



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 06:45 AM UTC

PDB ID : 6Z5R / pdb_00006z5r
EMDB ID : EMD-11080
Title : RC-LH1(16) complex from Rhodopseudomonas palustris
Authors : Swainsbury, D.J.K.; Qian, P.; Hitchcock, A.; Hunter, C.N.
Deposited on : 2020-05-27
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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 : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

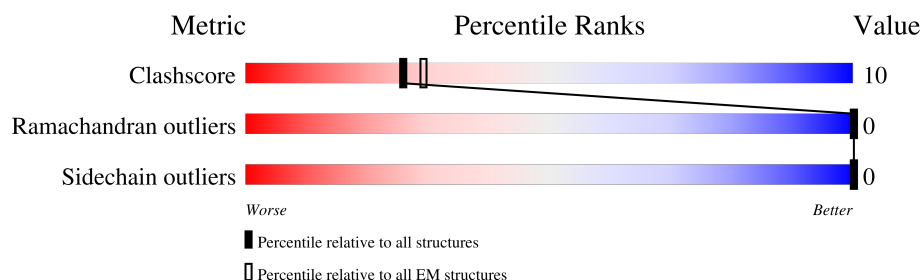
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 Å.

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



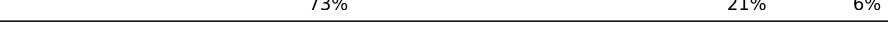
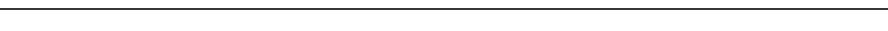
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	1	48	83% 12% .
1	3	48	75% 21% .
1	5	48	71% 23% . .
1	7	48	83% 12% .
1	9	48	50% 46% .
1	A	48	83% 12% .
1	C	48	73% 23% .
1	E	48	77% 19% .
1	G	48	75% 21% .

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Mol	Chain	Length	Quality of chain
1	J	48	
1	N	48	
1	P	48	
1	R	48	
1	T	48	
1	V	48	
1	Y	48	
2	0	52	
2	2	52	
2	4	52	
2	6	52	
2	8	52	
2	B	52	
2	D	52	
2	F	52	
2	I	52	
2	K	52	
2	O	52	
2	Q	52	
2	S	52	
2	U	52	
2	X	52	
2	Z	52	
3	H	255	
4	L	277	

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Mol	Chain	Length	Quality of chain
5	M	307	 89%11%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	BPH	L	302	X	-	-	-
11	BPH	M	405	X	-	-	-
14	QAK	M	407	X	-	-	-

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 25048 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 Light-harvesting complex 1 alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	46	Total	C	N	O	S	0	0
			397	274	67	55	1		
1	E	46	Total	C	N	O	S	0	0
			397	274	67	55	1		
1	G	46	Total	C	N	O	S	0	0
			397	274	67	55	1		
1	J	45	Total	C	N	O	S	0	0
			392	271	66	54	1		
1	N	46	Total	C	N	O	S	0	0
			397	274	67	55	1		
1	R	46	Total	C	N	O	S	0	0
			397	274	67	55	1		
1	T	48	Total	C	N	O	S	0	0
			411	283	70	57	1		
1	V	46	Total	C	N	O	S	0	0
			397	274	67	55	1		
1	P	46	Total	C	N	O	S	0	0
			397	274	67	55	1		
1	Y	45	Total	C	N	O		0	0
			387	268	66	53			
1	A	46	Total	C	N	O	S	0	0
			397	274	67	55	1		
1	1	46	Total	C	N	O	S	0	0
			397	274	67	55	1		
1	3	46	Total	C	N	O	S	0	0
			397	274	67	55	1		
1	5	46	Total	C	N	O	S	0	0
			397	274	67	55	1		
1	7	46	Total	C	N	O	S	0	0
			397	274	67	55	1		
1	9	46	Total	C	N	O	S	0	0
			397	274	67	55	1		

- Molecule 2 is a protein called Light-harvesting complex 1 beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	49	Total	C	N	O	S	1	0
			403	276	62	64	1		
2	F	49	Total	C	N	O	S	1	0
			403	276	62	64	1		
2	I	47	Total	C	N	O	S	0	0
			382	262	59	60	1		
2	K	47	Total	C	N	O	S	1	0
			393	271	60	61	1		
2	O	48	Total	C	N	O	S	1	0
			399	274	61	63	1		
2	S	48	Total	C	N	O	S	1	0
			399	274	61	63	1		
2	U	47	Total	C	N	O	S	1	0
			393	271	60	61	1		
2	X	47	Total	C	N	O	S	0	0
			382	262	59	60	1		
2	Q	48	Total	C	N	O	S	1	0
			399	274	61	63	1		
2	Z	48	Total	C	N	O	S	1	0
			399	274	61	63	1		
2	B	49	Total	C	N	O	S	1	0
			403	276	62	64	1		
2	2	48	Total	C	N	O	S	1	0
			399	274	61	63	1		
2	4	48	Total	C	N	O	S	1	0
			399	274	61	63	1		
2	6	50	Total	C	N	O	S	1	0
			411	280	63	67	1		
2	8	49	Total	C	N	O	S	1	0
			403	276	62	64	1		
2	0	49	Total	C	N	O	S	1	0
			403	276	62	64	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	247	Total	C	N	O	S	0	0
			1862	1201	314	342	5		

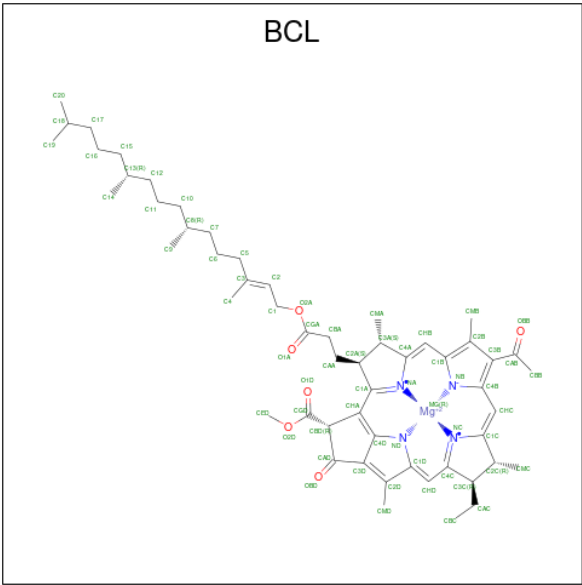
- Molecule 4 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	276	Total	C	N	O	S	0	0
			2185	1467	350	359	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	M	306	2433	1615	400	406	12	0	0

- Molecule 6 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
6	C	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
6	C	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
6	E	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
6	F	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
6	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
6	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
6	J	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
6	J	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
6	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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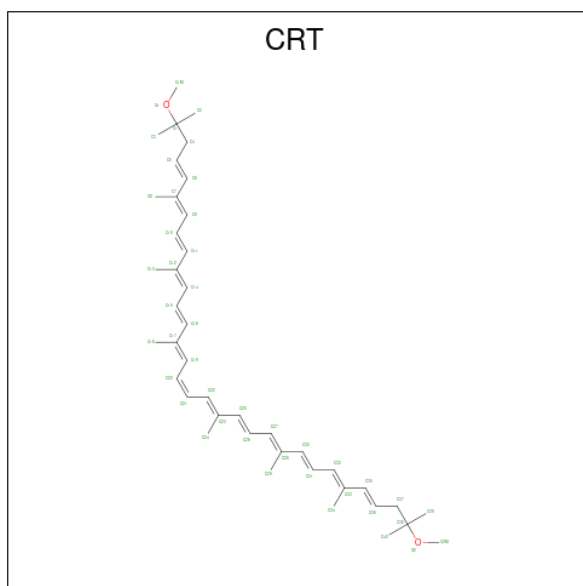
Mol	Chain	Residues	Atoms					AltConf
6	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	M	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	M	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	R	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	R	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	T	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	U	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	V	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	V	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	P	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	B	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	1	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	1	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	3	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	4	1	Total 66	C 55	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
6	5	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
6	5	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
6	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
6	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
6	9	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
6	0	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 7 is SPIRILLOXANTHIN (CCD ID: CRT) (formula: $C_{42}H_{60}O_2$) (labeled as "Ligand of Interest" by depositor).



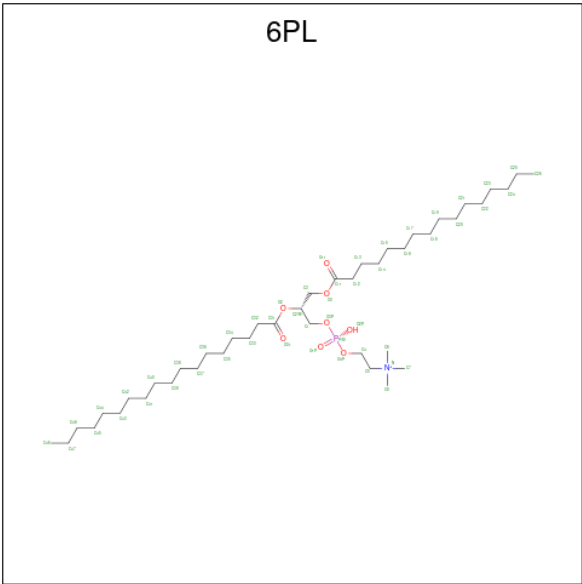
Mol	Chain	Residues	Atoms			AltConf
7	D	1	Total	C	O	0
			44	42	2	
7	G	1	Total	C	O	0
			44	42	2	
7	I	1	Total	C	O	0
			44	42	2	
7	K	1	Total	C	O	0
			44	42	2	
7	O	1	Total	C	O	0
			44	42	2	

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Mol	Chain	Residues	Atoms			AltConf
7	S	1	Total	C	O	0
			44	42	2	
7	U	1	Total	C	O	0
			44	42	2	
7	X	1	Total	C	O	0
			44	42	2	
7	Q	1	Total	C	O	0
			44	42	2	
7	Z	1	Total	C	O	0
			44	42	2	
7	B	1	Total	C	O	0
			44	42	2	
7	2	1	Total	C	O	0
			44	42	2	
7	4	1	Total	C	O	0
			44	42	2	
7	7	1	Total	C	O	0
			44	42	2	
7	8	1	Total	C	O	0
			44	42	2	
7	0	1	Total	C	O	0
			44	42	2	

- Molecule 8 is (4S,7R)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM 4-OXIDE (CCD ID: 6PL) (formula: C₄₂H₈₅NO₈P) (labeled as "Ligand of Interest" by depositor).



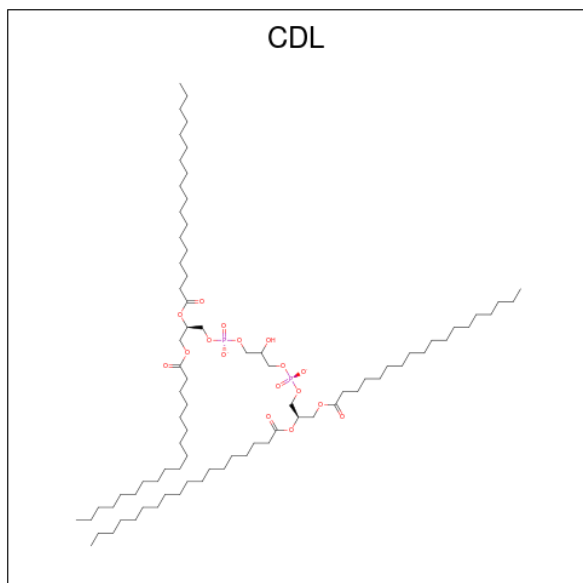
Mol	Chain	Residues	Atoms					AltConf
8	D	1	Total	C	N	O	P	0
			52	42	1	8	1	
8	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
8	F	1	Total	C	N	O	P	0
			52	42	1	8	1	
8	I	1	Total	C	N	O	P	0
			52	42	1	8	1	
8	I	1	Total	C	N	O	P	0
			52	42	1	8	1	
8	K	1	Total	C	N	O	P	0
			52	42	1	8	1	
8	O	1	Total	C	N	O	P	0
			47	37	1	8	1	
8	H	1	Total	C	N	O	P	0
			52	42	1	8	1	
8	L	1	Total	C	N	O	P	0
			52	42	1	8	1	
8	L	1	Total	C	N	O	P	0
			52	42	1	8	1	
8	M	1	Total	C	N	O	P	0
			52	42	1	8	1	
8	S	1	Total	C	N	O	P	0
			52	42	1	8	1	
8	U	1	Total	C	N	O	P	0
			52	42	1	8	1	
8	X	1	Total	C	N	O	P	0
			52	42	1	8	1	
8	P	1	Total	C	N	O	P	0
			52	42	1	8	1	
8	Q	1	Total	C	N	O	P	0
			48	38	1	8	1	
8	Z	1	Total	C	N	O	P	0
			52	42	1	8	1	
8	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
8	2	1	Total	C	N	O	P	0
			47	37	1	8	1	
8	4	1	Total	C	N	O	P	0
			52	42	1	8	1	
8	5	1	Total	C	N	O	P	0
			52	42	1	8	1	
8	6	1	Total	C	N	O	P	0
			52	42	1	8	1	

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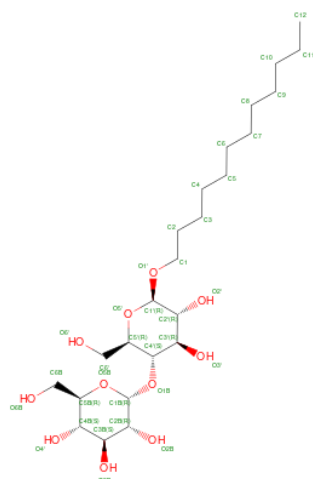
Mol	Chain	Residues	Atoms					AltConf
8	8	1	Total	C	N	O	P	0
			52	42	1	8	1	
8	0	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 9 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



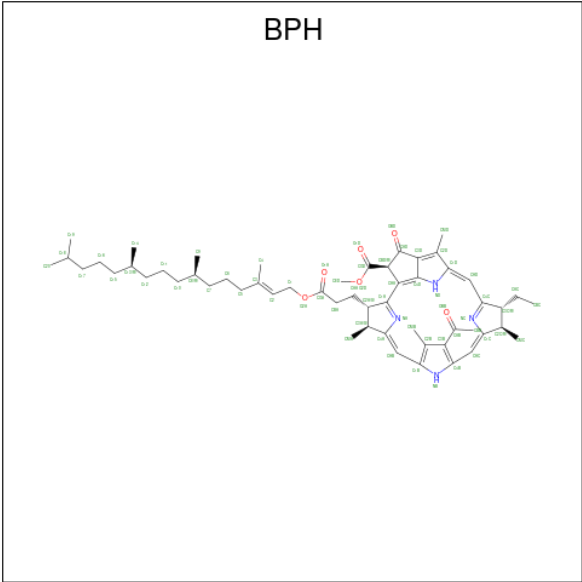
Mol	Chain	Residues	Atoms				AltConf
9	E	1	Total	C	O	P	0
			87	68	17	2	
9	G	1	Total	C	O	P	0
			100	81	17	2	
9	G	1	Total	C	O	P	0
			90	71	17	2	
9	L	1	Total	C	O	P	0
			100	81	17	2	
9	M	1	Total	C	O	P	0
			90	71	17	2	
9	M	1	Total	C	O	P	0
			84	65	17	2	

- Molecule 10 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).



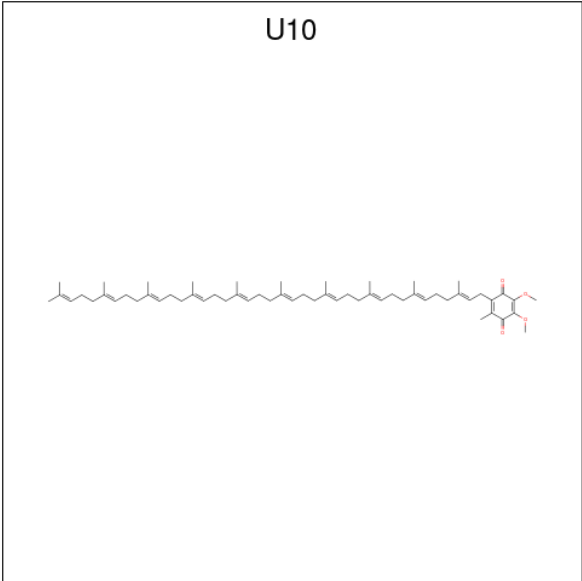
Id	Chain	Residues	Atoms			AltConf
10	F	1	Total 35	C 24	O 11	0
10	J	1	Total 35	C 24	O 11	0
10	O	1	Total 35	C 24	O 11	0
10	H	1	Total 35	C 24	O 11	0
10	L	1	Total 35	C 24	O 11	0
10	R	1	Total 35	C 24	O 11	0
10	P	1	Total 35	C 24	O 11	0
10	Z	1	Total 35	C 24	O 11	0
10	B	1	Total 35	C 24	O 11	0
10	2	1	Total 35	C 24	O 11	0
10	4	1	Total 35	C 24	O 11	0
10	6	1	Total 35	C 24	O 11	0

- Molecule 11 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
11	L	1	Total	C	N	O	0
			65	55	4	6	
11	M	1	Total	C	N	O	0
			65	55	4	6	

- Molecule 12 is UBIQUINONE-10 (CCD ID: U10) (formula: C₅₉H₉₀O₄) (labeled as "Ligand of Interest" by depositor).



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

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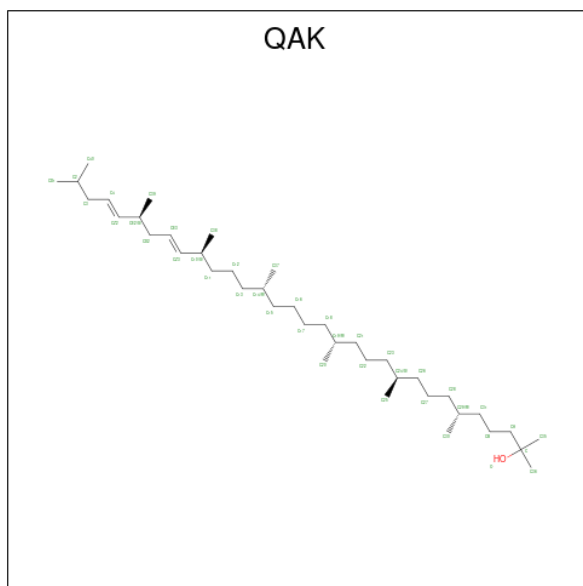
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Mol	Chain	Residues	Atoms			AltConf
12	L	1	Total	C	O	0
			63	59	4	
12	L	1	Total	C	O	0
			63	59	4	
12	M	1	Total	C	O	0
			48	44	4	
12	M	1	Total	C	O	0
			63	59	4	

- Molecule 13 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

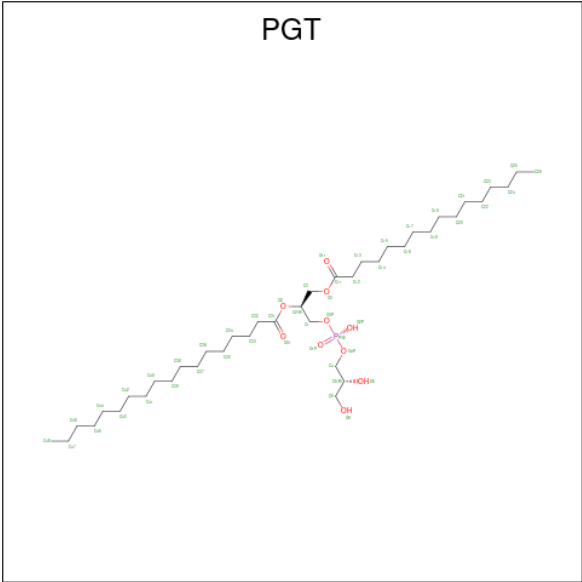
Mol	Chain	Residues	Atoms		AltConf
13	M	1	Total	Fe	0
			1	1	

- Molecule 14 is (6 {R},10 {S},14 {R},19 {R},23 {S},24 {E},27 {S},28 {E})-2,6,10,14,19,23,27,31-octamethyldotriaconta-24,28-dien-2-ol (CCD ID: QAK) (formula: C₄₀H₇₈O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
14	M	1	Total	C	O	0
			41	40	1	

- Molecule 15 is (1S)-2-{{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (CCD ID: PGT) (formula: C₄₀H₇₉O₁₀P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
15	7	1	Total	C	O	P	0
			51	40	10	1	
15	9	1	Total	C	O	P	0
			51	40	10	1	

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		AltConf
16	L	1	Total	O	0
			1	1	
16	M	2	Total	O	0
			2	2	

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. 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. 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: Light-harvesting complex 1 alpha chain

Chain C:  73% 23% .



- Molecule 1: Light-harvesting complex 1 alpha chain

Chain E:  77% 19% .



- Molecule 1: Light-harvesting complex 1 alpha chain

Chain G:  75% 21% .



- Molecule 1: Light-harvesting complex 1 alpha chain

Chain J:  81% 12% 6% .



- Molecule 1: Light-harvesting complex 1 alpha chain

Chain N:  73% 23% .

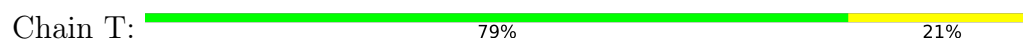


- Molecule 1: Light-harvesting complex 1 alpha chain

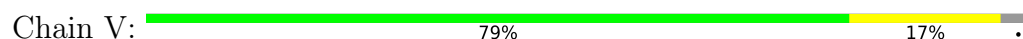
Chain R:  65% 31% .



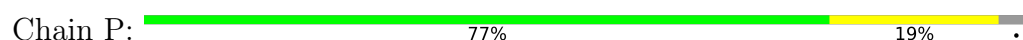
- Molecule 1: Light-harvesting complex 1 alpha chain



- Molecule 1: Light-harvesting complex 1 alpha chain



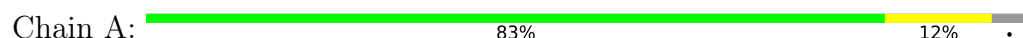
- Molecule 1: Light-harvesting complex 1 alpha chain



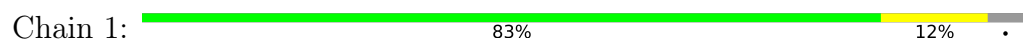
- Molecule 1: Light-harvesting complex 1 alpha chain



- Molecule 1: Light-harvesting complex 1 alpha chain



- Molecule 1: Light-harvesting complex 1 alpha chain



- Molecule 1: Light-harvesting complex 1 alpha chain





- Molecule 1: Light-harvesting complex 1 alpha chain

Chain 5: 71% 23% . .



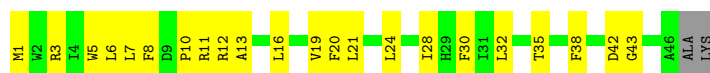
- Molecule 1: Light-harvesting complex 1 alpha chain

Chain 7: 83% 12% .



- Molecule 1: Light-harvesting complex 1 alpha chain

Chain 9: 50% 46% .



- Molecule 2: Light-harvesting complex 1 beta chain

Chain D: 73% 21% 6%



- Molecule 2: Light-harvesting complex 1 beta chain

Chain F: 79% 15% 6%



- Molecule 2: Light-harvesting complex 1 beta chain

Chain I: 77% 13% 10%



- Molecule 2: Light-harvesting complex 1 beta chain

Chain K: 75% 15% 10%



- Molecule 2: Light-harvesting complex 1 beta chain

Chain O: 69% 23% 8%



- Molecule 2: Light-harvesting complex 1 beta chain

Chain S: 79% 13% 8%



- Molecule 2: Light-harvesting complex 1 beta chain

Chain U: 71% 19% 10%



- Molecule 2: Light-harvesting complex 1 beta chain

Chain X: 65% 25% 10%



- Molecule 2: Light-harvesting complex 1 beta chain

Chain Q: 65% 27% 8%



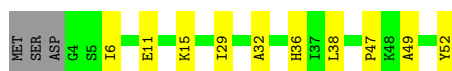
- Molecule 2: Light-harvesting complex 1 beta chain

Chain Z: 67% 25% 8%



- Molecule 2: Light-harvesting complex 1 beta chain

Chain B: 75% 19% 6%



- Molecule 2: Light-harvesting complex 1 beta chain



- Molecule 2: Light-harvesting complex 1 beta chain



- Molecule 2: Light-harvesting complex 1 beta chain



- Molecule 2: Light-harvesting complex 1 beta chain



- Molecule 2: Light-harvesting complex 1 beta chain



- Molecule 3: H subunit of photosynthetic reaction center complex

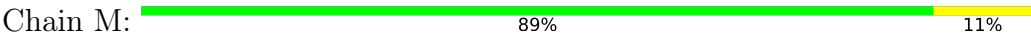


- Molecule 4: Reaction center protein L chain





• Molecule 5: Reaction center protein M chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	260752	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55.2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: QAK, FME, FE, BCL, LMT, BPH, PGT, CDL, CRT, 6PL, U10

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	1	0.16	0/401	0.29	0/546
1	3	0.15	0/401	0.29	0/546
1	5	0.15	0/401	0.31	0/546
1	7	0.15	0/401	0.34	0/546
1	9	0.17	0/401	0.33	0/546
1	A	0.18	0/401	0.31	0/546
1	C	0.18	0/401	0.31	0/546
1	E	0.18	0/401	0.36	0/546
1	G	0.18	0/401	0.31	0/546
1	J	0.17	0/396	0.32	0/539
1	N	0.17	0/401	0.31	0/546
1	P	0.16	0/401	0.32	0/546
1	R	0.17	0/401	0.38	0/546
1	T	0.18	0/415	0.31	0/564
1	V	0.16	0/401	0.31	0/546
1	Y	0.18	0/401	0.30	0/546
2	0	0.15	0/419	0.32	0/571
2	2	0.15	0/415	0.29	0/566
2	4	0.15	0/415	0.27	0/566
2	6	0.16	0/427	0.28	0/582
2	8	0.18	0/419	0.37	0/571
2	B	0.18	0/419	0.34	0/571
2	D	0.19	0/419	0.28	0/571
2	F	0.20	0/419	0.32	0/571
2	I	0.18	0/397	0.29	0/542
2	K	0.16	0/409	0.28	0/558
2	O	0.17	0/415	0.34	0/566
2	Q	0.17	0/415	0.28	0/566
2	S	0.18	0/415	0.28	0/566
2	U	0.17	0/409	0.32	0/558
2	X	0.17	0/397	0.33	0/542
2	Z	0.18	0/415	0.36	0/566

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	H	0.17	0/1913	0.37	0/2618
4	L	0.18	0/2271	0.32	0/3109
5	M	0.18	0/2524	0.32	0/3454
All	All	0.17	0/19757	0.32	0/26961

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	397	0	415	6	0
1	3	397	0	415	10	0
1	5	397	0	415	11	0
1	7	397	0	415	5	0
1	9	397	0	415	28	0
1	A	397	0	415	7	0
1	C	397	0	415	9	0
1	E	397	0	415	8	0
1	G	397	0	415	10	0
1	J	392	0	410	7	0
1	N	397	0	415	13	0
1	P	397	0	415	10	0
1	R	397	0	415	13	0
1	T	411	0	433	11	0
1	V	397	0	415	8	0
1	Y	387	0	404	13	0
2	0	403	0	396	12	0
2	2	399	0	393	7	0
2	4	399	0	393	21	0
2	6	411	0	400	15	0
2	8	403	0	396	16	0
2	B	403	0	396	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	403	0	396	12	0
2	F	403	0	396	9	0
2	I	382	0	380	9	0
2	K	393	0	388	7	0
2	O	399	0	393	11	0
2	Q	399	0	393	12	0
2	S	399	0	393	6	0
2	U	393	0	388	10	0
2	X	382	0	380	17	0
2	Z	399	0	393	12	0
3	H	1862	0	1873	20	0
4	L	2185	0	2130	17	0
5	M	2433	0	2379	28	0
6	0	66	0	74	4	0
6	1	132	0	148	10	0
6	3	66	0	74	2	0
6	4	66	0	74	6	0
6	5	132	0	148	10	0
6	7	132	0	148	5	0
6	9	66	0	74	1	0
6	A	66	0	74	8	0
6	B	66	0	74	6	0
6	C	132	0	148	6	0
6	E	66	0	74	1	0
6	F	66	0	74	4	0
6	G	132	0	148	8	0
6	J	132	0	148	5	0
6	L	132	0	148	5	0
6	M	132	0	148	4	0
6	N	132	0	148	4	0
6	P	66	0	74	4	0
6	Q	66	0	74	5	0
6	R	132	0	148	8	0
6	T	66	0	74	4	0
6	U	66	0	74	5	0
6	V	132	0	148	6	0
6	Y	132	0	148	12	0
7	0	44	0	60	5	0
7	2	44	0	60	5	0
7	4	44	0	60	11	0
7	7	44	0	60	2	0
7	8	44	0	60	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	44	0	60	4	0
7	D	44	0	60	5	0
7	G	44	0	60	4	0
7	I	44	0	60	2	0
7	K	44	0	60	2	0
7	O	44	0	60	4	0
7	Q	44	0	60	4	0
7	S	44	0	60	3	0
7	U	44	0	60	5	0
7	X	44	0	60	14	0
7	Z	44	0	60	7	0
8	0	52	0	84	3	0
8	2	47	0	71	7	0
8	4	52	0	84	5	0
8	5	52	0	84	2	0
8	6	52	0	84	4	0
8	8	52	0	84	4	0
8	B	52	0	84	4	0
8	D	52	0	84	5	0
8	E	52	0	84	6	0
8	F	52	0	84	3	0
8	H	52	0	84	0	0
8	I	104	0	168	10	0
8	K	52	0	84	3	0
8	L	104	0	168	10	0
8	M	52	0	84	5	0
8	O	47	0	71	4	0
8	P	52	0	84	4	0
8	Q	48	0	73	6	0
8	S	52	0	84	5	0
8	U	52	0	84	4	0
8	X	52	0	84	3	0
8	Z	52	0	84	4	0
9	E	87	0	127	7	0
9	G	190	0	289	21	0
9	L	100	0	156	9	0
9	M	174	0	251	10	0
10	2	35	0	45	2	0
10	4	35	0	45	3	0
10	6	35	0	46	3	0
10	B	35	0	45	2	0
10	F	35	0	45	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	H	35	0	45	4	0
10	J	35	0	45	7	0
10	L	35	0	45	0	0
10	O	35	0	45	1	0
10	P	35	0	44	2	0
10	R	35	0	45	3	0
10	Z	35	0	45	1	0
11	L	65	0	76	5	0
11	M	65	0	76	6	0
12	L	174	0	243	13	0
12	M	111	0	153	9	0
13	M	1	0	0	0	0
14	M	41	0	0	0	0
15	7	51	0	78	4	0
15	9	51	0	78	3	0
16	L	1	0	0	0	0
16	M	2	0	0	0	0
All	All	25048	0	26968	533	0

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

All (533) 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)
1:1:32:LEU:HD11	6:1:102:BCL:HHD	1.61	0.82
1:5:3:ARG:HB3	7:8:101:CRT:H23	1.65	0.77
2:8:17:PHE:HA	7:8:101:CRT:H6	1.67	0.75
9:L:310:CDL:H781	1:9:16:LEU:HD22	1.68	0.75
4:L:96:GLY:HA2	9:L:310:CDL:H632	1.67	0.74
1:Y:37:ARG:O	2:Z:43:ARG:NH1	2.22	0.73
6:N:101:BCL:H201	9:M:408:CDL:H611	1.70	0.73
6:1:101:BCL:HMA3	10:2:101:LMT:H121	1.69	0.72
1:Y:32:LEU:HD11	6:Y:102:BCL:HHD	1.71	0.72
4:L:31:TYR:O	4:L:104:ARG:NH2	2.23	0.72
2:X:17:PHE:HD1	7:X:101:CRT:H6	1.54	0.72
6:4:102:BCL:HAA1	8:4:104:6PL:H262	1.72	0.72
1:9:3:ARG:HG3	1:9:6:LEU:HD12	1.73	0.71
9:G:105:CDL:H602	6:J:101:BCL:H202	1.73	0.71
6:1:102:BCL:H152	8:2:103:6PL:H132	1.73	0.70
8:O:103:6PL:H73	2:Q:42:TRP:HB2	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:32:LEU:HD11	6:U:100:BCL:HHD	1.72	0.70
2:4:32:ALA:O	2:4:36:HIS:ND1	2.23	0.68
1:5:37:ARG:O	2:6:43:ARG:NH1	2.25	0.68
3:H:54:VAL:HG13	3:H:55:PRO:HD3	1.75	0.67
7:2:102:CRT:H2M3	1:3:29:HIS:HB3	1.75	0.67
3:H:16:VAL:HG13	9:M:408:CDL:H652	1.77	0.67
6:B:102:BCL:H152	8:B:104:6PL:H412	1.76	0.67
7:4:103:CRT:H35	6:5:101:BCL:HMB1	1.77	0.66
6:0:100:BCL:HAA1	8:0:102:6PL:H471	1.78	0.66
12:L:307:U10:H23	12:L:307:U10:H38	1.77	0.66
1:C:39:ASN:HD22	1:C:45:ARG:HH22	1.42	0.65
1:J:32:LEU:HD11	6:J:103:BCL:HHD	1.77	0.65
7:U:101:CRT:H2M3	1:V:29:HIS:HB3	1.77	0.65
9:G:105:CDL:H451	1:N:22:PHE:HZ	1.62	0.65
1:5:22:PHE:HB2	6:5:101:BCL:H72	1.78	0.65
1:T:4:ILE:HB	7:X:101:CRT:H82	1.79	0.65
2:8:49:ALA:O	2:0:43:ARG:NH2	2.29	0.65
1:5:32:LEU:HD11	6:5:103:BCL:HHD	1.79	0.65
2:K:32:ALA:O	2:K:36:HIS:ND1	2.21	0.65
2:0:32:ALA:O	2:0:36:HIS:ND1	2.23	0.64
6:4:102:BCL:H172	8:4:104:6PL:H171	1.78	0.64
11:L:302:BPH:HHC	11:L:302:BPH:HBB3	1.80	0.64
9:L:310:CDL:H782	1:A:15:VAL:HG13	1.80	0.64
2:8:32:ALA:O	2:8:36:HIS:ND1	2.30	0.64
10:J:102:LMT:H11	10:H:302:LMT:H21	1.80	0.63
7:O:102:CRT:H35	6:P:102:BCL:HMB2	1.81	0.63
2:D:43:ARG:HH12	2:B:49:ALA:HA	1.63	0.63
6:F:102:BCL:H171	8:I:101:6PL:H262	1.81	0.63
6:7:104:BCL:H152	8:8:102:6PL:H201	1.79	0.63
9:L:310:CDL:H711	1:9:12:ARG:HD3	1.80	0.63
8:L:304:6PL:H51	8:L:305:6PL:H61	1.78	0.63
6:0:100:BCL:H11	7:0:101:CRT:H25	1.80	0.62
2:2:40:TRP:CE2	8:2:103:6PL:H11	2.35	0.62
7:I:102:CRT:H2M3	1:J:29:HIS:HB3	1.80	0.62
2:8:48:LYS:HG3	2:8:49:ALA:H	1.62	0.62
2:K:47:PRO:O	2:O:43:ARG:NH2	2.33	0.62
3:H:13:THR:HG23	8:M:401:6PL:H442	1.82	0.62
2:4:17:PHE:HA	7:4:103:CRT:H6	1.82	0.62
6:R:103:BCL:H152	8:S:102:6PL:H422	1.80	0.61
9:L:310:CDL:H761	1:9:16:LEU:HD13	1.81	0.61
2:6:47:PRO:O	2:8:43:ARG:NH2	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:8:21:PHE:CD1	7:8:101:CRT:H14	2.35	0.61
6:Y:102:BCL:H152	8:Z:103:6PL:H201	1.82	0.61
2:6:32:ALA:O	2:6:36:HIS:ND1	2.19	0.61
9:G:105:CDL:H362	9:G:105:CDL:H131	1.84	0.60
12:L:303:U10:H162	6:L:308:BCL:H71	1.82	0.60
6:4:102:BCL:H8	8:4:104:6PL:H241	1.83	0.60
6:5:103:BCL:HAA1	8:6:102:6PL:H252	1.83	0.60
6:A:100:BCL:H203	6:A:100:BCL:H122	1.84	0.60
1:A:32:LEU:HD11	6:B:102:BCL:HHD	1.83	0.59
1:J:7:LEU:O	1:N:11:ARG:NH2	2.34	0.59
1:N:30:PHE:HB3	8:M:401:6PL:H162	1.84	0.59
5:M:66:VAL:HG22	12:M:410:U10:H71	1.85	0.59
11:M:405:BPH:HBB3	11:M:405:BPH:HHC	1.84	0.59
2:4:21:PHE:HD1	7:4:103:CRT:H14	1.67	0.59
1:R:45:ARG:HH21	10:R:102:LMT:H6'1	1.68	0.59
1:R:18:PHE:HB3	6:R:101:BCL:H92	1.85	0.59
1:R:22:PHE:HB2	6:R:101:BCL:H52	1.85	0.59
1:E:36:SER:OG	1:E:44:PRO:O	2.20	0.58
3:H:35:GLU:OE1	5:M:241:ARG:NH1	2.36	0.58
2:Q:40:TRP:HE1	8:Q:102:6PL:H52	1.68	0.58
1:R:3:ARG:NE	2:U:16:GLU:OE2	2.34	0.58
1:9:32:LEU:HD11	6:0:100:BCL:HHD	1.86	0.58
5:M:64:GLY:HA3	11:M:405:BPH:H5C1	1.85	0.58
5:M:137:SER:OG	5:M:143:GLY:O	2.21	0.58
1:E:11:ARG:HH22	8:E:102:6PL:H41	1.68	0.58
5:M:70:ILE:HG12	12:M:410:U10:H4M2	1.86	0.58
9:G:101:CDL:H421	8:L:305:6PL:H441	1.87	0.57
1:R:32:LEU:HD11	6:R:103:BCL:HHD	1.86	0.57
2:8:17:PHE:HB2	7:8:101:CRT:H32A	1.85	0.57
5:M:138:ARG:HG3	9:M:409:CDL:HB21	1.87	0.57
5:M:94:ALA:HB2	5:M:181:PRO:HG2	1.84	0.57
1:T:34:SER:O	1:T:45:ARG:NH2	2.36	0.57
2:X:17:PHE:HB2	7:X:101:CRT:H32A	1.86	0.57
2:X:32:ALA:O	2:X:36:HIS:ND1	2.30	0.57
1:9:42:ASP:OD1	1:9:43:GLY:N	2.38	0.57
4:L:43:ALA:HA	11:L:302:BPH:H9C3	1.86	0.57
11:M:405:BPH:HBC3	11:M:405:BPH:HHD	1.86	0.57
8:E:102:6PL:H261	9:E:103:CDL:H801	1.87	0.57
9:E:103:CDL:H571	9:G:101:CDL:H621	1.87	0.57
4:L:104:ARG:NH1	5:M:255:THR:O	2.37	0.57
1:Y:7:LEU:HD21	1:1:10:PRO:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:150:GLY:O	4:L:154:HIS:ND1	2.38	0.56
6:A:100:BCL:H102	6:A:100:BCL:H161	1.87	0.56
8:E:102:6PL:H42	8:E:102:6PL:H2	1.87	0.56
1:N:3:ARG:HA	1:N:6:LEU:HD13	1.88	0.56
9:M:409:CDL:H221	10:R:102:LMT:H112	1.87	0.56
2:S:43:ARG:NH2	2:Q:48:LYS:O	2.38	0.56
12:L:307:U10:H28	12:L:307:U10:H372	1.88	0.56
8:Q:102:6PL:H141	8:Q:102:6PL:H352	1.86	0.56
2:6:17:PHE:HB2	7:7:101:CRT:H32A	1.87	0.56
1:E:5:TRP:HE1	2:F:18:HIS:HD2	1.52	0.56
1:P:32:LEU:O	1:P:35:THR:HG22	2.05	0.56
1:C:18:PHE:HB3	6:C:101:BCL:H61	1.87	0.56
6:A:100:BCL:H172	1:9:20:PHE:HB3	1.86	0.56
2:U:32:ALA:O	2:U:36:HIS:ND1	2.27	0.56
8:B:104:6PL:H441	8:B:104:6PL:H252	1.88	0.56
1:G:22:PHE:HB2	6:G:103:BCL:H52	1.87	0.56
2:O:49:ALA:HA	2:Q:43:ARG:HH12	1.70	0.56
1:V:19:VAL:HG22	6:V:101:BCL:H122	1.88	0.56
6:A:100:BCL:HBB2	7:0:101:CRT:H403	1.88	0.56
9:G:105:CDL:HB22	9:G:105:CDL:HB32	1.86	0.56
4:L:266:TRP:HZ3	12:L:309:U10:H3M3	1.71	0.56
12:L:307:U10:H38	12:L:307:U10:H261	1.88	0.56
6:C:101:BCL:HBB2	7:B:103:CRT:H403	1.87	0.56
4:L:71:ASP:OD1	4:L:72:ALA:N	2.39	0.55
1:G:44:PRO:HG3	2:I:43:ARG:HH22	1.71	0.55
2:D:42:TRP:HB2	10:B:101:LMT:H11	1.88	0.55
1:G:5:TRP:HE1	2:I:18:HIS:HD2	1.55	0.55
5:M:70:ILE:HA	12:M:410:U10:H4M2	1.87	0.55
2:4:21:PHE:CE1	7:4:103:CRT:H16	2.42	0.55
7:Z:102:CRT:H403	6:1:101:BCL:HBB2	1.89	0.55
12:M:410:U10:H261	6:T:100:BCL:H192	1.88	0.55
8:I:103:6PL:H391	8:I:103:6PL:H191	1.87	0.55
2:X:17:PHE:CD1	7:X:101:CRT:H6	2.39	0.55
1:E:11:ARG:NH1	8:E:102:6PL:O1P	2.30	0.55
5:M:276:CYS:HB3	5:M:277:PRO:HD3	1.89	0.55
9:L:310:CDL:H771	1:9:8:PHE:HZ	1.71	0.54
1:9:1:FME:O	1:9:3:ARG:NH1	2.40	0.54
9:E:103:CDL:H811	9:G:101:CDL:H622	1.89	0.54
1:9:24:LEU:O	1:9:28:ILE:HG13	2.08	0.54
1:Y:7:LEU:HB2	7:2:102:CRT:H21A	1.89	0.54
2:K:40:TRP:HE1	8:K:102:6PL:H2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:205:GLU:OE2	5:M:24:ARG:NH1	2.41	0.54
1:P:32:LEU:HD11	6:Q:100:BCL:HHD	1.89	0.54
9:M:408:CDL:H861	8:P:103:6PL:H192	1.90	0.54
1:V:32:LEU:HD11	6:V:102:BCL:HHD	1.90	0.54
7:X:101:CRT:H372	1:Y:29:HIS:CG	2.43	0.54
8:S:102:6PL:H142	8:S:102:6PL:H322	1.89	0.54
8:M:401:6PL:H152	8:P:103:6PL:H131	1.90	0.53
12:M:410:U10:H211	1:T:23:GLY:HA3	1.89	0.53
8:F:103:6PL:H171	8:I:101:6PL:H231	1.90	0.53
6:Y:102:BCL:H11	7:Z:102:CRT:H25	1.91	0.53
1:A:29:HIS:CG	7:O:101:CRT:H372	2.43	0.53
2:6:38:LEU:HB3	10:6:101:LMT:H52	1.89	0.53
10:J:102:LMT:O2'	8:L:305:6PL:O31	2.16	0.53
2:U:21:PHE:CD1	7:U:101:CRT:H14	2.43	0.53
1:Y:18:PHE:HB3	6:Y:101:BCL:H61	1.90	0.53
1:7:14:LEU:HD11	2:8:17:PHE:HZ	1.73	0.53
8:6:102:6PL:H201	8:6:102:6PL:H372	1.91	0.53
7:Z:102:CRT:H372	1:1:29:HIS:CG	2.44	0.53
1:9:1:FME:SD	1:9:3:ARG:NH1	2.82	0.53
1:E:32:LEU:HD11	6:F:102:BCL:HHD	1.90	0.53
7:X:101:CRT:H403	6:Y:101:BCL:HBB2	1.90	0.53
6:A:100:BCL:H61	6:A:100:BCL:H13	1.91	0.53
1:P:22:PHE:HB2	6:P:102:BCL:H52	1.90	0.53
7:D:101:CRT:H35	6:E:101:BCL:HMB1	1.91	0.52
8:8:102:6PL:H381	8:8:102:6PL:H212	1.91	0.52
6:C:102:BCL:H11	7:D:101:CRT:H25	1.92	0.52
6:L:308:BCL:H42	12:L:309:U10:H512	1.91	0.52
6:Y:102:BCL:HAA1	8:Z:103:6PL:H262	1.91	0.52
2:Z:17:PHE:HB2	7:Z:102:CRT:H32A	1.92	0.52
8:2:103:6PL:H361	8:2:103:6PL:H131	1.90	0.52
1:5:27:ILE:HD11	8:5:102:6PL:H201	1.90	0.52
8:F:103:6PL:H431	8:F:103:6PL:H222	1.92	0.52
5:M:135:ARG:HH11	9:M:409:CDL:HA62	1.74	0.52
2:F:38:LEU:HB3	10:F:101:LMT:H12	1.91	0.52
1:G:30:PHE:HB3	8:L:305:6PL:H331	1.91	0.52
3:H:54:VAL:CG1	3:H:55:PRO:HD3	2.39	0.52
6:U:100:BCL:H151	8:U:102:6PL:H422	1.92	0.52
1:N:32:LEU:HD11	6:N:102:BCL:HHD	1.90	0.52
1:P:10:PRO:HB3	2:Q:17:PHE:CZ	2.45	0.52
8:6:102:6PL:H202	8:6:102:6PL:H391	1.90	0.52
1:9:28:ILE:HG12	7:O:101:CRT:H401	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:29:ILE:O	2:U:33:VAL:HG23	2.09	0.51
1:9:7:LEU:HA	2:0:6:ILE:HB	1.91	0.51
2:D:32:ALA:O	2:D:36:HIS:ND1	2.25	0.51
2:D:40:TRP:HZ2	8:D:102:6PL:H11	1.75	0.51
2:8:6:ILE:H	2:8:6:ILE:HD12	1.75	0.51
2:D:40:TRP:CD1	8:D:102:6PL:H401	2.46	0.51
7:O:102:CRT:H403	6:P:102:BCL:HBB2	1.92	0.51
15:7:103:PGT:H471	15:9:101:PGT:H381	1.93	0.51
1:C:32:LEU:HD11	6:C:102:BCL:HHD	1.92	0.51
3:H:110:GLY:HA3	3:H:241:ALA:HB2	1.93	0.51
1:9:32:LEU:O	1:9:35:THR:HG22	2.10	0.51
1:Y:7:LEU:HD22	7:2:102:CRT:H31A	1.93	0.51
3:H:20:PHE:HA	9:M:408:CDL:H621	1.93	0.51
2:X:37:ILE:HG22	2:X:41:MET:HE2	1.93	0.51
2:D:17:PHE:CD1	7:D:101:CRT:H6	2.46	0.51
2:X:21:PHE:HD1	7:X:101:CRT:H14	1.76	0.51
1:5:1:FME:HE1	7:8:101:CRT:H133	1.92	0.51
1:N:5:TRP:HE1	2:O:18:HIS:HD2	1.59	0.51
2:X:21:PHE:CE1	7:X:101:CRT:H16	2.46	0.51
2:D:41:MET:HG2	8:D:102:6PL:H352	1.93	0.50
3:H:1:MET:HG2	3:H:7:LEU:HD23	1.94	0.50
5:M:280:GLY:HA2	6:M:404:BCL:HED2	1.92	0.50
1:1:3:ARG:HB2	7:4:103:CRT:H5	1.93	0.50
2:4:19:SER:O	2:4:23:THR:HG23	2.10	0.50
2:B:32:ALA:O	2:B:36:HIS:ND1	2.29	0.50
1:G:19:VAL:HG12	9:G:101:CDL:H802	1.93	0.50
2:Z:40:TRP:CZ2	8:Z:103:6PL:H141	2.47	0.50
8:D:102:6PL:H221	8:D:102:6PL:H442	1.94	0.49
10:J:102:LMT:H4'	10:H:302:LMT:H1'	1.94	0.49
2:Z:45:TRP:HD1	2:Z:46:LEU:HG	1.77	0.49
1:9:7:LEU:HB2	2:0:6:ILE:HD12	1.93	0.49
2:0:37:ILE:HG22	2:0:41:MET:HE3	1.94	0.49
2:U:10:SER:HB2	2:U:13:GLU:HG2	1.93	0.49
2:Z:47:PRO:O	2:2:43:ARG:NH2	2.45	0.49
1:C:29:HIS:CG	7:B:103:CRT:H372	2.47	0.49
6:G:104:BCL:H152	8:I:103:6PL:H422	1.93	0.49
2:S:21:PHE:CD2	7:S:101:CRT:H14	2.48	0.49
2:B:11:GLU:O	2:B:15:LYS:HG2	2.12	0.49
2:4:42:TRP:HB2	10:4:101:LMT:H31	1.94	0.49
2:6:21:PHE:CD1	7:7:101:CRT:H14	2.47	0.49
1:Y:24:LEU:O	1:Y:28:ILE:HG13	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:105:CDL:H621	9:G:105:CDL:H191	1.93	0.49
1:Y:10:PRO:O	1:Y:14:LEU:HB2	2.13	0.49
1:3:32:LEU:HD11	6:4:102:BCL:HHD	1.93	0.49
7:B:103:CRT:H22A	1:9:3:ARG:HB2	1.94	0.49
6:1:102:BCL:H8	8:2:103:6PL:H432	1.94	0.49
8:2:103:6PL:H152	8:2:103:6PL:H342	1.95	0.49
3:H:153:VAL:HG12	3:H:159:VAL:HG22	1.94	0.49
1:3:20:PHE:HD2	1:3:21:LEU:HD12	1.77	0.49
2:X:21:PHE:CD1	7:X:101:CRT:H14	2.47	0.49
9:E:103:CDL:H791	9:G:101:CDL:H632	1.95	0.49
4:L:133:VAL:HG23	4:L:134:VAL:HG23	1.94	0.49
1:V:2:TRP:CE2	2:X:15:LYS:HE3	2.47	0.49
2:6:42:TRP:HB2	10:6:101:LMT:H31	1.94	0.49
9:E:103:CDL:H542	12:M:406:U10:H23	1.94	0.48
6:R:101:BCL:H171	1:P:20:PHE:HD1	1.78	0.48
8:U:102:6PL:H431	8:U:102:6PL:H231	1.95	0.48
10:J:102:LMT:H2'	10:J:102:LMT:H12	1.68	0.48
1:V:10:PRO:HB3	2:X:17:PHE:CZ	2.48	0.48
7:G:102:CRT:H35	6:G:103:BCL:HMB2	1.95	0.48
7:G:102:CRT:H291	6:G:103:BCL:H11	1.96	0.48
2:4:21:PHE:CD1	7:4:103:CRT:H14	2.48	0.48
8:K:102:6PL:H431	8:K:102:6PL:H242	1.96	0.48
2:4:38:LEU:HB3	10:4:101:LMT:H41	1.95	0.48
12:L:309:U10:H33	12:L:309:U10:H371	1.72	0.48
2:2:37:ILE:O	2:2:41:MET:HG3	2.13	0.48
2:4:21:PHE:CD1	7:4:103:CRT:H16	2.49	0.48
1:G:3:ARG:HB3	7:K:101:CRT:H23	1.96	0.48
3:H:131:PRO:HG3	3:H:167:TRP:CE2	2.49	0.48
10:R:102:LMT:H62	10:P:101:LMT:H62	1.96	0.48
9:G:105:CDL:H441	1:J:27:ILE:HD12	1.97	0.47
2:O:21:PHE:CD1	7:O:102:CRT:H14	2.49	0.47
3:H:167:TRP:HB2	3:H:177:TYR:HB2	1.96	0.47
4:L:130:VAL:HG11	9:L:310:CDL:H461	1.96	0.47
6:J:103:BCL:H8	8:K:102:6PL:H462	1.96	0.47
7:U:101:CRT:H35	6:V:101:BCL:HMB1	1.95	0.47
2:O:46:LEU:HD13	8:O:102:6PL:H182	1.95	0.47
2:D:37:ILE:HG22	2:D:41:MET:HE2	1.96	0.47
4:L:208:LYS:HG3	5:M:142:MET:HG2	1.96	0.47
6:U:100:BCL:H141	6:U:100:BCL:H161	1.69	0.47
6:A:100:BCL:H41	6:A:100:BCL:H62	1.56	0.47
2:O:19:SER:O	2:O:23:THR:HG23	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:307:U10:H251	12:L:307:U10:H272	1.70	0.47
2:X:27:LEU:O	2:X:31:VAL:HG23	2.15	0.47
1:9:10:PRO:HB3	2:0:17:PHE:CZ	2.50	0.47
2:D:17:PHE:HD1	7:D:101:CRT:H6	1.80	0.47
2:F:46:LEU:HD13	8:I:101:6PL:H361	1.97	0.47
6:N:101:BCL:HMA3	10:O:101:LMT:H121	1.96	0.47
5:M:116:LEU:HD23	1:T:30:PHE:HZ	1.79	0.47
9:M:408:CDL:H151	9:M:408:CDL:H351	1.95	0.47
8:S:102:6PL:H31	8:S:102:6PL:P	2.55	0.47
8:B:104:6PL:H32	8:B:104:6PL:H121	1.41	0.47
2:B:38:LEU:HB3	8:0:102:6PL:H192	1.96	0.47
8:O:103:6PL:H321	8:O:103:6PL:H171	1.97	0.47
5:M:128:LEU:HD11	6:T:100:BCL:H191	1.96	0.47
1:N:5:TRP:HE1	2:O:18:HIS:CD2	2.33	0.47
6:5:101:BCL:H61	6:5:101:BCL:H102	1.49	0.47
2:6:30:VAL:O	2:6:34:VAL:HG23	2.14	0.47
9:E:103:CDL:H1	9:G:101:CDL:HB32	1.97	0.46
2:Q:47:PRO:HB3	2:Q:52:TYR:CE1	2.50	0.46
2:U:13:GLU:HB2	7:U:101:CRT:H1M1	1.98	0.46
1:P:5:TRP:HE1	2:Q:18:HIS:HD2	1.63	0.46
11:M:405:BPH:HMA1	11:M:405:BPH:H143	1.98	0.46
2:X:20:ILE:HD13	7:X:101:CRT:H83	1.98	0.46
15:7:103:PGT:H151	15:7:103:PGT:H441	1.96	0.46
1:9:35:THR:HG23	1:9:38:PHE:H	1.80	0.46
2:S:43:ARG:NH1	2:Q:49:ALA:HA	2.30	0.46
2:F:49:ALA:HA	2:I:43:ARG:HH12	1.80	0.46
1:V:24:LEU:O	1:V:28:ILE:HG13	2.14	0.46
6:Q:100:BCL:H111	8:Q:102:6PL:H202	1.98	0.46
1:Y:4:ILE:HG22	1:Y:6:LEU:HB2	1.98	0.46
2:F:49:ALA:HA	2:I:43:ARG:NH1	2.31	0.46
6:F:102:BCL:H142	6:F:102:BCL:H112	1.73	0.46
12:L:307:U10:H422	12:L:307:U10:H401	1.56	0.46
2:Q:45:TRP:CD1	2:Q:46:LEU:HG	2.51	0.46
2:Z:21:PHE:CE1	7:Z:102:CRT:H16	2.51	0.46
1:G:23:GLY:O	1:G:26:ILE:HG22	2.16	0.46
9:G:105:CDL:H381	9:G:105:CDL:H162	1.97	0.46
2:K:21:PHE:CD2	7:K:101:CRT:H14	2.51	0.46
1:N:10:PRO:HB3	2:O:17:PHE:CZ	2.51	0.46
2:S:30:VAL:O	2:S:34:VAL:HG23	2.16	0.46
1:P:27:ILE:HD11	8:P:103:6PL:H241	1.98	0.46
1:G:32:LEU:HD11	6:G:104:BCL:HHD	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:104:BCL:H52	6:G:104:BCL:H12	1.79	0.45
1:V:20:PHE:HB2	6:Y:101:BCL:H143	1.98	0.45
2:Q:19:SER:O	2:Q:23:THR:HG23	2.16	0.45
7:S:101:CRT:H35	6:T:100:BCL:HMB1	1.99	0.45
2:I:32:ALA:O	2:I:36:HIS:ND1	2.25	0.45
1:C:5:TRP:HE1	2:D:18:HIS:HD2	1.64	0.45
6:J:103:BCL:H52	6:J:103:BCL:H12	1.73	0.45
6:Q:100:BCL:H12	6:Q:100:BCL:H52	1.68	0.45
6:7:104:BCL:H52	6:7:104:BCL:H12	1.75	0.45
10:F:101:LMT:H42	10:F:101:LMT:H71	1.75	0.45
8:M:401:6PL:H371	8:P:103:6PL:H122	1.99	0.45
6:U:100:BCL:H52	6:U:100:BCL:H12	1.73	0.45
1:9:1:FME:HB2	2:0:15:LYS:HE3	1.99	0.45
2:Z:45:TRP:CD1	2:Z:46:LEU:HG	2.52	0.45
1:C:12:ARG:HA	1:C:15:VAL:HG22	1.98	0.45
8:O:103:6PL:H321	8:O:103:6PL:H151	1.99	0.45
15:9:101:PGT:H261	6:9:102:BCL:H141	1.98	0.45
2:F:21:PHE:HE2	9:G:101:CDL:H211	1.81	0.45
9:G:101:CDL:H441	8:L:305:6PL:H451	1.99	0.45
8:I:103:6PL:H242	8:I:103:6PL:H202	1.98	0.45
1:T:5:TRP:HE1	2:U:18:HIS:HD2	1.64	0.45
2:X:21:PHE:CD1	7:X:101:CRT:H16	2.52	0.45
1:3:18:PHE:HB3	6:3:100:BCL:H72	1.98	0.45
2:4:13:GLU:HB3	7:4:103:CRT:H1M1	1.99	0.45
10:6:101:LMT:H1'	10:6:101:LMT:H22	1.74	0.45
8:E:102:6PL:H131	12:M:406:U10:H403	1.99	0.45
9:G:101:CDL:H592	9:G:101:CDL:H631	1.98	0.45
6:R:103:BCL:H52	6:R:103:BCL:H12	1.71	0.45
8:Q:102:6PL:H412	8:Q:102:6PL:H192	1.99	0.45
8:Z:103:6PL:H471	8:Z:103:6PL:H212	1.98	0.45
6:L:308:BCL:H51	6:L:308:BCL:H12	1.72	0.45
6:B:102:BCL:H122	8:B:104:6PL:H432	1.99	0.44
1:5:5:TRP:HE1	2:6:18:HIS:HD2	1.64	0.44
1:5:10:PRO:O	1:5:14:LEU:HB2	2.17	0.44
1:5:16:LEU:HD13	6:7:102:BCL:H143	1.99	0.44
6:1:102:BCL:H41	6:1:102:BCL:H62	1.69	0.44
5:M:75:MET:HE3	5:M:93:LEU:HB2	1.99	0.44
6:M:402:BCL:H13	6:M:402:BCL:H171	1.67	0.44
2:X:44:PRO:HD3	8:X:102:6PL:H41	1.99	0.44
1:5:24:LEU:HD23	6:5:103:BCL:HED3	1.99	0.44
1:G:44:PRO:HG3	2:I:43:ARG:NH2	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:7:4:ILE:HD12	1:7:4:ILE:H	1.83	0.44
3:H:200:ASP:HB3	3:H:201:PRO:HD3	1.99	0.44
12:M:406:U10:H272	12:M:406:U10:H251	1.70	0.44
7:4:103:CRT:H35	6:5:101:BCL:CMB	2.46	0.44
4:L:41:PHE:O	4:L:45:ILE:HG12	2.18	0.44
5:M:62:LEU:O	5:M:66:VAL:HG23	2.18	0.44
2:Z:30:VAL:O	2:Z:34:VAL:HG23	2.17	0.44
7:O:102:CRT:H2M3	1:P:29:HIS:HB3	2.00	0.44
1:A:29:HIS:CE1	6:B:102:BCL:HMD1	2.52	0.44
2:8:36:HIS:CE1	8:8:102:6PL:H251	2.53	0.44
1:9:1:FME:HE3	1:9:1:FME:HB3	1.56	0.44
6:C:102:BCL:H91	6:C:102:BCL:H111	1.70	0.43
10:J:102:LMT:H2'	10:H:302:LMT:O2'	2.18	0.43
8:L:304:6PL:H482	8:L:304:6PL:H412	2.00	0.43
12:L:307:U10:H322	1:9:20:PHE:CD2	2.53	0.43
1:Y:29:HIS:CE1	6:Y:102:BCL:HMD1	2.53	0.43
9:G:105:CDL:H271	1:J:27:ILE:HG12	2.00	0.43
8:S:102:6PL:H262	8:S:102:6PL:H222	2.00	0.43
2:X:37:ILE:HA	8:X:102:6PL:H391	2.00	0.43
2:4:40:TRP:CG	8:4:104:6PL:H431	2.53	0.43
1:T:29:HIS:CE1	6:U:100:BCL:HMD1	2.54	0.43
2:X:25:PHE:O	2:X:29:ILE:HG12	2.18	0.43
1:3:10:PRO:HB3	2:4:17:PHE:CZ	2.53	0.43
2:0:11:GLU:O	2:0:15:LYS:HG3	2.19	0.43
1:J:45:ARG:HA	1:J:45:ARG:NH2	2.34	0.43
9:L:310:CDL:H822	1:9:13:ALA:HB1	2.00	0.43
8:Q:102:6PL:H162	8:Q:102:6PL:H391	1.99	0.43
2:Z:10:SER:OG	2:Z:11:GLU:N	2.51	0.43
2:Z:21:PHE:CD1	7:Z:102:CRT:H14	2.53	0.43
1:C:29:HIS:CE1	6:C:102:BCL:HMD1	2.54	0.43
2:K:45:TRP:CD1	2:K:46:LEU:HG	2.53	0.43
1:N:27:ILE:HG12	8:M:401:6PL:H202	2.00	0.43
6:L:308:BCL:H152	6:L:308:BCL:H112	1.81	0.43
5:M:51:VAL:HG21	11:M:405:BPH:H202	1.99	0.43
6:Q:100:BCL:H152	8:Q:102:6PL:H372	2.01	0.43
2:B:6:ILE:HD12	2:B:6:ILE:H	1.83	0.43
1:1:5:TRP:HE1	2:2:18:HIS:HD2	1.66	0.43
2:8:48:LYS:HG3	2:8:49:ALA:N	2.32	0.43
11:L:302:BPH:HHC	11:L:302:BPH:CBB	2.48	0.43
5:M:284:ILE:HG12	6:M:404:BCL:HED3	2.00	0.43
1:R:42:ASP:OD2	1:P:35:THR:OG1	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:21:PHE:CD1	7:Q:101:CRT:H14	2.54	0.43
2:6:47:PRO:HB3	2:6:52:TYR:CZ	2.54	0.43
2:8:27:LEU:HA	2:8:30:VAL:HG12	2.01	0.43
1:C:3:ARG:HD3	7:G:102:CRT:H41	2.00	0.43
7:S:101:CRT:H2M3	1:T:29:HIS:HB3	2.01	0.43
10:P:101:LMT:H112	10:P:101:LMT:H81	1.78	0.43
2:Z:32:ALA:O	2:Z:36:HIS:ND1	2.25	0.43
2:B:47:PRO:HB3	2:B:52:TYR:CZ	2.54	0.43
7:2:102:CRT:H35	6:3:100:BCL:HMB2	2.01	0.43
2:4:48:LYS:C	2:6:43:ARG:HH21	2.27	0.43
2:6:45:TRP:HD1	2:6:46:LEU:HG	1.83	0.43
2:F:48:LYS:O	2:I:43:ARG:NH2	2.52	0.43
9:G:101:CDL:H602	8:L:305:6PL:H251	2.01	0.43
8:I:103:6PL:H2	8:I:103:6PL:H321	1.70	0.43
6:Y:102:BCL:H142	6:Y:102:BCL:H112	1.78	0.43
6:5:103:BCL:H91	6:5:103:BCL:H111	1.76	0.43
1:J:37:ARG:O	2:K:43:ARG:NH1	2.52	0.43
3:H:140:LEU:HD23	3:H:140:LEU:HA	1.90	0.43
2:F:22:VAL:HG22	9:G:101:CDL:H251	2.01	0.43
10:J:102:LMT:H6'2	10:H:302:LMT:H5'	2.00	0.43
6:T:100:BCL:H161	6:T:100:BCL:H141	1.74	0.43
2:U:36:HIS:CD2	8:U:102:6PL:H452	2.54	0.43
1:A:28:ILE:HG12	7:B:103:CRT:C40	2.48	0.43
2:4:17:PHE:CD1	7:4:103:CRT:H6	2.54	0.43
6:5:101:BCL:H162	6:5:101:BCL:H192	1.80	0.43
6:R:101:BCL:H192	6:R:101:BCL:H162	1.85	0.42
1:T:7:LEU:HG	7:X:101:CRT:H22A	2.01	0.42
2:X:17:PHE:CD1	7:X:101:CRT:H9	2.54	0.42
6:1:102:BCL:HAA1	8:2:103:6PL:H201	2.01	0.42
2:0:18:HIS:O	2:0:22:VAL:HG13	2.19	0.42
4:L:242:VAL:HG21	11:L:302:BPH:HBC3	2.01	0.42
1:R:24:LEU:O	1:R:28:ILE:HG13	2.19	0.42
6:V:102:BCL:H141	6:V:102:BCL:H161	1.76	0.42
2:6:45:TRP:CD1	2:6:46:LEU:HG	2.54	0.42
8:D:102:6PL:H221	8:D:102:6PL:H461	2.01	0.42
5:M:145:HIS:CD2	9:M:408:CDL:HA61	2.55	0.42
6:R:103:BCL:HAA1	8:S:102:6PL:H482	2.02	0.42
3:H:169:ASP:HB2	3:H:176:ARG:HG3	2.00	0.42
4:L:38:MET:HE1	9:L:310:CDL:H601	2.01	0.42
4:L:194:LEU:HD22	4:L:217:PHE:CE2	2.54	0.42
1:R:7:LEU:HD11	7:U:101:CRT:H31A	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:10:PRO:HB3	2:S:17:PHE:CE1	2.54	0.42
8:E:102:6PL:H73	3:H:91:TRP:CZ3	2.55	0.42
6:G:104:BCL:H18	8:I:103:6PL:H382	2.02	0.42
2:I:21:PHE:CD2	7:I:102:CRT:H14	2.54	0.42
5:M:179:VAL:O	5:M:182:HIS:ND1	2.51	0.42
6:Y:101:BCL:HMA3	10:Z:101:LMT:H122	2.00	0.42
6:1:102:BCL:HBB1	10:4:101:LMT:H62	2.02	0.42
1:3:5:TRP:HE1	2:4:18:HIS:CD2	2.37	0.42
2:D:26[A]:PHE:HD1	2:D:26[A]:PHE:HA	1.77	0.42
2:O:40:TRP:CD1	8:O:103:6PL:H172	2.54	0.42
7:4:103:CRT:H2M1	1:5:30:PHE:CE2	2.54	0.42
1:C:10:PRO:O	1:C:14:LEU:HB2	2.19	0.42
1:N:36:SER:HB2	1:N:46:ALA:HB3	2.01	0.42
1:A:22:PHE:CE1	6:A:100:BCL:H171	2.54	0.42
1:9:11:ARG:NH1	1:9:12:ARG:HH11	2.18	0.42
2:O:49:ALA:HA	2:Q:43:ARG:NH1	2.35	0.42
6:Y:102:BCL:H141	6:Y:102:BCL:H161	1.91	0.42
2:B:29:ILE:HD11	6:B:102:BCL:H2	2.01	0.42
1:G:24:LEU:HD23	6:G:104:BCL:HED3	2.02	0.42
2:O:45:TRP:CD1	2:O:46:LEU:HG	2.55	0.42
12:L:307:U10:H412	1:9:19:VAL:HG13	2.02	0.42
5:M:234:GLU:OE2	5:M:266:HIS:CE1	2.72	0.42
1:3:23:GLY:O	1:3:26:ILE:HG22	2.20	0.42
2:4:33:VAL:HG13	8:4:104:6PL:H481	2.02	0.42
8:5:102:6PL:H212	8:5:102:6PL:H172	2.02	0.42
2:8:40:TRP:CH2	8:8:102:6PL:H152	2.55	0.42
9:G:105:CDL:H451	1:N:22:PHE:CZ	2.48	0.42
2:K:45:TRP:HD1	2:K:46:LEU:HG	1.84	0.42
6:Y:102:BCL:H12	6:Y:102:BCL:H52	1.80	0.42
2:2:32:ALA:O	2:2:36:HIS:ND1	2.26	0.42
2:2:47:PRO:O	2:4:43:ARG:NH2	2.53	0.42
1:N:3:ARG:HD3	7:Q:101:CRT:H41	2.00	0.41
1:N:46:ALA:HB1	3:H:2:GLN:HB3	2.01	0.41
1:R:1:FME:HCN	1:R:3:ARG:HH21	1.84	0.41
1:1:7:LEU:HD21	1:3:10:PRO:HB2	2.01	0.41
6:1:101:BCL:H151	6:1:101:BCL:H18	1.97	0.41
9:E:103:CDL:H312	9:E:103:CDL:HA62	1.81	0.41
1:Y:10:PRO:HB3	2:Z:17:PHE:CZ	2.55	0.41
2:2:45:TRP:HD1	2:2:46:LEU:HG	1.86	0.41
1:7:23:GLY:HA2	15:7:103:PGT:H231	2.01	0.41
1:7:32:LEU:HD11	6:7:104:BCL:HHD	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:60:TRP:HZ3	8:L:304:6PL:H181	1.84	0.41
12:L:307:U10:H1M1	12:L:307:U10:H72	1.85	0.41
6:L:308:BCL:H43	11:M:405:BPH:HMA3	2.01	0.41
5:M:175:PRO:HA	5:M:176:PRO:HD3	1.94	0.41
1:P:35:THR:HG23	1:P:38:PHE:H	1.84	0.41
6:Q:100:BCL:H11	7:Q:101:CRT:H25	2.01	0.41
2:4:45:TRP:CD1	2:4:46:LEU:HG	2.55	0.41
3:H:151:PRO:HD2	3:H:203:GLY:O	2.20	0.41
1:7:5:TRP:HE1	2:8:18:HIS:HD2	1.69	0.41
6:7:104:BCL:HAA2	2:8:36:HIS:HE1	1.85	0.41
1:9:10:PRO:HB3	2:0:17:PHE:CE2	2.54	0.41
2:D:38:LEU:HB3	10:B:101:LMT:H42	2.02	0.41
1:E:24:LEU:O	1:E:28:ILE:HG13	2.21	0.41
6:F:102:BCL:H192	8:I:101:6PL:H241	2.02	0.41
3:H:130:VAL:HG12	3:H:131:PRO:O	2.20	0.41
12:L:309:U10:H502	12:L:309:U10:H261	2.03	0.41
12:M:410:U10:O2	1:T:27:ILE:HG21	2.21	0.41
1:3:29:HIS:CE1	6:4:102:BCL:HMD1	2.56	0.41
1:9:30:PHE:HD1	15:9:101:PGT:H31	1.86	0.41
6:0:100:BCL:H52	6:0:100:BCL:H12	1.77	0.41
2:F:41:MET:HG2	8:F:103:6PL:H341	2.02	0.41
6:J:103:BCL:H161	6:J:103:BCL:H141	1.67	0.41
5:M:270:TRP:CH2	9:M:408:CDL:H322	2.56	0.41
6:M:404:BCL:H192	6:M:404:BCL:H162	1.71	0.41
1:T:5:TRP:HE1	2:U:18:HIS:CD2	2.38	0.41
6:P:102:BCL:H161	6:P:102:BCL:H122	1.90	0.41
1:3:5:TRP:HE1	2:4:18:HIS:HD2	1.69	0.41
6:4:102:BCL:H12	6:4:102:BCL:H52	1.78	0.41
7:D:101:CRT:H2M1	1:E:30:PHE:CE2	2.56	0.41
1:R:23:GLY:O	1:R:26:ILE:HG22	2.20	0.41
1:R:32:LEU:HD23	1:R:32:LEU:HA	1.93	0.41
6:V:102:BCL:H172	8:X:102:6PL:H461	2.03	0.41
6:5:103:BCL:H52	6:5:103:BCL:H12	1.77	0.41
1:E:31:ILE:HG12	8:L:304:6PL:H341	2.03	0.41
10:F:101:LMT:H21	10:F:101:LMT:H1'	1.70	0.41
6:N:102:BCL:H52	6:N:102:BCL:H12	1.81	0.41
2:O:26[A]:PHE:O	2:O:30:VAL:HG13	2.21	0.41
3:H:132:LEU:HD23	3:H:132:LEU:HA	1.84	0.41
4:L:219:ASP:O	5:M:132:ARG:NH1	2.53	0.41
5:M:66:VAL:O	5:M:70:ILE:HG13	2.20	0.41
1:R:33:LEU:HD13	1:R:40:TRP:CH2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:25:PHE:O	2:S:29:ILE:HG12	2.20	0.41
6:V:102:BCL:H91	6:V:102:BCL:H111	1.83	0.41
1:Y:28:ILE:HG12	7:Z:102:CRT:H401	2.03	0.41
1:A:30:PHE:CE1	7:0:101:CRT:H2M1	2.56	0.41
6:A:100:BCL:H191	1:9:21:LEU:HD12	2.02	0.41
9:G:101:CDL:H742	3:H:54:VAL:HG11	2.03	0.41
6:B:102:BCL:H203	6:B:102:BCL:H13	2.02	0.41
2:6:40:TRP:CG	8:6:102:6PL:H342	2.56	0.41
15:7:103:PGT:H392	15:7:103:PGT:H421	1.97	0.41
2:I:19:SER:O	2:I:23:THR:HG23	2.21	0.40
8:I:101:6PL:H2	8:I:101:6PL:O2P	2.21	0.40
11:L:302:BPH:H112	11:L:302:BPH:H7C2	1.88	0.40
2:8:48:LYS:CG	2:8:49:ALA:H	2.31	0.40
7:G:102:CRT:H20	7:G:102:CRT:H181	1.95	0.40
10:J:102:LMT:H71	8:L:305:6PL:H192	2.02	0.40
1:9:5:TRP:HE1	2:0:18:HIS:CD2	2.39	0.40
5:M:192:LYS:HE3	5:M:193:TYR:CZ	2.55	0.40
2:U:40:TRP:CG	8:U:102:6PL:H201	2.56	0.40
7:2:102:CRT:H26	7:2:102:CRT:H241	1.98	0.40
2:4:43:ARG:HA	2:4:44:PRO:HD3	1.94	0.40
2:4:48:LYS:O	2:6:43:ARG:NH2	2.54	0.40
1:V:28:ILE:HG12	7:X:101:CRT:H401	2.04	0.40
7:Q:101:CRT:H20	7:Q:101:CRT:H181	1.96	0.40
6:1:102:BCL:H102	8:2:103:6PL:H181	2.02	0.40
10:2:101:LMT:H82	10:2:101:LMT:H52	1.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	44/48 (92%)	44 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	3	44/48 (92%)	43 (98%)	1 (2%)	0	100	100
1	5	44/48 (92%)	43 (98%)	1 (2%)	0	100	100
1	7	44/48 (92%)	42 (96%)	2 (4%)	0	100	100
1	9	44/48 (92%)	43 (98%)	1 (2%)	0	100	100
1	A	44/48 (92%)	44 (100%)	0	0	100	100
1	C	44/48 (92%)	44 (100%)	0	0	100	100
1	E	44/48 (92%)	42 (96%)	2 (4%)	0	100	100
1	G	44/48 (92%)	42 (96%)	2 (4%)	0	100	100
1	J	43/48 (90%)	42 (98%)	1 (2%)	0	100	100
1	N	44/48 (92%)	42 (96%)	2 (4%)	0	100	100
1	P	44/48 (92%)	43 (98%)	1 (2%)	0	100	100
1	R	44/48 (92%)	43 (98%)	1 (2%)	0	100	100
1	T	46/48 (96%)	45 (98%)	1 (2%)	0	100	100
1	V	44/48 (92%)	43 (98%)	1 (2%)	0	100	100
1	Y	43/48 (90%)	41 (95%)	2 (5%)	0	100	100
2	0	48/52 (92%)	45 (94%)	3 (6%)	0	100	100
2	2	47/52 (90%)	44 (94%)	3 (6%)	0	100	100
2	4	47/52 (90%)	45 (96%)	2 (4%)	0	100	100
2	6	49/52 (94%)	46 (94%)	3 (6%)	0	100	100
2	8	48/52 (92%)	44 (92%)	4 (8%)	0	100	100
2	B	48/52 (92%)	45 (94%)	3 (6%)	0	100	100
2	D	48/52 (92%)	45 (94%)	3 (6%)	0	100	100
2	F	48/52 (92%)	46 (96%)	2 (4%)	0	100	100
2	I	45/52 (86%)	42 (93%)	3 (7%)	0	100	100
2	K	46/52 (88%)	44 (96%)	2 (4%)	0	100	100
2	O	47/52 (90%)	44 (94%)	3 (6%)	0	100	100
2	Q	47/52 (90%)	45 (96%)	2 (4%)	0	100	100
2	S	47/52 (90%)	44 (94%)	3 (6%)	0	100	100
2	U	46/52 (88%)	43 (94%)	3 (6%)	0	100	100
2	X	45/52 (86%)	42 (93%)	3 (7%)	0	100	100
2	Z	47/52 (90%)	44 (94%)	3 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	H	245/255 (96%)	235 (96%)	10 (4%)	0	100	100
4	L	274/277 (99%)	270 (98%)	4 (2%)	0	100	100
5	M	304/307 (99%)	298 (98%)	6 (2%)	0	100	100
All	All	2280/2439 (94%)	2197 (96%)	83 (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	1	40/41 (98%)	40 (100%)	0	100	100
1	3	40/41 (98%)	40 (100%)	0	100	100
1	5	40/41 (98%)	40 (100%)	0	100	100
1	7	40/41 (98%)	40 (100%)	0	100	100
1	9	40/41 (98%)	40 (100%)	0	100	100
1	A	40/41 (98%)	40 (100%)	0	100	100
1	C	40/41 (98%)	40 (100%)	0	100	100
1	E	40/41 (98%)	40 (100%)	0	100	100
1	G	40/41 (98%)	40 (100%)	0	100	100
1	J	40/41 (98%)	40 (100%)	0	100	100
1	N	40/41 (98%)	40 (100%)	0	100	100
1	P	40/41 (98%)	40 (100%)	0	100	100
1	R	40/41 (98%)	40 (100%)	0	100	100
1	T	41/41 (100%)	41 (100%)	0	100	100
1	V	40/41 (98%)	40 (100%)	0	100	100
1	Y	40/41 (98%)	40 (100%)	0	100	100
2	0	41/43 (95%)	41 (100%)	0	100	100
2	2	41/43 (95%)	41 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	4	41/43 (95%)	41 (100%)	0	100	100
2	6	42/43 (98%)	42 (100%)	0	100	100
2	8	41/43 (95%)	41 (100%)	0	100	100
2	B	41/43 (95%)	41 (100%)	0	100	100
2	D	41/43 (95%)	41 (100%)	0	100	100
2	F	41/43 (95%)	41 (100%)	0	100	100
2	I	39/43 (91%)	39 (100%)	0	100	100
2	K	40/43 (93%)	40 (100%)	0	100	100
2	O	41/43 (95%)	41 (100%)	0	100	100
2	Q	41/43 (95%)	41 (100%)	0	100	100
2	S	41/43 (95%)	41 (100%)	0	100	100
2	U	40/43 (93%)	40 (100%)	0	100	100
2	X	39/43 (91%)	39 (100%)	0	100	100
2	Z	41/43 (95%)	41 (100%)	0	100	100
3	H	195/203 (96%)	195 (100%)	0	100	100
4	L	222/223 (100%)	222 (100%)	0	100	100
5	M	246/247 (100%)	246 (100%)	0	100	100
All	All	1955/2017 (97%)	1955 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	39	ASN
2	D	18	HIS
2	F	18	HIS
2	I	18	HIS
2	K	18	HIS
2	O	18	HIS
3	H	11	GLN
3	H	82	ASN
4	L	160	ASN
4	L	167	GLN
4	L	267	ASN
4	L	271	ASN

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Mol	Chain	Res	Type
5	M	5	GLN
5	M	12	GLN
5	M	74	ASN
5	M	202	HIS
2	S	18	HIS
2	U	18	HIS
2	Q	18	HIS
2	B	18	HIS
2	2	18	HIS
2	4	18	HIS
2	6	18	HIS
1	7	39	ASN
2	0	18	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

15 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
1	FME	G	1	1	8,9,10	0.97	0	8,9,11	0.83	0
1	FME	C	1	1	8,9,10	0.98	0	8,9,11	0.86	0
1	FME	1	1	1	8,9,10	0.97	0	8,9,11	0.91	0
1	FME	E	1	1	8,9,10	0.97	0	8,9,11	0.81	0
1	FME	J	1	1	8,9,10	0.98	0	8,9,11	0.91	0
1	FME	T	1	1	8,9,10	0.95	0	8,9,11	0.86	0
1	FME	P	1	1	8,9,10	1.01	0	8,9,11	0.70	0
1	FME	7	1	1	8,9,10	0.93	0	8,9,11	1.26	1 (12%)
1	FME	A	1	1	8,9,10	0.98	0	8,9,11	0.86	0
1	FME	3	1	1	8,9,10	0.95	0	8,9,11	0.95	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	FME	V	1	1	8,9,10	0.98	0	8,9,11	0.92	0
1	FME	5	1	1	8,9,10	0.95	0	8,9,11	1.11	1 (12%)
1	FME	R	1	1	8,9,10	0.98	0	8,9,11	0.86	0
1	FME	9	1	1	8,9,10	0.96	0	8,9,11	0.88	0
1	FME	N	1	1	8,9,10	1.00	0	8,9,11	0.91	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
1	FME	G	1	1	-	1/7/9/11	-
1	FME	C	1	1	-	3/7/9/11	-
1	FME	1	1	1	-	6/7/9/11	-
1	FME	E	1	1	-	3/7/9/11	-
1	FME	J	1	1	-	2/7/9/11	-
1	FME	T	1	1	-	1/7/9/11	-
1	FME	P	1	1	-	0/7/9/11	-
1	FME	7	1	1	-	3/7/9/11	-
1	FME	A	1	1	-	3/7/9/11	-
1	FME	3	1	1	-	1/7/9/11	-
1	FME	V	1	1	-	1/7/9/11	-
1	FME	5	1	1	-	3/7/9/11	-
1	FME	R	1	1	-	5/7/9/11	-
1	FME	9	1	1	-	3/7/9/11	-
1	FME	N	1	1	-	2/7/9/11	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	7	1	FME	C-CA-N	2.70	114.71	109.50
1	5	1	FME	C-CA-N	2.27	113.88	109.50
1	3	1	FME	C-CA-N	2.03	113.42	109.50

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	E	1	FME	CB-CA-N-CN
1	N	1	FME	N-CA-CB-CG
1	N	1	FME	C-CA-CB-CG
1	R	1	FME	C-CA-CB-CG
1	R	1	FME	O-C-CA-CB
1	A	1	FME	N-CA-CB-CG
1	1	1	FME	CB-CA-N-CN
1	1	1	FME	N-CA-CB-CG
1	1	1	FME	C-CA-CB-CG
1	1	1	FME	O-C-CA-CB
1	5	1	FME	O-C-CA-CB
1	9	1	FME	CA-CB-CG-SD
1	1	1	FME	CA-CB-CG-SD
1	7	1	FME	CA-CB-CG-SD
1	R	1	FME	N-CA-CB-CG
1	7	1	FME	N-CA-CB-CG
1	9	1	FME	N-CA-CB-CG
1	9	1	FME	CB-CG-SD-CE
1	A	1	FME	CA-CB-CG-SD
1	C	1	FME	N-CA-CB-CG
1	E	1	FME	N-CA-CB-CG
1	J	1	FME	N-CA-CB-CG
1	T	1	FME	N-CA-CB-CG
1	V	1	FME	N-CA-CB-CG
1	1	1	FME	CB-CG-SD-CE
1	A	1	FME	C-CA-CB-CG
1	7	1	FME	C-CA-CB-CG
1	R	1	FME	CB-CA-N-CN
1	C	1	FME	CB-CG-SD-CE
1	E	1	FME	CB-CG-SD-CE
1	R	1	FME	CB-CG-SD-CE
1	J	1	FME	CB-CG-SD-CE
1	G	1	FME	N-CA-CB-CG
1	5	1	FME	N-CA-CB-CG
1	5	1	FME	CB-CG-SD-CE
1	C	1	FME	CB-CA-N-CN
1	3	1	FME	N-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	5	1	FME	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	R	1	FME	1	0
1	9	1	FME	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 105 ligands modelled in this entry, 1 is monoatomic - leaving 104 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
8	6PL	Z	103	-	51,51,51	0.28	0	57,59,59	0.31	0
10	LMT	O	101	-	36,36,36	1.18	6 (16%)	47,47,47	1.08	2 (4%)
15	PGT	7	103	-	50,50,50	0.26	0	53,56,56	0.33	0
7	CRT	2	102	-	43,43,43	1.50	12 (27%)	48,54,54	1.75	16 (33%)
6	BCL	1	102	-	69,74,74	1.80	17 (24%)	79,115,115	2.20	24 (30%)
9	CDL	G	101	-	99,99,99	0.27	0	105,111,111	0.35	0
10	LMT	P	101	-	36,36,36	1.15	5 (13%)	47,47,47	0.98	2 (4%)
6	BCL	M	404	-	69,74,74	1.82	17 (24%)	79,115,115	2.29	25 (31%)
8	6PL	5	102	-	51,51,51	0.27	0	57,59,59	0.31	0
10	LMT	F	101	-	36,36,36	1.18	5 (13%)	47,47,47	1.03	1 (2%)
6	BCL	Y	101	-	69,74,74	1.77	17 (24%)	79,115,115	2.35	23 (29%)
7	CRT	I	102	-	43,43,43	1.50	12 (27%)	48,54,54	1.65	14 (29%)
8	6PL	Q	102	-	47,47,51	0.28	0	53,55,59	0.31	0
14	QAK	M	407	-	39,40,40	1.48	3 (7%)	46,49,49	0.94	3 (6%)
6	BCL	E	101	-	69,74,74	1.78	18 (26%)	79,115,115	2.30	21 (26%)
6	BCL	J	103	-	69,74,74	1.79	17 (24%)	79,115,115	2.24	22 (27%)
7	CRT	X	101	-	43,43,43	1.50	12 (27%)	48,54,54	1.73	16 (33%)
6	BCL	P	102	-	69,74,74	1.78	17 (24%)	79,115,115	2.31	22 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	BCL	L	301	-	69,74,74	1.79	17 (24%)	79,115,115	2.26	22 (27%)
12	U10	M	410	-	63,63,63	2.73	17 (26%)	78,79,79	1.78	22 (28%)
12	U10	L	303	-	48,48,63	2.75	14 (29%)	60,61,79	1.74	15 (25%)
6	BCL	5	103	-	69,74,74	1.79	17 (24%)	79,115,115	2.23	21 (26%)
6	BCL	A	100	-	69,74,74	1.78	18 (26%)	79,115,115	2.35	23 (29%)
7	CRT	G	102	-	43,43,43	1.51	12 (27%)	48,54,54	1.63	16 (33%)
6	BCL	3	100	-	69,74,74	1.79	18 (26%)	79,115,115	2.28	22 (27%)
9	CDL	M	409	-	83,83,99	0.29	0	89,95,111	0.38	0
8	6PL	P	103	-	51,51,51	0.28	0	57,59,59	0.37	0
8	6PL	4	104	-	51,51,51	0.28	0	57,59,59	0.35	0
7	CRT	8	101	-	43,43,43	1.52	12 (27%)	48,54,54	1.85	15 (31%)
6	BCL	R	101	-	69,74,74	1.78	17 (24%)	79,115,115	2.30	23 (29%)
10	LMT	2	101	-	36,36,36	1.15	3 (8%)	47,47,47	1.06	2 (4%)
7	CRT	U	101	-	43,43,43	1.50	12 (27%)	48,54,54	1.64	14 (29%)
6	BCL	F	102	-	69,74,74	1.80	17 (24%)	79,115,115	2.23	24 (30%)
6	BCL	U	100	-	69,74,74	1.80	17 (24%)	79,115,115	2.23	24 (30%)
8	6PL	X	102	-	51,51,51	0.28	0	57,59,59	0.34	0
8	6PL	I	101	-	51,51,51	0.28	0	57,59,59	0.37	0
8	6PL	8	102	-	51,51,51	0.28	0	57,59,59	0.31	0
8	6PL	0	102	-	51,51,51	0.28	0	57,59,59	0.40	0
8	6PL	L	305	-	51,51,51	0.30	0	57,59,59	0.34	0
8	6PL	E	102	-	51,51,51	0.29	0	57,59,59	0.28	0
12	U10	L	307	-	63,63,63	2.76	17 (26%)	78,79,79	1.74	20 (25%)
6	BCL	M	402	-	69,74,74	1.77	17 (24%)	79,115,115	2.25	23 (29%)
6	BCL	G	103	-	69,74,74	1.77	17 (24%)	79,115,115	2.36	23 (29%)
9	CDL	M	408	-	89,89,99	0.29	0	95,101,111	0.37	0
6	BCL	Y	102	-	69,74,74	1.79	17 (24%)	79,115,115	2.17	22 (27%)
7	CRT	4	103	-	43,43,43	1.50	12 (27%)	48,54,54	1.69	15 (31%)
8	6PL	2	103	-	46,46,51	0.29	0	52,54,59	0.32	0
6	BCL	J	101	-	69,74,74	1.78	17 (24%)	79,115,115	2.34	23 (29%)
6	BCL	N	101	-	69,74,74	1.78	17 (24%)	79,115,115	2.29	24 (30%)
7	CRT	Q	101	-	43,43,43	1.50	12 (27%)	48,54,54	1.61	15 (31%)
7	CRT	Z	102	-	43,43,43	1.50	12 (27%)	48,54,54	1.57	14 (29%)
6	BCL	Q	100	-	69,74,74	1.79	17 (24%)	79,115,115	2.22	22 (27%)
10	LMT	6	101	-	36,36,36	1.18	5 (13%)	47,47,47	1.05	1 (2%)
7	CRT	0	101	-	43,43,43	1.50	12 (27%)	48,54,54	1.61	14 (29%)
8	6PL	S	102	-	51,51,51	0.28	0	57,59,59	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	LMT	B	101	-	36,36,36	1.15	3 (8%)	47,47,47	0.99	1 (2%)
6	BCL	0	100	-	69,74,74	1.79	17 (24%)	79,115,115	2.27	24 (30%)
6	BCL	R	103	-	69,74,74	1.78	17 (24%)	79,115,115	2.21	23 (29%)
8	6PL	L	304	-	51,51,51	0.27	0	57,59,59	0.36	0
10	LMT	J	102	-	36,36,36	1.12	4 (11%)	47,47,47	1.12	3 (6%)
7	CRT	D	101	-	43,43,43	1.50	12 (27%)	48,54,54	1.63	16 (33%)
7	CRT	7	101	-	43,43,43	1.51	12 (27%)	48,54,54	1.62	14 (29%)
8	6PL	F	103	-	51,51,51	0.26	0	57,59,59	0.41	0
6	BCL	L	308	-	69,74,74	1.83	17 (24%)	79,115,115	2.23	21 (26%)
6	BCL	T	100	-	69,74,74	1.78	17 (24%)	79,115,115	2.34	25 (31%)
10	LMT	4	101	-	36,36,36	1.14	5 (13%)	47,47,47	1.17	5 (10%)
10	LMT	L	306	-	36,36,36	1.12	6 (16%)	47,47,47	1.02	2 (4%)
7	CRT	K	101	-	43,43,43	1.49	12 (27%)	48,54,54	1.62	13 (27%)
7	CRT	B	103	-	43,43,43	1.51	12 (27%)	48,54,54	1.56	14 (29%)
10	LMT	Z	101	-	36,36,36	1.14	4 (11%)	47,47,47	1.04	2 (4%)
6	BCL	C	102	-	69,74,74	1.79	17 (24%)	79,115,115	2.18	23 (29%)
6	BCL	C	101	-	69,74,74	1.78	17 (24%)	79,115,115	2.30	22 (27%)
6	BCL	4	102	-	69,74,74	1.81	17 (24%)	79,115,115	2.19	23 (29%)
8	6PL	D	102	-	51,51,51	0.28	0	57,59,59	0.30	0
7	CRT	S	101	-	43,43,43	1.50	11 (25%)	48,54,54	1.61	16 (33%)
8	6PL	M	401	-	51,51,51	0.28	0	57,59,59	0.33	0
6	BCL	N	102	-	69,74,74	1.80	17 (24%)	79,115,115	2.22	21 (26%)
10	LMT	H	302	-	36,36,36	1.13	5 (13%)	47,47,47	1.07	3 (6%)
10	LMT	R	102	-	36,36,36	1.15	5 (13%)	47,47,47	1.13	3 (6%)
8	6PL	B	104	-	51,51,51	0.28	0	57,59,59	0.38	0
9	CDL	E	103	-	86,86,99	0.29	0	92,98,111	0.38	0
7	CRT	O	102	-	43,43,43	1.50	10 (23%)	48,54,54	1.61	13 (27%)
8	6PL	K	102	-	51,51,51	0.27	0	57,59,59	0.34	0
6	BCL	7	104	-	69,74,74	1.79	17 (24%)	79,115,115	2.25	22 (27%)
9	CDL	L	310	-	99,99,99	0.27	0	105,111,111	0.31	0
12	U10	L	309	-	63,63,63	2.78	17 (26%)	78,79,79	1.82	23 (29%)
11	BPH	M	405	-	59,70,70	0.76	3 (5%)	59,101,101	0.89	3 (5%)
11	BPH	L	302	-	59,70,70	0.78	3 (5%)	59,101,101	0.91	3 (5%)
8	6PL	O	103	-	46,46,51	0.29	0	52,54,59	0.33	0
6	BCL	9	102	-	69,74,74	1.78	18 (26%)	79,115,115	2.37	24 (30%)
6	BCL	B	102	-	69,74,74	1.79	17 (24%)	79,115,115	2.19	23 (29%)
8	6PL	6	102	-	51,51,51	0.27	0	57,59,59	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	BCL	5	101	-	69,74,74	1.78	16 (23%)	79,115,115	2.27	24 (30%)
8	6PL	I	103	-	51,51,51	0.27	0	57,59,59	0.36	0
6	BCL	V	102	-	69,74,74	1.79	17 (24%)	79,115,115	2.20	23 (29%)
6	BCL	G	104	-	69,74,74	1.79	17 (24%)	79,115,115	2.20	21 (26%)
8	6PL	U	102	-	51,51,51	0.27	0	57,59,59	0.31	0
6	BCL	7	102	-	69,74,74	1.79	17 (24%)	79,115,115	2.30	22 (27%)
8	6PL	H	301	-	51,51,51	0.28	0	57,59,59	0.42	0
12	U10	M	406	-	48,48,63	2.75	14 (29%)	60,61,79	1.61	13 (21%)
6	BCL	1	101	-	69,74,74	1.78	18 (26%)	79,115,115	2.34	23 (29%)
6	BCL	V	101	-	69,74,74	1.77	17 (24%)	79,115,115	2.28	22 (27%)
15	PGT	9	101	-	50,50,50	0.27	0	53,56,56	0.35	0
9	CDL	G	105	-	89,89,99	0.30	0	95,101,111	0.45	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
8	6PL	Z	103	-	-	11/55/55/55	-
10	LMT	O	101	-	-	9/21/61/61	0/2/2/2
15	PGT	7	103	-	-	8/55/55/55	-
7	CRT	2	102	-	-	3/51/51/51	-
6	BCL	1	102	-	-	9/41/137/137	-
9	CDL	G	101	-	-	12/110/110/110	-
10	LMT	P	101	-	-	6/21/61/61	0/2/2/2
6	BCL	M	404	-	-	13/41/137/137	-
8	6PL	5	102	-	-	12/55/55/55	-
10	LMT	F	101	-	-	10/21/61/61	0/2/2/2
6	BCL	Y	101	-	-	11/41/137/137	-
7	CRT	I	102	-	-	0/51/51/51	-
8	6PL	Q	102	-	-	8/51/51/55	-
14	QAK	M	407	-	3/3/8/12	22/44/44/44	-
6	BCL	E	101	-	-	19/41/137/137	-
6	BCL	J	103	-	-	11/41/137/137	-
7	CRT	X	101	-	-	1/51/51/51	-
6	BCL	P	102	-	-	16/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BCL	L	301	-	-	11/41/137/137	-
12	U10	M	410	-	-	20/63/87/87	0/1/1/1
12	U10	L	303	-	-	18/45/69/87	0/1/1/1
6	BCL	5	103	-	-	8/41/137/137	-
6	BCL	A	100	-	-	20/41/137/137	-
7	CRT	G	102	-	-	0/51/51/51	-
6	BCL	3	100	-	-	19/41/137/137	-
9	CDL	M	409	-	-	6/94/94/110	-
8	6PL	P	103	-	-	11/55/55/55	-
8	6PL	4	104	-	-	5/55/55/55	-
7	CRT	8	101	-	-	1/51/51/51	-
6	BCL	R	101	-	-	16/41/137/137	-
10	LMT	2	101	-	-	13/21/61/61	0/2/2/2
7	CRT	U	101	-	-	0/51/51/51	-
6	BCL	F	102	-	-	15/41/137/137	-
6	BCL	U	100	-	-	16/41/137/137	-
8	6PL	X	102	-	-	5/55/55/55	-
8	6PL	I	101	-	-	11/55/55/55	-
8	6PL	8	102	-	-	6/55/55/55	-
8	6PL	0	102	-	-	7/55/55/55	-
8	6PL	L	305	-	-	8/55/55/55	-
8	6PL	E	102	-	-	11/55/55/55	-
12	U10	L	307	-	-	27/63/87/87	0/1/1/1
6	BCL	M	402	-	-	9/41/137/137	-
6	BCL	G	103	-	-	15/41/137/137	-
9	CDL	M	408	-	-	8/100/100/110	-
6	BCL	Y	102	-	-	16/41/137/137	-
7	CRT	4	103	-	-	0/51/51/51	-
8	6PL	2	103	-	-	11/50/50/55	-
6	BCL	J	101	-	-	14/41/137/137	-
6	BCL	N	101	-	-	16/41/137/137	-
7	CRT	Q	101	-	-	1/51/51/51	-
7	CRT	Z	102	-	-	0/51/51/51	-
6	BCL	Q	100	-	-	10/41/137/137	-
10	LMT	6	101	-	-	7/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	CRT	0	101	-	-	0/51/51/51	-
8	6PL	S	102	-	-	5/55/55/55	-
10	LMT	B	101	-	-	9/21/61/61	0/2/2/2
6	BCL	0	100	-	-	13/41/137/137	-
6	BCL	R	103	-	-	9/41/137/137	-
8	6PL	L	304	-	-	6/55/55/55	-
10	LMT	J	102	-	-	6/21/61/61	0/2/2/2
7	CRT	D	101	-	-	0/51/51/51	-
7	CRT	7	101	-	-	1/51/51/51	-
8	6PL	F	103	-	-	8/55/55/55	-
6	BCL	L	308	-	-	15/41/137/137	-
6	BCL	T	100	-	-	16/41/137/137	-
10	LMT	4	101	-	-	10/21/61/61	0/2/2/2
10	LMT	L	306	-	-	13/21/61/61	0/2/2/2
7	CRT	K	101	-	-	0/51/51/51	-
7	CRT	B	103	-	-	0/51/51/51	-
10	LMT	Z	101	-	-	11/21/61/61	0/2/2/2
6	BCL	C	102	-	-	12/41/137/137	-
6	BCL	C	101	-	-	15/41/137/137	-
6	BCL	4	102	-	-	9/41/137/137	-
8	6PL	D	102	-	-	4/55/55/55	-
7	CRT	S	101	-	-	0/51/51/51	-
8	6PL	M	401	-	-	8/55/55/55	-
6	BCL	N	102	-	-	8/41/137/137	-
10	LMT	H	302	-	-	10/21/61/61	0/2/2/2
10	LMT	R	102	-	-	15/21/61/61	0/2/2/2
8	6PL	B	104	-	-	7/55/55/55	-
9	CDL	E	103	-	-	10/97/97/110	-
7	CRT	O	102	-	-	1/51/51/51	-
8	6PL	K	102	-	-	11/55/55/55	-
6	BCL	7	104	-	-	15/41/137/137	-
9	CDL	L	310	-	-	18/110/110/110	-
12	U10	L	309	-	-	23/63/87/87	0/1/1/1
11	BPH	M	405	-	2/2/18/22	5/37/105/105	0/5/6/6
11	BPH	L	302	-	2/2/18/22	7/37/105/105	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	6PL	O	103	-	-	12/50/50/55	-
6	BCL	9	102	-	-	11/41/137/137	-
6	BCL	B	102	-	-	15/41/137/137	-
8	6PL	6	102	-	-	4/55/55/55	-
6	BCL	5	101	-	-	18/41/137/137	-
8	6PL	I	103	-	-	7/55/55/55	-
6	BCL	V	102	-	-	11/41/137/137	-
6	BCL	G	104	-	-	11/41/137/137	-
8	6PL	U	102	-	-	5/55/55/55	-
6	BCL	7	102	-	-	22/41/137/137	-
8	6PL	H	301	-	-	4/55/55/55	-
12	U10	M	406	-	-	10/45/69/87	0/1/1/1
6	BCL	1	101	-	-	12/41/137/137	-
6	BCL	V	101	-	-	22/41/137/137	-
15	PGT	9	101	-	-	5/55/55/55	-
9	CDL	G	105	-	-	16/100/100/110	-

All (949) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	410	U10	C38-C39	6.34	1.47	1.33
12	L	303	U10	C23-C24	6.34	1.47	1.33
12	L	309	U10	C38-C39	6.32	1.47	1.33
12	L	307	U10	C23-C24	6.31	1.47	1.33
12	M	410	U10	C43-C44	6.30	1.47	1.33
12	L	303	U10	C28-C29	6.30	1.47	1.33
12	L	307	U10	C33-C34	6.30	1.47	1.33
12	L	303	U10	C18-C19	6.28	1.47	1.33
12	L	309	U10	C13-C14	6.26	1.47	1.33
12	L	309	U10	C23-C24	6.25	1.47	1.33
12	L	309	U10	C18-C19	6.25	1.47	1.33
12	L	307	U10	C28-C29	6.24	1.47	1.33
12	M	406	U10	C8-C9	6.24	1.47	1.33
12	L	307	U10	C38-C39	6.23	1.47	1.33
12	L	309	U10	C43-C44	6.22	1.47	1.33
12	L	303	U10	C33-C34	6.21	1.47	1.33
12	L	307	U10	C48-C49	6.20	1.47	1.33
12	M	410	U10	C18-C19	6.20	1.47	1.33
12	L	307	U10	C18-C19	6.19	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	406	U10	C33-C34	6.19	1.47	1.33
12	L	309	U10	C48-C49	6.19	1.47	1.33
12	L	309	U10	C8-C9	6.19	1.47	1.33
12	L	309	U10	C33-C34	6.19	1.47	1.33
12	L	309	U10	C28-C29	6.18	1.47	1.33
12	M	406	U10	C28-C29	6.17	1.47	1.33
12	L	303	U10	C8-C9	6.17	1.47	1.33
12	M	410	U10	C13-C14	6.16	1.47	1.33
12	M	410	U10	C48-C49	6.15	1.47	1.33
12	M	406	U10	C23-C24	6.13	1.47	1.33
12	M	410	U10	C8-C9	6.13	1.47	1.33
12	L	307	U10	C13-C14	6.13	1.47	1.33
12	L	303	U10	C13-C14	6.12	1.47	1.33
12	L	307	U10	C43-C44	6.11	1.47	1.33
12	M	406	U10	C18-C19	6.10	1.47	1.33
12	M	406	U10	C13-C14	6.08	1.47	1.33
12	L	307	U10	C8-C9	6.07	1.47	1.33
12	M	410	U10	C23-C24	5.97	1.46	1.33
12	M	410	U10	C33-C34	5.96	1.46	1.33
12	M	410	U10	C28-C29	5.96	1.46	1.33
14	M	407	QAK	CZ2-C4	5.87	1.55	1.31
12	L	309	U10	O4-C4	-5.66	1.23	1.36
12	L	307	U10	O3-C3	-5.60	1.23	1.36
12	L	309	U10	O3-C3	-5.53	1.23	1.36
12	M	406	U10	O3-C3	-5.52	1.23	1.36
12	L	307	U10	O4-C4	-5.51	1.23	1.36
14	M	407	QAK	CZ3-CE3	5.51	1.54	1.31
12	L	303	U10	O4-C4	-5.50	1.23	1.36
12	M	406	U10	O4-C4	-5.47	1.23	1.36
12	M	410	U10	O4-C4	-5.46	1.23	1.36
12	M	410	U10	O3-C3	-5.46	1.23	1.36
12	L	303	U10	O3-C3	-5.40	1.23	1.36
6	M	404	BCL	O2D-CGD	5.12	1.45	1.33
6	V	102	BCL	O2D-CGD	5.06	1.45	1.33
12	M	406	U10	C38-C39	5.05	1.47	1.32
12	L	309	U10	C53-C54	5.05	1.47	1.32
6	1	102	BCL	O2D-CGD	5.04	1.45	1.33
12	L	307	U10	C53-C54	5.03	1.47	1.32
6	L	301	BCL	O2D-CGD	5.03	1.45	1.33
6	4	102	BCL	O2D-CGD	5.03	1.45	1.33
6	Q	100	BCL	O2D-CGD	5.01	1.45	1.33
6	P	102	BCL	O2D-CGD	5.00	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	0	100	BCL	O2D-CGD	5.00	1.45	1.33
6	R	103	BCL	O2D-CGD	5.00	1.45	1.33
6	5	103	BCL	O2D-CGD	4.98	1.45	1.33
6	A	100	BCL	O2D-CGD	4.98	1.45	1.33
6	Y	102	BCL	O2D-CGD	4.97	1.45	1.33
6	J	103	BCL	O2D-CGD	4.97	1.45	1.33
6	Y	101	BCL	O2D-CGD	4.97	1.45	1.33
6	U	100	BCL	O2D-CGD	4.97	1.45	1.33
12	L	303	U10	C38-C39	4.97	1.47	1.32
6	7	104	BCL	O2D-CGD	4.96	1.45	1.33
6	3	100	BCL	O2D-CGD	4.96	1.45	1.33
6	J	101	BCL	O2D-CGD	4.95	1.45	1.33
6	C	102	BCL	O2D-CGD	4.95	1.45	1.33
6	N	102	BCL	O2D-CGD	4.94	1.45	1.33
6	G	103	BCL	O2D-CGD	4.94	1.45	1.33
6	G	104	BCL	O2D-CGD	4.94	1.45	1.33
6	F	102	BCL	O2D-CGD	4.94	1.45	1.33
6	5	101	BCL	O2D-CGD	4.94	1.45	1.33
6	R	101	BCL	O2D-CGD	4.93	1.45	1.33
6	T	100	BCL	O2D-CGD	4.93	1.45	1.33
6	N	101	BCL	O2D-CGD	4.92	1.45	1.33
6	B	102	BCL	O2D-CGD	4.92	1.45	1.33
6	V	101	BCL	O2D-CGD	4.92	1.45	1.33
6	C	101	BCL	O2D-CGD	4.92	1.45	1.33
6	E	101	BCL	O2D-CGD	4.91	1.45	1.33
6	1	101	BCL	O2D-CGD	4.89	1.45	1.33
6	L	308	BCL	O2D-CGD	4.89	1.45	1.33
12	M	410	U10	C53-C54	4.88	1.47	1.32
6	M	402	BCL	O2D-CGD	4.87	1.45	1.33
6	9	102	BCL	O2D-CGD	4.87	1.45	1.33
6	7	102	BCL	O2D-CGD	4.86	1.45	1.33
6	L	308	BCL	C3D-C4D	-4.77	1.33	1.44
6	V	102	BCL	C3D-C4D	-4.74	1.33	1.44
6	M	404	BCL	C3D-C4D	-4.71	1.33	1.44
6	V	101	BCL	C3D-C4D	-4.70	1.33	1.44
6	1	102	BCL	C3D-C4D	-4.70	1.33	1.44
6	5	101	BCL	C3D-C4D	-4.70	1.33	1.44
6	7	102	BCL	C3D-C4D	-4.69	1.33	1.44
6	0	100	BCL	C3D-C4D	-4.69	1.33	1.44
6	Y	101	BCL	C3D-C4D	-4.68	1.33	1.44
6	N	102	BCL	C3D-C4D	-4.68	1.33	1.44
6	C	101	BCL	C3D-C4D	-4.68	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Q	100	BCL	C3D-C4D	-4.67	1.33	1.44
6	9	102	BCL	C3D-C4D	-4.67	1.33	1.44
6	G	104	BCL	C3D-C4D	-4.67	1.33	1.44
6	M	402	BCL	C3D-C4D	-4.67	1.33	1.44
6	U	100	BCL	C3D-C4D	-4.67	1.33	1.44
6	3	100	BCL	C3D-C4D	-4.66	1.33	1.44
6	F	102	BCL	C3D-C4D	-4.66	1.33	1.44
6	7	104	BCL	C3D-C4D	-4.66	1.33	1.44
6	1	101	BCL	C3D-C4D	-4.65	1.33	1.44
6	J	101	BCL	C3D-C4D	-4.65	1.33	1.44
6	C	102	BCL	C3D-C4D	-4.65	1.33	1.44
6	4	102	BCL	C3D-C4D	-4.64	1.33	1.44
6	E	101	BCL	C3D-C4D	-4.64	1.33	1.44
6	Y	102	BCL	C3D-C4D	-4.64	1.33	1.44
6	R	101	BCL	C3D-C4D	-4.64	1.33	1.44
6	L	301	BCL	C3D-C4D	-4.64	1.33	1.44
6	B	102	BCL	C3D-C4D	-4.64	1.33	1.44
6	N	101	BCL	C3D-C4D	-4.64	1.33	1.44
6	G	103	BCL	C3D-C4D	-4.63	1.33	1.44
6	A	100	BCL	C3D-C4D	-4.63	1.33	1.44
6	T	100	BCL	C3D-C4D	-4.62	1.33	1.44
6	5	103	BCL	C3D-C4D	-4.60	1.33	1.44
6	P	102	BCL	C3D-C4D	-4.60	1.33	1.44
6	J	103	BCL	C3D-C4D	-4.60	1.33	1.44
6	R	103	BCL	C3D-C4D	-4.59	1.33	1.44
6	N	102	BCL	O2A-CGA	4.31	1.45	1.33
6	G	104	BCL	O2A-CGA	4.31	1.45	1.33
6	4	102	BCL	O2A-CGA	4.29	1.45	1.33
6	J	103	BCL	O2A-CGA	4.28	1.45	1.33
6	V	102	BCL	O2A-CGA	4.28	1.45	1.33
6	L	301	BCL	O2A-CGA	4.27	1.45	1.33
6	N	101	BCL	O2A-CGA	4.26	1.45	1.33
6	5	103	BCL	O2A-CGA	4.26	1.45	1.33
6	M	402	BCL	O2A-CGA	4.25	1.45	1.33
6	M	404	BCL	O2A-CGA	4.25	1.45	1.33
6	P	102	BCL	O2A-CGA	4.24	1.45	1.33
6	R	101	BCL	O2A-CGA	4.24	1.45	1.33
6	1	101	BCL	O2A-CGA	4.23	1.45	1.33
6	C	101	BCL	O2A-CGA	4.22	1.45	1.33
6	7	104	BCL	O2A-CGA	4.22	1.45	1.33
6	R	103	BCL	O2A-CGA	4.22	1.45	1.33
6	J	101	BCL	O2A-CGA	4.21	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	102	BCL	O2A-CGA	4.21	1.45	1.33
6	Y	102	BCL	O2A-CGA	4.20	1.45	1.33
6	Y	101	BCL	O2A-CGA	4.20	1.45	1.33
6	9	102	BCL	O2A-CGA	4.20	1.45	1.33
6	C	102	BCL	O2A-CGA	4.20	1.45	1.33
6	T	100	BCL	O2A-CGA	4.19	1.45	1.33
6	E	101	BCL	O2A-CGA	4.18	1.45	1.33
6	1	102	BCL	O2A-CGA	4.18	1.45	1.33
6	7	102	BCL	O2A-CGA	4.18	1.45	1.33
6	F	102	BCL	O2A-CGA	4.18	1.45	1.33
6	3	100	BCL	O2A-CGA	4.18	1.45	1.33
6	U	100	BCL	O2A-CGA	4.17	1.45	1.33
6	Q	100	BCL	O2A-CGA	4.17	1.45	1.33
6	5	101	BCL	O2A-CGA	4.17	1.45	1.33
6	A	100	BCL	O2A-CGA	4.16	1.45	1.33
6	L	308	BCL	O2A-CGA	4.15	1.45	1.33
6	0	100	BCL	O2A-CGA	4.15	1.45	1.33
6	V	101	BCL	O2A-CGA	4.14	1.45	1.33
6	G	103	BCL	O2A-CGA	4.09	1.45	1.33
6	U	100	BCL	C3B-C4B	4.07	1.49	1.41
6	L	301	BCL	C3B-C4B	4.06	1.49	1.41
6	M	404	BCL	C3B-C4B	4.05	1.49	1.41
6	T	100	BCL	C3B-C4B	4.04	1.49	1.41
6	R	101	BCL	C3B-C4B	4.03	1.49	1.41
6	Y	101	BCL	C3B-C4B	4.02	1.49	1.41
6	G	104	BCL	C3B-C4B	4.02	1.49	1.41
6	7	102	BCL	C3B-C4B	4.01	1.49	1.41
6	5	103	BCL	C3B-C4B	4.00	1.49	1.41
6	F	102	BCL	C3B-C4B	3.99	1.49	1.41
6	N	102	BCL	C3B-C4B	3.99	1.49	1.41
6	N	101	BCL	C3B-C4B	3.99	1.49	1.41
6	P	102	BCL	C3B-C4B	3.98	1.49	1.41
6	L	308	BCL	C3B-C4B	3.96	1.48	1.41
6	G	103	BCL	C3B-C4B	3.96	1.48	1.41
6	9	102	BCL	C3B-C4B	3.95	1.48	1.41
6	E	101	BCL	C3B-C4B	3.95	1.48	1.41
6	Q	100	BCL	C3B-C4B	3.94	1.48	1.41
6	1	101	BCL	C3B-C4B	3.94	1.48	1.41
6	A	100	BCL	C3B-C4B	3.92	1.48	1.41
6	0	100	BCL	C3B-C4B	3.92	1.48	1.41
6	3	100	BCL	C3B-C4B	3.91	1.48	1.41
6	J	103	BCL	C3B-C4B	3.91	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	308	BCL	CHD-C1D	3.91	1.46	1.38
6	C	102	BCL	C3B-C4B	3.90	1.48	1.41
6	4	102	BCL	C3B-C4B	3.89	1.48	1.41
6	J	101	BCL	C3B-C4B	3.88	1.48	1.41
6	7	104	BCL	C3B-C4B	3.87	1.48	1.41
6	B	102	BCL	C3B-C4B	3.87	1.48	1.41
6	1	102	BCL	C3B-C4B	3.87	1.48	1.41
6	5	101	BCL	CHD-C1D	3.86	1.45	1.38
6	Y	102	BCL	C3B-C4B	3.84	1.48	1.41
6	C	101	BCL	C3B-C4B	3.82	1.48	1.41
6	5	101	BCL	C3B-C4B	3.78	1.48	1.41
6	V	101	BCL	C3B-C4B	3.78	1.48	1.41
6	R	103	BCL	C3B-C4B	3.78	1.48	1.41
6	7	102	BCL	CHD-C1D	3.76	1.45	1.38
6	P	102	BCL	CHD-C1D	3.75	1.45	1.38
6	3	100	BCL	CHD-C1D	3.72	1.45	1.38
6	R	101	BCL	CHD-C1D	3.71	1.45	1.38
6	U	100	BCL	CHD-C1D	3.71	1.45	1.38
6	J	101	BCL	CHD-C1D	3.71	1.45	1.38
6	5	103	BCL	CHD-C1D	3.69	1.45	1.38
6	4	102	BCL	CHD-C1D	3.69	1.45	1.38
6	Q	100	BCL	CHD-C1D	3.69	1.45	1.38
6	M	402	BCL	C3B-C4B	3.68	1.48	1.41
6	V	101	BCL	CHD-C1D	3.67	1.45	1.38
6	E	101	BCL	CHD-C1D	3.67	1.45	1.38
6	F	102	BCL	CHD-C1D	3.67	1.45	1.38
6	V	102	BCL	C3B-C4B	3.67	1.48	1.41
6	0	100	BCL	CHD-C1D	3.66	1.45	1.38
6	4	102	BCL	OBD-CAD	3.65	1.28	1.22
6	M	402	BCL	CHD-C1D	3.65	1.45	1.38
6	1	102	BCL	CHD-C1D	3.64	1.45	1.38
6	Y	102	BCL	OBD-CAD	3.64	1.28	1.22
6	G	104	BCL	OBD-CAD	3.63	1.28	1.22
6	V	102	BCL	CHD-C1D	3.61	1.45	1.38
6	5	103	BCL	OBD-CAD	3.61	1.28	1.22
6	N	102	BCL	OBD-CAD	3.60	1.28	1.22
6	N	101	BCL	CHD-C1D	3.60	1.45	1.38
6	E	101	BCL	OBD-CAD	3.60	1.28	1.22
6	M	402	BCL	OBD-CAD	3.60	1.28	1.22
6	Y	102	BCL	CHD-C1D	3.60	1.45	1.38
6	M	404	BCL	CHD-C1D	3.60	1.45	1.38
6	7	104	BCL	CHD-C1D	3.60	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	103	BCL	CHD-C1D	3.60	1.45	1.38
6	F	102	BCL	OBD-CAD	3.60	1.28	1.22
6	L	301	BCL	OBD-CAD	3.59	1.28	1.22
6	G	104	BCL	CHD-C1D	3.59	1.45	1.38
6	B	102	BCL	CHD-C1D	3.59	1.45	1.38
6	0	100	BCL	OBD-CAD	3.59	1.28	1.22
6	5	101	BCL	OBD-CAD	3.58	1.28	1.22
6	N	102	BCL	CHD-C1D	3.58	1.45	1.38
6	L	308	BCL	OBD-CAD	3.58	1.28	1.22
6	Q	100	BCL	OBD-CAD	3.57	1.28	1.22
6	3	100	BCL	OBD-CAD	3.57	1.28	1.22
6	C	102	BCL	OBD-CAD	3.57	1.28	1.22
6	C	101	BCL	CHD-C1D	3.57	1.45	1.38
6	Y	101	BCL	CHD-C1D	3.57	1.45	1.38
6	9	102	BCL	OBD-CAD	3.57	1.28	1.22
6	G	103	BCL	CHD-C1D	3.57	1.45	1.38
6	9	102	BCL	CHD-C1D	3.56	1.45	1.38
6	R	103	BCL	OBD-CAD	3.56	1.28	1.22
6	T	100	BCL	CHD-C1D	3.56	1.45	1.38
6	J	103	BCL	OBD-CAD	3.56	1.28	1.22
6	7	104	BCL	OBD-CAD	3.56	1.28	1.22
6	V	102	BCL	OBD-CAD	3.55	1.28	1.22
6	L	301	BCL	CHD-C1D	3.55	1.45	1.38
6	C	102	BCL	CHD-C1D	3.55	1.45	1.38
6	N	101	BCL	OBD-CAD	3.55	1.28	1.22
6	L	308	BCL	CHB-C1B	3.54	1.47	1.39
6	7	102	BCL	OBD-CAD	3.54	1.28	1.22
6	1	102	BCL	OBD-CAD	3.53	1.28	1.22
6	R	103	BCL	CHD-C1D	3.53	1.45	1.38
6	C	101	BCL	OBD-CAD	3.51	1.28	1.22
6	U	100	BCL	OBD-CAD	3.50	1.28	1.22
6	G	103	BCL	OBD-CAD	3.50	1.28	1.22
6	B	102	BCL	OBD-CAD	3.50	1.28	1.22
6	A	100	BCL	CHD-C1D	3.49	1.45	1.38
6	1	101	BCL	OBD-CAD	3.49	1.28	1.22
6	P	102	BCL	OBD-CAD	3.48	1.28	1.22
6	T	100	BCL	OBD-CAD	3.48	1.28	1.22
6	1	101	BCL	CHD-C1D	3.47	1.45	1.38
6	J	101	BCL	OBD-CAD	3.47	1.28	1.22
6	M	404	BCL	OBD-CAD	3.46	1.28	1.22
6	9	102	BCL	CHB-C1B	3.45	1.47	1.39
6	L	308	BCL	CHC-C4B	3.44	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	V	101	BCL	OBD-CAD	3.44	1.28	1.22
6	A	100	BCL	OBD-CAD	3.42	1.28	1.22
6	L	301	BCL	CHB-C1B	3.41	1.47	1.39
6	R	103	BCL	CHB-C1B	3.41	1.47	1.39
6	C	101	BCL	CHB-C1B	3.40	1.47	1.39
6	M	404	BCL	CHB-C1B	3.40	1.47	1.39
6	N	102	BCL	CHB-C1B	3.39	1.47	1.39
6	R	101	BCL	OBD-CAD	3.38	1.28	1.22
6	Y	101	BCL	OBD-CAD	3.38	1.28	1.22
6	M	402	BCL	CHB-C1B	3.38	1.47	1.39
6	J	101	BCL	CHB-C1B	3.37	1.47	1.39
6	5	103	BCL	CHB-C1B	3.37	1.47	1.39
12	L	307	U10	C4-C5	-3.36	1.39	1.48
12	L	303	U10	C4-C5	-3.35	1.39	1.48
6	4	102	BCL	CHB-C1B	3.35	1.46	1.39
12	L	309	U10	C4-C5	-3.35	1.39	1.48
6	5	101	BCL	CHB-C1B	3.35	1.46	1.39
6	0	100	BCL	CHB-C1B	3.35	1.46	1.39
6	7	104	BCL	CHB-C1B	3.34	1.46	1.39
6	1	101	BCL	CHB-C1B	3.33	1.46	1.39
6	1	102	BCL	CHC-C4B	3.33	1.46	1.39
12	M	410	U10	C4-C5	-3.33	1.39	1.48
6	G	104	BCL	CHB-C1B	3.32	1.46	1.39
6	V	102	BCL	CHB-C1B	3.31	1.46	1.39
6	N	101	BCL	CHB-C1B	3.29	1.46	1.39
6	G	104	BCL	CHC-C4B	3.28	1.46	1.39
12	M	406	U10	C3-C2	-3.28	1.39	1.48
6	4	102	BCL	CHC-C4B	3.28	1.46	1.39
6	B	102	BCL	CHC-C4B	3.28	1.46	1.39
6	R	101	BCL	CHB-C1B	3.28	1.46	1.39
6	L	301	BCL	CHC-C4B	3.28	1.46	1.39
6	1	102	BCL	CHB-C1B	3.27	1.46	1.39
6	P	102	BCL	CHB-C1B	3.27	1.46	1.39
6	Y	102	BCL	CHC-C4B	3.26	1.46	1.39
12	M	406	U10	C4-C5	-3.26	1.39	1.48
6	7	102	BCL	CHB-C1B	3.26	1.46	1.39
6	C	102	BCL	CHB-C1B	3.25	1.46	1.39
6	V	101	BCL	CHB-C1B	3.25	1.46	1.39
6	3	100	BCL	CHB-C1B	3.25	1.46	1.39
6	F	102	BCL	CHB-C1B	3.25	1.46	1.39
6	Q	100	BCL	CHB-C1B	3.25	1.46	1.39
12	M	410	U10	C3-C2	-3.25	1.39	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	307	U10	C3-C2	-3.24	1.39	1.48
6	F	102	BCL	CHC-C4B	3.24	1.46	1.39
6	M	404	BCL	CHC-C4B	3.24	1.46	1.39
6	A	100	BCL	CHB-C1B	3.24	1.46	1.39
12	L	309	U10	C3-C2	-3.24	1.39	1.48
6	Y	102	BCL	CHB-C1B	3.24	1.46	1.39
6	U	100	BCL	CHC-C4B	3.24	1.46	1.39
11	L	302	BPH	C4D-CHA	3.24	1.44	1.39
6	5	101	BCL	CHC-C4B	3.23	1.46	1.39
6	7	102	BCL	CHC-C4B	3.22	1.46	1.39
6	N	101	BCL	CHC-C4B	3.22	1.46	1.39
6	5	103	BCL	CHC-C4B	3.21	1.46	1.39
6	Y	101	BCL	CHB-C1B	3.21	1.46	1.39
6	C	102	BCL	CHC-C4B	3.21	1.46	1.39
6	V	102	BCL	CHC-C4B	3.21	1.46	1.39
6	Y	101	BCL	CHC-C4B	3.21	1.46	1.39
6	G	103	BCL	CHB-C1B	3.20	1.46	1.39
6	Q	100	BCL	CHC-C4B	3.20	1.46	1.39
6	N	102	BCL	CHC-C4B	3.20	1.46	1.39
6	3	100	BCL	CHC-C4B	3.20	1.46	1.39
6	T	100	BCL	CHB-C1B	3.20	1.46	1.39
6	J	103	BCL	CHB-C1B	3.19	1.46	1.39
6	B	102	BCL	CHB-C1B	3.19	1.46	1.39
6	U	100	BCL	CHB-C1B	3.18	1.46	1.39
6	J	103	BCL	CHC-C4B	3.17	1.46	1.39
6	E	101	BCL	CHC-C4B	3.17	1.46	1.39
6	0	100	BCL	CHC-C4B	3.17	1.46	1.39
6	T	100	BCL	CHC-C4B	3.16	1.46	1.39
6	A	100	BCL	CHC-C4B	3.15	1.46	1.39
6	7	104	BCL	CHC-C4B	3.14	1.46	1.39
6	R	103	BCL	CHC-C4B	3.14	1.46	1.39
6	P	102	BCL	CHC-C4B	3.14	1.46	1.39
6	R	101	BCL	CHC-C4B	3.11	1.46	1.39
6	G	103	BCL	CHC-C4B	3.11	1.46	1.39
6	E	101	BCL	CHB-C1B	3.11	1.46	1.39
6	M	402	BCL	CHC-C4B	3.10	1.46	1.39
12	L	303	U10	C3-C2	-3.10	1.39	1.48
6	C	101	BCL	CHC-C4B	3.10	1.46	1.39
6	Y	102	BCL	C3D-C2D	3.09	1.47	1.39
6	1	101	BCL	CHC-C4B	3.09	1.46	1.39
6	V	101	BCL	CHC-C4B	3.08	1.46	1.39
6	M	402	BCL	C3D-C2D	3.07	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	405	BPH	C4D-CHA	3.06	1.44	1.39
6	L	308	BCL	C3D-C2D	3.06	1.47	1.39
6	C	102	BCL	C3D-C2D	3.06	1.47	1.39
6	J	101	BCL	CHC-C4B	3.05	1.46	1.39
6	5	103	BCL	C3D-C2D	3.05	1.47	1.39
6	9	102	BCL	CHC-C4B	3.05	1.46	1.39
6	F	102	BCL	C3D-C2D	3.04	1.47	1.39
6	U	100	BCL	C3D-C2D	3.03	1.47	1.39
6	4	102	BCL	C3D-C2D	3.03	1.47	1.39
6	J	103	BCL	C3D-C2D	3.02	1.47	1.39
6	1	102	BCL	C3D-C2D	3.02	1.47	1.39
6	N	102	BCL	C3D-C2D	3.01	1.47	1.39
6	G	104	BCL	C3D-C2D	3.00	1.47	1.39
6	R	103	BCL	C3D-C2D	2.99	1.47	1.39
6	L	308	BCL	CHD-C4C	2.98	1.47	1.39
6	7	104	BCL	C3D-C2D	2.98	1.47	1.39
6	V	102	BCL	C3D-C2D	2.96	1.47	1.39
6	P	102	BCL	C3D-C2D	2.96	1.47	1.39
6	E	101	BCL	C3D-C2D	2.96	1.47	1.39
6	B	102	BCL	C3D-C2D	2.96	1.47	1.39
6	C	101	BCL	C3D-C2D	2.95	1.47	1.39
6	7	102	BCL	C3D-C2D	2.95	1.47	1.39
6	3	100	BCL	C3D-C2D	2.94	1.47	1.39
6	0	100	BCL	C3D-C2D	2.94	1.47	1.39
6	L	301	BCL	C3D-C2D	2.93	1.47	1.39
6	N	101	BCL	C3D-C2D	2.93	1.47	1.39
6	V	101	BCL	C3D-C2D	2.92	1.47	1.39
6	Q	100	BCL	C3D-C2D	2.92	1.46	1.39
6	R	101	BCL	C3D-C2D	2.91	1.46	1.39
6	J	101	BCL	C3D-C2D	2.91	1.46	1.39
6	M	404	BCL	C3D-C2D	2.91	1.46	1.39
6	5	101	BCL	C3D-C2D	2.90	1.46	1.39
6	T	100	BCL	C3D-C2D	2.89	1.46	1.39
6	A	100	BCL	C3D-C2D	2.88	1.46	1.39
6	1	101	BCL	C3D-C2D	2.87	1.46	1.39
6	Y	102	BCL	C1D-ND	-2.87	1.34	1.37
6	R	101	BCL	C1D-C2D	2.85	1.51	1.45
6	G	103	BCL	C3D-C2D	2.85	1.46	1.39
6	1	102	BCL	C1D-ND	-2.85	1.34	1.37
6	C	102	BCL	C1D-ND	-2.85	1.34	1.37
6	Y	101	BCL	C3D-C2D	2.84	1.46	1.39
6	J	103	BCL	C1D-ND	-2.84	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	9	102	BCL	C3D-C2D	2.84	1.46	1.39
6	L	308	BCL	C1D-C2D	2.83	1.50	1.45
6	M	402	BCL	C4B-NB	-2.83	1.34	1.37
6	C	102	BCL	C4B-NB	-2.82	1.34	1.37
6	E	101	BCL	CHD-C4C	2.82	1.47	1.39
6	4	102	BCL	C1D-ND	-2.82	1.34	1.37
6	5	101	BCL	CHD-C4C	2.82	1.47	1.39
6	N	102	BCL	C1D-ND	-2.81	1.34	1.37
6	7	102	BCL	CHD-C4C	2.81	1.47	1.39
6	U	100	BCL	C1D-ND	-2.80	1.34	1.37
6	3	100	BCL	CHD-C4C	2.80	1.47	1.39
6	J	101	BCL	CHD-C4C	2.80	1.47	1.39
6	9	102	BCL	C1D-C2D	2.80	1.50	1.45
6	Y	102	BCL	C4B-NB	-2.80	1.34	1.37
6	M	402	BCL	CHD-C4C	2.79	1.47	1.39
6	P	102	BCL	C1D-C2D	2.79	1.50	1.45
6	V	102	BCL	C1D-ND	-2.79	1.34	1.37
6	L	308	BCL	C4B-NB	-2.79	1.34	1.37
6	7	102	BCL	C1D-C2D	2.79	1.50	1.45
6	R	101	BCL	CHD-C4C	2.79	1.47	1.39
6	R	103	BCL	C4B-NB	-2.79	1.34	1.37
6	7	104	BCL	C4B-NB	-2.78	1.34	1.37
6	V	102	BCL	C4B-NB	-2.78	1.34	1.37
6	R	103	BCL	C1D-ND	-2.78	1.34	1.37
6	3	100	BCL	C1D-C2D	2.78	1.50	1.45
6	J	101	BCL	C4B-NB	-2.77	1.34	1.37
6	J	101	BCL	C1D-C2D	2.77	1.50	1.45
6	T	100	BCL	CHD-C4C	2.77	1.47	1.39
6	C	101	BCL	C4B-NB	-2.77	1.34	1.37
6	V	101	BCL	C1D-C2D	2.77	1.50	1.45
6	V	101	BCL	CHD-C4C	2.76	1.47	1.39
6	5	101	BCL	C1D-C2D	2.76	1.50	1.45
6	P	102	BCL	CHD-C4C	2.76	1.47	1.39
6	T	100	BCL	C1D-C2D	2.76	1.50	1.45
6	F	102	BCL	CHD-C4C	2.75	1.46	1.39
6	V	101	BCL	C4B-NB	-2.75	1.34	1.37
6	4	102	BCL	C4B-NB	-2.75	1.34	1.37
6	9	102	BCL	C4B-NB	-2.75	1.34	1.37
6	E	101	BCL	C4B-NB	-2.75	1.34	1.37
6	B	102	BCL	C1D-ND	-2.73	1.34	1.37
6	U	100	BCL	CHD-C4C	2.73	1.46	1.39
6	Q	100	BCL	CHD-C4C	2.73	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	0	100	BCL	CHD-C4C	2.73	1.46	1.39
6	1	101	BCL	C4B-NB	-2.73	1.34	1.37
6	7	104	BCL	CHD-C4C	2.73	1.46	1.39
6	B	102	BCL	C4B-NB	-2.72	1.34	1.37
6	N	102	BCL	C4B-NB	-2.72	1.34	1.37
6	G	103	BCL	C4B-NB	-2.72	1.34	1.37
6	Y	101	BCL	CHD-C4C	2.72	1.46	1.39
6	9	102	BCL	CHD-C4C	2.72	1.46	1.39
6	Q	100	BCL	C4B-NB	-2.71	1.34	1.37
6	1	102	BCL	C4B-NB	-2.71	1.34	1.37
6	5	101	BCL	C4B-NB	-2.71	1.34	1.37
6	Q	100	BCL	C1D-C2D	2.71	1.50	1.45
6	G	104	BCL	C4B-NB	-2.71	1.34	1.37
6	5	103	BCL	CHD-C4C	2.71	1.46	1.39
6	N	101	BCL	CHD-C4C	2.71	1.46	1.39
6	C	101	BCL	C1D-C2D	2.71	1.50	1.45
6	7	104	BCL	C1D-C2D	2.71	1.50	1.45
6	4	102	BCL	CHD-C4C	2.71	1.46	1.39
6	C	101	BCL	CHD-C4C	2.70	1.46	1.39
6	J	103	BCL	C4B-NB	-2.70	1.34	1.37
6	7	104	BCL	C1D-ND	-2.70	1.34	1.37
6	G	103	BCL	C1D-C2D	2.70	1.50	1.45
6	G	104	BCL	C1D-ND	-2.70	1.34	1.37
6	E	101	BCL	C1D-C2D	2.70	1.50	1.45
6	M	404	BCL	C1D-C2D	2.70	1.50	1.45
6	B	102	BCL	CHD-C4C	2.70	1.46	1.39
6	A	100	BCL	C4B-NB	-2.69	1.34	1.37
6	M	404	BCL	CHD-C4C	2.69	1.46	1.39
6	G	104	BCL	CHD-C4C	2.69	1.46	1.39
6	1	101	BCL	CHD-C4C	2.69	1.46	1.39
6	0	100	BCL	C4B-NB	-2.68	1.34	1.37
6	3	100	BCL	C4B-NB	-2.68	1.34	1.37
6	G	103	BCL	CHD-C4C	2.68	1.46	1.39
6	F	102	BCL	C1D-C2D	2.67	1.50	1.45
6	Q	100	BCL	C1D-ND	-2.67	1.34	1.37
6	L	301	BCL	CHD-C4C	2.67	1.46	1.39
6	A	100	BCL	CHD-C4C	2.67	1.46	1.39
6	M	402	BCL	C1D-C2D	2.67	1.50	1.45
6	N	102	BCL	CHD-C4C	2.67	1.46	1.39
12	L	307	U10	C6-C5	-2.67	1.39	1.46
6	5	103	BCL	C1D-ND	-2.67	1.34	1.37
6	J	103	BCL	CHD-C4C	2.67	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	7	102	BCL	C4B-NB	-2.66	1.34	1.37
6	Y	102	BCL	CHD-C4C	2.66	1.46	1.39
6	F	102	BCL	C1D-ND	-2.66	1.34	1.37
6	1	101	BCL	C1D-C2D	2.66	1.50	1.45
12	M	410	U10	C6-C5	-2.66	1.39	1.46
6	R	101	BCL	C4B-NB	-2.65	1.34	1.37
6	1	102	BCL	CHD-C4C	2.65	1.46	1.39
7	B	103	CRT	C16-C17	-2.65	1.40	1.46
6	Y	101	BCL	C1D-C2D	2.65	1.50	1.45
12	L	303	U10	C6-C5	-2.65	1.39	1.46
6	N	101	BCL	C1D-C2D	2.64	1.50	1.45
6	F	102	BCL	C4B-NB	-2.64	1.34	1.37
7	O	102	CRT	C25-C23	-2.63	1.40	1.46
6	0	100	BCL	C1D-C2D	2.63	1.50	1.45
6	0	100	BCL	C1D-ND	-2.63	1.34	1.37
6	A	100	BCL	C1D-C2D	2.63	1.50	1.45
6	V	102	BCL	CHD-C4C	2.63	1.46	1.39
6	L	308	BCL	MG-NA	-2.63	2.00	2.06
6	M	404	BCL	C1D-ND	-2.63	1.34	1.37
6	C	102	BCL	CHD-C4C	2.62	1.46	1.39
6	Y	101	BCL	C4B-NB	-2.62	1.34	1.37
6	U	100	BCL	C4B-NB	-2.62	1.34	1.37
6	L	308	BCL	C1B-C2B	2.62	1.49	1.43
6	U	100	BCL	C1D-C2D	2.61	1.50	1.45
7	8	101	CRT	C22-C23	2.61	1.41	1.35
6	M	404	BCL	C4B-NB	-2.61	1.34	1.37
12	M	406	U10	C6-C5	-2.61	1.39	1.46
12	L	309	U10	C6-C5	-2.60	1.39	1.46
6	R	103	BCL	CHD-C4C	2.60	1.46	1.39
6	T	100	BCL	C4B-NB	-2.60	1.34	1.37
6	L	301	BCL	C1D-C2D	2.59	1.50	1.45
10	R	102	LMT	O3'-C3'	-2.59	1.36	1.43
6	N	102	BCL	C1D-C2D	2.59	1.50	1.45
6	5	103	BCL	C4B-NB	-2.59	1.34	1.37
6	1	102	BCL	C1D-C2D	2.59	1.50	1.45
7	8	101	CRT	C19-C17	2.58	1.41	1.35
6	5	101	BCL	C1B-C2B	2.58	1.49	1.43
6	M	404	BCL	C1B-C2B	2.58	1.49	1.43
10	P	101	LMT	O3'-C3'	-2.58	1.36	1.43
6	5	103	BCL	C1D-C2D	2.58	1.50	1.45
7	Z	102	CRT	C30-C28	-2.58	1.40	1.46
10	2	101	LMT	O3'-C3'	-2.57	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	308	BCL	C1D-ND	-2.57	1.34	1.37
6	P	102	BCL	C4B-NB	-2.57	1.34	1.37
6	M	402	BCL	C1B-C2B	2.57	1.49	1.43
10	B	101	LMT	O3'-C3'	-2.56	1.36	1.43
7	U	101	CRT	C16-C17	-2.56	1.40	1.46
10	L	306	LMT	O3'-C3'	-2.56	1.36	1.43
7	O	102	CRT	C30-C28	-2.55	1.40	1.46
6	L	301	BCL	C1B-C2B	2.55	1.49	1.43
6	C	102	BCL	C1B-NB	-2.55	1.34	1.37
6	J	103	BCL	C1D-C2D	2.54	1.50	1.45
10	P	101	LMT	O2'-C2'	-2.54	1.36	1.43
7	I	102	CRT	C16-C17	-2.54	1.40	1.46
6	N	101	BCL	C4B-NB	-2.54	1.34	1.37
6	R	103	BCL	C1B-C2B	2.54	1.49	1.43
6	1	101	BCL	C1D-ND	-2.54	1.34	1.37
7	0	101	CRT	C30-C28	-2.53	1.40	1.46
7	G	102	CRT	C30-C28	-2.53	1.40	1.46
10	J	102	LMT	O3'-C3'	-2.53	1.36	1.43
7	Z	102	CRT	C16-C17	-2.53	1.40	1.46
7	8	101	CRT	C14-C12	2.52	1.41	1.35
7	B	103	CRT	C11-C12	-2.51	1.40	1.46
6	L	308	BCL	MG-NC	-2.51	2.00	2.06
6	J	101	BCL	C1B-C2B	2.51	1.49	1.43
6	A	100	BCL	C1D-ND	-2.51	1.34	1.37
10	O	101	LMT	O3'-C3'	-2.51	1.36	1.43
6	4	102	BCL	C1B-C2B	2.50	1.49	1.43
10	H	302	LMT	O3'-C3'	-2.50	1.36	1.43
6	9	102	BCL	C1D-ND	-2.50	1.34	1.37
6	4	102	BCL	C1D-C2D	2.50	1.50	1.45
6	R	101	BCL	C1D-ND	-2.50	1.34	1.37
6	R	103	BCL	C1D-C2D	2.50	1.50	1.45
7	O	102	CRT	C16-C17	-2.50	1.40	1.46
7	S	101	CRT	C30-C28	-2.49	1.40	1.46
7	I	102	CRT	C11-C12	-2.49	1.40	1.46
6	M	402	BCL	C1D-ND	-2.49	1.34	1.37
12	L	309	U10	C1-C2	-2.49	1.38	1.47
10	4	101	LMT	O3'-C3'	-2.49	1.36	1.43
10	Z	101	LMT	O3'-C3'	-2.49	1.36	1.43
6	B	102	BCL	C1D-C2D	2.49	1.50	1.45
10	F	101	LMT	O3'-C3'	-2.49	1.36	1.43
7	7	101	CRT	C16-C17	-2.49	1.40	1.46
6	M	404	BCL	MG-NA	-2.48	2.00	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	P	102	BCL	C1B-C2B	2.48	1.49	1.43
7	8	101	CRT	C9-C7	2.48	1.41	1.35
6	C	102	BCL	C1D-C2D	2.48	1.50	1.45
7	Q	101	CRT	C30-C28	-2.48	1.40	1.46
6	L	301	BCL	C1D-ND	-2.48	1.34	1.37
7	S	101	CRT	C25-C23	-2.48	1.40	1.46
6	7	102	BCL	C1B-C2B	2.48	1.48	1.43
7	G	102	CRT	C25-C23	-2.48	1.40	1.46
6	B	102	BCL	MG-NC	-2.47	2.00	2.06
12	M	406	U10	C1-C2	-2.47	1.38	1.47
7	B	103	CRT	C25-C23	-2.47	1.40	1.46
6	1	101	BCL	C1B-C2B	2.47	1.48	1.43
7	B	103	CRT	C30-C28	-2.47	1.40	1.46
6	L	308	BCL	C1B-NB	-2.47	1.34	1.37
6	1	102	BCL	MG-NC	-2.47	2.00	2.06
6	7	104	BCL	C1B-C2B	2.47	1.48	1.43
7	D	101	CRT	C16-C17	-2.47	1.40	1.46
6	C	101	BCL	C1B-C2B	2.47	1.48	1.43
6	L	301	BCL	C4B-NB	-2.47	1.34	1.37
6	9	102	BCL	C1B-C2B	2.46	1.48	1.43
6	J	103	BCL	C1B-NB	-2.46	1.34	1.37
7	Q	101	CRT	C16-C17	-2.46	1.40	1.46
7	7	101	CRT	C25-C23	-2.46	1.40	1.46
7	I	102	CRT	C25-C23	-2.46	1.40	1.46
6	4	102	BCL	C1B-NB	-2.46	1.34	1.37
7	Z	102	CRT	C25-C23	-2.45	1.40	1.46
6	G	104	BCL	C1B-C2B	2.45	1.48	1.43
6	V	102	BCL	C1B-C2B	2.45	1.48	1.43
6	0	100	BCL	C1B-C2B	2.45	1.48	1.43
7	7	101	CRT	C30-C28	-2.45	1.40	1.46
7	Z	102	CRT	C35-C33	-2.45	1.40	1.46
6	G	103	BCL	C1B-C2B	2.45	1.48	1.43
6	E	101	BCL	C1D-ND	-2.45	1.34	1.37
6	N	101	BCL	C1D-ND	-2.45	1.34	1.37
6	V	101	BCL	C1D-ND	-2.45	1.34	1.37
7	2	102	CRT	C19-C17	2.45	1.41	1.35
7	G	102	CRT	C35-C33	-2.44	1.40	1.46
7	D	101	CRT	C25-C23	-2.44	1.40	1.46
7	G	102	CRT	C16-C17	-2.44	1.40	1.46
6	5	103	BCL	C1B-C2B	2.44	1.48	1.43
6	T	100	BCL	C1D-ND	-2.44	1.34	1.37
6	M	404	BCL	C1B-NB	-2.44	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	7	101	CRT	C35-C33	-2.44	1.40	1.46
10	6	101	LMT	O3'-C3'	-2.44	1.36	1.43
6	5	103	BCL	MG-NC	-2.44	2.00	2.06
7	O	102	CRT	C35-C33	-2.44	1.40	1.46
6	U	100	BCL	C1B-NB	-2.44	1.34	1.37
7	Q	101	CRT	C35-C33	-2.43	1.40	1.46
6	0	100	BCL	MG-NC	-2.43	2.00	2.06
7	G	102	CRT	C11-C12	-2.43	1.40	1.46
7	Q	101	CRT	C25-C23	-2.43	1.40	1.46
6	7	102	BCL	C1D-ND	-2.43	1.34	1.37
7	2	102	CRT	C9-C7	2.43	1.41	1.35
12	M	406	U10	C6-C1	2.43	1.39	1.35
6	1	102	BCL	C1B-C2B	2.43	1.48	1.43
10	H	302	LMT	O2'-C2'	-2.43	1.36	1.43
6	Y	102	BCL	C1D-C2D	2.43	1.50	1.45
6	G	103	BCL	C1D-ND	-2.43	1.34	1.37
7	0	101	CRT	C35-C33	-2.43	1.40	1.46
10	J	102	LMT	O2B-C2B	-2.43	1.36	1.43
7	U	101	CRT	C30-C28	-2.43	1.40	1.46
6	Q	100	BCL	C1B-C2B	2.43	1.48	1.43
12	L	307	U10	C1-C2	-2.43	1.39	1.47
7	8	101	CRT	C27-C28	2.42	1.41	1.35
7	2	102	CRT	C22-C23	2.42	1.41	1.35
7	Q	101	CRT	C11-C12	-2.42	1.40	1.46
7	K	101	CRT	C16-C17	-2.42	1.40	1.46
7	S	101	CRT	C35-C33	-2.42	1.40	1.46
6	3	100	BCL	C1B-C2B	2.42	1.48	1.43
6	Y	102	BCL	C1B-C2B	2.42	1.48	1.43
7	X	101	CRT	C22-C23	2.42	1.41	1.35
7	U	101	CRT	C35-C33	-2.42	1.40	1.46
6	P	102	BCL	C1D-ND	-2.41	1.34	1.37
6	B	102	BCL	C1B-C2B	2.41	1.48	1.43
6	G	104	BCL	C1D-C2D	2.41	1.50	1.45
6	V	102	BCL	C1D-C2D	2.41	1.50	1.45
7	S	101	CRT	C16-C17	-2.41	1.40	1.46
6	F	102	BCL	MG-NC	-2.40	2.00	2.06
6	C	102	BCL	C1B-C2B	2.40	1.48	1.43
6	N	102	BCL	C1B-C2B	2.40	1.48	1.43
6	T	100	BCL	C1B-NB	-2.40	1.34	1.37
7	2	102	CRT	C27-C28	2.40	1.41	1.35
6	T	100	BCL	MG-NC	-2.40	2.00	2.06
7	X	101	CRT	C9-C7	2.40	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	V	102	BCL	C1B-NB	-2.40	1.34	1.37
6	4	102	BCL	MG-NC	-2.40	2.00	2.06
6	U	100	BCL	MG-NC	-2.40	2.00	2.06
7	B	103	CRT	C35-C33	-2.40	1.40	1.46
6	N	101	BCL	C1B-C2B	2.40	1.48	1.43
7	2	102	CRT	C14-C12	2.40	1.41	1.35
7	4	103	CRT	C30-C28	-2.40	1.40	1.46
6	J	101	BCL	C1D-ND	-2.40	1.34	1.37
6	1	102	BCL	C1B-NB	-2.40	1.34	1.37
6	R	101	BCL	C1B-C2B	2.39	1.48	1.43
7	I	102	CRT	C30-C28	-2.39	1.40	1.46
6	N	102	BCL	MG-NA	-2.39	2.00	2.06
6	C	101	BCL	C1D-ND	-2.39	1.34	1.37
7	X	101	CRT	C35-C33	-2.39	1.40	1.46
7	D	101	CRT	C30-C28	-2.39	1.40	1.46
12	M	410	U10	C1-C2	-2.39	1.39	1.47
6	U	100	BCL	C1B-C2B	2.39	1.48	1.43
7	X	101	CRT	C30-C28	-2.39	1.40	1.46
6	3	100	BCL	C1D-ND	-2.39	1.34	1.37
7	0	101	CRT	C11-C12	-2.39	1.40	1.46
7	B	103	CRT	C6-C7	-2.39	1.40	1.46
7	4	103	CRT	C9-C7	2.38	1.41	1.35
6	F	102	BCL	C1B-NB	-2.38	1.34	1.37
6	V	101	BCL	C1B-C2B	2.38	1.48	1.43
6	M	402	BCL	MG-NA	-2.38	2.00	2.06
7	U	101	CRT	C25-C23	-2.38	1.40	1.46
6	5	101	BCL	C1D-ND	-2.37	1.34	1.37
6	Y	102	BCL	C1B-NB	-2.37	1.34	1.37
7	K	101	CRT	C30-C28	-2.37	1.40	1.46
7	O	102	CRT	C11-C12	-2.37	1.40	1.46
10	F	101	LMT	O2'-C2'	-2.37	1.37	1.43
7	U	101	CRT	C11-C12	-2.37	1.40	1.46
7	7	101	CRT	C11-C12	-2.36	1.40	1.46
12	L	303	U10	C1-C2	-2.36	1.39	1.47
10	L	306	LMT	O2'-C2'	-2.36	1.37	1.43
6	B	102	BCL	C1B-NB	-2.36	1.34	1.37
7	I	102	CRT	C6-C7	-2.36	1.40	1.46
7	D	101	CRT	C11-C12	-2.36	1.40	1.46
6	J	103	BCL	MG-NC	-2.36	2.00	2.06
10	J	102	LMT	O2'-C2'	-2.36	1.37	1.43
6	1	101	BCL	C1B-NB	-2.36	1.34	1.37
6	A	100	BCL	C1B-C2B	2.36	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Y	102	BCL	MG-NC	-2.35	2.00	2.06
6	Y	101	BCL	MG-NC	-2.35	2.00	2.06
7	2	102	CRT	C30-C28	-2.35	1.40	1.46
6	A	100	BCL	C1B-NB	-2.35	1.34	1.37
6	A	100	BCL	MG-NC	-2.35	2.00	2.06
10	R	102	LMT	O2'-C2'	-2.35	1.37	1.43
6	F	102	BCL	C1B-C2B	2.35	1.48	1.43
7	4	103	CRT	C22-C23	2.35	1.41	1.35
6	7	102	BCL	MG-NC	-2.35	2.00	2.06
7	K	101	CRT	C6-C7	-2.34	1.40	1.46
6	Y	101	BCL	C1D-ND	-2.34	1.34	1.37
7	I	102	CRT	C35-C33	-2.34	1.40	1.46
6	1	102	BCL	MG-NA	-2.34	2.00	2.06
6	J	103	BCL	MG-NA	-2.34	2.00	2.06
6	E	101	BCL	C1B-NB	-2.34	1.34	1.37
6	C	102	BCL	MG-NC	-2.34	2.00	2.06
11	M	405	BPH	C3A-C2A	-2.33	1.52	1.54
7	0	101	CRT	C25-C23	-2.33	1.41	1.46
7	S	101	CRT	C11-C12	-2.33	1.41	1.46
6	R	103	BCL	MG-NA	-2.33	2.00	2.06
6	5	101	BCL	MG-NC	-2.33	2.00	2.06
6	M	404	BCL	MG-NC	-2.33	2.00	2.06
6	Q	100	BCL	C1B-NB	-2.33	1.34	1.37
6	R	103	BCL	MG-NC	-2.33	2.00	2.06
6	9	102	BCL	MG-NA	-2.33	2.00	2.06
7	4	103	CRT	C25-C23	-2.32	1.41	1.46
7	0	101	CRT	C16-C17	-2.32	1.41	1.46
6	E	101	BCL	C1B-C2B	2.32	1.48	1.43
7	X	101	CRT	C19-C17	2.32	1.41	1.35
7	X	101	CRT	C25-C23	-2.32	1.41	1.46
6	N	101	BCL	C1B-NB	-2.31	1.34	1.37
6	P	102	BCL	C1B-NB	-2.31	1.34	1.37
7	Z	102	CRT	C11-C12	-2.31	1.41	1.46
6	J	103	BCL	C1B-C2B	2.31	1.48	1.43
6	T	100	BCL	C1B-C2B	2.31	1.48	1.43
6	Q	100	BCL	MG-NC	-2.31	2.00	2.06
7	4	103	CRT	C16-C17	-2.31	1.41	1.46
7	8	101	CRT	C35-C33	-2.31	1.41	1.46
7	K	101	CRT	C35-C33	-2.31	1.41	1.46
6	B	102	BCL	MG-NA	-2.30	2.00	2.06
6	V	101	BCL	C1B-NB	-2.30	1.34	1.37
7	K	101	CRT	C11-C12	-2.30	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	X	101	CRT	C14-C12	2.30	1.41	1.35
6	7	104	BCL	MG-NA	-2.30	2.00	2.06
6	3	100	BCL	C1B-NB	-2.30	1.34	1.37
7	4	103	CRT	C19-C17	2.30	1.41	1.35
7	0	101	CRT	C9-C7	2.30	1.41	1.35
7	8	101	CRT	C30-C28	-2.30	1.41	1.46
6	0	100	BCL	C1B-NB	-2.30	1.34	1.37
6	N	101	BCL	MG-NC	-2.30	2.00	2.06
7	O	102	CRT	C6-C7	-2.29	1.41	1.46
7	Z	102	CRT	C6-C7	-2.29	1.41	1.46
7	2	102	CRT	C35-C33	-2.29	1.41	1.46
6	7	104	BCL	C1B-NB	-2.29	1.34	1.37
7	D	101	CRT	C35-C33	-2.29	1.41	1.46
10	H	302	LMT	O2B-C2B	-2.29	1.37	1.43
6	4	102	BCL	MG-NA	-2.29	2.00	2.06
7	D	101	CRT	C22-C23	2.29	1.41	1.35
6	Y	101	BCL	C1B-C2B	2.29	1.48	1.43
7	K	101	CRT	C25-C23	-2.29	1.41	1.46
6	5	103	BCL	MG-NA	-2.28	2.00	2.06
7	X	101	CRT	C27-C28	2.28	1.41	1.35
7	4	103	CRT	C35-C33	-2.28	1.41	1.46
7	X	101	CRT	C16-C17	-2.28	1.41	1.46
6	A	100	BCL	MG-NA	-2.28	2.00	2.06
7	G	102	CRT	C6-C7	-2.28	1.41	1.46
6	T	100	BCL	MG-NA	-2.28	2.00	2.06
6	J	101	BCL	MG-NC	-2.28	2.00	2.06
6	G	103	BCL	C1B-NB	-2.28	1.34	1.37
7	S	101	CRT	C6-C7	-2.27	1.41	1.46
6	Y	101	BCL	C1B-NB	-2.27	1.34	1.37
7	D	101	CRT	C6-C7	-2.27	1.41	1.46
7	K	101	CRT	C19-C17	2.27	1.41	1.35
6	0	100	BCL	MG-NA	-2.27	2.00	2.06
6	V	102	BCL	MG-NC	-2.27	2.00	2.06
7	Q	101	CRT	C6-C7	-2.27	1.41	1.46
6	R	103	BCL	C1B-NB	-2.27	1.34	1.37
7	8	101	CRT	C32-C33	2.27	1.41	1.35
7	7	101	CRT	C6-C7	-2.27	1.41	1.46
10	R	102	LMT	O3B-C3B	-2.26	1.37	1.43
7	0	101	CRT	C22-C23	2.26	1.41	1.35
7	U	101	CRT	C19-C17	2.26	1.41	1.35
6	1	101	BCL	MG-NC	-2.26	2.00	2.06
6	N	102	BCL	C1B-NB	-2.26	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	R	102	LMT	O2B-C2B	-2.26	1.37	1.43
10	J	102	LMT	O3B-C3B	-2.26	1.37	1.43
7	0	101	CRT	C14-C12	2.26	1.41	1.35
6	C	101	BCL	MG-NC	-2.25	2.00	2.06
6	E	101	BCL	MG-NC	-2.25	2.00	2.06
7	2	102	CRT	C32-C33	2.25	1.41	1.35
6	G	104	BCL	MG-NC	-2.25	2.00	2.06
6	V	102	BCL	MG-NA	-2.25	2.00	2.06
6	7	104	BCL	MG-NC	-2.25	2.00	2.06
7	S	101	CRT	C9-C7	2.25	1.41	1.35
6	M	402	BCL	MG-NC	-2.25	2.00	2.06
6	F	102	BCL	MG-NA	-2.25	2.00	2.06
7	K	101	CRT	C22-C23	2.25	1.41	1.35
6	G	104	BCL	C1B-NB	-2.25	1.34	1.37
6	Q	100	BCL	MG-NA	-2.24	2.00	2.06
10	H	302	LMT	O3B-C3B	-2.24	1.37	1.43
10	P	101	LMT	O3B-C3B	-2.24	1.37	1.43
7	U	101	CRT	C6-C7	-2.24	1.41	1.46
7	Z	102	CRT	C22-C23	2.24	1.41	1.35
6	J	101	BCL	MG-NA	-2.24	2.01	2.06
10	O	101	LMT	O2'-C2'	-2.24	1.37	1.43
6	L	301	BCL	MG-NC	-2.24	2.01	2.06
7	4	103	CRT	C14-C12	2.23	1.41	1.35
10	4	101	LMT	O3B-C3B	-2.23	1.37	1.43
7	G	102	CRT	C19-C17	2.23	1.41	1.35
10	F	101	LMT	O2B-C2B	-2.23	1.37	1.43
7	I	102	CRT	C27-C28	2.23	1.41	1.35
6	G	103	BCL	MG-NC	-2.23	2.01	2.06
10	B	101	LMT	O2B-C2B	-2.23	1.37	1.43
6	3	100	BCL	MG-NC	-2.23	2.01	2.06
7	G	102	CRT	C22-C23	2.23	1.41	1.35
6	U	100	BCL	MG-NA	-2.23	2.01	2.06
7	D	101	CRT	C14-C12	2.23	1.40	1.35
7	S	101	CRT	C22-C23	2.23	1.40	1.35
7	Z	102	CRT	C9-C7	2.23	1.40	1.35
6	7	102	BCL	MG-NA	-2.23	2.01	2.06
10	4	101	LMT	O2B-C2B	-2.23	1.37	1.43
7	U	101	CRT	C27-C28	2.22	1.40	1.35
6	7	102	BCL	C1B-NB	-2.22	1.34	1.37
7	D	101	CRT	C9-C7	2.22	1.40	1.35
7	7	101	CRT	C22-C23	2.22	1.40	1.35
7	U	101	CRT	C9-C7	2.22	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	U	101	CRT	C22-C23	2.22	1.40	1.35
6	Y	102	BCL	MG-NA	-2.22	2.01	2.06
7	4	103	CRT	C6-C7	-2.22	1.41	1.46
6	L	301	BCL	MG-NA	-2.22	2.01	2.06
6	G	104	BCL	MG-NA	-2.21	2.01	2.06
10	6	101	LMT	O2'-C2'	-2.21	1.37	1.43
7	K	101	CRT	C14-C12	2.21	1.40	1.35
7	4	103	CRT	C27-C28	2.21	1.40	1.35
10	P	101	LMT	O2B-C2B	-2.21	1.37	1.43
6	5	101	BCL	MG-NA	-2.21	2.01	2.06
6	3	100	BCL	MG-NA	-2.21	2.01	2.06
6	5	103	BCL	C1B-NB	-2.21	1.35	1.37
7	0	101	CRT	C6-C7	-2.21	1.41	1.46
7	G	102	CRT	C14-C12	2.21	1.40	1.35
10	O	101	LMT	O2B-C2B	-2.21	1.37	1.43
7	0	101	CRT	C19-C17	2.21	1.40	1.35
6	C	101	BCL	C1B-NB	-2.21	1.35	1.37
7	I	102	CRT	C22-C23	2.21	1.40	1.35
7	7	101	CRT	C19-C17	2.20	1.40	1.35
7	7	101	CRT	C9-C7	2.20	1.40	1.35
6	1	101	BCL	MG-NA	-2.20	2.01	2.06
7	Q	101	CRT	C22-C23	2.20	1.40	1.35
6	C	101	BCL	MG-NA	-2.20	2.01	2.06
6	N	102	BCL	MG-NC	-2.20	2.01	2.06
7	Z	102	CRT	C19-C17	2.20	1.40	1.35
6	E	101	BCL	MG-NA	-2.20	2.01	2.06
7	D	101	CRT	C27-C28	2.20	1.40	1.35
10	B	101	LMT	O3B-C3B	-2.20	1.37	1.43
7	2	102	CRT	C25-C23	-2.19	1.41	1.46
7	X	101	CRT	C32-C33	2.19	1.40	1.35
7	0	101	CRT	C27-C28	2.19	1.40	1.35
7	S	101	CRT	C19-C17	2.19	1.40	1.35
10	O	101	LMT	O3B-C3B	-2.19	1.37	1.43
7	O	102	CRT	C19-C17	2.19	1.40	1.35
6	V	101	BCL	MG-NC	-2.19	2.01	2.06
6	Y	101	BCL	MG-NA	-2.19	2.01	2.06
7	Q	101	CRT	C14-C12	2.18	1.40	1.35
10	4	101	LMT	O2'-C2'	-2.18	1.37	1.43
10	F	101	LMT	O3B-C3B	-2.18	1.37	1.43
10	Z	101	LMT	O3B-C3B	-2.18	1.37	1.43
6	R	101	BCL	MG-NC	-2.18	2.01	2.06
7	B	103	CRT	C22-C23	2.17	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	103	CRT	C27-C28	2.17	1.40	1.35
12	L	303	U10	C6-C1	2.17	1.39	1.35
7	K	101	CRT	C9-C7	2.17	1.40	1.35
7	4	103	CRT	C11-C12	-2.17	1.41	1.46
7	4	103	CRT	C32-C33	2.17	1.40	1.35
7	7	101	CRT	C27-C28	2.17	1.40	1.35
7	K	101	CRT	C27-C28	2.17	1.40	1.35
10	L	306	LMT	O2B-C2B	-2.17	1.37	1.43
7	G	102	CRT	C9-C7	2.17	1.40	1.35
11	L	302	BPH	C1B-C2B	2.17	1.42	1.39
6	V	101	BCL	MG-NA	-2.17	2.01	2.06
7	D	101	CRT	C19-C17	2.16	1.40	1.35
6	9	102	BCL	C1B-NB	-2.16	1.35	1.37
7	Q	101	CRT	C19-C17	2.16	1.40	1.35
10	2	101	LMT	O3B-C3B	-2.16	1.37	1.43
7	O	102	CRT	C22-C23	2.16	1.40	1.35
7	G	102	CRT	C32-C33	2.16	1.40	1.35
7	U	101	CRT	C14-C12	2.16	1.40	1.35
7	Q	101	CRT	C9-C7	2.16	1.40	1.35
6	R	101	BCL	C1B-NB	-2.16	1.35	1.37
10	L	306	LMT	O3B-C3B	-2.16	1.37	1.43
6	P	102	BCL	MG-NC	-2.15	2.01	2.06
7	I	102	CRT	C19-C17	2.15	1.40	1.35
7	I	102	CRT	C14-C12	2.15	1.40	1.35
6	L	301	BCL	C1B-NB	-2.14	1.35	1.37
10	O	101	LMT	O1'-C1'	-2.14	1.36	1.40
6	G	103	BCL	MG-NA	-2.14	2.01	2.06
7	X	101	CRT	C11-C12	-2.14	1.41	1.46
6	P	102	BCL	MG-NA	-2.14	2.01	2.06
7	7	101	CRT	C14-C12	2.14	1.40	1.35
6	C	102	BCL	MG-NA	-2.14	2.01	2.06
6	N	101	BCL	MG-NA	-2.14	2.01	2.06
7	Z	102	CRT	C14-C12	2.13	1.40	1.35
10	6	101	LMT	O3B-C3B	-2.13	1.37	1.43
7	G	102	CRT	C27-C28	2.13	1.40	1.35
10	Z	101	LMT	O2B-C2B	-2.13	1.37	1.43
12	L	309	U10	C6-C1	2.13	1.39	1.35
7	O	102	CRT	C9-C7	2.13	1.40	1.35
7	D	101	CRT	C32-C33	2.13	1.40	1.35
7	S	101	CRT	C14-C12	2.13	1.40	1.35
7	O	102	CRT	C14-C12	2.13	1.40	1.35
6	M	402	BCL	C1B-NB	-2.12	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	Z	102	CRT	C27-C28	2.12	1.40	1.35
6	R	101	BCL	MG-NA	-2.12	2.01	2.06
6	J	101	BCL	C1B-NB	-2.12	1.35	1.37
7	Q	101	CRT	C32-C33	2.12	1.40	1.35
10	2	101	LMT	O2'-C2'	-2.11	1.37	1.43
7	U	101	CRT	C32-C33	2.11	1.40	1.35
7	B	103	CRT	C19-C17	2.11	1.40	1.35
12	M	410	U10	C6-C1	2.11	1.39	1.35
10	R	102	LMT	O1'-C1'	-2.11	1.36	1.40
7	2	102	CRT	C16-C17	-2.11	1.41	1.46
7	K	101	CRT	C32-C33	2.11	1.40	1.35
7	X	101	CRT	C6-C7	-2.11	1.41	1.46
7	Q	101	CRT	C27-C28	2.10	1.40	1.35
12	L	307	U10	C6-C1	2.10	1.38	1.35
7	I	102	CRT	C32-C33	2.10	1.40	1.35
6	9	102	BCL	MG-NC	-2.10	2.01	2.06
7	2	102	CRT	C11-C12	-2.10	1.41	1.46
11	L	302	BPH	C3A-C2A	-2.10	1.52	1.54
7	8	101	CRT	C25-C23	-2.09	1.41	1.46
7	B	103	CRT	C32-C33	2.09	1.40	1.35
14	M	407	QAK	O-C	-2.09	1.39	1.44
7	Z	102	CRT	C32-C33	2.09	1.40	1.35
7	2	102	CRT	C6-C7	-2.09	1.41	1.46
7	7	101	CRT	C32-C33	2.08	1.40	1.35
10	4	101	LMT	O1'-C1'	-2.08	1.36	1.40
7	S	101	CRT	C27-C28	2.08	1.40	1.35
10	6	101	LMT	O2B-C2B	-2.08	1.37	1.43
10	Z	101	LMT	O2'-C2'	-2.07	1.37	1.43
7	8	101	CRT	C16-C17	-2.07	1.41	1.46
7	B	103	CRT	C14-C12	2.07	1.40	1.35
10	6	101	LMT	O1'-C1'	-2.07	1.36	1.40
10	P	101	LMT	O1'-C1'	-2.06	1.36	1.40
10	L	306	LMT	O1'-C1'	-2.05	1.36	1.40
7	I	102	CRT	C9-C7	2.04	1.40	1.35
7	8	101	CRT	C6-C7	-2.04	1.41	1.46
7	8	101	CRT	C11-C12	-2.03	1.41	1.46
10	L	306	LMT	O4'-C4B	-2.02	1.37	1.43
7	B	103	CRT	C9-C7	2.02	1.40	1.35
10	F	101	LMT	O1'-C1'	-2.02	1.36	1.40
6	E	101	BCL	CHB-C4A	-2.02	1.32	1.37
11	M	405	BPH	C1B-C2B	2.02	1.41	1.39
7	0	101	CRT	C32-C33	2.01	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	H	302	LMT	O4'-C4B	-2.01	1.38	1.43
6	9	102	BCL	CHC-C1C	-2.01	1.32	1.37
6	1	101	BCL	CHC-C1C	-2.01	1.32	1.37
10	O	101	LMT	O4'-C4B	-2.00	1.38	1.43
6	3	100	BCL	CHB-C4A	-2.00	1.32	1.37
6	A	100	BCL	CHC-C1C	-2.00	1.32	1.37

All (1183) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	9	102	BCL	CMD-C2D-C1D	8.36	139.45	124.73
6	5	101	BCL	CMD-C2D-C1D	8.35	139.43	124.73
6	T	100	BCL	CMD-C2D-C1D	8.34	139.42	124.73
6	G	103	BCL	CMD-C2D-C1D	8.32	139.37	124.73
6	Y	101	BCL	CMD-C2D-C1D	8.31	139.35	124.73
6	R	101	BCL	CMD-C2D-C1D	8.28	139.32	124.73
6	7	102	BCL	CMD-C2D-C1D	8.28	139.32	124.73
6	M	404	BCL	CMD-C2D-C1D	8.28	139.32	124.73
6	J	101	BCL	CMD-C2D-C1D	8.28	139.30	124.73
6	3	100	BCL	CMD-C2D-C1D	8.24	139.25	124.73
6	P	102	BCL	CMD-C2D-C1D	8.22	139.20	124.73
6	1	101	BCL	CMD-C2D-C1D	8.21	139.18	124.73
6	A	100	BCL	CMD-C2D-C1D	8.18	139.14	124.73
6	L	308	BCL	CMD-C2D-C1D	8.18	139.13	124.73
6	V	101	BCL	CMD-C2D-C1D	8.17	139.11	124.73
6	E	101	BCL	CMD-C2D-C1D	8.16	139.10	124.73
6	C	101	BCL	CMD-C2D-C1D	8.09	138.98	124.73
6	N	101	BCL	CMD-C2D-C1D	8.07	138.95	124.73
6	L	301	BCL	CMD-C2D-C1D	8.03	138.87	124.73
6	0	100	BCL	CMD-C2D-C1D	7.96	138.75	124.73
6	Q	100	BCL	CMD-C2D-C1D	7.86	138.56	124.73
6	7	104	BCL	CMD-C2D-C1D	7.80	138.46	124.73
6	F	102	BCL	CMD-C2D-C1D	7.79	138.44	124.73
6	M	402	BCL	CMD-C2D-C1D	7.66	138.23	124.73
6	5	103	BCL	CMD-C2D-C1D	7.66	138.22	124.73
6	R	103	BCL	CMD-C2D-C1D	7.64	138.19	124.73
6	J	103	BCL	CMD-C2D-C1D	7.64	138.18	124.73
6	1	102	BCL	CMD-C2D-C1D	7.61	138.14	124.73
6	N	102	BCL	CMD-C2D-C1D	7.58	138.08	124.73
6	4	102	BCL	CMD-C2D-C1D	7.47	137.88	124.73
6	B	102	BCL	CMD-C2D-C1D	7.46	137.87	124.73
6	U	100	BCL	CMD-C2D-C1D	7.46	137.86	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	V	102	BCL	CMD-C2D-C1D	7.43	137.81	124.73
6	G	104	BCL	CMD-C2D-C1D	7.35	137.67	124.73
6	C	102	BCL	CMD-C2D-C1D	7.18	137.37	124.73
6	Y	102	BCL	CMD-C2D-C1D	7.12	137.27	124.73
6	E	101	BCL	C2B-C1B-NB	6.88	117.46	110.33
6	T	100	BCL	C2B-C1B-NB	6.87	117.45	110.33
6	Y	101	BCL	C2B-C1B-NB	6.78	117.36	110.33
6	U	100	BCL	C2B-C1B-NB	6.74	117.32	110.33
6	J	103	BCL	C2B-C1B-NB	6.74	117.32	110.33
6	G	103	BCL	C2B-C1B-NB	6.72	117.29	110.33
6	P	102	BCL	C2B-C1B-NB	6.72	117.29	110.33
6	R	101	BCL	C2B-C1B-NB	6.69	117.26	110.33
6	7	102	BCL	C2B-C1B-NB	6.64	117.21	110.33
6	A	100	BCL	C2B-C1B-NB	6.63	117.20	110.33
6	N	101	BCL	C2B-C1B-NB	6.62	117.19	110.33
6	1	101	BCL	C2B-C1B-NB	6.61	117.18	110.33
6	V	101	BCL	C2B-C1B-NB	6.55	117.12	110.33
6	3	100	BCL	C2B-C1B-NB	6.55	117.12	110.33
6	0	100	BCL	C2B-C1B-NB	6.55	117.11	110.33
6	J	101	BCL	C2B-C1B-NB	6.51	117.07	110.33
6	C	102	BCL	C2B-C1B-NB	6.51	117.07	110.33
6	9	102	BCL	C2B-C1B-NB	6.50	117.07	110.33
6	L	301	BCL	C2B-C1B-NB	6.49	117.06	110.33
6	B	102	BCL	C2B-C1B-NB	6.49	117.06	110.33
6	7	104	BCL	C2B-C1B-NB	6.48	117.05	110.33
6	G	104	BCL	C2B-C1B-NB	6.47	117.03	110.33
6	5	103	BCL	C2B-C1B-NB	6.46	117.03	110.33
6	1	102	BCL	C2B-C1B-NB	6.45	117.02	110.33
6	F	102	BCL	C2B-C1B-NB	6.45	117.02	110.33
6	N	102	BCL	C2B-C1B-NB	6.45	117.01	110.33
6	C	101	BCL	C2B-C1B-NB	6.43	117.00	110.33
6	Q	100	BCL	C2B-C1B-NB	6.43	116.99	110.33
6	Y	102	BCL	C2B-C1B-NB	6.40	116.97	110.33
6	V	102	BCL	C2B-C1B-NB	6.39	116.95	110.33
6	R	103	BCL	C2B-C1B-NB	6.33	116.89	110.33
6	M	404	BCL	C2B-C1B-NB	6.31	116.87	110.33
6	4	102	BCL	C2B-C1B-NB	6.28	116.84	110.33
6	5	101	BCL	C2B-C1B-NB	6.25	116.80	110.33
6	M	404	BCL	CHD-C1D-ND	-6.17	116.12	124.80
6	M	402	BCL	C2B-C1B-NB	6.12	116.68	110.33
6	L	308	BCL	CHD-C1D-ND	-6.03	116.31	124.80
6	J	101	BCL	CHD-C1D-ND	-6.02	116.33	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	9	102	BCL	CHD-C1D-ND	-6.00	116.36	124.80
6	A	100	BCL	CHD-C1D-ND	-5.97	116.41	124.80
6	7	102	BCL	CHD-C1D-ND	-5.96	116.41	124.80
6	L	308	BCL	O2D-CGD-CBD	5.95	121.63	111.23
6	Y	101	BCL	CHD-C1D-ND	-5.93	116.46	124.80
6	T	100	BCL	CHD-C1D-ND	-5.91	116.49	124.80
6	P	102	BCL	CHD-C1D-ND	-5.86	116.55	124.80
6	R	101	BCL	CHD-C1D-ND	-5.86	116.56	124.80
6	C	101	BCL	CHD-C1D-ND	-5.84	116.58	124.80
6	M	402	BCL	CHD-C1D-ND	-5.83	116.60	124.80
6	L	301	BCL	CHD-C1D-ND	-5.82	116.61	124.80
6	F	102	BCL	CHD-C1D-ND	-5.82	116.62	124.80
6	E	101	BCL	CHD-C1D-ND	-5.81	116.63	124.80
6	V	101	BCL	CHD-C1D-ND	-5.81	116.63	124.80
6	J	103	BCL	CHD-C1D-ND	-5.80	116.63	124.80
6	G	103	BCL	CHD-C1D-ND	-5.78	116.67	124.80
6	5	103	BCL	CHD-C1D-ND	-5.78	116.67	124.80
6	Q	100	BCL	CHD-C1D-ND	-5.76	116.69	124.80
6	0	100	BCL	CHD-C1D-ND	-5.76	116.69	124.80
6	5	101	BCL	CHD-C1D-ND	-5.74	116.72	124.80
6	L	308	BCL	C2B-C1B-NB	5.74	116.28	110.33
6	7	104	BCL	CHD-C1D-ND	-5.74	116.73	124.80
6	U	100	BCL	CHD-C1D-ND	-5.73	116.73	124.80
6	M	402	BCL	O2D-CGD-CBD	5.73	121.25	111.23
6	1	101	BCL	CHD-C1D-ND	-5.72	116.75	124.80
6	N	101	BCL	CHD-C1D-ND	-5.71	116.77	124.80
6	3	100	BCL	CHD-C1D-ND	-5.69	116.79	124.80
6	N	102	BCL	CHD-C1D-ND	-5.69	116.80	124.80
6	1	102	BCL	CHD-C1D-ND	-5.68	116.81	124.80
6	R	103	BCL	CHD-C1D-ND	-5.62	116.90	124.80
6	B	102	BCL	CHD-C1D-ND	-5.56	116.98	124.80
6	4	102	BCL	CHD-C1D-ND	-5.55	116.98	124.80
6	G	104	BCL	CHD-C1D-ND	-5.51	117.04	124.80
6	V	102	BCL	CHD-C1D-ND	-5.51	117.04	124.80
6	9	102	BCL	O2D-CGD-CBD	5.49	120.83	111.23
6	Y	102	BCL	CHD-C1D-ND	-5.47	117.10	124.80
6	C	102	BCL	CHD-C1D-ND	-5.39	117.22	124.80
6	A	100	BCL	C3D-C2D-C1D	-5.23	98.69	105.83
6	1	101	BCL	O2D-CGD-CBD	5.19	120.30	111.23
6	1	101	BCL	C3D-C2D-C1D	-5.15	98.80	105.83
6	G	103	BCL	O2D-CGD-CBD	5.11	120.16	111.23
6	Y	101	BCL	C3D-C2D-C1D	-5.10	98.87	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	301	BCL	C3D-C2D-C1D	-5.04	98.95	105.83
6	V	101	BCL	O2D-CGD-CBD	5.03	120.02	111.23
6	3	100	BCL	O2D-CGD-CBD	5.02	120.01	111.23
6	3	100	BCL	C3D-C2D-C1D	-5.02	98.98	105.83
6	C	101	BCL	C3D-C2D-C1D	-5.02	98.98	105.83
6	G	103	BCL	C3D-C2D-C1D	-5.02	98.99	105.83
6	9	102	BCL	C3D-C2D-C1D	-5.01	98.99	105.83
6	Y	101	BCL	O2D-CGD-CBD	5.01	119.98	111.23
6	R	101	BCL	C3D-C2D-C1D	-5.00	99.01	105.83
6	T	100	BCL	C3D-C2D-C1D	-5.00	99.01	105.83
6	E	101	BCL	C3D-C2D-C1D	-4.99	99.02	105.83
6	C	101	BCL	O2D-CGD-CBD	4.99	119.95	111.23
6	J	101	BCL	O2D-CGD-CBD	4.98	119.94	111.23
6	M	404	BCL	C3D-C2D-C1D	-4.98	99.03	105.83
6	N	101	BCL	C3D-C2D-C1D	-4.97	99.05	105.83
6	P	102	BCL	C3D-C2D-C1D	-4.97	99.05	105.83
6	J	101	BCL	C3D-C2D-C1D	-4.96	99.07	105.83
6	V	101	BCL	C3D-C2D-C1D	-4.96	99.07	105.83
6	7	102	BCL	C3D-C2D-C1D	-4.95	99.08	105.83
6	N	101	BCL	O2D-CGD-CBD	4.95	119.88	111.23
6	R	101	BCL	O2D-CGD-CBD	4.94	119.87	111.23
6	E	101	BCL	O2D-CGD-CBD	4.94	119.86	111.23
6	7	104	BCL	O2D-CGD-CBD	4.90	119.79	111.23
6	7	102	BCL	O2D-CGD-CBD	4.89	119.78	111.23
6	F	102	BCL	O2D-CGD-CBD	4.88	119.75	111.23
6	0	100	BCL	C3D-C2D-C1D	-4.87	99.19	105.83
6	R	103	BCL	C3D-C2D-C1D	-4.85	99.21	105.83
6	T	100	BCL	O2D-CGD-CBD	4.84	119.70	111.23
6	A	100	BCL	O2D-CGD-CBD	4.84	119.70	111.23
6	5	103	BCL	O2D-CGD-CBD	4.84	119.70	111.23
6	J	103	BCL	C3D-C2D-C1D	-4.84	99.23	105.83
6	5	101	BCL	C3D-C2D-C1D	-4.83	99.23	105.83
6	P	102	BCL	O2D-CGD-CBD	4.83	119.67	111.23
6	5	101	BCL	O2D-CGD-CBD	4.80	119.61	111.23
12	L	309	U10	C7-C6-C1	-4.78	116.69	124.89
6	M	402	BCL	C3D-C2D-C1D	-4.78	99.31	105.83
6	U	100	BCL	O2D-CGD-CBD	4.76	119.56	111.23
7	8	101	CRT	C20-C21-C22	4.76	133.25	123.52
6	J	103	BCL	O2D-CGD-CBD	4.75	119.53	111.23
6	N	102	BCL	O2D-CGD-CBD	4.74	119.52	111.23
6	7	104	BCL	C3D-C2D-C1D	-4.74	99.36	105.83
6	F	102	BCL	C3D-C2D-C1D	-4.74	99.36	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	1	102	BCL	C3D-C2D-C1D	-4.73	99.37	105.83
6	N	102	BCL	C3D-C2D-C1D	-4.73	99.37	105.83
6	A	100	BCL	C1D-ND-C4D	-4.73	102.99	106.31
6	G	104	BCL	O2D-CGD-CBD	4.72	119.49	111.23
6	5	103	BCL	C3D-C2D-C1D	-4.72	99.39	105.83
6	V	102	BCL	C3D-C2D-C1D	-4.72	99.39	105.83
6	4	102	BCL	O2D-CGD-CBD	4.72	119.47	111.23
6	0	100	BCL	O2D-CGD-CBD	4.70	119.45	111.23
6	L	308	BCL	C3D-C2D-C1D	-4.70	99.41	105.83
6	U	100	BCL	C3D-C2D-C1D	-4.70	99.42	105.83
6	Y	102	BCL	C3D-C2D-C1D	-4.70	99.42	105.83
6	B	102	BCL	O2D-CGD-CBD	4.69	119.44	111.23
6	G	104	BCL	C3D-C2D-C1D	-4.68	99.45	105.83
6	Q	100	BCL	C3D-C2D-C1D	-4.68	99.45	105.83
6	C	102	BCL	C3D-C2D-C1D	-4.67	99.46	105.83
6	Y	102	BCL	O2D-CGD-CBD	4.66	119.37	111.23
6	4	102	BCL	C3D-C2D-C1D	-4.65	99.49	105.83
6	1	101	BCL	C1D-ND-C4D	-4.64	103.05	106.31
6	C	102	BCL	O2D-CGD-CBD	4.64	119.33	111.23
6	V	102	BCL	O2D-CGD-CBD	4.63	119.33	111.23
6	Q	100	BCL	O2D-CGD-CBD	4.61	119.29	111.23
6	B	102	BCL	C3D-C2D-C1D	-4.61	99.54	105.83
6	Y	101	BCL	C1D-ND-C4D	-4.59	103.09	106.31
6	9	102	BCL	C1D-ND-C4D	-4.57	103.11	106.31
7	X	101	CRT	C20-C21-C22	4.54	132.81	123.52
6	G	103	BCL	C1D-ND-C4D	-4.54	103.13	106.31
6	R	103	BCL	O2D-CGD-CBD	4.50	119.11	111.23
6	M	404	BCL	C3C-C4C-CHD	-4.47	113.96	123.39
6	C	101	BCL	C1D-ND-C4D	-4.47	103.18	106.31
6	A	100	BCL	C3C-C4C-CHD	-4.46	113.98	123.39
6	1	101	BCL	C3C-C4C-CHD	-4.46	114.00	123.39
6	M	404	BCL	O2D-CGD-CBD	4.45	119.00	111.23
7	I	102	CRT	C20-C21-C22	4.44	132.61	123.52
6	Y	101	BCL	C3C-C4C-CHD	-4.44	114.03	123.39
6	1	102	BCL	O2D-CGD-CBD	4.44	118.98	111.23
6	9	102	BCL	C3C-C4C-CHD	-4.43	114.06	123.39
6	L	301	BCL	C3C-C4C-CHD	-4.41	114.10	123.39
6	G	104	BCL	C3C-C4C-CHD	-4.38	114.15	123.39
6	P	102	BCL	C1D-ND-C4D	-4.38	103.24	106.31
6	T	100	BCL	C1D-ND-C4D	-4.38	103.24	106.31
6	J	101	BCL	C1D-ND-C4D	-4.38	103.24	106.31
6	G	103	BCL	C3C-C4C-CHD	-4.37	114.18	123.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	303	U10	C7-C8-C9	-4.36	119.33	126.83
6	M	402	BCL	C1D-ND-C4D	-4.34	103.27	106.31
7	2	102	CRT	C20-C21-C22	4.32	132.36	123.52
6	N	101	BCL	C1D-ND-C4D	-4.31	103.28	106.31
6	0	100	BCL	C1D-ND-C4D	-4.31	103.29	106.31
6	M	404	BCL	C1D-ND-C4D	-4.31	103.29	106.31
6	N	102	BCL	C3C-C4C-CHD	-4.30	114.32	123.39
6	G	104	BCL	C1D-ND-C4D	-4.30	103.30	106.31
6	7	102	BCL	C1D-ND-C4D	-4.28	103.31	106.31
6	R	101	BCL	C1D-ND-C4D	-4.28	103.31	106.31
6	J	101	BCL	C3B-C4B-NB	4.27	115.40	109.76
6	E	101	BCL	C1D-ND-C4D	-4.26	103.33	106.31
6	7	104	BCL	C3C-C4C-CHD	-4.25	114.42	123.39
6	A	100	BCL	C2D-C1D-ND	4.23	114.31	110.13
12	L	309	U10	C7-C8-C9	-4.23	119.55	126.83
6	L	301	BCL	C1D-ND-C4D	-4.23	103.35	106.31
6	V	102	BCL	C3C-C4C-CHD	-4.23	114.48	123.39
6	R	103	BCL	C3C-C4C-CHD	-4.23	114.48	123.39
6	B	102	BCL	C3C-C4C-CHD	-4.22	114.50	123.39
6	J	103	BCL	C3C-C4C-CHD	-4.21	114.51	123.39
6	T	100	BCL	C3C-C4C-CHD	-4.21	114.52	123.39
6	9	102	BCL	C3B-C4B-NB	4.21	115.31	109.76
6	P	102	BCL	C3B-C4B-NB	4.19	115.29	109.76
6	Q	100	BCL	C1D-ND-C4D	-4.19	103.37	106.31
6	R	103	BCL	C1D-ND-C4D	-4.19	103.38	106.31
6	5	103	BCL	C1D-ND-C4D	-4.19	103.38	106.31
6	V	101	BCL	C1D-ND-C4D	-4.18	103.38	106.31
6	L	301	BCL	C3B-C4B-NB	4.18	115.28	109.76
6	N	101	BCL	C3C-C4C-CHD	-4.17	114.61	123.39
6	G	103	BCL	C3B-C4B-NB	4.17	115.26	109.76
6	1	101	BCL	C3B-C4B-NB	4.16	115.25	109.76
6	N	102	BCL	C1D-ND-C4D	-4.16	103.39	106.31
6	7	104	BCL	C1D-ND-C4D	-4.16	103.39	106.31
6	G	103	BCL	C1-C2-C3	-4.16	119.39	126.20
6	1	102	BCL	C3C-C4C-CHD	-4.16	114.63	123.39
6	4	102	BCL	C3C-C4C-CHD	-4.15	114.63	123.39
6	C	101	BCL	C3B-C4B-NB	4.14	115.22	109.76
6	J	101	BCL	C1-C2-C3	-4.14	119.42	126.20
6	B	102	BCL	C1D-ND-C4D	-4.13	103.41	106.31
6	J	103	BCL	C1D-ND-C4D	-4.13	103.42	106.31
7	Z	102	CRT	C20-C21-C22	4.13	131.96	123.52
6	3	100	BCL	C1D-ND-C4D	-4.11	103.43	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	102	BCL	C3C-C4C-CHD	-4.10	114.74	123.39
6	V	102	BCL	C1D-ND-C4D	-4.10	103.44	106.31
6	1	101	BCL	C2D-C1D-ND	4.10	114.18	110.13
6	5	101	BCL	C1D-ND-C4D	-4.09	103.44	106.31
6	E	101	BCL	C3B-C4B-NB	4.09	115.16	109.76
6	C	101	BCL	C3C-C4C-CHD	-4.09	114.77	123.39
6	F	102	BCL	C1D-ND-C4D	-4.08	103.45	106.31
6	U	100	BCL	C1D-ND-C4D	-4.08	103.45	106.31
6	A	100	BCL	C3B-C4B-NB	4.08	115.14	109.76
6	3	100	BCL	C3B-C4B-NB	4.06	115.12	109.76
6	Y	102	BCL	C1D-ND-C4D	-4.06	103.46	106.31
6	0	100	BCL	C3B-C4B-NB	4.06	115.11	109.76
6	R	101	BCL	C3B-C4B-NB	4.05	115.11	109.76
7	U	101	CRT	C20-C21-C22	4.05	131.80	123.52
6	7	102	BCL	C3B-C4B-NB	4.04	115.09	109.76
6	R	101	BCL	C3C-C4C-CHD	-4.04	114.88	123.39
7	4	103	CRT	C20-C21-C22	4.03	131.77	123.52
6	7	104	BCL	C3B-C4B-NB	4.03	115.08	109.76
6	1	102	BCL	C1D-ND-C4D	-4.03	103.48	106.31
6	4	102	BCL	C1D-ND-C4D	-4.03	103.48	106.31
6	V	101	BCL	C3C-C4C-CHD	-4.03	114.90	123.39
6	0	100	BCL	C3C-C4C-CHD	-4.03	114.90	123.39
6	T	100	BCL	C3B-C4B-NB	4.02	115.07	109.76
6	N	101	BCL	C3B-C4B-NB	4.02	115.07	109.76
6	5	101	BCL	C3B-C4B-NB	4.02	115.07	109.76
6	M	402	BCL	C3C-C4C-CHD	-4.02	114.92	123.39
6	R	103	BCL	C3B-C4B-NB	4.02	115.06	109.76
6	Y	102	BCL	C3C-C4C-CHD	-4.02	114.93	123.39
6	V	101	BCL	C3B-C4B-NB	4.01	115.05	109.76
6	3	100	BCL	C3C-C4C-CHD	-4.00	114.96	123.39
6	9	102	BCL	C1-C2-C3	-4.00	119.65	126.20
7	O	102	CRT	C20-C21-C22	3.99	131.68	123.52
6	F	102	BCL	C3C-C4C-CHD	-3.98	114.99	123.39
6	U	100	BCL	C3C-C4C-CHD	-3.98	115.01	123.39
6	Q	100	BCL	C3C-C4C-CHD	-3.97	115.02	123.39
6	M	404	BCL	C3B-C4B-NB	3.97	115.00	109.76
6	L	301	BCL	O2D-CGD-CBD	3.97	118.17	111.23
7	K	101	CRT	C20-C21-C22	3.97	131.63	123.52
6	5	103	BCL	C3B-C4B-NB	3.95	114.98	109.76
6	Y	101	BCL	C2D-C1D-ND	3.95	114.04	110.13
7	D	101	CRT	C20-C21-C22	3.95	131.61	123.52
6	J	101	BCL	C3C-C4C-CHD	-3.94	115.08	123.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	N	102	BCL	C3B-C4B-NB	3.94	114.96	109.76
6	U	100	BCL	C3B-C4B-NB	3.94	114.96	109.76
6	Y	101	BCL	C3B-C4B-NB	3.94	114.96	109.76
6	C	102	BCL	C1D-ND-C4D	-3.93	103.56	106.31
6	C	102	BCL	C3B-C4B-NB	3.93	114.94	109.76
7	0	101	CRT	C20-C21-C22	3.92	131.55	123.52
6	G	103	BCL	C2D-C1D-ND	3.91	113.99	110.13
6	P	102	BCL	C3C-C4C-CHD	-3.91	115.16	123.39
6	E	101	BCL	C3C-C4C-CHD	-3.90	115.16	123.39
6	V	102	BCL	C3B-C4B-NB	3.90	114.91	109.76
6	F	102	BCL	C3B-C4B-NB	3.89	114.89	109.76
6	5	103	BCL	C3C-C4C-CHD	-3.88	115.21	123.39
6	L	301	BCL	C2D-C1D-ND	3.88	113.97	110.13
6	G	104	BCL	C3B-C4B-NB	3.87	114.87	109.76
6	9	102	BCL	C2D-C1D-ND	3.87	113.95	110.13
6	4	102	BCL	C3B-C4B-NB	3.86	114.86	109.76
6	R	103	BCL	C2D-C1D-ND	3.86	113.94	110.13
6	B	102	BCL	C3B-C4B-NB	3.85	114.84	109.76
6	5	101	BCL	C3C-C4C-CHD	-3.84	115.29	123.39
6	C	101	BCL	C2D-C1D-ND	3.84	113.93	110.13
6	7	102	BCL	C3C-C4C-CHD	-3.83	115.31	123.39
6	Y	102	BCL	C3B-C4B-NB	3.83	114.81	109.76
6	N	101	BCL	C2D-C1D-ND	3.82	113.91	110.13
6	J	103	BCL	C3B-C4B-NB	3.81	114.79	109.76
6	J	103	BCL	C2D-C1D-ND	3.81	113.90	110.13
6	Q	100	BCL	C3B-C4B-NB	3.81	114.79	109.76
6	T	100	BCL	C2D-C1D-ND	3.80	113.89	110.13
7	S	101	CRT	C20-C21-C22	3.80	131.29	123.52
6	M	404	BCL	C2D-C1D-ND	3.78	113.87	110.13
6	P	102	BCL	C2D-C1D-ND	3.78	113.87	110.13
6	E	101	BCL	C2D-C1D-ND	3.78	113.87	110.13
6	1	102	BCL	C3B-C4B-NB	3.76	114.72	109.76
6	M	402	BCL	C3D-C4D-ND	3.76	116.09	109.99
14	M	407	QAK	CD2-CE2-CZ2	3.74	114.70	110.75
6	0	100	BCL	C2D-C1D-ND	3.73	113.82	110.13
6	M	402	BCL	C3B-C4B-NB	3.73	114.67	109.76
6	J	101	BCL	C2D-C1D-ND	3.72	113.81	110.13
6	R	101	BCL	C2D-C1D-ND	3.72	113.81	110.13
6	G	104	BCL	C2D-C1D-ND	3.72	113.81	110.13
6	Y	102	BCL	C2D-C1D-ND	3.71	113.79	110.13
6	L	308	BCL	C3B-C4B-NB	3.70	114.64	109.76
7	7	101	CRT	C20-C21-C22	3.70	131.08	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	5	103	BCL	C2D-C1D-ND	3.69	113.78	110.13
6	3	100	BCL	C2D-C1D-ND	3.68	113.77	110.13
6	N	102	BCL	C2D-C1D-ND	3.67	113.76	110.13
6	7	102	BCL	C1-C2-C3	-3.67	120.19	126.20
6	7	102	BCL	C2D-C1D-ND	3.66	113.75	110.13
6	M	402	BCL	C2D-C1D-ND	3.66	113.75	110.13
6	V	102	BCL	C2D-C1D-ND	3.66	113.75	110.13
6	V	101	BCL	C1-C2-C3	-3.65	120.21	126.20
6	P	102	BCL	C1-C2-C3	-3.65	120.21	126.20
6	J	101	BCL	C3D-C4D-ND	3.65	115.92	109.99
6	7	102	BCL	C3D-C4D-ND	3.65	115.91	109.99
6	U	100	BCL	C3D-C4D-ND	3.64	115.91	109.99
6	Q	100	BCL	C3D-C4D-ND	3.64	115.91	109.99
6	G	104	BCL	C3D-C4D-ND	3.64	115.90	109.99
6	B	102	BCL	C3D-C4D-ND	3.63	115.89	109.99
6	V	101	BCL	C2D-C1D-ND	3.63	113.72	110.13
6	P	102	BCL	C3D-C4D-ND	3.63	115.89	109.99
6	L	308	BCL	CHC-C4B-NB	-3.63	118.61	124.05
6	5	103	BCL	C3D-C4D-ND	3.62	115.88	109.99
6	C	102	BCL	C2D-C1D-ND	3.62	113.71	110.13
6	C	101	BCL	C3D-C4D-ND	3.62	115.87	109.99
6	9	102	BCL	C3D-C4D-ND	3.61	115.86	109.99
6	1	102	BCL	C2D-C1D-ND	3.61	113.70	110.13
6	4	102	BCL	C2D-C1D-ND	3.61	113.70	110.13
6	0	100	BCL	C3D-C4D-ND	3.61	115.85	109.99
6	Y	102	BCL	C3D-C4D-ND	3.60	115.85	109.99
6	4	102	BCL	C3D-C4D-ND	3.60	115.84	109.99
6	7	104	BCL	C3D-C4D-ND	3.60	115.84	109.99
6	7	104	BCL	C2D-C1D-ND	3.60	113.69	110.13
6	1	101	BCL	C3D-C4D-ND	3.59	115.82	109.99
6	U	100	BCL	C2D-C1D-ND	3.59	113.68	110.13
6	1	102	BCL	C3D-C4D-ND	3.59	115.82	109.99
6	N	102	BCL	C3D-C4D-ND	3.59	115.81	109.99
6	F	102	BCL	C3D-C4D-ND	3.58	115.81	109.99
12	M	406	U10	C27-C28-C29	-3.58	119.43	127.62
6	T	100	BCL	C3D-C4D-ND	3.58	115.80	109.99
6	F	102	BCL	C2D-C1D-ND	3.58	113.67	110.13
6	V	101	BCL	C3D-C4D-ND	3.57	115.79	109.99
6	Y	101	BCL	C3D-C4D-ND	3.57	115.79	109.99
6	C	101	BCL	C1-C2-C3	-3.57	120.35	126.20
6	A	100	BCL	C3D-C4D-ND	3.57	115.78	109.99
6	M	404	BCL	C3D-C4D-ND	3.56	115.78	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	103	BCL	C3D-C4D-ND	3.56	115.78	109.99
6	R	101	BCL	C3D-C4D-ND	3.56	115.77	109.99
6	B	102	BCL	C2D-C1D-ND	3.56	113.65	110.13
12	L	307	U10	C7-C8-C9	-3.56	120.70	126.83
6	5	101	BCL	C3D-C4D-ND	3.56	115.77	109.99
7	G	102	CRT	C20-C21-C22	3.55	130.79	123.52
11	L	302	BPH	C4D-CHA-CBD	-3.55	106.75	108.45
7	Q	101	CRT	C20-C21-C22	3.55	130.78	123.52
12	M	410	U10	C22-C23-C24	-3.54	119.51	127.62
6	N	101	BCL	C3D-C4D-ND	3.54	115.74	109.99
6	Q	100	BCL	C1-C2-C3	-3.53	120.41	126.20
6	C	102	BCL	C1-C2-C3	-3.53	120.42	126.20
6	U	100	BCL	C1-C2-C3	-3.53	120.42	126.20
6	5	101	BCL	C1-C2-C3	-3.53	120.42	126.20
6	V	102	BCL	C3D-C4D-ND	3.52	115.72	109.99
6	E	101	BCL	C3D-C4D-ND	3.52	115.72	109.99
6	A	100	BCL	C1-C2-C3	-3.52	120.43	126.20
6	J	103	BCL	C3D-C4D-ND	3.51	115.70	109.99
12	L	309	U10	C27-C28-C29	-3.51	119.59	127.62
12	M	410	U10	C7-C8-C9	-3.51	120.79	126.83
6	C	102	BCL	C3D-C4D-ND	3.51	115.69	109.99
6	L	308	BCL	C3D-C4D-ND	3.50	115.68	109.99
6	R	103	BCL	C3D-C4D-ND	3.50	115.67	109.99
6	Q	100	BCL	C2D-C1D-ND	3.50	113.59	110.13
12	M	410	U10	C27-C28-C29	-3.49	119.63	127.62
7	2	102	CRT	C36-C35-C33	3.49	131.17	125.89
6	5	101	BCL	C2D-C1D-ND	3.48	113.57	110.13
6	E	101	BCL	C1-C2-C3	-3.48	120.49	126.20
6	3	100	BCL	C3D-C4D-ND	3.46	115.61	109.99
6	Y	101	BCL	C1-C2-C3	-3.45	120.54	126.20
6	1	102	BCL	C1-C2-C3	-3.43	120.57	126.20
6	L	308	BCL	C1D-ND-C4D	-3.43	103.90	106.31
6	L	301	BCL	C3D-C4D-ND	3.42	115.55	109.99
6	3	100	BCL	C1-C2-C3	-3.42	120.59	126.20
7	8	101	CRT	C36-C35-C33	3.41	131.05	125.89
12	M	410	U10	C42-C43-C44	-3.41	119.81	127.62
7	B	103	CRT	C20-C21-C22	3.41	130.50	123.52
12	L	307	U10	C32-C33-C34	-3.40	119.84	127.62
11	M	405	BPH	C4D-CHA-CBD	-3.40	106.82	108.45
12	L	303	U10	C27-C28-C29	-3.40	119.85	127.62
6	0	100	BCL	C1-C2-C3	-3.39	120.65	126.20
12	L	307	U10	C22-C23-C24	-3.38	119.89	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	R	101	BCL	C1-C2-C3	-3.38	120.66	126.20
12	L	307	U10	C42-C43-C44	-3.37	119.90	127.62
12	M	410	U10	C35-C34-C36	3.37	121.07	115.23
6	L	301	BCL	O2A-CGA-CBA	3.34	122.02	111.83
12	L	309	U10	C32-C33-C34	-3.34	119.98	127.62
6	V	102	BCL	C1-C2-C3	-3.33	120.74	126.20
12	M	410	U10	C12-C13-C14	-3.33	120.01	127.62
12	M	410	U10	C32-C33-C34	-3.32	120.02	127.62
12	L	307	U10	C15-C14-C16	3.32	121.00	115.23
12	L	303	U10	C12-C13-C14	-3.32	120.03	127.62
6	G	103	BCL	C4-C3-C5	3.30	120.95	115.23
10	6	101	LMT	C1'-O5'-C5'	-3.29	107.29	113.72
6	7	104	BCL	C1-C2-C3	-3.29	120.81	126.20
6	T	100	BCL	C1-C2-C3	-3.29	120.81	126.20
12	L	303	U10	C7-C6-C1	-3.28	119.26	124.89
12	M	406	U10	C12-C13-C14	-3.28	120.11	127.62
6	L	308	BCL	C3C-C4C-CHD	-3.23	116.58	123.39
6	R	103	BCL	C1-C2-C3	-3.23	120.91	126.20
6	R	101	BCL	O2A-CGA-CBA	3.22	121.64	111.83
12	L	309	U10	C42-C43-C44	-3.19	120.31	127.62
6	L	301	BCL	C1-C2-C3	-3.19	120.97	126.20
6	G	104	BCL	C1-C2-C3	-3.19	120.97	126.20
6	F	102	BCL	C1-C2-C3	-3.18	120.99	126.20
12	M	406	U10	C25-C24-C26	3.17	120.74	115.23
6	M	402	BCL	C1-C2-C3	-3.16	121.02	126.20
10	2	101	LMT	C3'-C4'-C5'	-3.16	103.92	110.93
6	5	101	BCL	O2A-CGA-CBA	3.16	121.47	111.83
6	Y	101	BCL	O2A-CGA-CBA	3.16	121.46	111.83
7	8	101	CRT	C15-C14-C12	3.15	131.70	127.28
10	J	102	LMT	C1'-O5'-C5'	-3.15	107.57	113.72
6	N	101	BCL	O2A-CGA-CBA	3.14	121.42	111.83
12	L	309	U10	C12-C13-C14	-3.14	120.43	127.62
6	C	101	BCL	C4-C3-C5	3.14	120.69	115.23
6	1	101	BCL	C1-C2-C3	-3.14	121.05	126.20
10	O	101	LMT	C1'-O5'-C5'	-3.14	107.60	113.72
6	J	103	BCL	C1-C2-C3	-3.13	121.06	126.20
12	L	307	U10	C25-C24-C26	3.12	120.65	115.23
6	3	100	BCL	C4-C3-C5	3.12	120.64	115.23
6	A	100	BCL	C4-C3-C5	3.10	120.61	115.23
12	M	410	U10	C7-C6-C1	-3.10	119.58	124.89
6	4	102	BCL	C1-C2-C3	-3.10	121.12	126.20
6	Y	102	BCL	C1-C2-C3	-3.09	121.14	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	307	U10	C20-C19-C21	3.09	120.59	115.23
6	E	101	BCL	C4-C3-C5	3.08	120.58	115.23
6	Y	101	BCL	C4-C3-C5	3.08	120.57	115.23
6	L	308	BCL	C2D-C1D-ND	3.08	113.17	110.13
12	M	406	U10	C17-C18-C19	-3.06	120.61	127.62
12	L	303	U10	C22-C23-C24	-3.06	120.61	127.62
6	U	100	BCL	O2A-CGA-CBA	3.06	121.17	111.83
12	M	406	U10	C35-C34-C36	3.05	120.53	115.23
12	L	307	U10	C47-C48-C49	-3.05	120.64	127.62
6	V	101	BCL	C4-C3-C5	3.05	120.52	115.23
7	X	101	CRT	C6-C7-C9	3.05	123.80	119.01
6	T	100	BCL	O2A-CGA-CBA	3.05	121.12	111.83
6	G	104	BCL	O2A-CGA-CBA	3.04	121.11	111.83
6	P	102	BCL	O2A-CGA-CBA	3.04	121.09	111.83
7	8	101	CRT	C31-C32-C33	3.03	131.53	127.28
10	4	101	LMT	C3'-C4'-C5'	-3.03	104.22	110.93
12	L	307	U10	C17-C18-C19	-3.02	120.71	127.62
6	9	102	BCL	C4-C3-C5	3.02	120.46	115.23
10	O	101	LMT	C3'-C4'-C5'	-3.01	104.26	110.93
12	M	410	U10	C25-C24-C26	3.00	120.44	115.23
6	L	308	BCL	CHB-C1B-NB	-3.00	119.55	124.05
12	L	309	U10	C47-C48-C49	-2.98	120.79	127.62
6	4	102	BCL	O2A-CGA-CBA	2.98	120.92	111.83
6	P	102	BCL	C4-C3-C5	2.98	120.39	115.23
6	C	102	BCL	O2A-CGA-CBA	2.97	120.89	111.83
6	7	102	BCL	O2A-CGA-CBA	2.97	120.88	111.83
6	M	402	BCL	C4-C3-C5	2.96	120.37	115.23
10	J	102	LMT	O1'-C1'-C2'	2.96	112.77	108.27
12	L	307	U10	C50-C49-C51	2.96	120.36	115.23
6	5	103	BCL	C1-C2-C3	-2.95	121.36	126.20
12	M	406	U10	C15-C14-C16	2.95	120.35	115.23
6	1	102	BCL	C4-C3-C5	2.94	120.33	115.23
6	3	100	BCL	O2A-CGA-CBA	2.94	120.80	111.83
6	Y	102	BCL	O2A-CGA-CBA	2.94	120.80	111.83
6	R	101	BCL	CHC-C1C-NC	2.94	128.64	124.40
12	L	309	U10	C50-C49-C51	2.94	120.32	115.23
6	5	103	BCL	O2A-CGA-CBA	2.93	120.78	111.83
6	1	101	BCL	O2A-CGA-CBA	2.93	120.78	111.83
6	N	102	BCL	C1-C2-C3	-2.93	121.39	126.20
6	M	404	BCL	O2A-CGA-CBA	2.93	120.78	111.83
6	L	301	BCL	C4-C3-C5	2.93	120.32	115.23
7	8	101	CRT	C6-C7-C9	2.93	123.61	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	309	U10	C22-C23-C24	-2.93	120.93	127.62
7	8	101	CRT	C21-C20-C19	2.92	129.50	123.52
6	L	308	BCL	O2A-CGA-CBA	2.92	120.74	111.83
6	J	103	BCL	CHB-C4A-NA	2.92	128.61	124.40
12	L	309	U10	C40-C39-C41	2.92	120.29	115.23
6	T	100	BCL	CHC-C1C-NC	2.91	128.60	124.40
6	J	101	BCL	CHC-C1C-NC	2.91	128.60	124.40
6	N	102	BCL	O2A-CGA-CBA	2.91	120.70	111.83
12	M	410	U10	C30-C29-C31	2.91	120.27	115.23
6	V	101	BCL	O2A-CGA-CBA	2.90	120.68	111.83
10	Z	101	LMT	C3'-C4'-C5'	-2.90	104.50	110.93
6	L	308	BCL	C4-C3-C5	2.90	120.26	115.23
6	T	100	BCL	C4-C3-C5	2.90	120.26	115.23
12	L	307	U10	C45-C44-C46	2.90	120.26	115.23
6	C	101	BCL	O2A-CGA-CBA	2.90	120.67	111.83
12	L	303	U10	C35-C34-C36	2.90	120.26	115.23
6	1	102	BCL	O2A-CGA-CBA	2.90	120.67	111.83
6	V	101	BCL	CHC-C1C-NC	2.90	128.58	124.40
12	L	309	U10	C20-C19-C21	2.90	120.25	115.23
6	V	102	BCL	O2A-CGA-CBA	2.89	120.64	111.83
6	1	101	BCL	C4-C3-C5	2.89	120.24	115.23
7	X	101	CRT	C8-C7-C9	-2.88	118.14	122.82
7	8	101	CRT	C25-C23-C22	2.88	123.54	119.01
7	4	103	CRT	C15-C14-C12	2.88	131.32	127.28
6	9	102	BCL	O2A-CGA-CBA	2.88	120.61	111.83
6	0	100	BCL	O2A-CGA-CBA	2.88	120.61	111.83
7	X	101	CRT	C25-C23-C22	2.88	123.53	119.01
12	L	303	U10	C32-C33-C34	-2.87	121.04	127.62
7	G	102	CRT	C21-C20-C19	2.87	129.40	123.52
12	M	410	U10	C17-C18-C19	-2.87	121.05	127.62
6	G	103	BCL	O2A-CGA-CBA	2.87	120.59	111.83
6	L	308	BCL	O2D-CGD-O1D	-2.87	118.27	123.85
12	M	406	U10	C20-C19-C21	2.87	120.20	115.23
11	M	405	BPH	C2B-C1B-NB	-2.87	107.36	109.43
6	J	101	BCL	O2A-CGA-CBA	2.87	120.57	111.83
6	E	101	BCL	O2A-CGA-CBA	2.86	120.57	111.83
6	N	101	BCL	C4-C3-C5	2.86	120.20	115.23
6	A	100	BCL	O2A-CGA-CBA	2.86	120.56	111.83
6	G	103	BCL	CHC-C1C-NC	2.86	128.53	124.40
12	M	410	U10	C50-C49-C51	2.86	120.19	115.23
6	9	102	BCL	CHC-C1C-NC	2.86	128.52	124.40
6	R	103	BCL	O2A-CGA-CBA	2.86	120.54	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	P	102	BCL	CHC-C1C-NC	2.85	128.51	124.40
6	7	102	BCL	C4-C3-C5	2.84	120.16	115.23
6	J	103	BCL	O2A-CGA-CBA	2.84	120.49	111.83
6	R	101	BCL	C4-C3-C5	2.84	120.15	115.23
12	L	307	U10	C40-C39-C41	2.84	120.15	115.23
7	2	102	CRT	C25-C23-C22	2.83	123.46	119.01
6	5	101	BCL	C4-C3-C5	2.83	120.14	115.23
6	F	102	BCL	O2A-CGA-CBA	2.83	120.46	111.83
6	M	404	BCL	CHC-C4B-NB	-2.83	119.81	124.05
12	L	309	U10	C35-C34-C36	2.82	120.13	115.23
7	0	101	CRT	C21-C20-C19	2.82	129.29	123.52
6	R	103	BCL	CHB-C4A-NA	2.82	128.47	124.40
11	L	302	BPH	C2B-C1B-NB	-2.82	107.39	109.43
6	E	101	BCL	CHC-C1C-NC	2.82	128.47	124.40
7	2	102	CRT	C24-C23-C22	-2.82	118.25	122.82
6	G	104	BCL	CHB-C4A-NA	2.82	128.46	124.40
7	I	102	CRT	C36-C35-C33	2.81	130.14	125.89
7	X	101	CRT	C24-C23-C22	-2.81	118.27	122.82
12	M	406	U10	C22-C23-C24	-2.81	121.20	127.62
7	8	101	CRT	C24-C23-C22	-2.81	118.27	122.82
7	8	101	CRT	C8-C7-C9	-2.80	118.27	122.82
12	L	307	U10	C10-C9-C11	2.80	120.09	115.23
6	A	100	BCL	CHC-C1C-NC	2.80	128.44	124.40
6	J	101	BCL	C4-C3-C5	2.80	120.09	115.23
6	7	104	BCL	CHB-C4A-NA	2.80	128.44	124.40
7	Q	101	CRT	C21-C20-C19	2.80	129.24	123.52
6	B	102	BCL	C1-C2-C3	-2.80	121.61	126.20
10	F	101	LMT	C1'-O5'-C5'	-2.79	108.27	113.72
6	9	102	BCL	O2D-CGD-O1D	-2.79	118.41	123.85
6	M	402	BCL	O2D-CGD-O1D	-2.79	118.41	123.85
6	U	100	BCL	C4-C3-C5	2.79	120.07	115.23
12	M	410	U10	C10-C9-C11	2.79	120.07	115.23
12	M	410	U10	C47-C48-C49	-2.78	121.25	127.62
12	L	303	U10	C30-C29-C31	2.78	120.06	115.23
6	L	301	BCL	CHC-C1C-NC	2.78	128.41	124.40
12	M	410	U10	C15-C14-C16	2.78	120.05	115.23
10	4	101	LMT	O5B-C5B-C4B	2.77	114.69	109.70
6	5	101	BCL	CMD-C2D-C3D	-2.77	121.33	127.69
6	V	102	BCL	CHB-C4A-NA	2.77	128.40	124.40
12	L	307	U10	C12-C13-C14	-2.77	121.29	127.62
12	L	309	U10	C15-C14-C16	2.77	120.03	115.23
6	J	103	BCL	CHC-C1C-NC	2.77	128.39	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Q	100	BCL	O2A-CGA-CBA	2.77	120.27	111.83
6	N	101	BCL	C1-C2-C3	-2.76	121.67	126.20
6	U	100	BCL	O2D-CGD-O1D	-2.76	118.47	123.85
7	7	101	CRT	C8-C7-C9	-2.76	118.34	122.82
12	M	406	U10	C32-C33-C34	-2.76	121.30	127.62
12	L	303	U10	C1M-C1-C6	-2.76	119.91	124.45
7	0	101	CRT	C24-C23-C22	-2.76	118.35	122.82
12	L	307	U10	C35-C34-C36	2.76	120.02	115.23
10	P	101	LMT	C1'-O5'-C5'	-2.76	108.33	113.72
6	B	102	BCL	O2D-CGD-O1D	-2.75	118.49	123.85
6	Q	100	BCL	C4-C3-C5	2.75	120.00	115.23
6	B	102	BCL	CHB-C4A-NA	2.75	128.37	124.40
12	L	307	U10	C30-C29-C31	2.75	120.00	115.23
6	3	100	BCL	CHC-C1C-NC	2.75	128.36	124.40
7	B	103	CRT	C21-C20-C19	2.74	129.13	123.52
6	U	100	BCL	CHC-C1C-NC	2.74	128.36	124.40
7	4	103	CRT	C36-C35-C33	2.74	130.03	125.89
7	I	102	CRT	C24-C23-C22	-2.74	118.37	122.82
7	U	101	CRT	C24-C23-C22	-2.74	118.37	122.82
12	M	410	U10	C20-C19-C21	2.74	119.98	115.23
6	Q	100	BCL	CHC-C1C-NC	2.74	128.35	124.40
6	1	101	BCL	CHC-C1C-NC	2.74	128.35	124.40
10	Z	101	LMT	C1'-O5'-C5'	-2.73	108.38	113.72
10	H	302	LMT	C3'-C4'-C5'	-2.73	104.89	110.93
7	X	101	CRT	C15-C14-C12	2.72	131.10	127.28
12	L	303	U10	C17-C18-C19	-2.72	121.40	127.62
6	U	100	BCL	CHB-C4A-NA	2.72	128.32	124.40
6	L	308	BCL	CMD-C2D-C3D	-2.72	121.46	127.69
6	7	104	BCL	CHC-C1C-NC	2.72	128.32	124.40
6	N	102	BCL	CHB-C4A-NA	2.71	128.32	124.40
7	4	103	CRT	C24-C23-C22	-2.71	118.42	122.82
6	7	104	BCL	O2A-CGA-CBA	2.71	120.10	111.83
7	0	101	CRT	C25-C23-C22	2.71	123.27	119.01
6	5	103	BCL	CHB-C4A-NA	2.71	128.31	124.40
6	F	102	BCL	CHC-C4B-NB	-2.71	119.99	124.05
6	Y	102	BCL	CHB-C4A-NA	2.70	128.30	124.40
6	V	102	BCL	C4-C3-C5	2.70	119.91	115.23
7	K	101	CRT	C8-C7-C9	-2.70	118.45	122.82
7	O	102	CRT	C8-C7-C9	-2.70	118.45	122.82
7	S	101	CRT	C24-C23-C22	-2.69	118.45	122.82
7	K	101	CRT	C24-C23-C22	-2.69	118.45	122.82
6	B	102	BCL	O2A-CGA-CBA	2.69	120.03	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	102	CRT	C8-C7-C9	-2.69	118.46	122.82
6	R	103	BCL	CHC-C1C-NC	2.69	128.28	124.40
7	2	102	CRT	C31-C32-C33	2.68	131.04	127.28
7	S	101	CRT	C21-C20-C19	2.68	129.01	123.52
12	L	309	U10	C25-C24-C26	2.68	119.89	115.23
10	4	101	LMT	C1'-O5'-C5'	-2.68	108.48	113.72
7	2	102	CRT	C21-C20-C19	2.68	129.00	123.52
6	Y	101	BCL	CHC-C1C-NC	2.68	128.27	124.40
10	R	102	LMT	C1'-O5'-C5'	-2.68	108.49	113.72
6	C	102	BCL	CHB-C4A-NA	2.68	128.27	124.40
6	N	102	BCL	O2D-CGD-O1D	-2.68	118.64	123.85
7	B	103	CRT	C8-C7-C9	-2.68	118.48	122.82
6	F	102	BCL	CHB-C4A-NA	2.68	128.26	124.40
6	9	102	BCL	CMD-C2D-C3D	-2.67	121.56	127.69
6	0	100	BCL	CHB-C4A-NA	2.67	128.26	124.40
7	7	101	CRT	C6-C7-C9	2.67	123.21	119.01
6	T	100	BCL	CMD-C2D-C3D	-2.67	121.57	127.69
6	Q	100	BCL	CHB-C4A-NA	2.67	128.25	124.40
6	C	101	BCL	O2D-CGD-O1D	-2.66	118.66	123.85
7	Q	101	CRT	C8-C7-C9	-2.66	118.50	122.82
6	G	104	BCL	CHC-C1C-NC	2.66	128.24	124.40
7	D	101	CRT	C24-C23-C22	-2.66	118.51	122.82
7	K	101	CRT	C6-C7-C9	2.66	123.19	119.01
7	0	101	CRT	C8-C7-C9	-2.66	118.51	122.82
6	7	102	BCL	CMD-C2D-C3D	-2.66	121.60	127.69
6	4	102	BCL	CHC-C4B-NB	-2.65	120.07	124.05
6	7	102	BCL	CHC-C4B-NB	-2.65	120.07	124.05
6	N	101	BCL	CHC-C1C-NC	2.65	128.22	124.40
7	Z	102	CRT	C24-C23-C22	-2.65	118.53	122.82
6	0	100	BCL	CHC-C1C-NC	2.64	128.22	124.40
10	H	302	LMT	C1'-O5'-C5'	-2.64	108.56	113.72
6	J	101	BCL	CMD-C2D-C3D	-2.64	121.63	127.69
12	L	309	U10	C30-C29-C31	2.64	119.81	115.23
7	O	102	CRT	C31-C32-C33	2.64	130.98	127.28
6	G	103	BCL	CMD-C2D-C3D	-2.64	121.64	127.69
7	7	101	CRT	C24-C23-C22	-2.64	118.54	122.82
6	M	404	BCL	C1-C2-C3	-2.64	121.88	126.20
6	7	102	BCL	CHC-C1C-NC	2.64	128.20	124.40
12	L	309	U10	C17-C18-C19	-2.63	121.59	127.62
6	M	404	BCL	CMD-C2D-C3D	-2.63	121.65	127.69
6	U	100	BCL	CHC-C4B-NB	-2.63	120.10	124.05
6	M	404	BCL	CHC-C1C-NC	2.63	128.20	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	5	103	BCL	CHC-C1C-NC	2.63	128.20	124.40
10	B	101	LMT	C1'-O5'-C5'	-2.63	108.58	113.72
6	N	102	BCL	CHC-C1C-NC	2.63	128.19	124.40
12	M	406	U10	C10-C9-C11	2.63	119.79	115.23
6	5	103	BCL	CHC-C4B-NB	-2.63	120.11	124.05
6	P	102	BCL	CHC-C4B-NB	-2.63	120.11	124.05
7	D	101	CRT	C21-C20-C19	2.62	128.88	123.52
6	R	101	BCL	CMD-C2D-C3D	-2.62	121.68	127.69
6	C	102	BCL	C4-C3-C5	2.62	119.78	115.23
6	Y	101	BCL	CHC-C4B-NB	-2.62	120.12	124.05
7	G	102	CRT	C24-C23-C22	-2.62	118.58	122.82
7	0	101	CRT	C18-C17-C19	-2.62	118.58	122.82
6	7	104	BCL	O2D-CGD-O1D	-2.61	118.76	123.85
6	Y	102	BCL	O2D-CGD-O1D	-2.61	118.76	123.85
6	Y	102	BCL	C4-C3-C5	2.61	119.76	115.23
12	L	309	U10	C1M-C1-C6	-2.61	120.16	124.45
6	C	101	BCL	CHC-C1C-NC	2.61	128.16	124.40
6	7	104	BCL	C4-C3-C5	2.60	119.74	115.23
6	G	103	BCL	O2D-CGD-O1D	-2.60	118.79	123.85
12	L	309	U10	C10-C9-C11	2.60	119.74	115.23
6	A	100	BCL	CHC-C4B-NB	-2.60	120.15	124.05
7	U	101	CRT	C25-C23-C22	2.60	123.09	119.01
6	9	102	BCL	CHB-C4A-NA	2.60	128.15	124.40
6	E	101	BCL	O2D-CGD-O1D	-2.59	118.80	123.85
6	C	102	BCL	O2D-CGD-O1D	-2.59	118.80	123.85
7	O	102	CRT	C24-C23-C22	-2.59	118.62	122.82
6	P	102	BCL	CMD-C2D-C3D	-2.59	121.75	127.69
6	R	103	BCL	C4-C3-C5	2.59	119.72	115.23
7	4	103	CRT	C25-C23-C22	2.59	123.08	119.01
7	U	101	CRT	C8-C7-C9	-2.59	118.62	122.82
7	Q	101	CRT	C24-C23-C22	-2.59	118.62	122.82
6	F	102	BCL	C4-C3-C5	2.59	119.72	115.23
6	G	104	BCL	CHC-C4B-NB	-2.59	120.17	124.05
6	0	100	BCL	O2D-CGD-O1D	-2.59	118.82	123.85
7	I	102	CRT	C25-C23-C22	2.58	123.08	119.01
6	M	402	BCL	O2A-CGA-CBA	2.58	119.72	111.83
6	Q	100	BCL	C2A-C1A-CHA	-2.58	119.38	123.87
10	4	101	LMT	O5B-C5B-C6B	2.58	112.84	106.44
7	U	101	CRT	C21-C20-C19	2.58	128.80	123.52
6	T	100	BCL	CHC-C4B-NB	-2.58	120.18	124.05
6	Y	101	BCL	CMD-C2D-C3D	-2.58	121.77	127.69
7	B	103	CRT	C24-C23-C22	-2.58	118.64	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	301	BCL	CHC-C4B-NB	-2.58	120.18	124.05
12	M	410	U10	C1M-C1-C6	-2.58	120.21	124.45
6	3	100	BCL	CMD-C2D-C3D	-2.58	121.78	127.69
6	9	102	BCL	CHC-C4B-NB	-2.58	120.18	124.05
6	5	103	BCL	O2D-CGD-O1D	-2.58	118.83	123.85
6	R	101	BCL	O2D-CGD-O1D	-2.57	118.84	123.85
6	5	101	BCL	CHC-C1C-NC	2.57	128.11	124.40
7	7	101	CRT	C21-C20-C19	2.57	128.78	123.52
7	S	101	CRT	C25-C23-C22	2.57	123.05	119.01
10	L	306	LMT	C1'-O5'-C5'	-2.57	108.70	113.72
12	L	303	U10	C20-C19-C21	2.57	119.69	115.23
6	J	103	BCL	C4-C3-C5	2.57	119.69	115.23
6	M	402	BCL	CHC-C1C-NC	2.57	128.10	124.40
6	1	102	BCL	CHB-C4A-NA	2.56	128.10	124.40
7	G	102	CRT	C31-C32-C33	2.56	130.87	127.28
7	7	101	CRT	C15-C14-C12	2.56	130.87	127.28
6	1	102	BCL	CHC-C1C-NC	2.56	128.09	124.40
6	V	101	BCL	CMD-C2D-C3D	-2.56	121.82	127.69
6	V	102	BCL	CHC-C1C-NC	2.56	128.09	124.40
6	V	101	BCL	O2D-CGD-O1D	-2.56	118.87	123.85
7	O	102	CRT	C6-C7-C9	2.55	123.03	119.01
7	S	101	CRT	C8-C7-C9	-2.55	118.68	122.82
12	L	303	U10	C25-C24-C26	2.55	119.65	115.23
6	F	102	BCL	O2D-CGD-O1D	-2.55	118.89	123.85
6	N	101	BCL	O2D-CGD-O1D	-2.55	118.89	123.85
6	F	102	BCL	CHC-C1C-NC	2.54	128.07	124.40
6	M	404	BCL	CHB-C1B-NB	-2.54	120.23	124.05
7	G	102	CRT	C15-C14-C12	2.54	130.84	127.28
7	G	102	CRT	C8-C7-C9	-2.54	118.70	122.82
7	2	102	CRT	C8-C7-C9	-2.54	118.70	122.82
6	E	101	BCL	CMD-C2D-C3D	-2.53	121.88	127.69
7	U	101	CRT	C31-C32-C33	2.53	130.83	127.28
6	1	101	BCL	C2A-C1A-CHA	-2.53	119.47	123.87
6	N	102	BCL	CHC-C4B-NB	-2.53	120.25	124.05
6	R	101	BCL	CHC-C4B-NB	-2.53	120.25	124.05
6	C	102	BCL	CHC-C4B-NB	-2.53	120.26	124.05
6	C	102	BCL	CHC-C1C-NC	2.53	128.05	124.40
6	C	101	BCL	CHC-C4B-NB	-2.53	120.26	124.05
7	G	102	CRT	C36-C35-C33	2.53	129.71	125.89
7	X	101	CRT	C29-C28-C27	-2.53	118.72	122.82
6	1	101	BCL	CHB-C4A-NA	2.53	128.04	124.40
6	L	308	BCL	C1-C2-C3	-2.53	122.06	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	2	102	CRT	C18-C17-C19	-2.52	118.73	122.82
6	G	103	BCL	CHC-C4B-NB	-2.52	120.26	124.05
6	G	103	BCL	CHB-C4A-NA	2.52	128.04	124.40
6	B	102	BCL	CHC-C1C-NC	2.52	128.04	124.40
7	I	102	CRT	C31-C32-C33	2.52	130.81	127.28
6	Y	101	BCL	C2A-C1A-CHA	-2.52	119.49	123.87
7	K	101	CRT	C25-C23-C22	2.52	122.97	119.01
10	2	101	LMT	C1'-O5'-C5'	-2.52	108.81	113.72
6	4	102	BCL	CHB-C4A-NA	2.52	128.03	124.40
6	T	100	BCL	O2D-CGD-O1D	-2.51	118.96	123.85
7	Q	101	CRT	C31-C32-C33	2.51	130.80	127.28
6	1	101	BCL	O2D-CGD-O1D	-2.51	118.97	123.85
6	C	101	BCL	CHB-C4A-NA	2.51	128.02	124.40
6	E	101	BCL	CHC-C4B-NB	-2.51	120.29	124.05
6	J	103	BCL	O2D-CGD-O1D	-2.51	118.97	123.85
12	M	406	U10	C30-C29-C31	2.50	119.58	115.23
7	I	102	CRT	C6-C7-C9	2.50	122.95	119.01
7	2	102	CRT	C29-C28-C27	-2.50	118.76	122.82
6	P	102	BCL	O2D-CGD-O1D	-2.50	118.98	123.85
7	G	102	CRT	C18-C17-C19	-2.50	118.77	122.82
6	3	100	BCL	CHC-C4B-NB	-2.50	120.30	124.05
6	Y	102	BCL	CHC-C1C-NC	2.50	128.00	124.40
6	4	102	BCL	C4-C3-C5	2.49	119.56	115.23
10	R	102	LMT	C3'-C4'-C5'	-2.49	105.42	110.93
7	4	103	CRT	C21-C20-C19	2.49	128.60	123.52
6	Q	100	BCL	CMD-C2D-C3D	-2.49	121.99	127.69
7	4	103	CRT	C8-C7-C9	-2.49	118.79	122.82
6	1	102	BCL	CHC-C4B-NB	-2.48	120.33	124.05
6	N	101	BCL	CMD-C2D-C3D	-2.48	122.00	127.69
6	5	101	BCL	CHB-C1B-NB	-2.48	120.33	124.05
6	7	104	BCL	CHC-C4B-NB	-2.48	120.33	124.05
6	J	101	BCL	CHC-C4B-NB	-2.48	120.33	124.05
12	M	410	U10	C40-C39-C41	2.48	119.53	115.23
7	2	102	CRT	C13-C12-C14	-2.48	118.80	122.82
6	1	101	BCL	CMD-C2D-C3D	-2.47	122.02	127.69
6	1	101	BCL	CHC-C4B-NB	-2.47	120.34	124.05
6	5	103	BCL	C4-C3-C5	2.47	119.51	115.23
12	L	307	U10	C1M-C1-C6	-2.47	120.39	124.45
6	C	101	BCL	CMD-C2D-C3D	-2.47	122.03	127.69
6	B	102	BCL	CHC-C4B-NB	-2.47	120.35	124.05
6	N	102	BCL	C4-C3-C5	2.46	119.51	115.23
6	0	100	BCL	CHC-C4B-NB	-2.46	120.36	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	402	BCL	C2A-C1A-CHA	-2.46	119.59	123.87
6	J	103	BCL	CHC-C4B-NB	-2.46	120.36	124.05
6	Q	100	BCL	CHC-C4B-NB	-2.46	120.36	124.05
6	0	100	BCL	C2A-C1A-CHA	-2.46	119.60	123.87
6	G	104	BCL	C4-C3-C5	2.46	119.49	115.23
7	Q	101	CRT	C6-C7-C9	2.46	122.87	119.01
10	R	102	LMT	O1B-C4'-C3'	2.46	113.47	107.23
12	M	410	U10	C56-C54-C55	2.45	120.24	114.59
6	0	100	BCL	CMD-C2D-C3D	-2.45	122.06	127.69
6	E	101	BCL	CMB-C2B-C3B	2.45	133.41	125.67
7	0	101	CRT	C13-C12-C14	-2.45	118.84	122.82
7	Z	102	CRT	C25-C23-C22	2.45	122.87	119.01
7	O	102	CRT	C36-C35-C33	2.45	129.60	125.89
6	7	104	BCL	C2A-C1A-CHA	-2.45	119.62	123.87
7	D	101	CRT	C18-C17-C19	-2.45	118.85	122.82
6	Y	101	BCL	CMB-C2B-C3B	2.45	133.39	125.67
7	Q	101	CRT	C18-C17-C19	-2.45	118.85	122.82
6	R	103	BCL	CHC-C4B-NB	-2.45	120.38	124.05
6	V	101	BCL	CHC-C4B-NB	-2.45	120.38	124.05
6	G	104	BCL	O2D-CGD-O1D	-2.44	119.09	123.85
6	R	103	BCL	O2D-CGD-O1D	-2.44	119.09	123.85
12	M	410	U10	C45-C44-C46	2.44	119.47	115.23
7	B	103	CRT	C34-C33-C32	-2.44	118.86	122.82
6	M	404	BCL	C4A-NA-C1A	2.44	107.79	106.68
7	8	101	CRT	C18-C17-C19	-2.44	118.87	122.82
7	Z	102	CRT	C15-C14-C12	2.44	130.69	127.28
6	C	102	BCL	CMB-C2B-C3B	2.43	133.35	125.67
7	0	101	CRT	C6-C7-C9	2.43	122.84	119.01
6	M	404	BCL	CED-O2D-CGD	2.43	121.43	115.92
7	D	101	CRT	C8-C7-C9	-2.43	118.88	122.82
7	O	102	CRT	C25-C23-C22	2.43	122.83	119.01
6	T	100	BCL	CMB-C2B-C3B	2.43	133.33	125.67
7	S	101	CRT	C18-C17-C19	-2.43	118.88	122.82
7	B	103	CRT	C18-C17-C19	-2.43	118.89	122.82
6	L	301	BCL	CED-O2D-CGD	2.43	121.42	115.92
12	L	307	U10	C37-C38-C39	-2.42	122.08	127.62
7	Z	102	CRT	C29-C28-C27	-2.42	118.89	122.82
6	9	102	BCL	C2A-C1A-CHA	-2.42	119.66	123.87
7	Z	102	CRT	C8-C7-C9	-2.42	118.89	122.82
7	7	101	CRT	C25-C23-C22	2.42	122.82	119.01
6	U	100	BCL	CMB-C2B-C3B	2.42	133.30	125.67
7	O	102	CRT	C15-C14-C12	2.42	130.67	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	M	405	BPH	CMA-C3A-C4A	-2.42	109.41	114.61
7	7	101	CRT	C31-C32-C33	2.42	130.66	127.28
7	2	102	CRT	C6-C7-C9	2.41	122.81	119.01
6	4	102	BCL	CHB-C1B-NB	-2.41	120.43	124.05
7	U	101	CRT	C13-C12-C14	-2.41	118.91	122.82
6	B	102	BCL	C4-C3-C5	2.41	119.41	115.23
6	L	308	BCL	CHD-C1D-C2D	2.41	130.50	125.49
6	A	100	BCL	CMD-C2D-C3D	-2.41	122.17	127.69
6	R	101	BCL	CHB-C4A-NA	2.41	127.88	124.40
7	4	103	CRT	C31-C32-C33	2.41	130.65	127.28
6	4	102	BCL	O2D-CGD-O1D	-2.40	119.17	123.85
6	7	104	BCL	CMD-C2D-C3D	-2.40	122.18	127.69
6	L	301	BCL	CMD-C2D-C3D	-2.40	122.18	127.69
7	0	101	CRT	C29-C28-C27	-2.40	118.93	122.82
6	5	103	BCL	C2A-C1A-CHA	-2.40	119.71	123.87
7	X	101	CRT	C34-C33-C32	-2.40	118.93	122.82
6	J	103	BCL	CMB-C2B-C3B	2.40	133.23	125.67
7	S	101	CRT	C34-C33-C32	-2.39	118.94	122.82
7	8	101	CRT	C26-C27-C28	2.39	130.63	127.28
6	F	102	BCL	CMD-C2D-C3D	-2.39	122.20	127.69
7	D	101	CRT	C25-C23-C22	2.39	122.77	119.01
6	3	100	BCL	O2D-CGD-O1D	-2.39	119.19	123.85
7	U	101	CRT	C18-C17-C19	-2.39	118.94	122.82
7	Q	101	CRT	C15-C14-C12	2.39	130.63	127.28
6	V	102	BCL	C2A-C1A-CHA	-2.39	119.72	123.87
7	0	101	CRT	C16-C17-C19	2.39	122.77	119.01
6	E	101	BCL	CHB-C4A-NA	2.39	127.85	124.40
6	A	100	BCL	CHB-C4A-NA	2.39	127.85	124.40
6	Y	101	BCL	O2D-CGD-O1D	-2.39	119.20	123.85
12	L	307	U10	C7-C6-C1	-2.39	120.80	124.89
7	K	101	CRT	C21-C20-C19	2.39	128.40	123.52
6	J	101	BCL	C2A-C1A-CHA	-2.39	119.73	123.87
7	Z	102	CRT	C34-C33-C32	-2.39	118.95	122.82
6	F	102	BCL	CMB-C2B-C3B	2.38	133.19	125.67
6	5	101	BCL	O2D-CGD-O1D	-2.38	119.21	123.85
7	D	101	CRT	C31-C32-C33	2.38	130.62	127.28
6	C	101	BCL	C2A-C1A-CHA	-2.38	119.73	123.87
7	K	101	CRT	C15-C14-C12	2.38	130.61	127.28
6	Y	101	BCL	CHB-C4A-NA	2.38	127.83	124.40
7	O	102	CRT	C21-C20-C19	2.38	128.38	123.52
7	4	103	CRT	C29-C28-C27	-2.37	118.97	122.82
6	0	100	BCL	C4-C3-C5	2.37	119.35	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	101	BCL	O2D-CGD-O1D	-2.37	119.23	123.85
7	B	103	CRT	C13-C12-C14	-2.37	118.98	122.82
7	7	101	CRT	C18-C17-C19	-2.37	118.98	122.82
6	P	102	BCL	CHB-C4A-NA	2.37	127.81	124.40
7	Q	101	CRT	C25-C23-C22	2.37	122.73	119.01
6	Q	100	BCL	O2D-CGD-O1D	-2.37	119.24	123.85
6	R	103	BCL	C2A-C1A-CHA	-2.36	119.76	123.87
7	O	102	CRT	C18-C17-C19	-2.36	118.99	122.82
7	B	103	CRT	C31-C32-C33	2.36	130.59	127.28
7	G	102	CRT	C25-C23-C22	2.36	122.72	119.01
6	A	100	BCL	O2D-CGD-O1D	-2.36	119.25	123.85
7	U	101	CRT	C26-C27-C28	2.36	130.59	127.28
6	7	102	BCL	O2D-CGD-O1D	-2.36	119.26	123.85
12	L	309	U10	C45-C44-C46	2.36	119.32	115.23
6	T	100	BCL	CHB-C4A-NA	2.36	127.80	124.40
6	Y	102	BCL	CHC-C4B-NB	-2.36	120.51	124.05
7	4	103	CRT	C34-C33-C32	-2.35	119.00	122.82
7	K	101	CRT	C34-C33-C32	-2.35	119.00	122.82
7	X	101	CRT	C13-C12-C14	-2.35	119.01	122.82
14	M	407	QAK	C3-C4-CZ2	-2.35	115.66	125.93
6	V	101	BCL	CHB-C4A-NA	2.35	127.79	124.40
7	4	103	CRT	C6-C7-C9	2.35	122.70	119.01
6	P	102	BCL	C2A-C1A-CHA	-2.35	119.79	123.87
6	Y	102	BCL	C2A-C1A-CHA	-2.35	119.79	123.87
7	K	101	CRT	C29-C28-C27	-2.34	119.02	122.82
7	B	103	CRT	C25-C23-C22	2.34	122.70	119.01
6	N	102	BCL	CMB-C2B-C3B	2.34	133.06	125.67
6	J	101	BCL	CHB-C4A-NA	2.34	127.78	124.40
6	R	101	BCL	C2A-C1A-CHA	-2.34	119.80	123.87
7	D	101	CRT	C15-C14-C12	2.34	130.56	127.28
7	K	101	CRT	C31-C32-C33	2.34	130.56	127.28
6	1	101	BCL	CMB-C2B-C3B	2.34	133.04	125.67
6	5	103	BCL	CMB-C2B-C3B	2.34	133.04	125.67
6	V	102	BCL	CHC-C4B-NB	-2.33	120.55	124.05
6	V	102	BCL	O2D-CGD-O1D	-2.33	119.31	123.85
7	U	101	CRT	C36-C35-C33	2.33	129.41	125.89
7	D	101	CRT	C34-C33-C32	-2.33	119.04	122.82
7	I	102	CRT	C18-C17-C19	-2.33	119.04	122.82
7	X	101	CRT	C18-C17-C19	-2.33	119.04	122.82
7	B	103	CRT	C6-C7-C9	2.33	122.67	119.01
6	G	103	BCL	C1D-CHD-C4C	-2.33	121.00	126.62
6	0	100	BCL	CHB-C1B-NB	-2.33	120.56	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	1	102	BCL	O2D-CGD-O1D	-2.33	119.32	123.85
6	1	101	BCL	CAC-C3C-C4C	-2.33	107.42	112.58
7	I	102	CRT	C13-C12-C14	-2.32	119.05	122.82
6	N	101	BCL	CHC-C4B-NB	-2.32	120.56	124.05
7	K	101	CRT	C18-C17-C19	-2.32	119.05	122.82
6	4	102	BCL	CHC-C1C-NC	2.32	127.75	124.40
6	N	101	BCL	CHB-C4A-NA	2.32	127.75	124.40
12	L	303	U10	C10-C9-C11	2.32	119.25	115.23
7	U	101	CRT	C34-C33-C32	-2.32	119.06	122.82
12	L	309	U10	C37-C38-C39	-2.32	122.31	127.62
6	5	101	BCL	CHC-C4B-NB	-2.32	120.57	124.05
10	P	101	LMT	C3'-C4'-C5'	-2.32	105.79	110.93
6	N	101	BCL	CMB-C2B-C3B	2.32	132.98	125.67
6	A	100	BCL	C2A-C1A-CHA	-2.32	119.85	123.87
6	M	404	BCL	C4-C3-C5	2.31	119.25	115.23
6	A	100	BCL	CMB-C2B-C3B	2.31	132.97	125.67
6	5	103	BCL	CMD-C2D-C3D	-2.31	122.39	127.69
7	U	101	CRT	C6-C7-C9	2.31	122.64	119.01
6	M	402	BCL	CHB-C4A-NA	2.31	127.73	124.40
7	X	101	CRT	C21-C20-C19	2.30	128.24	123.52
6	Q	100	BCL	CMB-C2B-C3B	2.30	132.93	125.67
7	0	101	CRT	C34-C33-C32	-2.30	119.09	122.82
6	P	102	BCL	CMB-C2B-C3B	2.30	132.93	125.67
6	U	100	BCL	C2A-C1A-CHA	-2.30	119.88	123.87
6	B	102	BCL	CMB-C2B-C3B	2.30	132.92	125.67
7	K	101	CRT	C13-C12-C14	-2.30	119.09	122.82
7	Z	102	CRT	C18-C17-C19	-2.30	119.09	122.82
11	L	302	BPH	CMA-C3A-C4A	-2.30	109.66	114.61
7	G	102	CRT	C29-C28-C27	-2.30	119.10	122.82
7	S	101	CRT	C13-C12-C14	-2.30	119.10	122.82
12	L	303	U10	C41-C39-C40	2.29	119.87	114.59
7	4	103	CRT	C18-C17-C19	-2.29	119.10	122.82
6	G	103	BCL	C2A-C1A-CHA	-2.29	119.89	123.87
7	Q	101	CRT	C29-C28-C27	-2.29	119.11	122.82
6	1	102	BCL	CHB-C1B-NB	-2.29	120.61	124.05
7	4	103	CRT	C10-C9-C7	2.29	130.49	127.28
6	M	404	BCL	CMB-C2B-C3B	2.29	132.89	125.67
6	Y	102	BCL	CMB-C2B-C3B	2.29	132.89	125.67
6	N	101	BCL	C2A-C1A-CHA	-2.29	119.90	123.87
6	7	102	BCL	CMB-C2B-C3B	2.29	132.88	125.67
6	G	104	BCL	CMB-C2B-C3B	2.28	132.88	125.67
6	R	101	BCL	CMB-C2B-C3B	2.28	132.88	125.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	104	BCL	C2A-C1A-CHA	-2.28	119.90	123.87
6	M	404	BCL	C1D-CHD-C4C	-2.28	121.11	126.62
6	B	102	BCL	C2A-C1A-CHA	-2.28	119.91	123.87
7	S	101	CRT	C6-C7-C9	2.28	122.60	119.01
7	Q	101	CRT	C13-C12-C14	-2.28	119.12	122.82
6	G	103	BCL	CMB-C2B-C3B	2.28	132.85	125.67
6	M	402	BCL	CMD-C2D-C3D	-2.28	122.47	127.69
6	L	301	BCL	O2A-CGA-O1A	-2.27	117.94	123.63
7	G	102	CRT	C6-C7-C9	2.27	122.58	119.01
6	V	102	BCL	CHB-C1B-NB	-2.27	120.64	124.05
7	S	101	CRT	C29-C28-C27	-2.27	119.14	122.82
7	D	101	CRT	C13-C12-C14	-2.27	119.14	122.82
6	3	100	BCL	CMB-C2B-C3B	2.27	132.82	125.67
7	D	101	CRT	C29-C28-C27	-2.27	119.14	122.82
6	L	301	BCL	CMB-C2B-C3B	2.27	132.82	125.67
6	1	102	BCL	CMD-C2D-C3D	-2.27	122.49	127.69
6	1	102	BCL	CMB-C2B-C3B	2.26	132.81	125.67
7	7	101	CRT	C29-C28-C27	-2.26	119.16	122.82
12	L	309	U10	C56-C54-C55	2.25	119.78	114.59
6	N	102	BCL	C2A-C1A-CHA	-2.25	119.95	123.87
7	O	102	CRT	C13-C12-C14	-2.25	119.17	122.82
6	J	103	BCL	C2A-C1A-CHA	-2.25	119.96	123.87
6	9	102	BCL	C1C-NC-C4C	-2.25	105.65	106.68
7	S	101	CRT	C31-C32-C33	2.25	130.43	127.28
7	8	101	CRT	C29-C28-C27	-2.25	119.17	122.82
12	L	303	U10	C15-C14-C16	2.25	119.13	115.23
7	7	101	CRT	C13-C12-C14	-2.25	119.17	122.82
7	I	102	CRT	C34-C33-C32	-2.25	119.18	122.82
6	1	102	BCL	C2A-C1A-CHA	-2.25	119.97	123.87
6	N	101	BCL	CAC-C3C-C4C	-2.25	107.60	112.58
7	G	102	CRT	C13-C12-C14	-2.24	119.18	122.82
7	O	102	CRT	C29-C28-C27	-2.24	119.18	122.82
6	N	102	BCL	CMD-C2D-C3D	-2.24	122.54	127.69
6	V	101	BCL	CMB-C2B-C3B	2.24	132.75	125.67
7	B	103	CRT	C29-C28-C27	-2.24	119.18	122.82
7	Z	102	CRT	C10-C9-C7	2.24	130.42	127.28
6	C	102	BCL	C2A-C1A-CHA	-2.24	119.98	123.87
6	L	308	BCL	O1D-CGD-CBD	-2.24	120.10	124.52
7	2	102	CRT	C30-C28-C27	2.24	122.53	119.01
12	M	410	U10	C37-C38-C39	-2.24	122.50	127.62
12	L	307	U10	C56-C54-C55	2.24	119.74	114.59
7	0	101	CRT	C31-C32-C33	2.24	130.42	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	404	BCL	O2D-CGD-O1D	-2.24	119.50	123.85
6	0	100	BCL	CMB-C2B-C3B	2.23	132.72	125.67
7	Q	101	CRT	C36-C35-C33	2.23	129.27	125.89
7	Q	101	CRT	C34-C33-C32	-2.23	119.20	122.82
7	7	101	CRT	C34-C33-C32	-2.23	119.20	122.82
7	S	101	CRT	C15-C14-C12	2.23	130.41	127.28
7	I	102	CRT	C15-C14-C12	2.23	130.41	127.28
6	B	102	BCL	CMD-C2D-C3D	-2.23	122.58	127.69
6	J	103	BCL	CMD-C2D-C3D	-2.22	122.59	127.69
7	I	102	CRT	C29-C28-C27	-2.22	119.22	122.82
6	R	103	BCL	CMD-C2D-C3D	-2.22	122.59	127.69
6	4	102	BCL	C2A-C1A-CHA	-2.22	120.01	123.87
6	4	102	BCL	CMB-C2B-C3B	2.22	132.68	125.67
7	8	101	CRT	C13-C12-C14	-2.22	119.23	122.82
6	M	402	BCL	C11-C10-C8	-2.22	108.60	115.97
7	D	101	CRT	C10-C9-C7	2.22	130.38	127.28
6	7	104	BCL	CMB-C2B-C3B	2.22	132.66	125.67
6	0	100	BCL	C6-C5-C3	-2.21	108.08	113.47
6	F	102	BCL	C2A-C1A-CHA	-2.21	120.03	123.87
6	C	102	BCL	C4D-CHA-C1A	-2.21	118.61	121.24
6	N	102	BCL	C1D-CHD-C4C	-2.21	121.30	126.62
6	G	104	BCL	C1D-CHD-C4C	-2.21	121.30	126.62
6	9	102	BCL	C1D-CHD-C4C	-2.20	121.31	126.62
6	M	402	BCL	C1D-CHD-C4C	-2.20	121.31	126.62
6	4	102	BCL	CMD-C2D-C3D	-2.20	122.64	127.69
6	V	101	BCL	C2A-C1A-CHA	-2.20	120.05	123.87
6	1	101	BCL	C1D-CHD-C4C	-2.20	121.31	126.62
6	R	103	BCL	C1D-CHD-C4C	-2.20	121.32	126.62
6	V	102	BCL	CMB-C2B-C3B	2.20	132.60	125.67
6	5	101	BCL	CAA-CBA-CGA	-2.20	106.97	113.21
6	5	103	BCL	C1D-CHD-C4C	-2.20	121.33	126.62
6	Q	100	BCL	C1D-CHD-C4C	-2.19	121.33	126.62
6	M	402	BCL	CHC-C4B-NB	-2.19	120.76	124.05
7	I	102	CRT	C26-C27-C28	2.18	130.34	127.28
6	L	308	BCL	CMB-C2B-C3B	2.18	132.56	125.67
6	J	101	BCL	C1D-CHD-C4C	-2.18	121.35	126.62
7	G	102	CRT	C34-C33-C32	-2.18	119.28	122.82
7	D	101	CRT	C26-C27-C28	2.18	130.34	127.28
6	T	100	BCL	CAC-C3C-C4C	-2.18	107.75	112.58
12	M	410	U10	C52-C53-C54	-2.18	120.38	127.64
6	B	102	BCL	C1D-CHD-C4C	-2.18	121.36	126.62
6	L	301	BCL	C1D-CHD-C4C	-2.18	121.37	126.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	T	100	BCL	C2A-C1A-CHA	-2.18	120.09	123.87
7	2	102	CRT	C34-C33-C32	-2.18	119.29	122.82
6	9	102	BCL	CMB-C2B-C3B	2.17	132.53	125.67
6	B	102	BCL	C4D-CHA-C1A	-2.17	118.65	121.24
7	0	101	CRT	C11-C12-C14	2.17	122.43	119.01
6	R	101	BCL	O2A-CGA-O1A	-2.17	118.19	123.63
7	X	101	CRT	C30-C28-C27	2.17	122.42	119.01
6	A	100	BCL	CAC-C3C-C4C	-2.17	107.77	112.58
7	O	102	CRT	C34-C33-C32	-2.17	119.30	122.82
6	L	301	BCL	CHB-C4A-NA	2.17	127.53	124.40
12	L	309	U10	C52-C53-C54	-2.17	120.41	127.64
6	U	100	BCL	CMD-C2D-C3D	-2.17	122.72	127.69
7	G	102	CRT	C26-C27-C28	2.17	130.32	127.28
7	U	101	CRT	C29-C28-C27	-2.17	119.31	122.82
6	V	102	BCL	C4D-CHA-C1A	-2.16	118.67	121.24
6	M	404	BCL	CHD-C1D-C2D	2.16	129.98	125.49
7	Z	102	CRT	C13-C12-C14	-2.16	119.32	122.82
12	M	406	U10	C7-C8-C9	-2.16	123.11	126.83
7	4	103	CRT	C13-C12-C14	-2.16	119.32	122.82
7	D	101	CRT	C16-C17-C19	2.16	122.40	119.01
6	V	101	BCL	C1D-CHD-C4C	-2.16	121.42	126.62
14	M	407	QAK	CD2-CE3-CZ3	-2.15	116.52	125.93
6	7	104	BCL	CHB-C1B-NB	-2.15	120.82	124.05
6	F	102	BCL	C4D-CHA-C1A	-2.15	118.68	121.24
6	R	103	BCL	CMB-C2B-C3B	2.15	132.45	125.67
7	7	101	CRT	C36-C35-C33	2.15	129.14	125.89
6	5	101	BCL	C2A-C3A-C4A	-2.15	98.40	101.87
6	0	100	BCL	C4D-CHA-C1A	-2.15	118.68	121.24
7	2	102	CRT	C16-C17-C19	2.15	122.39	119.01
6	B	102	BCL	CHB-C1B-NB	-2.14	120.83	124.05
6	E	101	BCL	C2A-C1A-CHA	-2.14	120.15	123.87
10	L	306	LMT	C3B-C4B-C5B	-2.14	106.35	110.23
6	R	103	BCL	CHB-C1B-NB	-2.14	120.84	124.05
6	7	102	BCL	CHB-C1B-NB	-2.14	120.84	124.05
6	A	100	BCL	C1D-CHD-C4C	-2.14	121.47	126.62
10	H	302	LMT	O1'-C1'-C2'	2.14	111.52	108.27
10	4	101	LMT	C1B-O5B-C5B	2.14	117.89	113.72
7	2	102	CRT	C11-C12-C14	2.13	122.36	119.01
6	Y	101	BCL	C1D-CHD-C4C	-2.13	121.48	126.62
6	V	102	BCL	CMD-C2D-C3D	-2.13	122.80	127.69
6	L	308	BCL	C1D-CHD-C4C	-2.13	121.48	126.62
7	8	101	CRT	C34-C33-C32	-2.13	119.37	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	2	102	CRT	C15-C14-C12	2.13	130.26	127.28
6	V	102	BCL	C1D-CHD-C4C	-2.12	121.50	126.62
7	G	102	CRT	C16-C17-C19	2.12	122.34	119.01
6	M	402	BCL	O1D-CGD-CBD	-2.12	120.34	124.52
7	B	103	CRT	C26-C27-C28	2.12	130.25	127.28
7	D	101	CRT	C36-C35-C33	2.12	129.09	125.89
7	B	103	CRT	C16-C17-C19	2.11	122.33	119.01
6	1	101	BCL	CHB-C1B-NB	-2.11	120.88	124.05
6	N	101	BCL	C1D-CHD-C4C	-2.11	121.52	126.62
6	0	100	BCL	C1D-CHD-C4C	-2.11	121.53	126.62
6	C	101	BCL	CMB-C2B-C3B	2.10	132.30	125.67
7	X	101	CRT	C31-C32-C33	2.10	130.23	127.28
6	7	104	BCL	C1D-CHD-C4C	-2.10	121.55	126.62
6	J	101	BCL	CHD-C1D-C2D	2.10	129.86	125.49
6	4	102	BCL	C4D-CHA-C1A	-2.10	118.74	121.24
6	4	102	BCL	C1D-CHD-C4C	-2.10	121.56	126.62
6	G	104	BCL	CMD-C2D-C3D	-2.10	122.88	127.69
6	1	102	BCL	C4D-CHA-C1A	-2.10	118.75	121.24
7	X	101	CRT	C4-C5-C6	2.09	127.86	124.91
6	J	101	BCL	CHB-C1B-NB	-2.09	120.91	124.05
6	Y	102	BCL	C1D-CHD-C4C	-2.09	121.57	126.62
12	L	309	U10	C6-C1-C2	2.09	120.82	119.17
6	J	101	BCL	CMB-C2B-C3B	2.09	132.26	125.67
6	Y	101	BCL	CHB-C1B-C2B	-2.09	121.36	127.43
6	3	100	BCL	C1D-CHD-C4C	-2.09	121.58	126.62
7	Z	102	CRT	C6-C7-C9	2.09	122.29	119.01
6	7	102	BCL	CHD-C1D-C2D	2.09	129.83	125.49
6	E	101	BCL	CHB-C1B-C2B	-2.09	121.37	127.43
6	1	102	BCL	CED-O2D-CGD	2.08	120.64	115.92
6	M	404	BCL	CAA-C2A-C3A	-2.08	107.37	113.00
7	8	101	CRT	C16-C17-C19	2.08	122.28	119.01
6	U	100	BCL	O2A-CGA-O1A	-2.08	118.42	123.63
6	J	103	BCL	C1D-CHD-C4C	-2.08	121.60	126.62
6	3	100	BCL	CHB-C1B-NB	-2.08	120.93	124.05
7	Q	101	CRT	C26-C27-C28	2.08	130.19	127.28
7	G	102	CRT	C10-C9-C7	2.08	130.19	127.28
6	L	301	BCL	C2A-C1A-CHA	-2.08	120.27	123.87
6	R	101	BCL	C1D-CHD-C4C	-2.07	121.62	126.62
7	U	101	CRT	C16-C17-C19	2.07	122.27	119.01
6	3	100	BCL	C2A-C1A-CHA	-2.07	120.27	123.87
6	J	103	BCL	CHB-C1B-C2B	-2.07	121.41	127.43
7	Z	102	CRT	C30-C28-C27	2.07	122.26	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	7	102	BCL	C2A-C1A-CHA	-2.07	120.28	123.87
6	Y	102	BCL	CHB-C1B-NB	-2.07	120.95	124.05
7	7	101	CRT	C26-C27-C28	2.07	130.18	127.28
6	T	100	BCL	C1D-CHD-C4C	-2.06	121.65	126.62
6	C	102	BCL	CHB-C1B-NB	-2.06	120.97	124.05
7	K	101	CRT	C26-C27-C28	2.06	130.16	127.28
6	7	102	BCL	C1D-CHD-C4C	-2.06	121.66	126.62
6	3	100	BCL	CHB-C4A-NA	2.05	127.36	124.40
6	P	102	BCL	CHB-C1B-NB	-2.05	120.97	124.05
7	Z	102	CRT	C21-C20-C19	2.05	127.72	123.52
6	G	103	BCL	CAC-C3C-C4C	-2.05	108.03	112.58
6	C	102	BCL	O2A-CGA-O1A	-2.05	118.50	123.63
6	C	101	BCL	CHB-C1B-NB	-2.05	120.97	124.05
7	S	101	CRT	C10-C9-C7	2.05	130.16	127.28
6	F	102	BCL	CHB-C1B-NB	-2.05	120.97	124.05
6	U	100	BCL	CHB-C1B-C2B	-2.05	121.48	127.43
6	Y	101	BCL	CAA-CBA-CGA	-2.05	107.40	113.21
7	X	101	CRT	C35-C33-C32	2.05	122.23	119.01
6	A	100	BCL	CHB-C1B-C2B	-2.04	121.49	127.43
7	S	101	CRT	C26-C27-C28	2.04	130.15	127.28
6	T	100	BCL	O2A-CGA-O1A	-2.04	118.52	123.63
6	N	101	BCL	O2A-CGA-O1A	-2.04	118.52	123.63
6	T	100	BCL	CHB-C1B-C2B	-2.04	121.50	127.43
6	5	101	BCL	C4D-CHA-C1A	-2.04	118.81	121.24
6	M	404	BCL	CHB-C4A-NA	2.04	127.34	124.40
7	Q	101	CRT	C16-C17-C19	2.04	122.21	119.01
6	5	101	BCL	O2A-CGA-O1A	-2.03	118.55	123.63
10	J	102	LMT	C3'-C4'-C5'	-2.03	106.43	110.93
7	D	101	CRT	C6-C7-C9	2.03	122.20	119.01
6	C	102	BCL	C1D-CHD-C4C	-2.03	121.73	126.62
6	5	101	BCL	CHD-C1D-C2D	2.03	129.70	125.49
6	C	101	BCL	C1D-CHD-C4C	-2.03	121.73	126.62
6	V	101	BCL	CHB-C1B-C2B	-2.03	121.54	127.43
7	X	101	CRT	C20-C19-C17	2.02	130.12	127.28
6	U	100	BCL	C4D-CHA-C1A	-2.02	118.83	121.24
6	F	102	BCL	CHD-C1D-C2D	2.02	129.69	125.49
6	F	102	BCL	C1D-CHD-C4C	-2.02	121.74	126.62
7	Z	102	CRT	C31-C32-C33	2.02	130.11	127.28
6	R	101	BCL	CHB-C1B-C2B	-2.02	121.56	127.43
6	9	102	BCL	C4A-NA-C1A	2.02	107.60	106.68
6	1	102	BCL	C1D-CHD-C4C	-2.02	121.75	126.62
6	Q	100	BCL	CHD-C1D-C2D	2.02	129.69	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	103	CRT	C35-C33-C32	2.02	122.18	119.01
7	I	102	CRT	C21-C20-C19	2.02	127.65	123.52
6	P	102	BCL	C1D-CHD-C4C	-2.02	121.76	126.62
7	4	103	CRT	C26-C27-C28	2.01	130.10	127.28
6	N	101	BCL	CHB-C1B-C2B	-2.01	121.59	127.43
6	G	103	BCL	CHB-C1B-NB	-2.01	121.03	124.05
6	9	102	BCL	CHD-C1D-C2D	2.01	129.67	125.49
6	Y	102	BCL	C4D-CHA-C1A	-2.01	118.85	121.24
6	U	100	BCL	C1D-CHD-C4C	-2.01	121.78	126.62
6	5	101	BCL	C1D-CHD-C4C	-2.01	121.78	126.62
6	T	100	BCL	CHB-C1B-NB	-2.01	121.04	124.05
6	M	402	BCL	C6-C5-C3	-2.01	108.58	113.47
7	S	101	CRT	C36-C35-C33	2.01	128.92	125.89
7	S	101	CRT	C16-C17-C19	2.01	122.16	119.01
7	0	101	CRT	C30-C28-C27	2.00	122.16	119.01
6	R	103	BCL	C4D-CHA-C1A	-2.00	118.86	121.24
12	M	406	U10	C41-C39-C40	2.00	119.19	114.59

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	L	302	BPH	C13
11	L	302	BPH	C8
11	M	405	BPH	C13
11	M	405	BPH	C8
14	M	407	QAK	C19
14	M	407	QAK	C14
14	M	407	QAK	C24

All (1027) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	101	BCL	C2C-C3C-CAC-CBC
6	C	101	BCL	C4C-C3C-CAC-CBC
6	C	101	BCL	C2-C3-C5-C6
6	C	101	BCL	C4-C3-C5-C6
6	C	102	BCL	C1A-C2A-CAA-CBA
6	C	102	BCL	C3A-C2A-CAA-CBA
6	C	102	BCL	C2C-C3C-CAC-CBC
6	C	102	BCL	C4C-C3C-CAC-CBC
6	E	101	BCL	C4C-C3C-CAC-CBC
6	E	101	BCL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
6	E	101	BCL	C4-C3-C5-C6
6	F	102	BCL	C1A-C2A-CAA-CBA
6	F	102	BCL	C3A-C2A-CAA-CBA
6	F	102	BCL	C4C-C3C-CAC-CBC
6	G	103	BCL	C4C-C3C-CAC-CBC
6	G	103	BCL	C2-C3-C5-C6
6	G	103	BCL	C4-C3-C5-C6
6	G	104	BCL	C1A-C2A-CAA-CBA
6	G	104	BCL	C3A-C2A-CAA-CBA
6	G	104	BCL	C11-C10-C8-C9
6	J	101	BCL	C4C-C3C-CAC-CBC
6	N	101	BCL	C1A-C2A-CAA-CBA
6	N	101	BCL	C3A-C2A-CAA-CBA
6	N	102	BCL	C1A-C2A-CAA-CBA
6	N	102	BCL	C3A-C2A-CAA-CBA
6	R	101	BCL	C1A-C2A-CAA-CBA
6	R	101	BCL	C3A-C2A-CAA-CBA
6	R	101	BCL	C4C-C3C-CAC-CBC
6	R	103	BCL	C1A-C2A-CAA-CBA
6	U	100	BCL	C1A-C2A-CAA-CBA
6	U	100	BCL	C3A-C2A-CAA-CBA
6	U	100	BCL	C2C-C3C-CAC-CBC
6	U	100	BCL	C4C-C3C-CAC-CBC
6	V	101	BCL	C1A-C2A-CAA-CBA
6	V	101	BCL	C4C-C3C-CAC-CBC
6	V	101	BCL	C2-C3-C5-C6
6	V	101	BCL	C4-C3-C5-C6
6	V	102	BCL	C1A-C2A-CAA-CBA
6	V	102	BCL	C3A-C2A-CAA-CBA
6	P	102	BCL	C2C-C3C-CAC-CBC
6	P	102	BCL	C4C-C3C-CAC-CBC
6	P	102	BCL	C4-C3-C5-C6
6	Q	100	BCL	C1A-C2A-CAA-CBA
6	Q	100	BCL	C3A-C2A-CAA-CBA
6	Q	100	BCL	C2C-C3C-CAC-CBC
6	Q	100	BCL	C4C-C3C-CAC-CBC
6	Y	102	BCL	C1A-C2A-CAA-CBA
6	Y	102	BCL	C3A-C2A-CAA-CBA
6	Y	102	BCL	C2C-C3C-CAC-CBC
6	Y	102	BCL	C4C-C3C-CAC-CBC
6	B	102	BCL	C1A-C2A-CAA-CBA
6	B	102	BCL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
6	B	102	BCL	C4C-C3C-CAC-CBC
6	1	102	BCL	C1A-C2A-CAA-CBA
6	1	102	BCL	C3A-C2A-CAA-CBA
6	3	100	BCL	C4C-C3C-CAC-CBC
6	4	102	BCL	C1A-C2A-CAA-CBA
6	4	102	BCL	C3A-C2A-CAA-CBA
6	4	102	BCL	C2C-C3C-CAC-CBC
6	4	102	BCL	C4C-C3C-CAC-CBC
6	5	101	BCL	C4C-C3C-CAC-CBC
6	5	103	BCL	C1A-C2A-CAA-CBA
6	5	103	BCL	C2C-C3C-CAC-CBC
6	5	103	BCL	C4C-C3C-CAC-CBC
6	7	102	BCL	C2C-C3C-CAC-CBC
6	7	102	BCL	C4C-C3C-CAC-CBC
6	7	104	BCL	C1A-C2A-CAA-CBA
6	7	104	BCL	C3A-C2A-CAA-CBA
6	7	104	BCL	C11-C10-C8-C9
6	0	100	BCL	C2C-C3C-CAC-CBC
6	0	100	BCL	C4C-C3C-CAC-CBC
7	X	101	CRT	C1-C4-C5-C6
7	2	102	CRT	C36-C37-C38-C40
7	7	101	CRT	C35-C36-C37-C38
7	8	101	CRT	C35-C36-C37-C38
8	D	102	6PL	C2-C1-O3P-P
8	D	102	6PL	C1-O3P-P-O4P
8	E	102	6PL	C12-C11-O3-C3
8	E	102	6PL	O11-C11-O3-C3
8	F	103	6PL	C5-C4-O4P-P
8	F	103	6PL	O31-C31-O2-C2
8	F	103	6PL	C32-C31-O2-C2
8	I	101	6PL	C2-C1-O3P-P
8	I	103	6PL	O31-C31-O2-C2
8	I	103	6PL	C32-C31-O2-C2
8	K	102	6PL	C12-C11-O3-C3
8	K	102	6PL	O11-C11-O3-C3
8	K	102	6PL	C4-O4P-P-O3P
8	K	102	6PL	C4-O4P-P-O1P
8	K	102	6PL	C4-O4P-P-O2P
8	L	304	6PL	C4-O4P-P-O2P
8	L	304	6PL	C5-C4-O4P-P
8	L	305	6PL	C4-O4P-P-O1P
8	L	305	6PL	C5-C4-O4P-P

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Mol	Chain	Res	Type	Atoms
8	S	102	6PL	C1-O3P-P-O2P
8	S	102	6PL	C1-O3P-P-O4P
8	S	102	6PL	O31-C31-O2-C2
8	S	102	6PL	C32-C31-O2-C2
8	U	102	6PL	C4-O4P-P-O1P
8	X	102	6PL	C1-O3P-P-O2P
8	X	102	6PL	C1-O3P-P-O4P
8	P	103	6PL	C2-C1-O3P-P
8	P	103	6PL	C4-O4P-P-O3P
8	P	103	6PL	C4-O4P-P-O2P
8	P	103	6PL	C5-C4-O4P-P
8	Z	103	6PL	C12-C11-O3-C3
8	Z	103	6PL	O11-C11-O3-C3
8	Z	103	6PL	C4-O4P-P-O1P
8	B	104	6PL	C12-C11-O3-C3
8	B	104	6PL	O31-C31-O2-C2
8	B	104	6PL	C32-C31-O2-C2
8	4	104	6PL	C1-O3P-P-O1P
8	5	102	6PL	C32-C31-O2-C2
8	6	102	6PL	C4-O4P-P-O1P
8	8	102	6PL	C12-C11-O3-C3
8	8	102	6PL	O11-C11-O3-C3
9	E	103	CDL	OA9-CA7-OA8-CA6
9	E	103	CDL	C31-CA7-OA8-CA6
9	E	103	CDL	CB4-CB3-OB5-PB2
9	G	101	CDL	OB9-CB7-OB8-CB6
9	G	101	CDL	C71-CB7-OB8-CB6
9	G	105	CDL	CA3-OA5-PA1-OA2
9	G	105	CDL	CA3-OA5-PA1-OA4
9	L	310	CDL	CA2-OA2-PA1-OA3
9	L	310	CDL	C1-CB2-OB2-PB2
9	L	310	CDL	CB2-OB2-PB2-OB4
9	L	310	CDL	OB9-CB7-OB8-CB6
9	L	310	CDL	C71-CB7-OB8-CB6
10	F	101	LMT	C2'-C1'-O1'-C1
10	F	101	LMT	O5'-C1'-O1'-C1
10	H	302	LMT	O5B-C1B-O1B-C4'
10	P	101	LMT	C2-C1-O1'-C1'
10	B	101	LMT	O5'-C1'-O1'-C1
10	2	101	LMT	C2-C1-O1'-C1'
12	L	303	U10	C28-C29-C31-C32
12	L	303	U10	C30-C29-C31-C32

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Mol	Chain	Res	Type	Atoms
12	L	307	U10	C22-C23-C24-C25
12	L	307	U10	C22-C23-C24-C26
12	L	307	U10	C24-C26-C27-C28
12	L	309	U10	C7-C8-C9-C10
12	L	309	U10	C7-C8-C9-C11
12	L	309	U10	C27-C28-C29-C30
12	L	309	U10	C27-C28-C29-C31
12	M	410	U10	C7-C8-C9-C10
12	M	410	U10	C7-C8-C9-C11
12	M	410	U10	C29-C31-C32-C33
12	M	410	U10	C37-C38-C39-C40
12	M	410	U10	C37-C38-C39-C41
14	M	407	QAK	C39-CE2-CZ2-C4
14	M	407	QAK	CZ3-C10-C11-C12
15	7	103	PGT	C1-O3P-P-O2P
15	7	103	PGT	C1-O3P-P-O4P
15	9	101	PGT	C5-C4-O4P-P
10	4	101	LMT	O5B-C1B-O1B-C4'
8	B	104	6PL	O11-C11-O3-C3
10	L	306	LMT	C4'-C5'-C6'-O6'
12	L	303	U10	C37-C38-C39-C40
10	R	102	LMT	C3'-C4'-O1B-C1B
10	Z	101	LMT	O5B-C5B-C6B-O6B
8	5	102	6PL	O31-C31-O2-C2
6	C	102	BCL	C3-C5-C6-C7
6	N	101	BCL	C3-C5-C6-C7
6	3	100	BCL	C3-C5-C6-C7
6	M	404	BCL	CBD-CGD-O2D-CED
6	N	101	BCL	C4-C3-C5-C6
6	L	301	BCL	C4-C3-C5-C6
6	R	101	BCL	C4-C3-C5-C6
6	T	100	BCL	C4-C3-C5-C6
6	Y	101	BCL	C4-C3-C5-C6
6	A	100	BCL	C4-C3-C5-C6
6	9	102	BCL	C4-C3-C5-C6
12	L	307	U10	C25-C24-C26-C27
12	L	307	U10	C40-C39-C41-C42
12	M	406	U10	C25-C24-C26-C27
12	M	406	U10	C35-C34-C36-C37
12	M	410	U10	C35-C34-C36-C37
6	N	101	BCL	C2-C3-C5-C6
6	L	301	BCL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
6	R	101	BCL	C2-C3-C5-C6
6	T	100	BCL	C2-C3-C5-C6
6	P	102	BCL	C2-C3-C5-C6
6	Y	101	BCL	C2-C3-C5-C6
6	A	100	BCL	C2-C3-C5-C6
6	9	102	BCL	C2-C3-C5-C6
12	L	307	U10	C23-C24-C26-C27
12	M	406	U10	C33-C34-C36-C37
6	J	103	BCL	C3-C5-C6-C7
6	F	102	BCL	C3-C5-C6-C7
6	L	308	BCL	C3-C5-C6-C7
6	M	404	BCL	C3-C5-C6-C7
6	V	102	BCL	C3-C5-C6-C7
6	7	104	BCL	C3-C5-C6-C7
10	O	101	LMT	C4B-C5B-C6B-O6B
10	R	102	LMT	C4B-C5B-C6B-O6B
10	R	102	LMT	O5B-C5B-C6B-O6B
10	Z	101	LMT	C4B-C5B-C6B-O6B
10	6	101	LMT	O5'-C5'-C6'-O6'
12	M	410	U10	C52-C53-C54-C55
6	1	102	BCL	C4-C3-C5-C6
6	7	102	BCL	C4-C3-C5-C6
12	L	309	U10	C40-C39-C41-C42
6	1	102	BCL	C2-C3-C5-C6
12	L	307	U10	C38-C39-C41-C42
12	L	309	U10	C38-C39-C41-C42
12	L	303	U10	C14-C16-C17-C18
12	L	303	U10	C24-C26-C27-C28
12	L	307	U10	C34-C36-C37-C38
12	L	307	U10	C44-C46-C47-C48
12	L	309	U10	C19-C21-C22-C23
12	L	309	U10	C29-C31-C32-C33
12	L	309	U10	C34-C36-C37-C38
12	L	309	U10	C49-C51-C52-C53
8	Q	102	6PL	C2-C1-O3P-P
10	L	306	LMT	O5'-C5'-C6'-O6'
10	H	302	LMT	C4'-C5'-C6'-O6'
10	6	101	LMT	C4B-C5B-C6B-O6B
10	L	306	LMT	O5'-C1'-O1'-C1
10	Z	101	LMT	O5'-C1'-O1'-C1
10	O	101	LMT	O5B-C5B-C6B-O6B
10	R	102	LMT	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
10	H	302	LMT	O5B-C5B-C6B-O6B
10	J	102	LMT	O5B-C5B-C6B-O6B
10	O	101	LMT	O5'-C5'-C6'-O6'
10	4	101	LMT	O5'-C5'-C6'-O6'
6	L	301	BCL	CBD-CGD-O2D-CED
12	L	303	U10	C37-C38-C39-C41
6	L	308	BCL	CBA-CGA-O2A-C1
10	J	102	LMT	C4B-C5B-C6B-O6B
10	4	101	LMT	C4'-C5'-C6'-O6'
10	R	102	LMT	C4'-C5'-C6'-O6'
12	M	406	U10	C23-C24-C26-C27
12	M	410	U10	C33-C34-C36-C37
12	M	410	U10	C52-C53-C54-C56
6	C	101	BCL	C11-C10-C8-C9
6	C	102	BCL	C11-C10-C8-C9
6	G	103	BCL	C11-C10-C8-C9
6	J	103	BCL	C11-C10-C8-C9
6	J	103	BCL	C14-C13-C15-C16
6	L	308	BCL	C11-C10-C8-C9
6	U	100	BCL	C11-C10-C8-C9
6	Y	101	BCL	C11-C10-C8-C9
6	3	100	BCL	C6-C7-C8-C9
6	4	102	BCL	C11-C10-C8-C9
6	5	103	BCL	C11-C10-C8-C9
6	0	100	BCL	C11-C10-C8-C9
14	M	407	QAK	C22-C23-C24-C25
14	M	407	QAK	C30-C29-C31-CB
10	H	302	LMT	C4B-C5B-C6B-O6B
10	J	102	LMT	C2'-C1'-O1'-C1
10	L	306	LMT	C2'-C1'-O1'-C1
10	B	101	LMT	C2'-C1'-O1'-C1
6	M	404	BCL	O1D-CGD-O2D-CED
10	H	302	LMT	O5'-C5'-C6'-O6'
10	O	101	LMT	C4'-C5'-C6'-O6'
10	6	101	LMT	O5B-C5B-C6B-O6B
6	E	101	BCL	CBA-CGA-O2A-C1
6	R	101	BCL	CBD-CGD-O2D-CED
6	F	102	BCL	C10-C11-C12-C13
6	T	100	BCL	C10-C11-C12-C13
6	A	100	BCL	C8-C10-C11-C12
6	5	101	BCL	C10-C11-C12-C13
6	9	102	BCL	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
10	Z	101	LMT	O5'-C5'-C6'-O6'
10	4	101	LMT	O5B-C5B-C6B-O6B
6	B	102	BCL	CBD-CGD-O2D-CED
6	M	402	BCL	C6-C7-C8-C10
6	5	101	BCL	C6-C7-C8-C10
10	2	101	LMT	O5'-C5'-C6'-O6'
12	L	303	U10	C29-C31-C32-C33
12	M	410	U10	C14-C16-C17-C18
12	M	410	U10	C34-C36-C37-C38
6	E	101	BCL	C3-C5-C6-C7
6	T	100	BCL	C5-C6-C7-C8
6	9	102	BCL	C13-C15-C16-C17
10	H	302	LMT	O1'-C1-C2-C3
6	L	308	BCL	O1A-CGA-O2A-C1
6	7	102	BCL	C8-C10-C11-C12
9	G	105	CDL	CB4-CB3-OB5-PB2
6	P	102	BCL	C2A-CAA-CBA-CGA
6	5	101	BCL	C15-C16-C17-C18
11	M	405	BPH	C5-C6-C7-C8
10	H	302	LMT	O5'-C1'-O1'-C1
10	R	102	LMT	O5'-C1'-O1'-C1
6	1	102	BCL	C15-C16-C17-C18
6	0	100	BCL	C15-C16-C17-C18
6	N	101	BCL	CBA-CGA-O2A-C1
10	4	101	LMT	C4B-C5B-C6B-O6B
10	6	101	LMT	C4'-C5'-C6'-O6'
6	E	101	BCL	C15-C16-C17-C18
6	A	100	BCL	C13-C15-C16-C17
6	3	100	BCL	C10-C11-C12-C13
14	M	407	QAK	C11-C12-C13-C14
6	R	103	BCL	C15-C16-C17-C18
6	Y	102	BCL	C10-C11-C12-C13
15	9	101	PGT	C32-C31-O2-C2
6	E	101	BCL	O1A-CGA-O2A-C1
6	0	100	BCL	C3-C5-C6-C7
15	9	101	PGT	O31-C31-O2-C2
6	G	103	BCL	C2A-CAA-CBA-CGA
6	C	102	BCL	C8-C10-C11-C12
6	C	102	BCL	C15-C16-C17-C18
6	E	101	BCL	C10-C11-C12-C13
6	N	102	BCL	C5-C6-C7-C8
6	P	102	BCL	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
6	T	100	BCL	C3-C5-C6-C7
6	J	101	BCL	C15-C16-C17-C18
6	R	101	BCL	C5-C6-C7-C8
6	B	102	BCL	C13-C15-C16-C17
6	7	102	BCL	C15-C16-C17-C18
6	R	103	BCL	C5-C6-C7-C8
6	U	100	BCL	C13-C15-C16-C17
6	Q	100	BCL	C5-C6-C7-C8
6	B	102	BCL	C15-C16-C17-C18
6	3	100	BCL	C15-C16-C17-C18
6	N	102	BCL	C11-C10-C8-C9
10	H	302	LMT	C2'-C1'-O1'-C1
10	R	102	LMT	C2'-C1'-O1'-C1
6	3	100	BCL	CBA-CGA-O2A-C1
6	C	101	BCL	C5-C6-C7-C8
10	B	101	LMT	C4B-C5B-C6B-O6B
8	S	102	6PL	C2-C1-O3P-P
9	G	105	CDL	C1-CB2-OB2-PB2
6	J	101	BCL	C2A-CAA-CBA-CGA
6	R	101	BCL	C2A-CAA-CBA-CGA
6	Y	101	BCL	C2A-CAA-CBA-CGA
12	M	406	U10	C37-C38-C39-C40
6	Y	102	BCL	C3-C5-C6-C7
6	J	103	BCL	C13-C15-C16-C17
8	O	103	6PL	C11-C12-C13-C14
10	O	101	LMT	C6-C7-C8-C9
6	7	102	BCL	C16-C17-C18-C19
10	P	101	LMT	C1-C2-C3-C4
8	Q	102	6PL	C35-C36-C37-C38
6	N	101	BCL	O1A-CGA-O2A-C1
10	F	101	LMT	C2-C1-O1'-C1'
10	H	302	LMT	C2-C3-C4-C5
10	B	101	LMT	C7-C8-C9-C10
6	0	100	BCL	C16-C17-C18-C19
6	Y	102	BCL	C8-C10-C11-C12
6	3	100	BCL	C13-C15-C16-C17
8	E	102	6PL	C32-C31-O2-C2
9	G	105	CDL	C72-C73-C74-C75
6	L	301	BCL	C11-C10-C8-C7
6	V	101	BCL	CBA-CGA-O2A-C1
6	A	100	BCL	C3-C5-C6-C7
6	C	101	BCL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
6	E	101	BCL	C3A-C2A-CAA-CBA
6	G	103	BCL	C3A-C2A-CAA-CBA
6	J	101	BCL	C3A-C2A-CAA-CBA
6	J	103	BCL	C3A-C2A-CAA-CBA
6	R	103	BCL	C3A-C2A-CAA-CBA
6	T	100	BCL	C3A-C2A-CAA-CBA
6	V	101	BCL	C3A-C2A-CAA-CBA
6	P	102	BCL	C3A-C2A-CAA-CBA
6	Y	101	BCL	C3A-C2A-CAA-CBA
6	A	100	BCL	C3A-C2A-CAA-CBA
6	1	101	BCL	C3A-C2A-CAA-CBA
6	3	100	BCL	C3A-C2A-CAA-CBA
6	5	101	BCL	C3A-C2A-CAA-CBA
6	5	103	BCL	C3A-C2A-CAA-CBA
6	9	102	BCL	C3A-C2A-CAA-CBA
6	0	100	BCL	C3A-C2A-CAA-CBA
10	Z	101	LMT	C1-C2-C3-C4
8	U	102	6PL	C13-C14-C15-C16
6	E	101	BCL	C8-C10-C11-C12
6	N	101	BCL	C8-C10-C11-C12
6	U	100	BCL	C15-C16-C17-C18
6	7	102	BCL	C16-C17-C18-C20
6	0	100	BCL	C16-C17-C18-C20
10	F	101	LMT	C3-C4-C5-C6
8	L	305	6PL	C38-C39-C40-C41
10	R	102	LMT	C2-C3-C4-C5
6	3	100	BCL	O1A-CGA-O2A-C1
14	M	407	QAK	C15-C16-C17-C18
8	B	104	6PL	C20-C21-C22-C23
12	L	307	U10	C32-C33-C34-C35
6	C	101	BCL	C2A-CAA-CBA-CGA
10	L	306	LMT	C3-C4-C5-C6
6	1	101	BCL	C8-C10-C11-C12
6	7	102	BCL	C2-C3-C5-C6
10	P	101	LMT	C2B-C1B-O1B-C4'
6	7	102	BCL	CBA-CGA-O2A-C1
6	V	102	BCL	C11-C10-C8-C9
6	B	102	BCL	C11-C10-C8-C9
10	O	101	LMT	C2-C3-C4-C5
10	L	306	LMT	C4-C5-C6-C7
10	6	101	LMT	C2-C3-C4-C5
6	V	101	BCL	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
6	L	308	BCL	C13-C15-C16-C17
6	Y	101	BCL	C15-C16-C17-C18
6	A	100	BCL	C15-C16-C17-C18
10	R	102	LMT	C5-C6-C7-C8
10	P	101	LMT	C3-C4-C5-C6
6	P	102	BCL	C3-C5-C6-C7
8	8	102	6PL	C32-C31-O2-C2
6	V	101	BCL	O1A-CGA-O2A-C1
10	B	101	LMT	O5B-C5B-C6B-O6B
8	E	102	6PL	O31-C31-O2-C2
12	L	307	U10	C15-C14-C16-C17
8	0	102	6PL	C37-C38-C39-C40
12	L	307	U10	C52-C53-C54-C55
10	Z	101	LMT	C2-C3-C4-C5
6	C	101	BCL	C10-C11-C12-C13
9	L	310	CDL	C41-C42-C43-C44
6	B	102	BCL	C5-C6-C7-C8
10	4	101	LMT	C1-C2-C3-C4
6	C	101	BCL	C8-C10-C11-C12
6	G	104	BCL	C15-C16-C17-C18
6	Y	101	BCL	C5-C6-C7-C8
6	7	102	BCL	C10-C11-C12-C13
6	L	301	BCL	O1D-CGD-O2D-CED
6	U	100	BCL	C3-C5-C6-C7
6	7	102	BCL	C3-C5-C6-C7
8	2	103	6PL	O2-C2-C3-O3
10	P	101	LMT	O5B-C1B-O1B-C4'
6	Q	100	BCL	C15-C16-C17-C18
6	G	103	BCL	C5-C6-C7-C8
9	G	105	CDL	CA4-CA3-OA5-PA1
12	L	307	U10	C45-C44-C46-C47
8	Z	103	6PL	C36-C37-C38-C39
10	R	102	LMT	C3-C4-C5-C6
6	L	308	BCL	CBD-CGD-O2D-CED
6	R	101	BCL	O1D-CGD-O2D-CED
6	7	102	BCL	O1A-CGA-O2A-C1
6	B	102	BCL	C3-C5-C6-C7
6	C	101	BCL	C1A-C2A-CAA-CBA
6	G	103	BCL	C1A-C2A-CAA-CBA
6	J	101	BCL	C1A-C2A-CAA-CBA
6	J	103	BCL	C1A-C2A-CAA-CBA
6	M	402	BCL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
6	T	100	BCL	C1A-C2A-CAA-CBA
6	P	102	BCL	C1A-C2A-CAA-CBA
6	Y	101	BCL	C1A-C2A-CAA-CBA
6	A	100	BCL	C1A-C2A-CAA-CBA
6	1	101	BCL	C1A-C2A-CAA-CBA
6	5	101	BCL	C1A-C2A-CAA-CBA
6	9	102	BCL	C1A-C2A-CAA-CBA
6	0	100	BCL	C1A-C2A-CAA-CBA
9	M	409	CDL	OA5-CA3-CA4-CA6
10	Z	101	LMT	C3-C4-C5-C6
6	G	103	BCL	C6-C7-C8-C10
6	N	101	BCL	C11-C10-C8-C7
6	R	101	BCL	C11-C10-C8-C7
6	R	103	BCL	C11-C10-C8-C7
6	A	100	BCL	C6-C7-C8-C10
6	3	100	BCL	C11-C10-C8-C7
6	5	101	BCL	C11-C10-C8-C7
6	5	101	BCL	C12-C13-C15-C16
6	7	104	BCL	C6-C7-C8-C10
11	M	405	BPH	C11-C10-C8-C7
6	E	101	BCL	C16-C17-C18-C19
6	7	104	BCL	C16-C17-C18-C19
6	Y	102	BCL	C15-C16-C17-C18
6	E	101	BCL	C2C-C3C-CAC-CBC
6	F	102	BCL	C2C-C3C-CAC-CBC
6	G	103	BCL	C2C-C3C-CAC-CBC
6	J	101	BCL	C2C-C3C-CAC-CBC
6	R	101	BCL	C2C-C3C-CAC-CBC
6	R	103	BCL	C2C-C3C-CAC-CBC
6	V	101	BCL	C2C-C3C-CAC-CBC
6	B	102	BCL	C2C-C3C-CAC-CBC
6	3	100	BCL	C2C-C3C-CAC-CBC
6	5	101	BCL	C2C-C3C-CAC-CBC
7	2	102	CRT	C36-C37-C38-C39
14	M	407	QAK	C40-C2-C3-C4
12	L	303	U10	C12-C11-C9-C8
6	1	101	BCL	C2A-CAA-CBA-CGA
6	C	101	BCL	C6-C7-C8-C9
6	F	102	BCL	C6-C7-C8-C9
6	F	102	BCL	C11-C12-C13-C14
6	G	103	BCL	C6-C7-C8-C9
6	M	402	BCL	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
6	V	101	BCL	C11-C10-C8-C9
6	5	101	BCL	C6-C7-C8-C9
6	5	101	BCL	C11-C10-C8-C9
6	5	101	BCL	C11-C12-C13-C14
6	9	102	BCL	C11-C10-C8-C9
11	M	405	BPH	C11-C10-C8-C9
14	M	407	QAK	C20-C19-C21-C22
10	B	101	LMT	C6-C7-C8-C9
6	T	100	BCL	CBA-CGA-O2A-C1
12	L	307	U10	C17-C18-C19-C20
10	L	306	LMT	C4B-C5B-C6B-O6B
12	M	406	U10	C37-C38-C39-C41
8	5	102	6PL	C1-C2-C3-O3
8	L	305	6PL	C19-C20-C21-C22
14	M	407	QAK	C11-C10-CZ3-CE3
9	M	408	CDL	O1-C1-CA2-OA2
6	5	101	BCL	CBA-CGA-O2A-C1
6	A	100	BCL	C16-C17-C18-C19
11	L	302	BPH	CHA-CBD-CGD-O1D
12	M	410	U10	C25-C24-C26-C27
12	L	307	U10	C43-C44-C46-C47
12	M	410	U10	C23-C24-C26-C27
10	2	101	LMT	O5B-C5B-C6B-O6B
8	H	301	6PL	C31-C32-C33-C34
9	E	103	CDL	CA7-C31-C32-C33
8	H	301	6PL	C32-C33-C34-C35
6	G	104	BCL	CBA-CGA-O2A-C1
6	7	104	BCL	C16-C17-C18-C20
8	0	102	6PL	O3P-C1-C2-O2
10	B	101	LMT	C3-C4-C5-C6
8	L	305	6PL	C41-C42-C43-C44
12	L	303	U10	C12-C11-C9-C10
8	4	104	6PL	C37-C38-C39-C40
6	E	101	BCL	C16-C17-C18-C20
8	2	103	6PL	O2-C31-C32-C33
8	I	101	6PL	C42-C43-C44-C45
10	R	102	LMT	C9-C10-C11-C12
6	N	101	BCL	C10-C11-C12-C13
8	8	102	6PL	O31-C31-O2-C2
10	F	101	LMT	C4'-C5'-C6'-O6'
8	O	103	6PL	C32-C31-O2-C2
6	V	102	BCL	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
10	2	101	LMT	C2B-C1B-O1B-C4'
6	3	100	BCL	C8-C10-C11-C12
6	B	102	BCL	O1D-CGD-O2D-CED
11	L	302	BPH	C4-C3-C5-C6
12	L	307	U10	C20-C19-C21-C22
10	J	102	LMT	C2-C1-O1'-C1'
10	6	101	LMT	C2-C1-O1'-C1'
6	L	301	BCL	C11-C10-C8-C9
6	M	404	BCL	C11-C10-C8-C9
6	R	101	BCL	C11-C10-C8-C9
6	R	103	BCL	C11-C10-C8-C9
6	T	100	BCL	C6-C7-C8-C9
6	Q	100	BCL	C11-C10-C8-C9
6	A	100	BCL	C6-C7-C8-C9
6	A	100	BCL	C11-C10-C8-C9
6	3	100	BCL	C11-C10-C8-C9
6	5	101	BCL	C14-C13-C15-C16
6	7	104	BCL	C6-C7-C8-C9
6	U	100	BCL	C8-C10-C11-C12
8	O	103	6PL	C2-C1-O3P-P
8	2	103	6PL	C2-C1-O3P-P
6	T	100	BCL	O1A-CGA-O2A-C1
10	4	101	LMT	C3-C4-C5-C6
10	2	101	LMT	C3-C4-C5-C6
9	M	409	CDL	OB5-CB3-CB4-CB6
9	G	101	CDL	C11-CA5-OA6-CA4
6	C	101	BCL	C6-C7-C8-C10
6	F	102	BCL	C6-C7-C8-C10
6	G	104	BCL	C11-C10-C8-C7
6	J	101	BCL	C12-C13-C15-C16
6	J	103	BCL	C6-C7-C8-C10
6	N	102	BCL	C6-C7-C8-C10
6	L	308	BCL	C11-C10-C8-C7
6	M	404	BCL	C11-C10-C8-C7
6	T	100	BCL	C6-C7-C8-C10
6	V	101	BCL	C11-C10-C8-C7
6	V	102	BCL	C6-C7-C8-C10
6	Q	100	BCL	C11-C10-C8-C7
6	Y	101	BCL	C6-C7-C8-C10
6	A	100	BCL	C11-C10-C8-C7
6	7	102	BCL	C6-C7-C8-C10
6	7	104	BCL	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
12	L	309	U10	C52-C53-C54-C55
6	A	100	BCL	C16-C17-C18-C20
6	L	308	BCL	C3A-C2A-CAA-CBA
12	L	307	U10	C12-C11-C9-C10
8	Q	102	6PL	O2-C31-C32-C33
12	L	307	U10	C13-C14-C16-C17
12	L	307	U10	C52-C53-C54-C56
8	O	103	6PL	C33-C34-C35-C36
6	G	104	BCL	O1A-CGA-O2A-C1
6	5	101	BCL	O1A-CGA-O2A-C1
9	G	105	CDL	C57-C58-C59-C60
10	4	101	LMT	O1'-C1-C2-C3
8	2	103	6PL	C1-C2-C3-O3
15	9	101	PGT	C14-C15-C16-C17
12	L	309	U10	C30-C29-C31-C32
8	O	103	6PL	O3-C11-C12-C13
11	L	302	BPH	C2-C3-C5-C6
12	L	307	U10	C12-C11-C9-C8
12	L	307	U10	C18-C19-C21-C22
10	R	102	LMT	C11-C10-C9-C8
15	7	103	PGT	O3P-C1-C2-O2
9	G	101	CDL	C74-C75-C76-C77
8	5	102	6PL	C21-C22-C23-C24
8	F	103	6PL	C40-C41-C42-C43
6	J	101	BCL	C13-C15-C16-C17
8	I	103	6PL	C21-C22-C23-C24
10	2	101	LMT	O1'-C1-C2-C3
8	P	103	6PL	O2-C2-C3-O3
9	E	103	CDL	OA6-CA4-CA6-OA8
10	F	101	LMT	C6-C7-C8-C9
14	M	407	QAK	C29-C31-CB-CA
12	L	303	U10	C5-C4-O4-C4M
6	T	100	BCL	C16-C17-C18-C19
6	M	404	BCL	C15-C16-C17-C18
6	J	101	BCL	C6-C7-C8-C9
6	V	101	BCL	C11-C12-C13-C14
6	B	102	BCL	C6-C7-C8-C9
6	7	102	BCL	C11-C10-C8-C9
6	7	104	BCL	C13-C15-C16-C17
6	F	102	BCL	C16-C17-C18-C19
12	L	307	U10	C19-C21-C22-C23
12	L	309	U10	C24-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
6	M	402	BCL	C4C-C3C-CAC-CBC
6	R	103	BCL	C4C-C3C-CAC-CBC
9	E	103	CDL	C37-C38-C39-C40
6	L	308	BCL	C5-C6-C7-C8
6	V	101	BCL	C3-C5-C6-C7
6	R	101	BCL	CBA-CGA-O2A-C1
8	P	103	6PL	O2-C31-C32-C33
6	C	102	BCL	C10-C11-C12-C13
9	M	408	CDL	CB2-C1-CA2-OA2
8	0	102	6PL	C42-C43-C44-C45
14	M	407	QAK	C19-C21-C22-C23
9	G	105	CDL	OA5-CA3-CA4-CA6
10	J	102	LMT	O5'-C5'-C6'-O6'
6	P	102	BCL	C5-C6-C7-C8
8	Z	103	6PL	C32-C33-C34-C35
6	C	101	BCL	C11-C10-C8-C7
6	E	101	BCL	C6-C7-C8-C10
6	J	101	BCL	C6-C7-C8-C10
6	V	101	BCL	C11-C12-C13-C15
6	P	102	BCL	C6-C7-C8-C10
6	B	102	BCL	C6-C7-C8-C10
6	4	102	BCL	C11-C10-C8-C7
6	5	103	BCL	C11-C10-C8-C7
6	7	102	BCL	C11-C10-C8-C7
6	7	102	BCL	C11-C12-C13-C15
6	0	100	BCL	C11-C10-C8-C7
14	M	407	QAK	C23-C24-C26-C27
14	M	407	QAK	C28-C29-C31-CB
9	G	105	CDL	C32-C31-CA7-OA8
10	Z	101	LMT	C4-C5-C6-C7
6	G	104	BCL	C5-C6-C7-C8
6	N	102	BCL	C10-C11-C12-C13
6	R	101	BCL	C10-C11-C12-C13
8	I	101	6PL	C17-C18-C19-C20
12	L	307	U10	C5-C4-O4-C4M
12	L	309	U10	C5-C4-O4-C4M
10	Z	101	LMT	O1'-C1-C2-C3
9	M	409	CDL	OA5-CA3-CA4-OA6
10	2	101	LMT	O5'-C1'-O1'-C1
12	L	307	U10	C39-C41-C42-C43
8	I	101	6PL	C5-C4-O4P-P
8	I	103	6PL	C5-C4-O4P-P

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Mol	Chain	Res	Type	Atoms
8	K	102	6PL	C5-C4-O4P-P
8	M	401	6PL	C5-C4-O4P-P
8	B	104	6PL	C5-C4-O4P-P
8	4	104	6PL	C5-C4-O4P-P
8	5	102	6PL	C5-C4-O4P-P
10	Z	101	LMT	C7-C8-C9-C10
6	V	102	BCL	C13-C15-C16-C17
6	E	101	BCL	C6-C7-C8-C9
6	V	102	BCL	C14-C13-C15-C16
8	U	102	6PL	O3-C11-C12-C13
6	R	101	BCL	O1A-CGA-O2A-C1
7	2	102	CRT	C36-C37-C38-O2
6	V	101	BCL	C15-C16-C17-C18
6	7	104	BCL	C5-C6-C7-C8
8	E	102	6PL	O4P-C4-C5-N
8	F	103	6PL	O4P-C4-C5-N
8	I	101	6PL	O4P-C4-C5-N
8	I	103	6PL	O4P-C4-C5-N
8	K	102	6PL	O4P-C4-C5-N
8	H	301	6PL	O4P-C4-C5-N
8	L	304	6PL	O4P-C4-C5-N
8	U	102	6PL	O4P-C4-C5-N
8	Q	102	6PL	O4P-C4-C5-N
8	Z	103	6PL	O4P-C4-C5-N
8	B	104	6PL	O4P-C4-C5-N
8	2	103	6PL	O4P-C4-C5-N
8	5	102	6PL	O4P-C4-C5-N
8	6	102	6PL	O4P-C4-C5-N
8	8	102	6PL	O4P-C4-C5-N
14	M	407	QAK	C38-C10-C11-C12
8	P	103	6PL	C33-C34-C35-C36
10	O	101	LMT	C7-C8-C9-C10
10	2	101	LMT	C2-C3-C4-C5
6	G	104	BCL	C3-C5-C6-C7
6	9	102	BCL	C3-C5-C6-C7
6	E	101	BCL	C1A-C2A-CAA-CBA
6	L	308	BCL	C1A-C2A-CAA-CBA
6	3	100	BCL	C1A-C2A-CAA-CBA
12	L	303	U10	C15-C14-C16-C17
12	L	303	U10	C20-C19-C21-C22
12	L	303	U10	C35-C34-C36-C37
12	L	309	U10	C50-C49-C51-C52

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Mol	Chain	Res	Type	Atoms
6	R	103	BCL	C3-C5-C6-C7
6	4	102	BCL	C3-C5-C6-C7
8	P	103	6PL	C35-C36-C37-C38
10	L	306	LMT	C2-C3-C4-C5
6	C	102	BCL	C6-C7-C8-C10
6	N	101	BCL	C6-C7-C8-C10
6	N	101	BCL	C11-C12-C13-C15
6	U	100	BCL	C6-C7-C8-C10
6	U	100	BCL	C11-C10-C8-C7
6	Y	101	BCL	C11-C10-C8-C7
6	Y	102	BCL	C6-C7-C8-C10
6	A	100	BCL	C11-C12-C13-C15
6	1	101	BCL	C6-C7-C8-C10
6	3	100	BCL	C6-C7-C8-C10
6	3	100	BCL	C12-C13-C15-C16
6	7	104	BCL	C11-C12-C13-C15
14	M	407	QAK	C22-C23-C24-C26
6	T	100	BCL	C16-C17-C18-C20
10	2	101	LMT	C7-C8-C9-C10
12	L	307	U10	C35-C34-C36-C37
12	M	406	U10	C30-C29-C31-C32
14	M	407	QAK	CD1-C2-C3-C4
6	J	103	BCL	C6-C7-C8-C9
6	N	101	BCL	C11-C10-C8-C9
6	P	102	BCL	C6-C7-C8-C9
6	7	102	BCL	C6-C7-C8-C9
6	7	102	BCL	C11-C12-C13-C14
14	M	407	QAK	C25-C24-C26-C27
8	E	102	6PL	C13-C14-C15-C16
8	E	102	6PL	C38-C39-C40-C41
10	6	101	LMT	C1-C2-C3-C4
6	L	308	BCL	O1D-CGD-O2D-CED
8	I	101	6PL	O2-C2-C3-O3
8	5	102	6PL	O2-C2-C3-O3
9	G	101	CDL	OB6-CB4-CB6-OB8
8	P	103	6PL	C1-C2-C3-O3
9	E	103	CDL	CA3-CA4-CA6-OA8
6	0	100	BCL	C13-C15-C16-C17
6	5	103	BCL	C3-C5-C6-C7
14	M	407	QAK	CD2-CE2-CZ2-C4
6	F	102	BCL	C13-C15-C16-C17
6	F	102	BCL	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
6	J	101	BCL	C3-C5-C6-C7
8	I	103	6PL	C38-C39-C40-C41
10	L	306	LMT	C11-C10-C9-C8
6	L	308	BCL	CHA-CBD-CGD-O1D
6	L	308	BCL	CHA-CBD-CGD-O2D
6	M	404	BCL	CHA-CBD-CGD-O1D
6	M	404	BCL	CHA-CBD-CGD-O2D
8	O	103	6PL	C1-O3P-P-O1P
8	O	103	6PL	C4-O4P-P-O1P
8	L	304	6PL	C4-O4P-P-O3P
8	L	305	6PL	C1-O3P-P-O1P
8	M	401	6PL	C1-O3P-P-O1P
8	X	102	6PL	C1-O3P-P-O1P
8	P	103	6PL	C1-O3P-P-O1P
8	Z	103	6PL	C1-O3P-P-O1P
8	Z	103	6PL	C4-O4P-P-O3P
8	Z	103	6PL	C4-O4P-P-O2P
8	2	103	6PL	C4-O4P-P-O1P
8	4	104	6PL	C4-O4P-P-O1P
8	5	102	6PL	C1-O3P-P-O1P
8	8	102	6PL	C4-O4P-P-O1P
8	0	102	6PL	C1-O3P-P-O1P
9	G	105	CDL	CA2-OA2-PA1-OA3
9	G	105	CDL	CA3-OA5-PA1-OA3
9	L	310	CDL	CA3-OA5-PA1-OA3
9	L	310	CDL	CB2-OB2-PB2-OB5
9	M	408	CDL	CB3-OB5-PB2-OB3
11	L	302	BPH	CHA-CBD-CGD-O2D
15	7	103	PGT	C4-O4P-P-O1P
10	2	101	LMT	O5B-C1B-O1B-C4'
10	J	102	LMT	C4'-C5'-C6'-O6'
9	M	409	CDL	C12-C11-CA5-OA6
8	X	102	6PL	C2-C1-O3P-P
8	M	401	6PL	C13-C14-C15-C16
9	L	310	CDL	C61-C62-C63-C64
9	M	408	CDL	C55-C56-C57-C58
6	B	102	BCL	C16-C17-C18-C19
6	M	402	BCL	C13-C15-C16-C17
6	R	101	BCL	C15-C16-C17-C18
10	4	101	LMT	C5-C6-C7-C8
12	L	307	U10	C33-C34-C36-C37
12	L	309	U10	C48-C49-C51-C52

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Mol	Chain	Res	Type	Atoms
6	Y	102	BCL	C16-C17-C18-C19
14	M	407	QAK	CE2-CD2-CE3-CZ3
10	H	302	LMT	C5'-C4'-O1B-C1B
9	G	101	CDL	C81-C82-C83-C84
6	J	101	BCL	C14-C13-C15-C16
6	N	101	BCL	C6-C7-C8-C9
6	N	102	BCL	C6-C7-C8-C9
6	V	102	BCL	C6-C7-C8-C9
6	Y	101	BCL	C6-C7-C8-C9
6	A	100	BCL	C11-C12-C13-C14
6	1	102	BCL	C11-C10-C8-C9
12	L	309	U10	C52-C53-C54-C56
8	Z	103	6PL	O3P-C1-C2-O2
9	G	105	CDL	OA5-CA3-CA4-OA6
9	M	408	CDL	C31-C32-C33-C34
10	R	102	LMT	O5B-C1B-O1B-C4'
8	M	401	6PL	O11-C11-O3-C3
10	4	101	LMT	C6-C7-C8-C9
12	M	410	U10	C45-C44-C46-C47
12	L	309	U10	C28-C29-C31-C32
8	M	401	6PL	C12-C11-O3-C3
8	H	301	6PL	C2-C3-O3-C11
9	G	101	CDL	OA7-CA5-OA6-CA4
8	4	104	6PL	C16-C17-C18-C19
8	L	305	6PL	C37-C38-C39-C40
6	9	102	BCL	C2A-CAA-CBA-CGA
10	L	306	LMT	C5'-C4'-O1B-C1B
6	7	102	BCL	C5-C6-C7-C8
12	M	410	U10	C9-C11-C12-C13
12	M	410	U10	C19-C21-C22-C23
10	F	101	LMT	C1-C2-C3-C4
6	L	301	BCL	C3-C5-C6-C7
8	O	103	6PL	O31-C31-O2-C2
6	L	301	BCL	C2A-CAA-CBA-CGA
6	V	102	BCL	C16-C17-C18-C19
8	I	101	6PL	C40-C41-C42-C43
12	L	303	U10	C13-C14-C16-C17
12	L	303	U10	C33-C34-C36-C37
12	L	303	U10	C3-C4-O4-C4M
8	2	103	6PL	C33-C34-C35-C36
9	M	408	CDL	C59-C60-C61-C62
10	Z	101	LMT	C4'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
9	G	101	CDL	C51-C52-C53-C54
12	M	410	U10	C5-C4-O4-C4M
12	L	307	U10	C47-C48-C49-C50
12	M	410	U10	C42-C43-C44-C45
6	E	101	BCL	C5-C6-C7-C8
6	V	101	BCL	C5-C6-C7-C8
6	Y	102	BCL	C2A-CAA-CBA-CGA
14	M	407	QAK	C-CA-CB-C31
6	M	402	BCL	C4-C3-C5-C6
12	M	410	U10	C43-C44-C46-C47
8	Q	102	6PL	O2-C2-C3-O3
12	M	406	U10	C28-C29-C31-C32
6	G	103	BCL	C10-C11-C12-C13
8	5	102	6PL	C18-C19-C20-C21
6	F	102	BCL	C2-C1-O2A-CGA
6	5	101	BCL	C2-C1-O2A-CGA
6	7	102	BCL	C2-C1-O2A-CGA
6	P	102	BCL	C16-C17-C18-C20
10	2	101	LMT	C4-C5-C6-C7
6	T	100	BCL	C13-C15-C16-C17
8	E	102	6PL	C12-C13-C14-C15
10	2	101	LMT	C4'-C5'-C6'-O6'
10	O	101	LMT	C4-C5-C6-C7
6	1	101	BCL	C16-C17-C18-C19
6	Q	100	BCL	C13-C15-C16-C17
12	M	406	U10	C5-C4-O4-C4M
12	L	309	U10	C44-C46-C47-C48
12	M	406	U10	C24-C26-C27-C28
6	E	101	BCL	C14-C13-C15-C16
6	F	102	BCL	C11-C10-C8-C9
6	M	402	BCL	C11-C12-C13-C14
6	U	100	BCL	C14-C13-C15-C16
6	Y	102	BCL	C11-C10-C8-C9
6	1	101	BCL	C6-C7-C8-C9
6	7	104	BCL	C11-C12-C13-C14
11	M	405	BPH	C6-C7-C8-C9
8	2	103	6PL	C31-C32-C33-C34
9	M	409	CDL	CA4-CA6-OA8-CA7
9	G	101	CDL	C60-C61-C62-C63
8	0	102	6PL	C32-C33-C34-C35
9	G	101	CDL	CA3-CA4-OA6-CA5
8	E	102	6PL	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
6	V	101	BCL	O1D-CGD-O2D-CED
14	M	407	QAK	C38-C10-CZ3-CE3
6	B	102	BCL	C16-C17-C18-C20
12	L	309	U10	C45-C44-C46-C47
6	M	402	BCL	C2-C3-C5-C6
6	G	104	BCL	C6-C7-C8-C10
6	V	101	BCL	C6-C7-C8-C10
6	1	101	BCL	C11-C10-C8-C7
6	1	102	BCL	C6-C7-C8-C10
9	L	310	CDL	C78-C79-C80-C81
6	A	100	BCL	C2A-CAA-CBA-CGA
8	0	102	6PL	O2-C2-C3-O3
15	9	101	PGT	O2-C2-C3-O3
8	L	305	6PL	C33-C34-C35-C36
10	L	306	LMT	O5B-C1B-O1B-C4'
10	B	101	LMT	C4'-C5'-C6'-O6'
10	L	306	LMT	C5-C6-C7-C8
10	F	101	LMT	O5'-C5'-C6'-O6'
6	J	103	BCL	C2-C1-O2A-CGA
6	M	404	BCL	C5-C6-C7-C8
6	M	404	BCL	C16-C17-C18-C19
10	R	102	LMT	C2B-C1B-O1B-C4'
14	M	407	QAK	C14-C15-C16-C17
8	Z	103	6PL	C40-C41-C42-C43
12	L	303	U10	C25-C24-C26-C27
12	M	410	U10	C12-C11-C9-C10
9	M	409	CDL	CA4-CA3-OA5-PA1
8	I	103	6PL	O3-C11-C12-C13
6	Y	102	BCL	C16-C17-C18-C20
12	L	309	U10	C14-C16-C17-C18
6	V	101	BCL	C10-C11-C12-C13
10	B	101	LMT	C2-C1-O1'-C1'
8	F	103	6PL	O3P-C1-C2-O2
10	R	102	LMT	C4-C5-C6-C7
6	L	301	BCL	C15-C16-C17-C18
8	O	103	6PL	O11-C11-C12-C13
10	P	101	LMT	C6-C7-C8-C9
6	J	101	BCL	C16-C17-C18-C19
6	P	102	BCL	C16-C17-C18-C19
6	9	102	BCL	C16-C17-C18-C19
8	M	401	6PL	C41-C42-C43-C44
8	L	304	6PL	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
12	L	309	U10	C35-C34-C36-C37
10	2	101	LMT	C11-C10-C9-C8
6	A	100	BCL	O1D-CGD-O2D-CED
10	F	101	LMT	C4-C5-C6-C7
11	L	302	BPH	C10-C11-C12-C13
9	L	310	CDL	C32-C33-C34-C35
8	O	103	6PL	C32-C33-C34-C35
6	U	100	BCL	C6-C7-C8-C9
6	P	102	BCL	C11-C10-C8-C9
6	Y	102	BCL	C6-C7-C8-C9
6	3	100	BCL	C14-C13-C15-C16
11	L	302	BPH	C11-C12-C13-C14
8	2	103	6PL	O31-C31-C32-C33
6	N	101	BCL	C2-C1-O2A-CGA
6	Y	102	BCL	C2-C1-O2A-CGA
6	0	100	BCL	C2-C1-O2A-CGA
8	L	304	6PL	C19-C20-C21-C22
8	2	103	6PL	C14-C15-C16-C17
6	M	404	BCL	C3A-C2A-CAA-CBA
8	I	101	6PL	C3-C2-O2-C31
8	5	102	6PL	C3-C2-O2-C31
9	E	103	CDL	CB6-CB4-OB6-CB5
6	C	101	BCL	C16-C17-C18-C19
12	L	303	U10	C18-C19-C21-C22
8	E	102	6PL	C2-C1-O3P-P
6	V	101	BCL	CBD-CGD-O2D-CED
10	O	101	LMT	C3-C4-C5-C6
6	1	101	BCL	C4-C3-C5-C6
8	O	103	6PL	O2-C31-C32-C33
8	D	102	6PL	C39-C40-C41-C42
6	7	104	BCL	C8-C10-C11-C12
6	C	102	BCL	C6-C7-C8-C9
6	N	101	BCL	C11-C12-C13-C14
6	V	102	BCL	C16-C17-C18-C20
8	M	401	6PL	C2-C3-O3-C11
15	7	103	PGT	O3P-C1-C2-C3
8	I	101	6PL	C11-C12-C13-C14
6	F	102	BCL	C2A-CAA-CBA-CGA
6	P	102	BCL	C11-C10-C8-C7
6	0	100	BCL	C6-C7-C8-C10
11	L	302	BPH	C11-C12-C13-C15
6	E	101	BCL	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
6	L	301	BCL	C2-C1-O2A-CGA
6	Q	100	BCL	C2-C1-O2A-CGA
6	1	102	BCL	C2-C1-O2A-CGA
6	4	102	BCL	C2-C1-O2A-CGA
11	M	405	BPH	C2C-C3C-CAC-CBC
6	L	308	BCL	CAA-CBA-CGA-O2A
8	I	101	6PL	C34-C35-C36-C37
6	1	101	BCL	C16-C17-C18-C20
6	5	101	BCL	C4-C3-C5-C6
9	L	310	CDL	C32-C31-CA7-OA8
12	L	309	U10	C33-C34-C36-C37
8	K	102	6PL	C32-C31-O2-C2
8	Q	102	6PL	C18-C19-C20-C21
8	Q	102	6PL	O31-C31-C32-C33
9	G	101	CDL	C15-C16-C17-C18
8	K	102	6PL	O3-C11-C12-C13
8	2	103	6PL	C40-C41-C42-C43
6	3	100	BCL	C16-C17-C18-C19
9	L	310	CDL	C38-C39-C40-C41
9	L	310	CDL	C40-C41-C42-C43
9	L	310	CDL	C12-C11-CA5-OA6
8	U	102	6PL	O11-C11-C12-C13
6	T	100	BCL	C11-C10-C8-C9
6	V	101	BCL	C6-C7-C8-C9
6	1	101	BCL	C11-C10-C8-C9
6	1	102	BCL	C6-C7-C8-C9
9	G	101	CDL	CB3-CB4-CB6-OB8
6	M	404	BCL	C1A-C2A-CAA-CBA
6	7	102	BCL	C1A-C2A-CAA-CBA
9	M	408	CDL	C75-C76-C77-C78
15	7	103	PGT	C32-C33-C34-C35
9	G	105	CDL	CB4-CB6-OB8-CB7
6	G	103	BCL	CAA-CBA-CGA-O2A
8	5	102	6PL	O2-C31-C32-C33
8	6	102	6PL	O3-C11-C12-C13
6	C	102	BCL	C2-C1-O2A-CGA
6	G	104	BCL	C2-C1-O2A-CGA
6	N	102	BCL	C2-C1-O2A-CGA
6	U	100	BCL	C2-C1-O2A-CGA
6	3	100	BCL	C2-C1-O2A-CGA
6	5	103	BCL	C2-C1-O2A-CGA
6	9	102	BCL	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
6	G	103	BCL	C11-C10-C8-C7
6	J	103	BCL	C12-C13-C15-C16
6	L	301	BCL	C6-C7-C8-C10
10	F	101	LMT	C5-C6-C7-C8
9	E	103	CDL	CA3-CA4-OA6-CA5
9	E	103	CDL	CA6-CA4-OA6-CA5
9	L	310	CDL	C32-C31-CA7-OA9
6	Y	102	BCL	C13-C15-C16-C17
6	J	103	BCL	C2C-C3C-CAC-CBC
8	K	102	6PL	C20-C21-C22-C23
6	4	102	BCL	C2A-CAA-CBA-CGA
6	J	101	BCL	C5-C6-C7-C8
8	M	401	6PL	C21-C22-C23-C24
6	1	101	BCL	C10-C11-C12-C13
6	7	102	BCL	C3A-C2A-CAA-CBA
6	A	100	BCL	C10-C11-C12-C13
8	P	103	6PL	O31-C31-C32-C33
8	E	102	6PL	C21-C22-C23-C24
8	I	101	6PL	C43-C44-C45-C46
9	G	105	CDL	C32-C31-CA7-OA9
6	M	402	BCL	C14-C13-C15-C16
9	L	310	CDL	C56-C57-C58-C59
6	U	100	BCL	O1A-CGA-O2A-C1
6	L	308	BCL	CAA-CBA-CGA-O1A
8	K	102	6PL	O11-C11-C12-C13
8	5	102	6PL	O31-C31-C32-C33
7	O	102	CRT	C35-C36-C37-C38
7	Q	101	CRT	C35-C36-C37-C38
9	G	105	CDL	C55-C56-C57-C58
8	D	102	6PL	C37-C38-C39-C40
10	L	306	LMT	C2B-C1B-O1B-C4'
8	X	102	6PL	C43-C44-C45-C46
6	G	103	BCL	CAA-CBA-CGA-O1A
9	L	310	CDL	C12-C11-CA5-OA7
8	0	102	6PL	O3-C11-C12-C13
8	O	103	6PL	O31-C31-C32-C33
8	Q	102	6PL	C34-C35-C36-C37
6	5	101	BCL	C5-C6-C7-C8
9	G	105	CDL	C34-C35-C36-C37
6	M	404	BCL	CAD-CBD-CGD-O2D
8	F	103	6PL	O3-C11-C12-C13
6	U	100	BCL	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
6	T	100	BCL	C2-C1-O2A-CGA
6	V	101	BCL	C2-C1-O2A-CGA
6	7	104	BCL	C2-C1-O2A-CGA
8	F	103	6PL	C33-C34-C35-C36
8	6	102	6PL	O11-C11-C12-C13
6	A	100	BCL	CAA-CBA-CGA-O2A
15	7	103	PGT	C13-C14-C15-C16
9	M	408	CDL	C11-CA5-OA6-CA4
15	7	103	PGT	C43-C44-C45-C46

There are no ring outliers.

100 monomers are involved in 357 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	Z	103	6PL	4	0
10	O	101	LMT	1	0
15	7	103	PGT	4	0
7	2	102	CRT	5	0
6	1	102	BCL	7	0
9	G	101	CDL	12	0
10	P	101	LMT	2	0
6	M	404	BCL	3	0
8	5	102	6PL	2	0
10	F	101	LMT	3	0
6	Y	101	BCL	4	0
7	I	102	CRT	2	0
8	Q	102	6PL	6	0
6	E	101	BCL	1	0
6	J	103	BCL	4	0
7	X	101	CRT	14	0
6	P	102	BCL	4	0
12	M	410	U10	6	0
12	L	303	U10	1	0
6	5	103	BCL	5	0
6	A	100	BCL	8	0
7	G	102	CRT	4	0
6	3	100	BCL	2	0
9	M	409	CDL	3	0
8	P	103	6PL	4	0
8	4	104	6PL	5	0
7	8	101	CRT	5	0
6	R	101	BCL	4	0

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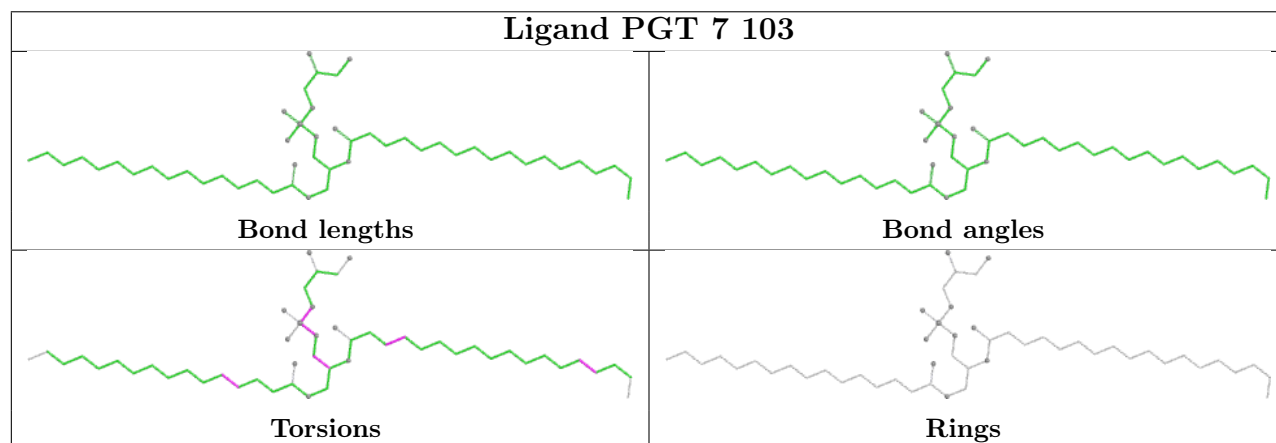
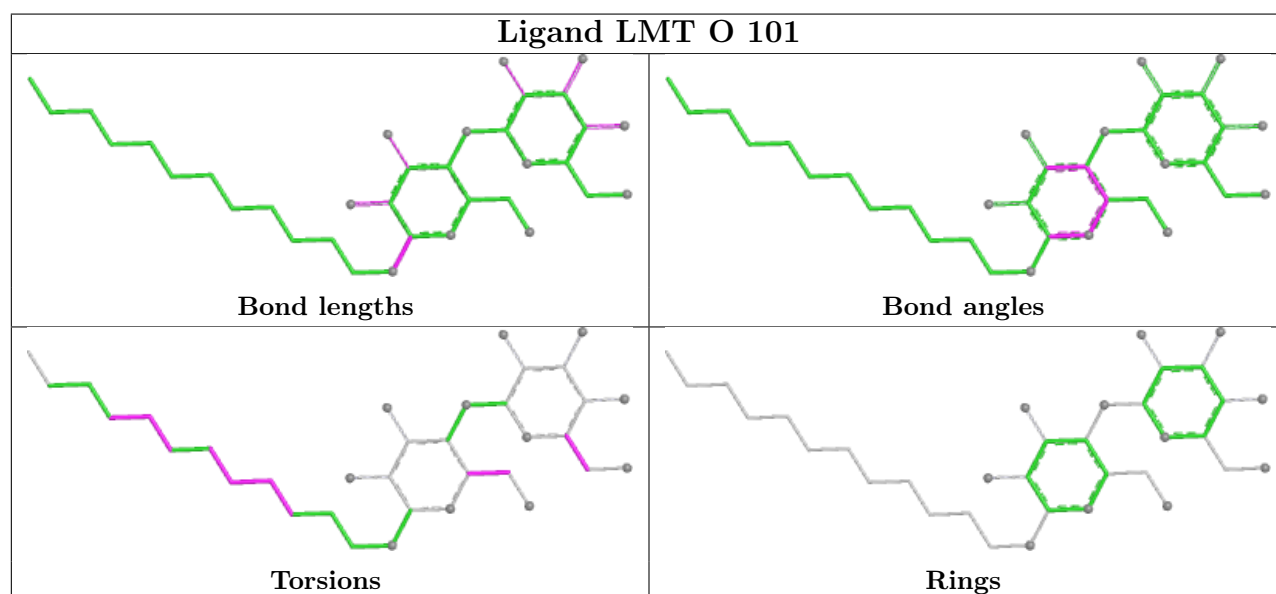
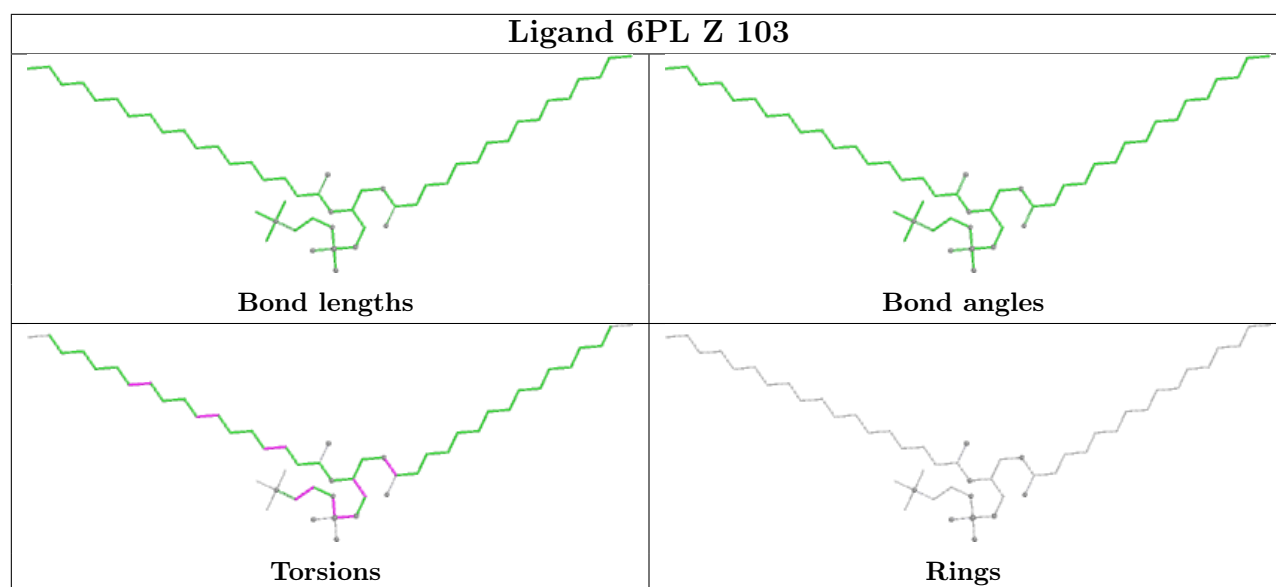
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	2	101	LMT	2	0
7	U	101	CRT	5	0
6	F	102	BCL	4	0
6	U	100	BCL	5	0
8	X	102	6PL	3	0
8	I	101	6PL	5	0
8	8	102	6PL	4	0
8	0	102	6PL	3	0
8	L	305	6PL	7	0
8	E	102	6PL	6	0
12	L	307	U10	8	0
6	M	402	BCL	1	0
6	G	103	BCL	3	0
9	M	408	CDL	7	0
6	Y	102	BCL	8	0
7	4	103	CRT	11	0
8	2	103	6PL	7	0
6	J	101	BCL	1	0
6	N	101	BCL	2	0
7	Q	101	CRT	4	0
7	Z	102	CRT	7	0
6	Q	100	BCL	5	0
10	6	101	LMT	3	0
7	0	101	CRT	5	0
8	S	102	6PL	5	0
10	B	101	LMT	2	0
6	0	100	BCL	4	0
6	R	103	BCL	4	0
8	L	304	6PL	4	0
10	J	102	LMT	7	0
7	D	101	CRT	5	0
7	7	101	CRT	2	0
8	F	103	6PL	3	0
6	L	308	BCL	5	0
6	T	100	BCL	4	0
10	4	101	LMT	3	0
7	K	101	CRT	2	0
7	B	103	CRT	4	0
10	Z	101	LMT	1	0
6	C	102	BCL	4	0
6	C	101	BCL	2	0
6	4	102	BCL	6	0

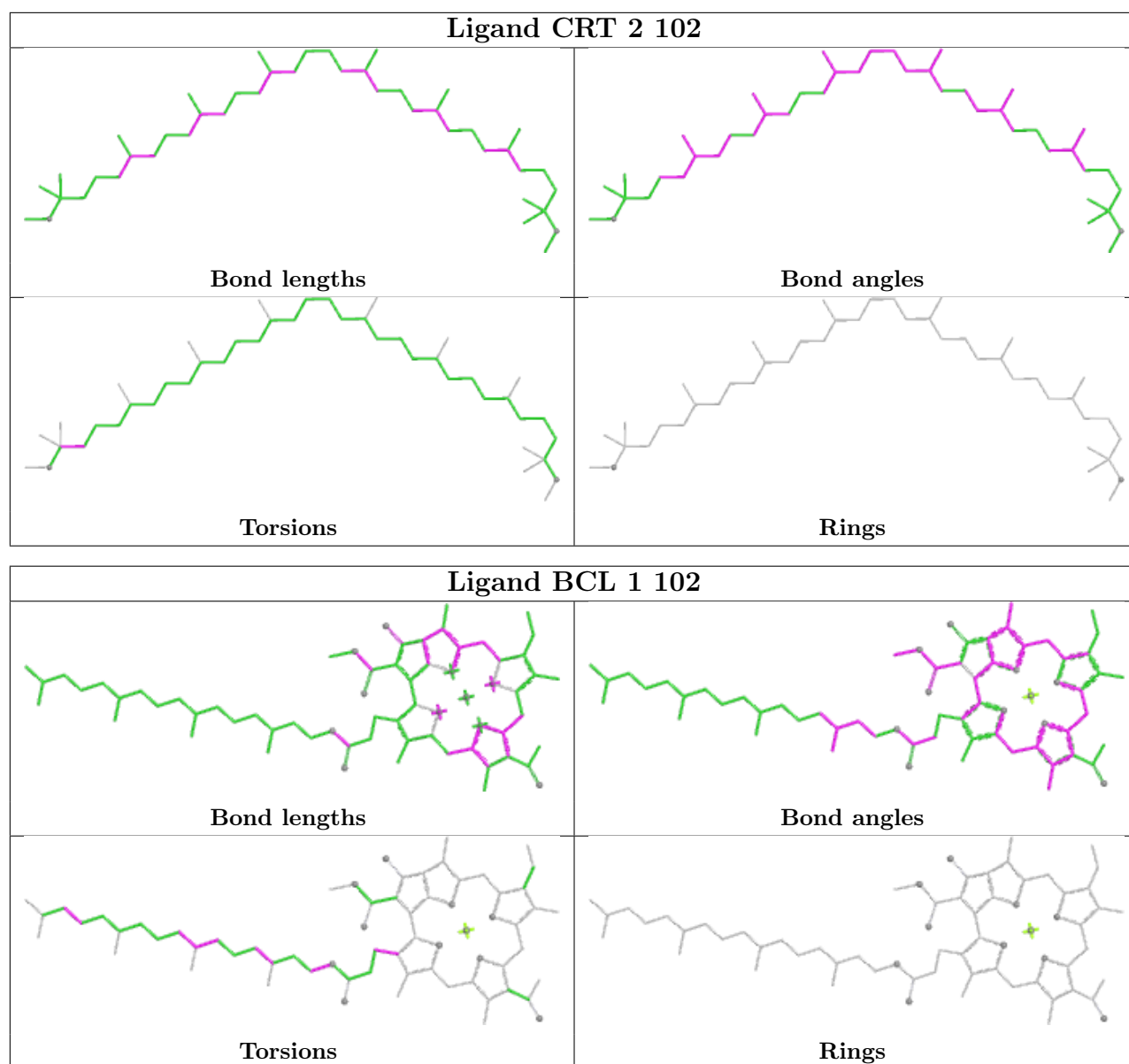
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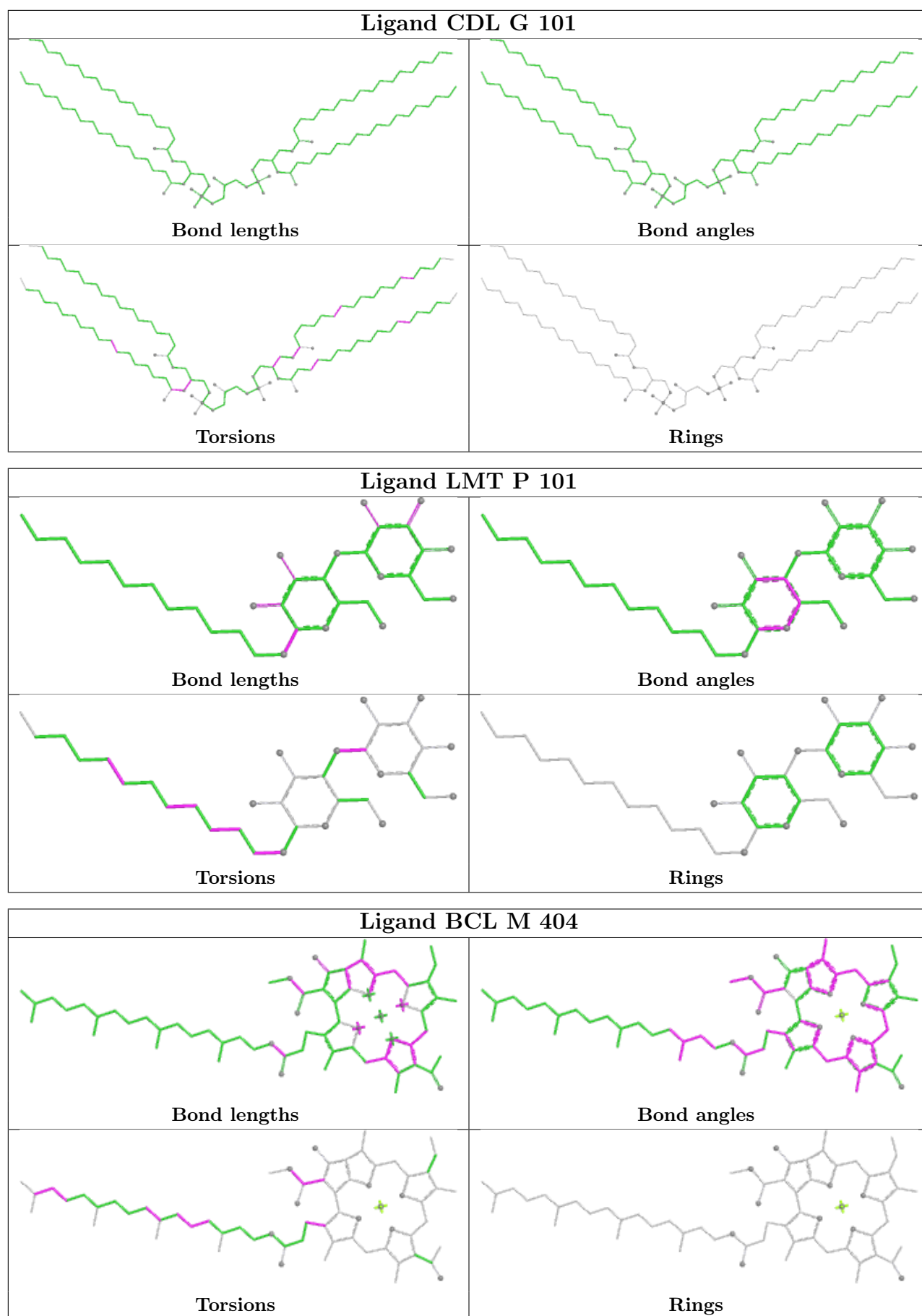
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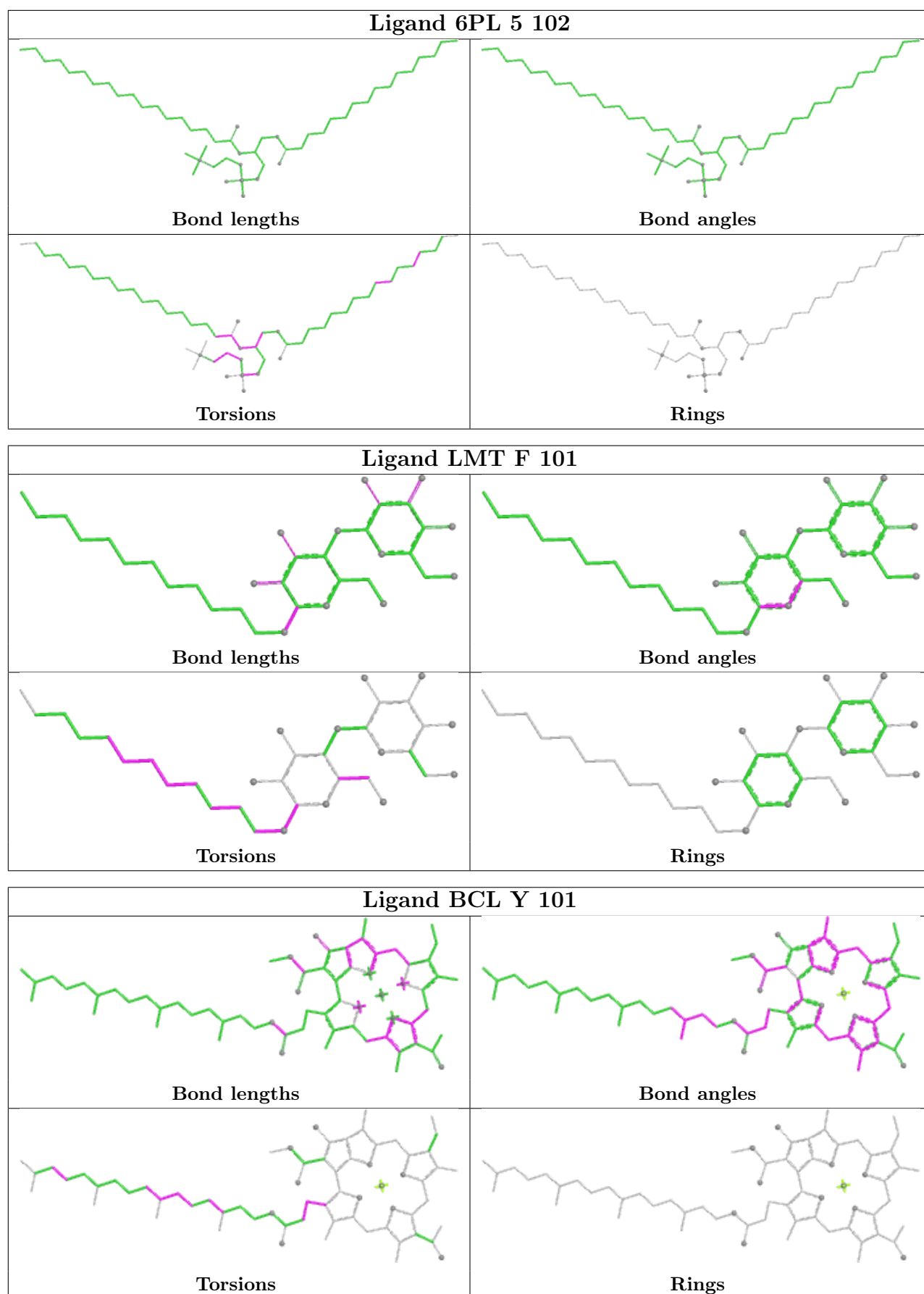
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	102	6PL	5	0
7	S	101	CRT	3	0
8	M	401	6PL	5	0
6	N	102	BCL	2	0
10	H	302	LMT	4	0
10	R	102	LMT	3	0
8	B	104	6PL	4	0
9	E	103	CDL	7	0
7	O	102	CRT	4	0
8	K	102	6PL	3	0
6	7	104	BCL	4	0
9	L	310	CDL	9	0
12	L	309	U10	4	0
11	M	405	BPH	6	0
11	L	302	BPH	5	0
8	O	103	6PL	4	0
6	9	102	BCL	1	0
6	B	102	BCL	6	0
8	6	102	6PL	4	0
6	5	101	BCL	5	0
8	I	103	6PL	5	0
6	V	102	BCL	4	0
6	G	104	BCL	5	0
8	U	102	6PL	4	0
6	7	102	BCL	1	0
12	M	406	U10	3	0
6	1	101	BCL	3	0
6	V	101	BCL	2	0
15	9	101	PGT	3	0
9	G	105	CDL	9	0

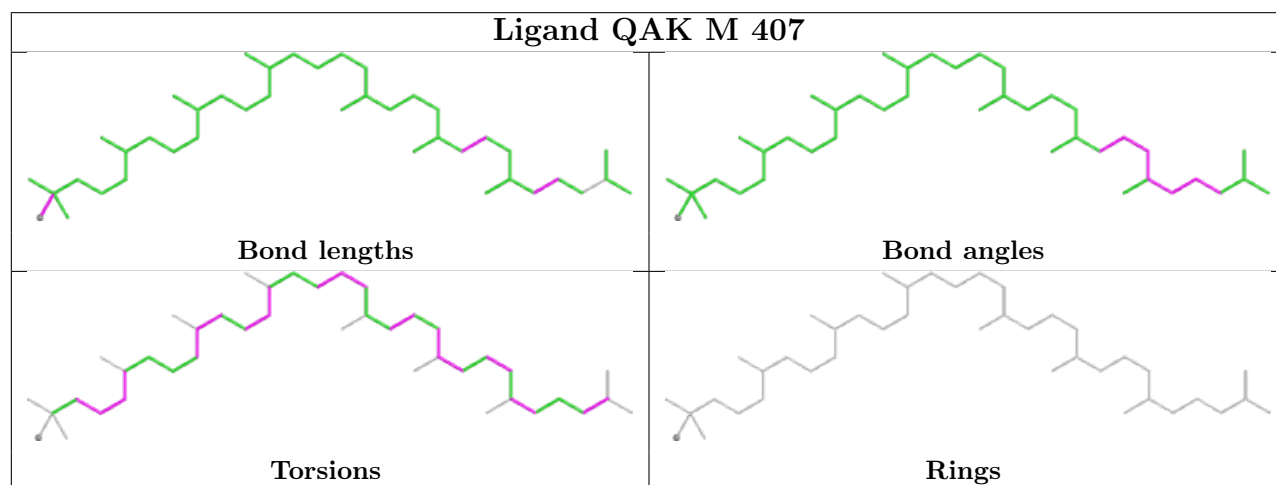
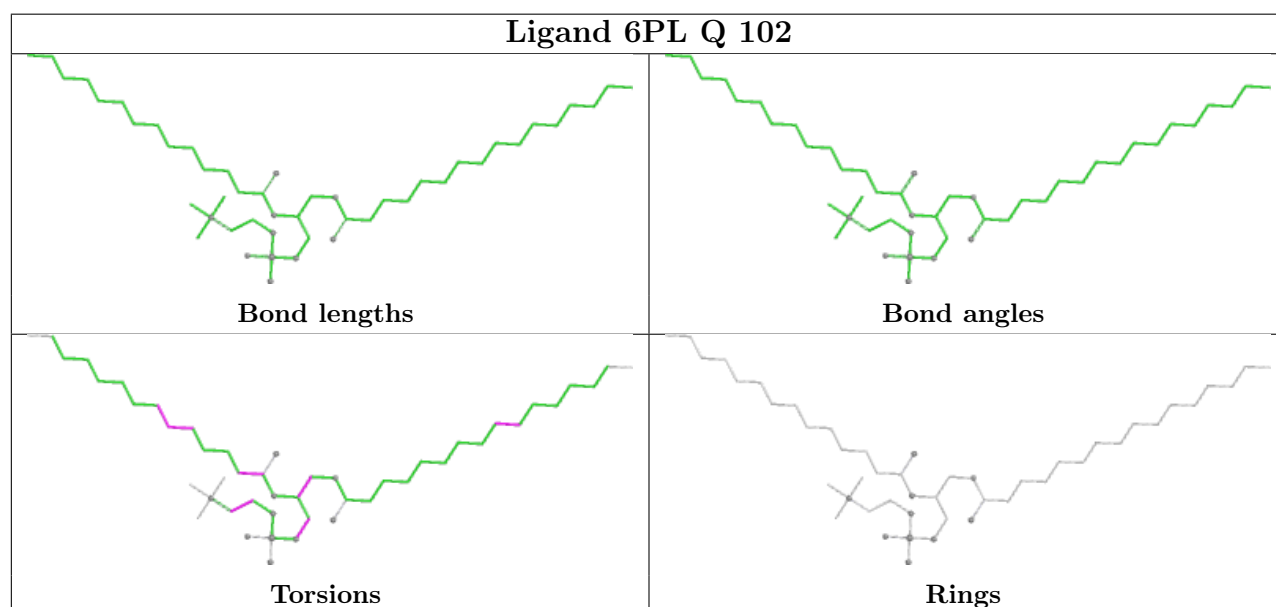
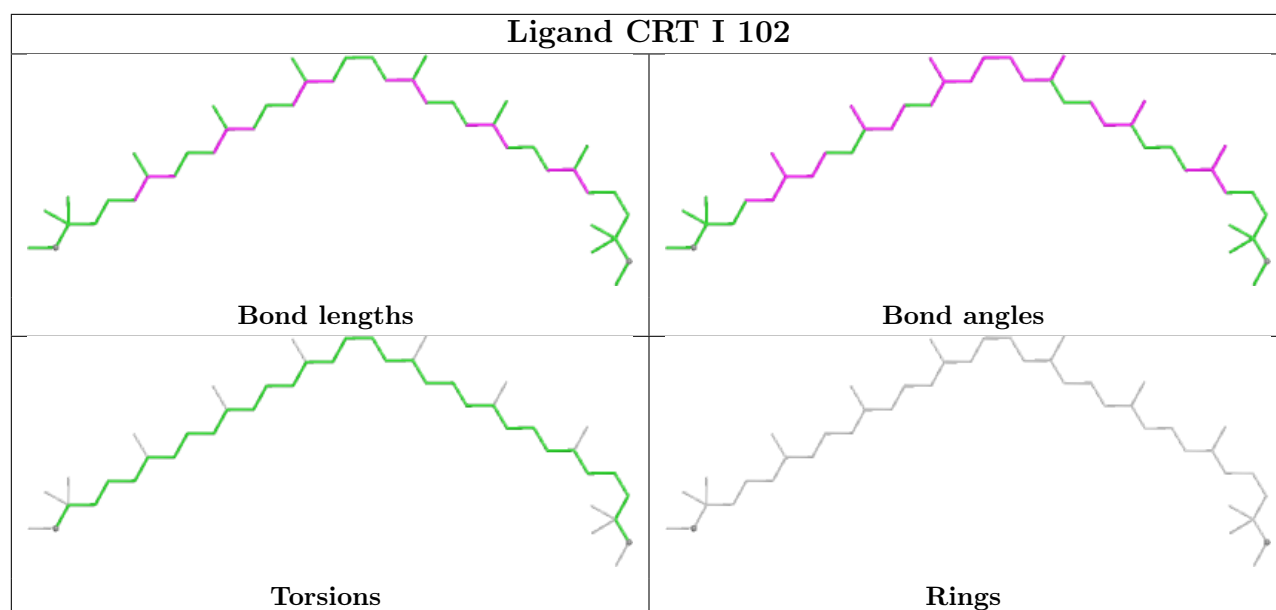
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

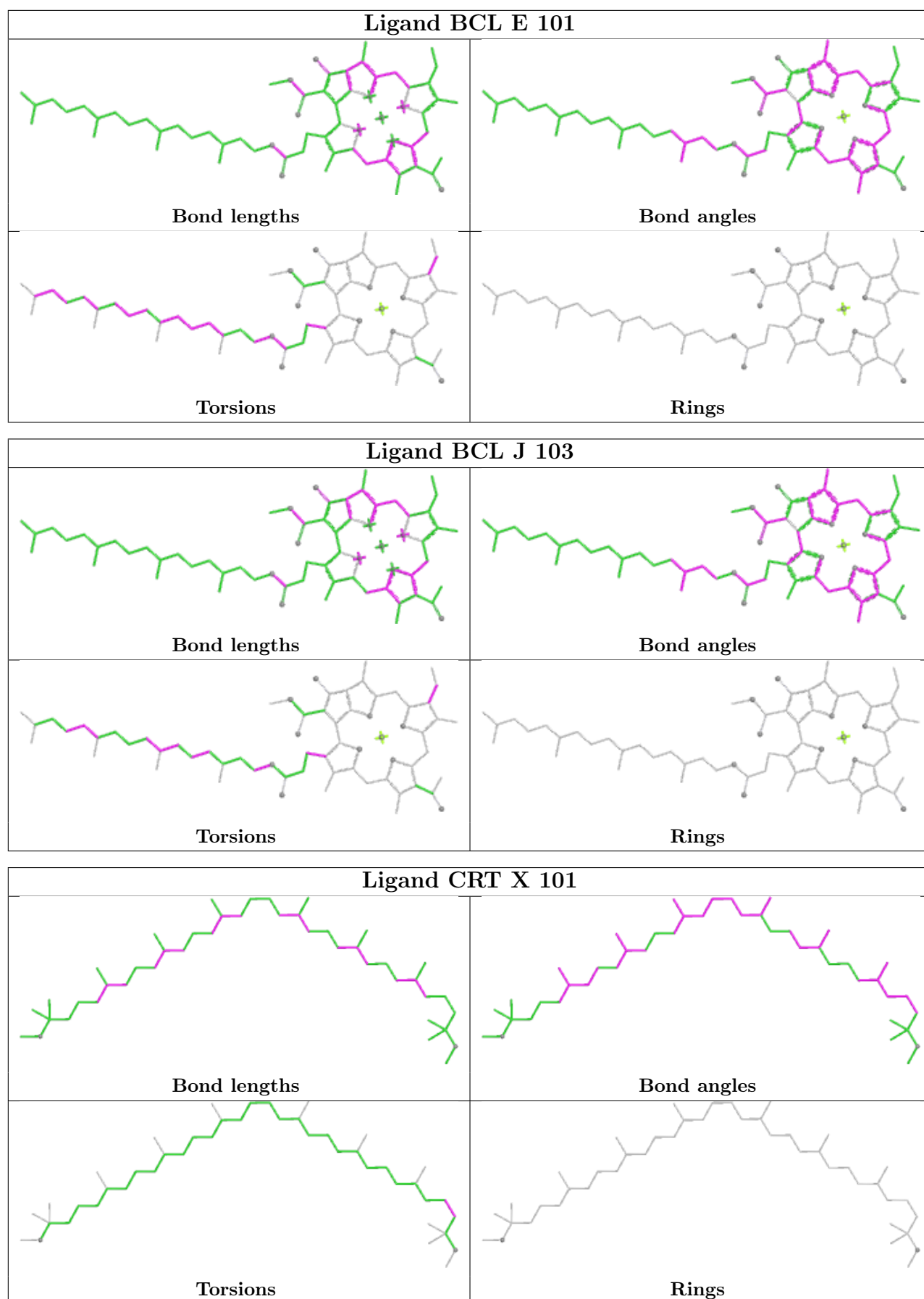


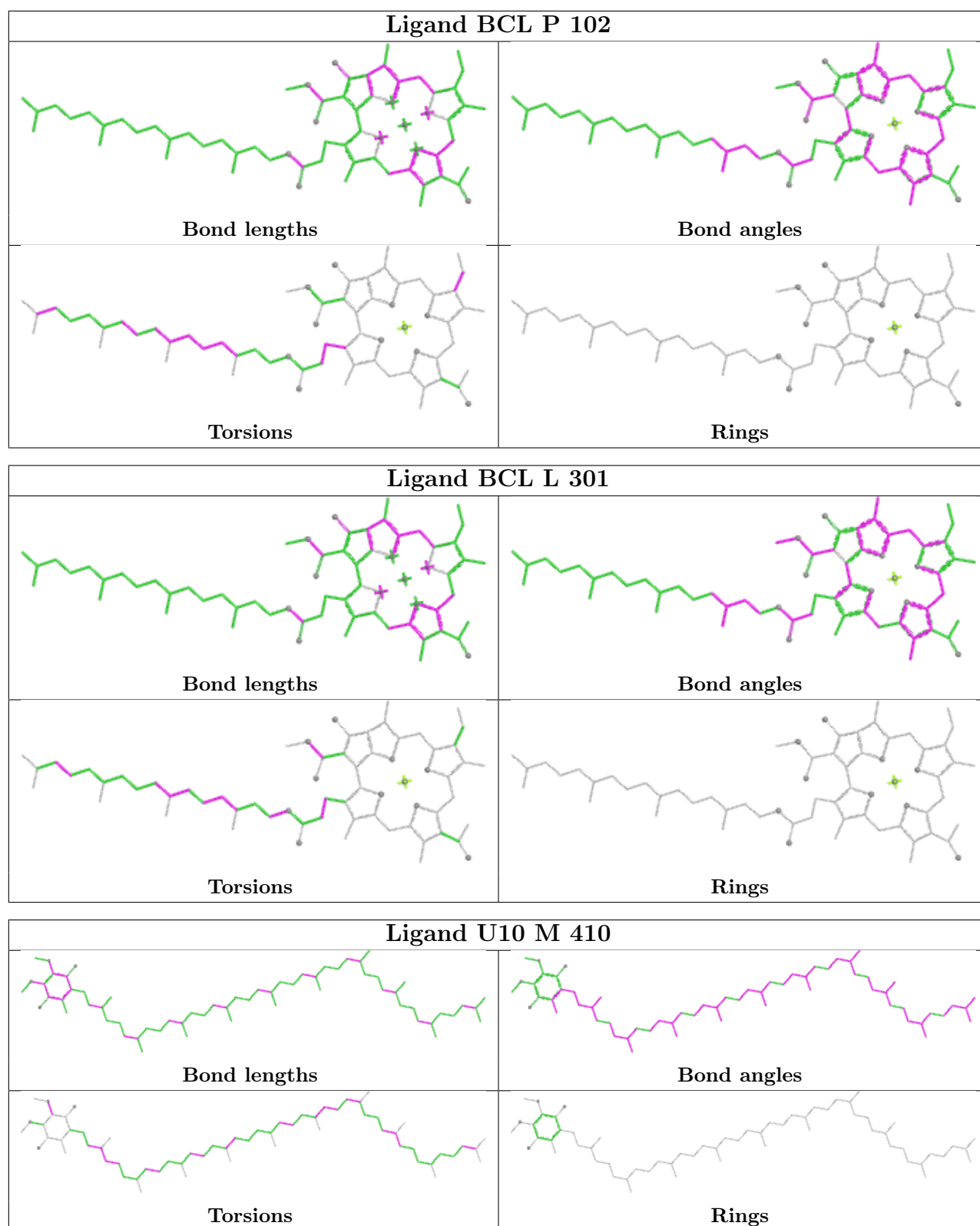


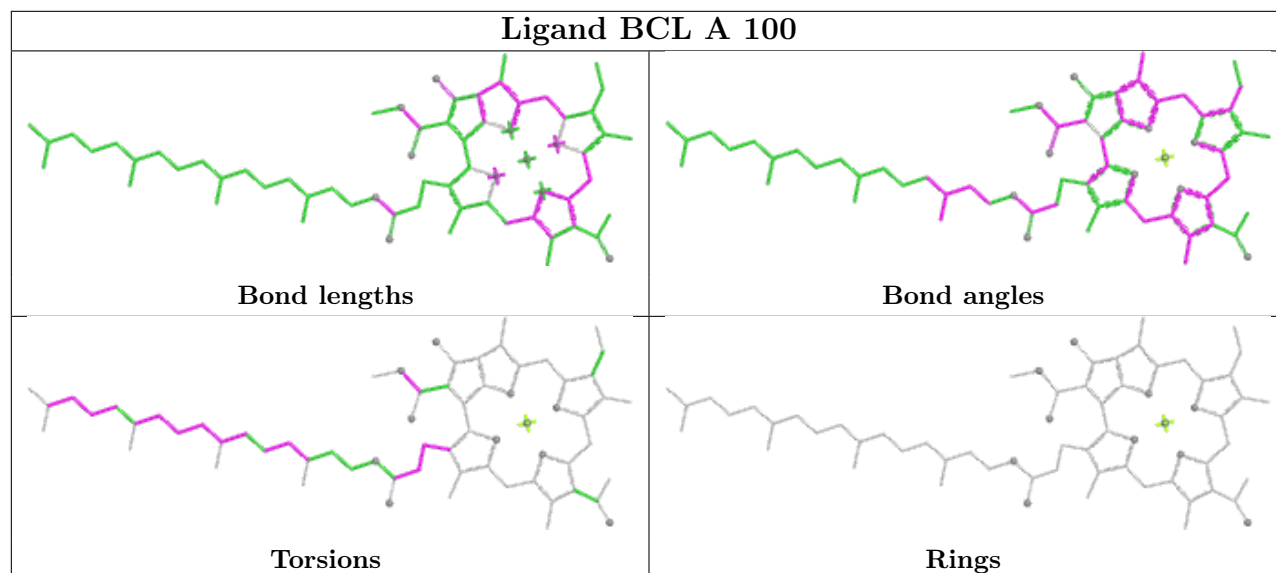
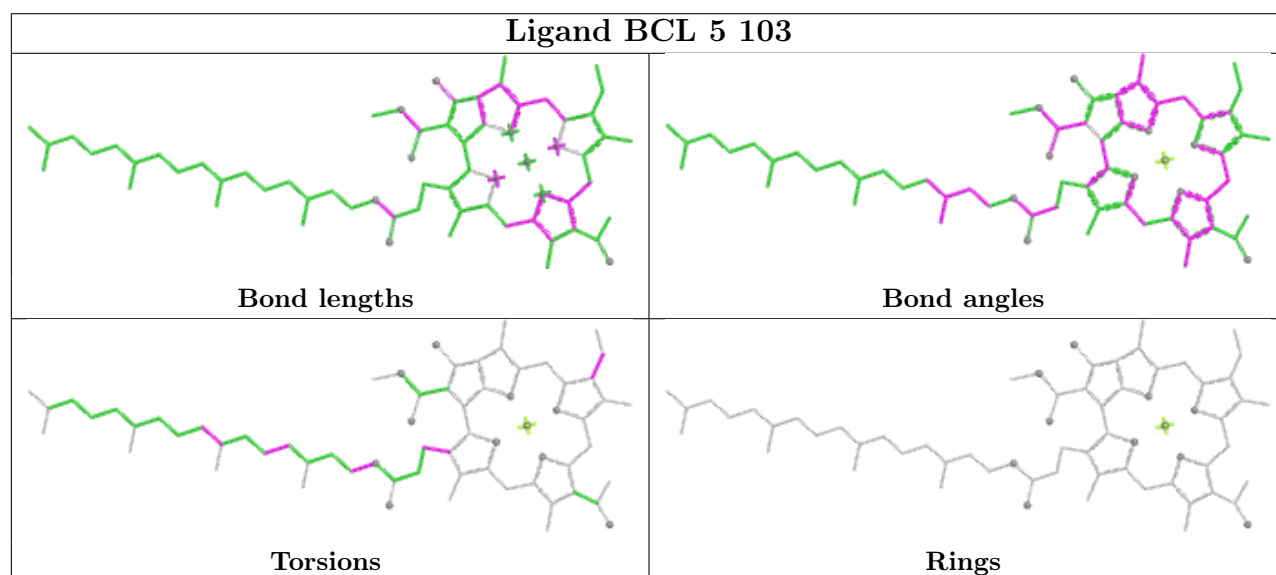
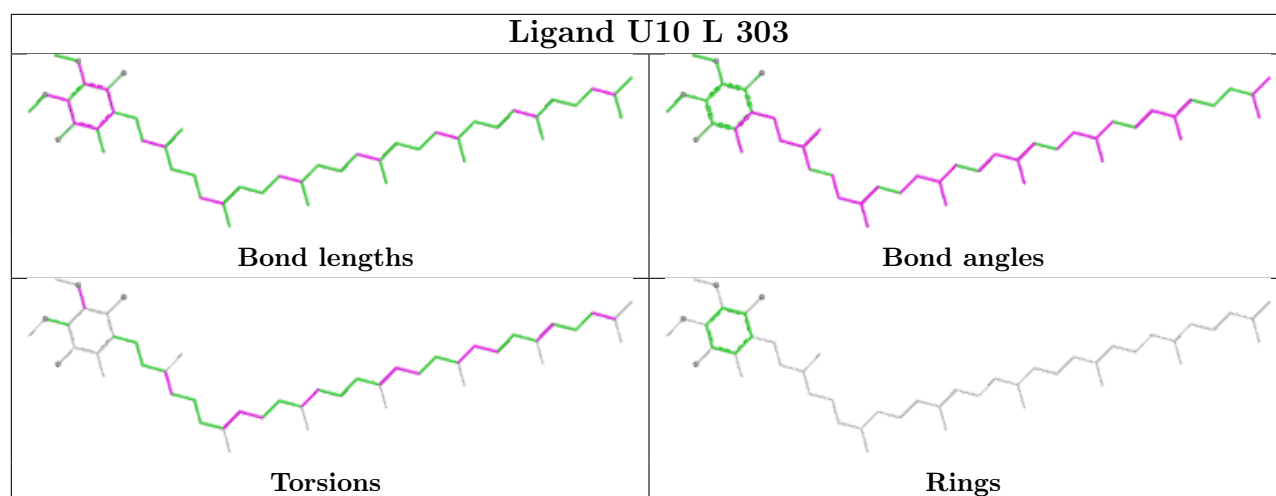


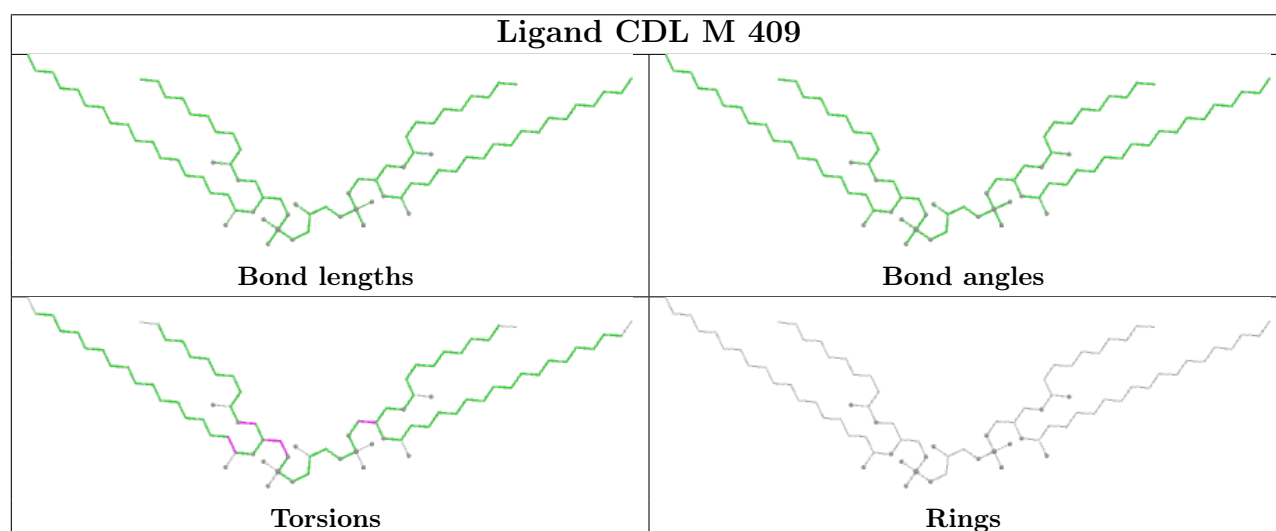
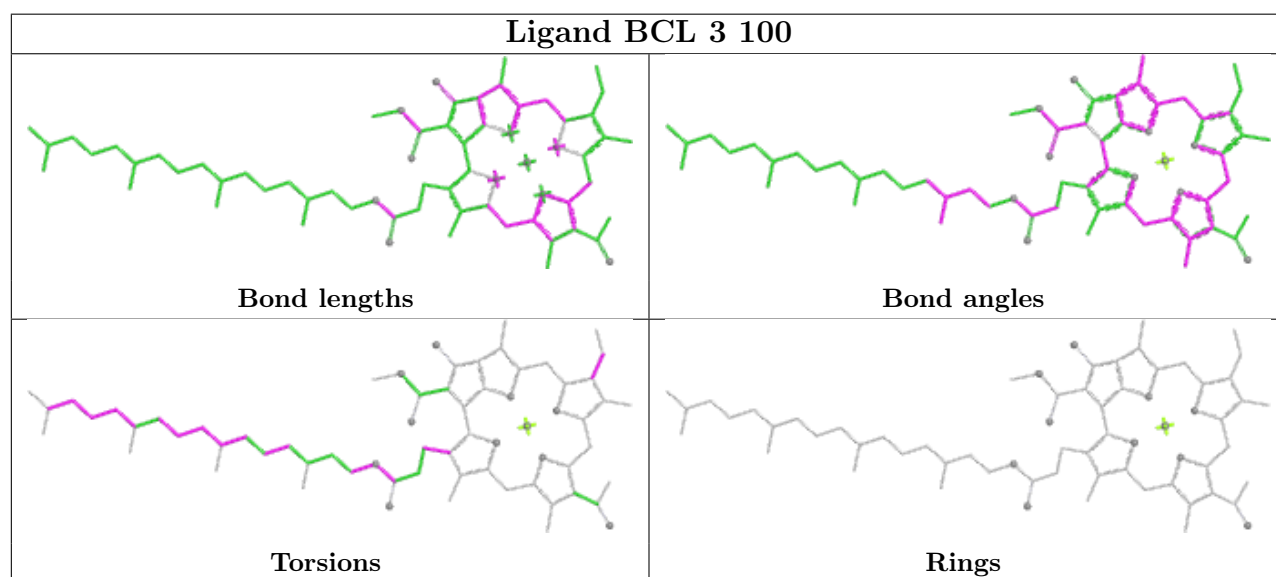
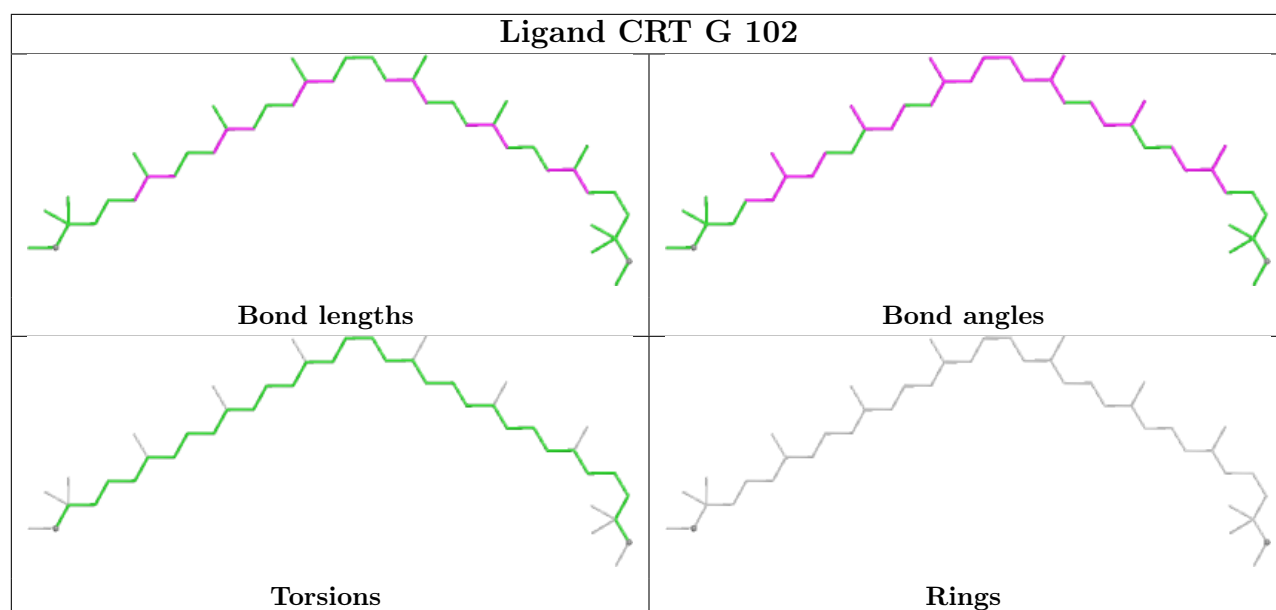


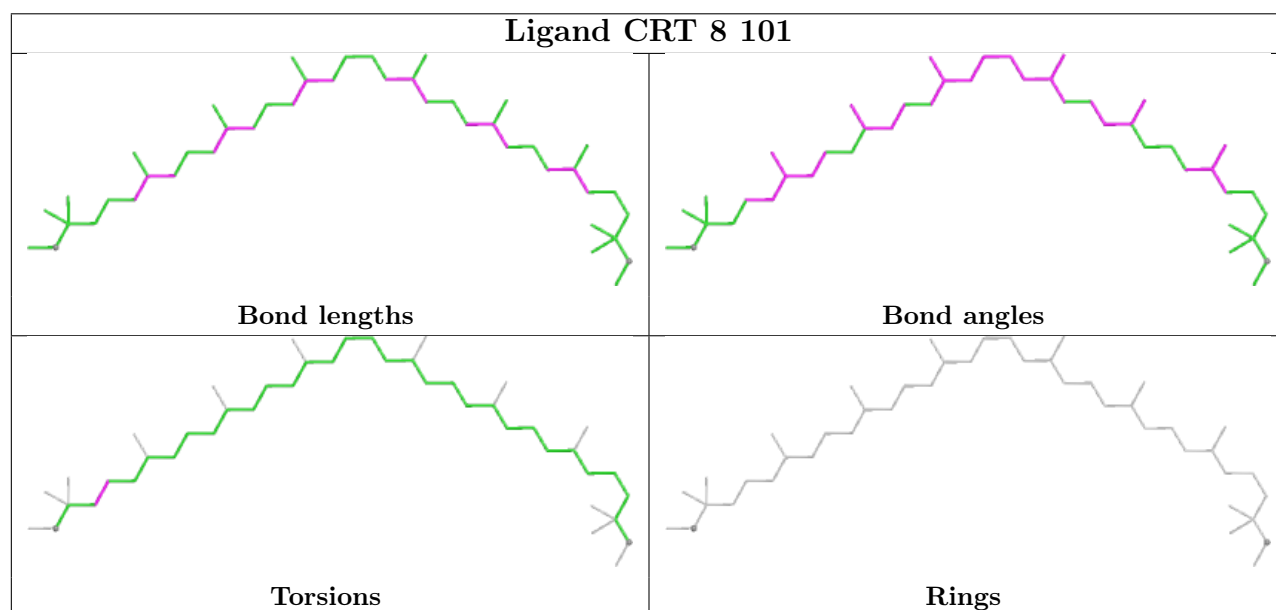
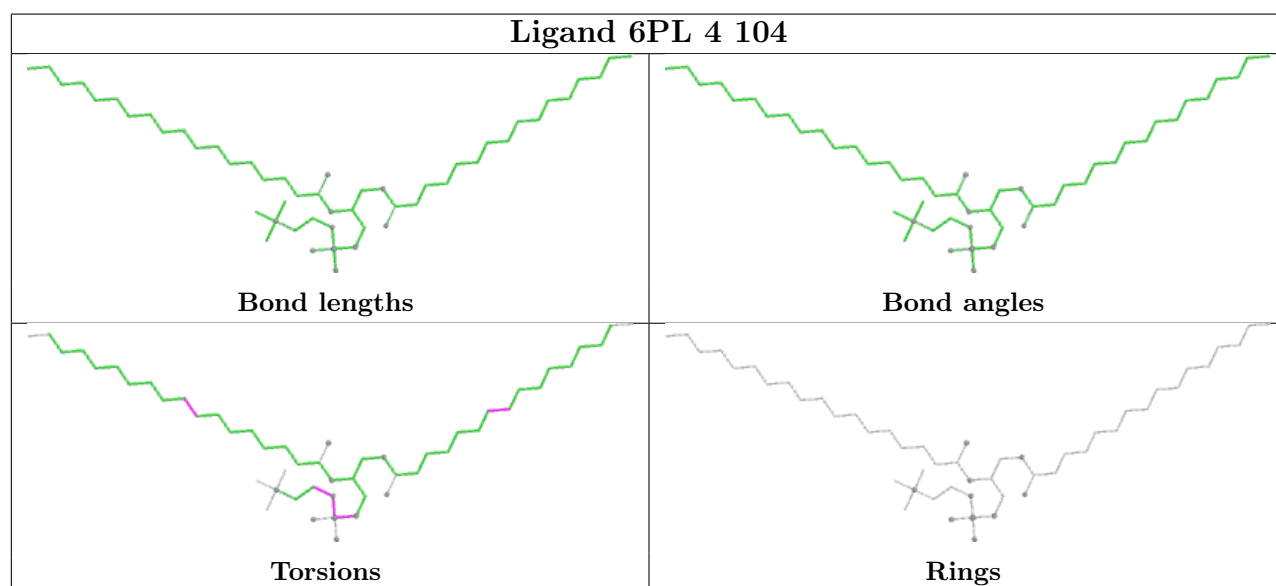
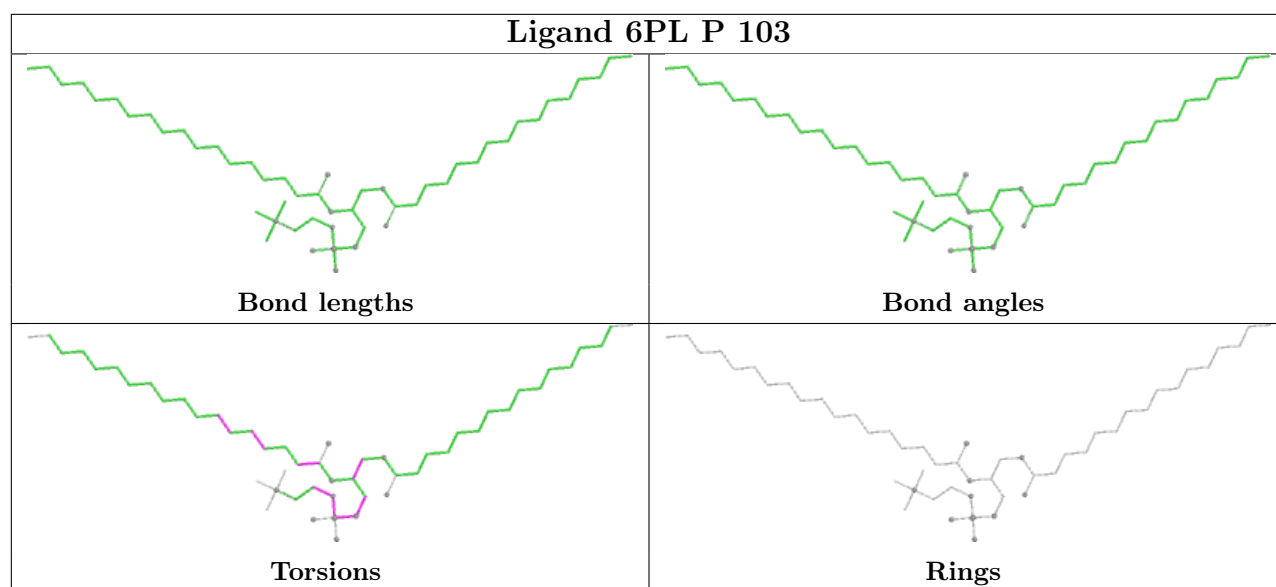


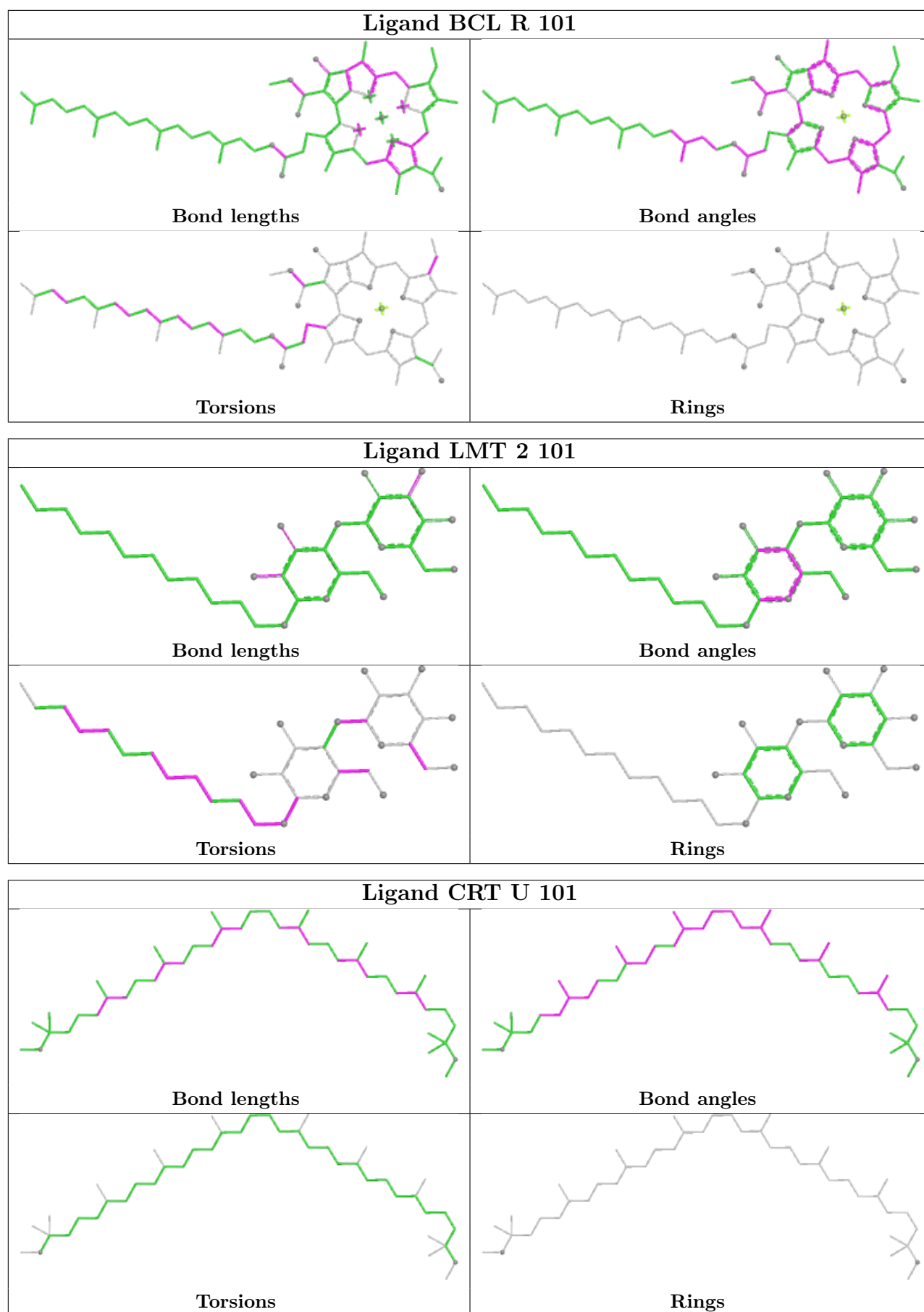


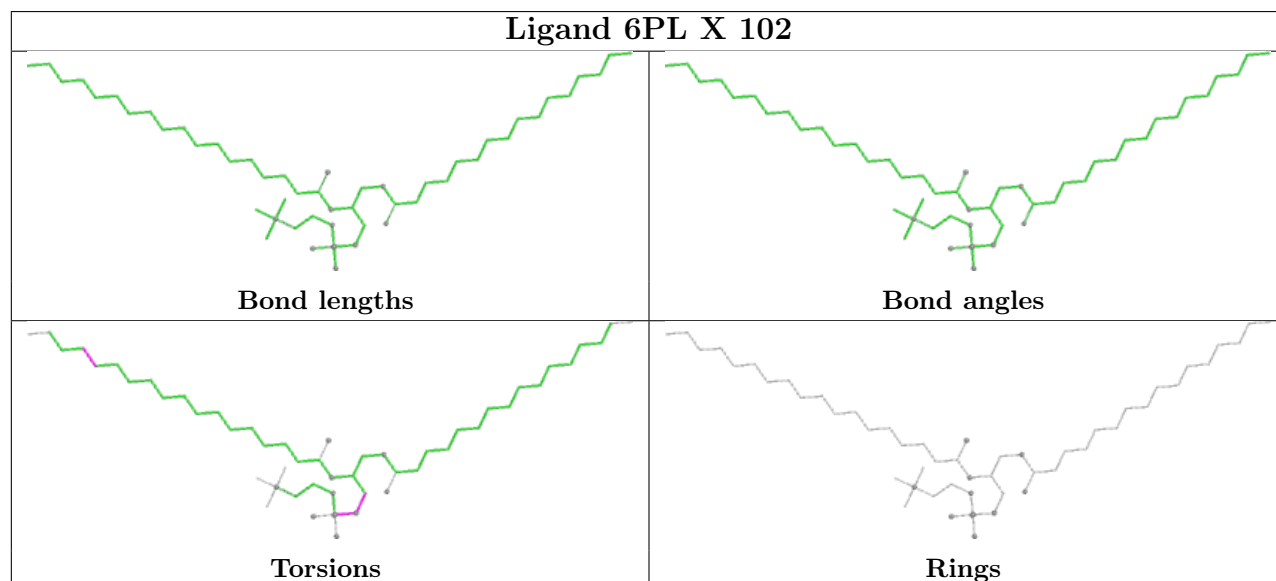
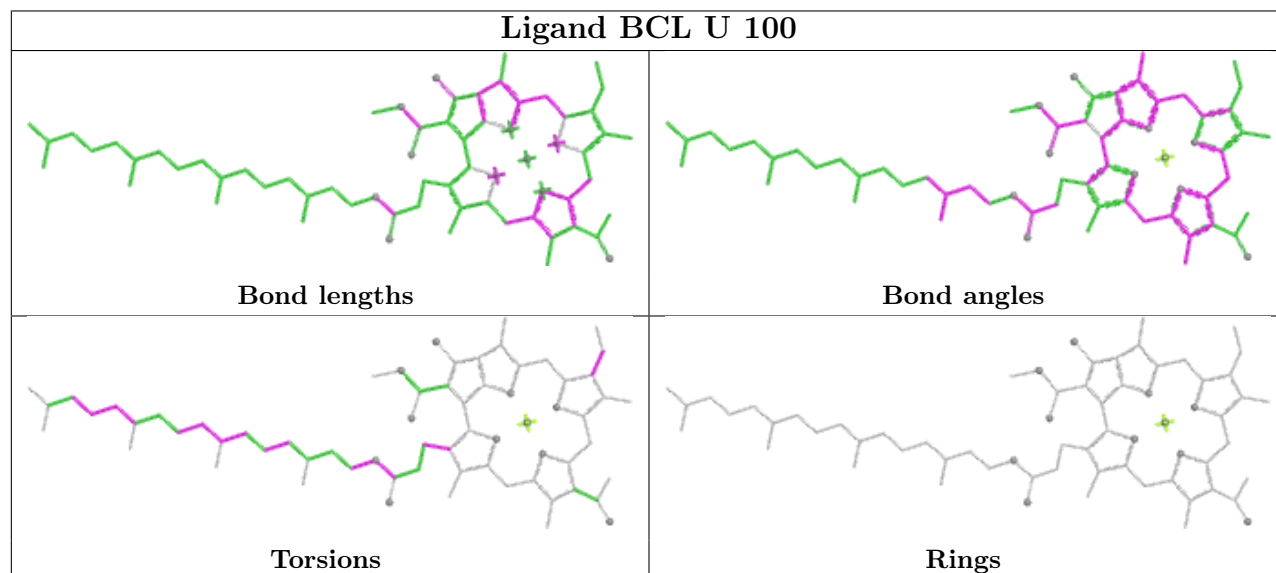
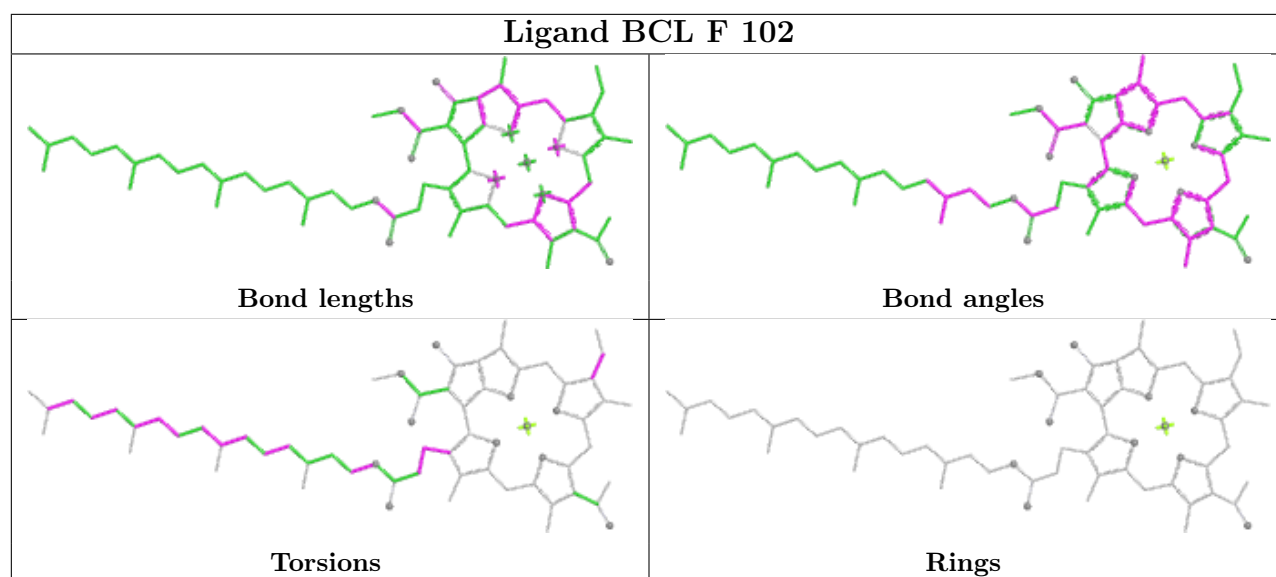


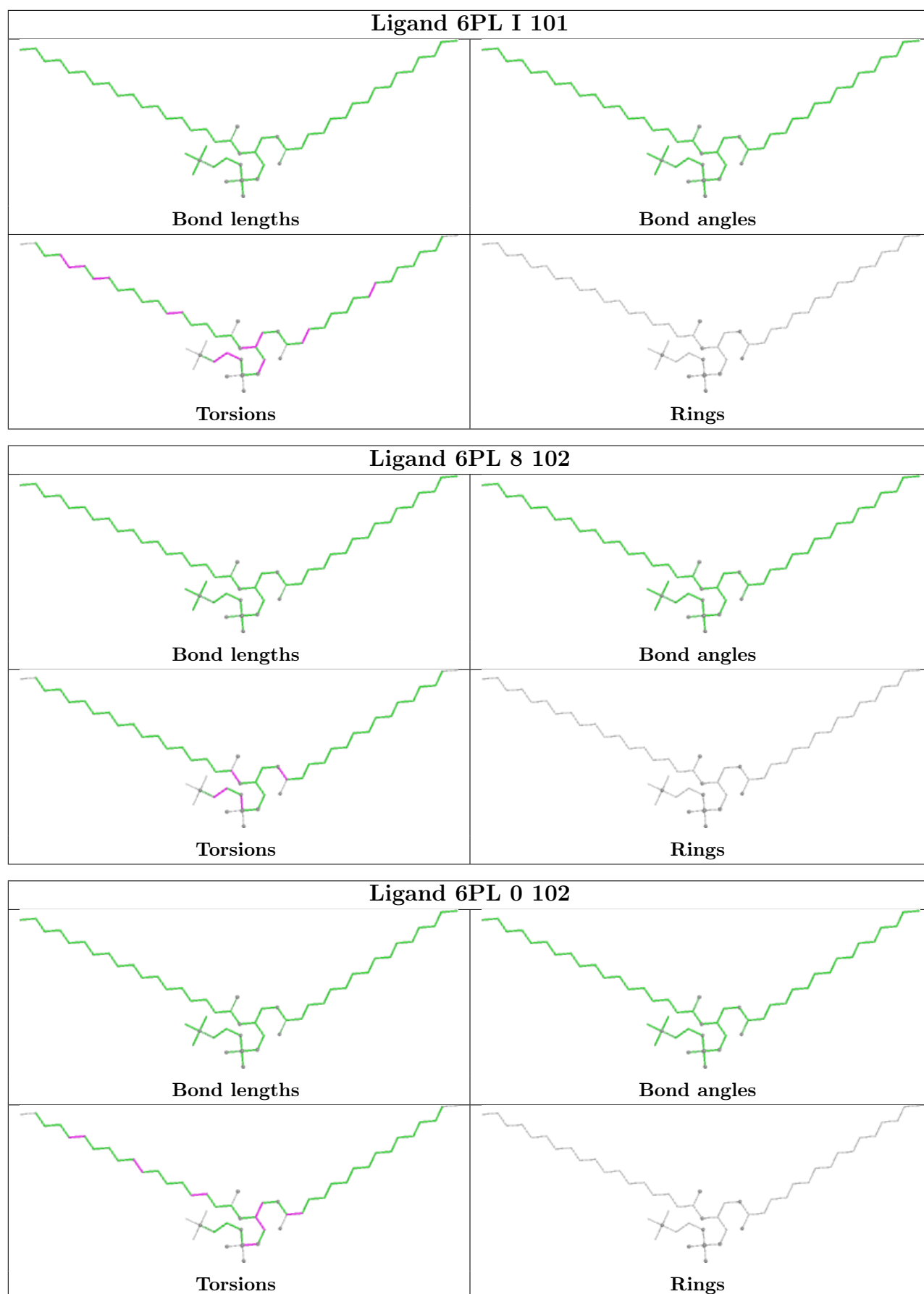


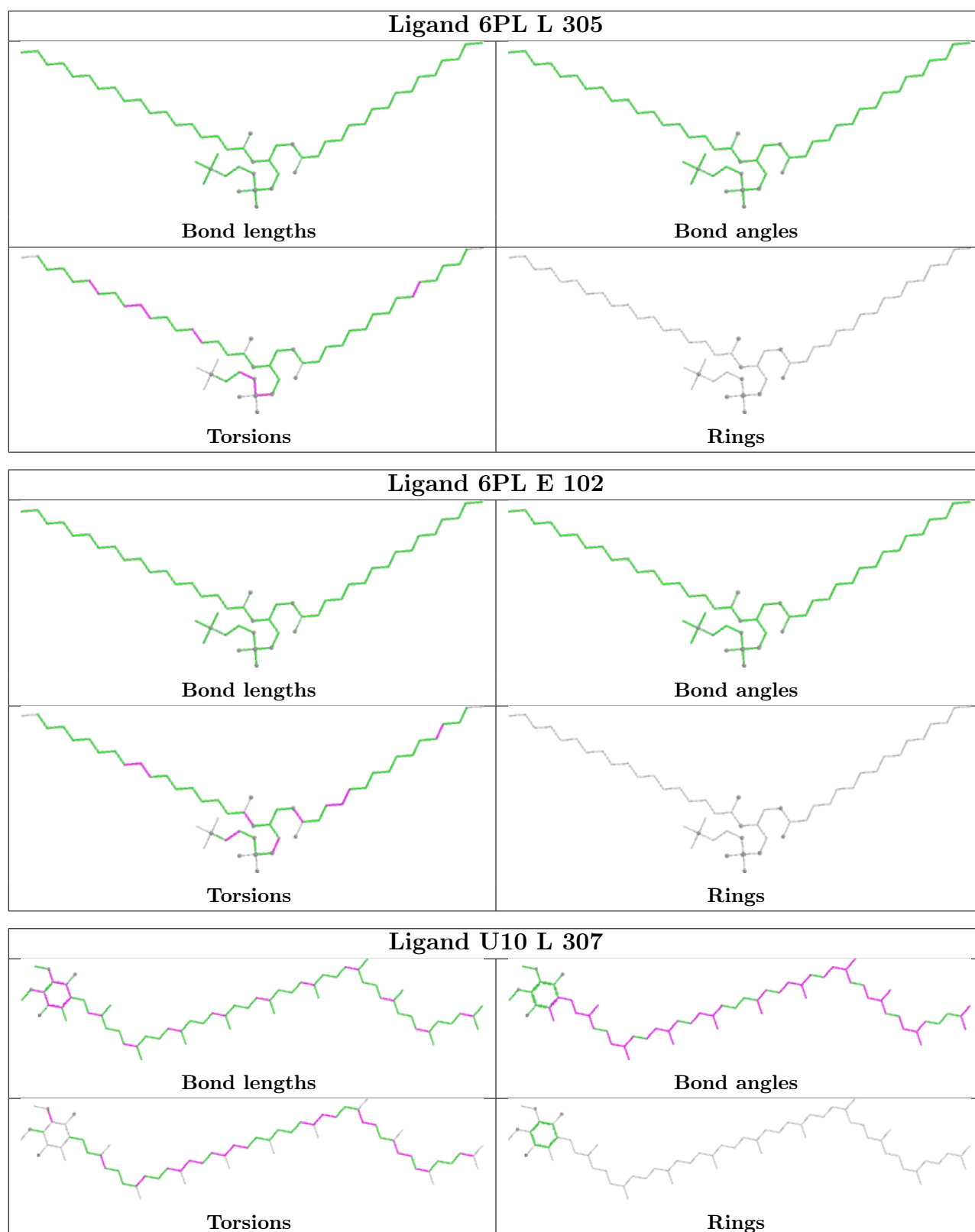


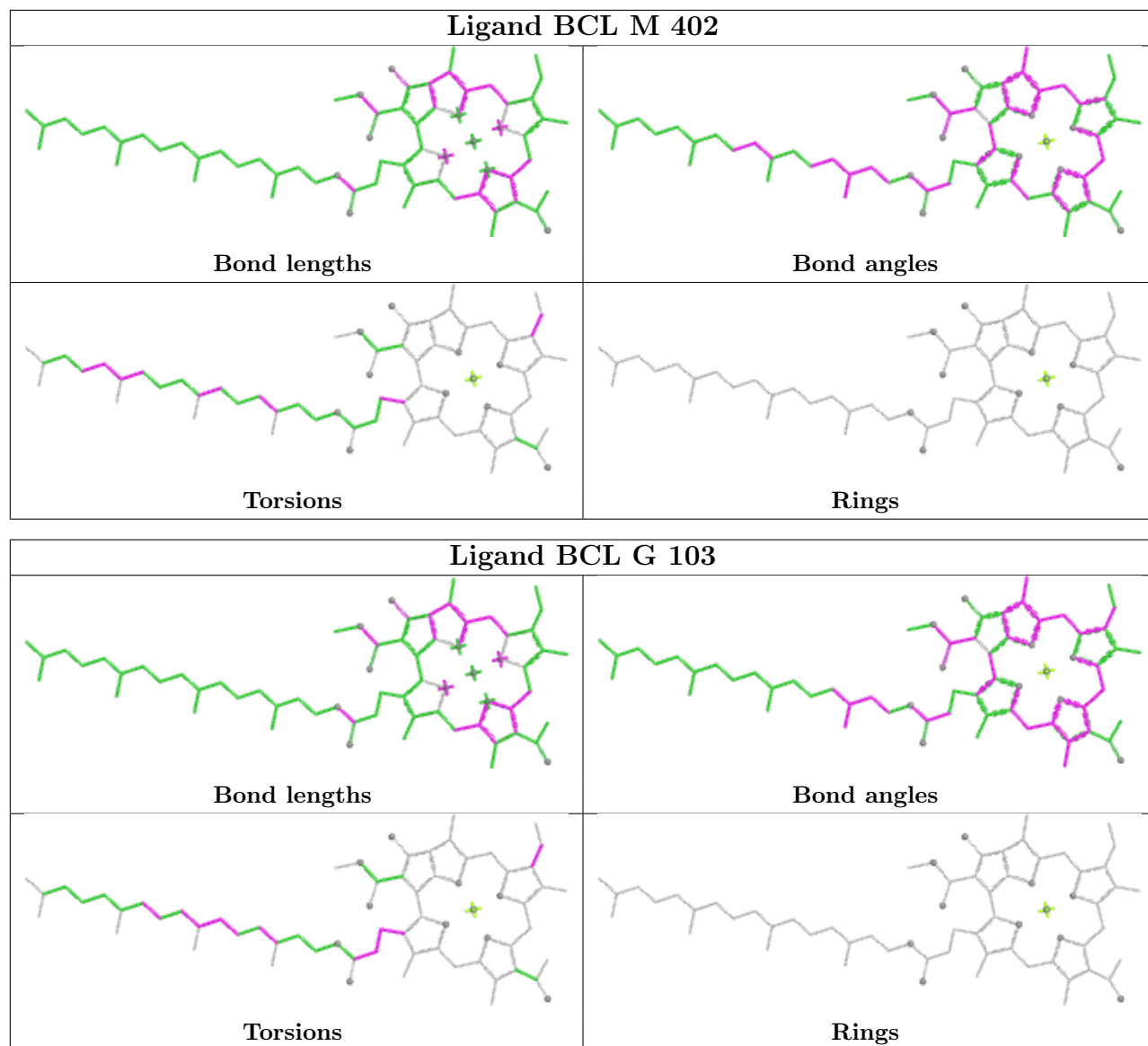


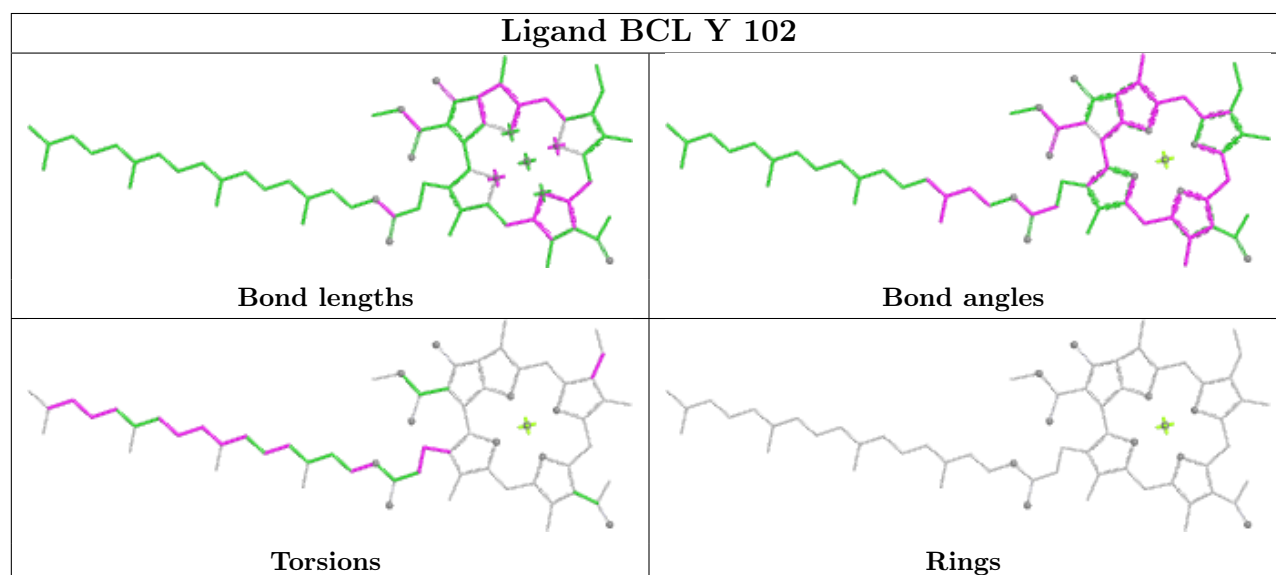
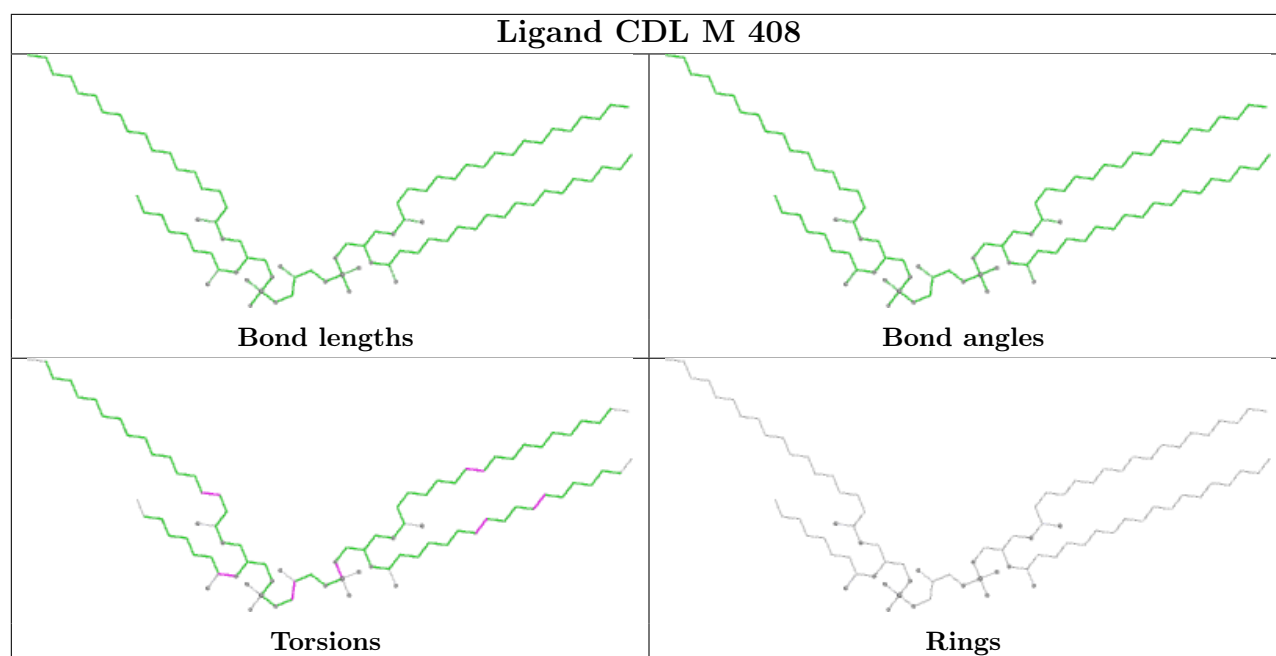


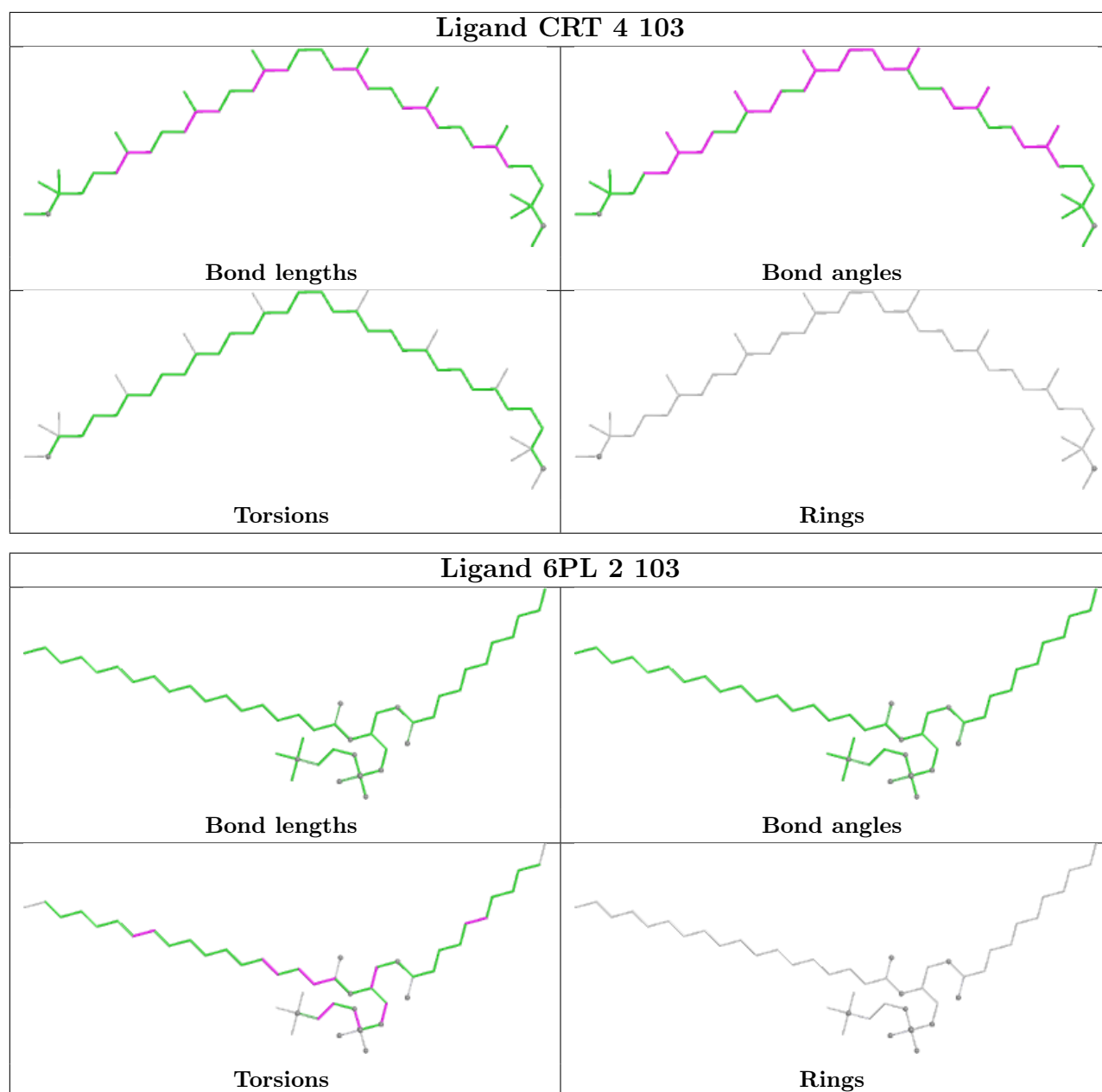


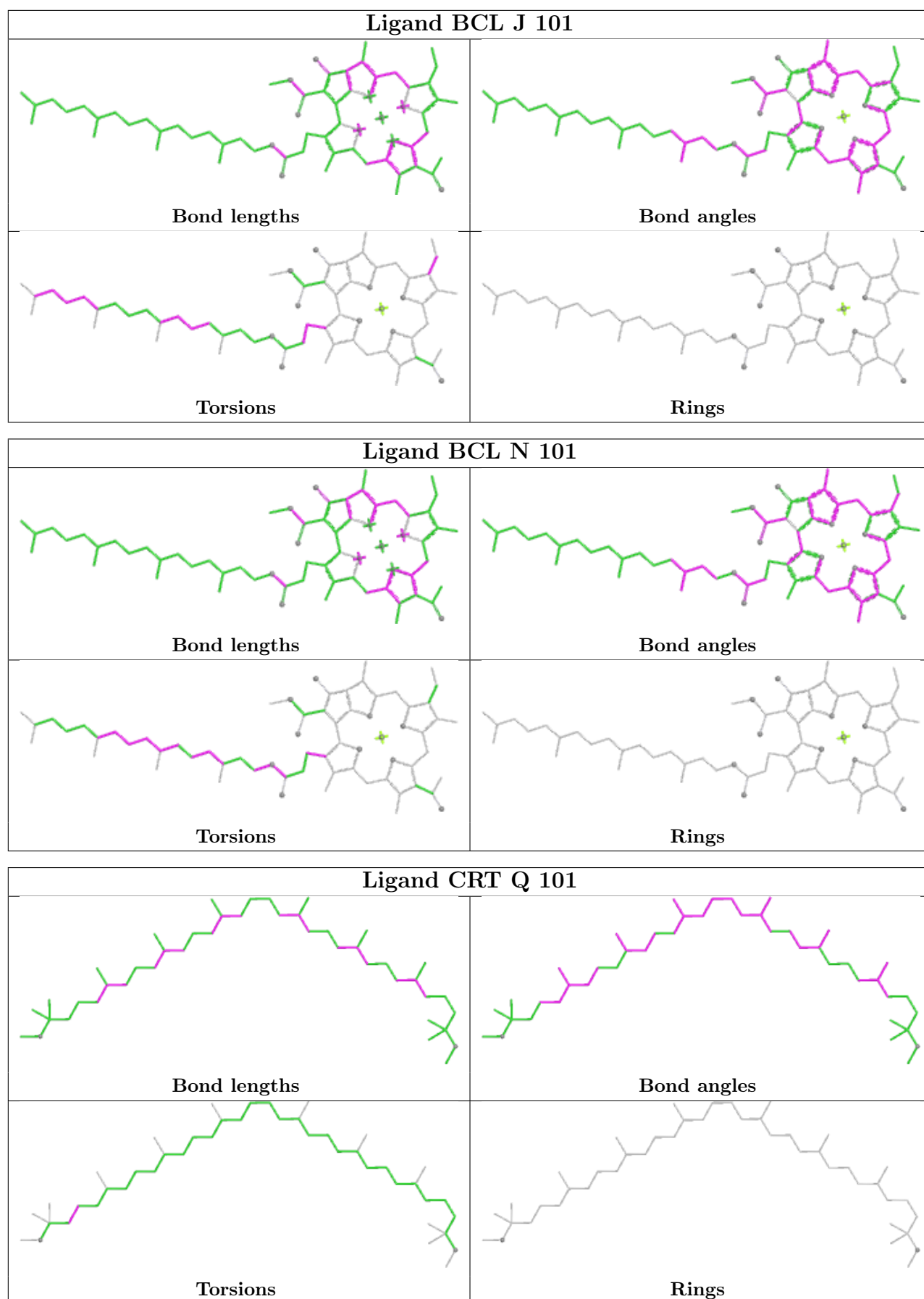


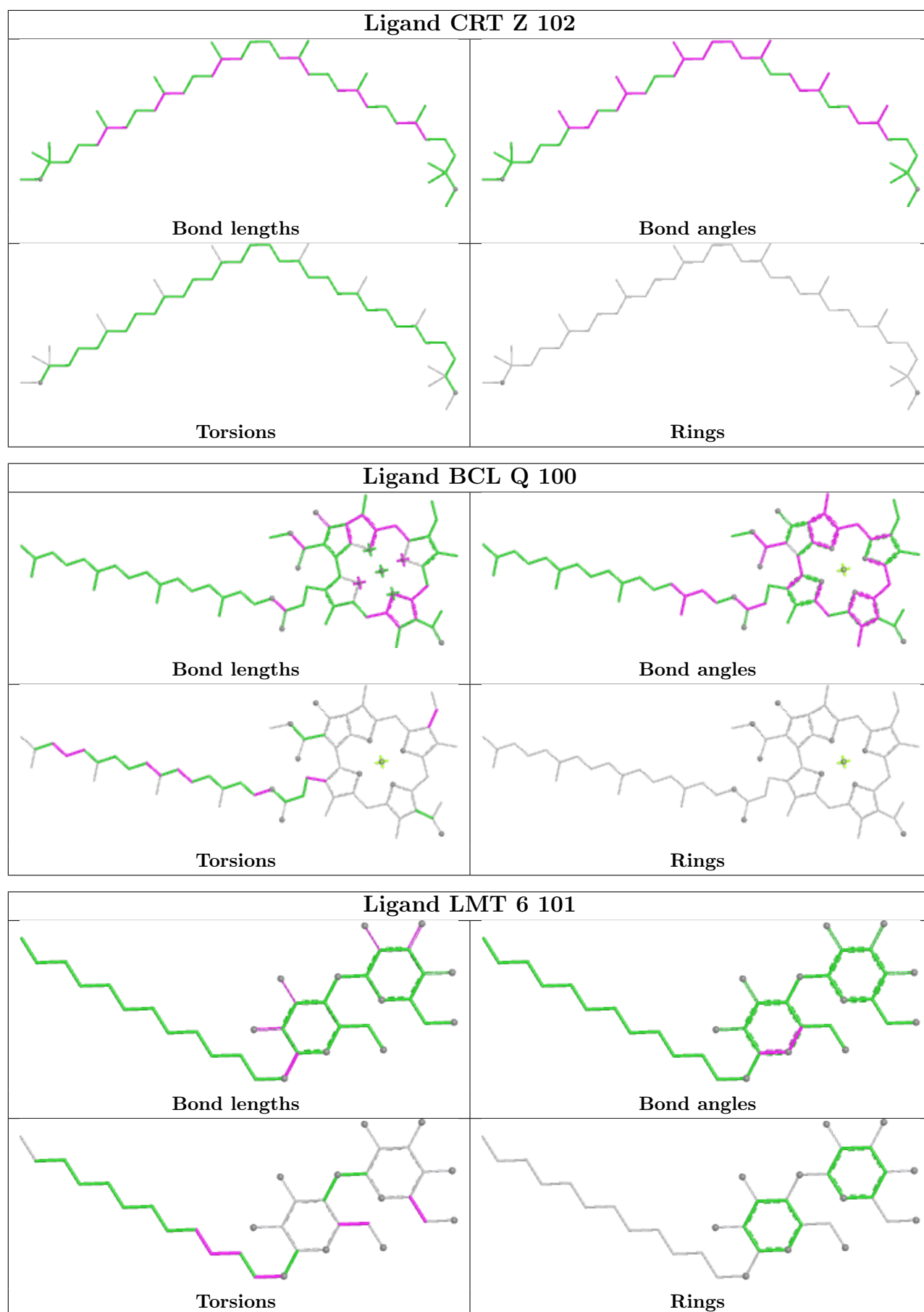


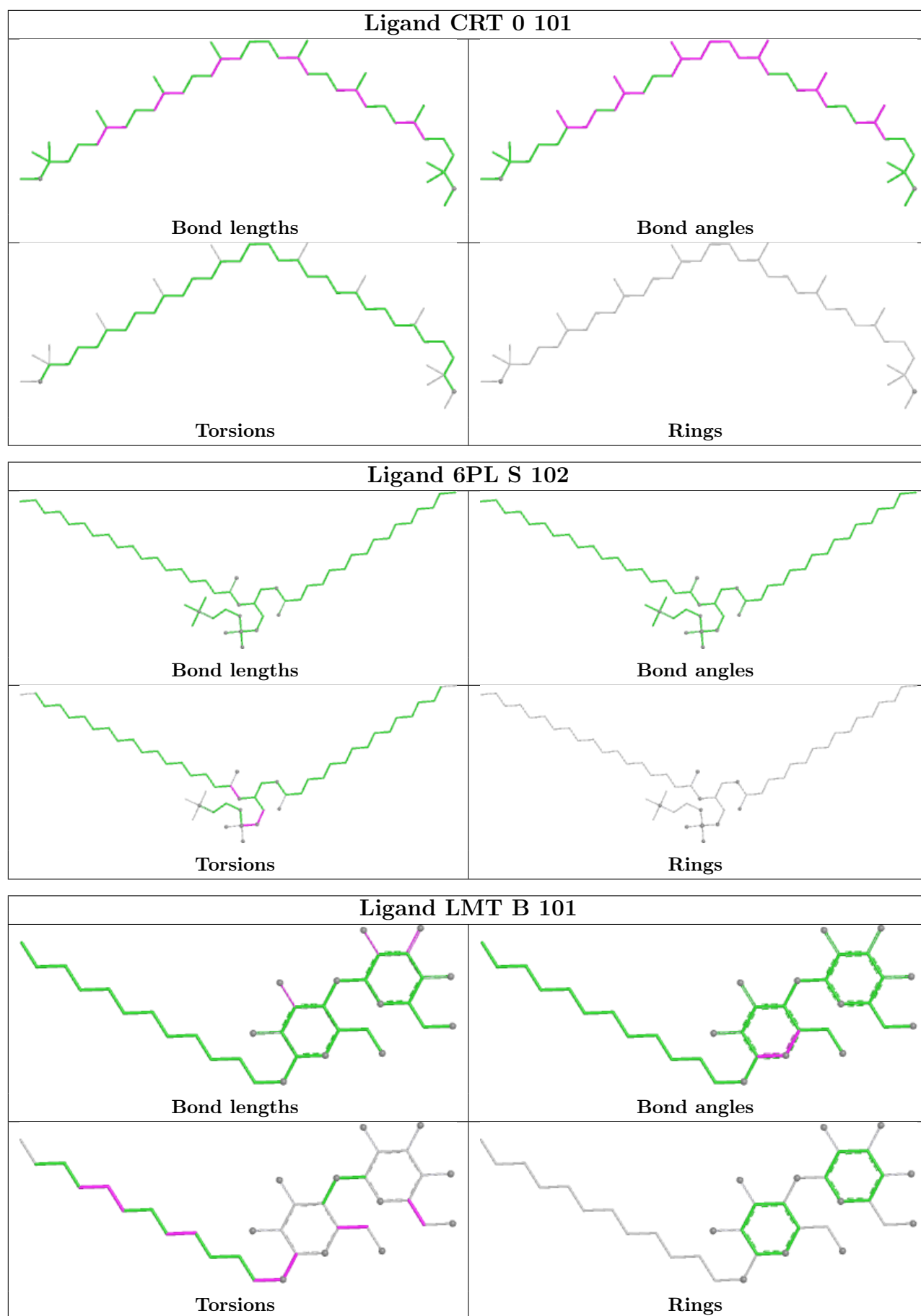


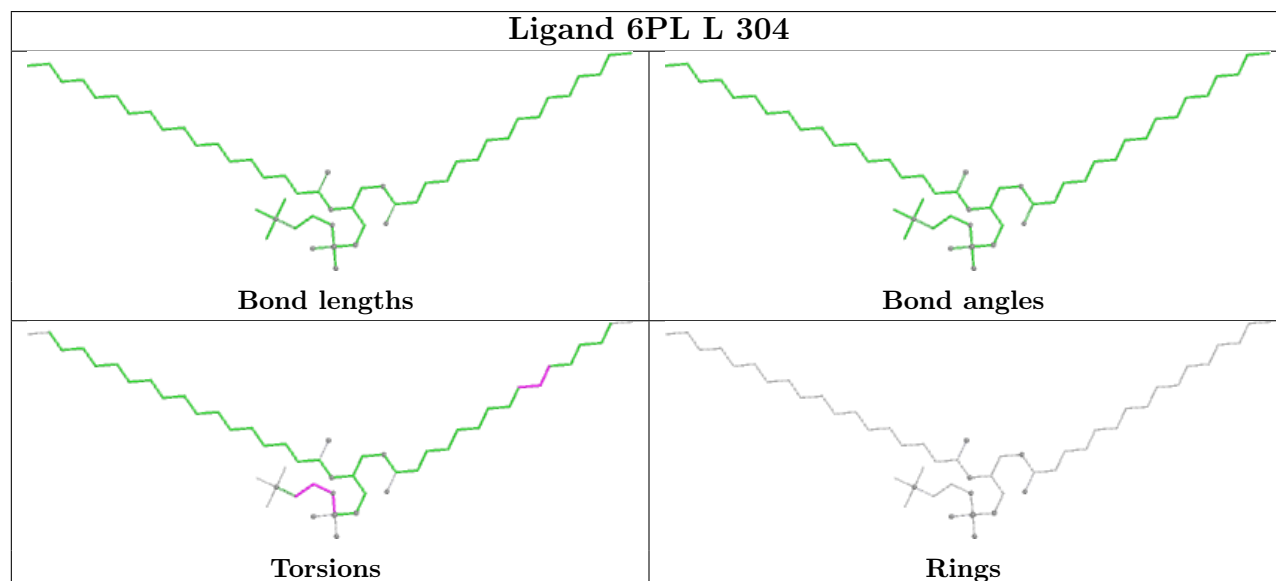
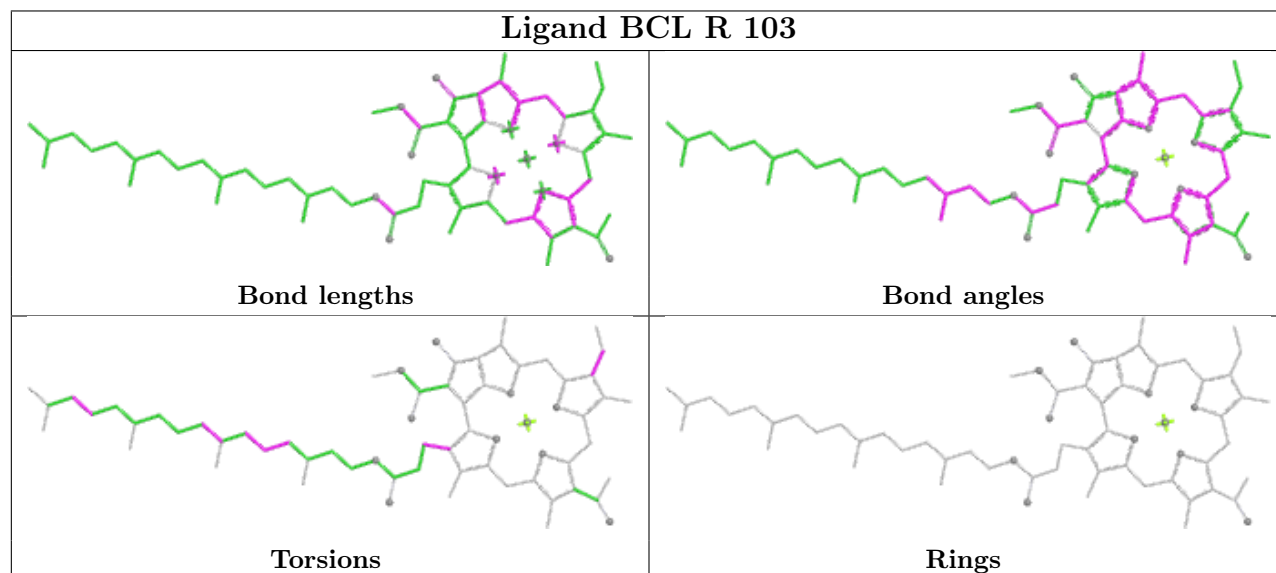
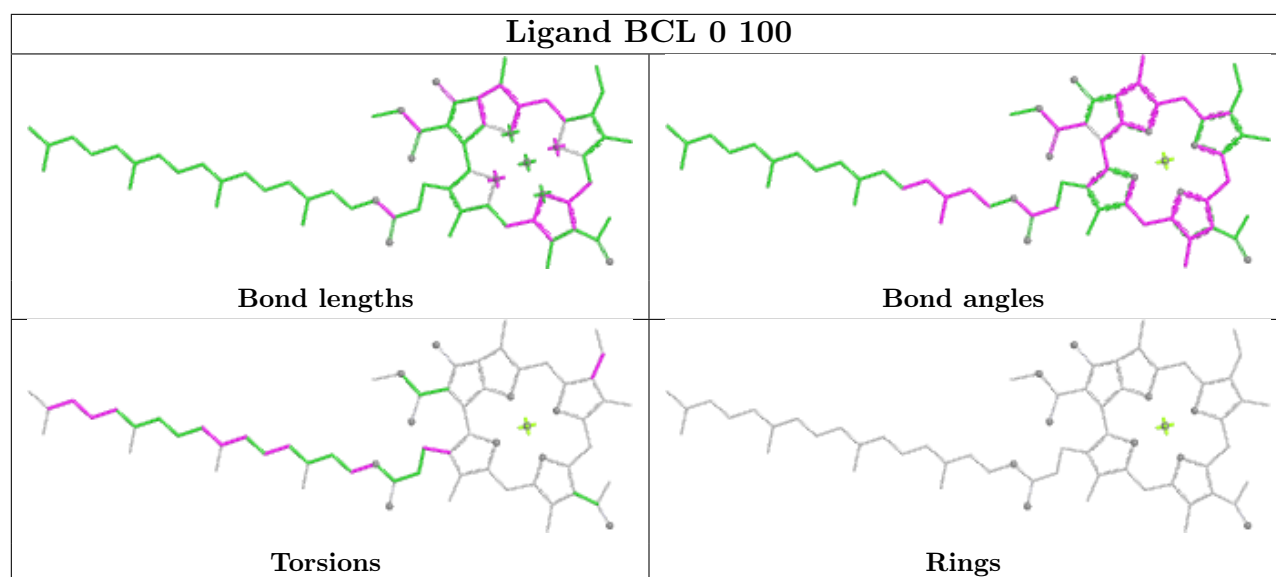


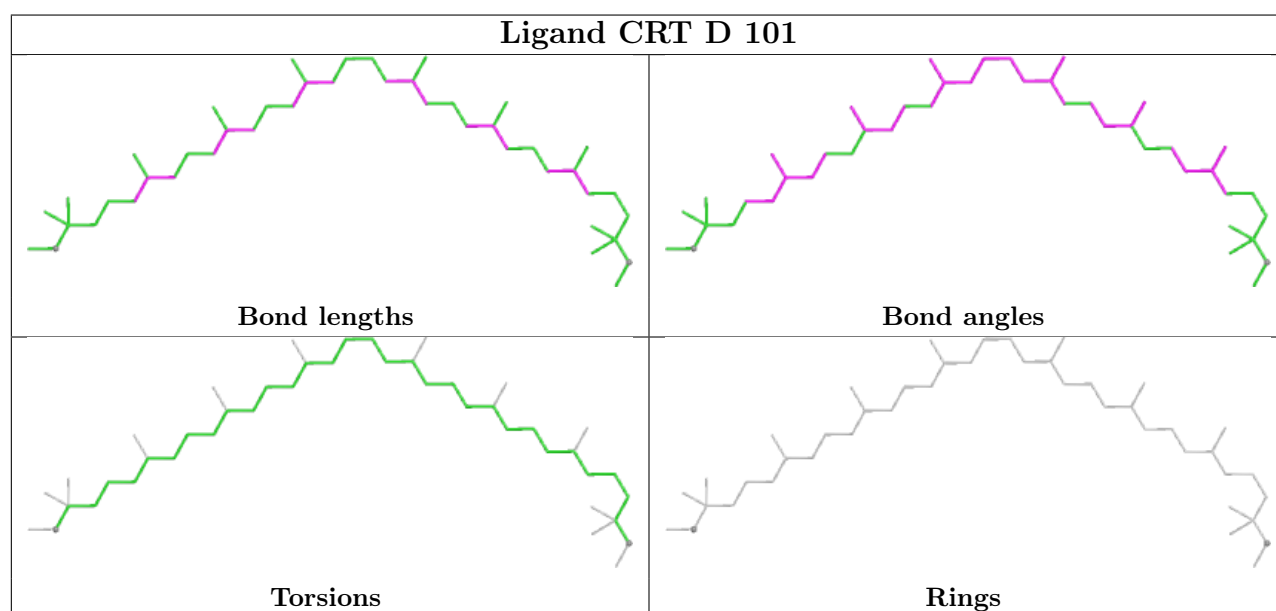
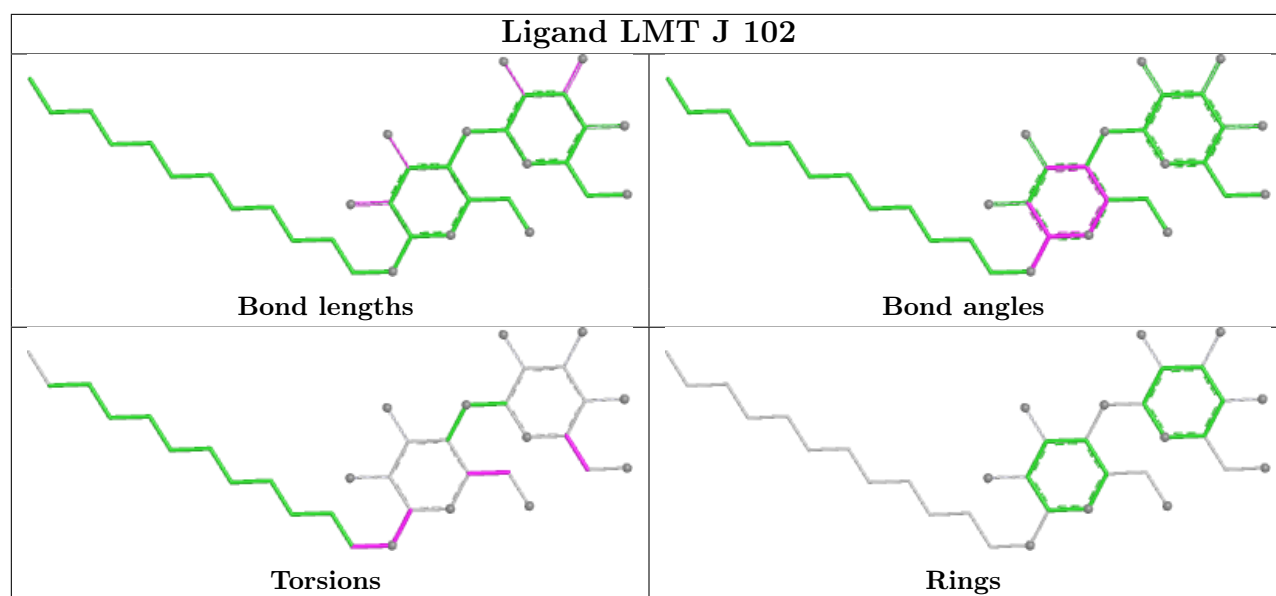


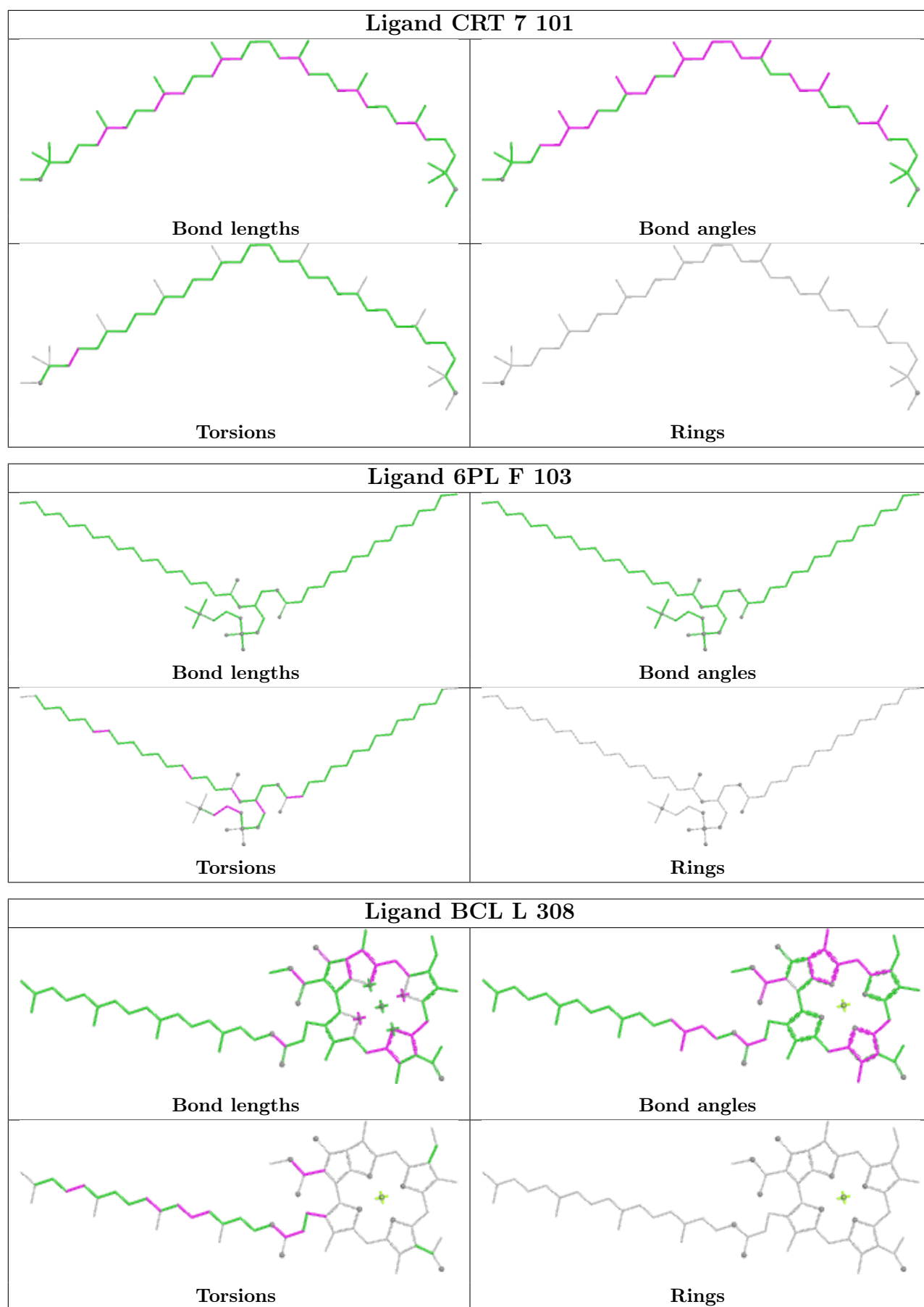


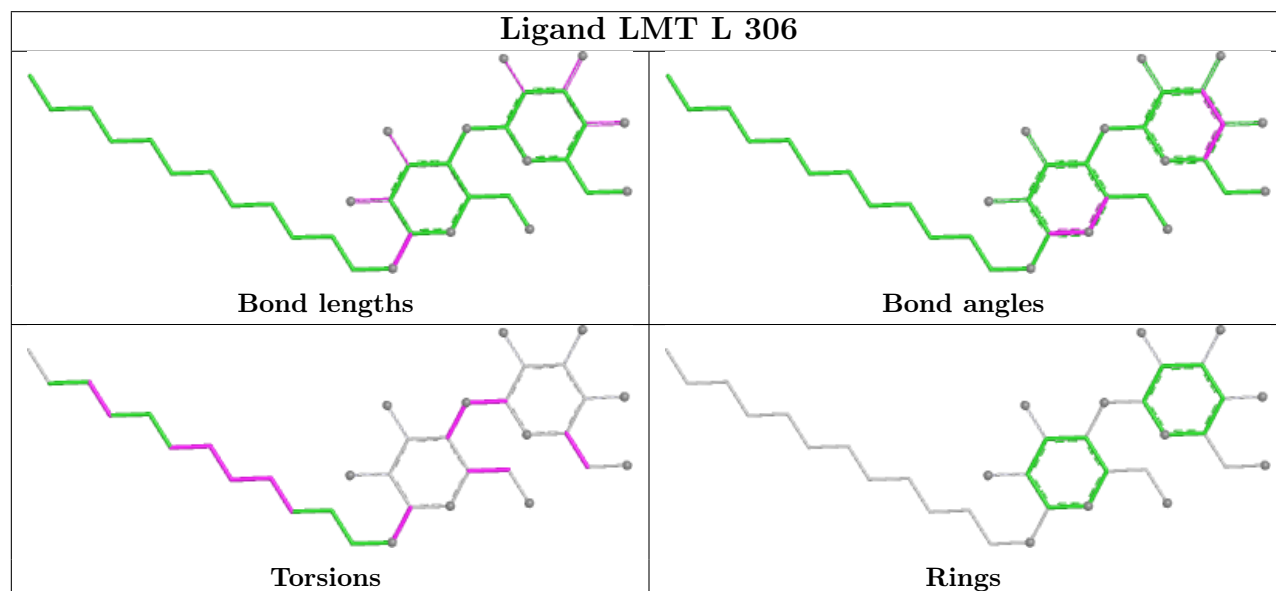
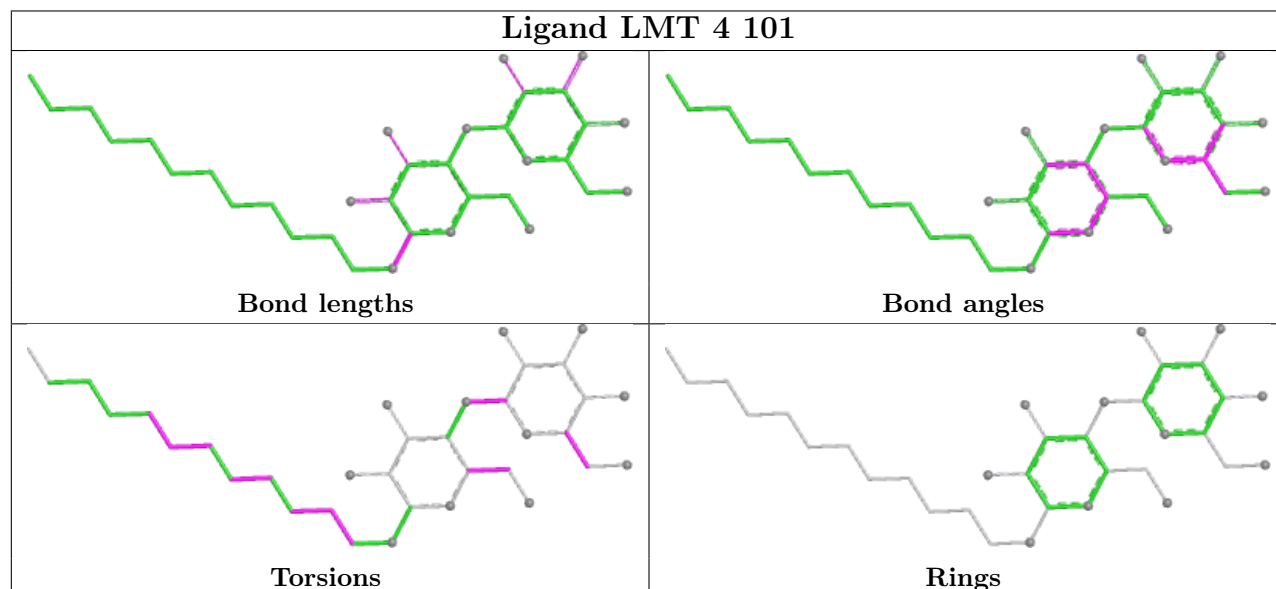
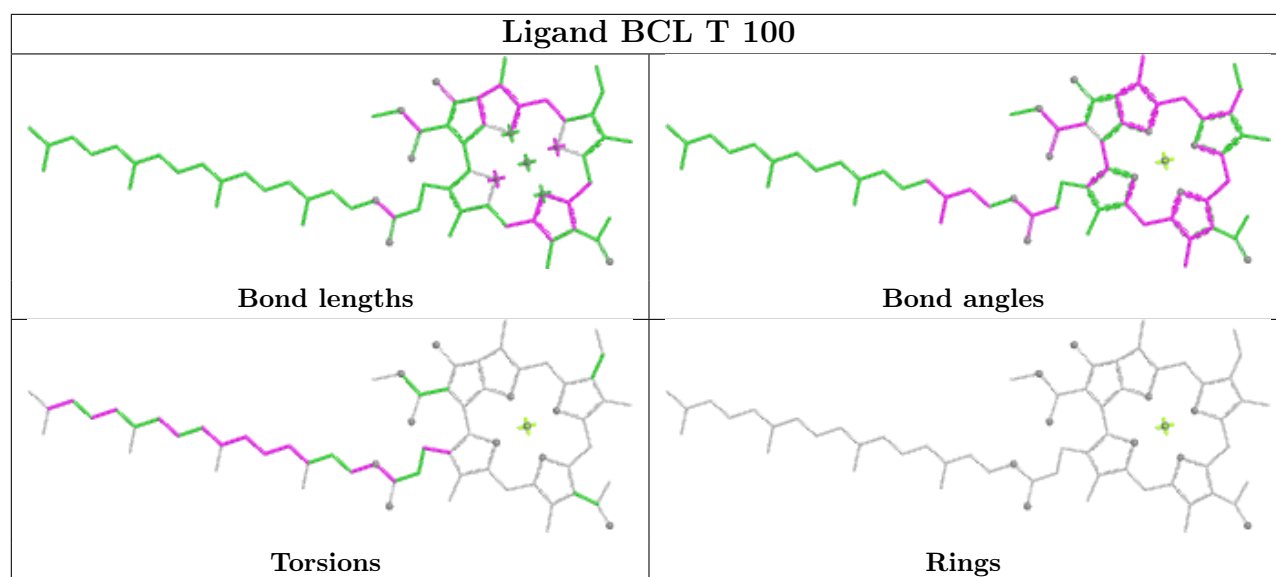


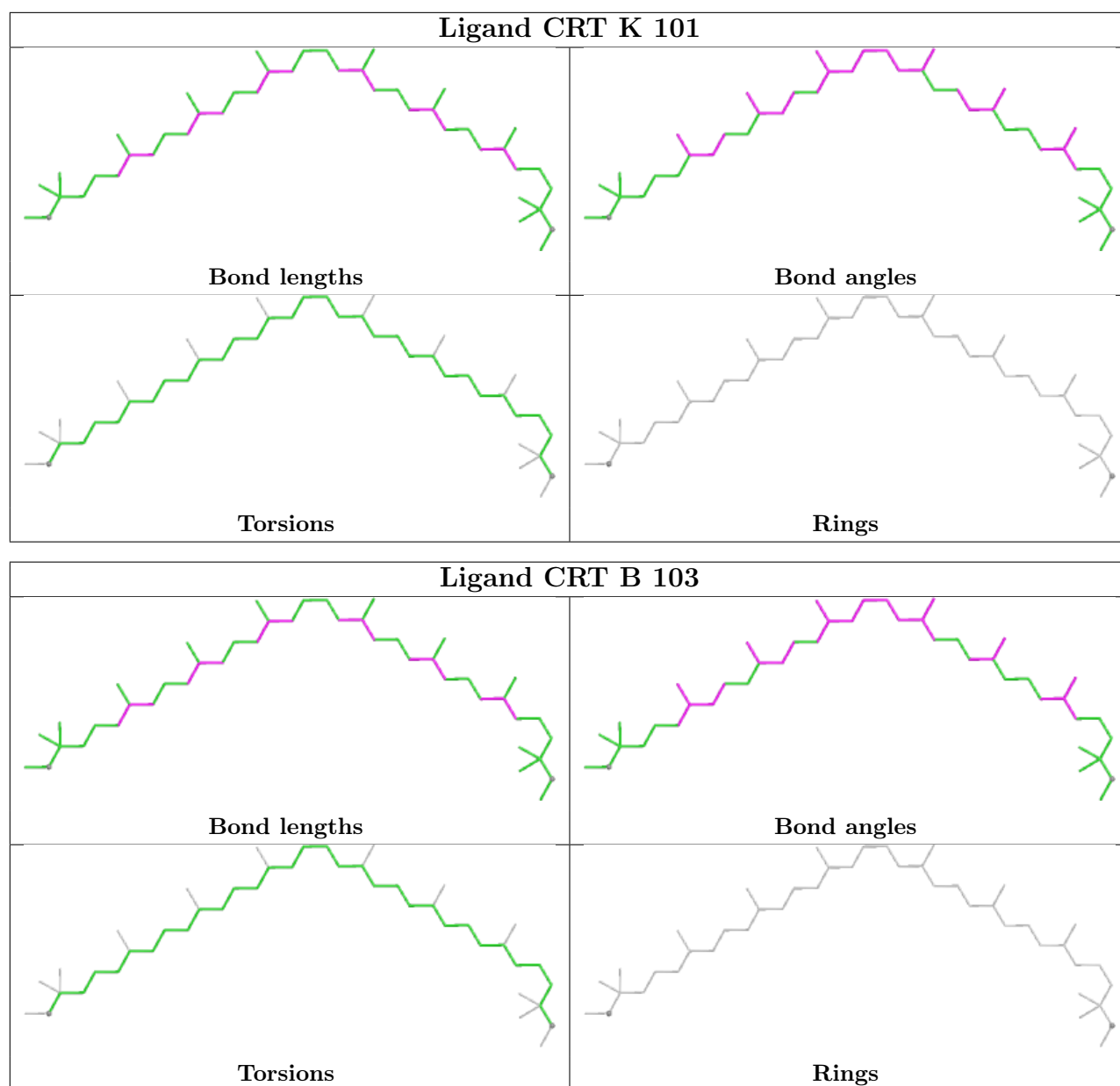


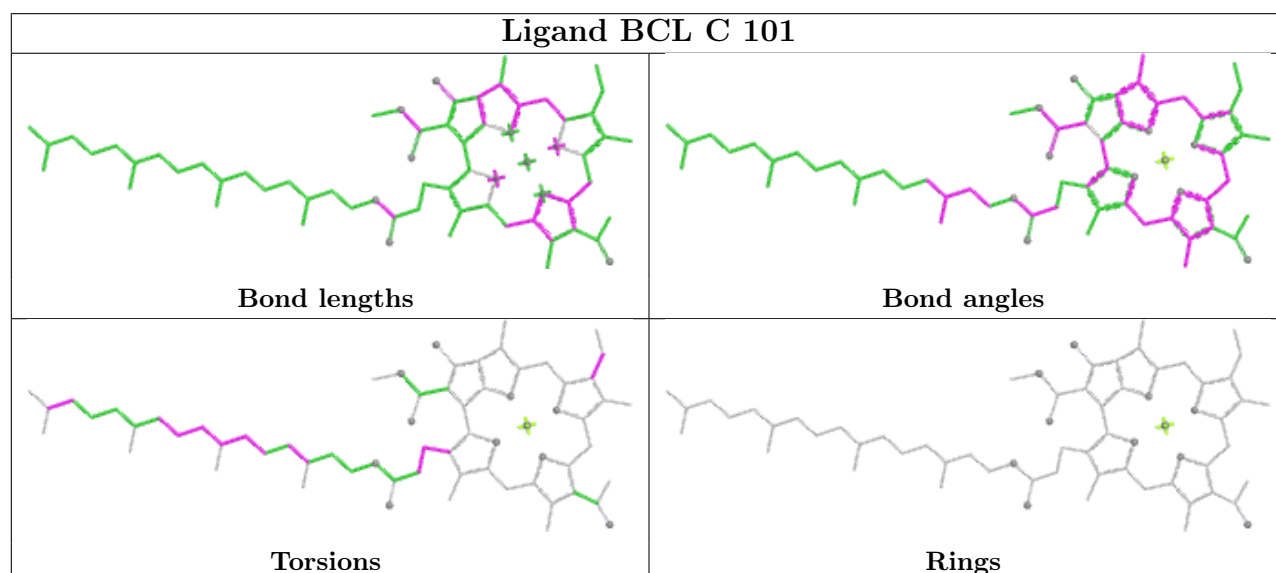
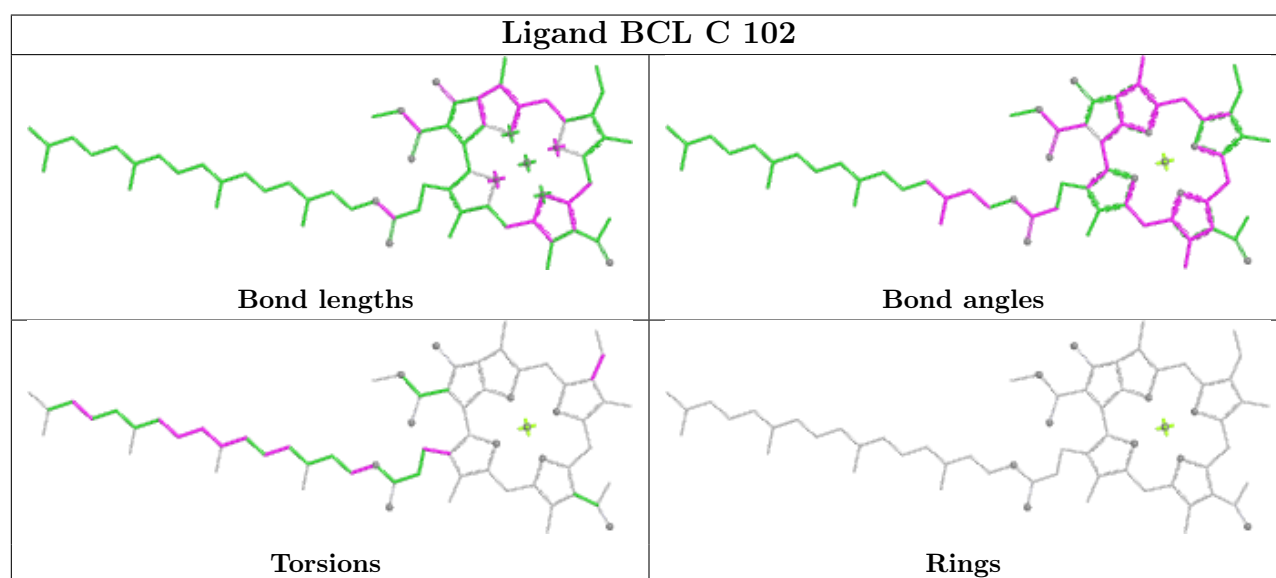
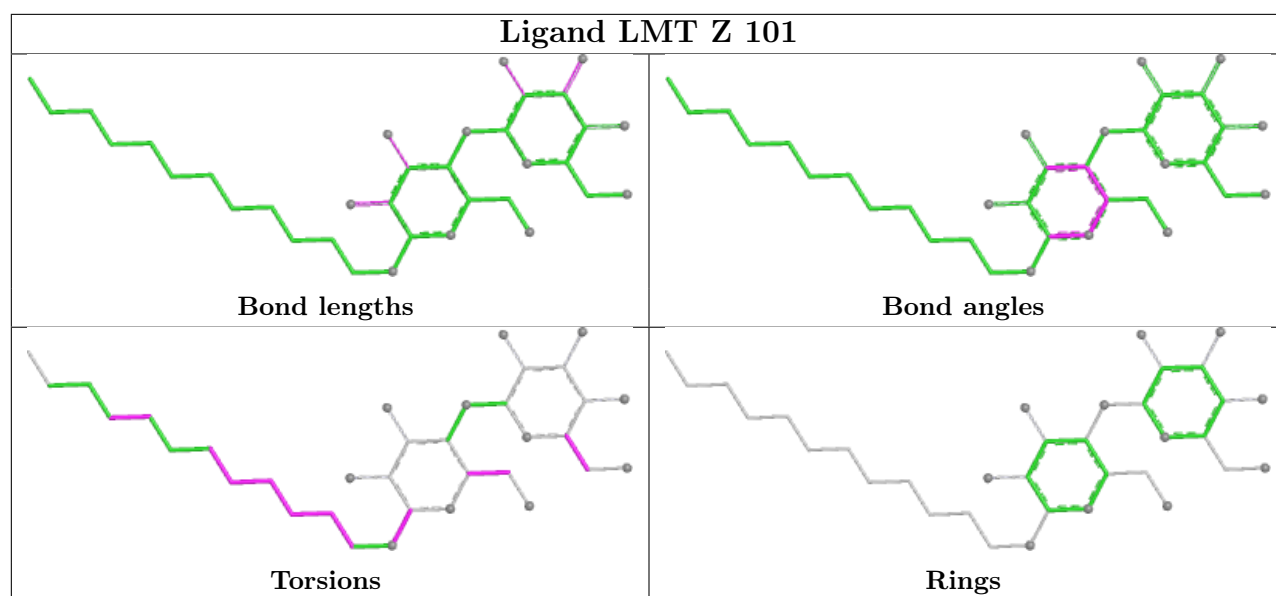


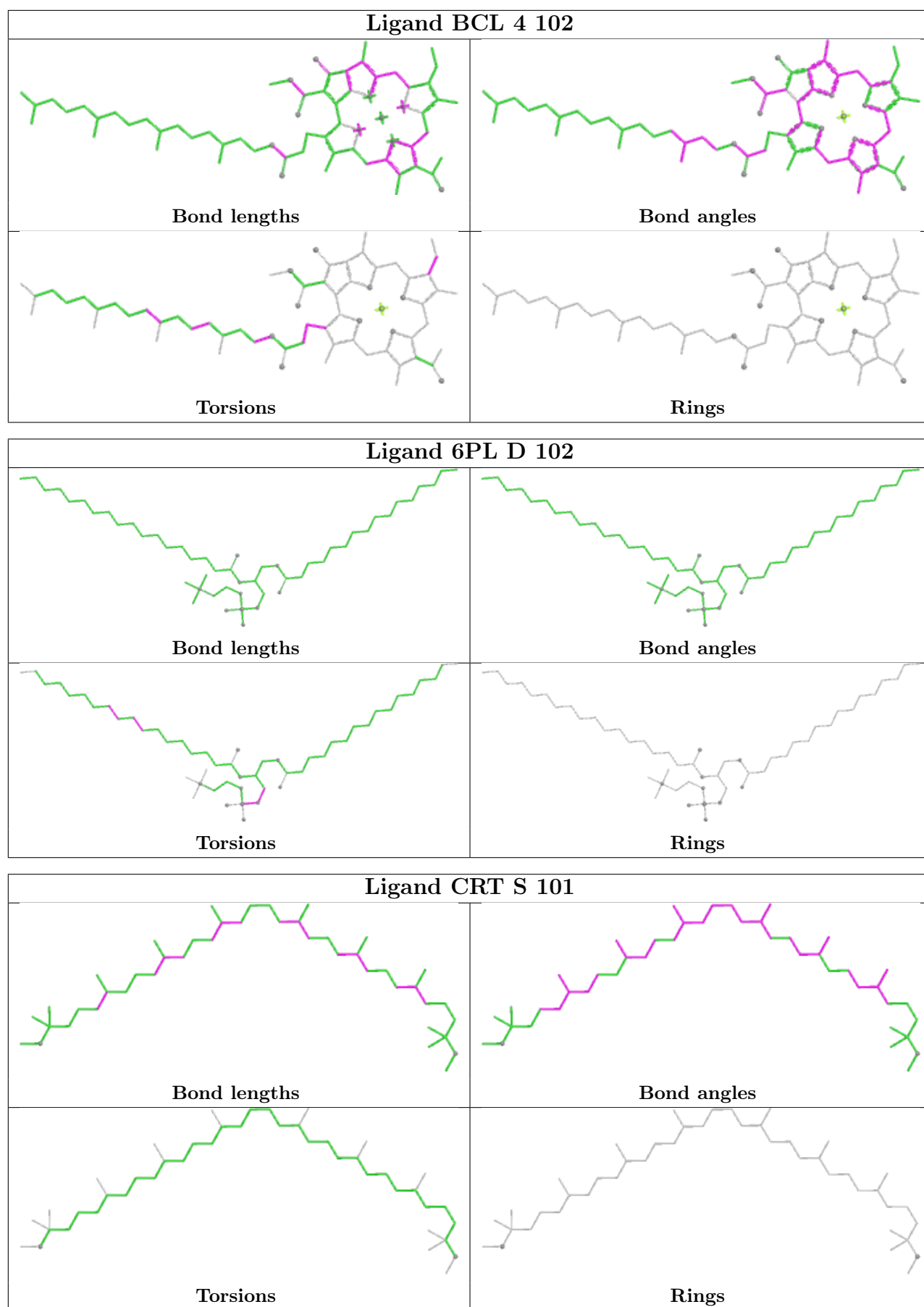


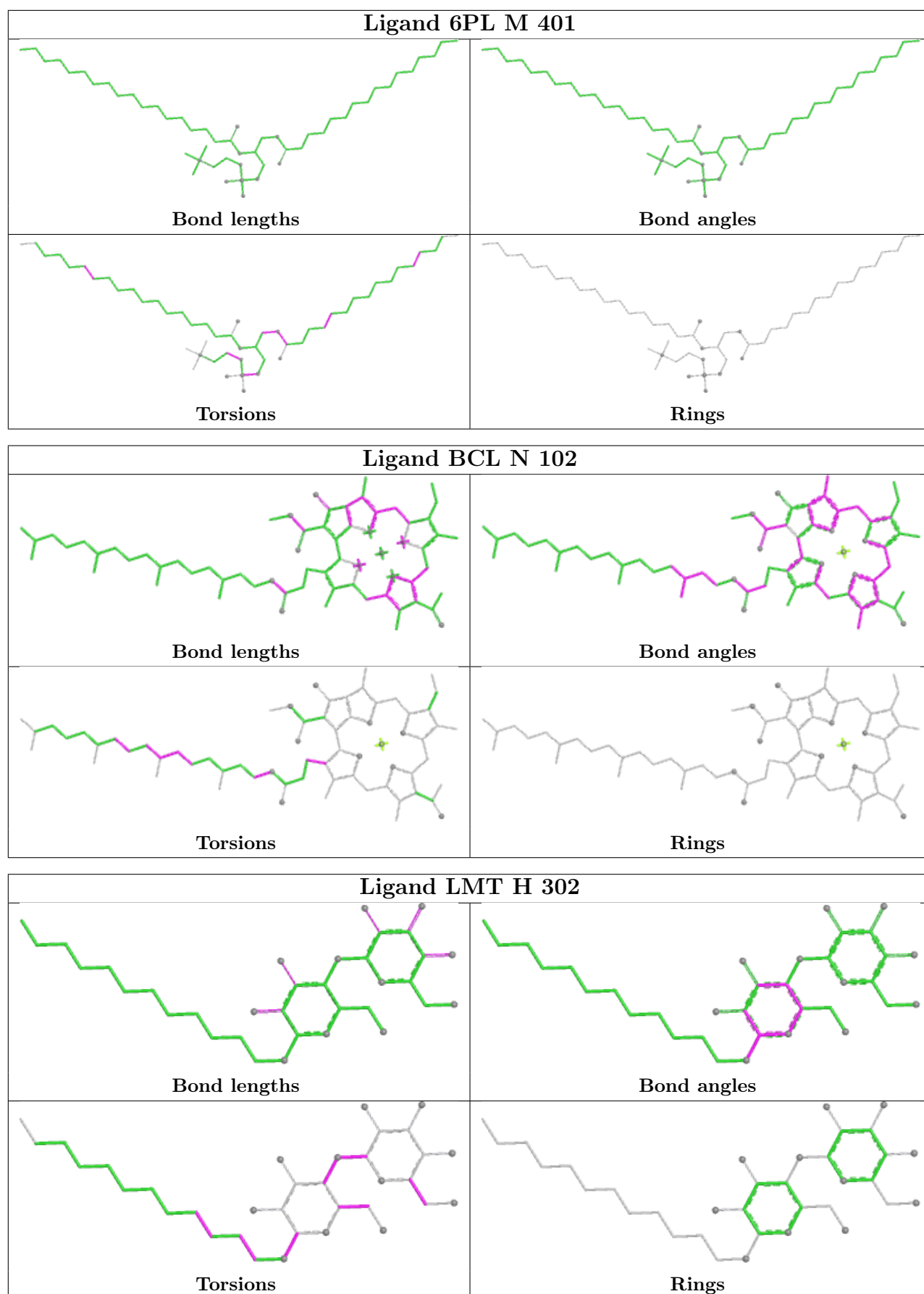


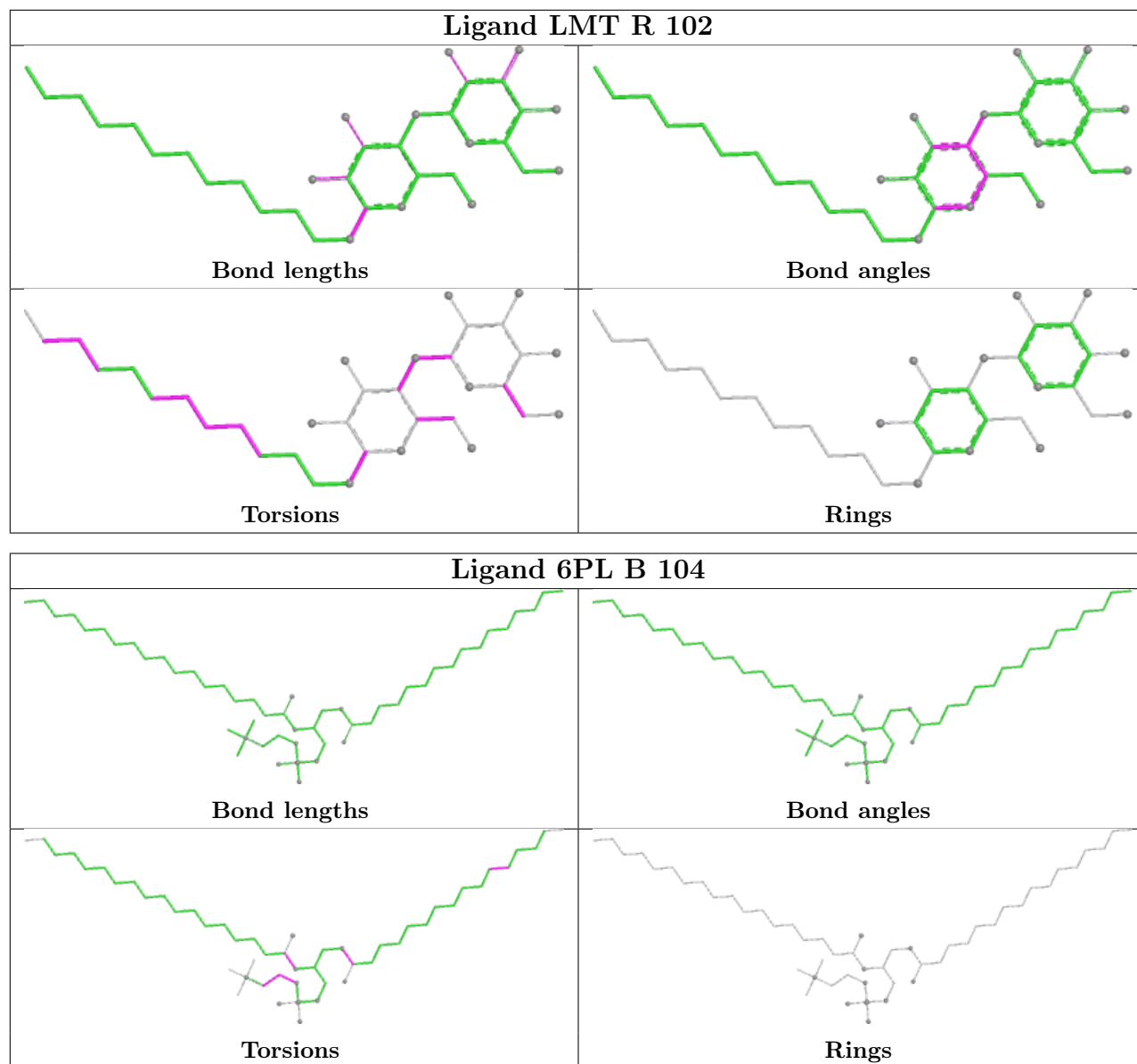


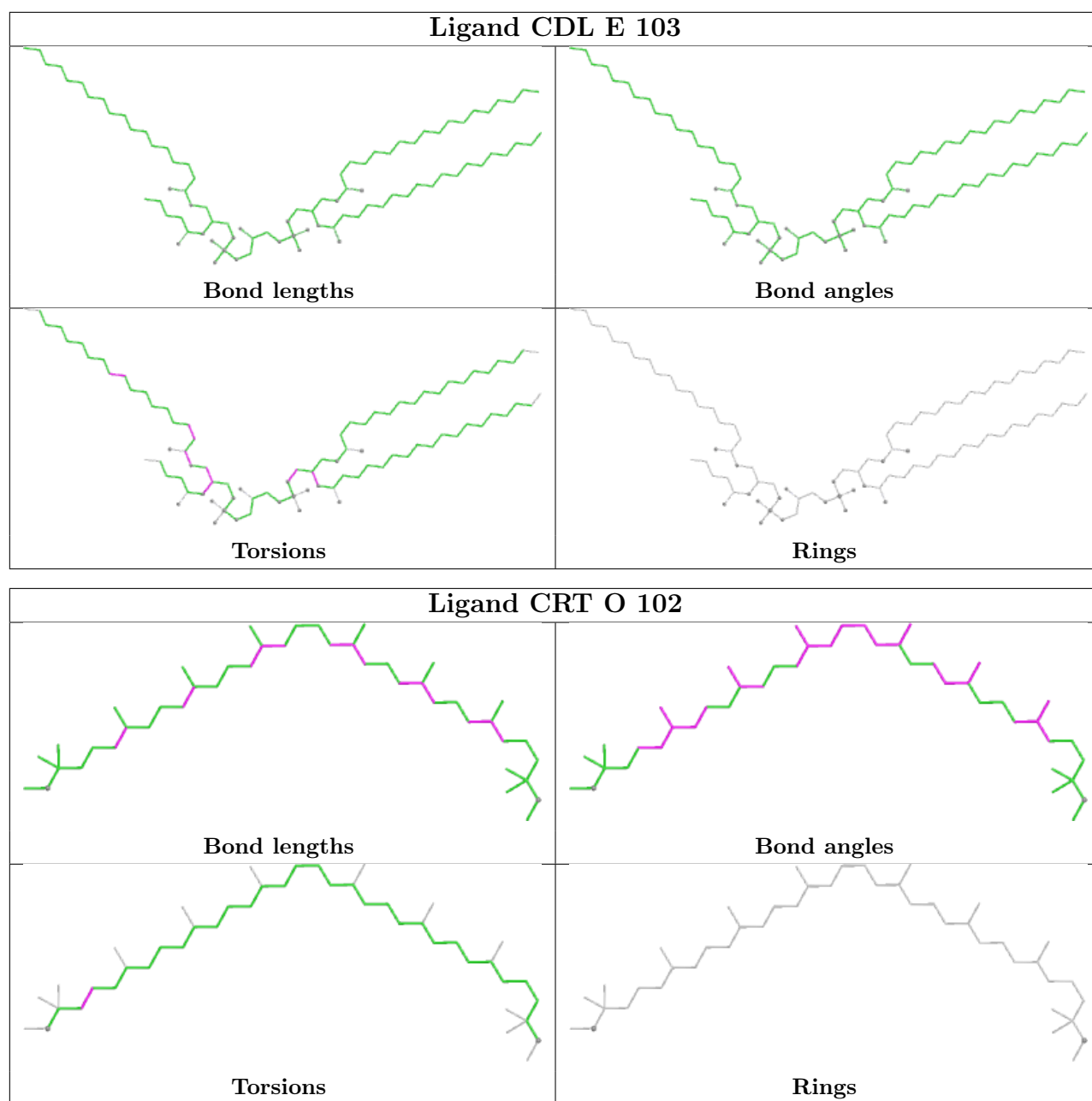


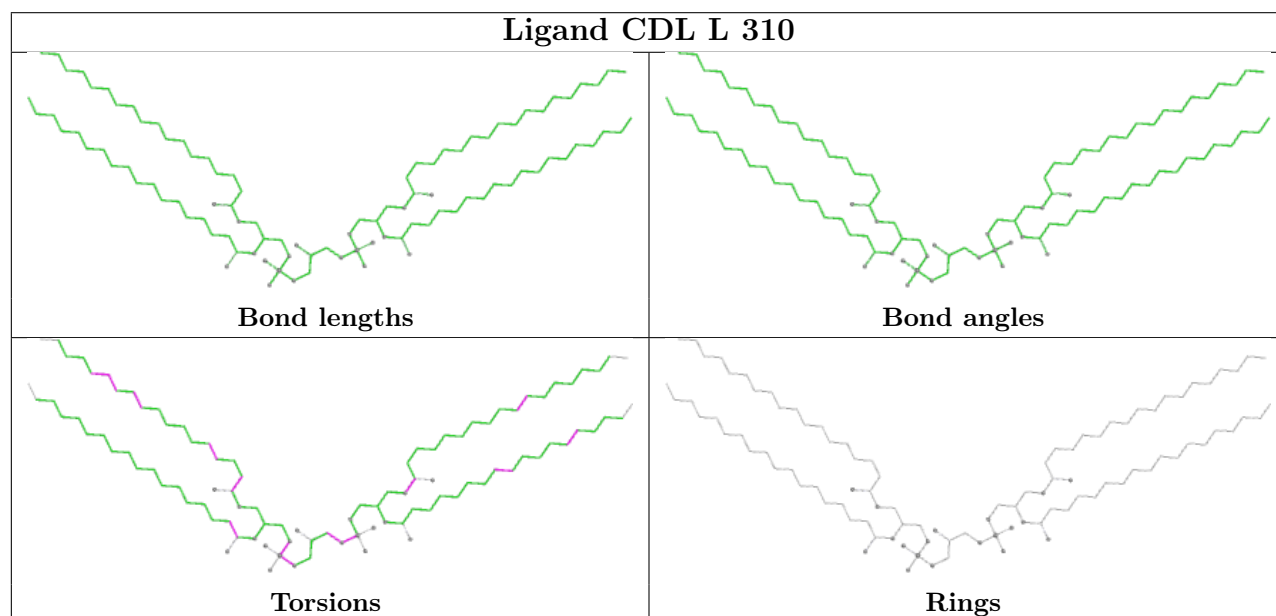
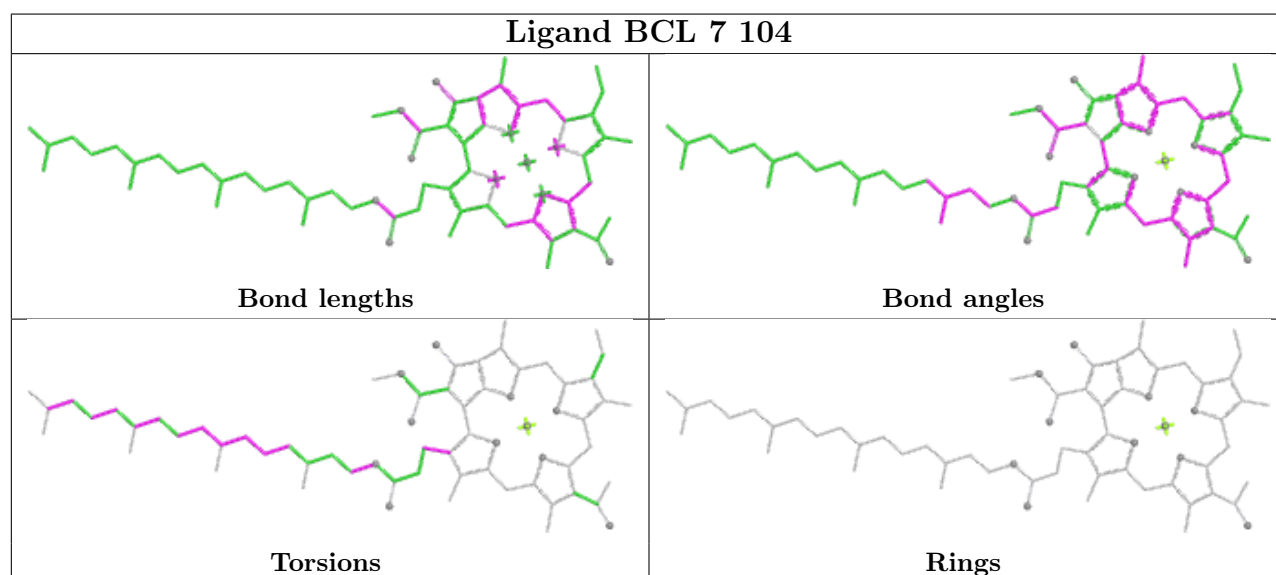
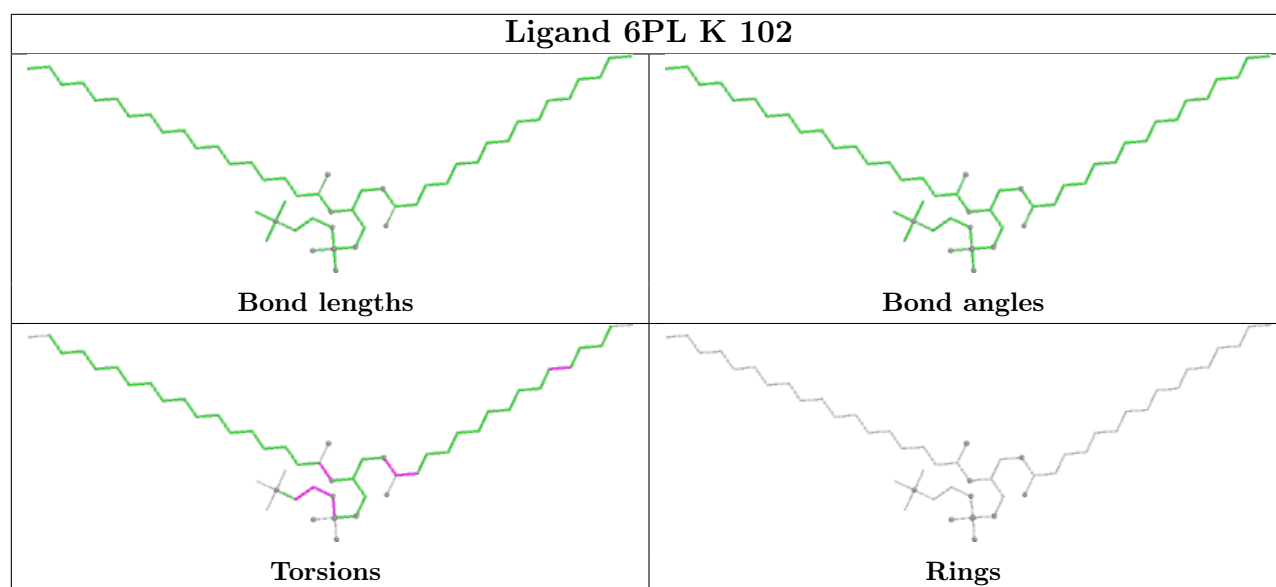


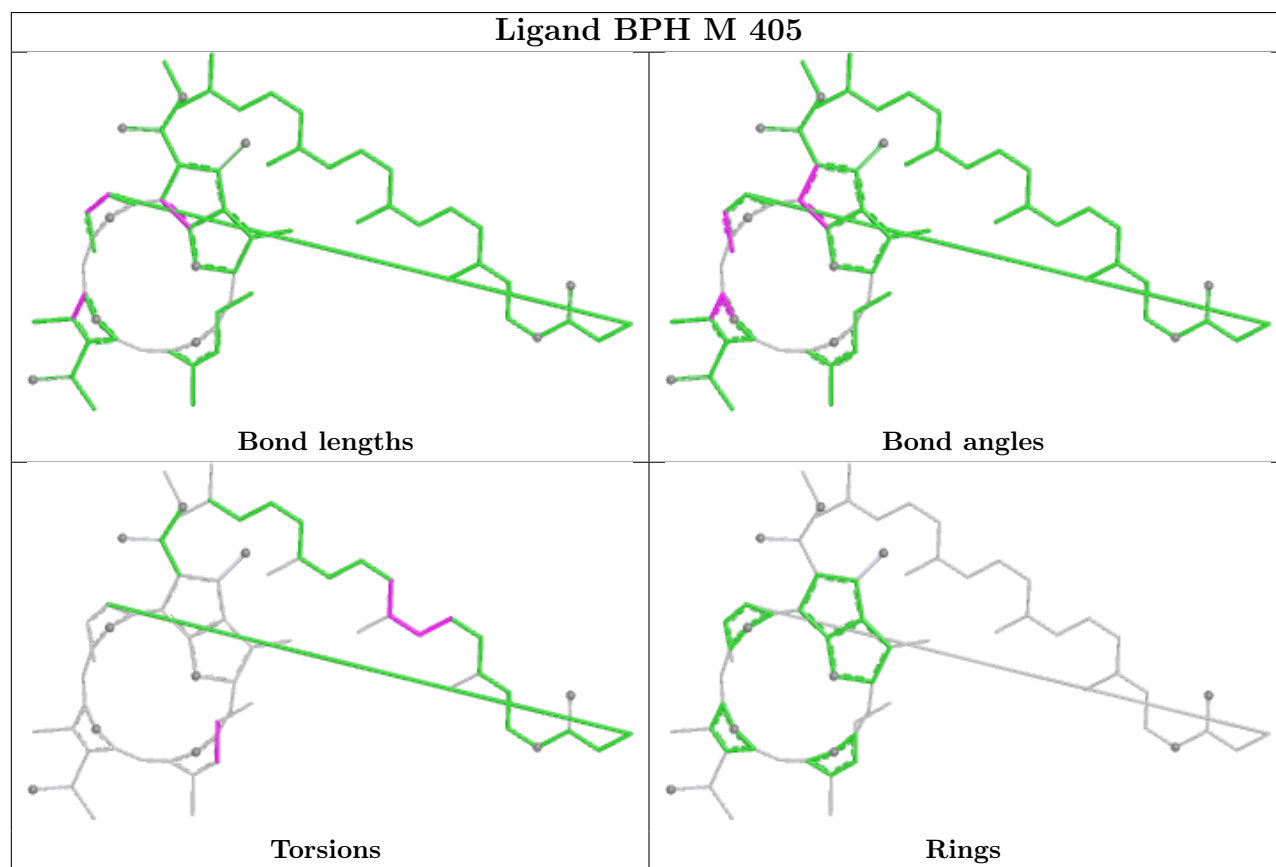
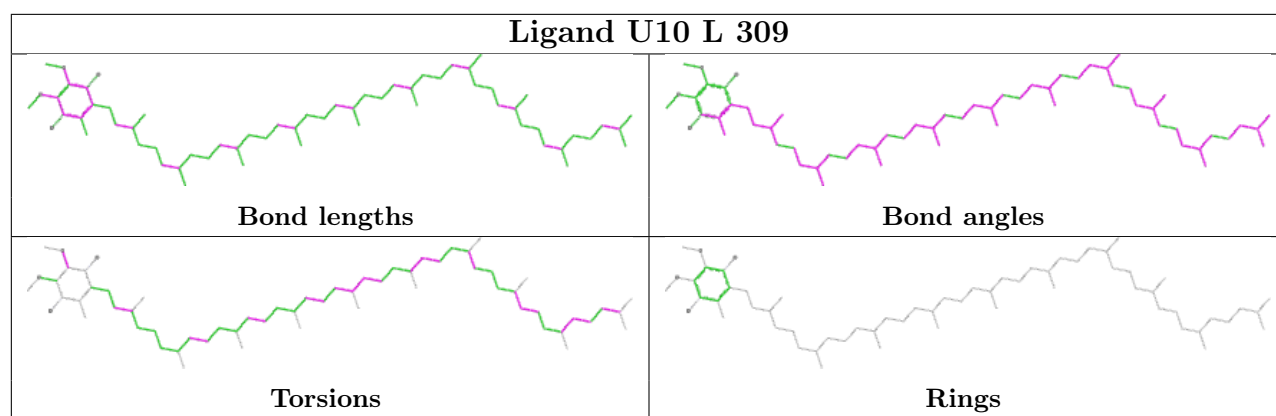




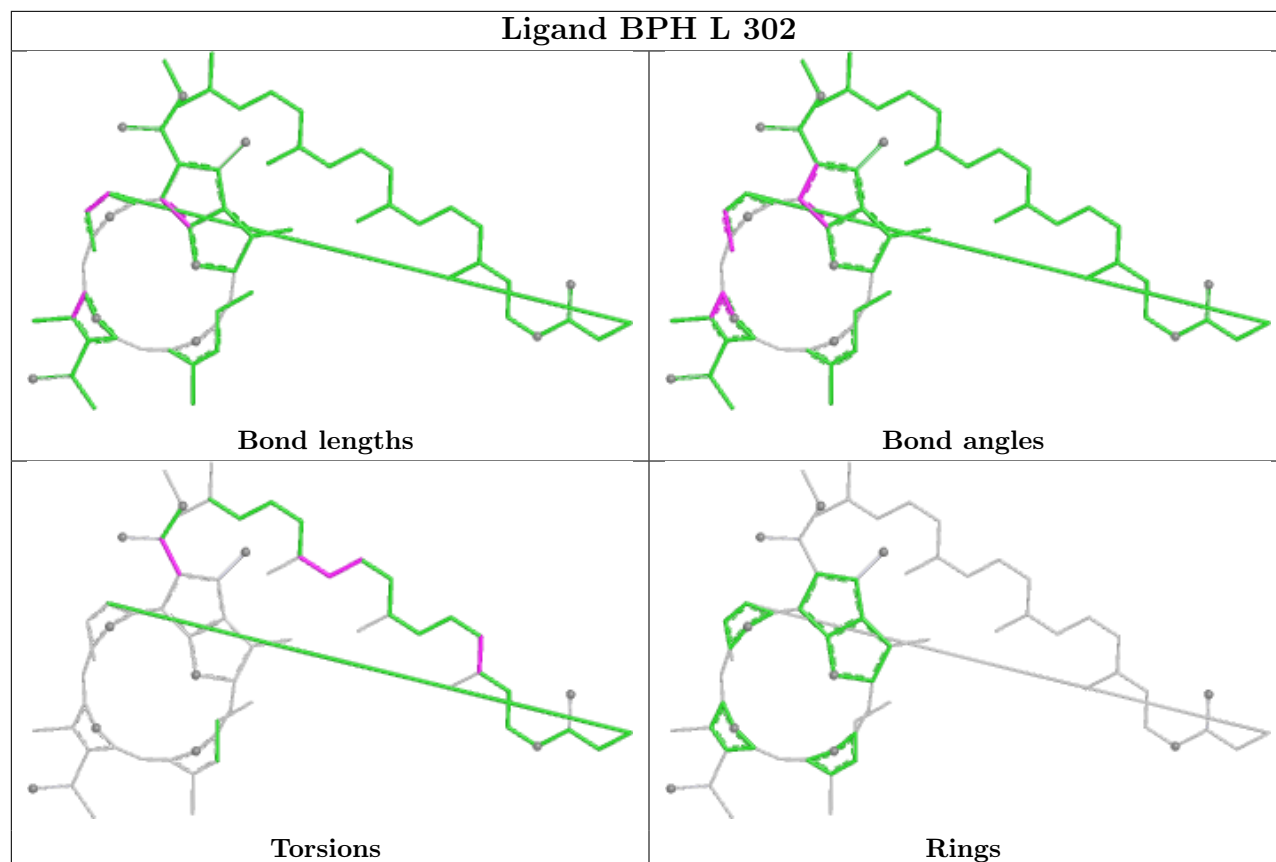




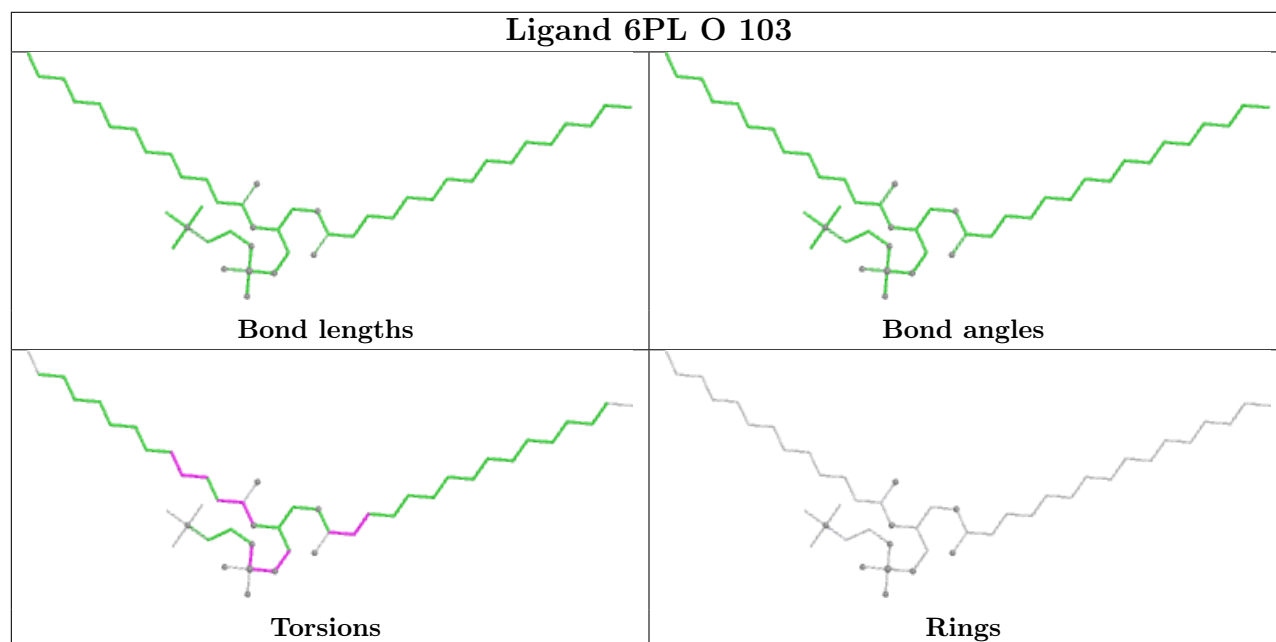


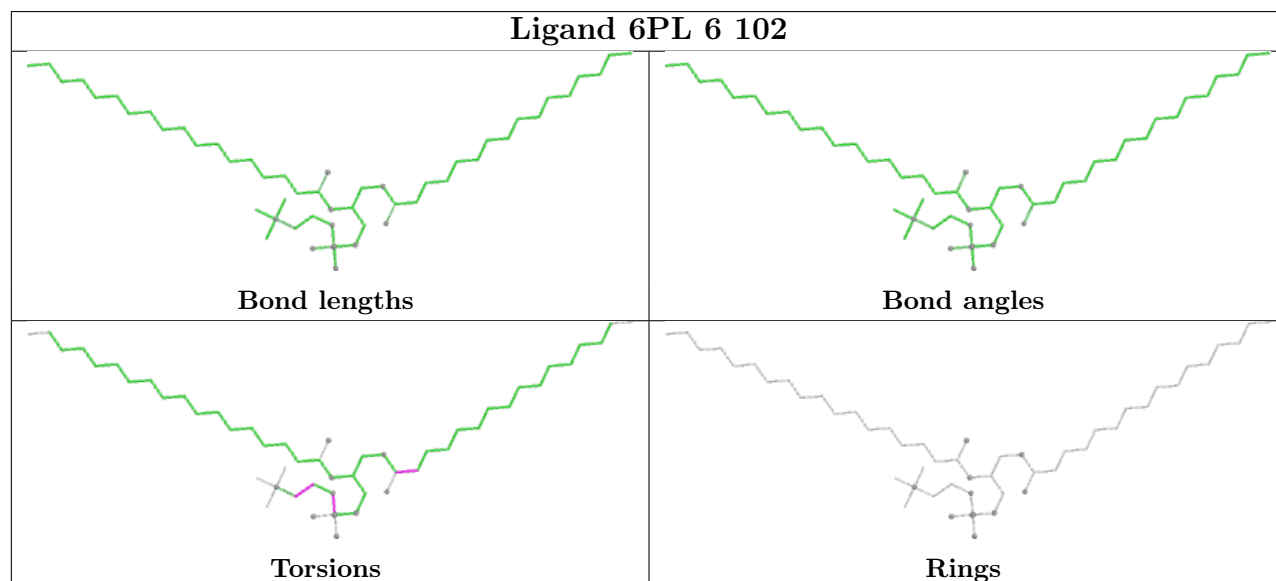
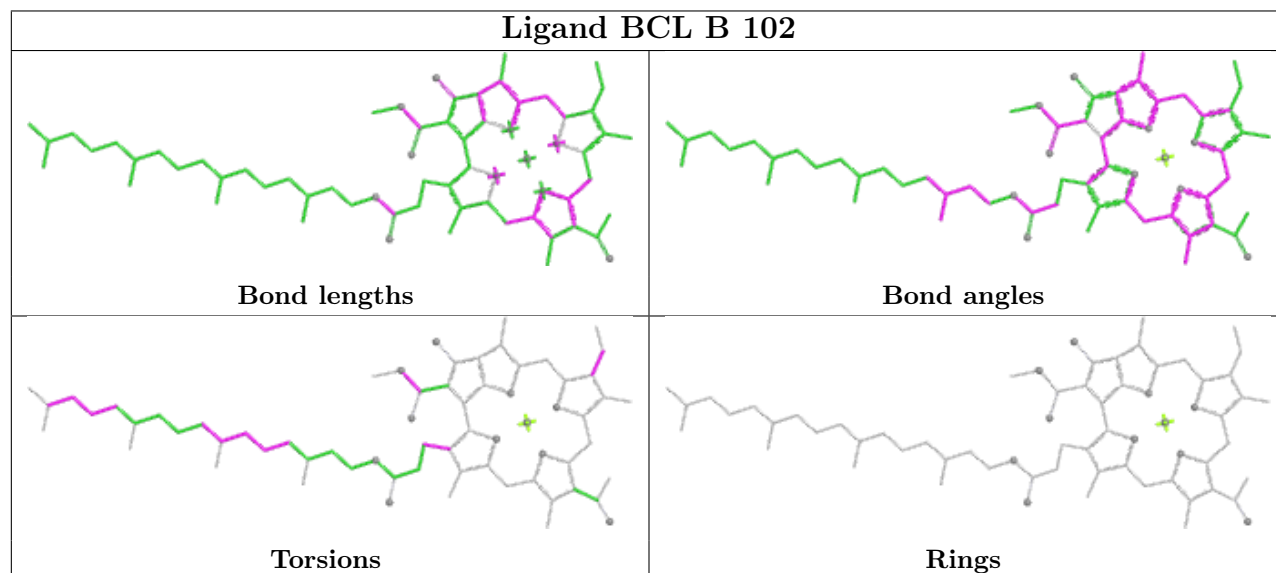
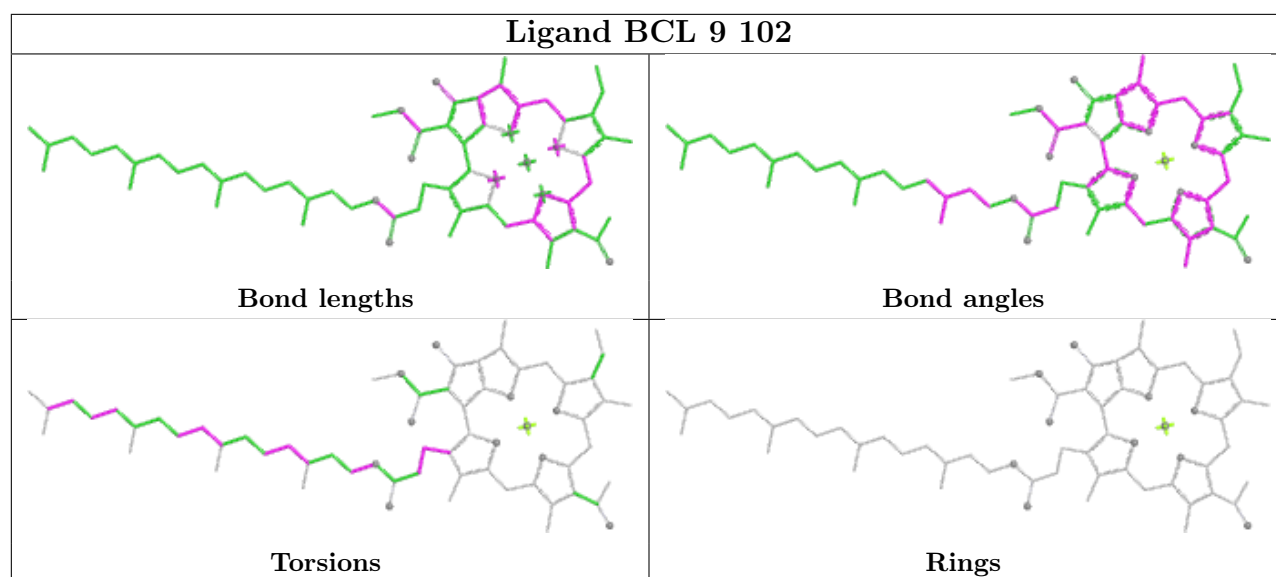


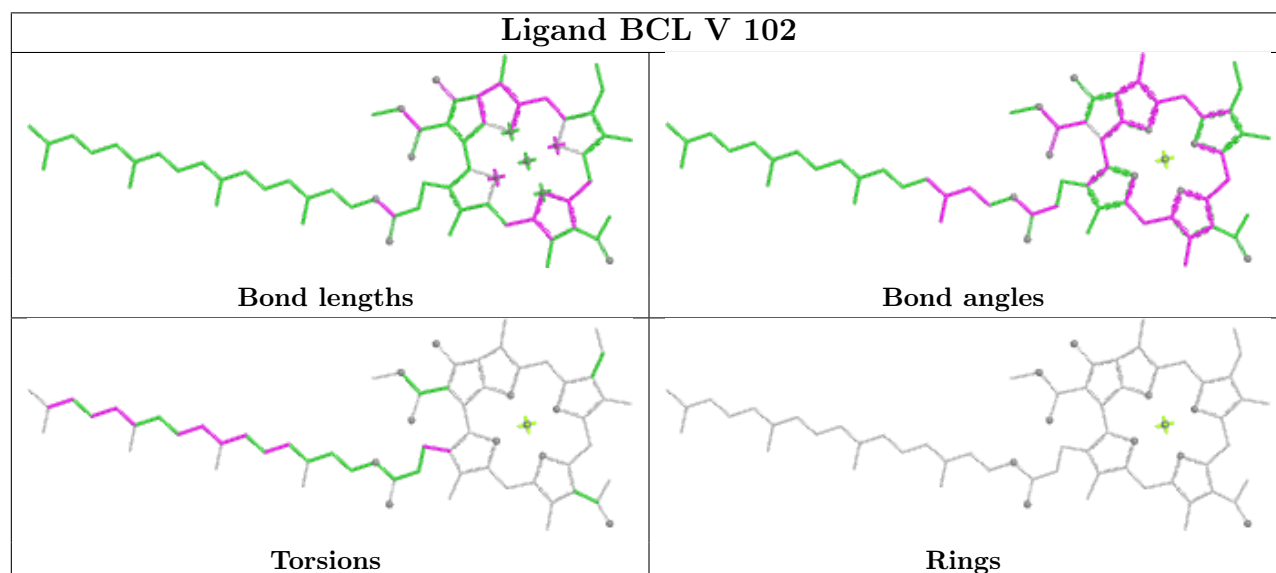
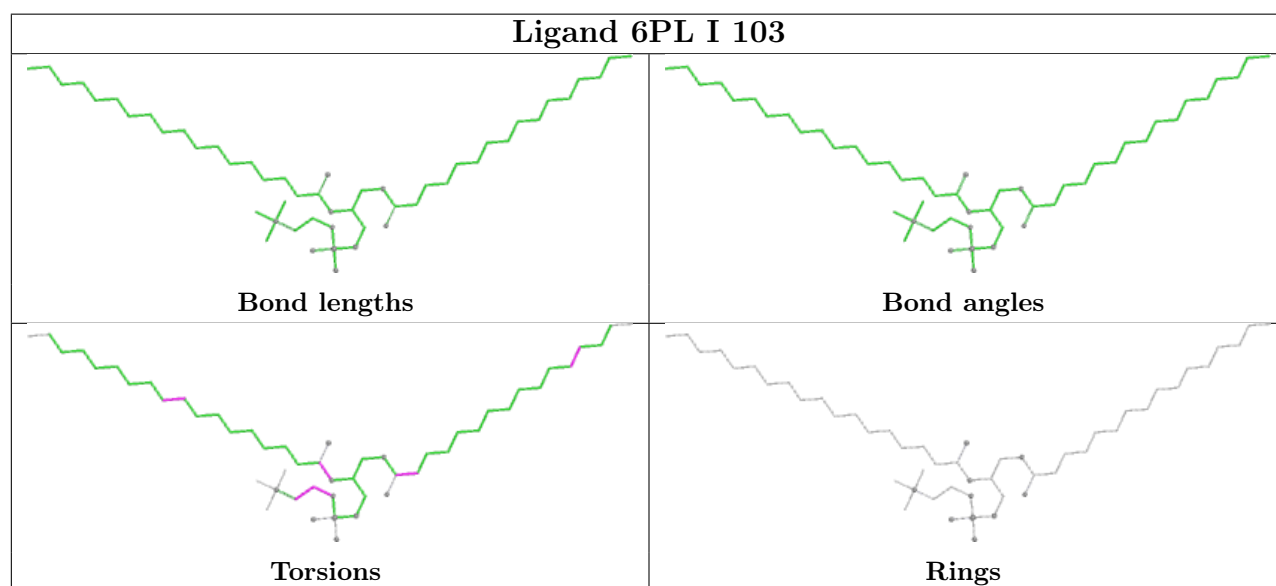
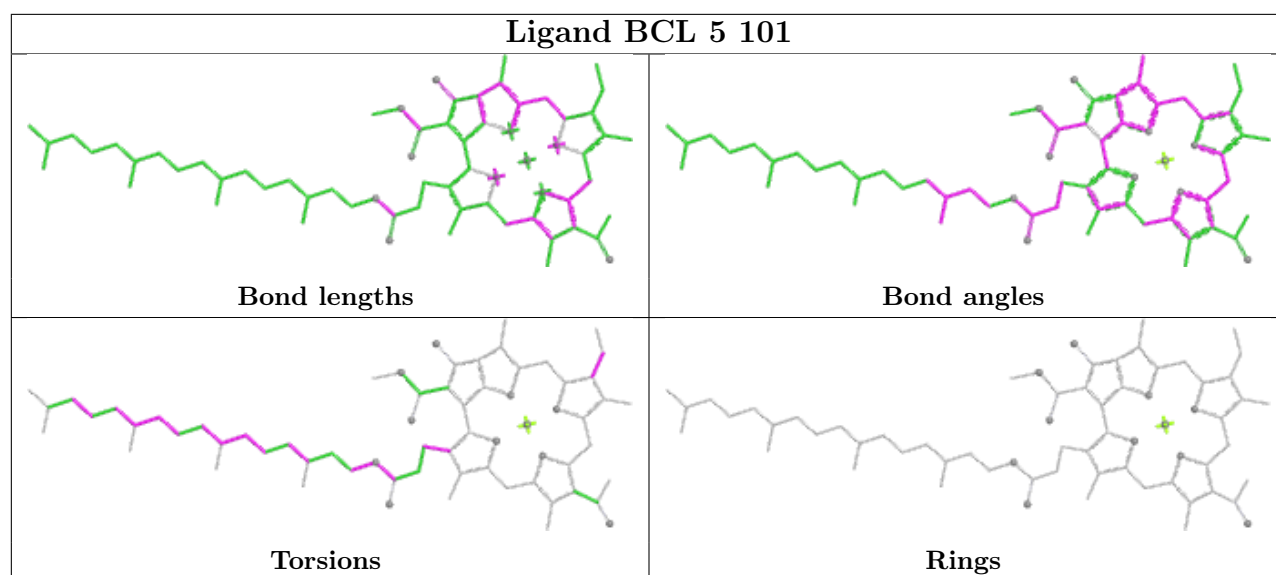
Ligand BPH L 302

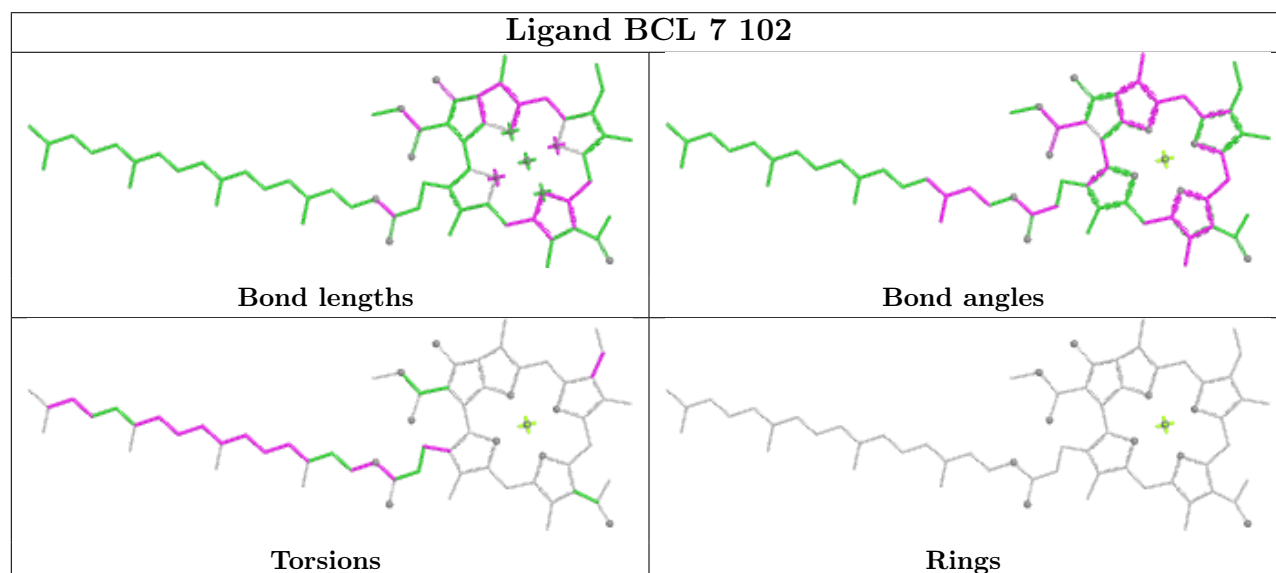
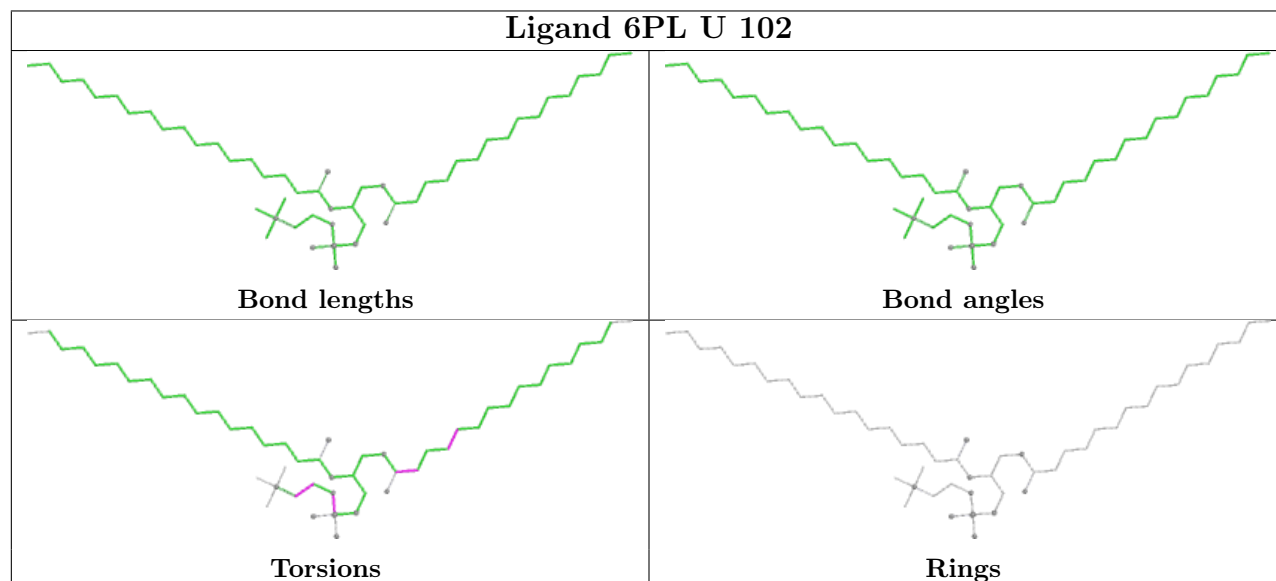
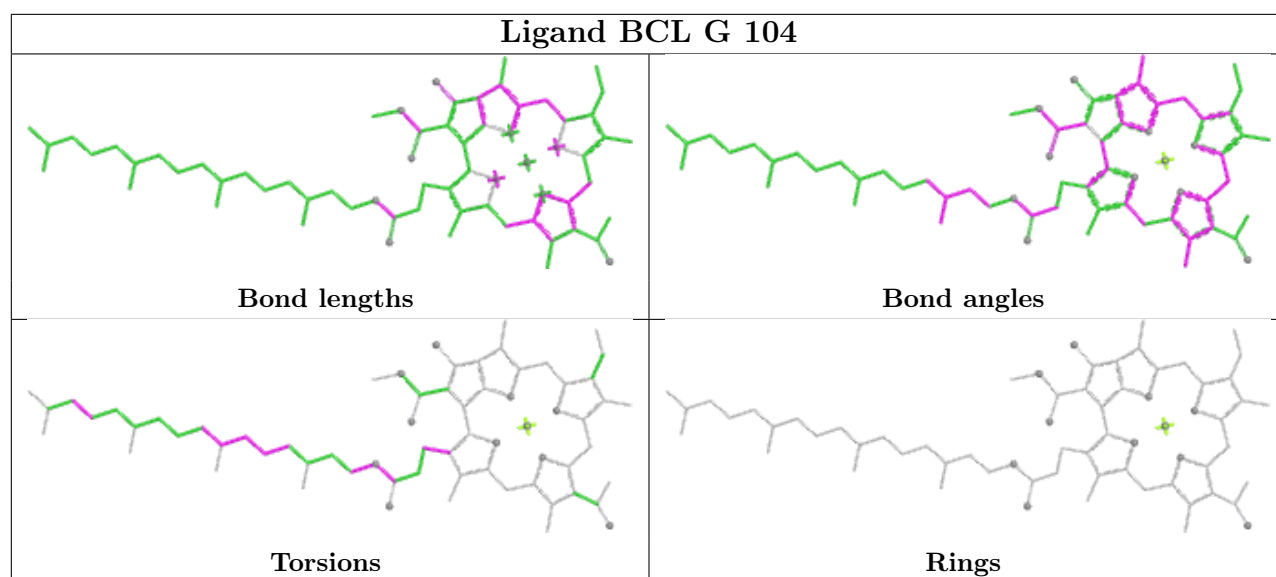


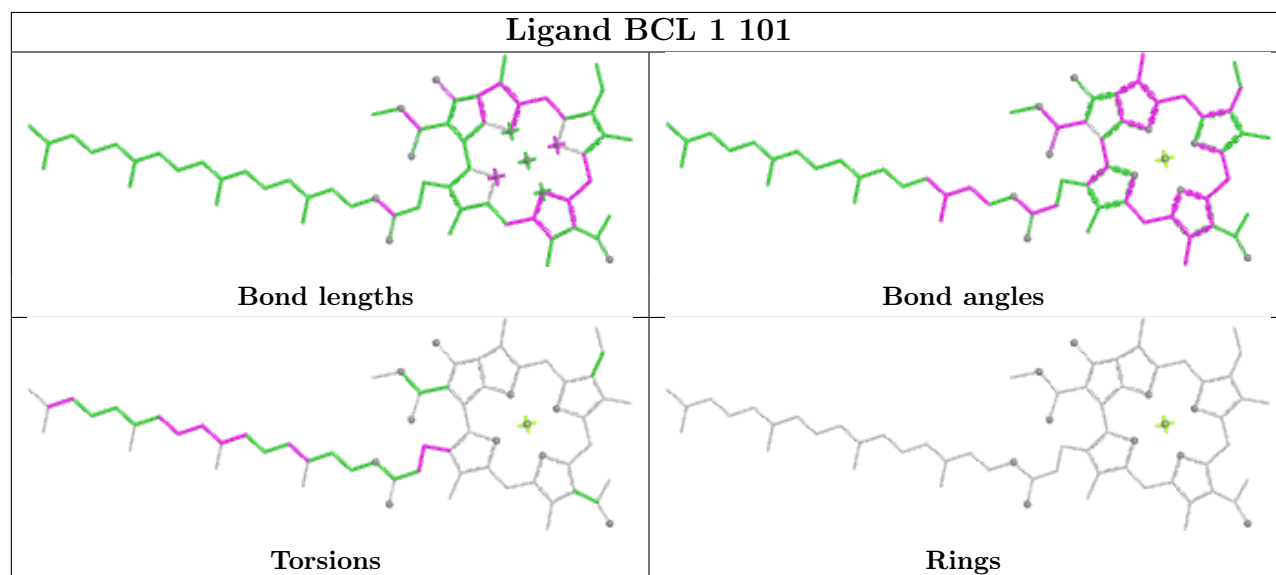
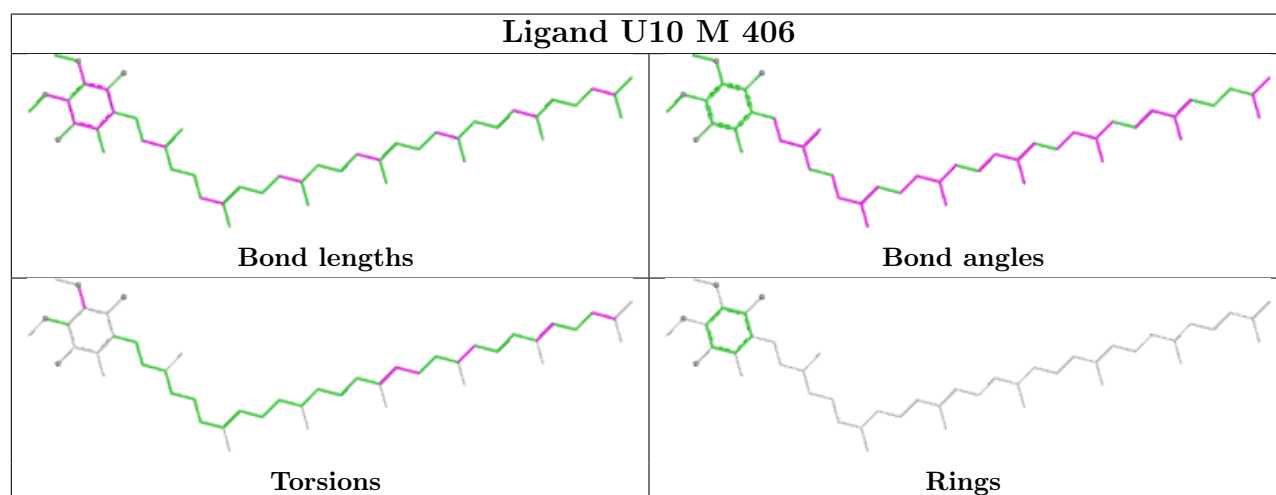
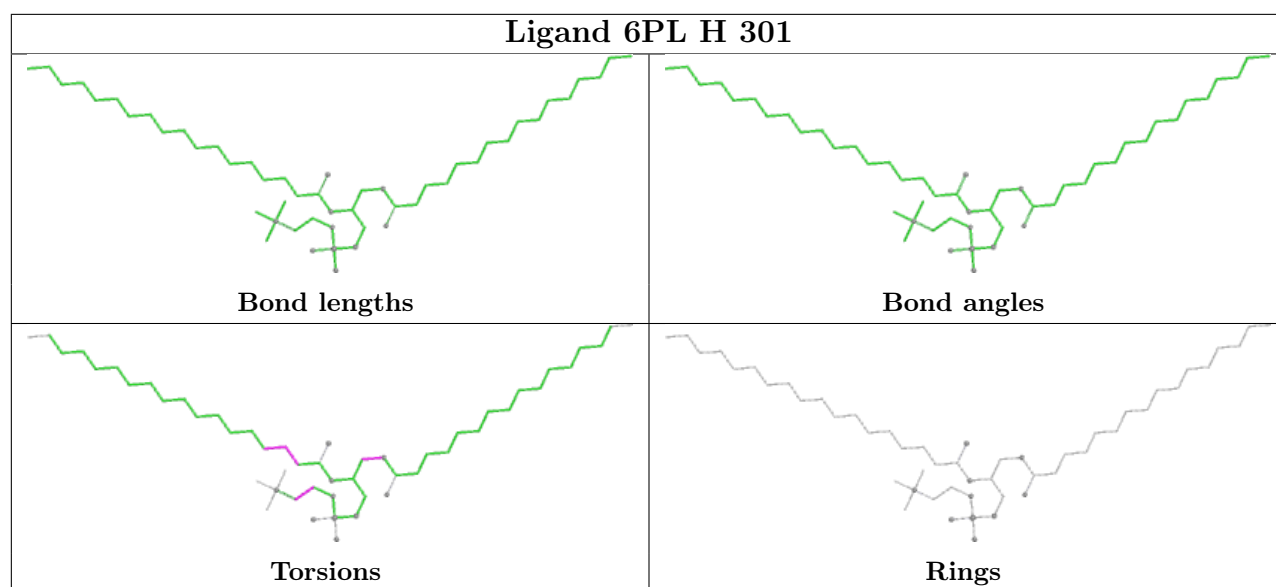
Ligand 6PL O 103

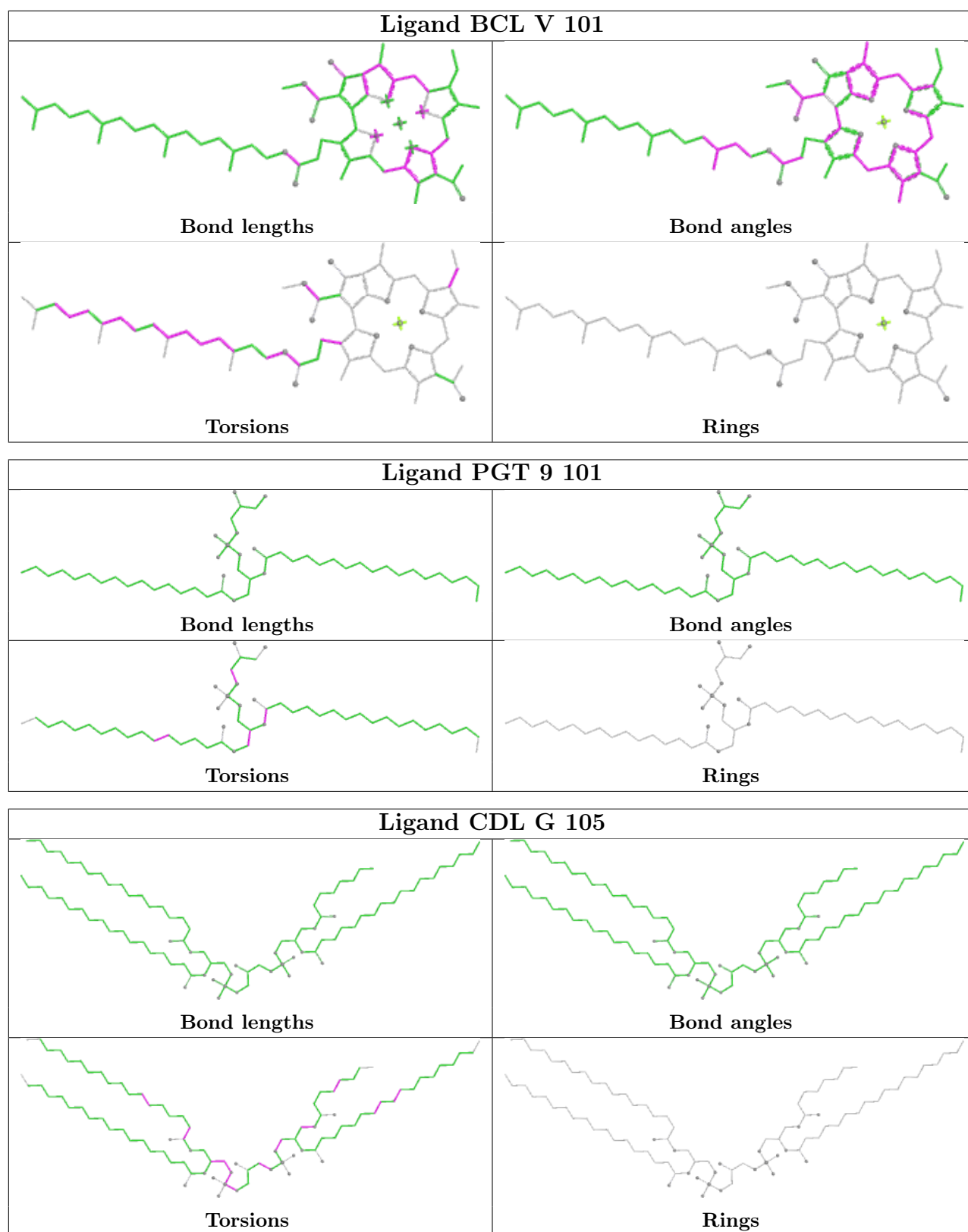












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11080. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.