



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 02:59 AM UTC

PDB ID : 8IUG / pdb_00008iug
EMDB ID : EMD-35721
Title : Cryo-EM structure of the RC-LH core complex from *roseiflexus castenholzii*
Authors : Wang, G.-L.; Qi, C.-H.; Yu, L.-J.
Deposited on : 2023-03-24
Resolution : 2.86 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

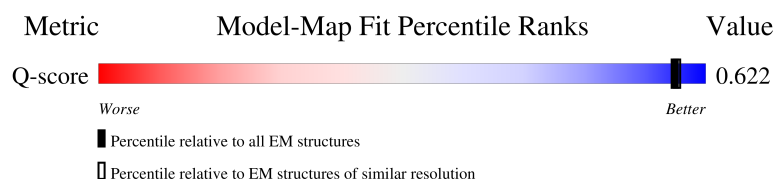
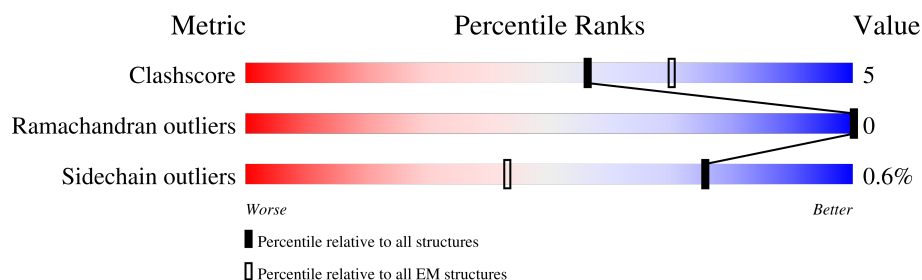
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.86 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.



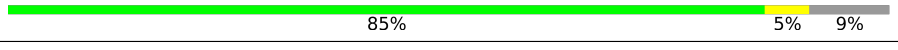
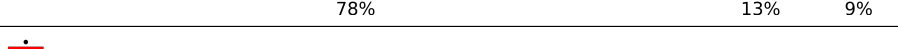
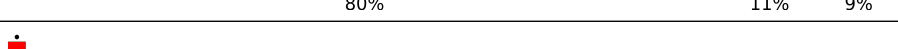
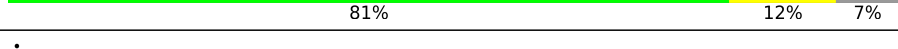
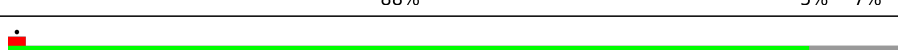
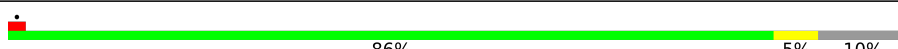
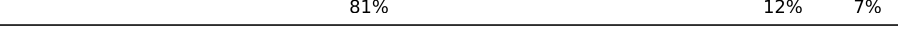
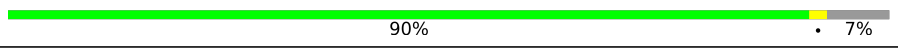
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12017 (2.36 - 3.36)

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

Mol	Chain	Length	Quality of chain
1	0	55	
1	2	55	
1	4	55	
1	6	55	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	8	55	
1	B	55	
1	E	55	
1	G	55	
1	I	55	
1	K	55	
1	O	55	
1	Q	55	
1	S	55	
1	U	55	
1	W	55	
2	1	42	
2	3	42	
2	5	42	
2	7	42	
2	9	42	
2	A	42	
2	D	42	
2	F	42	
2	H	42	
2	J	42	
2	N	42	
2	P	42	
2	R	42	
2	T	42	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	V	42	5% 81% 10% 10%
3	C	320	• 84% 13% ••
4	L	641	41% • 55%
4	M	641	43% 5% 52%
5	X	30	17% 93% 7%
6	Y	39	72% 10% 18%
7	Z	10	100%
8	h	63	62% 11% • 25%

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 25238 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 complex alpha/beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	50	Total 416	C 280	N 69	O 66	S 1	0	0
1	2	50	Total 416	C 280	N 69	O 66	S 1	0	0
1	4	50	Total 416	C 280	N 69	O 66	S 1	0	0
1	6	50	Total 416	C 280	N 69	O 66	S 1	0	0
1	8	50	Total 416	C 280	N 69	O 66	S 1	0	0
1	B	50	Total 416	C 280	N 69	O 66	S 1	0	0
1	E	50	Total 416	C 280	N 69	O 66	S 1	0	0
1	G	50	Total 416	C 280	N 69	O 66	S 1	0	0
1	I	50	Total 416	C 280	N 69	O 66	S 1	0	0
1	K	50	Total 416	C 280	N 69	O 66	S 1	0	0
1	O	50	Total 416	C 280	N 69	O 66	S 1	0	0
1	Q	50	Total 416	C 280	N 69	O 66	S 1	0	0
1	S	50	Total 416	C 280	N 69	O 66	S 1	0	0
1	U	50	Total 416	C 280	N 69	O 66	S 1	0	0
1	W	50	Total 416	C 280	N 69	O 66	S 1	0	0

- Molecule 2 is a protein called Alpha subunit of light-harvesting 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	3	39	Total	C	N	O	S	0	0
			308	205	52	50	1		
2	5	39	Total	C	N	O	S	0	0
			308	205	52	50	1		
2	7	39	Total	C	N	O	S	0	0
			308	205	52	50	1		
2	9	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	A	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	D	39	Total	C	N	O	S	0	0
			308	205	52	50	1		
2	F	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	H	39	Total	C	N	O	S	0	0
			308	205	52	50	1		
2	J	39	Total	C	N	O	S	0	0
			308	205	52	50	1		
2	N	39	Total	C	N	O	S	0	0
			308	205	52	50	1		
2	P	39	Total	C	N	O	S	0	0
			308	205	52	50	1		
2	R	39	Total	C	N	O	S	0	0
			308	205	52	50	1		
2	T	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	V	38	Total	C	N	O	S	0	0
			300	201	51	47	1		

- Molecule 3 is a protein called Cytochrome subunit of photosynthetic reaction center.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	316	Total	C	N	O	S	0	0
			2411	1537	408	444	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	286	Total	C	N	O	S	0	0
			2278	1527	367	376	8		
4	M	306	Total	C	N	O	S	0	0
			2488	1673	399	409	7		

- Molecule 5 is a protein called TMx polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	X	30	Total	C	N	O	S	1	0
			246	172	32	38	4		

- Molecule 6 is a protein called reaction center small polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Y	32	Total	C	N	O	S	0	0
			259	181	36	39	3		

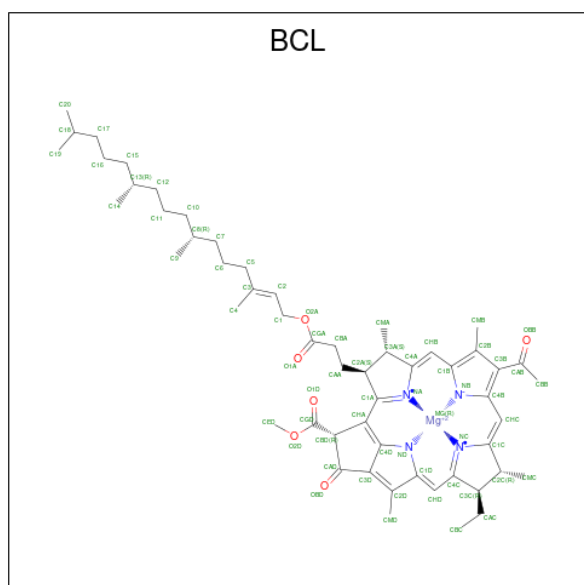
- Molecule 7 is a protein called reaction center unknown polypeptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	Z	10	Total	C	N	O	0	0
			51	31	10	10		

- Molecule 8 is a protein called reaction center small polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	47	Total	C	N	O	S	0	0
			362	242	59	60	1		

- Molecule 9 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
9	0	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	0	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	2	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	2	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	4	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	4	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	5	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	8	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	8	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	9	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	B	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	B	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	D	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	D	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	E	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	F	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

Continued on next page...

Continued from previous page...

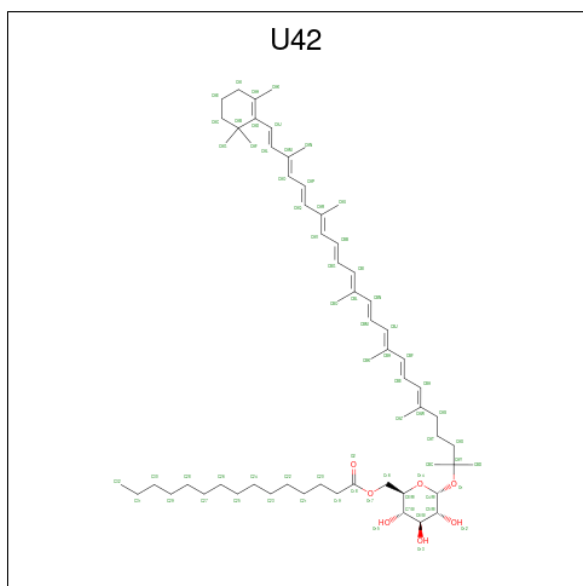
Mol	Chain	Residues	Atoms					AltConf
9	F	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	H	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	I	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	I	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	J	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	K	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	K	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	M	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	O	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	O	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	P	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	R	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	S	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	S	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	T	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
9	U	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	U	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	V	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 10 is [(2 {R},3 {S},4 {S},5 {R},6 {R})-6-[(6 {E},8 {E},10 {E},12 {E},14 {E},16 {E},18 {E},20 {E},22 {E},24 {E})-2,6,10,14,19,23-hexamethyl-25-(2,6,6-trimethylcyclohexen-1-yl)pentacos-6,8,10,12,14,16,18,20,22,24-decaen-2-yl]oxy-3,4,5-tris(oxidanyl)oxan-2-yl]methyl pentadecanoate (CCD ID: U42) (formula: C₆₁H₉₆O₇) (labeled as "Ligand of Interest" by depositor).



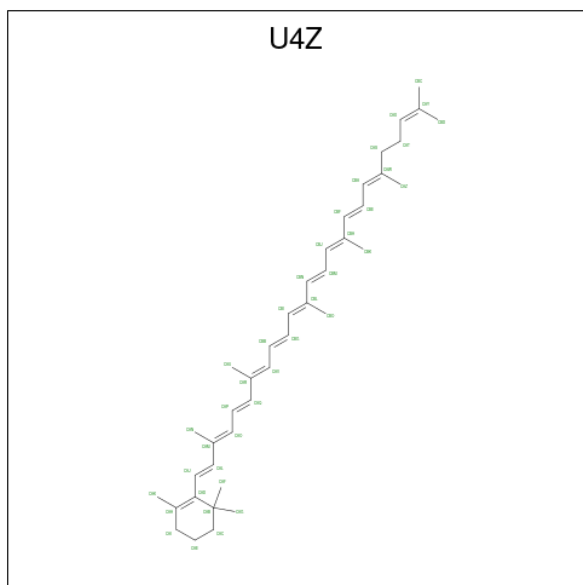
Mol	Chain	Residues	Atoms			AltConf
10	0	1	Total	C	O	0
			68	61	7	
10	4	1	Total	C	O	0
			68	61	7	
10	4	1	Total	C	O	0
			68	61	7	
10	8	1	Total	C	O	0
			68	61	7	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
10	B	1	Total	C	O	0
			68	61	7	
10	E	1	Total	C	O	0
			68	61	7	
10	G	1	Total	C	O	0
			68	61	7	
10	I	1	Total	C	O	0
			68	61	7	
10	I	1	Total	C	O	0
			68	61	7	
10	O	1	Total	C	O	0
			68	61	7	
10	Q	1	Total	C	O	0
			68	61	7	
10	S	1	Total	C	O	0
			68	61	7	
10	U	1	Total	C	O	0
			68	61	7	
10	U	1	Total	C	O	0
			68	61	7	

- Molecule 11 is gamma-Carotene (CCD ID: U4Z) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



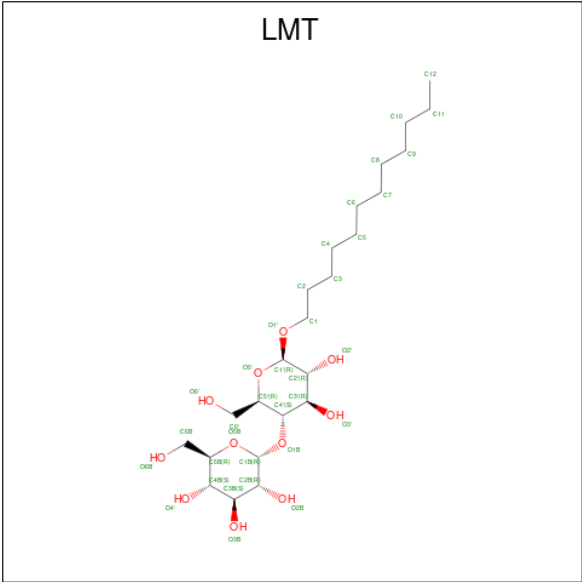
Mol	Chain	Residues	Atoms		AltConf
11	1	1	Total	C	0
			40	40	

Continued on next page...

Continued from previous page...

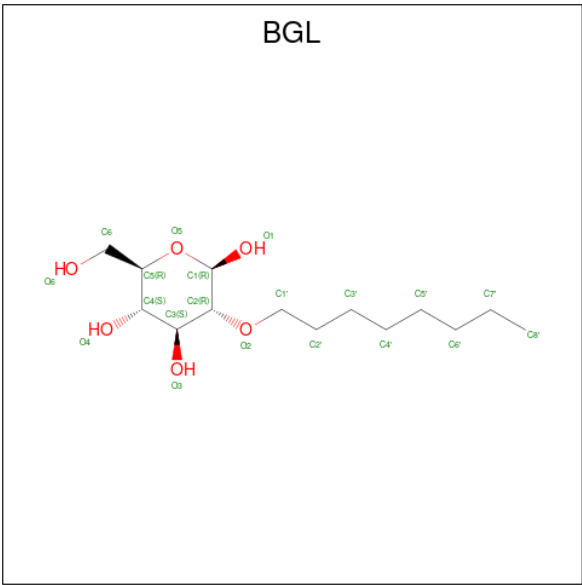
Mol	Chain	Residues	Atoms	AltConf
11	3	1	Total C 40 40	0
11	5	1	Total C 40 40	0
11	7	1	Total C 40 40	0
11	9	1	Total C 40 40	0
11	A	1	Total C 40 40	0
11	C	1	Total C 40 40	0
11	D	1	Total C 40 40	0
11	F	1	Total C 40 40	0
11	H	1	Total C 40 40	0
11	J	1	Total C 40 40	0
11	N	1	Total C 40 40	0
11	P	1	Total C 40 40	0
11	S	1	Total C 40 40	0
11	T	1	Total C 40 40	0
11	V	1	Total C 40 40	0

- Molecule 12 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
12	1	1	Total	C	O	0
			35	24	11	
12	D	1	Total	C	O	0
			35	24	11	
12	T	1	Total	C	O	0
			35	24	11	

- Molecule 13 is 2-O-octyl-beta-D-glucopyranose (CCD ID: BGL) (formula: C₁₄H₂₈O₆).



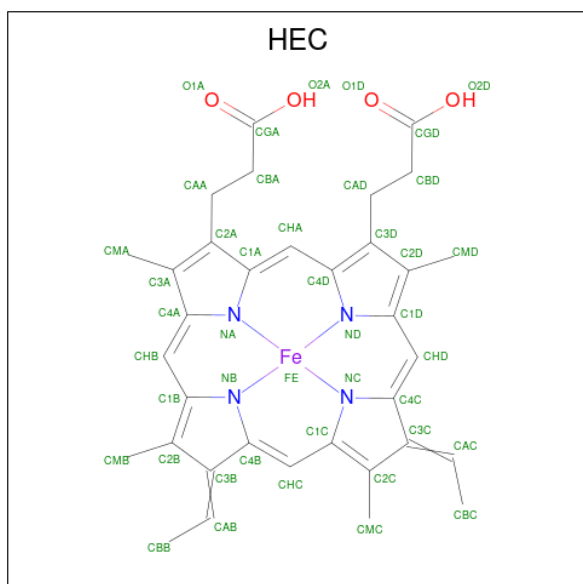
Mol	Chain	Residues	Atoms			AltConf
13	3	1	Total	C	O	0
			20	14	6	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
13	C	1	Total	C	O	0
			20	14	6	
13	C	1	Total	C	O	0
			20	14	6	
13	D	1	Total	C	O	0
			20	14	6	
13	F	1	Total	C	O	0
			20	14	6	
13	H	1	Total	C	O	0
			20	14	6	
13	H	1	Total	C	O	0
			20	14	6	
13	L	1	Total	C	O	0
			20	14	6	
13	L	1	Total	C	O	0
			20	14	6	
13	L	1	Total	C	O	0
			20	14	6	
13	L	1	Total	C	O	0
			20	14	6	
13	N	1	Total	C	O	0
			20	14	6	
13	Y	1	Total	C	O	0
			20	14	6	

- Molecule 14 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).

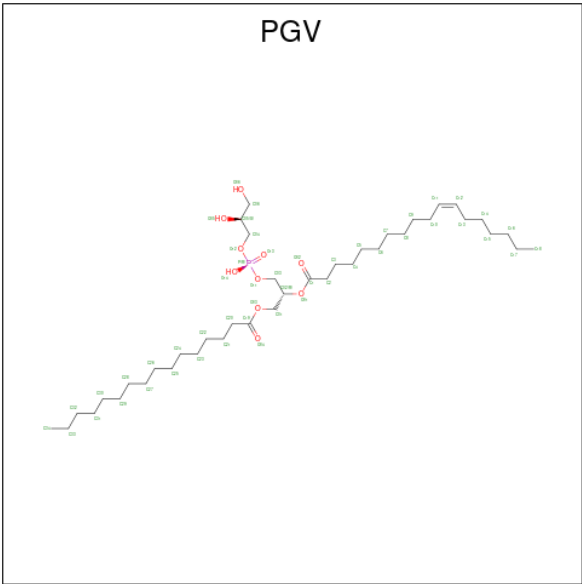


Mol	Chain	Residues	Atoms					AltConf
14	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
14	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
14	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
14	C	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 15 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
15	C	1	Total	Ca	0
			1	1	

- Molecule 16 is (1R)-2-{{[[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
16	C	1	Total	C	O	P	0
			41	30	10	1	
16	C	1	Total	C	O	P	0
			51	40	10	1	
16	L	1	Total	C	O	P	0
			51	40	10	1	
16	L	1	Total	C	O	P	0
			51	40	10	1	

Continued on next page...

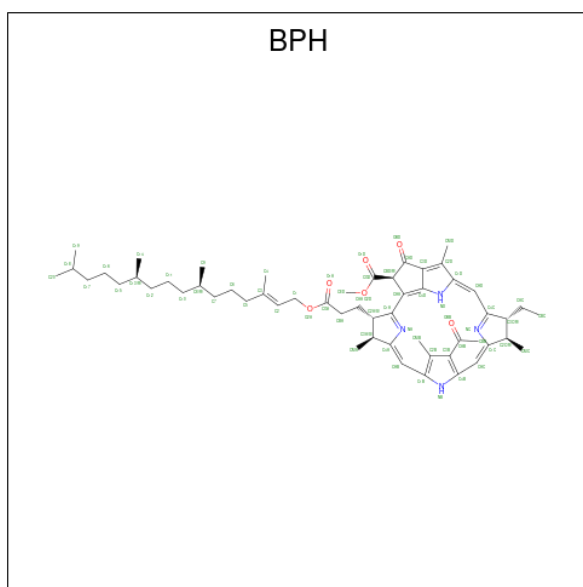
Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
16	L	1	Total	C	O	P	0
			51	40	10	1	
16	M	1	Total	C	O	P	0
			51	40	10	1	
16	M	1	Total	C	O	P	0
			51	40	10	1	
16	P	1	Total	C	O	P	0
			43	32	10	1	
16	P	1	Total	C	O	P	0
			51	40	10	1	

- Molecule 17 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

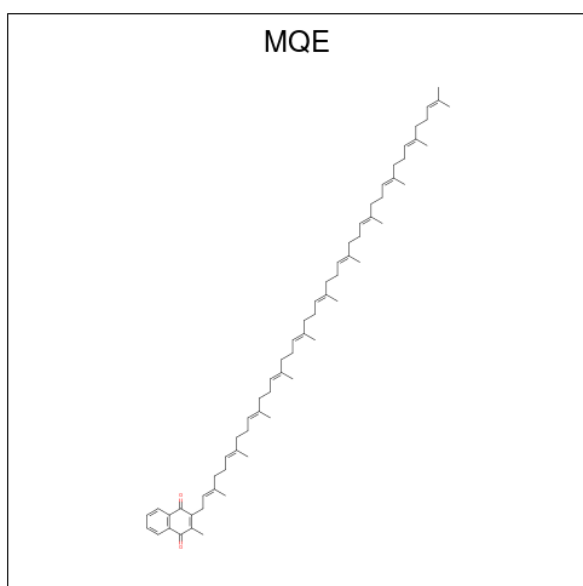
Mol	Chain	Residues	Atoms		AltConf
17	C	2	Total	C	0
			34	34	
17	H	4	Total	C	0
			52	52	
17	L	4	Total	C	0
			48	48	
17	M	1	Total	C	0
			12	12	
17	V	3	Total	C	0
			33	33	
17	Y	1	Total	C	0
			14	14	
17	h	2	Total	C	0
			24	24	

- Molecule 18 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



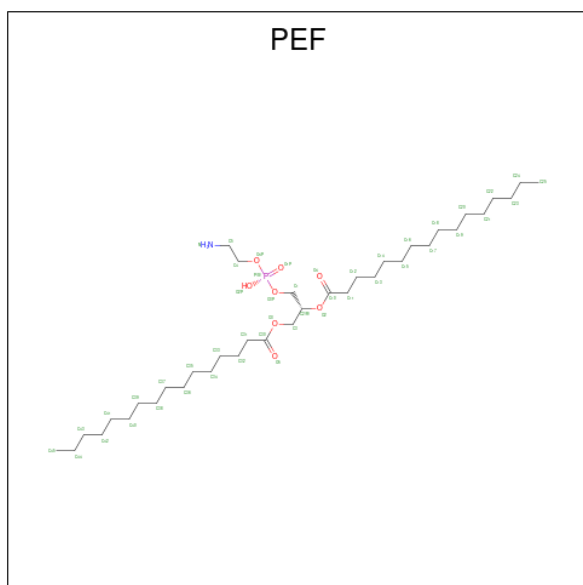
Mol	Chain	Residues	Atoms				AltConf
18	L	1	Total	C	N	O	0
			65	55	4	6	
18	L	1	Total	C	N	O	0
			65	55	4	6	
18	M	1	Total	C	N	O	0
			65	55	4	6	

- Molecule 19 is 2-methyl-3-[(2E,6E,10E,14E,18E,22E,26E,30E,34E,38E)-3,7,11,15,19,23,27,31,35,39,43-undecamethyltetraetraconta-2,6,10,14,18,22,26,30,34,38,42-undecaen-1-yl]naphthalene-1,4-dione (CCD ID: MQE) (formula: $C_{66}H_{96}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
19	L	1	Total	C	O	0
			53	51	2	
19	M	1	Total	C	O	0
			68	66	2	

- Molecule 20 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (CCD ID: PEF) (formula: $C_{37}H_{74}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
20	L	1	Total	C	N	O	P	0
			41	31	1	8	1	

- Molecule 21 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		AltConf
21	M	1	Total	Mn	0
			1	1	

- Molecule 22 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).

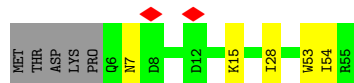
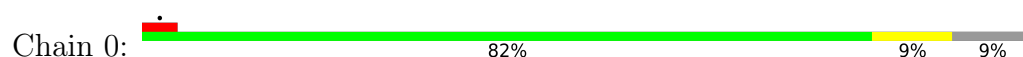


Mol	Chain	Residues	Atoms			AltConf
22	h	1	Total	C	O	0
			17	16	1	

3 Residue-property plots [i](#)

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

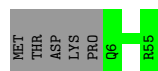
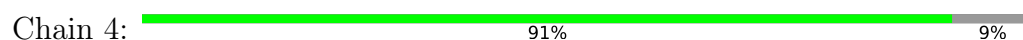
- Molecule 1: Antenna complex alpha/beta subunit



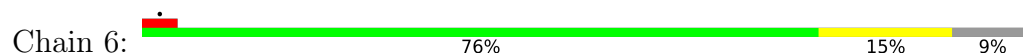
- Molecule 1: Antenna complex alpha/beta subunit



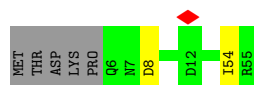
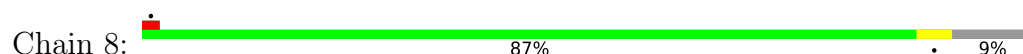
- Molecule 1: Antenna complex alpha/beta subunit



- Molecule 1: Antenna complex alpha/beta subunit

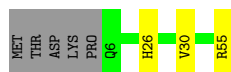


- Molecule 1: Antenna complex alpha/beta subunit



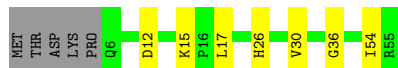
- Molecule 1: Antenna complex alpha/beta subunit

Chain B:  85% 5% 9%



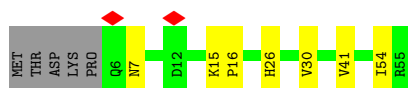
- Molecule 1: Antenna complex alpha/beta subunit

Chain E:  78% 13% 9%



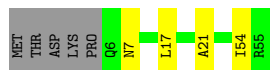
- Molecule 1: Antenna complex alpha/beta subunit

Chain G:  78% 13% 9%



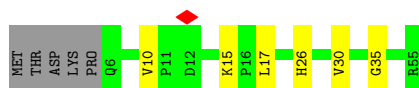
- Molecule 1: Antenna complex alpha/beta subunit

Chain I:  84% 7% 9%



- Molecule 1: Antenna complex alpha/beta subunit

Chain K:  80% 11% 9%



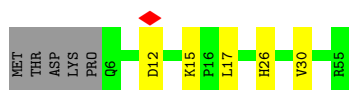
- Molecule 1: Antenna complex alpha/beta subunit

Chain O:  76% 15% 9%

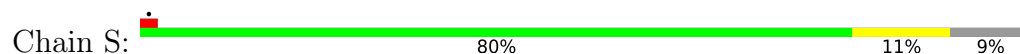


- Molecule 1: Antenna complex alpha/beta subunit

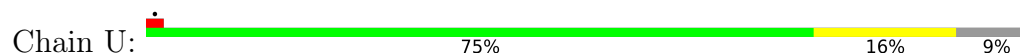
Chain Q:  82% 9% 9%



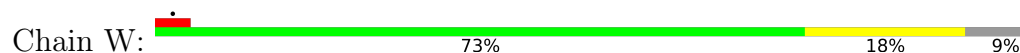
- Molecule 1: Antenna complex alpha/beta subunit



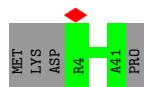
- Molecule 1: Antenna complex alpha/beta subunit



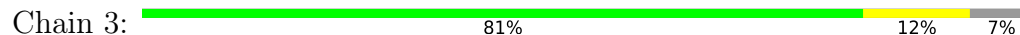
- Molecule 1: Antenna complex alpha/beta subunit



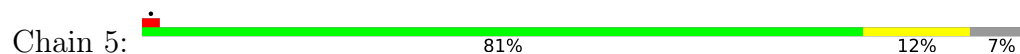
- Molecule 2: Alpha subunit of light-harvesting 1



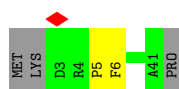
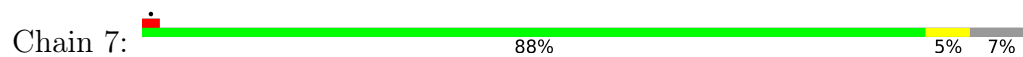
- Molecule 2: Alpha subunit of light-harvesting 1



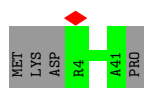
- Molecule 2: Alpha subunit of light-harvesting 1



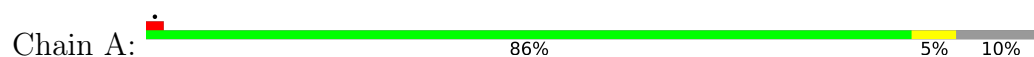
- Molecule 2: Alpha subunit of light-harvesting 1



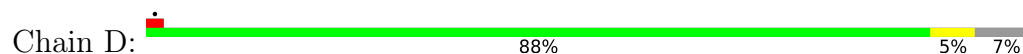
- Molecule 2: Alpha subunit of light-harvesting 1



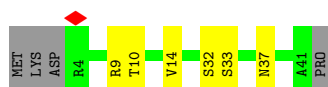
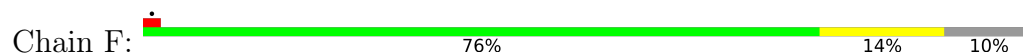
- Molecule 2: Alpha subunit of light-harvesting 1



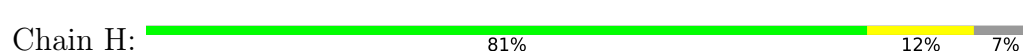
- Molecule 2: Alpha subunit of light-harvesting 1



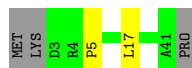
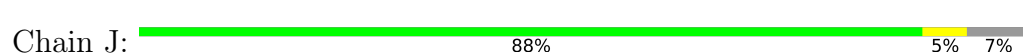
- Molecule 2: Alpha subunit of light-harvesting 1



- Molecule 2: Alpha subunit of light-harvesting 1



- Molecule 2: Alpha subunit of light-harvesting 1



- Molecule 2: Alpha subunit of light-harvesting 1

Chain N:  90% • 7%



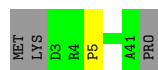
- Molecule 2: Alpha subunit of light-harvesting 1

Chain P:  79% 14% 7%



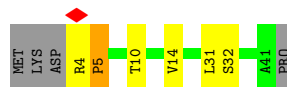
- Molecule 2: Alpha subunit of light-harvesting 1

Chain R:  90% • 7%



- Molecule 2: Alpha subunit of light-harvesting 1

Chain T:  76% 12% • 10%



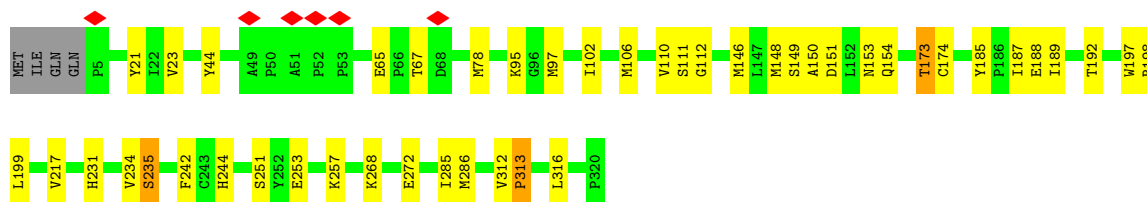
- Molecule 2: Alpha subunit of light-harvesting 1

Chain V:  5% 81% 10% 10%



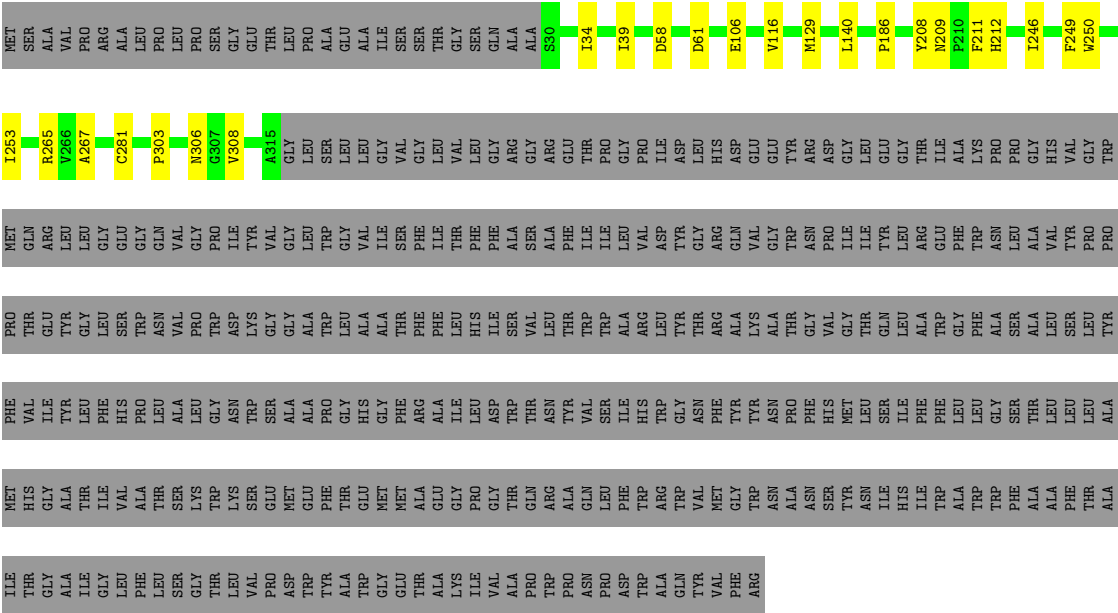
- Molecule 3: Cytochrome subunit of photosynthetic reaction center

Chain C:  84% 13% ••



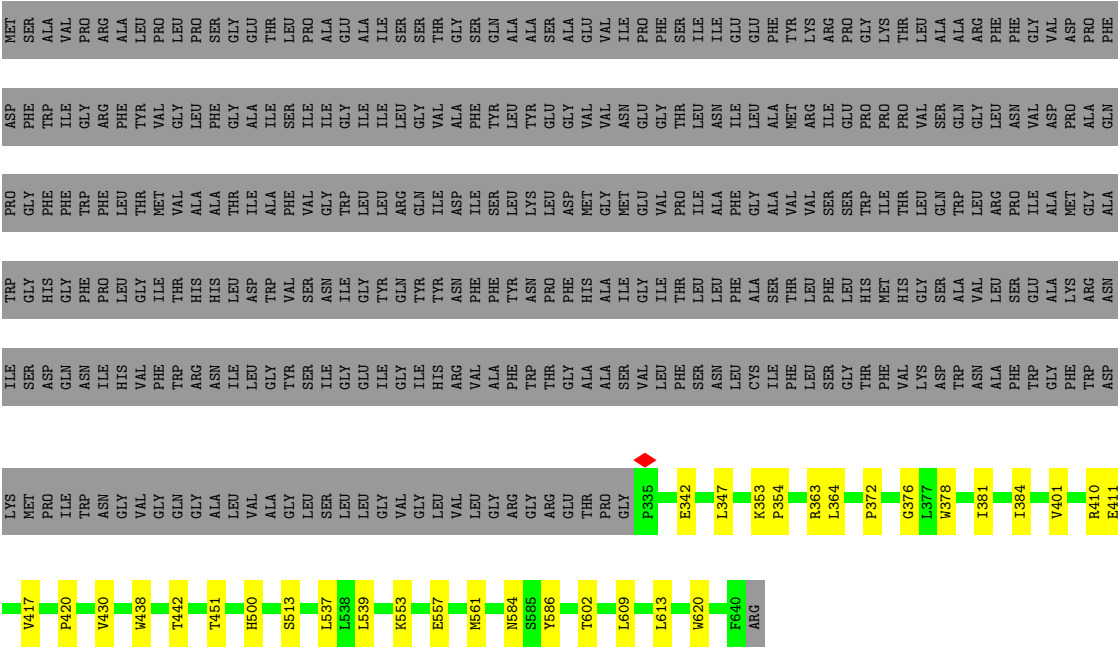
- Molecule 4: Reaction center protein L chain

Chain L:  41% • 55%



• Molecule 4: Reaction center protein L chain

Chain M: 43% 5%



• Molecule 5: TMx polypeptide

Chain X: 17% 93% 7%



• Molecule 6: reaction center small polypeptide

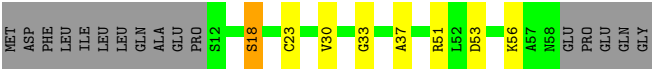


• Molecule 7: reaction center unknown polypeptide



There are no outlier residues recorded for this chain.

• Molecule 8: reaction center small polypeptide



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	639374	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.066	Depositor
Minimum map value	-1.238	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.047	Depositor
Recommended contour level	0.226	Depositor
Map size ($\text{\AA}$)	320.4, 320.4, 320.4	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.89, 0.89, 0.89	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BGL, LMT, HEC, U42, MQE, PEF, BPH, BCL, CA, MN, U4Z, LHG, UNL, PGV

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.21	0/432	0.31	0/597
1	2	0.28	0/432	0.37	0/597
1	4	0.29	0/432	0.40	0/597
1	6	0.30	0/432	0.41	0/597
1	8	0.30	0/432	0.42	0/597
1	B	0.18	0/432	0.30	0/597
1	E	0.19	0/432	0.31	0/597
1	G	0.20	0/432	0.31	0/597
1	I	0.20	0/432	0.29	0/597
1	K	0.21	0/432	0.31	0/597
1	O	0.19	0/432	0.29	0/597
1	Q	0.20	0/432	0.31	0/597
1	S	0.22	0/432	0.33	0/597
1	U	0.20	0/432	0.32	0/597
1	W	0.18	0/432	0.26	0/597
2	1	0.16	0/307	0.25	0/417
2	3	0.24	0/315	0.38	0/428
2	5	0.26	0/315	0.30	0/428
2	7	0.19	0/315	0.29	0/428
2	9	0.17	0/307	0.32	0/417
2	A	0.18	0/307	0.26	0/417
2	D	0.17	0/315	0.24	0/428
2	F	0.16	0/307	0.25	0/417
2	H	0.45	0/315	0.61	0/428
2	J	0.38	0/315	0.59	0/428
2	N	0.16	0/315	0.24	0/428
2	P	0.28	0/315	0.44	0/428
2	R	0.30	0/315	0.45	0/428
2	T	0.74	1/307 (0.3%)	0.37	0/417
2	V	0.16	0/307	0.35	0/417
3	C	0.61	1/2477 (0.0%)	0.47	2/3383 (0.1%)
4	L	0.37	0/2360	0.58	0/3220

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	M	0.23	0/2597	0.39	0/3566
5	X	0.13	0/253	0.22	0/341
6	Y	0.19	0/268	0.36	0/370
7	Z	1.06	0/51	1.30	0/70
8	h	0.18	0/374	0.30	0/513
All	All	0.34	2/19537 (0.0%)	0.41	2/26772 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	313	PRO	N-CD	-26.86	1.10	1.47
2	T	5	PRO	N-CD	-12.53	1.30	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	313	PRO	CA-N-CD	5.70	119.98	112.00
3	C	242	PHE	N-CA-C	-5.64	105.21	111.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	416	0	413	3	0
1	2	416	0	413	5	0
1	4	416	0	413	0	0
1	6	416	0	413	7	0
1	8	416	0	413	2	0
1	B	416	0	413	3	0
1	E	416	0	413	7	0
1	G	416	0	413	6	0
1	I	416	0	413	7	0
1	K	416	0	413	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	416	0	413	8	0
1	Q	416	0	413	3	0
1	S	416	0	413	5	0
1	U	416	0	413	5	0
1	W	416	0	413	8	0
2	1	300	0	316	0	0
2	3	308	0	320	3	0
2	5	308	0	320	5	0
2	7	308	0	320	2	0
2	9	300	0	316	0	0
2	A	300	0	316	3	0
2	D	308	0	320	2	0
2	F	300	0	316	4	0
2	H	308	0	320	4	0
2	J	308	0	320	2	0
2	N	308	0	320	1	0
2	P	308	0	320	8	0
2	R	308	0	320	1	0
2	T	300	0	316	5	0
2	V	300	0	316	3	0
3	C	2411	0	2367	34	0
4	L	2278	0	2235	17	0
4	M	2488	0	2373	23	0
5	X	246	0	261	2	0
6	Y	259	0	272	3	0
7	Z	51	0	49	0	0
8	h	362	0	366	8	0
9	0	132	0	148	1	0
9	1	66	0	74	3	0
9	2	132	0	148	3	0
9	3	66	0	74	0	0
9	4	132	0	148	4	0
9	5	66	0	74	1	0
9	6	132	0	148	0	0
9	7	66	0	74	0	0
9	8	132	0	148	10	0
9	9	66	0	74	0	0
9	A	66	0	72	0	0
9	B	132	0	148	1	0
9	D	132	0	148	1	0
9	E	66	0	74	2	0
9	F	132	0	148	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	G	66	0	74	1	0
9	H	66	0	74	0	0
9	I	132	0	148	2	0
9	J	66	0	74	0	0
9	K	132	0	148	1	0
9	L	132	0	148	0	0
9	M	66	0	74	2	0
9	N	66	0	74	1	0
9	O	132	0	148	4	0
9	P	66	0	72	1	0
9	Q	132	0	148	3	0
9	R	66	0	74	0	0
9	S	132	0	148	1	0
9	T	66	0	74	0	0
9	U	132	0	148	4	0
9	V	66	0	74	1	0
9	W	132	0	148	3	0
10	0	68	0	0	0	0
10	4	136	0	0	1	0
10	8	68	0	0	3	0
10	B	68	0	0	0	0
10	E	68	0	0	3	0
10	G	68	0	0	3	0
10	I	136	0	0	4	0
10	O	68	0	0	3	0
10	Q	68	0	0	1	0
10	S	68	0	0	2	0
10	U	136	0	0	4	0
11	1	40	0	0	0	0
11	3	40	0	0	0	0
11	5	40	0	0	0	0
11	7	40	0	0	0	0
11	9	40	0	0	0	0
11	A	40	0	0	0	0
11	C	40	0	0	0	0
11	D	40	0	0	0	0
11	F	40	0	0	0	0
11	H	40	0	0	0	0
11	J	40	0	0	0	0
11	N	40	0	0	0	0
11	P	40	0	0	0	0
11	S	40	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	T	40	0	0	0	0
11	V	40	0	0	0	0
12	1	35	0	46	1	0
12	D	35	0	46	2	0
12	T	35	0	46	2	0
13	3	20	0	28	1	0
13	C	40	0	56	2	0
13	D	20	0	28	0	0
13	F	20	0	28	2	0
13	H	40	0	56	1	0
13	L	80	0	112	0	0
13	N	20	0	28	0	0
13	Y	20	0	28	0	0
14	C	172	0	120	2	0
15	C	1	0	0	0	0
16	C	92	0	126	2	0
16	L	153	0	228	5	0
16	M	102	0	152	9	0
16	P	94	0	133	7	0
17	C	34	0	0	0	0
17	H	52	0	0	0	0
17	L	48	0	0	0	0
17	M	12	0	0	0	0
17	V	33	0	0	0	0
17	Y	14	0	0	0	0
17	h	24	0	0	0	0
18	L	130	0	150	5	0
18	M	65	0	76	0	0
19	L	53	0	0	0	0
19	M	68	0	0	0	0
20	L	41	0	58	1	0
21	M	1	0	0	0	0
22	h	17	0	31	2	0
All	All	25238	0	24018	240	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 5.

All (240) 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)
1:E:54:ILE:CG2	10:E:101:U42:CBD	2.35	1.05
1:O:54:ILE:HG22	10:O:101:U42:CBD	1.86	1.05
8:h:23:CYS:SG	22:h:101:LHG:C7	2.47	1.03
1:E:54:ILE:HG22	10:E:101:U42:CBD	1.91	1.00
1:O:54:ILE:CG2	10:O:101:U42:CBD	2.40	1.00
1:I:54:ILE:HG22	10:I:101:U42:CBD	1.92	0.99
1:S:54:ILE:HG22	10:S:101:U42:CBD	1.98	0.92
1:E:54:ILE:HG21	10:E:101:U42:CBD	2.01	0.90
10:U:104:U42:CBD	1:W:54:ILE:HG22	2.06	0.85
1:I:54:ILE:CG2	10:I:101:U42:CBD	2.54	0.84
2:T:10:THR:O	2:T:14:VAL:HG23	1.80	0.81
1:I:7:ASN:OD1	1:I:7:ASN:O	1.98	0.80
3:C:149:SER:O	3:C:153:ASN:OD1	2.00	0.80
3:C:150:ALA:O	3:C:154:GLN:HB2	1.82	0.80
3:C:268:LYS:O	3:C:272:GLU:HG2	1.83	0.78
1:S:54:ILE:CG2	10:S:101:U42:CBD	2.61	0.78
4:L:250:TRP:CE3	4:L:253:ILE:HD11	2.19	0.77
1:G:54:ILE:HG22	10:G:101:U42:CBD	2.15	0.77
10:U:104:U42:CBD	1:W:54:ILE:CG2	2.62	0.77
3:C:312:VAL:HG13	3:C:313:PRO:HD2	1.69	0.74
1:O:54:ILE:HG21	10:O:101:U42:CBD	2.16	0.74
2:F:9:ARG:NH1	2:H:5:PRO:O	2.20	0.73
3:C:192:THR:HG23	16:C:408:PGV:H012	1.72	0.72
10:4:104:U42:CBC	1:6:54:ILE:HG22	2.21	0.71
4:L:58:ASP:HB3	4:L:61:ASP:HB2	1.74	0.69
1:W:9:LEU:HD12	1:W:20:ASN:OD1	1.94	0.68
1:0:7:ASN:O	1:0:15:LYS:HE2	1.92	0.68
3:C:312:VAL:CG1	3:C:313:PRO:HD2	2.23	0.68
1:8:54:ILE:HG22	10:8:101:U42:CBC	2.24	0.67
3:C:65:GLU:O	3:C:67:THR:HG23	1.94	0.67
1:2:12:ASP:OD1	1:2:12:ASP:N	2.24	0.67
3:C:251:SER:OG	3:C:253:GLU:HG2	1.94	0.67
16:P:103:PGV:H162	16:P:104:PGV:H291	1.78	0.66
2:N:9:ARG:NH1	16:P:104:PGV:O02	2.29	0.65
1:G:26:HIS:O	1:G:30:VAL:HG13	1.97	0.65
4:L:106:GLU:HG3	4:L:186:PRO:HB3	1.80	0.64
4:M:609:LEU:HD22	4:M:613:LEU:HD12	1.80	0.63
4:M:381:ILE:HB	4:M:451:THR:HG21	1.80	0.63
2:A:17:LEU:HD23	4:M:384:ILE:HD12	1.80	0.62
2:P:9:ARG:HG3	16:P:103:PGV:H31	1.81	0.62
1:U:7:ASN:HB3	1:U:15:LYS:HD2	1.82	0.62
3:C:151:ASP:C	3:C:151:ASP:OD1	2.42	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:C:409:BGL:H5'1	13:C:410:BGL:H6'1	1.83	0.61
3:C:187:ILE:HG22	3:C:188:GLU:OE1	2.01	0.60
2:P:4:ARG:NH1	1:Q:17:LEU:O	2.35	0.60
16:L:1007:PGV:H031	16:P:103:PGV:H51	1.82	0.60
1:U:19:ASN:HB3	1:U:22:GLU:HG3	1.83	0.60
2:F:10:THR:O	2:F:14:VAL:HG23	2.02	0.60
1:W:27:ASP:O	1:W:31:LYS:HG2	2.03	0.59
2:F:32:SER:OG	13:F:104:BGL:H1'1	2.02	0.58
2:D:4:ARG:NH2	1:E:17:LEU:O	2.37	0.58
2:H:9:ARG:NH2	2:J:5:PRO:O	2.36	0.58
1:O:22:GLU:HG2	2:P:5:PRO:HG3	1.85	0.58
9:D:102:BCL:H52	1:E:36:GLY:HA3	1.86	0.57
4:L:211:PHE:HB2	4:L:281:CYS:HB3	1.86	0.57
2:F:33:SER:HA	13:F:104:BGL:H4	1.86	0.57
3:C:244:HIS:CE1	3:C:257:LYS:HE3	2.40	0.56
3:C:148:MET:HE2	3:C:285:ILE:HD11	1.88	0.56
4:M:420:PRO:HB3	4:M:430:VAL:HG11	1.87	0.55
10:U:104:U42:CBD	1:W:54:ILE:HG21	2.36	0.55
2:3:22:MET:HE1	2:3:25:LEU:HD23	1.89	0.55
4:M:557:GLU:O	4:M:561:MET:HG3	2.08	0.54
1:G:54:ILE:CG2	10:G:101:U42:CBD	2.84	0.54
1:G:41:VAL:HG22	10:G:101:U42:C32	2.38	0.54
2:V:36:PHE:O	2:V:39:LEU:N	2.30	0.54
1:K:10:VAL:HG23	1:K:15:LYS:HD3	1.90	0.54
4:L:249:PHE:O	4:L:253:ILE:HG12	2.08	0.54
2:T:4:ARG:O	2:T:4:ARG:NE	2.40	0.54
2:D:17:LEU:HD13	12:D:105:LMT:H82	1.89	0.54
1:I:7:ASN:OD1	1:I:7:ASN:C	2.52	0.53
1:2:12:ASP:HA	1:2:15:LYS:HG3	1.89	0.53
3:C:111:SER:HB2	14:C:402:HEC:HMC2	1.89	0.53
3:C:185:TYR:HA	3:C:189:ILE:HD11	1.91	0.53
16:M:706:PGV:H341	8:h:30:VAL:HG13	1.90	0.53
2:T:31:LEU:HD21	12:T:103:LMT:H6E	1.90	0.52
1:S:19:ASN:HB3	1:S:22:GLU:HG3	1.91	0.52
1:2:8:ASP:OD2	1:2:9:LEU:HD12	2.10	0.52
4:M:553:LYS:HB3	4:M:553:LYS:HZ3	1.75	0.52
10:8:101:U42:C32	9:8:102:BCL:HAA1	2.40	0.52
3:C:313:PRO:HG2	3:C:316:LEU:HD12	1.92	0.51
2:P:10:THR:HG22	16:P:103:PGV:H42	1.92	0.51
10:Q:101:U42:O15	10:Q:101:U42:O12	2.28	0.51
16:M:706:PGV:H131	16:M:706:PGV:H301	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:9:ARG:HG3	2:5:6:PHE:CZ	2.46	0.50
1:I:54:ILE:HG21	10:I:101:U42:CBD	2.37	0.50
2:5:3:ASP:N	2:5:3:ASP:OD1	2.44	0.50
1:6:39:ILE:HD11	9:8:103:BCL:H152	1.94	0.50
16:L:1007:PGV:H91	16:P:104:PGV:H131	1.94	0.50
2:A:22:MET:HE2	2:A:22:MET:HA	1.93	0.50
3:C:106:MET:HE1	3:C:146:MET:HE1	1.94	0.50
3:C:231:HIS:O	3:C:235:SER:OG	2.29	0.49
2:P:10:THR:O	2:P:14:VAL:HG23	2.11	0.49
12:D:105:LMT:H6D	4:M:378:TRP:HE1	1.78	0.49
4:M:584:ASN:HB3	4:M:586:TYR:H	1.77	0.49
1:0:28:ILE:HG12	9:B:103:BCL:H12	1.94	0.49
2:3:37:ASN:O	2:3:40:ARG:HG2	2.12	0.49
3:C:188:GLU:OE1	3:C:188:GLU:N	2.46	0.49
1:2:8:ASP:OD2	1:2:9:LEU:CD1	2.62	0.48
3:C:148:MET:CE	3:C:286:MET:HE3	2.43	0.48
16:C:408:PGV:H241	4:L:208:TYR:HA	1.95	0.48
9:V:101:BCL:H141	9:V:101:BCL:H161	1.69	0.48
2:A:17:LEU:HD21	4:M:381:ILE:HA	1.93	0.48
1:W:6:GLN:O	1:W:20:ASN:HB2	2.14	0.48
9:2:102:BCL:H8	9:2:102:BCL:H121	1.71	0.48
2:H:37:ASN:OD1	2:H:40:ARG:HD2	2.14	0.48
4:L:265:ARG:NH1	4:M:364:LEU:O	2.47	0.48
3:C:21:TYR:OH	13:C:409:BGL:O4	2.30	0.47
3:C:148:MET:CE	3:C:285:ILE:HD11	2.44	0.47
12:1:103:LMT:H1B	12:1:103:LMT:H3'	1.55	0.47
3:C:97:MET:HE3	3:C:102:ILE:HG12	1.97	0.47
4:M:620:TRP:HE1	8:h:18:SER:HB2	1.79	0.47
1:W:26:HIS:O	1:W:30:VAL:HG13	2.14	0.47
16:M:706:PGV:H262	16:M:706:PGV:H291	1.70	0.47
9:0:102:BCL:H122	9:0:102:BCL:H8	1.65	0.47
1:O:7:ASN:OD1	1:O:7:ASN:O	2.31	0.47
9:1:101:BCL:H112	9:1:101:BCL:H151	1.55	0.47
3:C:148:MET:HE1	3:C:286:MET:HE3	1.96	0.47
3:C:197:TRP:O	3:C:198:ARG:NH1	2.46	0.47
2:P:7:GLU:HG2	16:P:104:PGV:H042	1.97	0.47
1:6:28:ILE:HG23	9:8:103:BCL:H43	1.97	0.46
1:W:7:ASN:O	1:W:15:LYS:NZ	2.44	0.46
4:L:209:ASN:ND2	4:L:281:CYS:HB2	2.31	0.46
2:P:4:ARG:NH2	2:P:7:GLU:OE1	2.47	0.46
9:S:103:BCL:H91	9:S:103:BCL:H112	1.83	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:M:705:PGV:H271	16:M:705:PGV:H302	1.77	0.46
8:h:53:ASP:CG	8:h:56:LYS:HZ1	2.23	0.46
9:Q:103:BCL:H161	9:Q:103:BCL:H121	1.56	0.46
10:8:101:U42:CAI	9:8:103:BCL:H12	2.46	0.46
9:8:103:BCL:H143	9:8:103:BCL:H161	1.86	0.46
3:C:187:ILE:CG2	3:C:188:GLU:OE1	2.63	0.46
1:6:22:GLU:HG2	2:7:5:PRO:HG3	1.98	0.45
4:M:378:TRP:HE3	4:M:451:THR:HG23	1.81	0.45
2:T:4:ARG:N	2:T:5:PRO:HD2	2.30	0.45
3:C:44:TYR:HE2	6:Y:4:ILE:HD11	1.81	0.45
9:8:103:BCL:HHD	9:8:103:BCL:HAC2	1.82	0.45
3:C:173:THR:O	3:C:174:CYS:HB2	2.16	0.45
9:E:102:BCL:H162	9:E:102:BCL:H121	1.70	0.45
12:T:103:LMT:H1B	12:T:103:LMT:H3'	1.75	0.45
9:5:101:BCL:H93	9:5:101:BCL:H112	1.74	0.45
1:B:55:ARG:HG3	1:B:55:ARG:HH11	1.81	0.45
1:K:35:GLY:HA3	9:O:103:BCL:H121	1.99	0.45
2:5:32:SER:HB3	4:L:306:ASN:O	2.17	0.45
4:M:410:ARG:HG2	4:M:411:GLU:HG2	1.98	0.45
3:C:78:MET:HG3	14:C:402:HEC:CMB	2.47	0.45
16:M:706:PGV:H311	16:M:706:PGV:H282	1.61	0.45
9:Q:103:BCL:H143	9:Q:103:BCL:H112	1.74	0.45
9:U:103:BCL:H41	9:U:103:BCL:H62	1.69	0.45
10:I:101:U42:C32	9:I:102:BCL:HAA1	2.48	0.44
16:M:706:PGV:H302	16:M:706:PGV:H332	1.75	0.44
9:8:103:BCL:H122	9:8:103:BCL:H8	1.61	0.44
1:B:55:ARG:HG3	1:B:55:ARG:NH1	2.32	0.44
9:W:102:BCL:H143	9:W:102:BCL:H112	1.83	0.44
4:L:209:ASN:HB3	4:L:212:HIS:HB2	2.00	0.44
16:M:706:PGV:H242	8:h:37:ALA:HB1	1.99	0.44
4:M:353:LYS:HB2	4:M:354:PRO:HD3	1.99	0.44
9:P:101:BCL:H202	9:P:101:BCL:H161	1.68	0.44
9:4:102:BCL:H161	9:4:102:BCL:H141	1.73	0.44
3:C:185:TYR:OH	3:C:199:LEU:HB2	2.17	0.44
4:L:267:ALA:HB1	4:M:539:LEU:HG	1.99	0.44
1:U:9:LEU:HG	1:U:20:ASN:ND2	2.32	0.44
9:4:103:BCL:H61	9:4:103:BCL:H41	1.66	0.44
1:E:12:ASP:OD1	1:E:15:LYS:NZ	2.46	0.44
18:L:1003:BPH:H2	18:L:1003:BPH:H6C2	1.66	0.44
4:M:417:VAL:HG22	4:M:500:HIS:HB2	2.00	0.44
2:5:9:ARG:HG3	2:7:6:PHE:CZ	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:10:VAL:CG2	1:K:15:LYS:HD3	2.48	0.44
2:P:9:ARG:NH2	2:R:5:PRO:O	2.51	0.44
9:Q:103:BCL:H192	9:Q:103:BCL:H162	1.71	0.44
1:S:26:HIS:O	1:S:30:VAL:HG13	2.17	0.44
1:U:54:ILE:HG22	10:U:101:U42:CBD	2.48	0.43
1:I:21:ALA:HB1	1:K:17:LEU:HD21	1.99	0.43
8:h:53:ASP:HB3	8:h:56:LYS:NZ	2.32	0.43
9:8:103:BCL:H151	9:8:103:BCL:H111	1.79	0.43
16:L:1007:PGV:H71	16:L:1007:PGV:H41	1.76	0.43
4:M:347:LEU:O	4:M:376:GLY:HA2	2.18	0.43
9:2:101:BCL:H41	9:2:101:BCL:H61	1.52	0.43
16:L:1008:PGV:H152	2:V:18:LEU:HD13	2.01	0.43
9:M:701:BCL:H141	9:M:701:BCL:H161	1.68	0.43
9:U:103:BCL:H93	9:U:103:BCL:H112	1.75	0.43
4:M:513:SER:HB2	9:M:701:BCL:HHD	2.01	0.43
1:B:26:HIS:O	1:B:30:VAL:HG13	2.19	0.43
3:C:23:VAL:HG23	5:X:25:MET:HE1	2.01	0.43
3:C:148:MET:HE1	3:C:286:MET:CE	2.49	0.43
1:E:26:HIS:O	1:E:30:VAL:HG13	2.19	0.43
4:L:246:ILE:HD12	4:L:246:ILE:HA	1.93	0.43
9:1:101:BCL:H143	9:1:101:BCL:H161	1.73	0.43
1:6:31:LYS:HB2	9:8:103:BCL:H41	2.00	0.43
9:1:101:BCL:H142	9:4:103:BCL:HAC2	2.00	0.42
18:L:1005:BPH:H112	18:L:1005:BPH:H152	1.84	0.42
9:U:102:BCL:HBA1	9:U:102:BCL:H3A	1.81	0.42
22:h:101:LHG:H101	22:h:101:LHG:H131	1.75	0.42
3:C:95:LYS:HD2	3:C:95:LYS:HA	1.63	0.42
9:O:103:BCL:H8	9:O:103:BCL:H41	2.02	0.42
1:S:28:ILE:HG23	9:U:103:BCL:H2	2.01	0.42
2:V:26:ILE:HD12	9:W:101:BCL:O1D	2.19	0.42
1:8:8:ASP:OD1	1:8:8:ASP:C	2.61	0.42
9:W:102:BCL:H121	9:W:102:BCL:H162	1.73	0.42
4:L:140:LEU:HD21	20:L:1017:PEF:H162	2.01	0.42
4:M:363:ARG:NH2	6:Y:28:TRP:O	2.50	0.42
1:2:36:GLY:HA3	9:2:101:BCL:H52	2.02	0.42
1:O:9:LEU:HD12	1:O:20:ASN:HB2	2.02	0.42
13:3:103:BGL:H1'2	4:L:303:PRO:HD3	2.00	0.42
1:O:53:TRP:CD1	1:O:54:ILE:HG13	2.55	0.42
16:M:706:PGV:H132	8:h:33:GLY:HA3	2.02	0.42
1:O:7:ASN:O	1:O:15:LYS:NZ	2.53	0.42
16:L:1008:PGV:H272	16:L:1008:PGV:H242	1.81	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:O:102:BCL:H152	9:O:102:BCL:H112	1.86	0.42
3:C:106:MET:HA	3:C:110:VAL:HB	2.01	0.41
1:K:26:HIS:O	1:K:30:VAL:HG13	2.20	0.41
4:L:129:MET:HE3	4:L:129:MET:HB3	1.86	0.41
5:X:21:LEU:HD12	5:X:21:LEU:HA	1.87	0.41
4:L:34:ILE:O	8:h:51:ARG:NH1	2.53	0.41
1:Q:26:HIS:O	1:Q:30:VAL:HG13	2.20	0.41
4:M:438:TRP:O	4:M:442:THR:OG1	2.26	0.41
9:O:103:BCL:H143	9:O:103:BCL:H112	1.78	0.41
2:J:17:LEU:HD12	2:J:17:LEU:HA	1.94	0.41
1:G:15:LYS:N	1:G:16:PRO:HD2	2.36	0.41
9:G:102:BCL:H62	9:G:102:BCL:H101	1.69	0.41
9:E:102:BCL:H142	9:E:102:BCL:H112	1.82	0.41
1:U:26:HIS:O	1:U:30:VAL:HG13	2.21	0.41
2:H:4:ARG:HB3	1:I:17:LEU:HD23	2.02	0.41
1:6:15:LYS:N	1:6:16:PRO:HD2	2.36	0.41
3:C:110:VAL:C	3:C:112:GLY:H	2.29	0.41
1:G:7:ASN:HB3	1:G:15:LYS:HD2	2.02	0.41
16:M:705:PGV:H32	16:M:705:PGV:H61	1.95	0.41
1:Q:12:ASP:HA	1:Q:15:LYS:HG3	2.02	0.41
1:O:26:HIS:O	1:O:30:VAL:HG13	2.21	0.41
6:Y:9:MET:O	6:Y:13:VAL:HG23	2.21	0.41
2:5:4:ARG:HG2	1:6:17:LEU:HD23	2.02	0.40
4:L:116:VAL:O	2:T:32:SER:OG	2.39	0.40
4:M:342:GLU:HG3	4:M:372:PRO:HG2	2.02	0.40
9:8:102:BCL:H203	9:8:102:BCL:H162	1.76	0.40
9:I:103:BCL:H193	9:I:103:BCL:H162	1.85	0.40
18:L:1003:BPH:ND	4:M:537:LEU:HD13	2.36	0.40
18:L:1003:BPH:OBB	18:L:1003:BPH:HHC	2.21	0.40
9:4:103:BCL:H162	9:4:103:BCL:H122	1.38	0.40
9:K:102:BCL:H52	9:K:102:BCL:H11	1.67	0.40
13:H:103:BGL:H2'2	4:M:613:LEU:HD13	2.03	0.40
18:L:1005:BPH:HBC3	18:L:1005:BPH:H2C	1.91	0.40
9:N:101:BCL:H193	9:N:101:BCL:H162	1.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
1	2	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
1	4	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
1	6	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
1	8	48/55 (87%)	44 (92%)	4 (8%)	0	100	100
1	B	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
1	E	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
1	G	48/55 (87%)	46 (96%)	2 (4%)	0	100	100
1	I	48/55 (87%)	46 (96%)	2 (4%)	0	100	100
1	K	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
1	O	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
1	Q	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
1	S	48/55 (87%)	46 (96%)	2 (4%)	0	100	100
1	U	48/55 (87%)	46 (96%)	2 (4%)	0	100	100
1	W	48/55 (87%)	46 (96%)	2 (4%)	0	100	100
2	1	36/42 (86%)	34 (94%)	2 (6%)	0	100	100
2	3	37/42 (88%)	36 (97%)	1 (3%)	0	100	100
2	5	37/42 (88%)	35 (95%)	2 (5%)	0	100	100
2	7	37/42 (88%)	34 (92%)	3 (8%)	0	100	100
2	9	36/42 (86%)	36 (100%)	0	0	100	100
2	A	36/42 (86%)	33 (92%)	3 (8%)	0	100	100
2	D	37/42 (88%)	37 (100%)	0	0	100	100
2	F	36/42 (86%)	35 (97%)	1 (3%)	0	100	100
2	H	37/42 (88%)	37 (100%)	0	0	100	100
2	J	37/42 (88%)	37 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	N	37/42 (88%)	34 (92%)	3 (8%)	0	100	100
2	P	37/42 (88%)	35 (95%)	2 (5%)	0	100	100
2	R	37/42 (88%)	36 (97%)	1 (3%)	0	100	100
2	T	36/42 (86%)	36 (100%)	0	0	100	100
2	V	36/42 (86%)	33 (92%)	3 (8%)	0	100	100
3	C	314/320 (98%)	302 (96%)	12 (4%)	0	100	100
4	L	284/641 (44%)	269 (95%)	15 (5%)	0	100	100
4	M	304/641 (47%)	293 (96%)	11 (4%)	0	100	100
5	X	29/30 (97%)	28 (97%)	1 (3%)	0	100	100
6	Y	30/39 (77%)	29 (97%)	1 (3%)	0	100	100
7	Z	8/10 (80%)	6 (75%)	2 (25%)	0	100	100
8	h	45/63 (71%)	45 (100%)	0	0	100	100
All	All	2283/3199 (71%)	2197 (96%)	86 (4%)	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	0	44/49 (90%)	44 (100%)	0	100	100
1	2	44/49 (90%)	42 (96%)	2 (4%)	24	48
1	4	44/49 (90%)	44 (100%)	0	100	100
1	6	44/49 (90%)	44 (100%)	0	100	100
1	8	44/49 (90%)	44 (100%)	0	100	100
1	B	44/49 (90%)	44 (100%)	0	100	100
1	E	44/49 (90%)	44 (100%)	0	100	100
1	G	44/49 (90%)	44 (100%)	0	100	100
1	I	44/49 (90%)	44 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	44/49 (90%)	44 (100%)	0	100	100
1	O	44/49 (90%)	44 (100%)	0	100	100
1	Q	44/49 (90%)	44 (100%)	0	100	100
1	S	44/49 (90%)	44 (100%)	0	100	100
1	U	44/49 (90%)	44 (100%)	0	100	100
1	W	44/49 (90%)	44 (100%)	0	100	100
2	1	33/37 (89%)	33 (100%)	0	100	100
2	3	34/37 (92%)	34 (100%)	0	100	100
2	5	34/37 (92%)	34 (100%)	0	100	100
2	7	34/37 (92%)	34 (100%)	0	100	100
2	9	33/37 (89%)	33 (100%)	0	100	100
2	A	33/37 (89%)	33 (100%)	0	100	100
2	D	34/37 (92%)	34 (100%)	0	100	100
2	F	33/37 (89%)	32 (97%)	1 (3%)	36	61
2	H	34/37 (92%)	34 (100%)	0	100	100
2	J	34/37 (92%)	34 (100%)	0	100	100
2	N	34/37 (92%)	34 (100%)	0	100	100
2	P	34/37 (92%)	34 (100%)	0	100	100
2	R	34/37 (92%)	34 (100%)	0	100	100
2	T	33/37 (89%)	33 (100%)	0	100	100
2	V	33/37 (89%)	33 (100%)	0	100	100
3	C	258/262 (98%)	254 (98%)	4 (2%)	55	76
4	L	232/511 (45%)	230 (99%)	2 (1%)	70	84
4	M	244/511 (48%)	242 (99%)	2 (1%)	73	86
5	X	27/26 (104%)	27 (100%)	0	100	100
6	Y	29/36 (81%)	29 (100%)	0	100	100
7	Z	1/1 (100%)	1 (100%)	0	100	100
8	h	36/50 (72%)	35 (97%)	1 (3%)	38	62
All	All	1991/2687 (74%)	1979 (99%)	12 (1%)	76	89

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	2	10	VAL
1	2	12	ASP
3	C	173	THR
3	C	217	VAL
3	C	234	VAL
3	C	235	SER
2	F	37	ASN
4	L	39	ILE
4	L	308	VAL
4	M	401	VAL
4	M	602	THR
8	h	18	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	6	7	ASN
2	A	37	ASN
3	C	89	GLN
3	C	109	GLN
3	C	259	HIS
3	C	311	GLN
2	F	27	HIS
2	J	37	ASN
4	L	115	ASN
4	L	212	HIS
4	M	414	ASN
4	M	525	HIS
2	N	37	ASN
2	P	37	ASN
1	S	6	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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 133 ligands modelled in this entry, 2 are monoatomic and 17 are unknown - leaving 114 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
11	U4Z	S	104	-	40,40,40	1.48	9 (22%)	51,51,51	1.68	13 (25%)
10	U42	4	101	-	69,69,69	1.91	24 (34%)	88,89,89	1.79	22 (25%)
9	BCL	S	103	-	69,74,74	1.83	21 (30%)	79,115,115	2.48	30 (37%)
10	U42	G	101	-	69,69,69	1.92	23 (33%)	88,89,89	2.30	13 (14%)
19	MQE	M	704	-	69,69,69	0.35	0	85,87,87	0.72	2 (2%)
10	U42	4	104	-	69,69,69	1.72	18 (26%)	88,89,89	2.26	26 (29%)
9	BCL	V	101	-	69,74,74	1.75	18 (26%)	79,115,115	2.10	24 (30%)
9	BCL	E	102	-	69,74,74	1.83	18 (26%)	79,115,115	2.34	23 (29%)
11	U4Z	1	102	-	40,40,40	1.46	9 (22%)	51,51,51	1.60	14 (27%)
13	BGL	L	1015	-	20,20,20	1.07	2 (10%)	24,25,25	1.09	2 (8%)
10	U42	U	104	-	69,69,69	1.80	12 (17%)	88,89,89	2.25	27 (30%)
9	BCL	8	103	-	69,74,74	1.85	20 (28%)	79,115,115	2.25	25 (31%)
11	U4Z	7	102	-	40,40,40	1.46	10 (25%)	51,51,51	1.62	13 (25%)
9	BCL	Q	102	-	69,74,74	1.80	17 (24%)	79,115,115	2.14	23 (29%)
12	LMT	T	103	-	36,36,36	0.47	1 (2%)	47,47,47	0.97	3 (6%)
9	BCL	9	102	-	69,74,74	1.77	16 (23%)	79,115,115	2.28	24 (30%)
10	U42	0	103	-	69,69,69	2.20	16 (23%)	88,89,89	2.50	29 (32%)
14	HEC	C	403	3	46,50,50	1.83	4 (8%)	58,82,82	1.92	4 (6%)
9	BCL	O	102	-	69,74,74	1.78	17 (24%)	79,115,115	2.24	24 (30%)
13	BGL	N	103	-	20,20,20	1.01	1 (5%)	24,25,25	0.85	0
18	BPH	L	1003	-	59,70,70	2.59	14 (23%)	59,101,101	2.20	14 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	BGL	C	409	-	20,20,20	1.02	1 (5%)	24,25,25	0.88	0
9	BCL	L	1002	-	69,74,74	1.82	19 (27%)	79,115,115	2.27	24 (30%)
9	BCL	O	103	-	69,74,74	1.78	18 (26%)	79,115,115	2.37	22 (27%)
16	PGV	P	103	-	42,42,50	0.55	0	45,48,56	0.54	0
13	BGL	F	104	-	20,20,20	1.00	1 (5%)	24,25,25	0.93	0
22	LHG	h	101	-	16,16,48	1.07	1 (6%)	15,15,54	0.36	0
16	PGV	P	104	-	50,50,50	0.50	0	53,56,56	0.49	0
16	PGV	L	1008	-	50,50,50	0.49	0	53,56,56	0.46	0
11	U4Z	V	102	-	40,40,40	1.47	9 (22%)	51,51,51	1.68	13 (25%)
9	BCL	R	101	-	69,74,74	1.78	16 (23%)	79,115,115	2.23	23 (29%)
10	U42	E	101	-	69,69,69	1.99	19 (27%)	88,89,89	1.90	21 (23%)
11	U4Z	T	102	-	40,40,40	1.46	9 (22%)	51,51,51	1.62	13 (25%)
9	BCL	0	102	-	69,74,74	1.81	19 (27%)	79,115,115	2.49	27 (34%)
16	PGV	L	1006	-	50,50,50	0.51	0	53,56,56	0.45	0
9	BCL	D	101	-	69,74,74	1.80	18 (26%)	79,115,115	2.35	25 (31%)
9	BCL	U	103	-	69,74,74	1.80	20 (28%)	79,115,115	2.34	20 (25%)
11	U4Z	H	102	-	40,40,40	1.47	9 (22%)	51,51,51	1.64	14 (27%)
14	HEC	C	402	3	46,50,50	1.82	5 (10%)	58,82,82	1.87	4 (6%)
9	BCL	1	101	-	69,74,74	1.76	18 (26%)	79,115,115	2.40	22 (27%)
9	BCL	7	101	-	69,74,74	1.79	17 (24%)	79,115,115	2.22	21 (26%)
12	LMT	D	105	-	36,36,36	0.41	0	47,47,47	0.79	1 (2%)
9	BCL	2	102	-	69,74,74	1.84	22 (31%)	79,115,115	2.22	22 (27%)
11	U4Z	P	102	-	40,40,40	1.46	9 (22%)	51,51,51	1.60	13 (25%)
13	BGL	H	103	-	20,20,20	1.02	1 (5%)	24,25,25	0.80	0
13	BGL	L	1013	-	20,20,20	0.98	1 (5%)	24,25,25	0.90	0
9	BCL	2	101	-	69,74,74	1.80	16 (23%)	79,115,115	2.15	22 (27%)
9	BCL	T	101	-	69,74,74	1.76	17 (24%)	79,115,115	2.26	25 (31%)
12	LMT	1	103	-	36,36,36	0.39	0	47,47,47	0.73	1 (2%)
9	BCL	4	103	-	69,74,74	1.84	21 (30%)	79,115,115	2.56	29 (36%)
9	BCL	H	101	-	69,74,74	1.78	17 (24%)	79,115,115	2.33	24 (30%)
9	BCL	W	101	-	69,74,74	1.84	18 (26%)	79,115,115	2.15	24 (30%)
9	BCL	N	101	-	69,74,74	1.77	17 (24%)	79,115,115	2.22	21 (26%)
9	BCL	A	101	-	69,74,74	1.82	16 (23%)	79,115,115	2.25	20 (25%)
9	BCL	F	102	-	69,74,74	1.81	17 (24%)	79,115,115	2.11	23 (29%)
9	BCL	K	102	-	69,74,74	1.89	22 (31%)	79,115,115	2.44	26 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	PEF	L	1017	-	40,40,46	1.03	2 (5%)	43,45,51	1.07	2 (4%)
16	PGV	M	706	-	50,50,50	0.49	0	53,56,56	0.54	0
9	BCL	S	102	-	69,74,74	1.81	17 (24%)	79,115,115	2.25	27 (34%)
9	BCL	D	102	-	69,74,74	1.80	16 (23%)	79,115,115	2.12	23 (29%)
9	BCL	M	701	-	69,74,74	1.85	21 (30%)	79,115,115	2.42	25 (31%)
10	U42	S	101	-	69,69,69	1.97	18 (26%)	88,89,89	2.16	25 (28%)
10	U42	8	101	-	69,69,69	1.95	16 (23%)	88,89,89	2.27	23 (26%)
9	BCL	P	101	-	69,74,74	1.82	16 (23%)	79,115,115	2.28	22 (27%)
13	BGL	C	410	-	20,20,20	1.00	1 (5%)	24,25,25	0.90	0
11	U4Z	5	102	-	40,40,40	1.46	9 (22%)	51,51,51	1.63	13 (25%)
11	U4Z	J	102	-	40,40,40	1.48	9 (22%)	51,51,51	1.65	13 (25%)
9	BCL	W	102	-	69,74,74	1.80	20 (28%)	79,115,115	2.38	23 (29%)
11	U4Z	C	401	-	40,40,40	1.53	10 (25%)	51,51,51	2.21	17 (33%)
9	BCL	Q	103	-	69,74,74	1.81	20 (28%)	79,115,115	2.42	23 (29%)
16	PGV	C	407	-	40,40,50	0.55	0	43,46,56	0.52	0
9	BCL	4	102	-	69,74,74	1.81	17 (24%)	79,115,115	2.15	23 (29%)
9	BCL	J	101	-	69,74,74	1.78	18 (26%)	79,115,115	2.32	24 (30%)
10	U42	O	101	-	69,69,69	2.17	17 (24%)	88,89,89	2.04	23 (26%)
16	PGV	C	408	15	50,50,50	0.54	0	53,56,56	0.51	0
10	U42	U	101	-	69,69,69	1.89	19 (27%)	88,89,89	2.16	21 (23%)
9	BCL	L	1001	-	69,74,74	1.81	18 (26%)	79,115,115	2.31	22 (27%)
13	BGL	Y	101	-	20,20,20	1.03	1 (5%)	24,25,25	0.77	0
19	MQE	L	1004	-	54,54,69	0.38	0	67,69,87	0.96	4 (5%)
9	BCL	I	103	-	69,74,74	1.81	20 (28%)	79,115,115	2.34	22 (27%)
13	BGL	L	1011	-	20,20,20	1.09	1 (5%)	24,25,25	0.92	1 (4%)
10	U42	Q	101	-	69,69,69	2.00	21 (30%)	88,89,89	2.01	24 (27%)
9	BCL	8	102	-	69,74,74	1.80	17 (24%)	79,115,115	2.08	22 (27%)
11	U4Z	N	102	-	40,40,40	1.50	9 (22%)	51,51,51	1.64	13 (25%)
9	BCL	3	101	-	69,74,74	1.78	17 (24%)	79,115,115	2.23	24 (30%)
9	BCL	5	101	-	69,74,74	1.79	17 (24%)	79,115,115	2.25	24 (30%)
18	BPH	M	702	-	59,70,70	0.77	2 (3%)	59,101,101	1.00	4 (6%)
16	PGV	M	705	-	50,50,50	0.49	0	53,56,56	0.49	0
9	BCL	K	101	-	69,74,74	1.81	16 (23%)	79,115,115	2.12	23 (29%)
9	BCL	G	102	-	69,74,74	1.80	21 (30%)	79,115,115	2.36	26 (32%)
10	U42	I	104	-	69,69,69	1.82	22 (31%)	88,89,89	2.25	24 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	HEC	C	404	3	46,50,50	1.83	5 (10%)	58,82,82	1.93	5 (8%)
11	U4Z	9	101	-	40,40,40	1.46	10 (25%)	51,51,51	1.64	14 (27%)
9	BCL	I	102	-	69,74,74	1.78	16 (23%)	79,115,115	2.29	22 (27%)
9	BCL	6	102	-	69,74,74	1.79	19 (27%)	79,115,115	2.39	20 (25%)
9	BCL	U	102	-	69,74,74	1.79	17 (24%)	79,115,115	2.13	23 (29%)
10	U42	I	101	-	69,69,69	2.20	24 (34%)	88,89,89	2.50	23 (26%)
13	BGL	D	104	-	20,20,20	1.05	1 (5%)	24,25,25	0.77	0
9	BCL	6	101	-	69,74,74	1.80	17 (24%)	79,115,115	2.15	23 (29%)
10	U42	B	101	-	69,69,69	1.91	21 (30%)	88,89,89	2.19	27 (30%)
9	BCL	F	101	-	69,74,74	1.79	17 (24%)	79,115,115	2.26	25 (31%)
11	U4Z	F	103	-	40,40,40	1.48	9 (22%)	51,51,51	1.64	13 (25%)
14	HEC	C	405	3	46,50,50	1.84	3 (6%)	58,82,82	1.81	4 (6%)
9	BCL	0	101	-	69,74,74	1.81	16 (23%)	79,115,115	2.15	21 (26%)
11	U4Z	3	102	-	40,40,40	1.47	9 (22%)	51,51,51	1.64	13 (25%)
13	BGL	L	1012	-	20,20,20	1.05	1 (5%)	24,25,25	0.75	0
18	BPH	L	1005	-	59,70,70	0.86	3 (5%)	59,101,101	1.04	4 (6%)
9	BCL	B	102	-	69,74,74	1.79	16 (23%)	79,115,115	2.12	21 (26%)
11	U4Z	D	103	-	40,40,40	1.48	10 (25%)	51,51,51	1.64	13 (25%)
13	BGL	3	103	-	20,20,20	1.05	1 (5%)	24,25,25	0.80	0
16	PGV	L	1007	-	50,50,50	0.49	0	53,56,56	0.49	0
9	BCL	B	103	-	69,74,74	1.84	21 (30%)	79,115,115	2.42	26 (32%)
11	U4Z	A	102	-	40,40,40	1.45	9 (22%)	51,51,51	1.67	14 (27%)
13	BGL	H	107	-	20,20,20	1.05	1 (5%)	24,25,25	0.80	0

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
11	U4Z	S	104	-	-	3/36/53/53	0/1/1/1
10	U42	4	101	-	-	12/61/98/98	0/2/2/2
9	BCL	S	103	-	-	24/41/137/137	-
10	U42	G	101	-	-	14/61/98/98	0/2/2/2
19	MQE	M	704	-	-	7/65/85/85	0/2/2/2
10	U42	4	104	-	-	14/61/98/98	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BCL	V	101	-	-	16/41/137/137	-
9	BCL	E	102	-	-	21/41/137/137	-
11	U4Z	1	102	-	-	4/36/53/53	0/1/1/1
13	BGL	L	1015	-	-	8/11/31/31	0/1/1/1
10	U42	U	104	-	-	24/61/98/98	0/2/2/2
9	BCL	8	103	-	-	18/41/137/137	-
11	U4Z	7	102	-	-	2/36/53/53	0/1/1/1
9	BCL	Q	102	-	-	12/41/137/137	-
12	LMT	T	103	-	-	11/21/61/61	0/2/2/2
9	BCL	9	102	-	-	11/41/137/137	-
10	U42	0	103	-	-	13/61/98/98	0/2/2/2
14	HEC	C	403	3	-	4/14/54/54	-
9	BCL	O	102	-	-	11/41/137/137	-
13	BGL	N	103	-	-	5/11/31/31	0/1/1/1
18	BPH	L	1003	-	-	12/37/105/105	0/5/6/6
13	BGL	C	409	-	-	3/11/31/31	0/1/1/1
9	BCL	L	1002	-	-	12/41/137/137	-
9	BCL	O	103	-	-	14/41/137/137	-
16	PGV	P	103	-	-	17/47/47/55	-
13	BGL	F	104	-	-	4/11/31/31	0/1/1/1
22	LHG	h	101	-	-	11/14/14/53	-
16	PGV	P	104	-	-	20/55/55/55	-
16	PGV	L	1008	-	-	23/55/55/55	-
11	U4Z	V	102	-	-	4/36/53/53	0/1/1/1
9	BCL	R	101	-	-	15/41/137/137	-
10	U42	E	101	-	-	23/61/98/98	0/2/2/2
11	U4Z	T	102	-	-	4/36/53/53	0/1/1/1
9	BCL	0	102	-	-	16/41/137/137	-
16	PGV	L	1006	-	-	20/55/55/55	-
9	BCL	D	101	-	-	12/41/137/137	-
9	BCL	U	103	-	-	21/41/137/137	-
11	U4Z	H	102	-	-	2/36/53/53	0/1/1/1
14	HEC	C	402	3	-	8/14/54/54	-
9	BCL	1	101	-	-	16/41/137/137	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BCL	7	101	-	-	17/41/137/137	-
12	LMT	D	105	-	-	5/21/61/61	0/2/2/2
9	BCL	2	102	-	-	21/41/137/137	-
11	U4Z	P	102	-	-	4/36/53/53	0/1/1/1
13	BGL	H	103	-	-	0/11/31/31	0/1/1/1
13	BGL	L	1013	-	-	4/11/31/31	0/1/1/1
9	BCL	2	101	-	-	16/41/137/137	-
9	BCL	T	101	-	-	10/41/137/137	-
12	LMT	1	103	-	-	4/21/61/61	0/2/2/2
9	BCL	4	103	-	-	16/41/137/137	-
9	BCL	H	101	-	-	13/41/137/137	-
9	BCL	W	101	-	-	15/41/137/137	-
9	BCL	N	101	-	-	18/41/137/137	-
9	BCL	A	101	-	-	9/41/137/137	-
9	BCL	F	102	-	-	18/41/137/137	-
9	BCL	K	102	-	-	14/41/137/137	-
20	PEF	L	1017	-	-	7/44/44/50	-
16	PGV	M	706	-	-	20/55/55/55	-
9	BCL	S	102	-	-	16/41/137/137	-
9	BCL	D	102	-	-	18/41/137/137	-
9	BCL	M	701	-	-	25/41/137/137	-
10	U42	S	101	-	-	23/61/98/98	0/2/2/2
10	U42	8	101	-	-	14/61/98/98	0/2/2/2
9	BCL	P	101	-	-	13/41/137/137	-
13	BGL	C	410	-	-	3/11/31/31	0/1/1/1
11	U4Z	5	102	-	-	4/36/53/53	0/1/1/1
11	U4Z	J	102	-	-	4/36/53/53	0/1/1/1
9	BCL	W	102	-	-	18/41/137/137	-
11	U4Z	C	401	-	-	14/36/53/53	0/1/1/1
9	BCL	Q	103	-	-	18/41/137/137	-
16	PGV	C	407	-	-	16/45/45/55	-
9	BCL	4	102	-	-	13/41/137/137	-
9	BCL	J	101	-	-	13/41/137/137	-
10	U42	O	101	-	-	23/61/98/98	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	PGV	C	408	15	-	25/55/55/55	-
10	U42	U	101	-	-	21/61/98/98	0/2/2/2
9	BCL	L	1001	-	-	15/41/137/137	-
13	BGL	Y	101	-	-	6/11/31/31	0/1/1/1
19	MQE	L	1004	-	-	16/47/67/85	0/2/2/2
9	BCL	I	103	-	-	23/41/137/137	-
13	BGL	L	1011	-	-	4/11/31/31	0/1/1/1
10	U42	Q	101	-	-	20/61/98/98	0/2/2/2
9	BCL	8	102	-	-	13/41/137/137	-
11	U4Z	N	102	-	-	2/36/53/53	0/1/1/1
9	BCL	3	101	-	-	15/41/137/137	-
9	BCL	5	101	-	-	13/41/137/137	-
18	BPH	M	702	-	-	17/37/105/105	0/5/6/6
16	PGV	M	705	-	-	30/55/55/55	-
9	BCL	K	101	-	-	12/41/137/137	-
9	BCL	G	102	-	-	22/41/137/137	-
10	U42	I	104	-	-	12/61/98/98	0/2/2/2
14	HEC	C	404	3	-	6/14/54/54	-
11	U4Z	9	101	-	-	2/36/53/53	0/1/1/1
9	BCL	I	102	-	-	13/41/137/137	-
9	BCL	6	102	-	-	18/41/137/137	-
9	BCL	U	102	-	-	10/41/137/137	-
10	U42	I	101	-	-	19/61/98/98	0/2/2/2
13	BGL	D	104	-	-	2/11/31/31	0/1/1/1
9	BCL	6	101	-	-	11/41/137/137	-
10	U42	B	101	-	-	15/61/98/98	0/2/2/2
9	BCL	F	101	-	-	17/41/137/137	-
11	U4Z	F	103	-	-	4/36/53/53	0/1/1/1
14	HEC	C	405	3	-	4/14/54/54	-
9	BCL	0	101	-	-	11/41/137/137	-
11	U4Z	3	102	-	-	4/36/53/53	0/1/1/1
13	BGL	L	1012	-	-	4/11/31/31	0/1/1/1
18	BPH	L	1005	-	-	17/37/105/105	0/5/6/6
9	BCL	B	102	-	-	9/41/137/137	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	U4Z	D	103	-	-	4/36/53/53	0/1/1/1
13	BGL	3	103	-	-	4/11/31/31	0/1/1/1
16	PGV	L	1007	-	-	18/55/55/55	-
9	BCL	B	103	-	-	23/41/137/137	-
11	U4Z	A	102	-	-	4/36/53/53	0/1/1/1
13	BGL	H	107	-	-	5/11/31/31	0/1/1/1

All (1337) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	L	1003	BPH	C1B-C2B	8.61	1.49	1.39
18	L	1003	BPH	C1D-C2D	8.23	1.48	1.39
10	O	103	U42	CBO-CBL	-7.89	1.34	1.50
10	8	101	U42	CBK-CBH	-7.29	1.36	1.50
10	O	101	U42	CBF-CBH	-7.19	1.30	1.46
10	O	103	U42	CBK-CBH	-6.57	1.37	1.50
10	O	101	U42	CAN-CAM	-6.37	1.38	1.50
14	C	404	HEC	CAC-C3C	6.35	1.55	1.35
14	C	405	HEC	CAC-C3C	6.33	1.55	1.35
14	C	403	HEC	CAC-C3C	6.31	1.55	1.35
14	C	402	HEC	CAC-C3C	6.30	1.55	1.35
14	C	405	HEC	CAB-C3B	6.27	1.55	1.35
14	C	403	HEC	CAB-C3B	6.23	1.55	1.35
18	L	1003	BPH	C3B-C2B	6.15	1.50	1.39
10	I	101	U42	CBN-CBL	-6.15	1.32	1.46
14	C	402	HEC	CAB-C3B	6.15	1.55	1.35
10	E	101	U42	CBF-CBH	-6.13	1.32	1.46
14	C	404	HEC	CAB-C3B	6.11	1.54	1.35
18	L	1003	BPH	C4D-CHA	5.87	1.48	1.39
10	O	101	U42	CBK-CBH	-5.86	1.39	1.50
14	C	405	HEC	C3D-C2D	5.74	1.53	1.38
10	I	101	U42	CBK-CBH	-5.72	1.39	1.50
10	I	101	U42	CBO-CBL	-5.64	1.39	1.50
14	C	403	HEC	C3D-C2D	5.62	1.53	1.38
14	C	404	HEC	C3D-C2D	5.61	1.53	1.38
14	C	402	HEC	C3D-C2D	5.56	1.53	1.38
10	O	103	U42	CBN-CBL	-5.53	1.34	1.46
10	U	101	U42	CBK-CBH	-5.47	1.39	1.50
10	Q	101	U42	CBK-CBH	-5.45	1.39	1.50
10	I	101	U42	CBF-CBH	-5.42	1.34	1.46
10	S	101	U42	CBK-CBH	-5.41	1.39	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	L	1003	BPH	C3D-C2D	5.41	1.48	1.39
10	8	101	U42	CBF-CBH	-5.38	1.34	1.46
18	L	1003	BPH	C3B-C4B	5.37	1.50	1.41
10	G	101	U42	CBF-CBH	-5.34	1.34	1.46
10	8	101	U42	CBN-CBL	-5.24	1.34	1.46
9	M	701	BCL	O2D-CGD	5.18	1.46	1.33
9	6	102	BCL	C3D-C4D	-5.17	1.32	1.44
9	8	103	BCL	C3D-C4D	-5.14	1.32	1.44
9	I	103	BCL	C3D-C4D	-5.10	1.32	1.44
10	E	101	U42	CBK-CBH	-5.10	1.40	1.50
9	Q	103	BCL	C3D-C4D	-5.07	1.32	1.44
10	U	104	U42	CAC-CAE	-5.06	1.40	1.52
9	E	102	BCL	C3D-C4D	-5.02	1.32	1.44
9	0	102	BCL	O2D-CGD	5.02	1.45	1.33
9	U	103	BCL	C3D-C4D	-5.01	1.32	1.44
10	U	104	U42	CBK-CBH	-5.00	1.40	1.50
9	2	102	BCL	C3D-C4D	-4.98	1.33	1.44
9	G	102	BCL	C3D-C4D	-4.98	1.33	1.44
9	B	103	BCL	C3D-C4D	-4.98	1.33	1.44
9	V	101	BCL	O2D-CGD	4.97	1.45	1.33
9	W	102	BCL	C3D-C4D	-4.97	1.33	1.44
9	O	103	BCL	C3D-C4D	-4.97	1.33	1.44
9	2	101	BCL	O2D-CGD	4.97	1.45	1.33
9	L	1002	BCL	O2D-CGD	4.95	1.45	1.33
9	6	101	BCL	O2D-CGD	4.94	1.45	1.33
9	W	101	BCL	O2D-CGD	4.94	1.45	1.33
10	4	104	U42	CAN-CAM	-4.93	1.40	1.50
10	U	104	U42	CBF-CBH	-4.93	1.35	1.46
9	4	102	BCL	O2D-CGD	4.93	1.45	1.33
9	4	103	BCL	C3D-C4D	-4.93	1.33	1.44
10	O	101	U42	CAV-CAR	4.89	1.47	1.35
9	V	101	BCL	C3D-C4D	-4.88	1.33	1.44
9	0	102	BCL	C3D-C4D	-4.88	1.33	1.44
9	K	101	BCL	O2D-CGD	4.87	1.45	1.33
9	5	101	BCL	O2D-CGD	4.87	1.45	1.33
9	R	101	BCL	O2D-CGD	4.87	1.45	1.33
9	Q	102	BCL	O2D-CGD	4.87	1.45	1.33
9	L	1001	BCL	C3D-C4D	-4.86	1.33	1.44
10	0	103	U42	CBF-CBH	-4.86	1.35	1.46
9	K	102	BCL	C3D-C4D	-4.86	1.33	1.44
9	S	102	BCL	O2D-CGD	4.85	1.45	1.33
9	K	102	BCL	O2D-CGD	4.85	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	F	102	BCL	O2D-CGD	4.84	1.45	1.33
9	A	101	BCL	O2D-CGD	4.84	1.45	1.33
9	S	103	BCL	C3D-C4D	-4.83	1.33	1.44
9	P	101	BCL	O2D-CGD	4.83	1.45	1.33
9	8	102	BCL	O2D-CGD	4.83	1.45	1.33
9	F	101	BCL	O2D-CGD	4.82	1.45	1.33
9	U	102	BCL	O2D-CGD	4.82	1.45	1.33
9	T	101	BCL	O2D-CGD	4.81	1.45	1.33
9	D	102	BCL	O2D-CGD	4.81	1.45	1.33
9	B	103	BCL	O2D-CGD	4.80	1.45	1.33
9	O	102	BCL	O2D-CGD	4.80	1.45	1.33
9	R	101	BCL	C3D-C4D	-4.80	1.33	1.44
9	3	101	BCL	O2D-CGD	4.79	1.45	1.33
9	D	101	BCL	O2D-CGD	4.79	1.45	1.33
9	N	101	BCL	O2D-CGD	4.79	1.45	1.33
9	J	101	BCL	C3D-C4D	-4.79	1.33	1.44
9	9	102	BCL	O2D-CGD	4.78	1.45	1.33
9	L	1002	BCL	C3D-C4D	-4.77	1.33	1.44
9	4	103	BCL	O2D-CGD	4.77	1.45	1.33
9	7	101	BCL	O2D-CGD	4.77	1.45	1.33
9	M	701	BCL	C3D-C4D	-4.76	1.33	1.44
9	B	102	BCL	O2D-CGD	4.74	1.44	1.33
9	7	101	BCL	C3D-C4D	-4.74	1.33	1.44
10	Q	101	U42	CAN-CAM	-4.74	1.41	1.50
9	J	101	BCL	O2D-CGD	4.74	1.44	1.33
9	E	102	BCL	O2D-CGD	4.74	1.44	1.33
9	3	101	BCL	C3D-C4D	-4.73	1.33	1.44
9	9	102	BCL	C3D-C4D	-4.73	1.33	1.44
9	0	101	BCL	O2D-CGD	4.73	1.44	1.33
9	6	102	BCL	O2D-CGD	4.72	1.44	1.33
9	I	103	BCL	O2D-CGD	4.71	1.44	1.33
9	W	101	BCL	C3D-C4D	-4.70	1.33	1.44
9	2	101	BCL	C3D-C4D	-4.70	1.33	1.44
9	D	101	BCL	C3D-C4D	-4.70	1.33	1.44
9	H	101	BCL	O2D-CGD	4.69	1.44	1.33
9	H	101	BCL	C3D-C4D	-4.69	1.33	1.44
10	4	101	U42	CBN-CBL	-4.68	1.35	1.46
9	F	101	BCL	C3D-C4D	-4.68	1.33	1.44
9	K	101	BCL	C3D-C4D	-4.68	1.33	1.44
9	0	102	BCL	C3B-C4B	4.68	1.50	1.41
9	F	102	BCL	C3D-C4D	-4.68	1.33	1.44
9	W	102	BCL	O2D-CGD	4.68	1.44	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	Q	101	U42	CBF-CBH	-4.67	1.35	1.46
9	5	101	BCL	C3D-C4D	-4.67	1.33	1.44
9	0	101	BCL	C3D-C4D	-4.67	1.33	1.44
9	T	101	BCL	C3D-C4D	-4.67	1.33	1.44
9	D	102	BCL	C3D-C4D	-4.67	1.33	1.44
9	Q	103	BCL	O2D-CGD	4.66	1.44	1.33
18	L	1003	BPH	OBD-CAD	4.66	1.28	1.22
18	L	1003	BPH	O2D-CGD	4.65	1.44	1.33
9	L	1002	BCL	C3B-C4B	4.65	1.50	1.41
9	I	102	BCL	C3D-C4D	-4.65	1.33	1.44
9	N	101	BCL	C3D-C4D	-4.65	1.33	1.44
9	6	101	BCL	C3D-C4D	-4.64	1.33	1.44
9	8	102	BCL	C3D-C4D	-4.64	1.33	1.44
10	U	104	U42	CBO-CBL	-4.63	1.41	1.50
9	2	102	BCL	O2D-CGD	4.63	1.44	1.33
10	4	101	U42	CBK-CBH	-4.62	1.41	1.50
9	8	103	BCL	O2D-CGD	4.62	1.44	1.33
9	4	102	BCL	C3D-C4D	-4.61	1.33	1.44
9	L	1002	BCL	O2A-CGA	4.61	1.46	1.33
9	U	102	BCL	C3D-C4D	-4.61	1.33	1.44
9	S	102	BCL	C3D-C4D	-4.61	1.33	1.44
9	Q	102	BCL	C3D-C4D	-4.61	1.33	1.44
9	L	1001	BCL	C3B-C4B	4.61	1.50	1.41
9	B	102	BCL	C3D-C4D	-4.61	1.33	1.44
10	E	101	U42	CAV-CAR	4.60	1.46	1.35
9	U	103	BCL	O2D-CGD	4.58	1.44	1.33
10	B	101	U42	CBK-CBH	-4.58	1.41	1.50
9	S	103	BCL	O2D-CGD	4.57	1.44	1.33
9	G	102	BCL	O2D-CGD	4.57	1.44	1.33
9	1	101	BCL	O2D-CGD	4.56	1.44	1.33
9	O	102	BCL	C3D-C4D	-4.56	1.33	1.44
9	B	103	BCL	C3B-C4B	4.55	1.50	1.41
9	4	103	BCL	C3B-C4B	4.54	1.50	1.41
9	1	101	BCL	C3D-C4D	-4.53	1.34	1.44
9	I	102	BCL	O2D-CGD	4.53	1.44	1.33
9	O	103	BCL	O2D-CGD	4.53	1.44	1.33
9	0	101	BCL	C3B-C4B	4.52	1.50	1.41
9	6	101	BCL	C3B-C4B	4.52	1.50	1.41
9	Q	103	BCL	C3B-C4B	4.51	1.50	1.41
10	S	101	U42	CBO-CBL	-4.50	1.41	1.50
9	Q	102	BCL	C3B-C4B	4.49	1.50	1.41
9	S	103	BCL	C3B-C4B	4.49	1.50	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	Q	101	U42	CAU-CAR	-4.49	1.41	1.50
9	U	102	BCL	C3B-C4B	4.48	1.50	1.41
10	E	101	U42	CBI-CBL	4.48	1.46	1.35
10	G	101	U42	CBO-CBL	-4.46	1.41	1.50
9	B	102	BCL	C3B-C4B	4.45	1.49	1.41
9	Q	103	BCL	O2A-CGA	4.43	1.46	1.33
9	M	701	BCL	C3B-C4B	4.42	1.49	1.41
9	F	102	BCL	C3B-C4B	4.42	1.49	1.41
9	P	101	BCL	C3B-C4B	4.42	1.49	1.41
9	A	101	BCL	C3B-C4B	4.41	1.49	1.41
9	W	101	BCL	C3B-C4B	4.41	1.49	1.41
10	O	101	U42	CBN-CBL	-4.41	1.36	1.46
9	S	102	BCL	C3B-C4B	4.40	1.49	1.41
9	J	101	BCL	C3B-C4B	4.40	1.49	1.41
9	D	102	BCL	C3B-C4B	4.39	1.49	1.41
9	E	102	BCL	C3B-C4B	4.39	1.49	1.41
9	W	102	BCL	C3B-C4B	4.39	1.49	1.41
10	G	101	U42	CAN-CAM	-4.38	1.42	1.50
9	4	103	BCL	O2A-CGA	4.38	1.46	1.33
9	O	103	BCL	O2A-CGA	4.38	1.46	1.33
10	I	101	U42	CAN-CAM	-4.37	1.42	1.50
9	L	1001	BCL	O2A-CGA	4.36	1.46	1.33
10	B	101	U42	CAN-CAM	-4.36	1.42	1.50
9	K	101	BCL	O2A-CGA	4.35	1.46	1.33
9	K	101	BCL	C3B-C4B	4.34	1.49	1.41
9	G	102	BCL	O2A-CGA	4.33	1.46	1.33
9	F	101	BCL	C3B-C4B	4.33	1.49	1.41
9	2	101	BCL	C3B-C4B	4.33	1.49	1.41
10	S	101	U42	CAN-CAM	-4.32	1.42	1.50
9	I	103	BCL	C3B-C4B	4.31	1.49	1.41
9	M	701	BCL	O2A-CGA	4.29	1.45	1.33
9	D	101	BCL	C3B-C4B	4.29	1.49	1.41
9	2	102	BCL	O2A-CGA	4.28	1.45	1.33
9	4	102	BCL	C3B-C4B	4.28	1.49	1.41
9	K	102	BCL	C3B-C4B	4.28	1.49	1.41
9	A	101	BCL	CHD-C1D	4.27	1.46	1.38
10	4	101	U42	CBO-CBL	-4.27	1.42	1.50
20	L	1017	PEF	O3-C30	4.26	1.45	1.33
9	U	102	BCL	O2A-CGA	4.25	1.45	1.33
9	H	101	BCL	C3B-C4B	4.25	1.49	1.41
10	U	101	U42	CAN-CAM	-4.25	1.42	1.50
9	K	102	BCL	O2A-CGA	4.24	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	h	101	LHG	O7-C7	-4.24	1.20	1.42
9	P	101	BCL	C1D-ND	-4.24	1.32	1.37
9	2	101	BCL	O2A-CGA	4.24	1.45	1.33
9	U	103	BCL	C3B-C4B	4.23	1.49	1.41
9	I	102	BCL	C3B-C4B	4.23	1.49	1.41
10	I	104	U42	CBO-CBL	-4.22	1.42	1.50
10	0	103	U42	CAP-CAQ	4.22	1.45	1.34
10	4	101	U42	CBF-CBH	-4.22	1.36	1.46
9	V	101	BCL	O2A-CGA	4.22	1.45	1.33
9	W	102	BCL	O2A-CGA	4.22	1.45	1.33
9	8	103	BCL	C3B-C4B	4.20	1.49	1.41
9	D	102	BCL	O2A-CGA	4.20	1.45	1.33
9	O	102	BCL	C3B-C4B	4.19	1.49	1.41
9	8	102	BCL	C3B-C4B	4.19	1.49	1.41
9	S	103	BCL	O2A-CGA	4.18	1.45	1.33
9	E	102	BCL	O2A-CGA	4.17	1.45	1.33
9	L	1001	BCL	O2D-CGD	4.17	1.43	1.33
9	1	101	BCL	C3B-C4B	4.17	1.49	1.41
9	8	102	BCL	O2A-CGA	4.16	1.45	1.33
9	1	101	BCL	O2A-CGA	4.14	1.45	1.33
9	6	102	BCL	O2A-CGA	4.14	1.45	1.33
9	N	101	BCL	O2A-CGA	4.14	1.45	1.33
9	3	101	BCL	C3B-C4B	4.13	1.49	1.41
9	F	102	BCL	O2A-CGA	4.13	1.45	1.33
9	0	101	BCL	O2A-CGA	4.13	1.45	1.33
10	G	101	U42	CAC-CAE	-4.13	1.42	1.52
9	B	103	BCL	O2A-CGA	4.12	1.45	1.33
9	B	102	BCL	O2A-CGA	4.12	1.45	1.33
9	U	103	BCL	O2A-CGA	4.12	1.45	1.33
20	L	1017	PEF	O2-C10	4.11	1.45	1.34
9	Q	102	BCL	O2A-CGA	4.11	1.45	1.33
9	G	102	BCL	C3B-C4B	4.11	1.49	1.41
18	L	1003	BPH	O2A-CGA	4.10	1.45	1.33
9	A	101	BCL	O2A-CGA	4.10	1.45	1.33
9	6	101	BCL	O2A-CGA	4.10	1.45	1.33
10	I	101	U42	CAU-CAR	-4.10	1.42	1.50
9	H	101	BCL	O2A-CGA	4.10	1.45	1.33
9	4	102	BCL	O2A-CGA	4.10	1.45	1.33
9	P	101	BCL	CHD-C1D	4.09	1.46	1.38
9	I	103	BCL	O2A-CGA	4.09	1.45	1.33
9	7	101	BCL	C3B-C4B	4.09	1.49	1.41
9	D	101	BCL	O2A-CGA	4.09	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	9	102	BCL	C3B-C4B	4.08	1.49	1.41
9	P	101	BCL	O2A-CGA	4.08	1.45	1.33
9	F	101	BCL	O2A-CGA	4.07	1.45	1.33
9	R	101	BCL	O2A-CGA	4.07	1.45	1.33
9	O	103	BCL	C3B-C4B	4.07	1.49	1.41
9	I	102	BCL	O2A-CGA	4.07	1.45	1.33
9	6	102	BCL	C3B-C4B	4.06	1.49	1.41
10	B	101	U42	CBO-CBL	-4.06	1.42	1.50
10	S	101	U42	CAV-CAR	4.06	1.45	1.35
9	N	101	BCL	C3B-C4B	4.06	1.49	1.41
10	S	101	U42	CBF-CBH	-4.06	1.37	1.46
9	O	102	BCL	O2A-CGA	4.05	1.45	1.33
10	4	104	U42	CBF-CBH	-4.03	1.37	1.46
9	9	102	BCL	O2A-CGA	4.02	1.45	1.33
9	5	101	BCL	O2A-CGA	4.02	1.45	1.33
9	7	101	BCL	O2A-CGA	4.01	1.45	1.33
9	0	102	BCL	O2A-CGA	4.01	1.45	1.33
9	T	101	BCL	O2A-CGA	4.00	1.45	1.33
10	B	101	U42	CBF-CBH	-4.00	1.37	1.46
10	G	101	U42	CBN-CBL	-4.00	1.37	1.46
10	4	104	U42	CBK-CBH	-3.97	1.42	1.50
10	S	101	U42	CAL-CAM	-3.96	1.37	1.46
9	J	101	BCL	O2A-CGA	3.95	1.44	1.33
9	0	101	BCL	C1D-ND	-3.95	1.32	1.37
9	2	102	BCL	CHB-C1B	3.94	1.48	1.39
10	Q	101	U42	CAL-CAM	-3.94	1.37	1.46
10	U	101	U42	CBF-CBH	-3.94	1.37	1.46
10	B	101	U42	CBI-CBL	3.94	1.44	1.35
9	3	101	BCL	O2A-CGA	3.93	1.44	1.33
9	F	102	BCL	C1D-ND	-3.92	1.32	1.37
9	P	101	BCL	CHC-C4B	3.91	1.48	1.39
9	S	102	BCL	O2A-CGA	3.91	1.44	1.33
10	0	103	U42	CAN-CAM	-3.90	1.42	1.50
9	5	101	BCL	C3B-C4B	3.90	1.48	1.41
10	0	103	U42	CAX-CAY	3.89	1.58	1.53
9	4	102	BCL	C1D-ND	-3.89	1.32	1.37
10	B	101	U42	CAU-CAR	-3.89	1.43	1.50
9	2	101	BCL	C1D-ND	-3.88	1.32	1.37
10	0	103	U42	CAC-CAE	-3.87	1.43	1.52
10	U	101	U42	CBO-CBL	-3.87	1.43	1.50
9	R	101	BCL	C3B-C4B	3.87	1.48	1.41
9	A	101	BCL	C1D-ND	-3.86	1.32	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	101	BCL	CHC-C4B	3.85	1.48	1.39
10	O	101	U42	CBO-CBL	-3.83	1.43	1.50
9	8	102	BCL	C1D-ND	-3.83	1.32	1.37
9	8	103	BCL	O2A-CGA	3.82	1.44	1.33
10	Q	101	U42	CAC-CAE	-3.82	1.43	1.52
9	W	101	BCL	O2A-CGA	3.81	1.44	1.33
9	V	101	BCL	C3B-C4B	3.80	1.48	1.41
10	I	104	U42	CBI-CBL	3.80	1.44	1.35
9	D	102	BCL	C1D-ND	-3.79	1.32	1.37
11	C	401	U4Z	CBO-CBL	-3.77	1.43	1.50
10	O	101	U42	CBI-CBL	3.75	1.44	1.35
10	4	101	U42	C7-C8	-3.74	1.45	1.53
9	6	102	BCL	C4B-NB	-3.73	1.33	1.37
9	O	102	BCL	C1D-ND	-3.72	1.33	1.37
9	T	101	BCL	C3B-C4B	3.71	1.48	1.41
9	I	102	BCL	C1D-ND	-3.70	1.33	1.37
10	8	101	U42	CBO-CBL	-3.70	1.43	1.50
9	K	101	BCL	C1D-ND	-3.68	1.33	1.37
10	I	104	U42	CAN-CAM	-3.68	1.43	1.50
9	U	102	BCL	C1D-ND	-3.67	1.33	1.37
10	O	101	U42	CAL-CAM	-3.66	1.38	1.46
9	A	101	BCL	CHB-C1B	3.65	1.47	1.39
9	P	101	BCL	CHB-C1B	3.65	1.47	1.39
10	E	101	U42	C27-C26	-3.65	1.33	1.51
10	0	103	U42	CAO-CAM	3.64	1.44	1.35
10	Q	101	U42	CBO-CBL	-3.64	1.43	1.50
10	U	104	U42	CAV-CAR	3.64	1.44	1.35
9	P	101	BCL	C3D-C2D	3.64	1.48	1.39
10	0	103	U42	CAV-CAR	3.63	1.44	1.35
10	8	101	U42	CAV-CAR	3.63	1.44	1.35
9	8	103	BCL	CHB-C4A	-3.61	1.28	1.37
9	B	102	BCL	C1D-ND	-3.60	1.33	1.37
9	Q	102	BCL	C1D-ND	-3.60	1.33	1.37
10	S	101	U42	CBI-CBL	3.59	1.44	1.35
9	W	101	BCL	C1D-ND	-3.59	1.33	1.37
9	6	101	BCL	C1D-ND	-3.59	1.33	1.37
10	E	101	U42	CAC-CAE	-3.58	1.44	1.52
9	K	102	BCL	CHB-C1B	3.58	1.47	1.39
9	S	102	BCL	C1D-ND	-3.57	1.33	1.37
10	I	101	U42	CAC-CAE	-3.56	1.44	1.52
10	S	101	U42	CAU-CAR	-3.55	1.43	1.50
9	L	1002	BCL	CHC-C4B	3.54	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	101	BCL	C3D-C2D	3.54	1.48	1.39
10	O	101	U42	CAC-CAE	-3.54	1.44	1.52
10	I	104	U42	CBK-CBH	-3.54	1.43	1.50
10	Q	101	U42	CBN-CBL	-3.53	1.38	1.46
10	4	101	U42	CAV-CAR	3.53	1.44	1.35
10	4	104	U42	CAU-CAR	-3.51	1.43	1.50
9	4	103	BCL	C1B-NB	-3.47	1.33	1.37
9	S	102	BCL	CHC-C4B	3.47	1.47	1.39
9	U	103	BCL	CHB-C1B	3.46	1.47	1.39
10	G	101	U42	CBK-CBH	-3.45	1.43	1.50
9	7	101	BCL	C4B-NB	-3.45	1.33	1.37
9	O	103	BCL	C4B-NB	-3.45	1.33	1.37
9	P	101	BCL	OBD-CAD	3.44	1.28	1.22
9	A	101	BCL	OBD-CAD	3.44	1.28	1.22
9	6	101	BCL	CHC-C4B	3.44	1.47	1.39
9	2	102	BCL	C4B-NB	-3.43	1.33	1.37
9	P	101	BCL	C4B-NB	-3.42	1.33	1.37
9	U	102	BCL	CHC-C4B	3.40	1.47	1.39
10	4	104	U42	CBO-CBL	-3.40	1.44	1.50
9	A	101	BCL	C4B-NB	-3.40	1.33	1.37
9	S	103	BCL	C1B-NB	-3.39	1.33	1.37
10	U	101	U42	CAU-CAR	-3.39	1.44	1.50
11	V	102	U4Z	CAH-CAD	3.39	1.40	1.34
9	A	101	BCL	C1B-NB	-3.39	1.33	1.37
9	P	101	BCL	C1B-NB	-3.39	1.33	1.37
9	0	101	BCL	CHC-C4B	3.38	1.47	1.39
10	S	101	U42	CAC-CAE	-3.38	1.44	1.52
9	L	1001	BCL	CHD-C1D	3.37	1.45	1.38
10	I	104	U42	CBF-CBH	-3.36	1.38	1.46
9	W	102	BCL	CHB-C1B	3.36	1.47	1.39
10	I	101	U42	C27-C26	-3.36	1.35	1.51
9	L	1001	BCL	CHC-C4B	3.36	1.47	1.39
9	O	102	BCL	CHB-C1B	3.35	1.46	1.39
9	T	101	BCL	CHB-C1B	3.35	1.46	1.39
9	W	101	BCL	CHC-C4B	3.34	1.46	1.39
10	U	101	U42	CAC-CAE	-3.34	1.44	1.52
10	U	104	U42	CBI-CBL	3.33	1.43	1.35
10	E	101	U42	CAN-CAM	-3.33	1.44	1.50
9	2	101	BCL	CHB-C1B	3.33	1.46	1.39
9	F	102	BCL	OBD-CAD	3.32	1.28	1.22
9	H	101	BCL	CHB-C1B	3.32	1.46	1.39
9	T	101	BCL	C4B-NB	-3.31	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	6	102	BCL	C1B-NB	-3.31	1.33	1.37
10	B	101	U42	CAL-CAM	-3.31	1.38	1.46
9	Q	103	BCL	CHB-C1B	3.31	1.46	1.39
9	0	102	BCL	OBD-CAD	3.30	1.28	1.22
10	4	104	U42	CBN-CBL	-3.30	1.38	1.46
9	M	701	BCL	CHB-C1B	3.30	1.46	1.39
18	L	1005	BPH	C4D-CHA	3.30	1.44	1.39
11	F	103	U4Z	CAH-CAD	3.30	1.40	1.34
9	Q	103	BCL	C4B-NB	-3.29	1.33	1.37
9	8	103	BCL	CHB-C1B	3.29	1.46	1.39
9	V	101	BCL	CHC-C4B	3.29	1.46	1.39
9	4	102	BCL	OBD-CAD	3.29	1.28	1.22
9	R	101	BCL	C1D-ND	-3.28	1.33	1.37
18	L	1003	BPH	CHA-CBD	-3.28	1.47	1.51
11	N	102	U4Z	CAH-CAD	3.28	1.40	1.34
9	0	101	BCL	CHB-C1B	3.28	1.46	1.39
9	M	701	BCL	C1D-ND	-3.27	1.33	1.37
9	5	101	BCL	C4B-NB	-3.27	1.33	1.37
10	U	101	U42	CBN-CBL	-3.27	1.39	1.46
9	K	102	BCL	C4B-NB	-3.26	1.33	1.37
9	4	102	BCL	CHC-C4B	3.25	1.46	1.39
9	B	102	BCL	C3D-C2D	3.25	1.47	1.39
11	3	102	U4Z	CAH-CAD	3.25	1.40	1.34
10	I	101	U42	C20-C19	-3.25	1.40	1.52
9	2	102	BCL	CHD-C1D	3.25	1.44	1.38
9	B	102	BCL	CHC-C4B	3.24	1.46	1.39
9	I	103	BCL	CHB-C1B	3.24	1.46	1.39
9	F	102	BCL	CHC-C4B	3.24	1.46	1.39
9	I	102	BCL	CHC-C4B	3.24	1.46	1.39
9	V	101	BCL	CHD-C1D	3.24	1.44	1.38
9	3	101	BCL	CHD-C1D	3.24	1.44	1.38
9	R	101	BCL	C4B-NB	-3.23	1.33	1.37
9	0	102	BCL	C1B-NB	-3.23	1.33	1.37
9	D	102	BCL	C3D-C2D	3.23	1.47	1.39
9	K	101	BCL	OBD-CAD	3.23	1.28	1.22
13	L	1011	BGL	O5-C1	3.23	1.50	1.42
10	U	101	U42	CBI-CBL	3.23	1.43	1.35
10	I	104	U42	CAU-CAR	-3.23	1.44	1.50
9	D	102	BCL	CHC-C4B	3.22	1.46	1.39
9	O	103	BCL	CHB-C1B	3.22	1.46	1.39
9	G	102	BCL	CHD-C1D	3.22	1.44	1.38
9	R	101	BCL	CHB-C1B	3.22	1.46	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	8	102	BCL	CHC-C4B	3.21	1.46	1.39
9	8	102	BCL	CHB-C1B	3.21	1.46	1.39
9	Q	102	BCL	CHC-C4B	3.21	1.46	1.39
9	7	101	BCL	CHD-C1D	3.21	1.44	1.38
9	B	103	BCL	C4B-NB	-3.21	1.33	1.37
9	3	101	BCL	C4B-NB	-3.20	1.33	1.37
9	8	103	BCL	CHD-C1D	3.20	1.44	1.38
9	D	101	BCL	CHB-C1B	3.20	1.46	1.39
9	4	102	BCL	C1B-NB	-3.20	1.33	1.37
9	4	103	BCL	C4B-NB	-3.20	1.33	1.37
9	E	102	BCL	CHC-C4B	3.19	1.46	1.39
9	5	101	BCL	OBD-CAD	3.19	1.28	1.22
9	L	1002	BCL	CHD-C1D	3.19	1.44	1.38
9	W	101	BCL	CHB-C1B	3.18	1.46	1.39
11	S	104	U4Z	CAH-CAD	3.18	1.39	1.34
9	D	101	BCL	C1D-ND	-3.18	1.33	1.37
9	5	101	BCL	CHD-C1D	3.18	1.44	1.38
9	4	102	BCL	CHB-C1B	3.18	1.46	1.39
9	Q	102	BCL	OBD-CAD	3.18	1.28	1.22
9	S	102	BCL	OBD-CAD	3.17	1.27	1.22
10	0	103	U42	CBG-CBB	3.17	1.44	1.36
11	J	102	U4Z	CAH-CAD	3.17	1.39	1.34
9	L	1001	BCL	CHB-C1B	3.17	1.46	1.39
9	N	101	BCL	CHB-C1B	3.17	1.46	1.39
10	I	104	U42	C20-C19	-3.16	1.40	1.52
9	K	101	BCL	CHB-C1B	3.16	1.46	1.39
10	O	101	U42	CAQ-CAR	-3.16	1.39	1.46
9	K	101	BCL	CHC-C4B	3.16	1.46	1.39
9	D	101	BCL	CHC-C4B	3.15	1.46	1.39
9	B	103	BCL	C1B-NB	-3.15	1.33	1.37
9	I	102	BCL	OBD-CAD	3.15	1.27	1.22
10	U	104	U42	CAP-CAQ	3.15	1.42	1.34
10	U	104	U42	CBN-CBL	-3.15	1.39	1.46
9	2	101	BCL	CHC-C4B	3.15	1.46	1.39
9	B	102	BCL	CHB-C1B	3.15	1.46	1.39
11	5	102	U4Z	CAH-CAD	3.15	1.39	1.34
10	4	101	U42	CBI-CBL	3.15	1.43	1.35
9	D	102	BCL	CHB-C1B	3.15	1.46	1.39
9	1	101	BCL	OBD-CAD	3.14	1.27	1.22
9	8	103	BCL	C1B-NB	-3.14	1.33	1.37
9	8	102	BCL	C3D-C2D	3.14	1.47	1.39
9	2	101	BCL	C3D-C2D	3.14	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	E	102	BCL	CHB-C1B	3.14	1.46	1.39
9	5	101	BCL	C1D-ND	-3.14	1.33	1.37
9	G	102	BCL	C1B-NB	-3.14	1.33	1.37
9	G	102	BCL	CHB-C1B	3.14	1.46	1.39
9	6	101	BCL	OBD-CAD	3.13	1.27	1.22
9	H	101	BCL	C1D-ND	-3.13	1.33	1.37
9	K	101	BCL	C1B-NB	-3.13	1.33	1.37
9	O	102	BCL	CHC-C4B	3.13	1.46	1.39
9	H	101	BCL	OBD-CAD	3.12	1.27	1.22
9	F	101	BCL	CHB-C1B	3.12	1.46	1.39
13	3	103	BGL	O5-C1	3.12	1.50	1.42
9	5	101	BCL	C1B-NB	-3.12	1.33	1.37
9	U	102	BCL	CHB-C1B	3.12	1.46	1.39
9	I	102	BCL	C1B-NB	-3.11	1.33	1.37
9	M	701	BCL	OBD-CAD	3.11	1.27	1.22
9	9	102	BCL	CHB-C1B	3.11	1.46	1.39
9	B	102	BCL	C1B-NB	-3.11	1.33	1.37
9	N	101	BCL	C1D-ND	-3.11	1.33	1.37
9	D	101	BCL	OBD-CAD	3.11	1.27	1.22
9	0	102	BCL	C4B-NB	-3.10	1.33	1.37
11	P	102	U4Z	CAH-CAD	3.10	1.39	1.34
11	H	102	U4Z	CAH-CAD	3.10	1.39	1.34
9	F	101	BCL	OBD-CAD	3.10	1.27	1.22
9	L	1001	BCL	OBD-CAD	3.10	1.27	1.22
10	I	104	U42	CAV-CAR	3.09	1.43	1.35
13	L	1012	BGL	O5-C1	3.09	1.50	1.42
9	M	701	BCL	CHD-C1D	3.09	1.44	1.38
9	0	101	BCL	OBD-CAD	3.09	1.27	1.22
9	R	101	BCL	OBD-CAD	3.09	1.27	1.22
9	F	101	BCL	CHD-C1D	3.09	1.44	1.38
11	D	103	U4Z	CAH-CAD	3.09	1.39	1.34
9	E	102	BCL	C4B-NB	-3.09	1.33	1.37
9	M	701	BCL	CHC-C4B	3.08	1.46	1.39
10	S	101	U42	CBN-CBL	-3.08	1.39	1.46
9	N	101	BCL	OBD-CAD	3.08	1.27	1.22
9	J	101	BCL	CHC-C4B	3.08	1.46	1.39
9	F	102	BCL	CHB-C1B	3.08	1.46	1.39
9	J	101	BCL	CHD-C1D	3.08	1.44	1.38
9	J	101	BCL	C1D-ND	-3.08	1.33	1.37
9	V	101	BCL	C1D-ND	-3.08	1.33	1.37
9	6	101	BCL	C3D-C2D	3.08	1.47	1.39
9	6	101	BCL	C1B-NB	-3.07	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	T	101	BCL	CHD-C1D	3.06	1.44	1.38
9	U	102	BCL	C3D-C2D	3.06	1.47	1.39
10	E	101	U42	CBN-CBL	-3.06	1.39	1.46
9	Q	102	BCL	C3D-C2D	3.05	1.47	1.39
9	L	1001	BCL	C3D-C2D	3.05	1.47	1.39
9	1	101	BCL	C1D-ND	-3.05	1.33	1.37
9	F	102	BCL	C3D-C2D	3.05	1.47	1.39
9	7	101	BCL	C1B-NB	-3.05	1.33	1.37
9	S	102	BCL	C3D-C2D	3.05	1.47	1.39
9	I	102	BCL	CHB-C1B	3.05	1.46	1.39
9	I	103	BCL	C4B-NB	-3.05	1.33	1.37
9	6	101	BCL	CHB-C1B	3.05	1.46	1.39
9	G	102	BCL	C4B-NB	-3.05	1.33	1.37
11	1	102	U4Z	CAL-CAM	-3.05	1.39	1.46
9	K	101	BCL	C3D-C2D	3.05	1.47	1.39
9	U	103	BCL	CHC-C4B	3.04	1.46	1.39
13	C	409	BGL	O5-C1	3.04	1.50	1.42
9	I	103	BCL	CHC-C4B	3.04	1.46	1.39
9	L	1002	BCL	OBD-CAD	3.04	1.27	1.22
9	L	1002	BCL	CHB-C1B	3.04	1.46	1.39
9	E	102	BCL	CHD-C1D	3.04	1.44	1.38
9	1	101	BCL	CHD-C1D	3.04	1.44	1.38
10	Q	101	U42	CBI-CBL	3.03	1.42	1.35
9	O	102	BCL	C3D-C2D	3.03	1.47	1.39
9	W	101	BCL	C3D-C2D	3.03	1.47	1.39
9	7	101	BCL	C1D-ND	-3.03	1.33	1.37
9	S	102	BCL	C1B-NB	-3.03	1.33	1.37
9	H	101	BCL	CHC-C4B	3.03	1.46	1.39
9	O	103	BCL	C1D-ND	-3.03	1.33	1.37
9	N	101	BCL	CHC-C4B	3.02	1.46	1.39
10	O	101	U42	CAU-CAR	-3.02	1.44	1.50
9	5	101	BCL	CHB-C1B	3.02	1.46	1.39
9	S	103	BCL	C4B-NB	-3.02	1.33	1.37
9	Q	102	BCL	CHB-C1B	3.02	1.46	1.39
10	U	104	U42	CAO-CAM	3.02	1.42	1.35
9	I	102	BCL	C3D-C2D	3.02	1.47	1.39
9	F	101	BCL	CHC-C4B	3.02	1.46	1.39
9	0	101	BCL	C3D-C2D	3.02	1.47	1.39
9	O	102	BCL	OBD-CAD	3.02	1.27	1.22
9	U	102	BCL	OBD-CAD	3.02	1.27	1.22
11	T	102	U4Z	CAH-CAD	3.02	1.39	1.34
9	9	102	BCL	CHC-C4B	3.02	1.46	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	W	102	BCL	CHC-C4B	3.02	1.46	1.39
9	R	101	BCL	CHD-C1D	3.01	1.44	1.38
9	W	101	BCL	CHD-C1D	3.01	1.44	1.38
9	B	102	BCL	OBD-CAD	3.01	1.27	1.22
9	8	103	BCL	C4B-NB	-3.01	1.33	1.37
10	U	101	U42	CAV-CAR	3.01	1.42	1.35
9	2	102	BCL	C3B-C4B	3.01	1.47	1.41
10	U	101	U42	CBM-CBJ	-3.01	1.33	1.43
9	N	101	BCL	CHD-C1D	3.00	1.44	1.38
11	3	102	U4Z	CAL-CAM	-3.00	1.39	1.46
9	1	101	BCL	CHC-C4B	3.00	1.46	1.39
9	9	102	BCL	CHD-C1D	3.00	1.44	1.38
9	U	103	BCL	C4B-NB	-3.00	1.33	1.37
13	H	107	BGL	O5-C1	2.99	1.50	1.42
9	4	102	BCL	C3D-C2D	2.99	1.47	1.39
9	3	101	BCL	C1D-ND	-2.99	1.33	1.37
11	S	104	U4Z	CAL-CAM	-2.99	1.39	1.46
9	F	101	BCL	C3D-C2D	2.99	1.47	1.39
11	T	102	U4Z	CAL-CAM	-2.99	1.39	1.46
11	7	102	U4Z	CAL-CAM	-2.99	1.39	1.46
9	9	102	BCL	OBD-CAD	2.99	1.27	1.22
13	N	103	BGL	O5-C1	2.99	1.50	1.42
9	Q	103	BCL	C1B-NB	-2.98	1.33	1.37
9	3	101	BCL	C1B-NB	-2.98	1.33	1.37
9	K	101	BCL	CHD-C1D	2.98	1.44	1.38
13	Y	101	BGL	O5-C1	2.98	1.50	1.42
9	S	103	BCL	CHD-C1D	2.98	1.44	1.38
9	K	102	BCL	OBD-CAD	2.98	1.27	1.22
9	9	102	BCL	C4B-NB	-2.98	1.34	1.37
9	8	103	BCL	OBD-CAD	2.98	1.27	1.22
9	W	101	BCL	OBD-CAD	2.98	1.27	1.22
10	B	101	U42	CAV-CAR	2.98	1.42	1.35
9	F	102	BCL	C1B-NB	-2.97	1.34	1.37
9	D	102	BCL	C1B-NB	-2.97	1.34	1.37
9	W	101	BCL	C1B-NB	-2.97	1.34	1.37
10	8	101	U42	CBI-CBL	2.97	1.42	1.35
9	K	102	BCL	C1D-ND	-2.97	1.34	1.37
13	H	103	BGL	O5-C1	2.97	1.50	1.42
9	L	1001	BCL	C1B-NB	-2.97	1.34	1.37
9	7	101	BCL	C3D-C2D	2.97	1.47	1.39
9	B	103	BCL	CHD-C1D	2.97	1.44	1.38
9	H	101	BCL	C3D-C2D	2.97	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	V	101	BCL	CHB-C1B	2.97	1.46	1.39
9	1	101	BCL	CHB-C1B	2.97	1.46	1.39
9	9	102	BCL	C1D-ND	-2.96	1.34	1.37
9	V	101	BCL	C3D-C2D	2.96	1.47	1.39
9	4	103	BCL	C1D-ND	-2.96	1.34	1.37
11	1	102	U4Z	CAH-CAD	2.96	1.39	1.34
9	2	101	BCL	OBD-CAD	2.96	1.27	1.22
11	N	102	U4Z	CAL-CAM	-2.96	1.39	1.46
9	7	101	BCL	OBD-CAD	2.96	1.27	1.22
13	D	104	BGL	O5-C1	2.96	1.50	1.42
9	1	101	BCL	C1B-NB	-2.95	1.34	1.37
11	9	101	U4Z	CAL-CAM	-2.95	1.39	1.46
9	J	101	BCL	CHB-C1B	2.95	1.46	1.39
9	N	101	BCL	C3D-C2D	2.95	1.47	1.39
10	S	101	U42	C26-C25	-2.95	1.37	1.51
9	7	101	BCL	CHB-C1B	2.95	1.46	1.39
9	L	1001	BCL	C1D-ND	-2.95	1.34	1.37
9	J	101	BCL	OBD-CAD	2.95	1.27	1.22
9	K	102	BCL	CHC-C4B	2.94	1.46	1.39
9	O	102	BCL	C1B-NB	-2.94	1.34	1.37
10	I	101	U42	CBI-CBL	2.94	1.42	1.35
10	Q	101	U42	CAV-CAR	2.94	1.42	1.35
9	U	102	BCL	C1B-NB	-2.94	1.34	1.37
9	D	101	BCL	C1B-NB	-2.94	1.34	1.37
10	I	101	U42	C25-C24	-2.94	1.37	1.51
9	Q	103	BCL	CHC-C4B	2.93	1.46	1.39
9	H	101	BCL	CHD-C1D	2.93	1.44	1.38
13	C	410	BGL	O5-C1	2.93	1.50	1.42
9	8	103	BCL	C1D-ND	-2.93	1.34	1.37
13	F	104	BGL	O5-C1	2.93	1.50	1.42
11	J	102	U4Z	CAL-CAM	-2.93	1.39	1.46
9	3	101	BCL	CHC-C4B	2.93	1.46	1.39
9	B	103	BCL	CHC-C4B	2.93	1.46	1.39
11	H	102	U4Z	CAL-CAM	-2.93	1.39	1.46
9	F	101	BCL	C4B-NB	-2.93	1.34	1.37
9	K	102	BCL	C1B-NB	-2.93	1.34	1.37
11	5	102	U4Z	CAL-CAM	-2.93	1.39	1.46
11	P	102	U4Z	CAL-CAM	-2.92	1.39	1.46
11	D	103	U4Z	CAL-CAM	-2.92	1.39	1.46
9	G	102	BCL	CHC-C4B	2.92	1.46	1.39
9	2	102	BCL	C1D-ND	-2.92	1.34	1.37
9	A	101	BCL	CHD-C4C	2.92	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	3	101	BCL	CHB-C1B	2.92	1.46	1.39
9	S	103	BCL	OBD-CAD	2.92	1.27	1.22
9	8	103	BCL	CHC-C4B	2.91	1.46	1.39
10	U	101	U42	C20-C19	-2.91	1.41	1.52
9	9	102	BCL	C3D-C2D	2.91	1.46	1.39
9	Q	102	BCL	C1B-NB	-2.91	1.34	1.37
10	B	101	U42	CAC-CAE	-2.91	1.45	1.52
10	I	101	U42	CAV-CAR	2.91	1.42	1.35
9	8	102	BCL	OBD-CAD	2.91	1.27	1.22
9	M	701	BCL	C1B-NB	-2.91	1.34	1.37
9	M	701	BCL	C4B-NB	-2.91	1.34	1.37
9	R	101	BCL	CHC-C4B	2.91	1.45	1.39
10	0	103	U42	CAL-CAJ	2.91	1.41	1.33
9	U	103	BCL	CHD-C1D	2.90	1.44	1.38
9	J	101	BCL	C4B-NB	-2.90	1.34	1.37
9	0	102	BCL	CHD-C1D	2.90	1.44	1.38
9	9	102	BCL	C1B-NB	-2.90	1.34	1.37
11	F	103	U4Z	CAL-CAM	-2.90	1.39	1.46
10	8	101	U42	C20-C19	-2.90	1.41	1.52
9	8	102	BCL	C1B-NB	-2.90	1.34	1.37
10	I	101	U42	C19-C18	-2.90	1.42	1.50
9	D	101	BCL	C3D-C2D	2.90	1.46	1.39
9	W	102	BCL	C4B-NB	-2.90	1.34	1.37
13	L	1015	BGL	O5-C1	2.90	1.50	1.42
9	E	102	BCL	C1B-NB	-2.90	1.34	1.37
9	W	102	BCL	C1B-NB	-2.90	1.34	1.37
13	L	1013	BGL	O5-C1	2.89	1.49	1.42
9	T	101	BCL	C1D-ND	-2.89	1.34	1.37
9	J	101	BCL	C3D-C2D	2.89	1.46	1.39
9	4	103	BCL	CHD-C1D	2.89	1.44	1.38
9	S	103	BCL	CHC-C4B	2.88	1.45	1.39
9	P	101	BCL	CHD-C4C	2.88	1.47	1.39
9	1	101	BCL	C3D-C2D	2.88	1.46	1.39
11	A	102	U4Z	CAH-CAD	2.88	1.39	1.34
9	F	102	BCL	CHD-C1D	2.88	1.44	1.38
9	0	101	BCL	C1B-NB	-2.88	1.34	1.37
11	9	101	U4Z	CAH-CAD	2.88	1.39	1.34
9	Q	103	BCL	C1D-ND	-2.88	1.34	1.37
9	K	102	BCL	CHD-C1D	2.87	1.44	1.38
9	2	102	BCL	C3D-C2D	2.87	1.46	1.39
9	5	101	BCL	C3D-C2D	2.87	1.46	1.39
9	S	103	BCL	C1D-ND	-2.87	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	T	101	BCL	OBD-CAD	2.87	1.27	1.22
9	H	101	BCL	C4B-NB	-2.87	1.34	1.37
9	0	102	BCL	CHC-C4B	2.87	1.45	1.39
9	3	101	BCL	OBD-CAD	2.87	1.27	1.22
9	I	103	BCL	C1D-ND	-2.87	1.34	1.37
9	W	102	BCL	C1D-ND	-2.87	1.34	1.37
9	M	701	BCL	C3D-C2D	2.87	1.46	1.39
9	R	101	BCL	C1B-NB	-2.87	1.34	1.37
9	F	101	BCL	C1D-ND	-2.86	1.34	1.37
9	N	101	BCL	C4B-NB	-2.86	1.34	1.37
9	R	101	BCL	C3D-C2D	2.86	1.46	1.39
9	S	102	BCL	CHB-C1B	2.86	1.45	1.39
9	B	103	BCL	CHB-C1B	2.86	1.45	1.39
9	J	101	BCL	C1B-NB	-2.85	1.34	1.37
10	G	101	U42	C30-C29	-2.85	1.37	1.51
9	4	103	BCL	CHC-C4B	2.85	1.45	1.39
9	D	102	BCL	OBD-CAD	2.85	1.27	1.22
11	A	102	U4Z	CAL-CAM	-2.85	1.39	1.46
9	0	102	BCL	C1D-ND	-2.85	1.34	1.37
9	I	103	BCL	CHD-C1D	2.85	1.43	1.38
9	F	101	BCL	C1B-NB	-2.84	1.34	1.37
10	G	101	U42	CAU-CAR	-2.84	1.45	1.50
9	S	103	BCL	CHB-C1B	2.84	1.45	1.39
10	8	101	U42	CAN-CAM	-2.84	1.45	1.50
9	T	101	BCL	C3D-C2D	2.84	1.46	1.39
9	D	101	BCL	CHD-C1D	2.84	1.43	1.38
9	1	101	BCL	C4B-NB	-2.84	1.34	1.37
9	O	103	BCL	MG-NA	-2.83	1.99	2.06
10	8	101	U42	CAP-CAQ	2.83	1.42	1.34
18	L	1003	BPH	C1D-ND	-2.83	1.33	1.38
9	Q	103	BCL	CHD-C1D	2.82	1.43	1.38
9	W	102	BCL	CHD-C1D	2.82	1.43	1.38
9	U	103	BCL	C1B-NB	-2.82	1.34	1.37
10	4	104	U42	CAV-CAR	2.82	1.42	1.35
10	B	101	U42	C27-C26	-2.82	1.37	1.51
18	M	702	BPH	C4D-CHA	2.82	1.43	1.39
10	4	101	U42	CAC-CAE	-2.82	1.45	1.52
9	3	101	BCL	C3D-C2D	2.81	1.46	1.39
9	5	101	BCL	CHC-C4B	2.81	1.45	1.39
9	L	1002	BCL	C3D-C2D	2.81	1.46	1.39
9	U	102	BCL	CHD-C1D	2.80	1.43	1.38
10	4	101	U42	C27-C26	-2.80	1.37	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	8	101	U42	CAC-CAE	-2.80	1.46	1.52
10	E	101	U42	C20-C19	-2.80	1.41	1.52
9	T	101	BCL	CHC-C4B	2.80	1.45	1.39
9	U	103	BCL	C3D-C2D	2.80	1.46	1.39
10	4	101	U42	CAQ-CAR	-2.80	1.40	1.46
9	6	102	BCL	C1D-ND	-2.80	1.34	1.37
10	G	101	U42	CAL-CAM	-2.79	1.40	1.46
9	K	101	BCL	C4B-NB	-2.79	1.34	1.37
9	O	103	BCL	CHC-C4B	2.79	1.45	1.39
9	8	102	BCL	CHD-C1D	2.79	1.43	1.38
10	4	104	U42	CAL-CAM	-2.79	1.40	1.46
11	V	102	U4Z	CAL-CAM	-2.79	1.40	1.46
10	U	101	U42	C27-C26	-2.79	1.37	1.51
9	L	1002	BCL	C1D-ND	-2.78	1.34	1.37
9	2	101	BCL	MG-NA	-2.78	1.99	2.06
9	L	1002	BCL	C1B-NB	-2.78	1.34	1.37
9	6	102	BCL	CHD-C1D	2.78	1.43	1.38
9	D	101	BCL	C4B-NB	-2.78	1.34	1.37
9	S	102	BCL	CHD-C1D	2.78	1.43	1.38
10	E	101	U42	C26-C25	-2.77	1.38	1.51
9	8	103	BCL	C3D-C2D	2.77	1.46	1.39
9	4	102	BCL	C4B-NB	-2.77	1.34	1.37
9	O	103	BCL	C1B-NB	-2.77	1.34	1.37
9	I	102	BCL	CHD-C1D	2.77	1.43	1.38
9	L	1001	BCL	C4B-NB	-2.77	1.34	1.37
9	4	102	BCL	CHD-C1D	2.76	1.43	1.38
9	7	101	BCL	CHC-C4B	2.76	1.45	1.39
9	Q	102	BCL	CHD-C1D	2.76	1.43	1.38
10	B	101	U42	C28-C27	-2.76	1.38	1.51
10	U	104	U42	CAN-CAM	-2.76	1.45	1.50
9	4	103	BCL	OBD-CAD	2.76	1.27	1.22
9	K	102	BCL	C3D-C2D	2.76	1.46	1.39
9	B	103	BCL	C3D-C2D	2.76	1.46	1.39
9	E	102	BCL	C1D-ND	-2.76	1.34	1.37
10	U	104	U42	CBG-CBB	2.75	1.43	1.36
9	N	101	BCL	C1B-NB	-2.75	1.34	1.37
9	E	102	BCL	OBD-CAD	2.74	1.27	1.22
9	B	102	BCL	CHD-C1D	2.74	1.43	1.38
9	G	102	BCL	C3D-C2D	2.74	1.46	1.39
9	W	101	BCL	C3C-C4C	-2.74	1.48	1.51
10	4	101	U42	C20-C19	-2.74	1.42	1.52
9	V	101	BCL	OBD-CAD	2.74	1.27	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	I	104	U42	C27-C26	-2.74	1.38	1.51
9	L	1001	BCL	MG-NA	-2.74	1.99	2.06
11	7	102	U4Z	CAH-CAD	2.74	1.39	1.34
9	U	103	BCL	C1D-ND	-2.74	1.34	1.37
10	4	101	U42	C29-C28	-2.73	1.38	1.51
9	4	103	BCL	MG-NA	-2.73	1.99	2.06
9	G	102	BCL	C1D-ND	-2.73	1.34	1.37
9	I	102	BCL	C4B-NB	-2.73	1.34	1.37
9	W	102	BCL	CHB-C4A	-2.73	1.30	1.37
10	S	101	U42	C19-C18	-2.73	1.42	1.50
9	U	103	BCL	CHB-C4A	-2.73	1.30	1.37
9	H	101	BCL	C1B-NB	-2.72	1.34	1.37
9	8	102	BCL	C4B-NB	-2.72	1.34	1.37
9	W	101	BCL	MG-NC	-2.72	1.99	2.06
9	L	1001	BCL	CHD-C4C	2.72	1.46	1.39
9	6	101	BCL	CHD-C1D	2.72	1.43	1.38
9	6	101	BCL	C4B-NB	-2.71	1.34	1.37
9	S	103	BCL	C3D-C2D	2.71	1.46	1.39
9	D	102	BCL	CHD-C1D	2.71	1.43	1.38
9	W	102	BCL	C3D-C2D	2.71	1.46	1.39
9	6	102	BCL	CHB-C1B	2.71	1.45	1.39
18	L	1003	BPH	C4B-NB	-2.70	1.33	1.38
9	V	101	BCL	C4B-NB	-2.70	1.34	1.37
9	O	103	BCL	C3D-C2D	2.70	1.46	1.39
9	T	101	BCL	C1B-NB	-2.70	1.34	1.37
9	2	102	BCL	CHB-C4A	-2.70	1.30	1.37
9	2	101	BCL	CHD-C1D	2.69	1.43	1.38
9	W	101	BCL	C4B-NB	-2.69	1.34	1.37
9	Q	103	BCL	C3D-C2D	2.69	1.46	1.39
10	8	101	U42	CAU-CAR	-2.69	1.45	1.50
9	E	102	BCL	C3D-C2D	2.69	1.46	1.39
9	D	102	BCL	C4B-NB	-2.68	1.34	1.37
9	B	103	BCL	CHB-C4A	-2.68	1.31	1.37
10	G	101	U42	CAV-CAR	2.68	1.42	1.35
10	I	101	U42	C29-C28	-2.68	1.38	1.51
9	I	103	BCL	C3D-C2D	2.67	1.46	1.39
10	4	101	U42	C23-C22	-2.67	1.38	1.51
10	Q	101	U42	CAQ-CAR	-2.66	1.40	1.46
9	4	103	BCL	C3D-C2D	2.66	1.46	1.39
10	I	101	U42	C26-C25	-2.66	1.38	1.51
10	4	104	U42	CAB-CAD	-2.66	1.50	1.53
9	0	102	BCL	CHB-C1B	2.66	1.45	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	103	BCL	MG-NA	-2.65	2.00	2.06
9	K	102	BCL	CAA-C2A	-2.65	1.49	1.54
9	A	101	BCL	C4D-CHA	2.65	1.47	1.38
9	D	101	BCL	MG-NA	-2.65	2.00	2.06
9	V	101	BCL	C1B-NB	-2.64	1.34	1.37
9	2	102	BCL	CHC-C4B	2.64	1.45	1.39
10	B	101	U42	C20-C19	-2.64	1.42	1.52
9	I	103	BCL	C1B-NB	-2.64	1.34	1.37
9	6	102	BCL	MG-NA	-2.64	2.00	2.06
11	C	401	U4Z	CBF-CBH	-2.63	1.40	1.46
9	2	101	BCL	C4B-NB	-2.63	1.34	1.37
10	E	101	U42	C30-C29	-2.63	1.38	1.51
9	0	101	BCL	CHD-C1D	2.63	1.43	1.38
9	O	102	BCL	C4B-NB	-2.62	1.34	1.37
9	6	102	BCL	C3D-C2D	2.62	1.46	1.39
9	S	102	BCL	C4B-NB	-2.62	1.34	1.37
9	2	101	BCL	C1B-NB	-2.62	1.34	1.37
9	M	701	BCL	MG-NA	-2.61	2.00	2.06
9	S	103	BCL	CHB-C4A	-2.61	1.31	1.37
10	E	101	U42	CAL-CAM	-2.61	1.40	1.46
9	0	101	BCL	C4B-NB	-2.60	1.34	1.37
11	C	401	U4Z	CAH-CAD	2.60	1.38	1.34
9	I	103	BCL	OBD-CAD	2.59	1.26	1.22
10	G	101	U42	CBM-CBJ	-2.59	1.35	1.43
9	4	103	BCL	CHB-C1B	2.58	1.45	1.39
9	O	102	BCL	CHD-C1D	2.58	1.43	1.38
11	C	401	U4Z	CBB-CAV	-2.58	1.35	1.43
10	S	101	U42	C27-C26	-2.57	1.39	1.51
9	B	103	BCL	C1D-ND	-2.57	1.34	1.37
18	L	1003	BPH	C1B-NB	-2.57	1.34	1.38
9	8	103	BCL	CHD-C4C	2.57	1.46	1.39
9	O	103	BCL	OBD-CAD	2.57	1.26	1.22
10	S	101	U42	C20-C19	-2.56	1.42	1.52
10	I	104	U42	C6-C5	-2.56	1.45	1.52
18	L	1005	BPH	C3A-C2A	-2.56	1.52	1.54
10	Q	101	U42	C26-C25	-2.56	1.39	1.51
9	H	101	BCL	MG-NA	-2.56	2.00	2.06
9	Q	102	BCL	C4B-NB	-2.56	1.34	1.37
10	O	101	U42	C26-C25	-2.56	1.39	1.51
9	W	102	BCL	OBD-CAD	2.56	1.26	1.22
9	E	102	BCL	CHD-C4C	2.56	1.46	1.39
9	B	102	BCL	C4B-NB	-2.55	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	103	BCL	CHD-C4C	2.55	1.46	1.39
10	I	101	U42	CAP-CAQ	2.55	1.41	1.34
10	I	104	U42	CAC-CAE	-2.55	1.46	1.52
10	4	101	U42	C19-C18	-2.55	1.43	1.50
10	U	101	U42	C26-C25	-2.55	1.39	1.51
9	6	102	BCL	CHB-C4A	-2.55	1.31	1.37
9	0	102	BCL	C3D-C2D	2.55	1.45	1.39
9	K	102	BCL	CHB-C4A	-2.54	1.31	1.37
10	8	101	U42	CAO-CAM	2.54	1.41	1.35
9	G	102	BCL	CHB-C4A	-2.53	1.31	1.37
9	U	102	BCL	C4B-NB	-2.53	1.34	1.37
10	I	104	U42	C28-C27	-2.52	1.39	1.51
9	K	102	BCL	MG-NA	-2.52	2.00	2.06
10	4	104	U42	C28-C27	-2.52	1.39	1.51
10	U	101	U42	CAL-CAM	-2.52	1.40	1.46
9	O	103	BCL	CHD-C1D	2.52	1.43	1.38
9	4	103	BCL	C3C-C4C	-2.51	1.48	1.51
10	G	101	U42	C26-C25	-2.51	1.39	1.51
9	2	102	BCL	CHD-C4C	2.51	1.46	1.39
10	Q	101	U42	CBM-CBJ	-2.51	1.35	1.43
9	B	103	BCL	MG-NC	-2.51	2.00	2.06
9	W	101	BCL	MG-NA	-2.51	2.00	2.06
11	V	102	U4Z	CBI-CBL	2.50	1.41	1.35
9	P	101	BCL	C4D-CHA	2.50	1.47	1.38
9	2	102	BCL	C1B-C2B	2.50	1.49	1.43
11	N	102	U4Z	CBI-CBL	2.50	1.41	1.35
10	O	101	U42	CAL-CAJ	2.50	1.40	1.33
9	G	102	BCL	CHD-C4C	2.49	1.46	1.39
9	P	101	BCL	C1B-C2B	2.49	1.49	1.43
9	F	102	BCL	C4B-NB	-2.48	1.34	1.37
9	S	103	BCL	C3C-C4C	-2.48	1.48	1.51
9	Q	103	BCL	CHD-C4C	2.48	1.46	1.39
10	4	101	U42	C28-C27	-2.48	1.39	1.51
11	N	102	U4Z	CAQ-CAR	-2.48	1.40	1.46
10	I	101	U42	CAO-CAM	2.48	1.41	1.35
11	C	401	U4Z	CBN-CBL	-2.47	1.40	1.46
9	2	101	BCL	CHD-C4C	2.47	1.46	1.39
10	B	101	U42	CAL-CAJ	2.47	1.40	1.33
10	B	101	U42	C30-C29	-2.47	1.39	1.51
9	2	102	BCL	C1B-NB	-2.47	1.34	1.37
9	E	102	BCL	CHB-C4A	-2.46	1.31	1.37
9	4	103	BCL	CHD-C4C	2.46	1.46	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	G	101	U42	C20-C19	-2.45	1.43	1.52
11	J	102	U4Z	CBJ-CBH	2.45	1.41	1.35
9	8	103	BCL	C1B-C2B	2.45	1.48	1.43
9	B	103	BCL	CHD-C4C	2.45	1.46	1.39
11	1	102	U4Z	CAQ-CAR	-2.44	1.40	1.46
11	N	102	U4Z	CBJ-CBH	2.44	1.41	1.35
9	S	103	BCL	CHD-C4C	2.44	1.46	1.39
9	S	102	BCL	CAA-C2A	-2.44	1.49	1.54
11	S	104	U4Z	CBJ-CBH	2.44	1.41	1.35
9	U	103	BCL	CHD-C4C	2.44	1.46	1.39
9	2	102	BCL	CHC-C1C	-2.44	1.31	1.37
9	V	101	BCL	CHC-C1C	-2.44	1.31	1.37
9	Q	102	BCL	MG-NC	-2.43	2.00	2.06
9	B	103	BCL	OBD-CAD	2.43	1.26	1.22
9	A	101	BCL	C1B-C2B	2.43	1.48	1.43
11	C	401	U4Z	CAI-CAH	-2.42	1.46	1.51
11	1	102	U4Z	CBN-CBL	-2.42	1.40	1.46
9	2	102	BCL	MG-NA	-2.42	2.00	2.06
18	L	1003	BPH	C2C-C3C	-2.42	1.52	1.54
9	I	102	BCL	MG-NA	-2.42	2.00	2.06
10	Q	101	U42	C27-C26	-2.42	1.39	1.51
9	2	102	BCL	OBD-CAD	2.41	1.26	1.22
10	G	101	U42	C27-C26	-2.41	1.39	1.51
9	5	101	BCL	CHD-C4C	2.41	1.46	1.39
10	B	101	U42	CAO-CAM	2.41	1.41	1.35
9	Q	103	BCL	CHB-C4A	-2.41	1.31	1.37
11	J	102	U4Z	CAQ-CAR	-2.41	1.40	1.46
11	7	102	U4Z	CBN-CBL	-2.41	1.40	1.46
11	D	103	U4Z	CAQ-CAR	-2.41	1.40	1.46
9	K	102	BCL	CHD-C4C	2.41	1.45	1.39
11	F	103	U4Z	CBI-CBL	2.40	1.41	1.35
11	N	102	U4Z	CAV-CAR	2.40	1.41	1.35
9	W	102	BCL	CHD-C4C	2.40	1.45	1.39
9	J	101	BCL	CHD-C4C	2.40	1.45	1.39
10	4	104	U42	CAP-CAQ	2.40	1.40	1.34
9	7	101	BCL	CHD-C4C	2.40	1.45	1.39
9	3	101	BCL	CHD-C4C	2.40	1.45	1.39
10	4	104	U42	C27-C26	-2.40	1.39	1.51
9	G	102	BCL	OBD-CAD	2.40	1.26	1.22
11	7	102	U4Z	CAQ-CAR	-2.40	1.40	1.46
9	T	101	BCL	CHC-C1C	-2.40	1.31	1.37
9	4	102	BCL	MG-NA	-2.40	2.00	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	J	102	U4Z	CBI-CBL	2.40	1.41	1.35
9	L	1001	BCL	C1D-C2D	2.40	1.50	1.45
11	C	401	U4Z	CBI-CBL	2.40	1.41	1.35
11	V	102	U4Z	CAV-CAR	2.40	1.41	1.35
11	S	104	U4Z	CAV-CAR	2.39	1.41	1.35
11	9	101	U4Z	CAQ-CAR	-2.39	1.40	1.46
10	B	101	U42	CBN-CBL	-2.39	1.40	1.46
11	P	102	U4Z	CAQ-CAR	-2.39	1.40	1.46
9	K	102	BCL	C3C-C4C	-2.39	1.48	1.51
11	A	102	U4Z	CAV-CAR	2.39	1.41	1.35
11	F	103	U4Z	CAV-CAR	2.39	1.41	1.35
9	R	101	BCL	CHC-C1C	-2.39	1.31	1.37
11	5	102	U4Z	CBN-CBL	-2.39	1.40	1.46
9	B	102	BCL	MG-NC	-2.38	2.00	2.06
10	4	104	U42	CBM-CBJ	-2.38	1.35	1.43
11	P	102	U4Z	CBN-CBL	-2.38	1.40	1.46
11	F	103	U4Z	CAQ-CAR	-2.38	1.40	1.46
11	V	102	U4Z	CBJ-CBH	2.38	1.41	1.35
11	9	101	U4Z	CAV-CAR	2.38	1.41	1.35
11	D	103	U4Z	CAV-CAR	2.38	1.41	1.35
10	E	101	U42	C28-C27	-2.38	1.40	1.51
9	I	103	BCL	MG-NC	-2.38	2.00	2.06
9	U	103	BCL	OBD-CAD	2.37	1.26	1.22
9	E	102	BCL	MG-NC	-2.37	2.00	2.06
11	3	102	U4Z	CBN-CBL	-2.37	1.40	1.46
11	J	102	U4Z	CAV-CAR	2.37	1.41	1.35
10	0	103	U42	CBI-CBL	2.37	1.41	1.35
11	H	102	U4Z	CBJ-CBH	2.37	1.41	1.35
9	I	102	BCL	MG-NC	-2.37	2.00	2.06
10	E	101	U42	C25-C24	-2.36	1.40	1.51
9	U	103	BCL	C1B-C2B	2.36	1.48	1.43
11	H	102	U4Z	CBI-CBL	2.36	1.41	1.35
10	B	101	U42	C29-C28	-2.36	1.40	1.51
11	7	102	U4Z	CBF-CBH	-2.36	1.40	1.46
9	6	101	BCL	MG-NA	-2.36	2.00	2.06
9	T	101	BCL	CHD-C4C	2.36	1.45	1.39
9	8	102	BCL	MG-NA	-2.36	2.00	2.06
11	T	102	U4Z	CAQ-CAR	-2.36	1.40	1.46
9	0	101	BCL	MG-NC	-2.36	2.00	2.06
10	O	101	U42	CAT-CAS	-2.35	1.43	1.52
10	E	101	U42	CBM-CBJ	-2.35	1.35	1.43
11	S	104	U4Z	CAQ-CAR	-2.35	1.40	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	H	102	U4Z	CAQ-CAR	-2.35	1.40	1.46
9	D	101	BCL	C3C-C4C	-2.35	1.48	1.51
9	9	102	BCL	CHD-C4C	2.35	1.45	1.39
11	1	102	U4Z	CBF-CBH	-2.35	1.40	1.46
11	D	103	U4Z	CBI-CBL	2.35	1.41	1.35
9	L	1002	BCL	CHD-C4C	2.35	1.45	1.39
9	O	103	BCL	CHD-C4C	2.35	1.45	1.39
9	F	101	BCL	MG-NA	-2.35	2.00	2.06
9	L	1002	BCL	MG-NC	-2.35	2.00	2.06
11	D	103	U4Z	CBJ-CBH	2.35	1.41	1.35
9	0	102	BCL	CHD-C4C	2.35	1.45	1.39
9	9	102	BCL	MG-NA	-2.34	2.00	2.06
10	0	103	U42	C28-C27	-2.34	1.40	1.51
9	7	101	BCL	CHC-C1C	-2.34	1.31	1.37
9	U	102	BCL	MG-NC	-2.34	2.00	2.06
11	S	104	U4Z	CBI-CBL	2.34	1.41	1.35
9	Q	102	BCL	MG-NA	-2.34	2.00	2.06
11	F	103	U4Z	CBN-CBL	-2.34	1.40	1.46
10	G	101	U42	C19-C18	-2.34	1.43	1.50
9	0	102	BCL	MG-NC	-2.34	2.00	2.06
9	K	102	BCL	C1B-C2B	2.34	1.48	1.43
11	3	102	U4Z	CAQ-CAR	-2.34	1.41	1.46
11	H	102	U4Z	CBN-CBL	-2.33	1.41	1.46
11	9	101	U4Z	CBJ-CBH	2.33	1.41	1.35
10	I	101	U42	C22-C21	-2.33	1.40	1.51
11	H	102	U4Z	CAV-CAR	2.33	1.41	1.35
9	D	102	BCL	MG-NA	-2.33	2.00	2.06
11	A	102	U4Z	CBN-CBL	-2.33	1.41	1.46
9	U	103	BCL	MG-NC	-2.33	2.00	2.06
11	J	102	U4Z	CBN-CBL	-2.33	1.41	1.46
11	T	102	U4Z	CBN-CBL	-2.33	1.41	1.46
9	V	101	BCL	CHD-C4C	2.33	1.45	1.39
10	E	101	U42	CBG-CBB	2.33	1.42	1.36
10	I	104	U42	CAO-CAM	2.33	1.41	1.35
9	E	102	BCL	MG-NA	-2.33	2.00	2.06
9	6	102	BCL	CHD-C4C	2.33	1.45	1.39
9	W	101	BCL	CHD-C4C	2.33	1.45	1.39
11	A	102	U4Z	CBI-CBL	2.32	1.41	1.35
9	F	101	BCL	CHD-C4C	2.32	1.45	1.39
9	4	102	BCL	MG-NC	-2.32	2.00	2.06
9	D	102	BCL	MG-NC	-2.32	2.00	2.06
9	O	103	BCL	CHC-C1C	-2.32	1.31	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	6	102	BCL	MG-NC	-2.31	2.00	2.06
9	6	102	BCL	OBD-CAD	2.31	1.26	1.22
10	O	101	U42	C20-C19	-2.31	1.43	1.52
11	D	103	U4Z	CBF-CBH	-2.31	1.41	1.46
11	N	102	U4Z	CBF-CBH	-2.31	1.41	1.46
9	K	101	BCL	MG-NA	-2.31	2.00	2.06
11	5	102	U4Z	CAO-CAM	2.31	1.41	1.35
9	0	101	BCL	MG-NA	-2.31	2.00	2.06
9	T	101	BCL	MG-NA	-2.31	2.00	2.06
9	1	101	BCL	CHD-C4C	2.31	1.45	1.39
11	5	102	U4Z	CAQ-CAR	-2.31	1.41	1.46
9	9	102	BCL	CHC-C1C	-2.31	1.31	1.37
11	T	102	U4Z	CAV-CAR	2.31	1.41	1.35
9	E	102	BCL	C1D-C2D	2.30	1.49	1.45
9	8	103	BCL	CHC-C1C	-2.30	1.31	1.37
11	F	103	U4Z	CBF-CBH	-2.30	1.41	1.46
11	F	103	U4Z	CBJ-CBH	2.30	1.41	1.35
9	3	101	BCL	MG-NA	-2.30	2.00	2.06
9	8	102	BCL	MG-NC	-2.30	2.00	2.06
10	G	101	U42	CAO-CAM	2.30	1.41	1.35
9	5	101	BCL	MG-NA	-2.30	2.00	2.06
11	T	102	U4Z	CBJ-CBH	2.30	1.41	1.35
10	G	101	U42	C31-C30	-2.30	1.37	1.51
9	R	101	BCL	CHD-C4C	2.30	1.45	1.39
11	A	102	U4Z	CAQ-CAR	-2.30	1.41	1.46
9	1	101	BCL	MG-NA	-2.30	2.00	2.06
11	P	102	U4Z	CBI-CBL	2.30	1.41	1.35
9	W	102	BCL	C1B-C2B	2.30	1.48	1.43
11	H	102	U4Z	CBF-CBH	-2.29	1.41	1.46
9	5	101	BCL	CHC-C1C	-2.29	1.32	1.37
11	A	102	U4Z	CBJ-CBH	2.29	1.41	1.35
9	R	101	BCL	MG-NA	-2.29	2.00	2.06
11	D	103	U4Z	CBN-CBL	-2.29	1.41	1.46
9	E	102	BCL	C3A-C2A	-2.29	1.48	1.54
9	M	701	BCL	CHD-C4C	2.29	1.45	1.39
9	0	101	BCL	C1B-C2B	2.29	1.48	1.43
10	U	101	U42	C28-C27	-2.29	1.40	1.51
9	O	102	BCL	MG-NA	-2.29	2.00	2.06
11	V	102	U4Z	CAO-CAM	2.29	1.41	1.35
11	3	102	U4Z	CBI-CBL	2.29	1.41	1.35
11	5	102	U4Z	CBJ-CBH	2.29	1.41	1.35
9	K	102	BCL	MG-NC	-2.29	2.00	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	6	102	BCL	CHC-C4B	2.28	1.44	1.39
9	3	101	BCL	CHB-C4A	-2.28	1.32	1.37
10	G	101	U42	CAP-CAQ	2.28	1.40	1.34
10	S	101	U42	CAT-CAS	-2.28	1.43	1.52
9	S	102	BCL	CHD-C4C	2.28	1.45	1.39
10	S	101	U42	C30-C29	-2.28	1.40	1.51
9	Q	103	BCL	MG-NA	-2.28	2.00	2.06
11	7	102	U4Z	CBJ-CBH	2.28	1.41	1.35
11	T	102	U4Z	CBI-CBL	2.28	1.41	1.35
9	2	102	BCL	C3A-C2A	-2.28	1.48	1.54
9	8	103	BCL	MG-NA	-2.28	2.00	2.06
11	5	102	U4Z	CAV-CAR	2.28	1.41	1.35
11	5	102	U4Z	CBF-CBH	-2.28	1.41	1.46
11	J	102	U4Z	CBF-CBH	-2.28	1.41	1.46
10	Q	101	U42	C19-C18	-2.28	1.44	1.50
11	9	101	U4Z	CBI-CBL	2.28	1.41	1.35
9	2	102	BCL	CAA-C2A	-2.27	1.49	1.54
9	K	101	BCL	CHD-C4C	2.27	1.45	1.39
10	B	101	U42	C26-C25	-2.27	1.40	1.51
9	S	102	BCL	MG-NA	-2.27	2.00	2.06
9	7	101	BCL	MG-NA	-2.27	2.00	2.06
9	N	101	BCL	CHD-C4C	2.27	1.45	1.39
9	B	103	BCL	CAA-C2A	-2.27	1.50	1.54
9	B	102	BCL	MG-NA	-2.27	2.00	2.06
9	D	101	BCL	CHD-C4C	2.27	1.45	1.39
10	O	101	U42	C27-C26	-2.27	1.40	1.51
9	S	103	BCL	MG-NC	-2.27	2.00	2.06
10	I	101	U42	CAB-CAD	-2.27	1.50	1.53
9	2	102	BCL	C1D-C2D	2.27	1.49	1.45
11	9	101	U4Z	CBN-CBL	-2.27	1.41	1.46
10	U	101	U42	C30-C29	-2.27	1.40	1.51
9	O	103	BCL	CHB-C4A	-2.27	1.32	1.37
9	4	103	BCL	C1D-C2D	2.26	1.49	1.45
9	G	102	BCL	C1D-C2D	2.26	1.49	1.45
9	J	101	BCL	MG-NA	-2.26	2.00	2.06
9	F	102	BCL	MG-NA	-2.26	2.00	2.06
10	G	101	U42	CAB-CAD	-2.26	1.50	1.53
9	B	103	BCL	C1B-C2B	2.26	1.48	1.43
9	K	102	BCL	C3A-C2A	-2.26	1.48	1.54
10	Q	101	U42	C30-C29	-2.26	1.40	1.51
11	7	102	U4Z	CBI-CBL	2.26	1.41	1.35
9	H	101	BCL	CHD-C4C	2.26	1.45	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	L	1002	BCL	C4B-NB	-2.26	1.34	1.37
9	O	102	BCL	MG-NC	-2.26	2.00	2.06
9	I	103	BCL	CHB-C4A	-2.25	1.32	1.37
9	N	101	BCL	CHC-C1C	-2.25	1.32	1.37
11	C	401	U4Z	CAP-CAQ	2.25	1.40	1.34
9	B	103	BCL	C3A-C2A	-2.25	1.48	1.54
10	B	101	U42	CAQ-CAR	-2.25	1.41	1.46
10	I	101	U42	CBM-CBJ	-2.25	1.36	1.43
9	4	103	BCL	MG-NC	-2.25	2.00	2.06
9	A	101	BCL	C3D-C4D	-2.25	1.39	1.44
11	3	102	U4Z	CBJ-CBH	2.25	1.41	1.35
9	S	102	BCL	CHB-C4A	-2.25	1.32	1.37
10	I	104	U42	CBN-CBL	-2.25	1.41	1.46
9	P	101	BCL	C3D-C4D	-2.25	1.39	1.44
9	W	102	BCL	MG-NA	-2.25	2.00	2.06
11	9	101	U4Z	CBF-CBH	-2.24	1.41	1.46
11	D	103	U4Z	CAO-CAM	2.24	1.41	1.35
11	S	104	U4Z	CAO-CAM	2.24	1.41	1.35
9	V	101	BCL	MG-NC	-2.24	2.00	2.06
9	B	103	BCL	C1D-C2D	2.24	1.49	1.45
10	E	101	U42	C29-C28	-2.24	1.40	1.51
11	3	102	U4Z	CBF-CBH	-2.24	1.41	1.46
11	F	103	U4Z	CAO-CAM	2.23	1.41	1.35
10	8	101	U42	C27-C26	-2.23	1.40	1.51
9	0	102	BCL	MG-NA	-2.23	2.01	2.06
11	1	102	U4Z	CBI-CBL	2.23	1.41	1.35
11	7	102	U4Z	CAV-CAR	2.23	1.41	1.35
10	4	101	U42	CAN-CAM	-2.23	1.46	1.50
9	M	701	BCL	CHB-C4A	-2.23	1.32	1.37
10	I	101	U42	CAL-CAM	-2.23	1.41	1.46
11	P	102	U4Z	CAV-CAR	2.23	1.41	1.35
11	5	102	U4Z	CBI-CBL	2.23	1.40	1.35
11	3	102	U4Z	CAV-CAR	2.22	1.40	1.35
10	I	101	U42	C28-C27	-2.22	1.40	1.51
9	F	102	BCL	CHD-C4C	2.22	1.45	1.39
11	T	102	U4Z	CBF-CBH	-2.22	1.41	1.46
9	1	101	BCL	CHC-C1C	-2.22	1.32	1.37
11	P	102	U4Z	CBF-CBH	-2.22	1.41	1.46
11	3	102	U4Z	CAO-CAM	2.22	1.40	1.35
11	V	102	U4Z	CAQ-CAR	-2.21	1.41	1.46
9	Q	103	BCL	MG-NC	-2.21	2.01	2.06
10	B	101	U42	C23-C22	-2.21	1.40	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	K	101	BCL	MG-NC	-2.21	2.01	2.06
11	A	102	U4Z	CAO-CAM	2.21	1.40	1.35
9	T	101	BCL	C1B-C2B	2.21	1.48	1.43
9	B	102	BCL	CHD-C4C	2.21	1.45	1.39
9	S	102	BCL	MG-NC	-2.21	2.01	2.06
11	N	102	U4Z	CAO-CAM	2.21	1.40	1.35
9	F	101	BCL	CHC-C1C	-2.21	1.32	1.37
10	4	104	U42	CAC-CAE	-2.21	1.47	1.52
10	E	101	U42	C31-C30	-2.21	1.38	1.51
9	S	103	BCL	C1D-C2D	2.21	1.49	1.45
9	M	701	BCL	CHC-C1C	-2.21	1.32	1.37
10	4	101	U42	CAL-CAJ	2.20	1.39	1.33
11	V	102	U4Z	CBN-CBL	-2.20	1.41	1.46
9	B	103	BCL	MG-NA	-2.20	2.01	2.06
9	U	103	BCL	CBD-CAD	-2.20	1.46	1.56
9	U	102	BCL	CHD-C4C	2.20	1.45	1.39
10	I	101	U42	CAX-CAY	2.20	1.56	1.53
10	I	104	U42	C31-C30	-2.20	1.38	1.51
9	6	102	BCL	C1D-C2D	2.20	1.49	1.45
10	4	104	U42	CBG-CBI	-2.20	1.36	1.43
9	F	102	BCL	MG-NC	-2.20	2.01	2.06
11	S	104	U4Z	CBN-CBL	-2.20	1.41	1.46
9	8	103	BCL	C3A-C2A	-2.20	1.48	1.54
9	N	101	BCL	C1B-C2B	2.19	1.48	1.43
9	D	102	BCL	CHD-C4C	2.19	1.45	1.39
11	7	102	U4Z	CAO-CAM	2.19	1.40	1.35
9	6	101	BCL	MG-NC	-2.19	2.01	2.06
10	G	101	U42	CAT-CAS	-2.19	1.44	1.52
11	9	101	U4Z	CAO-CAM	2.19	1.40	1.35
9	I	102	BCL	CHD-C4C	2.19	1.45	1.39
9	S	103	BCL	C1B-C2B	2.19	1.48	1.43
9	6	101	BCL	CHD-C4C	2.19	1.45	1.39
9	Q	102	BCL	CHD-C4C	2.18	1.45	1.39
9	O	102	BCL	C1B-C2B	2.18	1.48	1.43
9	W	102	BCL	MG-NC	-2.18	2.01	2.06
11	P	102	U4Z	CBJ-CBH	2.18	1.40	1.35
9	S	103	BCL	MG-NA	-2.18	2.01	2.06
11	N	102	U4Z	CBN-CBL	-2.18	1.41	1.46
9	6	101	BCL	CHB-C4A	-2.18	1.32	1.37
9	H	101	BCL	CHC-C1C	-2.18	1.32	1.37
9	U	103	BCL	MG-NA	-2.18	2.01	2.06
10	4	101	U42	C22-C21	-2.18	1.41	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	K	102	BCL	CHC-C1C	-2.18	1.32	1.37
10	I	104	U42	C30-C29	-2.18	1.41	1.51
9	G	102	BCL	MG-NC	-2.17	2.01	2.06
11	A	102	U4Z	CBF-CBH	-2.17	1.41	1.46
9	M	701	BCL	C1B-C2B	2.17	1.48	1.43
9	2	102	BCL	MG-NC	-2.17	2.01	2.06
9	0	102	BCL	CHB-C4A	-2.17	1.32	1.37
9	Q	103	BCL	CHC-C1C	-2.17	1.32	1.37
9	0	102	BCL	C1B-C2B	2.17	1.48	1.43
10	B	101	U42	CBM-CBJ	-2.17	1.36	1.43
10	4	101	U42	CAT-CAS	-2.16	1.44	1.52
10	4	104	U42	CAT-CAS	-2.16	1.44	1.52
9	7	101	BCL	CHB-C4A	-2.16	1.32	1.37
11	1	102	U4Z	CBJ-CBH	2.16	1.40	1.35
9	U	102	BCL	MG-NA	-2.16	2.01	2.06
9	F	102	BCL	CHC-C1C	-2.15	1.32	1.37
9	8	102	BCL	CHC-C1C	-2.15	1.32	1.37
9	V	101	BCL	CHB-C4A	-2.15	1.32	1.37
9	K	102	BCL	C1D-C2D	2.15	1.49	1.45
11	P	102	U4Z	CAO-CAM	2.15	1.40	1.35
9	3	101	BCL	CHC-C1C	-2.15	1.32	1.37
10	4	101	U42	C26-C25	-2.15	1.41	1.51
9	K	101	BCL	CHC-C1C	-2.15	1.32	1.37
9	I	103	BCL	C1D-C2D	2.15	1.49	1.45
10	Q	101	U42	CBE-CBA	-2.15	1.36	1.43
9	G	102	BCL	CHC-C1C	-2.15	1.32	1.37
9	O	102	BCL	CHC-C1C	-2.15	1.32	1.37
11	V	102	U4Z	CBF-CBH	-2.15	1.41	1.46
10	I	104	U42	CBM-CBJ	-2.15	1.36	1.43
9	L	1002	BCL	C1B-C2B	2.15	1.48	1.43
11	J	102	U4Z	CAO-CAM	2.14	1.40	1.35
9	G	102	BCL	MG-NA	-2.14	2.01	2.06
10	I	104	U42	CBG-CBI	-2.14	1.36	1.43
11	H	102	U4Z	CAO-CAM	2.14	1.40	1.35
10	S	101	U42	CBM-CBJ	-2.14	1.36	1.43
9	J	101	BCL	CHC-C1C	-2.14	1.32	1.37
10	0	103	U42	CAL-CAM	-2.14	1.41	1.46
11	S	104	U4Z	CBF-CBH	-2.14	1.41	1.46
9	5	101	BCL	CHB-C4A	-2.14	1.32	1.37
9	W	102	BCL	CBD-CAD	-2.14	1.46	1.56
9	Q	102	BCL	CHB-C4A	-2.14	1.32	1.37
11	1	102	U4Z	CAV-CAR	2.14	1.40	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	8	102	BCL	CHD-C4C	2.13	1.45	1.39
11	7	102	U4Z	CAI-CAH	-2.13	1.47	1.51
9	F	101	BCL	CHB-C4A	-2.13	1.32	1.37
9	D	101	BCL	CHC-C1C	-2.13	1.32	1.37
9	4	103	BCL	CHB-C4A	-2.13	1.32	1.37
11	1	102	U4Z	CAO-CAM	2.13	1.40	1.35
9	7	101	BCL	MG-NC	-2.12	2.01	2.06
10	O	101	U42	CBM-CBJ	-2.12	1.36	1.43
10	I	104	U42	C29-C28	-2.12	1.41	1.51
10	4	101	U42	C25-C24	-2.12	1.41	1.51
9	0	102	BCL	CHC-C1C	-2.12	1.32	1.37
9	U	103	BCL	CHC-C1C	-2.12	1.32	1.37
11	C	401	U4Z	CAL-CAJ	2.12	1.39	1.33
9	I	103	BCL	CAA-C2A	-2.12	1.50	1.54
9	O	102	BCL	CHD-C4C	2.12	1.45	1.39
9	L	1001	BCL	CHB-C4A	-2.11	1.32	1.37
9	L	1002	BCL	CHB-C4A	-2.11	1.32	1.37
9	0	102	BCL	C1D-C2D	2.11	1.49	1.45
9	I	102	BCL	CHB-C4A	-2.11	1.32	1.37
9	N	101	BCL	MG-NA	-2.11	2.01	2.06
9	5	101	BCL	MG-NC	-2.11	2.01	2.06
9	G	102	BCL	C1B-C2B	2.11	1.48	1.43
10	U	101	U42	C25-C24	-2.10	1.41	1.51
9	P	101	BCL	C3B-C2B	2.10	1.49	1.42
10	U	101	U42	CAP-CAQ	2.10	1.40	1.34
10	I	104	U42	CBG-CBB	2.10	1.42	1.36
9	4	102	BCL	CHD-C4C	2.10	1.45	1.39
9	W	102	BCL	CHC-C1C	-2.10	1.32	1.37
9	A	101	BCL	C3B-C2B	2.10	1.49	1.42
9	1	101	BCL	CHB-C4A	-2.10	1.32	1.37
9	J	101	BCL	MG-NC	-2.10	2.01	2.06
9	M	701	BCL	C2C-C3C	-2.10	1.48	1.54
14	C	402	HEC	C3B-C2B	-2.10	1.34	1.41
9	1	101	BCL	C1B-C2B	2.10	1.48	1.43
9	F	102	BCL	CHB-C4A	-2.10	1.32	1.37
9	Q	103	BCL	OBD-CAD	2.09	1.26	1.22
9	8	102	BCL	C1B-C2B	2.09	1.48	1.43
9	S	103	BCL	CHC-C1C	-2.09	1.32	1.37
10	E	101	U42	CAU-CAR	-2.09	1.46	1.50
10	Q	101	U42	C22-C21	-2.09	1.41	1.51
9	B	102	BCL	CHB-C4A	-2.09	1.32	1.37
10	4	101	U42	C24-C23	-2.09	1.41	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	T	102	U4Z	CAO-CAM	2.09	1.40	1.35
9	8	103	BCL	C1D-C2D	2.09	1.49	1.45
9	Q	103	BCL	C1D-C2D	2.09	1.49	1.45
10	G	101	U42	CBG-CBI	-2.09	1.36	1.43
10	I	101	U42	C30-C29	-2.09	1.41	1.51
11	9	101	U4Z	CAI-CAH	-2.09	1.47	1.51
10	4	101	U42	O2-C18	-2.08	1.16	1.22
10	Q	101	U42	CAP-CAQ	2.08	1.40	1.34
9	Q	103	BCL	C1B-C2B	2.08	1.48	1.43
9	T	101	BCL	C3C-C4C	-2.08	1.49	1.51
9	W	102	BCL	C1D-C2D	2.08	1.49	1.45
9	Q	103	BCL	CBD-CAD	-2.08	1.47	1.56
9	6	102	BCL	CBD-CAD	-2.08	1.47	1.56
9	L	1001	BCL	MG-NC	-2.08	2.01	2.06
10	G	101	U42	C6-C5	-2.08	1.46	1.52
9	L	1002	BCL	C1D-C2D	2.08	1.49	1.45
9	W	101	BCL	CHB-C4A	-2.08	1.32	1.37
9	2	102	BCL	C3C-C4C	-2.07	1.49	1.51
9	G	102	BCL	CBD-CAD	-2.07	1.47	1.56
10	0	103	U42	C27-C26	-2.07	1.41	1.51
9	F	101	BCL	C3C-C4C	-2.07	1.49	1.51
10	G	101	U42	O2-C18	-2.07	1.16	1.22
9	0	101	BCL	CHD-C4C	2.07	1.45	1.39
9	D	101	BCL	CHB-C4A	-2.07	1.32	1.37
14	C	404	HEC	C3B-C2B	-2.07	1.34	1.41
9	O	103	BCL	C2C-C3C	-2.07	1.48	1.54
11	C	401	U4Z	CBJ-CBH	2.06	1.40	1.35
10	Q	101	U42	C25-C24	-2.06	1.41	1.51
9	4	102	BCL	C1B-C2B	2.06	1.48	1.43
10	8	101	U42	O1-CAY	-2.06	1.44	1.46
10	U	101	U42	CAB-CAD	-2.06	1.51	1.53
9	D	102	BCL	CHB-C4A	-2.06	1.32	1.37
9	M	701	BCL	MG-NC	-2.05	2.01	2.06
14	C	402	HEC	C3C-C2C	-2.05	1.34	1.41
9	M	701	BCL	C1D-C2D	2.05	1.49	1.45
10	I	104	U42	CAP-CAQ	2.05	1.40	1.34
9	V	101	BCL	C1B-C2B	2.05	1.47	1.43
9	2	101	BCL	MG-NC	-2.05	2.01	2.06
10	4	104	U42	C24-C23	-2.04	1.41	1.51
9	6	101	BCL	C3C-C4C	-2.04	1.49	1.51
9	O	103	BCL	C4D-CHA	2.04	1.45	1.38
13	L	1015	BGL	C3-C2	-2.04	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	J	101	BCL	CHB-C4A	-2.04	1.32	1.37
10	Q	101	U42	C20-C19	-2.04	1.44	1.52
9	2	101	BCL	CHB-C4A	-2.04	1.32	1.37
11	D	103	U4Z	CAI-CAH	-2.04	1.47	1.51
9	L	1002	BCL	MG-NA	-2.04	2.01	2.06
18	M	702	BPH	C3A-C2A	-2.03	1.53	1.54
18	L	1005	BPH	C4D-ND	-2.03	1.35	1.38
12	T	103	LMT	O1'-C1'	2.03	1.43	1.40
9	8	103	BCL	MG-NC	-2.03	2.01	2.06
9	D	101	BCL	MG-NC	-2.03	2.01	2.06
14	C	404	HEC	CMB-C2B	2.03	1.54	1.50
9	S	103	BCL	C3A-C2A	-2.03	1.49	1.54
10	U	104	U42	CAL-CAJ	2.03	1.39	1.33
9	6	102	BCL	CHC-C1C	-2.03	1.32	1.37
9	U	102	BCL	CHC-C1C	-2.03	1.32	1.37
9	U	102	BCL	C1B-C2B	2.03	1.47	1.43
10	4	101	U42	CAO-CAM	2.03	1.40	1.35
10	I	104	U42	O1-CAY	-2.03	1.44	1.46
9	I	103	BCL	CHC-C1C	-2.02	1.32	1.37
9	J	101	BCL	C2C-C3C	-2.02	1.49	1.54
14	C	403	HEC	CMC-C2C	2.02	1.54	1.50
9	N	101	BCL	CHB-C4A	-2.02	1.32	1.37
9	U	103	BCL	C1D-C2D	2.02	1.49	1.45
9	G	102	BCL	C3C-C4C	-2.02	1.49	1.51
9	4	103	BCL	C1B-C2B	2.02	1.47	1.43
10	S	101	U42	CAO-CAM	2.02	1.40	1.35
9	H	101	BCL	C3C-C4C	-2.02	1.49	1.51
9	B	103	BCL	CHC-C1C	-2.02	1.32	1.37
9	4	103	BCL	C2C-C3C	-2.02	1.49	1.54
9	4	102	BCL	CHC-C1C	-2.02	1.32	1.37
9	V	101	BCL	MG-NA	-2.01	2.01	2.06
9	4	103	BCL	CHC-C1C	-2.01	1.32	1.37
9	R	101	BCL	C2C-C3C	-2.01	1.49	1.54
9	L	1001	BCL	CHC-C1C	-2.01	1.32	1.37
9	3	101	BCL	MG-NC	-2.01	2.01	2.06
9	I	103	BCL	C1B-C2B	2.01	1.47	1.43
9	Q	102	BCL	C3C-C4C	-2.01	1.49	1.51
9	H	101	BCL	C4D-CHA	2.01	1.45	1.38
10	4	104	U42	CAL-CAJ	2.01	1.39	1.33
9	W	101	BCL	CHC-C1C	-2.00	1.32	1.37
9	1	101	BCL	MG-NC	-2.00	2.01	2.06
10	8	101	U42	C22-C21	-2.00	1.41	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	L	1002	BCL	C4D-CHA	2.00	1.45	1.38
9	9	102	BCL	MG-NC	-2.00	2.01	2.06
10	8	101	U42	CAL-CAM	-2.00	1.41	1.46
9	M	701	BCL	C4D-CHA	2.00	1.45	1.38

All (1726) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	G	101	U42	CAL-CAM-CAO	12.16	138.14	119.01
10	I	101	U42	CAL-CAM-CAO	10.47	135.47	119.01
10	4	104	U42	CAL-CAM-CAO	10.23	135.10	119.01
10	8	101	U42	CAL-CAM-CAO	9.55	134.04	119.01
10	U	101	U42	CAL-CAM-CAO	9.10	133.33	119.01
9	1	101	BCL	O2D-CGD-CBD	8.81	126.62	111.23
10	I	104	U42	CAL-CAM-CAO	8.80	132.85	119.01
14	C	404	HEC	CBB-CAB-C3B	-8.70	110.04	127.43
9	6	102	BCL	CMD-C2D-C1D	8.58	139.83	124.73
9	I	102	BCL	O2D-CGD-CBD	8.50	126.10	111.23
9	0	102	BCL	CMD-C2D-C1D	8.40	139.52	124.73
9	4	103	BCL	CMD-C2D-C1D	8.38	139.49	124.73
14	C	403	HEC	CBC-CAC-C3C	-8.36	110.72	127.43
9	E	102	BCL	CMD-C2D-C1D	8.30	139.35	124.73
10	I	104	U42	CBB-CBG-CBI	8.29	140.48	123.52
9	G	102	BCL	CMD-C2D-C1D	8.24	139.24	124.73
9	4	103	BCL	C2B-C1B-NB	8.17	118.80	110.33
9	I	103	BCL	CMD-C2D-C1D	8.15	139.08	124.73
9	K	102	BCL	CMD-C2D-C1D	8.10	138.99	124.73
10	S	101	U42	CAJ-CAL-CAM	8.09	138.20	126.23
9	W	102	BCL	CMD-C2D-C1D	8.09	138.97	124.73
9	Q	103	BCL	CMD-C2D-C1D	8.06	138.92	124.73
9	B	103	BCL	CMD-C2D-C1D	8.05	138.90	124.73
14	C	402	HEC	CBC-CAC-C3C	-8.02	111.41	127.43
14	C	402	HEC	CBB-CAB-C3B	-7.98	111.48	127.43
9	S	103	BCL	CMD-C2D-C1D	7.98	138.78	124.73
9	O	103	BCL	CMD-C2D-C1D	7.97	138.77	124.73
9	8	103	BCL	CMD-C2D-C1D	7.97	138.76	124.73
9	0	102	BCL	C2B-C1B-NB	7.94	118.56	110.33
14	C	403	HEC	CBB-CAB-C3B	-7.90	111.65	127.43
18	L	1003	BPH	O2D-CGD-CBD	7.89	119.61	110.95
9	U	103	BCL	CMD-C2D-C1D	7.80	138.46	124.73
10	U	104	U42	CAL-CAM-CAO	7.74	131.18	119.01
9	2	102	BCL	CMD-C2D-C1D	7.71	138.31	124.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	L	1002	BCL	CMD-C2D-C1D	7.65	138.20	124.73
10	I	101	U42	CAJ-CAL-CAM	7.63	137.52	126.23
14	C	405	HEC	CBC-CAC-C3C	-7.59	112.26	127.43
9	S	103	BCL	C2B-C1B-NB	7.54	118.14	110.33
10	G	101	U42	CAN-CAM-CAL	-7.51	106.62	118.09
10	4	101	U42	CBB-CBG-CBI	7.49	138.84	123.52
10	G	101	U42	CAJ-CAL-CAM	7.43	137.23	126.23
9	B	103	BCL	C2B-C1B-NB	7.40	118.00	110.33
14	C	405	HEC	CBB-CAB-C3B	-7.36	112.73	127.43
9	L	1001	BCL	CMD-C2D-C1D	7.26	137.51	124.73
9	M	701	BCL	CMD-C2D-C1D	7.19	137.39	124.73
9	M	701	BCL	O2D-CGD-CBD	7.17	123.76	111.23
9	6	101	BCL	C2B-C1B-NB	7.10	117.69	110.33
9	S	102	BCL	C2B-C1B-NB	7.05	117.64	110.33
10	U	104	U42	CBB-CBG-CBI	7.04	137.92	123.52
9	L	1002	BCL	C2B-C1B-NB	7.01	117.59	110.33
14	C	404	HEC	CBC-CAC-C3C	-7.00	113.44	127.43
10	I	101	U42	CBB-CBG-CBI	7.00	137.84	123.52
10	0	103	U42	CBB-CBG-CBI	6.90	137.63	123.52
9	H	101	BCL	CMD-C2D-C1D	6.87	136.83	124.73
9	J	101	BCL	C2B-C1B-NB	6.87	117.45	110.33
9	U	102	BCL	C2B-C1B-NB	6.86	117.44	110.33
9	M	701	BCL	C2B-C1B-NB	6.81	117.39	110.33
9	F	101	BCL	C2B-C1B-NB	6.81	117.39	110.33
18	L	1003	BPH	C2B-C1B-NB	6.77	114.33	109.43
9	D	101	BCL	C2B-C1B-NB	6.76	117.33	110.33
9	F	101	BCL	CMD-C2D-C1D	6.75	136.61	124.73
9	Q	102	BCL	C2B-C1B-NB	6.74	117.32	110.33
9	J	101	BCL	CMD-C2D-C1D	6.73	136.58	124.73
9	7	101	BCL	C2B-C1B-NB	6.71	117.28	110.33
9	F	102	BCL	C2B-C1B-NB	6.70	117.28	110.33
9	W	101	BCL	C2B-C1B-NB	6.68	117.25	110.33
9	T	101	BCL	CMD-C2D-C1D	6.68	136.48	124.73
9	L	1001	BCL	C2B-C1B-NB	6.67	117.25	110.33
10	0	103	U42	CBG-CBB-CAV	6.64	137.10	123.52
9	1	101	BCL	CMD-C2D-C1D	6.64	136.41	124.73
9	V	101	BCL	C2B-C1B-NB	6.63	117.20	110.33
9	7	101	BCL	CMD-C2D-C1D	6.63	136.41	124.73
9	5	101	BCL	CMD-C2D-C1D	6.62	136.39	124.73
9	Q	103	BCL	C2B-C1B-NB	6.62	117.19	110.33
9	I	103	BCL	C2B-C1B-NB	6.62	117.19	110.33
9	3	101	BCL	C2B-C1B-NB	6.61	117.19	110.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	101	BCL	CAC-C3C-C4C	6.60	127.23	112.58
9	B	102	BCL	C2B-C1B-NB	6.59	117.16	110.33
9	3	101	BCL	CMD-C2D-C1D	6.59	136.34	124.73
9	D	101	BCL	CMD-C2D-C1D	6.56	136.28	124.73
9	I	102	BCL	C2B-C1B-NB	6.56	117.13	110.33
9	G	102	BCL	C2B-C1B-NB	6.55	117.12	110.33
9	K	101	BCL	C2B-C1B-NB	6.55	117.11	110.33
9	D	102	BCL	C2B-C1B-NB	6.54	117.11	110.33
9	E	102	BCL	C2B-C1B-NB	6.54	117.10	110.33
9	P	101	BCL	C4A-NA-C1A	-6.53	103.70	106.68
9	2	101	BCL	C2B-C1B-NB	6.52	117.09	110.33
9	9	102	BCL	CMD-C2D-C1D	6.50	136.18	124.73
9	W	102	BCL	C2B-C1B-NB	6.50	117.07	110.33
9	L	1001	BCL	O2D-CGD-CBD	6.49	122.57	111.23
9	N	101	BCL	C2B-C1B-NB	6.49	117.05	110.33
9	P	101	BCL	CAC-C3C-C4C	6.48	126.98	112.58
9	0	101	BCL	C2B-C1B-NB	6.45	117.02	110.33
9	1	101	BCL	C2B-C1B-NB	6.45	117.01	110.33
9	6	102	BCL	C2B-C1B-NB	6.44	117.00	110.33
9	5	101	BCL	C2B-C1B-NB	6.43	117.00	110.33
9	8	102	BCL	C2B-C1B-NB	6.43	116.99	110.33
9	N	101	BCL	CMD-C2D-C1D	6.41	136.02	124.73
9	9	102	BCL	O2D-CGD-CBD	6.41	122.43	111.23
9	H	101	BCL	C2B-C1B-NB	6.41	116.97	110.33
9	4	102	BCL	C2B-C1B-NB	6.40	116.97	110.33
10	B	101	U42	CBB-CBG-CBI	6.36	136.53	123.52
9	9	102	BCL	C2B-C1B-NB	6.34	116.91	110.33
9	O	103	BCL	C2B-C1B-NB	6.33	116.89	110.33
9	P	101	BCL	O2D-CGD-CBD	6.32	122.27	111.23
9	R	101	BCL	O2D-CGD-CBD	6.29	122.22	111.23
9	A	101	BCL	CMC-C2C-C1C	6.26	128.59	111.77
9	O	102	BCL	C2B-C1B-NB	6.25	116.81	110.33
9	K	102	BCL	O2D-CGD-CBD	6.24	122.15	111.23
11	C	401	U4Z	CBN-CBL-CBI	6.24	128.82	119.01
10	8	101	U42	CAJ-CAL-CAM	6.24	135.47	126.23
9	U	103	BCL	C2B-C1B-NB	6.23	116.79	110.33
9	P	101	BCL	CMC-C2C-C1C	6.22	128.49	111.77
9	R	101	BCL	CMD-C2D-C1D	6.21	135.66	124.73
10	I	104	U42	CAQ-CAR-CAV	6.20	128.76	119.01
9	D	101	BCL	O2D-CGD-CBD	6.19	122.05	111.23
9	3	101	BCL	O2D-CGD-CBD	6.18	122.04	111.23
10	0	103	U42	CAJ-CAL-CAM	6.16	135.35	126.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	0	103	U42	CAP-CAO-CAM	6.16	135.92	127.28
9	N	101	BCL	O2D-CGD-CBD	6.13	121.95	111.23
9	K	102	BCL	C2B-C1B-NB	6.13	116.68	110.33
9	V	101	BCL	CMD-C2D-C1D	6.12	135.51	124.73
10	0	103	U42	CAL-CAM-CAO	6.11	128.62	119.01
9	A	101	BCL	O2D-CGD-CBD	6.11	121.91	111.23
9	T	101	BCL	O2D-CGD-CBD	6.09	121.87	111.23
11	C	401	U4Z	CBO-CBL-CBI	-6.08	112.97	122.82
10	U	104	U42	CAJ-CAL-CAM	6.06	135.19	126.23
9	R	101	BCL	C2B-C1B-NB	6.00	116.55	110.33
9	T	101	BCL	C2B-C1B-NB	6.00	116.55	110.33
9	O	103	BCL	C3D-C2D-C1D	-5.98	97.67	105.83
9	J	101	BCL	O2D-CGD-CBD	5.97	121.67	111.23
10	I	101	U42	CAN-CAM-CAL	-5.96	108.98	118.09
9	4	103	BCL	CHD-C1D-ND	-5.95	116.43	124.80
9	6	102	BCL	CHD-C1D-ND	-5.94	116.45	124.80
10	O	101	U42	CBB-CBG-CBI	5.93	135.66	123.52
9	E	102	BCL	CHD-C1D-ND	-5.92	116.47	124.80
9	K	102	BCL	CHD-C1D-ND	-5.92	116.48	124.80
9	I	103	BCL	CHD-C1D-ND	-5.91	116.48	124.80
9	B	103	BCL	CHD-C1D-ND	-5.91	116.49	124.80
10	S	101	U42	CBB-CBG-CBI	5.90	135.60	123.52
9	H	101	BCL	O2D-CGD-CBD	5.87	121.50	111.23
10	B	101	U42	CBE-CBA-CAW	-5.87	119.44	127.69
9	S	103	BCL	CHD-C1D-ND	-5.86	116.56	124.80
9	F	101	BCL	O2D-CGD-CBD	5.85	121.46	111.23
9	5	101	BCL	O2D-CGD-CBD	5.84	121.44	111.23
9	G	102	BCL	CHD-C1D-ND	-5.84	116.59	124.80
9	0	102	BCL	CHD-C1D-ND	-5.83	116.60	124.80
9	6	102	BCL	C3D-C2D-C1D	-5.83	97.87	105.83
9	Q	103	BCL	C3D-C2D-C1D	-5.82	97.88	105.83
10	I	101	U42	CBG-CBI-CBL	5.80	135.42	127.28
9	8	103	BCL	C2B-C1B-NB	5.79	116.33	110.33
10	4	104	U42	CAJ-CAL-CAM	5.78	134.78	126.23
9	O	103	BCL	CHD-C1D-ND	-5.76	116.69	124.80
10	0	103	U42	CBE-CBA-CAW	-5.74	119.62	127.69
10	8	101	U42	CBG-CBI-CBL	5.74	135.33	127.28
10	O	101	U42	CAJ-CAL-CAM	5.73	134.71	126.23
9	D	102	BCL	O2D-CGD-CBD	5.71	121.21	111.23
10	E	101	U42	CBB-CBG-CBI	5.71	135.19	123.52
9	8	103	BCL	CHD-C1D-ND	-5.70	116.78	124.80
9	7	101	BCL	O2D-CGD-CBD	5.70	121.19	111.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	I	101	U42	CAQ-CAR-CAV	5.69	127.97	119.01
9	Q	103	BCL	CHD-C1D-ND	-5.69	116.79	124.80
9	W	102	BCL	C3D-C2D-C1D	-5.68	98.08	105.83
9	I	103	BCL	C3D-C2D-C1D	-5.66	98.11	105.83
9	L	1001	BCL	CHD-C1D-ND	-5.64	116.86	124.80
9	2	102	BCL	CHD-C1D-ND	-5.63	116.88	124.80
9	W	102	BCL	CHD-C1D-ND	-5.61	116.91	124.80
9	B	103	BCL	C3D-C2D-C1D	-5.61	98.18	105.83
9	U	103	BCL	C3D-C2D-C1D	-5.60	98.18	105.83
9	U	103	BCL	CHD-C1D-ND	-5.58	116.94	124.80
9	2	101	BCL	CMD-C2D-C1D	5.58	134.55	124.73
9	4	103	BCL	C3D-C2D-C1D	-5.57	98.23	105.83
9	B	103	BCL	O2D-CGD-CBD	5.56	120.95	111.23
10	Q	101	U42	CAJ-CAL-CAM	5.55	134.44	126.23
18	L	1003	BPH	CMC-C2C-C1C	5.54	126.54	114.61
9	K	101	BCL	O2D-CGD-CBD	5.53	120.89	111.23
9	E	102	BCL	C3D-C2D-C1D	-5.52	98.30	105.83
9	0	102	BCL	O2D-CGD-CBD	5.50	120.85	111.23
10	U	104	U42	CBG-CBI-CBL	5.50	134.99	127.28
9	0	102	BCL	C3D-C2D-C1D	-5.47	98.36	105.83
9	H	101	BCL	CHD-C1D-ND	-5.47	117.10	124.80
9	S	103	BCL	C3D-C2D-C1D	-5.46	98.38	105.83
9	S	103	BCL	O2D-CGD-CBD	5.45	120.77	111.23
10	O	101	U42	CBG-CBB-CAV	5.41	134.58	123.52
9	2	102	BCL	O2D-CGD-CBD	5.40	120.67	111.23
10	B	101	U42	CAQ-CAR-CAV	5.40	127.50	119.01
9	Q	103	BCL	O2D-CGD-CBD	5.39	120.65	111.23
9	G	102	BCL	C3D-C2D-C1D	-5.38	98.49	105.83
9	K	102	BCL	C3D-C2D-C1D	-5.37	98.51	105.83
10	S	101	U42	CAC-CAB-CAD	5.36	118.23	110.44
10	U	101	U42	CAN-CAM-CAO	-5.34	114.17	122.82
9	U	103	BCL	O2D-CGD-CBD	5.34	120.56	111.23
10	B	101	U42	CAL-CAM-CAO	5.32	127.38	119.01
10	O	101	U42	CAL-CAM-CAO	5.31	127.37	119.01
10	O	101	U42	CAC-CAB-CAD	5.30	118.13	110.44
10	O	101	U42	CBG-CBI-CBL	5.29	134.69	127.28
10	Q	101	U42	CAL-CAM-CAO	5.27	127.30	119.01
10	4	104	U42	CAN-CAM-CAL	-5.27	110.04	118.09
9	P	101	BCL	C2B-C1B-NB	5.25	115.78	110.33
9	2	102	BCL	C3D-C2D-C1D	-5.25	98.66	105.83
9	W	101	BCL	O2D-CGD-CBD	5.25	120.40	111.23
9	H	101	BCL	C3D-C2D-C1D	-5.25	98.67	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	W	101	BCL	CMD-C2D-C1D	5.24	133.95	124.73
9	A	101	BCL	C4A-NA-C1A	-5.24	104.29	106.68
10	E	101	U42	CBG-CBI-CBL	5.23	134.61	127.28
9	F	102	BCL	O2D-CGD-CBD	5.21	120.34	111.23
9	L	1002	BCL	C3D-C2D-C1D	-5.19	98.75	105.83
9	O	102	BCL	C2D-C1D-ND	5.19	115.26	110.13
9	8	103	BCL	C3D-C2D-C1D	-5.18	98.76	105.83
9	2	101	BCL	CHD-C1D-ND	-5.18	117.51	124.80
10	U	101	U42	CBB-CBG-CBI	5.17	134.10	123.52
9	L	1002	BCL	CHD-C1D-ND	-5.17	117.52	124.80
9	U	102	BCL	O2D-CGD-CBD	5.14	120.22	111.23
10	G	101	U42	CBG-CBI-CBL	5.13	134.48	127.28
9	S	102	BCL	CMD-C2D-C1D	5.13	133.75	124.73
9	M	701	BCL	CHD-C1D-ND	-5.13	117.59	124.80
9	4	102	BCL	O2D-CGD-CBD	5.12	120.19	111.23
9	D	101	BCL	C3D-C2D-C1D	-5.10	98.87	105.83
9	1	101	BCL	C3D-C2D-C1D	-5.10	98.87	105.83
9	5	101	BCL	CHD-C1D-ND	-5.09	117.64	124.80
9	O	103	BCL	C4A-NA-C1A	5.09	109.00	106.68
9	J	101	BCL	C3D-C2D-C1D	-5.08	98.90	105.83
10	I	104	U42	CAO-CAP-CAQ	5.07	137.88	123.20
9	9	102	BCL	C3D-C2D-C1D	-5.06	98.93	105.83
9	2	101	BCL	O2D-CGD-CBD	5.04	120.04	111.23
9	O	102	BCL	C1D-ND-C4D	-5.03	102.79	106.31
9	O	102	BCL	C3C-C4C-CHD	-5.02	112.80	123.39
9	D	101	BCL	CHD-C1D-ND	-5.02	117.73	124.80
9	7	101	BCL	C3D-C2D-C1D	-5.02	98.98	105.83
9	F	101	BCL	C3D-C2D-C1D	-5.02	98.98	105.83
9	6	102	BCL	C3B-C4B-NB	5.01	116.37	109.76
9	8	102	BCL	O2D-CGD-CBD	5.01	119.98	111.23
10	U	104	U42	CBB-CAV-CAR	4.99	134.28	127.28
10	I	104	U42	CAN-CAM-CAO	-4.98	114.75	122.82
9	6	101	BCL	C3C-C4C-CHD	-4.97	112.91	123.39
9	J	101	BCL	CHD-C1D-ND	-4.97	117.81	124.80
9	T	101	BCL	C3D-C2D-C1D	-4.95	99.07	105.83
9	0	101	BCL	C3C-C4C-CHD	-4.95	112.96	123.39
9	O	102	BCL	C1-C2-C3	-4.93	118.11	126.20
9	B	102	BCL	O2D-CGD-CBD	4.93	119.85	111.23
9	W	102	BCL	O2D-CGD-CBD	4.92	119.83	111.23
9	H	101	BCL	C3C-C4C-CHD	-4.92	113.03	123.39
10	4	104	U42	CAN-CAM-CAO	-4.91	114.85	122.82
9	0	101	BCL	O2D-CGD-CBD	4.91	119.82	111.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	Q	102	BCL	C3C-C4C-CHD	-4.91	113.04	123.39
10	U	101	U42	CAO-CAP-CAQ	4.90	137.40	123.20
9	4	103	BCL	O2D-CGD-CBD	4.88	119.76	111.23
9	N	101	BCL	C3D-C2D-C1D	-4.88	99.18	105.83
9	7	101	BCL	CHD-C1D-ND	-4.87	117.94	124.80
9	1	101	BCL	CHD-C1D-ND	-4.87	117.95	124.80
10	4	104	U42	CBG-CBB-CAV	4.87	133.48	123.52
10	G	101	U42	CBE-CBA-CAW	-4.87	120.85	127.69
9	3	101	BCL	CHD-C1D-ND	-4.86	117.97	124.80
9	V	101	BCL	C3D-C2D-C1D	-4.85	99.21	105.83
9	5	101	BCL	C3D-C2D-C1D	-4.84	99.23	105.83
9	F	101	BCL	CHD-C1D-ND	-4.83	118.00	124.80
9	P	101	BCL	C1D-CHD-C4C	-4.83	114.98	126.62
9	D	102	BCL	C3C-C4C-CHD	-4.82	113.22	123.39
10	8	101	U42	CAN-CAM-CAL	-4.82	110.72	118.09
9	S	102	BCL	O2D-CGD-CBD	4.82	119.65	111.23
11	J	102	U4Z	CBB-CBG-CBI	4.82	133.37	123.52
9	3	101	BCL	C3D-C2D-C1D	-4.81	99.27	105.83
9	K	101	BCL	CMD-C2D-C1D	4.81	133.20	124.73
10	O	101	U42	CBB-CAV-CAR	4.81	134.02	127.28
10	U	101	U42	CAJ-CAL-CAM	4.80	133.34	126.23
9	G	102	BCL	O2D-CGD-CBD	4.80	119.62	111.23
9	2	101	BCL	C3D-C2D-C1D	-4.79	99.29	105.83
10	U	104	U42	CAN-CAM-CAO	-4.79	115.06	122.82
9	B	102	BCL	C3C-C4C-CHD	-4.79	113.30	123.39
9	O	103	BCL	C3C-C4C-CHD	-4.78	113.31	123.39
18	L	1005	BPH	C4D-CHA-CBD	-4.77	106.17	108.45
9	A	101	BCL	C1D-CHD-C4C	-4.77	115.11	126.62
9	9	102	BCL	CHD-C1D-ND	-4.77	118.09	124.80
9	E	102	BCL	O2D-CGD-CBD	4.77	119.57	111.23
9	V	101	BCL	O2D-CGD-CBD	4.77	119.56	111.23
9	T	101	BCL	CHD-C1D-ND	-4.77	118.10	124.80
9	0	101	BCL	C2D-C1D-ND	4.76	114.84	110.13
9	D	101	BCL	C3C-C4C-CHD	-4.76	113.35	123.39
9	Q	102	BCL	CMD-C2D-C1D	4.76	133.11	124.73
9	O	102	BCL	C3D-C2D-C1D	-4.76	99.34	105.83
9	W	102	BCL	C3C-C4C-CHD	-4.76	113.36	123.39
9	Q	103	BCL	C3C-C4C-CHD	-4.75	113.37	123.39
9	S	102	BCL	C3C-C4C-CHD	-4.75	113.37	123.39
9	B	102	BCL	C3D-C2D-C1D	-4.75	99.35	105.83
9	L	1001	BCL	O2D-CGD-O1D	-4.74	114.61	123.85
9	R	101	BCL	C3D-C2D-C1D	-4.74	99.36	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	101	U42	CBG-CBI-CBL	4.71	133.89	127.28
9	M	701	BCL	C3D-C2D-C1D	-4.71	99.40	105.83
9	0	101	BCL	CMD-C2D-C1D	4.71	133.02	124.73
9	B	102	BCL	C2D-C1D-ND	4.71	114.78	110.13
10	G	101	U42	CAN-CAM-CAO	-4.71	115.19	122.82
9	S	103	BCL	C3C-C4C-CHD	-4.70	113.48	123.39
10	8	101	U42	CAN-CAM-CAO	-4.70	115.20	122.82
10	S	101	U42	CAQ-CAR-CAV	4.70	126.40	119.01
9	I	102	BCL	CMD-C2D-C1D	4.69	132.98	124.73
9	O	102	BCL	O2D-CGD-CBD	4.68	119.41	111.23
9	U	103	BCL	C3C-C4C-CHD	-4.68	113.53	123.39
9	4	102	BCL	C3C-C4C-CHD	-4.68	113.53	123.39
10	Q	101	U42	CBB-CAV-CAR	4.68	133.84	127.28
9	2	102	BCL	C2B-C1B-NB	4.67	115.17	110.33
10	Q	101	U42	CBG-CBB-CAV	4.67	133.07	123.52
9	U	102	BCL	CMD-C2D-C1D	4.66	132.94	124.73
9	I	102	BCL	C3C-C4C-CHD	-4.66	113.56	123.39
9	0	101	BCL	C3D-C2D-C1D	-4.66	99.47	105.83
9	2	101	BCL	C1D-ND-C4D	-4.65	103.05	106.31
9	I	103	BCL	C3C-C4C-CHD	-4.65	113.58	123.39
9	8	102	BCL	C3C-C4C-CHD	-4.65	113.59	123.39
9	2	101	BCL	C2D-C1D-ND	4.65	114.73	110.13
9	F	102	BCL	CMD-C2D-C1D	4.64	132.91	124.73
9	6	101	BCL	C3D-C2D-C1D	-4.64	99.50	105.83
10	B	101	U42	CAX-CAT-CAS	4.64	123.48	112.33
9	A	101	BCL	C2B-C1B-NB	4.63	115.13	110.33
9	U	102	BCL	C3C-C4C-CHD	-4.63	113.62	123.39
9	N	101	BCL	CHD-C1D-ND	-4.62	118.30	124.80
9	6	101	BCL	O2D-CGD-CBD	4.62	119.31	111.23
9	Q	102	BCL	C2D-C1D-ND	4.62	114.70	110.13
9	0	101	BCL	C1D-ND-C4D	-4.62	103.07	106.31
9	D	102	BCL	C3D-C2D-C1D	-4.62	99.53	105.83
10	B	101	U42	CBG-CBB-CAV	4.61	132.95	123.52
9	6	101	BCL	C2D-C1D-ND	4.61	114.69	110.13
9	Q	102	BCL	C3D-C2D-C1D	-4.61	99.54	105.83
9	M	701	BCL	C1C-NC-C4C	-4.61	104.58	106.68
9	F	102	BCL	C3C-C4C-CHD	-4.60	113.69	123.39
9	4	103	BCL	C3C-C4C-CHD	-4.60	113.70	123.39
9	O	103	BCL	C2D-C1D-ND	4.60	114.68	110.13
9	Q	102	BCL	O2D-CGD-CBD	4.60	119.27	111.23
9	4	103	BCL	C4A-NA-C1A	4.59	108.78	106.68
9	A	101	BCL	CHD-C1D-ND	-4.58	118.36	124.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	E	101	U42	CBB-CAV-CAR	4.58	133.70	127.28
9	E	102	BCL	C3C-C4C-CHD	-4.57	113.75	123.39
9	4	102	BCL	C2D-C1D-ND	4.57	114.65	110.13
9	Q	102	BCL	C1D-ND-C4D	-4.57	103.11	106.31
11	C	401	U4Z	CBB-CBG-CBI	4.57	132.87	123.52
9	0	102	BCL	C1D-ND-C4D	-4.56	103.11	106.31
10	I	101	U42	CAN-CAM-CAO	-4.55	115.44	122.82
9	W	101	BCL	C3D-C2D-C1D	-4.54	99.63	105.83
9	8	103	BCL	O2D-CGD-CBD	4.54	119.17	111.23
9	S	102	BCL	C3D-C2D-C1D	-4.54	99.64	105.83
9	Q	103	BCL	C1-C2-C3	-4.54	118.77	126.20
9	Q	103	BCL	C2D-C1D-ND	4.53	114.61	110.13
9	J	101	BCL	C3C-C4C-CHD	-4.53	113.84	123.39
9	W	101	BCL	CHD-C1D-ND	-4.53	118.43	124.80
9	V	101	BCL	CHD-C1D-ND	-4.53	118.43	124.80
10	E	101	U42	CBG-CBB-CAV	4.52	132.76	123.52
9	R	101	BCL	CHD-C1D-ND	-4.52	118.44	124.80
9	1	101	BCL	C2D-C1D-ND	4.51	114.59	110.13
9	W	102	BCL	C2D-C1D-ND	4.51	114.59	110.13
11	N	102	U4Z	CBB-CBG-CBI	4.51	132.75	123.52
9	D	102	BCL	C2D-C1D-ND	4.51	114.59	110.13
9	S	102	BCL	C1D-ND-C4D	-4.50	103.15	106.31
9	K	101	BCL	C3C-C4C-CHD	-4.50	113.91	123.39
9	I	103	BCL	C1D-ND-C4D	-4.49	103.16	106.31
9	4	102	BCL	C3D-C2D-C1D	-4.49	99.70	105.83
10	4	104	U42	CAQ-CAR-CAV	4.49	126.07	119.01
9	B	103	BCL	C3C-C4C-CHD	-4.49	113.93	123.39
9	L	1001	BCL	C3D-C2D-C1D	-4.48	99.71	105.83
9	S	102	BCL	C2D-C1D-ND	4.48	114.56	110.13
9	E	102	BCL	C1D-ND-C4D	-4.48	103.17	106.31
9	4	102	BCL	CMD-C2D-C1D	4.48	132.62	124.73
9	6	102	BCL	O2D-CGD-CBD	4.48	119.06	111.23
9	I	103	BCL	O2D-CGD-CBD	4.47	119.05	111.23
9	U	103	BCL	C1D-ND-C4D	-4.47	103.17	106.31
10	I	101	U42	CAX-CAT-CAS	4.47	123.08	112.33
10	U	101	U42	CBB-CAV-CAR	4.47	133.55	127.28
9	9	102	BCL	C3C-C4C-CHD	-4.47	113.97	123.39
9	T	101	BCL	C3C-C4C-CHD	-4.46	113.98	123.39
9	H	101	BCL	C2D-C1D-ND	4.46	114.54	110.13
9	1	101	BCL	C3C-C4C-CHD	-4.46	113.99	123.39
9	P	101	BCL	C1C-NC-C4C	-4.46	104.64	106.68
10	8	101	U42	CBB-CBG-CBI	4.45	132.62	123.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	R	101	BCL	C3C-C4C-CHD	-4.44	114.03	123.39
9	U	103	BCL	C2D-C1D-ND	4.44	114.52	110.13
9	6	101	BCL	CMD-C2D-C1D	4.43	132.54	124.73
9	D	101	BCL	C2D-C1D-ND	4.43	114.51	110.13
9	U	102	BCL	C3D-C2D-C1D	-4.43	99.78	105.83
9	I	103	BCL	C2D-C1D-ND	4.43	114.51	110.13
9	D	102	BCL	CMD-C2D-C1D	4.43	132.52	124.73
9	0	102	BCL	C2D-C1D-ND	4.42	114.50	110.13
9	I	102	BCL	C3D-C2D-C1D	-4.41	99.81	105.83
9	0	102	BCL	C3C-C4C-CHD	-4.40	114.11	123.39
9	W	102	BCL	C1D-ND-C4D	-4.40	103.22	106.31
9	8	102	BCL	C3D-C2D-C1D	-4.40	99.82	105.83
9	F	101	BCL	C3C-C4C-CHD	-4.40	114.12	123.39
9	4	102	BCL	C1D-ND-C4D	-4.39	103.23	106.31
9	8	103	BCL	C3B-C4B-NB	4.39	115.55	109.76
9	8	102	BCL	C2D-C1D-ND	4.39	114.47	110.13
9	Q	103	BCL	C1D-ND-C4D	-4.37	103.24	106.31
9	6	102	BCL	C2D-C1D-ND	4.37	114.45	110.13
9	K	102	BCL	C3C-C4C-CHD	-4.37	114.18	123.39
9	U	102	BCL	C2D-C1D-ND	4.37	114.45	110.13
9	J	101	BCL	C2D-C1D-ND	4.36	114.44	110.13
9	6	102	BCL	C1D-ND-C4D	-4.34	103.26	106.31
10	U	101	U42	CBG-CBI-CBL	4.34	133.36	127.28
9	B	102	BCL	C1D-ND-C4D	-4.34	103.27	106.31
10	G	101	U42	CBB-CAV-CAR	4.34	133.36	127.28
9	2	102	BCL	C3C-C4C-CHD	-4.33	114.27	123.39
9	4	103	BCL	C2D-C1D-ND	4.33	114.41	110.13
9	7	101	BCL	C3B-C4B-NB	4.33	115.47	109.76
18	L	1003	BPH	C4A-C3A-C2A	-4.33	98.72	102.84
9	T	101	BCL	C3B-C4B-NB	4.32	115.46	109.76
10	S	101	U42	CBG-CBB-CAV	4.32	132.36	123.52
9	N	101	BCL	C3C-C4C-CHD	-4.32	114.28	123.39
11	H	102	U4Z	CBB-CBG-CBI	4.32	132.35	123.52
9	2	101	BCL	C3C-C4C-CHD	-4.32	114.29	123.39
9	3	101	BCL	C3C-C4C-CHD	-4.31	114.31	123.39
9	K	101	BCL	C3D-C2D-C1D	-4.31	99.95	105.83
9	6	101	BCL	C1D-ND-C4D	-4.30	103.29	106.31
9	N	101	BCL	C3B-C4B-NB	4.30	115.43	109.76
9	O	103	BCL	O2D-CGD-CBD	4.30	118.75	111.23
9	L	1002	BCL	C3C-C4C-CHD	-4.29	114.35	123.39
9	M	701	BCL	C3B-C4B-NB	4.28	115.41	109.76
9	9	102	BCL	C2D-C1D-ND	4.28	114.37	110.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	0	103	U42	CBF-CBH-CBJ	4.28	125.74	119.01
9	O	102	BCL	CMD-C2D-C1D	4.28	132.27	124.73
9	F	102	BCL	C3D-C2D-C1D	-4.28	100.00	105.83
9	F	102	BCL	C2D-C1D-ND	4.27	114.36	110.13
11	F	103	U4Z	CBB-CBG-CBI	4.27	132.26	123.52
10	0	103	U42	CBB-CAV-CAR	4.27	133.27	127.28
9	Q	103	BCL	C3B-C4B-NB	4.27	115.39	109.76
9	S	103	BCL	C3B-C4B-NB	4.27	115.39	109.76
9	W	101	BCL	C2D-C1D-ND	4.26	114.34	110.13
10	0	103	U42	CBN-CBL-CBI	4.26	125.71	119.01
9	K	102	BCL	C2D-C1D-ND	4.26	114.34	110.13
9	0	102	BCL	C3B-C4B-NB	4.26	115.38	109.76
9	S	103	BCL	C2D-C1D-ND	4.26	114.34	110.13
9	B	103	BCL	C2D-C1D-ND	4.25	114.34	110.13
9	B	103	BCL	C1D-ND-C4D	-4.24	103.33	106.31
9	F	101	BCL	C3B-C4B-NB	4.24	115.36	109.76
9	8	102	BCL	CMD-C2D-C1D	4.23	132.19	124.73
9	K	102	BCL	C3B-C4B-NB	4.23	115.34	109.76
10	U	104	U42	CAO-CAP-CAQ	4.22	135.44	123.20
9	J	101	BCL	C1D-ND-C4D	-4.22	103.35	106.31
10	Q	101	U42	CBB-CBG-CBI	4.22	132.15	123.52
11	D	103	U4Z	CBB-CBG-CBI	4.22	132.15	123.52
9	F	102	BCL	C1D-ND-C4D	-4.21	103.36	106.31
9	A	101	BCL	C1C-NC-C4C	-4.21	104.76	106.68
9	T	101	BCL	C2D-C1D-ND	4.21	114.29	110.13
9	V	101	BCL	C3C-C4C-CHD	-4.20	114.53	123.39
9	E	102	BCL	C2D-C1D-ND	4.20	114.29	110.13
9	K	102	BCL	C1D-ND-C4D	-4.20	103.36	106.31
9	I	102	BCL	C2D-C1D-ND	4.20	114.28	110.13
9	G	102	BCL	C3B-C4B-NB	4.20	115.30	109.76
9	B	102	BCL	CMD-C2D-C1D	4.20	132.12	124.73
9	5	101	BCL	C3B-C4B-NB	4.19	115.29	109.76
9	U	102	BCL	C1D-ND-C4D	-4.19	103.37	106.31
9	4	103	BCL	C1D-ND-C4D	-4.18	103.38	106.31
9	S	102	BCL	CHD-C1D-ND	-4.16	118.94	124.80
11	V	102	U4Z	CBB-CBG-CBI	4.16	132.03	123.52
10	I	104	U42	CBG-CBB-CAV	4.16	132.03	123.52
9	6	102	BCL	C1-C2-C3	-4.16	119.38	126.20
9	D	102	BCL	CHD-C1D-ND	-4.16	118.95	124.80
9	K	101	BCL	C1D-ND-C4D	-4.16	103.40	106.31
9	K	101	BCL	CHD-C1D-ND	-4.15	118.96	124.80
9	5	101	BCL	C3C-C4C-CHD	-4.15	114.64	123.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	Q	102	BCL	CHD-C1D-ND	-4.15	118.96	124.80
9	B	103	BCL	C3B-C4B-NB	4.15	115.23	109.76
9	L	1002	BCL	C2D-C1D-ND	4.15	114.23	110.13
9	R	101	BCL	C3B-C4B-NB	4.14	115.23	109.76
9	6	102	BCL	C3C-C4C-CHD	-4.14	114.66	123.39
9	7	101	BCL	C3C-C4C-CHD	-4.14	114.66	123.39
9	K	101	BCL	C2D-C1D-ND	4.14	114.22	110.13
9	1	101	BCL	C1D-ND-C4D	-4.14	103.41	106.31
10	Q	101	U42	CAN-CAM-CAO	-4.14	116.11	122.82
9	M	701	BCL	C4A-NA-C1A	4.12	108.56	106.68
19	L	1004	MQE	CAY-CAX-CBK	-4.12	117.83	124.89
9	N	101	BCL	C2D-C1D-ND	4.12	114.20	110.13
9	8	103	BCL	C3C-C4C-CHD	-4.12	114.71	123.39
9	W	102	BCL	C3B-C4B-NB	4.12	115.19	109.76
9	7	101	BCL	C2D-C1D-ND	4.12	114.20	110.13
11	S	104	U4Z	CBB-CBG-CBI	4.11	131.93	123.52
9	W	101	BCL	C1D-ND-C4D	-4.11	103.43	106.31
9	B	102	BCL	CHD-C1D-ND	-4.11	119.02	124.80
9	1	101	BCL	C3B-C4B-NB	4.11	115.18	109.76
9	O	102	BCL	C3B-C4B-NB	4.10	115.17	109.76
9	D	101	BCL	C1D-ND-C4D	-4.10	103.43	106.31
9	D	101	BCL	C3B-C4B-NB	4.10	115.17	109.76
9	O	103	BCL	C3B-C4B-NB	4.10	115.17	109.76
9	0	101	BCL	CHD-C1D-ND	-4.10	119.03	124.80
9	S	103	BCL	C1D-ND-C4D	-4.10	103.44	106.31
9	F	101	BCL	C2D-C1D-ND	4.09	114.17	110.13
9	I	102	BCL	CHD-C1D-ND	-4.09	119.05	124.80
9	9	102	BCL	C1D-ND-C4D	-4.09	103.44	106.31
11	7	102	U4Z	CBB-CBG-CBI	4.09	131.88	123.52
9	2	102	BCL	C3B-C4B-NB	4.09	115.15	109.76
9	L	1002	BCL	O2D-CGD-CBD	4.08	118.36	111.23
9	V	101	BCL	C2D-C1D-ND	4.08	114.16	110.13
9	4	103	BCL	C3B-C4B-NB	4.08	115.14	109.76
10	8	101	U42	CAX-CAT-CAS	4.07	122.11	112.33
9	U	103	BCL	C3B-C4B-NB	4.07	115.13	109.76
10	O	101	U42	CAQ-CAR-CAV	4.07	125.41	119.01
9	G	102	BCL	C3C-C4C-CHD	-4.07	114.81	123.39
10	I	101	U42	CAU-CAR-CAV	-4.07	116.23	122.82
9	9	102	BCL	C3B-C4B-NB	4.06	115.12	109.76
9	S	102	BCL	CAA-CBA-CGA	-4.06	101.69	113.21
9	M	701	BCL	C3C-C4C-CHD	-4.05	114.84	123.39
9	D	102	BCL	C1D-ND-C4D	-4.04	103.48	106.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	T	101	BCL	C1D-ND-C4D	-4.03	103.48	106.31
9	V	101	BCL	C1D-ND-C4D	-4.03	103.49	106.31
9	U	102	BCL	CHD-C1D-ND	-4.02	119.14	124.80
9	J	101	BCL	C3B-C4B-NB	4.02	115.07	109.76
10	I	104	U42	CAU-CAR-CAV	-4.02	116.31	122.82
9	H	101	BCL	C1C-NC-C4C	-4.01	104.85	106.68
10	4	104	U42	CAU-CAR-CAV	-4.01	116.32	122.82
10	E	101	U42	CAL-CAM-CAO	4.01	125.31	119.01
9	L	1002	BCL	C1D-ND-C4D	-4.01	103.50	106.31
9	H	101	BCL	C1D-ND-C4D	-4.00	103.50	106.31
9	4	102	BCL	CHD-C1D-ND	-4.00	119.17	124.80
9	8	102	BCL	C1D-ND-C4D	-4.00	103.51	106.31
9	R	101	BCL	C2D-C1D-ND	3.99	114.07	110.13
10	I	101	U42	CAO-CAP-CAQ	3.99	134.75	123.20
9	S	103	BCL	CHC-C4B-NB	-3.99	118.07	124.05
9	B	103	BCL	CHC-C4B-NB	-3.98	118.08	124.05
19	L	1004	MQE	CAY-CAX-CBQ	3.97	122.76	118.58
10	U	101	U42	CAQ-CAR-CAV	3.97	125.25	119.01
10	4	101	U42	CAN-CAM-CAO	-3.97	116.39	122.82
9	O	102	BCL	CHD-C1D-ND	-3.96	119.23	124.80
9	F	102	BCL	CHD-C1D-ND	-3.96	119.24	124.80
9	1	101	BCL	O1D-CGD-CBD	-3.94	116.75	124.52
9	H	101	BCL	C3B-C4B-NB	3.94	114.95	109.76
11	A	102	U4Z	CBB-CBG-CBI	3.93	131.57	123.52
10	0	103	U42	CBM-CBJ-CBH	3.93	132.79	127.28
9	L	1001	BCL	C1D-ND-C4D	-3.93	103.56	106.31
9	5	101	BCL	C2D-C1D-ND	3.93	114.01	110.13
9	3	101	BCL	C3B-C4B-NB	3.92	114.94	109.76
9	6	102	BCL	CHC-C4B-NB	-3.92	118.17	124.05
9	M	701	BCL	CHC-C4B-NB	-3.92	118.17	124.05
9	3	101	BCL	C2D-C1D-ND	3.92	114.00	110.13
9	4	103	BCL	CHC-C4B-NB	-3.92	118.17	124.05
9	I	103	BCL	C3B-C4B-NB	3.92	114.93	109.76
9	0	102	BCL	CHC-C4B-NB	-3.91	118.18	124.05
10	B	101	U42	CAU-CAR-CAV	-3.91	116.48	122.82
9	E	102	BCL	C3B-C4B-NB	3.90	114.91	109.76
10	I	104	U42	CBG-CBI-CBL	3.90	132.75	127.28
9	K	101	BCL	C3B-C4B-NB	3.90	114.91	109.76
9	G	102	BCL	C2D-C1D-ND	3.90	113.98	110.13
9	3	101	BCL	C1D-ND-C4D	-3.89	103.58	106.31
9	O	103	BCL	CHC-C4B-NB	-3.88	118.22	124.05
9	Q	103	BCL	CHC-C4B-NB	-3.88	118.22	124.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	401	U4Z	CAO-CAP-CAQ	3.88	134.45	123.20
11	1	102	U4Z	CBG-CBB-CAV	3.88	131.46	123.52
9	L	1001	BCL	C3C-C4C-CHD	-3.87	115.23	123.39
10	0	103	U42	CAB-CAD-CAH	-3.87	117.35	122.64
10	B	101	U42	O14-C4-O1	3.87	121.70	109.61
9	A	101	BCL	C1D-ND-C4D	3.87	109.03	106.31
9	I	102	BCL	C1D-ND-C4D	-3.87	103.60	106.31
10	I	101	U42	CBB-CAV-CAR	3.86	132.69	127.28
10	S	101	U42	CAL-CAM-CAO	3.86	125.08	119.01
10	0	103	U42	CAQ-CAR-CAV	3.85	125.07	119.01
11	P	102	U4Z	CBB-CBG-CBI	3.85	131.40	123.52
9	6	101	BCL	CHD-C1D-ND	-3.85	119.39	124.80
10	S	101	U42	CBB-CAV-CAR	3.85	132.68	127.28
9	W	101	BCL	C3C-C4C-CHD	-3.85	115.28	123.39
9	F	101	BCL	C1D-ND-C4D	-3.84	103.61	106.31
10	0	103	U42	CBJ-CBM-CBN	-3.84	112.07	123.20
10	B	101	U42	CAJ-CAL-CAM	3.84	131.92	126.23
10	4	101	U42	CAJ-CAL-CAM	3.84	131.92	126.23
9	8	102	BCL	C3B-C4B-NB	3.83	114.82	109.76
11	T	102	U4Z	CBB-CBG-CBI	3.83	131.35	123.52
10	S	101	U42	CAP-CAO-CAM	3.81	132.63	127.28
14	C	404	HEC	C4D-ND-C1D	3.81	112.04	105.82
11	C	401	U4Z	CAQ-CAR-CAV	3.81	125.01	119.01
9	2	102	BCL	C1-C2-C3	-3.81	119.96	126.20
9	B	102	BCL	C3B-C4B-NB	3.81	114.78	109.76
10	E	101	U42	CBA-CBE-CBF	-3.80	112.18	123.20
9	B	103	BCL	C1-C2-C3	-3.80	119.97	126.20
9	L	1002	BCL	C3B-C4B-NB	3.80	114.77	109.76
9	7	101	BCL	C1D-ND-C4D	-3.80	103.65	106.31
10	Q	101	U42	CAQ-CAR-CAV	3.80	124.98	119.01
9	L	1001	BCL	CHC-C4B-NB	-3.79	118.36	124.05
9	9	102	BCL	O2D-CGD-O1D	-3.79	116.47	123.85
9	G	102	BCL	C1D-ND-C4D	-3.79	103.65	106.31
10	8	101	U42	CBG-CBB-CAV	3.79	131.27	123.52
10	4	104	U42	CAX-CAT-CAS	3.79	121.43	112.33
10	E	101	U42	CAQ-CAR-CAV	3.78	124.96	119.01
9	4	102	BCL	C3B-C4B-NB	3.78	114.75	109.76
9	N	101	BCL	C1D-ND-C4D	-3.78	103.66	106.31
10	8	101	U42	CAQ-CAR-CAV	3.76	124.92	119.01
9	L	1001	BCL	C3D-C4D-ND	3.76	116.09	109.99
11	9	101	U4Z	CBB-CBG-CBI	3.75	131.20	123.52
9	F	102	BCL	C3B-C4B-NB	3.75	114.71	109.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	L	1017	PEF	O2-C10-C11	3.74	119.57	111.48
14	C	405	HEC	C4D-ND-C1D	3.74	111.92	105.82
10	B	101	U42	CBB-CAV-CAR	3.73	132.52	127.28
11	3	102	U4Z	CBB-CBG-CBI	3.73	131.16	123.52
10	O	101	U42	CAN-CAM-CAO	-3.73	116.77	122.82
9	I	102	BCL	O1D-CGD-CBD	-3.73	117.16	124.52
10	I	104	U42	CAN-CAM-CAL	-3.73	112.39	118.09
10	S	101	U42	CAB-CAD-CAH	-3.72	117.55	122.64
9	8	102	BCL	CHD-C1D-ND	-3.72	119.56	124.80
9	1	101	BCL	O2D-CGD-O1D	-3.72	116.61	123.85
9	0	101	BCL	C3B-C4B-NB	3.72	114.66	109.76
9	D	102	BCL	C3B-C4B-NB	3.72	114.66	109.76
10	0	103	U42	CBG-CBI-CBL	3.72	132.49	127.28
10	S	101	U42	CAB-CAD-CAJ	3.71	125.72	115.65
9	L	1001	BCL	O2A-CGA-CBA	3.71	123.14	111.83
10	S	101	U42	CAU-CAR-CAV	-3.69	116.83	122.82
9	G	102	BCL	C1-C2-C3	-3.69	120.15	126.20
9	R	101	BCL	C1D-ND-C4D	-3.68	103.73	106.31
9	I	102	BCL	O2D-CGD-O1D	-3.67	116.70	123.85
9	2	102	BCL	C2D-C1D-ND	3.67	113.76	110.13
9	M	701	BCL	C2D-C1D-ND	3.66	113.75	110.13
10	U	101	U42	CAN-CAM-CAL	-3.66	112.49	118.09
9	U	102	BCL	O2D-CGD-O1D	-3.66	116.73	123.85
9	D	102	BCL	O2D-CGD-O1D	-3.65	116.74	123.85
10	E	101	U42	CAN-CAM-CAO	-3.64	116.92	122.82
9	8	103	BCL	CAA-CBA-CGA	-3.64	102.88	113.21
10	4	104	U42	CBB-CAV-CAR	3.64	132.38	127.28
10	8	101	U42	CBB-CAV-CAR	3.63	132.38	127.28
9	L	1002	BCL	CHC-C4B-NB	-3.63	118.60	124.05
10	G	101	U42	CAO-CAP-CAQ	3.63	133.72	123.20
9	5	101	BCL	C1D-ND-C4D	-3.63	103.77	106.31
9	I	102	BCL	C1-C2-C3	-3.63	120.25	126.20
14	C	403	HEC	C4D-ND-C1D	3.63	111.73	105.82
9	T	101	BCL	C1C-NC-C4C	-3.62	105.03	106.68
9	2	101	BCL	C3D-C4D-ND	3.61	115.86	109.99
9	K	102	BCL	CHC-C4B-NB	-3.61	118.63	124.05
9	0	101	BCL	C1-C2-C3	-3.61	120.28	126.20
10	Q	101	U42	CBG-CBI-CBL	3.61	132.34	127.28
18	M	702	BPH	C4D-CHA-CBD	-3.60	106.73	108.45
9	M	701	BCL	C1D-ND-C4D	-3.60	103.78	106.31
10	E	101	U42	CAC-CAB-CAD	3.60	115.67	110.44
10	U	104	U42	CAU-CAR-CAV	-3.60	116.98	122.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	C	402	HEC	C4D-ND-C1D	3.60	111.69	105.82
10	4	104	U42	CBG-CBI-CBL	3.60	132.33	127.28
9	R	101	BCL	C1C-NC-C4C	-3.60	105.04	106.68
10	Q	101	U42	CAB-CAD-CAH	-3.60	117.72	122.64
10	0	103	U42	CAU-CAR-CAV	-3.59	117.00	122.82
9	I	102	BCL	C3B-C4B-NB	3.59	114.49	109.76
9	E	102	BCL	CHC-C4B-NB	-3.59	118.67	124.05
9	6	101	BCL	C1-C2-C3	-3.58	120.34	126.20
9	O	102	BCL	C4-C3-C5	3.58	121.44	115.23
9	Q	102	BCL	C3B-C4B-NB	3.57	114.47	109.76
9	4	103	BCL	CHC-C1C-NC	3.57	129.55	124.40
9	D	101	BCL	O2D-CGD-O1D	-3.57	116.91	123.85
9	U	102	BCL	C3B-C4B-NB	3.57	114.47	109.76
9	W	102	BCL	CHC-C4B-NB	-3.56	118.70	124.05
9	D	101	BCL	CHC-C4B-NB	-3.56	118.70	124.05
9	V	101	BCL	C3B-C4B-NB	3.56	114.45	109.76
9	8	102	BCL	C1-C2-C3	-3.56	120.37	126.20
9	Q	103	BCL	O2D-CGD-O1D	-3.56	116.93	123.85
11	5	102	U4Z	CBB-CBG-CBI	3.56	130.79	123.52
9	F	102	BCL	C1-C2-C3	-3.55	120.38	126.20
9	S	103	BCL	C4-C3-C2	-3.55	114.51	123.63
18	L	1003	BPH	C4D-CHA-CBD	-3.55	106.75	108.45
9	6	101	BCL	C3B-C4B-NB	3.55	114.44	109.76
9	U	103	BCL	O2D-CGD-O1D	-3.55	116.95	123.85
9	2	102	BCL	O2D-CGD-O1D	-3.54	116.95	123.85
9	J	101	BCL	CHC-C4B-NB	-3.54	118.74	124.05
10	U	104	U42	CAQ-CAR-CAV	3.54	124.58	119.01
9	I	103	BCL	CHC-C4B-NB	-3.54	118.74	124.05
10	U	101	U42	CBG-CBB-CAV	3.53	130.75	123.52
9	3	101	BCL	O2D-CGD-O1D	-3.53	116.97	123.85
9	D	101	BCL	C4A-NA-C1A	3.53	108.29	106.68
9	W	101	BCL	C3B-C4B-NB	3.53	114.42	109.76
9	T	101	BCL	O2D-CGD-O1D	-3.53	116.98	123.85
9	2	102	BCL	C1D-ND-C4D	-3.53	103.84	106.31
9	7	101	BCL	CHC-C4B-NB	-3.52	118.77	124.05
9	0	101	BCL	C3D-C4D-ND	3.51	115.70	109.99
9	4	102	BCL	C1-C2-C3	-3.51	120.44	126.20
9	S	103	BCL	O2D-CGD-O1D	-3.51	117.01	123.85
9	F	101	BCL	CHC-C4B-NB	-3.49	118.81	124.05
9	S	102	BCL	C3D-C4D-ND	3.49	115.66	109.99
11	C	401	U4Z	CAB-CAD-CAJ	3.49	125.11	115.65
9	K	101	BCL	C3D-C4D-ND	3.48	115.65	109.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	8	103	BCL	C2D-C1D-ND	3.48	113.57	110.13
9	F	102	BCL	C3D-C4D-ND	3.48	115.64	109.99
9	V	101	BCL	C1C-NC-C4C	-3.48	105.09	106.68
9	J	101	BCL	O2D-CGD-O1D	-3.48	117.08	123.85
10	8	101	U42	CBM-CBJ-CBH	3.48	132.15	127.28
9	Q	102	BCL	C3D-C4D-ND	3.47	115.62	109.99
9	6	101	BCL	CHC-C4B-NB	-3.47	118.85	124.05
9	2	101	BCL	C3B-C4B-NB	3.46	114.33	109.76
9	K	102	BCL	C1-C2-C3	-3.46	120.52	126.20
9	R	101	BCL	O2D-CGD-O1D	-3.46	117.12	123.85
9	H	101	BCL	O2D-CGD-O1D	-3.45	117.12	123.85
9	B	102	BCL	O2D-CGD-O1D	-3.45	117.13	123.85
10	4	104	U42	CBJ-CBM-CBN	3.44	133.18	123.20
9	O	102	BCL	C3D-C4D-ND	3.44	115.58	109.99
9	N	101	BCL	O2D-CGD-O1D	-3.44	117.16	123.85
10	S	101	U42	CBG-CBI-CBL	3.43	132.09	127.28
9	L	1001	BCL	C3B-C4B-NB	3.43	114.28	109.76
11	5	102	U4Z	CBG-CBB-CAV	3.43	130.53	123.52
9	O	103	BCL	C1D-ND-C4D	-3.42	103.91	106.31
11	A	102	U4Z	CAB-CAD-CAH	-3.42	117.97	122.64
11	7	102	U4Z	CAI-CAH-CAD	-3.42	118.09	122.70
9	E	102	BCL	C1-C2-C3	-3.41	120.61	126.20
13	L	1015	BGL	O5-C5-C4	3.41	115.84	109.70
9	W	102	BCL	CAA-CBA-CGA	-3.41	103.53	113.21
19	M	704	MQE	CAY-CAX-CBQ	-3.41	114.99	118.58
9	B	102	BCL	C3D-C4D-ND	3.41	115.52	109.99
9	W	101	BCL	C3D-C4D-ND	3.40	115.51	109.99
10	O	101	U42	O15-C7-C8	3.40	117.69	109.32
9	F	101	BCL	O2D-CGD-O1D	-3.40	117.23	123.85
9	3	101	BCL	CHC-C4B-NB	-3.40	118.95	124.05
9	E	102	BCL	C3D-C4D-ND	3.40	115.51	109.99
10	U	101	U42	CAU-CAR-CAV	-3.39	117.32	122.82
10	Q	101	U42	O14-C4-O1	3.39	120.20	109.61
9	O	103	BCL	C1C-NC-C4C	-3.39	105.13	106.68
9	4	102	BCL	C3D-C4D-ND	3.38	115.49	109.99
11	V	102	U4Z	CAN-CAM-CAO	-3.38	117.34	122.82
10	4	104	U42	CAO-CAP-CAQ	3.38	132.99	123.20
9	A	101	BCL	O2D-CGD-O1D	-3.38	117.28	123.85
18	L	1003	BPH	C1A-C2A-C3A	-3.38	99.63	102.84
9	O	102	BCL	O2D-CGD-O1D	-3.37	117.28	123.85
11	7	102	U4Z	CAB-CAD-CAH	-3.37	118.03	122.64
9	G	102	BCL	CHC-C4B-NB	-3.37	118.99	124.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	0	102	BCL	C4A-NA-C1A	3.37	108.22	106.68
9	U	102	BCL	C3D-C4D-ND	3.37	115.46	109.99
9	2	101	BCL	CHC-C4B-NB	-3.37	119.00	124.05
9	S	103	BCL	CHC-C1C-NC	3.36	129.25	124.40
9	S	102	BCL	C3B-C4B-NB	3.36	114.19	109.76
9	U	103	BCL	CHC-C4B-NB	-3.35	119.02	124.05
9	W	101	BCL	O2D-CGD-O1D	-3.35	117.32	123.85
11	1	102	U4Z	CAN-CAM-CAO	-3.34	117.41	122.82
9	6	102	BCL	C4-C3-C5	3.34	121.02	115.23
9	V	101	BCL	C3D-C4D-ND	3.34	115.41	109.99
9	8	102	BCL	C3D-C4D-ND	3.34	115.41	109.99
10	Q	101	U42	CBN-CBL-CBI	3.33	124.25	119.01
9	D	102	BCL	CHC-C4B-NB	-3.33	119.05	124.05
9	P	101	BCL	C1-C2-C3	-3.33	120.74	126.20
9	8	103	BCL	O2D-CGD-O1D	-3.33	117.37	123.85
9	I	102	BCL	C4-C3-C5	3.33	121.00	115.23
9	7	101	BCL	O2D-CGD-O1D	-3.33	117.38	123.85
11	1	102	U4Z	CAI-CAH-CAD	-3.32	118.21	122.70
9	L	1001	BCL	C2D-C1D-ND	3.32	113.41	110.13
9	M	701	BCL	C1-C2-C3	-3.32	120.76	126.20
9	M	701	BCL	O2D-CGD-O1D	-3.31	117.40	123.85
9	D	102	BCL	C3D-C4D-ND	3.31	115.37	109.99
9	P	101	BCL	O2D-CGD-O1D	-3.31	117.40	123.85
18	L	1003	BPH	CMC-C2C-C3C	3.31	126.91	114.13
10	4	104	U42	O17-C16-C8	3.31	115.39	108.41
9	Q	102	BCL	C1-C2-C3	-3.31	120.78	126.20
11	9	101	U4Z	CAB-CAD-CAH	-3.31	118.12	122.64
9	H	101	BCL	C4A-NA-C1A	3.31	108.19	106.68
11	N	102	U4Z	CAN-CAM-CAO	-3.30	117.47	122.82
11	T	102	U4Z	CAN-CAM-CAO	-3.30	117.47	122.82
11	A	102	U4Z	CAN-CAM-CAO	-3.30	117.47	122.82
11	A	102	U4Z	CBG-CBB-CAV	3.29	130.26	123.52
10	0	103	U42	CAN-CAM-CAO	-3.29	117.48	122.82
9	6	101	BCL	C3D-C4D-ND	3.29	115.33	109.99
10	S	101	U42	CBM-CBJ-CBH	3.28	131.88	127.28
9	M	701	BCL	C3D-C4D-ND	3.28	115.32	109.99
10	4	101	U42	O17-C16-C8	-3.28	101.48	108.41
11	A	102	U4Z	CAI-CAH-CAD	-3.28	118.27	122.70
9	5	101	BCL	C1C-NC-C4C	-3.28	105.18	106.68
9	H	101	BCL	CHC-C4B-NB	-3.28	119.13	124.05
11	P	102	U4Z	CAN-CAM-CAO	-3.28	117.50	122.82
9	B	102	BCL	CHC-C4B-NB	-3.28	119.13	124.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	U	103	BCL	C4-C3-C2	-3.28	115.21	123.63
11	S	104	U4Z	CAN-CAM-CAO	-3.28	117.51	122.82
9	G	102	BCL	O2D-CGD-O1D	-3.28	117.47	123.85
11	J	102	U4Z	CAN-CAM-CAO	-3.27	117.52	122.82
9	L	1002	BCL	CED-O2D-CGD	3.27	123.33	115.92
9	2	102	BCL	C3D-C4D-ND	3.27	115.30	109.99
11	H	102	U4Z	CAN-CAM-CAO	-3.27	117.53	122.82
10	E	101	U42	CAB-CAD-CAH	-3.26	118.18	122.64
11	9	101	U4Z	CAI-CAH-CAD	-3.26	118.30	122.70
9	S	102	BCL	CHC-C4B-NB	-3.26	119.16	124.05
9	5	101	BCL	CHC-C4B-NB	-3.26	119.16	124.05
9	I	103	BCL	CAA-CBA-CGA	-3.25	103.97	113.21
11	D	103	U4Z	CAN-CAM-CAO	-3.25	117.55	122.82
9	U	103	BCL	C3D-C4D-ND	3.25	115.27	109.99
9	S	103	BCL	CAA-CBA-CGA	-3.25	103.99	113.21
9	L	1002	BCL	O2A-CGA-CBA	3.25	121.73	111.83
9	Q	102	BCL	C4-C3-C5	3.24	120.86	115.23
11	5	102	U4Z	CAN-CAM-CAO	-3.24	117.56	122.82
9	A	101	BCL	CMC-C2C-C3C	3.24	126.50	113.98
18	L	1003	BPH	O2D-CGD-O1D	-3.24	117.55	123.85
10	0	103	U42	CBK-CBH-CBJ	-3.23	117.58	122.82
11	V	102	U4Z	CBG-CBB-CAV	3.23	130.14	123.52
9	4	103	BCL	O2A-CGA-CBA	3.23	121.67	111.83
9	M	701	BCL	CED-O2D-CGD	3.22	123.23	115.92
11	7	102	U4Z	CAN-CAM-CAO	-3.22	117.59	122.82
11	F	103	U4Z	CAN-CAM-CAO	-3.22	117.60	122.82
9	K	102	BCL	C4-C3-C5	3.22	120.81	115.23
9	9	102	BCL	CHC-C4B-NB	-3.21	119.23	124.05
11	3	102	U4Z	CAN-CAM-CAO	-3.21	117.61	122.82
9	5	101	BCL	O2D-CGD-O1D	-3.21	117.60	123.85
11	C	401	U4Z	CAU-CAR-CAV	-3.21	117.61	122.82
9	4	102	BCL	CHC-C4B-NB	-3.21	119.23	124.05
9	N	101	BCL	CHC-C4B-NB	-3.21	119.23	124.05
10	E	101	U42	CAB-CAD-CAJ	3.21	124.35	115.65
11	S	104	U4Z	CBG-CBB-CAV	3.20	130.08	123.52
10	B	101	U42	CAN-CAM-CAO	-3.20	117.63	122.82
9	S	102	BCL	C4D-CHA-C1A	-3.20	117.42	121.24
9	I	102	BCL	C3D-C4D-ND	3.20	115.19	109.99
10	Q	101	U42	CBM-CBJ-CBH	3.20	131.76	127.28
10	8	101	U42	CAO-CAP-CAQ	3.20	132.46	123.20
9	K	101	BCL	CHC-C4B-NB	-3.19	119.26	124.05
10	U	104	U42	CBG-CBB-CAV	3.19	130.06	123.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	401	U4Z	CAN-CAM-CAO	-3.19	117.64	122.82
9	Q	102	BCL	CHC-C4B-NB	-3.19	119.26	124.05
11	9	101	U4Z	CBG-CBB-CAV	3.19	130.05	123.52
11	3	102	U4Z	CBG-CBB-CAV	3.19	130.05	123.52
9	1	101	BCL	C1C-NC-C4C	-3.19	105.22	106.68
9	K	102	BCL	C3D-C4D-ND	3.18	115.16	109.99
10	B	101	U42	CAP-CAO-CAM	3.18	131.74	127.28
9	2	101	BCL	O2A-CGA-CBA	3.18	121.54	111.83
18	L	1003	BPH	C3D-C4D-ND	3.18	111.78	107.71
9	F	102	BCL	O2D-CGD-O1D	-3.18	117.66	123.85
9	4	102	BCL	C4-C3-C5	3.18	120.74	115.23
10	I	104	U42	CBB-CAV-CAR	3.18	131.73	127.28
9	K	101	BCL	O2D-CGD-O1D	-3.17	117.68	123.85
9	J	101	BCL	C3D-C4D-ND	3.16	115.13	109.99
9	O	102	BCL	CHC-C4B-NB	-3.16	119.31	124.05
11	T	102	U4Z	CAI-CAH-CAD	-3.16	118.44	122.70
10	B	101	U42	CAC-CAB-CAD	3.16	115.03	110.44
9	J	101	BCL	C1-C2-C3	-3.16	121.02	126.20
9	9	102	BCL	C1C-NC-C4C	-3.16	105.24	106.68
11	D	103	U4Z	CAI-CAH-CAD	-3.16	118.44	122.70
9	P	101	BCL	C3C-C4C-CHD	-3.16	116.74	123.39
9	N	101	BCL	C1C-NC-C4C	-3.15	105.24	106.68
10	8	101	U42	CAC-CAB-CAD	3.15	115.02	110.44
9	W	101	BCL	CHC-C4B-NB	-3.15	119.32	124.05
11	H	102	U4Z	CAI-CAH-CAD	-3.15	118.45	122.70
10	0	103	U42	CAX-CAT-CAS	3.15	119.90	112.33
9	S	102	BCL	O2D-CGD-O1D	-3.15	117.72	123.85
9	I	102	BCL	CHC-C4B-NB	-3.15	119.33	124.05
9	G	102	BCL	O2A-CGA-CBA	3.14	121.42	111.83
11	9	101	U4Z	CAN-CAM-CAO	-3.14	117.73	122.82
9	L	1001	BCL	CMB-C2B-C3B	3.14	135.58	125.67
9	8	102	BCL	O2D-CGD-O1D	-3.14	117.74	123.85
9	8	103	BCL	C1D-ND-C4D	-3.13	104.11	106.31
9	3	101	BCL	C3D-C4D-ND	3.13	115.08	109.99
9	I	103	BCL	C3D-C4D-ND	3.13	115.08	109.99
9	E	102	BCL	O2D-CGD-O1D	-3.13	117.75	123.85
11	3	102	U4Z	CAI-CAH-CAD	-3.13	118.47	122.70
9	0	101	BCL	CHC-C4B-NB	-3.13	119.36	124.05
9	0	102	BCL	CHC-C1C-NC	3.13	128.91	124.40
9	0	102	BCL	C3D-C4D-ND	3.13	115.07	109.99
9	A	101	BCL	CBC-CAC-C3C	-3.13	106.78	113.41
9	B	103	BCL	C3D-C4D-ND	3.13	115.07	109.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	K	102	BCL	C1C-NC-C4C	-3.13	105.25	106.68
9	B	102	BCL	C1-C2-C3	-3.12	121.09	126.20
10	O	101	U42	CAP-CAO-CAM	3.12	131.65	127.28
11	5	102	U4Z	CAI-CAH-CAD	-3.12	118.49	122.70
9	6	102	BCL	C3D-C4D-ND	3.11	115.05	109.99
9	R	101	BCL	CHC-C4B-NB	-3.11	119.38	124.05
10	U	104	U42	CAJ-CAD-CAH	3.11	128.72	121.56
11	J	102	U4Z	CAI-CAH-CAD	-3.11	118.50	122.70
11	P	102	U4Z	CAI-CAH-CAD	-3.11	118.50	122.70
9	8	103	BCL	CHC-C4B-NB	-3.11	119.38	124.05
10	4	104	U42	CAC-CAB-CAD	3.11	114.95	110.44
9	N	101	BCL	C3D-C4D-ND	3.11	115.03	109.99
10	4	101	U42	CBK-CBH-CBJ	-3.11	117.78	122.82
9	0	101	BCL	O2D-CGD-O1D	-3.11	117.80	123.85
9	4	103	BCL	O2D-CGD-O1D	-3.11	117.80	123.85
10	4	101	U42	CAQ-CAR-CAV	3.10	123.89	119.01
9	Q	103	BCL	C3D-C4D-ND	3.10	115.03	109.99
9	O	102	BCL	C4D-CHA-C1A	-3.10	117.55	121.24
9	A	101	BCL	C4-C3-C5	3.10	120.61	115.23
9	S	103	BCL	O2A-CGA-CBA	3.10	121.29	111.83
9	9	102	BCL	C3D-C4D-ND	3.10	115.02	109.99
11	1	102	U4Z	CBB-CBG-CBI	3.10	129.85	123.52
9	W	102	BCL	C3D-C4D-ND	3.09	115.02	109.99
9	P	101	BCL	CMC-C2C-C3C	3.09	125.94	113.98
9	4	102	BCL	C4D-CHA-C1A	-3.09	117.56	121.24
9	7	101	BCL	C3D-C4D-ND	3.09	115.01	109.99
10	4	101	U42	CAL-CAM-CAO	3.09	123.87	119.01
11	T	102	U4Z	CBG-CBB-CAV	3.09	129.84	123.52
9	F	101	BCL	C3D-C4D-ND	3.09	115.01	109.99
9	O	103	BCL	CHC-C1C-NC	3.09	128.86	124.40
9	F	102	BCL	CHC-C4B-NB	-3.09	119.42	124.05
9	P	101	BCL	CBC-CAC-C3C	-3.08	106.87	113.41
9	K	101	BCL	C1-C2-C3	-3.08	121.15	126.20
10	4	101	U42	CBB-CAV-CAR	3.08	131.60	127.28
9	1	101	BCL	CHC-C4B-NB	-3.08	119.43	124.05
10	I	104	U42	CBM-CBJ-CBH	3.06	131.57	127.28
10	S	101	U42	CAY-O1-C4	-3.06	113.51	119.78
19	L	1004	MQE	CBL-CAY-CAX	3.06	119.62	112.08
9	D	101	BCL	C3D-C4D-ND	3.06	114.96	109.99
10	0	103	U42	CAP-CAQ-CAR	3.06	134.75	126.36
9	G	102	BCL	CAA-C2A-C3A	-3.06	104.74	113.00
9	4	103	BCL	C3D-C4D-ND	3.06	114.95	109.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	103	BCL	O2D-CGD-O1D	-3.06	117.90	123.85
9	O	103	BCL	C1D-CHD-C4C	-3.05	119.26	126.62
9	R	101	BCL	C3D-C4D-ND	3.05	114.95	109.99
10	8	101	U42	CBN-CBL-CBI	3.05	123.81	119.01
10	0	103	U42	CBM-CBN-CBL	3.05	134.73	126.36
11	F	103	U4Z	CBG-CBB-CAV	3.05	129.76	123.52
10	U	101	U42	CBN-CBL-CBI	3.05	123.80	119.01
9	G	102	BCL	C3D-C4D-ND	3.04	114.93	109.99
9	T	101	BCL	C3D-C4D-ND	3.04	114.93	109.99
9	8	102	BCL	C4-C3-C5	3.04	120.51	115.23
11	S	104	U4Z	CAI-CAH-CAD	-3.04	118.59	122.70
10	B	101	U42	CAY-O1-C4	-3.04	113.56	119.78
10	U	101	U42	C6-C7-C8	-3.04	104.72	110.23
9	1	101	BCL	C3D-C4D-ND	3.04	114.92	109.99
9	4	102	BCL	O2D-CGD-O1D	-3.04	117.94	123.85
11	C	401	U4Z	CAN-CAM-CAL	3.04	122.73	118.09
9	S	103	BCL	C3D-C4D-ND	3.03	114.92	109.99
9	5	101	BCL	C3D-C4D-ND	3.03	114.92	109.99
10	8	101	U42	CAU-CAR-CAV	-3.03	117.90	122.82
10	G	101	U42	CAU-CAR-CAV	-3.03	117.91	122.82
9	W	101	BCL	C4D-CHA-C1A	-3.02	117.64	121.24
10	U	104	U42	CAC-CAB-CAD	3.02	114.83	110.44
11	J	102	U4Z	CBN-CBL-CBI	3.02	123.76	119.01
9	1	101	BCL	C1-C2-C3	-3.02	121.25	126.20
9	W	101	BCL	C1-C2-C3	-3.02	121.25	126.20
9	F	102	BCL	C4D-CHA-C1A	-3.02	117.64	121.24
9	R	101	BCL	O2A-CGA-CBA	3.02	121.04	111.83
9	B	103	BCL	O2D-CGD-O1D	-3.01	117.98	123.85
10	S	101	U42	CAN-CAM-CAO	-3.01	117.94	122.82
9	B	102	BCL	C4-C3-C5	3.01	120.45	115.23
9	S	102	BCL	CMB-C2B-C3B	3.01	135.16	125.67
9	H	101	BCL	C3D-C4D-ND	3.01	114.88	109.99
11	V	102	U4Z	CAE-CAI-CAH	3.01	119.42	114.06
9	R	101	BCL	C1-C2-C3	-3.00	121.27	126.20
9	U	102	BCL	CHC-C4B-NB	-3.00	119.54	124.05
9	L	1002	BCL	C3D-C4D-ND	3.00	114.87	109.99
10	8	101	U42	O14-C4-O1	3.00	118.97	109.61
9	F	102	BCL	C4-C3-C5	2.99	120.42	115.23
9	O	103	BCL	C4-C3-C2	-2.99	115.94	123.63
9	S	102	BCL	C4-C3-C5	2.99	120.42	115.23
9	W	102	BCL	O2D-CGD-O1D	-2.99	118.03	123.85
20	L	1017	PEF	O3-C30-C31	2.99	120.94	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	Q	102	BCL	C4D-CHA-C1A	-2.99	117.68	121.24
9	W	102	BCL	C4-C3-C2	-2.98	115.96	123.63
9	N	101	BCL	O2A-CGA-CBA	2.98	120.93	111.83
9	S	102	BCL	O2A-CGA-CBA	2.98	120.93	111.83
9	U	103	BCL	O2A-CGA-CBA	2.98	120.93	111.83
9	P	101	BCL	C1D-ND-C4D	2.98	108.41	106.31
9	W	102	BCL	C4-C3-C5	2.98	120.40	115.23
10	U	104	U42	CBM-CBJ-CBH	2.98	131.46	127.28
10	4	101	U42	CBG-CBB-CAV	2.98	129.61	123.52
11	F	103	U4Z	CAE-CAI-CAH	2.97	119.36	114.06
9	U	102	BCL	O2A-CGA-CBA	2.97	120.89	111.83
11	V	102	U4Z	CAI-CAH-CAD	-2.97	118.69	122.70
11	N	102	U4Z	CAI-CAH-CAD	-2.96	118.70	122.70
10	S	101	U42	CAO-CAP-CAQ	2.96	131.78	123.20
10	0	103	U42	CAC-CAB-CAD	2.96	114.74	110.44
10	I	101	U42	CAC-CAB-CAD	2.96	114.74	110.44
9	8	102	BCL	CHC-C4B-NB	-2.96	119.61	124.05
10	E	101	U42	CBN-CBL-CBI	2.96	123.66	119.01
10	0	103	U42	O17-C16-C8	2.95	114.65	108.41
9	Q	103	BCL	C1-O2A-CGA	2.95	123.80	116.65
9	6	101	BCL	C4D-CHA-C1A	-2.95	117.73	121.24
9	6	101	BCL	CMB-C2B-C3B	2.94	134.96	125.67
9	8	103	BCL	C1-C2-C3	-2.94	121.38	126.20
10	Q	101	U42	CAX-CAT-CAS	2.94	119.39	112.33
10	U	101	U42	CBE-CBF-CBH	2.94	134.42	126.36
9	6	101	BCL	O2D-CGD-O1D	-2.94	118.13	123.85
10	Q	101	U42	CBC-CAY-CAX	2.94	116.34	111.12
11	P	102	U4Z	CBG-CBB-CAV	2.93	129.52	123.52
11	F	103	U4Z	CAI-CAH-CAD	-2.93	118.74	122.70
18	M	702	BPH	C2B-C1B-NB	-2.93	107.31	109.43
9	K	102	BCL	CAA-C2A-C3A	-2.93	105.08	113.00
10	4	104	U42	CAP-CAQ-CAR	2.93	134.38	126.36
10	U	104	U42	C4-O14-C8	2.92	119.42	113.72
9	I	102	BCL	C4D-CHA-C1A	-2.92	117.76	121.24
10	O	101	U42	CAB-CAD-CAH	-2.92	118.65	122.64
9	8	102	BCL	C4D-CHA-C1A	-2.92	117.77	121.24
10	I	104	U42	CBN-CBL-CBI	2.91	123.59	119.01
9	2	101	BCL	C4-C3-C5	2.91	120.28	115.23
9	W	101	BCL	C1D-CHD-C4C	-2.91	119.60	126.62
9	O	103	BCL	O2D-CGD-O1D	-2.91	118.18	123.85
9	U	102	BCL	CMB-C2B-C3B	2.91	134.84	125.67
9	4	103	BCL	C4-C3-C5	2.91	120.28	115.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	0	101	BCL	C4D-CHA-C1A	-2.91	117.78	121.24
9	D	102	BCL	C4-C3-C5	2.90	120.27	115.23
9	G	102	BCL	C4-C3-C5	2.90	120.27	115.23
11	F	103	U4Z	CBN-CBL-CBI	2.90	123.57	119.01
9	B	103	BCL	CHC-C1C-NC	2.90	128.59	124.40
11	1	102	U4Z	CAQ-CAR-CAV	2.90	123.56	119.01
9	T	101	BCL	CHC-C4B-NB	-2.90	119.71	124.05
9	4	103	BCL	C1C-NC-C4C	-2.89	105.36	106.68
10	4	101	U42	CBN-CBL-CBI	2.89	123.56	119.01
9	4	103	BCL	C1-C2-C3	-2.89	121.46	126.20
10	Q	101	U42	CAU-CAR-CAV	-2.89	118.13	122.82
9	2	102	BCL	CAA-CBA-CGA	-2.89	105.00	113.21
9	A	101	BCL	O2A-CGA-CBA	2.89	120.64	111.83
9	M	701	BCL	O1D-CGD-CBD	-2.89	118.82	124.52
10	Q	101	U42	C7-C6-C5	-2.89	105.76	110.83
10	U	104	U42	CAN-CAM-CAL	-2.89	113.68	118.09
9	F	101	BCL	C1-C2-C3	-2.88	121.47	126.20
11	N	102	U4Z	CBN-CBL-CBI	2.88	123.54	119.01
11	J	102	U4Z	CBO-CBL-CBI	-2.88	118.16	122.82
9	T	101	BCL	O2A-CGA-CBA	2.87	120.60	111.83
9	K	102	BCL	O2D-CGD-O1D	-2.87	118.26	123.85
11	S	104	U4Z	CBO-CBL-CBI	-2.87	118.17	122.82
10	4	104	U42	CAY-O1-C4	-2.87	113.91	119.78
9	Q	103	BCL	O2A-CGA-CBA	2.86	120.57	111.83
14	C	404	HEC	C2A-C1A-NA	-2.86	107.56	110.32
9	K	102	BCL	C1-O2A-CGA	2.86	123.58	116.65
9	S	102	BCL	C6-C5-C3	-2.86	106.50	113.47
9	5	101	BCL	C1-C2-C3	-2.86	121.52	126.20
9	V	101	BCL	O2A-CGA-CBA	2.86	120.54	111.83
9	2	101	BCL	CHC-C1C-NC	2.85	128.52	124.40
9	8	103	BCL	C3D-C4D-ND	2.85	114.62	109.99
9	T	101	BCL	C4A-NA-C1A	2.85	107.98	106.68
11	H	102	U4Z	CBN-CBL-CBI	2.85	123.49	119.01
10	B	101	U42	CAB-CAD-CAH	-2.85	118.74	122.64
9	D	102	BCL	CMB-C2B-C3B	2.85	134.65	125.67
10	S	101	U42	CBN-CBL-CBI	2.85	123.48	119.01
9	B	102	BCL	CMB-C2B-C3B	2.85	134.64	125.67
10	I	104	U42	O14-C8-C7	2.84	114.82	109.70
9	W	101	BCL	CMB-C2B-C3B	2.84	134.63	125.67
11	S	104	U4Z	CBN-CBL-CBI	2.84	123.48	119.01
9	Q	102	BCL	CMB-C2B-C3B	2.84	134.63	125.67
9	P	101	BCL	CHD-C1D-ND	-2.84	120.81	124.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	N	102	U4Z	CAE-CAI-CAH	2.84	119.11	114.06
10	I	101	U42	CAJ-CAD-CAH	2.84	128.09	121.56
11	3	102	U4Z	CBN-CBL-CBI	2.84	123.47	119.01
11	3	102	U4Z	CBO-CBL-CBI	-2.83	118.22	122.82
9	W	102	BCL	C1C-NC-C4C	-2.83	105.39	106.68
11	7	102	U4Z	CBN-CBL-CBI	2.83	123.47	119.01
9	E	102	BCL	CAA-CBA-CGA	-2.83	105.16	113.21
10	Q	101	U42	O17-C16-C8	2.83	114.39	108.41
9	L	1002	BCL	C1-O2A-CGA	2.83	123.50	116.65
10	G	101	U42	CAQ-CAR-CAV	2.83	123.45	119.01
9	W	102	BCL	O2A-CGA-CBA	2.82	120.45	111.83
10	4	101	U42	CAC-CAB-CAD	2.82	114.53	110.44
11	H	102	U4Z	CBO-CBL-CBI	-2.82	118.25	122.82
9	4	103	BCL	C1D-CHD-C4C	-2.82	119.82	126.62
10	E	101	U42	CAP-CAO-CAM	2.82	131.23	127.28
9	I	103	BCL	CHC-C1C-NC	2.81	128.46	124.40
11	1	102	U4Z	CAU-CAR-CAV	-2.81	118.26	122.82
9	0	102	BCL	C1-C2-C3	-2.81	121.59	126.20
11	3	102	U4Z	CAE-CAI-CAH	2.81	119.06	114.06
10	4	101	U42	CAX-CAT-CAS	2.81	119.08	112.33
9	8	103	BCL	CHC-C1C-NC	2.81	128.45	124.40
9	D	101	BCL	C1-C2-C3	-2.81	121.60	126.20
10	I	104	U42	C6-C7-C8	2.81	115.32	110.23
9	U	103	BCL	CHB-C4A-NA	2.81	128.45	124.40
10	Q	101	U42	CAB-CAD-CAJ	2.81	123.26	115.65
11	7	102	U4Z	CBO-CBL-CBI	-2.81	118.27	122.82
9	D	101	BCL	C1C-NC-C4C	-2.80	105.40	106.68
9	I	103	BCL	C6-C5-C3	-2.80	106.64	113.47
9	0	102	BCL	C4-C3-C5	2.80	120.09	115.23
9	Q	102	BCL	O2D-CGD-O1D	-2.80	118.39	123.85
9	K	101	BCL	C4D-CHA-C1A	-2.80	117.90	121.24
10	B	101	U42	CBK-CBH-CBJ	-2.80	118.28	122.82
11	D	103	U4Z	CBO-CBL-CBI	-2.80	118.28	122.82
9	K	101	BCL	CMB-C2B-C3B	2.79	134.48	125.67
9	U	102	BCL	C4D-CHA-C1A	-2.79	117.91	121.24
11	V	102	U4Z	CBK-CBH-CBJ	-2.79	118.29	122.82
9	D	101	BCL	C1-O2A-CGA	2.79	123.41	116.65
9	M	701	BCL	C1-O2A-CGA	2.79	123.41	116.65
9	2	101	BCL	O2D-CGD-O1D	-2.79	118.42	123.85
9	G	102	BCL	CHC-C1C-NC	2.79	128.43	124.40
11	A	102	U4Z	CBN-CBL-CBI	2.79	123.39	119.01
10	0	103	U42	CAN-CAM-CAL	-2.78	113.83	118.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	U	101	U42	CBK-CBH-CBJ	-2.78	118.31	122.82
11	T	102	U4Z	CAB-CAD-CAH	-2.78	118.83	122.64
11	C	401	U4Z	CAI-CAH-CAD	-2.78	118.94	122.70
9	K	101	BCL	C4-C3-C5	2.78	120.06	115.23
11	S	104	U4Z	CAE-CAI-CAH	2.78	119.01	114.06
9	L	1002	BCL	C4-C3-C2	-2.78	116.49	123.63
9	B	103	BCL	C1D-CHD-C4C	-2.78	119.92	126.62
9	9	102	BCL	C1-C2-C3	-2.78	121.64	126.20
11	N	102	U4Z	CBO-CBL-CBI	-2.78	118.32	122.82
9	N	101	BCL	C4-C3-C5	2.78	120.05	115.23
11	T	102	U4Z	CBN-CBL-CBI	2.78	123.38	119.01
9	0	101	BCL	C4-C3-C5	2.77	120.04	115.23
11	C	401	U4Z	CAB-CAD-CAH	-2.77	118.86	122.64
9	I	102	BCL	CMB-C2B-C3B	2.77	134.40	125.67
9	7	101	BCL	C4-C3-C5	2.76	120.03	115.23
9	4	103	BCL	CMB-C2B-C3B	2.76	134.39	125.67
11	9	101	U4Z	CBO-CBL-CBI	-2.76	118.34	122.82
11	D	103	U4Z	CAB-CAD-CAH	-2.76	118.86	122.64
11	T	102	U4Z	CBO-CBL-CBI	-2.76	118.35	122.82
9	M	701	BCL	O2A-CGA-CBA	2.76	120.24	111.83
11	7	102	U4Z	CBG-CBB-CAV	2.76	129.16	123.52
9	0	102	BCL	C1D-CHD-C4C	-2.76	119.97	126.62
11	A	102	U4Z	CBO-CBL-CBI	-2.75	118.35	122.82
11	F	103	U4Z	CBO-CBL-CBI	-2.75	118.36	122.82
9	4	102	BCL	CMB-C2B-C3B	2.75	134.33	125.67
9	G	102	BCL	C1D-CHD-C4C	-2.74	120.00	126.62
9	F	102	BCL	CMB-C2B-C3B	2.74	134.32	125.67
11	3	102	U4Z	CBK-CBH-CBJ	-2.74	118.38	122.82
9	7	101	BCL	O2A-CGA-CBA	2.74	120.19	111.83
11	V	102	U4Z	CBF-CBH-CBJ	2.74	123.32	119.01
9	T	101	BCL	C1-C2-C3	-2.74	121.71	126.20
9	T	101	BCL	CHB-C4A-NA	2.74	128.35	124.40
9	V	101	BCL	C1-C2-C3	-2.74	121.71	126.20
9	T	101	BCL	C4-C3-C5	2.73	119.97	115.23
9	S	103	BCL	CAA-C2A-C3A	-2.73	105.62	113.00
10	Q	101	U42	CAC-CAB-CAD	2.73	114.41	110.44
11	9	101	U4Z	CBN-CBL-CBI	2.73	123.30	119.01
11	D	103	U4Z	CBN-CBL-CBI	2.73	123.30	119.01
9	6	102	BCL	CHB-C4A-NA	2.73	128.34	124.40
9	L	1002	BCL	CMB-C2B-C3B	2.73	134.27	125.67
11	J	102	U4Z	CAE-CAI-CAH	2.73	118.91	114.06
10	I	104	U42	CAY-O1-C4	-2.72	114.20	119.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	G	101	U42	CAP-CAQ-CAR	2.72	133.83	126.36
11	V	102	U4Z	CBO-CBL-CBI	-2.72	118.41	122.82
11	5	102	U4Z	CAE-CAI-CAH	2.72	118.91	114.06
11	N	102	U4Z	CBG-CBB-CAV	2.72	129.09	123.52
10	4	101	U42	CBF-CBH-CBJ	2.72	123.28	119.01
11	C	401	U4Z	CBF-CBH-CBJ	2.72	123.28	119.01
11	C	401	U4Z	CBK-CBH-CBJ	-2.71	118.42	122.82
9	4	102	BCL	CHB-C4A-NA	2.71	128.32	124.40
9	8	102	BCL	CHB-C4A-NA	2.71	128.31	124.40
11	H	102	U4Z	CAE-CAI-CAH	2.71	118.89	114.06
9	M	701	BCL	C1D-CHD-C4C	-2.71	120.08	126.62
9	K	102	BCL	O2A-CGA-CBA	2.71	120.09	111.83
9	9	102	BCL	C4-C3-C5	2.71	119.93	115.23
9	R	101	BCL	C4-C3-C5	2.71	119.93	115.23
9	U	102	BCL	C1-C2-C3	-2.71	121.76	126.20
11	P	102	U4Z	CBO-CBL-CBI	-2.70	118.43	122.82
10	U	104	U42	CAK-CAH-CAD	2.70	127.44	124.48
10	U	104	U42	CBN-CBL-CBI	2.70	123.26	119.01
9	P	101	BCL	O2A-CGA-CBA	2.70	120.07	111.83
11	H	102	U4Z	CBG-CBB-CAV	2.70	129.04	123.52
9	D	101	BCL	C4-C3-C5	2.70	119.92	115.23
10	O	101	U42	CBJ-CBM-CBN	2.70	131.02	123.20
9	U	103	BCL	C4-C3-C5	2.70	119.91	115.23
9	Q	103	BCL	CHC-C1C-NC	2.70	128.29	124.40
10	G	101	U42	CBB-CBG-CBI	2.70	129.03	123.52
9	K	102	BCL	CAA-CBA-CGA	-2.70	105.55	113.21
9	B	102	BCL	O2A-CGA-CBA	2.69	120.05	111.83
10	I	101	U42	CBN-CBL-CBI	2.69	123.24	119.01
11	V	102	U4Z	CBN-CBL-CBI	2.69	123.24	119.01
10	U	104	U42	O14-C8-C16	2.69	112.03	106.69
9	0	102	BCL	CHB-C1B-NB	-2.69	120.01	124.05
11	D	103	U4Z	CBG-CBB-CAV	2.69	129.02	123.52
9	S	103	BCL	C1D-CHD-C4C	-2.69	120.14	126.62
11	3	102	U4Z	CBF-CBH-CBJ	2.69	123.23	119.01
9	E	102	BCL	CMB-C2B-C3B	2.69	134.14	125.67
9	6	101	BCL	CHB-C4A-NA	2.69	128.28	124.40
11	5	102	U4Z	CBO-CBL-CBI	-2.69	118.47	122.82
9	6	101	BCL	C4-C3-C5	2.69	119.89	115.23
11	P	102	U4Z	CAE-CAI-CAH	2.68	118.84	114.06
11	A	102	U4Z	CBK-CBH-CBJ	-2.68	118.47	122.82
11	T	102	U4Z	CAE-CAI-CAH	2.68	118.84	114.06
9	4	103	BCL	CHB-C1B-C2B	-2.68	119.64	127.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	1	103	LMT	C1B-O1B-C4'	-2.68	111.62	117.98
9	N	101	BCL	C1-C2-C3	-2.68	121.81	126.20
9	0	102	BCL	O2D-CGD-O1D	-2.68	118.64	123.85
11	P	102	U4Z	CBK-CBH-CBJ	-2.68	118.48	122.82
9	H	101	BCL	CHC-C1C-NC	2.67	128.26	124.40
9	8	102	BCL	C1D-CHD-C4C	-2.67	120.17	126.62
9	5	101	BCL	C4A-NA-C1A	2.67	107.90	106.68
10	4	104	U42	CAC-CAE-CAI	2.67	117.15	111.28
9	H	101	BCL	C1-C2-C3	-2.67	121.82	126.20
10	S	101	U42	CAK-CAH-CAD	-2.67	121.57	124.48
9	P	101	BCL	C3B-C4B-NB	2.67	113.28	109.76
9	1	101	BCL	CHB-C4A-NA	2.67	128.25	124.40
18	M	702	BPH	C1A-C2A-C3A	-2.67	100.30	102.84
9	F	101	BCL	CMB-C2B-C3B	2.66	134.07	125.67
9	D	101	BCL	CHC-C1C-NC	2.66	128.24	124.40
11	T	102	U4Z	CBK-CBH-CBJ	-2.66	118.51	122.82
9	W	102	BCL	CHB-C4A-NA	2.66	128.24	124.40
9	W	101	BCL	C4-C3-C5	2.66	119.84	115.23
9	S	103	BCL	CAA-C2A-C1A	2.66	120.69	111.97
9	J	101	BCL	CMB-C2B-C3B	2.66	134.06	125.67
11	5	102	U4Z	CBK-CBH-CBJ	-2.66	118.51	122.82
9	J	101	BCL	O2A-CGA-CBA	2.66	119.94	111.83
9	0	101	BCL	CMB-C2B-C3B	2.66	134.05	125.67
9	3	101	BCL	C1C-NC-C4C	-2.66	105.47	106.68
10	I	104	U42	CAX-CAT-CAS	2.66	118.71	112.33
9	D	102	BCL	C4D-CHA-C1A	-2.65	118.08	121.24
9	P	101	BCL	C4-C3-C5	2.65	119.83	115.23
9	D	101	BCL	C1D-CHD-C4C	-2.65	120.22	126.62
9	S	103	BCL	C4A-NA-C1A	2.65	107.89	106.68
19	M	704	MQE	CAY-CBL-CBB	2.65	131.40	126.83
11	5	102	U4Z	CAU-CAR-CAV	-2.65	118.52	122.82
9	V	101	BCL	CHC-C1C-NC	2.65	128.22	124.40
11	S	104	U4Z	CAU-CAR-CAV	-2.65	118.53	122.82
9	Q	103	BCL	C1D-CHD-C4C	-2.65	120.24	126.62
9	2	102	BCL	O2A-CGA-CBA	2.65	119.90	111.83
11	5	102	U4Z	CBN-CBL-CBI	2.64	123.17	119.01
11	S	104	U4Z	CBK-CBH-CBJ	-2.64	118.53	122.82
14	C	405	HEC	C2A-C1A-NA	-2.64	107.77	110.32
9	6	102	BCL	CMB-C2B-C3B	2.64	134.01	125.67
9	W	101	BCL	CHB-C4A-NA	2.64	128.21	124.40
11	V	102	U4Z	CAU-CAR-CAV	-2.64	118.54	122.82
9	Q	102	BCL	CHB-C4A-NA	2.64	128.20	124.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	V	102	U4Z	CAQ-CAR-CAV	2.63	123.15	119.01
9	D	101	BCL	CMB-C2B-C3B	2.63	133.98	125.67
11	P	102	U4Z	CBN-CBL-CBI	2.63	123.15	119.01
9	1	101	BCL	O2A-CGA-CBA	2.63	119.86	111.83
11	F	103	U4Z	CBK-CBH-CBJ	-2.63	118.55	122.82
9	O	102	BCL	O2A-CGA-CBA	2.63	119.86	111.83
9	O	102	BCL	C1C-NC-C4C	-2.63	105.48	106.68
9	8	103	BCL	CHB-C4A-NA	2.63	128.19	124.40
11	S	104	U4Z	CAQ-CAR-CAV	2.63	123.14	119.01
9	H	101	BCL	O2A-CGA-CBA	2.62	119.83	111.83
9	7	101	BCL	C1C-NC-C4C	-2.62	105.48	106.68
10	8	101	U42	C21-C20-C19	-2.62	103.49	113.13
9	2	102	BCL	CAA-C2A-C3A	-2.62	105.91	113.00
9	D	101	BCL	CBA-CAA-C2A	-2.62	105.99	113.79
10	I	104	U42	O13-C6-C5	-2.62	104.20	110.38
9	B	102	BCL	C1D-CHD-C4C	-2.62	120.30	126.62
9	I	102	BCL	CHB-C4A-NA	2.62	128.18	124.40
9	U	102	BCL	CHB-C4A-NA	2.62	128.18	124.40
9	F	101	BCL	O2A-CGA-CBA	2.62	119.81	111.83
9	H	101	BCL	CMB-C2B-C3B	2.61	133.91	125.67
18	L	1005	BPH	C2B-C1B-NB	-2.61	107.54	109.43
9	V	101	BCL	CHB-C4A-NA	2.61	128.17	124.40
9	O	102	BCL	CMB-C2B-C3B	2.61	133.90	125.67
9	6	102	BCL	O2D-CGD-O1D	-2.61	118.77	123.85
9	K	101	BCL	CHB-C4A-NA	2.61	128.16	124.40
10	U	104	U42	CAE-CAI-CAH	2.61	118.70	114.06
9	L	1002	BCL	CHC-C1C-NC	2.60	128.16	124.40
9	8	103	BCL	C4-C3-C5	2.60	119.75	115.23
9	2	102	BCL	C1C-NC-C4C	-2.60	105.49	106.68
11	9	101	U4Z	CBK-CBH-CBJ	-2.60	118.60	122.82
10	Q	101	U42	CAP-CAO-CAM	2.60	130.93	127.28
11	A	102	U4Z	CBF-CBH-CBJ	2.60	123.10	119.01
11	C	401	U4Z	CBG-CBB-CAV	2.60	128.84	123.52
9	I	103	BCL	C1-C2-C3	-2.60	121.94	126.20
9	6	102	BCL	O2A-CGA-CBA	2.60	119.75	111.83
9	8	103	BCL	CAA-C2A-C3A	-2.60	105.98	113.00
11	J	102	U4Z	CBG-CBB-CAV	2.60	128.83	123.52
10	8	101	U42	CAP-CAQ-CAR	2.59	133.47	126.36
9	L	1001	BCL	C4-C3-C5	2.59	119.73	115.23
9	I	103	BCL	CMB-C2B-C3B	2.59	133.85	125.67
9	D	102	BCL	C1-C2-C3	-2.59	121.95	126.20
9	0	102	BCL	O2A-CGA-CBA	2.59	119.72	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	S	102	BCL	CHB-C4A-NA	2.59	128.13	124.40
9	2	101	BCL	CMB-C2B-C3B	2.59	133.82	125.67
10	8	101	U42	CBK-CBH-CBJ	-2.58	118.63	122.82
9	8	103	BCL	C1C-NC-C4C	-2.58	105.50	106.68
9	G	102	BCL	C1C-NC-C4C	-2.58	105.50	106.68
9	I	102	BCL	C1D-CHD-C4C	-2.58	120.39	126.62
9	L	1001	BCL	C1D-CHD-C4C	-2.58	120.39	126.62
11	5	102	U4Z	CAB-CAD-CAH	-2.58	119.11	122.64
10	O	101	U42	CAY-O1-C4	-2.58	114.50	119.78
11	D	103	U4Z	CAE-CAI-CAH	2.58	118.65	114.06
9	9	102	BCL	O2A-CGA-CBA	2.58	119.69	111.83
10	U	104	U42	CAB-CAD-CAH	-2.58	119.11	122.64
11	S	104	U4Z	CAB-CAD-CAH	-2.58	119.11	122.64
11	5	102	U4Z	CBF-CBH-CBJ	2.58	123.06	119.01
9	0	101	BCL	O2A-CGA-CBA	2.58	119.69	111.83
9	K	102	BCL	C1D-CHD-C4C	-2.58	120.41	126.62
11	T	102	U4Z	CAU-CAR-CAV	-2.58	118.64	122.82
11	H	102	U4Z	CAB-CAD-CAH	-2.57	119.12	122.64
9	6	101	BCL	C1D-CHD-C4C	-2.57	120.41	126.62
9	V	101	BCL	O2D-CGD-O1D	-2.57	118.84	123.85
10	B	101	U42	C4-C5-C6	-2.57	104.60	110.01
9	B	103	BCL	CAA-C2A-C3A	-2.57	106.05	113.00
11	3	102	U4Z	CAU-CAR-CAV	-2.57	118.65	122.82
14	C	403	HEC	C2A-C1A-NA	-2.57	107.84	110.32
9	3	101	BCL	CHB-C4A-NA	2.57	128.11	124.40
10	O	101	U42	CAP-CAQ-CAR	2.57	133.40	126.36
9	J	101	BCL	C4-C3-C5	2.56	119.68	115.23
9	M	701	BCL	CMB-C2B-C3B	2.56	133.75	125.67
9	U	102	BCL	C1D-CHD-C4C	-2.56	120.44	126.62
10	U	104	U42	CAX-CAT-CAS	2.56	118.49	112.33
9	R	101	BCL	C1D-CHD-C4C	-2.56	120.44	126.62
9	O	103	BCL	O2A-CGA-CBA	2.56	119.64	111.83
11	J	102	U4Z	CBK-CBH-CBJ	-2.56	118.67	122.82
10	4	101	U42	CBM-CBJ-CBH	2.56	130.87	127.28
10	E	101	U42	CAJ-CAL-CAM	2.56	130.02	126.23
11	P	102	U4Z	CBF-CBH-CBJ	2.56	123.03	119.01
11	7	102	U4Z	CBK-CBH-CBJ	-2.55	118.68	122.82
9	L	1001	BCL	C1-O2A-CGA	2.55	122.83	116.65
9	5	101	BCL	O2A-CGA-CBA	2.55	119.61	111.83
11	C	401	U4Z	CAJ-CAD-CAH	-2.55	115.68	121.56
11	1	102	U4Z	CBO-CBL-CBI	-2.55	118.69	122.82
9	F	101	BCL	CHB-C4A-NA	2.55	128.08	124.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	3	101	BCL	C1D-CHD-C4C	-2.55	120.48	126.62
11	D	103	U4Z	CAU-CAR-CAV	-2.55	118.69	122.82
11	D	103	U4Z	CBK-CBH-CBJ	-2.55	118.69	122.82
11	1	102	U4Z	CAE-CAI-CAH	2.55	118.59	114.06
9	U	103	BCL	C1D-CHD-C4C	-2.54	120.48	126.62
11	F	103	U4Z	CBF-CBH-CBJ	2.54	123.01	119.01
9	9	102	BCL	C1-O2A-CGA	2.54	122.81	116.65
9	L	1001	BCL	CHC-C1C-NC	2.54	128.07	124.40
9	Q	103	BCL	CMB-C2B-C3B	2.54	133.69	125.67
10	E	101	U42	CAU-CAR-CAV	-2.54	118.70	122.82
9	O	103	BCL	C4-C3-C5	2.54	119.63	115.23
11	P	102	U4Z	CAB-CAD-CAH	-2.54	119.17	122.64
9	L	1002	BCL	C4D-CHA-C1A	-2.54	118.22	121.24
9	R	101	BCL	C4A-NA-C1A	2.54	107.84	106.68
9	E	102	BCL	C1D-CHD-C4C	-2.54	120.50	126.62
18	L	1003	BPH	CBC-CAC-C3C	-2.53	108.79	113.78
10	U	104	U42	CAP-CAQ-CAR	2.53	133.31	126.36
10	U	101	U42	O14-C8-C7	2.53	114.26	109.70
9	H	101	BCL	C4-C3-C5	2.53	119.62	115.23
9	3	101	BCL	CMB-C2B-C3B	2.53	133.65	125.67
9	G	102	BCL	CMB-C2B-C3B	2.53	133.64	125.67
9	4	102	BCL	C1D-CHD-C4C	-2.53	120.53	126.62
9	Q	102	BCL	C1D-CHD-C4C	-2.53	120.53	126.62
9	U	102	BCL	C4-C3-C5	2.53	119.61	115.23
9	D	102	BCL	C1D-CHD-C4C	-2.52	120.53	126.62
9	J	101	BCL	CHB-C4A-NA	2.52	128.04	124.40
9	N	101	BCL	CHB-C4A-NA	2.52	128.04	124.40
9	4	102	BCL	C1C-NC-C4C	-2.52	105.53	106.68
9	7	101	BCL	CMB-C2B-C3B	2.52	133.62	125.67
9	U	103	BCL	CHC-C1C-NC	2.52	128.04	124.40
11	J	102	U4Z	CAU-CAR-CAV	-2.52	118.73	122.82
11	1	102	U4Z	CBK-CBH-CBJ	-2.52	118.74	122.82
9	4	103	BCL	O2A-CGA-O1A	-2.52	117.33	123.63
11	3	102	U4Z	CAB-CAD-CAH	-2.51	119.20	122.64
9	9	102	BCL	CMB-C2B-C3B	2.51	133.60	125.67
9	5	101	BCL	C4-C3-C5	2.51	119.59	115.23
10	8	101	U42	CAY-O1-C4	-2.51	114.64	119.78
11	N	102	U4Z	CAU-CAR-CAV	-2.51	118.75	122.82
9	I	103	BCL	C1D-CHD-C4C	-2.51	120.57	126.62
9	L	1001	BCL	CHB-C1B-C2B	-2.51	120.15	127.43
11	5	102	U4Z	CAQ-CAR-CAV	2.51	122.95	119.01
9	2	102	BCL	C2A-C3A-C4A	-2.51	97.82	101.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	J	101	BCL	C4D-CHA-C1A	-2.50	118.26	121.24
9	D	101	BCL	CHB-C4A-NA	2.50	128.01	124.40
9	5	101	BCL	CMB-C2B-C3B	2.50	133.56	125.67
11	9	101	U4Z	CAU-CAR-CAV	-2.50	118.77	122.82
11	N	102	U4Z	CBK-CBH-CBJ	-2.50	118.77	122.82
9	M	701	BCL	CHB-C4A-NA	2.50	128.01	124.40
9	K	102	BCL	O1D-CGD-CBD	-2.50	119.59	124.52
9	9	102	BCL	CHB-C4A-NA	2.50	128.01	124.40
11	J	102	U4Z	CAB-CAD-CAH	-2.50	119.22	122.64
11	N	102	U4Z	CAQ-CAR-CAV	2.50	122.94	119.01
10	I	101	U42	CBG-CBB-CAV	2.50	128.63	123.52
10	G	101	U42	O13-C6-C5	-2.49	104.50	110.38
10	4	104	U42	O14-C4-O1	2.49	117.40	109.61
14	C	402	HEC	C2A-C1A-NA	-2.49	107.92	110.32
9	U	103	BCL	O2A-CGA-O1A	-2.49	117.39	123.63
9	5	101	BCL	CHB-C4A-NA	2.49	128.00	124.40
9	N	101	BCL	CMB-C2B-C3B	2.49	133.53	125.67
11	A	102	U4Z	CAU-CAR-CAV	-2.49	118.78	122.82
10	U	104	U42	CAL-CAJ-CAD	2.49	133.65	127.00
18	L	1003	BPH	C3B-C4B-NB	2.49	111.67	108.05
9	1	101	BCL	C1D-CHD-C4C	-2.49	120.62	126.62
9	O	102	BCL	CHB-C4A-NA	2.49	127.99	124.40
9	A	101	BCL	C3C-C4C-CHD	-2.49	118.15	123.39
9	I	103	BCL	C4-C3-C5	2.49	119.54	115.23
9	0	102	BCL	CAA-CBA-CGA	-2.48	106.16	113.21
9	S	103	BCL	C6-C5-C3	-2.48	107.42	113.47
9	9	102	BCL	C1D-CHD-C4C	-2.48	120.63	126.62
10	S	101	U42	O1-CAY-CBC	-2.48	91.99	108.91
11	9	101	U4Z	CAE-CAI-CAH	2.48	118.48	114.06
9	N	101	BCL	C1D-CHD-C4C	-2.48	120.64	126.62
9	7	101	BCL	CHB-C4A-NA	2.48	127.98	124.40
11	H	102	U4Z	CBK-CBH-CBJ	-2.48	118.80	122.82
9	2	102	BCL	CHC-C1C-NC	2.48	127.97	124.40
9	G	102	BCL	CAA-C2A-C1A	2.48	120.09	111.97
9	T	101	BCL	C1D-CHD-C4C	-2.47	120.65	126.62
11	7	102	U4Z	CAU-CAR-CAV	-2.47	118.81	122.82
9	0	101	BCL	C1D-CHD-C4C	-2.47	120.65	126.62
9	A	101	BCL	C3B-C4B-NB	2.47	113.02	109.76
9	W	102	BCL	C1D-CHD-C4C	-2.47	120.66	126.62
9	K	102	BCL	CHC-C1C-NC	2.47	127.97	124.40
11	P	102	U4Z	CAU-CAR-CAV	-2.47	118.81	122.82
9	2	102	BCL	C1D-CHD-C4C	-2.47	120.67	126.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	103	U4Z	CAU-CAR-CAV	-2.47	118.82	122.82
10	0	103	U42	C4-C5-C6	2.47	115.20	110.01
9	3	101	BCL	C1-C2-C3	-2.47	122.15	126.20
9	E	102	BCL	CHB-C1B-C2B	-2.47	120.26	127.43
11	C	401	U4Z	CAE-CAI-CAH	2.47	118.45	114.06
9	B	103	BCL	CMB-C2B-C3B	2.46	133.43	125.67
11	S	104	U4Z	CBF-CBH-CBJ	2.46	122.87	119.01
9	5	101	BCL	C1D-CHD-C4C	-2.46	120.69	126.62
9	S	102	BCL	CBA-CAA-C2A	-2.46	106.48	113.79
9	E	102	BCL	CHC-C1C-NC	2.46	127.94	124.40
11	J	102	U4Z	CAQ-CAR-CAV	2.45	122.87	119.01
11	T	102	U4Z	CAQ-CAR-CAV	2.45	122.87	119.01
9	B	102	BCL	CHB-C4A-NA	2.45	127.94	124.40
9	F	101	BCL	C1D-CHD-C4C	-2.45	120.71	126.62
9	3	101	BCL	C4-C3-C5	2.45	119.48	115.23
11	1	102	U4Z	CAB-CAD-CAH	-2.45	119.29	122.64
9	H	101	BCL	C1D-CHD-C4C	-2.45	120.72	126.62
11	D	103	U4Z	CBF-CBH-CBJ	2.45	122.86	119.01
9	8	102	BCL	CMB-C2B-C3B	2.44	133.38	125.67
9	2	101	BCL	CHB-C4A-NA	2.44	127.93	124.40
9	W	102	BCL	CHC-C1C-NC	2.44	127.93	124.40
10	I	101	U42	CAC-CAE-CAI	2.44	116.65	111.28
9	R	101	BCL	CHB-C4A-NA	2.44	127.92	124.40
10	I	101	U42	CBK-CBH-CBJ	-2.44	118.86	122.82
9	0	101	BCL	CHB-C4A-NA	2.44	127.92	124.40
9	R	101	BCL	CMB-C2B-C3B	2.44	133.36	125.67
11	H	102	U4Z	CAU-CAR-CAV	-2.44	118.86	122.82
11	T	102	U4Z	CBF-CBH-CBJ	2.44	122.84	119.01
9	6	102	BCL	C1D-CHD-C4C	-2.43	120.75	126.62
10	U	101	U42	CAC-CAB-CAD	2.43	113.97	110.44
9	B	103	BCL	CAA-CBA-CGA	-2.43	106.30	113.21
9	F	101	BCL	C1C-NC-C4C	-2.43	105.57	106.68
9	J	101	BCL	CHC-C1C-NC	2.43	127.91	124.40
9	0	102	BCL	CMD-C2D-C3D	-2.43	122.12	127.69
9	B	102	BCL	C4D-CHA-C1A	-2.43	118.35	121.24
11	3	102	U4Z	CAQ-CAR-CAV	2.42	122.82	119.01
18	L	1003	BPH	O2A-CGA-CBA	2.42	119.21	111.83
9	K	102	BCL	C6-C7-C8	-2.42	107.92	115.97
9	8	102	BCL	O2A-CGA-CBA	2.42	119.21	111.83
9	4	103	BCL	CAA-C2A-C1A	2.42	119.90	111.97
9	W	102	BCL	CMB-C2B-C3B	2.42	133.30	125.67
9	O	102	BCL	C1D-CHD-C4C	-2.42	120.79	126.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	102	U4Z	CAE-CAI-CAH	2.42	118.36	114.06
10	B	101	U42	CBN-CBL-CBI	2.42	122.81	119.01
9	K	101	BCL	C1D-CHD-C4C	-2.41	120.80	126.62
11	D	103	U4Z	CAQ-CAR-CAV	2.41	122.81	119.01
10	B	101	U42	CBE-CBF-CBH	2.41	132.98	126.36
9	K	102	BCL	CMB-C2B-C3B	2.41	133.27	125.67
10	4	101	U42	CAP-CAO-CAM	2.41	130.66	127.28
10	B	101	U42	O15-C7-C8	2.41	115.26	109.32
12	T	103	LMT	O5'-C5'-C6'	2.40	112.39	106.44
11	9	101	U4Z	CBF-CBH-CBJ	2.40	122.78	119.01
9	S	102	BCL	C1D-CHD-C4C	-2.40	120.83	126.62
9	W	101	BCL	CBC-CAC-C3C	-2.40	108.33	113.41
9	F	101	BCL	CHC-C1C-NC	2.40	127.86	124.40
9	V	101	BCL	C1D-CHD-C4C	-2.39	120.84	126.62
9	S	102	BCL	CHB-C1B-C2B	-2.39	120.48	127.43
9	6	101	BCL	O2A-CGA-CBA	2.39	119.12	111.83
9	F	101	BCL	C4-C3-C5	2.39	119.38	115.23
10	E	101	U42	CAE-CAI-CAH	2.39	118.31	114.06
9	O	103	BCL	C1-O2A-CGA	2.39	122.43	116.65
10	I	104	U42	CAL-CAJ-CAD	2.38	133.37	127.00
11	J	102	U4Z	CBF-CBH-CBJ	2.38	122.75	119.01
10	Q	101	U42	CBE-CBA-CAW	-2.38	124.35	127.69
9	3	101	BCL	O2A-CGA-CBA	2.38	119.08	111.83
11	9	101	U4Z	CAQ-CAR-CAV	2.38	122.75	119.01
10	Q	101	U42	O14-C8-C16	2.38	111.41	106.69
9	B	103	BCL	O2A-CGA-CBA	2.37	119.08	111.83
9	F	102	BCL	CHB-C4A-NA	2.37	127.83	124.40
9	F	102	BCL	C1D-CHD-C4C	-2.37	120.91	126.62
9	0	102	BCL	CHB-C4A-NA	2.37	127.81	124.40
9	B	102	BCL	CHC-C1C-NC	2.36	127.81	124.40
9	G	102	BCL	CMD-C2D-C3D	-2.36	122.27	127.69
10	4	104	U42	CAJ-CAD-CAH	2.36	126.99	121.56
10	4	104	U42	CBN-CBL-CBI	2.36	122.72	119.01
9	I	102	BCL	CHC-C1C-NC	2.36	127.81	124.40
9	4	103	BCL	CMD-C2D-C3D	-2.36	122.28	127.69
9	G	102	BCL	CHB-C4A-NA	2.36	127.80	124.40
9	M	701	BCL	CHB-C1B-NB	-2.36	120.51	124.05
9	5	101	BCL	CHC-C1C-NC	2.35	127.80	124.40
9	6	102	BCL	CMD-C2D-C3D	-2.35	122.29	127.69
10	O	101	U42	CBE-CBF-CBH	2.35	132.82	126.36
9	J	101	BCL	C1D-CHD-C4C	-2.35	120.95	126.62
9	A	101	BCL	CHA-C4D-ND	2.35	137.40	132.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	U	104	U42	CAP-CAO-CAM	2.35	130.57	127.28
9	O	103	BCL	C3D-C4D-ND	2.35	113.80	109.99
9	H	101	BCL	C1-O2A-CGA	2.35	122.33	116.65
9	D	102	BCL	CHC-C1C-NC	2.35	127.79	124.40
9	O	103	BCL	CMB-C2B-C3B	2.34	133.06	125.67
9	E	102	BCL	C4-C3-C5	2.34	119.29	115.23
9	6	101	BCL	C6-C5-C3	-2.34	107.77	113.47
10	I	101	U42	CBM-CBJ-CBH	2.34	130.56	127.28
10	O	101	U42	O14-C8-C7	-2.34	105.48	109.70
9	W	101	BCL	C6-C5-C3	-2.34	107.77	113.47
10	E	101	U42	CAP-CAQ-CAR	2.34	132.78	126.36
9	4	103	BCL	C1-O2A-CGA	2.34	122.31	116.65
11	V	102	U4Z	CAB-CAD-CAH	-2.34	119.44	122.64
9	4	103	BCL	C6-C7-C8	-2.33	108.21	115.97
9	K	101	BCL	O2A-CGA-CBA	2.33	118.95	111.83
9	E	102	BCL	CMD-C2D-C3D	-2.33	122.35	127.69
9	H	101	BCL	C6-C5-C3	-2.33	107.80	113.47
9	A	101	BCL	C2C-C3C-C4C	-2.33	97.86	101.34
19	L	1004	MQE	OAA-CBQ-CBP	-2.33	117.85	121.57
9	I	103	BCL	O2A-CGA-CBA	2.32	118.92	111.83
9	F	102	BCL	CHC-C1C-NC	2.32	127.75	124.40
13	L	1015	BGL	C3-C4-C5	2.32	114.43	110.23
10	4	101	U42	CBE-CBA-CAW	-2.32	124.43	127.69
9	Q	102	BCL	O2A-CGA-CBA	2.32	118.90	111.83
9	S	103	BCL	CMB-C2B-C3B	2.32	132.97	125.67
9	8	103	BCL	O2A-CGA-CBA	2.32	118.90	111.83
11	1	102	U4Z	CBN-CBL-CBI	2.32	122.65	119.01
11	7	102	U4Z	CBF-CBH-CBJ	2.31	122.65	119.01
9	S	103	BCL	C5-C3-C2	2.31	126.36	121.17
9	U	103	BCL	CMB-C2B-C3B	2.31	132.96	125.67
9	D	102	BCL	CHB-C4A-NA	2.31	127.74	124.40
12	T	103	LMT	C1'-C2'-C3'	2.31	114.87	110.01
10	O	101	U42	CBE-CBA-CAW	2.31	130.94	127.69
9	F	102	BCL	O2A-CGA-CBA	2.31	118.87	111.83
10	0	103	U42	CBO-CBL-CBI	-2.30	119.08	122.82
9	F	102	BCL	C1C-NC-C4C	-2.30	105.63	106.68
9	J	101	BCL	CBA-CAA-C2A	-2.30	106.95	113.79
9	S	103	BCL	C1C-NC-C4C	-2.30	105.63	106.68
9	J	101	BCL	CHB-C1B-C2B	-2.30	120.76	127.43
10	4	104	U42	CBB-CBG-CBI	2.30	128.22	123.52
9	Q	102	BCL	CHB-C1B-C2B	-2.30	120.76	127.43
11	A	102	U4Z	CAQ-CAR-CAV	2.29	122.62	119.01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	H	102	U4Z	CBE-CBA-CAW	2.29	130.91	127.69
9	G	102	BCL	CHB-C1B-C2B	-2.29	120.78	127.43
10	0	103	U42	O1-CAY-CBD	-2.29	93.31	108.91
10	4	101	U42	O15-C7-C8	-2.29	103.69	109.32
9	8	103	BCL	CMB-C2B-C3B	2.29	132.88	125.67
9	7	101	BCL	C1D-CHD-C4C	-2.29	121.10	126.62
9	Q	102	BCL	CED-O2D-CGD	2.28	121.09	115.92
11	F	103	U4Z	CAB-CAD-CAH	-2.28	119.52	122.64
9	6	101	BCL	CHB-C1B-C2B	-2.28	120.81	127.43
9	D	101	BCL	O2A-CGA-CBA	2.28	118.78	111.83
9	Q	103	BCL	CHB-C4A-NA	2.28	127.69	124.40
9	V	101	BCL	CMB-C2B-C3B	2.28	132.85	125.67
9	O	102	BCL	C2A-C1A-CHA	-2.28	119.92	123.87
11	N	102	U4Z	CBF-CBH-CBJ	2.27	122.59	119.01
10	0	103	U42	CAB-CAD-CAJ	2.27	121.82	115.65
10	O	101	U42	CBA-CBE-CBF	-2.27	116.62	123.20
9	J	101	BCL	C6-C5-C3	-2.27	107.94	113.47
9	8	103	BCL	CMD-C2D-C3D	-2.27	122.48	127.69
10	O	101	U42	CAB-CAD-CAJ	2.27	121.81	115.65
11	F	103	U4Z	CAQ-CAR-CAV	2.27	122.58	119.01
9	K	101	BCL	C11-C12-C13	-2.27	108.43	115.97
9	2	101	BCL	CHB-C1B-C2B	-2.27	120.84	127.43
10	4	104	U42	CBE-CBA-CAW	-2.27	124.50	127.69
10	I	101	U42	O15-C7-C8	2.27	114.90	109.32
10	8	101	U42	CAJ-CAD-CAH	2.26	126.77	121.56
10	4	101	U42	C7-C6-C5	2.26	114.80	110.83
9	K	102	BCL	CMD-C2D-C3D	-2.26	122.50	127.69
10	B	101	U42	CAP-CAQ-CAR	2.26	132.57	126.36
9	3	101	BCL	C11-C12-C13	-2.26	108.45	115.97
12	D	105	LMT	C1B-O1B-C4'	-2.26	112.63	117.98
11	N	102	U4Z	CAB-CAD-CAH	-2.26	119.55	122.64
11	7	102	U4Z	CAQ-CAR-CAV	2.26	122.56	119.01
9	Q	103	BCL	C4-C3-C2	-2.26	117.83	123.63
11	P	102	U4Z	CAQ-CAR-CAV	2.25	122.56	119.01
9	S	103	BCL	CHB-C1B-C2B	-2.25	120.88	127.43
9	0	102	BCL	CMB-C2B-C3B	2.25	132.77	125.67
10	U	101	U42	CAT-CAX-CAY	2.25	124.94	114.09
9	1	101	BCL	C4D-CHA-C1A	-2.25	118.56	121.24
10	E	101	U42	CBE-CBF-CBH	2.25	132.53	126.36
9	S	103	BCL	C4-C3-C5	2.25	119.13	115.23
9	L	1002	BCL	C1D-CHD-C4C	-2.25	121.19	126.62
9	D	102	BCL	CHB-C1B-C2B	-2.25	120.91	127.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	102	BCL	CHB-C1B-C2B	-2.24	120.92	127.43
9	4	102	BCL	O2A-CGA-CBA	2.24	118.66	111.83
9	3	101	BCL	C4D-CHA-C1A	-2.24	118.57	121.24
9	B	103	BCL	CHB-C1B-C2B	-2.24	120.93	127.43
9	3	101	BCL	C6-C5-C3	-2.23	108.03	113.47
9	H	101	BCL	CHB-C1B-C2B	-2.23	120.95	127.43
9	G	102	BCL	C4-C3-C2	-2.23	117.90	123.63
9	4	102	BCL	CED-O2D-CGD	2.23	120.97	115.92
18	L	1003	BPH	CMB-C2B-C3B	2.23	129.13	124.68
9	3	101	BCL	CHB-C1B-C2B	-2.23	120.96	127.43
9	K	101	BCL	C1-O2A-CGA	2.23	122.04	116.65
9	1	101	BCL	CMB-C2B-C3B	2.23	132.69	125.67
9	9	102	BCL	CHC-C1C-NC	2.23	127.61	124.40
10	S	101	U42	CAP-CAQ-CAR	2.23	132.46	126.36
10	0	103	U42	CAE-CAI-CAH	2.22	118.02	114.06
11	V	102	U4Z	CAK-CAH-CAD	2.22	126.91	124.48
11	H	102	U4Z	CAQ-CAR-CAV	2.22	122.50	119.01
13	L	1011	BGL	O5-C5-C4	2.22	113.70	109.70
10	B	101	U42	CBK-CBH-CBF	2.22	121.47	118.09
9	Q	103	BCL	CHB-C1B-C2B	-2.22	120.99	127.43
9	S	102	BCL	CHC-C1C-NC	2.21	127.59	124.40
11	7	102	U4Z	CAE-CAI-CAH	2.21	117.99	114.06
9	2	101	BCL	C4D-CHA-C1A	-2.21	118.61	121.24
10	U	101	U42	CAP-CAQ-CAR	2.20	132.41	126.36
9	5	101	BCL	C1-O2A-CGA	2.20	121.98	116.65
9	L	1002	BCL	CHB-C1B-C2B	-2.20	121.04	127.43
9	Q	102	BCL	CHC-C1C-NC	2.20	127.58	124.40
9	U	102	BCL	CHB-C1B-C2B	-2.19	121.06	127.43
9	K	101	BCL	CHC-C1C-NC	2.19	127.57	124.40
9	R	101	BCL	C4D-CHA-C1A	-2.19	118.63	121.24
9	8	102	BCL	CHC-C1C-NC	2.19	127.56	124.40
9	5	101	BCL	CHB-C1B-C2B	-2.19	121.06	127.43
9	S	102	BCL	C2A-C1A-CHA	-2.19	120.06	123.87
11	1	102	U4Z	CAK-CAH-CAD	2.19	126.87	124.48
10	4	104	U42	CBE-CBF-CBH	2.19	132.36	126.36
9	W	101	BCL	O2A-CGA-O1A	-2.19	118.16	123.63
9	P	101	BCL	CHA-C4D-ND	2.19	137.06	132.55
9	F	101	BCL	C6-C5-C3	-2.18	108.15	113.47
9	S	103	BCL	CHB-C1B-NB	-2.18	120.77	124.05
9	D	101	BCL	CHB-C1B-C2B	-2.18	121.10	127.43
9	A	101	BCL	CHA-C1A-NA	-2.18	121.46	126.39
10	I	104	U42	O1-CAY-CBC	-2.18	94.07	108.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	4	101	U42	CAU-CAR-CAV	-2.18	119.29	122.82
18	L	1005	BPH	C2D-C1D-ND	-2.17	107.86	109.43
10	I	101	U42	CAY-O1-C4	-2.17	115.33	119.78
9	I	103	BCL	CHB-C1B-C2B	-2.17	121.12	127.43
9	W	101	BCL	CHB-C1B-C2B	-2.17	121.12	127.43
9	T	101	BCL	C4D-CHA-C1A	-2.17	118.66	121.24
9	I	102	BCL	CHB-C1B-C2B	-2.17	121.13	127.43
9	L	1001	BCL	CMD-C2D-C3D	-2.17	122.71	127.69
9	7	101	BCL	C4D-CHA-C1A	-2.17	118.66	121.24
9	E	102	BCL	O2A-CGA-CBA	2.17	118.44	111.83
10	I	104	U42	C4-C5-C6	-2.17	105.45	110.01
10	O	101	U42	CAU-CAR-CAV	-2.16	119.31	122.82
9	B	103	BCL	CED-O2D-CGD	2.16	120.82	115.92
11	3	102	U4Z	CAK-CAH-CAD	2.16	126.84	124.48
9	L	1002	BCL	C4-C3-C5	2.16	118.98	115.23
9	B	103	BCL	C11-C12-C13	-2.16	108.79	115.97
9	9	102	BCL	C4D-CHA-C1A	-2.16	118.67	121.24
9	F	101	BCL	CHB-C1B-C2B	-2.15	121.17	127.43
9	D	102	BCL	O2A-CGA-CBA	2.15	118.40	111.83
9	M	701	BCL	CHC-C1C-NC	2.15	127.51	124.40
11	1	102	U4Z	CBF-CBH-CBJ	2.15	122.39	119.01
9	W	101	BCL	CHC-C1C-NC	2.15	127.50	124.40
9	4	102	BCL	C1-O2A-CGA	2.15	121.85	116.65
18	L	1003	BPH	CMA-C3A-C4A	-2.14	110.00	114.61
9	0	102	BCL	CED-O2D-CGD	2.14	120.77	115.92
9	Q	103	BCL	C1C-NC-C4C	-2.14	105.70	106.68
11	D	103	U4Z	CAK-CAH-CAD	2.14	126.82	124.48
9	2	102	BCL	CHC-C4B-C3B	-2.14	123.22	131.72
9	Q	103	BCL	CAA-C2A-C1A	2.14	118.98	111.97
9	L	1002	BCL	CHB-C4A-NA	2.14	127.49	124.40
9	0	102	BCL	CHB-C1B-C2B	-2.14	121.22	127.43
9	T	101	BCL	C1-O2A-CGA	2.14	121.82	116.65
10	S	101	U42	CAJ-CAD-CAH	-2.14	116.64	121.56
9	0	102	BCL	C1C-NC-C4C	-2.13	105.70	106.68
9	J	101	BCL	C1C-NC-C4C	-2.13	105.71	106.68
9	7	101	BCL	CHB-C1B-C2B	-2.13	121.24	127.43
9	B	103	BCL	C4-C3-C5	2.13	118.93	115.23
9	2	102	BCL	C4-C3-C5	2.13	118.93	115.23
9	U	102	BCL	CHC-C1C-NC	2.13	127.47	124.40
9	I	103	BCL	CMD-C2D-C3D	-2.13	122.81	127.69
9	H	101	BCL	CHB-C4A-NA	2.13	127.47	124.40
9	N	101	BCL	CHC-C1C-NC	2.13	127.47	124.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	R	101	BCL	C6-C5-C3	-2.13	108.28	113.47
11	9	101	U4Z	CAK-CAH-CAD	2.13	126.81	124.48
10	4	101	U42	O14-C8-C7	-2.13	105.86	109.70
9	U	102	BCL	C1C-NC-C4C	-2.13	105.71	106.68
9	2	101	BCL	CED-O2D-CGD	2.13	120.74	115.92
11	H	102	U4Z	CBF-CBH-CBJ	2.13	122.35	119.01
9	P	101	BCL	O1D-CGD-CBD	-2.13	120.33	124.52
9	F	101	BCL	C1-O2A-CGA	2.12	121.79	116.65
9	B	103	BCL	CHB-C1B-NB	-2.12	120.86	124.05
9	E	102	BCL	C2A-C3A-C4A	-2.12	98.44	101.87
9	F	102	BCL	CHB-C1B-C2B	-2.12	121.27	127.43
9	F	101	BCL	CBA-CAA-C2A	-2.12	107.48	113.79
10	4	101	U42	CAC-CAE-CAI	2.12	115.93	111.28
9	R	101	BCL	CED-O2D-CGD	2.12	120.71	115.92
9	Q	102	BCL	C1-O2A-CGA	2.12	121.77	116.65
9	S	103	BCL	CHB-C4A-NA	2.11	127.45	124.40
9	2	101	BCL	C1D-CHD-C4C	-2.11	121.52	126.62
11	J	102	U4Z	CAK-CAH-CAD	2.11	126.79	124.48
9	S	103	BCL	CMD-C2D-C3D	-2.11	122.84	127.69
9	O	102	BCL	CED-O2D-CGD	2.11	120.70	115.92
9	8	103	BCL	C1D-CHD-C4C	-2.11	121.53	126.62
9	1	101	BCL	CHC-C1C-NC	2.11	127.44	124.40
9	2	101	BCL	O2A-CGA-O1A	-2.11	118.35	123.63
9	8	102	BCL	C1C-NC-C4C	-2.11	105.72	106.68
10	U	104	U42	CBM-CBN-CBL	2.11	132.14	126.36
11	1	102	U4Z	CAL-CAM-CAO	2.11	122.32	119.01
10	4	104	U42	CAG-CAB-CAD	-2.11	106.94	110.24
9	G	102	BCL	O2A-CGA-O1A	-2.11	118.36	123.63
10	0	103	U42	CAC-CAE-CAI	2.10	115.89	111.28
9	T	101	BCL	CMB-C2B-C3B	2.10	132.28	125.67
9	K	101	BCL	CHB-C1B-C2B	-2.10	121.34	127.43
9	N	101	BCL	C4D-CHA-C1A	-2.10	118.75	121.24
9	V	101	BCL	CHB-C1B-C2B	-2.09	121.34	127.43
11	C	401	U4Z	CBB-CAV-CAR	-2.09	124.34	127.28
9	L	1001	BCL	O2A-CGA-O1A	-2.09	118.39	123.63
9	K	102	BCL	CED-O2D-CGD	2.09	120.66	115.92
9	O	102	BCL	CHC-C1C-NC	2.09	127.42	124.40
9	U	102	BCL	C2A-C1A-CHA	-2.09	120.24	123.87
9	V	101	BCL	CED-O2D-CGD	2.09	120.65	115.92
10	U	104	U42	O17-C16-C8	2.09	112.82	108.41
9	5	101	BCL	CBA-CAA-C2A	-2.09	107.58	113.79
10	8	101	U42	CBO-CBL-CBN	-2.09	114.90	118.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	6	101	BCL	CED-O2D-CGD	2.09	120.65	115.92
9	6	101	BCL	CHC-C1C-NC	2.09	127.41	124.40
10	Q	101	U42	CBE-CBF-CBH	2.09	132.08	126.36
9	9	102	BCL	C4A-NA-C1A	2.08	107.63	106.68
9	V	101	BCL	C1-O2A-CGA	2.08	121.69	116.65
9	0	101	BCL	CHC-C1C-NC	2.08	127.41	124.40
10	O	101	U42	CBN-CBL-CBI	2.08	122.28	119.01
9	8	102	BCL	C6-C5-C3	-2.08	108.40	113.47
11	7	102	U4Z	CAK-CAH-CAD	2.08	126.75	124.48
9	B	103	BCL	CMD-C2D-C3D	-2.08	122.92	127.69
11	F	103	U4Z	CAK-CAH-CAD	2.08	126.75	124.48
11	N	102	U4Z	CAK-CAH-CAD	2.08	126.75	124.48
10	Q	101	U42	CAP-CAQ-CAR	2.08	132.06	126.36
12	T	103	LMT	C1B-O1B-C4'	-2.08	113.05	117.98
9	0	101	BCL	CHB-C1B-C2B	-2.08	121.40	127.43
10	U	104	U42	CBK-CBH-CBJ	-2.08	119.45	122.82
9	T	101	BCL	CHC-C1C-NC	2.08	127.39	124.40
9	A	101	BCL	CHC-C1C-NC	2.07	127.39	124.40
14	C	404	HEC	CAA-CBA-CGA	-2.07	108.16	113.67
10	S	101	U42	CAX-CAT-CAS	2.07	117.31	112.33
9	E	102	BCL	CHB-C4A-NA	2.07	127.39	124.40
9	S	102	BCL	C1-C2-C3	-2.07	122.80	126.20
9	1	101	BCL	C4A-NA-C1A	2.07	107.62	106.68
9	W	102	BCL	CMD-C2D-C3D	-2.07	122.94	127.69
18	M	702	BPH	C2D-C1D-ND	-2.07	107.93	109.43
9	D	102	BCL	C11-C12-C13	-2.07	109.08	115.97
9	4	103	BCL	C6-C5-C3	-2.07	108.42	113.47
11	S	104	U4Z	CAK-CAH-CAD	2.07	126.74	124.48
18	L	1005	BPH	C1A-C2A-C3A	-2.07	100.87	102.84
10	4	104	U42	CAB-CAD-CAJ	-2.07	110.04	115.65
9	F	102	BCL	C2A-C1A-CHA	-2.07	120.28	123.87
9	D	102	BCL	O2A-CGA-O1A	-2.07	118.45	123.63
10	I	104	U42	CAU-CAR-CAQ	-2.07	114.93	118.09
9	F	101	BCL	C4D-CHA-C1A	-2.07	118.78	121.24
10	S	101	U42	CAG-CAB-CAF	-2.07	102.72	108.63
9	8	103	BCL	C6-C7-C8	-2.06	109.10	115.97
10	I	104	U42	CAC-CAB-CAD	2.06	113.44	110.44
10	S	101	U42	CBO-CBL-CBI	-2.06	119.47	122.82
9	6	102	BCL	CHB-C1B-C2B	-2.06	121.44	127.43
10	8	101	U42	CAK-CAH-CAD	2.06	126.73	124.48
10	U	101	U42	C4-O14-C8	2.06	117.75	113.72
11	P	102	U4Z	CAK-CAH-CAD	2.06	126.73	124.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	102	BCL	O2A-CGA-CBA	2.06	118.11	111.83
10	O	101	U42	CAG-CAB-CAF	-2.06	102.74	108.63
9	7	101	BCL	C1-C2-C3	-2.06	122.83	126.20
9	V	101	BCL	C4D-CHA-C1A	-2.06	118.79	121.24
11	T	102	U4Z	CAK-CAH-CAD	2.05	126.73	124.48
10	E	101	U42	CAY-O1-C4	-2.05	115.57	119.78
11	H	102	U4Z	CAK-CAH-CAD	2.05	126.72	124.48
11	9	101	U4Z	CAN-CAM-CAL	2.05	121.22	118.09
10	I	101	U42	CAK-CAH-CAD	2.05	126.72	124.48
10	E	101	U42	CBO-CBL-CBN	-2.05	114.96	118.09
10	I	101	U42	CAB-CAD-CAH	-2.05	119.84	122.64
9	D	101	BCL	C4D-CHA-C1A	-2.05	118.80	121.24
9	8	103	BCL	CHB-C1B-NB	-2.05	120.98	124.05
10	4	104	U42	C6-C7-C8	2.05	113.94	110.23
9	P	101	BCL	CMD-C2D-C1D	2.04	128.33	124.73
10	I	104	U42	CBA-CBE-CBF	2.04	129.12	123.20
9	O	102	BCL	O2A-CGA-O1A	-2.04	118.52	123.63
9	L	1002	BCL	O2D-CGD-O1D	-2.04	119.88	123.85
10	E	101	U42	CAX-CAT-CAS	2.04	117.23	112.33
9	S	102	BCL	CED-O2D-CGD	2.04	120.54	115.92
9	2	102	BCL	CMD-C2D-C3D	-2.04	123.01	127.69
9	S	103	BCL	O2A-CGA-O1A	-2.04	118.53	123.63
10	4	101	U42	CBJ-CBM-CBN	-2.04	117.30	123.20
9	M	701	BCL	C4-C3-C5	2.03	118.76	115.23
9	4	102	BCL	CHB-C1B-C2B	-2.03	121.52	127.43
11	5	102	U4Z	CAK-CAH-CAD	2.03	126.70	124.48
9	V	101	BCL	O2A-CGA-O1A	-2.03	118.54	123.63
10	B	101	U42	CAO-CAP-CAQ	2.03	129.09	123.20
9	P	101	BCL	CHA-C1A-NA	-2.03	121.79	126.39
11	A	102	U4Z	CAN-CAM-CAL	2.03	121.19	118.09
9	0	102	BCL	O1D-CGD-CBD	-2.03	120.51	124.52
10	B	101	U42	CAN-CAM-CAL	-2.03	114.98	118.09
9	4	103	BCL	CHB-C4A-NA	2.03	127.33	124.40
9	O	103	BCL	CHB-C1B-C2B	-2.03	121.54	127.43
10	U	101	U42	O17-C16-C8	-2.03	104.13	108.41
9	L	1001	BCL	CHD-C1D-C2D	2.03	129.71	125.49
9	B	103	BCL	C7-C6-C5	-2.02	107.86	113.26
9	L	1002	BCL	CMD-C2D-C3D	-2.02	123.05	127.69
9	V	101	BCL	CHC-C4B-NB	-2.02	121.02	124.05
9	3	101	BCL	CHC-C1C-NC	2.02	127.31	124.40
10	B	101	U42	CAB-CAD-CAJ	2.02	121.12	115.65
10	B	101	U42	CBC-CAY-CAX	2.02	114.71	111.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	T	101	BCL	O2A-CGA-O1A	-2.02	118.59	123.63
9	P	101	BCL	C2A-C1A-CHA	-2.02	120.37	123.87
9	4	103	BCL	CBA-CAA-C2A	2.01	119.78	113.79
9	W	102	BCL	C6-C7-C8	-2.01	109.28	115.97
10	I	104	U42	O15-C7-C8	-2.01	104.37	109.32
10	I	101	U42	CAL-CAJ-CAD	2.01	132.37	127.00
9	9	102	BCL	CHB-C1B-C2B	-2.01	121.59	127.43
11	A	102	U4Z	CAK-CAH-CAD	2.01	126.67	124.48
9	T	101	BCL	CHB-C1B-NB	-2.01	121.04	124.05
9	S	102	BCL	C5-C3-C2	-2.00	116.67	121.17
10	S	101	U42	CBE-CBF-CBH	2.00	131.85	126.36
9	W	101	BCL	CED-O2D-CGD	2.00	120.45	115.92

There are no chirality outliers.

All (1427) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	0	102	BCL	C4C-C3C-CAC-CBC
9	0	102	BCL	CHA-CBD-CGD-O2D
9	1	101	BCL	C1A-C2A-CAA-CBA
9	1	101	BCL	C3A-C2A-CAA-CBA
9	1	101	BCL	C2C-C3C-CAC-CBC
9	1	101	BCL	C4C-C3C-CAC-CBC
9	1	101	BCL	C14-C13-C15-C16
9	2	102	BCL	CBD-CGD-O2D-CED
9	3	101	BCL	C4C-C3C-CAC-CBC
9	4	103	BCL	C4C-C3C-CAC-CBC
9	6	102	BCL	C4C-C3C-CAC-CBC
9	7	101	BCL	C4C-C3C-CAC-CBC
9	8	103	BCL	C2C-C3C-CAC-CBC
9	8	103	BCL	C4C-C3C-CAC-CBC
9	8	103	BCL	CBD-CGD-O2D-CED
9	9	102	BCL	C2C-C3C-CAC-CBC
9	9	102	BCL	C4C-C3C-CAC-CBC
9	A	101	BCL	C2C-C3C-CAC-CBC
9	A	101	BCL	C4C-C3C-CAC-CBC
9	B	103	BCL	C1A-C2A-CAA-CBA
9	B	103	BCL	C3A-C2A-CAA-CBA
9	B	103	BCL	C2C-C3C-CAC-CBC
9	B	103	BCL	C4C-C3C-CAC-CBC
9	D	101	BCL	C2C-C3C-CAC-CBC
9	D	101	BCL	C4C-C3C-CAC-CBC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	D	101	BCL	C14-C13-C15-C16
9	D	102	BCL	C1A-C2A-CAA-CBA
9	E	102	BCL	C2C-C3C-CAC-CBC
9	E	102	BCL	C4C-C3C-CAC-CBC
9	G	102	BCL	C1A-C2A-CAA-CBA
9	G	102	BCL	C3A-C2A-CAA-CBA
9	G	102	BCL	C4C-C3C-CAC-CBC
9	G	102	BCL	CBD-CGD-O2D-CED
9	G	102	BCL	C11-C10-C8-C9
9	H	101	BCL	C2C-C3C-CAC-CBC
9	H	101	BCL	C4C-C3C-CAC-CBC
9	I	102	BCL	CHA-CBD-CGD-O1D
9	I	102	BCL	CHA-CBD-CGD-O2D
9	I	103	BCL	C1A-C2A-CAA-CBA
9	I	103	BCL	C3A-C2A-CAA-CBA
9	I	103	BCL	CBD-CGD-O2D-CED
9	J	101	BCL	C2C-C3C-CAC-CBC
9	J	101	BCL	C4C-C3C-CAC-CBC
9	K	102	BCL	C1A-C2A-CAA-CBA
9	K	102	BCL	C3A-C2A-CAA-CBA
9	K	102	BCL	C2-C1-O2A-CGA
9	K	102	BCL	C4C-C3C-CAC-CBC
9	L	1001	BCL	C1A-C2A-CAA-CBA
9	L	1001	BCL	C4C-C3C-CAC-CBC
9	L	1002	BCL	C1A-C2A-CAA-CBA
9	L	1002	BCL	C3A-C2A-CAA-CBA
9	O	103	BCL	CBD-CGD-O2D-CED
9	P	101	BCL	C4C-C3C-CAC-CBC
9	Q	103	BCL	C1A-C2A-CAA-CBA
9	Q	103	BCL	C2C-C3C-CAC-CBC
9	R	101	BCL	C2C-C3C-CAC-CBC
9	R	101	BCL	C4C-C3C-CAC-CBC
9	S	103	BCL	C4C-C3C-CAC-CBC
9	T	101	BCL	C1A-C2A-CAA-CBA
9	T	101	BCL	C3A-C2A-CAA-CBA
9	U	103	BCL	C2C-C3C-CAC-CBC
9	U	103	BCL	C4C-C3C-CAC-CBC
9	V	101	BCL	C1A-C2A-CAA-CBA
9	V	101	BCL	C3A-C2A-CAA-CBA
9	W	101	BCL	C1A-C2A-CAA-CBA
9	W	101	BCL	C4C-C3C-CAC-CBC
9	W	101	BCL	C14-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	W	102	BCL	C2C-C3C-CAC-CBC
9	W	102	BCL	C4C-C3C-CAC-CBC
9	W	102	BCL	C2-C3-C5-C6
9	W	102	BCL	C4-C3-C5-C6
9	W	102	BCL	C11-C10-C8-C9
10	0	103	U42	CAO-CAP-CAQ-CAR
10	0	103	U42	CAT-CAX-CAY-CBC
10	0	103	U42	CAT-CAX-CAY-CBD
10	4	101	U42	CAT-CAX-CAY-CBC
10	4	101	U42	CAT-CAX-CAY-CBD
10	4	101	U42	CAT-CAX-CAY-O1
10	E	101	U42	CAS-CAT-CAX-CAY
10	E	101	U42	CAT-CAX-CAY-CBC
10	E	101	U42	CAX-CAY-O1-C4
10	E	101	U42	CBC-CAY-O1-C4
10	E	101	U42	CBD-CAY-O1-C4
10	G	101	U42	CAT-CAS-CAW-CAZ
10	G	101	U42	CAT-CAX-CAY-CBC
10	G	101	U42	CAT-CAX-CAY-O1
10	G	101	U42	CAX-CAY-O1-C4
10	G	101	U42	CBC-CAY-O1-C4
10	G	101	U42	CBD-CAY-O1-C4
10	I	101	U42	C5-C4-O1-CAY
10	I	101	U42	CAT-CAX-CAY-CBC
10	I	101	U42	CAT-CAX-CAY-CBD
10	I	101	U42	CAX-CAY-O1-C4
10	I	101	U42	CBC-CAY-O1-C4
10	I	104	U42	CAX-CAY-O1-C4
10	I	104	U42	CBC-CAY-O1-C4
10	I	104	U42	CBD-CAY-O1-C4
10	O	101	U42	CAX-CAY-O1-C4
10	O	101	U42	CBC-CAY-O1-C4
10	O	101	U42	CBD-CAY-O1-C4
10	O	101	U42	CBJ-CBM-CBN-CBL
10	Q	101	U42	CAT-CAX-CAY-CBC
10	Q	101	U42	CAX-CAY-O1-C4
10	S	101	U42	CAT-CAX-CAY-CBC
10	S	101	U42	CAX-CAY-O1-C4
10	S	101	U42	CBC-CAY-O1-C4
10	S	101	U42	CBD-CAY-O1-C4
10	U	101	U42	C19-C18-O17-C16
10	U	101	U42	O2-C18-O17-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	U	101	U42	CAX-CAY-O1-C4
10	U	101	U42	CBD-CAY-O1-C4
10	U	104	U42	C5-C4-O1-CAY
10	U	104	U42	O14-C4-O1-CAY
10	U	104	U42	CAT-CAS-CAW-CAZ
10	U	104	U42	CAT-CAS-CAW-CBA
10	U	104	U42	CAT-CAX-CAY-CBC
10	U	104	U42	CAT-CAX-CAY-O1
10	U	104	U42	CAX-CAY-O1-C4
10	U	104	U42	CBC-CAY-O1-C4
10	U	104	U42	CBD-CAY-O1-C4
11	C	401	U4Z	CAB-CAD-CAJ-CAL
11	C	401	U4Z	CAH-CAD-CAJ-CAL
11	C	401	U4Z	CAL-CAM-CAO-CAP
11	C	401	U4Z	CAN-CAM-CAO-CAP
11	C	401	U4Z	CAS-CAW-CBA-CBE
11	C	401	U4Z	CAZ-CAW-CBA-CBE
11	C	401	U4Z	CAT-CAX-CAY-CBC
11	C	401	U4Z	CBF-CBH-CBJ-CBM
11	C	401	U4Z	CBK-CBH-CBJ-CBM
11	V	102	U4Z	CAH-CAD-CAJ-CAL
14	C	402	HEC	C2B-C3B-CAB-CBB
14	C	402	HEC	C4B-C3B-CAB-CBB
14	C	402	HEC	C2C-C3C-CAC-CBC
14	C	403	HEC	C2B-C3B-CAB-CBB
14	C	403	HEC	C4B-C3B-CAB-CBB
14	C	403	HEC	C2C-C3C-CAC-CBC
14	C	404	HEC	C2B-C3B-CAB-CBB
14	C	404	HEC	C4B-C3B-CAB-CBB
14	C	404	HEC	C2C-C3C-CAC-CBC
14	C	404	HEC	C4C-C3C-CAC-CBC
14	C	405	HEC	C2B-C3B-CAB-CBB
14	C	405	HEC	C4B-C3B-CAB-CBB
14	C	405	HEC	C2C-C3C-CAC-CBC
14	C	405	HEC	C4C-C3C-CAC-CBC
16	C	407	PGV	C03-O11-P-O12
16	C	407	PGV	C03-O11-P-O14
16	C	407	PGV	C04-O12-P-O13
16	C	407	PGV	C04-C05-C06-O06
16	C	407	PGV	O05-C05-C06-O06
16	C	408	PGV	C03-O11-P-O12
16	C	408	PGV	C03-O11-P-O13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
16	C	408	PGV	C03-O11-P-O14
16	C	408	PGV	C04-C05-C06-O06
16	C	408	PGV	O05-C05-C06-O06
16	L	1006	PGV	C03-O11-P-O13
16	L	1006	PGV	O12-C04-C05-C06
16	L	1007	PGV	C03-O11-P-O12
16	L	1007	PGV	C03-O11-P-O14
16	L	1007	PGV	C04-O12-P-O13
16	L	1007	PGV	O12-C04-C05-O05
16	L	1008	PGV	C03-O11-P-O12
16	L	1008	PGV	C03-O11-P-O13
16	L	1008	PGV	C03-O11-P-O14
16	L	1008	PGV	C04-O12-P-O13
16	M	705	PGV	C03-O11-P-O12
16	M	705	PGV	C03-O11-P-O13
16	M	705	PGV	C03-O11-P-O14
16	M	705	PGV	C04-O12-P-O13
16	M	706	PGV	C03-O11-P-O12
16	P	103	PGV	O12-C04-C05-C06
16	P	103	PGV	O12-C04-C05-O05
16	P	104	PGV	C03-O11-P-O12
16	P	104	PGV	O03-C01-C02-O01
16	P	104	PGV	C04-C05-C06-O06
18	L	1003	BPH	O2A-C1-C2-C3
18	L	1005	BPH	C2C-C3C-CAC-CBC
19	L	1004	MQE	CAL-CAE-CAR-CBV
19	L	1004	MQE	CBK-CAX-CAY-CBL
19	L	1004	MQE	CBQ-CAX-CAY-CBL
20	L	1017	PEF	C1-O3P-P-O1P
9	8	103	BCL	O1D-CGD-O2D-CED
9	G	102	BCL	O1D-CGD-O2D-CED
9	B	103	BCL	CBD-CGD-O2D-CED
9	K	102	BCL	CBD-CGD-O2D-CED
9	M	701	BCL	CBD-CGD-O2D-CED
9	Q	103	BCL	CBD-CGD-O2D-CED
9	8	103	BCL	O1A-CGA-O2A-C1
9	W	101	BCL	O1A-CGA-O2A-C1
11	C	401	U4Z	CAT-CAX-CAY-CBD
9	M	701	BCL	O1D-CGD-O2D-CED
9	8	103	BCL	CBA-CGA-O2A-C1
9	W	101	BCL	CBA-CGA-O2A-C1
9	2	102	BCL	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	4	103	BCL	O1A-CGA-O2A-C1
9	B	102	BCL	O1A-CGA-O2A-C1
9	B	103	BCL	O1A-CGA-O2A-C1
16	C	407	PGV	O04-C19-O03-C01
9	2	102	BCL	O1D-CGD-O2D-CED
9	O	103	BCL	O1D-CGD-O2D-CED
13	L	1013	BGL	O5-C5-C6-O6
10	8	101	U42	O17-C16-C8-O14
10	G	101	U42	O17-C16-C8-O14
10	I	104	U42	O17-C16-C8-O14
10	O	101	U42	O17-C16-C8-O14
10	Q	101	U42	O17-C16-C8-O14
10	S	101	U42	O17-C16-C8-O14
9	4	103	BCL	CBD-CGD-O2D-CED
9	I	103	BCL	O1D-CGD-O2D-CED
13	L	1015	BGL	C4-C5-C6-O6
9	0	101	BCL	C3-C5-C6-C7
9	2	101	BCL	C3-C5-C6-C7
9	3	101	BCL	C3-C5-C6-C7
9	6	101	BCL	C3-C5-C6-C7
9	B	102	BCL	C3-C5-C6-C7
9	B	103	BCL	C3-C5-C6-C7
9	O	103	BCL	C3-C5-C6-C7
9	R	101	BCL	C3-C5-C6-C7
9	S	103	BCL	C3-C5-C6-C7
9	U	102	BCL	C3-C5-C6-C7
9	U	103	BCL	C3-C5-C6-C7
9	W	102	BCL	C3-C5-C6-C7
18	M	702	BPH	C3-C5-C6-C7
10	0	103	U42	C8-C16-O17-C18
9	4	103	BCL	CBA-CGA-O2A-C1
9	K	102	BCL	CBA-CGA-O2A-C1
16	C	407	PGV	C20-C19-O03-C01
9	1	101	BCL	CBD-CGD-O2D-CED
9	E	102	BCL	CBD-CGD-O2D-CED
9	O	102	BCL	CBD-CGD-O2D-CED
9	V	101	BCL	CBD-CGD-O2D-CED
9	W	102	BCL	CBD-CGD-O2D-CED
16	C	408	PGV	C2-C1-O01-C02
9	2	101	BCL	C4-C3-C5-C6
9	6	102	BCL	C4-C3-C5-C6
9	D	102	BCL	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	U	103	BCL	C4-C3-C5-C6
10	O	101	U42	CAT-CAS-CAW-CAZ
10	S	101	U42	CAT-CAS-CAW-CAZ
11	1	102	U4Z	CAT-CAS-CAW-CAZ
19	L	1004	MQE	CAM-CAG-CAW-CBY
19	L	1004	MQE	CAO-CAH-CAV-CBX
9	6	102	BCL	C2-C3-C5-C6
9	U	103	BCL	C2-C3-C5-C6
10	G	101	U42	CAT-CAS-CAW-CBA
10	O	101	U42	CAT-CAS-CAW-CBA
10	S	101	U42	CAT-CAS-CAW-CBA
19	L	1004	MQE	CAL-CAE-CAR-CBD
19	L	1004	MQE	CAM-CAG-CAW-CBH
19	L	1004	MQE	CAO-CAH-CAV-CBF
9	0	102	BCL	CBD-CGD-O2D-CED
9	I	102	BCL	C3-C5-C6-C7
9	J	101	BCL	C3-C5-C6-C7
9	N	101	BCL	C3-C5-C6-C7
9	V	101	BCL	C3-C5-C6-C7
10	O	101	U42	CAW-CAS-CAT-CAX
12	T	103	LMT	C3'-C4'-O1B-C1B
9	2	102	BCL	CBA-CGA-O2A-C1
9	8	102	BCL	CBA-CGA-O2A-C1
9	B	102	BCL	CBA-CGA-O2A-C1
9	B	103	BCL	CBA-CGA-O2A-C1
9	I	102	BCL	CBA-CGA-O2A-C1
9	I	103	BCL	CBA-CGA-O2A-C1
10	0	103	U42	C19-C18-O17-C16
13	L	1015	BGL	O5-C5-C6-O6
10	S	101	U42	O17-C16-C8-C7
9	4	102	BCL	O1A-CGA-O2A-C1
9	I	102	BCL	O1A-CGA-O2A-C1
9	K	101	BCL	O1A-CGA-O2A-C1
9	K	102	BCL	O1A-CGA-O2A-C1
9	U	103	BCL	O1A-CGA-O2A-C1
10	0	103	U42	O2-C18-O17-C16
16	C	408	PGV	O02-C1-O01-C02
13	Y	101	BGL	C4-C5-C6-O6
9	9	102	BCL	C3-C5-C6-C7
9	S	102	BCL	C3-C5-C6-C7
9	9	102	BCL	CBD-CGD-O2D-CED
9	H	101	BCL	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	I	102	BCL	CBD-CGD-O2D-CED
18	M	702	BPH	CBD-CGD-O2D-CED
10	I	101	U42	O17-C16-C8-O14
16	C	408	PGV	O12-C04-C05-O05
9	B	103	BCL	O1D-CGD-O2D-CED
9	6	101	BCL	CBA-CGA-O2A-C1
9	F	102	BCL	CBA-CGA-O2A-C1
9	K	101	BCL	CBA-CGA-O2A-C1
9	Q	102	BCL	CBA-CGA-O2A-C1
9	U	103	BCL	CBA-CGA-O2A-C1
9	6	101	BCL	O1A-CGA-O2A-C1
9	8	102	BCL	O1A-CGA-O2A-C1
9	Q	102	BCL	O1A-CGA-O2A-C1
13	L	1012	BGL	C4-C5-C6-O6
9	Q	103	BCL	O1D-CGD-O2D-CED
9	S	102	BCL	CBD-CGD-O2D-CED
13	N	103	BGL	O5-C5-C6-O6
13	N	103	BGL	C4-C5-C6-O6
9	K	102	BCL	O1D-CGD-O2D-CED
13	3	103	BGL	O5-C5-C6-O6
13	L	1013	BGL	C4-C5-C6-O6
9	0	101	BCL	CBA-CGA-O2A-C1
9	4	102	BCL	CBA-CGA-O2A-C1
9	4	103	BCL	C4-C3-C5-C6
9	L	1002	BCL	C4-C3-C5-C6
9	O	103	BCL	C4-C3-C5-C6
9	S	103	BCL	C4-C3-C5-C6
10	E	101	U42	CAT-CAS-CAW-CAZ
10	I	101	U42	CAT-CAS-CAW-CAZ
19	L	1004	MQE	CAS-CAN-CBB-CCA
9	2	101	BCL	C2-C3-C5-C6
9	4	103	BCL	C2-C3-C5-C6
9	D	102	BCL	C2-C3-C5-C6
10	E	101	U42	CAT-CAS-CAW-CBA
9	I	103	BCL	O1A-CGA-O2A-C1
19	L	1004	MQE	CAP-CAC-CAI-CBD
19	L	1004	MQE	CBB-CAN-CAS-CBH
19	M	704	MQE	CBM-CBJ-CBO-CCB
13	C	409	BGL	O5-C5-C6-O6
9	0	101	BCL	O1A-CGA-O2A-C1
9	0	102	BCL	CBA-CGA-O2A-C1
9	W	102	BCL	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	2	101	BCL	CBD-CGD-O2D-CED
9	F	101	BCL	CBD-CGD-O2D-CED
13	L	1011	BGL	O5-C5-C6-O6
13	L	1012	BGL	O5-C5-C6-O6
13	Y	101	BGL	O5-C5-C6-O6
9	F	102	BCL	O1A-CGA-O2A-C1
10	Q	101	U42	O2-C18-O17-C16
13	C	410	BGL	O5-C5-C6-O6
9	L	1002	BCL	CBD-CGD-O2D-CED
12	1	103	LMT	C3'-C4'-O1B-C1B
13	3	103	BGL	C4-C5-C6-O6
9	3	101	BCL	O1A-CGA-O2A-C1
16	C	408	PGV	O12-C04-C05-C06
16	M	705	PGV	O12-C04-C05-C06
16	P	104	PGV	O12-C04-C05-C06
9	3	101	BCL	CBA-CGA-O2A-C1
10	Q	101	U42	C19-C18-O17-C16
16	L	1007	PGV	C4-C5-C6-C7
13	F	104	BGL	O5-C5-C6-O6
22	h	101	LHG	C10-C11-C12-C13
10	O	101	U42	O17-C16-C8-C7
10	Q	101	U42	O17-C16-C8-C7
9	4	103	BCL	O1D-CGD-O2D-CED
10	O	101	U42	C23-C24-C25-C26
11	1	102	U4Z	CAT-CAS-CAW-CBA
19	L	1004	MQE	CAS-CAN-CBB-CBL
9	A	101	BCL	C3-C5-C6-C7
10	E	101	U42	CAW-CAS-CAT-CAX
9	D	102	BCL	CBD-CGD-O2D-CED
9	8	103	BCL	C14-C13-C15-C16
9	M	701	BCL	C11-C10-C8-C9
9	M	701	BCL	C14-C13-C15-C16
9	S	103	BCL	C6-C7-C8-C9
9	S	103	BCL	C11-C10-C8-C9
9	U	103	BCL	C11-C10-C8-C9
18	L	1005	BPH	C6-C7-C8-C9
16	M	706	PGV	C28-C29-C30-C31
9	6	101	BCL	CBD-CGD-O2D-CED
10	4	104	U42	CAJ-CAL-CAM-CAN
10	8	101	U42	CAJ-CAL-CAM-CAN
10	G	101	U42	CAJ-CAL-CAM-CAN
10	U	101	U42	CAJ-CAL-CAM-CAN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	C	401	U4Z	CAJ-CAL-CAM-CAN
10	4	104	U42	CAJ-CAL-CAM-CAO
10	8	101	U42	CAJ-CAL-CAM-CAO
10	G	101	U42	CAJ-CAL-CAM-CAO
10	U	101	U42	CAJ-CAL-CAM-CAO
13	C	410	BGL	C4-C5-C6-O6
13	L	1011	BGL	C4-C5-C6-O6
18	L	1003	BPH	CBD-CGD-O2D-CED
10	I	104	U42	O17-C16-C8-C7
9	O	102	BCL	O1D-CGD-O2D-CED
9	7	101	BCL	C13-C15-C16-C17
9	P	101	BCL	C10-C11-C12-C13
9	W	102	BCL	C10-C11-C12-C13
18	M	702	BPH	C13-C15-C16-C17
16	P	104	PGV	O05-C05-C06-O06
9	D	101	BCL	CBD-CGD-O2D-CED
9	4	103	BCL	C12-C13-C15-C16
9	P	101	BCL	C6-C7-C8-C10
9	Q	102	BCL	C12-C13-C15-C16
12	1	103	LMT	C5'-C4'-O1B-C1B
9	U	103	BCL	C8-C10-C11-C12
9	W	102	BCL	O1D-CGD-O2D-CED
16	L	1007	PGV	C1-C2-C3-C4
10	G	101	U42	O17-C16-C8-C7
12	D	105	LMT	O5'-C5'-C6'-O6'
19	L	1004	MQE	CAV-CAH-CAO-CBI
9	I	102	BCL	C10-C11-C12-C13
12	T	103	LMT	O5B-C5B-C6B-O6B
9	F	102	BCL	CBD-CGD-O2D-CED
9	J	101	BCL	CBD-CGD-O2D-CED
9	V	101	BCL	O1D-CGD-O2D-CED
9	2	101	BCL	C5-C6-C7-C8
9	G	102	BCL	C8-C10-C11-C12
9	G	102	BCL	C13-C15-C16-C17
9	I	103	BCL	C10-C11-C12-C13
9	P	101	BCL	C15-C16-C17-C18
9	Q	102	BCL	C15-C16-C17-C18
9	3	101	BCL	C2A-CAA-CBA-CGA
9	B	103	BCL	C2A-CAA-CBA-CGA
9	O	103	BCL	C2A-CAA-CBA-CGA
9	V	101	BCL	C2A-CAA-CBA-CGA
9	0	102	BCL	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	1	101	BCL	C5-C6-C7-C8
9	2	101	BCL	C10-C11-C12-C13
9	6	102	BCL	C13-C15-C16-C17
9	8	103	BCL	C13-C15-C16-C17
9	S	102	BCL	C10-C11-C12-C13
16	P	104	PGV	C19-C20-C21-C22
9	0	102	BCL	O1D-CGD-O2D-CED
9	0	102	BCL	O1A-CGA-O2A-C1
9	W	102	BCL	O1A-CGA-O2A-C1
10	U	104	U42	CAW-CAS-CAT-CAX
9	4	103	BCL	C10-C11-C12-C13
9	5	101	BCL	C8-C10-C11-C12
9	8	102	BCL	C13-C15-C16-C17
9	8	103	BCL	C5-C6-C7-C8
9	B	103	BCL	C5-C6-C7-C8
9	F	101	BCL	C13-C15-C16-C17
9	I	102	BCL	C5-C6-C7-C8
9	J	101	BCL	C8-C10-C11-C12
9	M	701	BCL	C13-C15-C16-C17
9	M	701	BCL	C15-C16-C17-C18
9	O	103	BCL	C5-C6-C7-C8
9	Q	103	BCL	C10-C11-C12-C13
9	V	101	BCL	C13-C15-C16-C17
16	L	1006	PGV	O12-C04-C05-O05
16	L	1008	PGV	O12-C04-C05-O05
16	M	705	PGV	O12-C04-C05-O05
16	P	104	PGV	O12-C04-C05-O05
9	S	103	BCL	CBA-CGA-O2A-C1
10	U	104	U42	C19-C18-O17-C16
9	3	101	BCL	CBD-CGD-O2D-CED
12	T	103	LMT	C4B-C5B-C6B-O6B
9	K	102	BCL	C15-C16-C17-C18
13	L	1015	BGL	O2-C1'-C2'-C3'
10	4	104	U42	C21-C22-C23-C24
12	D	105	LMT	O1'-C1-C2-C3
9	Q	103	BCL	C3-C5-C6-C7
9	1	101	BCL	O1D-CGD-O2D-CED
9	9	102	BCL	O1D-CGD-O2D-CED
9	E	102	BCL	O1D-CGD-O2D-CED
18	M	702	BPH	O1D-CGD-O2D-CED
9	1	101	BCL	C13-C15-C16-C17
9	D	102	BCL	C13-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	L	1001	BCL	C13-C15-C16-C17
9	S	102	BCL	C5-C6-C7-C8
9	W	102	BCL	C5-C6-C7-C8
10	I	101	U42	CAT-CAS-CAW-CBA
9	H	101	BCL	O1D-CGD-O2D-CED
9	F	101	BCL	C8-C10-C11-C12
9	I	103	BCL	C5-C6-C7-C8
18	L	1005	BPH	C8-C10-C11-C12
9	2	101	BCL	CBA-CGA-O2A-C1
9	P	101	BCL	C3-C5-C6-C7
9	2	102	BCL	C15-C16-C17-C18
9	N	101	BCL	C15-C16-C17-C18
10	U	104	U42	O2-C18-O17-C16
9	O	102	BCL	C2A-CAA-CBA-CGA
9	D	102	BCL	CBA-CGA-O2A-C1
9	G	102	BCL	CBA-CGA-O2A-C1
10	8	101	U42	C19-C18-O17-C16
10	8	101	U42	C21-C22-C23-C24
9	4	102	BCL	C13-C15-C16-C17
9	O	103	BCL	C10-C11-C12-C13
9	U	102	BCL	C13-C15-C16-C17
10	U	101	U42	O17-C16-C8-O14
9	6	102	BCL	C5-C6-C7-C8
9	8	102	BCL	C15-C16-C17-C18
9	F	102	BCL	C13-C15-C16-C17
9	L	1002	BCL	C15-C16-C17-C18
9	P	101	BCL	C5-C6-C7-C8
9	U	103	BCL	C10-C11-C12-C13
9	V	101	BCL	C15-C16-C17-C18
13	L	1011	BGL	O2-C1'-C2'-C3'
9	0	101	BCL	C5-C6-C7-C8
9	B	103	BCL	C15-C16-C17-C18
9	D	101	BCL	C8-C10-C11-C12
9	S	102	BCL	C15-C16-C17-C18
9	S	103	BCL	C8-C10-C11-C12
18	L	1005	BPH	C10-C11-C12-C13
9	O	103	BCL	C2-C3-C5-C6
10	S	101	U42	CAW-CAS-CAT-CAX
9	S	102	BCL	O1D-CGD-O2D-CED
9	7	101	BCL	C8-C10-C11-C12
16	C	408	PGV	C1-C2-C3-C4
9	S	103	BCL	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	S	103	BCL	CBD-CGD-O2D-CED
9	6	101	BCL	C10-C11-C12-C13
9	E	102	BCL	C15-C16-C17-C18
9	U	102	BCL	C5-C6-C7-C8
10	E	101	U42	CBE-CBF-CBH-CBK
10	I	101	U42	CAJ-CAL-CAM-CAN
16	M	706	PGV	C26-C27-C28-C29
10	I	101	U42	CAJ-CAL-CAM-CAO
10	U	104	U42	CAJ-CAL-CAM-CAO
11	C	401	U4Z	CAJ-CAL-CAM-CAO
9	7	101	BCL	C2A-CAA-CBA-CGA
9	E	102	BCL	C2A-CAA-CBA-CGA
16	L	1008	PGV	C04-C05-C06-O06
16	M	706	PGV	C04-C05-C06-O06
9	2	102	BCL	C16-C17-C18-C20
9	6	102	BCL	C3-C5-C6-C7
9	R	101	BCL	C10-C11-C12-C13
9	D	101	BCL	C15-C16-C17-C18
9	S	103	BCL	C2-C3-C5-C6
9	I	102	BCL	O1D-CGD-O2D-CED
9	6	102	BCL	CBA-CGA-O2A-C1
16	P	104	PGV	C4-C5-C6-C7
9	1	101	BCL	C16-C17-C18-C19
9	9	102	BCL	C16-C17-C18-C20
9	E	102	BCL	C16-C17-C18-C19
9	F	102	BCL	C16-C17-C18-C20
9	H	101	BCL	C16-C17-C18-C20
9	L	1001	BCL	C16-C17-C18-C19
13	H	107	BGL	C1'-C2'-C3'-C4'
9	D	102	BCL	O1A-CGA-O2A-C1
9	G	102	BCL	O1A-CGA-O2A-C1
9	M	701	BCL	C8-C10-C11-C12
10	U	104	U42	O17-C16-C8-C7
10	B	101	U42	C24-C25-C26-C27
13	N	103	BGL	O2-C1'-C2'-C3'
10	O	101	U42	CAV-CBB-CBG-CBI
10	U	101	U42	CAV-CBB-CBG-CBI
10	4	101	U42	C20-C21-C22-C23
10	4	101	U42	C26-C27-C28-C29
10	Q	101	U42	C24-C25-C26-C27
9	0	101	BCL	C15-C16-C17-C18
9	M	701	BCL	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	Q	102	BCL	C8-C10-C11-C12
9	S	103	BCL	C5-C6-C7-C8
10	G	101	U42	C27-C28-C29-C30
20	L	1017	PEF	C18-C19-C20-C21
22	h	101	LHG	C18-C19-C20-C21
10	U	104	U42	C27-C28-C29-C30
22	h	101	LHG	C11-C10-C9-C8
16	M	706	PGV	O05-C05-C06-O06
10	U	101	U42	CAW-CAS-CAT-CAX
9	2	102	BCL	C16-C17-C18-C19
9	3	101	BCL	C16-C17-C18-C19
9	F	101	BCL	C16-C17-C18-C19
9	H	101	BCL	C16-C17-C18-C19
9	M	701	BCL	C16-C17-C18-C19
9	M	701	BCL	C16-C17-C18-C20
9	T	101	BCL	C16-C17-C18-C20
9	V	101	BCL	C16-C17-C18-C19
9	V	101	BCL	C16-C17-C18-C20
9	I	103	BCL	C8-C10-C11-C12
9	S	103	BCL	C15-C16-C17-C18
16	L	1007	PGV	C2-C1-O01-C02
13	F	104	BGL	C4-C5-C6-O6
9	6	101	BCL	C11-C12-C13-C15
9	Q	103	BCL	C6-C7-C8-C10
10	4	101	U42	C28-C29-C30-C31
16	M	706	PGV	C29-C30-C31-C32
10	8	101	U42	O2-C18-O17-C16
9	H	101	BCL	C3-C5-C6-C7
9	2	102	BCL	C3A-C2A-CAA-CBA
9	3	101	BCL	C3A-C2A-CAA-CBA
9	D	102	BCL	C3A-C2A-CAA-CBA
9	Q	103	BCL	C3A-C2A-CAA-CBA
9	W	101	BCL	C3A-C2A-CAA-CBA
10	4	104	U42	C27-C28-C29-C30
13	H	107	BGL	C4'-C5'-C6'-C7'
9	L	1002	BCL	C2-C3-C5-C6
9	U	102	BCL	CBD-CGD-O2D-CED
9	U	103	BCL	CBD-CGD-O2D-CED
9	T	101	BCL	C13-C15-C16-C17
9	W	102	BCL	C13-C15-C16-C17
18	L	1003	BPH	C10-C11-C12-C13
13	Y	101	BGL	O2-C1'-C2'-C3'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	5	101	BCL	C16-C17-C18-C19
9	E	102	BCL	C16-C17-C18-C20
9	Q	102	BCL	C16-C17-C18-C19
18	L	1005	BPH	C16-C17-C18-C19
18	L	1005	BPH	C16-C17-C18-C20
9	2	101	BCL	O1A-CGA-O2A-C1
10	E	101	U42	C25-C26-C27-C28
16	L	1008	PGV	C23-C24-C25-C26
16	P	103	PGV	C22-C23-C24-C25
22	h	101	LHG	C11-C12-C13-C14
16	M	705	PGV	C7-C8-C9-C10
16	L	1007	PGV	O12-C04-C05-C06
10	S	101	U42	C20-C21-C22-C23
16	C	408	PGV	C20-C21-C22-C23
16	L	1008	PGV	C20-C21-C22-C23
10	O	101	U42	C25-C26-C27-C28
16	C	407	PGV	C20-C21-C22-C23
13	N	103	BGL	C1'-C2'-C3'-C4'
10	B	101	U42	C27-C28-C29-C30
16	L	1008	PGV	C22-C23-C24-C25
9	F	101	BCL	O1D-CGD-O2D-CED
10	U	101	U42	C21-C22-C23-C24
10	U	104	U42	C28-C29-C30-C31
9	9	102	BCL	C16-C17-C18-C19
9	L	1001	BCL	C16-C17-C18-C20
10	0	103	U42	CAB-CAD-CAJ-CAL
10	0	103	U42	CAH-CAD-CAJ-CAL
10	4	101	U42	CAB-CAD-CAJ-CAL
10	4	101	U42	CAH-CAD-CAJ-CAL
10	B	101	U42	CAB-CAD-CAJ-CAL
10	B	101	U42	CAH-CAD-CAJ-CAL
10	I	101	U42	CAB-CAD-CAJ-CAL
10	I	101	U42	CAH-CAD-CAJ-CAL
10	O	101	U42	CAB-CAD-CAJ-CAL
10	O	101	U42	CAH-CAD-CAJ-CAL
10	Q	101	U42	CAB-CAD-CAJ-CAL
10	Q	101	U42	CAH-CAD-CAJ-CAL
10	S	101	U42	CAH-CAD-CAJ-CAL
10	U	104	U42	CAB-CAD-CAJ-CAL
10	U	104	U42	CAH-CAD-CAJ-CAL
11	1	102	U4Z	CAB-CAD-CAJ-CAL
11	1	102	U4Z	CAH-CAD-CAJ-CAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	3	102	U4Z	CAB-CAD-CAJ-CAL
11	3	102	U4Z	CAH-CAD-CAJ-CAL
11	5	102	U4Z	CAB-CAD-CAJ-CAL
11	5	102	U4Z	CAH-CAD-CAJ-CAL
11	7	102	U4Z	CAB-CAD-CAJ-CAL
11	7	102	U4Z	CAH-CAD-CAJ-CAL
11	9	101	U4Z	CAB-CAD-CAJ-CAL
11	9	101	U4Z	CAH-CAD-CAJ-CAL
11	A	102	U4Z	CAB-CAD-CAJ-CAL
11	A	102	U4Z	CAH-CAD-CAJ-CAL
11	D	103	U4Z	CAB-CAD-CAJ-CAL
11	D	103	U4Z	CAH-CAD-CAJ-CAL
11	F	103	U4Z	CAB-CAD-CAJ-CAL
11	F	103	U4Z	CAH-CAD-CAJ-CAL
11	H	102	U4Z	CAB-CAD-CAJ-CAL
11	H	102	U4Z	CAH-CAD-CAJ-CAL
11	J	102	U4Z	CAB-CAD-CAJ-CAL
11	J	102	U4Z	CAH-CAD-CAJ-CAL
11	N	102	U4Z	CAB-CAD-CAJ-CAL
11	N	102	U4Z	CAH-CAD-CAJ-CAL
11	P	102	U4Z	CAB-CAD-CAJ-CAL
11	P	102	U4Z	CAH-CAD-CAJ-CAL
11	S	104	U4Z	CAB-CAD-CAJ-CAL
11	S	104	U4Z	CAH-CAD-CAJ-CAL
11	T	102	U4Z	CAB-CAD-CAJ-CAL
11	T	102	U4Z	CAH-CAD-CAJ-CAL
11	V	102	U4Z	CAB-CAD-CAJ-CAL
9	0	101	BCL	CBD-CGD-O2D-CED
9	7	101	BCL	CBD-CGD-O2D-CED
9	E	102	BCL	C10-C11-C12-C13
9	N	101	BCL	C8-C10-C11-C12
18	M	702	BPH	C15-C16-C17-C18
9	8	103	BCL	C3-C5-C6-C7
9	G	102	BCL	C3-C5-C6-C7
9	G	102	BCL	C10-C11-C12-C13
10	O	101	U42	C19-C20-C21-C22
16	M	705	PGV	C21-C22-C23-C24
22	h	101	LHG	C12-C13-C14-C15
9	6	102	BCL	O1A-CGA-O2A-C1
9	8	102	BCL	CBD-CGD-O2D-CED
16	L	1007	PGV	O02-C1-O01-C02
10	U	101	U42	CAT-CAS-CAW-CAZ

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	B	103	BCL	C10-C11-C12-C13
9	U	102	BCL	C15-C16-C17-C18
9	2	101	BCL	O1D-CGD-O2D-CED
9	E	102	BCL	C6-C7-C8-C9
9	T	101	BCL	C11-C12-C13-C14
9	L	1002	BCL	O1D-CGD-O2D-CED
10	4	101	U42	C22-C23-C24-C25
16	M	706	PGV	C27-C28-C29-C30
16	P	104	PGV	C22-C23-C24-C25
10	U	104	U42	O17-C16-C8-O14
9	B	102	BCL	C10-C11-C12-C13
9	1	101	BCL	C16-C17-C18-C20
9	F	102	BCL	C16-C17-C18-C19
16	L	1008	PGV	C2-C1-O01-C02
16	L	1007	PGV	C3-C4-C5-C6
16	L	1008	PGV	O02-C1-O01-C02
22	h	101	LHG	C16-C17-C18-C19
10	I	104	U42	CAJ-CAL-CAM-CAN
10	U	104	U42	CAJ-CAL-CAM-CAN
9	8	102	BCL	C3-C5-C6-C7
10	I	104	U42	CAJ-CAL-CAM-CAO
13	L	1015	BGL	C2'-C3'-C4'-C5'
9	R	101	BCL	C2A-CAA-CBA-CGA
9	N	101	BCL	C16-C17-C18-C20
9	Q	102	BCL	C16-C17-C18-C20
9	T	101	BCL	C16-C17-C18-C19
18	L	1005	BPH	CBD-CGD-O2D-CED
16	C	408	PGV	C22-C23-C24-C25
16	M	705	PGV	C24-C25-C26-C27
10	U	101	U42	C23-C24-C25-C26
10	B	101	U42	C26-C27-C28-C29
9	4	102	BCL	C8-C10-C11-C12
9	F	101	BCL	C15-C16-C17-C18
13	Y	101	BGL	C1'-C2'-C3'-C4'
16	P	103	PGV	C1-C2-C3-C4
16	L	1007	PGV	C2-C3-C4-C5
16	P	103	PGV	O01-C02-C03-O11
9	D	102	BCL	C5-C6-C7-C8
12	T	103	LMT	C5'-C4'-O1B-C1B
10	8	101	U42	O17-C16-C8-C7
10	Q	101	U42	C25-C26-C27-C28
10	S	101	U42	C18-C19-C20-C21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
16	P	104	PGV	C1-C2-C3-C4
9	I	103	BCL	C15-C16-C17-C18
12	T	103	LMT	O5'-C5'-C6'-O6'
13	L	1013	BGL	C2'-C3'-C4'-C5'
16	C	408	PGV	C28-C29-C30-C31
9	D	102	BCL	C15-C16-C17-C18
10	I	101	U42	O17-C16-C8-C7
12	1	103	LMT	C3-C4-C5-C6
16	L	1008	PGV	C4-C5-C6-C7
9	O	103	BCL	C2-C1-O2A-CGA
18	L	1003	BPH	C2C-C3C-CAC-CBC
9	6	102	BCL	C8-C10-C11-C12
9	S	103	BCL	C10-C11-C12-C13
10	I	104	U42	C24-C25-C26-C27
22	h	101	LHG	O7-C7-C8-C9
10	B	101	U42	O17-C16-C8-O14
10	E	101	U42	O17-C16-C8-O14
16	L	1007	PGV	C14-C15-C16-C17
9	K	101	BCL	CBD-CGD-O2D-CED
13	L	1012	BGL	C4'-C5'-C6'-C7'
9	D	101	BCL	O1D-CGD-O2D-CED
20	L	1017	PEF	C15-C16-C17-C18
9	J	101	BCL	C16-C17-C18-C19
9	2	102	BCL	C1A-C2A-CAA-CBA
9	3	101	BCL	C1A-C2A-CAA-CBA
9	4	103	BCL	C1A-C2A-CAA-CBA
9	6	102	BCL	C1A-C2A-CAA-CBA
9	S	103	BCL	C1A-C2A-CAA-CBA
9	O	103	BCL	C15-C16-C17-C18
9	Q	103	BCL	C5-C6-C7-C8
10	4	104	U42	C23-C24-C25-C26
10	8	101	U42	C26-C27-C28-C29
9	0	101	BCL	C11-C10-C8-C7
9	4	102	BCL	C11-C12-C13-C15
9	8	102	BCL	C11-C10-C8-C7
9	8	102	BCL	C12-C13-C15-C16
9	B	103	BCL	C12-C13-C15-C16
9	D	101	BCL	C11-C10-C8-C7
9	E	102	BCL	C11-C10-C8-C7
9	G	102	BCL	C12-C13-C15-C16
9	I	103	BCL	C6-C7-C8-C10
9	J	101	BCL	C11-C12-C13-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	M	701	BCL	C6-C7-C8-C10
9	N	101	BCL	C11-C10-C8-C7
9	N	101	BCL	C11-C12-C13-C15
9	O	103	BCL	C6-C7-C8-C10
9	S	102	BCL	C12-C13-C15-C16
9	W	101	BCL	C11-C12-C13-C15
9	W	102	BCL	C6-C7-C8-C10
18	L	1003	BPH	C11-C10-C8-C7
16	C	408	PGV	C25-C26-C27-C28
9	0	102	BCL	C2C-C3C-CAC-CBC
9	3	101	BCL	C2C-C3C-CAC-CBC
9	4	103	BCL	C2C-C3C-CAC-CBC
9	6	102	BCL	C2C-C3C-CAC-CBC
9	7	101	BCL	C2C-C3C-CAC-CBC
9	F	101	BCL	C2C-C3C-CAC-CBC
9	G	102	BCL	C2C-C3C-CAC-CBC
9	K	102	BCL	C2C-C3C-CAC-CBC
9	N	101	BCL	C2C-C3C-CAC-CBC
9	P	101	BCL	C2C-C3C-CAC-CBC
9	S	103	BCL	C2C-C3C-CAC-CBC
9	T	101	BCL	C2C-C3C-CAC-CBC
9	W	101	BCL	C2C-C3C-CAC-CBC
13	C	409	BGL	C4-C5-C6-O6
10	S	101	U42	CAS-CAT-CAX-CAY
9	5	101	BCL	C15-C16-C17-C18
10	S	101	U42	C19-C20-C21-C22
13	H	107	BGL	C4-C5-C6-O6
9	B	102	BCL	C15-C16-C17-C18
9	0	101	BCL	C11-C10-C8-C9
9	6	101	BCL	C11-C12-C13-C14
9	6	102	BCL	C11-C12-C13-C14
9	D	101	BCL	C11-C10-C8-C9
9	D	102	BCL	C11-C12-C13-C14
9	H	101	BCL	C14-C13-C15-C16
9	I	103	BCL	C6-C7-C8-C9
9	L	1001	BCL	C14-C13-C15-C16
9	N	101	BCL	C11-C12-C13-C14
9	O	103	BCL	C11-C10-C8-C9
9	Q	102	BCL	C6-C7-C8-C9
9	S	102	BCL	C14-C13-C15-C16
9	V	101	BCL	C6-C7-C8-C9
9	W	102	BCL	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	L	1003	BPH	C11-C10-C8-C9
10	4	104	U42	C19-C18-O17-C16
13	N	103	BGL	C2'-C1'-O2-C2
10	0	103	U42	C29-C30-C31-C32
16	C	408	PGV	O03-C01-C02-C03
16	L	1007	PGV	O03-C01-C02-C03
16	P	103	PGV	O03-C01-C02-C03
16	M	705	PGV	C5-C6-C7-C8
9	6	101	BCL	O1D-CGD-O2D-CED
16	M	705	PGV	C11-C10-C9-C8
9	2	102	BCL	C13-C15-C16-C17
9	7	101	BCL	C15-C16-C17-C18
9	Q	103	BCL	C8-C10-C11-C12
10	O	101	U42	C20-C21-C22-C23
13	D	104	BGL	C4'-C5'-C6'-C7'
16	C	408	PGV	C27-C28-C29-C30
9	D	102	BCL	O1D-CGD-O2D-CED
9	J	101	BCL	O1D-CGD-O2D-CED
9	N	101	BCL	CBA-CGA-O2A-C1
16	M	705	PGV	C20-C19-O03-C01
16	L	1006	PGV	C6-C7-C8-C9
10	E	101	U42	CAU-CAR-CAV-CBB
9	8	102	BCL	C8-C10-C11-C12
9	B	103	BCL	C2-C3-C5-C6
9	0	101	BCL	C13-C15-C16-C17
10	U	104	U42	C21-C22-C23-C24
9	O	102	BCL	C10-C11-C12-C13
10	I	101	U42	C28-C29-C30-C31
9	3	101	BCL	O1D-CGD-O2D-CED
9	S	102	BCL	C2A-CAA-CBA-CGA
13	Y	101	BGL	C1-C2-O2-C1'
22	h	101	LHG	C19-C20-C21-C22
18	L	1003	BPH	O1D-CGD-O2D-CED
9	O	102	BCL	CBA-CGA-O2A-C1
9	I	103	BCL	C13-C15-C16-C17
16	M	706	PGV	C2-C3-C4-C5
10	U	101	U42	O14-C4-O1-CAY
9	J	101	BCL	C16-C17-C18-C20
9	F	101	BCL	C3-C5-C6-C7
10	O	101	U42	CBF-CBH-CBJ-CBM
10	I	104	U42	C28-C29-C30-C31
16	P	104	PGV	C27-C28-C29-C30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	B	101	U42	C25-C26-C27-C28
9	A	101	BCL	CBA-CGA-O2A-C1
16	P	103	PGV	C4-C5-C6-C7
10	U	101	U42	C5-C4-O1-CAY
10	E	101	U42	C27-C28-C29-C30
10	G	101	U42	C19-C20-C21-C22
10	Q	101	U42	C22-C23-C24-C25
9	B	103	BCL	C4-C3-C5-C6
9	Q	103	BCL	C4-C3-C5-C6
9	Q	103	BCL	C2-C3-C5-C6
10	S	101	U42	C25-C26-C27-C28
13	D	104	BGL	C5'-C6'-C7'-C8'
16	L	1006	PGV	C26-C27-C28-C29
16	C	407	PGV	O03-C01-C02-O01
16	C	408	PGV	O03-C01-C02-O01
16	L	1006	PGV	O03-C01-C02-O01
16	M	705	PGV	C4-C5-C6-C7
10	Q	101	U42	C29-C30-C31-C32
13	L	1015	BGL	C1'-C2'-C3'-C4'
10	S	101	U42	C23-C24-C25-C26
16	P	104	PGV	C11-C10-C9-C8
10	U	104	U42	C29-C30-C31-C32
16	M	705	PGV	C2-C1-O01-C02
13	C	410	BGL	C2'-C3'-C4'-C5'
10	8	101	U42	CAV-CBB-CBG-CBI
9	F	102	BCL	O1D-CGD-O2D-CED
10	U	101	U42	O17-C16-C8-C7
9	7	101	BCL	C16-C17-C18-C19
9	E	102	BCL	C4-C3-C5-C6
9	V	101	BCL	C4-C3-C5-C6
9	2	102	BCL	C8-C10-C11-C12
10	Q	101	U42	C28-C29-C30-C31
12	T	103	LMT	C11-C10-C9-C8
16	L	1008	PGV	O05-C05-C06-O06
16	L	1006	PGV	C9-C10-C11-C12
9	4	102	BCL	C11-C12-C13-C14
9	4	103	BCL	C11-C12-C13-C14
9	4	103	BCL	C14-C13-C15-C16
9	6	102	BCL	C14-C13-C15-C16
9	8	102	BCL	C14-C13-C15-C16
9	E	102	BCL	C11-C10-C8-C9
9	E	102	BCL	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	J	101	BCL	C11-C12-C13-C14
9	K	102	BCL	C11-C10-C8-C9
9	N	101	BCL	C11-C10-C8-C9
9	S	102	BCL	C11-C12-C13-C14
9	W	101	BCL	C11-C12-C13-C14
10	4	101	U42	C25-C26-C27-C28
9	4	103	BCL	C13-C15-C16-C17
9	9	102	BCL	C13-C15-C16-C17
9	D	102	BCL	C8-C10-C11-C12
16	P	103	PGV	C3-C4-C5-C6
9	A	101	BCL	C5-C6-C7-C8
10	S	101	U42	C21-C22-C23-C24
9	7	101	BCL	C3-C5-C6-C7
10	U	101	U42	C29-C30-C31-C32
16	C	407	PGV	C01-C02-C03-O11
16	C	408	PGV	C01-C02-C03-O11
16	L	1008	PGV	C01-C02-C03-O11
16	P	103	PGV	C01-C02-C03-O11
16	P	104	PGV	C01-C02-C03-O11
9	7	101	BCL	O1D-CGD-O2D-CED
10	B	101	U42	CAT-CAX-CAY-CBC
10	E	101	U42	CAT-CAX-CAY-CBD
10	G	101	U42	CAT-CAX-CAY-CBD
10	I	104	U42	CAT-CAX-CAY-CBC
10	Q	101	U42	CAT-CAX-CAY-CBD
22	h	101	LHG	C14-C15-C16-C17
9	2	102	BCL	C6-C7-C8-C10
9	2	102	BCL	C11-C10-C8-C7
9	4	103	BCL	C11-C12-C13-C15
9	6	102	BCL	C11-C12-C13-C15
9	6	102	BCL	C12-C13-C15-C16
9	7	101	BCL	C11-C10-C8-C7
9	D	102	BCL	C11-C12-C13-C15
9	F	101	BCL	C6-C7-C8-C10
9	F	101	BCL	C11-C12-C13-C15
9	G	102	BCL	C11-C10-C8-C7
9	H	101	BCL	C11-C10-C8-C7
9	H	101	BCL	C12-C13-C15-C16
9	K	102	BCL	C11-C10-C8-C7
9	L	1001	BCL	C12-C13-C15-C16
9	M	701	BCL	C11-C10-C8-C7
9	S	102	BCL	C11-C12-C13-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	U	103	BCL	C6-C7-C8-C10
9	U	103	BCL	C11-C10-C8-C7
9	U	103	BCL	C11-C12-C13-C15
9	W	101	BCL	C12-C13-C15-C16
18	M	702	BPH	C11-C10-C8-C7
9	V	101	BCL	C8-C10-C11-C12
9	8	103	BCL	C4-C3-C5-C6
9	V	101	BCL	C2-C3-C5-C6
10	U	104	U42	C20-C21-C22-C23
10	O	103	U42	C26-C27-C28-C29
9	N	101	BCL	O1A-CGA-O2A-C1
10	4	104	U42	O2-C18-O17-C16
9	F	102	BCL	C8-C10-C11-C12
11	C	401	U4Z	CAM-CAO-CAP-CAQ
9	L	1001	BCL	C3-C5-C6-C7
13	3	103	BGL	C5'-C6'-C7'-C8'
16	M	705	PGV	O04-C19-O03-C01
16	L	1007	PGV	C11-C10-C9-C8
10	B	101	U42	O17-C16-C8-C7
16	P	103	PGV	C13-C14-C15-C16
16	C	407	PGV	O03-C01-C02-C03
16	L	1006	PGV	O03-C01-C02-C03
10	4	104	U42	CAV-CBB-CBG-CBI
9	S	102	BCL	C13-C15-C16-C17
18	M	702	BPH	C1A-C2A-CAA-CBA
10	O	101	U42	C21-C22-C23-C24
9	P	101	BCL	C4-C3-C5-C6
18	L	1003	BPH	C4-C3-C5-C6
9	O	102	BCL	O1A-CGA-O2A-C1
9	8	103	BCL	C16-C17-C18-C19
16	C	408	PGV	O01-C02-C03-O11
16	P	104	PGV	O01-C02-C03-O11
10	S	101	U42	CAB-CAD-CAJ-CAL
9	D	102	BCL	C3-C5-C6-C7
18	L	1005	BPH	C3-C5-C6-C7
10	8	101	U42	CAZ-CAW-CBA-CBE
10	E	101	U42	O17-C16-C8-C7
9	5	101	BCL	C16-C17-C18-C20
9	H	101	BCL	C8-C10-C11-C12
16	M	706	PGV	O03-C01-C02-O01
16	L	1006	PGV	C5-C6-C7-C8
18	L	1005	BPH	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
16	L	1008	PGV	C21-C22-C23-C24
9	8	103	BCL	C2-C3-C5-C6
9	E	102	BCL	C2-C3-C5-C6
9	P	101	BCL	C2-C3-C5-C6
18	L	1003	BPH	C2-C3-C5-C6
10	I	101	U42	CBD-CAY-O1-C4
10	U	101	U42	CBC-CAY-O1-C4
18	M	702	BPH	C1-C2-C3-C5
9	7	101	BCL	C16-C17-C18-C20
18	M	702	BPH	C16-C17-C18-C20
9	S	103	BCL	O1D-CGD-O2D-CED
9	F	101	BCL	C6-C7-C8-C9
9	G	102	BCL	C14-C13-C15-C16
9	M	701	BCL	C6-C7-C8-C9
9	O	103	BCL	C6-C7-C8-C9
9	Q	102	BCL	C14-C13-C15-C16
9	R	101	BCL	C11-C12-C13-C14
9	U	103	BCL	C11-C12-C13-C14
18	M	702	BPH	C11-C10-C8-C9
10	4	104	U42	C24-C25-C26-C27
13	L	1011	BGL	C3'-C4'-C5'-C6'
16	M	706	PGV	C7-C8-C9-C10
13	H	107	BGL	O2-C1'-C2'-C3'
9	8	102	BCL	O1D-CGD-O2D-CED
10	B	101	U42	C22-C23-C24-C25
9	3	101	BCL	C16-C17-C18-C20
9	F	101	BCL	C16-C17-C18-C20
22	h	101	LHG	C7-C8-C9-C10
9	U	103	BCL	O1D-CGD-O2D-CED
10	4	101	U42	C27-C28-C29-C30
9	2	102	BCL	C4C-C3C-CAC-CBC
9	N	101	BCL	C4C-C3C-CAC-CBC
9	Q	103	BCL	C4C-C3C-CAC-CBC
10	E	101	U42	CAT-CAX-CAY-O1
10	I	101	U42	CAT-CAX-CAY-O1
10	Q	101	U42	CAT-CAX-CAY-O1
9	N	101	BCL	C2A-CAA-CBA-CGA
16	M	705	PGV	C20-C21-C22-C23
10	I	101	U42	C29-C30-C31-C32
10	E	101	U42	C26-C27-C28-C29
16	C	407	PGV	C2-C3-C4-C5
16	M	706	PGV	C21-C22-C23-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	N	101	BCL	C16-C17-C18-C19
9	G	102	BCL	C5-C6-C7-C8
9	K	101	BCL	C13-C15-C16-C17
13	L	1013	BGL	O2-C1'-C2'-C3'
9	Q	103	BCL	C15-C16-C17-C18
10	O	101	U42	CBG-CBI-CBL-CBO
10	S	101	U42	CAN-CAM-CAO-CAP
9	D	102	BCL	C10-C11-C12-C13
9	6	101	BCL	C15-C16-C17-C18
9	B	102	BCL	C13-C15-C16-C17
9	2	101	BCL	C6-C7-C8-C10
9	5	101	BCL	C6-C7-C8-C10
9	B	103	BCL	C11-C12-C13-C15
9	J	101	BCL	C11-C10-C8-C7
9	S	103	BCL	C11-C10-C8-C7
9	S	103	BCL	C11-C12-C13-C15
9	V	101	BCL	C6-C7-C8-C10
18	M	702	BPH	C12-C13-C15-C16
9	6	102	BCL	C10-C11-C12-C13
9	A	101	BCL	O1A-CGA-O2A-C1
10	S	101	U42	C29-C30-C31-C32
16	L	1006	PGV	C29-C30-C31-C32
16	M	706	PGV	C24-C25-C26-C27
9	G	102	BCL	C2A-CAA-CBA-CGA
10	I	101	U42	C26-C27-C28-C29
16	M	705	PGV	O02-C1-O01-C02
9	I	103	BCL	C4-C3-C5-C6
18	L	1005	BPH	C4-C3-C5-C6
18	L	1005	BPH	C15-C16-C17-C18
16	L	1006	PGV	O01-C02-C03-O11
16	M	706	PGV	C30-C31-C32-C33
16	P	104	PGV	O03-C01-C02-C03
9	L	1001	BCL	CBD-CGD-O2D-CED
9	U	103	BCL	C16-C17-C18-C20
10	8	101	U42	C23-C24-C25-C26
10	O	101	U42	C29-C30-C31-C32
9	1	101	BCL	C10-C11-C12-C13
10	B	101	U42	C23-C24-C25-C26
16	M	705	PGV	C25-C26-C27-C28
16	L	1007	PGV	O03-C01-C02-O01
9	0	102	BCL	C11-C12-C13-C14
9	B	103	BCL	C14-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	J	101	BCL	C11-C10-C8-C9
9	Q	103	BCL	C11-C12-C13-C14
9	U	103	BCL	C6-C7-C8-C9
16	C	408	PGV	C2-C3-C4-C5
9	K	101	BCL	C8-C10-C11-C12
9	4	102	BCL	C15-C16-C17-C18
18	M	702	BPH	C16-C17-C18-C19
13	C	409	BGL	C2'-C3'-C4'-C5'
11	P	102	U4Z	CAT-CAS-CAW-CAZ
19	M	704	MQE	CAL-CAE-CAR-CBV
10	U	101	U42	CAT-CAS-CAW-CBA
10	4	104	U42	C29-C30-C31-C32
9	B	103	BCL	C16-C17-C18-C19
16	L	1006	PGV	C28-C29-C30-C31
12	D	105	LMT	C4'-C5'-C6'-O6'
10	U	101	U42	C25-C26-C27-C28
9	0	101	BCL	O1D-CGD-O2D-CED
9	8	103	BCL	C16-C17-C18-C20
9	D	101	BCL	C16-C17-C18-C20
16	M	705	PGV	C31-C32-C33-C34
9	U	102	BCL	O1D-CGD-O2D-CED
11	3	102	U4Z	CAT-CAS-CAW-CAZ
11	D	103	U4Z	CAT-CAS-CAW-CAZ
11	T	102	U4Z	CAT-CAS-CAW-CAZ
16	P	104	PGV	C21-C22-C23-C24
16	L	1006	PGV	C15-C16-C17-C18
16	L	1008	PGV	C11-C10-C9-C8
16	L	1006	PGV	C01-C02-C03-O11
9	0	102	BCL	C11-C12-C13-C15
9	7	101	BCL	C12-C13-C15-C16
9	F	102	BCL	C11-C12-C13-C15
9	L	1001	BCL	C11-C10-C8-C7
9	R	101	BCL	C11-C12-C13-C15
9	S	103	BCL	C6-C7-C8-C10
9	S	103	BCL	C12-C13-C15-C16
9	W	101	BCL	C11-C10-C8-C7
18	L	1005	BPH	C6-C7-C8-C10
10	I	104	U42	C25-C26-C27-C28
9	O	103	BCL	C8-C10-C11-C12
10	I	104	U42	C26-C27-C28-C29
9	K	101	BCL	O1D-CGD-O2D-CED
9	2	102	BCL	C2C-C3C-CAC-CBC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	I	103	BCL	C2C-C3C-CAC-CBC
9	L	1002	BCL	C2C-C3C-CAC-CBC
9	M	701	BCL	C2C-C3C-CAC-CBC
10	4	101	U42	C21-C22-C23-C24
9	L	1001	BCL	C3A-C2A-CAA-CBA
14	C	402	HEC	C4C-C3C-CAC-CBC
14	C	403	HEC	C4C-C3C-CAC-CBC
16	C	407	PGV	C6-C7-C8-C9
16	L	1008	PGV	O01-C02-C03-O11
9	2	101	BCL	C6-C7-C8-C9
9	5	101	BCL	C6-C7-C8-C9
9	F	101	BCL	C11-C12-C13-C14
9	H	101	BCL	C11-C10-C8-C9
9	W	101	BCL	C11-C10-C8-C9
18	M	702	BPH	C14-C13-C15-C16
16	L	1008	PGV	C24-C25-C26-C27
9	G	102	BCL	C16-C17-C18-C19
9	E	102	BCL	C8-C10-C11-C12
13	L	1015	BGL	C2'-C1'-O2-C2
16	P	103	PGV	O03-C01-C02-O01
9	A	101	BCL	C16-C17-C18-C20
11	P	102	U4Z	CAT-CAS-CAW-CBA
9	N	101	BCL	CBD-CGD-O2D-CED
18	L	1003	BPH	C4C-C3C-CAC-CBC
10	0	103	U42	C21-C22-C23-C24
9	F	102	BCL	C3-C5-C6-C7
9	O	102	BCL	C3-C5-C6-C7
13	3	103	BGL	O2-C1'-C2'-C3'
9	0	102	BCL	CHA-CBD-CGD-O1D
9	1	101	BCL	CHA-CBD-CGD-O1D
9	1	101	BCL	CHA-CBD-CGD-O2D
9	B	103	BCL	CHA-CBD-CGD-O1D
9	B	103	BCL	CHA-CBD-CGD-O2D
9	M	701	BCL	CHA-CBD-CGD-O1D
9	M	701	BCL	CHA-CBD-CGD-O2D
10	E	101	U42	CAM-CAO-CAP-CAQ
16	M	706	PGV	C03-O11-P-O13
16	M	706	PGV	C04-O12-P-O13
16	P	104	PGV	C03-O11-P-O13
18	L	1003	BPH	CHA-CBD-CGD-O1D
18	L	1003	BPH	CHA-CBD-CGD-O2D
20	L	1017	PEF	C1-O3P-P-O2P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	L	1017	PEF	C1-O3P-P-O4P
16	L	1006	PGV	C7-C8-C9-C10
11	J	102	U4Z	CAT-CAS-CAW-CAZ
10	E	101	U42	CAH-CAD-CAJ-CAL
9	I	103	BCL	C2-C3-C5-C6
19	M	704	MQE	CAL-CAE-CAR-CBD
9	5	101	BCL	C5-C6-C7-C8
16	C	408	PGV	C19-C20-C21-C22
16	C	408	PGV	C5-C6-C7-C8
11	C	401	U4Z	CBI-CBL-CBN-CBM
16	M	706	PGV	C3-C4-C5-C6
9	M	701	BCL	C2A-CAA-CBA-CGA
16	L	1006	PGV	C2-C1-O01-C02
16	P	103	PGV	C20-C21-C22-C23
9	3	101	BCL	C15-C16-C17-C18
10	I	101	U42	O14-C4-O1-CAY
9	A	101	BCL	C16-C17-C18-C19
9	U	103	BCL	C16-C17-C18-C19
16	M	705	PGV	C01-C02-C03-O11
10	Q	101	U42	C27-C28-C29-C30
9	2	102	BCL	C6-C7-C8-C9
9	2	102	BCL	C11-C10-C8-C9
9	5	101	BCL	C11-C10-C8-C9
9	7	101	BCL	C11-C10-C8-C9
9	B	103	BCL	C11-C12-C13-C14
9	D	102	BCL	C11-C10-C8-C9
9	F	102	BCL	C6-C7-C8-C9
9	F	102	BCL	C11-C10-C8-C9
9	F	102	BCL	C11-C12-C13-C14
9	Q	103	BCL	C6-C7-C8-C9
9	S	103	BCL	C11-C12-C13-C14
9	F	101	BCL	C12-C13-C15-C16
9	I	102	BCL	C11-C12-C13-C15
9	L	1002	BCL	C12-C13-C15-C16
9	M	701	BCL	CBA-CGA-O2A-C1
12	T	103	LMT	C3-C4-C5-C6
9	R	101	BCL	CBD-CGD-O2D-CED
19	M	704	MQE	CAK-CAF-CAT-CBW
18	L	1005	BPH	C2-C3-C5-C6
16	M	705	PGV	C02-C03-O11-P
10	4	104	U42	O17-C18-C19-C20
13	F	104	BGL	C2'-C3'-C4'-C5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	B	103	BCL	C16-C17-C18-C20
14	C	404	HEC	C1A-C2A-CAA-CBA
9	N	101	BCL	O1D-CGD-O2D-CED
16	C	407	PGV	C11-C10-C9-C8
10	O	101	U42	C22-C23-C24-C25
9	I	103	BCL	C16-C17-C18-C19
11	D	103	U4Z	CAT-CAS-CAW-CBA
11	J	102	U4Z	CAT-CAS-CAW-CBA
11	T	102	U4Z	CAT-CAS-CAW-CBA
9	7	101	BCL	C14-C13-C15-C16
9	I	102	BCL	C11-C12-C13-C14
9	I	103	BCL	C11-C12-C13-C14
9	J	101	BCL	C14-C13-C15-C16
9	L	1001	BCL	C11-C10-C8-C9
9	V	101	BCL	C14-C13-C15-C16
9	B	102	BCL	CBD-CGD-O2D-CED
16	M	706	PGV	C19-C20-C21-C22
9	P	101	BCL	C16-C17-C18-C20
9	M	701	BCL	C4-C3-C5-C6
9	W	101	BCL	C4-C3-C5-C6
19	L	1004	MQE	CAJ-CAD-CAQ-CBU
9	K	102	BCL	CAA-CBA-CGA-O2A
10	4	104	U42	C26-C27-C28-C29
16	L	1007	PGV	O01-C02-C03-O11
9	B	102	BCL	C5-C6-C7-C8
9	M	701	BCL	O1A-CGA-O2A-C1
10	S	101	U42	CAT-CAX-CAY-CBD
10	U	104	U42	CAT-CAX-CAY-CBD
16	L	1006	PGV	C20-C21-C22-C23
9	G	102	BCL	C6-C7-C8-C10
9	I	103	BCL	C11-C10-C8-C7
9	K	101	BCL	C11-C12-C13-C15
9	U	102	BCL	C11-C10-C8-C7
18	L	1005	BPH	C11-C12-C13-C15
9	7	101	BCL	C5-C6-C7-C8
9	L	1001	BCL	C15-C16-C17-C18
9	E	102	BCL	O1A-CGA-O2A-C1
16	L	1006	PGV	O02-C1-O01-C02
9	I	103	BCL	C16-C17-C18-C20
9	P	101	BCL	C16-C17-C18-C19
10	Q	101	U42	C23-C24-C25-C26
11	F	103	U4Z	CAT-CAS-CAW-CAZ

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	V	102	U4Z	CAT-CAS-CAW-CAZ
12	T	103	LMT	C6-C7-C8-C9
9	4	102	BCL	C10-C11-C12-C13
9	8	102	BCL	C5-C6-C7-C8
16	M	705	PGV	C23-C24-C25-C26
9	I	102	BCL	C2-C1-O2A-CGA
18	M	702	BPH	C2C-C3C-CAC-CBC
16	M	705	PGV	C28-C29-C30-C31
9	H	101	BCL	C15-C16-C17-C18
9	T	101	BCL	C8-C10-C11-C12
9	2	102	BCL	C4-C3-C5-C6
11	A	102	U4Z	CAT-CAS-CAW-CAZ
11	3	102	U4Z	CAT-CAS-CAW-CBA
16	L	1008	PGV	O12-C04-C05-C06
9	5	101	BCL	O1D-CGD-O2D-CED
9	5	101	BCL	CBD-CGD-O2D-CED
9	P	101	BCL	C8-C10-C11-C12
9	Q	103	BCL	O1A-CGA-O2A-C1
9	0	102	BCL	C14-C13-C15-C16
9	2	101	BCL	C11-C10-C8-C9
9	2	102	BCL	C11-C12-C13-C14
9	I	103	BCL	C11-C10-C8-C9
9	K	101	BCL	C11-C12-C13-C14
9	P	101	BCL	C11-C10-C8-C9
18	M	702	BPH	C6-C7-C8-C9
13	F	104	BGL	C4'-C5'-C6'-C7'
9	3	101	BCL	C8-C10-C11-C12
18	M	702	BPH	C1-C2-C3-C4
10	4	104	U42	O17-C16-C8-O14
9	F	102	BCL	C2A-CAA-CBA-CGA
13	L	1012	BGL	C3'-C4'-C5'-C6'
9	5	101	BCL	C1A-C2A-CAA-CBA
9	9	102	BCL	C1A-C2A-CAA-CBA
9	O	102	BCL	C1A-C2A-CAA-CBA
9	U	103	BCL	C1A-C2A-CAA-CBA
9	6	102	BCL	C16-C17-C18-C19
16	P	103	PGV	C7-C8-C9-C10
9	R	101	BCL	O1D-CGD-O2D-CED
10	8	101	U42	CAB-CAD-CAJ-CAL
10	E	101	U42	CAB-CAD-CAJ-CAL
16	L	1008	PGV	C5-C6-C7-C8
16	P	103	PGV	C11-C10-C9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	S	101	U42	C22-C23-C24-C25
12	T	103	LMT	C5-C6-C7-C8
11	5	102	U4Z	CAT-CAS-CAW-CAZ
9	M	701	BCL	C2-C3-C5-C6
11	V	102	U4Z	CAT-CAS-CAW-CBA
9	2	101	BCL	C11-C12-C13-C15
9	I	103	BCL	C11-C12-C13-C15
9	R	101	BCL	C6-C7-C8-C10
9	R	101	BCL	C11-C10-C8-C7
9	S	102	BCL	C6-C7-C8-C10
16	P	104	PGV	C6-C7-C8-C9
19	L	1004	MQE	CAR-CAE-CAL-CBF
19	M	704	MQE	CAR-CAE-CAL-CBF
9	5	101	BCL	C2C-C3C-CAC-CBC
9	Q	103	BCL	CBA-CGA-O2A-C1
9	8	103	BCL	C8-C10-C11-C12
9	F	102	BCL	C4-C3-C5-C6
9	E	102	BCL	C5-C6-C7-C8
9	W	101	BCL	C2-C3-C5-C6
11	5	102	U4Z	CAT-CAS-CAW-CBA
11	A	102	U4Z	CAT-CAS-CAW-CBA
11	F	103	U4Z	CAT-CAS-CAW-CBA
19	L	1004	MQE	CAJ-CAD-CAQ-CBE
10	Q	101	U42	CBC-CAY-O1-C4
10	Q	101	U42	CBD-CAY-O1-C4
9	2	101	BCL	C11-C12-C13-C14
9	U	102	BCL	C11-C10-C8-C9
10	U	101	U42	C20-C21-C22-C23
13	L	1015	BGL	C3'-C4'-C5'-C6'
12	D	105	LMT	C5-C6-C7-C8
16	C	407	PGV	C24-C25-C26-C27
9	4	102	BCL	C4-C3-C5-C6
9	2	102	BCL	C2-C3-C5-C6
9	F	102	BCL	C2-C3-C5-C6
9	F	101	BCL	C4C-C3C-CAC-CBC
9	K	101	BCL	C4C-C3C-CAC-CBC
9	T	101	BCL	C4C-C3C-CAC-CBC
12	T	103	LMT	C2-C3-C4-C5
9	E	102	BCL	CBA-CGA-O2A-C1
10	8	101	U42	O17-C18-C19-C20
20	L	1017	PEF	C12-C13-C14-C15
16	C	407	PGV	O01-C02-C03-O11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
16	M	705	PGV	C19-C20-C21-C22
10	O	101	U42	C27-C28-C29-C30
9	B	102	BCL	O1D-CGD-O2D-CED
16	M	705	PGV	C22-C23-C24-C25
9	4	102	BCL	C2-C3-C5-C6
18	L	1005	BPH	C5-C6-C7-C8
9	W	102	BCL	C11-C10-C8-C7
16	P	103	PGV	C5-C6-C7-C8
9	G	102	BCL	C11-C12-C13-C14
9	S	103	BCL	C14-C13-C15-C16
16	L	1006	PGV	C30-C31-C32-C33
16	C	408	PGV	C12-C13-C14-C15
9	0	102	BCL	C10-C11-C12-C13
9	4	102	BCL	C2-C1-O2A-CGA
9	L	1002	BCL	C2-C1-O2A-CGA
9	N	101	BCL	C2-C1-O2A-CGA
22	h	101	LHG	C17-C18-C19-C20
9	K	101	BCL	C15-C16-C17-C18
10	E	101	U42	C23-C24-C25-C26
16	M	705	PGV	C27-C28-C29-C30
9	5	101	BCL	C3A-C2A-CAA-CBA
9	9	102	BCL	C3A-C2A-CAA-CBA
9	N	101	BCL	C4-C3-C5-C6
9	O	102	BCL	C3A-C2A-CAA-CBA
19	M	704	MQE	CAK-CAF-CAT-CBG
9	L	1001	BCL	O1D-CGD-O2D-CED
10	0	103	U42	CBA-CBE-CBF-CBH
13	L	1015	BGL	C4'-C5'-C6'-C7'
10	Q	101	U42	O14-C4-O1-CAY
16	L	1006	PGV	C25-C26-C27-C28
9	9	102	BCL	C10-C11-C12-C13
9	S	103	BCL	C16-C17-C18-C19
10	B	101	U42	C28-C29-C30-C31
11	S	104	U4Z	CAW-CAS-CAT-CAX
16	L	1008	PGV	C27-C28-C29-C30
14	C	402	HEC	CAD-CBD-CGD-O2D
10	0	103	U42	C5-C4-O1-CAY
10	E	101	U42	C5-C4-O1-CAY
16	L	1007	PGV	C9-C10-C11-C12
16	P	104	PGV	C9-C10-C11-C12
9	F	101	BCL	C14-C13-C15-C16
9	M	701	BCL	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	L	1002	BCL	C13-C15-C16-C17
10	B	101	U42	C29-C30-C31-C32
10	B	101	U42	C21-C22-C23-C24
9	S	103	BCL	C2A-CAA-CBA-CGA
9	0	102	BCL	C12-C13-C15-C16
9	1	101	BCL	C12-C13-C15-C16
9	8	103	BCL	C12-C13-C15-C16
9	D	101	BCL	C12-C13-C15-C16
9	G	102	BCL	C11-C12-C13-C15
9	M	701	BCL	C12-C13-C15-C16
10	E	101	U42	C22-C23-C24-C25
9	4	102	BCL	C3-C5-C6-C7
10	4	104	U42	C28-C29-C30-C31
16	M	705	PGV	C9-C10-C11-C12
9	2	102	BCL	C2-C1-O2A-CGA
9	6	101	BCL	C2-C1-O2A-CGA
9	F	102	BCL	C2-C1-O2A-CGA
9	K	101	BCL	C2-C1-O2A-CGA
9	M	701	BCL	C2-C1-O2A-CGA
9	Q	102	BCL	C2-C1-O2A-CGA
16	L	1008	PGV	O01-C1-C2-C3
16	M	706	PGV	C22-C23-C24-C25
13	H	107	BGL	O5-C5-C6-O6
9	1	101	BCL	C2A-CAA-CBA-CGA
9	A	101	BCL	C2A-CAA-CBA-CGA
9	8	103	BCL	CAA-CBA-CGA-O2A
16	M	706	PGV	O03-C19-C20-C21
12	1	103	LMT	C1-C2-C3-C4
9	0	102	BCL	C8-C10-C11-C12
10	U	101	U42	CAU-CAR-CAV-CBB
16	C	408	PGV	O01-C1-C2-C3
9	3	101	BCL	C14-C13-C15-C16
9	L	1002	BCL	C14-C13-C15-C16
9	R	101	BCL	C6-C7-C8-C9
9	R	101	BCL	C11-C10-C8-C9
9	W	102	BCL	CAA-CBA-CGA-O2A
9	E	102	BCL	C1A-C2A-CAA-CBA
9	F	101	BCL	C1A-C2A-CAA-CBA
9	S	102	BCL	C1A-C2A-CAA-CBA
10	S	101	U42	C27-C28-C29-C30
14	C	402	HEC	CAD-CBD-CGD-O1D
14	C	402	HEC	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	4	102	BCL	C16-C17-C18-C19
12	T	103	LMT	O5B-C1B-O1B-C4'
9	2	101	BCL	CAA-CBA-CGA-O2A
9	S	102	BCL	CAA-CBA-CGA-O2A
10	B	101	U42	CAT-CAX-CAY-CBD
9	0	101	BCL	C2-C1-O2A-CGA
9	7	101	BCL	C2-C1-O2A-CGA
9	8	102	BCL	C2-C1-O2A-CGA
9	D	101	BCL	C2-C1-O2A-CGA
9	R	101	BCL	C2-C1-O2A-CGA
9	U	103	BCL	C2-C1-O2A-CGA
9	U	102	BCL	CAA-CBA-CGA-O2A
9	M	701	BCL	C11-C12-C13-C15
9	T	101	BCL	C12-C13-C15-C16
9	F	102	BCL	C10-C11-C12-C13
9	W	101	BCL	C16-C17-C18-C20
18	L	1005	BPH	O2A-C1-C2-C3
16	M	705	PGV	O01-C1-C2-C3
9	L	1001	BCL	C2C-C3C-CAC-CBC
9	0	102	BCL	C16-C17-C18-C20
10	O	101	U42	C24-C25-C26-C27
13	Y	101	BGL	C4'-C5'-C6'-C7'
19	M	704	MQE	CAW-CAG-CAM-CBG
9	4	103	BCL	C3A-C2A-CAA-CBA
9	6	102	BCL	C3A-C2A-CAA-CBA
9	E	102	BCL	C3A-C2A-CAA-CBA
16	P	104	PGV	C20-C21-C22-C23
16	L	1007	PGV	C31-C32-C33-C34
9	D	102	BCL	C2A-CAA-CBA-CGA
9	O	102	BCL	C11-C10-C8-C9
9	S	102	BCL	C6-C7-C8-C9
9	2	101	BCL	CAA-CBA-CGA-O1A
10	8	101	U42	C27-C28-C29-C30
16	L	1008	PGV	O02-C1-C2-C3
14	C	404	HEC	C3A-C2A-CAA-CBA
9	W	102	BCL	CAA-CBA-CGA-O1A
16	P	103	PGV	O02-C1-O01-C02
16	M	706	PGV	O04-C19-C20-C21
20	L	1017	PEF	O3-C30-C31-C32
16	C	408	PGV	O02-C1-C2-C3
16	M	705	PGV	O02-C1-C2-C3
9	Q	102	BCL	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	I	102	BCL	C13-C15-C16-C17
12	D	105	LMT	C3'-C4'-O1B-C1B
9	I	103	BCL	CAD-CBD-CGD-O2D
9	K	102	BCL	CAD-CBD-CGD-O2D
18	L	1005	BPH	C4C-C3C-CAC-CBC
18	M	702	BPH	C4C-C3C-CAC-CBC
9	O	102	BCL	C8-C10-C11-C12
9	R	101	BCL	C13-C15-C16-C17
9	K	101	BCL	C10-C11-C12-C13
9	Q	102	BCL	C10-C11-C12-C13
9	8	103	BCL	CAA-CBA-CGA-O1A
16	M	705	PGV	C13-C14-C15-C16
14	C	402	HEC	CAA-CBA-CGA-O2A
9	6	101	BCL	C13-C15-C16-C17
16	P	103	PGV	C2-C1-O01-C02
9	U	102	BCL	CAA-CBA-CGA-O1A

There are no ring outliers.

58 monomers are involved in 112 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	S	103	BCL	1	0
10	G	101	U42	3	0
10	4	104	U42	1	0
9	V	101	BCL	1	0
9	E	102	BCL	2	0
10	U	104	U42	3	0
9	8	103	BCL	8	0
12	T	103	LMT	2	0
9	O	102	BCL	1	0
18	L	1003	BPH	3	0
13	C	409	BGL	2	0
9	O	103	BCL	3	0
16	P	103	PGV	4	0
13	F	104	BGL	2	0
22	h	101	LHG	2	0
16	P	104	PGV	4	0
16	L	1008	PGV	2	0
10	E	101	U42	3	0
9	0	102	BCL	1	0
9	U	103	BCL	3	0
14	C	402	HEC	2	0

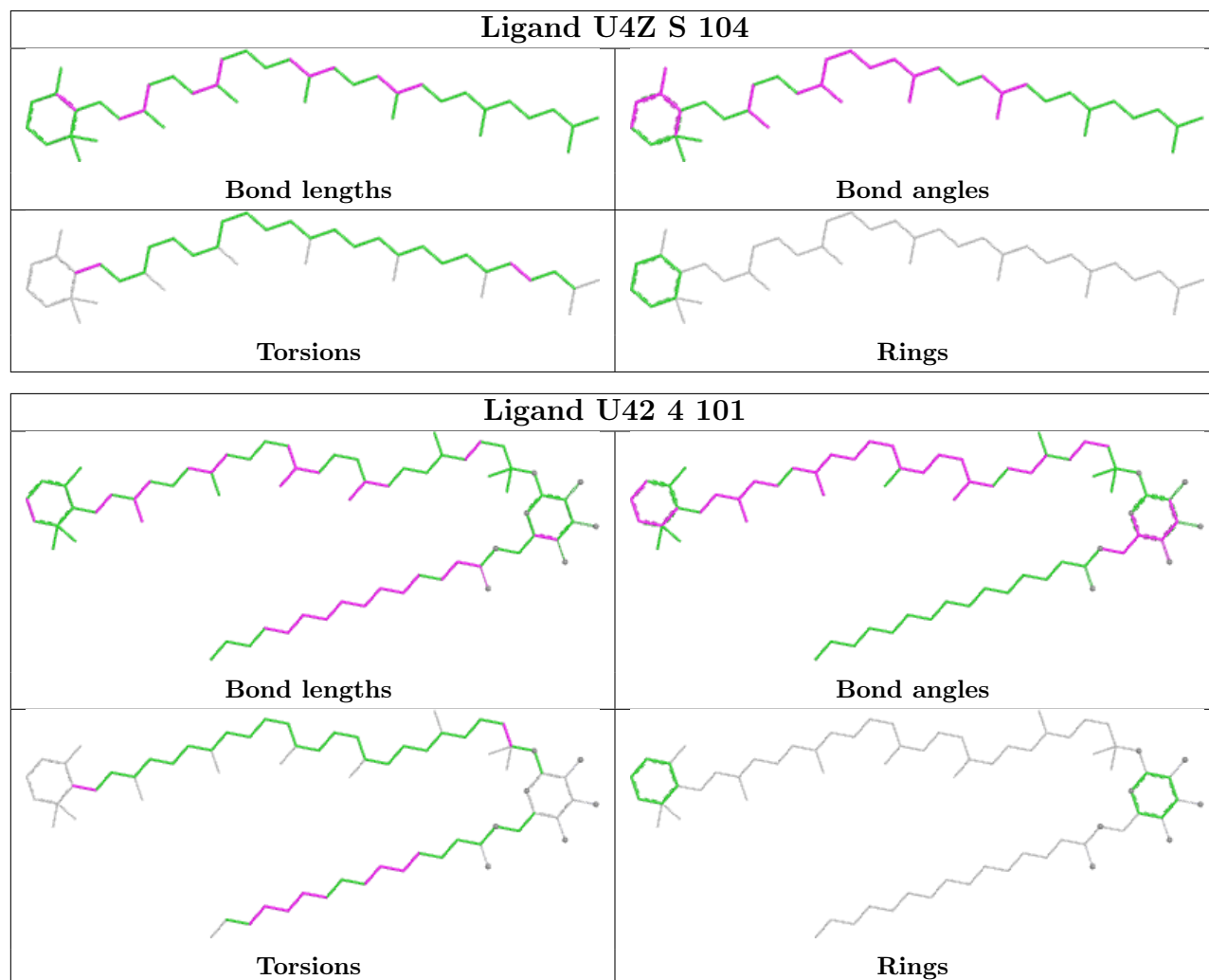
Continued on next page...

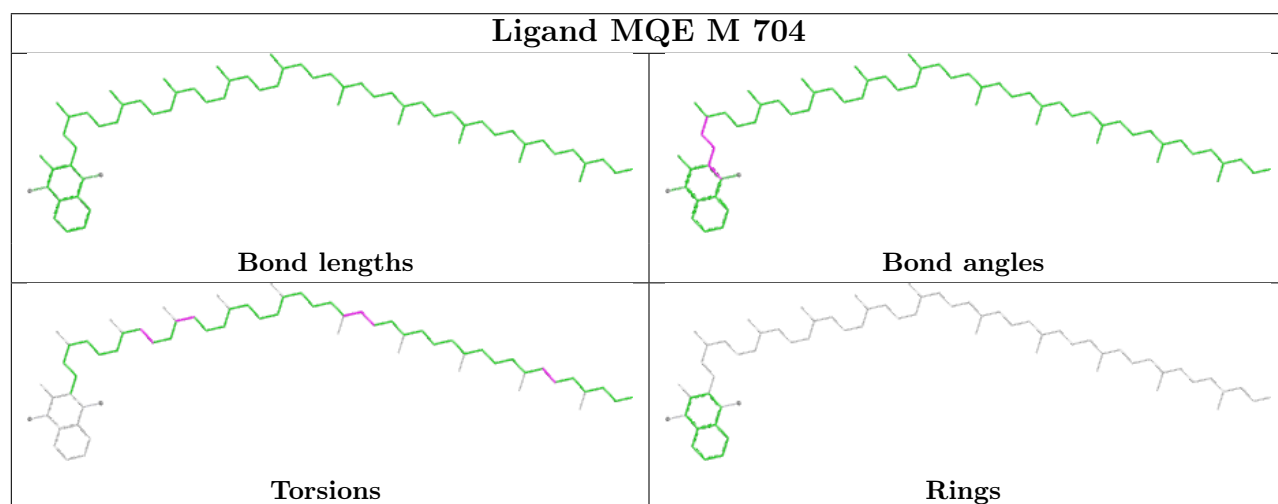
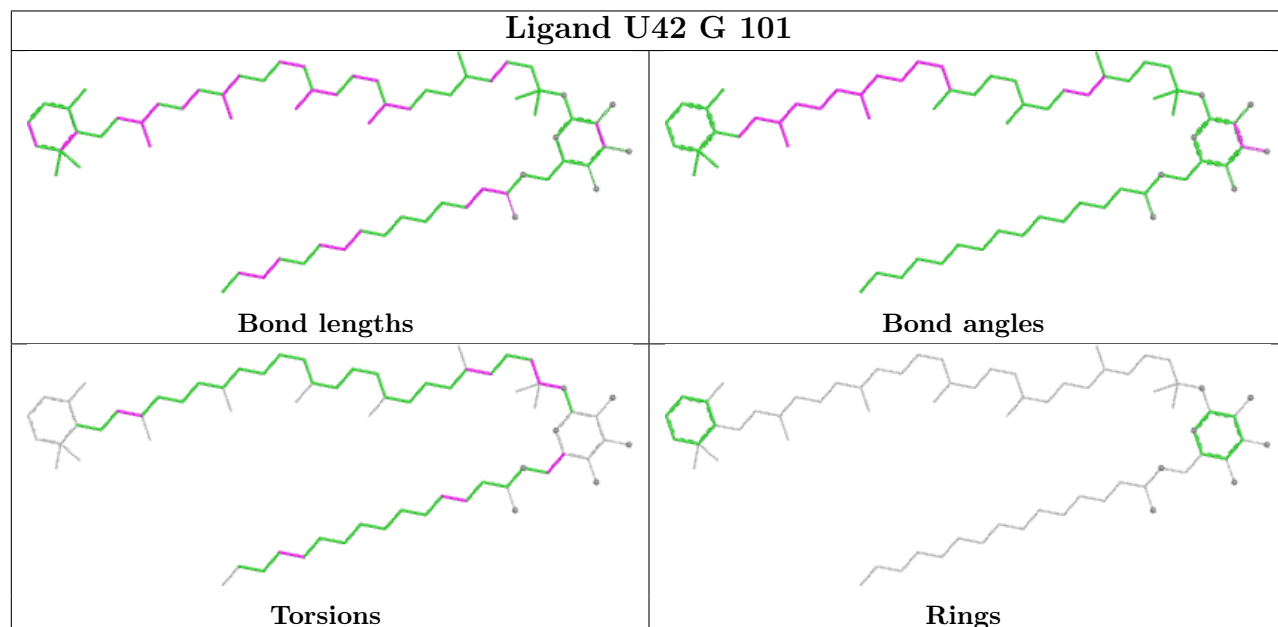
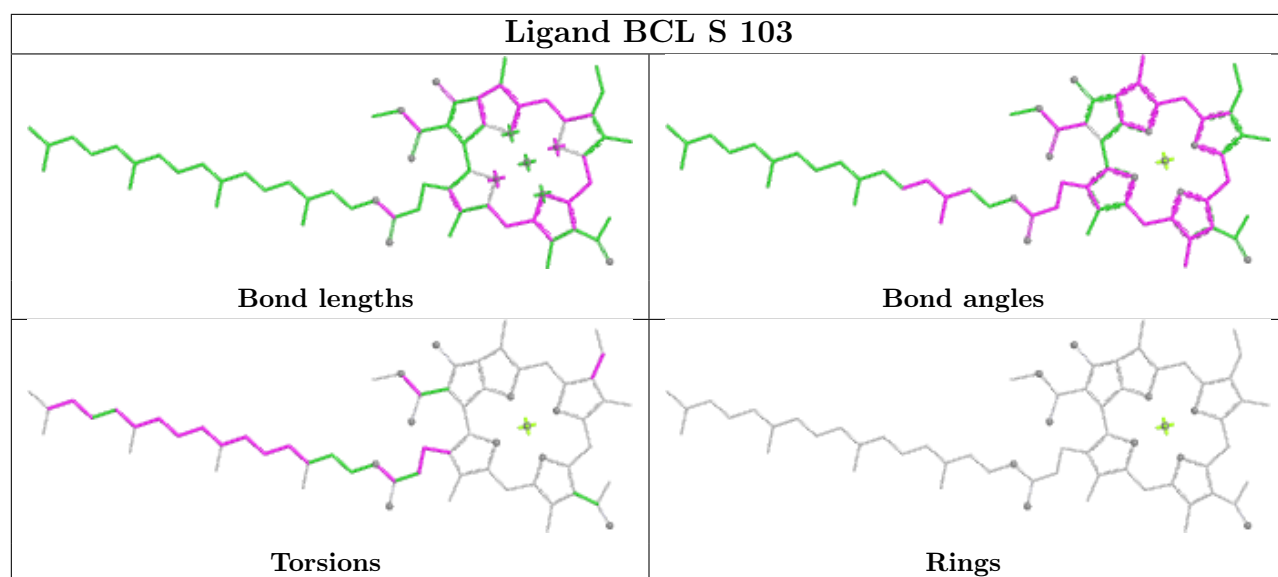
Continued from previous page...

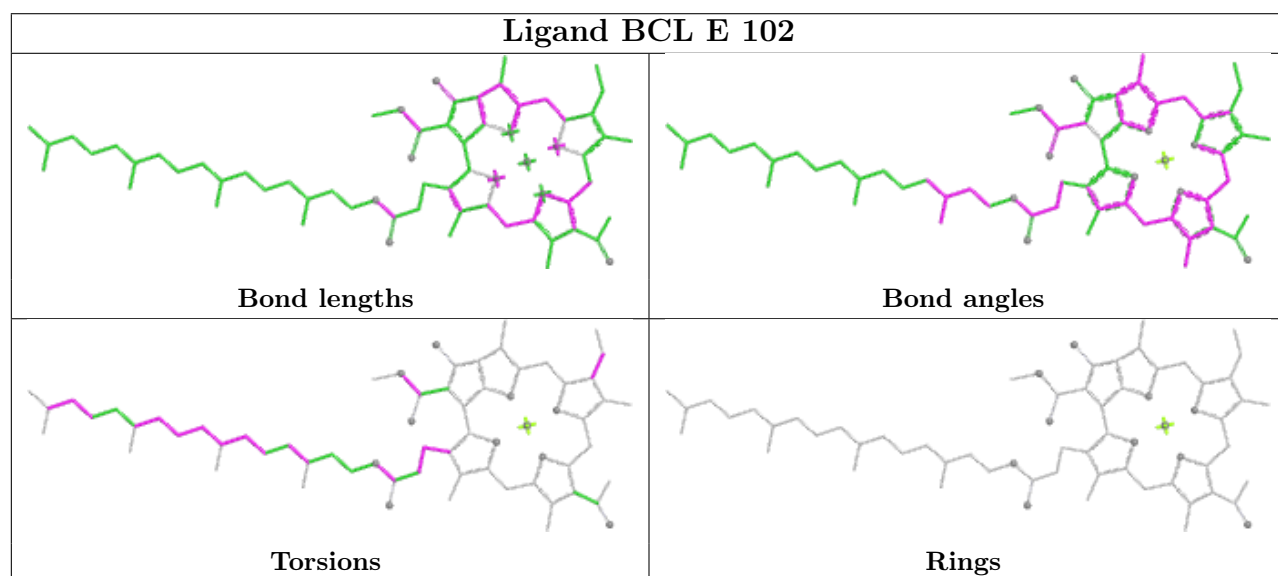
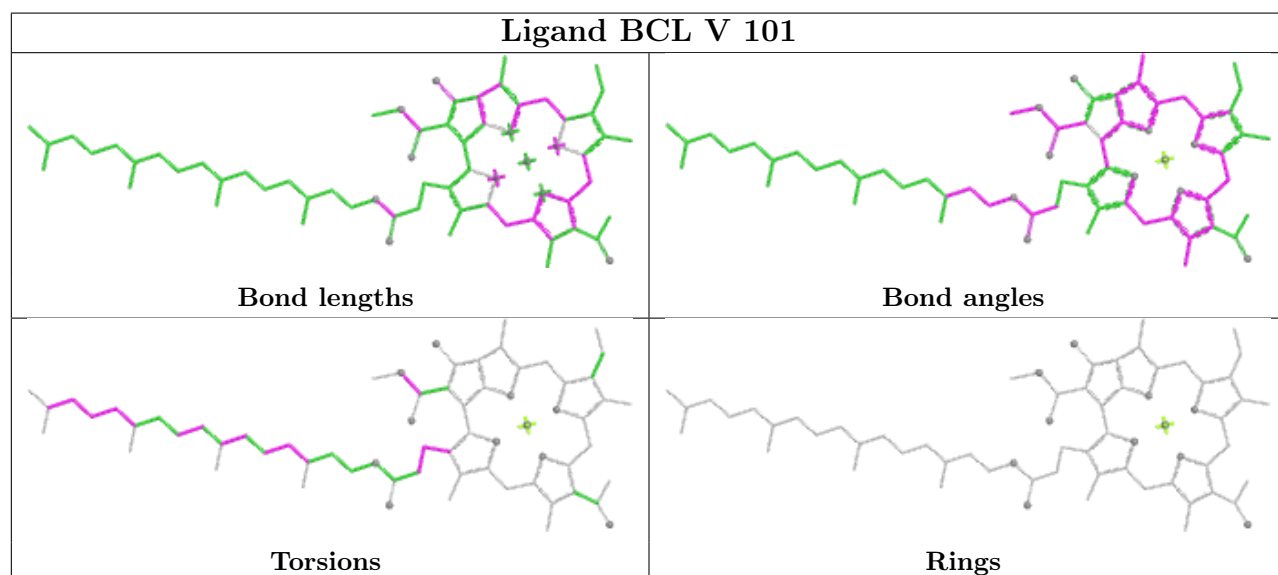
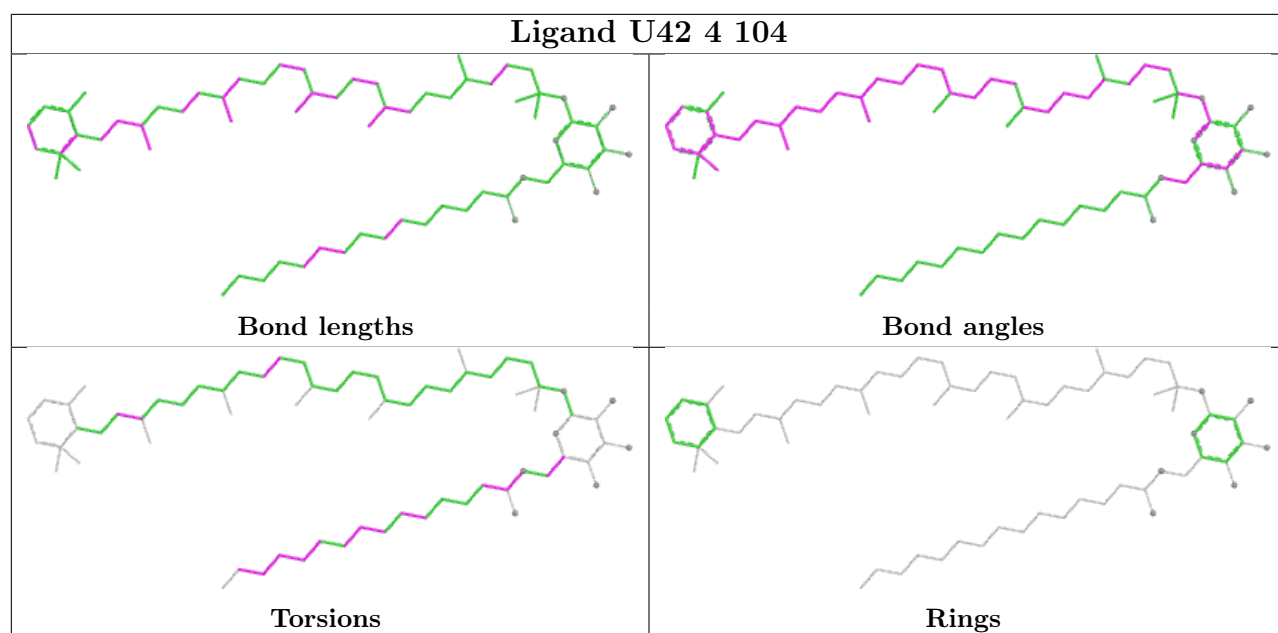
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	1	101	BCL	3	0
12	D	105	LMT	2	0
9	2	102	BCL	1	0
13	H	103	BGL	1	0
9	2	101	BCL	2	0
12	1	103	LMT	1	0
9	4	103	BCL	3	0
9	W	101	BCL	1	0
9	N	101	BCL	1	0
9	K	102	BCL	1	0
20	L	1017	PEF	1	0
16	M	706	PGV	7	0
9	D	102	BCL	1	0
9	M	701	BCL	2	0
10	S	101	U42	2	0
10	8	101	U42	3	0
9	P	101	BCL	1	0
13	C	410	BGL	1	0
9	W	102	BCL	2	0
9	Q	103	BCL	3	0
9	4	102	BCL	1	0
10	O	101	U42	3	0
16	C	408	PGV	2	0
10	U	101	U42	1	0
9	I	103	BCL	1	0
10	Q	101	U42	1	0
9	8	102	BCL	2	0
9	5	101	BCL	1	0
16	M	705	PGV	2	0
9	G	102	BCL	1	0
9	I	102	BCL	1	0
9	U	102	BCL	1	0
10	I	101	U42	4	0
18	L	1005	BPH	2	0
13	3	103	BGL	1	0
16	L	1007	PGV	3	0
9	B	103	BCL	1	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.

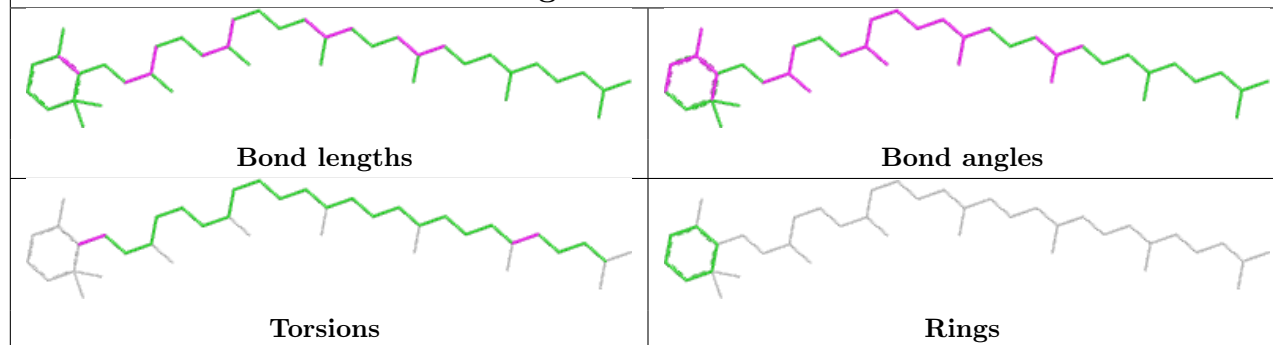
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.



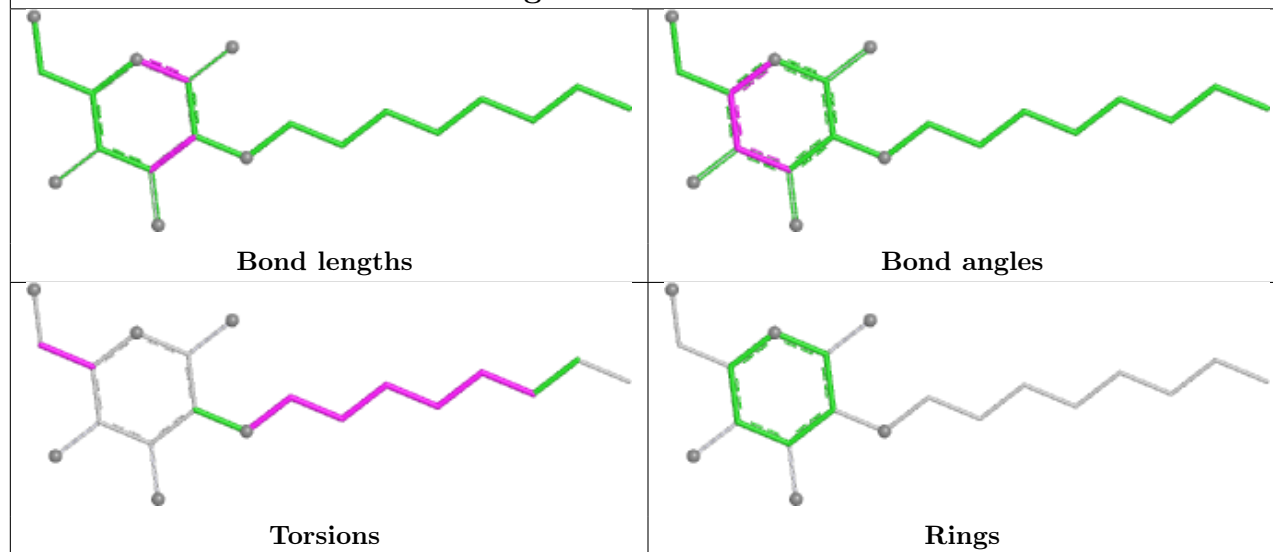




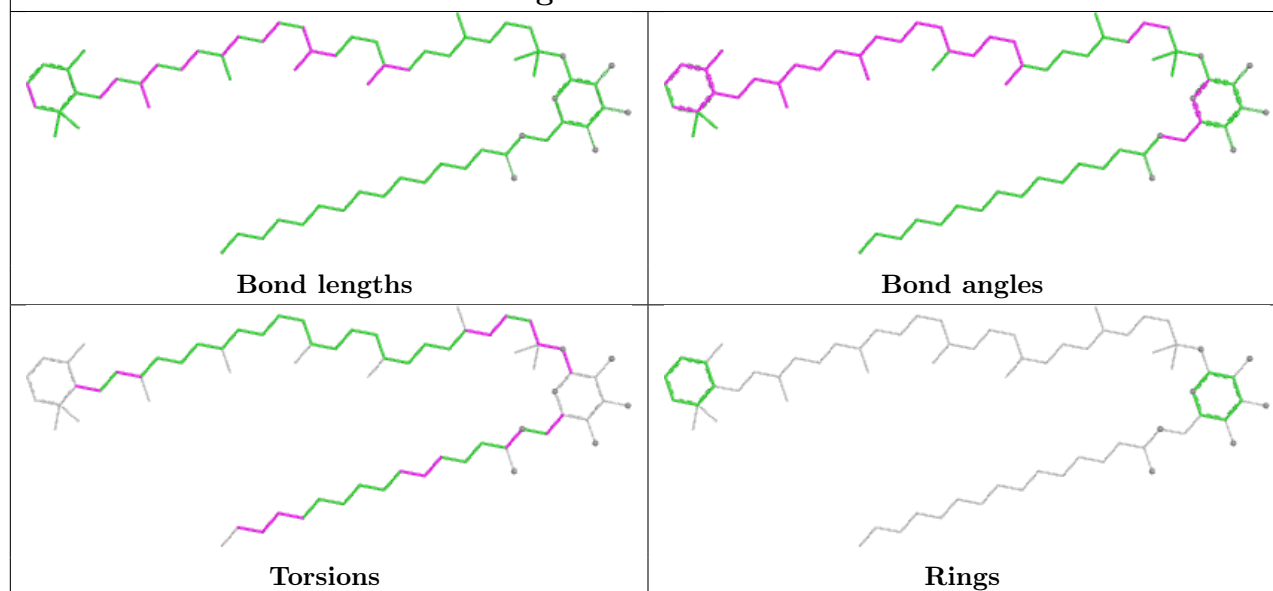
Ligand U4Z 1 102

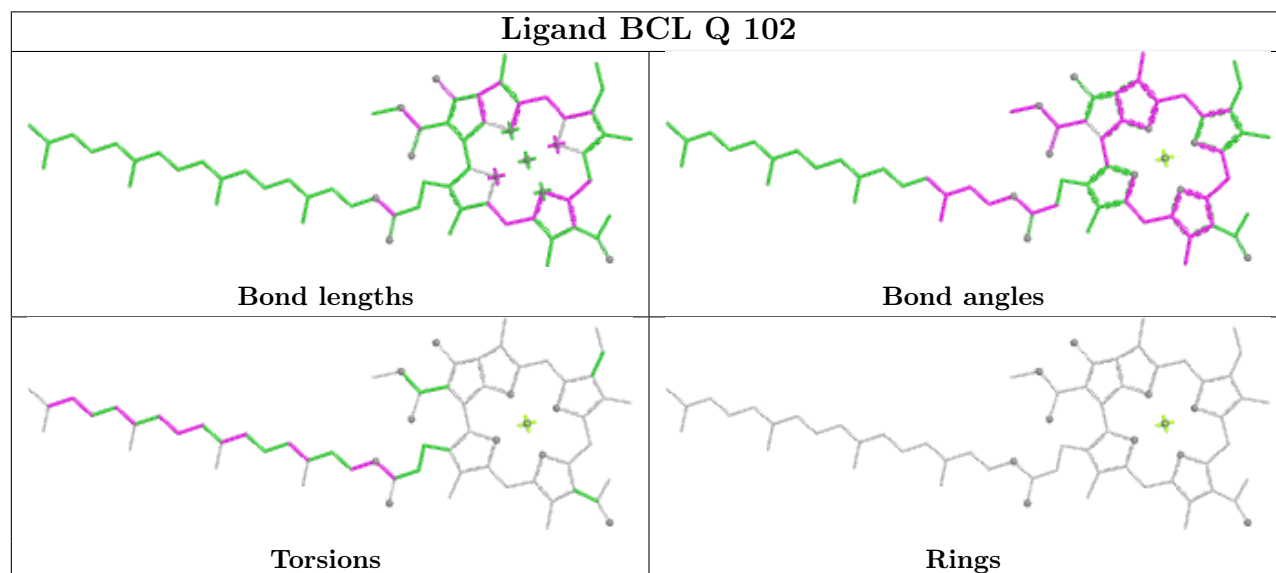
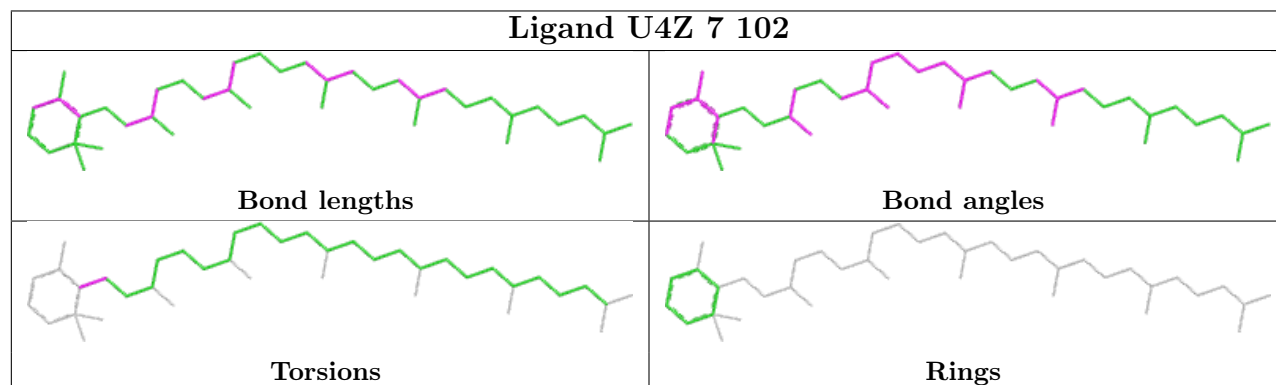
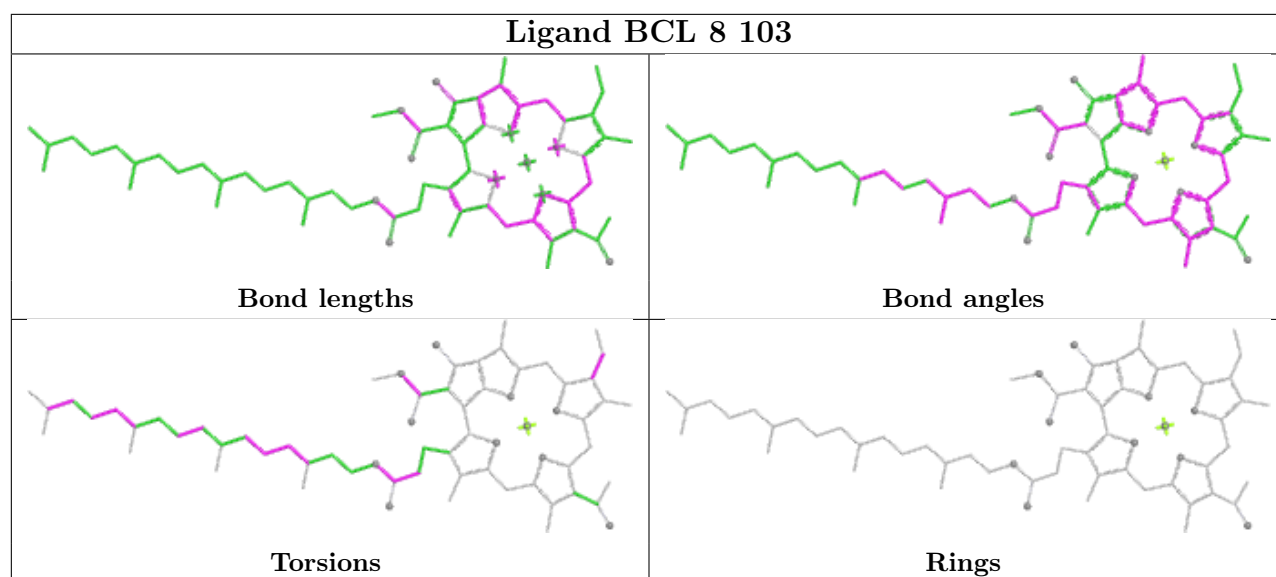


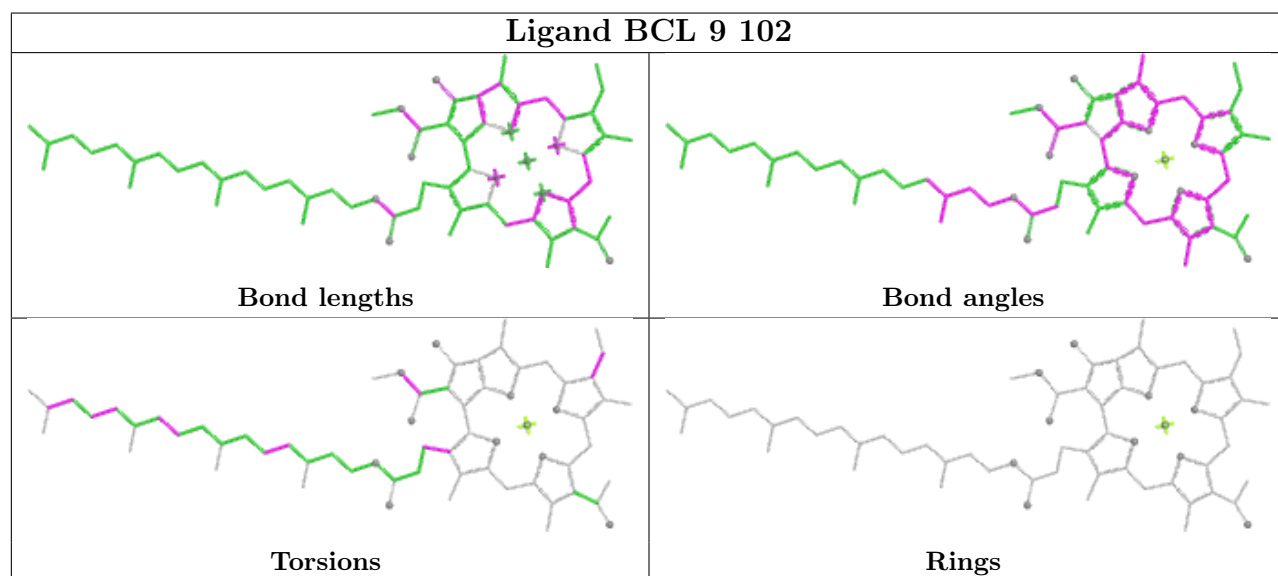
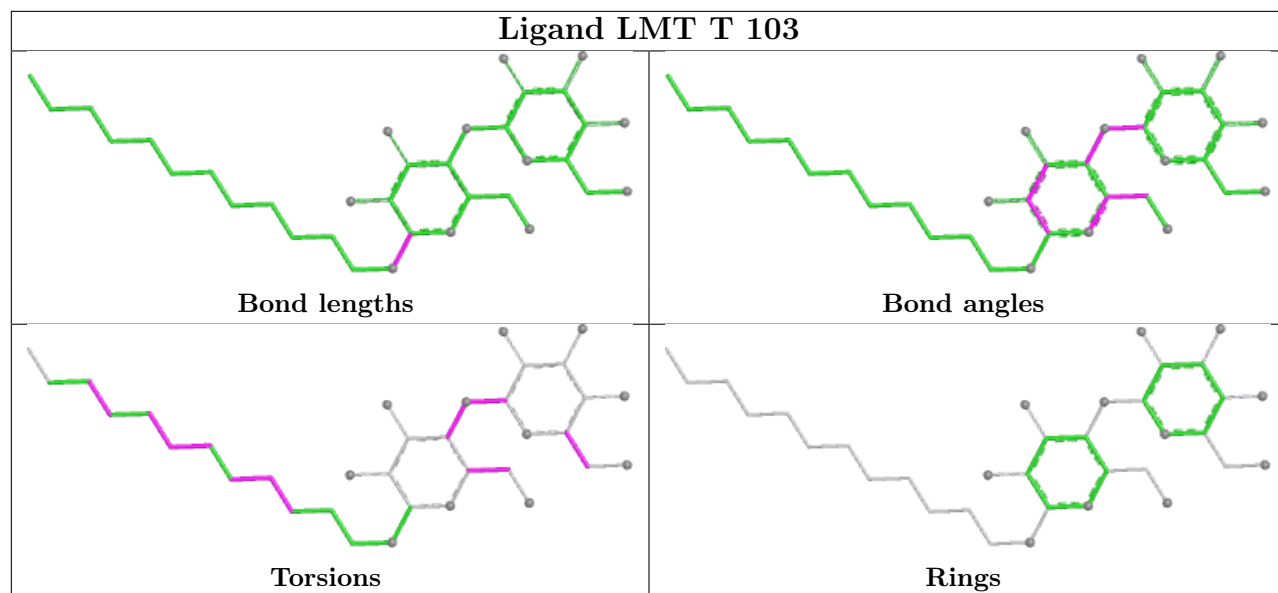
Ligand BGL L 1015



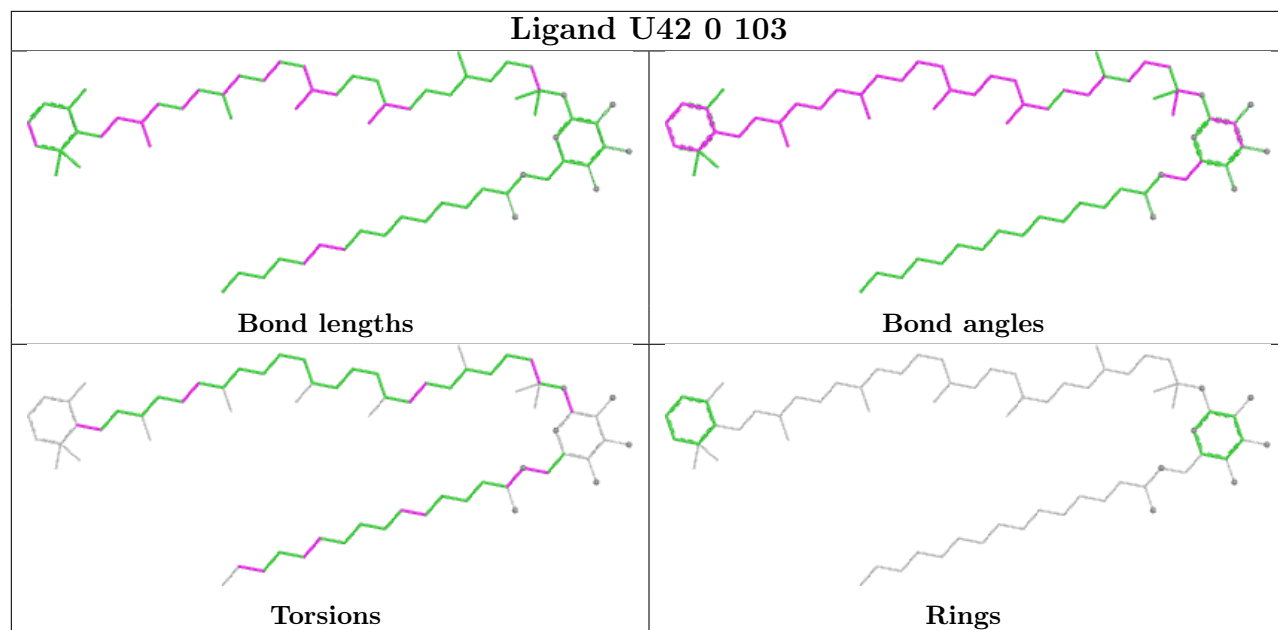
Ligand U42 U 104



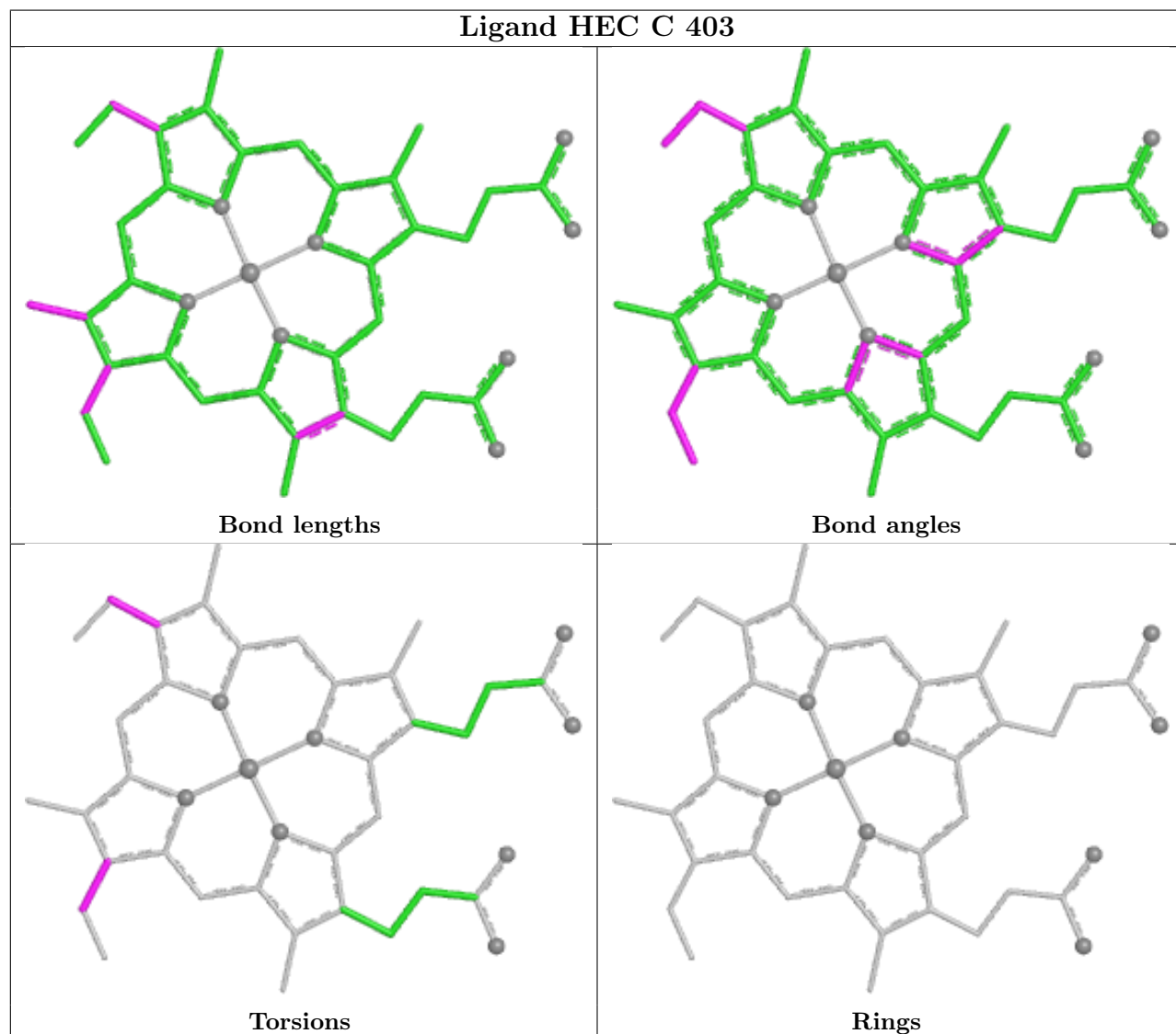


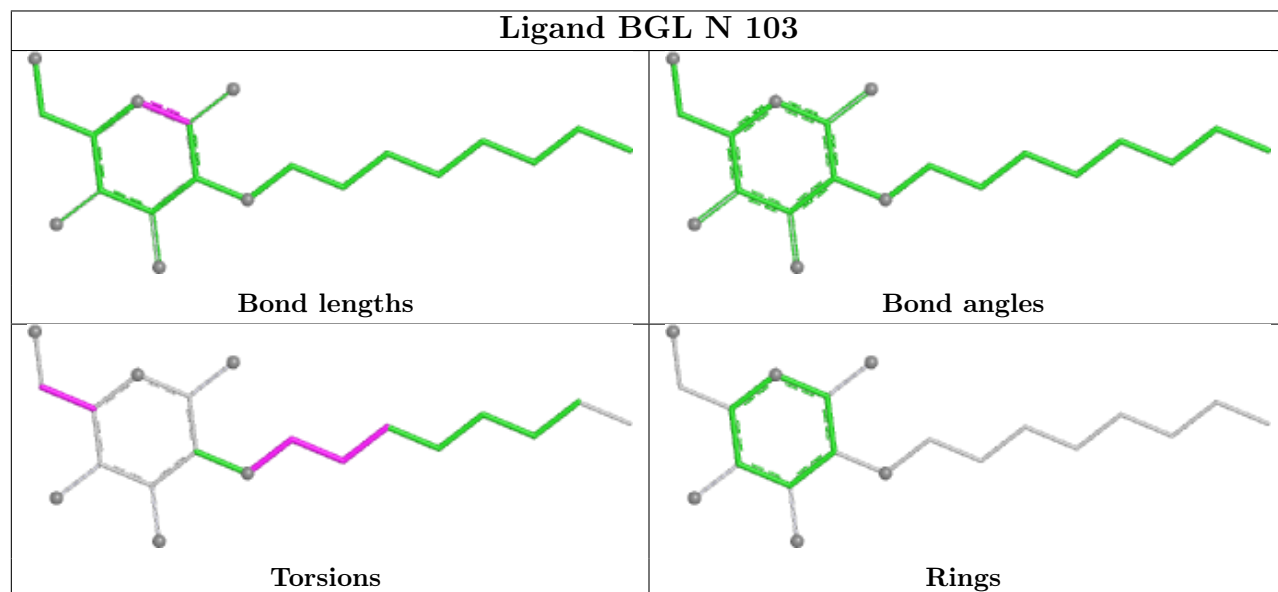
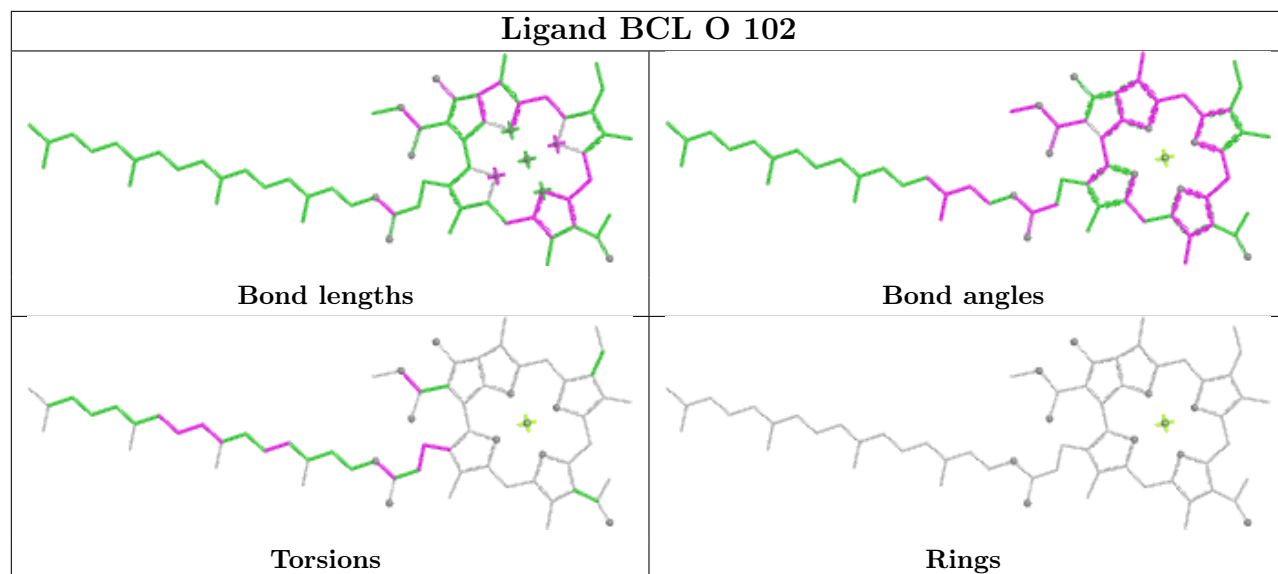


Ligand U42 0 103

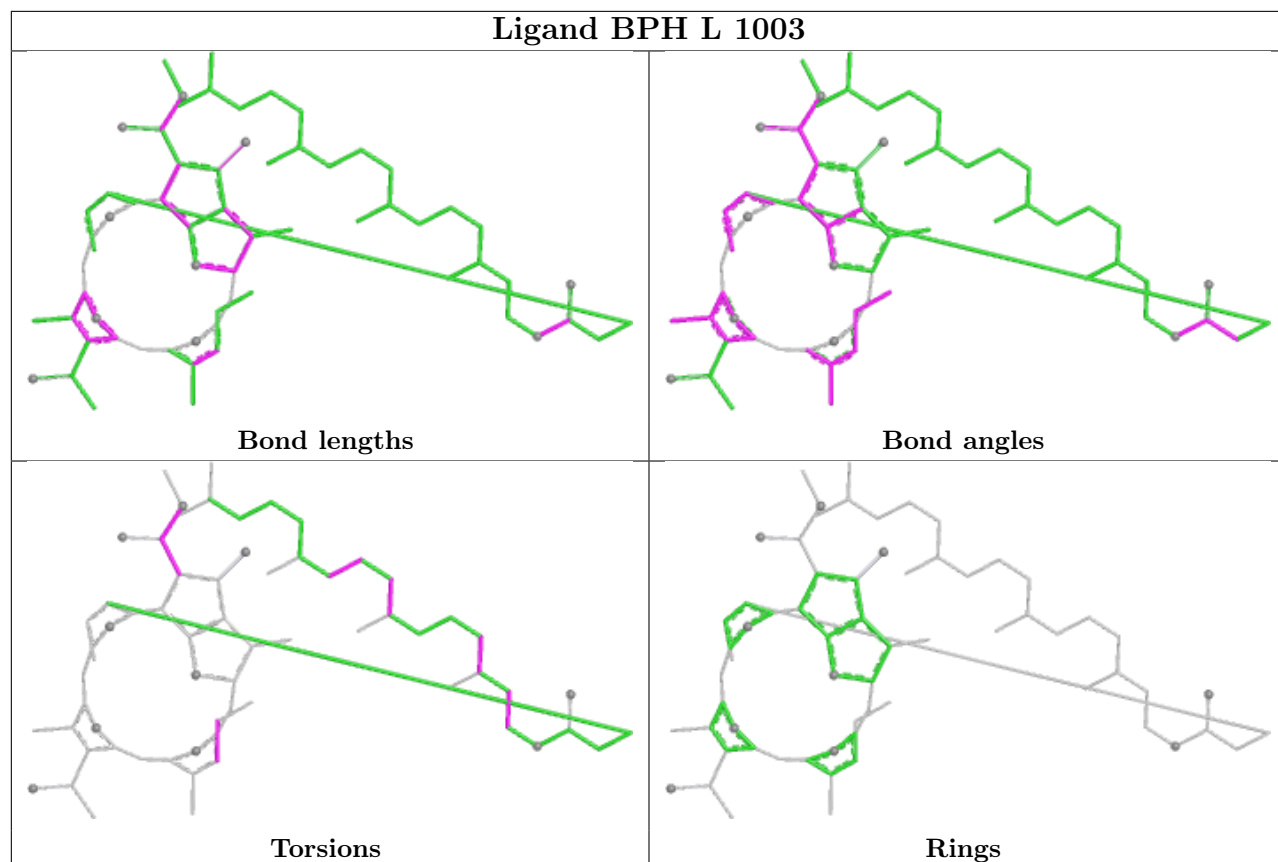


Ligand HEC C 403

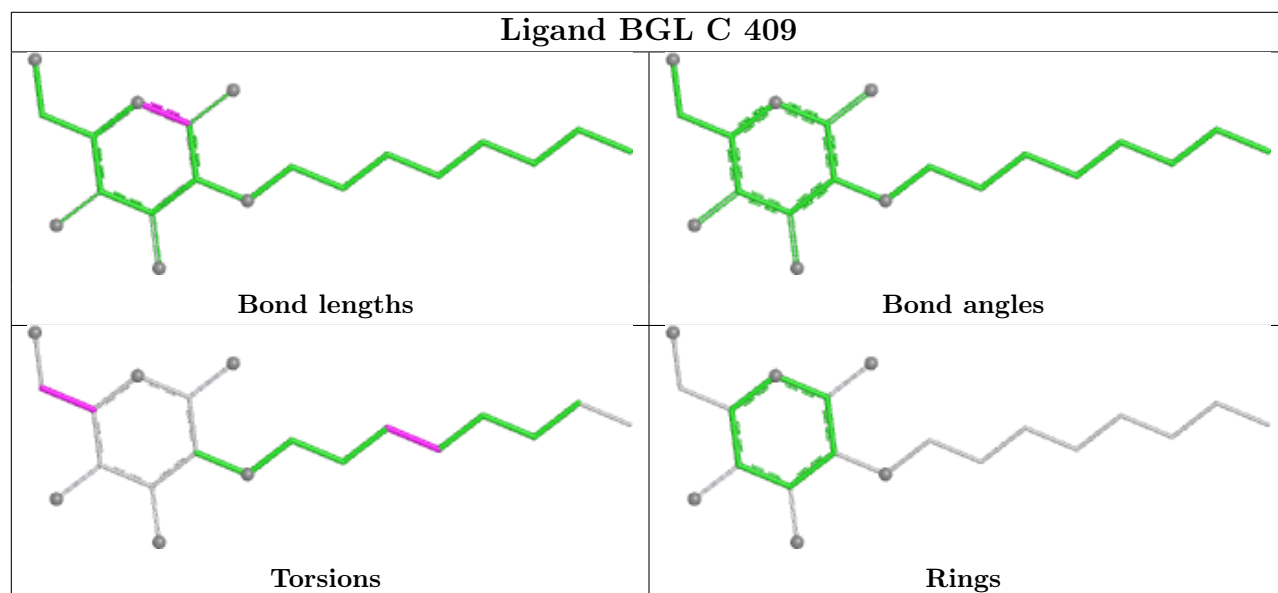


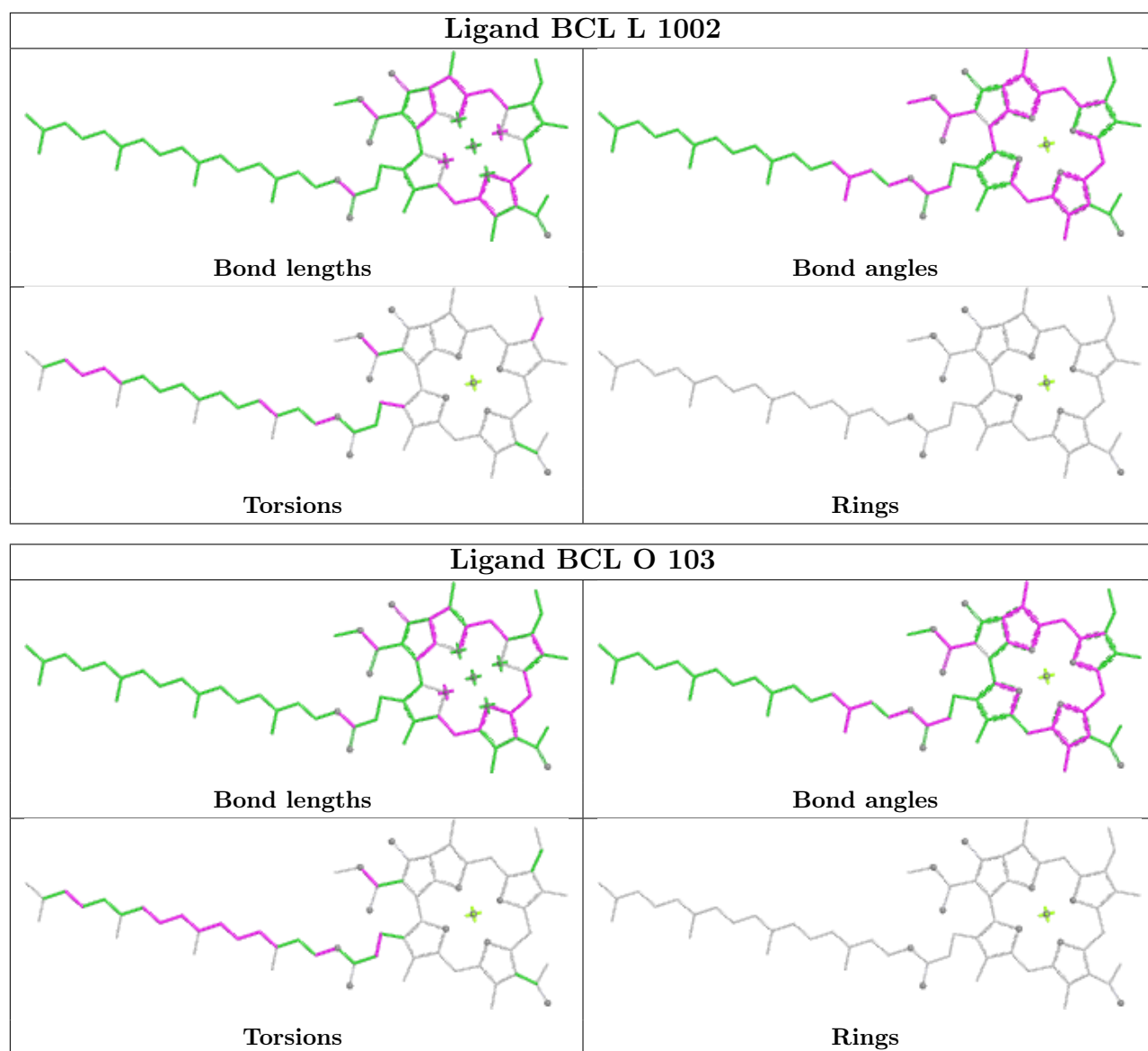


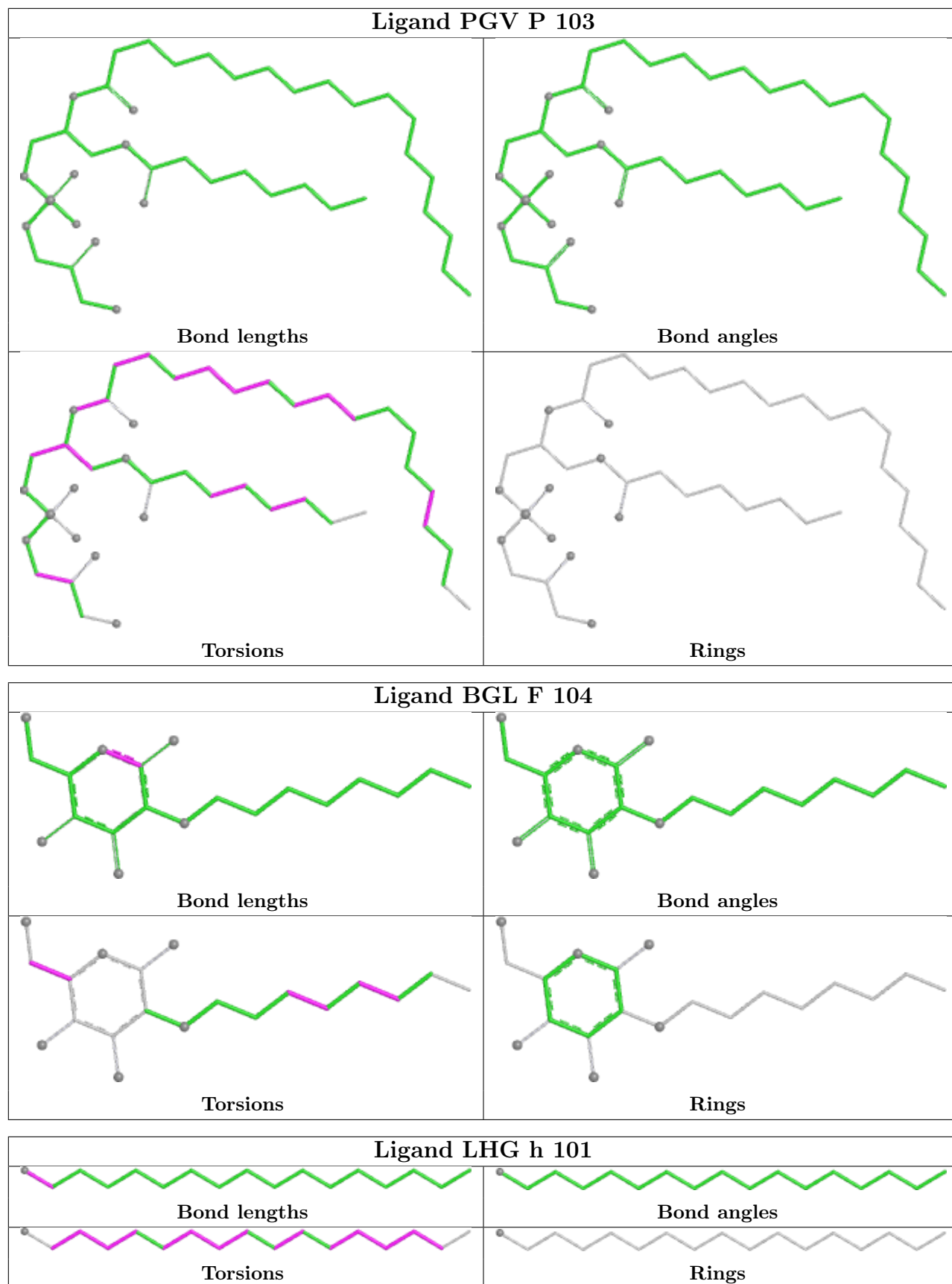
Ligand BPH L 1003

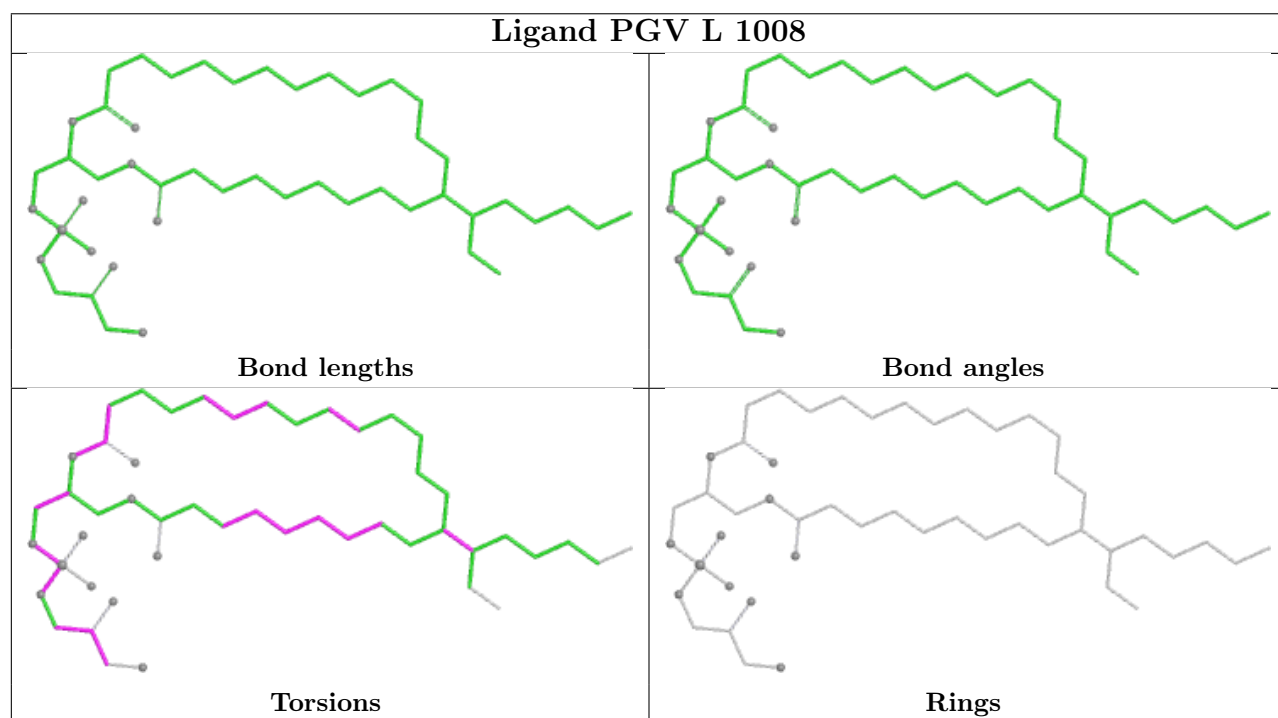
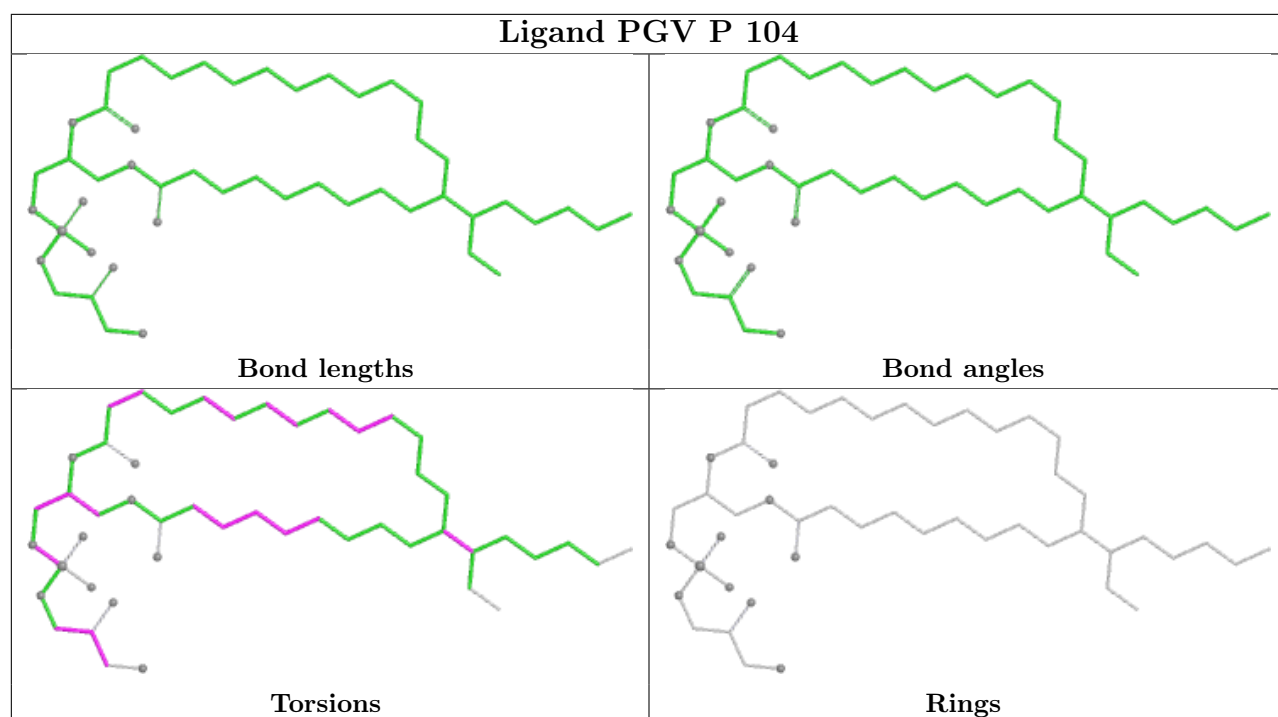


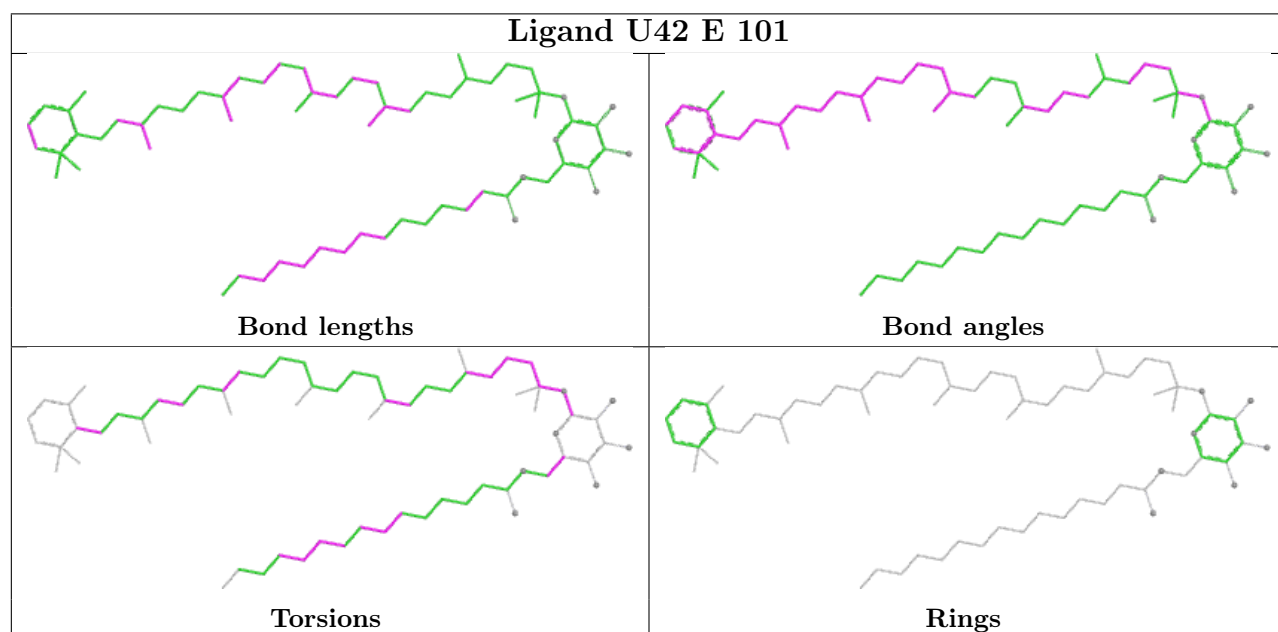
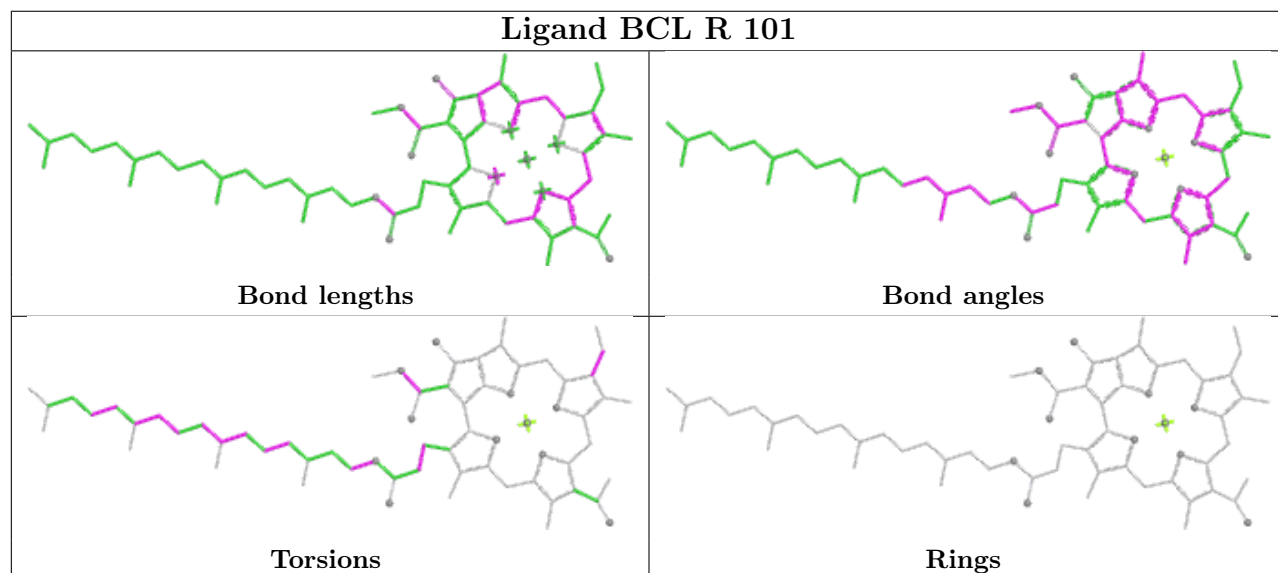
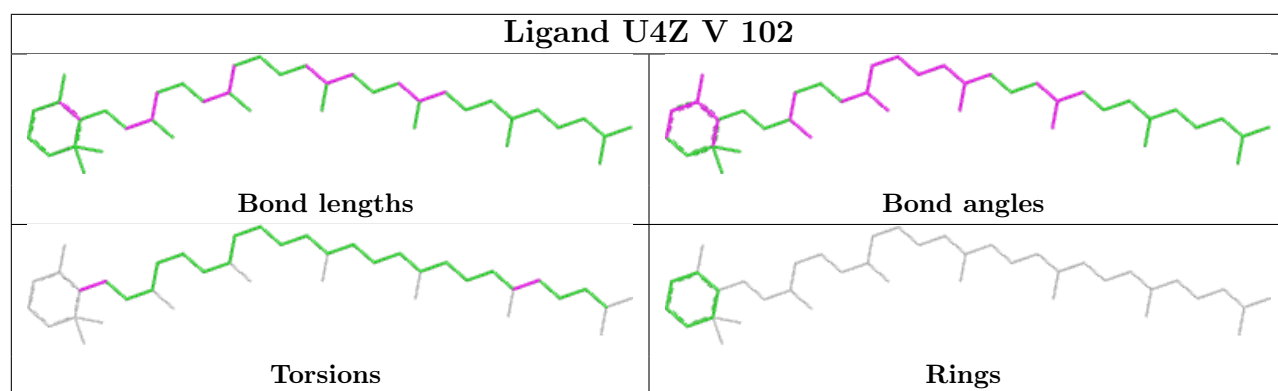
Ligand BGL C 409

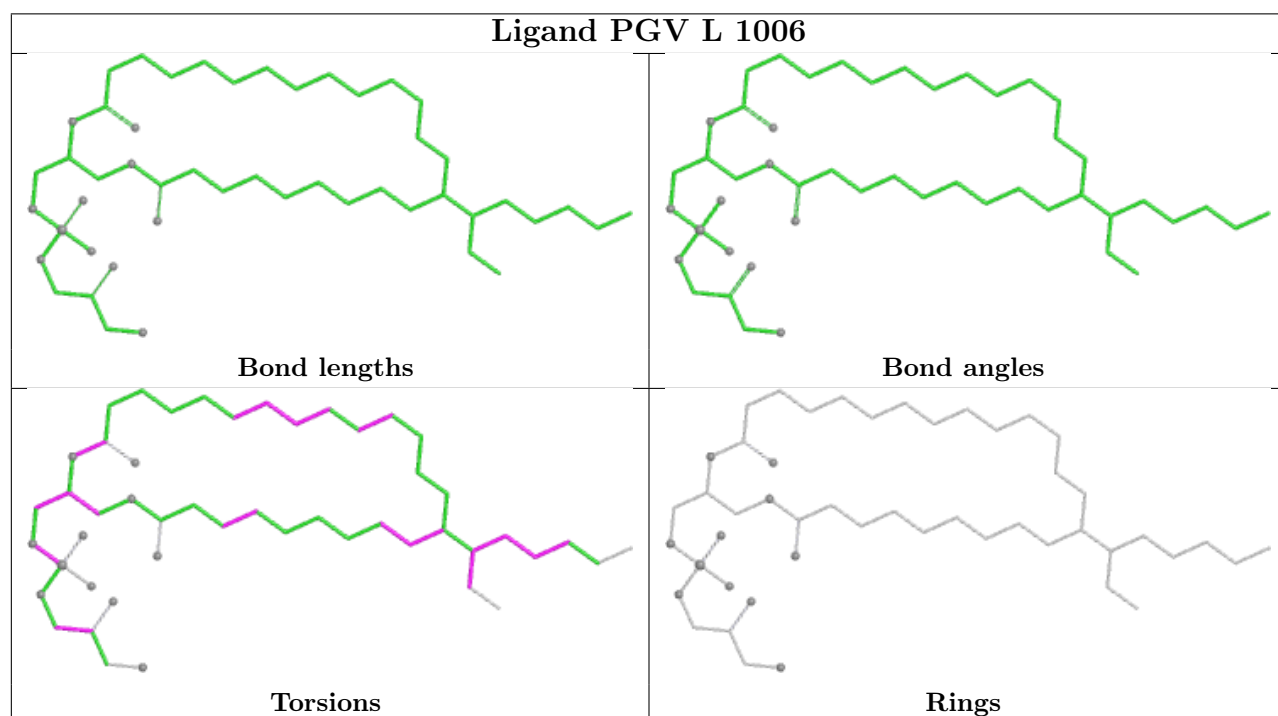
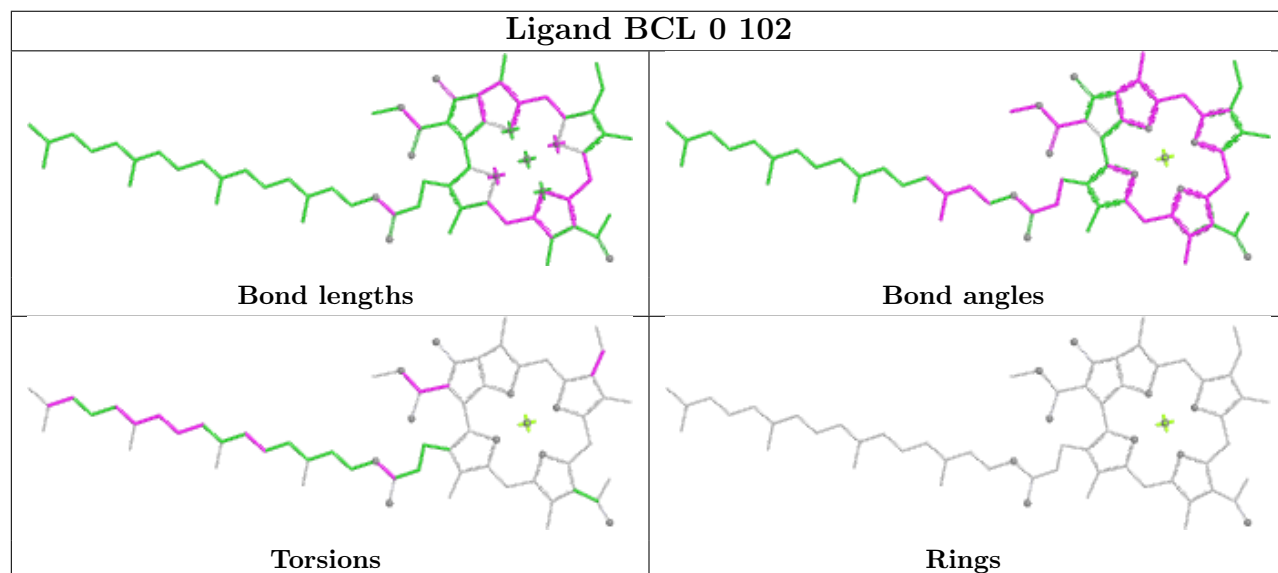
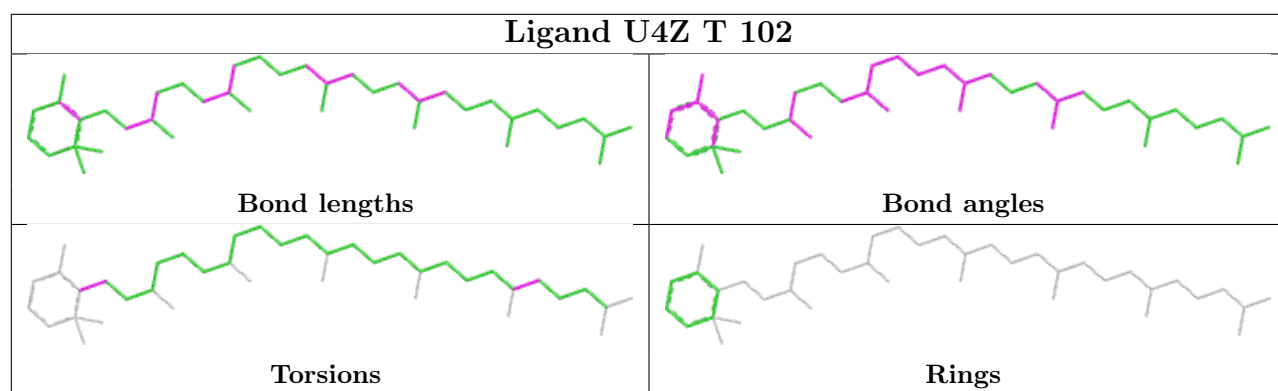


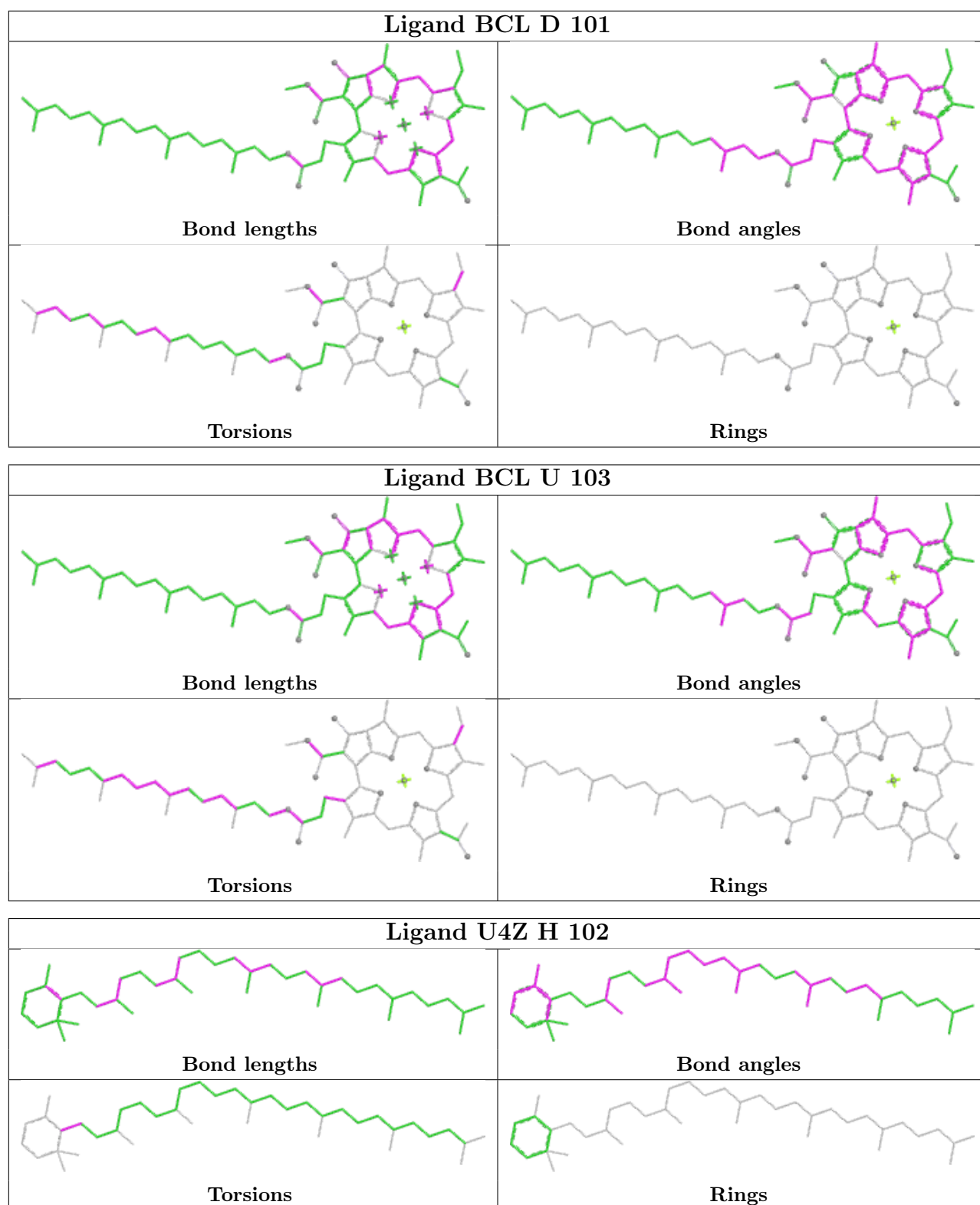


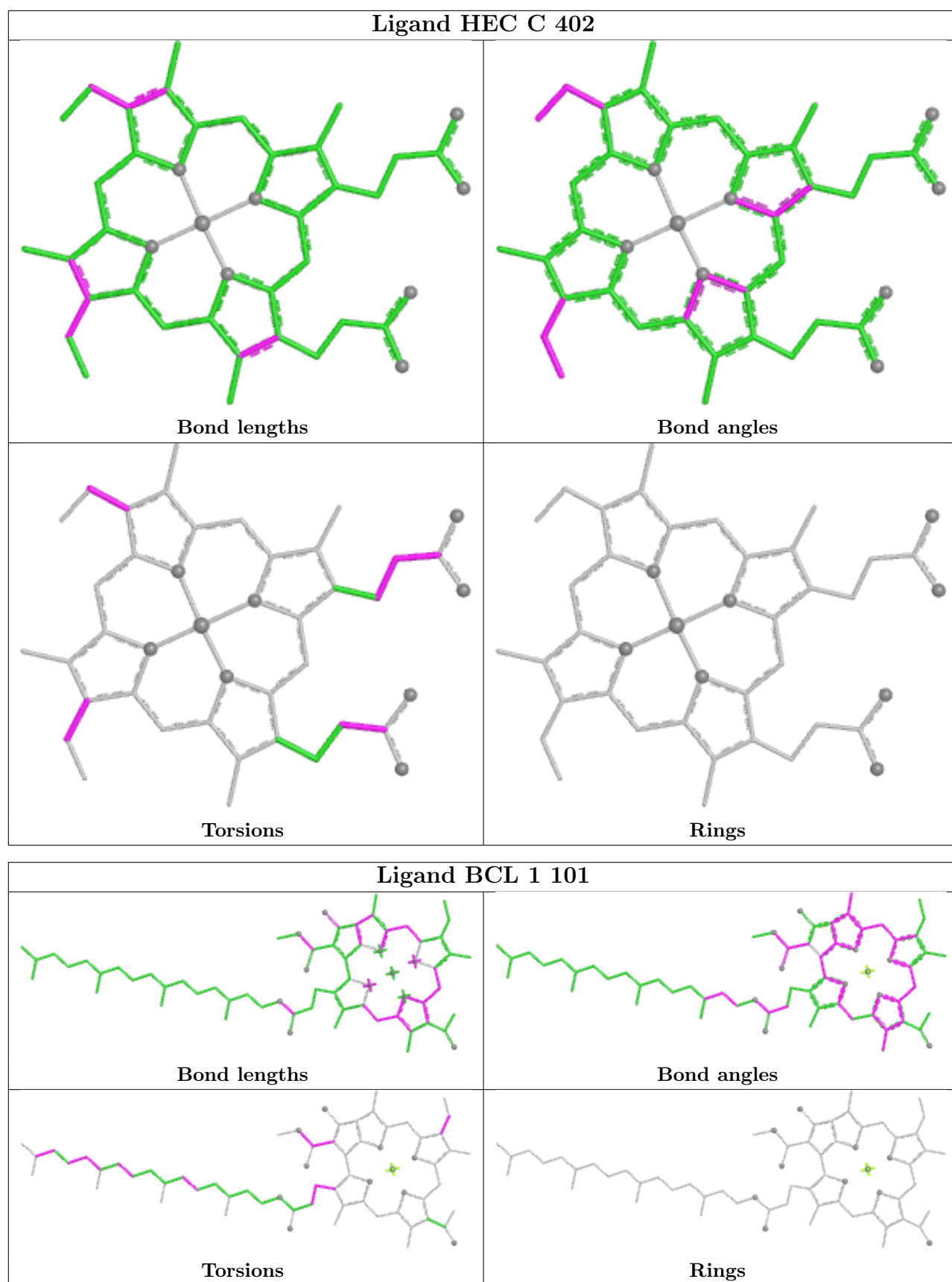


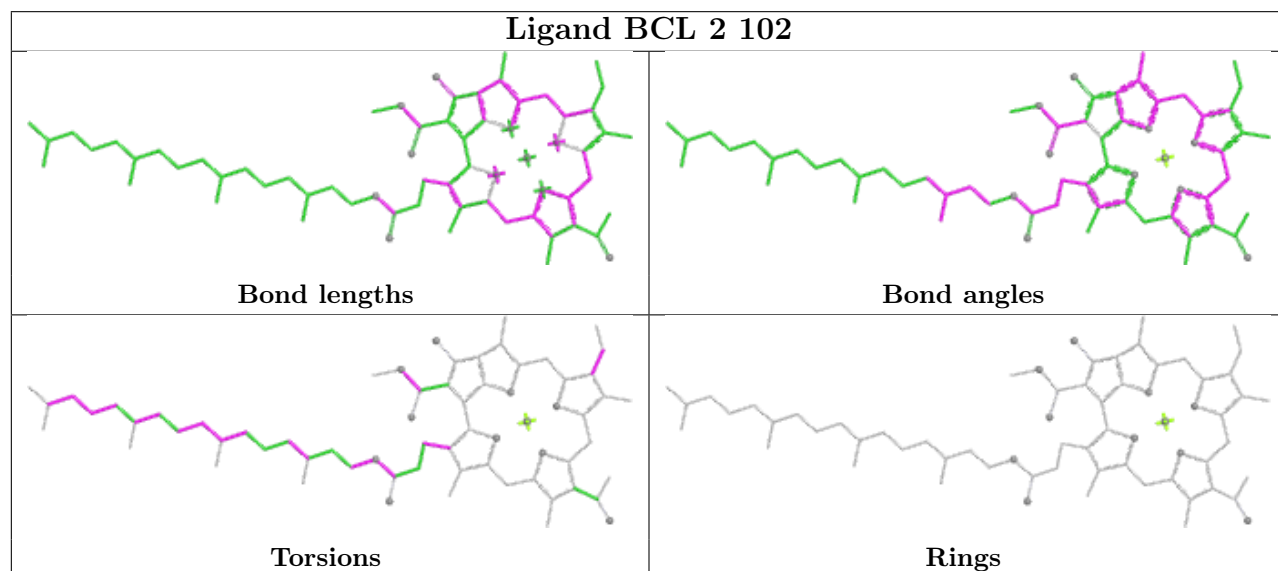
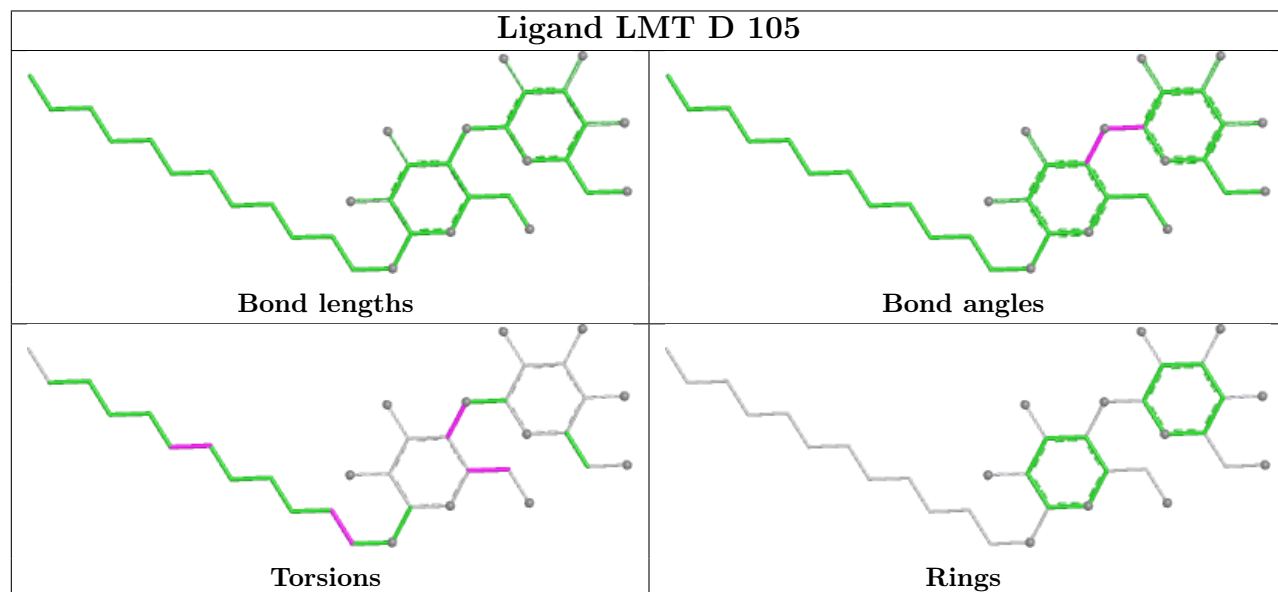
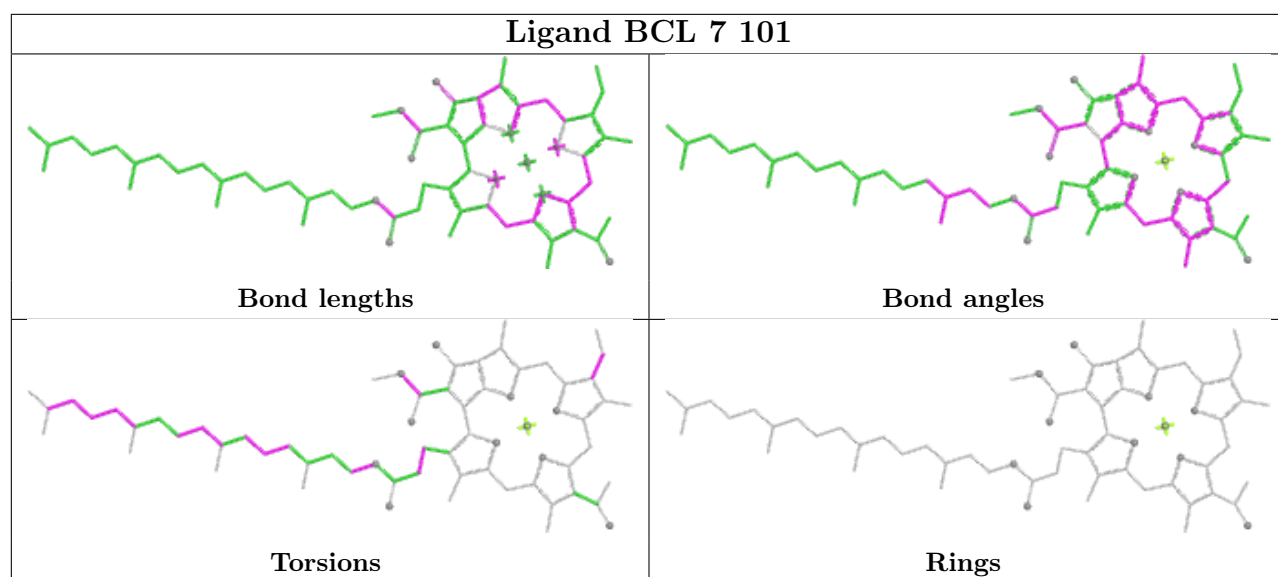








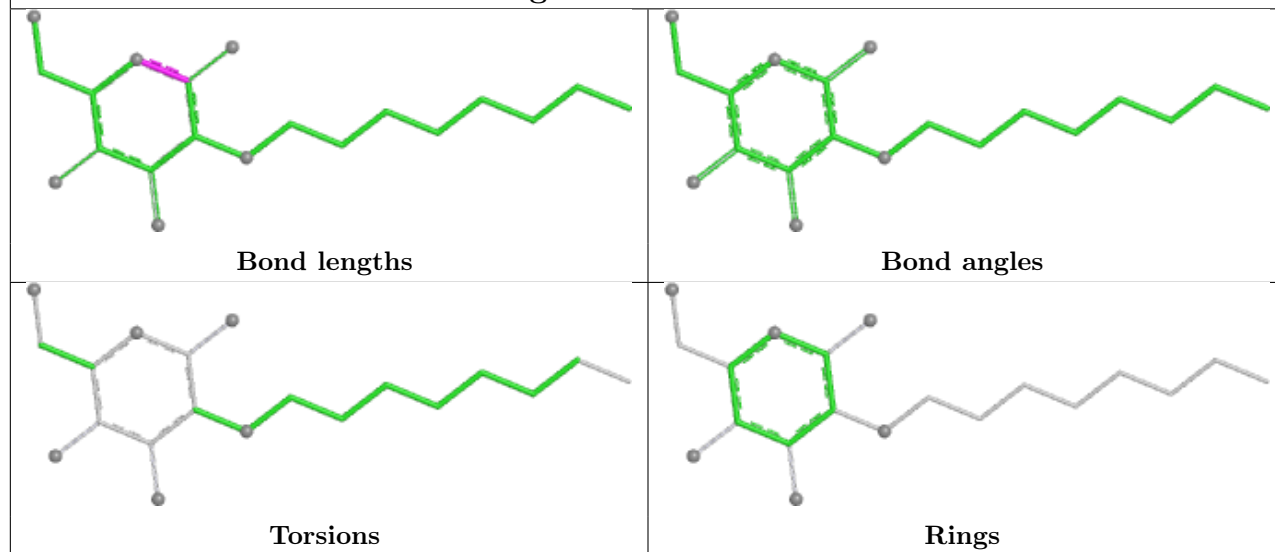




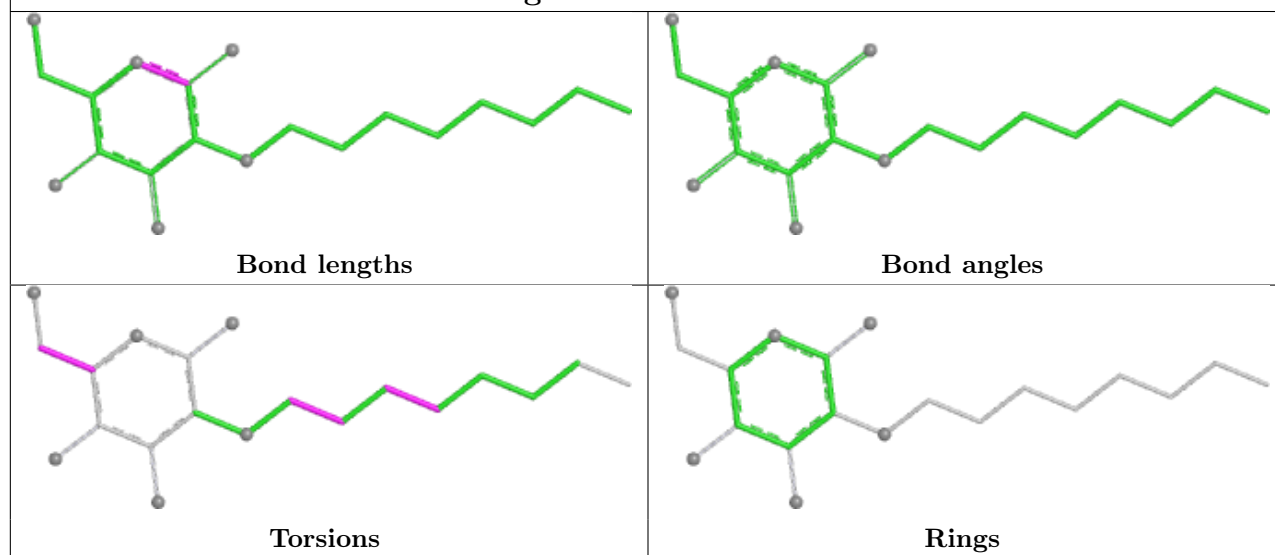
Ligand U4Z P 102

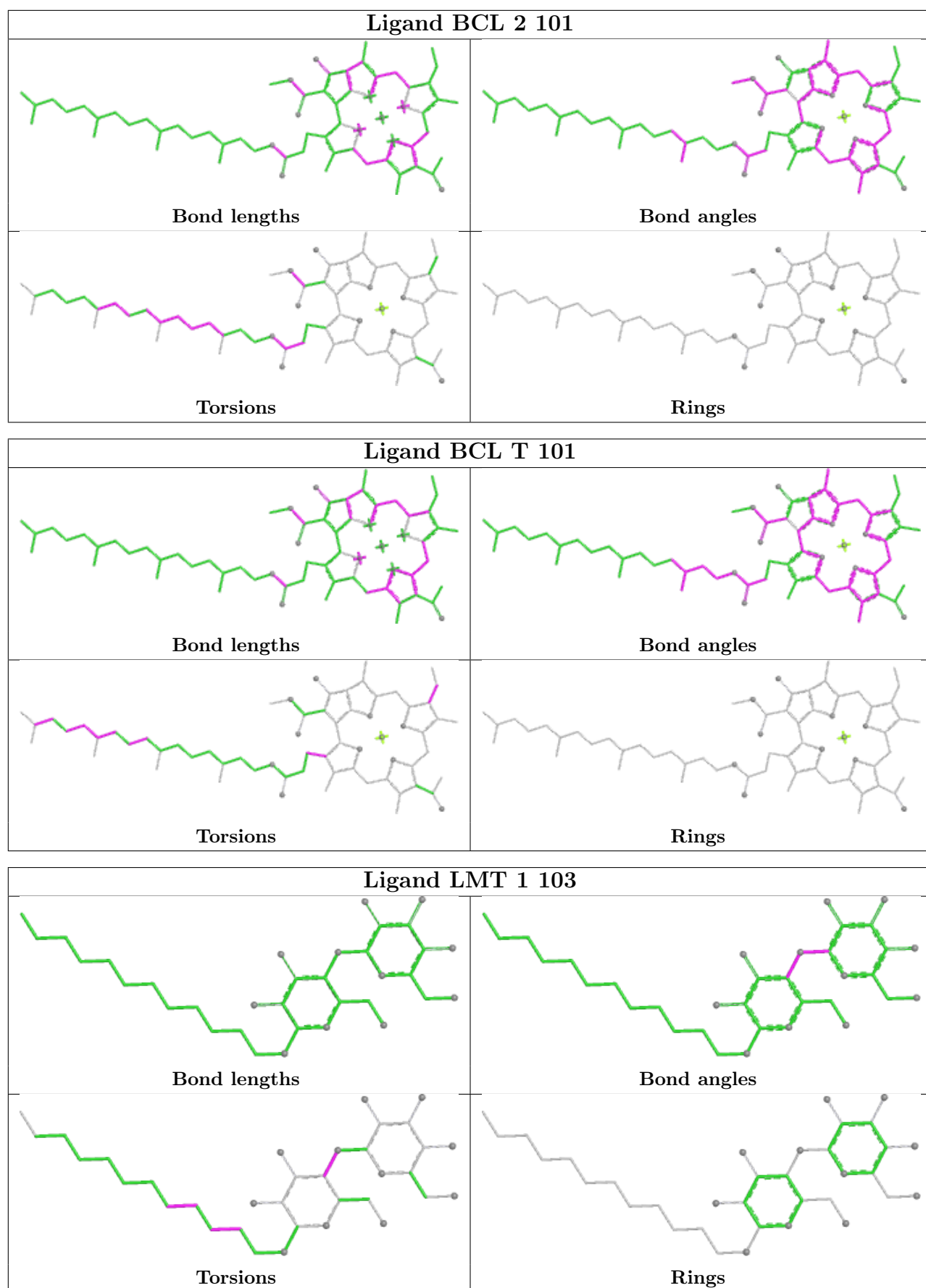


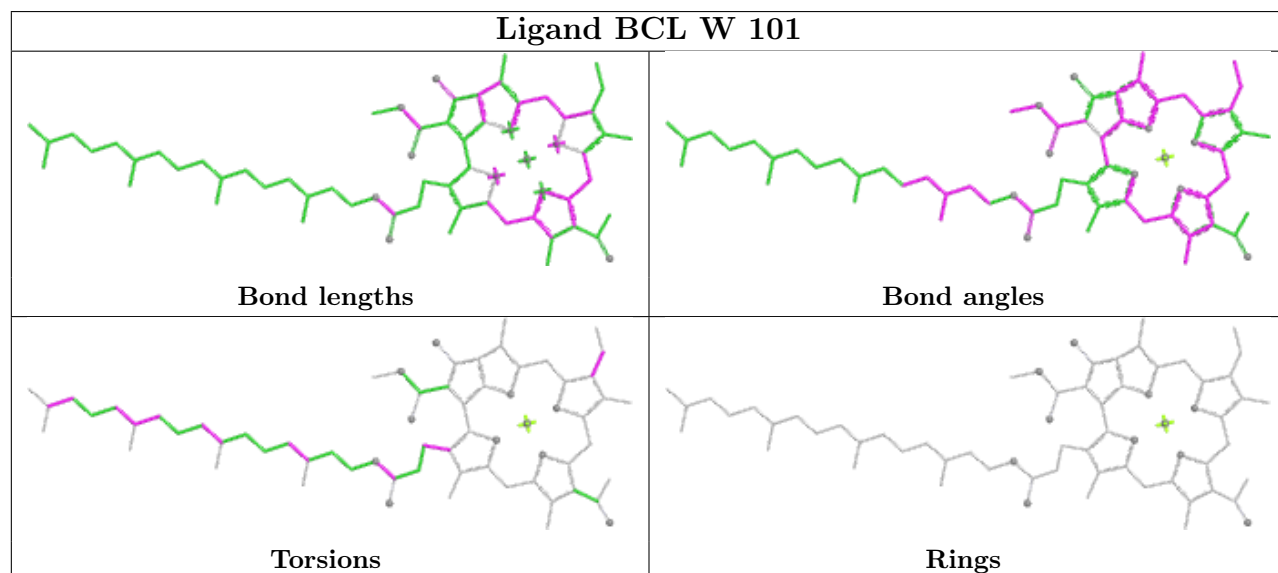
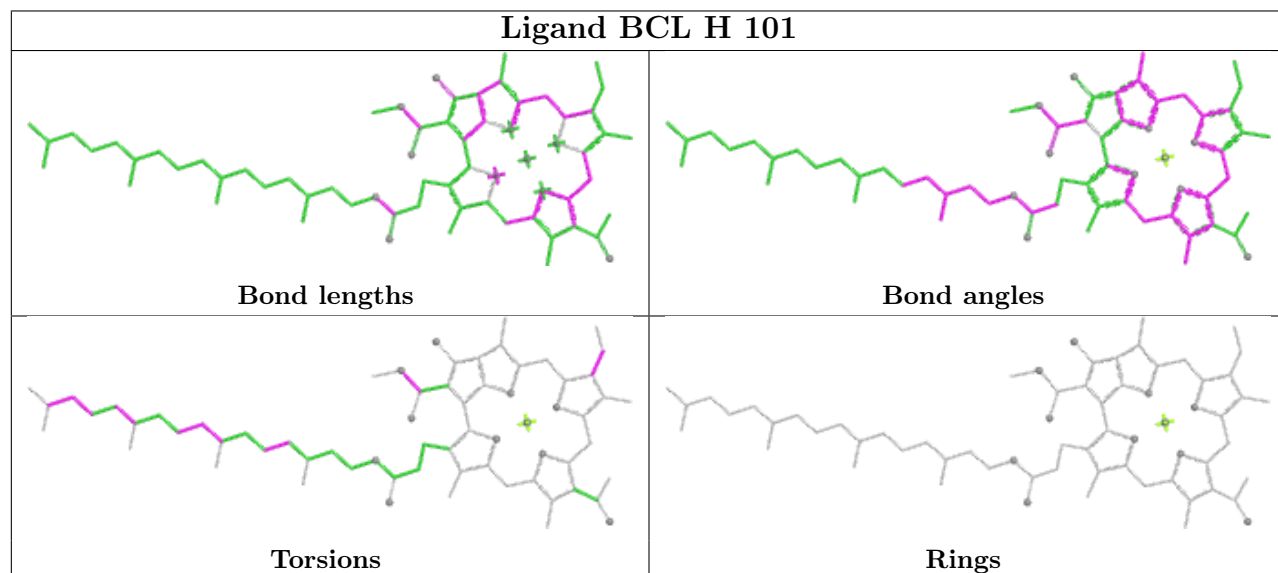
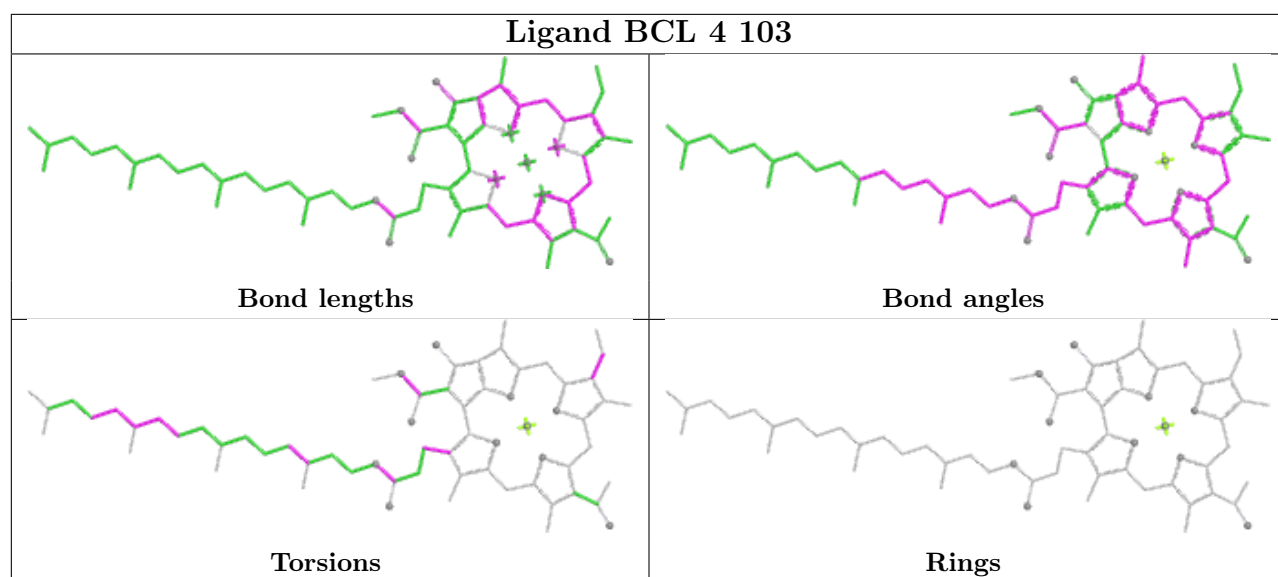
Ligand BGL H 103

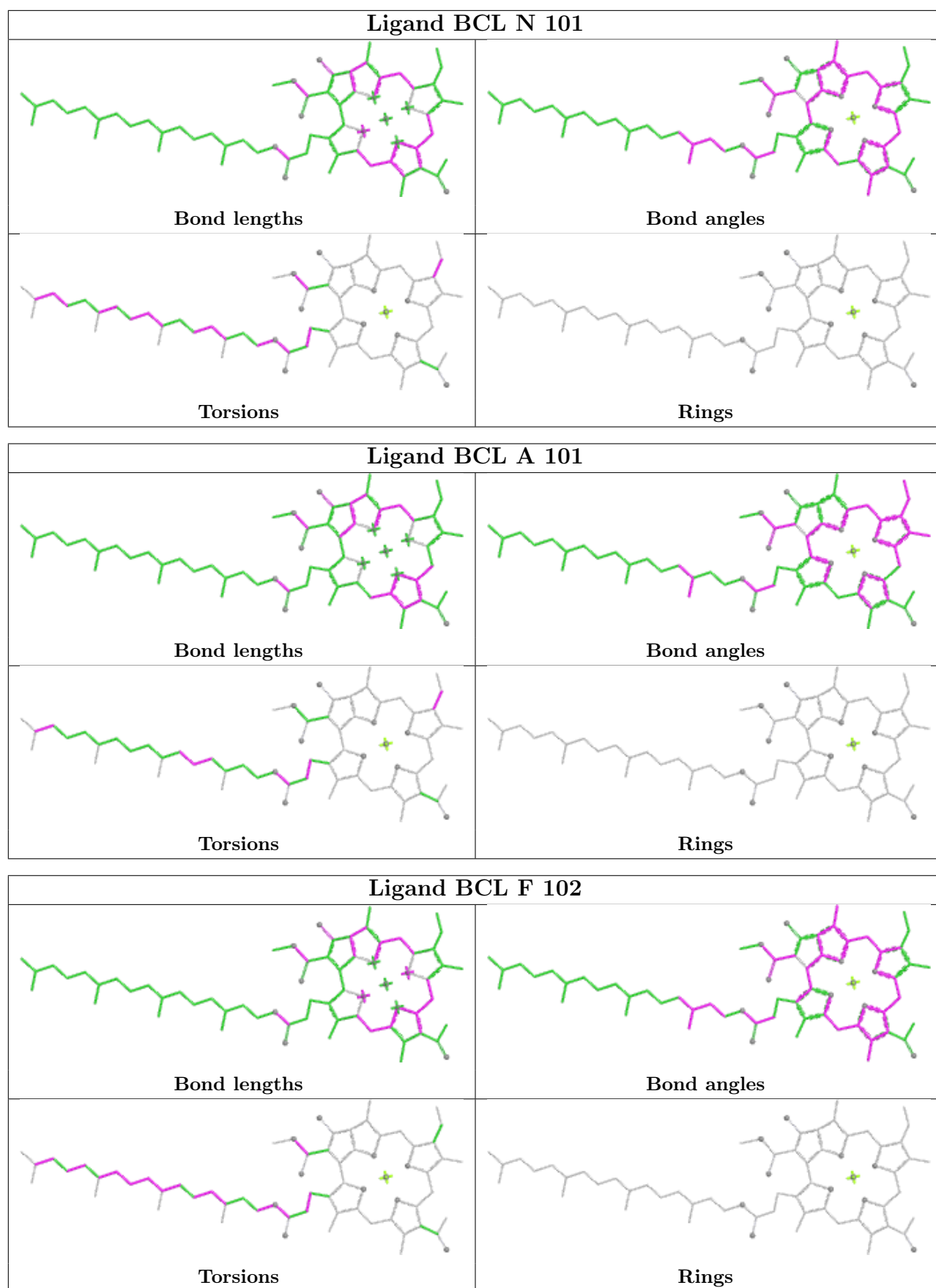


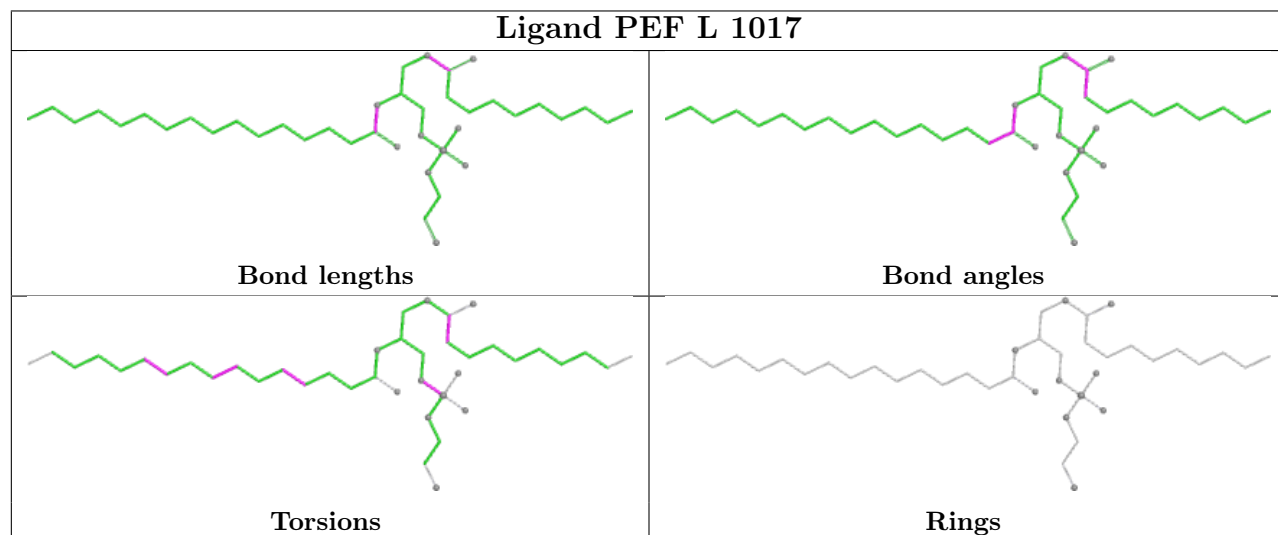
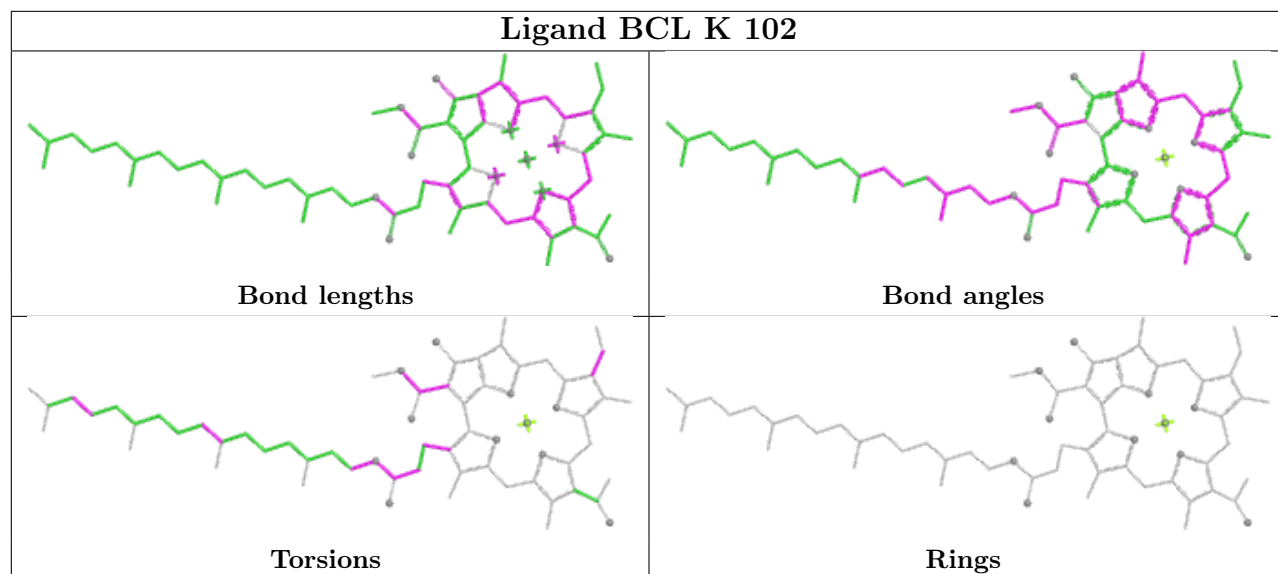
Ligand BGL L 1013

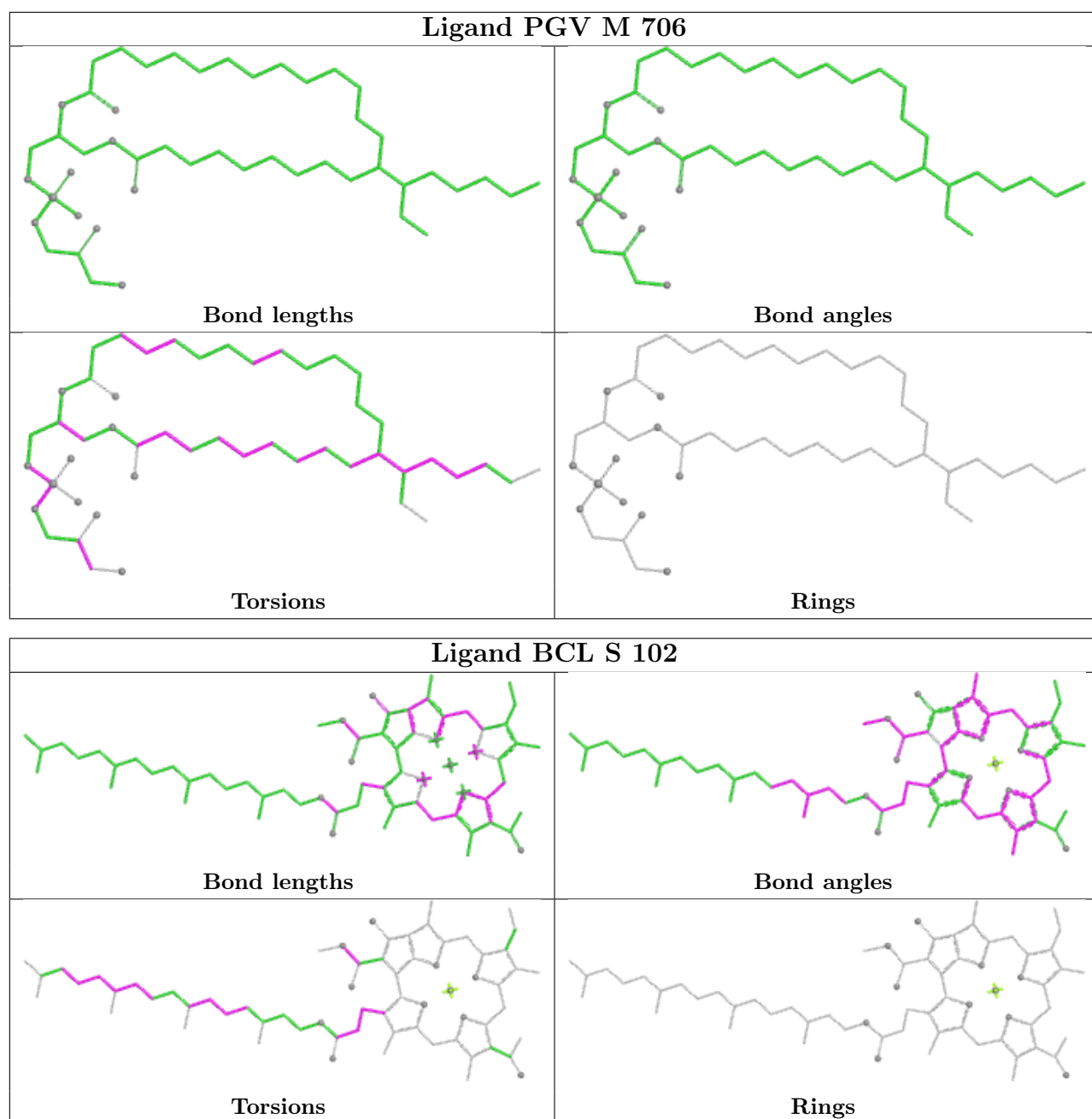


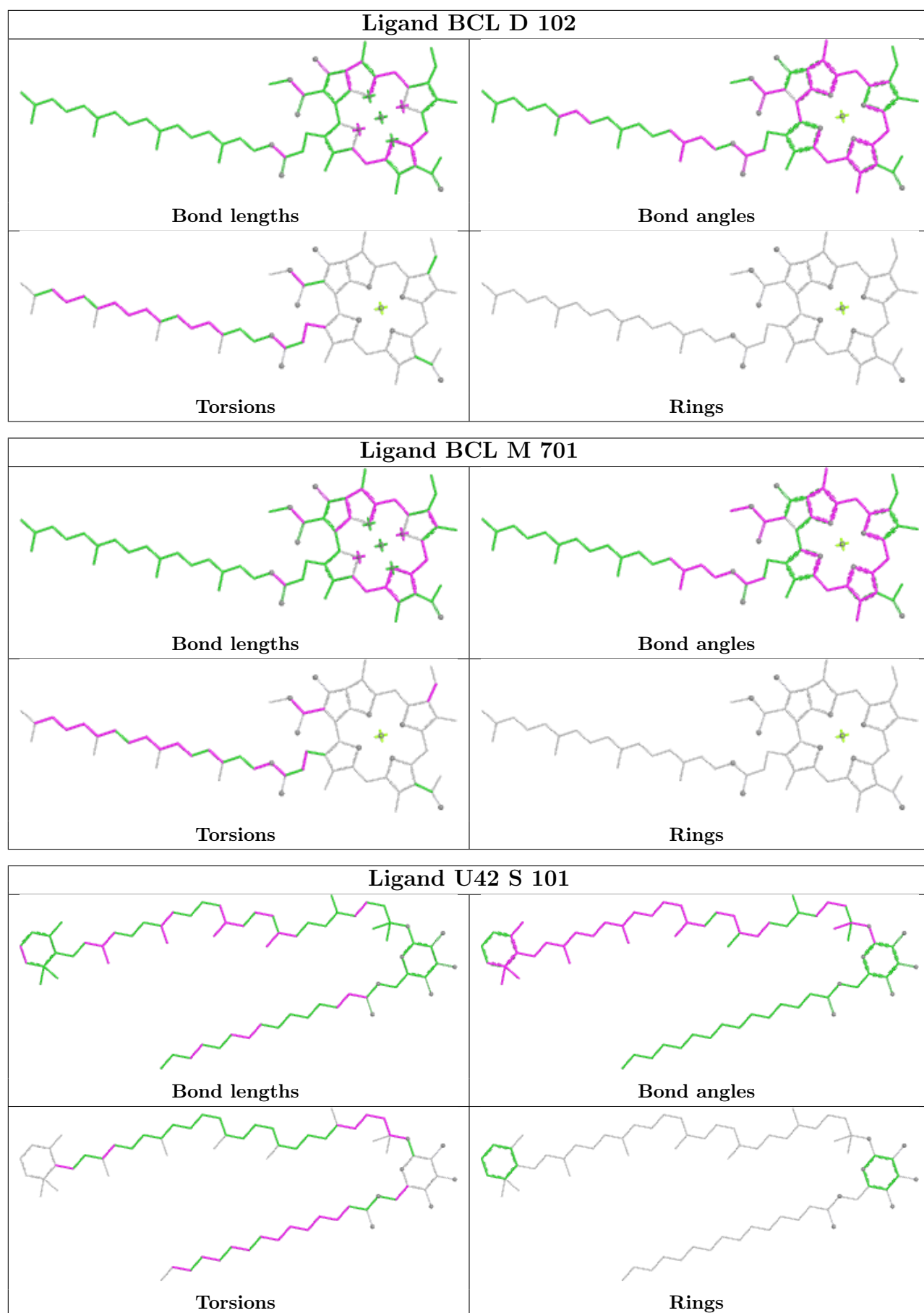


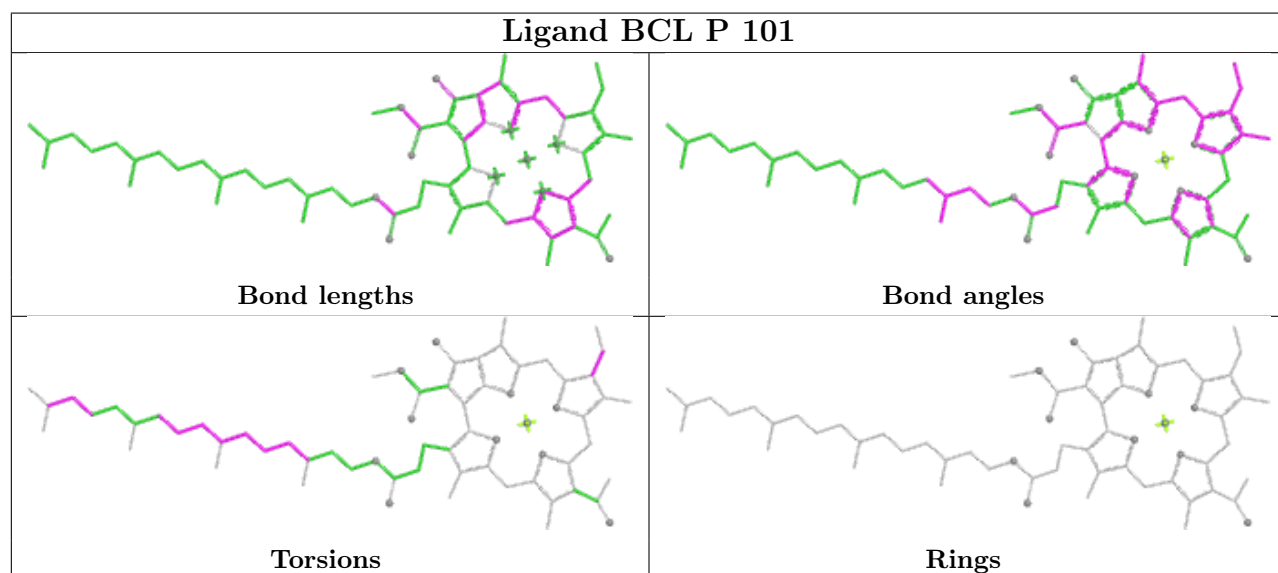
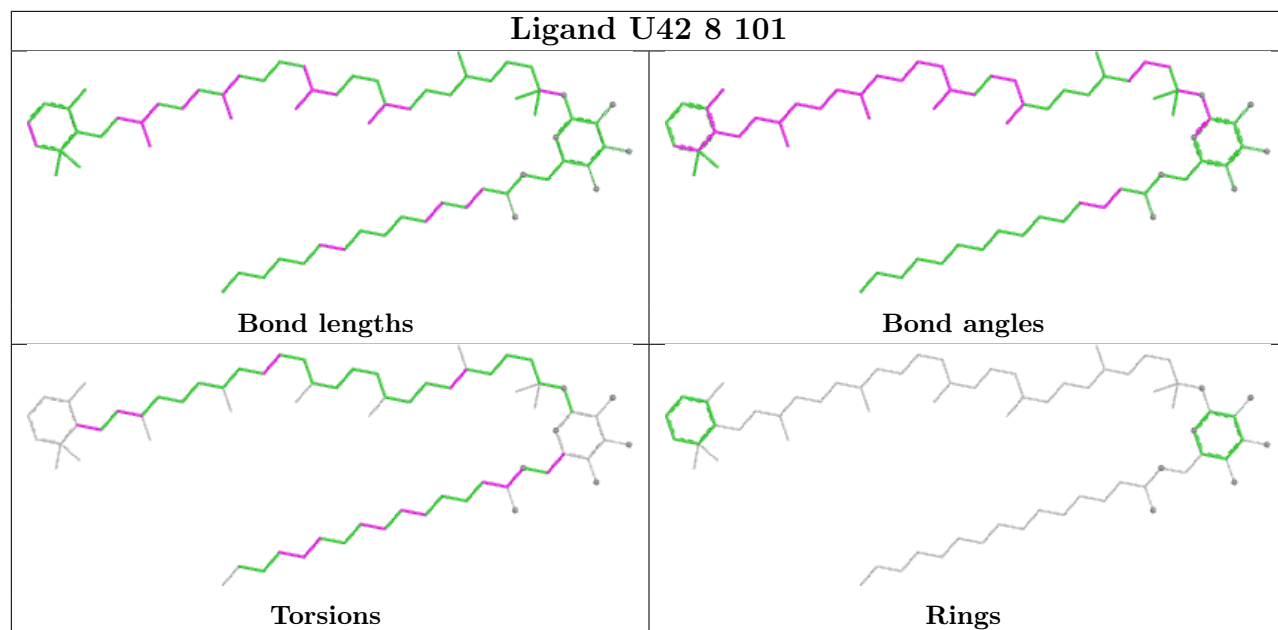


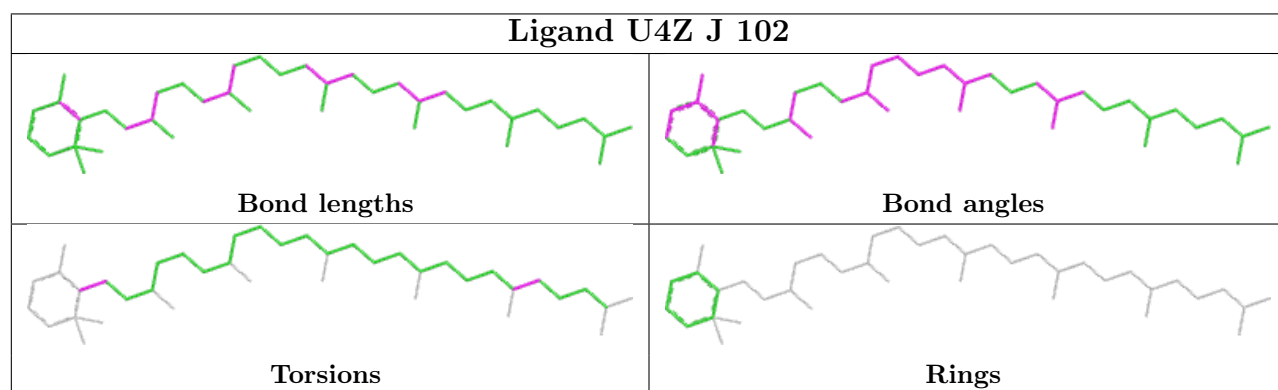
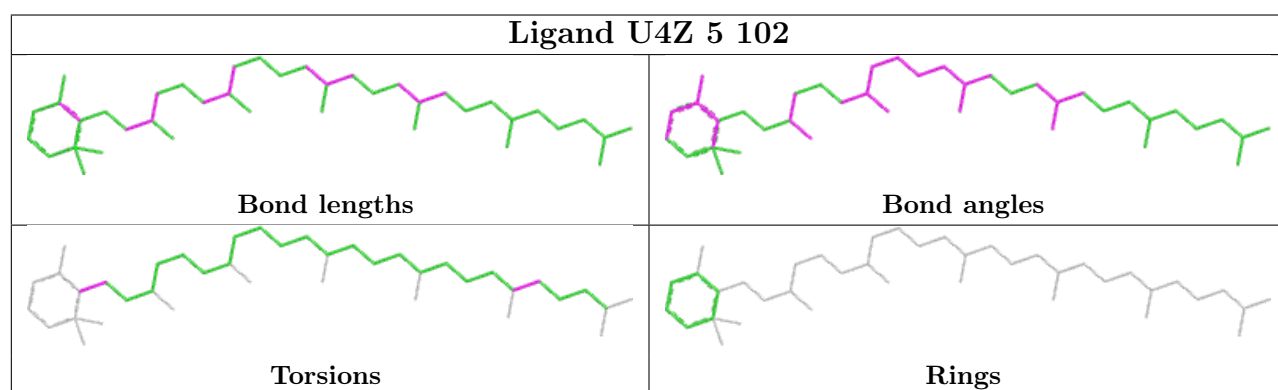
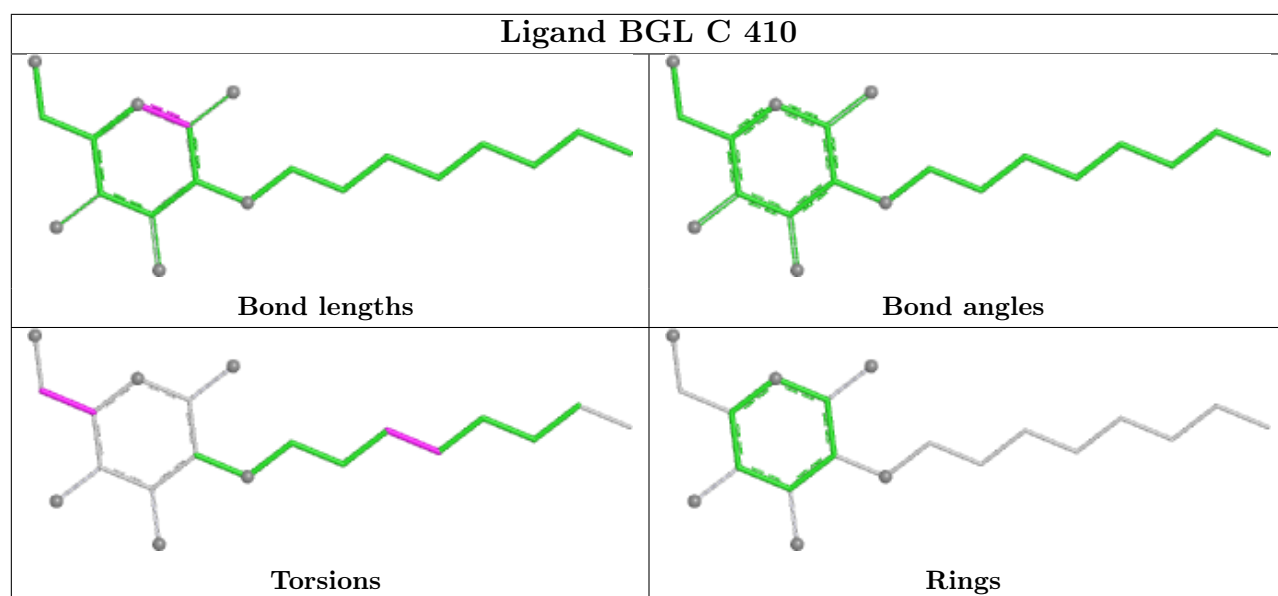


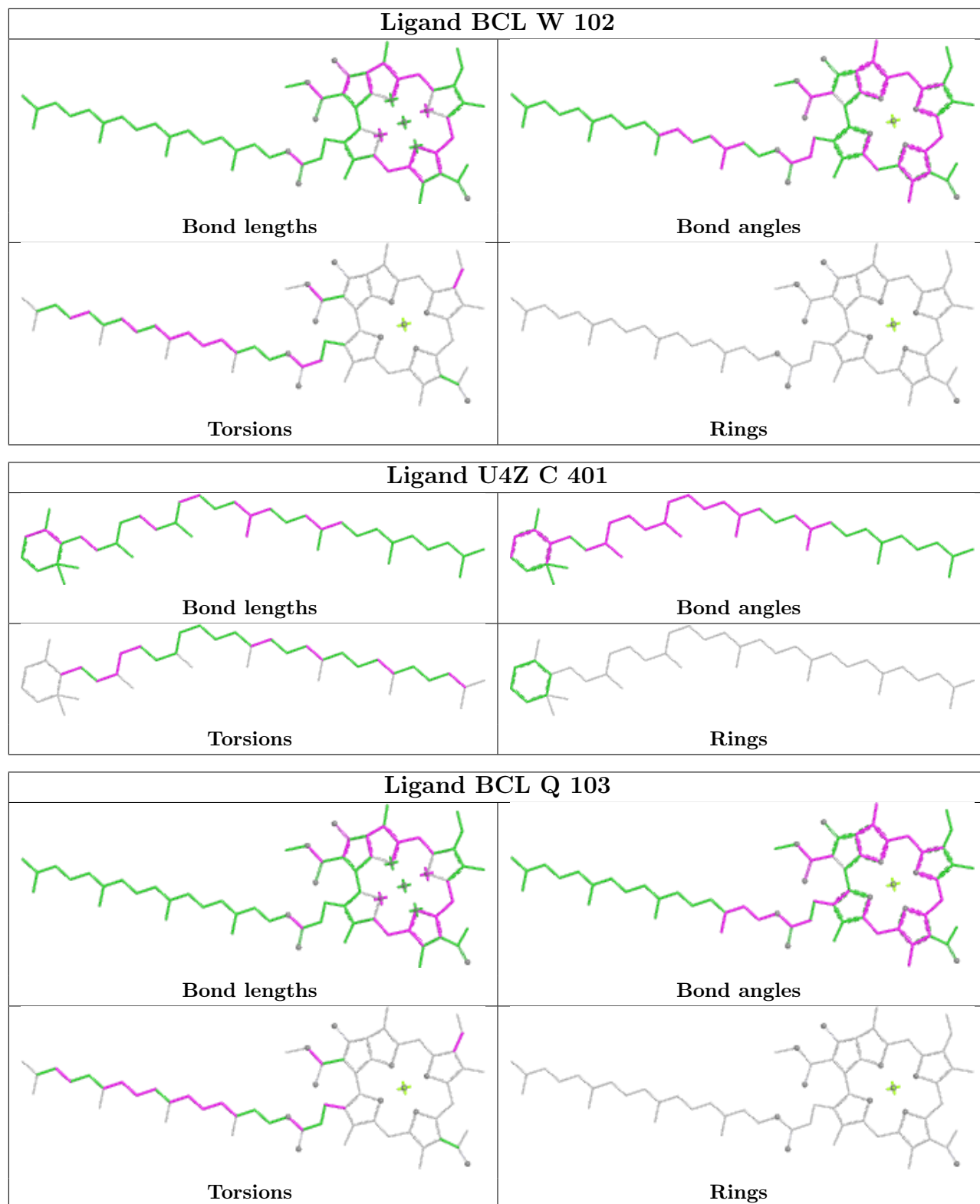


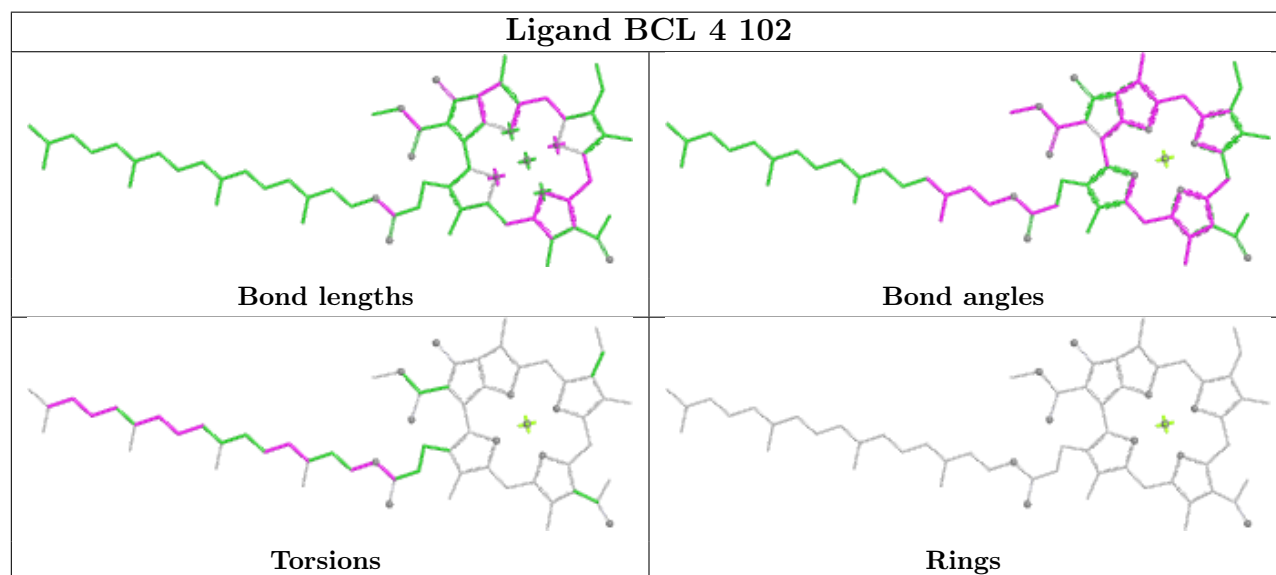
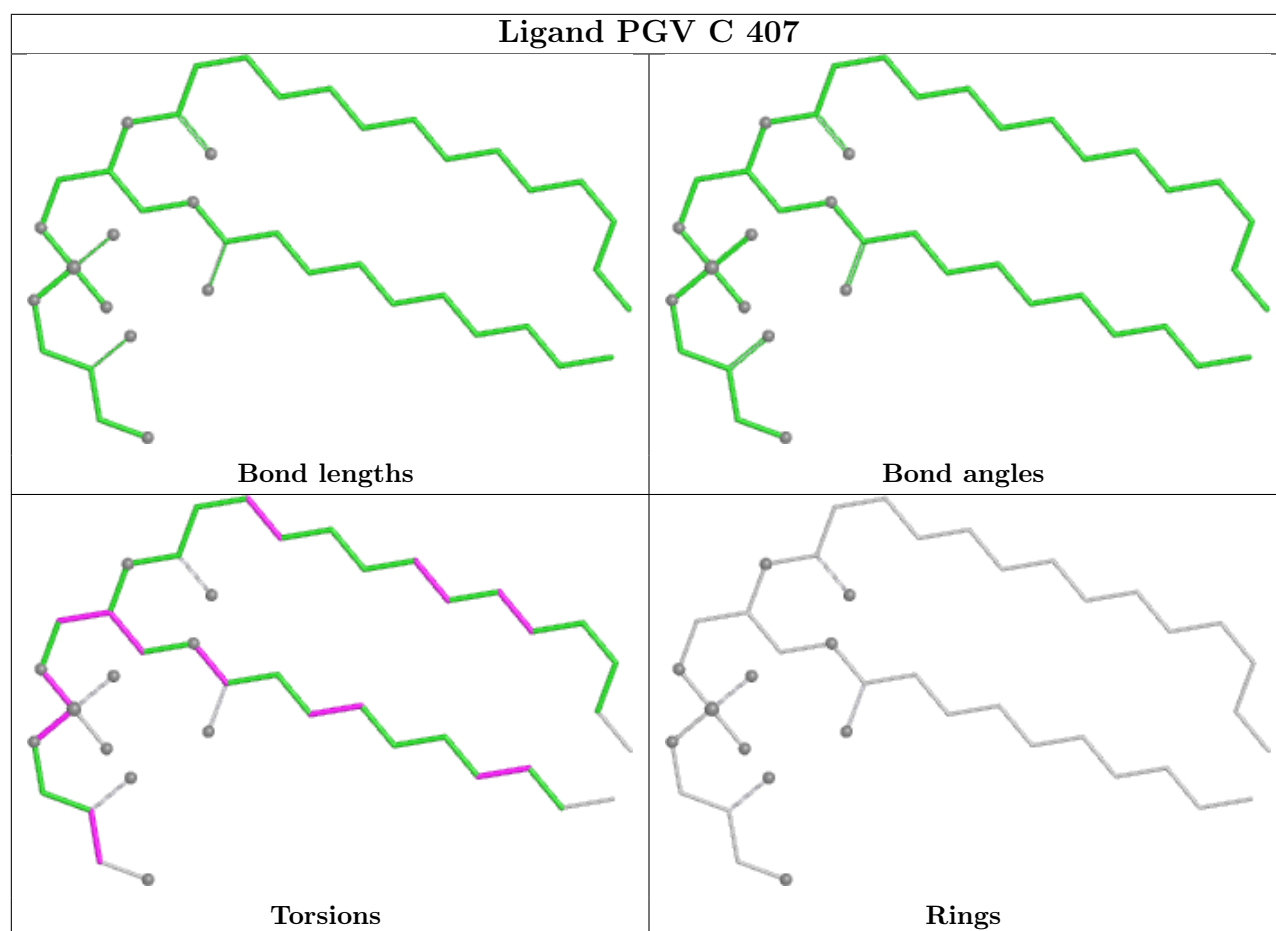


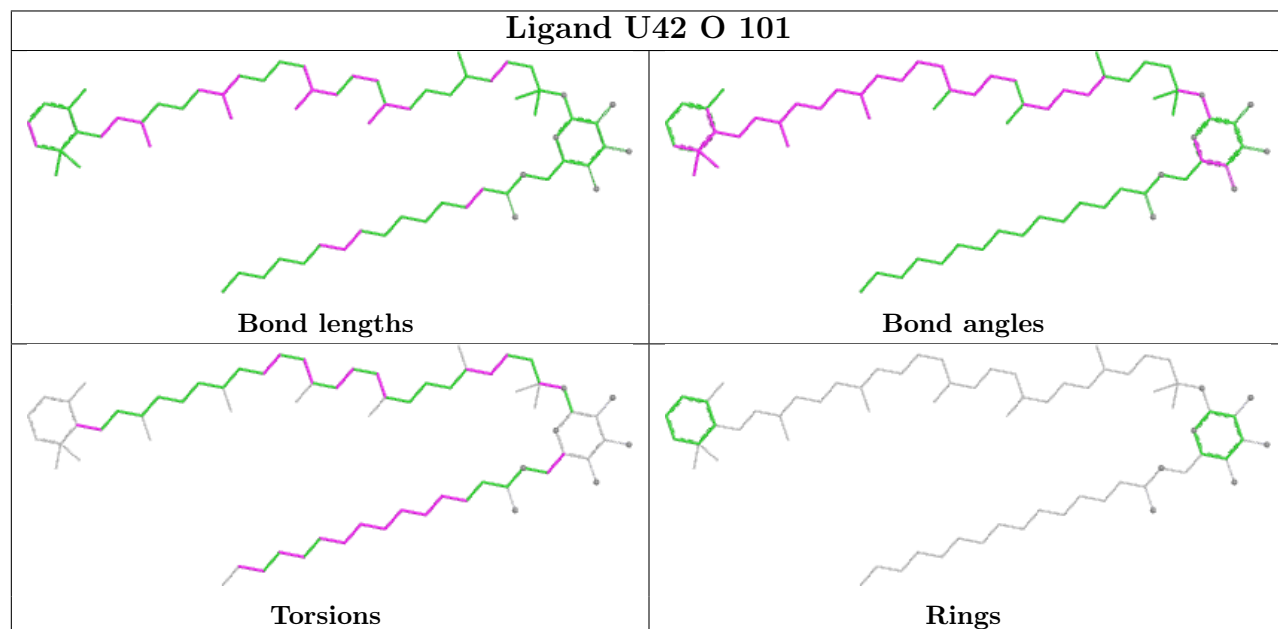
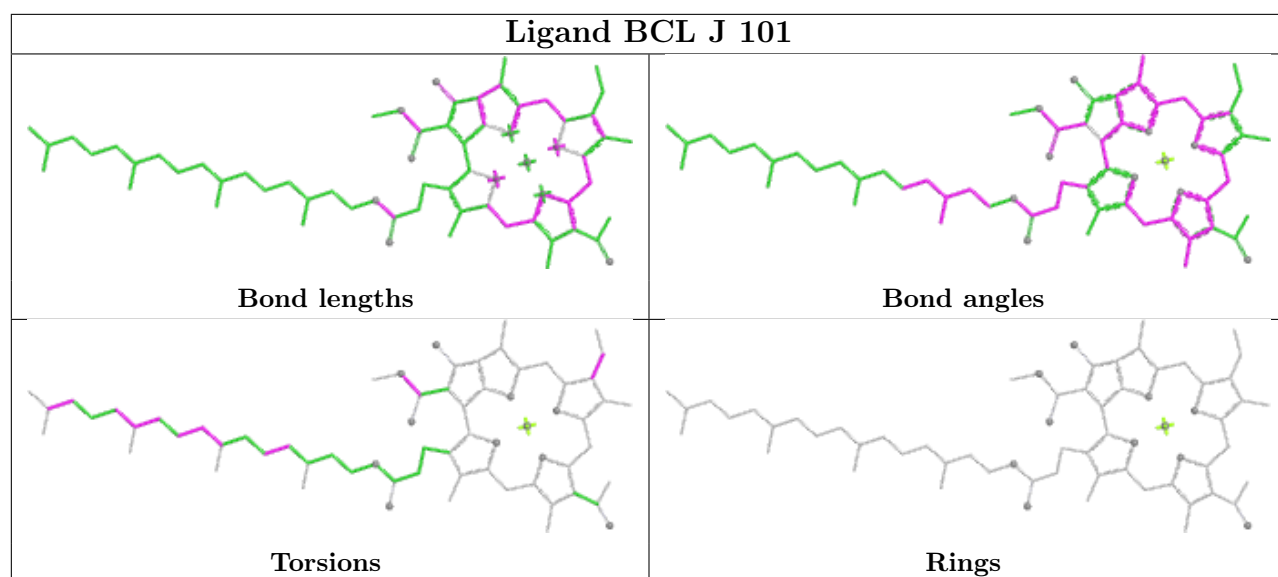


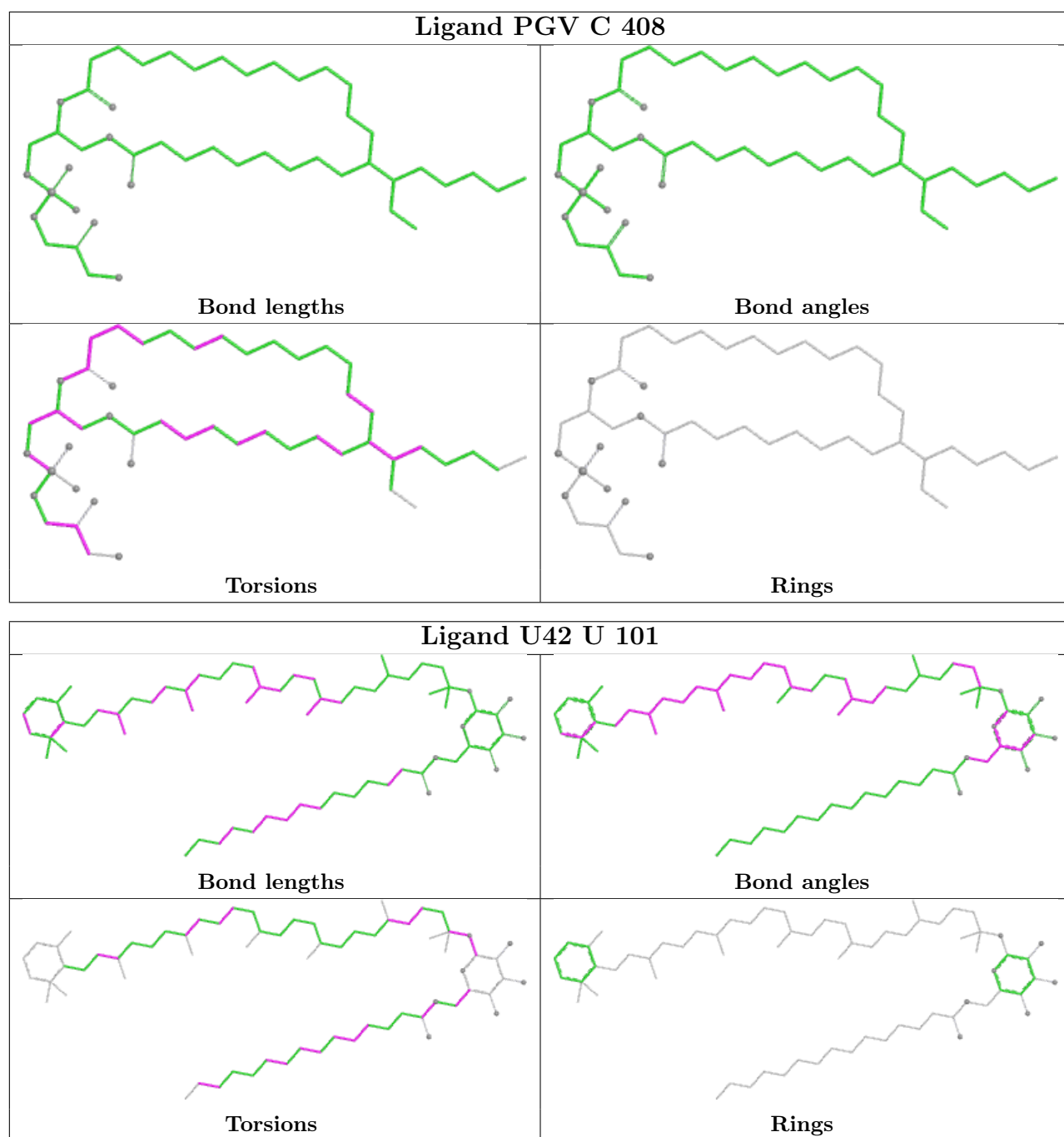


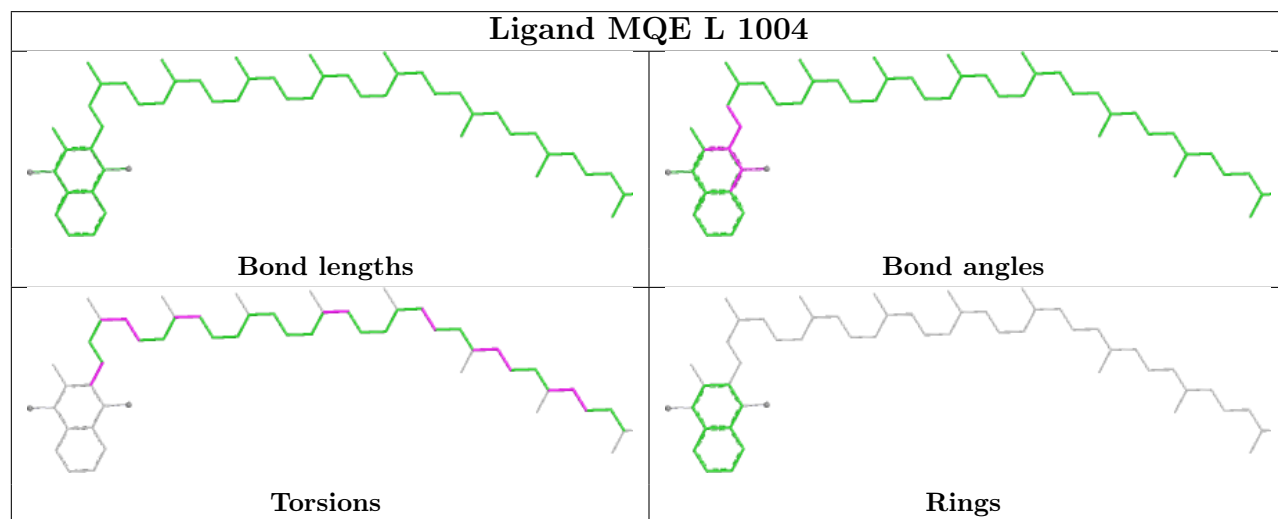
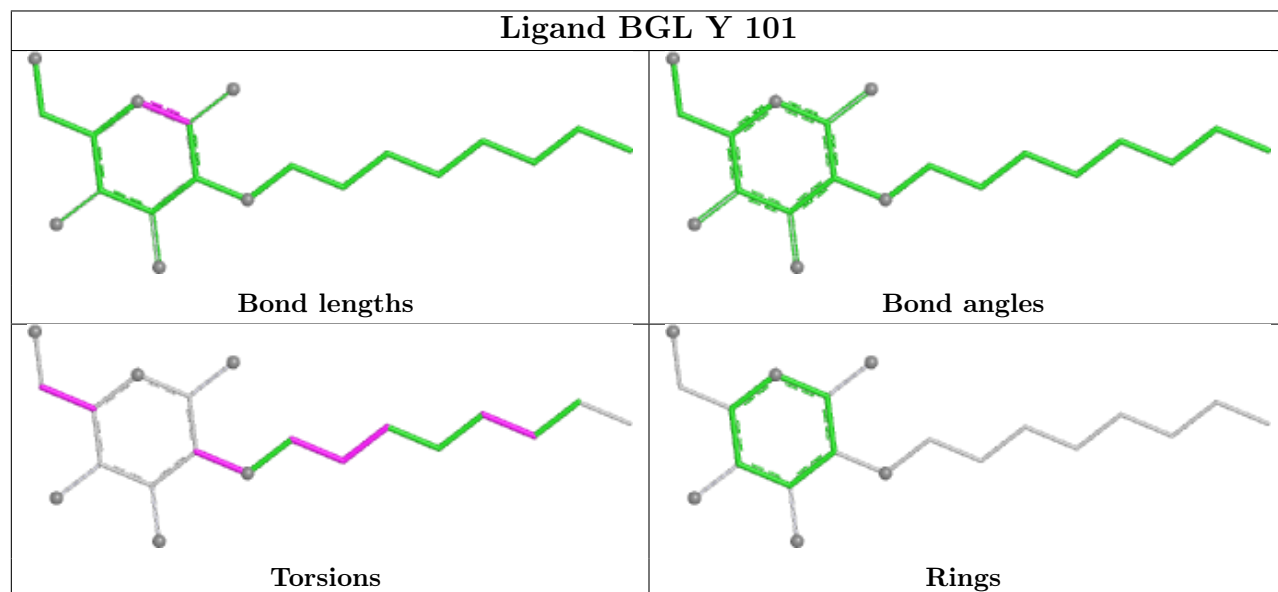
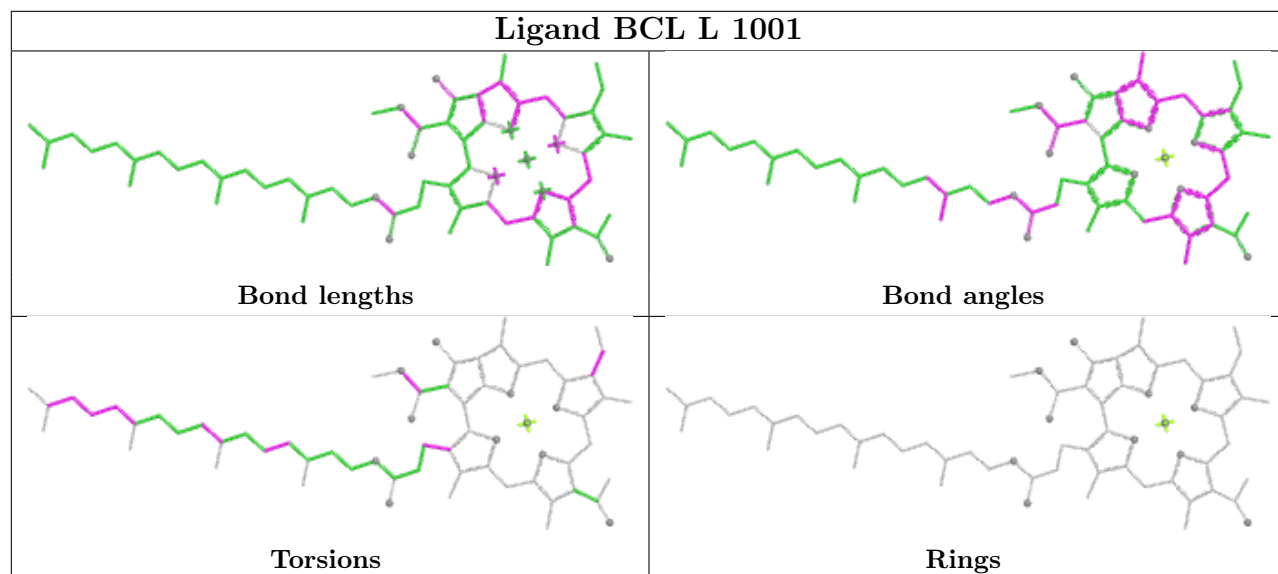


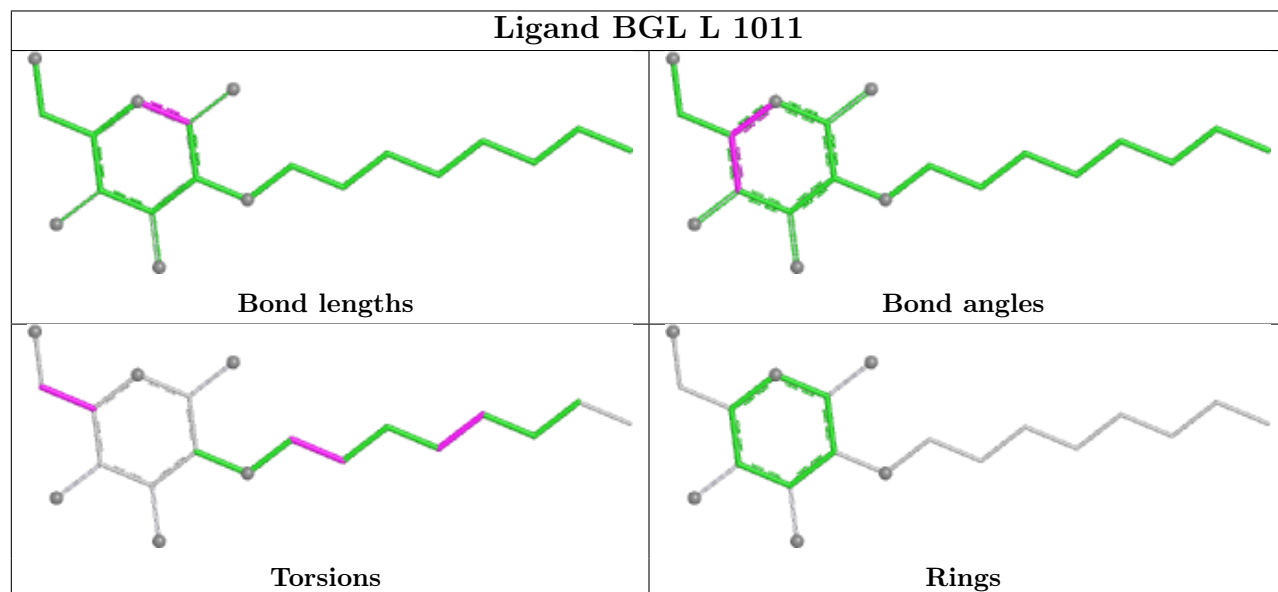
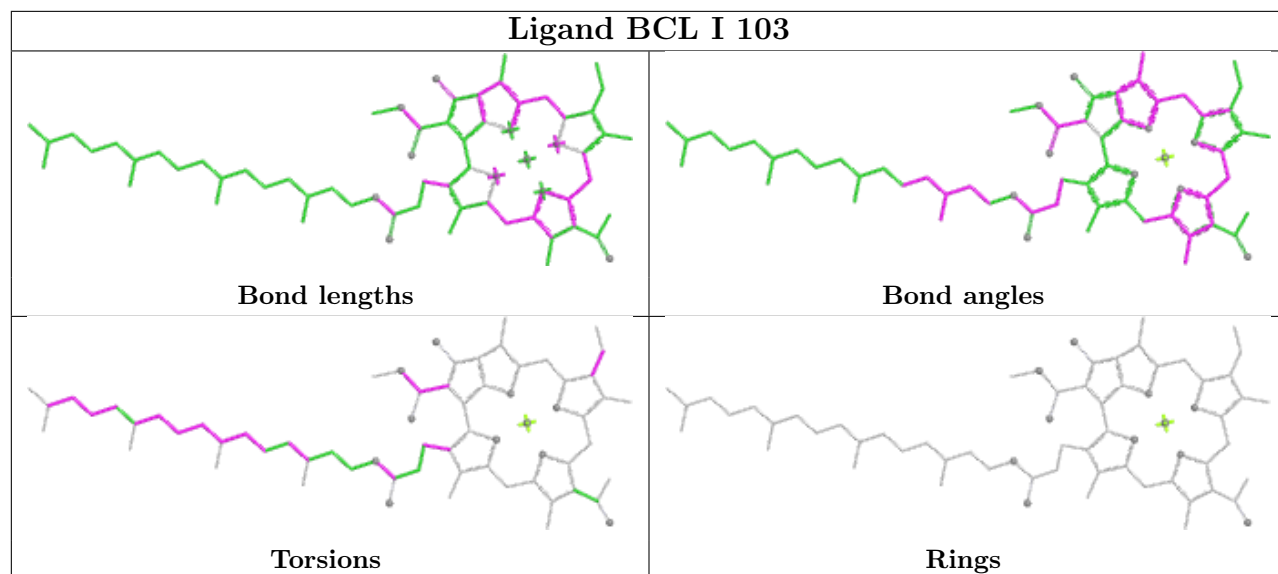


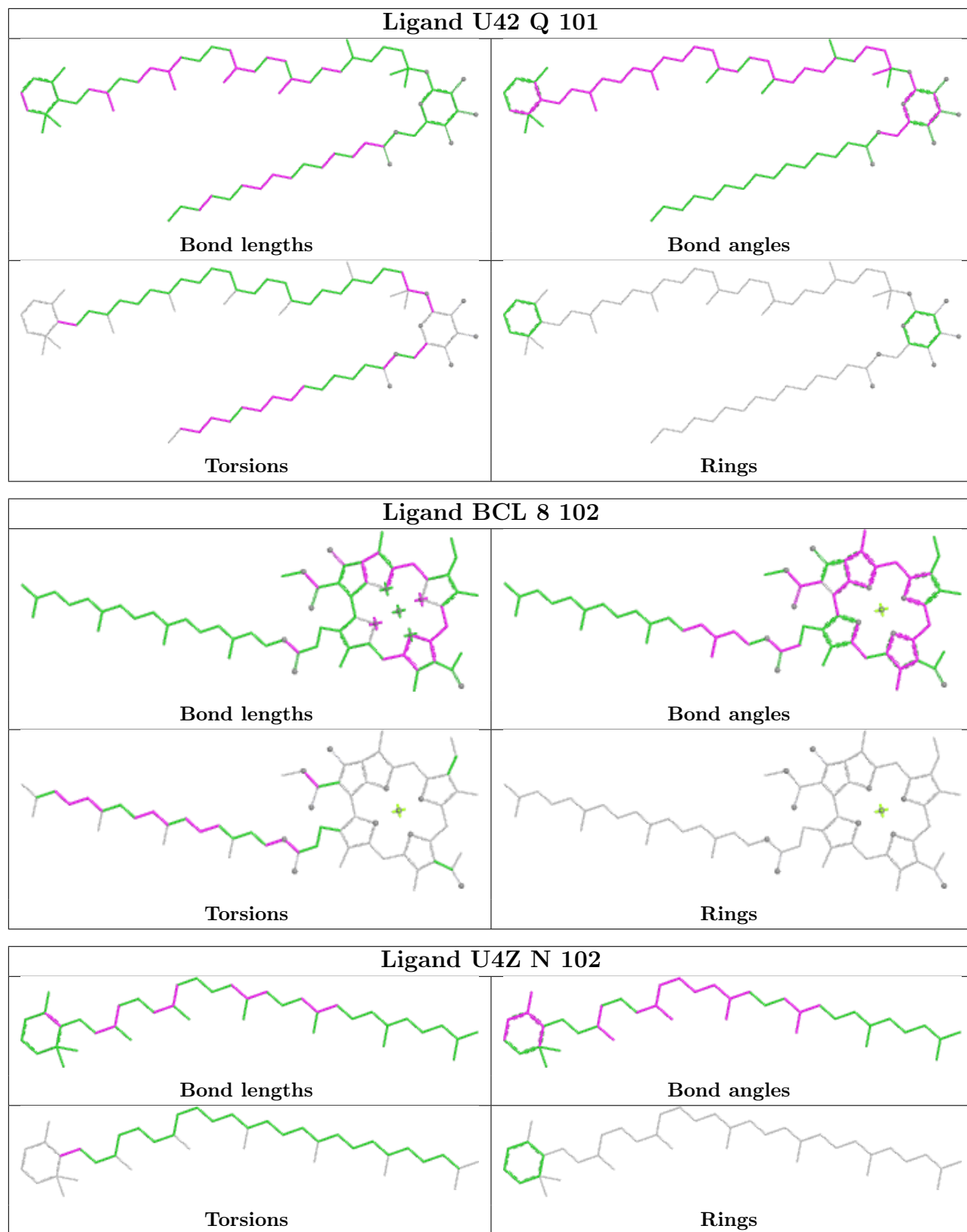


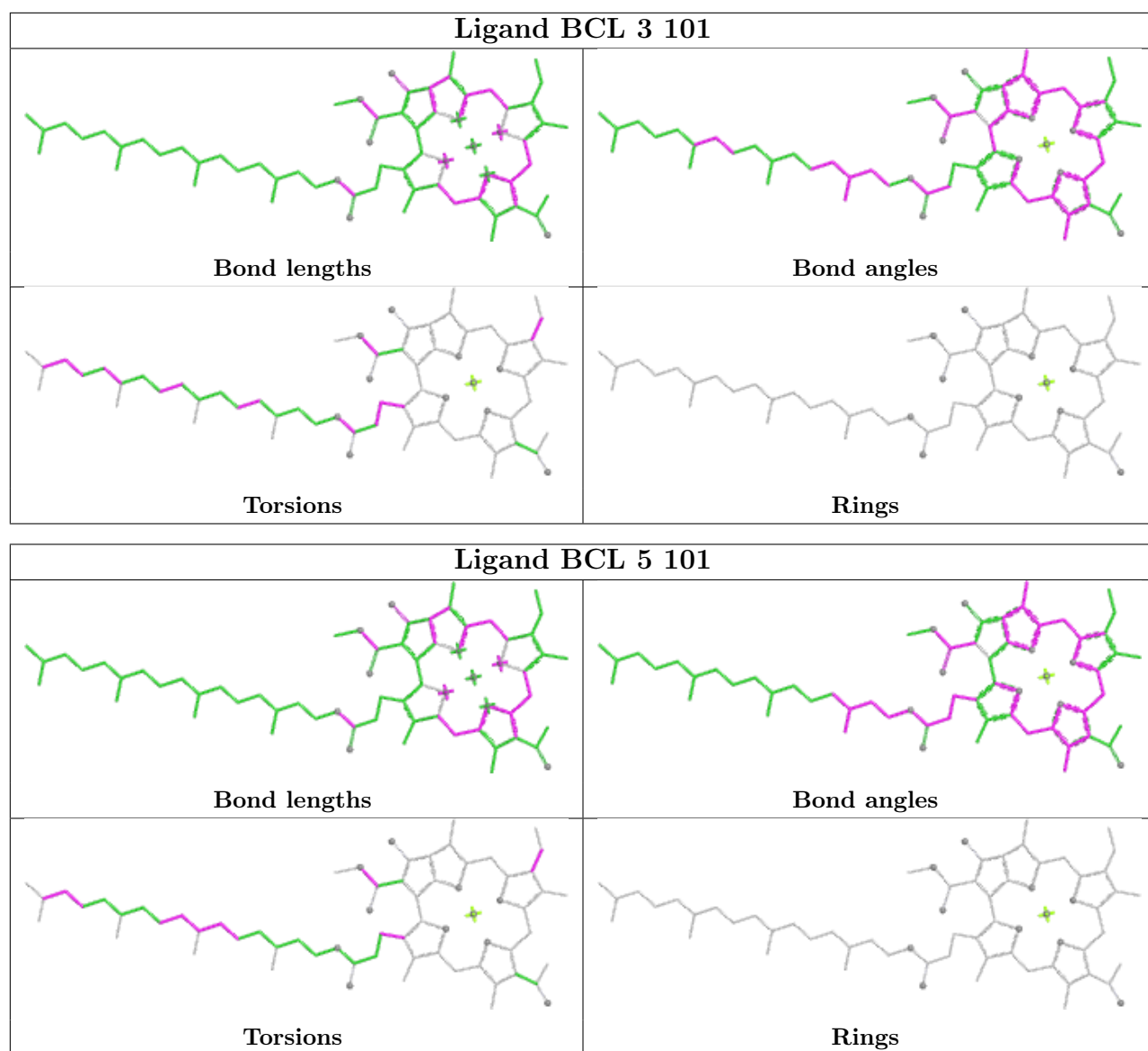


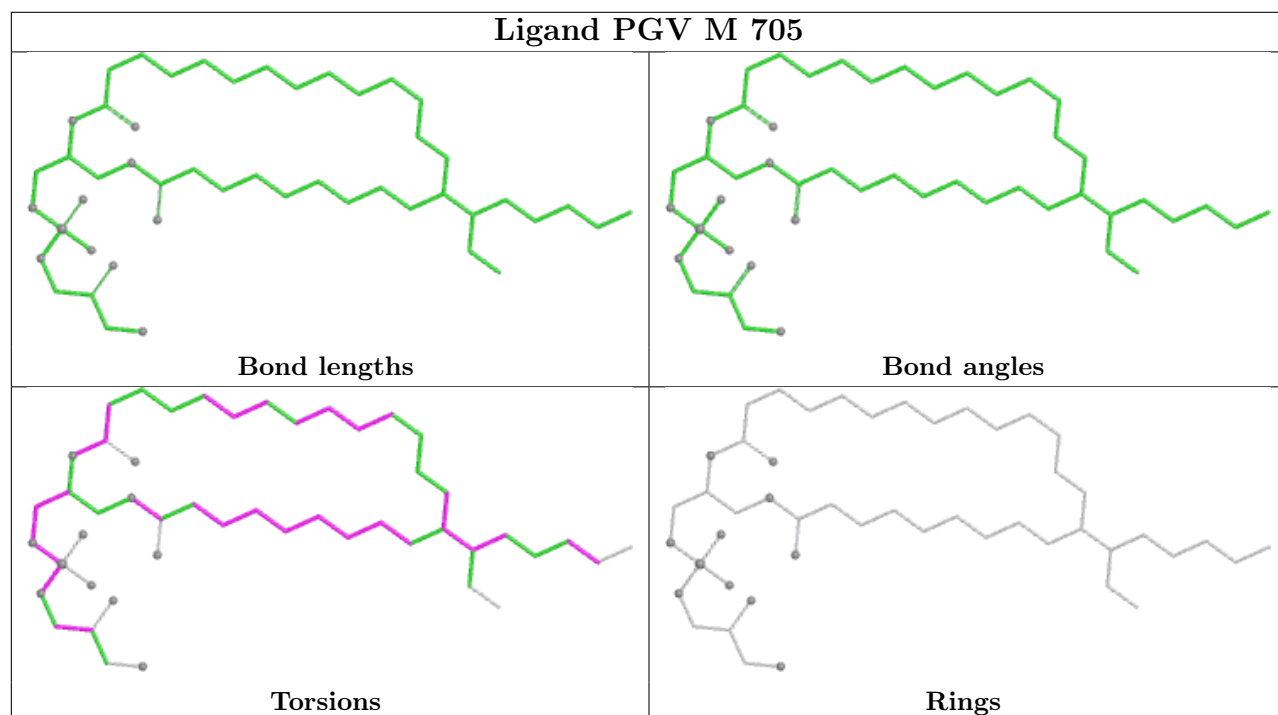
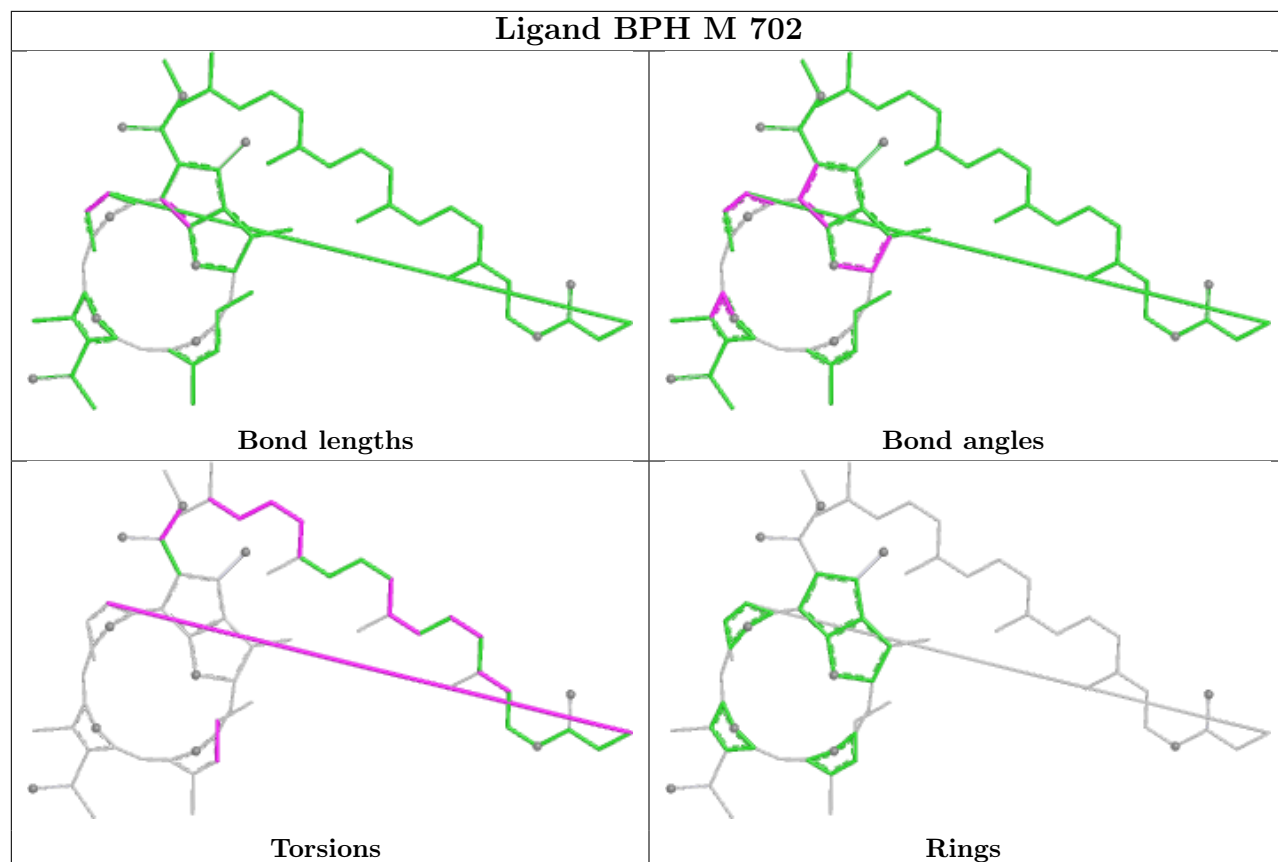


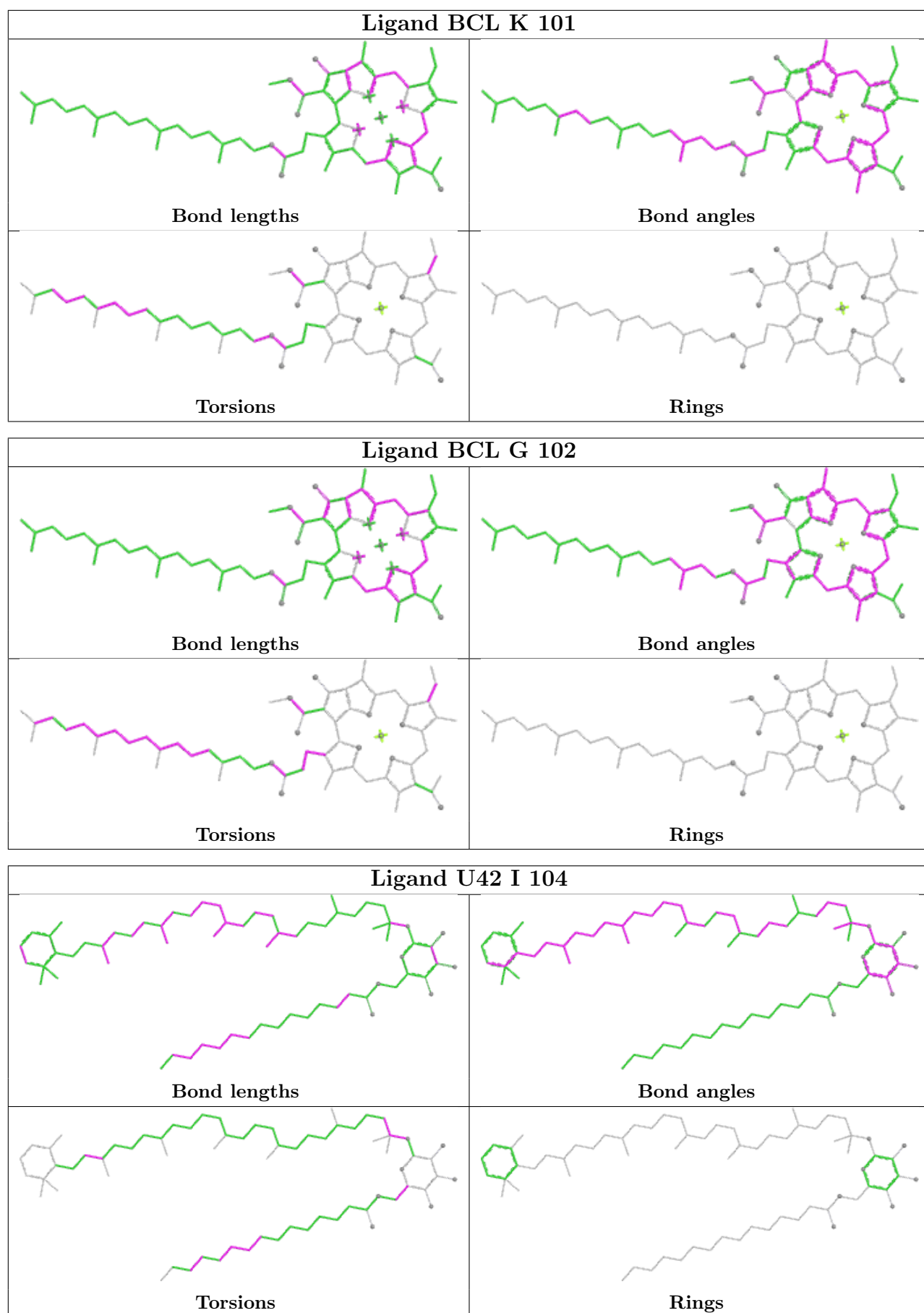


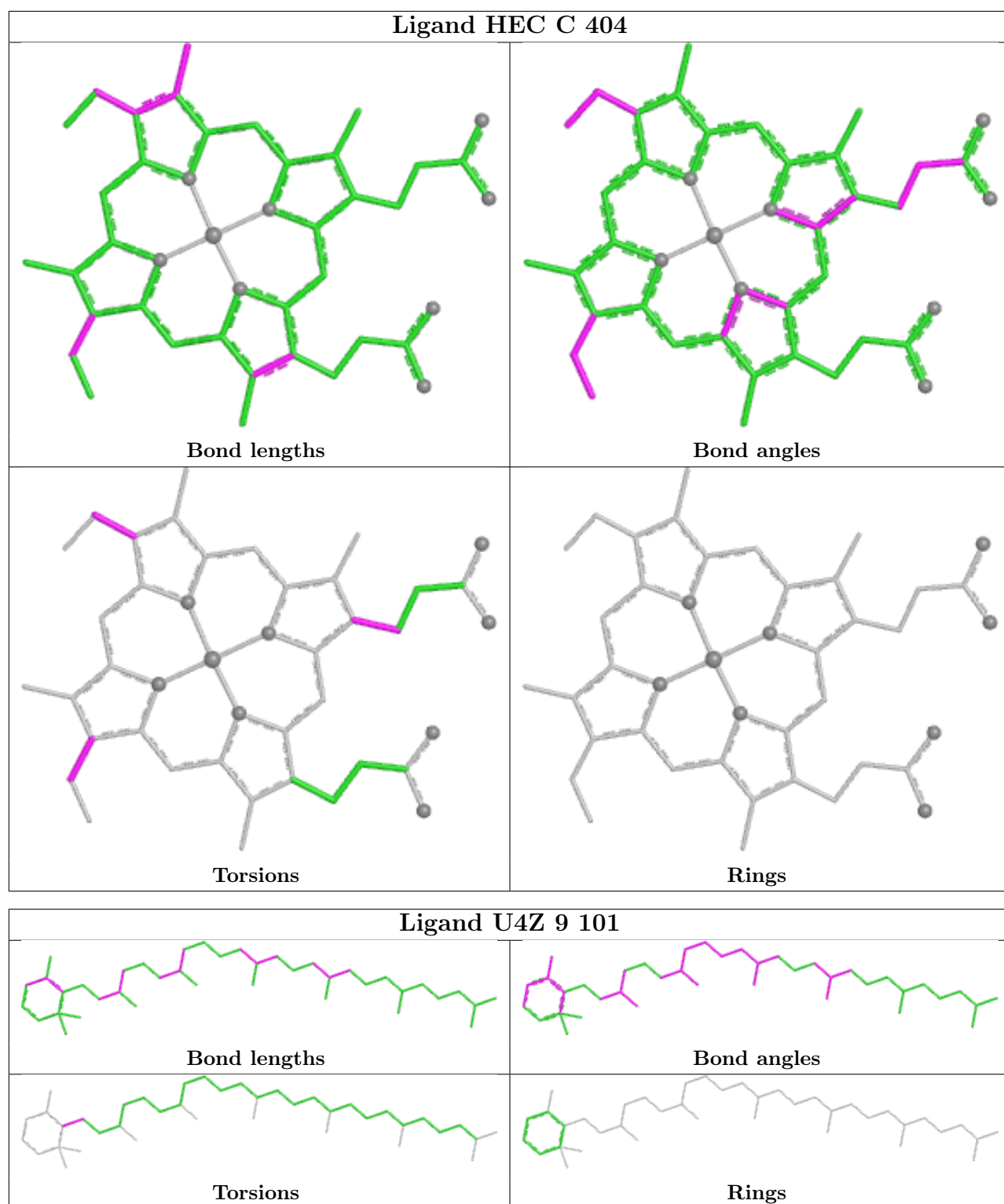


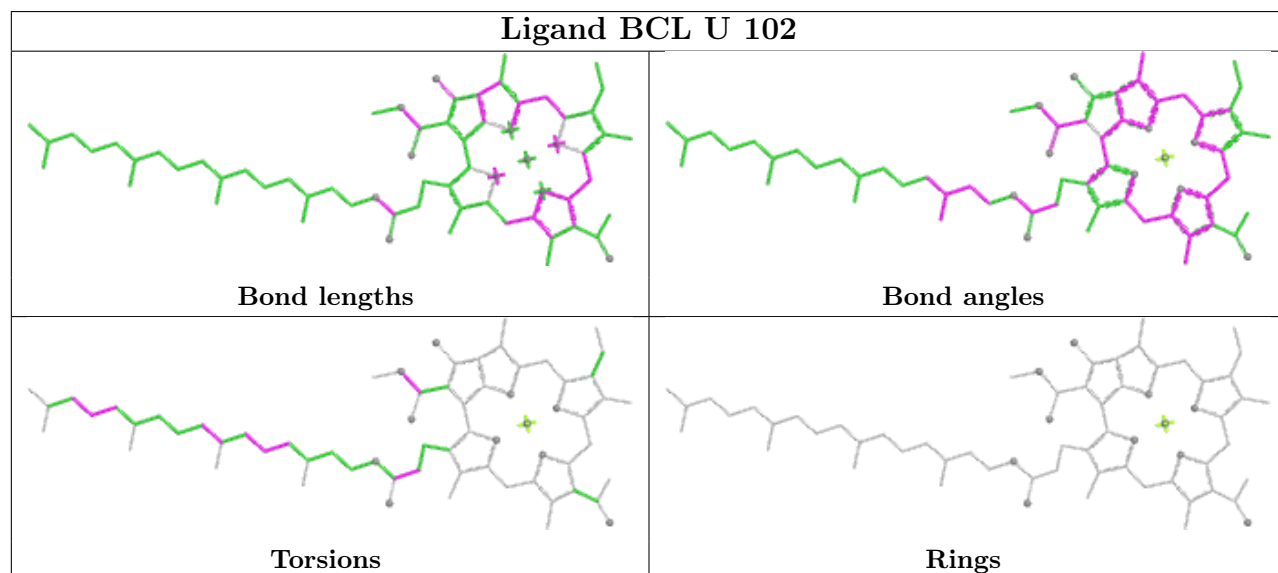
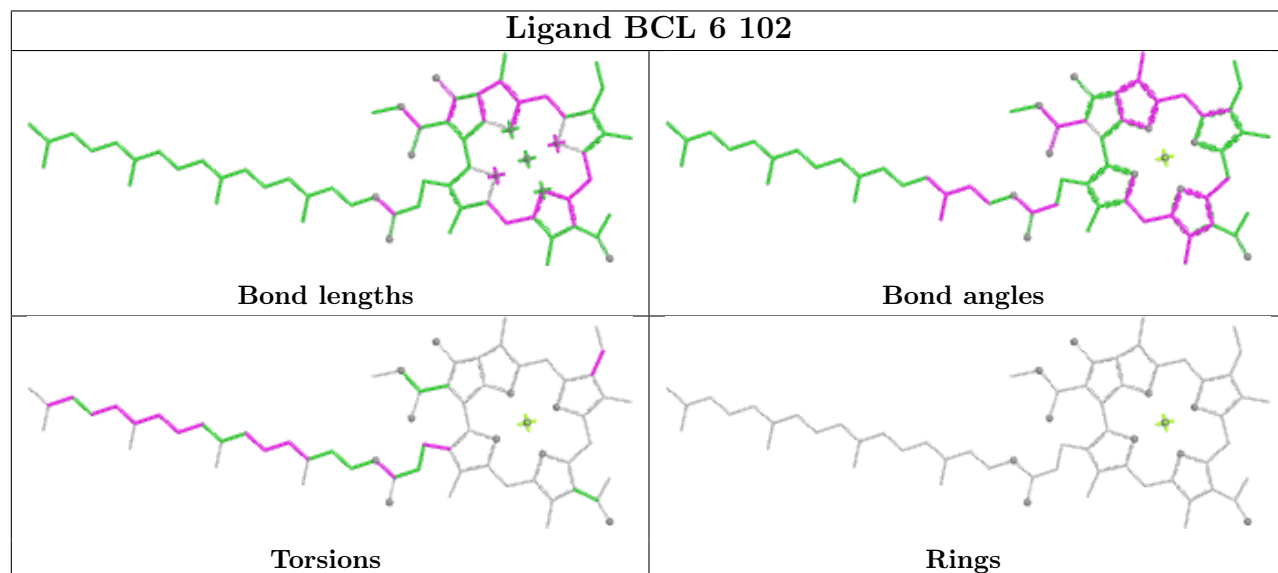
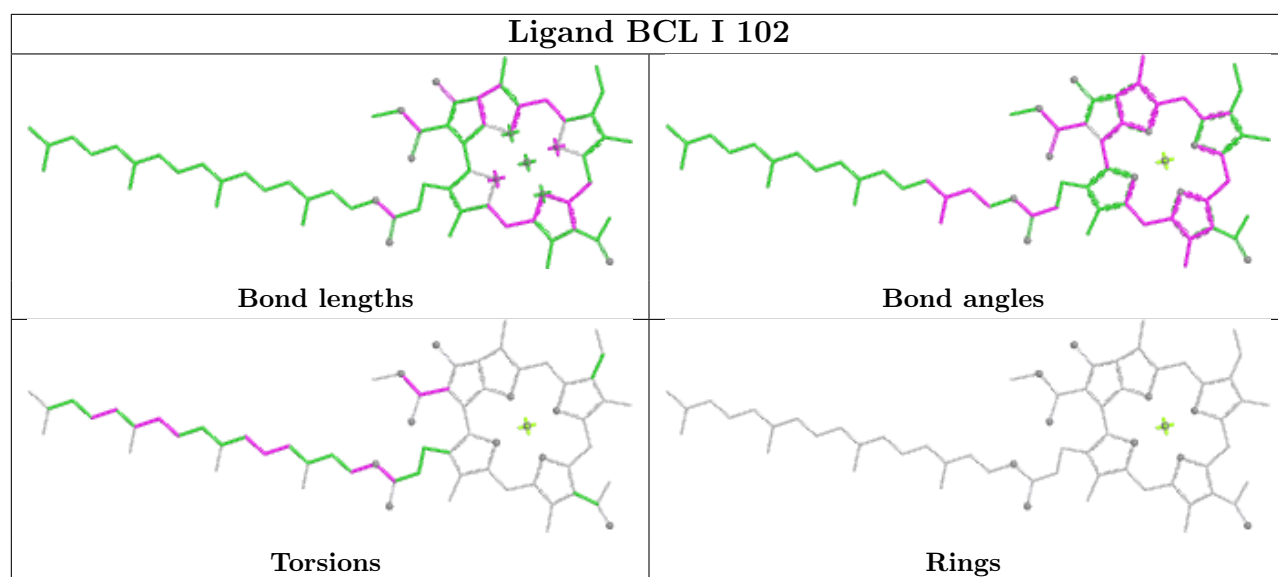


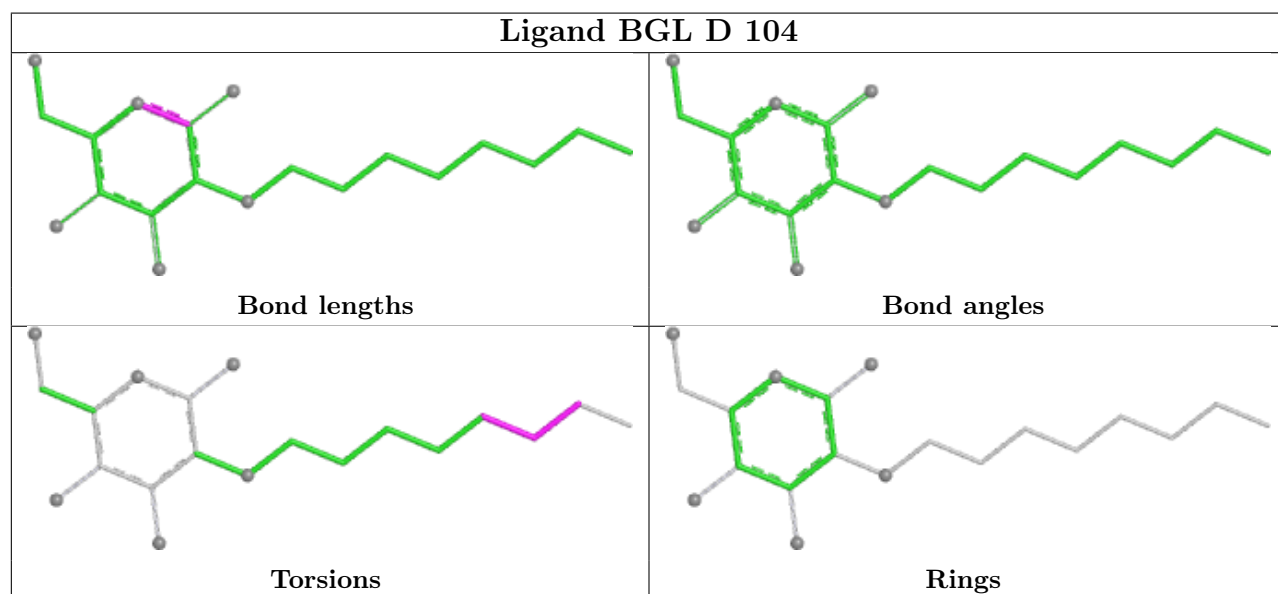
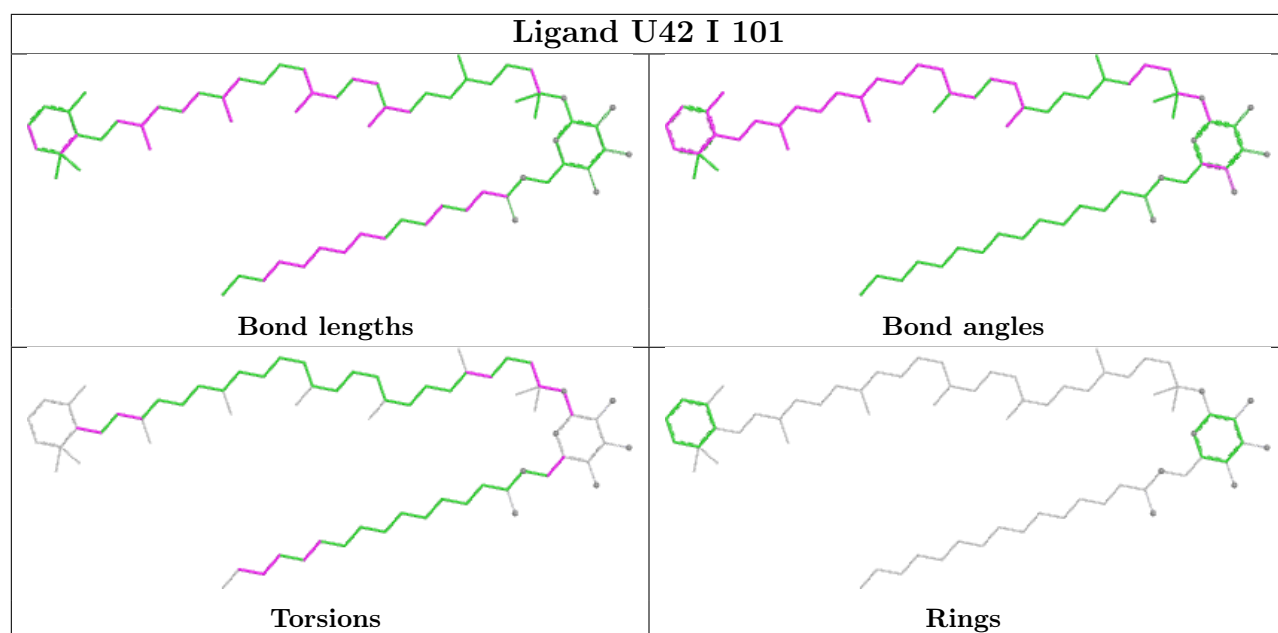


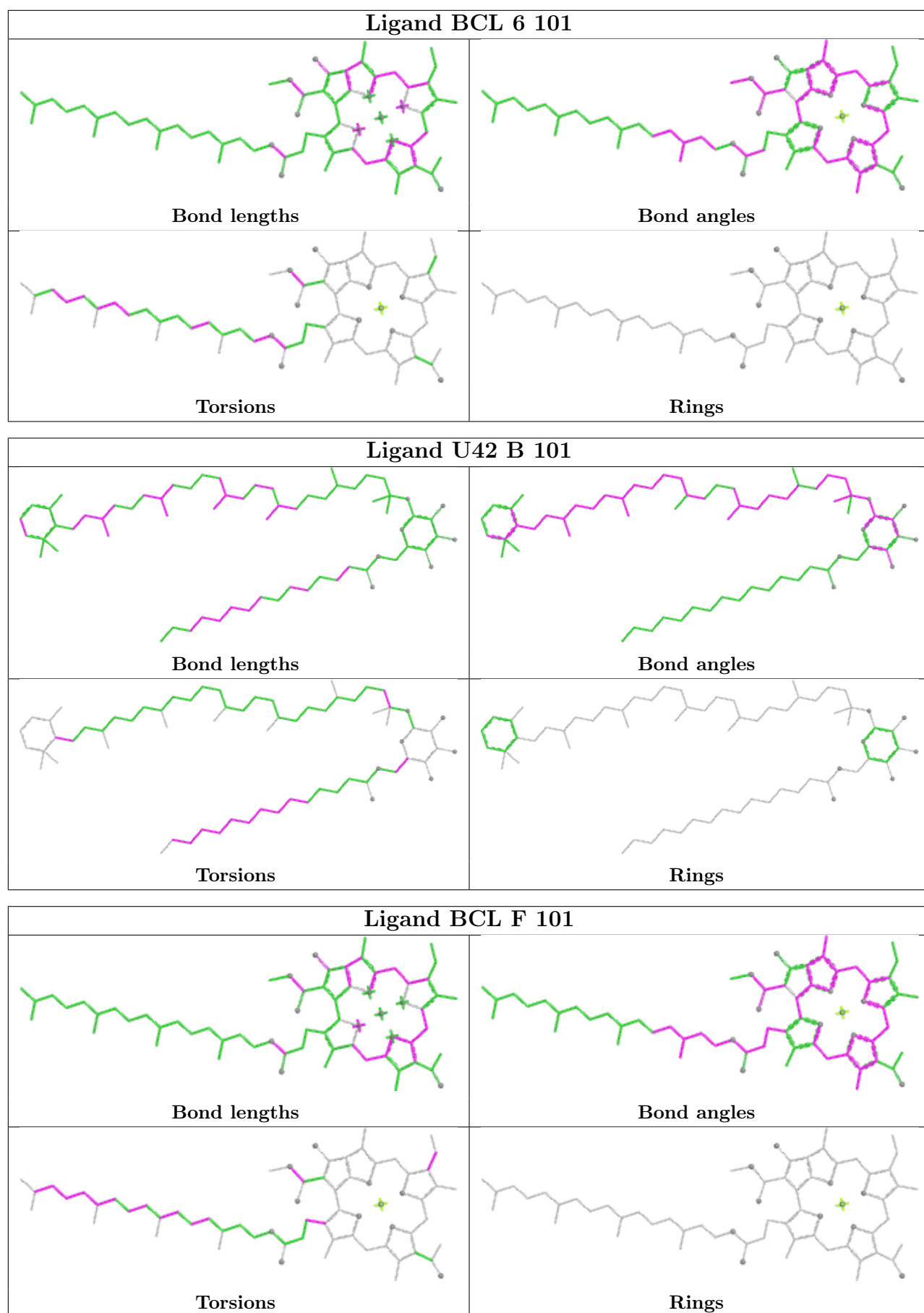




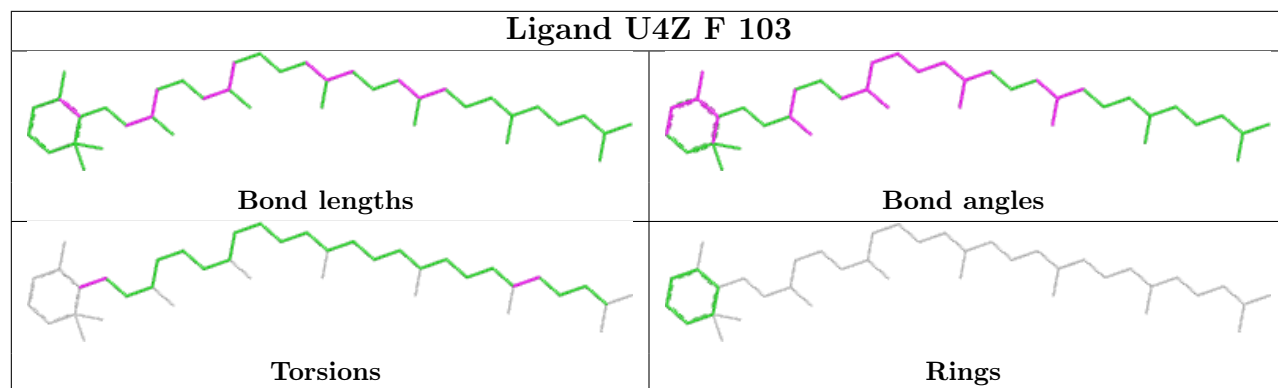




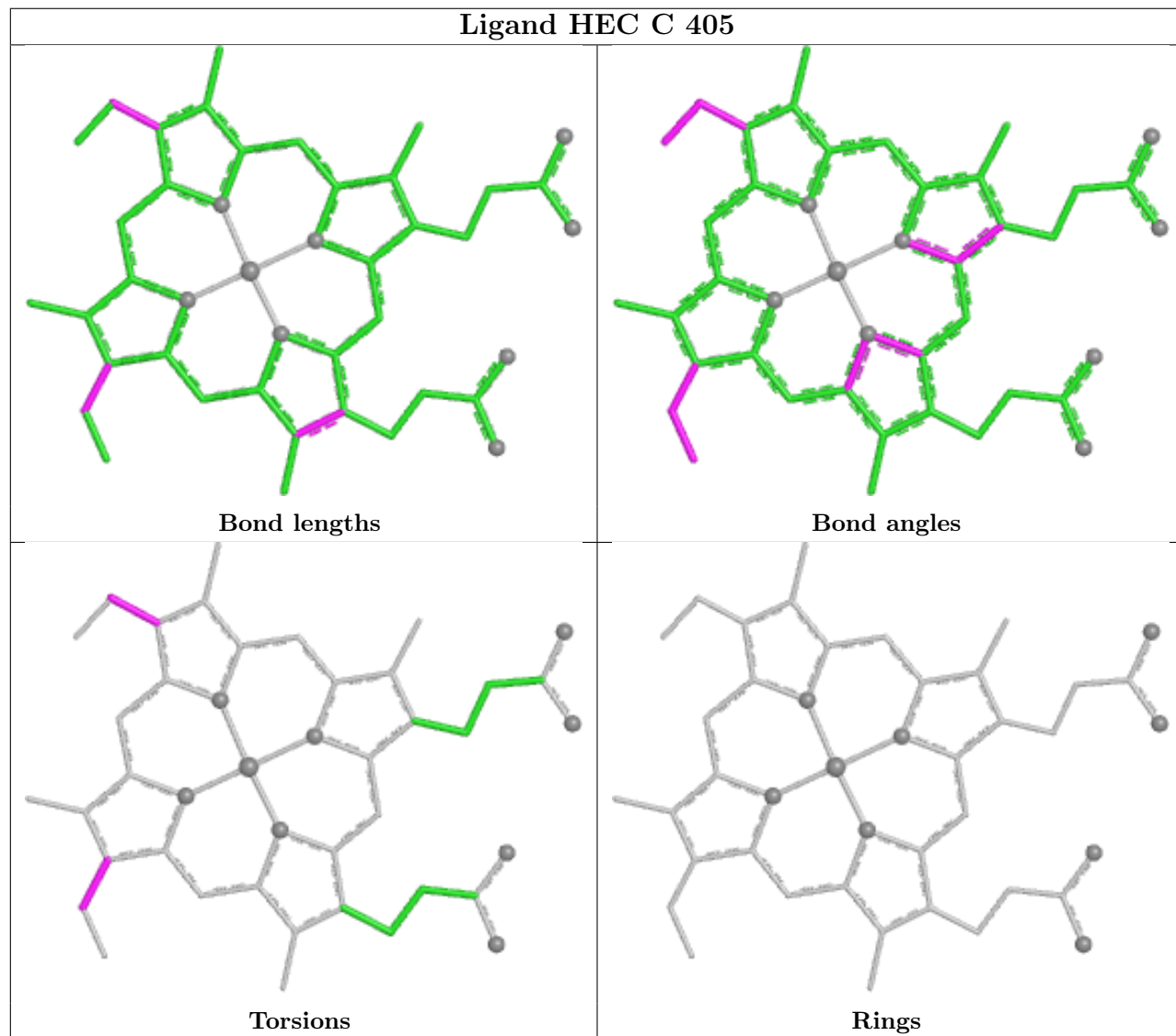


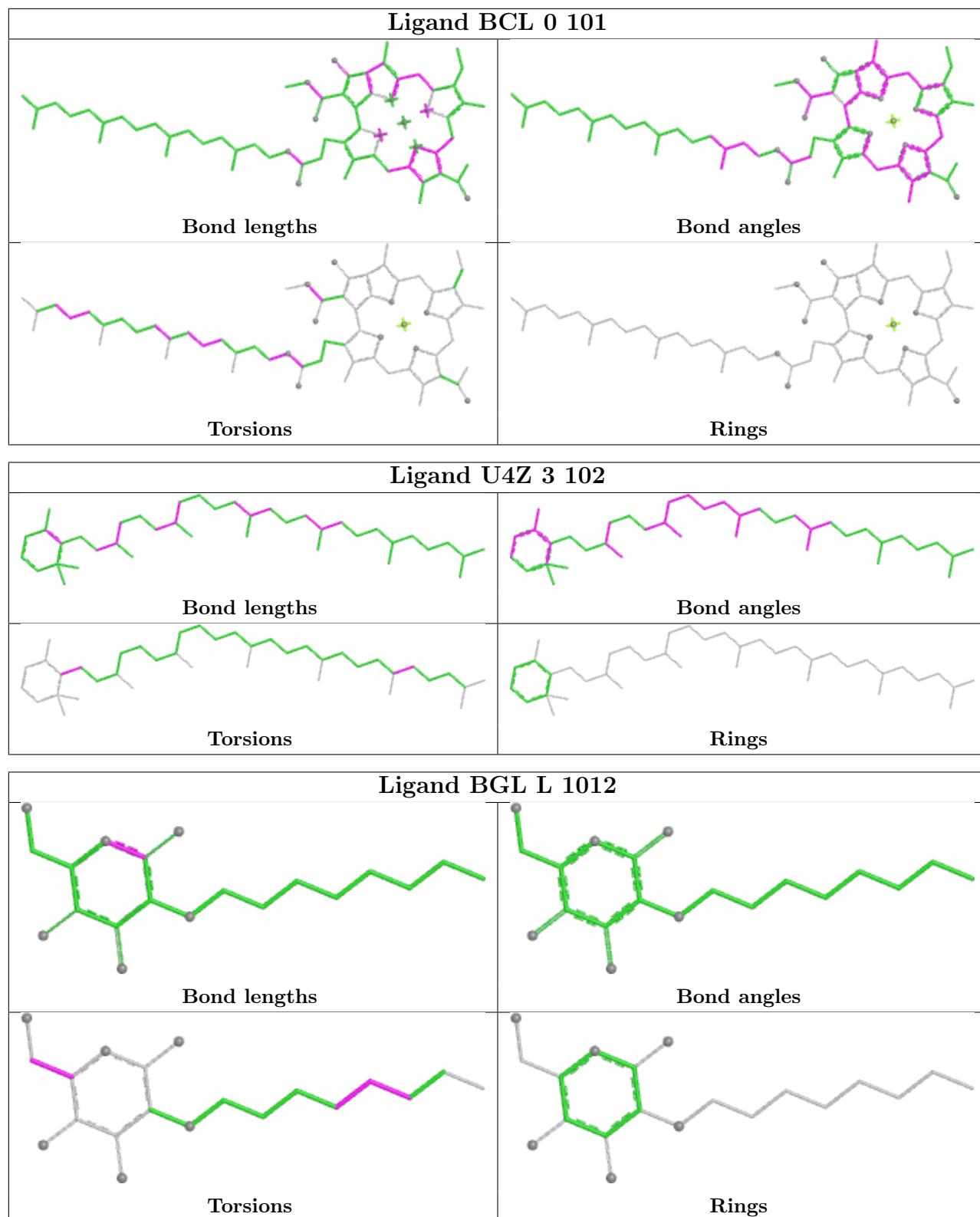


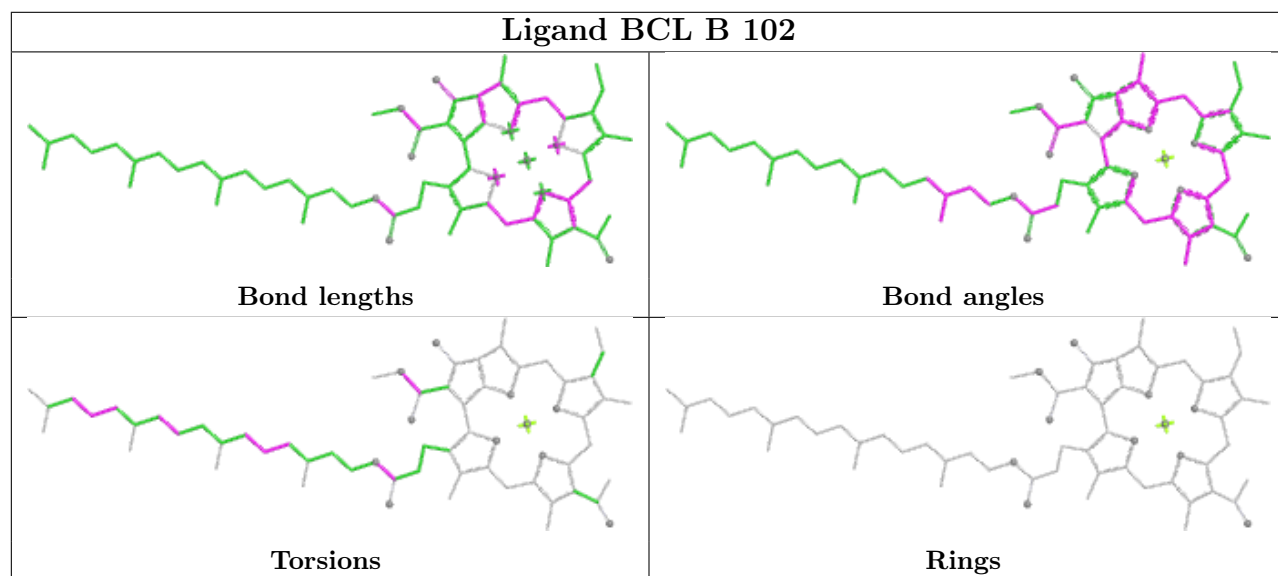
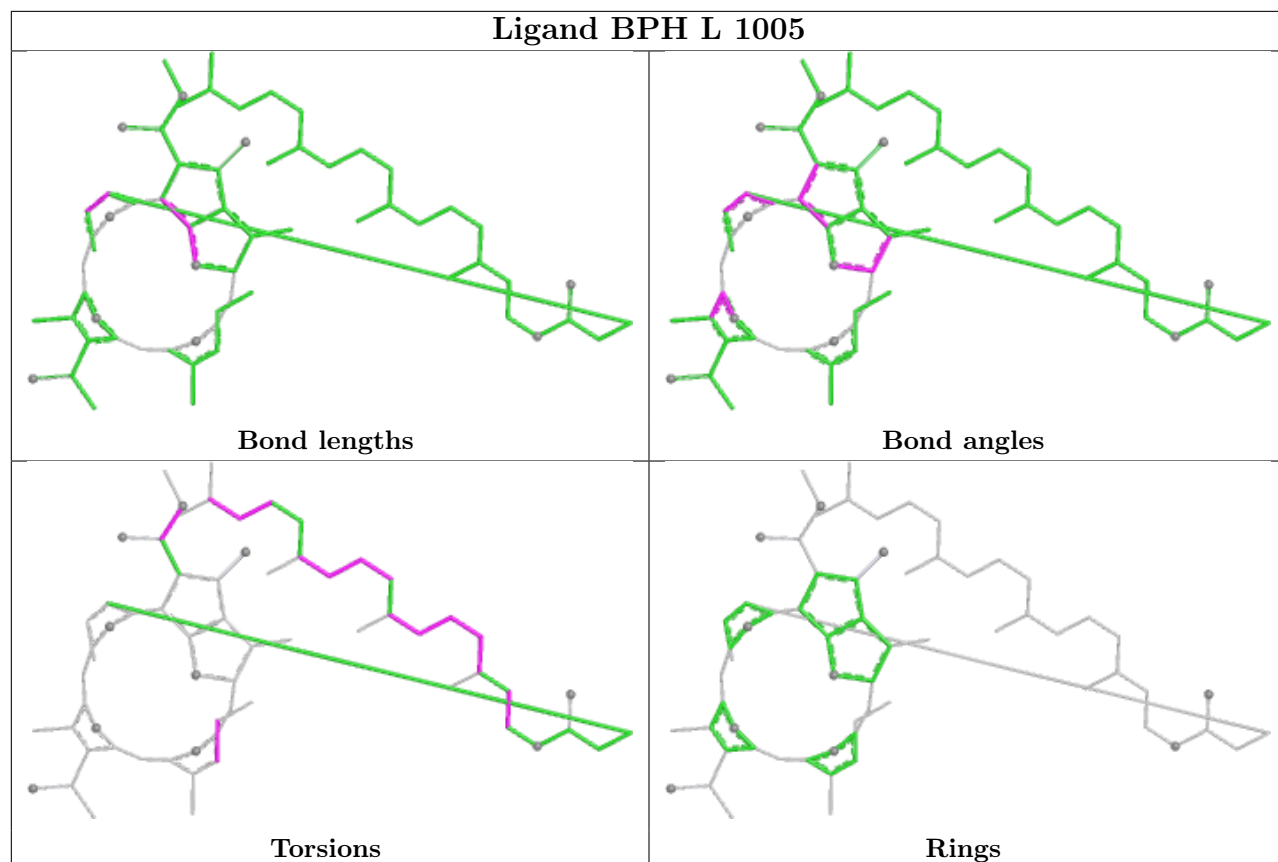
Ligand U4Z F 103



Ligand HEC C 405



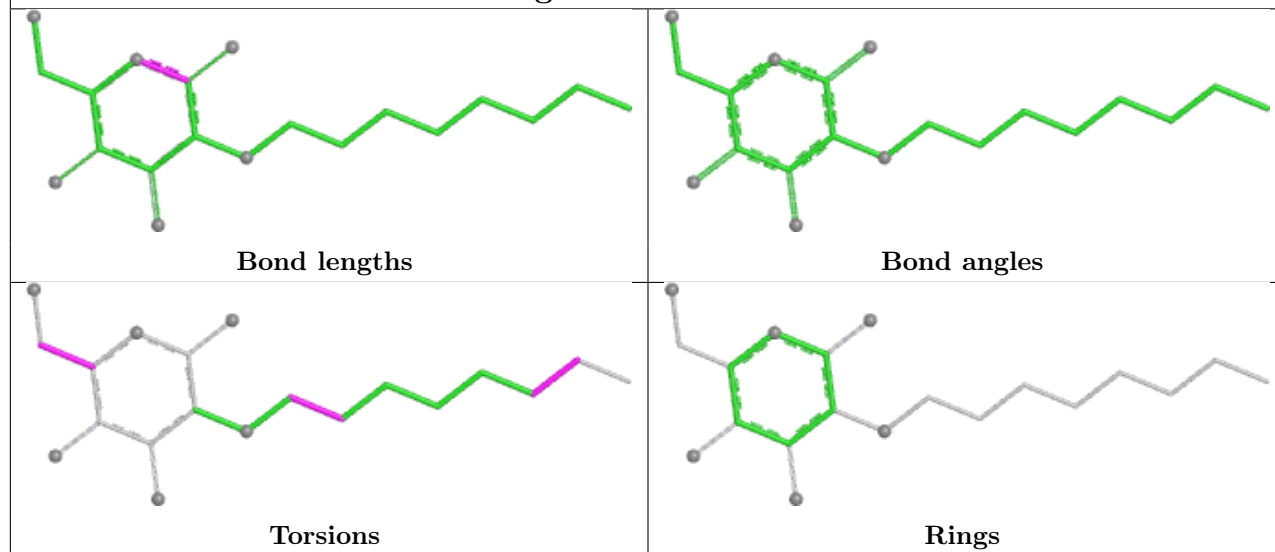




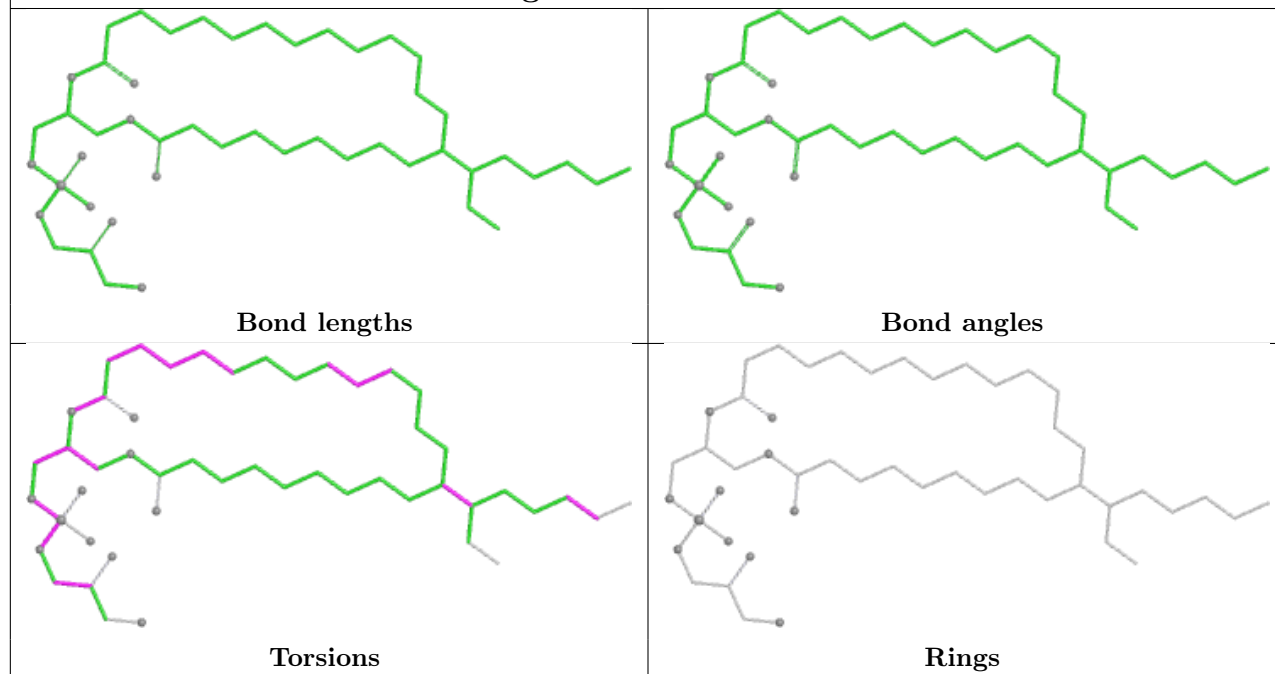
Ligand U4Z D 103

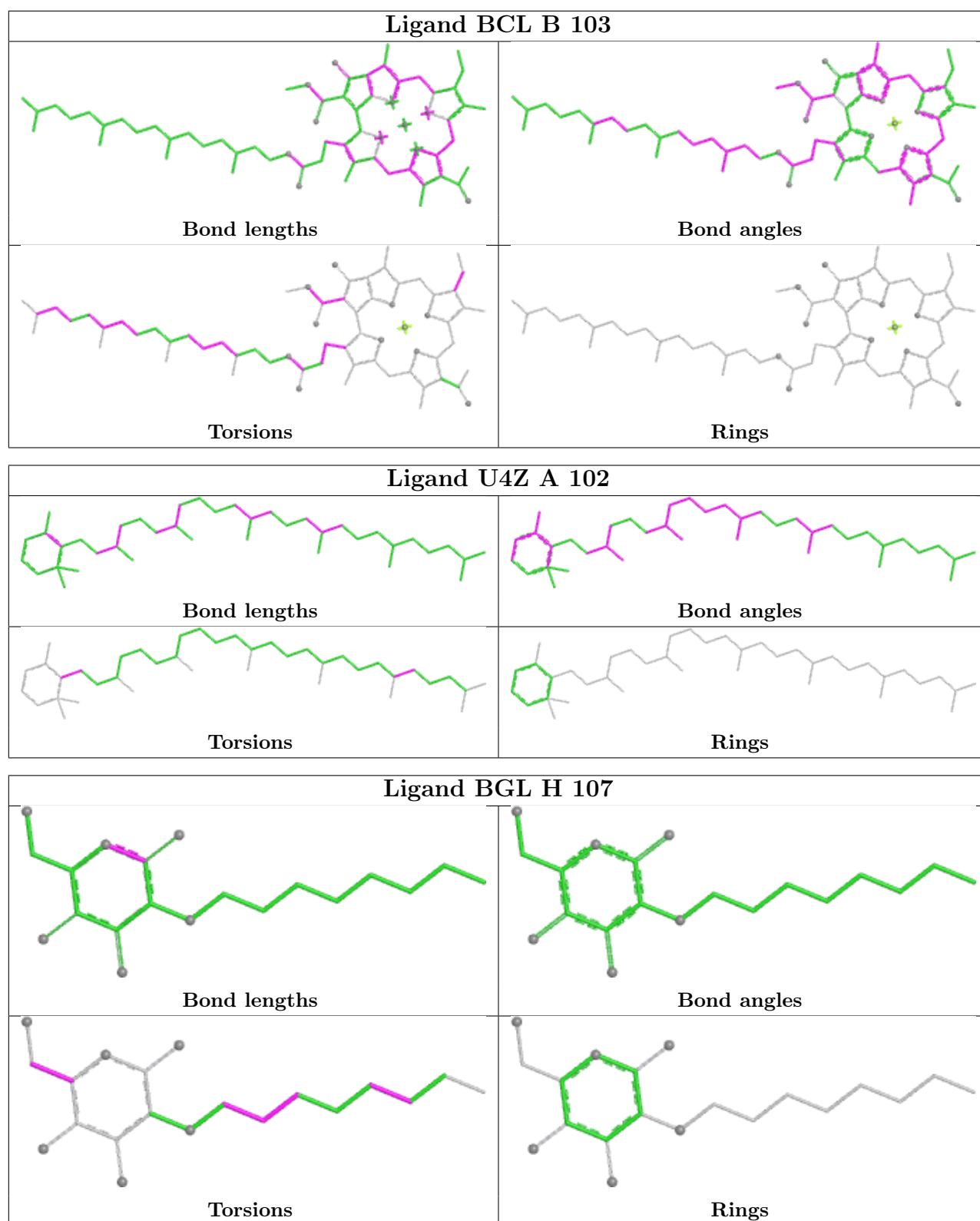


Ligand BGL 3 103



Ligand PGV L 1007





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

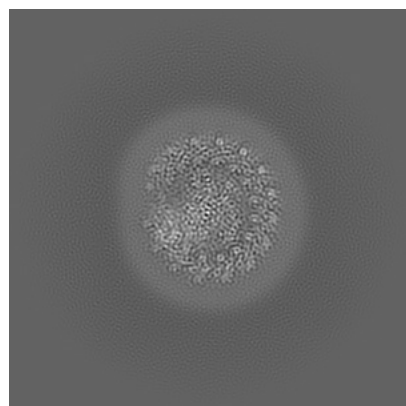
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35721. These allow visual inspection of the internal detail of the map and identification of artifacts.

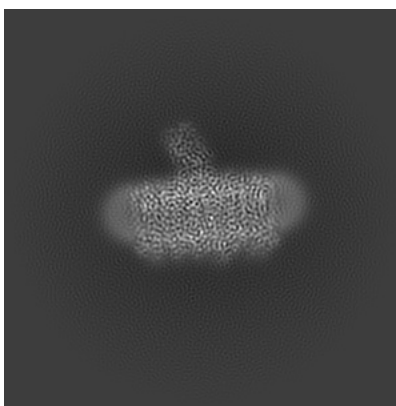
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

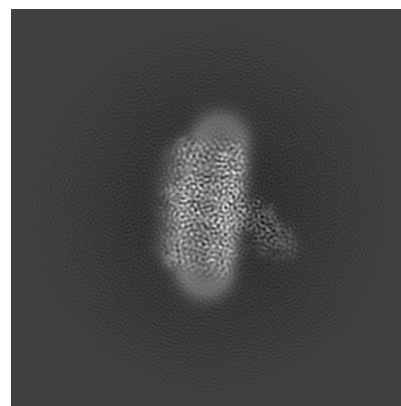
6.1.1 Primary map



X

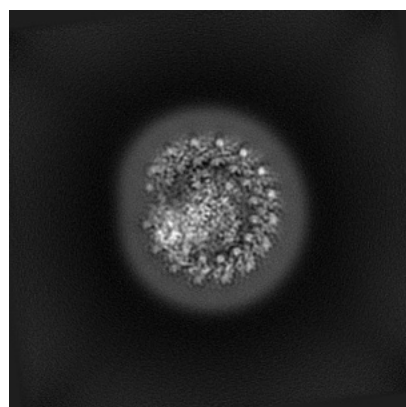


Y

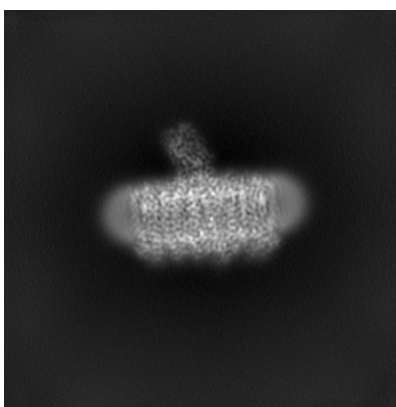


Z

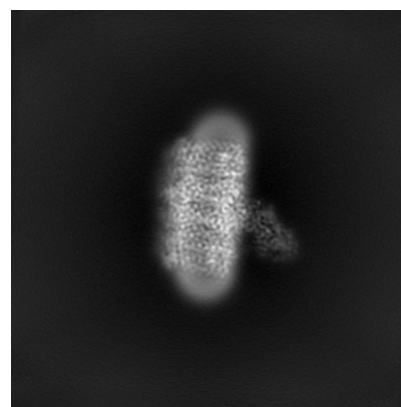
6.1.2 Raw map



X



Y

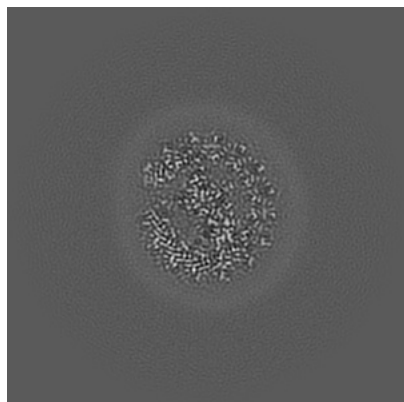


Z

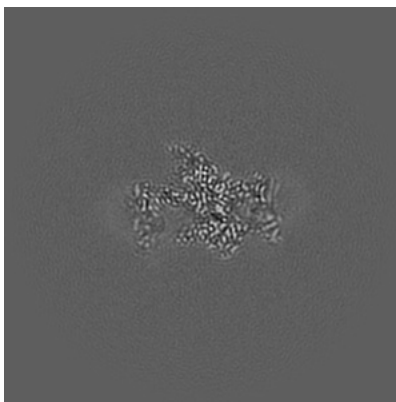
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

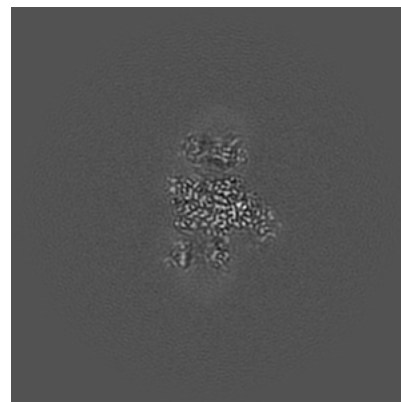
6.2.1 Primary map



X Index: 180

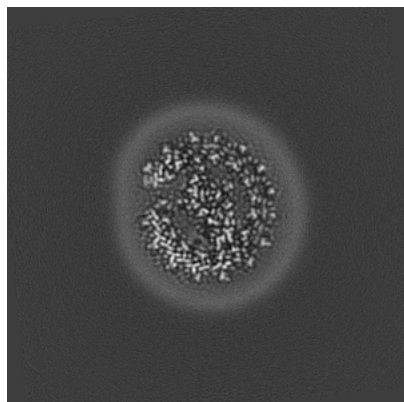


Y Index: 180

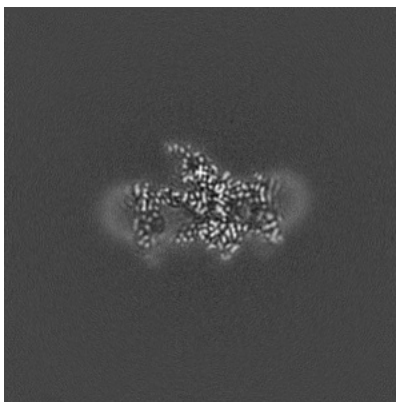


Z Index: 180

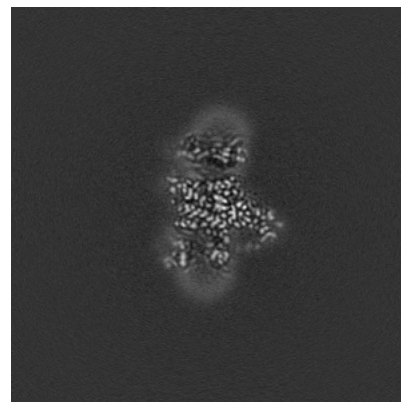
6.2.2 Raw map



X Index: 180



Y Index: 180

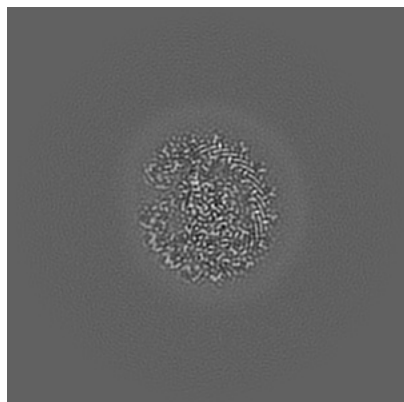


Z Index: 180

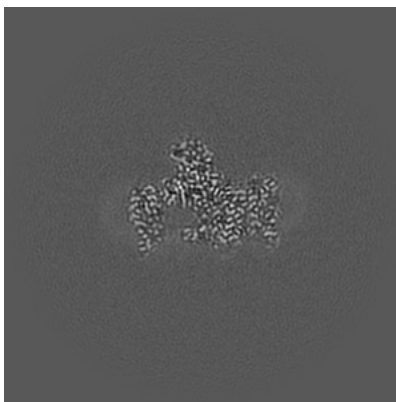
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

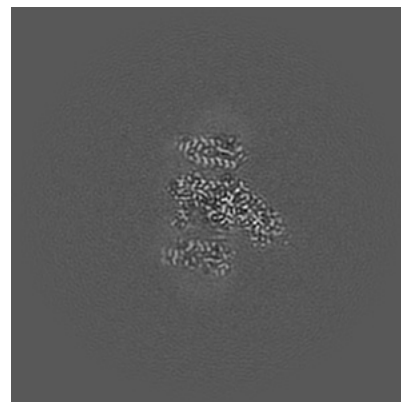
6.3.1 Primary map



X Index: 192

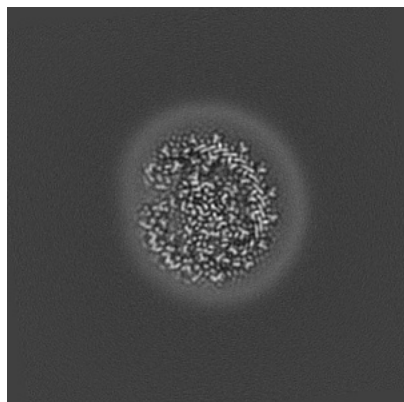


Y Index: 171

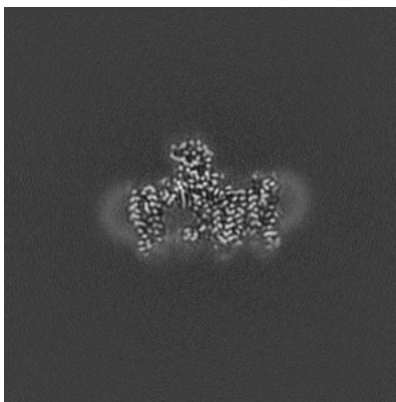


Z Index: 173

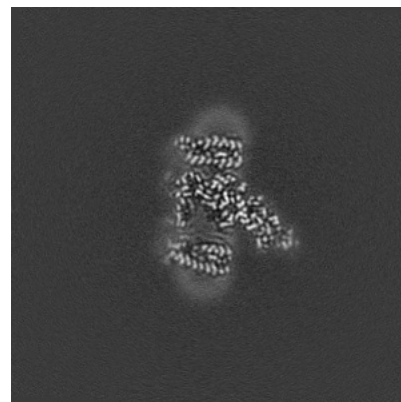
6.3.2 Raw map



X Index: 192



Y Index: 171

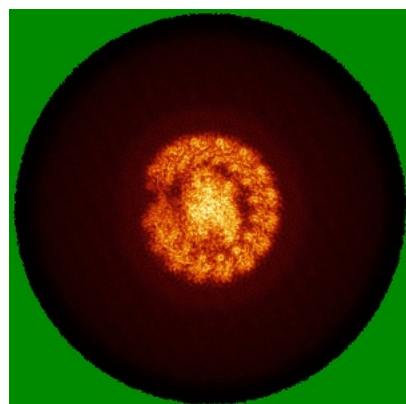


Z Index: 169

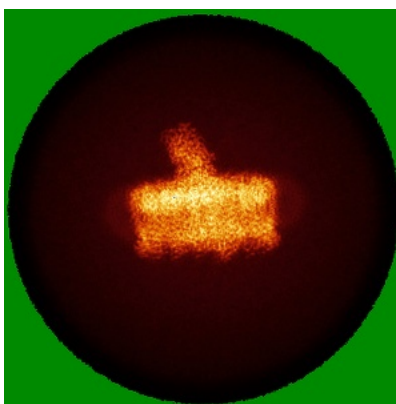
The images above show the largest variance slices of the map in three orthogonal directions.

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

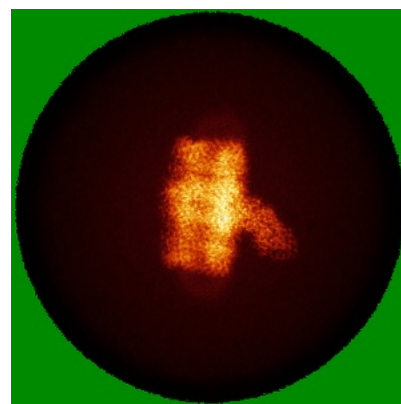
6.4.1 Primary map



X

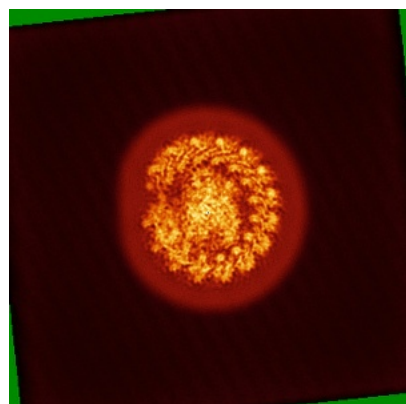


Y

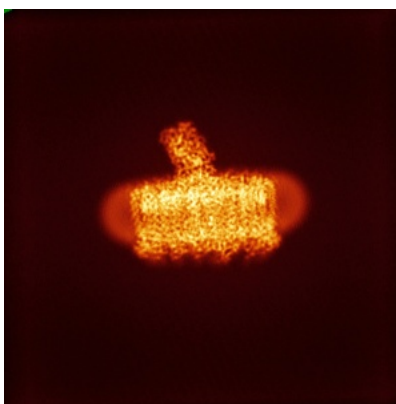


Z

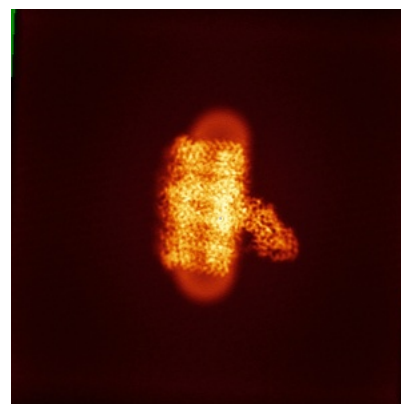
6.4.2 Raw map



X



Y

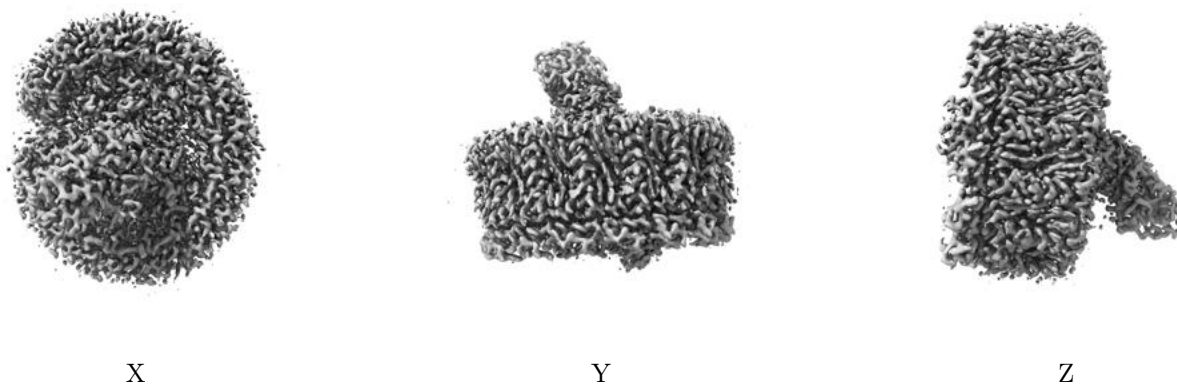


Z

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.

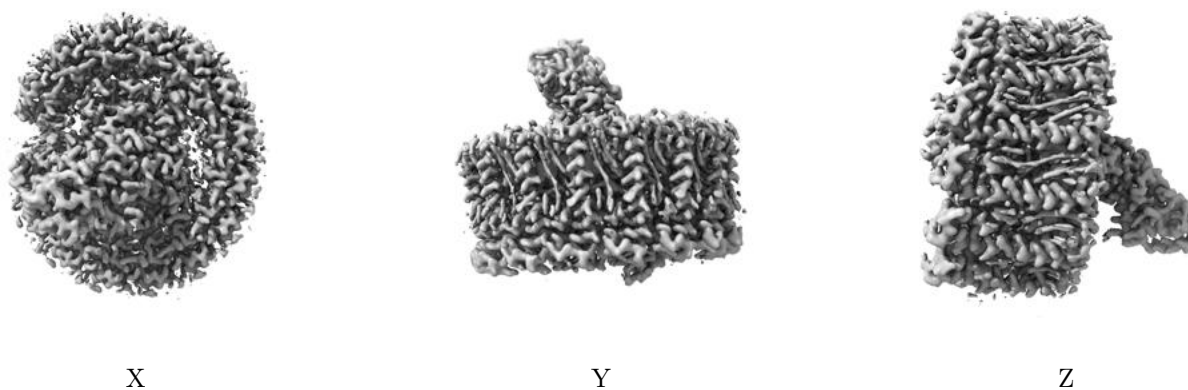
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.226. 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.

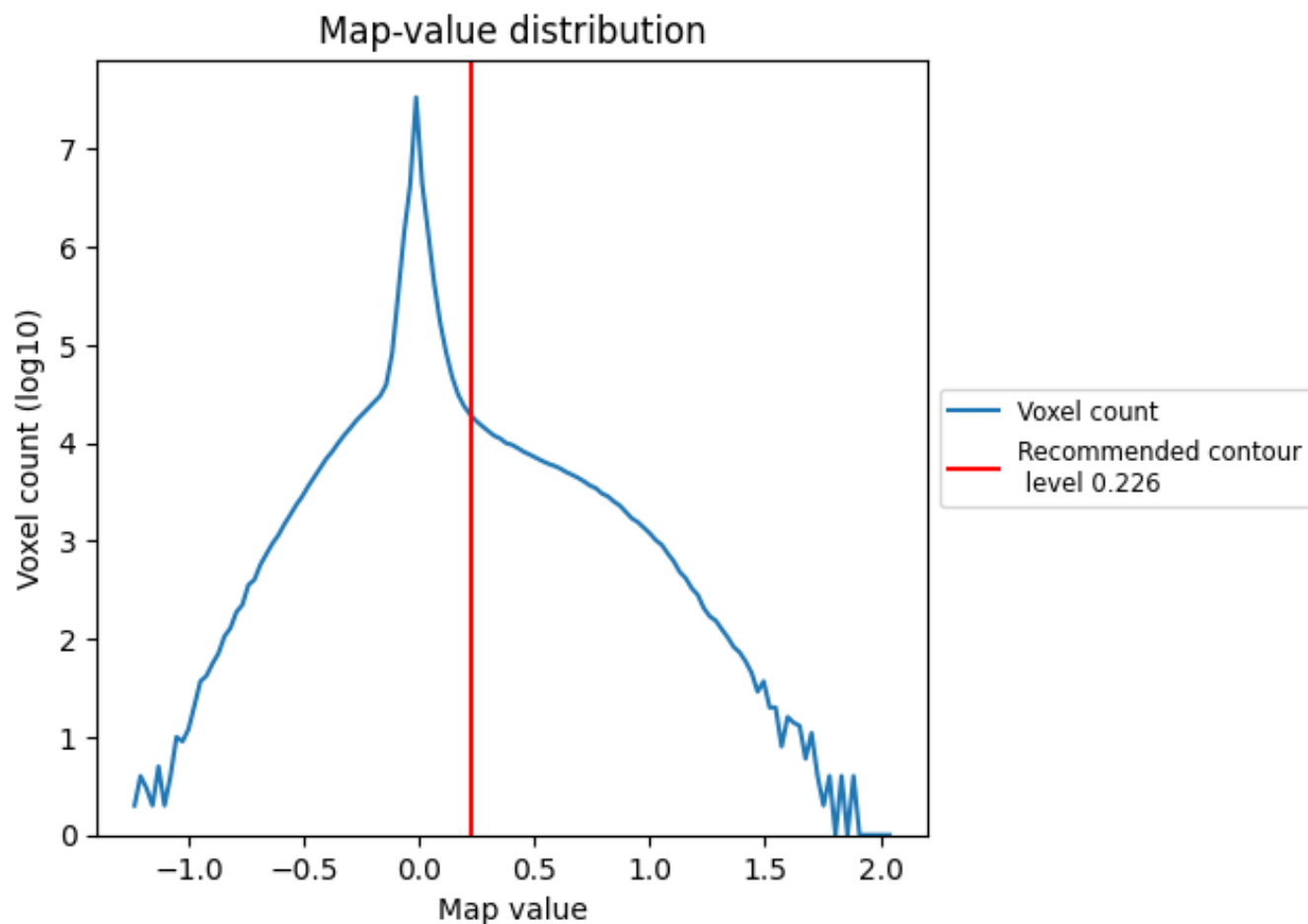
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

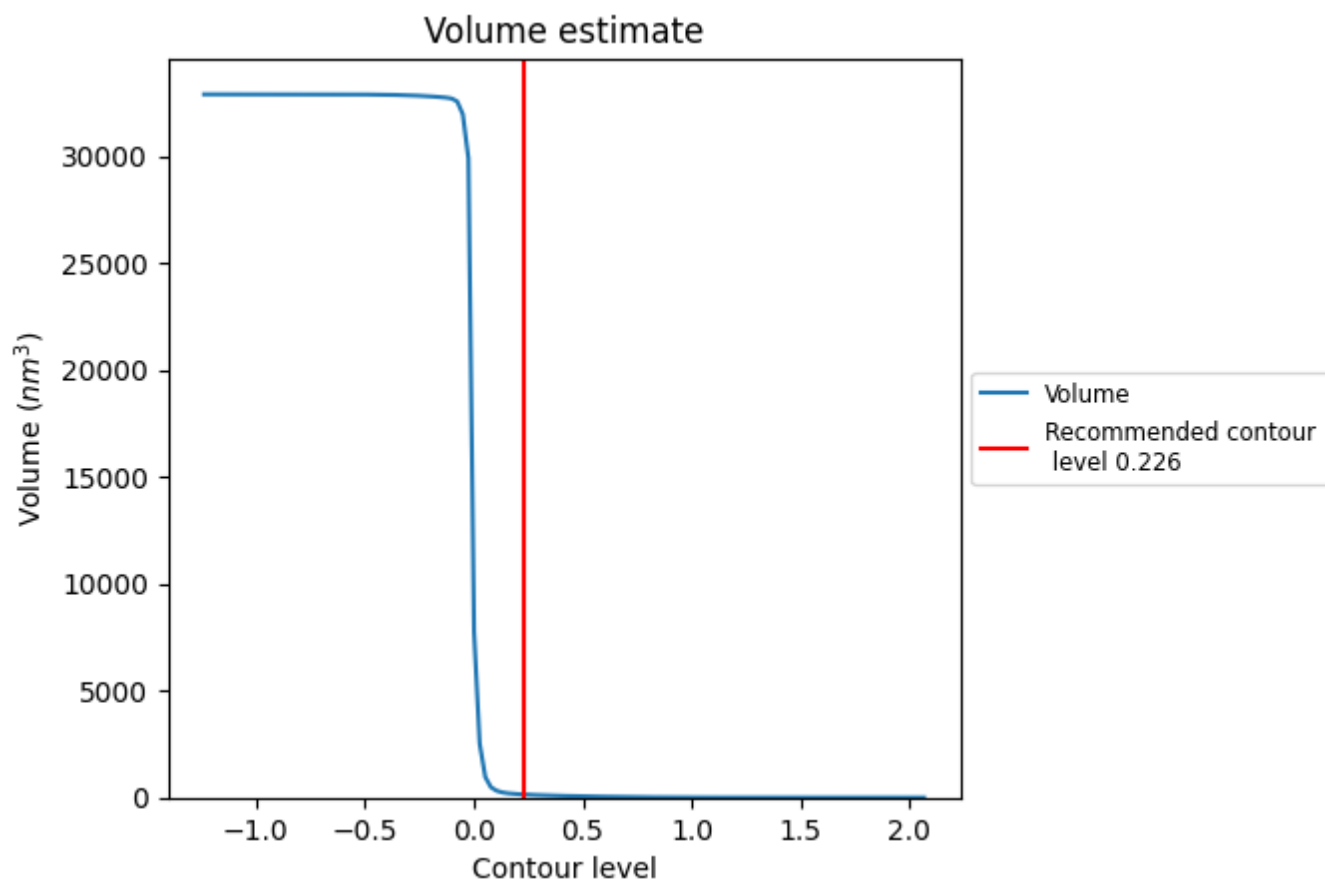
This section contains the results of statistical analysis of the map.

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.

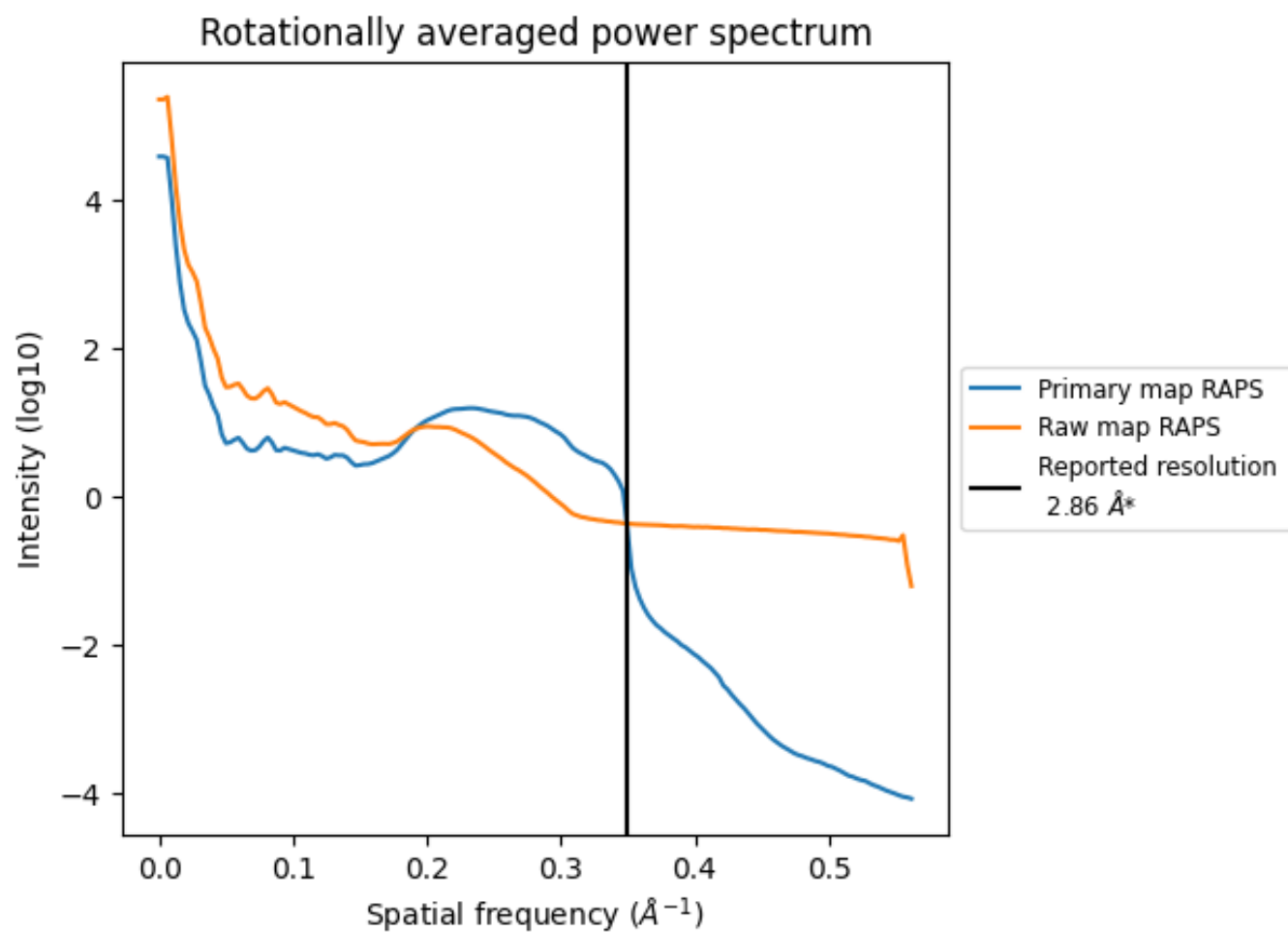
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 146 nm³; this corresponds to an approximate mass of 132 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 ⓘ

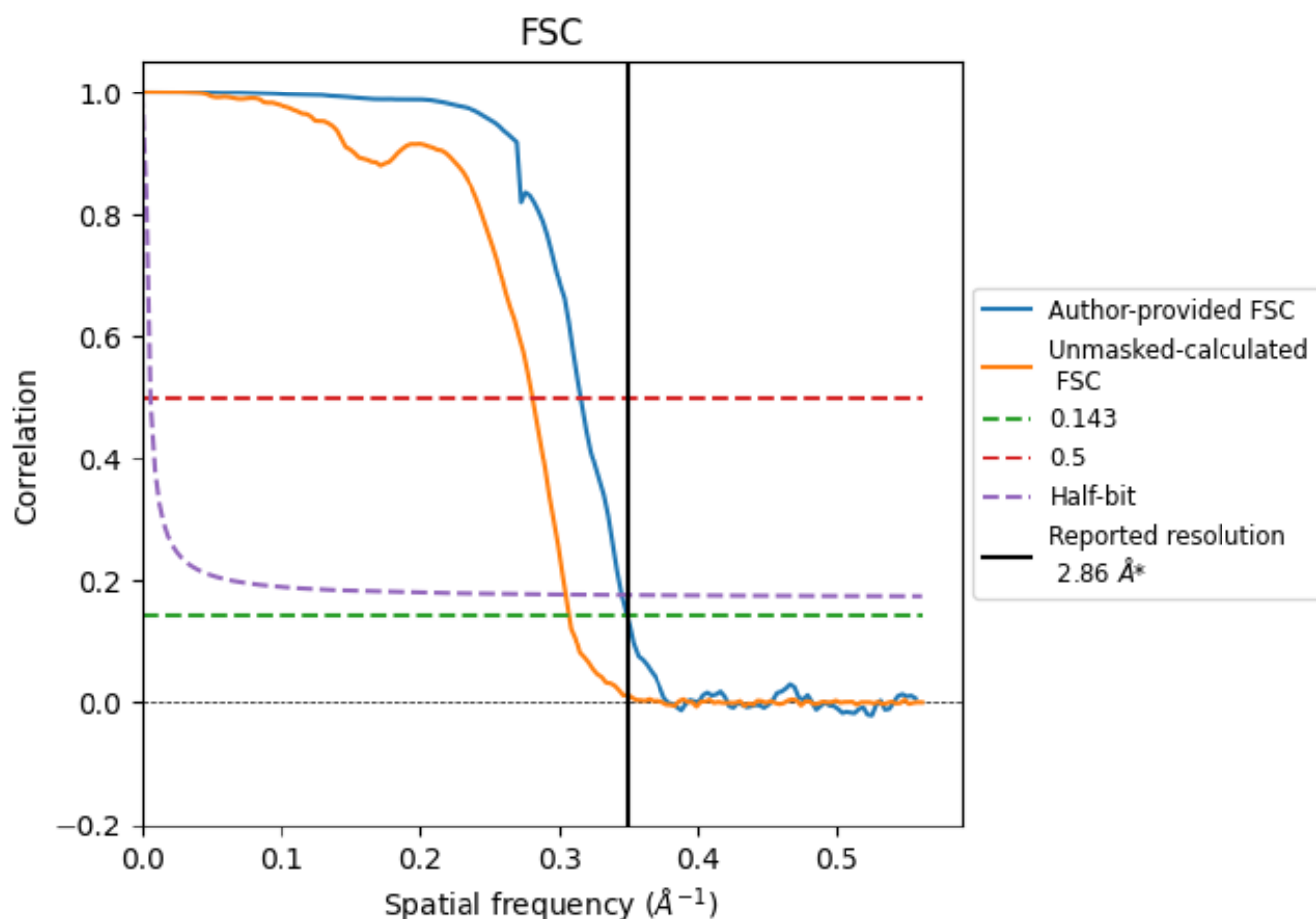


*Reported resolution corresponds to spatial frequency of $0.350 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.350 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

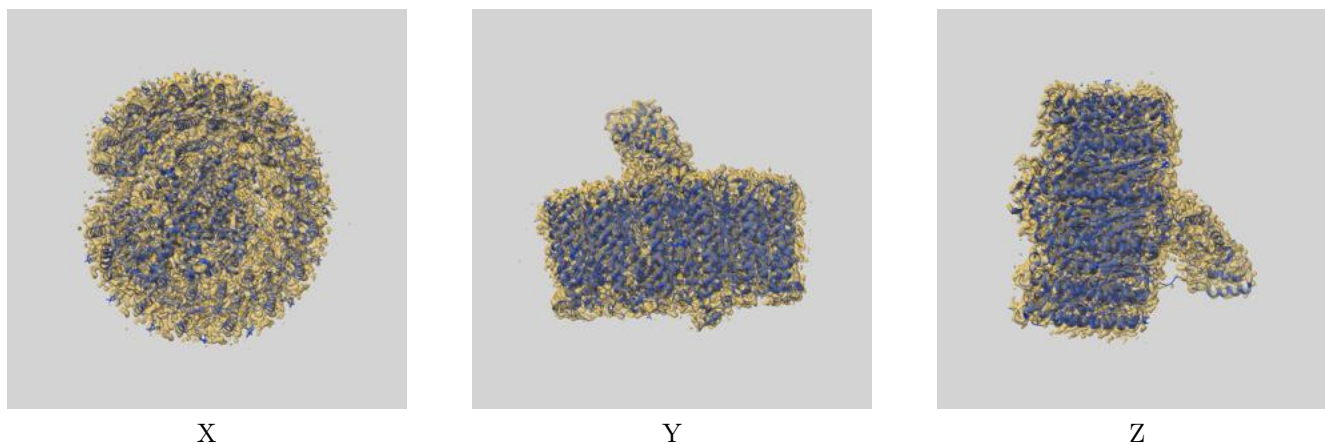
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.86	-	-
Author-provided FSC curve	2.86	3.17	2.90
Unmasked-calculated*	3.25	3.56	3.28

*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 3.25 differs from the reported value 2.86 by more than 10 %

9 Map-model fit [i](#)

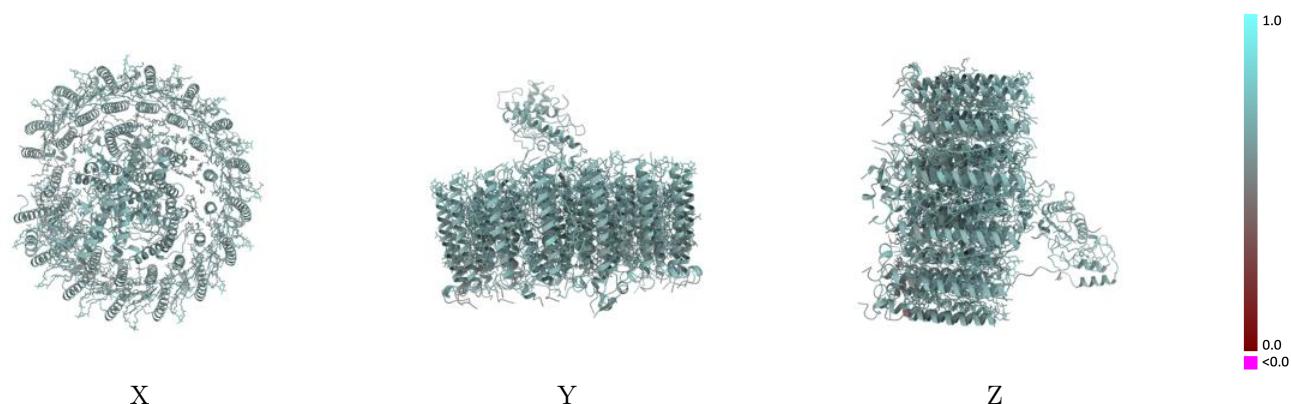
This section contains information regarding the fit between EMDB map EMD-35721 and PDB model 8IUG. Per-residue inclusion information can be found in section [3](#) on page [20](#).

9.1 Map-model overlay [i](#)



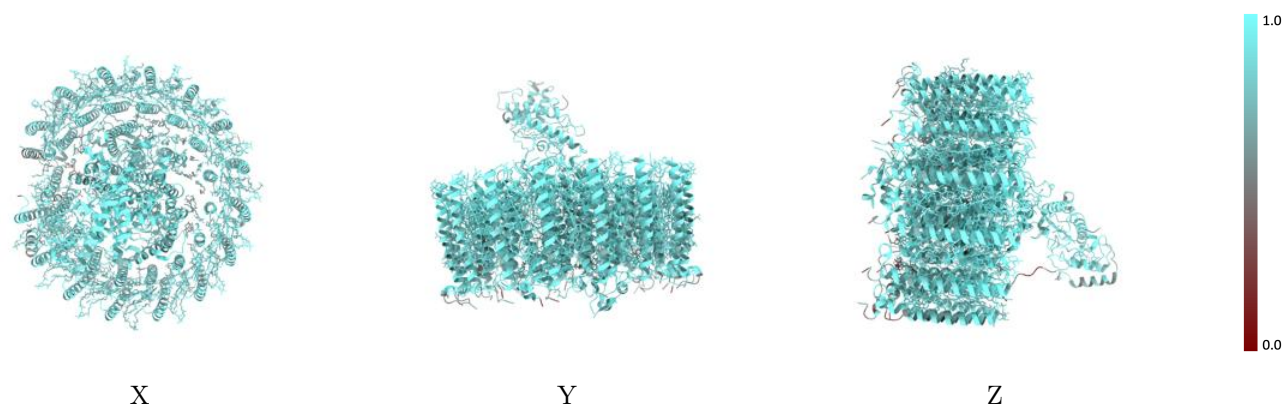
The images above show the 3D surface view of the map at the recommended contour level 0.226 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



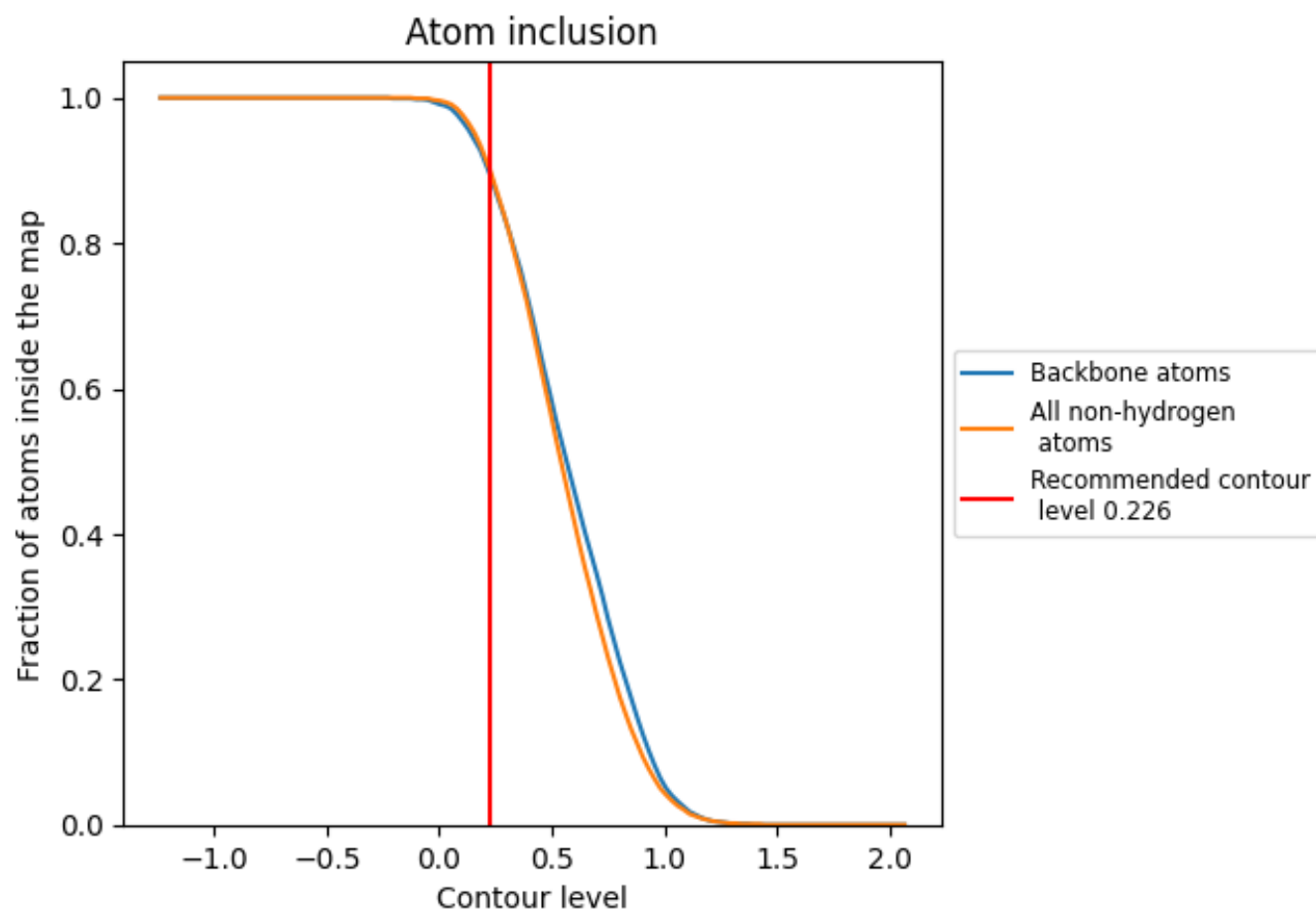
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.226).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 90% 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 (0.226) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9000	 0.6220
0	 0.8560	 0.6100
1	 0.8530	 0.6070
2	 0.8570	 0.5980
3	 0.9190	 0.6220
4	 0.8790	 0.6190
5	 0.9180	 0.6260
6	 0.8850	 0.6120
7	 0.9000	 0.6250
8	 0.8710	 0.6090
9	 0.9080	 0.6230
A	 0.9210	 0.6260
B	 0.8800	 0.6100
C	 0.8780	 0.6150
D	 0.8980	 0.6170
E	 0.8820	 0.6100
F	 0.9200	 0.6220
G	 0.8820	 0.6160
H	 0.8780	 0.6180
I	 0.8850	 0.6220
J	 0.9480	 0.6430
K	 0.8950	 0.6130
L	 0.9390	 0.6390
M	 0.9480	 0.6420
N	 0.9260	 0.6310
O	 0.8960	 0.6170
P	 0.9010	 0.6290
Q	 0.8830	 0.6150
R	 0.9390	 0.6340
S	 0.9020	 0.6220
T	 0.9090	 0.6150
U	 0.8710	 0.6140
V	 0.8730	 0.6110
W	 0.8520	 0.6020
X	 0.6620	 0.5670



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Y	 0.9070	 0.6180
Z	 0.9410	 0.6260
h	 0.9340	 0.6330