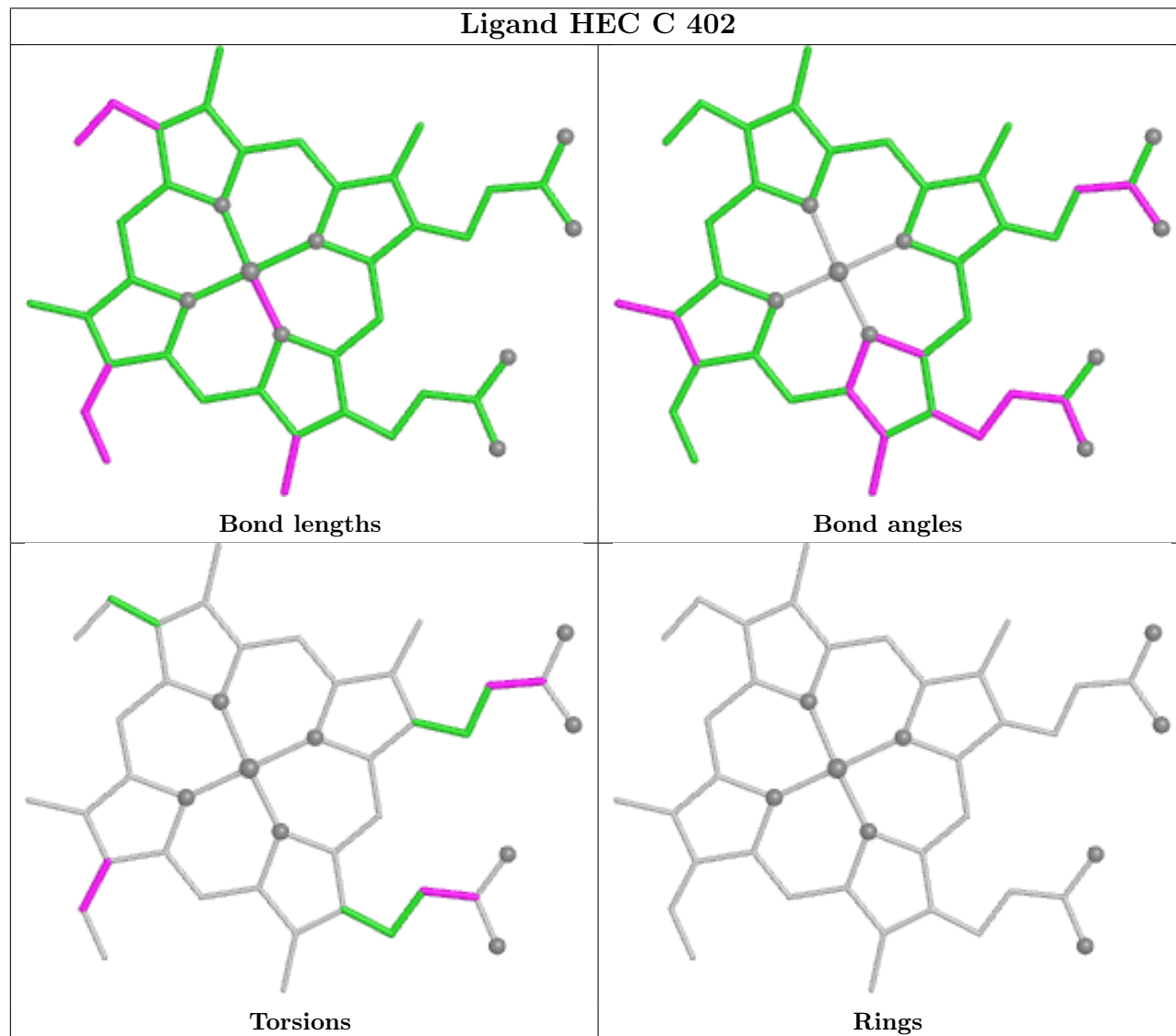


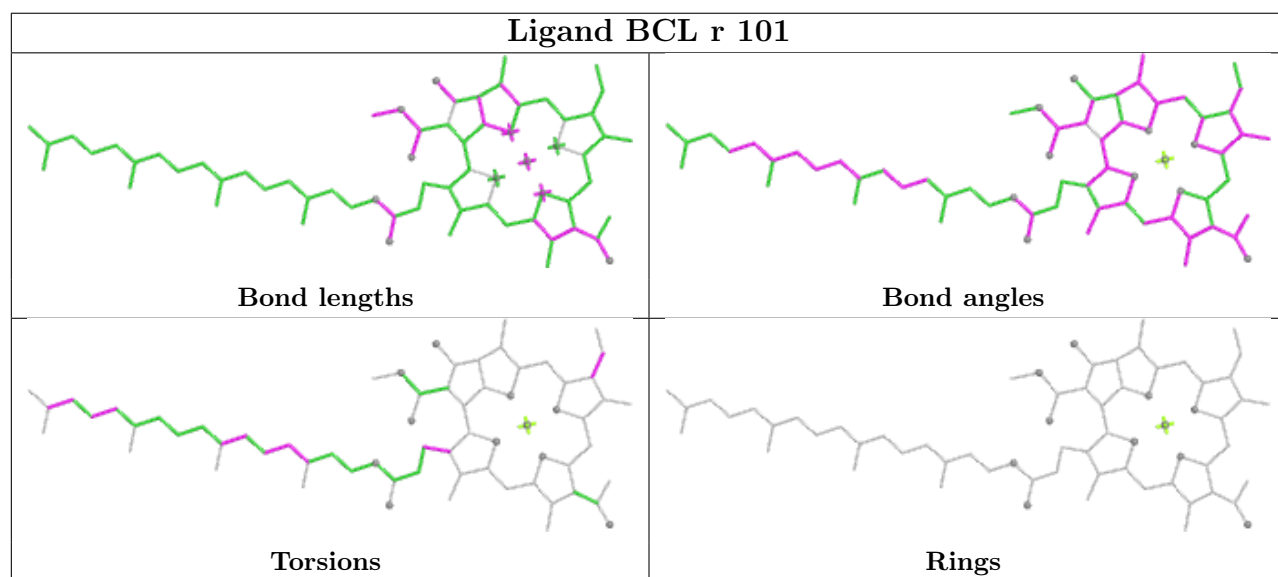
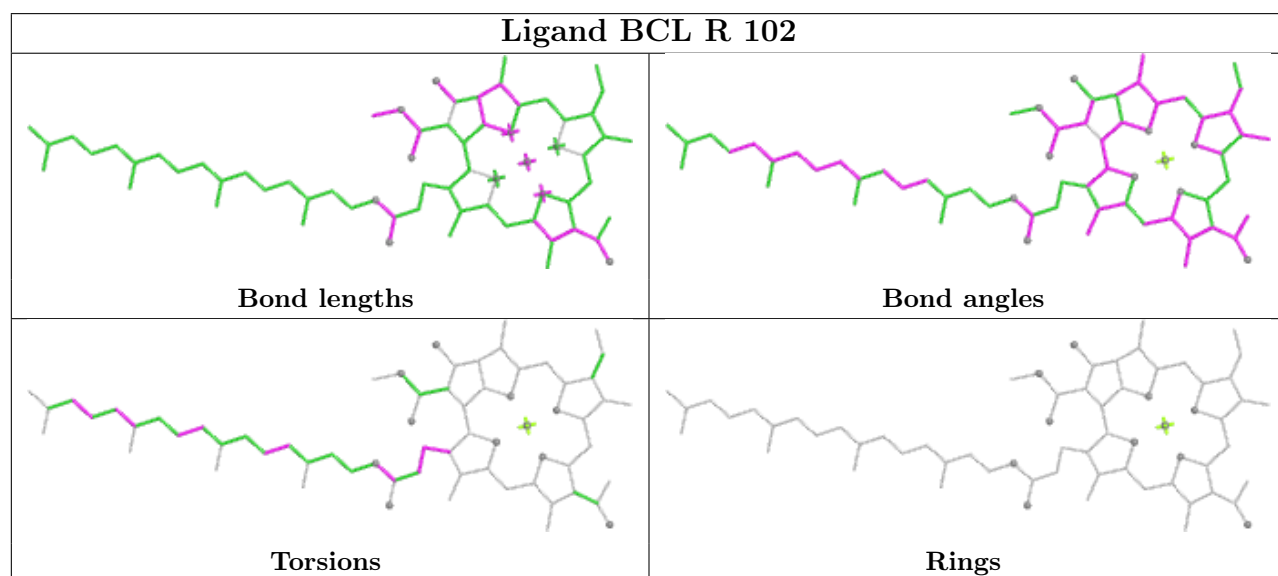
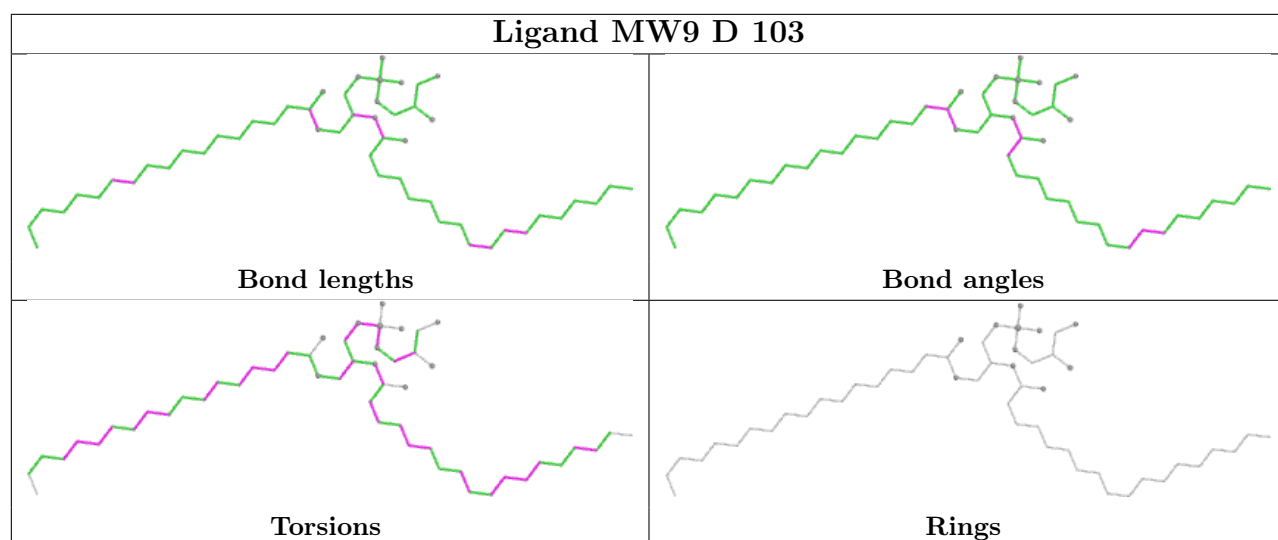


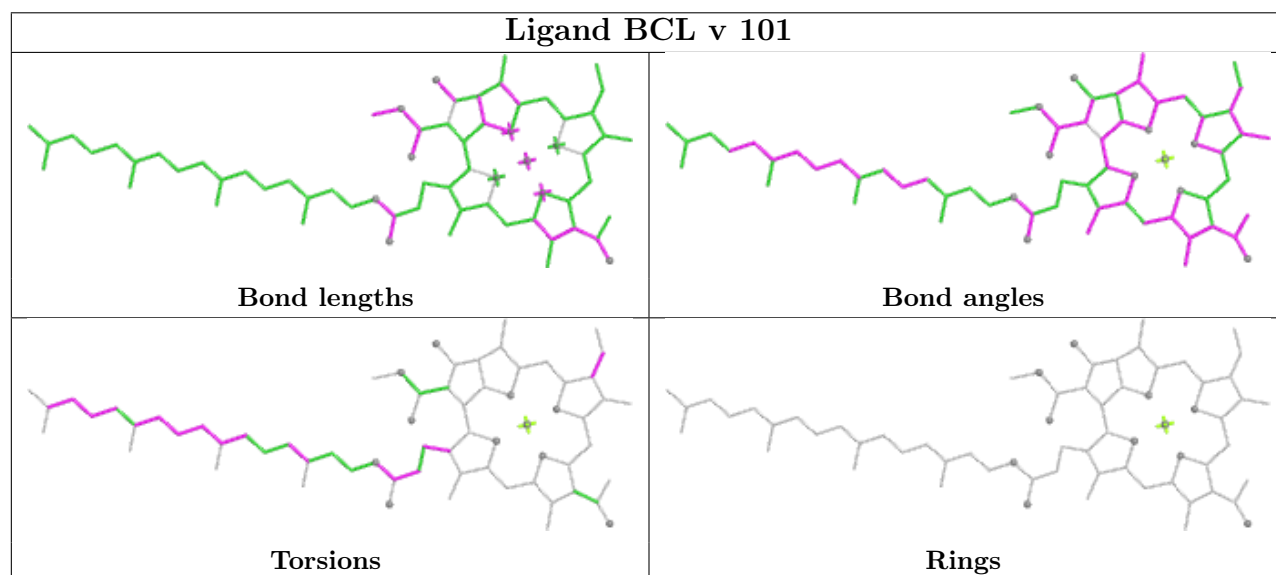
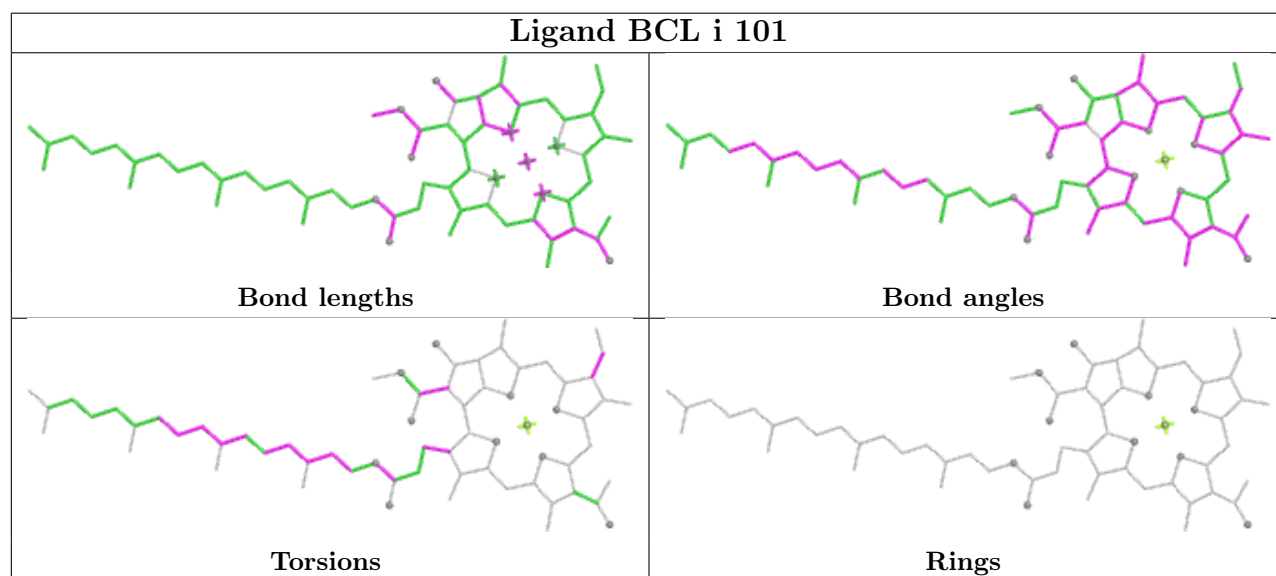
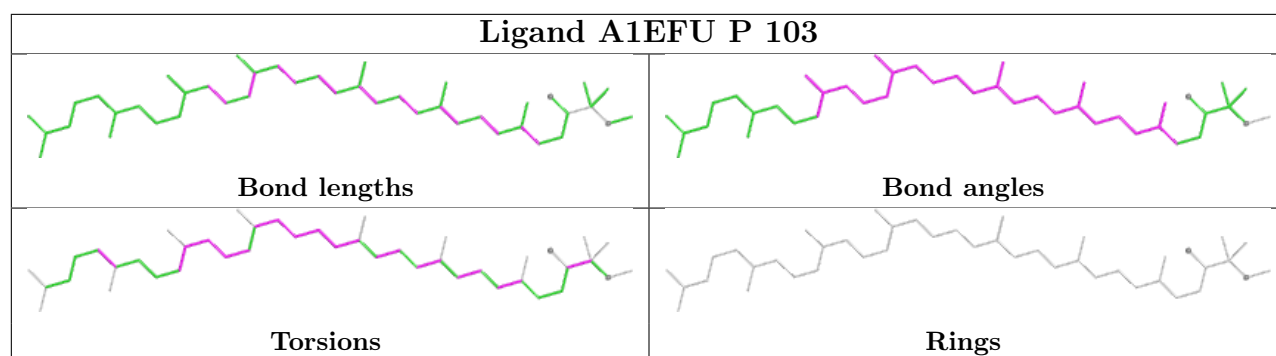
Ligand BCL P 102

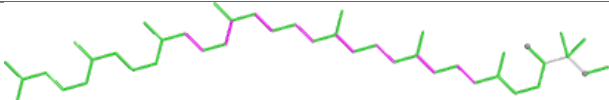
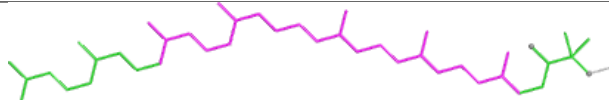
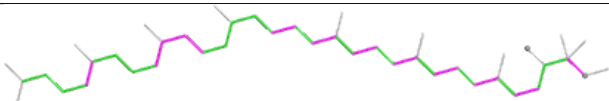
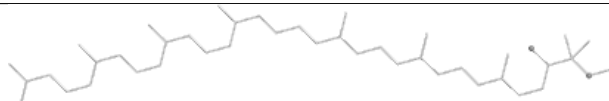


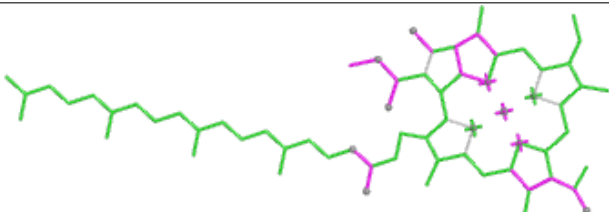
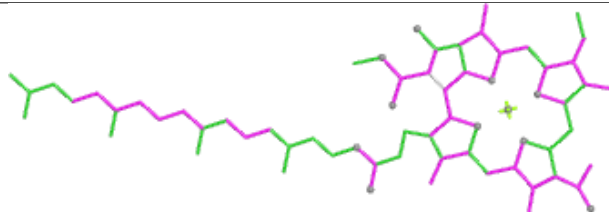
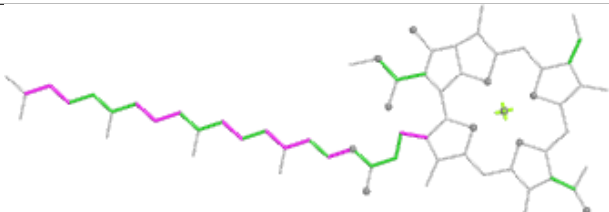
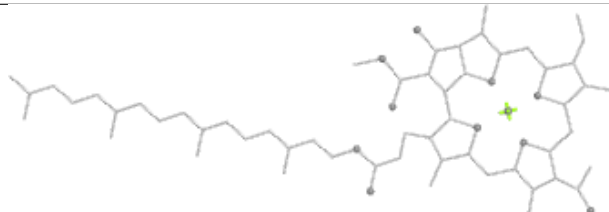
Ligand HEC C 402

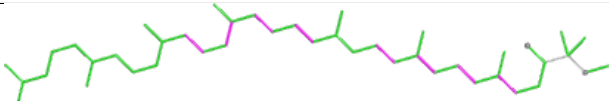
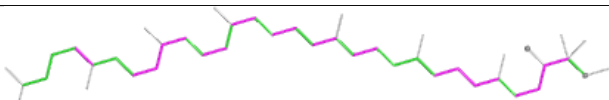
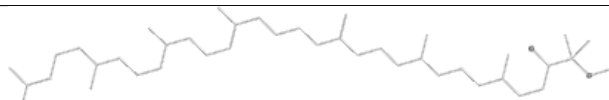


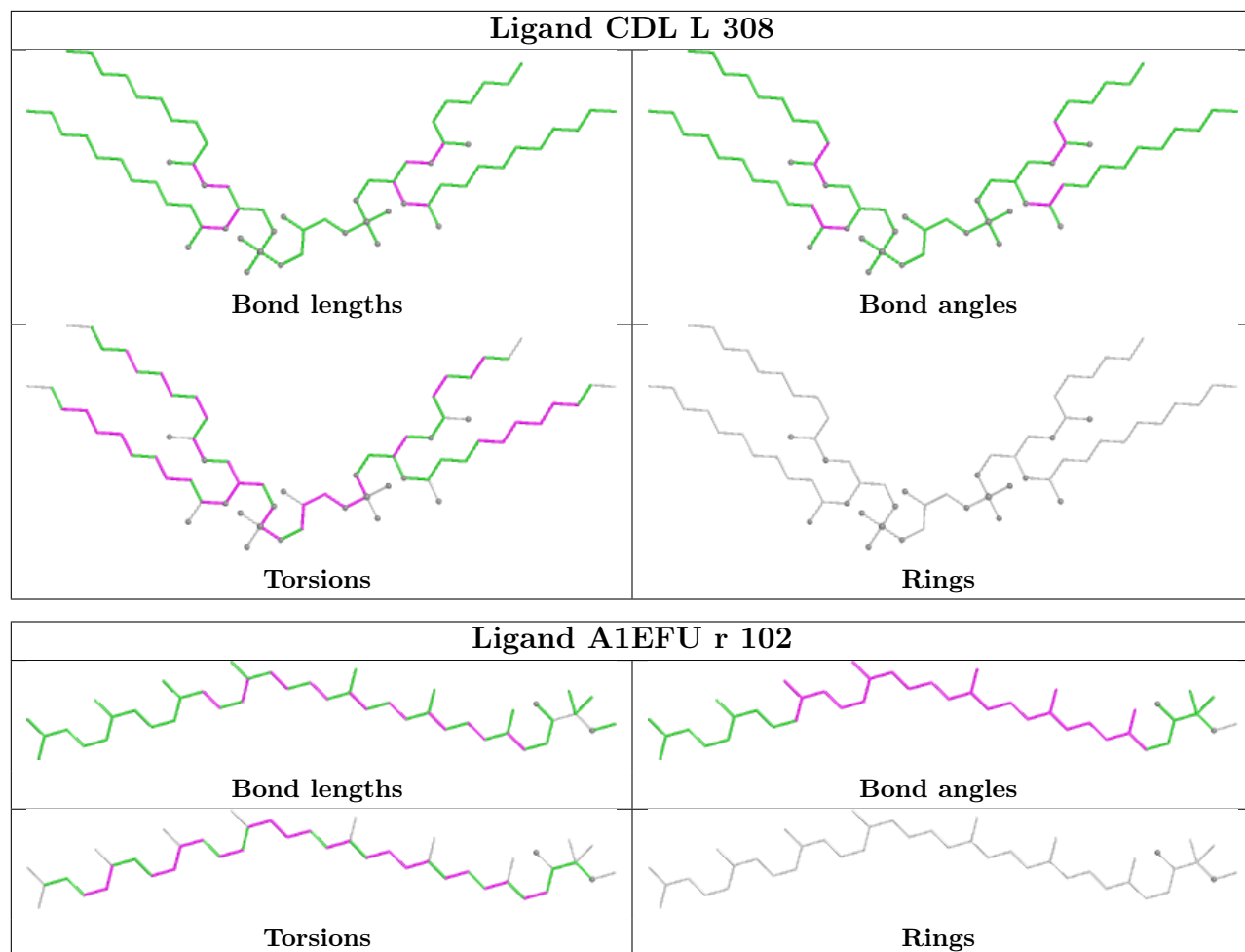




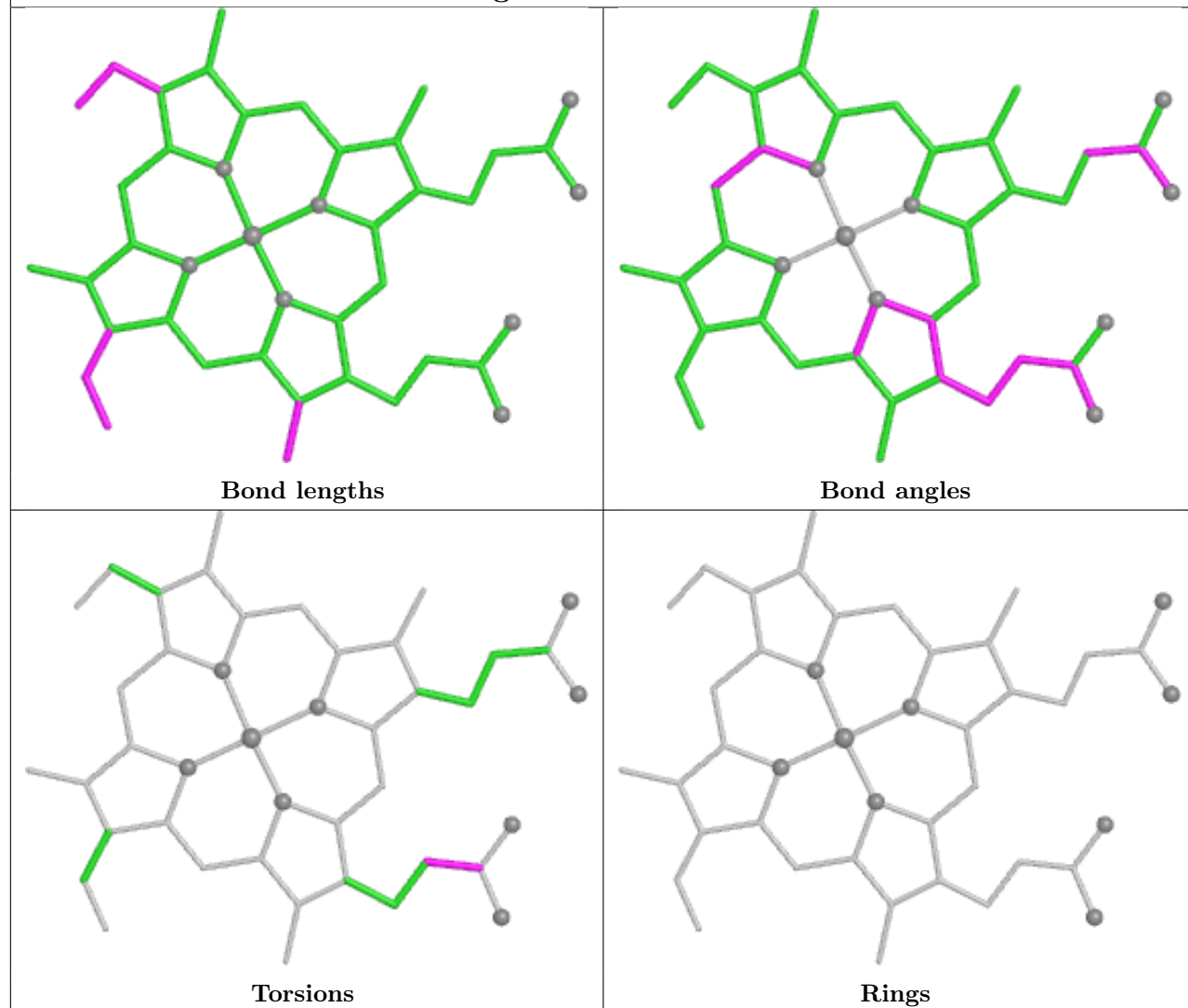
Ligand A1EFU M 407	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL e 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

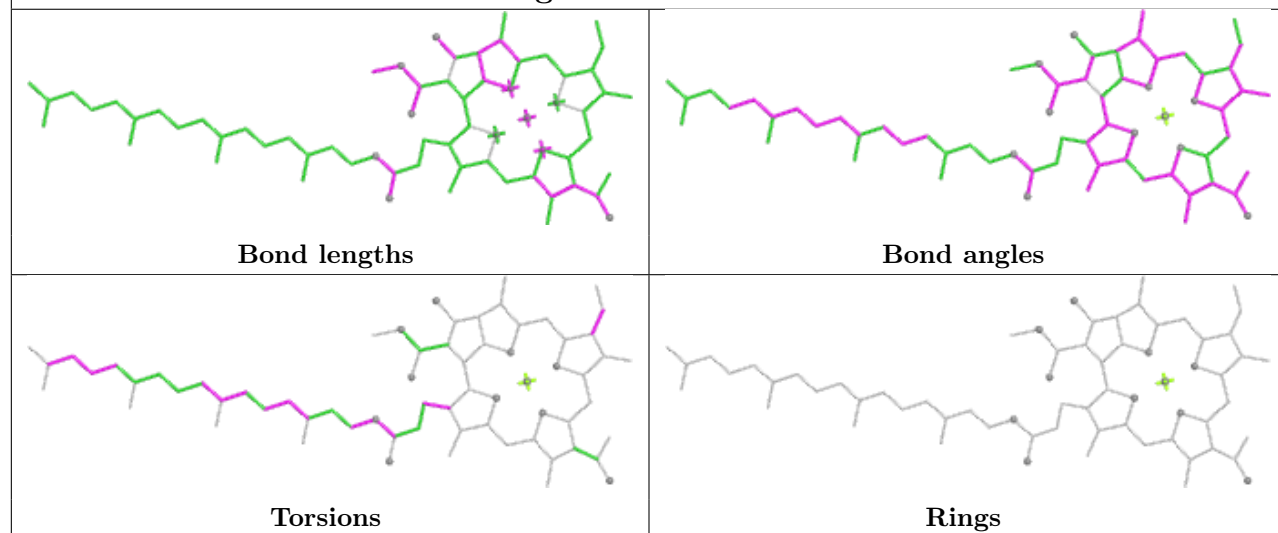
Ligand A1EFU v 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

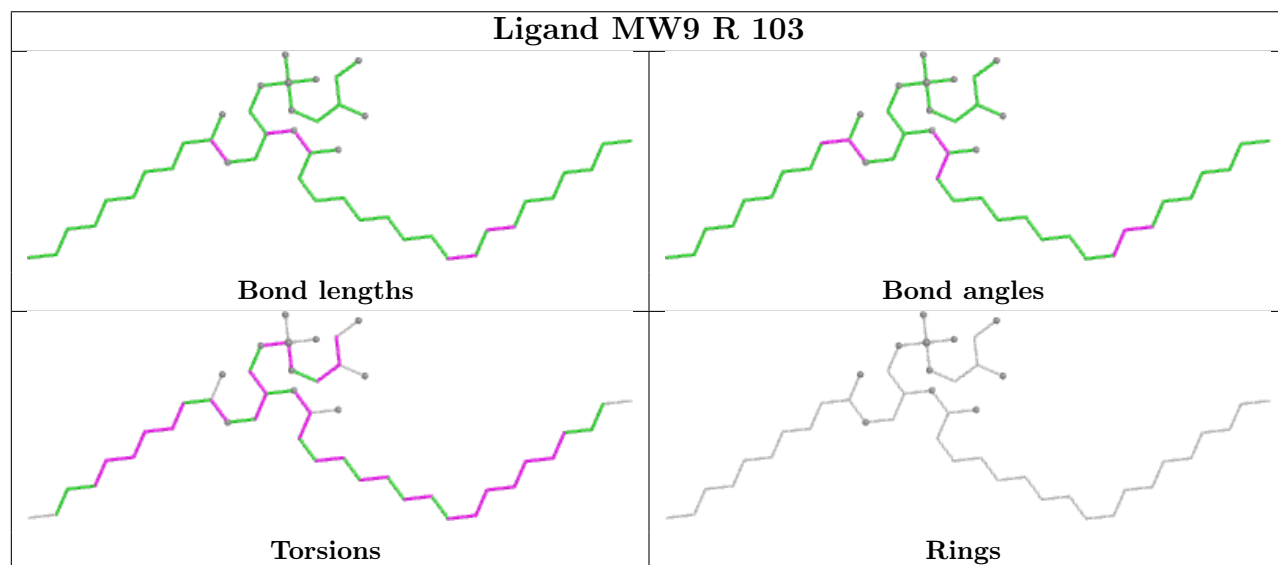
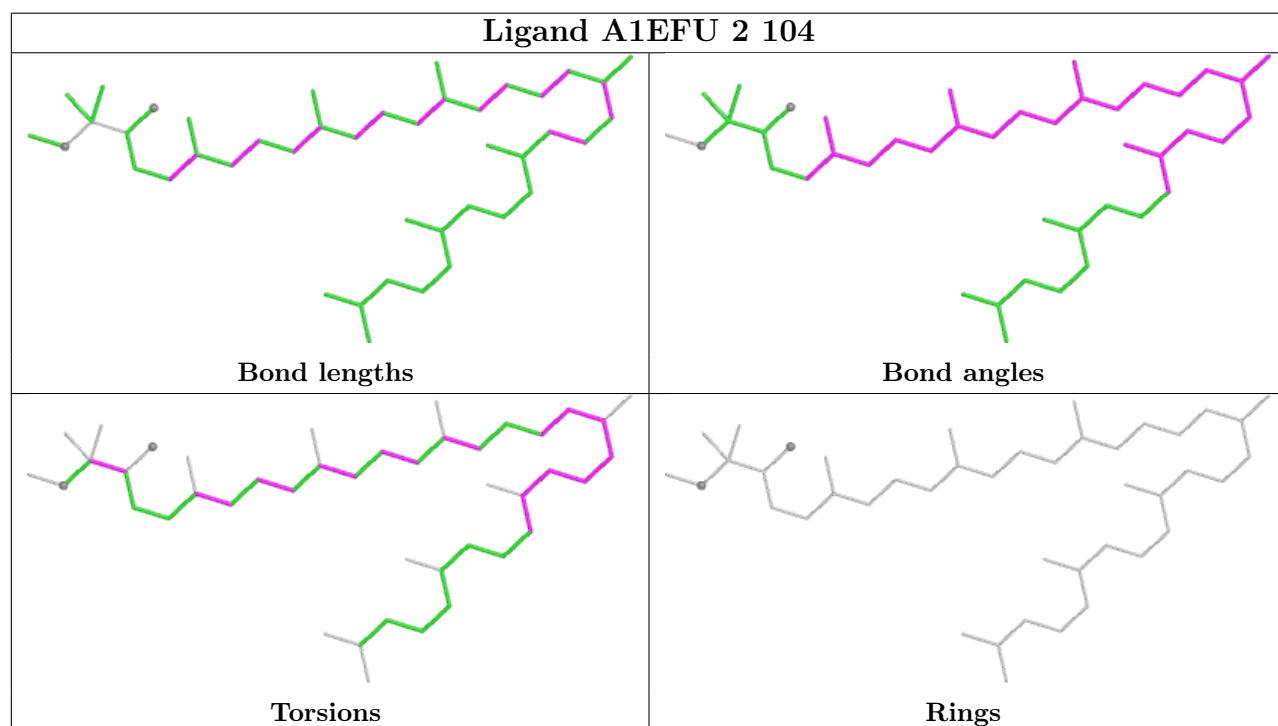
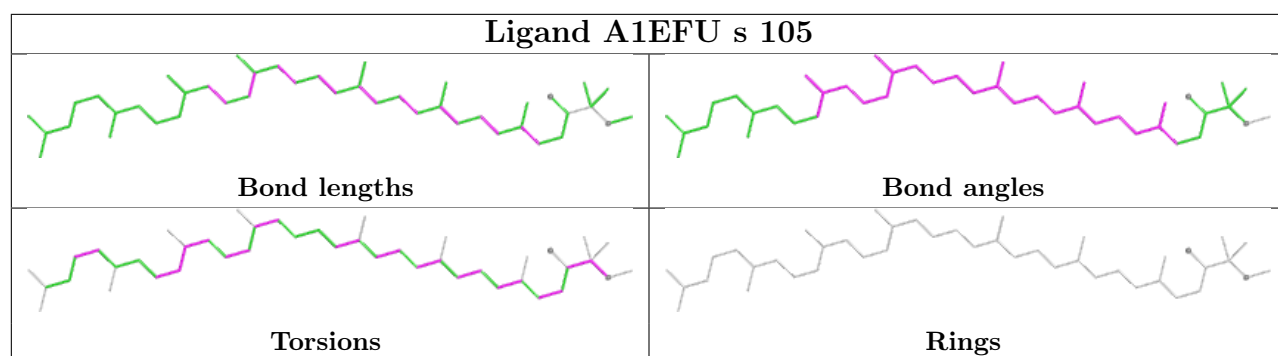


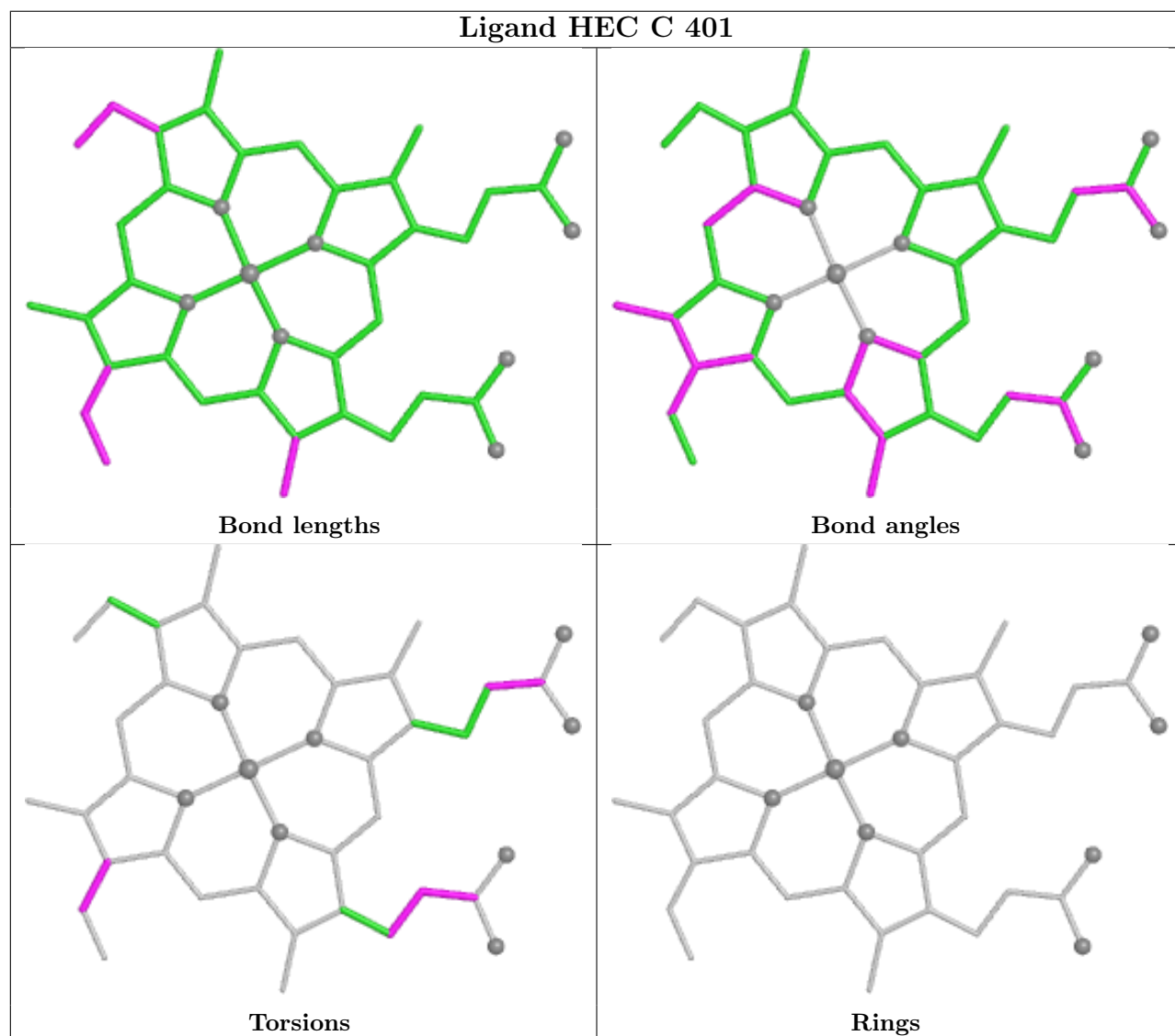
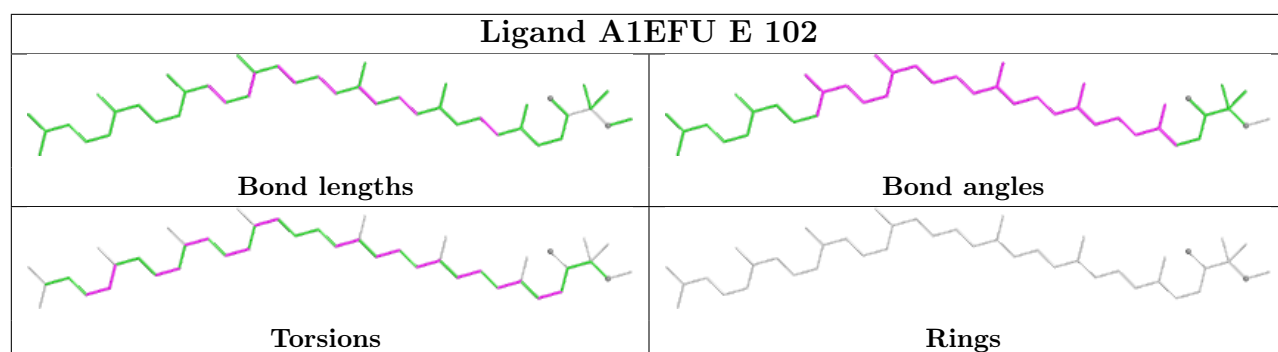
Ligand HEC C 403

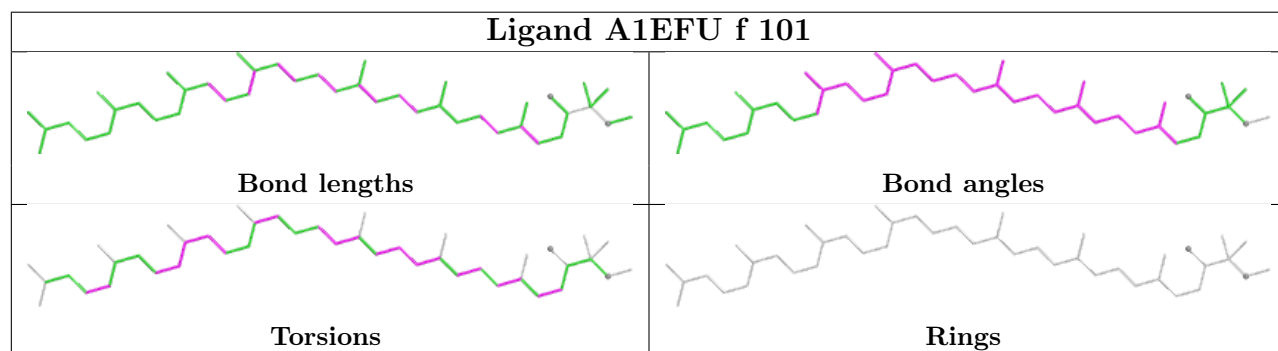
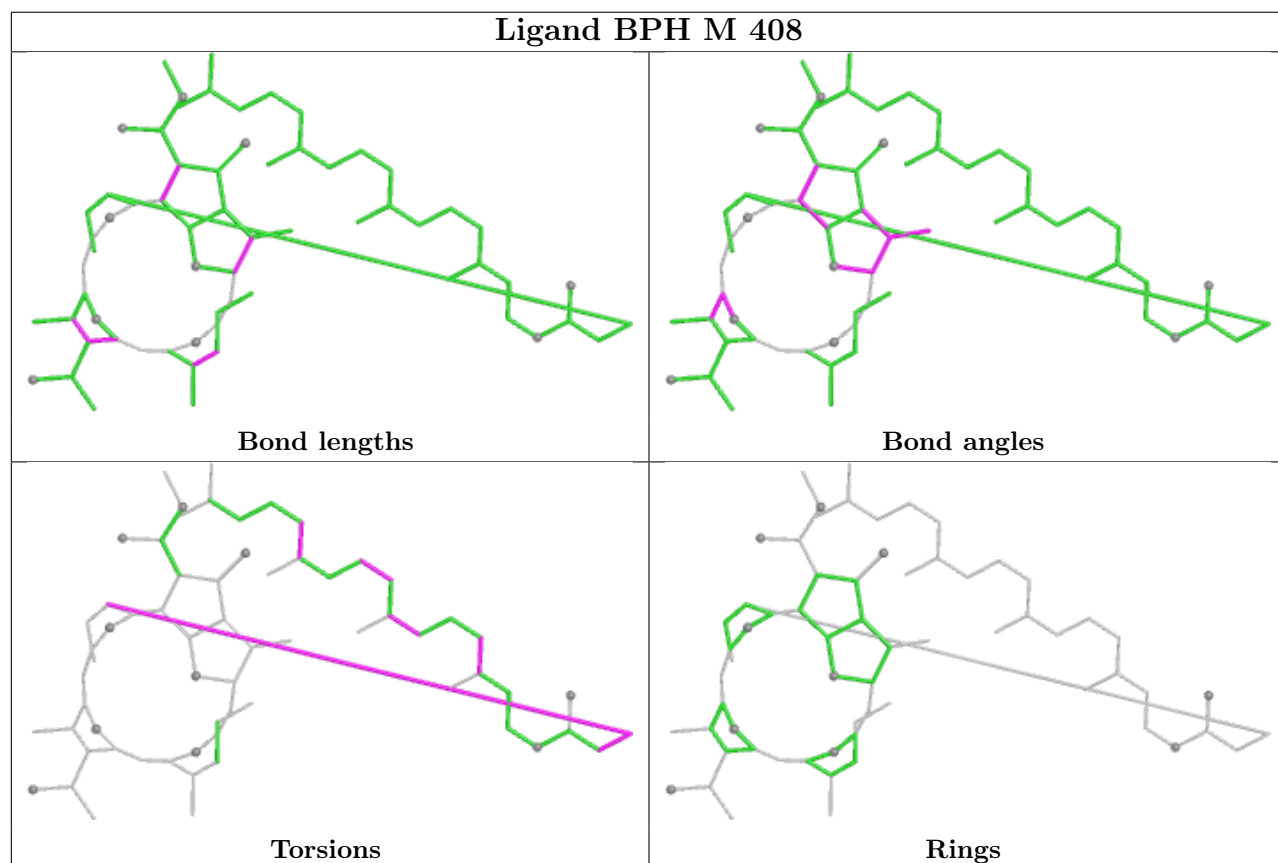
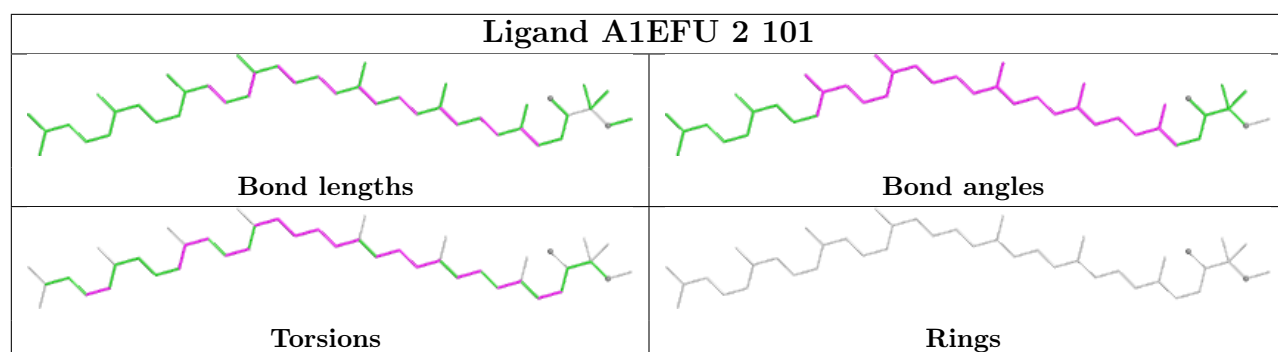


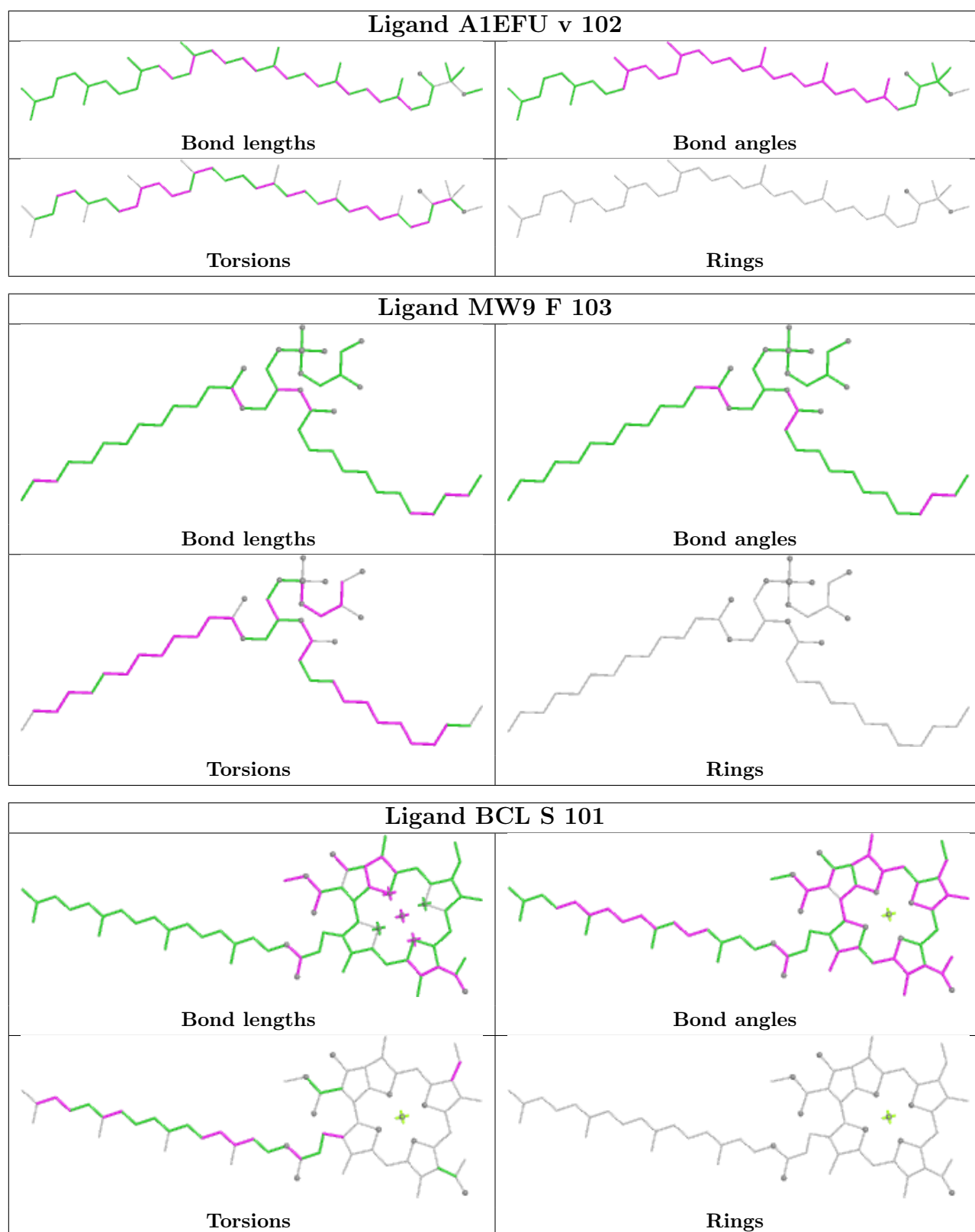
Ligand BCL L 301

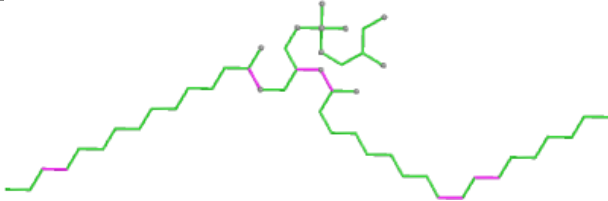
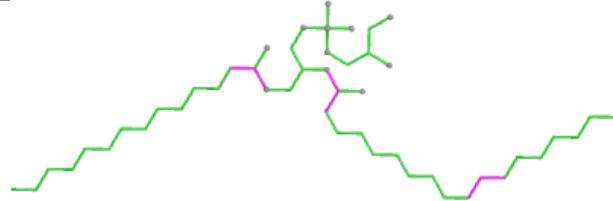
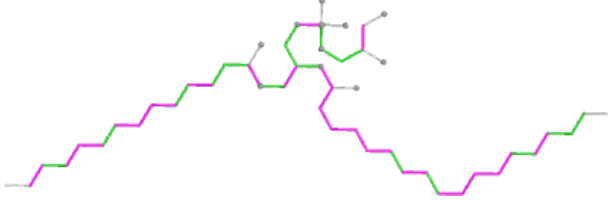
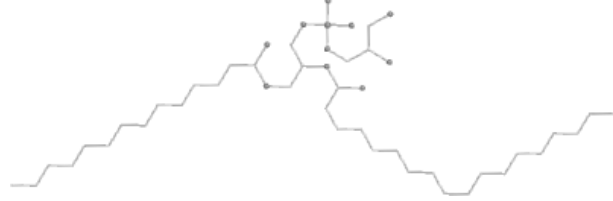


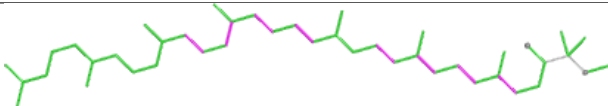
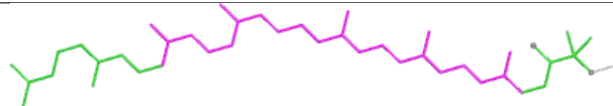
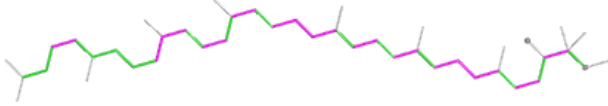
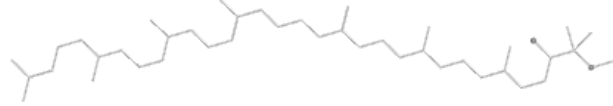


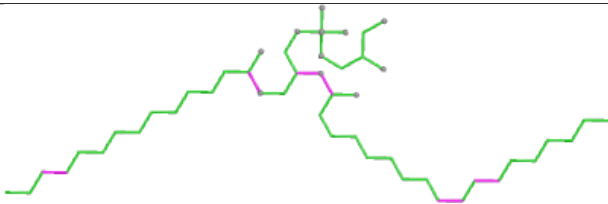
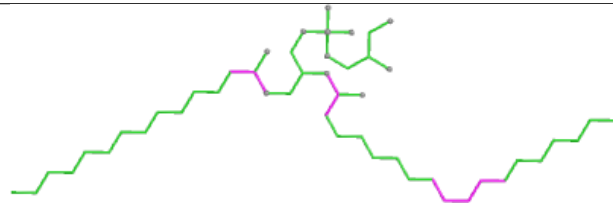
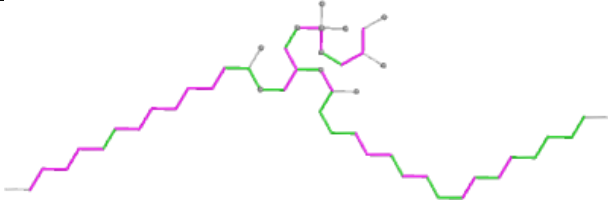
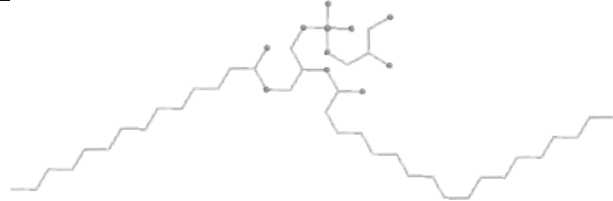


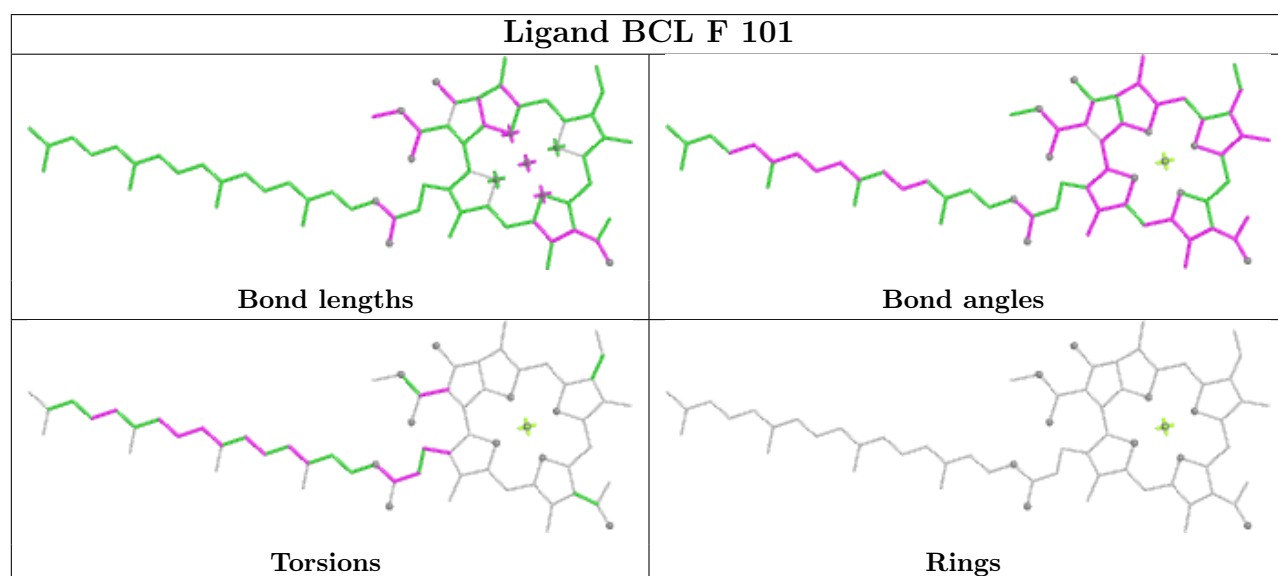
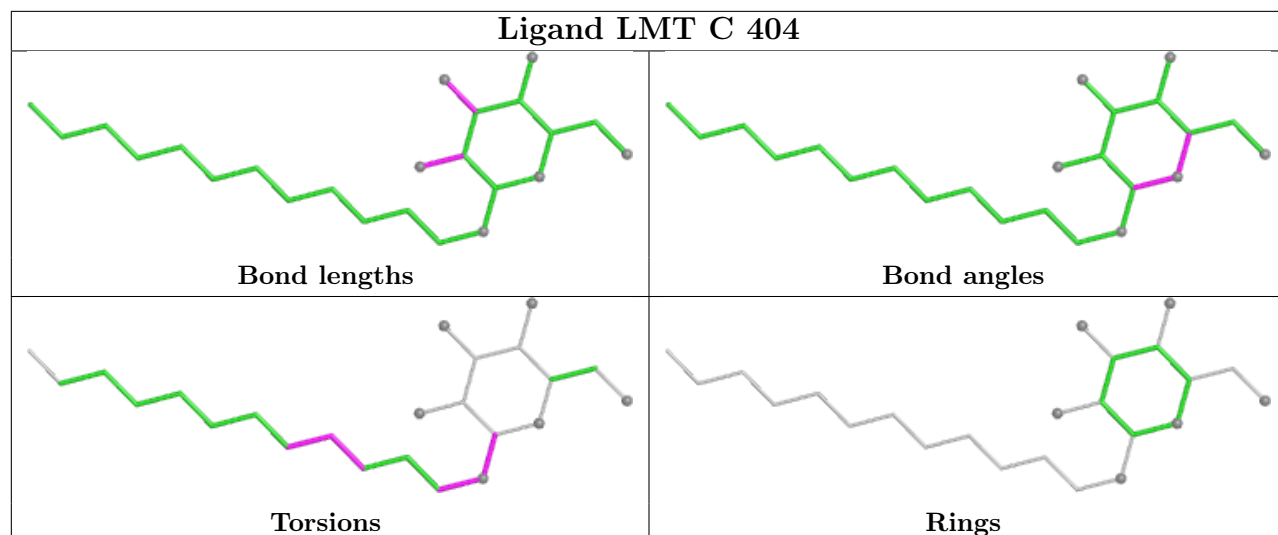


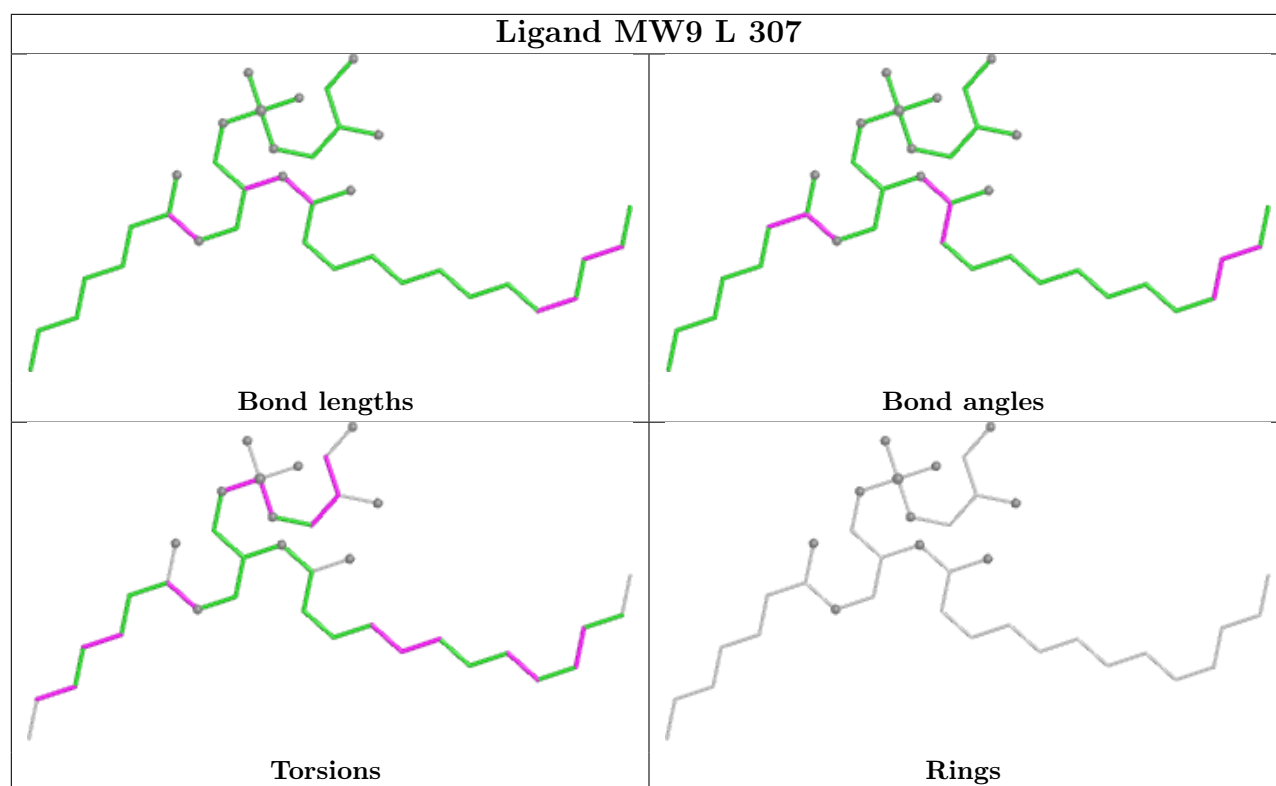


Ligand MW9 M 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand A1EFU B 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand MW9 G 103	
	
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.

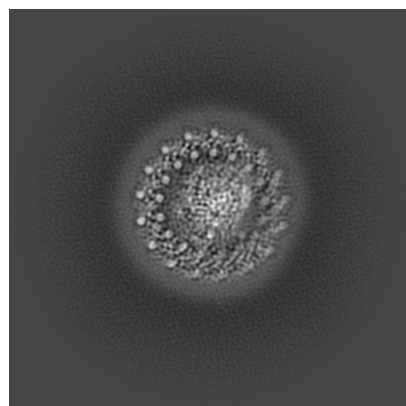
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62419. These allow visual inspection of the internal detail of the map and identification of artifacts.

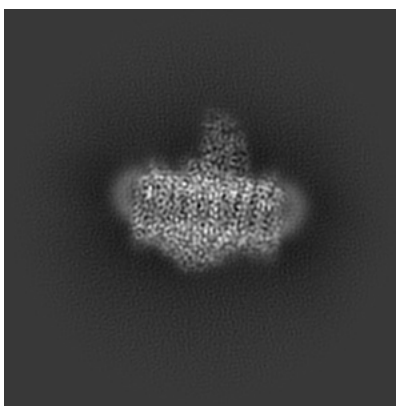
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

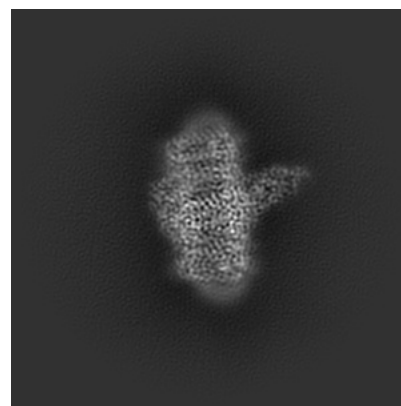
6.1.1 Primary map



X

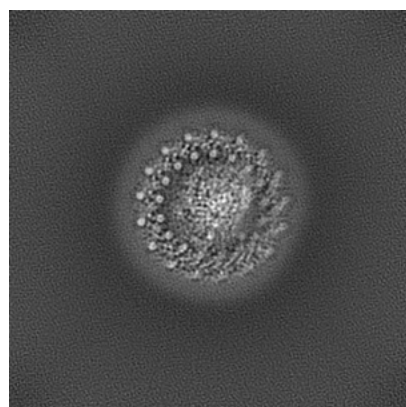


Y

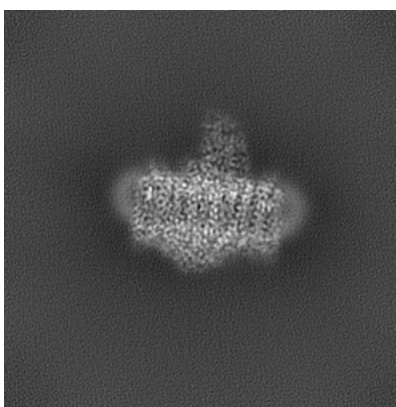


Z

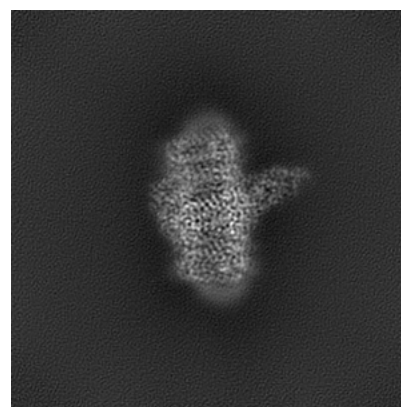
6.1.2 Raw map



X



Y

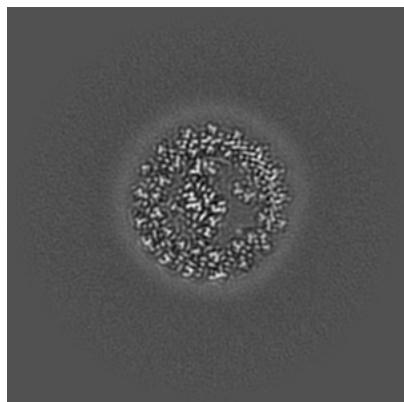


Z

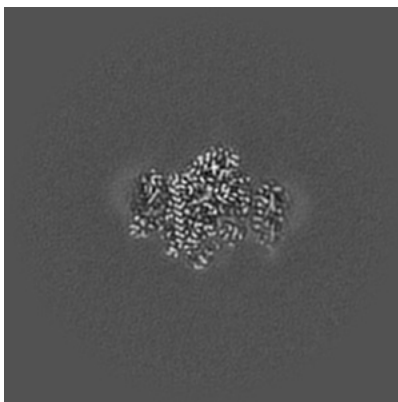
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

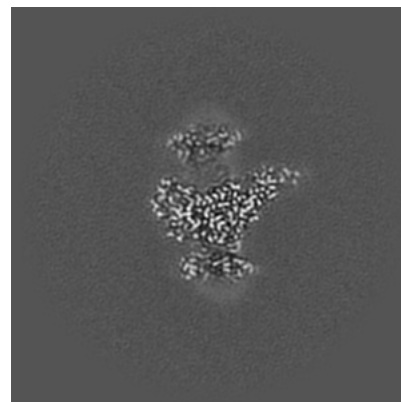
6.2.1 Primary map



X Index: 128

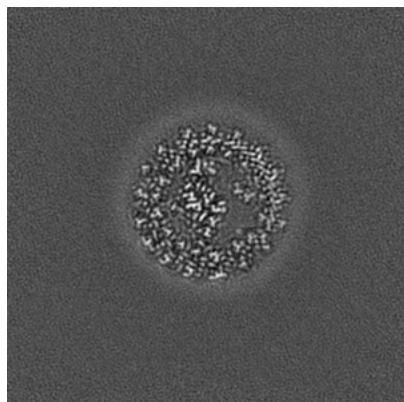


Y Index: 128

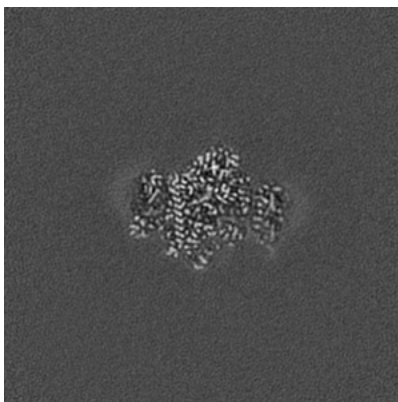


Z Index: 128

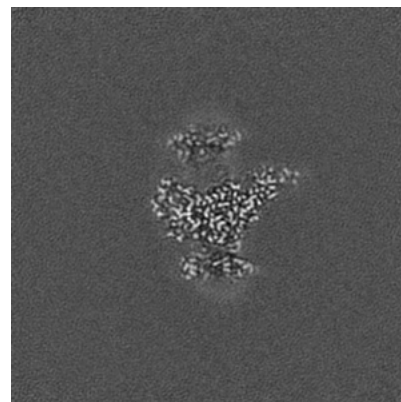
6.2.2 Raw map



X Index: 128



Y Index: 128

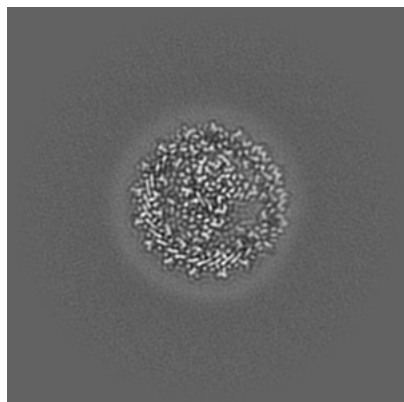


Z Index: 128

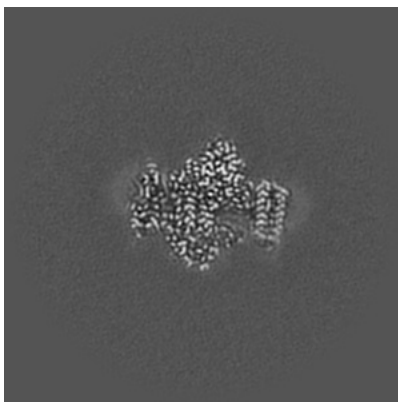
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

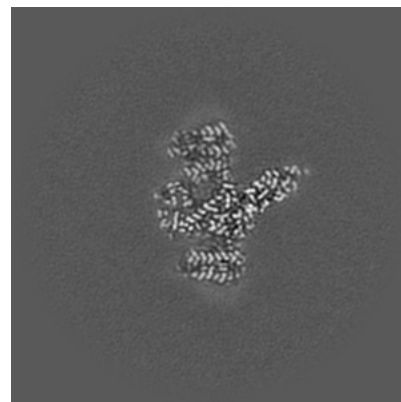
6.3.1 Primary map



X Index: 137

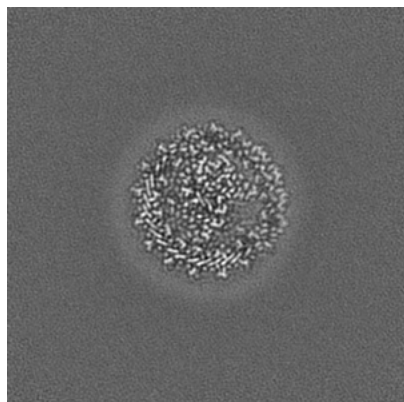


Y Index: 131

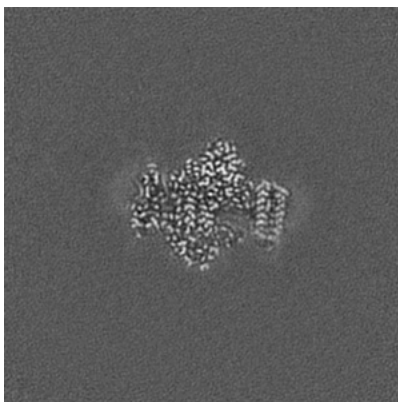


Z Index: 135

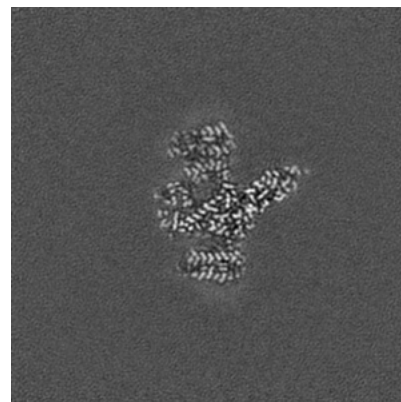
6.3.2 Raw map



X Index: 137



Y Index: 131

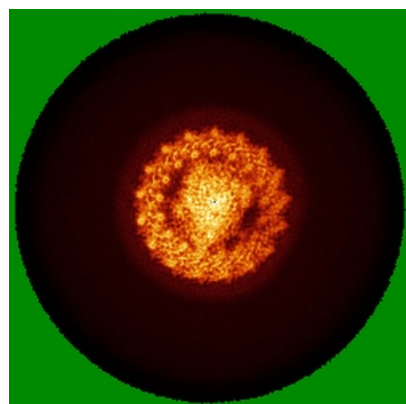


Z Index: 135

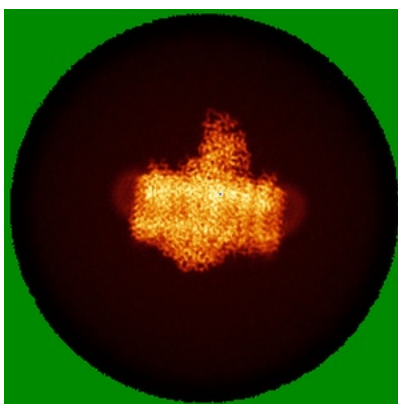
The images above show the largest variance slices of the map in three orthogonal directions.

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

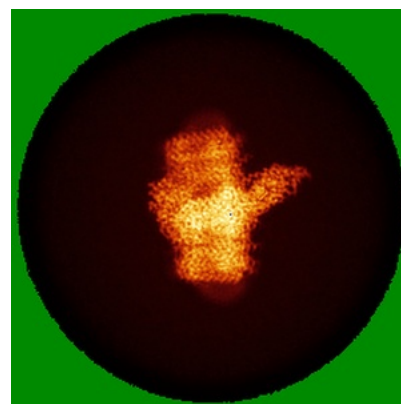
6.4.1 Primary map



X

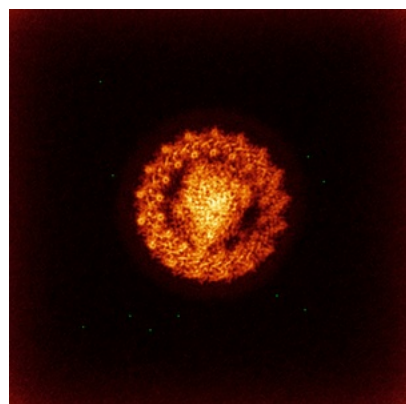


Y

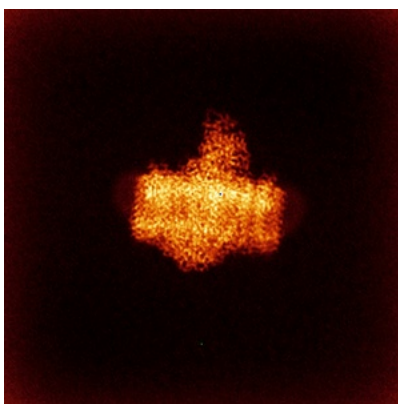


Z

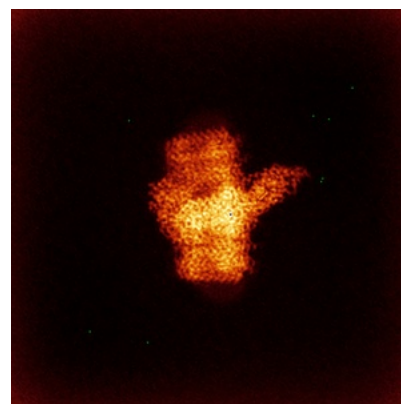
6.4.2 Raw map



X



Y

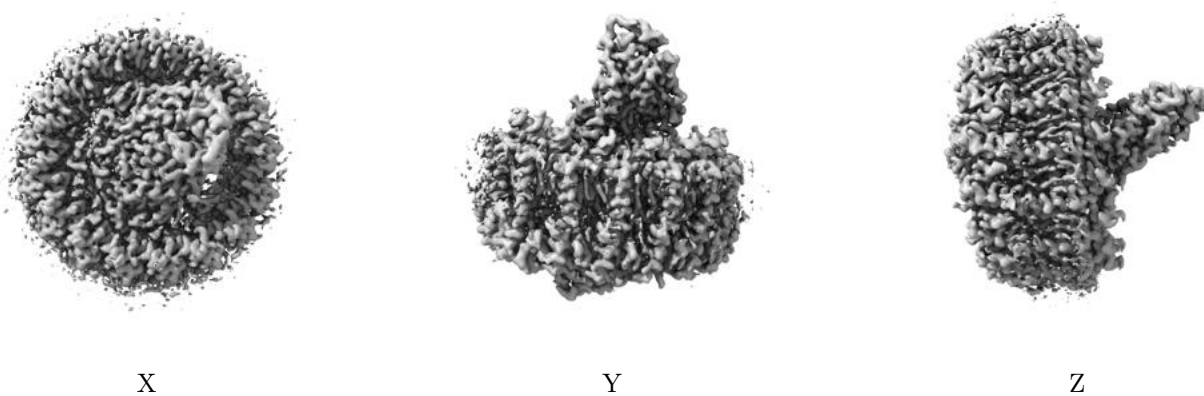


Z

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

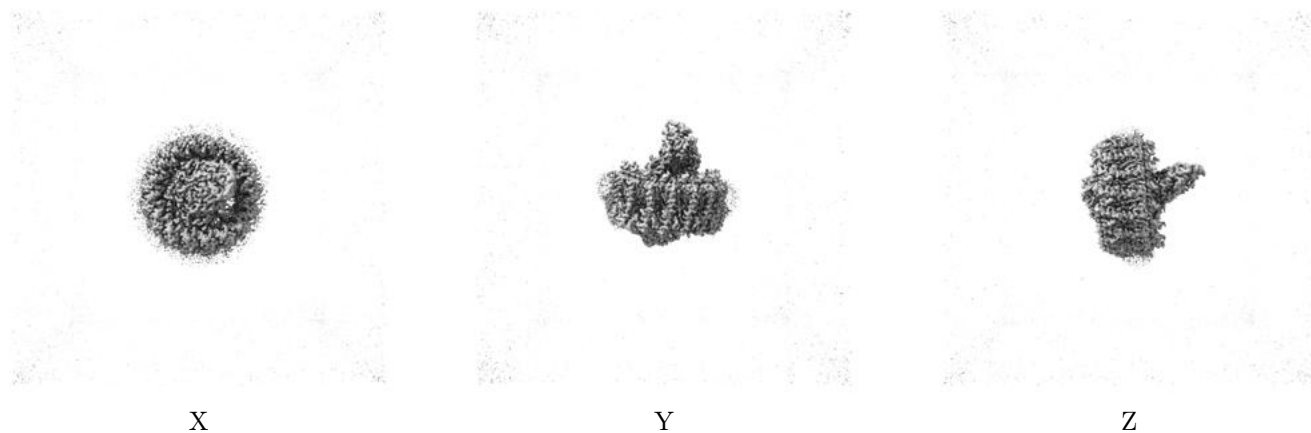
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

6.5.2 Raw map



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

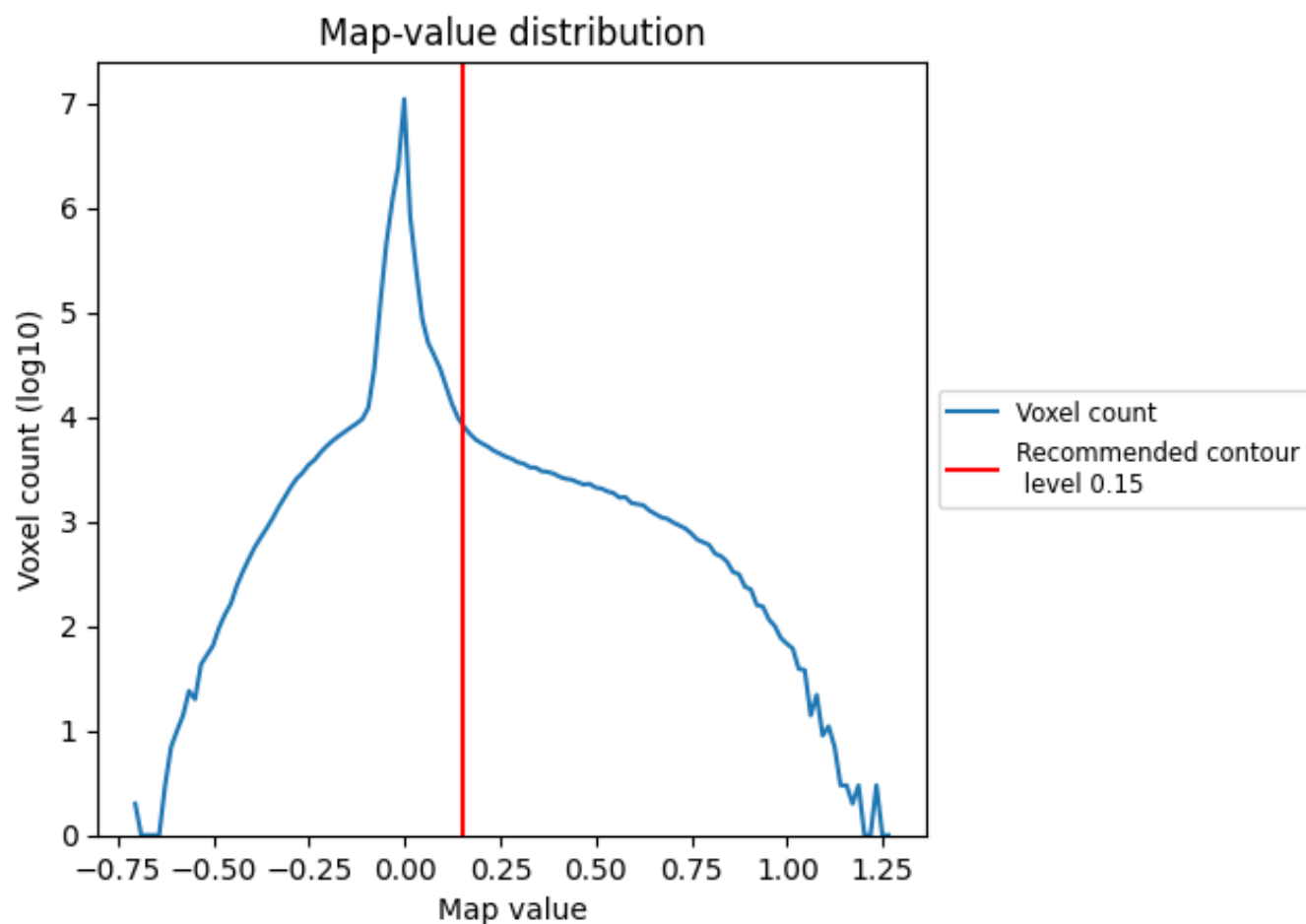
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

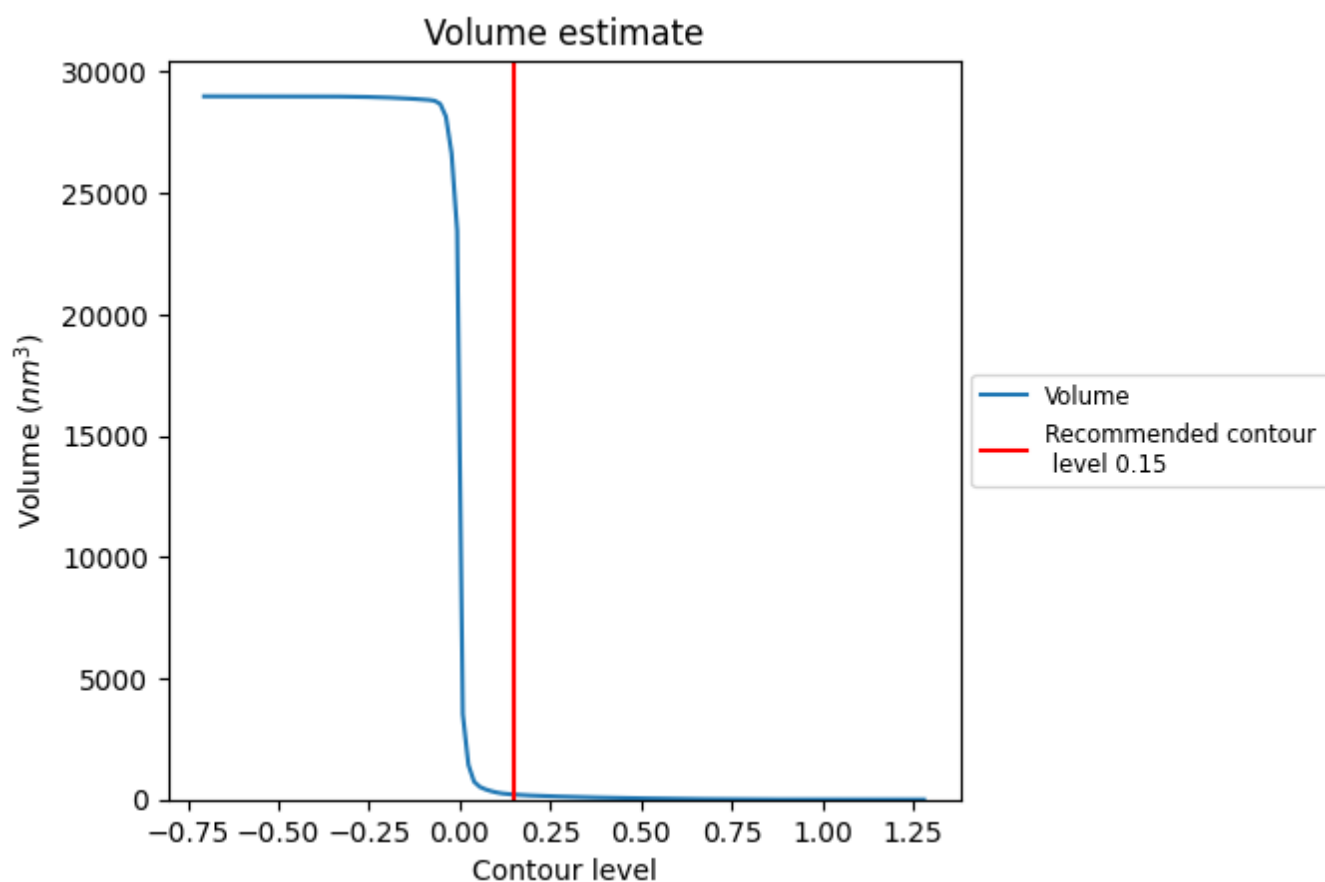
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

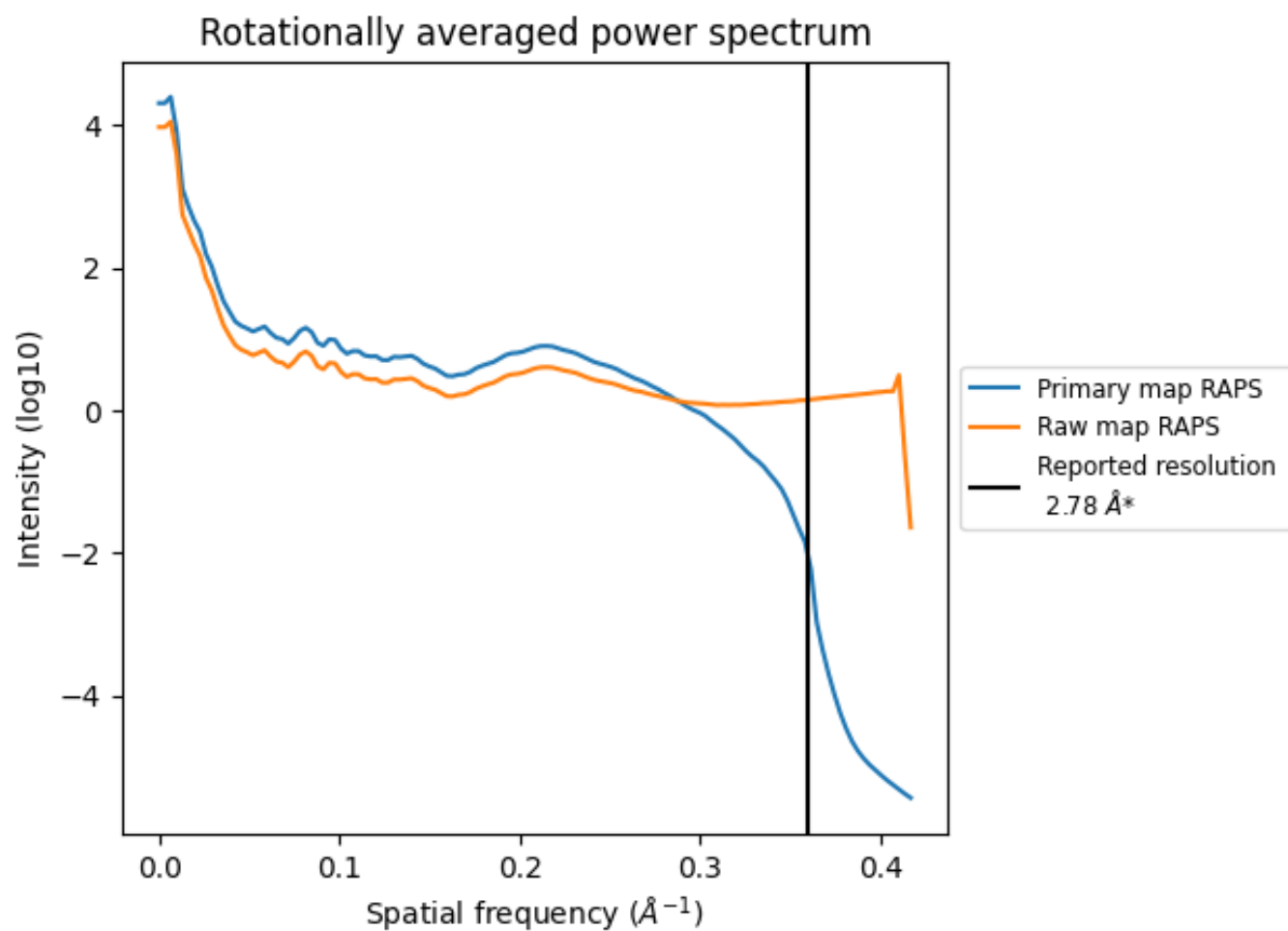
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 206 nm³; this corresponds to an approximate mass of 186 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 ⓘ

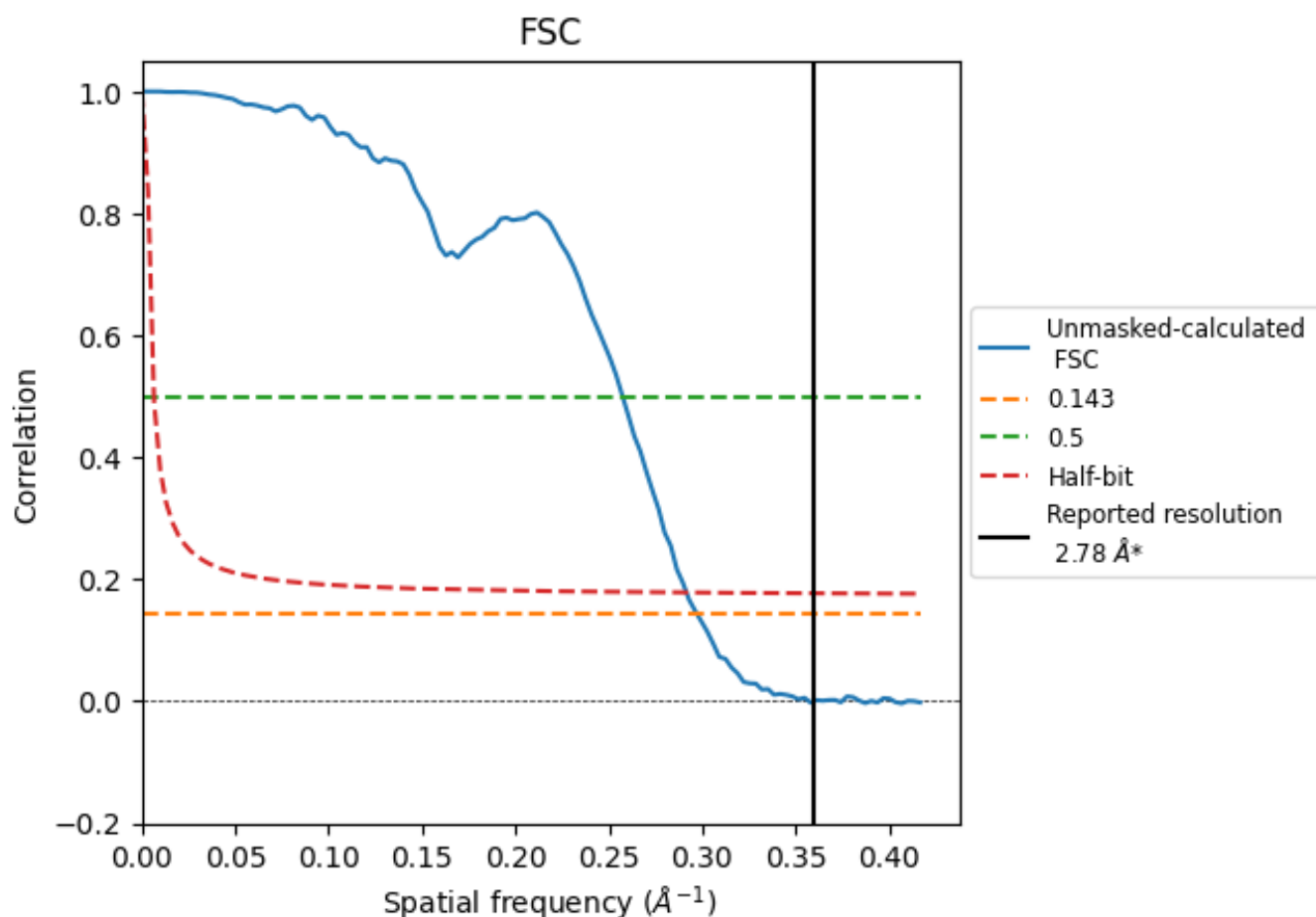


*Reported resolution corresponds to spatial frequency of 0.360 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.360 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

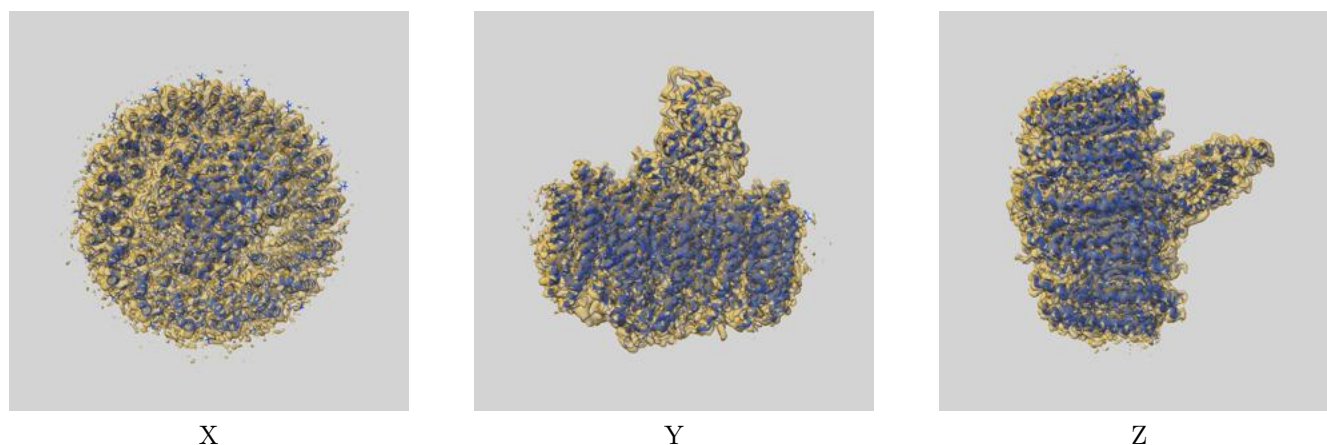
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.78	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.36	3.89	3.43

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.36 differs from the reported value 2.78 by more than 10 %

9 Map-model fit [i](#)

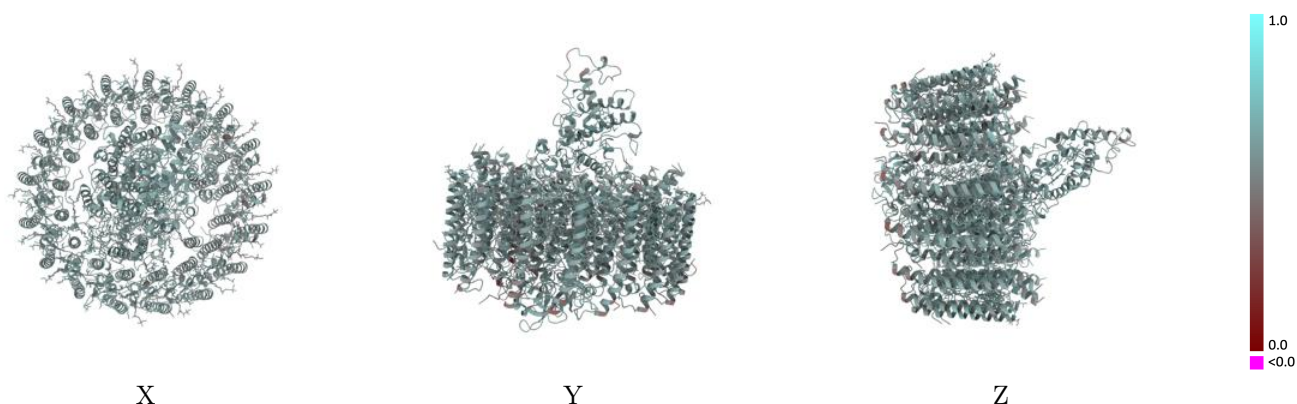
This section contains information regarding the fit between EMDB map EMD-62419 and PDB model 9KM0. Per-residue inclusion information can be found in section 3 on page 17.

9.1 Map-model overlay [i](#)



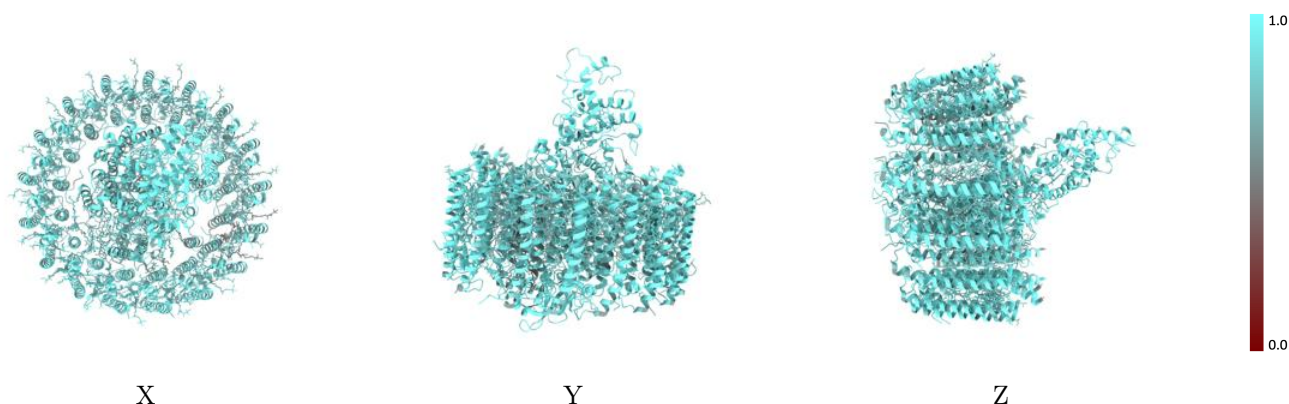
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



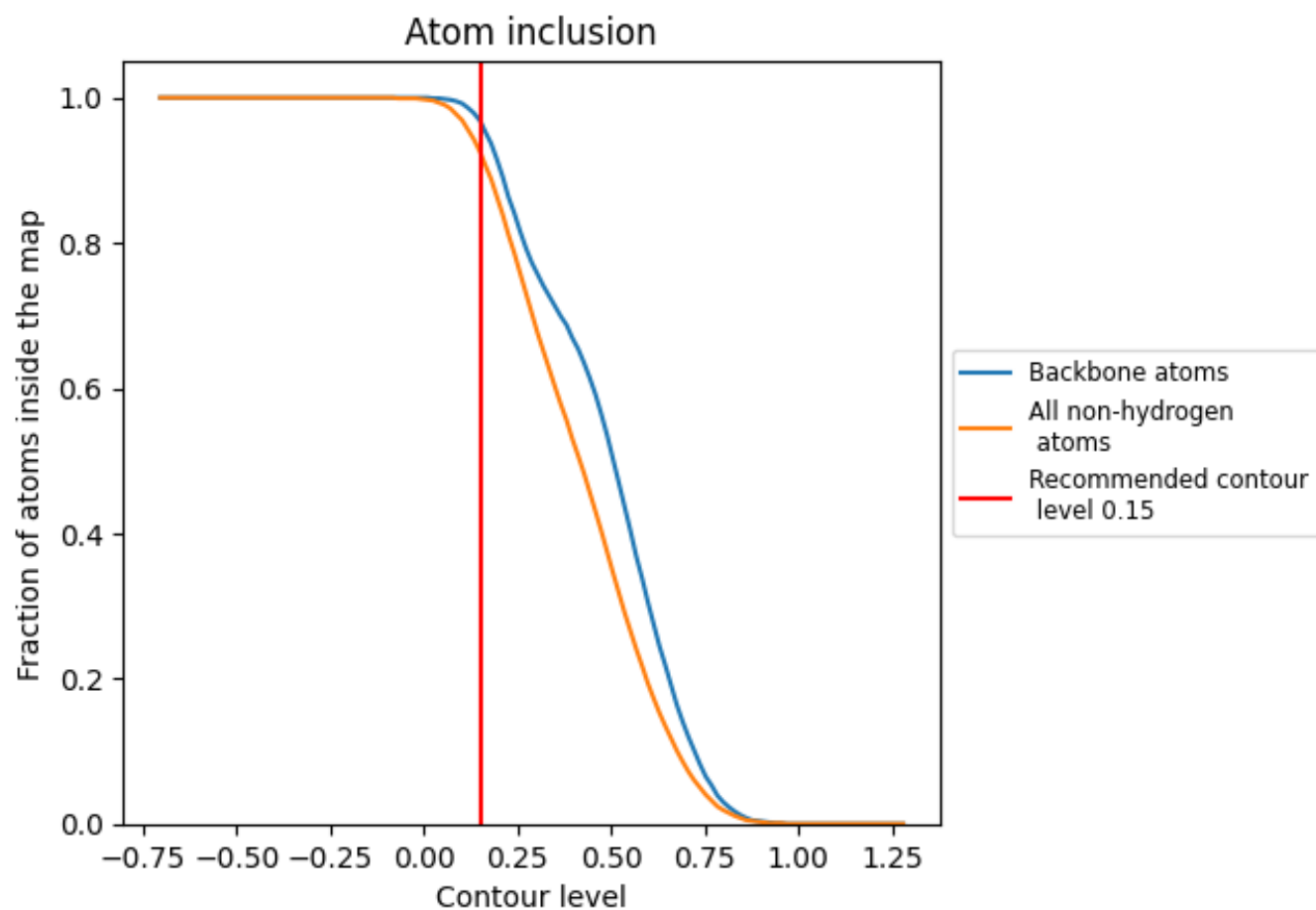
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

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

Chain	Atom inclusion	Q-score
All	 0.9250	 0.5750
1	 0.9340	 0.5750
2	 0.8890	 0.5530
A	 0.8850	 0.5670
B	 0.9360	 0.5750
C	 0.9350	 0.5720
D	 0.9050	 0.5810
E	 0.9570	 0.5800
F	 0.9440	 0.5990
G	 0.9230	 0.5870
H	 0.9420	 0.5880
I	 0.9480	 0.5870
J	 0.9340	 0.5790
K	 0.9390	 0.5750
L	 0.9530	 0.5970
M	 0.9530	 0.5930
N	 0.9170	 0.5660
O	 0.8750	 0.5580
P	 0.8960	 0.5640
Q	 0.9370	 0.5800
R	 0.9130	 0.5690
S	 0.8930	 0.5590
T	 0.8840	 0.5580
V	 0.8320	 0.5240
a	 0.8770	 0.5400
b	 0.9440	 0.5700
d	 0.9540	 0.5710
e	 0.9590	 0.5860
f	 0.9600	 0.5860
g	 0.9550	 0.5740
i	 0.9530	 0.5810
j	 0.9210	 0.5670
k	 0.9240	 0.5550
n	 0.9080	 0.5620
p	 0.9040	 0.5390



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
q	 0.8990	 0.5580
r	 0.8980	 0.5590
s	 0.8680	 0.5570
t	 0.8970	 0.5390
v	 0.7820	 0.5200