



Full wwPDB EM Validation Report ⓘ

Apr 12, 2026 – 12:17 AM JST

PDB ID : 9WQV / pdb_00009wqv
EMDB ID : EMD-66181
Title : Cryo-EM structure of LH1-RC from Rhodovulum sulfidophilum
Authors : Yue, X.-Y.; Wang, G.-L.; Yu, L.-J.
Deposited on : 2025-09-11
Resolution : 1.81 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 : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.48.1

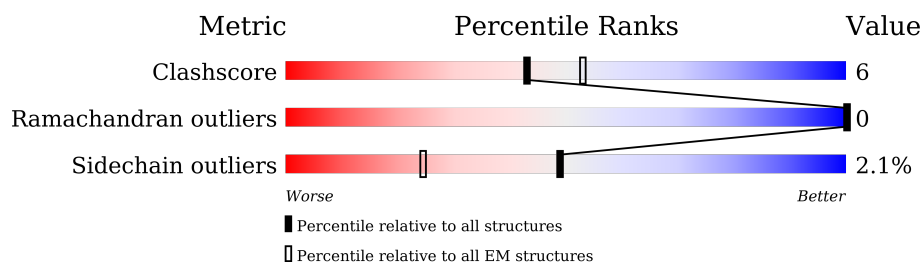
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 1.81 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.













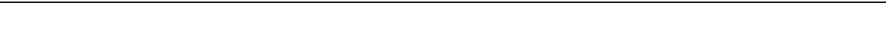

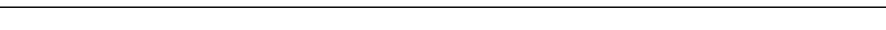
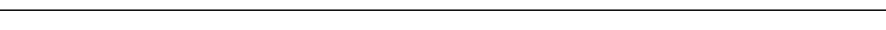











Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	0	48	
1	2	48	
1	4	48	
1	6	48	
1	8	48	
1	B	48	
1	E	48	
1	G	48	
1	J	48	

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Mol	Chain	Length	Quality of chain
1	N	48	 85% 8% 6%
1	P	48	 88% 8% .
1	R	48	 88% 6% 6%
1	T	48	 81% 10% 8%
1	V	48	 81% 12% 6%
1	X	48	 85% 6% . 6%
1	Z	48	 73% 10% 17%
2	1	54	 69% 17% 6% 9%
2	3	54	 63% 19% . 15%
2	5	54	 78% 20% .
2	7	54	 80% 19% .
2	9	54	 83% 15% .
2	A	54	 87% 11% .
2	D	54	 87% 9% . .
2	F	54	 85% 13% .
2	I	54	 85% 13% .
2	K	54	 87% 11% .
2	O	54	 89% 9% .
2	Q	54	 83% 15% .
2	S	54	 85% 13% .
2	U	54	 85% 11% . .
2	W	54	 81% 15% . .
2	Y	54	 74% 17% . 6%
3	C	356	 91% 8% .
4	H	260	 92% 8%

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Mol	Chain	Length	Quality of chain
5	L	284	<div><div></div><div>92%</div><div>8%</div></div>
6	M	321	<div><div></div><div>87%</div><div>11%</div><div>••</div></div>
7	a	229	<div><div></div><div>41%</div><div>5%</div><div>•</div><div>52%</div></div>

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 28553 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	45	Total	C	N	O	S	0	0
			362	240	57	64	1		
1	2	41	Total	C	N	O	S	0	0
			326	216	53	56	1		
1	4	43	Total	C	N	O	S	0	0
			348	233	55	59	1		
1	6	45	Total	C	N	O	S	0	0
			362	240	57	64	1		
1	8	45	Total	C	N	O	S	0	0
			362	240	57	64	1		
1	B	45	Total	C	N	O	S	0	0
			362	240	57	64	1		
1	E	45	Total	C	N	O	S	0	0
			362	240	57	64	1		
1	G	45	Total	C	N	O	S	0	0
			362	240	57	64	1		
1	J	45	Total	C	N	O	S	0	0
			362	240	57	64	1		
1	N	45	Total	C	N	O	S	0	0
			362	240	57	64	1		
1	P	46	Total	C	N	O	S	0	0
			371	245	58	67	1		
1	R	45	Total	C	N	O	S	0	0
			362	240	57	64	1		
1	T	44	Total	C	N	O	S	0	0
			356	237	56	62	1		
1	V	45	Total	C	N	O	S	0	0
			362	240	57	64	1		
1	X	45	Total	C	N	O	S	0	0
			362	240	57	64	1		
1	Z	40	Total	C	N	O	S	0	0
			324	216	52	55	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	49	Total	C	N	O	S	0	0
			411	283	64	62	2		
2	3	46	Total	C	N	O	S	0	0
			393	272	60	58	3		
2	5	53	Total	C	N	O	S	0	0
			435	297	68	67	3		
2	7	53	Total	C	N	O	S	0	0
			435	297	68	67	3		
2	9	53	Total	C	N	O	S	1	0
			443	302	71	67	3		
2	A	53	Total	C	N	O	S	0	0
			435	297	68	67	3		
2	D	53	Total	C	N	O	S	0	0
			435	297	68	67	3		
2	F	53	Total	C	N	O	S	0	0
			435	297	68	67	3		
2	I	53	Total	C	N	O	S	0	0
			435	297	68	67	3		
2	K	53	Total	C	N	O	S	0	0
			435	297	68	67	3		
2	O	53	Total	C	N	O	S	0	0
			435	297	68	67	3		
2	Q	53	Total	C	N	O	S	0	0
			435	297	68	67	3		
2	S	53	Total	C	N	O	S	0	0
			435	297	68	67	3		
2	U	53	Total	C	N	O	S	0	0
			435	297	68	67	3		
2	W	53	Total	C	N	O	S	0	0
			435	297	68	67	3		
2	Y	51	Total	C	N	O	S	0	0
			420	288	66	64	2		

- Molecule 3 is a protein called Photosynthetic reaction center cytochrome c subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	352	Total	C	N	O	S	0	0
			2715	1701	454	541	19		

- Molecule 4 is a protein called photosynthetic reaction center subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	260	Total	C	N	O	S	0	0
			2026	1303	341	371	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	283	Total	C	N	O	S	0	0
			2241	1505	357	368	11		

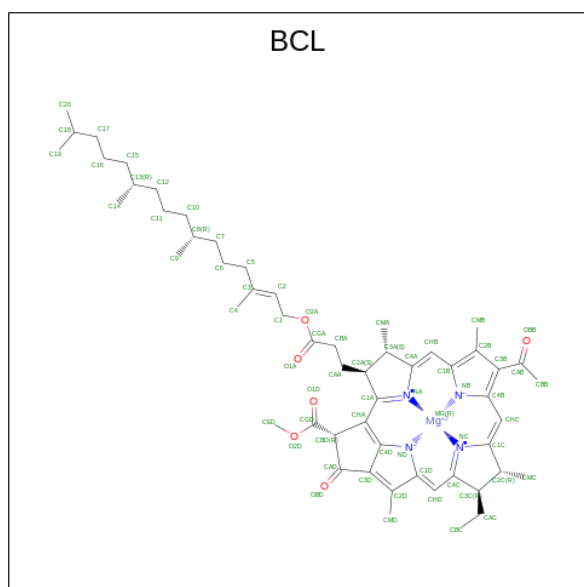
- Molecule 6 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	M	317	Total	C	N	O	S	1	0
			2568	1707	415	431	15		

- Molecule 7 is a protein called NADH:ubiquinone oxidoreductase 41 kd complex i subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	a	110	Total	C	N	O	S	0	0
			827	544	143	135	5		

- Molecule 8 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
8	0	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	2	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
8	3	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
8	4	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	5	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	8	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	9	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	B	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	D	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	E	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	F	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	I	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	J	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	K	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	L	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	L	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	L	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	M	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
8	O	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	P	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	R	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	S	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	T	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	U	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	V	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	W	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	X	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	Z	1	Total 66	C 55	Mg 1	N 4	O 6	0

- Molecule 9 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

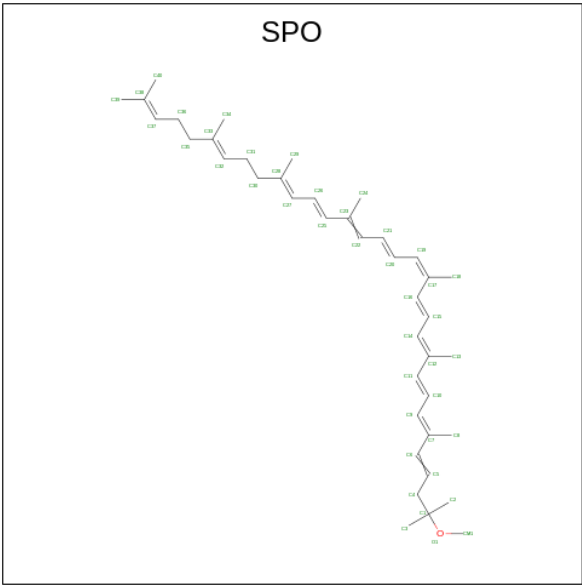
Mol	Chain	Residues	Atoms		AltConf
9	0	1	Total 18	C 18	0
9	6	1	Total 18	C 18	0
9	8	1	Total 18	C 18	0
9	B	1	Total 18	C 18	0
9	D	1	Total 18	C 18	0
9	E	1	Total 18	C 18	0
9	G	1	Total 18	C 18	0

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Mol	Chain	Residues	Atoms	AltConf
9	J	1	Total C 18 18	0
9	N	1	Total C 18 18	0
9	P	1	Total C 18 18	0
9	R	1	Total C 18 18	0
9	T	1	Total C 18 18	0
9	V	1	Total C 18 18	0

- Molecule 10 is SPHEROIDENE (CCD ID: SPO) (formula: C₄₁H₆₀O) (labeled as "Ligand of Interest" by depositor).



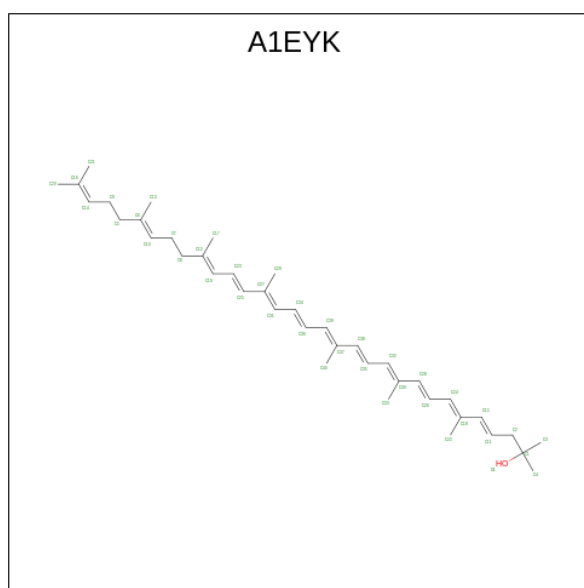
Mol	Chain	Residues	Atoms	AltConf
10	4	1	Total C O 42 41 1	0
10	5	1	Total C O 42 41 1	0
10	7	1	Total C O 42 41 1	0
10	9	1	Total C O 42 41 1	0
10	A	1	Total C O 42 41 1	0

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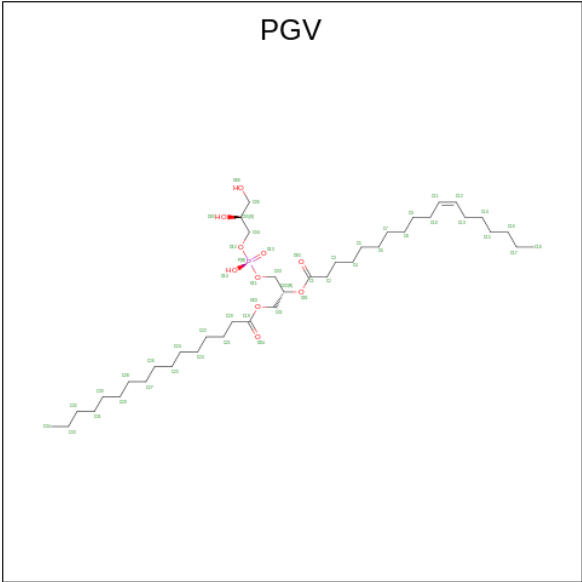
Mol	Chain	Residues	Atoms			AltConf
10	D	1	Total	C	O	0
			42	41	1	
10	F	1	Total	C	O	0
			42	41	1	
10	I	1	Total	C	O	0
			42	41	1	
10	K	1	Total	C	O	0
			42	41	1	
10	M	1	Total	C	O	0
			42	41	1	
10	O	1	Total	C	O	0
			42	41	1	
10	Q	1	Total	C	O	0
			42	41	1	
10	S	1	Total	C	O	0
			42	41	1	
10	U	1	Total	C	O	0
			42	41	1	
10	U	1	Total	C	O	0
			42	41	1	
10	Y	1	Total	C	O	0
			42	41	1	

- Molecule 11 is (4 {E},6 {E},8 {E},10 {E},12 {E},14 {E},16 {E},18 {E},20 {E},22 {E},26 {E})-2,6,10,14,19,23,27,31-octamethyldotriaconta-4,6,8,10,12,14,16,18,20,22,26,30-dodecaen-2-ol (CCD ID: A1EYK) (formula: C₄₀H₅₈O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
11	5	1	Total	C	O	0
			41	40	1	
11	7	1	Total	C	O	0
			41	40	1	
11	9	1	Total	C	O	0
			41	40	1	
11	A	1	Total	C	O	0
			41	40	1	
11	D	1	Total	C	O	0
			41	40	1	
11	F	1	Total	C	O	0
			41	40	1	
11	I	1	Total	C	O	0
			41	40	1	
11	K	1	Total	C	O	0
			41	40	1	
11	O	1	Total	C	O	0
			41	40	1	
11	Q	1	Total	C	O	0
			41	40	1	
11	S	1	Total	C	O	0
			41	40	1	
11	U	1	Total	C	O	0
			41	40	1	
11	W	1	Total	C	O	0
			41	40	1	
11	Z	1	Total	C	O	0
			41	40	1	

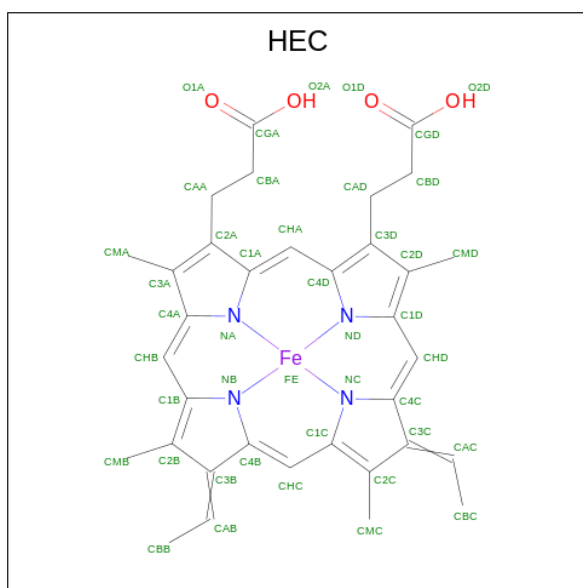
- Molecule 12 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms				AltConf
13	A	1	Total	C	O	P	0
			47	36	10	1	
13	D	1	Total	C	O	P	0
			32	23	8	1	
13	F	1	Total	C	O	P	0
			51	40	10	1	
13	H	1	Total	C	O	P	0
			34	23	10	1	
13	H	1	Total	C	O	P	0
			33	22	10	1	
13	H	1	Total	C	O	P	0
			42	31	10	1	
13	H	1	Total	C	O	P	0
			42	31	10	1	
13	H	1	Total	C	O	P	0
			36	27	8	1	
13	L	1	Total	C	O	P	0
			43	32	10	1	
13	M	1	Total	C	O	P	0
			40	31	8	1	
13	M	1	Total	C	O	P	0
			45	34	10	1	
13	M	1	Total	C	O	P	0
			43	32	10	1	
13	M	1	Total	C	O	P	0
			33	22	10	1	

- Molecule 14 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₄FeN₄O₄) (labeled as "Ligand of

Interest" by depositor).



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

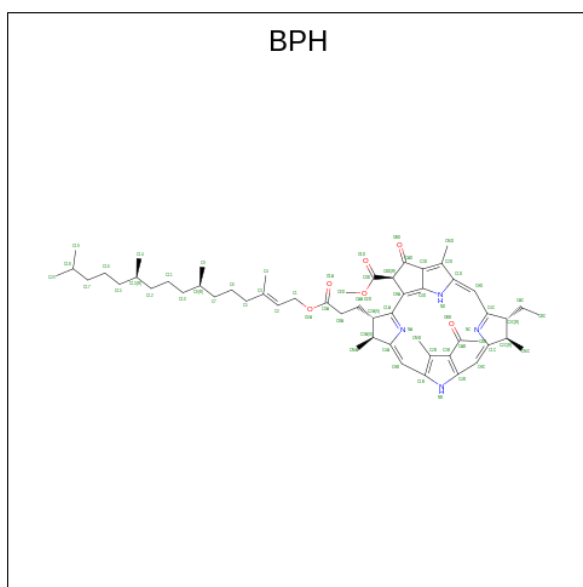
- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
15	C	2	Total	Mg	0
			2	2	
15	M	2	Total	Mg	0
			2	2	

- Molecule 16 is FE (III) ION (CCD ID: FE) (formula: Fe).

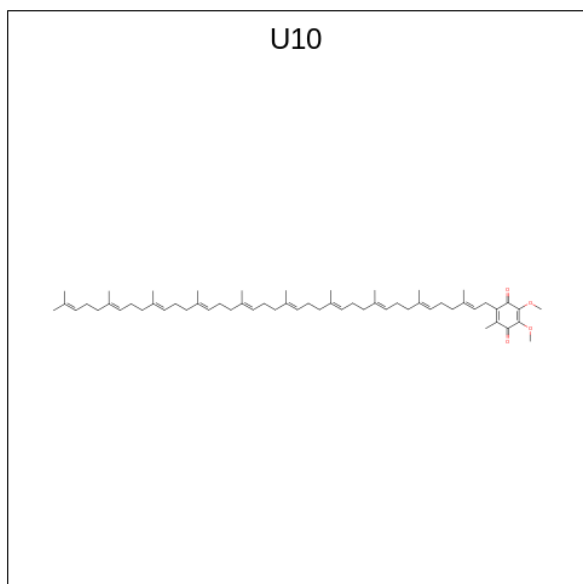
Mol	Chain	Residues	Atoms		AltConf
16	C	1	Total	Fe	0
			1	1	
16	M	1	Total	Fe	0
			1	1	

- Molecule 17 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: C₅₅H₇₆N₄O₆) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 18 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
18	L	1	Total	C	O	0
			63	59	4	

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Mol	Chain	Residues	Atoms			AltConf
18	M	1	Total	C	O	0
			25	21	4	
18	M	1	Total	C	O	0
			63	59	4	
18	M	1	Total	C	O	0
			28	24	4	

- Molecule 19 is water.

Mol	Chain	Residues	Atoms		AltConf
19	0	3	Total	O	0
			3	3	
19	6	1	Total	O	0
			1	1	
19	7	3	Total	O	0
			3	3	
19	8	2	Total	O	0
			2	2	
19	9	5	Total	O	0
			5	5	
19	A	12	Total	O	0
			12	12	
19	B	7	Total	O	0
			7	7	
19	C	184	Total	O	0
			184	184	
19	D	5	Total	O	0
			5	5	
19	E	2	Total	O	0
			2	2	
19	F	6	Total	O	0
			6	6	
19	G	2	Total	O	0
			2	2	
19	H	65	Total	O	0
			65	65	
19	I	10	Total	O	0
			10	10	
19	J	4	Total	O	0
			4	4	
19	K	8	Total	O	0
			8	8	

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Mol	Chain	Residues	Atoms		AltConf
19	L	57	Total 57	O 57	0
19	M	76	Total 76	O 76	0
19	N	5	Total 5	O 5	0
19	O	5	Total 5	O 5	0
19	P	3	Total 3	O 3	0
19	Q	11	Total 11	O 11	0
19	R	2	Total 2	O 2	0
19	S	14	Total 14	O 14	0
19	T	2	Total 2	O 2	0
19	U	7	Total 7	O 7	0
19	V	1	Total 1	O 1	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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: Antenna pigment protein beta chain

Chain 0: 




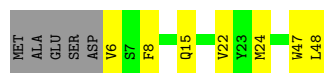
- Molecule 1: Antenna pigment protein beta chain

Chain 2: 




- Molecule 1: Antenna pigment protein beta chain

Chain 4: 




- Molecule 1: Antenna pigment protein beta chain

Chain 6: 




- Molecule 1: Antenna pigment protein beta chain

Chain 8: 



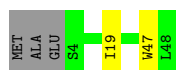
- Molecule 1: Antenna pigment protein beta chain

Chain B: 



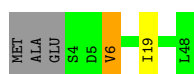
- Molecule 1: Antenna pigment protein beta chain

Chain E: 90% 6%



- Molecule 1: Antenna pigment protein beta chain

Chain G: 90% 6%



- Molecule 1: Antenna pigment protein beta chain

Chain J: 88% 6% 6%



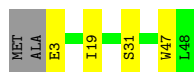
- Molecule 1: Antenna pigment protein beta chain

Chain N: 85% 8% 6%



- Molecule 1: Antenna pigment protein beta chain

Chain P: 88% 8% 4%



- Molecule 1: Antenna pigment protein beta chain

Chain R: 88% 6% 6%



- Molecule 1: Antenna pigment protein beta chain

Chain T: 81% 10% 8%



- Molecule 1: Antenna pigment protein beta chain

Chain V: 81% 12% 6%



- Molecule 1: Antenna pigment protein beta chain

Chain X: 85% 6% 6%



- Molecule 1: Antenna pigment protein beta chain

Chain Z: 73% 10% 17%



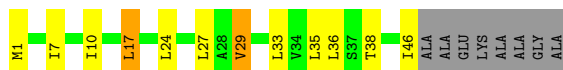
- Molecule 2: Antenna pigment protein alpha chain

Chain 1: 69% 17% 6% 9%



- Molecule 2: Antenna pigment protein alpha chain

Chain 3: 63% 19% 15%



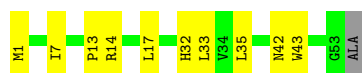
- Molecule 2: Antenna pigment protein alpha chain

Chain 5: 78% 20% 2%



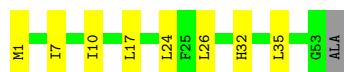
- Molecule 2: Antenna pigment protein alpha chain

Chain 7: 80% 19% 1%



- Molecule 2: Antenna pigment protein alpha chain

Chain 9: 83% 15% .



- Molecule 2: Antenna pigment protein alpha chain

Chain A: 87% 11% .



- Molecule 2: Antenna pigment protein alpha chain

Chain D: 87% 9% . .



- Molecule 2: Antenna pigment protein alpha chain

Chain F: 85% 13% .



- Molecule 2: Antenna pigment protein alpha chain

Chain I: 85% 13% .



- Molecule 2: Antenna pigment protein alpha chain

Chain K: 87% 11% .



- Molecule 2: Antenna pigment protein alpha chain

Chain O: 89% 9% .



- Molecule 2: Antenna pigment protein alpha chain

Chain Q: 83% 15% .



- Molecule 2: Antenna pigment protein alpha chain

Chain S: 85% 13% .



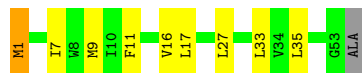
- Molecule 2: Antenna pigment protein alpha chain

Chain U: 85% 11% ..



- Molecule 2: Antenna pigment protein alpha chain

Chain W: 81% 15% ..



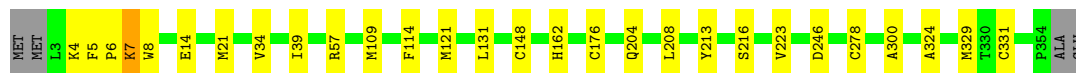
- Molecule 2: Antenna pigment protein alpha chain

Chain Y: 74% 17% 6%



- Molecule 3: Photosynthetic reaction center cytochrome c subunit

Chain C: 91% 8% .



- Molecule 4: photosynthetic reaction center subunit H

Chain H: 92% 8%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	108964	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A1EYK, HEC, MG, U10, BCL, LMT, BPH, FE, SPO, UNL, FME, PGV

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.09	0/374	0.19	0/512
1	2	0.11	0/337	0.41	0/462
1	4	0.08	0/360	0.23	0/493
1	6	0.08	0/374	0.18	0/512
1	8	0.09	0/374	0.18	0/512
1	B	0.09	0/374	0.19	0/512
1	E	0.09	0/374	0.18	0/512
1	G	0.09	0/374	0.18	0/512
1	J	0.09	0/374	0.18	0/512
1	N	0.09	0/374	0.19	0/512
1	P	0.08	0/383	0.18	0/524
1	R	0.08	0/374	0.18	0/512
1	T	0.10	0/368	0.20	0/504
1	V	0.09	0/374	0.19	0/512
1	X	0.08	0/374	0.21	0/512
1	Z	0.10	0/335	0.29	0/459
2	1	0.09	0/423	0.28	0/574
2	3	0.08	0/395	0.24	0/537
2	5	0.10	0/437	0.21	0/593
2	7	0.09	0/437	0.23	0/593
2	9	0.10	0/448	0.23	0/607
2	A	0.10	0/437	0.22	0/593
2	D	0.10	0/437	0.21	0/593
2	F	0.11	0/437	0.22	0/593
2	I	0.10	0/437	0.20	0/593
2	K	0.10	0/437	0.21	0/593
2	O	0.10	0/437	0.21	0/593
2	Q	0.11	0/437	0.25	0/593
2	S	0.09	0/437	0.22	0/593
2	U	0.08	0/437	0.22	0/593
2	W	0.08	0/437	0.25	0/593
2	Y	0.08	0/432	0.32	0/586

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	C	0.12	0/2782	0.30	0/3795
4	H	0.13	0/2084	0.26	0/2827
5	L	0.12	0/2330	0.28	0/3183
6	M	0.13	0/2667	0.29	0/3642
7	a	0.11	0/852	0.31	0/1161
All	All	0.11	0/23554	0.25	0/32102

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	0	362	0	347	4	0
1	2	326	0	308	5	0
1	4	348	0	338	8	0
1	6	362	0	347	5	0
1	8	362	0	347	7	0
1	B	362	0	347	5	0
1	E	362	0	347	3	0
1	G	362	0	347	2	0
1	J	362	0	347	4	0
1	N	362	0	347	4	0
1	P	371	0	353	3	0
1	R	362	0	347	3	0
1	T	356	0	342	5	0
1	V	362	0	347	5	0
1	X	362	0	347	4	0
1	Z	324	0	315	5	0
2	1	411	0	431	11	0
2	3	393	0	413	14	0
2	5	435	0	455	9	0
2	7	435	0	455	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	9	443	0	468	7	0
2	A	435	0	455	5	0
2	D	435	0	455	5	0
2	F	435	0	455	5	0
2	I	435	0	455	7	0
2	K	435	0	455	7	0
2	O	435	0	455	4	0
2	Q	435	0	455	7	0
2	S	435	0	455	5	0
2	U	435	0	455	6	0
2	W	435	0	455	9	0
2	Y	420	0	439	9	0
3	C	2715	0	2561	24	0
4	H	2026	0	1992	14	0
5	L	2241	0	2176	17	0
6	M	2568	0	2469	28	0
7	a	827	0	841	11	0
8	0	66	0	74	5	0
8	1	66	0	74	7	0
8	2	66	0	74	3	0
8	3	47	0	35	0	0
8	4	66	0	74	5	0
8	5	66	0	74	6	0
8	6	66	0	74	3	0
8	7	66	0	74	2	0
8	8	66	0	74	6	0
8	9	66	0	74	2	0
8	A	66	0	74	3	0
8	B	66	0	74	6	0
8	D	66	0	74	2	0
8	E	66	0	74	5	0
8	F	66	0	74	1	0
8	G	66	0	74	4	0
8	I	66	0	74	0	0
8	J	66	0	74	3	0
8	K	66	0	74	2	0
8	L	198	0	222	7	0
8	M	66	0	74	4	0
8	N	66	0	74	4	0
8	O	66	0	74	2	0
8	P	66	0	74	5	0
8	Q	66	0	74	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	R	66	0	74	5	0
8	S	66	0	74	1	0
8	T	66	0	74	6	0
8	U	66	0	74	2	0
8	V	66	0	74	5	0
8	W	66	0	74	0	0
8	X	66	0	74	8	0
8	Y	66	0	74	2	0
8	Z	66	0	74	5	0
9	0	18	0	0	0	0
9	6	18	0	0	0	0
9	8	18	0	0	0	0
9	B	18	0	0	0	0
9	D	18	0	0	0	0
9	E	18	0	0	0	0
9	G	18	0	0	0	0
9	J	18	0	0	0	0
9	N	18	0	0	0	0
9	P	18	0	0	0	0
9	R	18	0	0	0	0
9	T	18	0	0	0	0
9	V	18	0	0	0	0
10	4	42	0	60	13	0
10	5	42	0	60	4	0
10	7	42	0	60	6	0
10	9	42	0	60	4	0
10	A	42	0	60	9	0
10	D	42	0	60	7	0
10	F	42	0	60	5	0
10	I	42	0	60	4	0
10	K	42	0	60	5	0
10	M	42	0	60	4	0
10	O	42	0	60	7	0
10	Q	42	0	60	4	0
10	S	42	0	60	5	0
10	U	84	0	120	11	0
10	Y	42	0	60	10	0
11	5	41	0	0	0	0
11	7	41	0	0	0	0
11	9	41	0	0	0	0
11	A	41	0	0	0	0
11	D	41	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	F	41	0	0	0	0
11	I	41	0	0	0	0
11	K	41	0	0	0	0
11	O	41	0	0	0	0
11	Q	41	0	0	0	0
11	S	41	0	0	0	0
11	U	41	0	0	0	0
11	W	41	0	0	0	0
11	Z	41	0	0	0	0
12	7	27	0	27	4	0
12	9	27	0	27	1	0
12	D	35	0	46	2	0
12	F	28	0	29	0	0
12	K	27	0	27	1	0
12	L	54	0	54	0	0
12	M	53	0	64	0	0
12	O	27	0	27	0	0
13	A	47	0	65	3	0
13	D	32	0	38	1	0
13	F	51	0	76	2	0
13	H	187	0	229	6	0
13	L	43	0	59	2	0
13	M	161	0	200	4	0
14	C	129	0	92	8	0
15	C	2	0	0	0	0
15	M	2	0	0	0	0
16	C	1	0	0	0	0
16	M	1	0	0	0	0
17	L	65	0	76	5	0
17	M	65	0	76	6	0
18	L	63	0	90	4	0
18	M	116	0	148	6	0
19	0	3	0	0	0	0
19	6	1	0	0	0	0
19	7	3	0	0	0	0
19	8	2	0	0	0	0
19	9	5	0	0	0	0
19	A	12	0	0	0	0
19	B	7	0	0	0	0
19	C	184	0	0	1	0
19	D	5	0	0	0	0
19	E	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	F	6	0	0	0	0
19	G	2	0	0	0	0
19	H	65	0	0	0	0
19	I	10	0	0	0	0
19	J	4	0	0	0	0
19	K	8	0	0	0	0
19	L	57	0	0	0	0
19	M	76	0	0	0	0
19	N	5	0	0	0	0
19	O	5	0	0	0	0
19	P	3	0	0	0	0
19	Q	11	0	0	0	0
19	R	2	0	0	0	0
19	S	14	0	0	0	0
19	T	2	0	0	0	0
19	U	7	0	0	0	0
19	V	1	0	0	0	0
All	All	28553	0	27758	357	0

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

All (357) 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)
3:C:278:CYS:SG	14:C:402:HEC:HAC	1.77	1.24
3:C:278:CYS:SG	14:C:402:HEC:CAC	2.30	1.19
3:C:331:CYS:SG	14:C:403:HEC:CAC	2.50	1.00
3:C:331:CYS:SG	14:C:403:HEC:HAC	2.05	0.95
3:C:204:GLN:OE1	19:C:502:HOH:O	1.89	0.89
2:3:27:LEU:HD11	10:4:101:SPO:H6	1.61	0.82
3:C:176:CYS:SG	14:C:401:HEC:CAC	2.71	0.78
3:C:176:CYS:SG	14:C:401:HEC:HAC	2.26	0.76
12:9:104:LMT:H6E	5:L:81:LEU:H	1.53	0.72
8:L:308:BCL:H102	8:M:403:BCL:H171	1.71	0.72
2:5:17:LEU:HD11	10:5:102:SPO:H342	1.75	0.68
2:A:17:LEU:HD11	10:A:102:SPO:H342	1.75	0.68
2:7:17:LEU:HD11	10:7:102:SPO:H342	1.74	0.67
3:C:121:MET:HE1	3:C:131:LEU:HD21	1.75	0.67
13:M:409:PGV:H51	13:M:409:PGV:H202	1.77	0.67
2:I:17:LEU:HD11	10:I:102:SPO:H342	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:M:404:BPH:HHC	17:M:404:BPH:HBB3	1.77	0.66
2:K:6:LYS:HD3	10:O:102:SPO:H393	1.78	0.65
6:M:64:GLY:HA3	17:M:404:BPH:H6C1	1.79	0.65
6:M:156:LEU:HD23	8:M:403:BCL:H42	1.79	0.65
2:S:17:LEU:HD11	10:S:102:SPO:H342	1.79	0.65
2:7:33:LEU:HD22	12:7:104:LMT:H1'	1.80	0.64
2:1:32:HIS:HB3	10:Y:102:SPO:H32A	1.80	0.63
2:9:17:LEU:HD11	10:9:102:SPO:H342	1.80	0.63
2:Q:17:LEU:HD11	10:Q:102:SPO:H342	1.79	0.63
2:U:17:LEU:HD11	10:U:102:SPO:H342	1.79	0.63
2:3:27:LEU:HD21	10:4:101:SPO:H9	1.82	0.62
2:Y:43:TRP:CZ2	8:Y:101:BCL:HHC	2.34	0.62
3:C:329:MET:HG2	5:L:280:VAL:HG21	1.82	0.62
2:U:3:LYS:HE3	2:U:6:LYS:HE2	1.82	0.62
2:K:17:LEU:HD11	10:K:102:SPO:H342	1.82	0.62
13:M:411:PGV:H22	2:W:33:LEU:HD22	1.82	0.61
1:4:47:TRP:CD1	1:4:48:LEU:HG	2.35	0.61
2:K:42:ASN:HD21	12:K:104:LMT:H6D	1.65	0.61
2:Q:35:LEU:HD11	8:R:101:BCL:HHD	1.81	0.61
17:L:302:BPH:HHC	17:L:302:BPH:HBB3	1.81	0.61
6:M:17:SER:HB2	6:M:34:MET:SD	2.41	0.61
2:Q:24:LEU:HB2	8:Q:101:BCL:H42	1.83	0.60
2:Y:24:LEU:HD13	8:Z:102:BCL:HED1	1.84	0.60
8:1:101:BCL:HBD	8:1:101:BCL:HBA2	1.82	0.60
2:7:13:PRO:HG2	1:8:19:ILE:HD13	1.83	0.60
10:U:104:SPO:H342	2:W:17:LEU:HD11	1.84	0.59
3:C:278:CYS:SG	14:C:402:HEC:C3C	2.91	0.59
10:Q:102:SPO:H392	1:R:19:ILE:HA	1.84	0.59
2:D:17:LEU:HD11	10:D:103:SPO:H342	1.85	0.59
6:M:124:ILE:HD13	13:M:408:PGV:H11	1.83	0.59
2:F:17:LEU:HD11	10:F:102:SPO:H342	1.85	0.58
10:D:103:SPO:H6	8:F:101:BCL:HMB2	1.85	0.58
3:C:109:MET:HE3	3:C:114:PHE:HA	1.85	0.58
8:1:101:BCL:HBB2	10:Y:102:SPO:H31	1.86	0.58
10:O:102:SPO:H392	1:P:19:ILE:HA	1.85	0.58
10:I:102:SPO:H392	1:J:19:ILE:HA	1.86	0.57
2:I:7:ILE:HD13	10:K:102:SPO:H311	1.86	0.57
17:M:404:BPH:HBC3	17:M:404:BPH:HHD	1.86	0.57
2:O:17:LEU:HD11	10:O:102:SPO:H342	1.85	0.57
10:4:101:SPO:H393	7:a:10:PHE:HB3	1.87	0.57
2:9:24:LEU:HB2	8:9:101:BCL:H42	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:102:BCL:H102	13:H:301:PGV:H201	1.86	0.56
10:A:102:SPO:H392	1:B:19:ILE:HA	1.87	0.56
12:D:101:LMT:H5B	12:D:101:LMT:H6D	1.87	0.56
6:M:65:CYS:HB2	17:M:404:BPH:H172	1.87	0.56
2:W:35:LEU:HD11	8:X:101:BCL:HHD	1.88	0.55
2:Q:32:HIS:CE1	8:R:101:BCL:HMD3	2.41	0.55
7:a:3:ILE:HG22	7:a:63:THR:HG22	1.89	0.55
2:F:3:LYS:HE2	2:F:6:LYS:HE2	1.89	0.55
2:F:32:HIS:CE1	8:G:101:BCL:HMD3	2.41	0.55
2:1:43:TRP:CZ2	8:1:101:BCL:HHC	2.41	0.55
2:1:6:LYS:HG2	7:a:2:ASN:HB2	1.89	0.54
10:S:102:SPO:H392	1:T:19:ILE:HA	1.90	0.54
1:2:24:MET:HE3	1:2:28:TRP:HZ3	1.73	0.54
1:4:15:GLN:HB2	3:C:8:TRP:CZ2	2.43	0.54
2:3:7:ILE:HD13	10:5:102:SPO:H311	1.90	0.53
2:O:35:LEU:HD11	8:P:101:BCL:HHD	1.90	0.53
1:2:47:TRP:HD1	1:2:48:LEU:HG	1.73	0.53
1:0:19:ILE:HA	10:9:102:SPO:H392	1.91	0.53
2:K:35:LEU:HD11	8:N:101:BCL:HHD	1.89	0.53
6:M:161:GLY:HA3	10:M:406:SPO:H292	1.90	0.53
5:L:49:MET:HB3	5:L:86:LEU:HD11	1.91	0.52
10:5:102:SPO:H392	1:6:19:ILE:HA	1.89	0.52
2:U:35:LEU:HD11	8:V:101:BCL:HHD	1.90	0.52
2:7:35:LEU:HD11	8:8:101:BCL:HHD	1.90	0.52
8:A:101:BCL:HHD	1:B:41:VAL:HG21	1.92	0.52
1:X:47:TRP:CD1	1:X:48:LEU:HG	2.44	0.52
10:4:101:SPO:H32A	2:5:32:HIS:HB3	1.92	0.52
2:Q:7:ILE:HD13	10:S:102:SPO:H311	1.92	0.52
10:D:103:SPO:H392	1:E:19:ILE:HA	1.92	0.52
1:0:47:TRP:CD1	1:0:48:LEU:HG	2.45	0.51
2:W:27:LEU:HD23	8:X:101:BCL:HED3	1.90	0.51
3:C:5:PHE:CZ	7:a:10:PHE:HB2	2.45	0.51
1:B:47:TRP:CD1	1:B:48:LEU:HG	2.45	0.51
10:K:102:SPO:H392	1:N:19:ILE:HA	1.91	0.51
6:M:94:ALA:HB2	6:M:181:PRO:HG2	1.93	0.51
7:a:3:ILE:HD12	7:a:61:CYS:HA	1.92	0.51
8:1:101:BCL:H13	2:Y:16:VAL:HG13	1.93	0.51
1:4:22:VAL:HG21	3:C:6:PRO:HD3	1.93	0.51
1:Z:47:TRP:CD1	1:Z:48:LEU:HG	2.46	0.51
5:L:40:ILE:HG21	18:M:405:U10:H402	1.92	0.50
8:1:101:BCL:CHB	10:Y:102:SPO:H6	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:7:7:ILE:HD13	10:9:102:SPO:H311	1.93	0.50
13:M:411:PGV:H41	2:W:33:LEU:HD13	1.94	0.50
13:H:304:PGV:H341	13:H:305:PGV:H262	1.92	0.50
2:A:35:LEU:HD11	8:B:101:BCL:HHD	1.94	0.50
1:2:41:VAL:HG13	1:2:47:TRP:HZ3	1.76	0.50
2:5:32:HIS:NE2	8:5:101:BCL:NB	2.59	0.50
13:A:104:PGV:H061	4:H:50:PRO:HD2	1.94	0.50
2:I:11:PHE:HZ	2:K:17:LEU:HB2	1.76	0.50
4:H:169:TRP:HB2	4:H:179:TYR:HB2	1.93	0.49
4:H:201:LYS:HG2	6:M:4:TYR:HB2	1.95	0.49
3:C:246:ASP:HB2	4:H:2:VAL:HG21	1.95	0.49
13:H:303:PGV:H161	18:M:405:U10:H552	1.95	0.49
6:M:59:VAL:HG13	2:Q:22:VAL:HG21	1.94	0.49
2:D:32:HIS:CE1	8:E:101:BCL:HMD3	2.47	0.49
10:F:102:SPO:H392	1:G:19:ILE:HA	1.93	0.49
8:0:101:BCL:HMD3	2:9:32:HIS:CE1	2.48	0.49
1:T:47:TRP:CD1	1:T:48:LEU:HG	2.48	0.49
2:1:44:LEU:HD23	2:Y:38:THR:HG21	1.94	0.49
13:F:105:PGV:H152	2:I:26:LEU:HD12	1.95	0.49
2:7:42:ASN:HD21	12:7:104:LMT:H3B	1.77	0.48
1:E:47:TRP:CE2	8:E:101:BCL:H2C	2.48	0.48
1:N:47:TRP:CD1	1:N:48:LEU:HG	2.48	0.48
1:P:31:SER:HB3	8:P:101:BCL:H72	1.94	0.48
8:S:101:BCL:H102	8:S:101:BCL:H61	1.52	0.48
10:I:102:SPO:H41	2:K:32:HIS:CG	2.48	0.48
13:A:104:PGV:H152	18:M:405:U10:H561	1.95	0.48
2:D:35:LEU:HD11	8:E:101:BCL:HHD	1.96	0.48
4:H:35:MET:HE2	4:H:57:LEU:HD23	1.96	0.48
1:J:47:TRP:CD1	1:J:48:LEU:HG	2.48	0.48
10:O:102:SPO:H6	8:Q:101:BCL:HMB2	1.96	0.48
10:U:102:SPO:H392	1:V:19:ILE:HA	1.96	0.48
2:A:7:ILE:HD13	10:D:103:SPO:H311	1.95	0.48
1:8:47:TRP:CD1	1:8:48:LEU:HG	2.49	0.48
2:Y:27:LEU:HD23	8:Z:102:BCL:HED3	1.95	0.48
2:3:17:LEU:HD12	10:4:101:SPO:H402	1.95	0.47
1:G:6:VAL:HG11	1:J:19:ILE:HD11	1.96	0.47
2:S:4:PHE:HB3	8:U:101:BCL:H201	1.96	0.47
1:4:47:TRP:HD1	1:4:48:LEU:HG	1.77	0.47
8:8:101:BCL:HBA1	8:8:101:BCL:H3A	1.68	0.47
8:P:101:BCL:HBA1	8:P:101:BCL:H3A	1.70	0.47
10:7:102:SPO:H392	1:8:19:ILE:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:31:SER:OG	8:V:101:BCL:H2	2.13	0.47
1:6:9:THR:HG23	1:6:11:LEU:H	1.79	0.47
2:W:1:FME:HG3	1:Z:25:SER:HB2	1.96	0.47
10:4:101:SPO:H81	8:5:101:BCL:HAA1	1.96	0.47
2:5:10:ILE:HG23	2:7:14:ARG:HG2	1.96	0.47
4:H:148:ASP:HB3	7:a:85:ARG:HE	1.79	0.47
8:L:301:BCL:H2	17:L:302:BPH:HBB3	1.95	0.47
2:9:7:ILE:HD13	10:A:102:SPO:H311	1.96	0.47
2:W:9:MET:HA	1:X:11:LEU:HD11	1.97	0.47
1:4:8:PHE:CE1	2:5:14:ARG:HD2	2.50	0.47
6:M:72:GLY:HA3	10:M:406:SPO:H23	1.96	0.47
8:E:101:BCL:HBA1	8:E:101:BCL:H3A	1.74	0.46
8:K:101:BCL:HHD	1:N:41:VAL:HG21	1.97	0.46
17:M:404:BPH:H4C1	17:M:404:BPH:H7C1	1.98	0.46
18:M:410:U10:H102	18:M:410:U10:H1M1	1.97	0.46
8:G:101:BCL:H93	8:G:101:BCL:H61	1.72	0.46
2:3:29:VAL:HG23	7:a:25:LEU:HD12	1.96	0.46
2:O:32:HIS:CE1	8:P:101:BCL:HMD1	2.50	0.46
3:C:39:ILE:HD13	7:a:39:LEU:HA	1.97	0.46
8:8:101:BCL:H111	8:8:101:BCL:H143	1.70	0.46
2:A:32:HIS:CE1	8:B:101:BCL:HMD1	2.51	0.46
3:C:57:ARG:HB3	5:L:71:ASP:OD1	2.15	0.46
2:S:32:HIS:CE1	8:T:101:BCL:HMD1	2.51	0.46
1:0:14:GLU:O	1:0:18:GLU:HG2	2.16	0.46
1:8:47:TRP:CE2	8:8:101:BCL:H2C	2.51	0.46
13:H:303:PGV:H062	13:H:303:PGV:H012	1.97	0.46
8:Z:102:BCL:HBA1	8:Z:102:BCL:H3A	1.71	0.46
2:5:45:THR:O	2:5:49:GLU:HG2	2.16	0.46
1:N:47:TRP:CE2	8:N:101:BCL:H2C	2.51	0.46
1:V:47:TRP:CD1	1:V:48:LEU:HG	2.50	0.46
2:1:35:LEU:HG	2:1:41:PHE:HB3	1.98	0.46
1:4:6:VAL:HG11	1:6:19:ILE:HD11	1.98	0.46
2:F:11:PHE:HZ	2:I:17:LEU:HB2	1.80	0.46
6:M:76:LEU:HD13	6:M:86:LEU:HD22	1.98	0.46
3:C:7:LYS:HD2	3:C:8:TRP:N	2.32	0.45
8:X:101:BCL:H192	8:X:101:BCL:H162	1.71	0.45
8:0:101:BCL:H111	8:0:101:BCL:H143	1.69	0.45
17:L:302:BPH:HHC	17:L:302:BPH:CBB	2.45	0.45
6:M:160:LEU:HD23	6:M:284:ILE:HG21	1.98	0.45
2:3:27:LEU:HD11	10:4:101:SPO:H9	1.98	0.45
3:C:7:LYS:HD2	3:C:8:TRP:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:98:PRO:HG3	6:M:107:PRO:HG3	1.98	0.45
6:M:223:ILE:O	6:M:227:THR:HG23	2.16	0.45
10:Y:102:SPO:H22	1:Z:23:TYR:CE1	2.52	0.45
2:3:33:LEU:HD11	7:a:28:ALA:HB1	1.98	0.45
18:L:303:U10:H201	18:L:303:U10:H23	1.98	0.45
2:1:6:LYS:HD3	2:1:9:MET:HE3	1.99	0.45
10:A:102:SPO:H6	8:D:102:BCL:HMB2	1.99	0.45
3:C:162:HIS:CE1	3:C:300:ALA:HB2	2.52	0.45
4:H:41:LEU:HB3	5:L:2:ALA:HB1	1.99	0.45
10:D:103:SPO:H32	10:D:103:SPO:H362	1.68	0.45
2:I:32:HIS:CE1	8:J:101:BCL:HMD1	2.52	0.45
10:I:102:SPO:H20	10:I:102:SPO:H181	1.79	0.45
2:K:32:HIS:CE1	8:N:101:BCL:HMD1	2.52	0.45
6:M:4:TYR:CZ	6:M:6:ASN:HA	2.52	0.45
10:U:104:SPO:H20	10:U:104:SPO:H181	1.79	0.45
2:1:6:LYS:HZ3	2:1:6:LYS:HB2	1.81	0.45
2:7:42:ASN:ND2	12:7:104:LMT:H3B	2.32	0.45
2:D:12:ASP:HB3	13:D:105:PGV:O13	2.16	0.45
2:U:24:LEU:HB2	8:U:101:BCL:H42	1.99	0.45
10:4:101:SPO:H27	10:4:101:SPO:H241	1.99	0.45
2:A:19:ALA:HB2	13:A:104:PGV:H221	1.99	0.45
6:M:202:HIS:CE1	6:M:206:ILE:HD11	2.52	0.45
10:M:406:SPO:H10	10:M:406:SPO:H81	1.84	0.44
6:M:55:TYR:HB3	2:Q:18:VAL:HG11	2.00	0.44
6:M:74:ASN:HD21	6:M:114:TRP:CD1	2.35	0.44
1:T:47:TRP:CD2	8:T:101:BCL:H2C	2.52	0.44
8:T:101:BCL:H192	8:T:101:BCL:H162	1.74	0.44
10:Y:102:SPO:H10	10:Y:102:SPO:H81	1.83	0.44
12:7:104:LMT:H6'2	5:L:77:SER:HB2	1.98	0.44
12:D:101:LMT:H51	13:L:304:PGV:H212	1.99	0.44
8:G:101:BCL:H91	8:G:101:BCL:H112	1.86	0.44
8:Y:101:BCL:H143	8:Y:101:BCL:H111	1.76	0.44
6:M:229:PHE:HB2	6:M:244:ALA:HB2	1.99	0.44
2:1:13:PRO:HB2	2:Y:10:ILE:HD12	2.00	0.44
2:9:10:ILE:CG1	10:A:102:SPO:H37	2.47	0.44
13:F:105:PGV:H262	13:F:105:PGV:H231	1.87	0.44
13:H:303:PGV:H102	13:H:303:PGV:H131	1.57	0.44
8:X:101:BCL:H41	8:X:101:BCL:H62	1.54	0.44
7:a:3:ILE:HD11	7:a:12:PHE:HB2	2.00	0.44
10:S:102:SPO:H362	10:S:102:SPO:H32	1.72	0.44
10:K:102:SPO:H6	8:O:101:BCL:HMB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:L:303:U10:H471	18:L:303:U10:H43	1.79	0.43
1:B:6:VAL:HG21	1:E:19:ILE:HD11	1.99	0.43
8:Q:101:BCL:HHD	8:Q:101:BCL:HAC1	1.82	0.43
3:C:208:LEU:HB2	6:M:89:GLN:NE2	2.34	0.43
1:J:47:TRP:CD2	8:J:101:BCL:H2C	2.54	0.43
8:R:101:BCL:H61	8:R:101:BCL:H102	1.42	0.43
10:U:102:SPO:H20	10:U:102:SPO:H181	1.81	0.43
8:2:101:BCL:H162	8:2:101:BCL:H192	1.74	0.43
2:3:27:LEU:HD21	10:4:101:SPO:H11	2.00	0.43
10:4:101:SPO:H26	10:4:101:SPO:H301	1.73	0.43
8:J:101:BCL:H141	8:J:101:BCL:H162	1.81	0.43
6:M:226:VAL:HG23	6:M:231:GLY:HA3	1.99	0.43
1:R:47:TRP:CD2	8:R:101:BCL:H2C	2.54	0.43
10:U:102:SPO:H361	1:V:22:VAL:HG11	2.00	0.43
8:6:101:BCL:H93	8:6:101:BCL:H61	1.77	0.43
2:7:43:TRP:CZ2	8:7:101:BCL:HHC	2.54	0.43
10:A:102:SPO:H32	10:A:102:SPO:H362	1.68	0.43
10:D:103:SPO:HM11	2:F:33:LEU:HG	2.01	0.43
6:M:97:PRO:HD3	6:M:176:PRO:HA	2.01	0.43
8:M:403:BCL:H41	8:M:403:BCL:H62	1.53	0.43
1:P:47:TRP:CE2	8:P:101:BCL:H2C	2.53	0.43
1:X:8:PHE:HD2	2:Y:14:ARG:HH21	1.65	0.43
2:5:10:ILE:CG1	10:7:102:SPO:H37	2.48	0.43
10:S:102:SPO:H20	10:S:102:SPO:H181	1.82	0.43
8:V:101:BCL:H93	8:V:101:BCL:H61	1.69	0.43
2:3:27:LEU:HD23	8:4:102:BCL:HED2	2.01	0.43
10:7:102:SPO:H20	10:7:102:SPO:H181	1.80	0.43
8:B:101:BCL:HBA1	8:B:101:BCL:H3A	1.74	0.43
4:H:260:PHE:HB3	5:L:18:ILE:HD13	2.00	0.43
1:V:11:LEU:HD21	1:V:19:ILE:HD12	2.00	0.43
2:W:11:PHE:HB3	2:W:16:VAL:HG21	1.99	0.43
8:1:101:BCL:HHB	10:Y:102:SPO:H6	2.00	0.43
3:C:216:SER:HB3	3:C:223:VAL:HG12	2.01	0.43
2:1:9:MET:HA	1:2:12:THR:HG23	2.00	0.43
8:L:307:BCL:H13	8:L:307:BCL:H172	1.76	0.43
10:O:102:SPO:H32	10:O:102:SPO:H362	1.69	0.43
1:B:47:TRP:CD2	8:B:101:BCL:H2C	2.55	0.42
10:D:103:SPO:H20	10:D:103:SPO:H181	1.83	0.42
4:H:113:ALA:HB2	4:H:245:GLY:HA3	2.01	0.42
5:L:131:THR:HA	5:L:135:PHE:HB2	2.01	0.42
8:V:101:BCL:HBA1	8:V:101:BCL:H3A	1.69	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:101:BCL:HHD	1:8:41:VAL:HG21	2.00	0.42
10:F:102:SPO:H20	10:F:102:SPO:H181	1.85	0.42
6:M:76:LEU:HG	6:M:81:TRP:HA	2.01	0.42
10:4:101:SPO:H10	8:5:101:BCL:H3A	2.01	0.42
6:M:197:TYR:CE1	8:M:403:BCL:HMC2	2.53	0.42
8:O:101:BCL:H61	8:O:101:BCL:H102	1.44	0.42
8:T:101:BCL:HBA1	8:T:101:BCL:H3A	1.68	0.42
10:Y:102:SPO:H15	10:Y:102:SPO:H131	1.88	0.42
10:4:101:SPO:H31	8:5:101:BCL:HBB2	2.00	0.42
2:D:10:ILE:HD11	10:F:102:SPO:H403	2.01	0.42
8:N:101:BCL:H192	8:N:101:BCL:H161	1.81	0.42
2:3:24:LEU:HD22	8:4:102:BCL:HED1	2.02	0.42
2:7:32:HIS:CE1	8:8:101:BCL:HMD1	2.54	0.42
10:K:102:SPO:H32	10:K:102:SPO:H362	1.71	0.42
8:L:307:BCL:O1D	6:M:203:ALA:HB1	2.20	0.42
6:M:81:TRP:CH2	2:S:34:VAL:HG22	2.55	0.42
10:O:102:SPO:H20	10:O:102:SPO:H181	1.80	0.42
8:5:101:BCL:HBC3	8:5:101:BCL:H2C	1.85	0.42
8:A:101:BCL:H143	8:A:101:BCL:H111	1.79	0.42
5:L:247:VAL:HA	5:L:250:ILE:HG22	2.01	0.42
10:U:104:SPO:H26	10:U:104:SPO:H241	1.91	0.42
1:Z:47:TRP:CZ2	8:Z:102:BCL:HHC	2.55	0.42
10:F:102:SPO:HM11	2:I:33:LEU:HG	2.02	0.42
2:9:10:ILE:HG12	10:A:102:SPO:H37	2.01	0.42
5:L:133:GLU:OE1	5:L:146:ALA:HB1	2.20	0.42
5:L:245:SER:OG	8:L:301:BCL:HMA2	2.20	0.42
10:U:104:SPO:C16	8:X:101:BCL:H12	2.50	0.42
2:5:43:TRP:CE3	8:5:101:BCL:HBC3	2.54	0.42
10:A:102:SPO:C16	8:B:101:BCL:H12	2.50	0.41
4:H:135:LEU:HD13	4:H:170:VAL:HG21	2.02	0.41
10:Q:102:SPO:H26	10:Q:102:SPO:H241	1.90	0.41
1:X:47:TRP:CE2	8:X:101:BCL:H2C	2.55	0.41
2:1:32:HIS:CG	10:Y:102:SPO:H41	2.55	0.41
2:3:27:LEU:CD2	10:4:101:SPO:H11	2.50	0.41
8:A:101:BCL:H151	8:A:101:BCL:H18	1.92	0.41
10:M:406:SPO:H20	10:M:406:SPO:H181	1.79	0.41
8:X:101:BCL:H162	8:X:101:BCL:H141	1.81	0.41
10:Y:102:SPO:H392	1:Z:19:ILE:HG12	2.02	0.41
10:5:102:SPO:H26	10:5:102:SPO:H241	1.88	0.41
8:E:101:BCL:H93	8:E:101:BCL:H61	1.78	0.41
6:M:98:PRO:HB3	6:M:107:PRO:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:M:405:U10:H412	18:M:405:U10:H371	1.91	0.41
8:4:102:BCL:HBA1	8:4:102:BCL:H3A	1.79	0.41
13:L:304:PGV:H291	13:L:304:PGV:H321	1.90	0.41
2:3:36:LEU:HD13	7:a:32:TYR:HB3	2.02	0.41
1:6:31:SER:OG	8:6:101:BCL:H2	2.19	0.41
10:7:102:SPO:H32	10:7:102:SPO:H362	1.73	0.41
3:C:208:LEU:HD23	3:C:213:TYR:HA	2.01	0.41
3:C:324:ALA:HB3	14:C:401:HEC:HAD2	2.02	0.41
4:H:260:PHE:HB3	5:L:18:ILE:CD1	2.50	0.41
5:L:242:VAL:HG21	17:L:302:BPH:HBC3	2.03	0.41
8:L:308:BCL:HMA1	8:L:308:BCL:H142	2.02	0.41
2:U:6:LYS:HE3	10:U:104:SPO:H393	2.01	0.41
13:H:305:PGV:H242	13:H:305:PGV:H211	1.77	0.41
8:K:101:BCL:H62	8:K:101:BCL:H41	1.70	0.41
5:L:37:VAL:HA	18:M:405:U10:H403	2.03	0.41
17:L:302:BPH:H141	8:L:307:BCL:HBB3	2.03	0.41
2:O:7:ILE:HD13	10:Q:102:SPO:H311	2.02	0.41
10:U:104:SPO:H32	10:U:104:SPO:H362	1.80	0.41
8:0:101:BCL:HHD	2:9:35:LEU:HD11	2.03	0.41
10:7:102:SPO:H6	8:9:101:BCL:HMB2	2.01	0.41
5:L:136:ARG:HB3	5:L:137:PRO:HD3	2.03	0.41
2:3:10:ILE:HA	1:4:8:PHE:CE1	2.55	0.41
18:L:303:U10:H171	18:L:303:U10:H211	1.92	0.41
10:O:102:SPO:H26	10:O:102:SPO:H241	1.92	0.41
2:U:27:LEU:HD23	8:V:101:BCL:HED3	2.03	0.41
8:0:101:BCL:HBA1	8:0:101:BCL:H3A	1.76	0.41
2:1:17:LEU:HB3	2:Y:11:PHE:HZ	1.86	0.41
1:2:41:VAL:HG21	8:2:101:BCL:HBC1	2.03	0.41
8:4:102:BCL:H13	8:4:102:BCL:H102	1.91	0.41
1:6:6:VAL:HG21	1:8:19:ILE:HD11	2.02	0.41
4:H:226:LYS:HD2	4:H:235:GLU:OE2	2.21	0.41
6:M:65:CYS:HB2	17:M:404:BPH:H143	2.03	0.41
1:T:47:TRP:CE2	8:T:101:BCL:H2C	2.55	0.41
8:X:101:BCL:HBA1	8:X:101:BCL:H3A	1.65	0.41
2:3:35:LEU:HD11	8:4:102:BCL:HHD	2.03	0.41
8:G:101:BCL:HBA1	8:G:101:BCL:H3A	1.76	0.41
4:H:82:ARG:HH21	4:H:115:TRP:H	1.68	0.41
18:L:303:U10:H271	18:L:303:U10:H251	1.84	0.41
2:S:10:ILE:CG1	10:U:102:SPO:H37	2.51	0.41
1:T:31:SER:HB3	8:T:101:BCL:H72	2.02	0.41
8:B:101:BCL:H192	8:B:101:BCL:H162	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:102:BCL:H162	8:Z:102:BCL:H192	1.72	0.40
1:R:47:TRP:CE2	8:R:101:BCL:H2C	2.56	0.40
1:0:47:TRP:CD2	8:0:101:BCL:H2C	2.56	0.40
8:1:101:BCL:H203	2:Y:7:ILE:HG21	2.03	0.40
1:4:24:MET:HA	1:4:24:MET:HE2	2.03	0.40
2:5:3:LYS:HD2	2:5:6:LYS:HE3	2.02	0.40
10:A:102:SPO:H20	10:A:102:SPO:H181	1.82	0.40
8:2:101:BCL:H93	8:2:101:BCL:H61	1.80	0.40
10:9:102:SPO:H26	10:9:102:SPO:H241	1.92	0.40
8:6:101:BCL:H62	8:6:101:BCL:H41	1.91	0.40
1:8:47:TRP:CD2	8:8:101:BCL:H2C	2.57	0.40
4:H:260:PHE:HD2	5:L:18:ILE:HD12	1.87	0.40
2:W:7:ILE:HD13	10:Y:102:SPO:H311	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	43/48 (90%)	43 (100%)	0	0	100	100
1	2	39/48 (81%)	37 (95%)	2 (5%)	0	100	100
1	4	41/48 (85%)	41 (100%)	0	0	100	100
1	6	43/48 (90%)	43 (100%)	0	0	100	100
1	8	43/48 (90%)	43 (100%)	0	0	100	100
1	B	43/48 (90%)	43 (100%)	0	0	100	100
1	E	43/48 (90%)	42 (98%)	1 (2%)	0	100	100
1	G	43/48 (90%)	42 (98%)	1 (2%)	0	100	100
1	J	43/48 (90%)	42 (98%)	1 (2%)	0	100	100
1	N	43/48 (90%)	42 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	P	44/48 (92%)	43 (98%)	1 (2%)	0	100	100
1	R	43/48 (90%)	43 (100%)	0	0	100	100
1	T	42/48 (88%)	42 (100%)	0	0	100	100
1	V	43/48 (90%)	43 (100%)	0	0	100	100
1	X	43/48 (90%)	43 (100%)	0	0	100	100
1	Z	38/48 (79%)	35 (92%)	3 (8%)	0	100	100
2	1	47/54 (87%)	47 (100%)	0	0	100	100
2	3	44/54 (82%)	44 (100%)	0	0	100	100
2	5	51/54 (94%)	51 (100%)	0	0	100	100
2	7	51/54 (94%)	51 (100%)	0	0	100	100
2	9	52/54 (96%)	52 (100%)	0	0	100	100
2	A	51/54 (94%)	51 (100%)	0	0	100	100
2	D	51/54 (94%)	51 (100%)	0	0	100	100
2	F	51/54 (94%)	51 (100%)	0	0	100	100
2	I	51/54 (94%)	51 (100%)	0	0	100	100
2	K	51/54 (94%)	51 (100%)	0	0	100	100
2	O	51/54 (94%)	51 (100%)	0	0	100	100
2	Q	51/54 (94%)	51 (100%)	0	0	100	100
2	S	51/54 (94%)	51 (100%)	0	0	100	100
2	U	51/54 (94%)	51 (100%)	0	0	100	100
2	W	51/54 (94%)	51 (100%)	0	0	100	100
2	Y	49/54 (91%)	49 (100%)	0	0	100	100
3	C	350/356 (98%)	341 (97%)	9 (3%)	0	100	100
4	H	258/260 (99%)	254 (98%)	4 (2%)	0	100	100
5	L	281/284 (99%)	275 (98%)	6 (2%)	0	100	100
6	M	316/321 (98%)	308 (98%)	8 (2%)	0	100	100
7	a	108/229 (47%)	107 (99%)	1 (1%)	0	100	100
All	All	2794/3082 (91%)	2756 (99%)	38 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	37/39 (95%)	37 (100%)	0	100	100
1	2	31/39 (80%)	28 (90%)	3 (10%)	6	0
1	4	35/39 (90%)	35 (100%)	0	100	100
1	6	37/39 (95%)	37 (100%)	0	100	100
1	8	37/39 (95%)	37 (100%)	0	100	100
1	B	37/39 (95%)	37 (100%)	0	100	100
1	E	37/39 (95%)	37 (100%)	0	100	100
1	G	37/39 (95%)	36 (97%)	1 (3%)	40	22
1	J	37/39 (95%)	37 (100%)	0	100	100
1	N	37/39 (95%)	37 (100%)	0	100	100
1	P	38/39 (97%)	37 (97%)	1 (3%)	41	24
1	R	37/39 (95%)	36 (97%)	1 (3%)	40	22
1	T	36/39 (92%)	35 (97%)	1 (3%)	38	21
1	V	37/39 (95%)	37 (100%)	0	100	100
1	X	37/39 (95%)	36 (97%)	1 (3%)	40	22
1	Z	32/39 (82%)	32 (100%)	0	100	100
2	1	43/43 (100%)	37 (86%)	6 (14%)	3	0
2	3	41/43 (95%)	37 (90%)	4 (10%)	6	0
2	5	43/43 (100%)	42 (98%)	1 (2%)	45	29
2	7	43/43 (100%)	43 (100%)	0	100	100
2	9	44/43 (102%)	43 (98%)	1 (2%)	45	29
2	A	43/43 (100%)	43 (100%)	0	100	100
2	D	43/43 (100%)	42 (98%)	1 (2%)	45	29
2	F	43/43 (100%)	43 (100%)	0	100	100
2	I	43/43 (100%)	43 (100%)	0	100	100
2	K	43/43 (100%)	43 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	O	43/43 (100%)	43 (100%)	0	100	100
2	Q	43/43 (100%)	43 (100%)	0	100	100
2	S	43/43 (100%)	42 (98%)	1 (2%)	45	29
2	U	43/43 (100%)	42 (98%)	1 (2%)	45	29
2	W	43/43 (100%)	43 (100%)	0	100	100
2	Y	43/43 (100%)	39 (91%)	4 (9%)	7	0
3	C	295/298 (99%)	289 (98%)	6 (2%)	50	35
4	H	210/210 (100%)	207 (99%)	3 (1%)	62	50
5	L	224/225 (100%)	221 (99%)	3 (1%)	65	52
6	M	256/257 (100%)	252 (98%)	4 (2%)	58	45
7	a	80/162 (49%)	73 (91%)	7 (9%)	8	1
All	All	2331/2464 (95%)	2281 (98%)	50 (2%)	49	32

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	6	LYS
2	1	17	LEU
2	1	25	PHE
2	1	27	LEU
2	1	33	LEU
2	1	44	LEU
1	2	12	THR
1	2	14	GLU
1	2	29	LEU
2	3	17	LEU
2	3	29	VAL
2	3	38	THR
2	3	46	ILE
2	5	36	LEU
2	9	26	LEU
3	C	4	LYS
3	C	7	LYS
3	C	14	GLU
3	C	21	MET
3	C	34	VAL
3	C	148	CYS
2	D	12	ASP

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Mol	Chain	Res	Type
1	G	6	VAL
4	H	182	LEU
4	H	205	PHE
4	H	237	ASP
5	L	39	THR
5	L	217	PHE
5	L	248	CYS
6	M	34	MET
6	M	61	LEU
6	M	89	GLN
6	M	216	PHE
1	P	3	GLU
1	R	6	VAL
2	S	26	LEU
1	T	11	LEU
2	U	6	LYS
1	X	11	LEU
2	Y	3	LYS
2	Y	10	ILE
2	Y	17	LEU
2	Y	24	LEU
7	a	6	THR
7	a	9	ARG
7	a	10	PHE
7	a	12	PHE
7	a	36	LEU
7	a	39	LEU
7	a	76	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	302	GLN
1	G	17	GLN
1	J	17	GLN
5	L	240	ASN
6	M	25	ASN
6	M	74	ASN
1	T	15	GLN
7	a	2	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

14 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	$\# Z > 2$
2	FME	Q	1	2	8,9,10	0.51	0	7,9,11	1.04	1 (14%)
2	FME	S	1	2	8,9,10	0.50	0	7,9,11	0.96	1 (14%)
2	FME	I	1	2	8,9,10	0.50	0	7,9,11	0.95	1 (14%)
2	FME	A	1	2	8,9,10	0.51	0	7,9,11	0.98	1 (14%)
2	FME	F	1	2	8,9,10	0.52	0	7,9,11	0.96	1 (14%)
2	FME	3	1	2	8,9,10	0.51	0	7,9,11	1.26	1 (14%)
2	FME	K	1	2	8,9,10	0.51	0	7,9,11	0.98	1 (14%)
2	FME	7	1	2	8,9,10	0.52	0	7,9,11	1.00	1 (14%)
2	FME	O	1	2	8,9,10	0.52	0	7,9,11	0.97	1 (14%)
2	FME	U	1	2	8,9,10	0.52	0	7,9,11	0.94	1 (14%)
2	FME	9	1	2	8,9,10	0.51	0	7,9,11	0.96	1 (14%)
2	FME	W	1	2	8,9,10	0.52	0	7,9,11	1.00	1 (14%)
2	FME	5	1	2	8,9,10	0.52	0	7,9,11	0.94	1 (14%)
2	FME	D	1	2	8,9,10	0.50	0	7,9,11	0.98	1 (14%)

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
2	FME	Q	1	2	-	0/7/9/11	-
2	FME	S	1	2	-	0/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FME	I	1	2	-	0/7/9/11	-
2	FME	A	1	2	-	1/7/9/11	-
2	FME	F	1	2	-	0/7/9/11	-
2	FME	3	1	2	-	1/7/9/11	-
2	FME	K	1	2	-	1/7/9/11	-
2	FME	7	1	2	-	2/7/9/11	-
2	FME	O	1	2	-	0/7/9/11	-
2	FME	U	1	2	-	0/7/9/11	-
2	FME	9	1	2	-	1/7/9/11	-
2	FME	W	1	2	-	2/7/9/11	-
2	FME	5	1	2	-	0/7/9/11	-
2	FME	D	1	2	-	1/7/9/11	-

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3	1	FME	O-C-CA	-2.57	118.05	124.78
2	Q	1	FME	O-C-CA	-2.56	118.07	124.78
2	W	1	FME	O-C-CA	-2.52	118.18	124.78
2	7	1	FME	O-C-CA	-2.51	118.21	124.78
2	K	1	FME	O-C-CA	-2.50	118.24	124.78
2	A	1	FME	O-C-CA	-2.49	118.25	124.78
2	D	1	FME	O-C-CA	-2.48	118.28	124.78
2	F	1	FME	O-C-CA	-2.47	118.30	124.78
2	9	1	FME	O-C-CA	-2.47	118.30	124.78
2	S	1	FME	O-C-CA	-2.47	118.30	124.78
2	O	1	FME	O-C-CA	-2.46	118.34	124.78
2	I	1	FME	O-C-CA	-2.44	118.39	124.78
2	5	1	FME	O-C-CA	-2.42	118.43	124.78
2	U	1	FME	O-C-CA	-2.41	118.46	124.78

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	3	1	FME	CB-CA-N-CN
2	7	1	FME	O1-CN-N-CA
2	7	1	FME	CB-CA-N-CN
2	9	1	FME	O1-CN-N-CA
2	A	1	FME	O1-CN-N-CA

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Mol	Chain	Res	Type	Atoms
2	D	1	FME	O1-CN-N-CA
2	K	1	FME	O1-CN-N-CA
2	W	1	FME	O1-CN-N-CA
2	W	1	FME	CB-CA-N-CN

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	W	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 117 ligands modelled in this entry, 13 are unknown and 6 are monoatomic - leaving 98 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	A1EYK	Q	103	-	39,40,40	1.70	11 (28%)	47,49,49	0.77	0
8	BCL	U	101	2	64,74,74	1.68	12 (18%)	78,115,115	2.34	23 (29%)
8	BCL	W	101	2	64,74,74	1.69	14 (21%)	78,115,115	2.33	20 (25%)
8	BCL	M	403	6	64,74,74	1.72	14 (21%)	78,115,115	2.31	22 (28%)
8	BCL	F	101	2	64,74,74	1.68	12 (18%)	78,115,115	2.31	23 (29%)
13	PGV	H	305	-	35,35,50	1.11	2 (5%)	38,40,56	1.23	4 (10%)
8	BCL	S	101	2	64,74,74	1.66	13 (20%)	78,115,115	2.30	22 (28%)
8	BCL	3	101	2	45,55,74	2.17	14 (31%)	55,92,115	2.58	16 (29%)
10	SPO	U	104	-	40,41,41	0.64	0	47,50,50	1.73	13 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	BCL	O	101	2	64,74,74	1.68	12 (18%)	78,115,115	2.32	22 (28%)
8	BCL	9	101	2	64,74,74	1.68	13 (20%)	78,115,115	2.31	23 (29%)
11	A1EYK	S	103	-	39,40,40	1.69	11 (28%)	47,49,49	0.83	0
8	BCL	0	101	1	64,74,74	1.68	14 (21%)	78,115,115	2.17	21 (26%)
8	BCL	P	101	1	64,74,74	1.68	14 (21%)	78,115,115	2.16	19 (24%)
8	BCL	5	101	2	64,74,74	1.70	14 (21%)	78,115,115	2.20	23 (29%)
18	U10	L	303	-	63,63,63	0.58	2 (3%)	76,79,79	0.50	0
13	PGV	M	411	-	31,31,50	1.15	2 (6%)	33,36,56	1.22	3 (9%)
10	SPO	9	102	-	40,41,41	0.62	0	47,50,50	1.66	10 (21%)
13	PGV	L	304	-	42,42,50	0.99	2 (4%)	45,48,56	1.04	4 (8%)
10	SPO	K	102	-	40,41,41	0.62	0	47,50,50	1.70	11 (23%)
10	SPO	U	102	-	40,41,41	0.63	0	47,50,50	1.76	13 (27%)
10	SPO	Y	102	-	40,41,41	0.64	0	47,50,50	1.84	11 (23%)
14	HEC	C	402	3	32,50,50	1.56	4 (12%)	24,82,82	1.35	1 (4%)
17	BPH	M	404	-	51,70,70	0.50	1 (1%)	52,101,101	0.68	1 (1%)
13	PGV	A	104	-	46,46,50	0.95	2 (4%)	49,52,56	1.03	3 (6%)
18	U10	M	402	-	25,25,63	0.90	2 (8%)	30,33,79	0.73	0
8	BCL	Q	101	2	64,74,74	1.68	13 (20%)	78,115,115	2.42	23 (29%)
8	BCL	E	101	1	64,74,74	1.68	14 (21%)	78,115,115	2.17	18 (23%)
12	LMT	L	306	-	28,28,36	0.44	0	39,39,47	0.75	1 (2%)
11	A1EYK	I	103	-	39,40,40	1.71	11 (28%)	47,49,49	0.86	2 (4%)
8	BCL	L	308	6	64,74,74	1.71	14 (21%)	78,115,115	2.24	22 (28%)
10	SPO	I	102	-	40,41,41	0.62	0	47,50,50	1.73	11 (23%)
8	BCL	4	102	1	64,74,74	1.82	14 (21%)	78,115,115	2.24	20 (25%)
12	LMT	K	104	-	28,28,36	0.45	0	39,39,47	0.79	1 (2%)
12	LMT	M	414	-	29,29,36	0.46	0	40,40,47	0.69	1 (2%)
10	SPO	S	102	-	40,41,41	0.63	0	47,50,50	1.70	10 (21%)
13	PGV	M	408	-	44,44,50	0.96	2 (4%)	47,50,56	1.09	3 (6%)
12	LMT	F	104	-	29,29,36	0.48	0	40,40,47	1.16	4 (10%)
10	SPO	A	102	-	40,41,41	0.63	0	47,50,50	1.63	10 (21%)
13	PGV	F	105	-	50,50,50	0.91	2 (4%)	53,56,56	0.95	2 (3%)
8	BCL	K	101	2	64,74,74	1.69	13 (20%)	78,115,115	2.31	20 (25%)
12	LMT	D	101	-	36,36,36	0.37	0	47,47,47	0.84	2 (4%)
8	BCL	J	101	1	64,74,74	1.67	14 (21%)	78,115,115	2.18	19 (24%)
12	LMT	M	413	-	25,25,36	0.44	0	30,30,47	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	BCL	D	102	2	64,74,74	1.67	13 (20%)	78,115,115	2.31	23 (29%)
8	BCL	6	101	1	64,74,74	1.69	14 (21%)	78,115,115	2.17	21 (26%)
8	BCL	1	101	2	64,74,74	1.77	14 (21%)	78,115,115	2.18	19 (24%)
8	BCL	2	101	1	64,74,74	1.83	14 (21%)	78,115,115	2.16	19 (24%)
11	A1EYK	O	103	-	39,40,40	1.70	11 (28%)	47,49,49	0.81	0
12	LMT	L	305	-	28,28,36	0.49	0	39,39,47	1.13	5 (12%)
11	A1EYK	9	103	-	39,40,40	1.73	10 (25%)	47,49,49	1.30	4 (8%)
10	SPO	O	102	-	40,41,41	0.62	0	47,50,50	1.70	11 (23%)
11	A1EYK	D	104	-	39,40,40	1.71	11 (28%)	47,49,49	0.79	1 (2%)
8	BCL	X	101	1	64,74,74	1.71	14 (21%)	78,115,115	2.15	19 (24%)
13	PGV	M	407	-	39,39,50	1.06	2 (5%)	43,44,56	1.22	4 (9%)
8	BCL	N	101	1	64,74,74	1.67	13 (20%)	78,115,115	2.21	20 (25%)
12	LMT	7	104	-	28,28,36	0.50	0	39,39,47	1.08	2 (5%)
8	BCL	V	101	1	64,74,74	1.69	14 (21%)	78,115,115	2.21	20 (25%)
13	PGV	H	301	-	33,33,50	1.12	2 (6%)	36,39,56	1.19	3 (8%)
12	LMT	O	104	-	28,28,36	0.48	0	39,39,47	0.94	1 (2%)
13	PGV	H	302	-	32,32,50	1.13	2 (6%)	35,38,56	1.14	3 (8%)
13	PGV	M	409	-	42,42,50	1.02	2 (4%)	45,48,56	1.01	2 (4%)
11	A1EYK	K	103	-	39,40,40	1.71	11 (28%)	47,49,49	0.80	0
12	LMT	9	104	-	28,28,36	0.51	0	39,39,47	0.98	2 (5%)
11	A1EYK	A	103	-	39,40,40	1.68	11 (28%)	47,49,49	0.81	1 (2%)
8	BCL	7	101	2	64,74,74	1.68	12 (18%)	78,115,115	2.25	23 (29%)
8	BCL	Y	101	2	64,74,74	1.74	14 (21%)	78,115,115	2.23	19 (24%)
11	A1EYK	5	103	-	39,40,40	1.73	11 (28%)	47,49,49	0.85	0
8	BCL	Z	102	1	64,74,74	1.80	15 (23%)	78,115,115	2.19	22 (28%)
8	BCL	T	101	1	64,74,74	1.67	14 (21%)	78,115,115	2.20	20 (25%)
10	SPO	Q	102	-	40,41,41	0.62	0	47,50,50	1.69	10 (21%)
8	BCL	8	101	1	64,74,74	1.67	14 (21%)	78,115,115	2.20	21 (26%)
14	HEC	C	401	3	32,50,50	1.57	4 (12%)	24,82,82	1.47	4 (16%)
17	BPH	L	302	-	51,70,70	0.51	0	52,101,101	0.60	0
10	SPO	4	101	-	40,41,41	0.66	0	47,50,50	2.01	15 (31%)
10	SPO	D	103	-	40,41,41	0.62	0	47,50,50	1.65	11 (23%)
8	BCL	R	101	1	64,74,74	1.67	13 (20%)	78,115,115	2.16	20 (25%)
8	BCL	L	307	5	64,74,74	1.68	14 (21%)	78,115,115	2.21	20 (25%)
11	A1EYK	Z	101	-	39,40,40	1.69	10 (25%)	47,49,49	1.31	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	A1EYK	F	103	-	39,40,40	1.69	11 (28%)	47,49,49	0.82	1 (2%)
13	PGV	H	304	-	41,41,50	1.00	2 (4%)	44,47,56	1.16	4 (9%)
13	PGV	H	303	-	41,41,50	1.01	2 (4%)	44,47,56	1.09	3 (6%)
10	SPO	M	406	-	40,41,41	0.62	0	47,50,50	1.71	8 (17%)
8	BCL	L	301	5	64,74,74	1.68	14 (21%)	78,115,115	2.25	20 (25%)
11	A1EYK	U	103	-	39,40,40	1.70	10 (25%)	47,49,49	1.30	5 (10%)
8	BCL	I	101	2	64,74,74	1.67	12 (18%)	78,115,115	2.35	23 (29%)
14	HEC	C	403	3	32,50,50	1.56	4 (12%)	24,82,82	1.29	1 (4%)
10	SPO	F	102	-	40,41,41	0.61	0	47,50,50	1.65	10 (21%)
8	BCL	G	101	1	64,74,74	1.67	14 (21%)	78,115,115	2.16	20 (25%)
8	BCL	B	101	1	64,74,74	1.68	14 (21%)	78,115,115	2.16	17 (21%)
18	U10	M	405	-	63,63,63	0.61	2 (3%)	76,79,79	0.52	0
10	SPO	5	102	-	40,41,41	0.63	0	47,50,50	1.71	11 (23%)
13	PGV	D	105	-	31,31,50	1.14	2 (6%)	34,36,56	1.07	3 (8%)
8	BCL	A	101	2	64,74,74	1.69	12 (18%)	78,115,115	2.29	23 (29%)
18	U10	M	410	-	28,28,63	0.83	2 (7%)	34,37,79	0.72	0
11	A1EYK	W	102	-	39,40,40	1.80	10 (25%)	47,49,49	1.56	6 (12%)
11	A1EYK	7	103	-	39,40,40	1.69	11 (28%)	47,49,49	0.81	0
10	SPO	7	102	-	40,41,41	0.62	0	47,50,50	1.70	10 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	A1EYK	Q	103	-	-	2/44/44/44	-
8	BCL	U	101	2	-	9/37/137/137	-
8	BCL	W	101	2	-	16/37/137/137	-
8	BCL	M	403	6	-	11/37/137/137	-
8	BCL	F	101	2	-	6/37/137/137	-
13	PGV	H	305	-	-	5/37/37/55	-
8	BCL	S	101	2	-	6/37/137/137	-
8	BCL	3	101	2	-	8/15/115/137	-
10	SPO	U	104	-	-	4/47/47/47	-
8	BCL	O	101	2	-	8/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCL	9	101	2	-	11/37/137/137	-
11	A1EYK	S	103	-	-	2/44/44/44	-
8	BCL	0	101	1	-	9/37/137/137	-
8	BCL	P	101	1	-	10/37/137/137	-
8	BCL	5	101	2	-	12/37/137/137	-
18	U10	L	303	-	-	12/63/87/87	0/1/1/1
13	PGV	M	411	-	-	10/35/35/55	-
10	SPO	9	102	-	-	3/47/47/47	-
13	PGV	L	304	-	-	12/47/47/55	-
10	SPO	K	102	-	-	3/47/47/47	-
10	SPO	U	102	-	-	3/47/47/47	-
10	SPO	Y	102	-	-	4/47/47/47	-
14	HEC	C	402	3	-	2/10/54/54	-
17	BPH	M	404	-	-	6/37/105/105	0/5/6/6
13	PGV	A	104	-	-	9/51/51/55	-
18	U10	M	402	-	-	5/18/42/87	0/1/1/1
8	BCL	Q	101	2	-	11/37/137/137	-
8	BCL	E	101	1	-	9/37/137/137	-
12	LMT	L	306	-	-	1/13/53/61	0/2/2/2
11	A1EYK	I	103	-	-	1/44/44/44	-
8	BCL	L	308	6	-	9/37/137/137	-
10	SPO	I	102	-	-	3/47/47/47	-
8	BCL	4	102	1	-	10/37/137/137	-
12	LMT	K	104	-	-	3/13/53/61	0/2/2/2
12	LMT	M	414	-	-	4/14/54/61	0/2/2/2
10	SPO	S	102	-	-	3/47/47/47	-
13	PGV	M	408	-	-	12/49/49/55	-
12	LMT	F	104	-	-	5/14/54/61	0/2/2/2
10	SPO	A	102	-	-	1/47/47/47	-
13	PGV	F	105	-	-	23/55/55/55	-
8	BCL	K	101	2	-	13/37/137/137	-
12	LMT	D	101	-	-	3/21/61/61	0/2/2/2
8	BCL	J	101	1	-	8/37/137/137	-
12	LMT	M	413	-	-	5/17/37/61	0/1/1/2
8	BCL	D	102	2	-	8/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCL	6	101	1	-	11/37/137/137	-
8	BCL	1	101	2	-	15/37/137/137	-
8	BCL	2	101	1	-	14/37/137/137	-
11	A1EYK	O	103	-	-	2/44/44/44	-
12	LMT	L	305	-	-	3/13/53/61	0/2/2/2
11	A1EYK	9	103	-	-	4/44/44/44	-
10	SPO	O	102	-	-	3/47/47/47	-
11	A1EYK	D	104	-	-	2/44/44/44	-
8	BCL	X	101	1	-	14/37/137/137	-
13	PGV	M	407	-	-	4/41/41/55	-
8	BCL	N	101	1	-	6/37/137/137	-
12	LMT	7	104	-	-	4/13/53/61	0/2/2/2
8	BCL	V	101	1	-	10/37/137/137	-
13	PGV	H	301	-	-	13/38/38/55	-
12	LMT	O	104	-	-	2/13/53/61	0/2/2/2
13	PGV	H	302	-	-	17/37/37/55	-
13	PGV	M	409	-	-	16/47/47/55	-
11	A1EYK	K	103	-	-	1/44/44/44	-
12	LMT	9	104	-	-	1/13/53/61	0/2/2/2
11	A1EYK	A	103	-	-	1/44/44/44	-
8	BCL	7	101	2	-	11/37/137/137	-
8	BCL	Y	101	2	-	10/37/137/137	-
11	A1EYK	5	103	-	-	2/44/44/44	-
8	BCL	Z	102	1	-	7/37/137/137	-
8	BCL	T	101	1	-	6/37/137/137	-
10	SPO	Q	102	-	-	3/47/47/47	-
8	BCL	8	101	1	-	9/37/137/137	-
14	HEC	C	401	3	-	2/10/54/54	-
17	BPH	L	302	-	-	5/37/105/105	0/5/6/6
10	SPO	4	101	-	-	11/47/47/47	-
10	SPO	D	103	-	-	1/47/47/47	-
8	BCL	R	101	1	-	10/37/137/137	-
8	BCL	L	307	5	-	8/37/137/137	-
11	A1EYK	Z	101	-	-	1/44/44/44	-
11	A1EYK	F	103	-	-	1/44/44/44	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	PGV	H	304	-	-	11/46/46/55	-
13	PGV	H	303	-	-	15/46/46/55	-
10	SPO	M	406	-	-	5/47/47/47	-
8	BCL	L	301	5	-	12/37/137/137	-
11	A1EYK	U	103	-	-	4/44/44/44	-
8	BCL	I	101	2	-	10/37/137/137	-
14	HEC	C	403	3	-	0/10/54/54	-
10	SPO	F	102	-	-	3/47/47/47	-
8	BCL	G	101	1	-	8/37/137/137	-
8	BCL	B	101	1	-	10/37/137/137	-
18	U10	M	405	-	-	9/63/87/87	0/1/1/1
10	SPO	5	102	-	-	3/47/47/47	-
13	PGV	D	105	-	-	9/35/35/55	-
8	BCL	A	101	2	-	16/37/137/137	-
18	U10	M	410	-	-	2/21/45/87	0/1/1/1
11	A1EYK	W	102	-	-	6/44/44/44	-
11	A1EYK	7	103	-	-	1/44/44/44	-
10	SPO	7	102	-	-	2/47/47/47	-

All (683) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	403	BCL	O2D-CGD	5.30	1.46	1.33
8	1	101	BCL	O2D-CGD	5.23	1.46	1.33
8	4	102	BCL	C3B-C2B	5.21	1.48	1.39
8	L	301	BCL	O2D-CGD	5.20	1.45	1.33
8	3	101	BCL	C3B-C2B	5.20	1.48	1.39
8	3	101	BCL	O2D-CGD	5.17	1.45	1.33
8	2	101	BCL	O2D-CGD	5.16	1.45	1.33
8	O	101	BCL	O2D-CGD	5.16	1.45	1.33
8	Y	101	BCL	O2D-CGD	5.15	1.45	1.33
8	W	101	BCL	O2D-CGD	5.15	1.45	1.33
8	5	101	BCL	O2D-CGD	5.14	1.45	1.33
8	9	101	BCL	O2D-CGD	5.14	1.45	1.33
8	6	101	BCL	O2D-CGD	5.14	1.45	1.33
8	U	101	BCL	O2D-CGD	5.14	1.45	1.33
8	P	101	BCL	O2D-CGD	5.14	1.45	1.33
8	4	102	BCL	O2D-CGD	5.14	1.45	1.33
8	Z	102	BCL	C3B-C2B	5.14	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	R	101	BCL	O2D-CGD	5.13	1.45	1.33
8	Q	101	BCL	O2D-CGD	5.13	1.45	1.33
8	N	101	BCL	O2D-CGD	5.13	1.45	1.33
8	V	101	BCL	O2D-CGD	5.12	1.45	1.33
8	X	101	BCL	O2D-CGD	5.12	1.45	1.33
8	D	102	BCL	O2D-CGD	5.12	1.45	1.33
8	F	101	BCL	O2D-CGD	5.12	1.45	1.33
8	T	101	BCL	O2D-CGD	5.12	1.45	1.33
8	7	101	BCL	O2D-CGD	5.11	1.45	1.33
8	0	101	BCL	O2D-CGD	5.11	1.45	1.33
8	A	101	BCL	O2D-CGD	5.11	1.45	1.33
8	Z	102	BCL	O2D-CGD	5.11	1.45	1.33
8	E	101	BCL	O2D-CGD	5.10	1.45	1.33
8	B	101	BCL	O2D-CGD	5.10	1.45	1.33
8	J	101	BCL	O2D-CGD	5.09	1.45	1.33
8	S	101	BCL	O2D-CGD	5.09	1.45	1.33
8	8	101	BCL	O2D-CGD	5.09	1.45	1.33
8	G	101	BCL	O2D-CGD	5.07	1.45	1.33
8	K	101	BCL	O2D-CGD	5.06	1.45	1.33
8	I	101	BCL	O2D-CGD	5.06	1.45	1.33
11	W	102	A1EYK	C32-C30	5.04	1.42	1.35
8	L	307	BCL	O2D-CGD	5.04	1.45	1.33
8	1	101	BCL	C3B-C2B	4.97	1.48	1.39
8	M	403	BCL	C3B-C2B	4.95	1.48	1.39
8	W	101	BCL	C3B-C2B	4.93	1.48	1.39
8	2	101	BCL	C3B-C2B	4.93	1.48	1.39
8	O	101	BCL	C3B-C2B	4.92	1.48	1.39
8	L	308	BCL	C3B-C2B	4.91	1.48	1.39
8	L	308	BCL	O2D-CGD	4.90	1.45	1.33
8	D	102	BCL	C3B-C2B	4.90	1.48	1.39
8	E	101	BCL	C3B-C2B	4.89	1.48	1.39
8	K	101	BCL	C3B-C2B	4.88	1.48	1.39
8	A	101	BCL	C3B-C2B	4.88	1.48	1.39
8	U	101	BCL	C3B-C2B	4.88	1.48	1.39
8	9	101	BCL	C3B-C2B	4.87	1.48	1.39
8	V	101	BCL	C3B-C2B	4.87	1.48	1.39
8	F	101	BCL	C3B-C2B	4.86	1.48	1.39
8	Q	101	BCL	C3B-C2B	4.86	1.48	1.39
8	P	101	BCL	C3B-C2B	4.86	1.48	1.39
8	B	101	BCL	C3B-C2B	4.82	1.48	1.39
8	S	101	BCL	C3B-C2B	4.82	1.48	1.39
8	I	101	BCL	C3B-C2B	4.82	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	301	BCL	C3B-C2B	4.81	1.48	1.39
8	J	101	BCL	C3B-C2B	4.79	1.48	1.39
8	Y	101	BCL	C3B-C2B	4.79	1.48	1.39
8	N	101	BCL	C3B-C2B	4.78	1.48	1.39
8	X	101	BCL	C3B-C2B	4.78	1.48	1.39
8	T	101	BCL	C3B-C2B	4.76	1.48	1.39
8	0	101	BCL	C3B-C2B	4.76	1.48	1.39
8	6	101	BCL	C3B-C2B	4.74	1.47	1.39
8	8	101	BCL	C3B-C2B	4.74	1.47	1.39
8	G	101	BCL	C3B-C2B	4.74	1.47	1.39
8	R	101	BCL	C3B-C2B	4.73	1.47	1.39
8	7	101	BCL	C3B-C2B	4.72	1.47	1.39
8	3	101	BCL	C3D-C4D	-4.70	1.33	1.44
8	5	101	BCL	C3B-C2B	4.70	1.47	1.39
8	L	307	BCL	C3B-C2B	4.70	1.47	1.39
8	Z	102	BCL	C3D-C4D	-4.68	1.33	1.44
8	2	101	BCL	C3D-C4D	-4.68	1.33	1.44
8	4	102	BCL	C3D-C4D	-4.65	1.33	1.44
8	L	308	BCL	C3D-C4D	-4.63	1.33	1.44
8	Y	101	BCL	C3D-C4D	-4.61	1.33	1.44
8	V	101	BCL	C3D-C4D	-4.59	1.33	1.44
8	6	101	BCL	C3D-C4D	-4.58	1.33	1.44
8	2	101	BCL	CHD-C1D	4.58	1.47	1.38
8	K	101	BCL	C3D-C4D	-4.58	1.33	1.44
8	L	301	BCL	C3D-C4D	-4.57	1.33	1.44
8	7	101	BCL	C3D-C4D	-4.56	1.33	1.44
8	L	307	BCL	C3D-C4D	-4.56	1.33	1.44
8	X	101	BCL	C3D-C4D	-4.55	1.33	1.44
8	1	101	BCL	C3D-C4D	-4.55	1.33	1.44
8	N	101	BCL	C3D-C4D	-4.55	1.33	1.44
8	8	101	BCL	C3D-C4D	-4.54	1.33	1.44
8	5	101	BCL	C3D-C4D	-4.54	1.33	1.44
8	A	101	BCL	C3D-C4D	-4.54	1.33	1.44
8	B	101	BCL	C3D-C4D	-4.54	1.33	1.44
8	O	101	BCL	C3D-C4D	-4.53	1.33	1.44
8	U	101	BCL	C3D-C4D	-4.53	1.33	1.44
8	0	101	BCL	C3D-C4D	-4.53	1.34	1.44
8	T	101	BCL	C3D-C4D	-4.53	1.34	1.44
8	S	101	BCL	C3D-C4D	-4.52	1.34	1.44
8	E	101	BCL	C3D-C4D	-4.52	1.34	1.44
8	J	101	BCL	C3D-C4D	-4.51	1.34	1.44
8	P	101	BCL	C3D-C4D	-4.51	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	403	BCL	C3D-C4D	-4.50	1.34	1.44
8	I	101	BCL	C3D-C4D	-4.50	1.34	1.44
8	G	101	BCL	C3D-C4D	-4.50	1.34	1.44
8	R	101	BCL	C3D-C4D	-4.50	1.34	1.44
8	W	101	BCL	C3D-C4D	-4.50	1.34	1.44
8	D	102	BCL	C3D-C4D	-4.48	1.34	1.44
8	9	101	BCL	C3D-C4D	-4.48	1.34	1.44
8	F	101	BCL	C3D-C4D	-4.46	1.34	1.44
8	Q	101	BCL	C3D-C4D	-4.46	1.34	1.44
8	3	101	BCL	CHD-C1D	4.45	1.47	1.38
8	M	403	BCL	O2A-CGA	4.41	1.46	1.33
14	C	402	HEC	CBC-CAC	-4.35	1.33	1.49
8	4	102	BCL	CHD-C1D	4.34	1.46	1.38
14	C	403	HEC	CBC-CAC	-4.34	1.33	1.49
14	C	401	HEC	CBC-CAC	-4.34	1.33	1.49
8	Z	102	BCL	O2A-CGA	4.33	1.46	1.33
8	L	307	BCL	O2A-CGA	4.32	1.46	1.33
13	M	409	PGV	O03-C19	4.32	1.46	1.33
8	1	101	BCL	O2A-CGA	4.32	1.46	1.33
8	K	101	BCL	O2A-CGA	4.31	1.45	1.33
8	X	101	BCL	O2A-CGA	4.31	1.45	1.33
8	2	101	BCL	O2A-CGA	4.29	1.45	1.33
8	L	308	BCL	O2A-CGA	4.29	1.45	1.33
8	J	101	BCL	O2A-CGA	4.27	1.45	1.33
14	C	401	HEC	CBB-CAB	-4.27	1.33	1.49
14	C	403	HEC	CBB-CAB	-4.26	1.33	1.49
8	W	101	BCL	O2A-CGA	4.26	1.45	1.33
13	H	302	PGV	O03-C19	4.25	1.45	1.33
8	A	101	BCL	O2A-CGA	4.25	1.45	1.33
8	Y	101	BCL	O2A-CGA	4.25	1.45	1.33
8	6	101	BCL	O2A-CGA	4.24	1.45	1.33
13	M	407	PGV	O03-C19	4.24	1.45	1.33
8	5	101	BCL	O2A-CGA	4.24	1.45	1.33
13	M	411	PGV	O03-C19	4.24	1.45	1.33
8	4	102	BCL	O2A-CGA	4.24	1.45	1.33
8	0	101	BCL	O2A-CGA	4.23	1.45	1.33
8	9	101	BCL	O2A-CGA	4.23	1.45	1.33
13	M	409	PGV	O01-C1	4.23	1.46	1.34
8	G	101	BCL	O2A-CGA	4.23	1.45	1.33
8	Q	101	BCL	O2A-CGA	4.23	1.45	1.33
8	L	301	BCL	O2A-CGA	4.22	1.45	1.33
14	C	402	HEC	CBB-CAB	-4.22	1.33	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	O	101	BCL	O2A-CGA	4.22	1.45	1.33
13	L	304	PGV	O03-C19	4.22	1.45	1.33
8	F	101	BCL	O2A-CGA	4.21	1.45	1.33
13	A	104	PGV	O03-C19	4.21	1.45	1.33
8	1	101	BCL	CHD-C1D	4.19	1.46	1.38
8	U	101	BCL	O2A-CGA	4.19	1.45	1.33
8	D	102	BCL	O2A-CGA	4.19	1.45	1.33
13	H	303	PGV	O03-C19	4.19	1.45	1.33
8	7	101	BCL	O2A-CGA	4.19	1.45	1.33
13	F	105	PGV	O03-C19	4.19	1.45	1.33
8	Z	102	BCL	CHD-C1D	4.18	1.46	1.38
8	I	101	BCL	O2A-CGA	4.18	1.45	1.33
8	S	101	BCL	O2A-CGA	4.18	1.45	1.33
8	R	101	BCL	O2A-CGA	4.18	1.45	1.33
13	D	105	PGV	O03-C19	4.18	1.45	1.33
13	H	301	PGV	O03-C19	4.17	1.45	1.33
8	8	101	BCL	O2A-CGA	4.16	1.45	1.33
11	5	103	A1EYK	C39-C37	4.16	1.41	1.35
8	E	101	BCL	O2A-CGA	4.16	1.45	1.33
11	W	102	A1EYK	C39-C37	4.16	1.41	1.35
8	T	101	BCL	O2A-CGA	4.15	1.45	1.33
8	P	101	BCL	O2A-CGA	4.15	1.45	1.33
11	W	102	A1EYK	C31-C27	4.14	1.41	1.35
11	9	103	A1EYK	C39-C37	4.14	1.41	1.35
13	H	304	PGV	O03-C19	4.13	1.45	1.33
11	I	103	A1EYK	C39-C37	4.13	1.41	1.35
8	V	101	BCL	O2A-CGA	4.13	1.45	1.33
13	M	408	PGV	O03-C19	4.13	1.45	1.33
13	H	305	PGV	O01-C1	4.12	1.45	1.34
13	H	301	PGV	O01-C1	4.12	1.45	1.34
11	U	103	A1EYK	C31-C27	4.12	1.41	1.35
13	F	105	PGV	O01-C1	4.10	1.45	1.34
11	Q	103	A1EYK	C39-C37	4.10	1.41	1.35
11	D	104	A1EYK	C39-C37	4.10	1.41	1.35
13	H	305	PGV	O03-C19	4.09	1.45	1.33
13	H	304	PGV	O01-C1	4.09	1.45	1.34
8	N	101	BCL	O2A-CGA	4.09	1.45	1.33
13	D	105	PGV	O01-C1	4.08	1.45	1.34
13	H	303	PGV	O01-C1	4.07	1.45	1.34
11	U	103	A1EYK	C39-C37	4.07	1.41	1.35
11	K	103	A1EYK	C39-C37	4.07	1.41	1.35
13	A	104	PGV	O01-C1	4.07	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	5	103	A1EYK	C31-C27	4.06	1.41	1.35
14	C	403	HEC	C2B-C3B	-4.05	1.36	1.40
11	9	103	A1EYK	C32-C30	4.05	1.41	1.35
11	D	104	A1EYK	C31-C27	4.05	1.41	1.35
11	9	103	A1EYK	C31-C27	4.05	1.41	1.35
11	Z	101	A1EYK	C24-C18	4.05	1.41	1.35
11	W	102	A1EYK	C24-C18	4.04	1.41	1.35
11	Z	101	A1EYK	C39-C37	4.03	1.41	1.35
13	M	411	PGV	O01-C1	4.03	1.45	1.34
11	Z	101	A1EYK	C31-C27	4.03	1.41	1.35
8	3	101	BCL	O2A-CGA	4.03	1.45	1.33
11	O	103	A1EYK	C39-C37	4.03	1.41	1.35
13	M	408	PGV	O01-C1	4.02	1.45	1.34
14	C	401	HEC	C2B-C3B	-4.01	1.36	1.40
11	S	103	A1EYK	C39-C37	4.01	1.41	1.35
11	Z	101	A1EYK	C32-C30	4.01	1.41	1.35
11	U	103	A1EYK	C32-C30	4.00	1.41	1.35
8	Y	101	BCL	CHD-C1D	4.00	1.46	1.38
13	M	407	PGV	O01-C1	4.00	1.45	1.34
13	L	304	PGV	O01-C1	4.00	1.45	1.34
11	F	103	A1EYK	C32-C30	4.00	1.41	1.35
11	I	103	A1EYK	C32-C30	4.00	1.41	1.35
11	5	103	A1EYK	C32-C30	3.99	1.41	1.35
13	H	302	PGV	O01-C1	3.99	1.45	1.34
14	C	402	HEC	C2B-C3B	-3.99	1.36	1.40
11	5	103	A1EYK	C24-C18	3.99	1.41	1.35
8	B	101	BCL	O2A-CGA	3.99	1.45	1.33
11	K	103	A1EYK	C31-C27	3.98	1.41	1.35
11	I	103	A1EYK	C31-C27	3.97	1.41	1.35
11	I	103	A1EYK	C24-C18	3.96	1.41	1.35
11	K	103	A1EYK	C32-C30	3.96	1.41	1.35
11	7	103	A1EYK	C32-C30	3.95	1.41	1.35
11	D	104	A1EYK	C32-C30	3.95	1.41	1.35
11	O	103	A1EYK	C31-C27	3.94	1.41	1.35
11	Q	103	A1EYK	C32-C30	3.94	1.41	1.35
11	S	103	A1EYK	C31-C27	3.93	1.41	1.35
11	O	103	A1EYK	C32-C30	3.92	1.41	1.35
11	Q	103	A1EYK	C31-C27	3.92	1.41	1.35
11	A	103	A1EYK	C31-C27	3.91	1.41	1.35
11	K	103	A1EYK	C24-C18	3.91	1.41	1.35
11	F	103	A1EYK	C39-C37	3.91	1.41	1.35
11	7	103	A1EYK	C39-C37	3.90	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	103	A1EYK	C31-C27	3.89	1.40	1.35
11	O	103	A1EYK	C24-C18	3.88	1.40	1.35
11	7	103	A1EYK	C31-C27	3.88	1.40	1.35
11	F	103	A1EYK	C24-C18	3.88	1.40	1.35
11	7	103	A1EYK	C24-C18	3.87	1.40	1.35
11	9	103	A1EYK	C24-C18	3.85	1.40	1.35
11	U	103	A1EYK	C24-C18	3.84	1.40	1.35
11	Q	103	A1EYK	C24-C18	3.83	1.40	1.35
11	S	103	A1EYK	C32-C30	3.83	1.40	1.35
11	D	104	A1EYK	C24-C18	3.83	1.40	1.35
11	A	103	A1EYK	C32-C30	3.81	1.40	1.35
11	A	103	A1EYK	C39-C37	3.81	1.40	1.35
8	5	101	BCL	CHD-C1D	3.79	1.45	1.38
11	A	103	A1EYK	C24-C18	3.79	1.40	1.35
8	L	308	BCL	CHD-C1D	3.79	1.45	1.38
8	X	101	BCL	CHD-C1D	3.79	1.45	1.38
8	1	101	BCL	OBD-CAD	3.73	1.28	1.22
11	S	103	A1EYK	C24-C18	3.73	1.40	1.35
8	7	101	BCL	CHD-C1D	3.70	1.45	1.38
8	6	101	BCL	CHD-C1D	3.69	1.45	1.38
8	Y	101	BCL	OBD-CAD	3.68	1.28	1.22
8	2	101	BCL	OBD-CAD	3.65	1.28	1.22
8	0	101	BCL	OBD-CAD	3.65	1.28	1.22
8	3	101	BCL	OBD-CAD	3.65	1.28	1.22
8	T	101	BCL	OBD-CAD	3.64	1.28	1.22
8	4	102	BCL	OBD-CAD	3.63	1.28	1.22
8	W	101	BCL	CHD-C1D	3.63	1.45	1.38
8	5	101	BCL	OBD-CAD	3.63	1.28	1.22
8	M	403	BCL	CHD-C1D	3.63	1.45	1.38
8	8	101	BCL	OBD-CAD	3.62	1.28	1.22
8	X	101	BCL	OBD-CAD	3.62	1.28	1.22
8	6	101	BCL	OBD-CAD	3.61	1.28	1.22
8	U	101	BCL	OBD-CAD	3.61	1.28	1.22
8	L	301	BCL	OBD-CAD	3.61	1.28	1.22
8	V	101	BCL	OBD-CAD	3.61	1.28	1.22
8	L	301	BCL	CHD-C1D	3.61	1.45	1.38
8	W	101	BCL	OBD-CAD	3.61	1.28	1.22
8	G	101	BCL	OBD-CAD	3.60	1.28	1.22
8	V	101	BCL	CHD-C1D	3.59	1.45	1.38
8	I	101	BCL	OBD-CAD	3.59	1.28	1.22
8	M	403	BCL	OBD-CAD	3.59	1.28	1.22
8	P	101	BCL	OBD-CAD	3.58	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	101	BCL	OBD-CAD	3.57	1.28	1.22
8	P	101	BCL	CHD-C1D	3.57	1.45	1.38
8	G	101	BCL	CHD-C1D	3.57	1.45	1.38
8	E	101	BCL	CHD-C1D	3.57	1.45	1.38
8	J	101	BCL	CHD-C1D	3.57	1.45	1.38
8	N	101	BCL	OBD-CAD	3.56	1.28	1.22
8	R	101	BCL	OBD-CAD	3.56	1.28	1.22
8	S	101	BCL	OBD-CAD	3.56	1.28	1.22
8	F	101	BCL	OBD-CAD	3.55	1.28	1.22
8	Q	101	BCL	OBD-CAD	3.55	1.28	1.22
8	L	307	BCL	CHD-C1D	3.55	1.45	1.38
8	J	101	BCL	OBD-CAD	3.55	1.28	1.22
8	Z	102	BCL	OBD-CAD	3.55	1.28	1.22
8	U	101	BCL	CHD-C1D	3.55	1.45	1.38
8	0	101	BCL	CHD-C1D	3.55	1.45	1.38
8	F	101	BCL	CHD-C1D	3.54	1.45	1.38
8	8	101	BCL	CHD-C1D	3.54	1.45	1.38
8	K	101	BCL	CHD-C1D	3.53	1.45	1.38
8	9	101	BCL	OBD-CAD	3.53	1.28	1.22
8	K	101	BCL	OBD-CAD	3.53	1.28	1.22
8	A	101	BCL	OBD-CAD	3.53	1.28	1.22
8	D	102	BCL	OBD-CAD	3.53	1.28	1.22
8	N	101	BCL	CHD-C1D	3.52	1.45	1.38
8	E	101	BCL	OBD-CAD	3.52	1.28	1.22
8	9	101	BCL	CHD-C1D	3.52	1.45	1.38
8	O	101	BCL	OBD-CAD	3.51	1.28	1.22
8	S	101	BCL	CHD-C1D	3.50	1.45	1.38
8	T	101	BCL	CHD-C1D	3.49	1.45	1.38
8	R	101	BCL	CHD-C1D	3.49	1.45	1.38
8	O	101	BCL	CHD-C1D	3.49	1.45	1.38
8	7	101	BCL	OBD-CAD	3.49	1.28	1.22
8	A	101	BCL	CHD-C1D	3.49	1.45	1.38
8	B	101	BCL	CHD-C1D	3.47	1.45	1.38
8	L	308	BCL	OBD-CAD	3.46	1.28	1.22
8	D	102	BCL	CHD-C1D	3.46	1.45	1.38
8	L	307	BCL	OBD-CAD	3.45	1.28	1.22
8	I	101	BCL	CHD-C1D	3.40	1.45	1.38
8	2	101	BCL	MG-NC	-3.34	1.98	2.06
8	Q	101	BCL	CHD-C1D	3.33	1.44	1.38
8	2	101	BCL	C3D-C2D	3.27	1.48	1.39
8	3	101	BCL	C3D-C2D	3.23	1.48	1.39
8	2	101	BCL	CHD-C4C	3.20	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	3	101	BCL	CHD-C4C	3.17	1.48	1.39
8	4	102	BCL	C3D-C2D	3.17	1.47	1.39
8	Z	102	BCL	C3D-C2D	3.16	1.47	1.39
8	4	102	BCL	CHD-C4C	3.15	1.48	1.39
11	9	103	A1EYK	C23-C25	3.13	1.42	1.34
8	L	307	BCL	C3D-C2D	3.12	1.47	1.39
8	1	101	BCL	C3D-C2D	3.10	1.47	1.39
8	2	101	BCL	C1D-C2D	3.10	1.51	1.45
8	4	102	BCL	C1D-C2D	3.05	1.51	1.45
14	C	401	HEC	C4B-C3B	3.04	1.48	1.43
8	R	101	BCL	C3D-C2D	3.04	1.47	1.39
8	Y	101	BCL	C3D-C2D	3.02	1.47	1.39
8	3	101	BCL	C1D-C2D	3.02	1.51	1.45
8	Z	102	BCL	CHD-C4C	3.01	1.47	1.39
8	J	101	BCL	C3D-C2D	3.01	1.47	1.39
8	2	101	BCL	MG-NA	-3.01	1.99	2.06
8	B	101	BCL	C3D-C2D	3.00	1.47	1.39
8	0	101	BCL	C3D-C2D	3.00	1.47	1.39
8	X	101	BCL	C3D-C2D	3.00	1.47	1.39
8	E	101	BCL	C3D-C2D	2.99	1.47	1.39
8	5	101	BCL	C3D-C2D	2.99	1.47	1.39
8	L	308	BCL	C3D-C2D	2.99	1.47	1.39
8	G	101	BCL	C3D-C2D	2.99	1.47	1.39
8	Y	101	BCL	C1D-C2D	2.97	1.51	1.45
8	N	101	BCL	C3D-C2D	2.97	1.47	1.39
8	P	101	BCL	C3D-C2D	2.97	1.47	1.39
8	4	102	BCL	MG-NC	-2.97	1.99	2.06
8	6	101	BCL	C3D-C2D	2.97	1.47	1.39
8	1	101	BCL	CHD-C4C	2.97	1.47	1.39
8	T	101	BCL	C3D-C2D	2.96	1.47	1.39
8	1	101	BCL	C1D-C2D	2.95	1.51	1.45
8	3	101	BCL	MG-NC	-2.94	1.99	2.06
8	V	101	BCL	C3D-C2D	2.93	1.47	1.39
8	8	101	BCL	C3D-C2D	2.93	1.47	1.39
8	3	101	BCL	MG-NA	-2.92	1.99	2.06
11	W	102	A1EYK	C23-C25	2.92	1.42	1.34
8	7	101	BCL	C3D-C2D	2.92	1.47	1.39
14	C	403	HEC	C4B-C3B	2.91	1.48	1.43
8	I	101	BCL	C3D-C2D	2.91	1.47	1.39
8	Q	101	BCL	C3D-C2D	2.91	1.47	1.39
8	G	101	BCL	C1D-ND	-2.91	1.34	1.37
8	A	101	BCL	C3D-C2D	2.91	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	U	101	BCL	C3D-C2D	2.90	1.47	1.39
8	Z	102	BCL	MG-NA	-2.90	1.99	2.06
8	Y	101	BCL	CHD-C4C	2.90	1.47	1.39
8	F	101	BCL	C3D-C2D	2.89	1.47	1.39
8	B	101	BCL	C1D-ND	-2.89	1.34	1.37
8	M	403	BCL	C3D-C2D	2.89	1.47	1.39
8	S	101	BCL	C3D-C2D	2.89	1.47	1.39
14	C	402	HEC	C4B-C3B	2.89	1.48	1.43
8	K	101	BCL	C3D-C2D	2.87	1.47	1.39
8	O	101	BCL	C3D-C2D	2.87	1.47	1.39
8	W	101	BCL	C3D-C2D	2.87	1.47	1.39
8	D	102	BCL	C3D-C2D	2.86	1.46	1.39
8	P	101	BCL	C1D-ND	-2.86	1.34	1.37
8	5	101	BCL	CHD-C4C	2.86	1.47	1.39
8	4	102	BCL	MG-NA	-2.86	1.99	2.06
8	J	101	BCL	C1D-ND	-2.86	1.34	1.37
8	9	101	BCL	C3D-C2D	2.85	1.46	1.39
8	0	101	BCL	C1D-ND	-2.85	1.34	1.37
8	R	101	BCL	C1D-ND	-2.85	1.34	1.37
8	L	307	BCL	C1D-ND	-2.84	1.34	1.37
8	L	301	BCL	C3D-C2D	2.84	1.46	1.39
8	L	308	BCL	CHD-C4C	2.83	1.47	1.39
8	E	101	BCL	C1D-ND	-2.83	1.34	1.37
8	Z	102	BCL	MG-NC	-2.80	1.99	2.06
8	V	101	BCL	C1D-ND	-2.80	1.34	1.37
8	6	101	BCL	C1D-ND	-2.79	1.34	1.37
8	1	101	BCL	MG-NC	-2.78	1.99	2.06
8	X	101	BCL	CHD-C4C	2.78	1.47	1.39
8	N	101	BCL	C1D-ND	-2.78	1.34	1.37
8	Z	102	BCL	C1D-C2D	2.77	1.50	1.45
8	T	101	BCL	C1D-ND	-2.77	1.34	1.37
8	I	101	BCL	C1D-ND	-2.76	1.34	1.37
8	5	101	BCL	C1D-C2D	2.76	1.50	1.45
8	L	308	BCL	C1D-C2D	2.75	1.50	1.45
8	Z	102	BCL	C1D-ND	-2.75	1.34	1.37
8	Q	101	BCL	C1D-ND	-2.74	1.34	1.37
8	W	101	BCL	C1D-C2D	2.73	1.50	1.45
8	8	101	BCL	C1D-ND	-2.73	1.34	1.37
8	W	101	BCL	CHD-C4C	2.73	1.46	1.39
8	M	403	BCL	CHD-C4C	2.72	1.46	1.39
8	3	101	BCL	C1D-ND	-2.72	1.34	1.37
8	7	101	BCL	CHD-C4C	2.71	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	4	102	BCL	C1D-ND	-2.71	1.34	1.37
8	U	101	BCL	C1D-C2D	2.70	1.50	1.45
8	L	301	BCL	CHD-C4C	2.68	1.46	1.39
8	O	101	BCL	C1D-C2D	2.68	1.50	1.45
8	A	101	BCL	C1D-ND	-2.68	1.34	1.37
8	D	102	BCL	C1D-C2D	2.67	1.50	1.45
8	X	101	BCL	C1D-C2D	2.67	1.50	1.45
8	9	101	BCL	CHD-C4C	2.67	1.46	1.39
8	F	101	BCL	CHD-C4C	2.66	1.46	1.39
11	9	103	A1EYK	C35-C38	2.66	1.41	1.34
8	6	101	BCL	CHD-C4C	2.66	1.46	1.39
8	F	101	BCL	C1D-C2D	2.66	1.50	1.45
8	K	101	BCL	CHD-C4C	2.66	1.46	1.39
8	L	301	BCL	C1D-C2D	2.66	1.50	1.45
11	5	103	A1EYK	C35-C38	2.66	1.41	1.34
8	O	101	BCL	CHD-C4C	2.65	1.46	1.39
8	9	101	BCL	C1D-C2D	2.65	1.50	1.45
8	U	101	BCL	CHD-C4C	2.65	1.46	1.39
8	K	101	BCL	C1D-ND	-2.64	1.34	1.37
8	A	101	BCL	CHD-C4C	2.64	1.46	1.39
8	A	101	BCL	C1D-C2D	2.64	1.50	1.45
8	K	101	BCL	C1D-C2D	2.64	1.50	1.45
8	X	101	BCL	C1D-ND	-2.64	1.34	1.37
8	V	101	BCL	CHD-C4C	2.63	1.46	1.39
8	M	403	BCL	C1D-C2D	2.63	1.50	1.45
8	L	308	BCL	C1D-ND	-2.62	1.34	1.37
18	M	402	U10	C3-C2	-2.62	1.41	1.48
11	I	103	A1EYK	C35-C38	2.62	1.41	1.34
8	I	101	BCL	CHD-C4C	2.62	1.46	1.39
8	2	101	BCL	C1D-ND	-2.62	1.34	1.37
8	S	101	BCL	C1D-C2D	2.62	1.50	1.45
11	5	103	A1EYK	C23-C25	2.61	1.41	1.34
11	W	102	A1EYK	C35-C38	2.61	1.41	1.34
8	D	102	BCL	CHD-C4C	2.61	1.46	1.39
8	S	101	BCL	CHD-C4C	2.61	1.46	1.39
8	7	101	BCL	C1D-C2D	2.60	1.50	1.45
11	K	103	A1EYK	C35-C38	2.60	1.41	1.34
11	U	103	A1EYK	C35-C38	2.60	1.41	1.34
8	Q	101	BCL	CHD-C4C	2.60	1.46	1.39
8	N	101	BCL	CHD-C4C	2.60	1.46	1.39
11	7	103	A1EYK	C35-C38	2.60	1.41	1.34
11	Z	101	A1EYK	C23-C25	2.60	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	307	BCL	CHD-C4C	2.60	1.46	1.39
8	E	101	BCL	CHD-C4C	2.60	1.46	1.39
8	I	101	BCL	C1D-C2D	2.59	1.50	1.45
8	8	101	BCL	CHD-C4C	2.59	1.46	1.39
11	Z	101	A1EYK	C35-C38	2.59	1.41	1.34
11	Q	103	A1EYK	C35-C38	2.59	1.41	1.34
8	B	101	BCL	CHD-C4C	2.59	1.46	1.39
8	U	101	BCL	C1D-ND	-2.58	1.34	1.37
11	F	103	A1EYK	C35-C38	2.58	1.41	1.34
8	Q	101	BCL	C1D-C2D	2.58	1.50	1.45
8	J	101	BCL	CHD-C4C	2.58	1.46	1.39
11	D	104	A1EYK	C35-C38	2.58	1.41	1.34
11	Z	101	A1EYK	C26-C28	2.58	1.41	1.34
8	Q	101	BCL	MG-NA	-2.58	2.00	2.06
8	P	101	BCL	CHD-C4C	2.58	1.46	1.39
8	D	102	BCL	C1D-ND	-2.58	1.34	1.37
8	O	101	BCL	C1D-ND	-2.58	1.34	1.37
8	T	101	BCL	CHD-C4C	2.57	1.46	1.39
11	5	103	A1EYK	C26-C28	2.57	1.41	1.34
8	0	101	BCL	CHD-C4C	2.57	1.46	1.39
11	U	103	A1EYK	C23-C25	2.57	1.41	1.34
11	I	103	A1EYK	C23-C25	2.57	1.41	1.34
8	9	101	BCL	C1D-ND	-2.56	1.34	1.37
11	D	104	A1EYK	C23-C25	2.56	1.41	1.34
11	K	103	A1EYK	C26-C28	2.56	1.41	1.34
8	7	101	BCL	C1D-ND	-2.56	1.34	1.37
11	F	103	A1EYK	C26-C28	2.56	1.41	1.34
8	G	101	BCL	CHD-C4C	2.55	1.46	1.39
11	Q	103	A1EYK	C26-C28	2.55	1.41	1.34
11	I	103	A1EYK	C26-C28	2.55	1.41	1.34
8	2	101	BCL	C4B-CHC	2.54	1.48	1.41
11	U	103	A1EYK	C26-C28	2.54	1.41	1.34
8	F	101	BCL	C1D-ND	-2.54	1.34	1.37
11	7	103	A1EYK	C26-C28	2.54	1.41	1.34
11	S	103	A1EYK	C23-C25	2.53	1.41	1.34
8	R	101	BCL	CHD-C4C	2.53	1.46	1.39
11	O	103	A1EYK	C35-C38	2.53	1.41	1.34
8	S	101	BCL	C1D-ND	-2.53	1.34	1.37
11	S	103	A1EYK	C35-C38	2.53	1.41	1.34
8	M	403	BCL	C1D-ND	-2.53	1.34	1.37
8	V	101	BCL	C1D-C2D	2.53	1.50	1.45
11	W	102	A1EYK	C26-C28	2.52	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	103	A1EYK	C23-C25	2.52	1.41	1.34
11	9	103	A1EYK	C26-C28	2.52	1.41	1.34
11	F	103	A1EYK	C23-C25	2.52	1.41	1.34
11	O	103	A1EYK	C23-C25	2.51	1.41	1.34
11	O	103	A1EYK	C26-C28	2.50	1.41	1.34
11	A	103	A1EYK	C35-C38	2.50	1.41	1.34
11	Q	103	A1EYK	C23-C25	2.49	1.41	1.34
11	7	103	A1EYK	C23-C25	2.49	1.41	1.34
8	2	101	BCL	C1B-CHB	2.49	1.47	1.41
8	4	102	BCL	C4B-CHC	2.49	1.47	1.41
11	S	103	A1EYK	C26-C28	2.48	1.41	1.34
11	D	104	A1EYK	C26-C28	2.48	1.41	1.34
8	Y	101	BCL	MG-NC	-2.48	2.00	2.06
18	M	405	U10	C4-C5	-2.48	1.41	1.48
11	A	103	A1EYK	C26-C28	2.48	1.41	1.34
8	Y	101	BCL	MG-NA	-2.47	2.00	2.06
8	6	101	BCL	C1D-C2D	2.47	1.50	1.45
8	1	101	BCL	MG-NA	-2.47	2.00	2.06
11	D	104	A1EYK	C15-C18	-2.47	1.40	1.45
8	8	101	BCL	C1D-C2D	2.46	1.50	1.45
8	L	301	BCL	C1D-ND	-2.46	1.34	1.37
8	3	101	BCL	C1B-CHB	2.46	1.47	1.41
11	A	103	A1EYK	C23-C25	2.46	1.40	1.34
8	Z	102	BCL	C1B-CHB	2.45	1.47	1.41
8	N	101	BCL	C1D-C2D	2.44	1.50	1.45
18	L	303	U10	C4-C5	-2.44	1.41	1.48
11	9	103	A1EYK	C15-C18	-2.44	1.40	1.45
8	1	101	BCL	C1B-CHB	2.44	1.47	1.41
18	M	410	U10	C4-C5	-2.42	1.41	1.48
11	S	103	A1EYK	C15-C18	-2.42	1.40	1.45
8	T	101	BCL	C1D-C2D	2.42	1.50	1.45
8	L	307	BCL	C1D-C2D	2.42	1.50	1.45
8	W	101	BCL	C1D-ND	-2.41	1.34	1.37
11	S	103	A1EYK	C28-C30	-2.41	1.40	1.45
11	9	103	A1EYK	C28-C30	-2.40	1.40	1.45
11	A	103	A1EYK	C28-C30	-2.40	1.40	1.45
11	7	103	A1EYK	C15-C18	-2.40	1.40	1.45
11	A	103	A1EYK	C15-C18	-2.40	1.40	1.45
8	3	101	BCL	C4B-CHC	2.40	1.47	1.41
8	5	101	BCL	MG-NA	-2.38	2.00	2.06
8	Y	101	BCL	C1D-ND	-2.38	1.34	1.37
11	A	103	A1EYK	C25-C27	-2.38	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	104	A1EYK	C28-C30	-2.38	1.40	1.45
8	5	101	BCL	MG-NC	-2.38	2.00	2.06
11	I	103	A1EYK	C15-C18	-2.38	1.40	1.45
11	Q	103	A1EYK	C28-C30	-2.38	1.40	1.45
11	U	103	A1EYK	C28-C30	-2.37	1.40	1.45
8	J	101	BCL	C1D-C2D	2.37	1.50	1.45
11	5	103	A1EYK	C15-C18	-2.37	1.40	1.45
8	5	101	BCL	C1D-ND	-2.37	1.34	1.37
11	A	103	A1EYK	C38-C37	-2.36	1.40	1.45
8	B	101	BCL	C1D-C2D	2.36	1.50	1.45
11	O	103	A1EYK	C15-C18	-2.36	1.40	1.45
11	K	103	A1EYK	C25-C27	-2.36	1.40	1.45
11	Q	103	A1EYK	C15-C18	-2.35	1.40	1.45
11	F	103	A1EYK	C15-C18	-2.35	1.40	1.45
8	E	101	BCL	C1D-C2D	2.35	1.50	1.45
8	I	101	BCL	MG-NA	-2.35	2.00	2.06
11	O	103	A1EYK	C28-C30	-2.35	1.40	1.45
11	F	103	A1EYK	C28-C30	-2.34	1.40	1.45
8	1	101	BCL	C4B-CHC	2.34	1.47	1.41
8	0	101	BCL	C1D-C2D	2.34	1.49	1.45
11	K	103	A1EYK	C15-C18	-2.34	1.40	1.45
11	K	103	A1EYK	C28-C30	-2.34	1.40	1.45
11	W	102	A1EYK	C38-C37	-2.34	1.40	1.45
8	P	101	BCL	C1D-C2D	2.33	1.49	1.45
8	L	308	BCL	MG-NA	-2.33	2.00	2.06
8	Q	101	BCL	C1B-CHB	2.32	1.47	1.41
8	5	101	BCL	C1B-CHB	2.32	1.47	1.41
11	S	103	A1EYK	C38-C37	-2.32	1.41	1.45
8	Z	102	BCL	C4B-CHC	2.31	1.47	1.41
11	I	103	A1EYK	C28-C30	-2.31	1.41	1.45
8	4	102	BCL	C1B-CHB	2.31	1.47	1.41
11	5	103	A1EYK	C28-C30	-2.31	1.41	1.45
11	O	103	A1EYK	C38-C37	-2.31	1.41	1.45
11	Q	103	A1EYK	C25-C27	-2.30	1.41	1.45
8	X	101	BCL	MG-NC	-2.30	2.00	2.06
18	M	402	U10	C4-C5	-2.29	1.42	1.48
8	F	101	BCL	C1B-CHB	2.29	1.47	1.41
8	X	101	BCL	MG-NA	-2.29	2.00	2.06
18	M	405	U10	C3-C2	-2.29	1.42	1.48
11	O	103	A1EYK	C25-C27	-2.29	1.41	1.45
11	K	103	A1EYK	C38-C37	-2.29	1.41	1.45
11	W	102	A1EYK	C15-C18	-2.29	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	Y	101	BCL	C1B-CHB	2.29	1.47	1.41
11	7	103	A1EYK	C28-C30	-2.29	1.41	1.45
11	7	103	A1EYK	C25-C27	-2.29	1.41	1.45
11	W	102	A1EYK	C28-C30	-2.29	1.41	1.45
11	U	103	A1EYK	C25-C27	-2.28	1.41	1.45
8	A	101	BCL	MG-NA	-2.28	2.00	2.06
8	G	101	BCL	C1D-C2D	2.27	1.49	1.45
11	I	103	A1EYK	C38-C37	-2.26	1.41	1.45
8	L	308	BCL	C1B-CHB	2.26	1.47	1.41
8	R	101	BCL	C1D-C2D	2.26	1.49	1.45
11	F	103	A1EYK	C25-C27	-2.26	1.41	1.45
11	U	103	A1EYK	C38-C37	-2.26	1.41	1.45
11	S	103	A1EYK	C25-C27	-2.26	1.41	1.45
8	L	308	BCL	MG-NC	-2.25	2.00	2.06
11	Q	103	A1EYK	C38-C37	-2.25	1.41	1.45
11	F	103	A1EYK	C38-C37	-2.25	1.41	1.45
11	I	103	A1EYK	C25-C27	-2.25	1.41	1.45
11	9	103	A1EYK	C38-C37	-2.24	1.41	1.45
8	I	101	BCL	C1B-CHB	2.24	1.47	1.41
18	L	303	U10	C3-C2	-2.24	1.42	1.48
8	1	101	BCL	C1D-ND	-2.24	1.35	1.37
11	7	103	A1EYK	C38-C37	-2.24	1.41	1.45
11	D	104	A1EYK	C25-C27	-2.24	1.41	1.45
8	U	101	BCL	MG-NA	-2.24	2.01	2.06
8	A	101	BCL	C1B-CHB	2.23	1.47	1.41
8	B	101	BCL	MG-NA	-2.23	2.01	2.06
8	M	403	BCL	C4B-CHC	2.23	1.47	1.41
8	6	101	BCL	MG-NC	-2.23	2.01	2.06
8	F	101	BCL	MG-NA	-2.23	2.01	2.06
11	5	103	A1EYK	C38-C37	-2.23	1.41	1.45
11	D	104	A1EYK	C38-C37	-2.22	1.41	1.45
11	Z	101	A1EYK	C25-C27	-2.22	1.41	1.45
8	K	101	BCL	C1B-CHB	2.21	1.47	1.41
11	Z	101	A1EYK	C28-C30	-2.21	1.41	1.45
11	Z	101	A1EYK	C38-C37	-2.21	1.41	1.45
11	5	103	A1EYK	C25-C27	-2.21	1.41	1.45
8	X	101	BCL	C1B-CHB	2.20	1.47	1.41
8	V	101	BCL	MG-NC	-2.20	2.01	2.06
8	S	101	BCL	C1B-CHB	2.20	1.47	1.41
8	O	101	BCL	C1B-CHB	2.20	1.47	1.41
8	K	101	BCL	MG-NA	-2.19	2.01	2.06
8	M	403	BCL	MG-NC	-2.19	2.01	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	9	101	BCL	C1B-CHB	2.19	1.47	1.41
8	L	307	BCL	C1B-CHB	2.19	1.47	1.41
8	D	102	BCL	C1B-CHB	2.19	1.47	1.41
8	L	307	BCL	MG-NC	-2.19	2.01	2.06
8	O	101	BCL	MG-NA	-2.18	2.01	2.06
8	9	101	BCL	MG-NA	-2.18	2.01	2.06
8	L	307	BCL	MG-NA	-2.18	2.01	2.06
18	M	410	U10	C3-C2	-2.17	1.42	1.48
8	V	101	BCL	MG-NA	-2.17	2.01	2.06
8	E	101	BCL	C4B-CHC	2.17	1.47	1.41
8	U	101	BCL	C1B-CHB	2.17	1.47	1.41
8	8	101	BCL	C1B-CHB	2.16	1.47	1.41
8	B	101	BCL	C1B-CHB	2.15	1.47	1.41
8	E	101	BCL	C1B-CHB	2.15	1.47	1.41
8	0	101	BCL	C1B-CHB	2.15	1.47	1.41
8	7	101	BCL	C1B-CHB	2.15	1.47	1.41
8	M	403	BCL	MG-NA	-2.15	2.01	2.06
8	V	101	BCL	C1B-CHB	2.14	1.46	1.41
8	Y	101	BCL	C4B-CHC	2.13	1.46	1.41
8	D	102	BCL	MG-NA	-2.13	2.01	2.06
8	P	101	BCL	C4B-CHC	2.13	1.46	1.41
8	7	101	BCL	MG-NA	-2.13	2.01	2.06
8	6	101	BCL	C1B-CHB	2.13	1.46	1.41
8	G	101	BCL	C1B-CHB	2.13	1.46	1.41
8	T	101	BCL	C1B-CHB	2.12	1.46	1.41
8	M	403	BCL	C1B-CHB	2.12	1.46	1.41
8	0	101	BCL	C4B-CHC	2.12	1.46	1.41
8	E	101	BCL	MG-NA	-2.12	2.01	2.06
8	W	101	BCL	MG-NA	-2.12	2.01	2.06
8	R	101	BCL	C1B-CHB	2.12	1.46	1.41
8	N	101	BCL	C1B-CHB	2.12	1.46	1.41
8	B	101	BCL	MG-NC	-2.11	2.01	2.06
8	6	101	BCL	C4B-CHC	2.11	1.46	1.41
8	L	308	BCL	C4B-CHC	2.11	1.46	1.41
8	P	101	BCL	C1B-CHB	2.10	1.46	1.41
8	6	101	BCL	MG-NA	-2.10	2.01	2.06
8	V	101	BCL	C4B-CHC	2.10	1.46	1.41
8	J	101	BCL	C1B-CHB	2.09	1.46	1.41
8	N	101	BCL	C4B-CHC	2.09	1.46	1.41
8	L	301	BCL	MG-NC	-2.09	2.01	2.06
8	5	101	BCL	C4B-CHC	2.09	1.46	1.41
8	B	101	BCL	C4B-CHC	2.09	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	T	101	BCL	C4B-CHC	2.09	1.46	1.41
8	L	301	BCL	C4B-CHC	2.09	1.46	1.41
8	8	101	BCL	C4B-CHC	2.09	1.46	1.41
8	T	101	BCL	MG-NC	-2.08	2.01	2.06
8	E	101	BCL	MG-NC	-2.08	2.01	2.06
8	W	101	BCL	C1B-CHB	2.08	1.46	1.41
8	G	101	BCL	C4B-CHC	2.07	1.46	1.41
8	Q	101	BCL	C4D-CHA	2.07	1.45	1.38
8	L	301	BCL	C1B-CHB	2.07	1.46	1.41
8	T	101	BCL	MG-NA	-2.06	2.01	2.06
8	S	101	BCL	MG-NA	-2.05	2.01	2.06
8	J	101	BCL	C4B-CHC	2.05	1.46	1.41
8	X	101	BCL	C4B-CHC	2.05	1.46	1.41
8	W	101	BCL	C4B-CHC	2.05	1.46	1.41
8	R	101	BCL	C4B-CHC	2.04	1.46	1.41
8	8	101	BCL	MG-NC	-2.04	2.01	2.06
8	P	101	BCL	MG-NA	-2.03	2.01	2.06
8	Z	102	BCL	C4D-CHA	2.03	1.45	1.38
8	0	101	BCL	MG-NC	-2.03	2.01	2.06
8	J	101	BCL	MG-NC	-2.03	2.01	2.06
8	J	101	BCL	MG-NA	-2.02	2.01	2.06
8	9	101	BCL	C4B-CHC	2.02	1.46	1.41
8	K	101	BCL	C4B-CHC	2.02	1.46	1.41
8	8	101	BCL	MG-NA	-2.02	2.01	2.06
8	D	102	BCL	C4B-CHC	2.02	1.46	1.41
8	0	101	BCL	MG-NA	-2.02	2.01	2.06
8	L	307	BCL	C4B-CHC	2.01	1.46	1.41
8	G	101	BCL	MG-NC	-2.01	2.01	2.06
8	R	101	BCL	MG-NA	-2.01	2.01	2.06
17	M	404	BPH	C3A-C2A	-2.01	1.52	1.54
8	P	101	BCL	MG-NC	-2.01	2.01	2.06
8	N	101	BCL	MG-NA	-2.01	2.01	2.06
8	S	101	BCL	C4B-CHC	2.01	1.46	1.41
8	L	301	BCL	MG-NA	-2.01	2.01	2.06
8	G	101	BCL	MG-NA	-2.00	2.01	2.06
8	W	101	BCL	MG-NC	-2.00	2.01	2.06

All (1010) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	2	101	BCL	CHD-C1D-ND	-9.17	116.03	124.45
8	4	102	BCL	CHD-C1D-ND	-9.16	116.04	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	3	101	BCL	CHD-C1D-ND	-9.00	116.19	124.45
8	5	101	BCL	CHD-C1D-ND	-8.71	116.45	124.45
8	1	101	BCL	CHD-C1D-ND	-8.69	116.47	124.45
8	Q	101	BCL	CHD-C1D-ND	-8.67	116.48	124.45
8	Y	101	BCL	CHD-C1D-ND	-8.59	116.56	124.45
8	L	308	BCL	CHD-C1D-ND	-8.58	116.56	124.45
8	M	403	BCL	CHD-C1D-ND	-8.44	116.70	124.45
8	I	101	BCL	CHD-C1D-ND	-8.42	116.71	124.45
8	U	101	BCL	CHD-C1D-ND	-8.39	116.75	124.45
8	9	101	BCL	CHD-C1D-ND	-8.38	116.75	124.45
8	W	101	BCL	CHD-C1D-ND	-8.37	116.76	124.45
8	F	101	BCL	CHD-C1D-ND	-8.35	116.78	124.45
8	D	102	BCL	CHD-C1D-ND	-8.34	116.79	124.45
8	O	101	BCL	CHD-C1D-ND	-8.34	116.79	124.45
8	A	101	BCL	CHD-C1D-ND	-8.33	116.80	124.45
8	Z	102	BCL	CHD-C1D-ND	-8.30	116.83	124.45
8	K	101	BCL	CHD-C1D-ND	-8.30	116.83	124.45
8	S	101	BCL	CHD-C1D-ND	-8.27	116.86	124.45
8	Y	101	BCL	CMD-C2D-C1D	8.19	139.14	124.71
8	4	102	BCL	CMD-C2D-C1D	8.18	139.13	124.71
8	W	101	BCL	CMD-C2D-C1D	8.17	139.11	124.71
8	7	101	BCL	CHD-C1D-ND	-8.17	116.95	124.45
8	M	403	BCL	CMD-C2D-C1D	8.17	139.11	124.71
8	L	307	BCL	CHD-C1D-ND	-8.17	116.95	124.45
8	L	301	BCL	CMD-C2D-C1D	8.17	139.10	124.71
8	L	301	BCL	CHD-C1D-ND	-8.13	116.98	124.45
8	U	101	BCL	CMD-C2D-C1D	8.11	139.01	124.71
8	D	102	BCL	CMD-C2D-C1D	8.10	138.98	124.71
8	3	101	BCL	CMD-C2D-C1D	8.07	138.94	124.71
8	1	101	BCL	CMD-C2D-C1D	8.07	138.93	124.71
8	L	308	BCL	CMD-C2D-C1D	8.05	138.90	124.71
8	9	101	BCL	CMD-C2D-C1D	8.01	138.83	124.71
8	O	101	BCL	CMD-C2D-C1D	8.01	138.82	124.71
8	K	101	BCL	CMD-C2D-C1D	8.01	138.82	124.71
8	X	101	BCL	CHD-C1D-ND	-7.98	117.12	124.45
8	7	101	BCL	CMD-C2D-C1D	7.97	138.77	124.71
8	F	101	BCL	CMD-C2D-C1D	7.95	138.73	124.71
8	S	101	BCL	CMD-C2D-C1D	7.93	138.68	124.71
8	2	101	BCL	CMD-C2D-C1D	7.92	138.68	124.71
8	5	101	BCL	CMD-C2D-C1D	7.91	138.65	124.71
8	Q	101	BCL	CMD-C2D-C1D	7.89	138.61	124.71
8	V	101	BCL	CHD-C1D-ND	-7.88	117.21	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	101	BCL	CMD-C2D-C1D	7.86	138.56	124.71
8	I	101	BCL	CMD-C2D-C1D	7.84	138.54	124.71
8	T	101	BCL	CHD-C1D-ND	-7.76	117.33	124.45
8	8	101	BCL	CHD-C1D-ND	-7.72	117.36	124.45
8	E	101	BCL	CHD-C1D-ND	-7.69	117.39	124.45
8	B	101	BCL	CHD-C1D-ND	-7.68	117.40	124.45
8	J	101	BCL	CHD-C1D-ND	-7.67	117.41	124.45
8	6	101	BCL	CHD-C1D-ND	-7.64	117.43	124.45
8	N	101	BCL	CHD-C1D-ND	-7.64	117.43	124.45
8	Z	102	BCL	CMD-C2D-C1D	7.62	138.13	124.71
8	X	101	BCL	CMD-C2D-C1D	7.58	138.07	124.71
8	P	101	BCL	CHD-C1D-ND	-7.52	117.54	124.45
8	0	101	BCL	CHD-C1D-ND	-7.51	117.55	124.45
8	G	101	BCL	CHD-C1D-ND	-7.47	117.59	124.45
8	R	101	BCL	CHD-C1D-ND	-7.40	117.65	124.45
8	8	101	BCL	CMD-C2D-C1D	7.39	137.74	124.71
8	6	101	BCL	CMD-C2D-C1D	7.33	137.64	124.71
8	V	101	BCL	CMD-C2D-C1D	7.33	137.63	124.71
8	E	101	BCL	CMD-C2D-C1D	7.16	137.34	124.71
8	T	101	BCL	CMD-C2D-C1D	7.16	137.33	124.71
8	N	101	BCL	CMD-C2D-C1D	7.13	137.28	124.71
8	J	101	BCL	CMD-C2D-C1D	7.11	137.24	124.71
8	0	101	BCL	CMD-C2D-C1D	7.09	137.21	124.71
8	P	101	BCL	CMD-C2D-C1D	7.01	137.07	124.71
8	G	101	BCL	CMD-C2D-C1D	6.98	137.01	124.71
8	B	101	BCL	CMD-C2D-C1D	6.92	136.91	124.71
8	L	307	BCL	CMD-C2D-C1D	6.91	136.90	124.71
8	R	101	BCL	CMD-C2D-C1D	6.87	136.83	124.71
11	9	103	A1EYK	C29-C27-C25	5.60	126.90	118.08
11	W	102	A1EYK	C29-C27-C25	5.55	126.83	118.08
8	I	101	BCL	C2D-C1D-ND	5.41	114.09	110.10
8	R	101	BCL	C2D-C1D-ND	5.40	114.08	110.10
8	U	101	BCL	C2D-C1D-ND	5.35	114.05	110.10
8	J	101	BCL	C2D-C1D-ND	5.34	114.04	110.10
8	K	101	BCL	C2D-C1D-ND	5.33	114.03	110.10
8	D	102	BCL	C2D-C1D-ND	5.30	114.01	110.10
8	Q	101	BCL	C2D-C1D-ND	5.30	114.01	110.10
8	L	307	BCL	C2D-C1D-ND	5.29	114.00	110.10
8	O	101	BCL	C2D-C1D-ND	5.24	113.97	110.10
8	B	101	BCL	C2D-C1D-ND	5.23	113.96	110.10
10	4	101	SPO	C5-C6-C7	5.22	133.78	125.89
8	9	101	BCL	C2D-C1D-ND	5.21	113.94	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	W	101	BCL	C2D-C1D-ND	5.21	113.94	110.10
8	L	307	BCL	O2D-CGD-CBD	5.19	120.49	111.27
8	S	101	BCL	C2D-C1D-ND	5.19	113.93	110.10
8	G	101	BCL	C2D-C1D-ND	5.18	113.92	110.10
8	E	101	BCL	C2D-C1D-ND	5.18	113.92	110.10
8	L	301	BCL	C2D-C1D-ND	5.18	113.92	110.10
8	T	101	BCL	C2D-C1D-ND	5.16	113.91	110.10
8	N	101	BCL	C2D-C1D-ND	5.14	113.89	110.10
8	0	101	BCL	C2D-C1D-ND	5.12	113.88	110.10
8	8	101	BCL	C2D-C1D-ND	5.11	113.87	110.10
11	U	103	A1EYK	C22-C18-C15	5.10	126.11	118.08
8	P	101	BCL	C2D-C1D-ND	5.10	113.86	110.10
8	M	403	BCL	C3D-C2D-C1D	-5.09	98.88	105.83
8	L	301	BCL	C3D-C2D-C1D	-5.06	98.93	105.83
8	1	101	BCL	O2D-CGD-CBD	5.05	120.24	111.27
8	M	403	BCL	C2D-C1D-ND	5.05	113.83	110.10
8	2	101	BCL	O2D-CGD-CBD	5.02	120.18	111.27
8	K	101	BCL	C3D-C2D-C1D	-5.01	98.99	105.83
8	U	101	BCL	C3D-C2D-C1D	-5.01	98.99	105.83
8	V	101	BCL	C2D-C1D-ND	5.01	113.80	110.10
8	F	101	BCL	C2D-C1D-ND	5.01	113.80	110.10
8	W	101	BCL	C3D-C2D-C1D	-5.00	99.01	105.83
8	D	102	BCL	C3D-C2D-C1D	-4.99	99.02	105.83
8	Z	102	BCL	C4B-CHC-C1C	-4.99	120.23	130.12
8	A	101	BCL	C2D-C1D-ND	4.98	113.78	110.10
8	I	101	BCL	C3D-C2D-C1D	-4.98	99.03	105.83
8	3	101	BCL	C1B-CHB-C4A	-4.98	120.25	130.12
8	O	101	BCL	C3D-C2D-C1D	-4.96	99.07	105.83
8	Z	102	BCL	O2D-CGD-CBD	4.94	120.05	111.27
8	L	308	BCL	C3D-C2D-C1D	-4.93	99.10	105.83
8	7	101	BCL	C2D-C1D-ND	4.92	113.73	110.10
8	S	101	BCL	C3D-C2D-C1D	-4.91	99.13	105.83
8	Q	101	BCL	C3D-C2D-C1D	-4.91	99.13	105.83
8	A	101	BCL	C3D-C2D-C1D	-4.90	99.14	105.83
8	9	101	BCL	C3D-C2D-C1D	-4.90	99.15	105.83
8	F	101	BCL	C3D-C2D-C1D	-4.90	99.15	105.83
11	Z	101	A1EYK	C22-C18-C15	4.88	125.76	118.08
8	7	101	BCL	C3D-C2D-C1D	-4.87	99.18	105.83
8	6	101	BCL	C2D-C1D-ND	4.86	113.68	110.10
8	L	307	BCL	C3D-C2D-C1D	-4.84	99.22	105.83
8	5	101	BCL	C3D-C2D-C1D	-4.84	99.23	105.83
8	Y	101	BCL	C3D-C2D-C1D	-4.79	99.30	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	101	BCL	CHD-C4C-NC	4.77	130.37	125.08
8	L	308	BCL	O2D-CGD-CBD	4.77	119.74	111.27
8	R	101	BCL	C3D-C2D-C1D	-4.73	99.38	105.83
8	J	101	BCL	C3D-C2D-C1D	-4.72	99.40	105.83
8	Q	101	BCL	C1C-NC-C4C	-4.69	104.60	106.71
8	E	101	BCL	C3D-C2D-C1D	-4.69	99.43	105.83
8	L	308	BCL	C2D-C1D-ND	4.69	113.56	110.10
8	I	101	BCL	C3C-C4C-CHD	-4.69	113.38	123.39
8	K	101	BCL	CHD-C4C-NC	4.68	130.28	125.08
8	O	101	BCL	CHD-C4C-NC	4.68	130.27	125.08
8	8	101	BCL	C3D-C2D-C1D	-4.68	99.45	105.83
8	1	101	BCL	C3D-C2D-C1D	-4.67	99.45	105.83
8	Q	101	BCL	C3C-C4C-CHD	-4.66	113.43	123.39
8	N	101	BCL	C3D-C2D-C1D	-4.66	99.47	105.83
8	U	101	BCL	CHD-C4C-NC	4.66	130.25	125.08
8	Q	101	BCL	CHD-C4C-NC	4.66	130.25	125.08
8	X	101	BCL	C3D-C2D-C1D	-4.65	99.49	105.83
8	X	101	BCL	C2D-C1D-ND	4.65	113.53	110.10
8	T	101	BCL	C3D-C2D-C1D	-4.64	99.49	105.83
8	V	101	BCL	C3D-C2D-C1D	-4.63	99.51	105.83
8	4	102	BCL	C1B-CHB-C4A	-4.63	120.94	130.12
8	W	101	BCL	CHD-C4C-NC	4.63	130.22	125.08
8	P	101	BCL	C3D-C2D-C1D	-4.63	99.51	105.83
8	3	101	BCL	O2D-CGD-CBD	4.62	119.47	111.27
8	B	101	BCL	C3D-C2D-C1D	-4.61	99.53	105.83
8	G	101	BCL	C3D-C2D-C1D	-4.61	99.55	105.83
8	5	101	BCL	C2D-C1D-ND	4.60	113.50	110.10
8	0	101	BCL	C3D-C2D-C1D	-4.60	99.56	105.83
8	6	101	BCL	C3D-C2D-C1D	-4.59	99.56	105.83
8	Y	101	BCL	O2D-CGD-CBD	4.59	119.42	111.27
8	5	101	BCL	O2D-CGD-CBD	4.57	119.39	111.27
8	M	403	BCL	CHD-C4C-NC	4.56	130.15	125.08
8	D	102	BCL	CHD-C4C-NC	4.56	130.14	125.08
8	O	101	BCL	C3C-C4C-CHD	-4.55	113.66	123.39
8	B	101	BCL	CHD-C4C-NC	4.54	130.12	125.08
10	Y	102	SPO	C21-C22-C23	-4.54	120.83	127.31
8	4	102	BCL	C3D-C2D-C1D	-4.53	99.64	105.83
8	T	101	BCL	CHD-C4C-NC	4.53	130.11	125.08
8	K	101	BCL	C3C-C4C-CHD	-4.52	113.73	123.39
8	U	101	BCL	C3C-C4C-CHD	-4.52	113.74	123.39
8	T	101	BCL	C3C-C4C-CHD	-4.50	113.77	123.39
8	K	101	BCL	O2D-CGD-CBD	4.50	119.26	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	3	101	BCL	C3D-C2D-C1D	-4.50	99.69	105.83
8	X	101	BCL	O2D-CGD-CBD	4.50	119.26	111.27
8	Z	102	BCL	C3D-C2D-C1D	-4.50	99.69	105.83
8	A	101	BCL	CHD-C4C-NC	4.50	130.07	125.08
8	S	101	BCL	CHD-C4C-NC	4.49	130.06	125.08
8	9	101	BCL	CHD-C4C-NC	4.48	130.05	125.08
8	D	102	BCL	C3C-C4C-CHD	-4.48	113.82	123.39
8	V	101	BCL	O2D-CGD-CBD	4.47	119.22	111.27
8	F	101	BCL	O2D-CGD-CBD	4.46	119.19	111.27
8	S	101	BCL	C3C-C4C-CHD	-4.46	113.87	123.39
8	E	101	BCL	CHD-C4C-NC	4.45	130.02	125.08
8	6	101	BCL	O2D-CGD-CBD	4.45	119.18	111.27
8	B	101	BCL	C1D-ND-C4D	-4.45	103.18	106.33
8	8	101	BCL	CHD-C4C-NC	4.44	130.01	125.08
8	U	101	BCL	CMB-C2B-C3B	4.44	132.99	124.68
8	B	101	BCL	C3C-C4C-CHD	-4.44	113.90	123.39
10	7	102	SPO	C21-C22-C23	-4.44	120.97	127.31
8	8	101	BCL	O2D-CGD-CBD	4.44	119.15	111.27
8	G	101	BCL	O2D-CGD-CBD	4.43	119.14	111.27
8	W	101	BCL	C3C-C4C-CHD	-4.43	113.93	123.39
8	0	101	BCL	CHD-C4C-NC	4.43	129.99	125.08
8	A	101	BCL	C3C-C4C-CHD	-4.43	113.93	123.39
8	0	101	BCL	C3C-C4C-CHD	-4.43	113.94	123.39
8	Q	101	BCL	CMB-C2B-C3B	4.42	132.95	124.68
8	9	101	BCL	C3C-C4C-CHD	-4.42	113.94	123.39
8	8	101	BCL	C3C-C4C-CHD	-4.42	113.95	123.39
8	J	101	BCL	C3C-C4C-CHD	-4.42	113.96	123.39
8	T	101	BCL	C1D-ND-C4D	-4.41	103.20	106.33
8	I	101	BCL	O2D-CGD-CBD	4.41	119.11	111.27
8	Q	101	BCL	O2D-CGD-CBD	4.41	119.11	111.27
8	W	101	BCL	CMB-C2B-C3B	4.41	132.93	124.68
8	V	101	BCL	CMB-C2B-C3B	4.41	132.93	124.68
8	E	101	BCL	C3C-C4C-CHD	-4.41	113.98	123.39
8	F	101	BCL	CMB-C2B-C3B	4.40	132.92	124.68
8	J	101	BCL	CHD-C4C-NC	4.40	129.96	125.08
8	R	101	BCL	C3C-C4C-CHD	-4.40	114.00	123.39
8	3	101	BCL	C4B-CHC-C1C	-4.40	121.41	130.12
8	9	101	BCL	CMB-C2B-C3B	4.38	132.88	124.68
8	N	101	BCL	C3C-C4C-CHD	-4.38	114.03	123.39
8	G	101	BCL	C3C-C4C-CHD	-4.38	114.03	123.39
8	J	101	BCL	C1D-ND-C4D	-4.38	103.22	106.33
8	W	101	BCL	O2D-CGD-CBD	4.38	119.05	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	2	101	BCL	C3D-C2D-C1D	-4.38	99.85	105.83
8	M	403	BCL	CMB-C2B-C3B	4.38	132.87	124.68
8	T	101	BCL	O2D-CGD-CBD	4.38	119.05	111.27
8	V	101	BCL	CHD-C4C-NC	4.38	129.94	125.08
8	V	101	BCL	C1D-ND-C4D	-4.38	103.23	106.33
8	N	101	BCL	C1D-ND-C4D	-4.38	103.23	106.33
8	3	101	BCL	C1C-NC-C4C	4.37	108.67	106.71
8	L	301	BCL	CMB-C2B-C3B	4.37	132.86	124.68
8	P	101	BCL	C3C-C4C-CHD	-4.37	114.06	123.39
8	B	101	BCL	O2D-CGD-CBD	4.36	119.02	111.27
8	U	101	BCL	C1D-ND-C4D	-4.36	103.24	106.33
8	G	101	BCL	CHD-C4C-NC	4.36	129.92	125.08
8	R	101	BCL	CHD-C4C-NC	4.35	129.91	125.08
8	P	101	BCL	CMB-C2B-C3B	4.35	132.81	124.68
8	8	101	BCL	C1D-ND-C4D	-4.34	103.25	106.33
8	K	101	BCL	C1D-ND-C4D	-4.34	103.25	106.33
8	R	101	BCL	O2D-CGD-CBD	4.33	118.97	111.27
8	N	101	BCL	CHD-C4C-NC	4.33	129.89	125.08
11	W	102	A1EYK	C25-C27-C31	-4.33	112.30	118.94
8	R	101	BCL	C1D-ND-C4D	-4.33	103.26	106.33
8	Q	101	BCL	C4A-NA-C1A	4.32	108.65	106.71
8	D	102	BCL	CMB-C2B-C3B	4.31	132.73	124.68
8	N	101	BCL	CMB-C2B-C3B	4.31	132.73	124.68
8	I	101	BCL	CMB-C2B-C3B	4.30	132.72	124.68
8	A	101	BCL	O2D-CGD-CBD	4.30	118.91	111.27
8	P	101	BCL	CHD-C4C-NC	4.30	129.85	125.08
8	O	101	BCL	CMB-C2B-C3B	4.29	132.71	124.68
8	N	101	BCL	O2D-CGD-CBD	4.29	118.89	111.27
8	7	101	BCL	CHD-C4C-NC	4.29	129.84	125.08
10	I	102	SPO	C20-C19-C17	-4.29	121.19	127.31
8	L	308	BCL	CMB-C2B-C3B	4.29	132.70	124.68
8	O	101	BCL	C1D-ND-C4D	-4.29	103.29	106.33
8	A	101	BCL	CMB-C2B-C3B	4.28	132.69	124.68
8	U	101	BCL	O2D-CGD-CBD	4.28	118.88	111.27
8	0	101	BCL	C1D-ND-C4D	-4.28	103.30	106.33
8	W	101	BCL	C1D-ND-C4D	-4.28	103.30	106.33
8	S	101	BCL	CMB-C2B-C3B	4.27	132.67	124.68
8	E	101	BCL	O2D-CGD-CBD	4.27	118.85	111.27
8	P	101	BCL	O2D-CGD-CBD	4.26	118.84	111.27
8	J	101	BCL	O2D-CGD-CBD	4.26	118.84	111.27
8	4	102	BCL	C1C-NC-C4C	4.26	108.62	106.71
8	B	101	BCL	CMB-C2B-C3B	4.26	132.64	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	9	101	BCL	C1D-ND-C4D	-4.25	103.31	106.33
8	G	101	BCL	CMB-C2B-C3B	4.25	132.62	124.68
13	M	407	PGV	O01-C1-C2	4.25	120.65	111.50
8	D	102	BCL	C1D-ND-C4D	-4.24	103.32	106.33
8	T	101	BCL	CMB-C2B-C3B	4.23	132.60	124.68
8	Z	102	BCL	C1B-CHB-C4A	-4.23	121.74	130.12
8	S	101	BCL	C1D-ND-C4D	-4.23	103.33	106.33
8	J	101	BCL	CMB-C2B-C3B	4.23	132.59	124.68
8	K	101	BCL	CMB-C2B-C3B	4.23	132.59	124.68
8	E	101	BCL	CMB-C2B-C3B	4.23	132.59	124.68
8	V	101	BCL	C3C-C4C-CHD	-4.23	114.36	123.39
13	H	301	PGV	O01-C1-C2	4.22	120.60	111.50
8	S	101	BCL	O2D-CGD-CBD	4.21	118.76	111.27
8	I	101	BCL	C1D-ND-C4D	-4.21	103.34	106.33
8	6	101	BCL	CHD-C4C-NC	4.21	129.75	125.08
8	G	101	BCL	C1D-ND-C4D	-4.20	103.35	106.33
8	F	101	BCL	CHD-C4C-NC	4.20	129.75	125.08
8	E	101	BCL	C1D-ND-C4D	-4.20	103.35	106.33
8	6	101	BCL	CMB-C2B-C3B	4.20	132.53	124.68
8	L	307	BCL	C1D-ND-C4D	-4.19	103.36	106.33
8	7	101	BCL	C3C-C4C-CHD	-4.19	114.43	123.39
8	M	403	BCL	C3C-C4C-CHD	-4.19	114.44	123.39
8	O	101	BCL	O2D-CGD-CBD	4.19	118.71	111.27
13	M	408	PGV	O01-C1-C2	4.19	120.53	111.50
8	7	101	BCL	O2D-CGD-CBD	4.19	118.71	111.27
8	F	101	BCL	C3C-C4C-CHD	-4.18	114.45	123.39
8	8	101	BCL	CMB-C2B-C3B	4.18	132.50	124.68
10	5	102	SPO	C21-C22-C23	-4.18	121.34	127.31
10	Q	102	SPO	C21-C22-C23	-4.17	121.36	127.31
10	O	102	SPO	C21-C22-C23	-4.17	121.36	127.31
8	P	101	BCL	C1D-ND-C4D	-4.17	103.38	106.33
8	L	301	BCL	C1D-ND-C4D	-4.16	103.38	106.33
13	H	305	PGV	O01-C1-C2	4.13	120.39	111.50
10	I	102	SPO	C21-C22-C23	-4.12	121.43	127.31
8	0	101	BCL	O2D-CGD-CBD	4.12	118.59	111.27
8	Y	101	BCL	C2D-C1D-ND	4.11	113.14	110.10
10	U	104	SPO	C21-C22-C23	-4.11	121.44	127.31
8	L	307	BCL	CMB-C2B-C3B	4.10	132.35	124.68
8	0	101	BCL	CMB-C2B-C3B	4.09	132.33	124.68
8	L	307	BCL	CHD-C4C-NC	4.08	129.61	125.08
10	K	102	SPO	C21-C22-C23	-4.08	121.48	127.31
10	U	102	SPO	C21-C22-C23	-4.08	121.49	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	M	406	SPO	C20-C19-C17	-4.07	121.50	127.31
10	Y	102	SPO	C20-C19-C17	-4.07	121.50	127.31
13	H	304	PGV	O01-C1-C2	4.07	120.27	111.50
10	S	102	SPO	C21-C22-C23	-4.06	121.51	127.31
8	4	102	BCL	CMB-C2B-C3B	4.06	132.28	124.68
8	6	101	BCL	C3C-C4C-CHD	-4.06	114.73	123.39
8	6	101	BCL	C1D-ND-C4D	-4.06	103.45	106.33
8	4	102	BCL	O2D-CGD-CBD	4.05	118.47	111.27
10	U	104	SPO	C20-C19-C17	-4.05	121.53	127.31
8	D	102	BCL	O2D-CGD-CBD	4.05	118.46	111.27
8	L	301	BCL	C3C-C4C-CHD	-4.05	114.75	123.39
8	X	101	BCL	CHD-C4C-NC	4.03	129.55	125.08
8	2	101	BCL	C1B-CHB-C4A	-4.02	122.15	130.12
8	R	101	BCL	CMB-C2B-C3B	4.02	132.20	124.68
8	9	101	BCL	O2D-CGD-CBD	4.02	118.41	111.27
8	L	301	BCL	CHD-C4C-NC	4.00	129.52	125.08
10	9	102	SPO	C21-C22-C23	-4.00	121.61	127.31
8	Y	101	BCL	CHD-C4C-NC	3.99	129.51	125.08
10	U	102	SPO	C20-C19-C17	-3.99	121.61	127.31
8	Q	101	BCL	C1D-ND-C4D	-3.99	103.50	106.33
8	X	101	BCL	CMB-C2B-C3B	3.99	132.14	124.68
8	L	308	BCL	CHD-C4C-NC	3.98	129.50	125.08
13	A	104	PGV	O01-C1-C2	3.97	120.06	111.50
8	L	307	BCL	C3C-C4C-CHD	-3.96	114.94	123.39
10	O	102	SPO	C20-C19-C17	-3.95	121.67	127.31
10	4	101	SPO	C20-C19-C17	-3.95	121.67	127.31
13	H	303	PGV	O01-C1-C2	3.94	120.00	111.50
10	K	102	SPO	C20-C19-C17	-3.94	121.69	127.31
13	M	411	PGV	O01-C1-C2	3.93	119.97	111.50
11	Z	101	A1EYK	C22-C18-C24	-3.92	117.43	122.92
10	Y	102	SPO	C10-C9-C7	-3.91	121.72	127.31
8	7	101	BCL	CMB-C2B-C3B	3.91	132.00	124.68
13	L	304	PGV	O01-C1-C2	3.91	119.92	111.50
10	A	102	SPO	C21-C22-C23	-3.90	121.74	127.31
10	7	102	SPO	C20-C19-C17	-3.90	121.75	127.31
10	5	102	SPO	C20-C19-C17	-3.90	121.75	127.31
8	F	101	BCL	C1D-ND-C4D	-3.90	103.57	106.33
8	7	101	BCL	C1D-ND-C4D	-3.89	103.57	106.33
8	1	101	BCL	CMB-C2B-C3B	3.88	131.93	124.68
10	F	102	SPO	C21-C22-C23	-3.88	121.78	127.31
10	Q	102	SPO	C20-C19-C17	-3.87	121.78	127.31
8	A	101	BCL	C1D-ND-C4D	-3.87	103.59	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	9	102	SPO	C20-C19-C17	-3.86	121.81	127.31
10	4	101	SPO	C8-C7-C6	3.85	124.15	118.08
13	H	302	PGV	O01-C1-C2	3.84	119.78	111.50
8	X	101	BCL	C1D-ND-C4D	-3.82	103.62	106.33
10	D	103	SPO	C21-C22-C23	-3.81	121.88	127.31
8	4	102	BCL	CHD-C4C-NC	3.81	129.30	125.08
10	S	102	SPO	C20-C19-C17	-3.81	121.88	127.31
8	1	101	BCL	C2D-C1D-ND	3.80	112.90	110.10
12	7	104	LMT	C1B-O1B-C4'	-3.77	108.63	117.96
10	4	101	SPO	C24-C23-C25	3.77	124.02	118.08
8	M	403	BCL	C1D-ND-C4D	-3.75	103.67	106.33
8	Y	101	BCL	C1-C2-C3	-3.73	119.60	126.04
8	X	101	BCL	C3C-C4C-CHD	-3.73	115.43	123.39
10	D	103	SPO	C20-C19-C17	-3.72	122.00	127.31
8	5	101	BCL	CMB-C2B-C3B	3.70	131.60	124.68
8	L	308	BCL	C1D-ND-C4D	-3.69	103.72	106.33
10	A	102	SPO	C20-C19-C17	-3.66	122.09	127.31
11	W	102	A1EYK	C34-C36-C39	3.64	130.94	123.47
8	5	101	BCL	C1D-ND-C4D	-3.63	103.75	106.33
10	M	406	SPO	C10-C9-C7	-3.62	122.14	127.31
8	N	101	BCL	C1-C2-C3	-3.62	119.78	126.04
8	Y	101	BCL	C4B-CHC-C1C	-3.61	122.96	130.12
8	K	101	BCL	C1-C2-C3	-3.61	119.79	126.04
8	B	101	BCL	C3D-C4D-ND	3.61	116.07	110.24
8	M	403	BCL	O2A-C1-C2	3.60	118.11	108.64
8	V	101	BCL	C3D-C4D-ND	3.59	116.04	110.24
11	U	103	A1EYK	C11-C15-C18	3.58	131.31	125.89
10	M	406	SPO	C21-C22-C23	-3.58	122.20	127.31
8	1	101	BCL	C1-C2-C3	-3.57	119.87	126.04
8	Z	102	BCL	CHD-C4C-NC	3.55	129.02	125.08
10	F	102	SPO	C20-C19-C17	-3.55	122.25	127.31
8	3	101	BCL	CHD-C4C-NC	3.55	129.01	125.08
8	T	101	BCL	C3D-C4D-ND	3.54	115.97	110.24
11	9	103	A1EYK	C29-C27-C31	-3.53	117.97	122.92
11	U	103	A1EYK	C22-C18-C24	-3.53	117.97	122.92
11	Z	101	A1EYK	C11-C15-C18	3.53	131.23	125.89
8	L	307	BCL	C3D-C4D-ND	3.53	115.95	110.24
8	N	101	BCL	C3D-C4D-ND	3.53	115.94	110.24
8	L	307	BCL	C1-C2-C3	-3.52	119.95	126.04
8	L	308	BCL	C3C-C4C-CHD	-3.52	115.88	123.39
8	F	101	BCL	C1C-NC-C4C	-3.51	105.13	106.71
14	C	401	HEC	CBA-CAA-C2A	-3.51	106.69	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	0	101	BCL	C3D-C4D-ND	3.50	115.91	110.24
12	9	104	LMT	C1B-O1B-C4'	-3.49	109.32	117.96
10	4	101	SPO	C9-C10-C11	-3.49	112.33	123.22
8	J	101	BCL	C3D-C4D-ND	3.49	115.88	110.24
8	8	101	BCL	C3D-C4D-ND	3.48	115.86	110.24
8	A	101	BCL	C1-C2-C3	-3.47	120.04	126.04
8	L	301	BCL	O2D-CGD-CBD	3.47	117.43	111.27
10	4	101	SPO	C21-C22-C23	-3.44	122.40	127.31
8	Y	101	BCL	C3C-C4C-CHD	-3.43	116.06	123.39
8	2	101	BCL	CMB-C2B-C3B	3.43	131.10	124.68
8	R	101	BCL	C3D-C4D-ND	3.43	115.79	110.24
8	P	101	BCL	C3D-C4D-ND	3.43	115.78	110.24
8	M	403	BCL	O2D-CGD-CBD	3.43	117.36	111.27
8	G	101	BCL	C3D-C4D-ND	3.42	115.77	110.24
8	3	101	BCL	CMB-C2B-C3B	3.42	131.07	124.68
8	6	101	BCL	C3D-C4D-ND	3.42	115.76	110.24
8	E	101	BCL	C3D-C4D-ND	3.41	115.75	110.24
8	Y	101	BCL	CMB-C2B-C3B	3.39	131.03	124.68
10	M	406	SPO	C34-C33-C35	3.38	120.96	115.27
8	Z	102	BCL	C2D-C1D-ND	3.36	112.58	110.10
8	X	101	BCL	C3D-C4D-ND	3.34	115.65	110.24
8	L	308	BCL	C3D-C4D-ND	3.33	115.62	110.24
13	F	105	PGV	O01-C1-C2	3.32	118.65	111.50
8	L	308	BCL	C1-C2-C3	-3.31	120.31	126.04
13	M	409	PGV	O01-C1-C2	3.31	118.64	111.50
8	U	101	BCL	C3D-C4D-ND	3.30	115.58	110.24
8	K	101	BCL	C3D-C4D-ND	3.30	115.57	110.24
8	4	102	BCL	C2D-C1D-ND	3.29	112.53	110.10
8	O	101	BCL	C3D-C4D-ND	3.29	115.56	110.24
8	M	403	BCL	O2A-CGA-CBA	3.28	122.20	111.91
8	W	101	BCL	C3D-C4D-ND	3.27	115.53	110.24
8	S	101	BCL	C3D-C4D-ND	3.27	115.52	110.24
8	9	101	BCL	C3D-C4D-ND	3.25	115.49	110.24
8	L	301	BCL	C3D-C4D-ND	3.24	115.48	110.24
8	Q	101	BCL	C1-C2-C3	-3.24	120.44	126.04
10	Y	102	SPO	C15-C14-C12	-3.24	122.69	127.31
12	O	104	LMT	C1B-O1B-C4'	-3.23	109.96	117.96
8	Z	102	BCL	CMB-C2B-C3B	3.23	130.72	124.68
8	I	101	BCL	C3D-C4D-ND	3.23	115.46	110.24
8	D	102	BCL	C3D-C4D-ND	3.22	115.45	110.24
10	9	102	SPO	C31-C32-C33	-3.22	119.91	127.66
10	D	103	SPO	C31-C32-C33	-3.21	119.93	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	D	105	PGV	O01-C1-C2	3.20	119.73	110.80
8	7	101	BCL	C3D-C4D-ND	3.20	115.41	110.24
8	I	101	BCL	C1C-NC-C4C	-3.20	105.27	106.71
8	5	101	BCL	C3D-C4D-ND	3.18	115.39	110.24
8	Y	101	BCL	C1D-ND-C4D	-3.17	104.09	106.33
10	A	102	SPO	C31-C32-C33	-3.16	120.05	127.66
8	A	101	BCL	C3D-C4D-ND	3.16	115.35	110.24
10	5	102	SPO	C31-C32-C33	-3.16	120.06	127.66
10	7	102	SPO	C31-C32-C33	-3.15	120.08	127.66
8	3	101	BCL	C2D-C1D-ND	3.14	112.42	110.10
10	U	102	SPO	C31-C32-C33	-3.14	120.10	127.66
8	Z	102	BCL	C4A-NA-C1A	3.13	108.11	106.71
10	M	406	SPO	C5-C6-C7	-3.12	121.17	125.89
8	F	101	BCL	C3D-C4D-ND	3.12	115.29	110.24
10	F	102	SPO	C31-C32-C33	-3.12	120.15	127.66
8	F	101	BCL	C4-C3-C5	3.12	120.52	115.27
10	Y	102	SPO	C34-C33-C35	3.11	120.51	115.27
10	K	102	SPO	C31-C32-C33	-3.11	120.17	127.66
8	Y	101	BCL	C3D-C4D-ND	3.10	115.25	110.24
10	O	102	SPO	C31-C32-C33	-3.10	120.21	127.66
8	L	301	BCL	O2A-CGA-CBA	3.08	121.58	111.91
8	1	101	BCL	C3D-C4D-ND	3.08	115.22	110.24
10	Q	102	SPO	C31-C32-C33	-3.08	120.24	127.66
8	Q	101	BCL	C3D-C4D-ND	3.08	115.22	110.24
10	S	102	SPO	C31-C32-C33	-3.08	120.25	127.66
8	M	403	BCL	C3D-C4D-ND	3.07	115.20	110.24
8	2	101	BCL	C3D-C4D-ND	3.06	115.19	110.24
8	U	101	BCL	C1-C2-C3	-3.06	120.75	126.04
8	4	102	BCL	C3C-C4C-CHD	-3.05	116.87	123.39
8	9	101	BCL	C1-C2-C3	-3.05	120.76	126.04
8	R	101	BCL	CHB-C4A-NA	3.05	128.72	124.51
10	I	102	SPO	C31-C32-C33	-3.04	120.34	127.66
13	M	411	PGV	C02-O01-C1	-3.02	110.35	117.79
8	4	102	BCL	C3D-C4D-ND	3.02	115.13	110.24
8	J	101	BCL	CHB-C4A-NA	3.02	128.68	124.51
8	M	403	BCL	CED-O2D-CGD	3.01	122.75	115.94
8	6	101	BCL	CHB-C4A-NA	3.01	128.67	124.51
12	L	305	LMT	C1'-C2'-C3'	3.00	116.25	110.00
8	4	102	BCL	C4B-CHC-C1C	-3.00	124.17	130.12
8	1	101	BCL	C4B-CHC-C1C	-3.00	124.17	130.12
8	T	101	BCL	CHB-C4A-NA	3.00	128.65	124.51
8	K	101	BCL	O2A-CGA-CBA	2.99	121.31	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	3	101	BCL	C3D-C4D-ND	2.99	115.08	110.24
10	U	104	SPO	C31-C32-C33	-2.99	120.46	127.66
8	0	101	BCL	C1-C2-C3	-2.98	120.88	126.04
8	V	101	BCL	CHB-C4A-NA	2.98	128.63	124.51
8	Q	101	BCL	O2A-CGA-CBA	2.97	121.24	111.91
8	2	101	BCL	CHD-C1D-C2D	2.97	131.72	125.48
8	2	101	BCL	C1-C2-C3	-2.96	120.92	126.04
8	L	301	BCL	C4-C3-C5	2.96	120.25	115.27
12	F	104	LMT	O1B-C1B-C2B	2.95	115.75	108.10
8	N	101	BCL	C4-C3-C5	2.95	120.24	115.27
8	0	101	BCL	CHB-C4A-NA	2.95	128.59	124.51
8	F	101	BCL	C4A-NA-C1A	2.95	108.03	106.71
10	4	101	SPO	C29-C28-C30	2.95	120.23	115.27
8	O	101	BCL	C4-C3-C5	2.94	120.22	115.27
8	G	101	BCL	CHB-C4A-NA	2.94	128.58	124.51
8	B	101	BCL	CHB-C4A-NA	2.94	128.58	124.51
8	5	101	BCL	CHD-C4C-NC	2.94	128.34	125.08
10	I	102	SPO	C29-C28-C30	2.93	120.20	115.27
8	Z	102	BCL	C3C-C4C-CHD	-2.93	117.14	123.39
8	5	101	BCL	C1-C2-C3	-2.92	120.99	126.04
8	2	101	BCL	C2D-C1D-ND	2.92	112.26	110.10
10	4	101	SPO	C6-C7-C9	-2.92	114.46	118.94
8	P	101	BCL	CHB-C4A-NA	2.92	128.55	124.51
8	8	101	BCL	CHB-C4A-NA	2.92	128.54	124.51
8	9	101	BCL	C1C-NC-C4C	-2.91	105.40	106.71
8	S	101	BCL	O2A-CGA-CBA	2.91	121.03	111.91
8	5	101	BCL	O2A-CGA-CBA	2.90	121.02	111.91
8	2	101	BCL	C1C-NC-C4C	2.90	108.01	106.71
13	M	407	PGV	C02-O01-C1	-2.90	110.66	117.79
10	F	102	SPO	C29-C28-C30	2.89	120.14	115.27
8	1	101	BCL	C1D-CHD-C4C	-2.89	119.66	126.62
10	K	102	SPO	C29-C28-C30	2.89	120.13	115.27
8	5	101	BCL	C1D-CHD-C4C	-2.88	119.66	126.62
8	S	101	BCL	C4-C3-C5	2.88	120.12	115.27
8	1	101	BCL	O2A-CGA-CBA	2.88	120.95	111.91
8	V	101	BCL	C4-C3-C5	2.88	120.12	115.27
8	I	101	BCL	C4A-NA-C1A	2.88	108.00	106.71
10	U	104	SPO	C29-C28-C30	2.88	120.11	115.27
8	W	101	BCL	C1-C2-C3	-2.87	121.07	126.04
8	Q	101	BCL	CHC-C1C-NC	2.87	128.48	124.51
10	S	102	SPO	C29-C28-C30	2.87	120.10	115.27
10	U	102	SPO	C29-C28-C30	2.87	120.10	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	N	101	BCL	CHB-C4A-NA	2.87	128.48	124.51
8	W	101	BCL	CHB-C4A-NA	2.87	128.47	124.51
10	5	102	SPO	C29-C28-C30	2.86	120.09	115.27
8	W	101	BCL	C4-C3-C5	2.86	120.08	115.27
8	F	101	BCL	O2A-CGA-CBA	2.86	120.87	111.91
10	O	102	SPO	C29-C28-C30	2.86	120.08	115.27
8	I	101	BCL	C4-C3-C5	2.85	120.07	115.27
8	I	101	BCL	O2A-CGA-CBA	2.85	120.85	111.91
8	Z	102	BCL	C1-C2-C3	-2.84	121.12	126.04
8	7	101	BCL	C1-C2-C3	-2.84	121.12	126.04
10	Y	102	SPO	C29-C28-C30	2.84	120.05	115.27
10	7	102	SPO	C29-C28-C30	2.84	120.05	115.27
8	Y	101	BCL	C1B-CHB-C4A	-2.83	124.50	130.12
8	4	102	BCL	CHD-C1D-C2D	2.83	131.41	125.48
8	G	101	BCL	C4-C3-C5	2.83	120.03	115.27
8	1	101	BCL	C1D-ND-C4D	-2.82	104.33	106.33
8	7	101	BCL	O2A-CGA-CBA	2.82	120.75	111.91
8	Z	102	BCL	C3D-C4D-ND	2.82	114.80	110.24
8	U	101	BCL	O2A-CGA-CBA	2.81	120.74	111.91
8	O	101	BCL	CHC-C1C-NC	2.81	128.40	124.51
13	M	411	PGV	O03-C19-C20	2.81	120.74	111.91
8	3	101	BCL	CHD-C1D-C2D	2.81	131.38	125.48
10	U	104	SPO	C5-C6-C7	-2.81	121.65	125.89
8	A	101	BCL	C1C-NC-C4C	-2.81	105.44	106.71
10	D	103	SPO	C29-C28-C30	2.81	119.99	115.27
8	6	101	BCL	C4-C3-C5	2.80	119.98	115.27
8	9	101	BCL	O2A-CGA-CBA	2.80	120.70	111.91
8	M	403	BCL	C1-C2-C3	2.80	130.88	126.04
8	A	101	BCL	O2A-CGA-CBA	2.80	120.69	111.91
8	W	101	BCL	CHC-C1C-NC	2.80	128.38	124.51
10	9	102	SPO	C29-C28-C30	2.79	119.97	115.27
10	U	102	SPO	C10-C9-C7	-2.79	123.32	127.31
8	5	101	BCL	C4-C3-C5	2.79	119.97	115.27
8	J	101	BCL	C4-C3-C5	2.79	119.96	115.27
10	O	102	SPO	C9-C10-C11	-2.78	114.53	123.22
8	Y	101	BCL	O2A-CGA-CBA	2.78	120.63	111.91
8	4	102	BCL	CMD-C2D-C3D	-2.78	121.22	127.61
8	X	101	BCL	C4B-CHC-C1C	-2.78	124.62	130.12
8	D	102	BCL	C4-C3-C5	2.77	119.94	115.27
8	O	101	BCL	C1C-NC-C4C	-2.77	105.46	106.71
8	M	403	BCL	C5-C3-C2	-2.77	115.51	121.12
13	H	303	PGV	C02-O01-C1	-2.77	110.97	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	102	BCL	C1-C2-C3	-2.77	121.25	126.04
8	4	102	BCL	C4-C3-C5	2.76	119.92	115.27
8	E	101	BCL	C4-C3-C5	2.76	119.92	115.27
8	1	101	BCL	C4-C3-C5	2.76	119.92	115.27
8	0	101	BCL	C4-C3-C5	2.76	119.91	115.27
8	D	102	BCL	O2A-CGA-CBA	2.76	120.56	111.91
12	L	305	LMT	C1-O1'-C1'	-2.76	109.27	113.84
10	I	102	SPO	C9-C10-C11	-2.76	114.61	123.22
8	S	101	BCL	C1-C2-C3	-2.76	121.28	126.04
13	M	409	PGV	O03-C19-C20	2.76	120.56	111.91
13	H	301	PGV	C02-O01-C1	-2.75	111.01	117.79
10	K	102	SPO	C9-C10-C11	-2.75	114.62	123.22
8	P	101	BCL	C4-C3-C5	2.75	119.90	115.27
8	F	101	BCL	CHC-C1C-NC	2.75	128.32	124.51
8	8	101	BCL	C1-C2-C3	-2.75	121.28	126.04
8	K	101	BCL	C4-C3-C5	2.75	119.90	115.27
10	D	103	SPO	C9-C10-C11	-2.75	114.64	123.22
8	7	101	BCL	C4-C3-C5	2.74	119.89	115.27
8	N	101	BCL	C2A-C1A-CHA	-2.74	119.06	123.86
8	2	101	BCL	C4-C3-C5	2.74	119.88	115.27
8	Z	102	BCL	C4-C3-C5	2.74	119.88	115.27
8	I	101	BCL	CHC-C1C-NC	2.74	128.30	124.51
10	A	102	SPO	C9-C10-C11	-2.74	114.68	123.22
8	K	101	BCL	CHB-C4A-NA	2.73	128.29	124.51
10	F	102	SPO	C9-C10-C11	-2.73	114.69	123.22
8	Z	102	BCL	C1C-NC-C4C	2.73	107.93	106.71
10	Q	102	SPO	C29-C28-C30	2.73	119.86	115.27
10	4	101	SPO	C24-C23-C22	-2.73	119.10	122.92
8	J	101	BCL	C1-C2-C3	-2.73	121.33	126.04
10	5	102	SPO	C9-C10-C11	-2.72	114.72	123.22
8	L	301	BCL	CHC-C1C-NC	2.72	128.28	124.51
13	M	408	PGV	C02-O01-C1	-2.72	111.09	117.79
8	L	308	BCL	C4-C3-C5	2.72	119.84	115.27
8	D	102	BCL	CHB-C4A-NA	2.72	128.27	124.51
8	3	101	BCL	CMD-C2D-C3D	-2.71	121.37	127.61
8	P	101	BCL	C1-C2-C3	-2.71	121.35	126.04
8	O	101	BCL	C1-C2-C3	-2.71	121.36	126.04
8	I	101	BCL	C1-C2-C3	-2.71	121.36	126.04
8	U	101	BCL	CHB-C4A-NA	2.70	128.25	124.51
10	7	102	SPO	C9-C10-C11	-2.70	114.78	123.22
8	O	101	BCL	CHB-C4A-NA	2.70	128.25	124.51
8	E	101	BCL	C1-C2-C3	-2.70	121.38	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	102	SPO	C29-C28-C30	2.69	119.80	115.27
8	E	101	BCL	CHB-C4A-NA	2.69	128.23	124.51
11	W	102	A1EYK	C33-C30-C32	2.69	126.69	122.92
8	N	101	BCL	C1-O2A-CGA	2.69	123.49	116.44
8	S	101	BCL	CHB-C4A-NA	2.69	128.22	124.51
13	H	302	PGV	O03-C19-C20	2.68	120.33	111.91
8	X	101	BCL	C1B-CHB-C4A	-2.68	124.81	130.12
8	8	101	BCL	C2A-C1A-CHA	-2.68	119.17	123.86
8	V	101	BCL	C1-C2-C3	-2.68	121.41	126.04
8	W	101	BCL	O2A-CGA-CBA	2.68	120.31	111.91
8	L	308	BCL	C4B-CHC-C1C	-2.67	124.82	130.12
8	2	101	BCL	CMD-C2D-C3D	-2.67	121.47	127.61
8	Q	101	BCL	C1D-CHD-C4C	-2.67	120.19	126.62
10	9	102	SPO	C9-C10-C11	-2.66	114.90	123.22
8	L	301	BCL	CED-O2D-CGD	2.66	121.96	115.94
13	H	304	PGV	O03-C19-C20	2.66	120.26	111.91
8	9	101	BCL	CHB-C4A-NA	2.66	128.19	124.51
8	Z	102	BCL	O2D-CGD-O1D	-2.66	118.64	123.84
8	U	101	BCL	CHC-C1C-NC	2.65	128.18	124.51
8	B	101	BCL	C2A-C1A-CHA	-2.65	119.22	123.86
8	U	101	BCL	C1C-NC-C4C	-2.65	105.51	106.71
8	T	101	BCL	C2A-C1A-CHA	-2.65	119.23	123.86
12	L	306	LMT	C1B-O1B-C4'	-2.65	111.41	117.96
13	H	304	PGV	C02-O01-C1	-2.64	111.29	117.79
8	T	101	BCL	C4-C3-C5	2.64	119.71	115.27
8	U	101	BCL	C4-C3-C5	2.64	119.70	115.27
8	N	101	BCL	CHC-C1C-NC	2.64	128.16	124.51
8	Y	101	BCL	CMD-C2D-C3D	-2.63	121.56	127.61
13	L	304	PGV	O03-C19-C20	2.63	120.16	111.91
8	8	101	BCL	C1-O2A-CGA	2.63	123.33	116.44
12	K	104	LMT	C1B-O1B-C4'	-2.62	111.48	117.96
8	F	101	BCL	C1-C2-C3	-2.62	121.52	126.04
8	6	101	BCL	C1-C2-C3	-2.62	121.52	126.04
8	I	101	BCL	CHB-C4A-NA	2.61	128.13	124.51
8	Y	101	BCL	C4-C3-C5	2.61	119.67	115.27
13	A	104	PGV	O03-C19-C20	2.61	120.11	111.91
8	1	101	BCL	CMD-C2D-C3D	-2.61	121.61	127.61
10	Q	102	SPO	C9-C10-C11	-2.61	115.08	123.22
8	S	101	BCL	C1C-NC-C4C	-2.61	105.53	106.71
8	7	101	BCL	CHB-C4A-NA	2.61	128.12	124.51
8	2	101	BCL	C1D-CHD-C4C	-2.60	120.34	126.62
8	D	102	BCL	C1C-NC-C4C	-2.60	105.54	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	V	101	BCL	C2A-C1A-CHA	-2.60	119.31	123.86
12	M	414	LMT	C1B-O1B-C4'	-2.60	111.53	117.96
8	L	307	BCL	C4-C3-C5	2.60	119.64	115.27
14	C	402	HEC	CBA-CAA-C2A	-2.59	108.23	112.60
12	L	305	LMT	C2'-C3'-C4'	2.59	115.59	109.68
8	L	307	BCL	CHC-C1C-NC	2.59	128.09	124.51
8	O	101	BCL	C2A-C1A-CHA	-2.58	119.34	123.86
8	T	101	BCL	CHC-C1C-NC	2.58	128.08	124.51
8	M	403	BCL	C4-C3-C5	2.57	119.60	115.27
8	G	101	BCL	C2A-C1A-CHA	-2.57	119.36	123.86
13	F	105	PGV	O03-C19-C20	2.57	119.98	111.91
8	8	101	BCL	CHC-C1C-NC	2.57	128.07	124.51
10	U	102	SPO	C5-C6-C7	-2.57	122.01	125.89
10	U	104	SPO	C10-C9-C7	-2.57	123.65	127.31
8	K	101	BCL	CHC-C1C-NC	2.56	128.05	124.51
8	D	102	BCL	CHC-C1C-NC	2.56	128.05	124.51
8	J	101	BCL	CHC-C1C-NC	2.56	128.05	124.51
8	G	101	BCL	CHC-C1C-NC	2.55	128.04	124.51
8	T	101	BCL	C1-C2-C3	-2.55	121.64	126.04
13	H	305	PGV	O14-P-O13	2.55	120.65	110.68
10	U	102	SPO	C14-C15-C16	-2.55	115.27	123.22
8	O	101	BCL	O2A-CGA-CBA	2.54	119.89	111.91
8	X	101	BCL	O2A-CGA-CBA	2.54	119.88	111.91
8	L	301	BCL	CHB-C4A-NA	2.54	128.02	124.51
8	P	101	BCL	C2A-C1A-CHA	-2.54	119.42	123.86
8	A	101	BCL	CHB-C4A-NA	2.53	128.01	124.51
10	Y	102	SPO	C40-C38-C39	2.53	120.20	114.60
8	I	101	BCL	C1D-CHD-C4C	-2.53	120.52	126.62
8	S	101	BCL	CHC-C1C-NC	2.53	128.01	124.51
8	1	101	BCL	CHD-C4C-NC	2.53	127.88	125.08
11	W	102	A1EYK	C35-C32-C30	2.53	130.92	127.31
8	9	101	BCL	CHC-C1C-NC	2.53	128.00	124.51
10	Q	102	SPO	C14-C15-C16	-2.52	115.34	123.22
8	3	101	BCL	C3C-C4C-CHD	-2.52	118.00	123.39
8	F	101	BCL	CHB-C4A-NA	2.52	128.00	124.51
8	G	101	BCL	C1-C2-C3	-2.52	121.68	126.04
8	R	101	BCL	CHC-C1C-NC	2.52	127.99	124.51
8	R	101	BCL	C2A-C1A-CHA	-2.51	119.47	123.86
8	2	101	BCL	C4D-CHA-C1A	-2.50	118.20	121.25
8	A	101	BCL	C4-C3-C5	2.50	119.48	115.27
10	O	102	SPO	C14-C15-C16	-2.50	115.41	123.22
13	H	301	PGV	O03-C19-C20	2.50	119.75	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	V	101	BCL	CHC-C1C-NC	2.50	127.97	124.51
8	6	101	BCL	C2A-C1A-CHA	-2.50	119.49	123.86
10	4	101	SPO	C13-C12-C11	2.50	122.01	118.08
8	Q	101	BCL	C4-C3-C5	2.49	119.47	115.27
8	J	101	BCL	C2A-C1A-CHA	-2.49	119.50	123.86
8	B	101	BCL	CHC-C1C-NC	2.49	127.96	124.51
8	R	101	BCL	C1-C2-C3	-2.49	121.73	126.04
8	W	101	BCL	CMD-C2D-C3D	-2.49	121.89	127.61
8	L	307	BCL	O2D-CGD-O1D	-2.49	118.97	123.84
10	7	102	SPO	C14-C15-C16	-2.49	115.46	123.22
11	9	103	A1EYK	C25-C27-C31	-2.48	115.13	118.94
10	Y	102	SPO	C31-C32-C33	-2.48	121.68	127.66
13	H	305	PGV	O03-C19-C20	2.48	119.69	111.91
13	H	302	PGV	C02-O01-C1	-2.48	111.69	117.79
8	X	101	BCL	C4-C3-C5	2.48	119.44	115.27
10	S	102	SPO	C10-C9-C7	-2.48	123.78	127.31
10	D	103	SPO	C14-C15-C16	-2.47	115.50	123.22
8	0	101	BCL	CHC-C1C-NC	2.47	127.93	124.51
8	P	101	BCL	CHC-C1C-NC	2.47	127.93	124.51
8	2	101	BCL	C4B-CHC-C1C	-2.47	125.22	130.12
10	M	406	SPO	C40-C38-C39	2.47	120.06	114.60
8	L	308	BCL	C4A-NA-C1A	2.47	107.82	106.71
8	6	101	BCL	CHC-C1C-NC	2.47	127.92	124.51
10	S	102	SPO	C14-C15-C16	-2.47	115.52	123.22
8	F	101	BCL	C1D-CHD-C4C	-2.47	120.67	126.62
10	S	102	SPO	C9-C10-C11	-2.46	115.53	123.22
8	L	307	BCL	C1D-CHD-C4C	-2.46	120.68	126.62
8	8	101	BCL	C4-C3-C5	2.46	119.41	115.27
8	4	102	BCL	C1-C2-C3	-2.46	121.79	126.04
8	L	301	BCL	CMD-C2D-C3D	-2.46	121.97	127.61
12	L	305	LMT	O1B-C4'-C3'	2.45	113.80	107.28
8	1	101	BCL	CHD-C1D-C2D	2.45	130.62	125.48
11	9	103	A1EYK	C34-C36-C39	2.45	128.48	123.47
8	U	101	BCL	CMD-C2D-C3D	-2.44	122.00	127.61
8	L	301	BCL	C1-C2-C3	-2.44	121.82	126.04
8	L	308	BCL	CMD-C2D-C3D	-2.44	122.00	127.61
8	D	102	BCL	CMD-C2D-C3D	-2.44	122.00	127.61
13	H	303	PGV	O03-C19-C20	2.44	119.56	111.91
8	M	403	BCL	CMD-C2D-C3D	-2.44	122.01	127.61
8	9	101	BCL	CMD-C2D-C3D	-2.43	122.02	127.61
10	A	102	SPO	C14-C15-C16	-2.43	115.63	123.22
8	Z	102	BCL	CHD-C1D-C2D	2.43	130.58	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	101	BCL	CHC-C1C-NC	2.42	127.86	124.51
8	L	308	BCL	O2A-CGA-CBA	2.42	119.52	111.91
8	5	101	BCL	C4A-NA-C1A	2.42	107.80	106.71
8	M	403	BCL	CHB-C4A-NA	2.42	127.86	124.51
8	7	101	BCL	CMD-C2D-C3D	-2.42	122.05	127.61
8	Q	101	BCL	CHB-C4A-NA	2.42	127.86	124.51
8	9	101	BCL	C1D-CHD-C4C	-2.42	120.79	126.62
10	5	102	SPO	C14-C15-C16	-2.41	115.68	123.22
8	1	101	BCL	O2D-CGD-O1D	-2.41	119.12	123.84
10	A	102	SPO	C40-C38-C39	2.41	119.94	114.60
12	D	101	LMT	O1'-C1'-C2'	2.41	112.07	108.30
10	U	104	SPO	C9-C10-C11	-2.41	115.71	123.22
8	U	101	BCL	C1D-CHD-C4C	-2.40	120.82	126.62
13	M	407	PGV	O03-C19-C20	2.40	119.45	111.91
10	5	102	SPO	C5-C6-C7	-2.40	122.26	125.89
8	T	101	BCL	C1-O2A-CGA	2.40	122.74	116.44
8	B	101	BCL	C4-C3-C5	2.40	119.31	115.27
8	L	307	BCL	O2A-CGA-CBA	2.40	119.44	111.91
8	9	101	BCL	C4-C3-C5	2.40	119.31	115.27
8	2	101	BCL	O2A-CGA-CBA	2.40	119.43	111.91
10	F	102	SPO	C14-C15-C16	-2.40	115.74	123.22
8	5	101	BCL	C3C-C4C-CHD	-2.39	118.28	123.39
8	L	307	BCL	C2A-C1A-CHA	-2.39	119.67	123.86
10	5	102	SPO	C13-C12-C11	2.39	121.85	118.08
8	2	101	BCL	CHD-C4C-NC	2.39	127.73	125.08
8	O	101	BCL	CMD-C2D-C3D	-2.39	122.11	127.61
8	5	101	BCL	CMD-C2D-C3D	-2.39	122.11	127.61
8	R	101	BCL	C4-C3-C5	2.39	119.29	115.27
8	G	101	BCL	O2D-CGD-O1D	-2.39	119.17	123.84
8	F	101	BCL	CMD-C2D-C3D	-2.39	122.12	127.61
8	L	308	BCL	O2D-CGD-O1D	-2.39	119.17	123.84
10	U	104	SPO	C14-C15-C16	-2.38	115.80	123.22
12	F	104	LMT	C1B-O1B-C4'	2.37	123.84	117.96
10	I	102	SPO	C8-C7-C6	2.37	121.81	118.08
8	Z	102	BCL	CMD-C2D-C3D	-2.37	122.17	127.61
10	4	101	SPO	C36-C37-C38	-2.36	119.69	127.75
8	E	101	BCL	O2D-CGD-O1D	-2.36	119.23	123.84
8	K	101	BCL	CMD-C2D-C3D	-2.36	122.19	127.61
8	S	101	BCL	CMD-C2D-C3D	-2.36	122.19	127.61
10	U	102	SPO	C40-C38-C39	2.36	119.81	114.60
13	M	408	PGV	O03-C19-C20	2.35	119.30	111.91
8	7	101	BCL	C4B-CHC-C1C	-2.35	125.46	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	5	101	BCL	C1C-NC-C4C	-2.35	105.65	106.71
8	O	101	BCL	C1D-CHD-C4C	-2.35	120.95	126.62
10	U	104	SPO	C34-C33-C35	2.35	119.22	115.27
13	M	407	PGV	O14-P-O13	2.35	119.86	110.68
8	2	101	BCL	O2D-CGD-O1D	-2.34	119.26	123.84
8	A	101	BCL	C1D-CHD-C4C	-2.34	120.98	126.62
8	L	301	BCL	O2A-CGA-O1A	-2.33	117.71	123.59
8	R	101	BCL	C1C-NC-C4C	-2.33	105.66	106.71
12	F	104	LMT	C1-O1'-C1'	-2.33	109.98	113.84
8	T	101	BCL	O2D-CGD-O1D	-2.33	119.28	123.84
8	Q	101	BCL	CMD-C2D-C3D	-2.33	122.25	127.61
8	S	101	BCL	C2A-C1A-CHA	-2.33	119.79	123.86
8	B	101	BCL	O2D-CGD-O1D	-2.33	119.28	123.84
8	B	101	BCL	C1-O2A-CGA	2.32	122.54	116.44
8	5	101	BCL	CHC-C1C-NC	2.32	127.72	124.51
10	D	103	SPO	C40-C38-C39	2.32	119.72	114.60
10	7	102	SPO	C40-C38-C39	2.32	119.72	114.60
8	5	101	BCL	CHB-C4A-NA	2.32	127.72	124.51
10	U	102	SPO	C9-C10-C11	-2.32	115.99	123.22
10	I	102	SPO	C40-C38-C39	2.31	119.72	114.60
10	Q	102	SPO	C40-C38-C39	2.31	119.71	114.60
10	S	102	SPO	C40-C38-C39	2.31	119.71	114.60
8	P	101	BCL	C1-O2A-CGA	2.31	122.51	116.44
10	D	103	SPO	C13-C12-C11	2.31	121.72	118.08
8	A	101	BCL	CMD-C2D-C3D	-2.31	122.30	127.61
8	R	101	BCL	O2D-CGD-O1D	-2.31	119.33	123.84
10	9	102	SPO	C14-C15-C16	-2.31	116.02	123.22
8	J	101	BCL	C1-O2A-CGA	2.30	122.49	116.44
10	K	102	SPO	C13-C12-C11	2.30	121.70	118.08
8	D	102	BCL	C1D-CHD-C4C	-2.30	121.07	126.62
13	A	104	PGV	C02-O01-C1	-2.30	112.12	117.79
10	F	102	SPO	C40-C38-C39	2.30	119.69	114.60
10	O	102	SPO	C13-C12-C11	2.30	121.70	118.08
10	9	102	SPO	C40-C38-C39	2.30	119.68	114.60
10	Y	102	SPO	C5-C6-C7	-2.30	122.42	125.89
8	G	101	BCL	C1C-NC-C4C	-2.30	105.67	106.71
8	6	101	BCL	O2D-CGD-O1D	-2.30	119.35	123.84
8	Z	102	BCL	O2A-CGA-CBA	2.30	119.12	111.91
12	D	101	LMT	C1-O1'-C1'	-2.30	110.03	113.84
8	V	101	BCL	O2D-CGD-O1D	-2.30	119.35	123.84
10	O	102	SPO	C40-C38-C39	2.29	119.67	114.60
13	H	304	PGV	C03-C02-C01	-2.29	106.37	111.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	8	101	BCL	O2D-CGD-O1D	-2.29	119.36	123.84
8	Y	101	BCL	CHD-C1D-C2D	2.29	130.28	125.48
8	E	101	BCL	C2A-C1A-CHA	-2.29	119.86	123.86
8	X	101	BCL	O2D-CGD-O1D	-2.29	119.36	123.84
8	E	101	BCL	C1-O2A-CGA	2.28	122.44	116.44
8	M	403	BCL	CHC-C1C-NC	2.28	127.67	124.51
8	7	101	BCL	C1D-CHD-C4C	-2.28	121.11	126.62
10	U	104	SPO	C40-C38-C39	2.28	119.65	114.60
8	M	403	BCL	CAA-C2A-C3A	-2.28	106.53	112.78
10	I	102	SPO	C14-C15-C16	-2.28	116.10	123.22
8	7	101	BCL	CHC-C1C-NC	2.28	127.67	124.51
8	L	307	BCL	C1C-NC-C4C	-2.28	105.68	106.71
8	Q	101	BCL	C4B-CHC-C1C	-2.28	125.61	130.12
8	K	101	BCL	C1D-CHD-C4C	-2.27	121.14	126.62
10	4	101	SPO	C14-C15-C16	-2.27	116.13	123.22
8	9	101	BCL	CED-O2D-CGD	2.27	121.07	115.94
8	W	101	BCL	C1D-CHD-C4C	-2.27	121.15	126.62
10	K	102	SPO	C40-C38-C39	2.25	119.58	114.60
8	L	307	BCL	CHB-C4A-NA	2.25	127.63	124.51
8	M	403	BCL	C1D-CHD-C4C	-2.25	121.19	126.62
10	K	102	SPO	C14-C15-C16	-2.25	116.19	123.22
8	I	101	BCL	CMD-C2D-C3D	-2.25	122.43	127.61
8	W	101	BCL	C1C-NC-C4C	-2.25	105.69	106.71
8	Y	101	BCL	C1D-CHD-C4C	-2.25	121.20	126.62
8	3	101	BCL	C4A-NA-C1A	2.25	107.72	106.71
8	X	101	BCL	CMD-C2D-C3D	-2.25	122.44	127.61
8	O	101	BCL	C4A-NA-C1A	2.25	107.72	106.71
8	F	101	BCL	O2D-CGD-O1D	-2.24	119.45	123.84
8	D	102	BCL	CED-O2D-CGD	2.24	121.01	115.94
8	4	102	BCL	C1-O2A-CGA	2.24	122.33	116.44
13	L	304	PGV	C02-O01-C1	-2.24	112.27	117.79
12	7	104	LMT	C1B-C2B-C3B	2.24	114.67	110.00
8	S	101	BCL	C1D-CHD-C4C	-2.24	121.21	126.62
10	Q	102	SPO	C13-C12-C11	2.24	121.61	118.08
10	S	102	SPO	C13-C12-C11	2.24	121.61	118.08
10	5	102	SPO	C40-C38-C39	2.24	119.55	114.60
8	N	101	BCL	O2D-CGD-O1D	-2.24	119.46	123.84
10	I	102	SPO	C20-C21-C22	-2.23	118.90	123.47
10	M	406	SPO	C15-C14-C12	-2.23	124.12	127.31
8	5	101	BCL	O2D-CGD-O1D	-2.23	119.47	123.84
8	Q	101	BCL	O2D-CGD-O1D	-2.23	119.47	123.84
10	U	102	SPO	C15-C14-C12	-2.23	124.12	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	101	BCL	C4A-NA-C1A	2.23	107.71	106.71
8	E	101	BCL	CHC-C1C-NC	2.23	127.59	124.51
8	6	101	BCL	C1D-CHD-C4C	-2.23	121.25	126.62
8	Q	101	BCL	O2A-CGA-O1A	-2.22	117.98	123.59
8	O	101	BCL	C2A-C1A-CHA	-2.22	119.97	123.86
8	J	101	BCL	O2D-CGD-O1D	-2.22	119.49	123.84
8	P	101	BCL	O2D-CGD-O1D	-2.22	119.50	123.84
10	4	101	SPO	C34-C33-C35	2.21	118.99	115.27
8	I	101	BCL	C4B-CHC-C1C	-2.21	125.74	130.12
10	Q	102	SPO	C34-C33-C35	2.21	118.98	115.27
8	O	101	BCL	CED-O2D-CGD	2.20	120.92	115.94
8	0	101	BCL	C1D-CHD-C4C	-2.20	121.31	126.62
8	3	101	BCL	O2D-CGD-O1D	-2.20	119.53	123.84
8	W	101	BCL	C2A-C1A-CHA	-2.20	120.01	123.86
8	D	102	BCL	C2A-C1A-CHA	-2.20	120.02	123.86
8	0	101	BCL	C1-O2A-CGA	2.20	122.21	116.44
8	B	101	BCL	C1D-CHD-C4C	-2.19	121.33	126.62
8	L	308	BCL	C1D-CHD-C4C	-2.19	121.33	126.62
8	K	101	BCL	O2D-CGD-O1D	-2.19	119.56	123.84
8	0	101	BCL	O2D-CGD-O1D	-2.19	119.56	123.84
8	G	101	BCL	C1D-CHD-C4C	-2.19	121.35	126.62
8	S	101	BCL	O2A-CGA-O1A	-2.19	118.08	123.59
10	A	102	SPO	C13-C12-C11	2.18	121.52	118.08
10	4	101	SPO	C40-C38-C39	2.18	119.42	114.60
8	R	101	BCL	C1-O2A-CGA	2.18	122.17	116.44
8	L	301	BCL	C2A-C1A-CHA	-2.18	120.05	123.86
8	Y	101	BCL	O2D-CGD-O1D	-2.18	119.58	123.84
10	7	102	SPO	C13-C12-C11	2.18	121.51	118.08
11	W	102	A1EYK	C40-C37-C39	-2.18	119.87	122.92
10	U	102	SPO	C20-C21-C22	-2.18	119.01	123.47
8	5	101	BCL	CHD-C1D-C2D	2.17	130.04	125.48
11	I	103	A1EYK	C36-C34-C31	2.17	127.93	123.47
10	U	102	SPO	C13-C12-C11	2.17	121.50	118.08
8	4	102	BCL	C1D-ND-C4D	-2.17	104.79	106.33
8	5	101	BCL	C4B-CHC-C1C	-2.17	125.82	130.12
8	T	101	BCL	C1D-CHD-C4C	-2.17	121.39	126.62
11	A	103	A1EYK	C36-C34-C31	2.17	127.92	123.47
8	X	101	BCL	C1D-CHD-C4C	-2.17	121.39	126.62
10	M	406	SPO	C29-C28-C30	2.17	118.91	115.27
8	X	101	BCL	C2A-C1A-CHA	-2.16	120.08	123.86
10	O	102	SPO	C8-C7-C6	2.16	121.48	118.08
8	8	101	BCL	C1C-NC-C4C	-2.16	105.73	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	R	101	BCL	C1D-CHD-C4C	-2.16	121.41	126.62
8	A	101	BCL	O2D-CGD-O1D	-2.16	119.62	123.84
13	D	105	PGV	O03-C19-C20	2.16	118.68	111.91
8	V	101	BCL	C4D-CHA-C1A	-2.16	118.63	121.25
11	U	103	A1EYK	C36-C34-C31	2.15	127.89	123.47
10	5	102	SPO	C34-C33-C35	2.15	118.89	115.27
10	K	102	SPO	C34-C33-C35	2.15	118.89	115.27
8	M	403	BCL	O2A-CGA-O1A	-2.15	118.17	123.59
8	6	101	BCL	C4D-CHA-C1A	-2.15	118.63	121.25
10	D	103	SPO	C34-C33-C35	2.15	118.89	115.27
13	H	305	PGV	C02-O01-C1	-2.15	112.50	117.79
8	S	101	BCL	CED-O2D-CGD	2.15	120.80	115.94
8	G	101	BCL	C1-O2A-CGA	2.15	122.08	116.44
8	8	101	BCL	C1D-CHD-C4C	-2.15	121.44	126.62
8	P	101	BCL	C1D-CHD-C4C	-2.15	121.44	126.62
8	J	101	BCL	C1D-CHD-C4C	-2.15	121.44	126.62
8	9	101	BCL	C4A-NA-C1A	2.14	107.67	106.71
10	U	102	SPO	C34-C33-C35	2.14	118.88	115.27
8	L	308	BCL	CHC-C1C-NC	2.14	127.47	124.51
10	O	102	SPO	C34-C33-C35	2.14	118.87	115.27
10	F	102	SPO	C13-C12-C11	2.14	121.45	118.08
8	L	301	BCL	C1D-CHD-C4C	-2.14	121.47	126.62
8	9	101	BCL	C4B-CHC-C1C	-2.14	125.89	130.12
8	0	101	BCL	C1C-NC-C4C	-2.13	105.75	106.71
10	I	102	SPO	C34-C33-C35	2.13	118.86	115.27
8	Z	102	BCL	C1D-CHD-C4C	-2.13	121.48	126.62
10	9	102	SPO	C13-C12-C11	2.13	121.43	118.08
8	F	101	BCL	O2A-CGA-O1A	-2.13	118.22	123.59
11	F	103	A1EYK	C36-C34-C31	2.12	127.83	123.47
8	I	101	BCL	O2D-CGD-O1D	-2.12	119.69	123.84
8	E	101	BCL	C1D-CHD-C4C	-2.12	121.50	126.62
17	M	404	BPH	CMA-C3A-C4A	-2.12	109.74	114.38
11	I	103	A1EYK	C29-C27-C31	-2.12	119.95	122.92
10	I	102	SPO	C15-C14-C12	-2.12	124.29	127.31
10	K	102	SPO	C15-C14-C12	-2.12	124.29	127.31
8	F	101	BCL	CED-O2D-CGD	2.12	120.72	115.94
10	U	104	SPO	C13-C12-C11	2.12	121.41	118.08
8	U	101	BCL	C2A-C1A-CHA	-2.11	120.16	123.86
12	9	104	LMT	O5B-C1B-C2B	2.11	114.82	110.35
8	N	101	BCL	C1D-CHD-C4C	-2.11	121.53	126.62
8	W	101	BCL	O2D-CGD-O1D	-2.11	119.72	123.84
8	U	101	BCL	O2D-CGD-O1D	-2.11	119.72	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	J	101	BCL	C1C-NC-C4C	-2.10	105.76	106.71
8	R	101	BCL	CED-O2D-CGD	2.10	120.70	115.94
8	0	101	BCL	CED-O2D-CGD	2.10	120.69	115.94
8	K	101	BCL	C1C-NC-C4C	-2.10	105.76	106.71
8	S	101	BCL	O2D-CGD-O1D	-2.10	119.73	123.84
10	S	102	SPO	C34-C33-C35	2.10	118.80	115.27
8	A	101	BCL	CED-O2D-CGD	2.10	120.68	115.94
8	1	101	BCL	C3C-C4C-CHD	-2.10	118.91	123.39
8	N	101	BCL	CED-O2D-CGD	2.10	120.68	115.94
8	6	101	BCL	CMD-C2D-C3D	-2.09	122.80	127.61
10	F	102	SPO	C34-C33-C35	2.09	118.79	115.27
8	7	101	BCL	C1C-NC-C4C	-2.09	105.77	106.71
8	7	101	BCL	CED-O2D-CGD	2.09	120.67	115.94
8	L	308	BCL	CHD-C1D-C2D	2.09	129.87	125.48
13	L	304	PGV	O01-C1-O02	-2.09	118.65	123.70
13	D	105	PGV	C02-O01-C1	-2.09	112.65	117.79
8	I	101	BCL	CED-O2D-CGD	2.09	120.66	115.94
8	8	101	BCL	CMD-C2D-C3D	-2.09	122.81	127.61
8	9	101	BCL	C2A-C1A-CHA	-2.09	120.21	123.86
8	V	101	BCL	C1D-CHD-C4C	-2.08	121.59	126.62
8	L	308	BCL	CHB-C4A-NA	2.08	127.39	124.51
8	I	101	BCL	O2A-CGA-O1A	-2.08	118.34	123.59
10	A	102	SPO	C8-C7-C6	2.08	121.35	118.08
8	D	102	BCL	C4A-NA-C1A	2.08	107.64	106.71
11	D	104	A1EYK	C36-C34-C31	2.08	127.73	123.47
8	7	101	BCL	O2D-CGD-O1D	-2.08	119.77	123.84
12	L	305	LMT	O1'-C1'-C2'	2.08	111.54	108.30
10	O	102	SPO	C20-C21-C22	-2.07	119.23	123.47
8	0	101	BCL	O2A-CGA-CBA	2.07	118.39	111.91
8	V	101	BCL	CMD-C2D-C3D	-2.07	122.86	127.61
8	6	101	BCL	O2A-CGA-CBA	2.06	118.38	111.91
8	X	101	BCL	CHC-C1C-NC	2.06	127.36	124.51
10	7	102	SPO	C34-C33-C35	2.06	118.73	115.27
8	K	101	BCL	C2A-C1A-CHA	-2.06	120.26	123.86
10	7	102	SPO	C5-C6-C7	-2.05	122.79	125.89
10	Y	102	SPO	C21-C20-C19	-2.05	119.27	123.47
8	6	101	BCL	C1-O2A-CGA	2.05	121.83	116.44
8	Z	102	BCL	C4D-CHA-C1A	-2.05	118.75	121.25
14	C	401	HEC	CMB-C2B-C1B	-2.05	125.31	128.46
8	L	308	BCL	C2A-C1A-CHA	-2.05	120.27	123.86
8	F	101	BCL	C4B-CHC-C1C	-2.05	126.06	130.12
8	D	102	BCL	O2A-CGA-O1A	-2.05	118.42	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	T	101	BCL	CED-O2D-CGD	2.05	120.57	115.94
10	9	102	SPO	C34-C33-C35	2.04	118.71	115.27
8	N	101	BCL	C4D-CHA-C1A	-2.04	118.77	121.25
14	C	403	HEC	CAA-CBA-CGA	-2.04	108.04	113.76
8	4	102	BCL	C4D-CHA-C1A	-2.04	118.77	121.25
8	8	101	BCL	CED-O2D-CGD	2.04	120.55	115.94
8	Z	102	BCL	C1D-ND-C4D	-2.04	104.89	106.33
10	U	104	SPO	C15-C14-C12	-2.04	124.40	127.31
12	F	104	LMT	O1B-C4'-C3'	2.04	112.70	107.28
8	G	101	BCL	CED-O2D-CGD	2.04	120.54	115.94
8	5	101	BCL	CED-O2D-CGD	2.04	120.54	115.94
8	U	101	BCL	O2A-CGA-O1A	-2.03	118.46	123.59
10	U	104	SPO	C36-C37-C38	-2.03	120.80	127.75
8	Q	101	BCL	CED-O2D-CGD	2.03	120.53	115.94
10	D	103	SPO	C8-C7-C6	2.03	121.28	118.08
10	K	102	SPO	C20-C21-C22	-2.03	119.31	123.47
8	P	101	BCL	CED-O2D-CGD	2.03	120.53	115.94
10	F	102	SPO	C8-C7-C6	2.03	121.27	118.08
8	U	101	BCL	CED-O2D-CGD	2.03	120.53	115.94
8	V	101	BCL	O2A-CGA-CBA	2.03	118.27	111.91
10	Q	102	SPO	C5-C6-C7	-2.03	122.83	125.89
11	U	103	A1EYK	C29-C27-C31	-2.03	120.09	122.92
14	C	401	HEC	CMC-C2C-C1C	-2.02	125.36	128.46
10	Y	102	SPO	C36-C37-C38	-2.02	120.84	127.75
10	A	102	SPO	C34-C33-C35	2.02	118.67	115.27
8	4	102	BCL	O2A-CGA-CBA	2.02	118.24	111.91
8	O	101	BCL	O2D-CGD-O1D	-2.02	119.89	123.84
14	C	401	HEC	CAD-CBD-CGD	-2.02	108.10	113.76
8	7	101	BCL	O2A-CGA-O1A	-2.02	118.50	123.59
8	T	101	BCL	C1C-NC-C4C	-2.02	105.80	106.71
8	A	101	BCL	C4B-CHC-C1C	-2.01	126.13	130.12
8	L	307	BCL	C4B-CHC-C1C	-2.01	126.13	130.12
8	A	101	BCL	C6-C5-C3	-2.01	108.18	113.45
10	4	101	SPO	C20-C21-C22	-2.01	119.36	123.47
8	9	101	BCL	O2A-CGA-O1A	-2.01	118.53	123.59
8	D	102	BCL	O2D-CGD-O1D	-2.01	119.92	123.84
8	1	101	BCL	CAA-C2A-C3A	-2.01	107.29	112.78
10	D	103	SPO	C20-C21-C22	-2.01	119.37	123.47
10	5	102	SPO	C10-C9-C7	-2.00	124.45	127.31
8	U	101	BCL	C4B-CHC-C1C	-2.00	126.15	130.12
10	9	102	SPO	C5-C6-C7	-2.00	122.87	125.89
8	7	101	BCL	C2A-C1A-CHA	-2.00	120.36	123.86

There are no chirality outliers.

All (676) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	0	101	BCL	C3A-C2A-CAA-CBA
8	1	101	BCL	C1A-C2A-CAA-CBA
8	1	101	BCL	C4C-C3C-CAC-CBC
8	1	101	BCL	C2-C3-C5-C6
8	1	101	BCL	C4-C3-C5-C6
8	2	101	BCL	C2C-C3C-CAC-CBC
8	2	101	BCL	C4C-C3C-CAC-CBC
8	2	101	BCL	CHA-CBD-CGD-O1D
8	2	101	BCL	CHA-CBD-CGD-O2D
8	3	101	BCL	C2C-C3C-CAC-CBC
8	3	101	BCL	C4C-C3C-CAC-CBC
8	4	102	BCL	C1A-C2A-CAA-CBA
8	5	101	BCL	C2C-C3C-CAC-CBC
8	6	101	BCL	C1A-C2A-CAA-CBA
8	6	101	BCL	C3A-C2A-CAA-CBA
8	8	101	BCL	C3A-C2A-CAA-CBA
8	B	101	BCL	C1A-C2A-CAA-CBA
8	E	101	BCL	C1A-C2A-CAA-CBA
8	E	101	BCL	C3A-C2A-CAA-CBA
8	E	101	BCL	C11-C10-C8-C9
8	G	101	BCL	C3A-C2A-CAA-CBA
8	I	101	BCL	C11-C12-C13-C14
8	J	101	BCL	C3A-C2A-CAA-CBA
8	J	101	BCL	C11-C10-C8-C9
8	M	403	BCL	O2A-C1-C2-C3
8	M	403	BCL	C2-C3-C5-C6
8	M	403	BCL	C4-C3-C5-C6
8	N	101	BCL	C3A-C2A-CAA-CBA
8	P	101	BCL	C1A-C2A-CAA-CBA
8	P	101	BCL	C3A-C2A-CAA-CBA
8	R	101	BCL	C1A-C2A-CAA-CBA
8	R	101	BCL	C3A-C2A-CAA-CBA
8	T	101	BCL	C1A-C2A-CAA-CBA
8	T	101	BCL	C3A-C2A-CAA-CBA
8	T	101	BCL	C11-C10-C8-C9
8	V	101	BCL	C1A-C2A-CAA-CBA
8	X	101	BCL	C1A-C2A-CAA-CBA
8	X	101	BCL	C3A-C2A-CAA-CBA
8	X	101	BCL	O2A-C1-C2-C3
8	Y	101	BCL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
8	Z	102	BCL	C1A-C2A-CAA-CBA
10	4	101	SPO	C2-C1-C4-C5
10	4	101	SPO	C1-C4-C5-C6
10	4	101	SPO	C22-C23-C25-C26
10	4	101	SPO	C24-C23-C25-C26
10	I	102	SPO	C10-C11-C12-C13
10	I	102	SPO	C10-C11-C12-C14
10	M	406	SPO	C2-C1-C4-C5
10	M	406	SPO	C3-C1-C4-C5
10	M	406	SPO	C32-C33-C35-C36
10	M	406	SPO	C34-C33-C35-C36
10	U	104	SPO	C33-C35-C36-C37
10	Y	102	SPO	C32-C33-C35-C36
10	Y	102	SPO	C34-C33-C35-C36
11	5	103	A1EYK	C15-C11-C2-C1
11	I	103	A1EYK	C15-C11-C2-C1
11	K	103	A1EYK	C15-C11-C2-C1
11	O	103	A1EYK	C15-C11-C2-C1
11	S	103	A1EYK	C15-C11-C2-C1
11	U	103	A1EYK	C15-C11-C2-C1
11	W	102	A1EYK	C39-C37-C38-C35
11	W	102	A1EYK	C40-C37-C38-C35
11	Z	101	A1EYK	C15-C11-C2-C1
13	A	104	PGV	C03-O11-P-O14
13	D	105	PGV	C03-O11-P-O14
13	F	105	PGV	C03-O11-P-O13
13	F	105	PGV	C04-O12-P-O14
13	H	302	PGV	C03-O11-P-O14
13	H	302	PGV	C04-O12-P-O14
13	H	303	PGV	C03-O11-P-O12
13	H	303	PGV	C03-O11-P-O14
13	H	303	PGV	C04-O12-P-O11
13	H	304	PGV	C03-O11-P-O12
13	L	304	PGV	C04-O12-P-O14
13	M	407	PGV	C03-O11-P-O12
13	M	408	PGV	C04-O12-P-O13
13	M	408	PGV	C04-O12-P-O14
13	M	409	PGV	C03-O11-P-O12
13	M	409	PGV	C04-O12-P-O14
13	M	409	PGV	C2-C1-O01-C02
18	L	303	U10	C39-C41-C42-C43
18	M	405	U10	C49-C51-C52-C53

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Mol	Chain	Res	Type	Atoms
8	4	102	BCL	CBD-CGD-O2D-CED
8	M	403	BCL	O1A-CGA-O2A-C1
12	F	104	LMT	C2B-C1B-O1B-C4'
8	M	403	BCL	CBA-CGA-O2A-C1
12	L	305	LMT	C3'-C4'-O1B-C1B
13	M	409	PGV	O02-C1-O01-C02
8	S	101	BCL	C3-C5-C6-C7
8	Y	101	BCL	CBA-CGA-O2A-C1
8	K	101	BCL	C4-C3-C5-C6
8	K	101	BCL	C2-C3-C5-C6
8	M	403	BCL	C3-C5-C6-C7
8	Y	101	BCL	O1A-CGA-O2A-C1
11	W	102	A1EYK	C30-C32-C35-C38
12	L	305	LMT	O5'-C5'-C6'-O6'
13	H	301	PGV	O12-C04-C05-O05
13	H	303	PGV	O12-C04-C05-O05
8	A	101	BCL	CBA-CGA-O2A-C1
8	O	101	BCL	C3-C5-C6-C7
8	X	101	BCL	C4-C3-C5-C6
11	W	102	A1EYK	C17-C12-C8-C7
18	L	303	U10	C25-C24-C26-C27
18	M	410	U10	C12-C11-C9-C10
8	X	101	BCL	C2-C3-C5-C6
11	W	102	A1EYK	C19-C12-C8-C7
18	L	303	U10	C23-C24-C26-C27
18	M	410	U10	C12-C11-C9-C8
8	4	102	BCL	O1D-CGD-O2D-CED
8	A	101	BCL	O1A-CGA-O2A-C1
10	4	101	SPO	C28-C30-C31-C32
10	9	102	SPO	C33-C35-C36-C37
10	A	102	SPO	C33-C35-C36-C37
10	D	103	SPO	C33-C35-C36-C37
10	F	102	SPO	C33-C35-C36-C37
10	I	102	SPO	C33-C35-C36-C37
10	K	102	SPO	C33-C35-C36-C37
10	O	102	SPO	C33-C35-C36-C37
10	Q	102	SPO	C33-C35-C36-C37
10	Y	102	SPO	C33-C35-C36-C37
8	K	101	BCL	CBA-CGA-O2A-C1
13	H	301	PGV	O12-C04-C05-C06
13	H	303	PGV	O12-C04-C05-C06
8	K	101	BCL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
12	L	305	LMT	C4'-C5'-C6'-O6'
8	7	101	BCL	C15-C16-C17-C18
8	Q	101	BCL	C15-C16-C17-C18
8	2	101	BCL	C6-C7-C8-C9
8	4	102	BCL	C11-C10-C8-C9
8	5	101	BCL	C14-C13-C15-C16
8	6	101	BCL	C6-C7-C8-C9
8	B	101	BCL	C11-C10-C8-C9
8	L	308	BCL	C11-C10-C8-C9
8	P	101	BCL	C11-C10-C8-C9
8	P	101	BCL	C11-C12-C13-C14
8	X	101	BCL	C11-C10-C8-C9
10	4	101	SPO	C5-C6-C7-C8
8	F	101	BCL	C15-C16-C17-C18
8	Y	101	BCL	C13-C15-C16-C17
13	H	301	PGV	C1-C2-C3-C4
8	7	101	BCL	C13-C15-C16-C17
8	9	101	BCL	C15-C16-C17-C18
13	M	407	PGV	C1-C2-C3-C4
12	M	413	LMT	C4'-C5'-C6'-O6'
8	O	101	BCL	C15-C16-C17-C18
8	X	101	BCL	C3-C5-C6-C7
12	7	104	LMT	O5B-C5B-C6B-O6B
8	N	101	BCL	C10-C11-C12-C13
8	K	101	BCL	C6-C7-C8-C10
8	R	101	BCL	C6-C7-C8-C10
8	Q	101	BCL	C5-C6-C7-C8
12	K	104	LMT	O5'-C1'-O1'-C1
10	5	102	SPO	C33-C35-C36-C37
10	7	102	SPO	C33-C35-C36-C37
10	S	102	SPO	C33-C35-C36-C37
10	U	102	SPO	C33-C35-C36-C37
13	H	302	PGV	O12-C04-C05-O05
8	R	101	BCL	C8-C10-C11-C12
13	H	301	PGV	C19-C20-C21-C22
8	9	101	BCL	C13-C15-C16-C17
8	N	101	BCL	C15-C16-C17-C18
13	A	104	PGV	C03-O11-P-O12
13	D	105	PGV	C03-O11-P-O12
13	F	105	PGV	C04-O12-P-O11
13	H	301	PGV	C03-O11-P-O12
13	H	302	PGV	C03-O11-P-O12

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Mol	Chain	Res	Type	Atoms
13	L	304	PGV	C04-O12-P-O11
13	M	408	PGV	C04-O12-P-O11
13	M	409	PGV	C04-O12-P-O11
8	1	101	BCL	CBA-CGA-O2A-C1
13	A	104	PGV	C1-C2-C3-C4
13	H	302	PGV	O12-C04-C05-C06
18	M	402	U10	C12-C13-C14-C16
8	X	101	BCL	CBA-CGA-O2A-C1
13	F	105	PGV	C2-C1-O01-C02
13	M	409	PGV	C01-C02-O01-C1
13	F	105	PGV	O02-C1-O01-C02
8	1	101	BCL	C8-C10-C11-C12
8	3	101	BCL	CBD-CGD-O2D-CED
12	F	104	LMT	C5'-C4'-O1B-C1B
13	M	411	PGV	O12-C04-C05-O05
8	U	101	BCL	C13-C15-C16-C17
10	U	104	SPO	C34-C33-C35-C36
13	H	302	PGV	C2-C3-C4-C5
8	L	301	BCL	C11-C10-C8-C9
13	H	303	PGV	C6-C7-C8-C9
8	W	101	BCL	C2A-CAA-CBA-CGA
8	1	101	BCL	O1A-CGA-O2A-C1
13	L	304	PGV	C27-C28-C29-C30
13	M	408	PGV	C25-C26-C27-C28
13	F	105	PGV	C04-C05-C06-O06
13	M	408	PGV	C04-C05-C06-O06
13	H	303	PGV	C11-C10-C9-C8
8	X	101	BCL	O1A-CGA-O2A-C1
8	S	101	BCL	C13-C15-C16-C17
8	3	101	BCL	C3A-C2A-CAA-CBA
8	A	101	BCL	C3A-C2A-CAA-CBA
8	K	101	BCL	C3A-C2A-CAA-CBA
8	V	101	BCL	C3A-C2A-CAA-CBA
8	Z	102	BCL	C3A-C2A-CAA-CBA
12	7	104	LMT	C2-C1-O1'-C1'
12	K	104	LMT	C2-C1-O1'-C1'
13	H	301	PGV	C3-C4-C5-C6
8	B	101	BCL	O2A-C1-C2-C3
12	F	104	LMT	C3'-C4'-O1B-C1B
17	M	404	BPH	C3-C5-C6-C7
12	M	413	LMT	C1-C2-C3-C4
8	M	403	BCL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
13	H	301	PGV	C2-C3-C4-C5
12	F	104	LMT	O5'-C5'-C6'-O6'
13	A	104	PGV	C3-C4-C5-C6
13	M	408	PGV	C5-C6-C7-C8
8	B	101	BCL	CBA-CGA-O2A-C1
8	0	101	BCL	C10-C11-C12-C13
8	M	403	BCL	C5-C6-C7-C8
8	U	101	BCL	C15-C16-C17-C18
12	M	413	LMT	O5'-C5'-C6'-O6'
8	2	101	BCL	CBD-CGD-O2D-CED
8	L	301	BCL	C4-C3-C5-C6
8	2	101	BCL	C6-C7-C8-C10
8	6	101	BCL	C6-C7-C8-C10
8	I	101	BCL	C11-C12-C13-C15
8	L	301	BCL	C11-C10-C8-C7
8	O	101	BCL	C6-C7-C8-C10
8	S	101	BCL	C6-C7-C8-C10
8	X	101	BCL	C6-C7-C8-C10
8	Z	102	BCL	C11-C10-C8-C7
10	U	104	SPO	C32-C33-C35-C36
8	B	101	BCL	O1A-CGA-O2A-C1
13	M	409	PGV	C20-C19-O03-C01
12	D	101	LMT	O1'-C1-C2-C3
13	H	303	PGV	C1-C2-C3-C4
8	5	101	BCL	C15-C16-C17-C18
13	H	302	PGV	C2-C1-O01-C02
13	M	411	PGV	C2-C1-O01-C02
13	M	411	PGV	O02-C1-O01-C02
12	O	104	LMT	O5B-C5B-C6B-O6B
10	4	101	SPO	C29-C28-C30-C31
8	L	301	BCL	C2-C3-C5-C6
8	8	101	BCL	C6-C7-C8-C9
8	Q	101	BCL	C6-C7-C8-C9
8	R	101	BCL	C6-C7-C8-C9
8	Z	102	BCL	C11-C10-C8-C9
8	Q	101	BCL	C8-C10-C11-C12
8	0	101	BCL	C1A-C2A-CAA-CBA
8	3	101	BCL	C1A-C2A-CAA-CBA
8	8	101	BCL	C1A-C2A-CAA-CBA
8	A	101	BCL	C1A-C2A-CAA-CBA
8	G	101	BCL	C1A-C2A-CAA-CBA
8	J	101	BCL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
8	K	101	BCL	C1A-C2A-CAA-CBA
8	N	101	BCL	C1A-C2A-CAA-CBA
8	Y	101	BCL	C1A-C2A-CAA-CBA
12	D	101	LMT	C6-C7-C8-C9
13	D	105	PGV	C01-C02-C03-O11
11	9	103	A1EYK	C15-C11-C2-C1
11	Q	103	A1EYK	C15-C11-C2-C1
12	M	414	LMT	O5'-C5'-C6'-O6'
12	O	104	LMT	O5'-C5'-C6'-O6'
13	H	302	PGV	O02-C1-O01-C02
8	1	101	BCL	C2C-C3C-CAC-CBC
8	D	102	BCL	C8-C10-C11-C12
13	H	304	PGV	C2-C1-O01-C02
13	H	304	PGV	C21-C22-C23-C24
8	P	101	BCL	C10-C11-C12-C13
12	M	414	LMT	O5B-C5B-C6B-O6B
8	8	101	BCL	C10-C11-C12-C13
8	W	101	BCL	CBD-CGD-O2D-CED
12	9	104	LMT	O5'-C5'-C6'-O6'
12	K	104	LMT	O1'-C1-C2-C3
8	V	101	BCL	C5-C6-C7-C8
8	V	101	BCL	CBA-CGA-O2A-C1
8	8	101	BCL	C2-C1-O2A-CGA
12	L	306	LMT	O5'-C5'-C6'-O6'
13	M	407	PGV	C03-O11-P-O13
8	R	101	BCL	CBA-CGA-O2A-C1
8	W	101	BCL	C13-C15-C16-C17
8	W	101	BCL	C15-C16-C17-C18
13	H	305	PGV	O03-C01-C02-O01
13	M	409	PGV	O04-C19-O03-C01
10	4	101	SPO	C3-C1-C4-C5
8	2	101	BCL	C11-C10-C8-C7
8	9	101	BCL	C6-C7-C8-C10
8	A	101	BCL	C6-C7-C8-C10
8	E	101	BCL	C11-C10-C8-C7
8	I	101	BCL	C6-C7-C8-C10
8	K	101	BCL	C11-C10-C8-C7
8	N	101	BCL	C11-C10-C8-C7
8	P	101	BCL	C11-C10-C8-C7
8	Q	101	BCL	C6-C7-C8-C10
8	R	101	BCL	C11-C10-C8-C7
8	W	101	BCL	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
8	Y	101	BCL	C11-C10-C8-C7
17	M	404	BPH	C6-C7-C8-C10
8	F	101	BCL	C3-C5-C6-C7
8	2	101	BCL	C11-C10-C8-C9
8	5	101	BCL	C11-C10-C8-C9
8	7	101	BCL	C6-C7-C8-C9
8	9	101	BCL	C6-C7-C8-C9
8	9	101	BCL	C11-C10-C8-C9
8	A	101	BCL	C6-C7-C8-C9
8	D	102	BCL	C6-C7-C8-C9
8	D	102	BCL	C11-C10-C8-C9
8	I	101	BCL	C6-C7-C8-C9
8	K	101	BCL	C11-C10-C8-C9
8	N	101	BCL	C11-C10-C8-C9
8	S	101	BCL	C11-C10-C8-C9
8	U	101	BCL	C6-C7-C8-C9
8	U	101	BCL	C11-C10-C8-C9
8	W	101	BCL	C11-C10-C8-C9
8	Y	101	BCL	C11-C10-C8-C9
17	M	404	BPH	C6-C7-C8-C9
10	M	406	SPO	O1-C1-C4-C5
8	3	101	BCL	O1D-CGD-O2D-CED
8	R	101	BCL	O1A-CGA-O2A-C1
8	O	101	BCL	CBA-CGA-O2A-C1
13	M	409	PGV	C19-C20-C21-C22
8	A	101	BCL	C8-C10-C11-C12
13	F	105	PGV	C26-C27-C28-C29
8	4	102	BCL	C3A-C2A-CAA-CBA
8	B	101	BCL	C3A-C2A-CAA-CBA
8	7	101	BCL	C8-C10-C11-C12
13	H	304	PGV	C25-C26-C27-C28
8	V	101	BCL	O1A-CGA-O2A-C1
13	F	105	PGV	C20-C19-O03-C01
13	H	302	PGV	O03-C01-C02-C03
13	H	305	PGV	O03-C01-C02-C03
17	L	302	BPH	O2A-C1-C2-C3
8	O	101	BCL	C8-C10-C11-C12
13	M	408	PGV	O05-C05-C06-O06
8	F	101	BCL	C8-C10-C11-C12
8	1	101	BCL	C15-C16-C17-C18
13	L	304	PGV	O12-C04-C05-O05
8	O	101	BCL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
13	H	304	PGV	O02-C1-O01-C02
8	9	101	BCL	C8-C10-C11-C12
8	0	101	BCL	C6-C7-C8-C9
8	0	101	BCL	C11-C10-C8-C9
8	1	101	BCL	C6-C7-C8-C9
8	1	101	BCL	C11-C10-C8-C9
8	A	101	BCL	C11-C12-C13-C14
8	I	101	BCL	C11-C10-C8-C9
8	K	101	BCL	C6-C7-C8-C9
8	L	307	BCL	C11-C10-C8-C9
8	O	101	BCL	C11-C10-C8-C9
8	R	101	BCL	C11-C10-C8-C9
8	V	101	BCL	C6-C7-C8-C9
8	W	101	BCL	C6-C7-C8-C9
17	M	404	BPH	C14-C13-C15-C16
13	H	303	PGV	C05-C04-O12-P
13	F	105	PGV	C22-C23-C24-C25
13	D	105	PGV	C21-C22-C23-C24
8	2	101	BCL	O1D-CGD-O2D-CED
8	L	307	BCL	C4C-C3C-CAC-CBC
8	K	101	BCL	C10-C11-C12-C13
8	X	101	BCL	C15-C16-C17-C18
13	H	304	PGV	C19-C20-C21-C22
13	M	409	PGV	C22-C23-C24-C25
10	U	102	SPO	C34-C33-C35-C36
8	1	101	BCL	C6-C7-C8-C10
8	1	101	BCL	C11-C10-C8-C7
8	5	101	BCL	C11-C10-C8-C7
8	7	101	BCL	C6-C7-C8-C10
8	9	101	BCL	C11-C10-C8-C7
8	A	101	BCL	C11-C10-C8-C7
8	B	101	BCL	C11-C10-C8-C7
8	D	102	BCL	C6-C7-C8-C10
8	D	102	BCL	C11-C10-C8-C7
8	F	101	BCL	C11-C10-C8-C7
8	I	101	BCL	C11-C10-C8-C7
8	J	101	BCL	C11-C10-C8-C7
8	O	101	BCL	C11-C10-C8-C7
8	Q	101	BCL	C11-C10-C8-C7
8	S	101	BCL	C11-C10-C8-C7
8	T	101	BCL	C11-C10-C8-C7
8	U	101	BCL	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
8	U	101	BCL	C11-C10-C8-C7
8	W	101	BCL	C6-C7-C8-C10
8	X	101	BCL	C11-C10-C8-C7
8	9	101	BCL	C5-C6-C7-C8
8	W	101	BCL	CBA-CGA-O2A-C1
13	H	305	PGV	C03-O11-P-O14
12	D	101	LMT	C7-C8-C9-C10
17	L	302	BPH	CAD-CBD-CGD-O2D
18	M	402	U10	C12-C13-C14-C15
8	V	101	BCL	C10-C11-C12-C13
13	D	105	PGV	O01-C02-C03-O11
8	U	101	BCL	C8-C10-C11-C12
13	L	304	PGV	C2-C3-C4-C5
13	M	409	PGV	O12-C04-C05-C06
13	F	105	PGV	O04-C19-O03-C01
13	F	105	PGV	O03-C01-C02-O01
10	Q	102	SPO	C34-C33-C35-C36
18	L	303	U10	C50-C49-C51-C52
8	W	101	BCL	O1A-CGA-O2A-C1
12	7	104	LMT	C4B-C5B-C6B-O6B
10	Q	102	SPO	C32-C33-C35-C36
10	U	102	SPO	C32-C33-C35-C36
8	5	101	BCL	C6-C7-C8-C9
8	7	101	BCL	C11-C10-C8-C9
8	Q	101	BCL	C11-C10-C8-C9
8	Y	101	BCL	C6-C7-C8-C9
8	6	101	BCL	C10-C11-C12-C13
13	H	301	PGV	O02-C1-O01-C02
8	L	301	BCL	CBA-CGA-O2A-C1
8	2	101	BCL	C15-C16-C17-C18
10	4	101	SPO	C27-C28-C30-C31
18	L	303	U10	C48-C49-C51-C52
13	F	105	PGV	C04-O12-P-O13
13	H	301	PGV	C03-O11-P-O13
13	H	302	PGV	C03-O11-P-O13
13	H	303	PGV	C03-O11-P-O13
13	H	303	PGV	C04-O12-P-O14
13	H	304	PGV	C03-O11-P-O14
13	M	409	PGV	C03-O11-P-O14
8	I	101	BCL	C16-C17-C18-C19
8	Y	101	BCL	C8-C10-C11-C12
12	M	413	LMT	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
8	B	101	BCL	C5-C6-C7-C8
8	I	101	BCL	C8-C10-C11-C12
8	L	308	BCL	C15-C16-C17-C18
13	L	304	PGV	C20-C21-C22-C23
13	M	411	PGV	O12-C04-C05-C06
8	4	102	BCL	C11-C10-C8-C7
8	5	101	BCL	C6-C7-C8-C10
8	7	101	BCL	C11-C10-C8-C7
8	L	307	BCL	C6-C7-C8-C10
8	L	308	BCL	C6-C7-C8-C10
8	Y	101	BCL	C6-C7-C8-C10
13	H	302	PGV	O01-C02-C03-O11
13	H	301	PGV	C2-C1-O01-C02
8	L	301	BCL	O1A-CGA-O2A-C1
8	Z	102	BCL	C15-C16-C17-C18
8	A	101	BCL	C2A-CAA-CBA-CGA
8	L	307	BCL	C16-C17-C18-C19
13	L	304	PGV	O03-C01-C02-C03
13	L	304	PGV	O03-C01-C02-O01
8	A	101	BCL	C11-C10-C8-C9
8	B	101	BCL	C6-C7-C8-C9
8	F	101	BCL	C11-C10-C8-C9
8	J	101	BCL	C6-C7-C8-C9
8	K	101	BCL	C14-C13-C15-C16
8	M	403	BCL	C11-C10-C8-C9
18	L	303	U10	C19-C21-C22-C23
13	M	411	PGV	C19-C20-C21-C22
8	6	101	BCL	O1A-CGA-O2A-C1
10	4	101	SPO	C23-C25-C26-C27
11	9	103	A1EYK	C19-C23-C25-C27
11	W	102	A1EYK	C19-C23-C25-C27
18	L	303	U10	C12-C11-C9-C10
18	M	405	U10	C45-C44-C46-C47
8	L	307	BCL	C13-C15-C16-C17
8	P	101	BCL	C16-C17-C18-C19
13	F	105	PGV	C23-C24-C25-C26
13	H	302	PGV	C01-C02-C03-O11
8	6	101	BCL	CBA-CGA-O2A-C1
8	2	101	BCL	C2-C1-O2A-CGA
8	A	101	BCL	C2-C1-O2A-CGA
17	L	302	BPH	C2-C1-O2A-CGA
12	7	104	LMT	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
13	H	303	PGV	C14-C15-C16-C17
8	W	101	BCL	C16-C17-C18-C19
13	M	411	PGV	O03-C01-C02-O01
13	A	104	PGV	C04-O12-P-O11
13	F	105	PGV	C03-O11-P-O12
13	H	301	PGV	C04-O12-P-O11
13	H	302	PGV	C04-O12-P-O11
13	H	304	PGV	C04-O12-P-O11
13	L	304	PGV	C03-O11-P-O12
8	4	102	BCL	C5-C6-C7-C8
11	D	104	A1EYK	C9-C5-C6-C13
8	8	101	BCL	C6-C7-C8-C10
10	K	102	SPO	C32-C33-C35-C36
8	V	101	BCL	C11-C12-C13-C14
17	L	302	BPH	C16-C17-C18-C20
8	7	101	BCL	C2A-CAA-CBA-CGA
13	M	411	PGV	C04-C05-C06-O06
13	H	301	PGV	C05-C04-O12-P
8	L	307	BCL	C15-C16-C17-C18
13	F	105	PGV	C4-C5-C6-C7
13	F	105	PGV	C28-C29-C30-C31
8	I	101	BCL	C16-C17-C18-C20
8	6	101	BCL	C16-C17-C18-C19
10	U	104	SPO	C28-C30-C31-C32
10	K	102	SPO	C34-C33-C35-C36
18	L	303	U10	C40-C39-C41-C42
8	W	101	BCL	C8-C10-C11-C12
10	F	102	SPO	C32-C33-C35-C36
13	M	409	PGV	C2-C3-C4-C5
14	C	402	HEC	CAA-CBA-CGA-O1A
8	L	301	BCL	C2-C1-O2A-CGA
8	X	101	BCL	C2-C1-O2A-CGA
13	F	105	PGV	C21-C22-C23-C24
8	1	101	BCL	C3A-C2A-CAA-CBA
8	Q	101	BCL	C4-C3-C5-C6
13	H	302	PGV	C3-C4-C5-C6
8	8	101	BCL	C11-C10-C8-C9
8	8	101	BCL	C11-C12-C13-C14
8	D	102	BCL	C11-C12-C13-C14
8	L	307	BCL	C6-C7-C8-C9
14	C	401	HEC	CAA-CBA-CGA-O1A
13	F	105	PGV	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
13	H	304	PGV	O03-C01-C02-C03
13	H	303	PGV	O02-C1-O01-C02
8	J	101	BCL	C16-C17-C18-C19
13	F	105	PGV	C13-C14-C15-C16
10	4	101	SPO	C5-C6-C7-C9
11	U	103	A1EYK	C9-C5-C6-C13
8	7	101	BCL	C1A-C2A-CAA-CBA
8	W	101	BCL	C1A-C2A-CAA-CBA
8	L	308	BCL	C11-C10-C8-C7
8	L	308	BCL	C11-C12-C13-C15
8	P	101	BCL	C11-C12-C13-C15
17	M	404	BPH	C12-C13-C15-C16
8	E	101	BCL	C16-C17-C18-C19
8	M	403	BCL	C16-C17-C18-C19
12	F	104	LMT	C2-C3-C4-C5
8	5	101	BCL	C16-C17-C18-C19
8	Q	101	BCL	C13-C15-C16-C17
14	C	401	HEC	CAA-CBA-CGA-O2A
8	0	101	BCL	C4-C3-C5-C6
10	F	102	SPO	C34-C33-C35-C36
10	O	102	SPO	C32-C33-C35-C36
13	M	409	PGV	O12-C04-C05-O05
13	D	105	PGV	C27-C28-C29-C30
12	M	414	LMT	C3'-C4'-O1B-C1B
13	H	304	PGV	C30-C31-C32-C33
13	H	304	PGV	C20-C21-C22-C23
13	H	302	PGV	O03-C01-C02-O01
14	C	402	HEC	CAA-CBA-CGA-O2A
18	L	303	U10	C51-C52-C53-C54
13	L	304	PGV	O12-C04-C05-C06
18	M	405	U10	C35-C34-C36-C37
8	Z	102	BCL	C2-C1-O2A-CGA
8	Q	101	BCL	C2-C3-C5-C6
11	D	104	A1EYK	C9-C5-C6-C10
18	L	303	U10	C12-C11-C9-C8
13	M	411	PGV	C1-C2-C3-C4
8	G	101	BCL	C5-C6-C7-C8
13	H	305	PGV	C24-C25-C26-C27
8	E	101	BCL	O1A-CGA-O2A-C1
10	Y	102	SPO	C29-C28-C30-C31
10	9	102	SPO	C32-C33-C35-C36
18	M	405	U10	C43-C44-C46-C47

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Mol	Chain	Res	Type	Atoms
8	L	301	BCL	O1D-CGD-O2D-CED
8	L	301	BCL	C15-C16-C17-C18
13	M	408	PGV	C6-C7-C8-C9
13	M	409	PGV	C23-C24-C25-C26
8	D	102	BCL	C2A-CAA-CBA-CGA
18	L	303	U10	C5-C4-O4-C4M
8	T	101	BCL	C16-C17-C18-C19
13	L	304	PGV	C01-C02-C03-O11
8	6	101	BCL	C4-C3-C5-C6
18	M	405	U10	C30-C29-C31-C32
8	0	101	BCL	C6-C7-C8-C10
8	A	101	BCL	C11-C12-C13-C15
8	B	101	BCL	C6-C7-C8-C10
8	V	101	BCL	C6-C7-C8-C10
11	U	103	A1EYK	C9-C5-C6-C10
13	F	105	PGV	O05-C05-C06-O06
13	M	409	PGV	C29-C30-C31-C32
8	9	101	BCL	C2A-CAA-CBA-CGA
13	H	303	PGV	C2-C1-O01-C02
13	H	305	PGV	C23-C24-C25-C26
8	E	101	BCL	CBA-CGA-O2A-C1
13	M	407	PGV	C03-O11-P-O14
8	9	101	BCL	C4-C3-C5-C6
18	M	402	U10	C12-C11-C9-C10
18	M	402	U10	C15-C14-C16-C17
8	W	101	BCL	C16-C17-C18-C20
8	4	102	BCL	C6-C7-C8-C9
8	G	101	BCL	C6-C7-C8-C9
8	L	308	BCL	C6-C7-C8-C9
8	P	101	BCL	C6-C7-C8-C9
13	H	302	PGV	C1-C2-C3-C4
8	7	101	BCL	C3A-C2A-CAA-CBA
8	W	101	BCL	C3A-C2A-CAA-CBA
13	M	408	PGV	C11-C12-C13-C14
12	M	414	LMT	C5'-C4'-O1B-C1B
8	L	301	BCL	CAD-CBD-CGD-O2D
8	L	307	BCL	CAD-CBD-CGD-O2D
17	M	404	BPH	CAD-CBD-CGD-O2D
10	O	102	SPO	C34-C33-C35-C36
10	5	102	SPO	C32-C33-C35-C36
10	S	102	SPO	C32-C33-C35-C36
18	M	405	U10	C5-C4-O4-C4M

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Mol	Chain	Res	Type	Atoms
13	M	408	PGV	C9-C10-C11-C12
13	L	304	PGV	O01-C02-C03-O11
8	L	301	BCL	CBD-CGD-O2D-CED
8	0	101	BCL	O2A-C1-C2-C3
8	4	102	BCL	O2A-C1-C2-C3
8	6	101	BCL	O2A-C1-C2-C3
8	8	101	BCL	O2A-C1-C2-C3
8	E	101	BCL	O2A-C1-C2-C3
8	G	101	BCL	O2A-C1-C2-C3
8	J	101	BCL	O2A-C1-C2-C3
8	P	101	BCL	O2A-C1-C2-C3
8	R	101	BCL	O2A-C1-C2-C3
8	T	101	BCL	O2A-C1-C2-C3
8	V	101	BCL	O2A-C1-C2-C3
8	U	101	BCL	C2A-CAA-CBA-CGA
13	D	105	PGV	C20-C21-C22-C23
13	M	408	PGV	C7-C8-C9-C10
8	L	308	BCL	CHA-CBD-CGD-O1D
8	L	308	BCL	CHA-CBD-CGD-O2D
10	7	102	SPO	C32-C33-C35-C36
13	M	411	PGV	C01-C02-C03-O11
13	F	105	PGV	O03-C19-C20-C21
13	D	105	PGV	O03-C01-C02-O01
8	2	101	BCL	C2A-CAA-CBA-CGA
8	5	101	BCL	C2A-CAA-CBA-CGA
8	A	101	BCL	C12-C13-C15-C16
8	G	101	BCL	C12-C13-C15-C16
8	J	101	BCL	C6-C7-C8-C10
18	M	405	U10	C28-C29-C31-C32
8	G	101	BCL	C14-C13-C15-C16
8	L	308	BCL	C11-C12-C13-C14
12	M	413	LMT	C5-C6-C7-C8
13	A	104	PGV	C21-C22-C23-C24
13	D	105	PGV	C29-C30-C31-C32
8	3	101	BCL	CAA-CBA-CGA-O2A
11	5	103	A1EYK	C16-C14-C9-C5
11	7	103	A1EYK	C6-C10-C7-C8
11	9	103	A1EYK	C6-C10-C7-C8
11	F	103	A1EYK	C6-C10-C7-C8
11	O	103	A1EYK	C6-C10-C7-C8
11	Q	103	A1EYK	C6-C10-C7-C8
11	S	103	A1EYK	C6-C10-C7-C8

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Mol	Chain	Res	Type	Atoms
11	U	103	A1EYK	C16-C14-C9-C5
18	M	405	U10	C51-C52-C53-C54
13	A	104	PGV	C12-C13-C14-C15
13	A	104	PGV	C2-C3-C4-C5
8	5	101	BCL	C1A-C2A-CAA-CBA
8	9	101	BCL	C1A-C2A-CAA-CBA
8	D	102	BCL	C1A-C2A-CAA-CBA
8	F	101	BCL	C1A-C2A-CAA-CBA
8	Q	101	BCL	C1A-C2A-CAA-CBA
8	S	101	BCL	C1A-C2A-CAA-CBA
8	U	101	BCL	C1A-C2A-CAA-CBA
13	M	408	PGV	O03-C19-C20-C21
11	A	103	A1EYK	C6-C10-C7-C8
18	M	405	U10	C46-C47-C48-C49
8	Z	102	BCL	C16-C17-C18-C19
10	9	102	SPO	C34-C33-C35-C36
13	H	303	PGV	C15-C16-C17-C18
13	A	104	PGV	C04-O12-P-O13
13	H	301	PGV	C04-O12-P-O13
13	H	302	PGV	C04-O12-P-O13
8	G	101	BCL	C16-C17-C18-C19
8	L	301	BCL	C16-C17-C18-C19
8	7	101	BCL	O1A-CGA-O2A-C1
8	2	101	BCL	C5-C6-C7-C8
8	A	101	BCL	C15-C16-C17-C18
8	5	101	BCL	C16-C17-C18-C20
13	F	105	PGV	O04-C19-C20-C21
8	E	101	BCL	C4-C3-C5-C6
18	L	303	U10	C26-C27-C28-C29
18	M	402	U10	C13-C14-C16-C17
8	4	102	BCL	CAD-CBD-CGD-O1D
8	W	101	BCL	CAD-CBD-CGD-O1D
8	A	101	BCL	C14-C13-C15-C16
8	1	101	BCL	CAA-CBA-CGA-O2A
8	0	101	BCL	C2-C3-C5-C6
8	5	101	BCL	C3A-C2A-CAA-CBA
8	K	101	BCL	C12-C13-C15-C16
13	M	411	PGV	O01-C02-C03-O11
17	L	302	BPH	C11-C12-C13-C15
13	F	105	PGV	C1-C2-C3-C4
8	M	403	BCL	CAA-CBA-CGA-O2A
8	6	101	BCL	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
11	9	103	A1EYK	C16-C14-C9-C5
8	3	101	BCL	CAA-CBA-CGA-O1A
8	X	101	BCL	C16-C17-C18-C19
8	I	101	BCL	C10-C11-C12-C13
10	5	102	SPO	C34-C33-C35-C36
10	S	102	SPO	C34-C33-C35-C36

There are no ring outliers.

72 monomers are involved in 257 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	U	101	BCL	2	0
8	M	403	BCL	4	0
8	F	101	BCL	1	0
13	H	305	PGV	2	0
8	S	101	BCL	1	0
10	U	104	SPO	6	0
8	O	101	BCL	2	0
8	9	101	BCL	2	0
8	0	101	BCL	5	0
8	P	101	BCL	5	0
8	5	101	BCL	6	0
18	L	303	U10	4	0
13	M	411	PGV	2	0
10	9	102	SPO	4	0
13	L	304	PGV	2	0
10	K	102	SPO	5	0
10	U	102	SPO	5	0
10	Y	102	SPO	10	0
14	C	402	HEC	3	0
17	M	404	BPH	6	0
13	A	104	PGV	3	0
8	Q	101	BCL	3	0
8	E	101	BCL	5	0
8	L	308	BCL	2	0
10	I	102	SPO	4	0
8	4	102	BCL	5	0
12	K	104	LMT	1	0
10	S	102	SPO	5	0
13	M	408	PGV	1	0
10	A	102	SPO	9	0
13	F	105	PGV	2	0

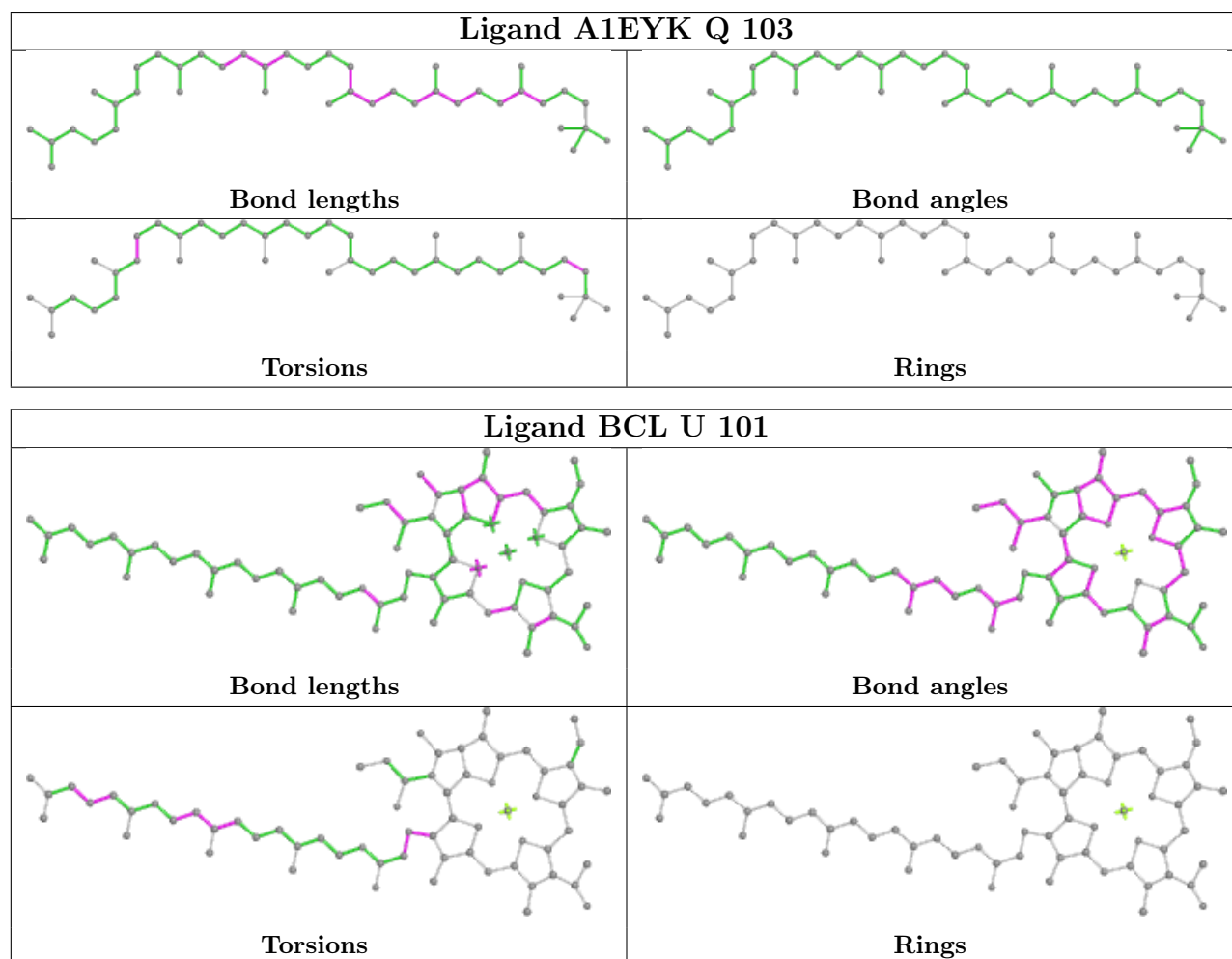
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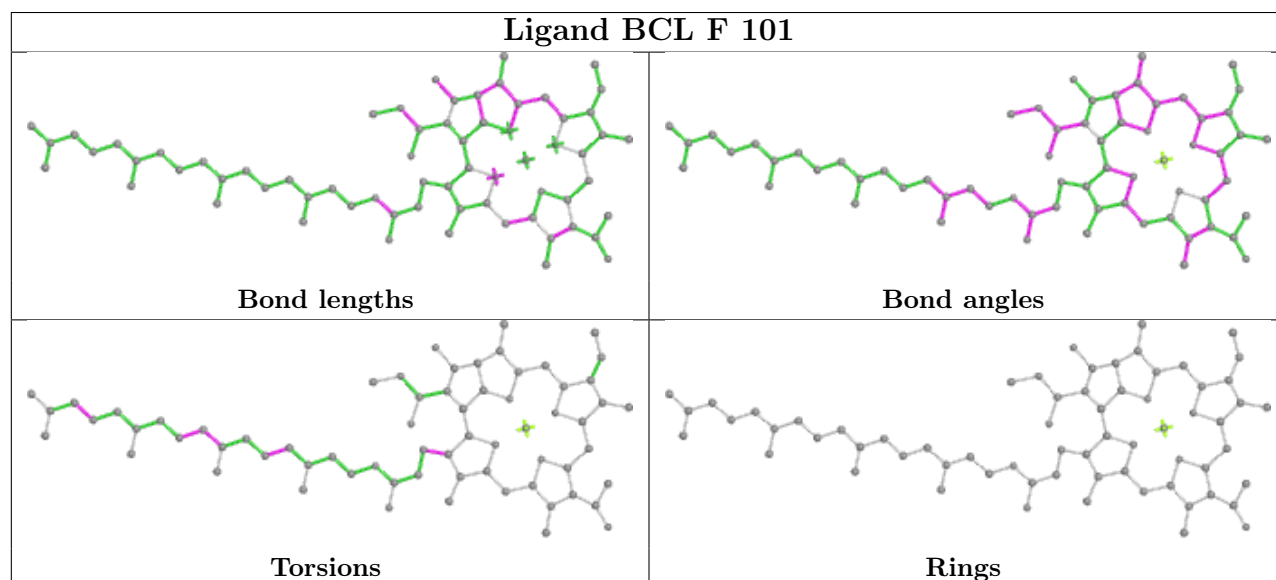
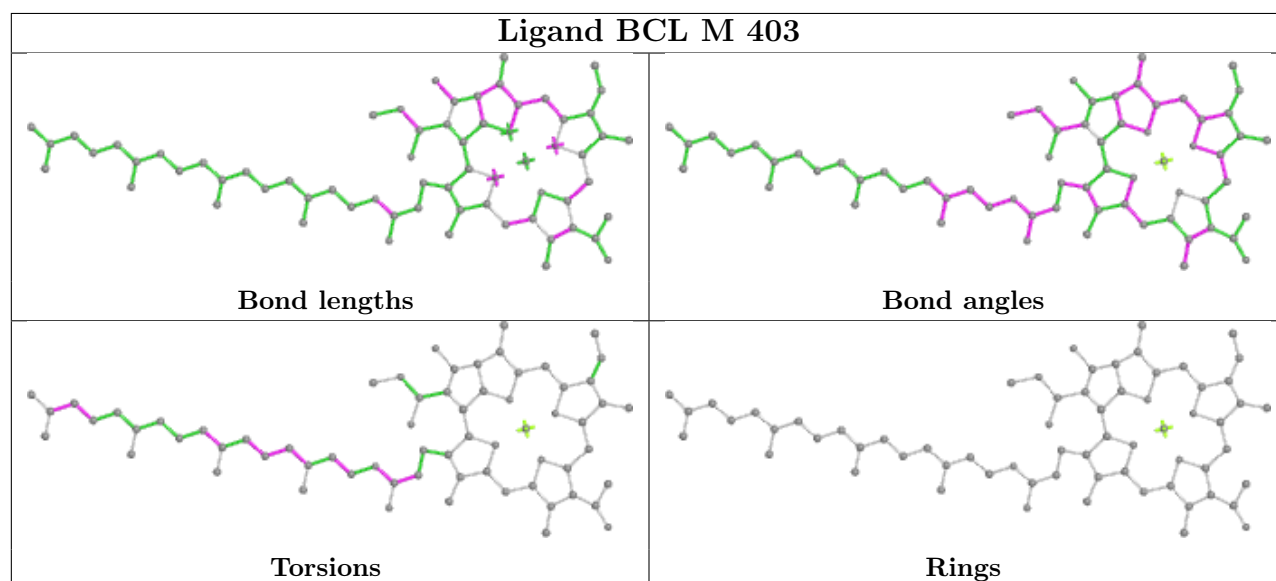
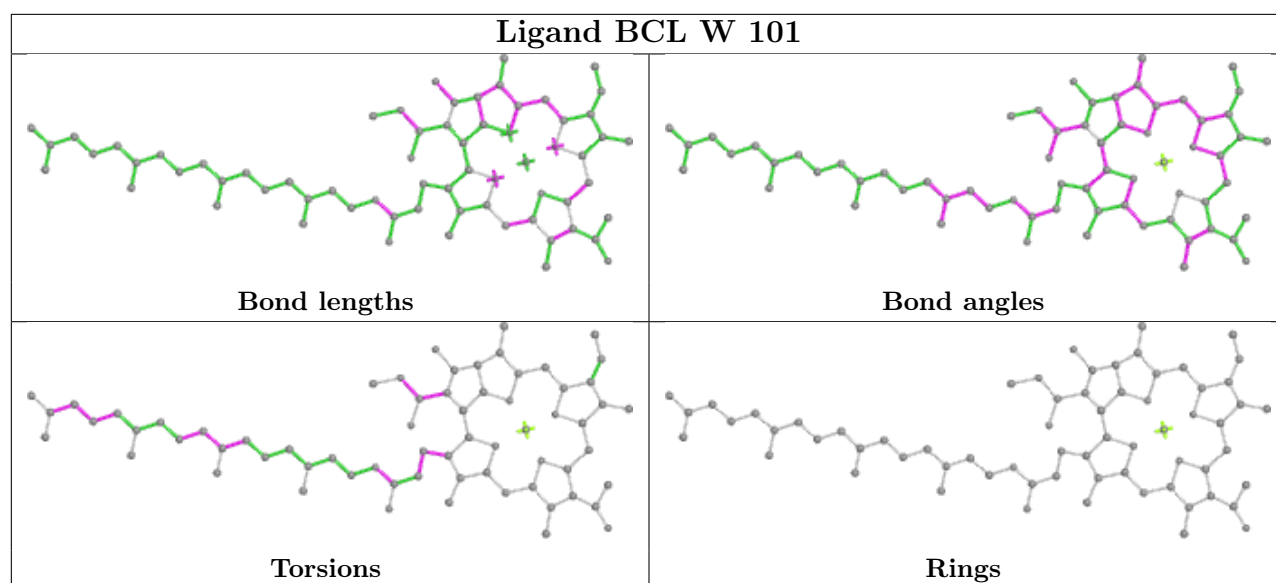
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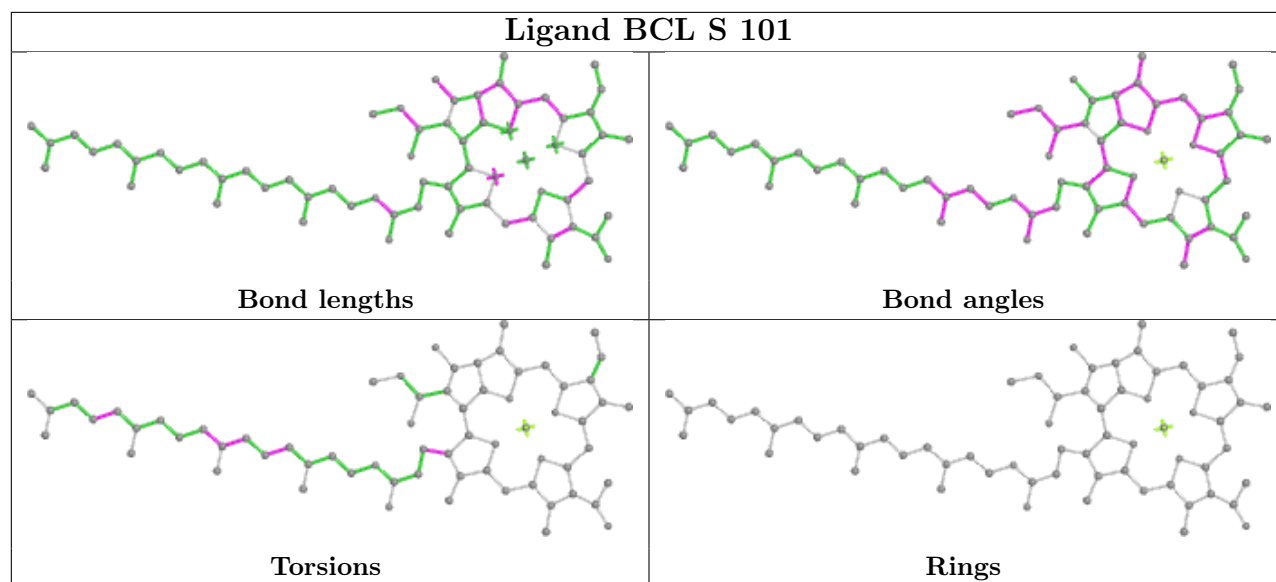
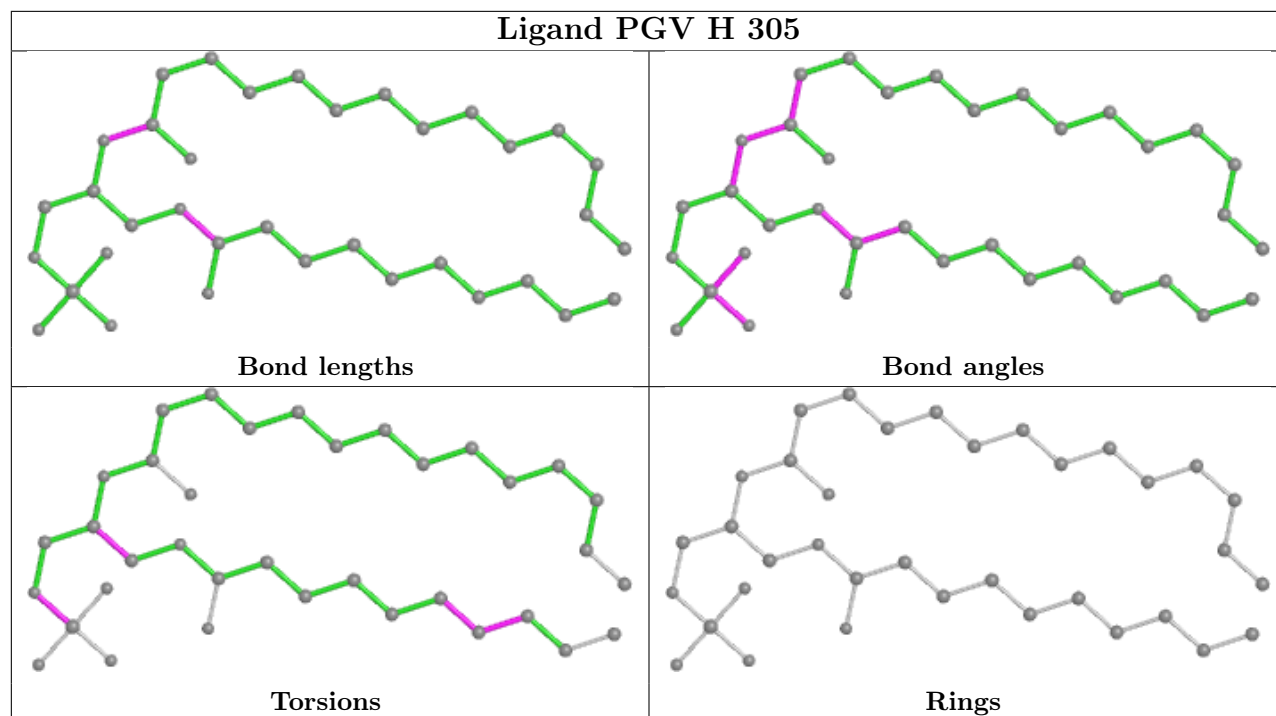
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	K	101	BCL	2	0
12	D	101	LMT	2	0
8	J	101	BCL	3	0
8	D	102	BCL	2	0
8	6	101	BCL	3	0
8	1	101	BCL	7	0
8	2	101	BCL	3	0
10	O	102	SPO	7	0
8	X	101	BCL	8	0
8	N	101	BCL	4	0
12	7	104	LMT	4	0
8	V	101	BCL	5	0
13	H	301	PGV	1	0
13	M	409	PGV	1	0
12	9	104	LMT	1	0
8	7	101	BCL	2	0
8	Y	101	BCL	2	0
8	Z	102	BCL	5	0
8	T	101	BCL	6	0
10	Q	102	SPO	4	0
8	8	101	BCL	6	0
14	C	401	HEC	3	0
17	L	302	BPH	5	0
10	4	101	SPO	13	0
10	D	103	SPO	7	0
8	R	101	BCL	5	0
8	L	307	BCL	3	0
13	H	304	PGV	1	0
13	H	303	PGV	3	0
10	M	406	SPO	4	0
8	L	301	BCL	2	0
14	C	403	HEC	2	0
10	F	102	SPO	5	0
8	G	101	BCL	4	0
8	B	101	BCL	6	0
18	M	405	U10	5	0
10	5	102	SPO	4	0
13	D	105	PGV	1	0
8	A	101	BCL	3	0
18	M	410	U10	1	0
10	7	102	SPO	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

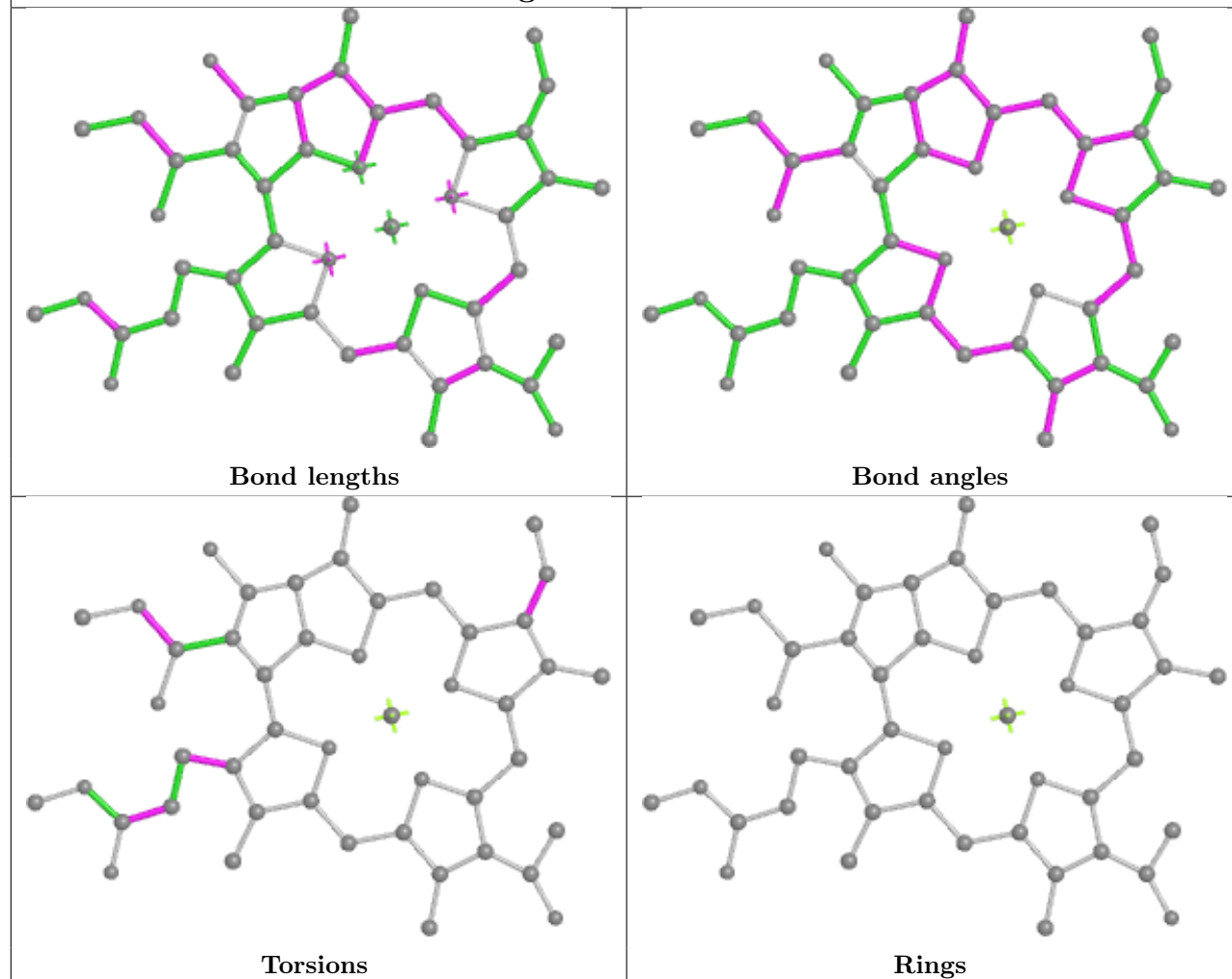
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within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



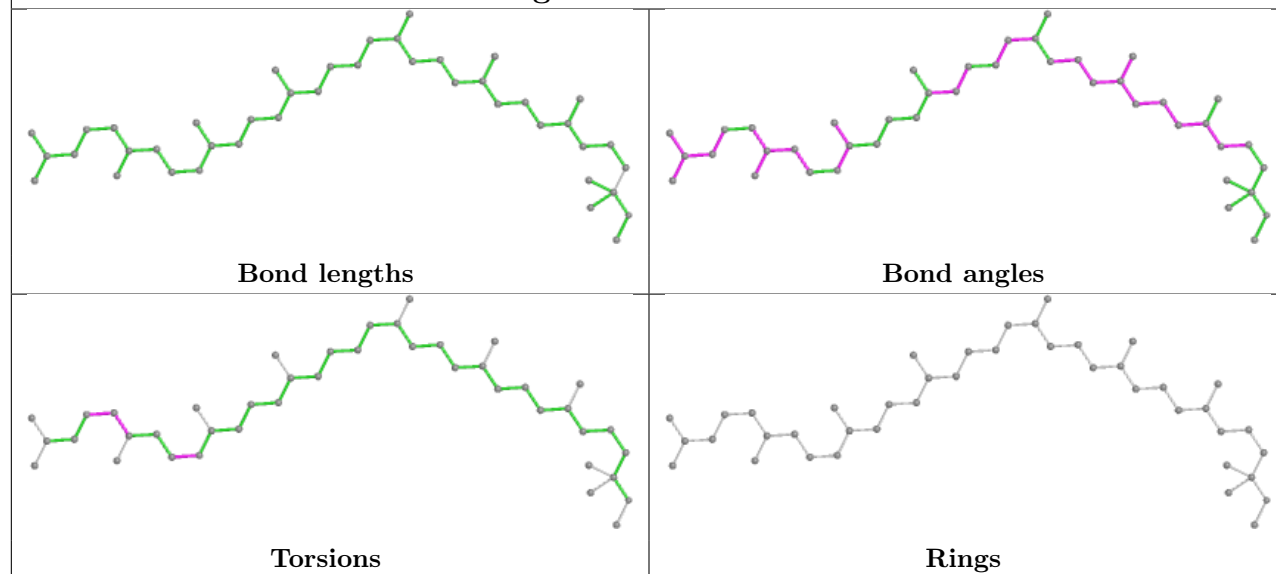


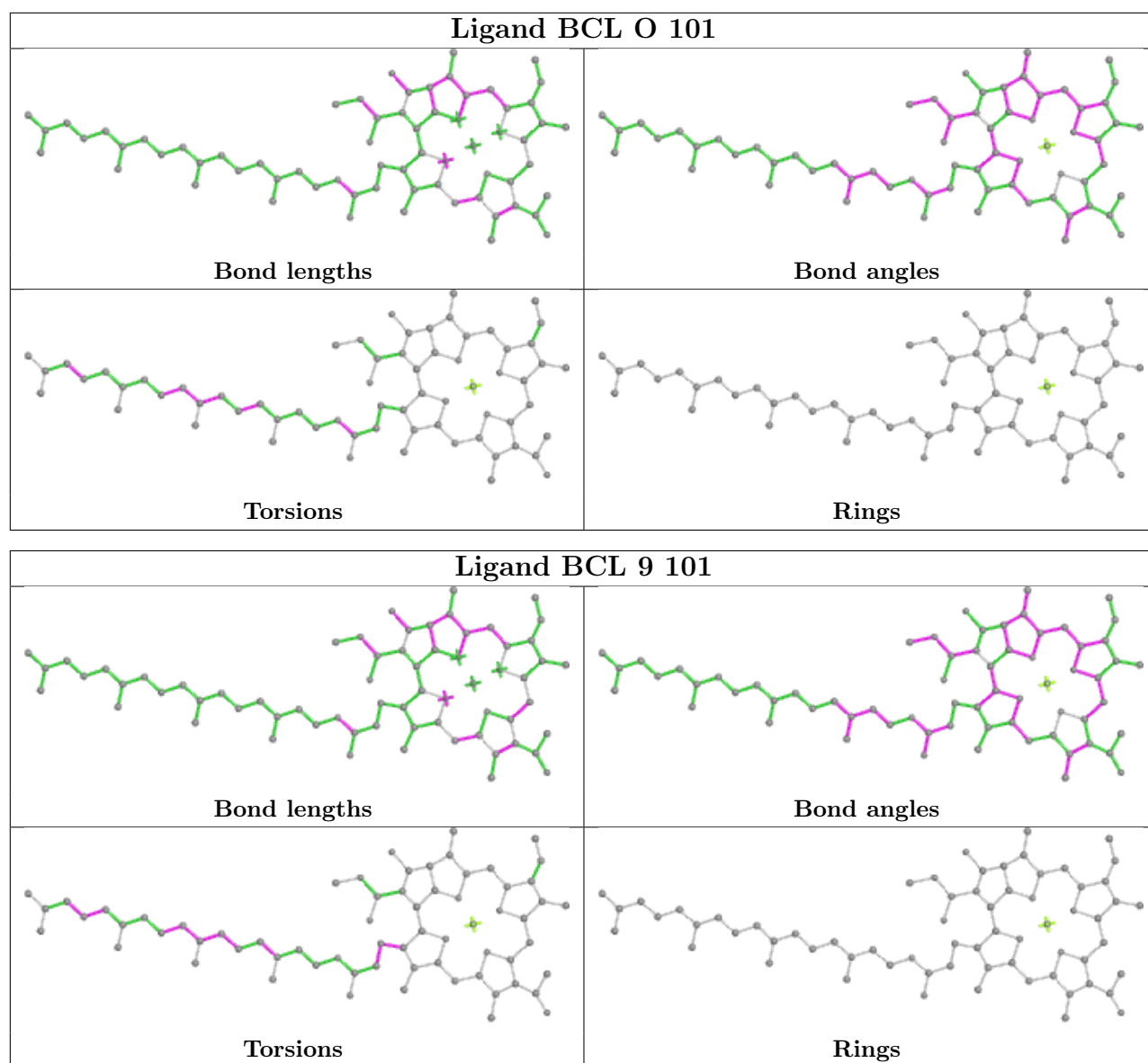


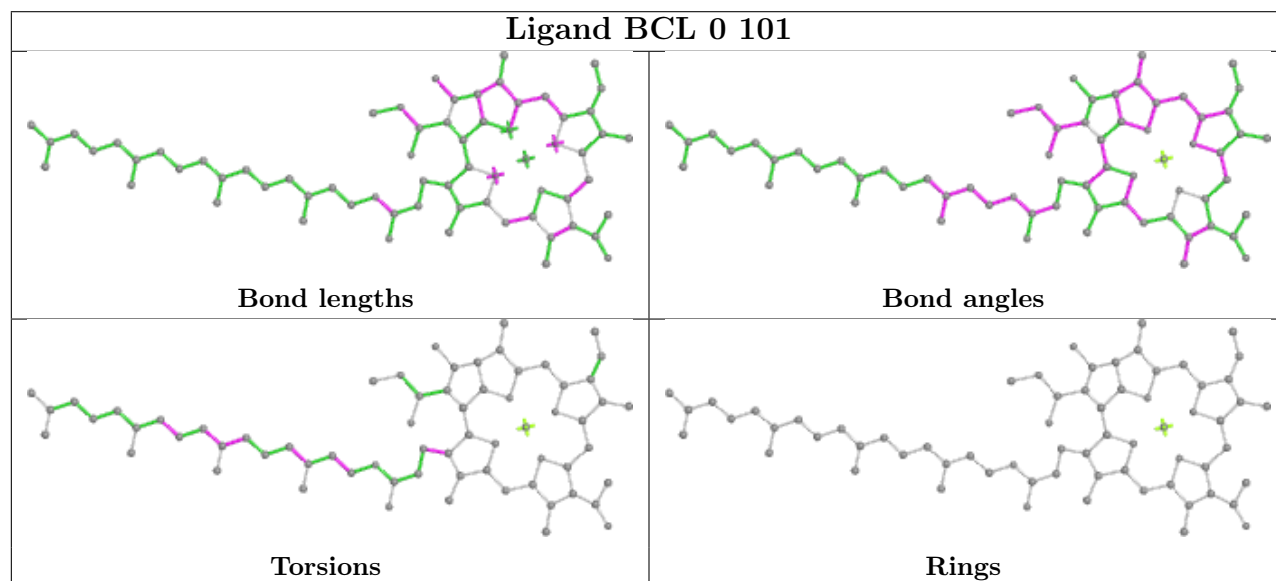
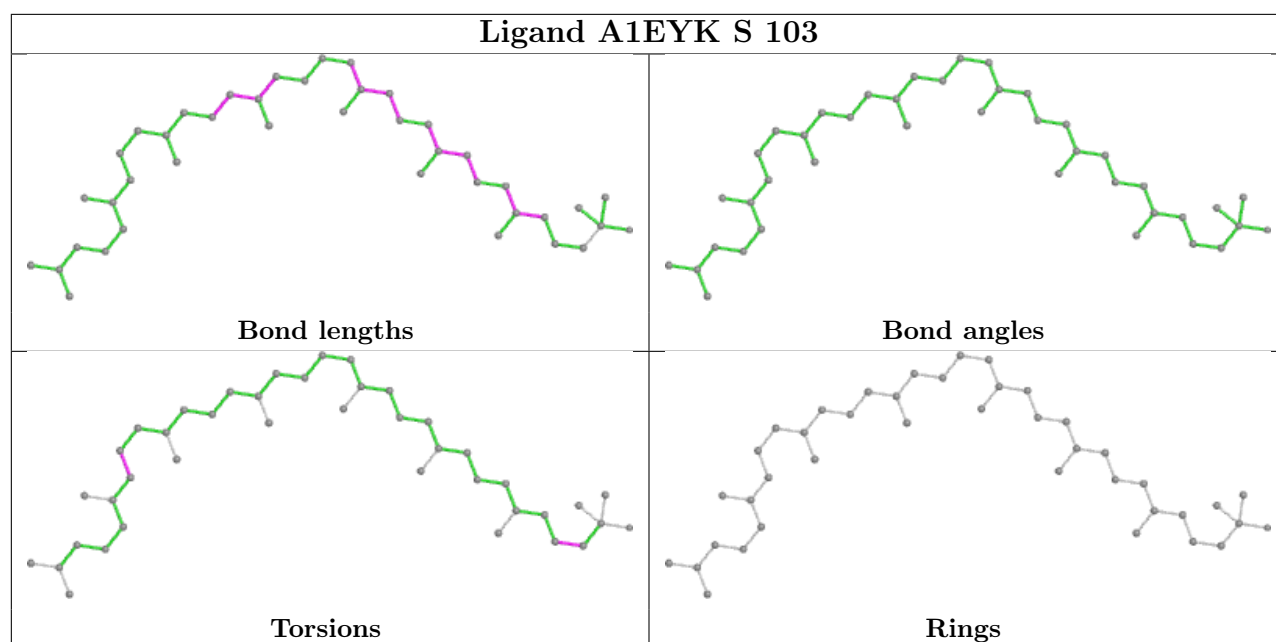
Ligand BCL 3 101

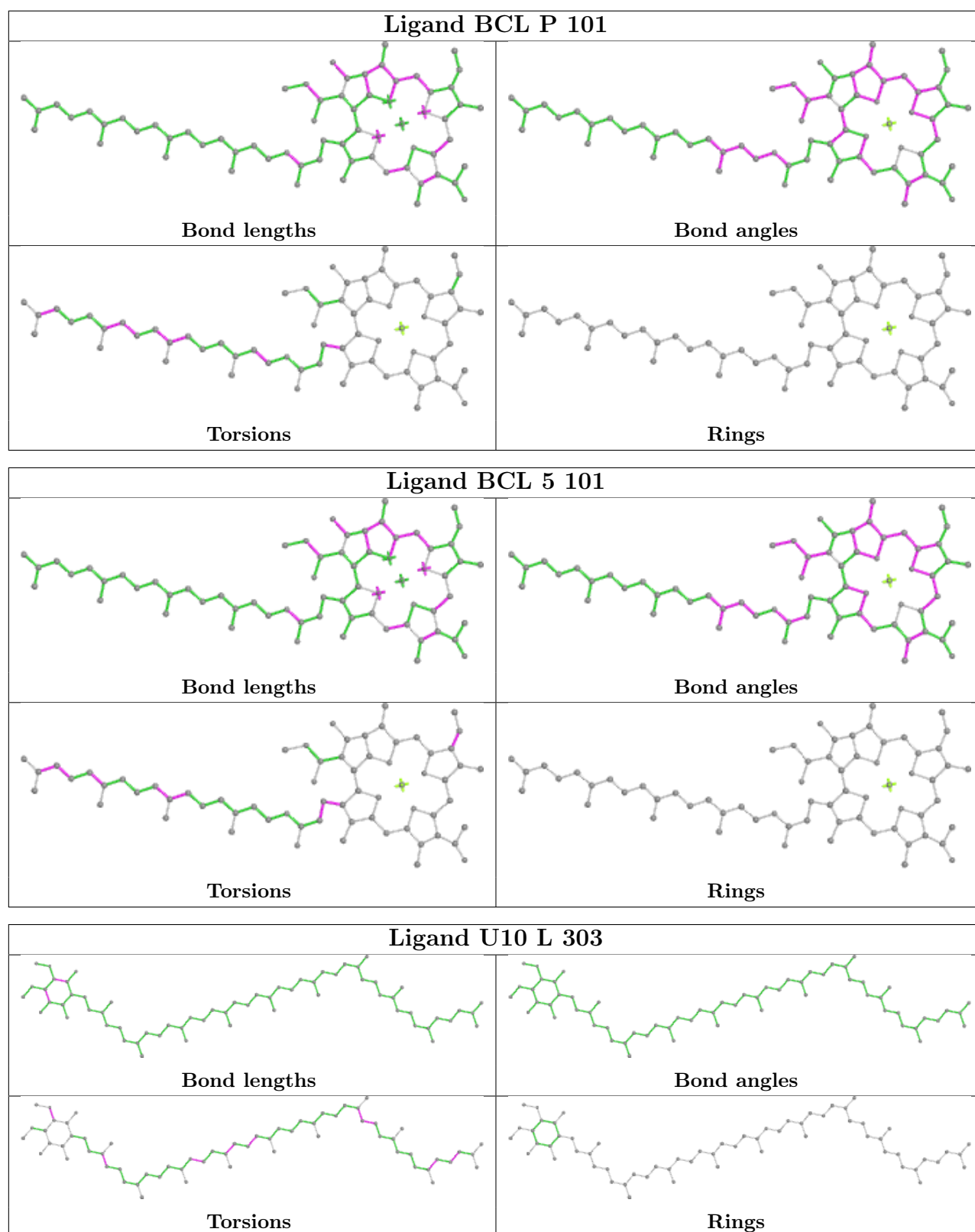


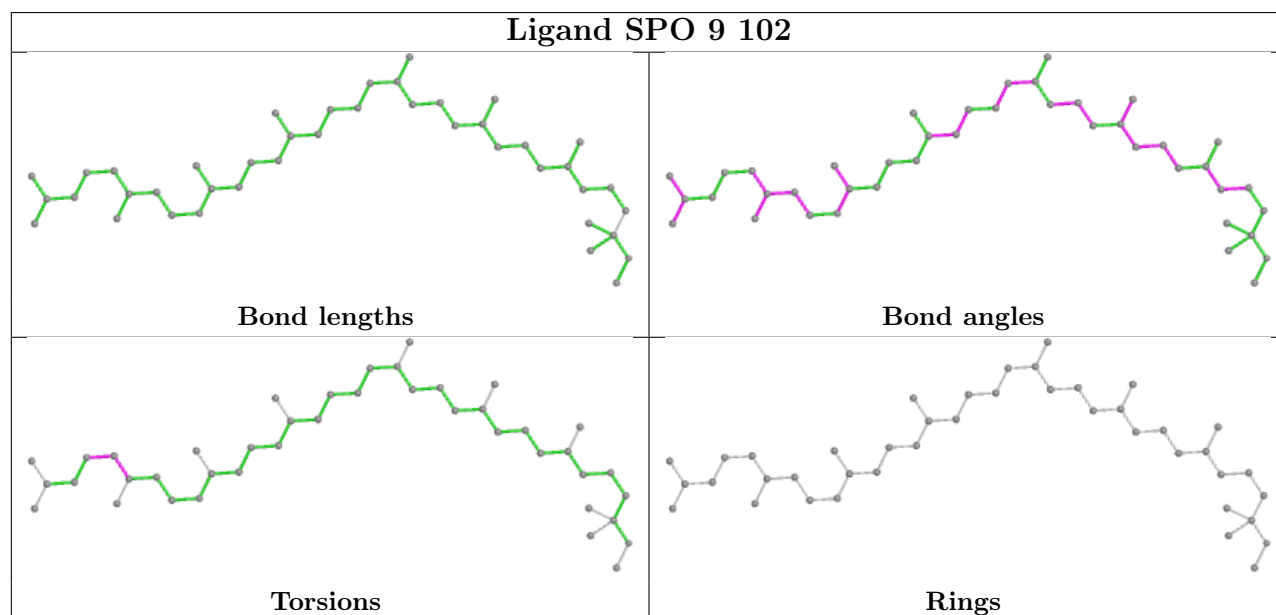
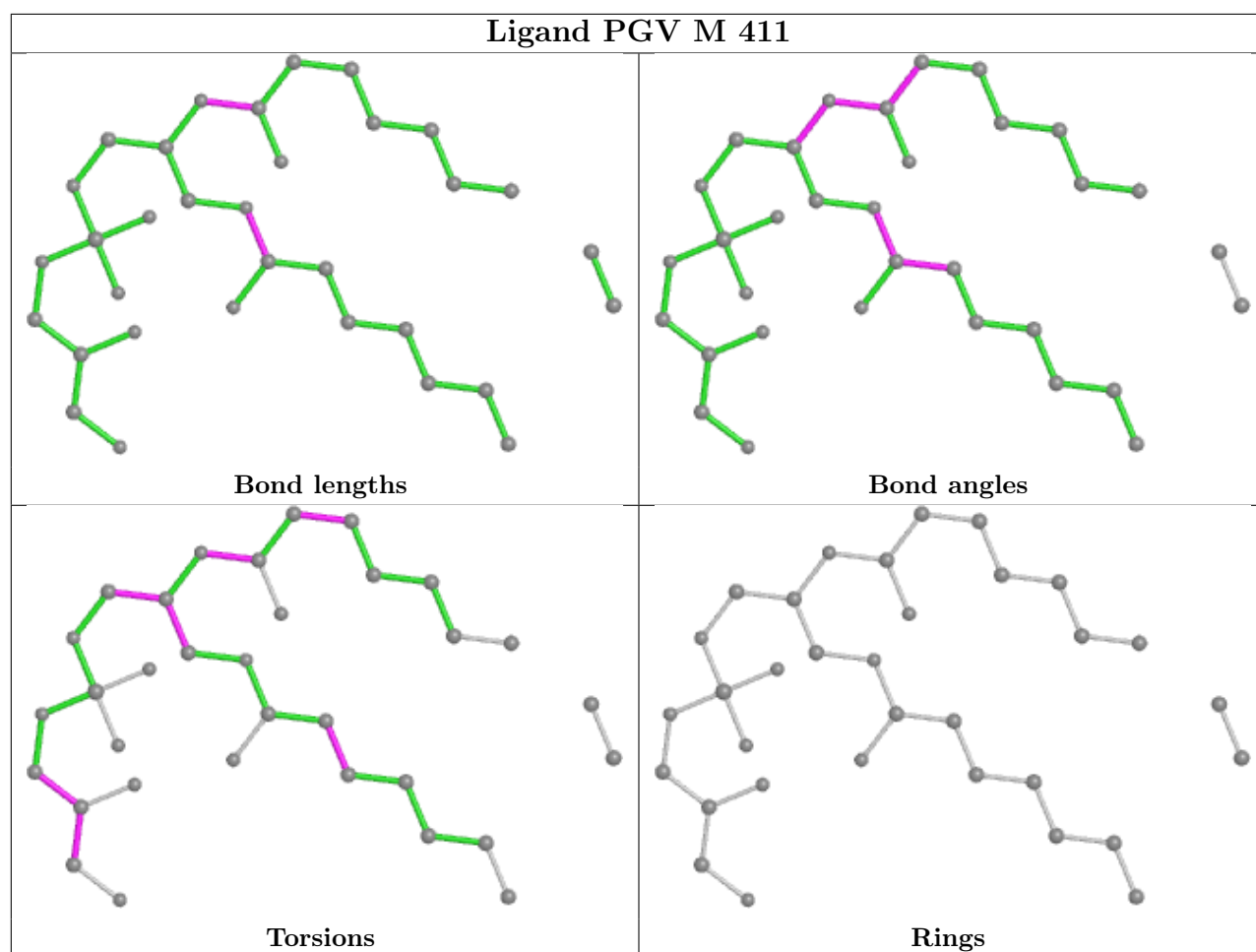
Ligand SPO U 104

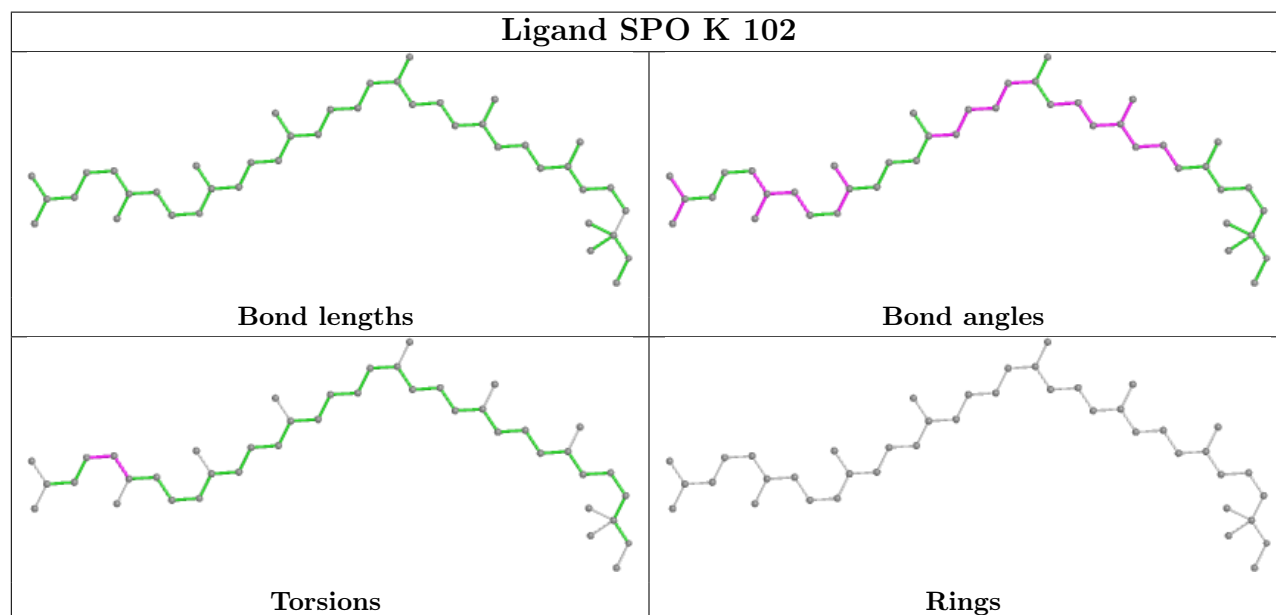
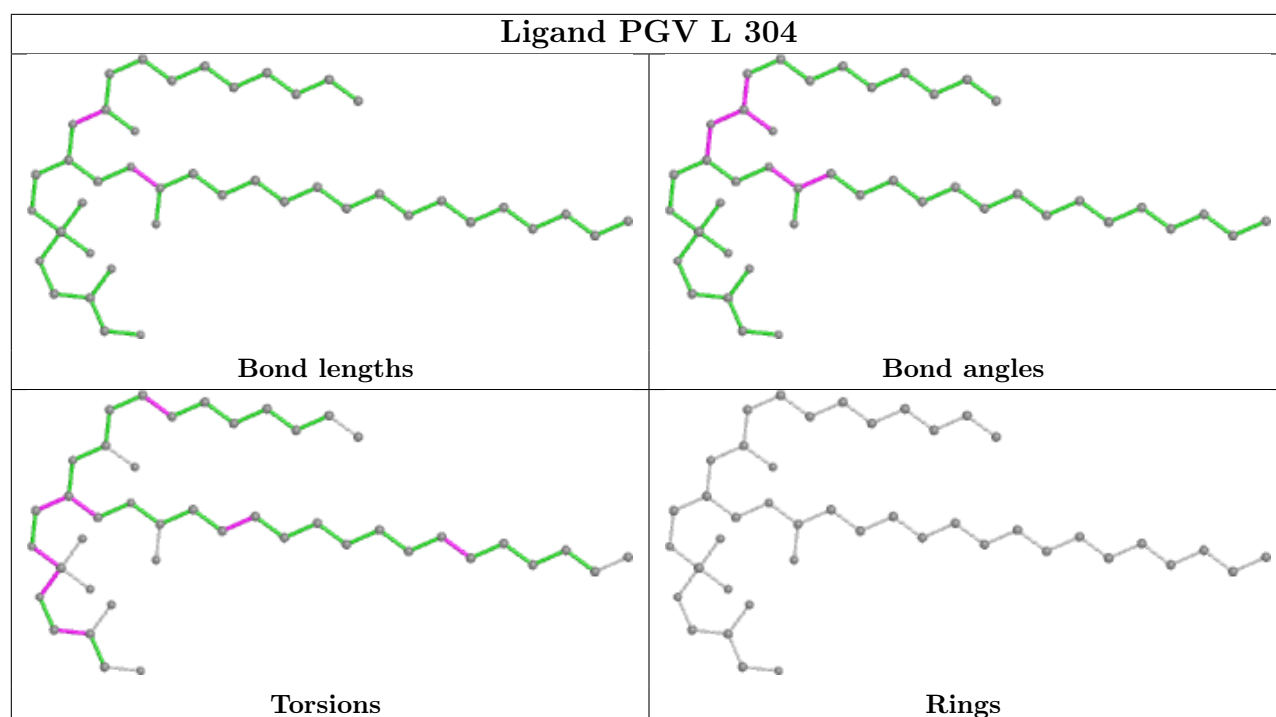


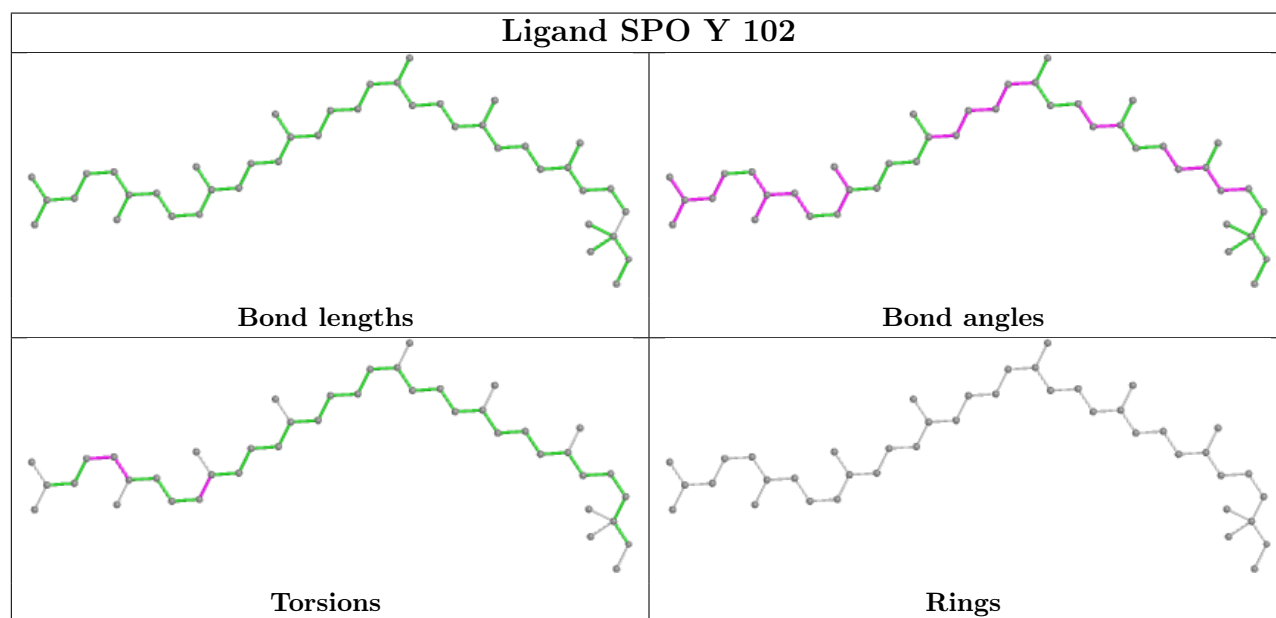
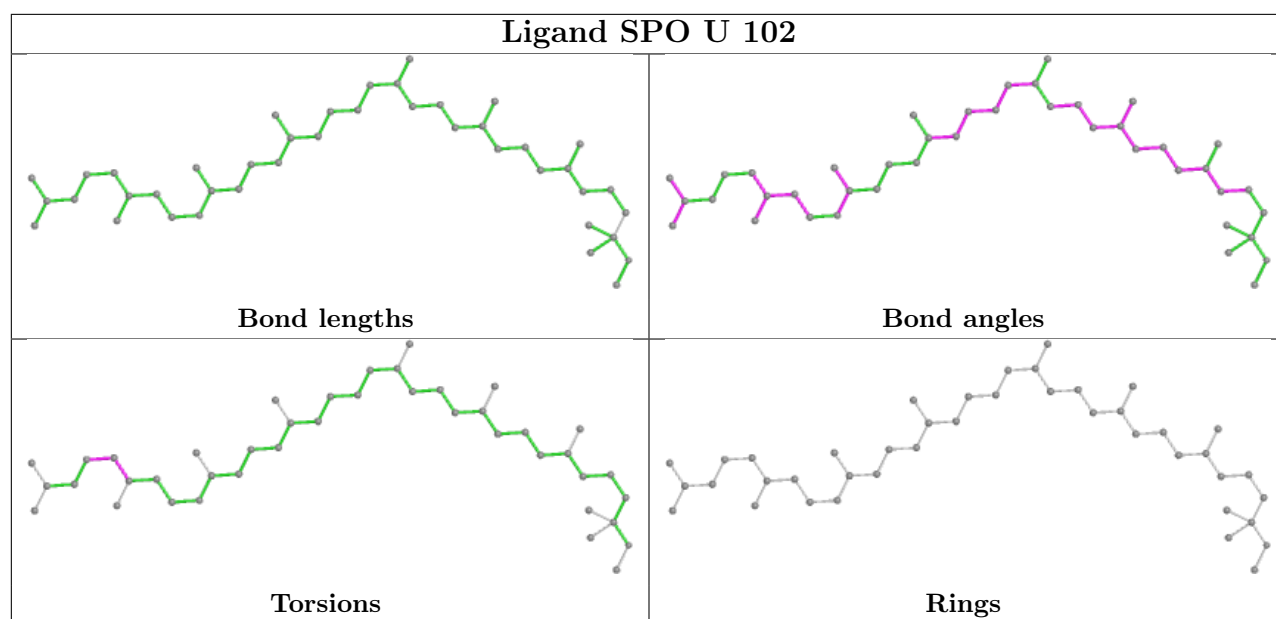


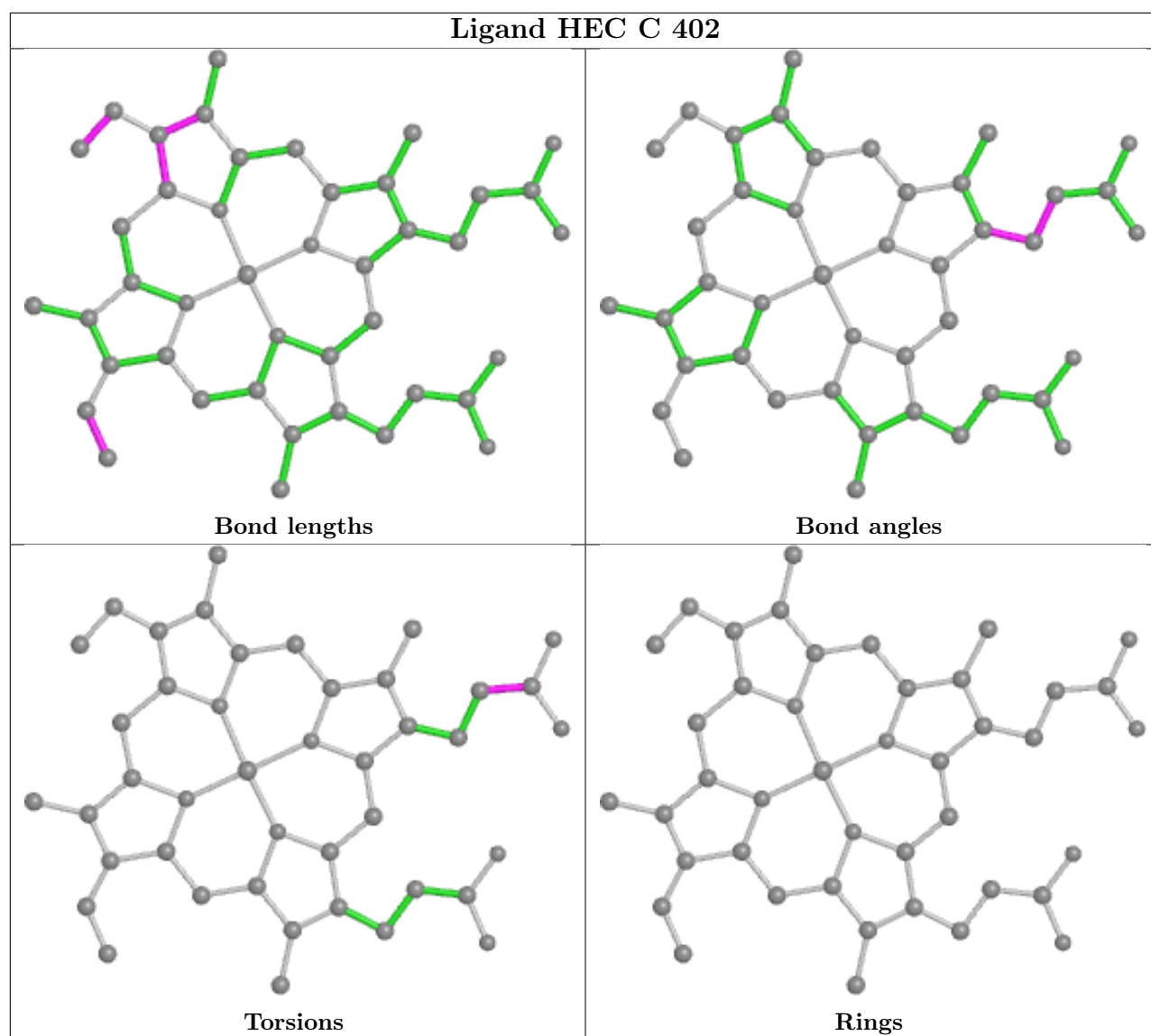




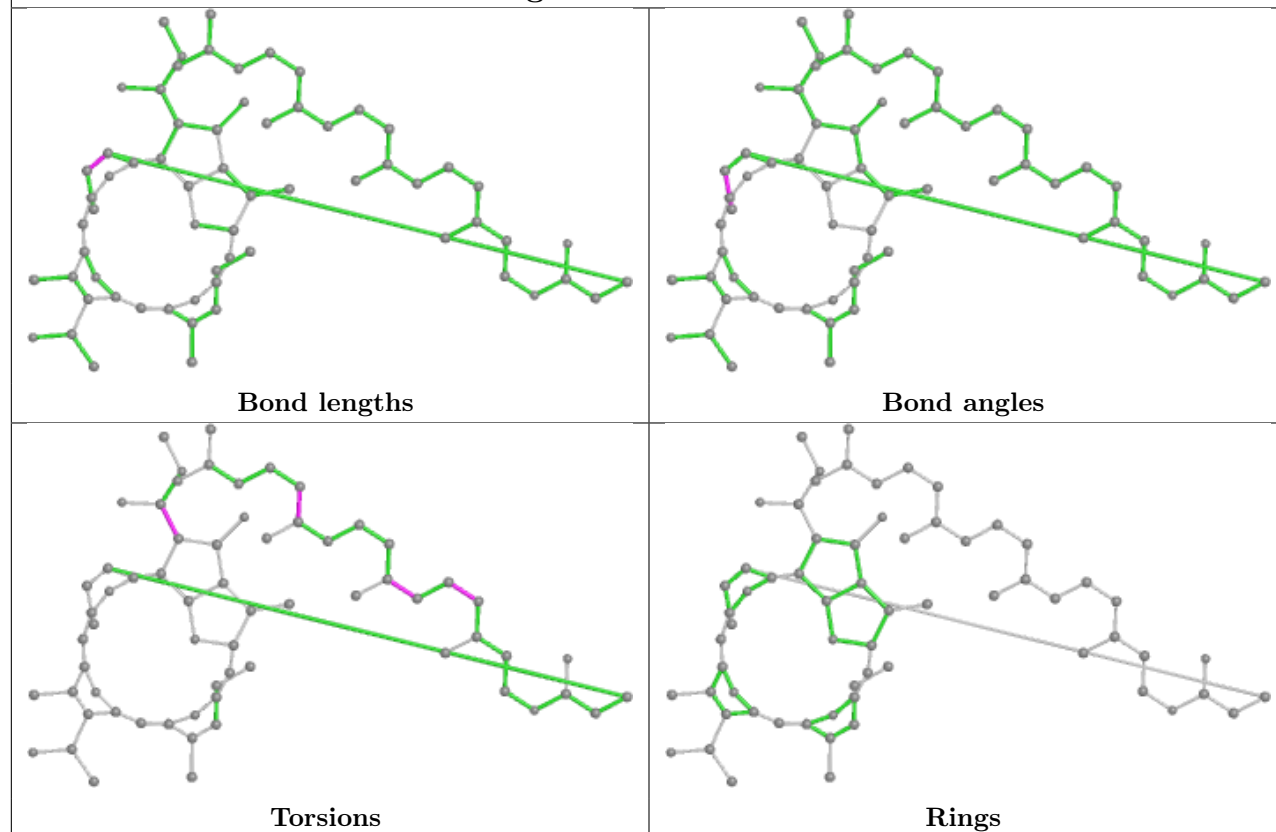




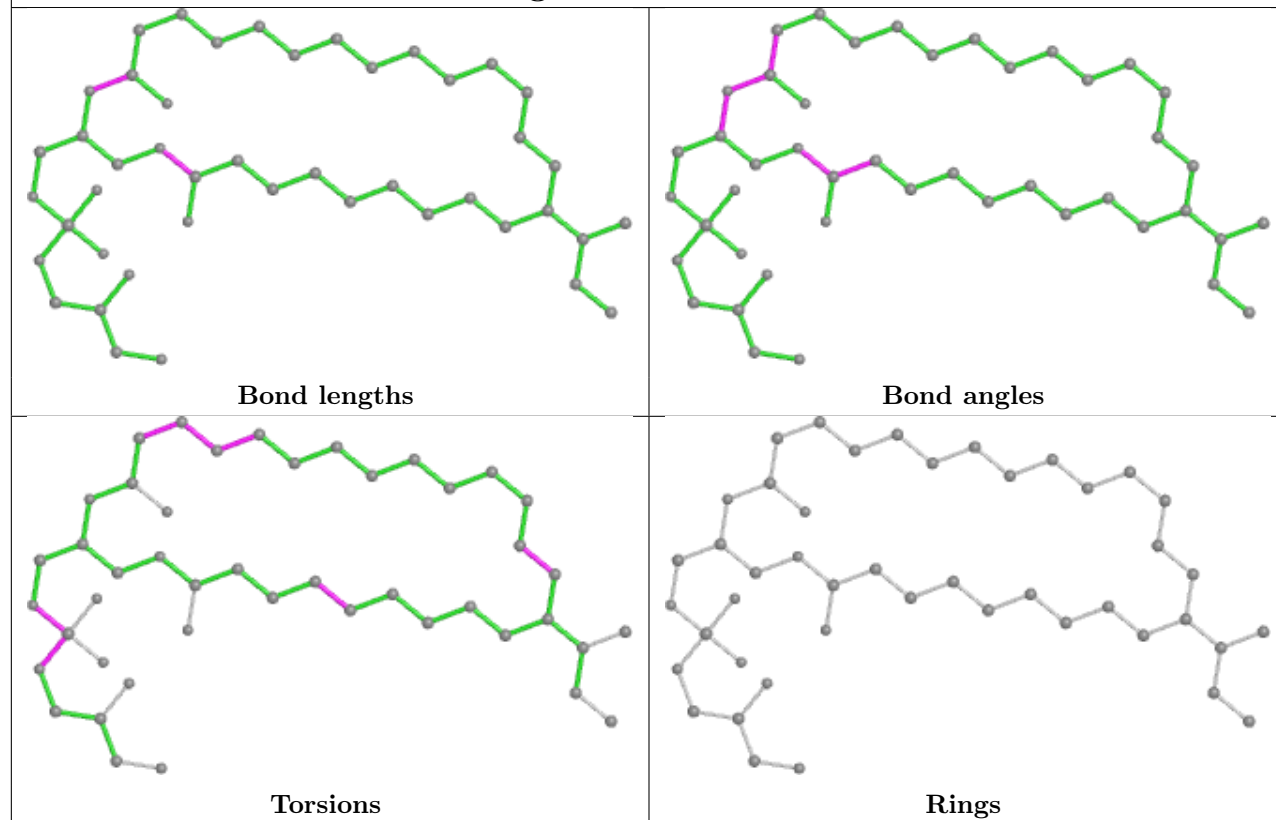


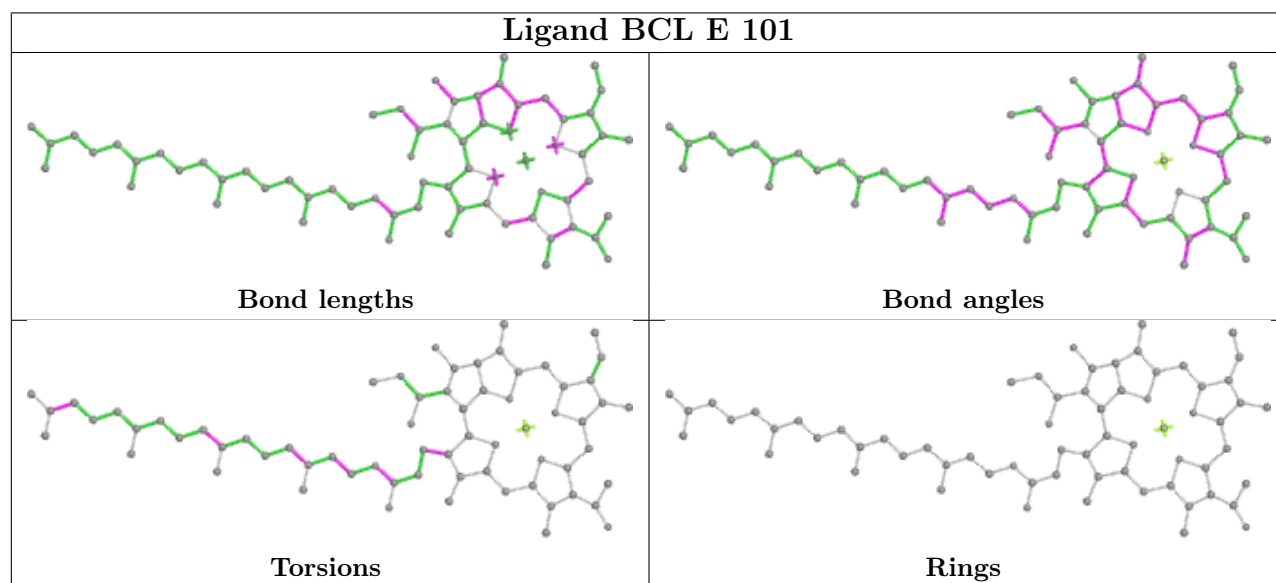
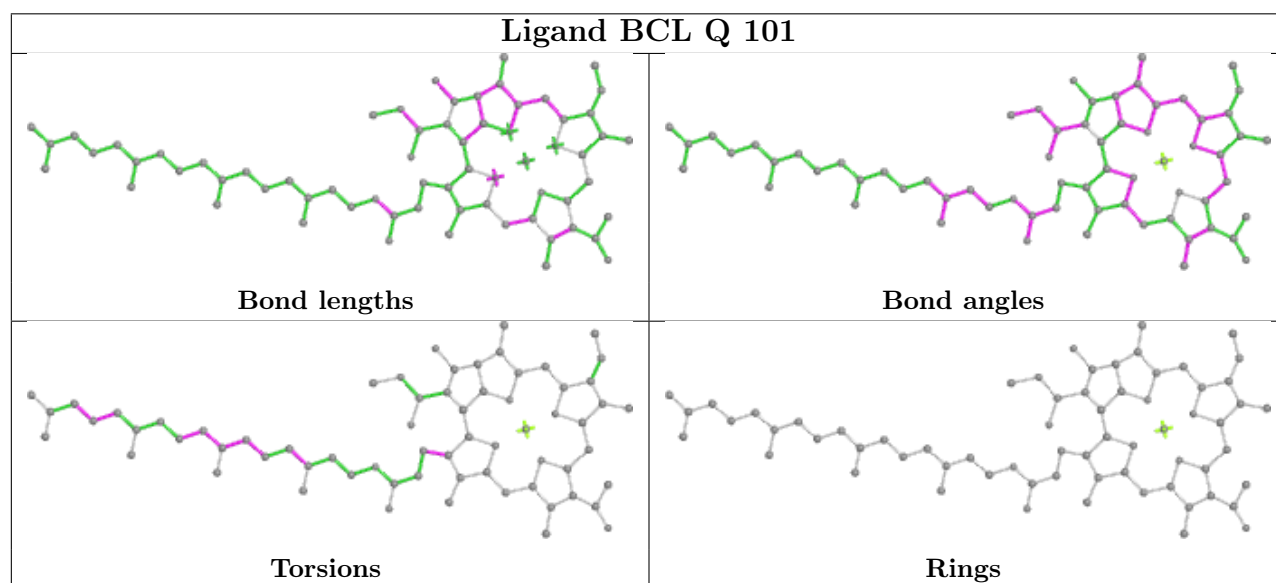
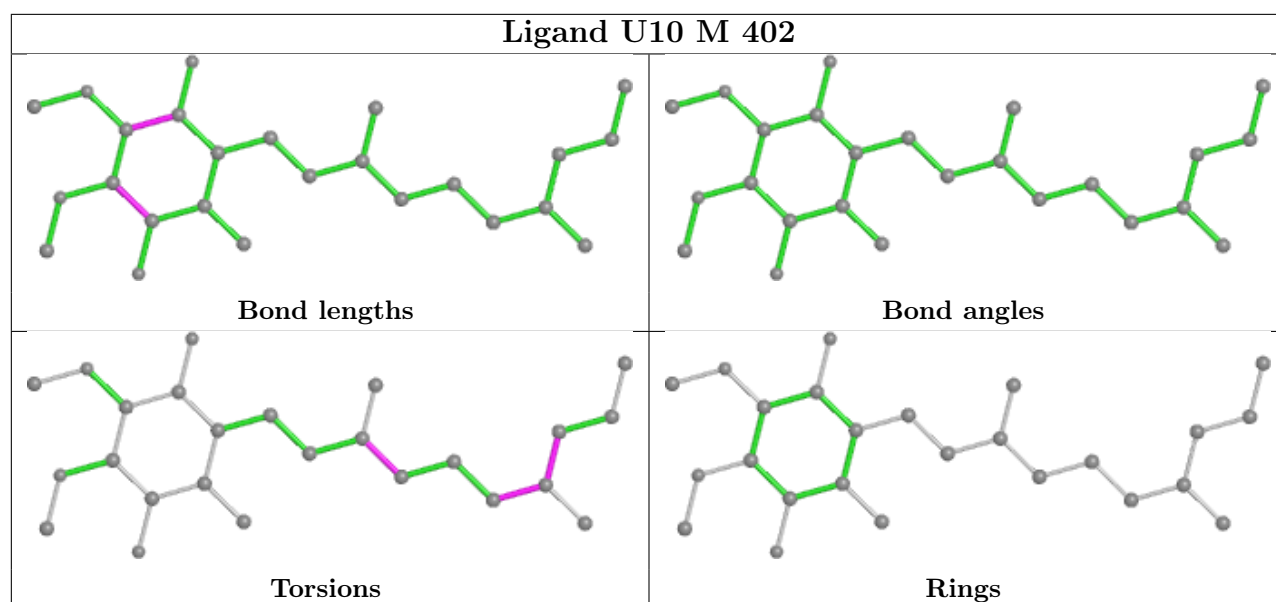


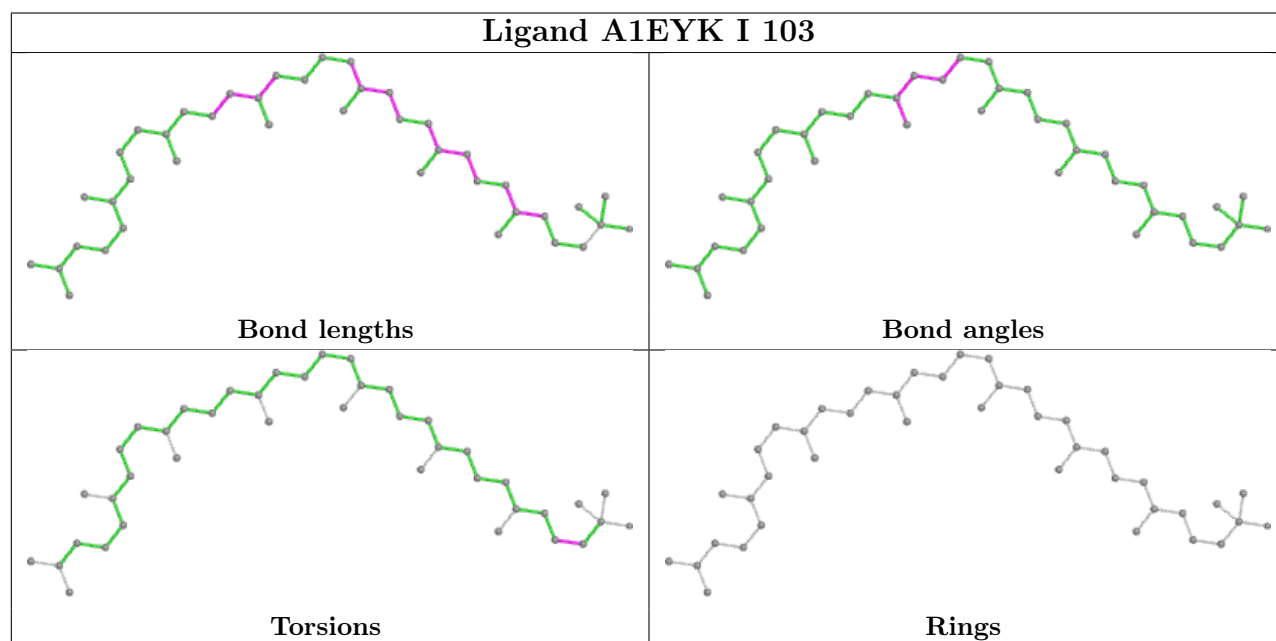
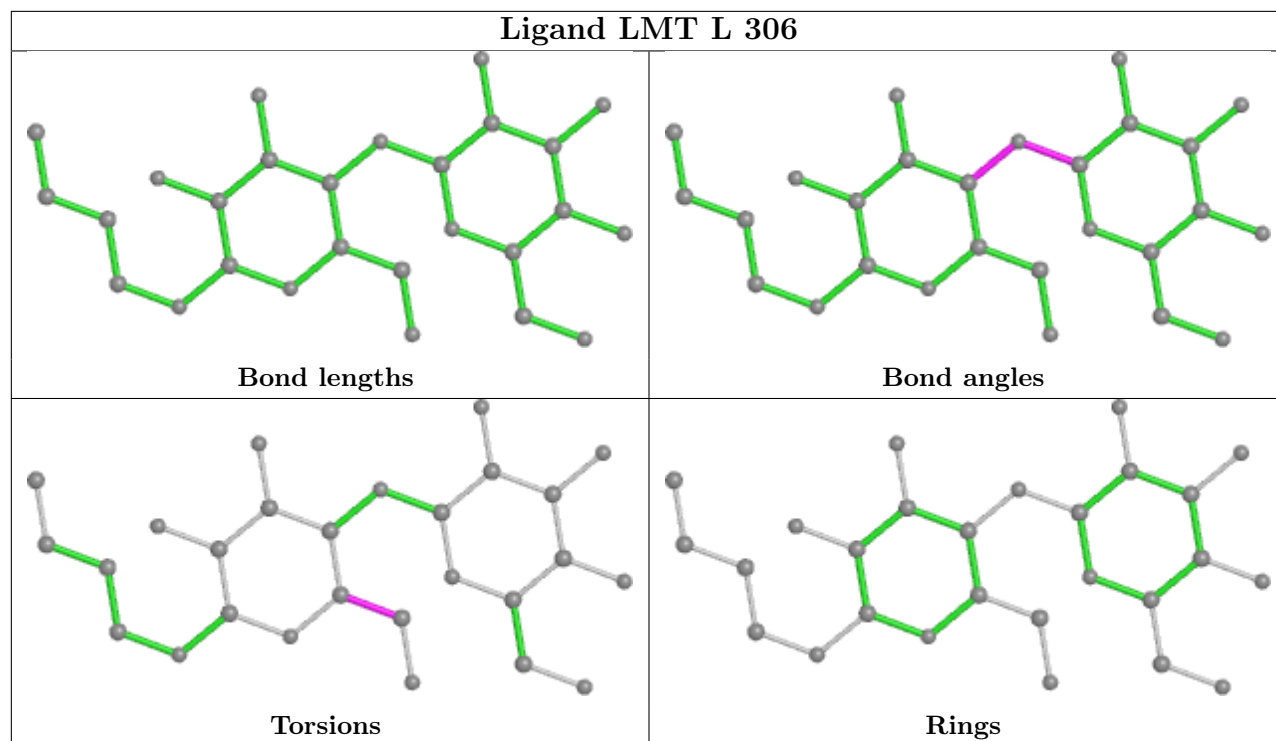
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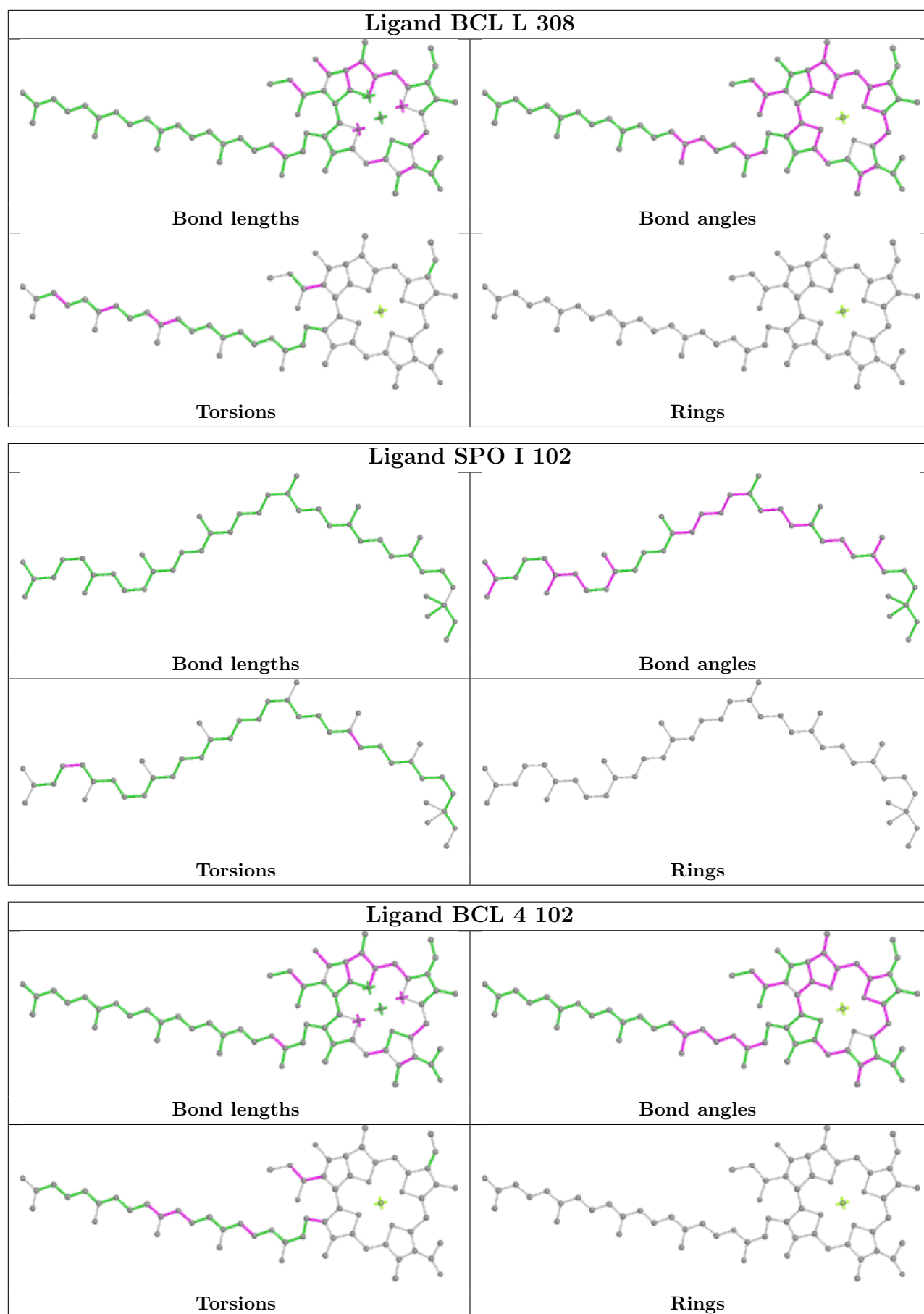


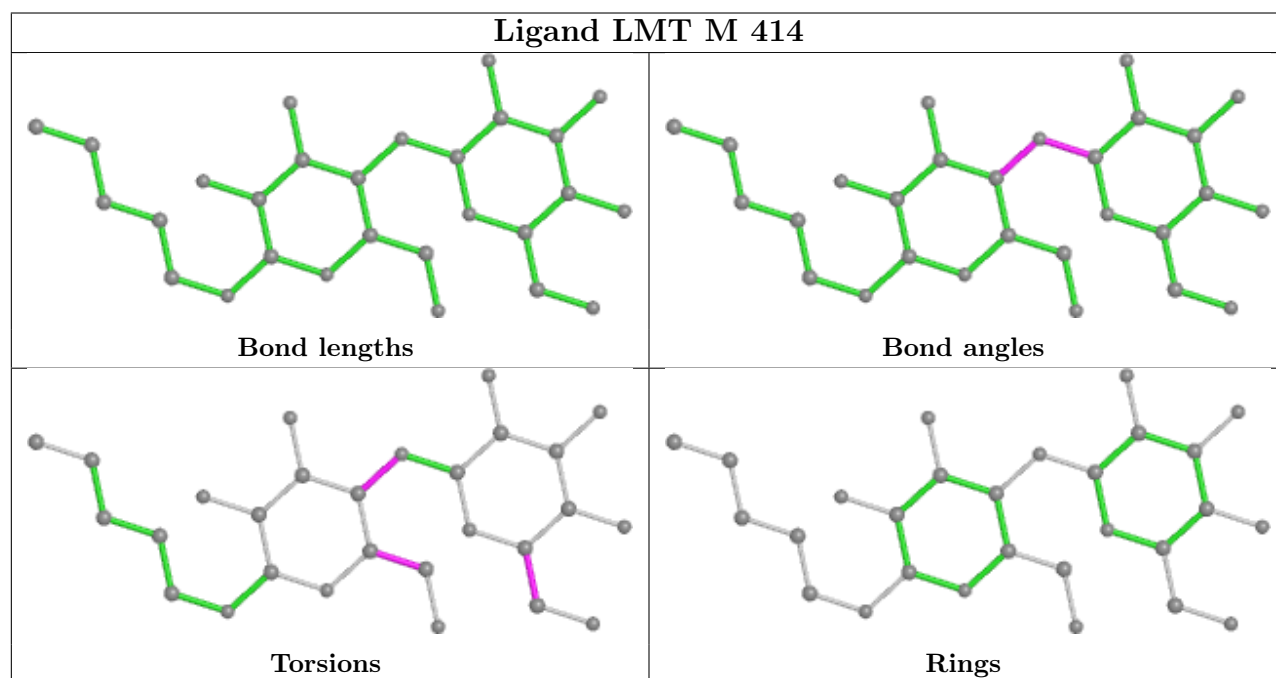
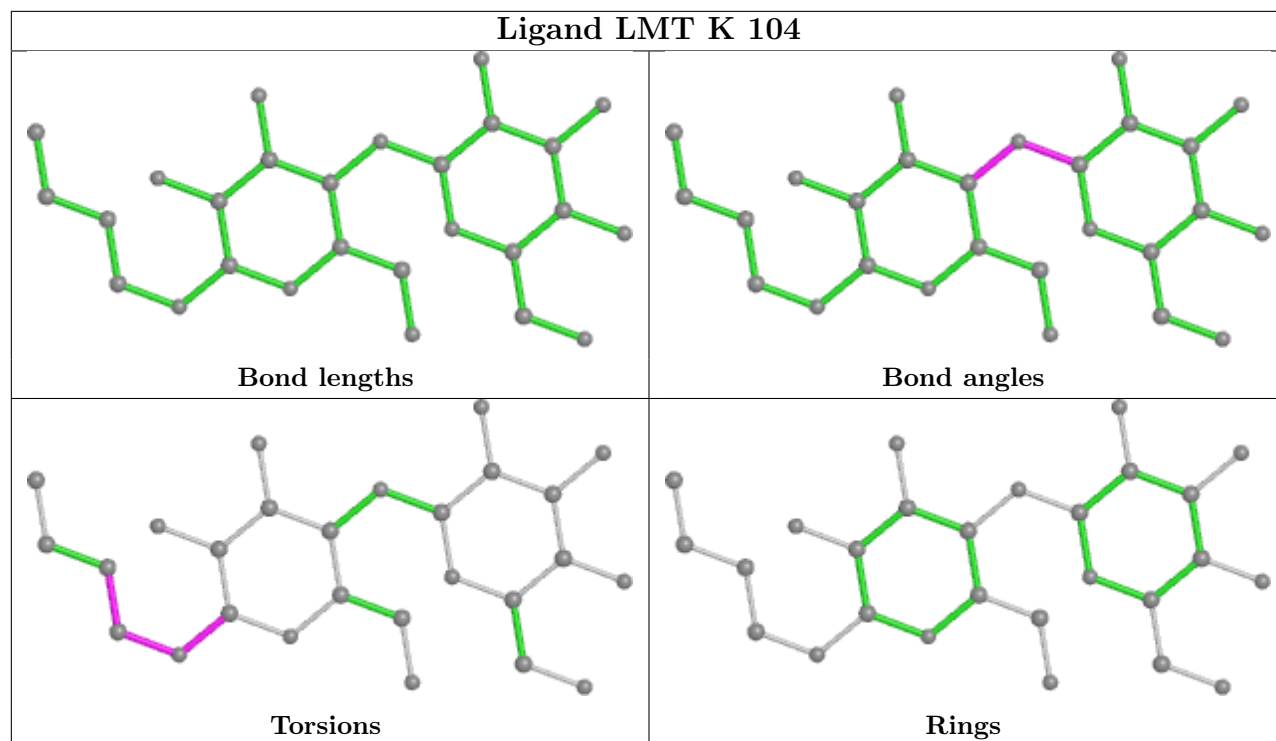
Ligand PGV A 104



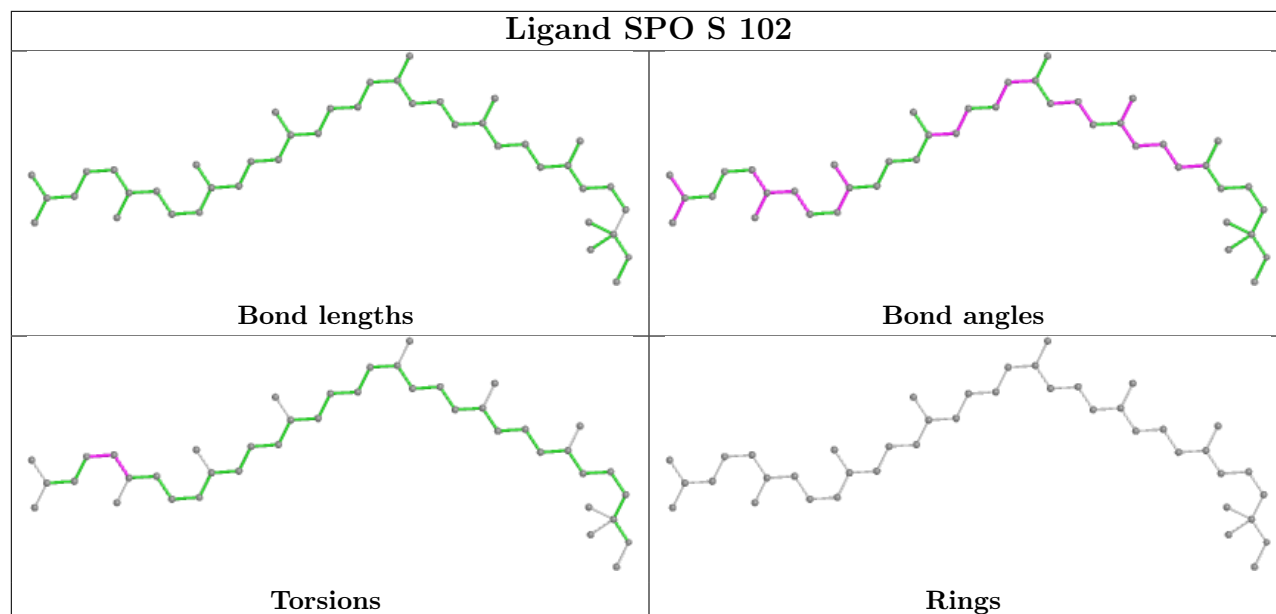




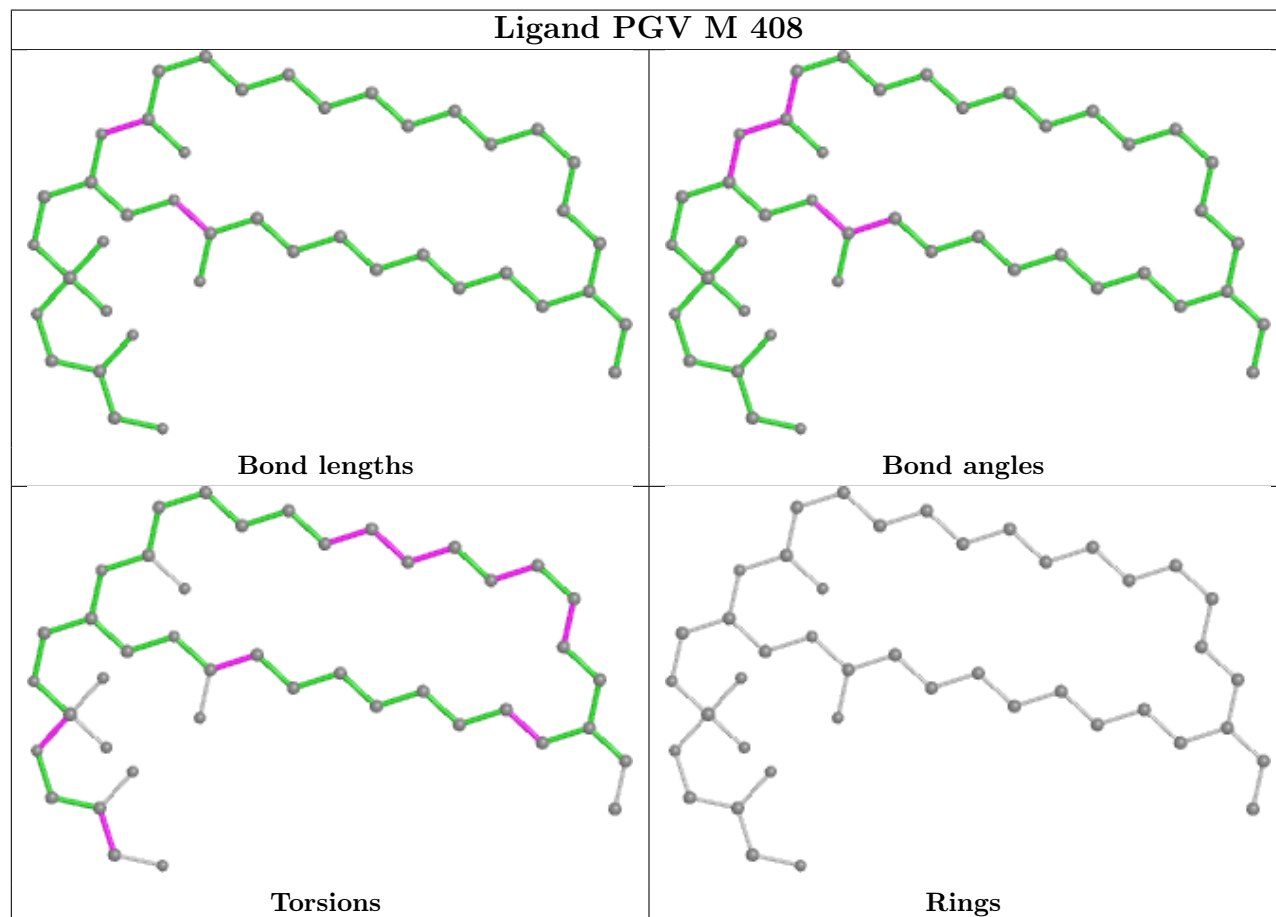


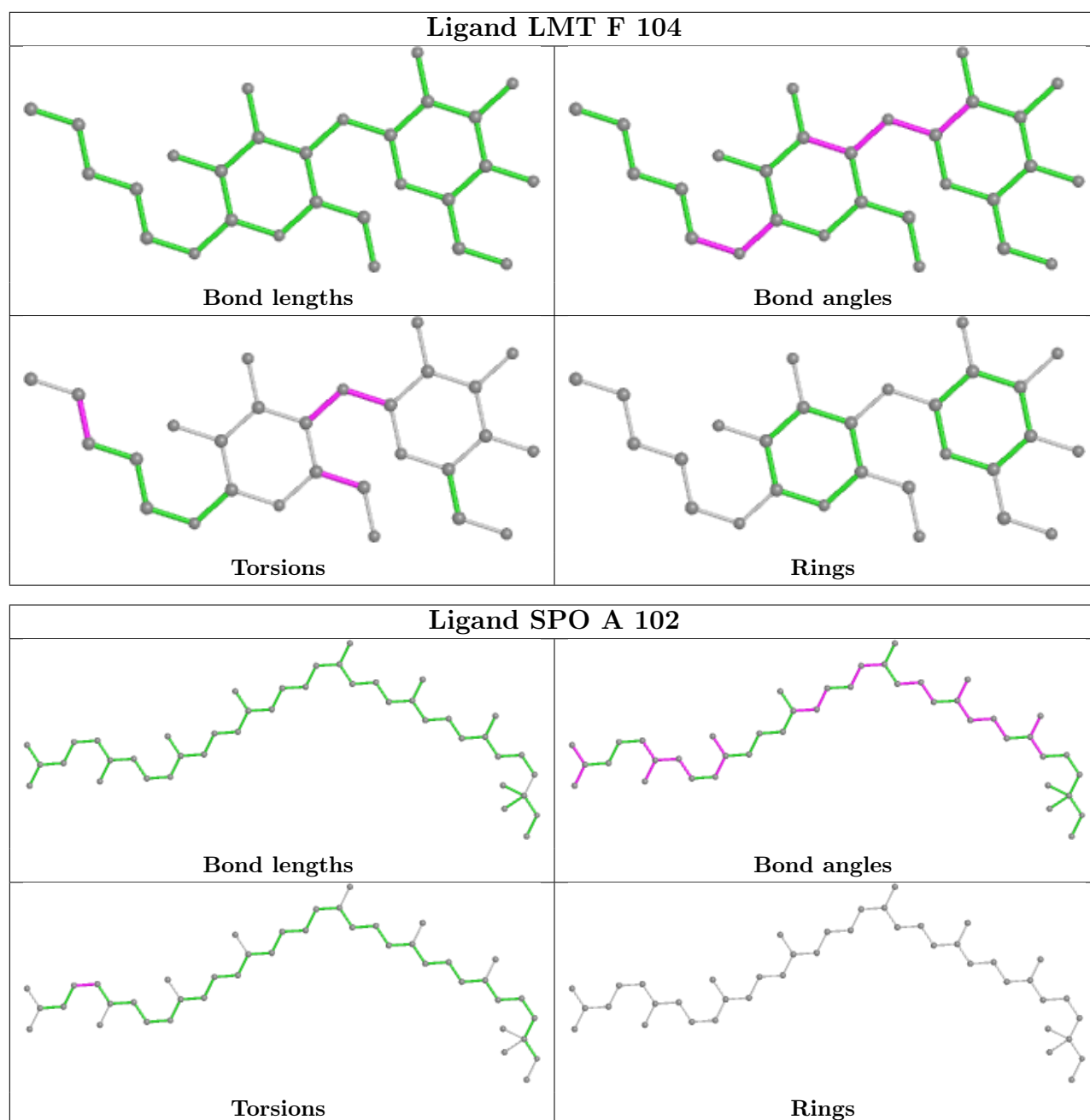


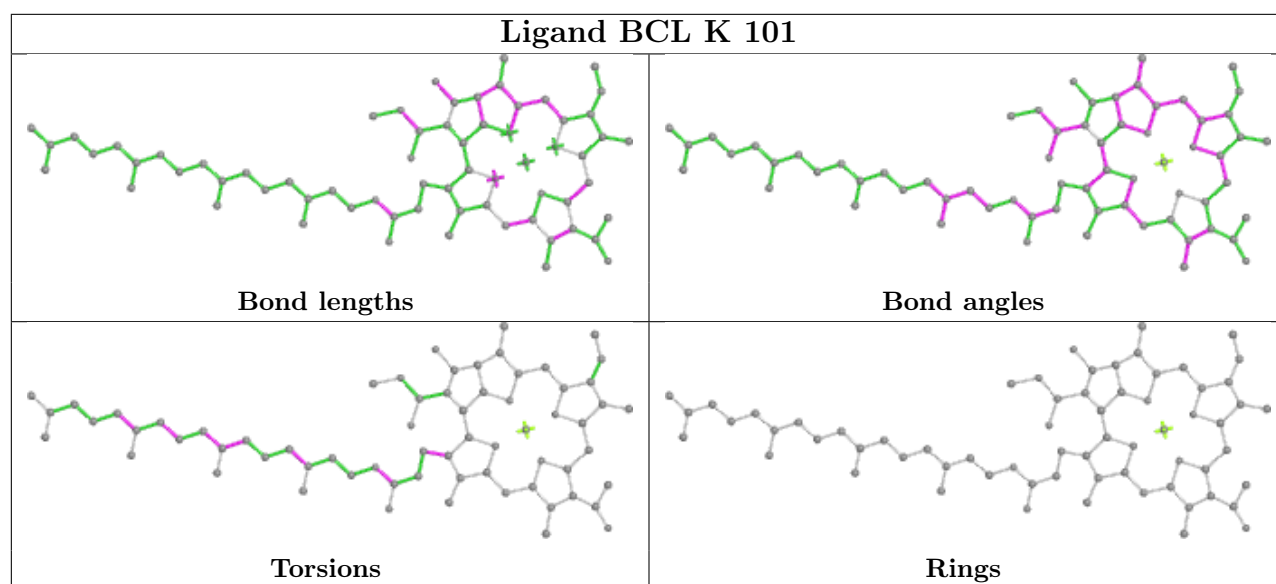
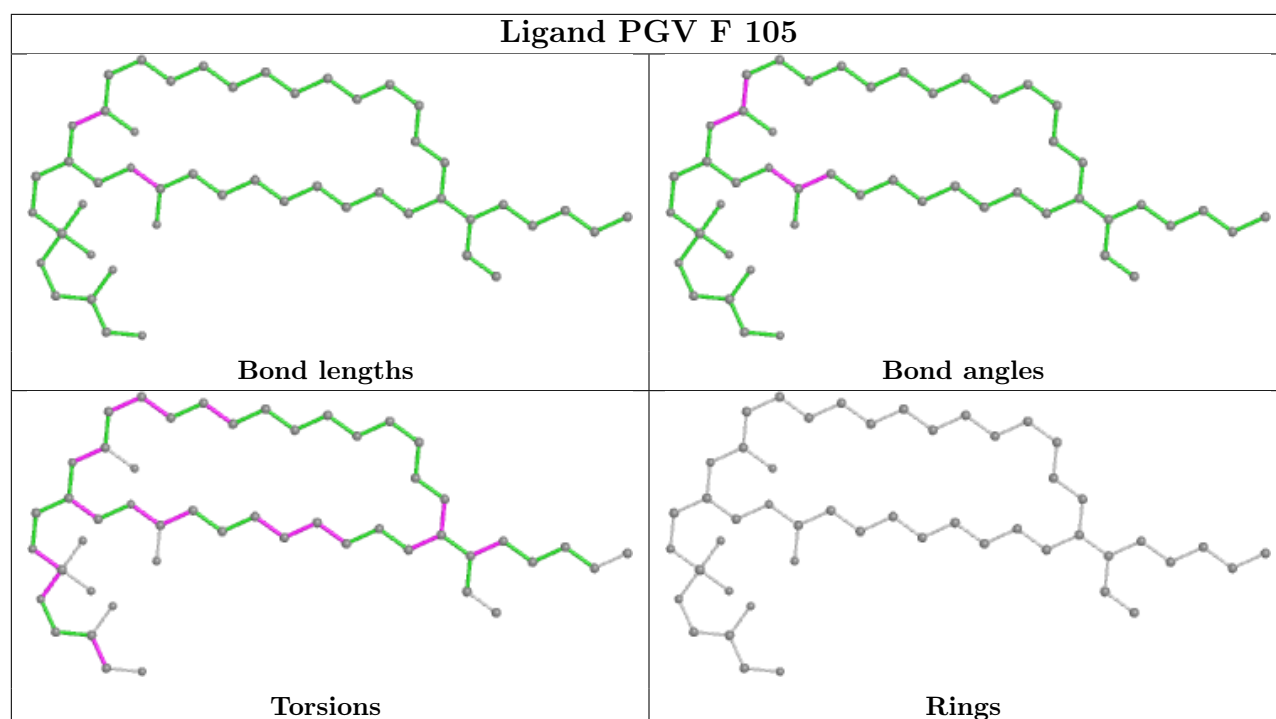
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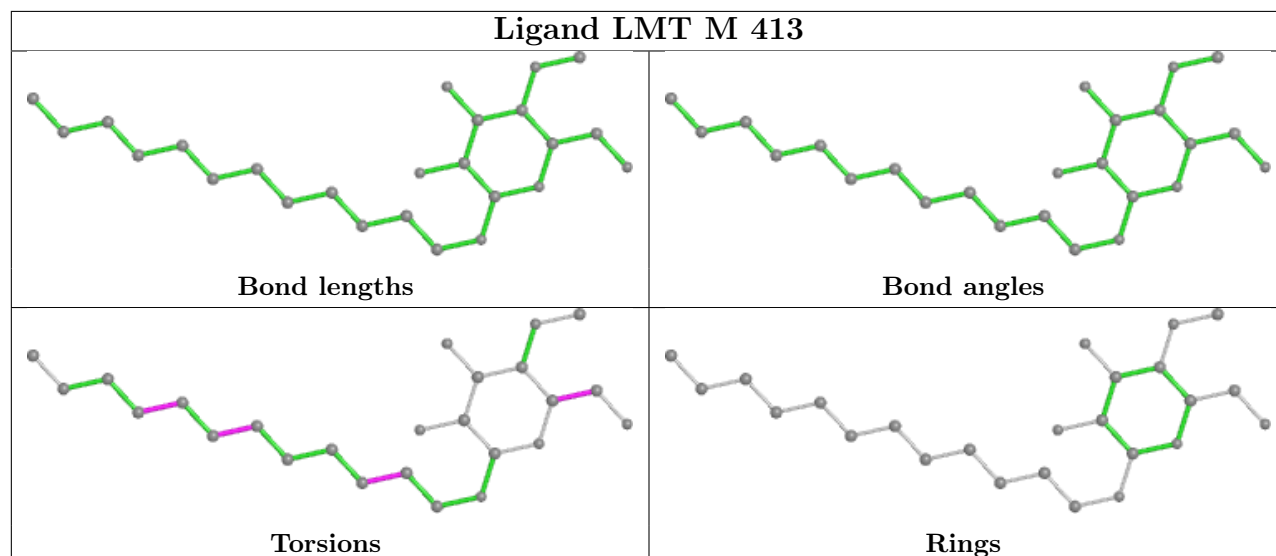
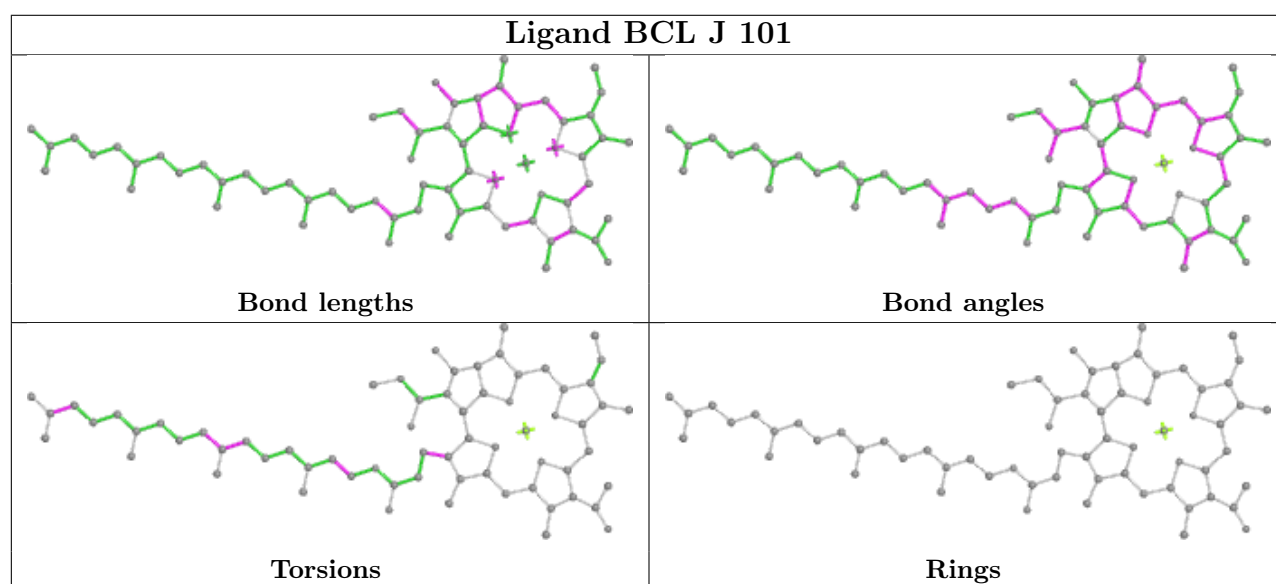
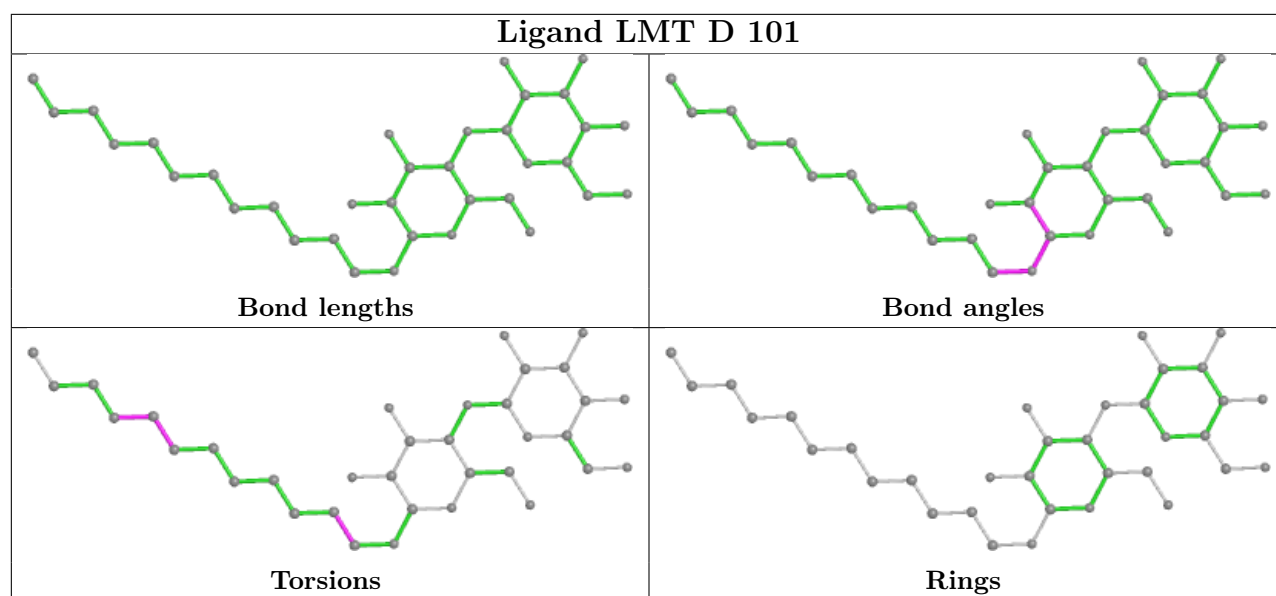


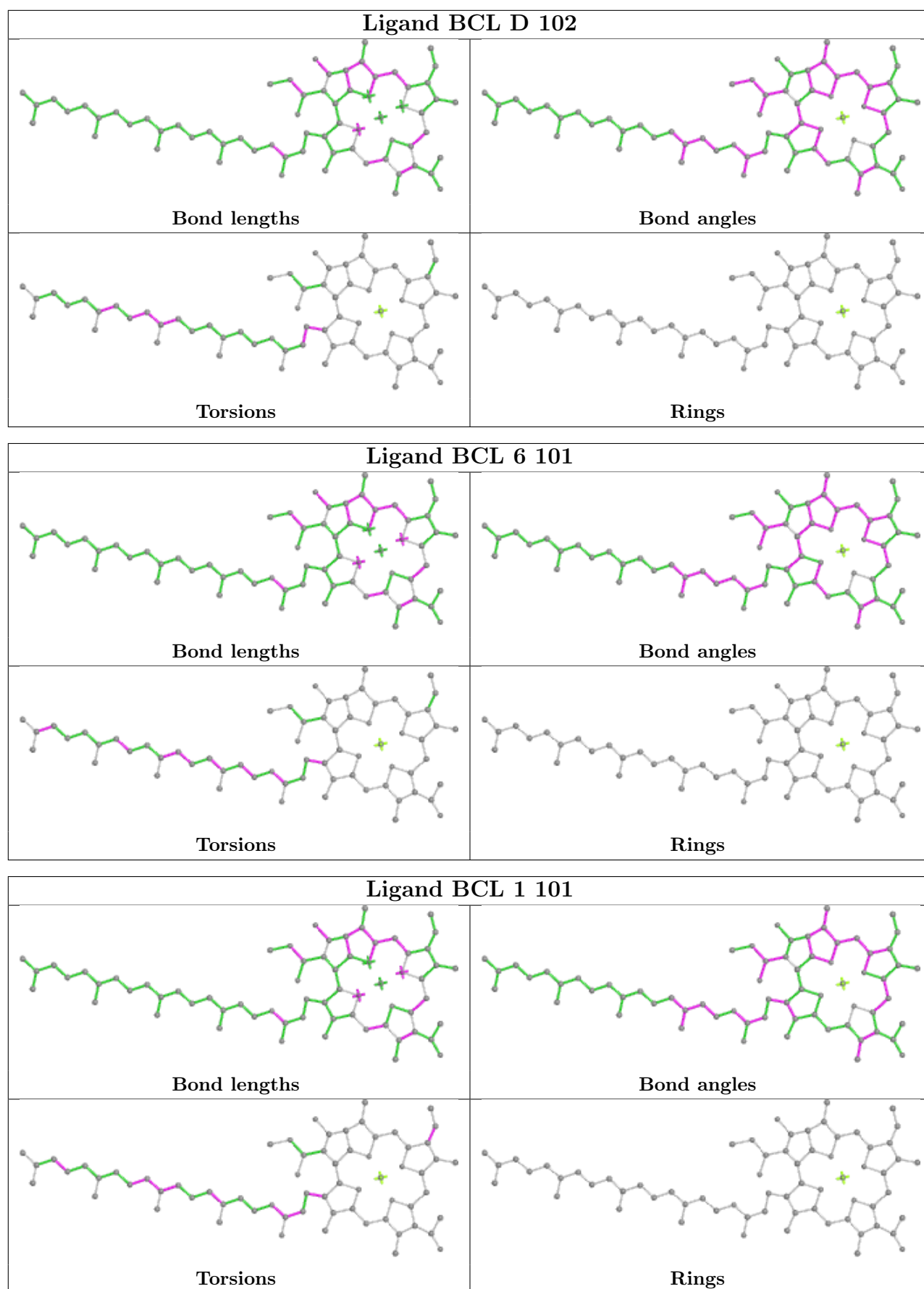
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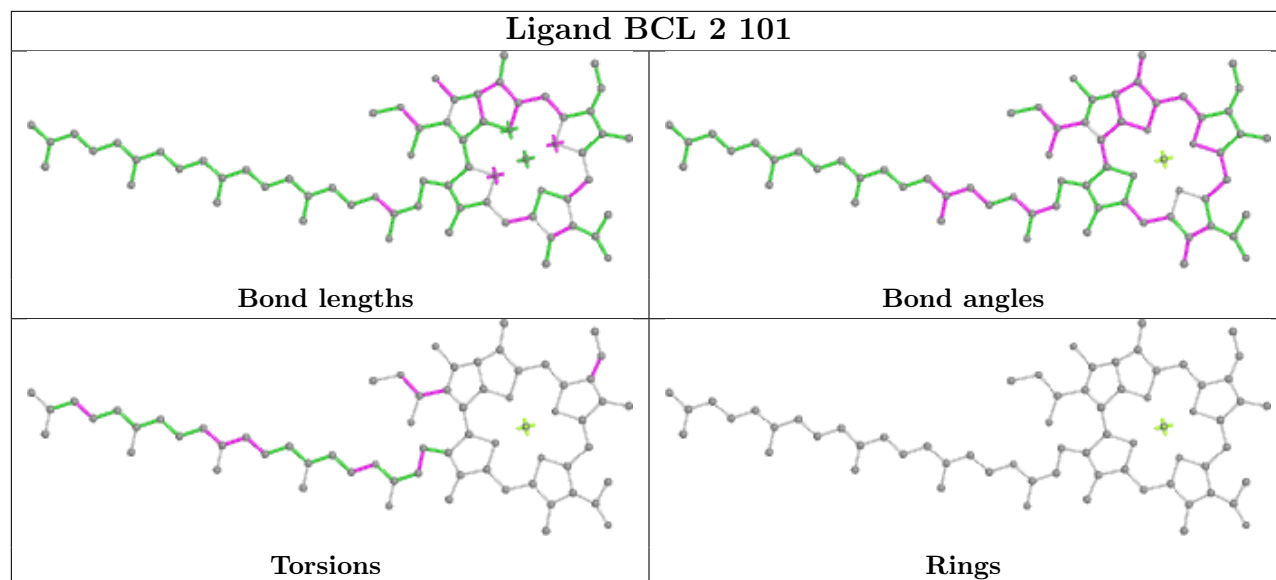




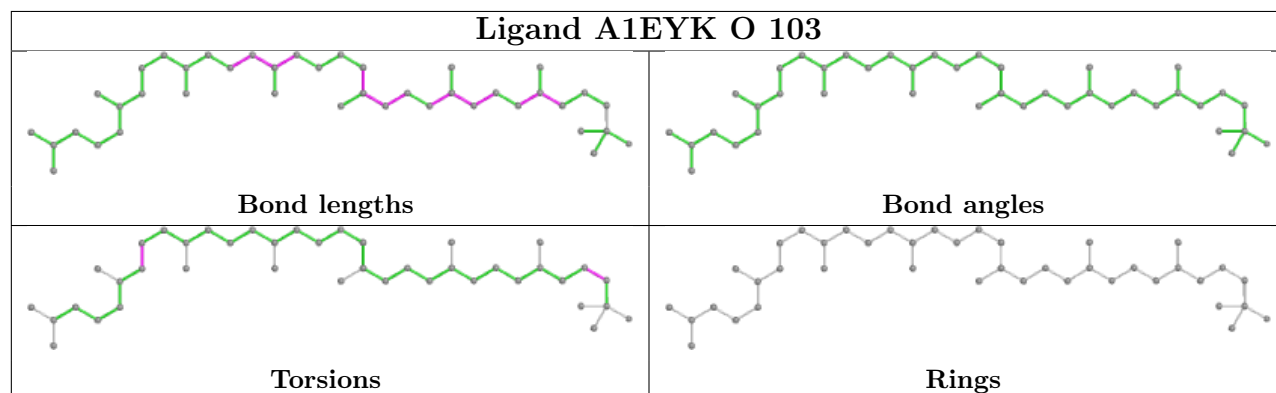




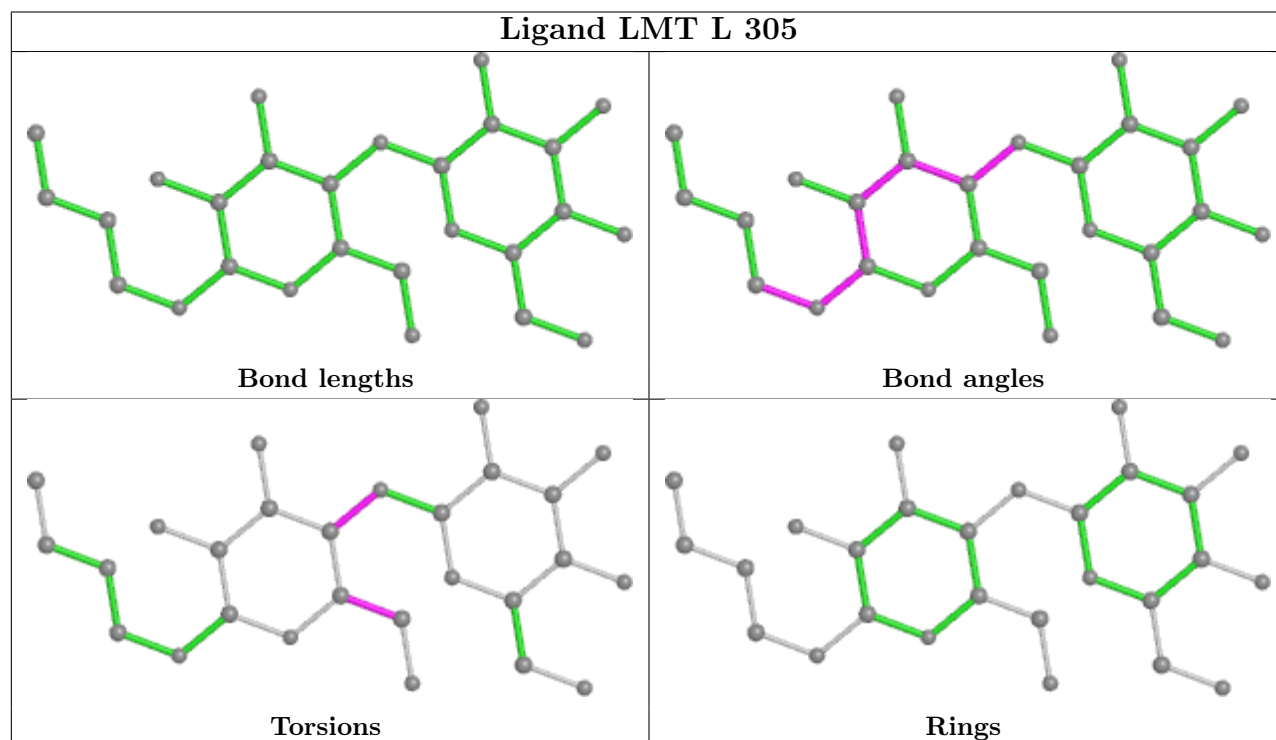
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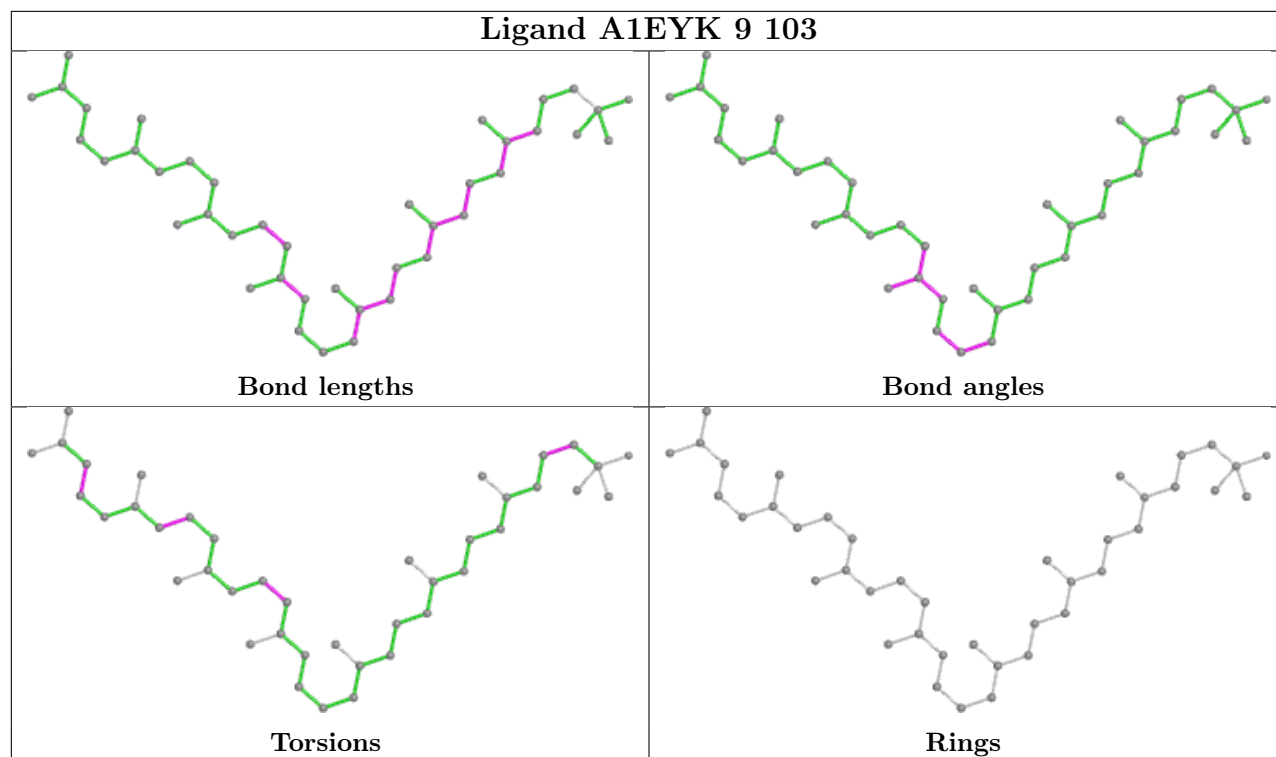
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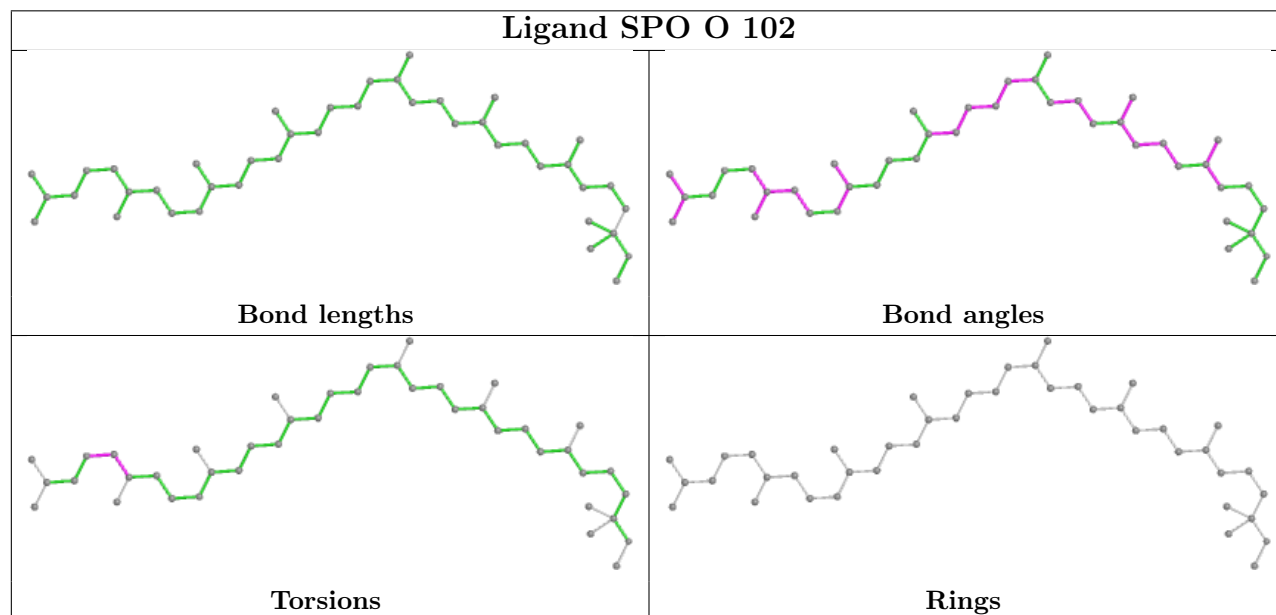
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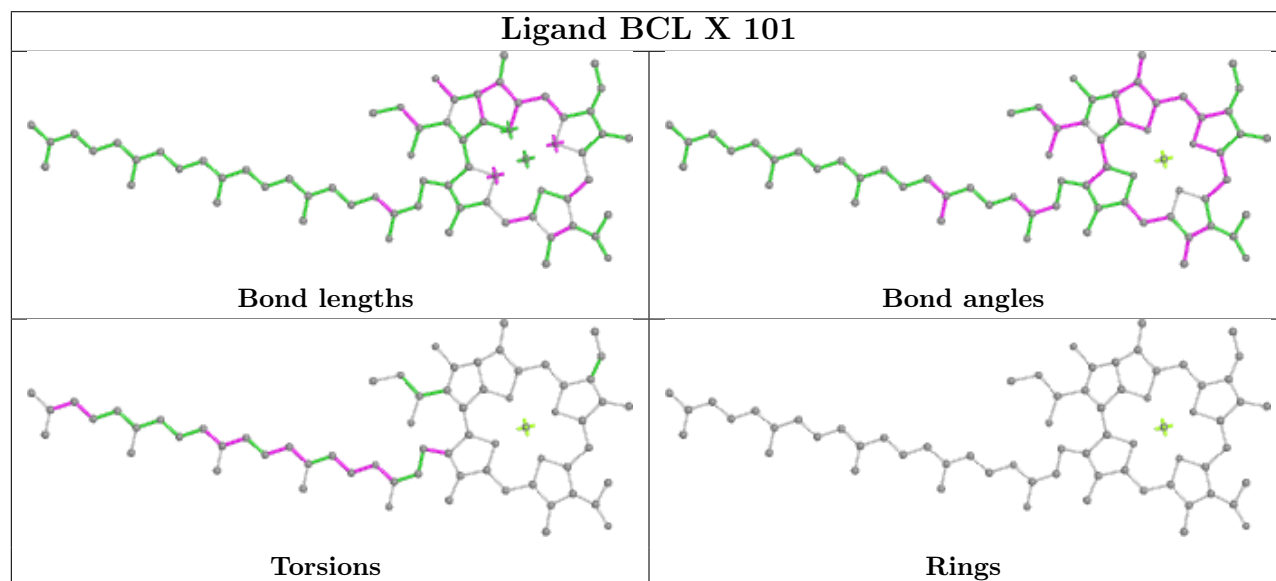
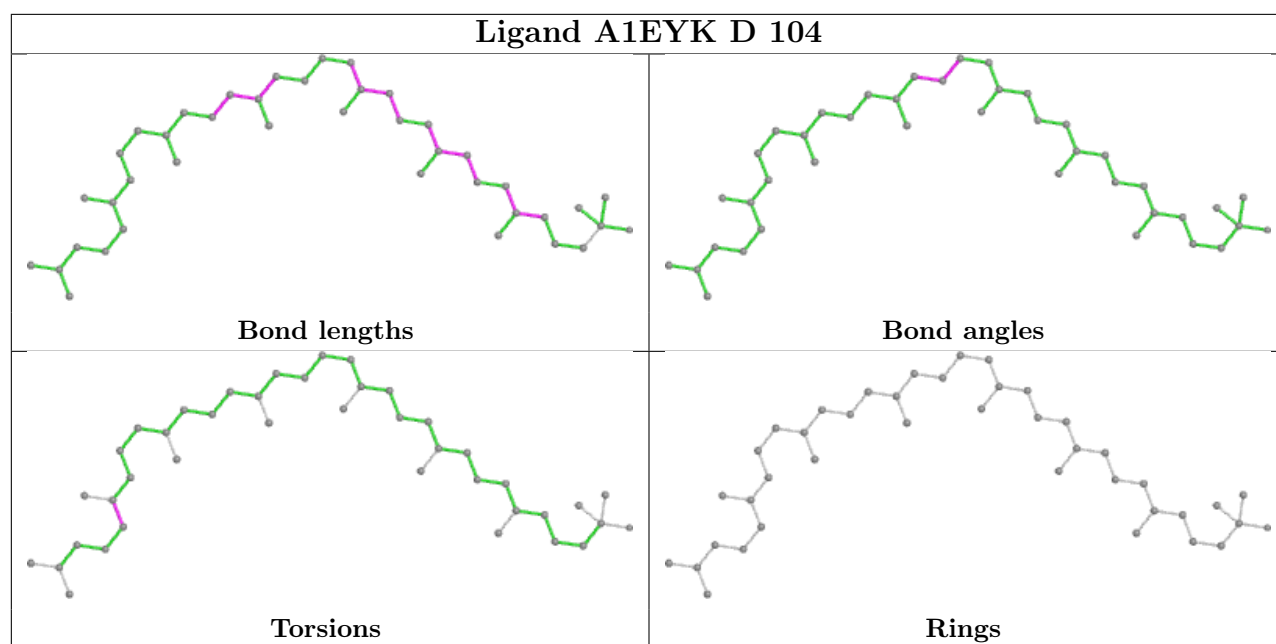


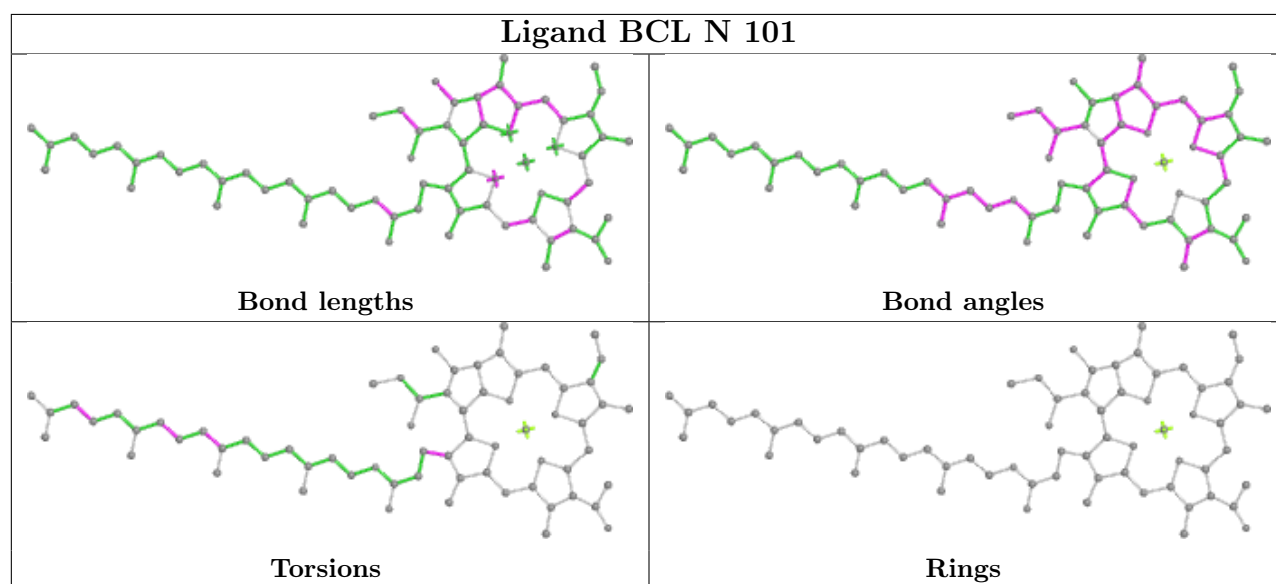
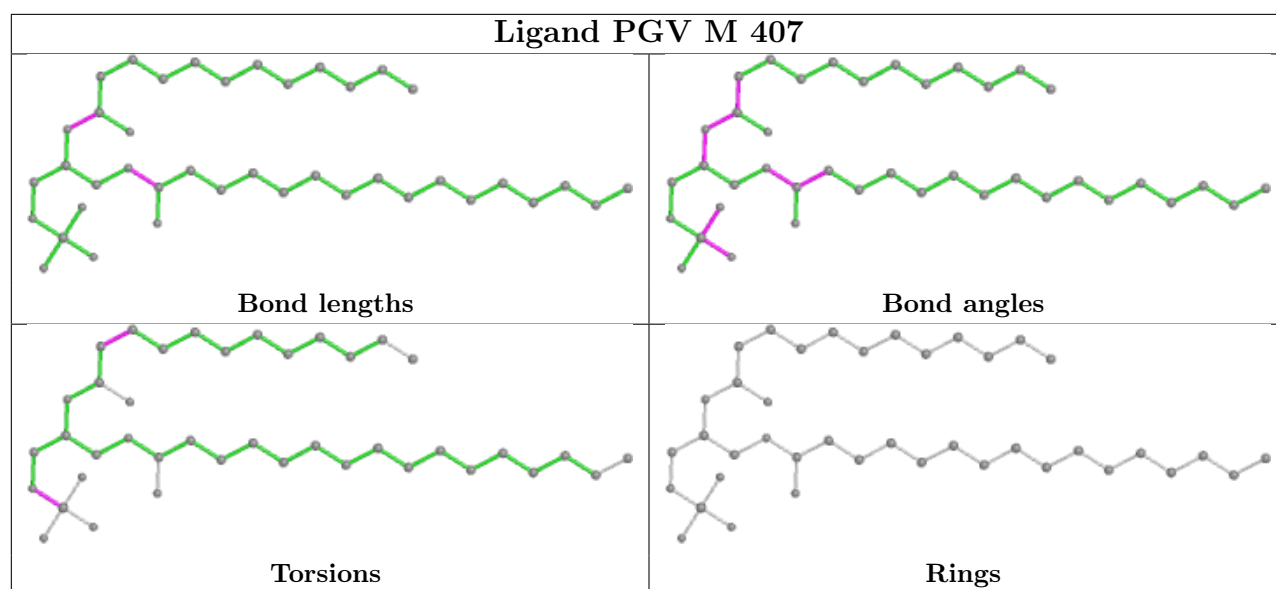
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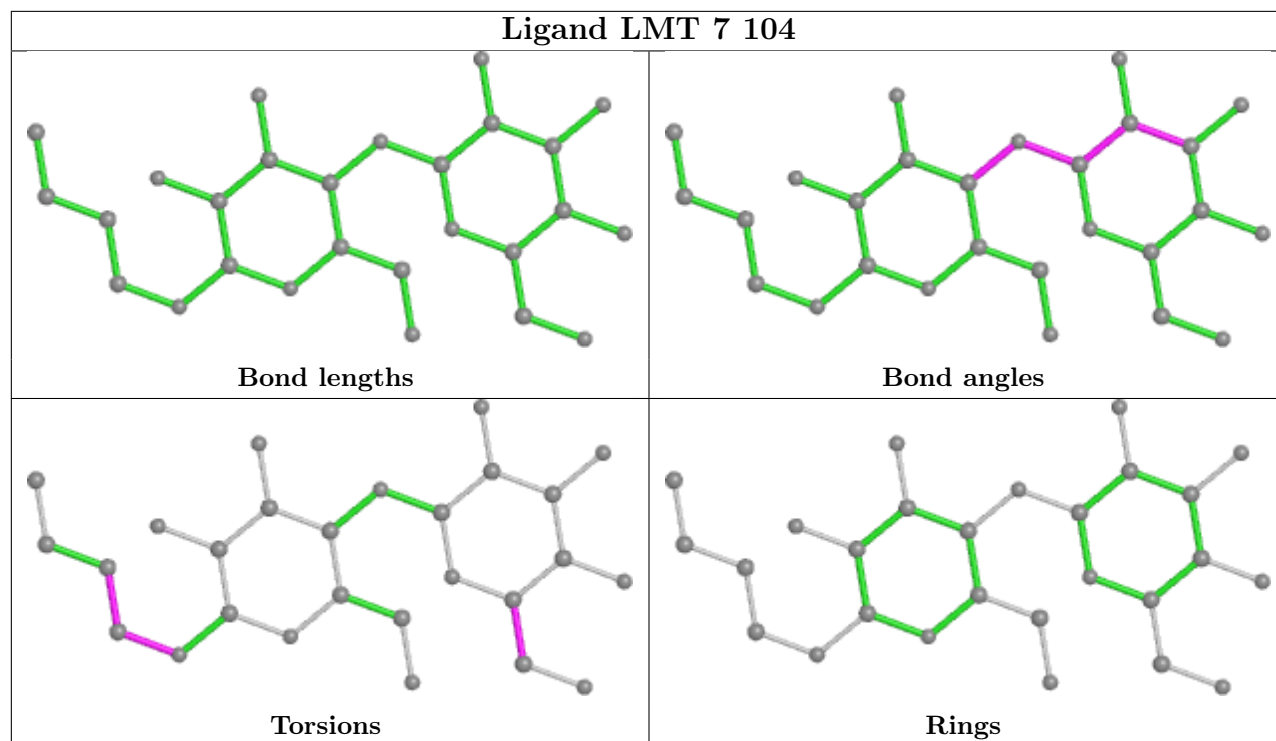
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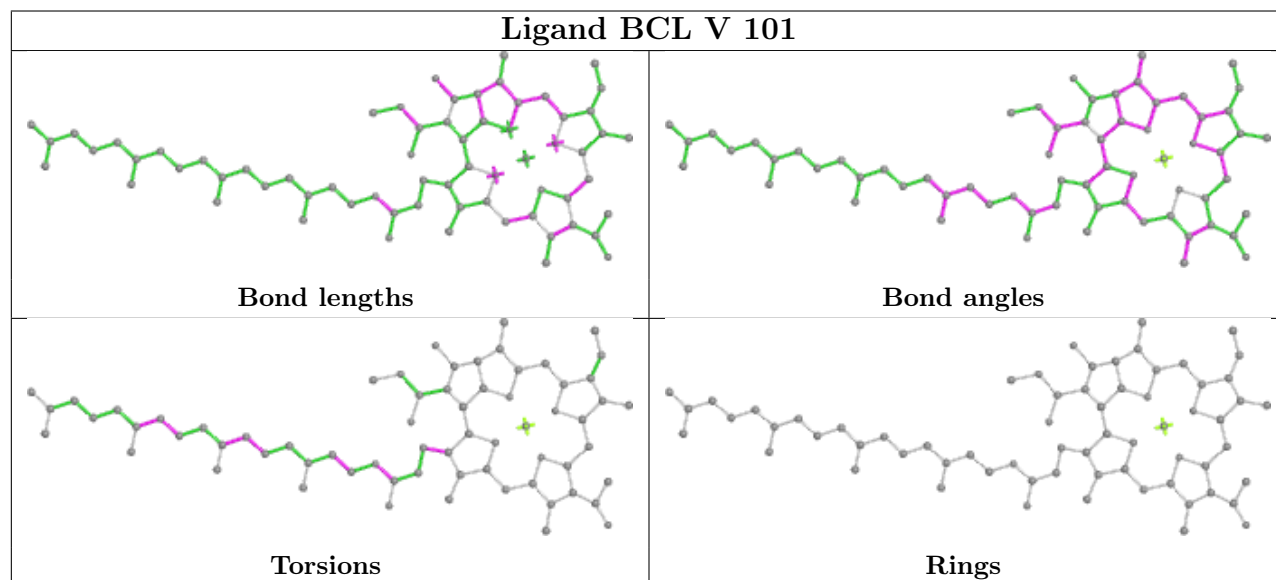


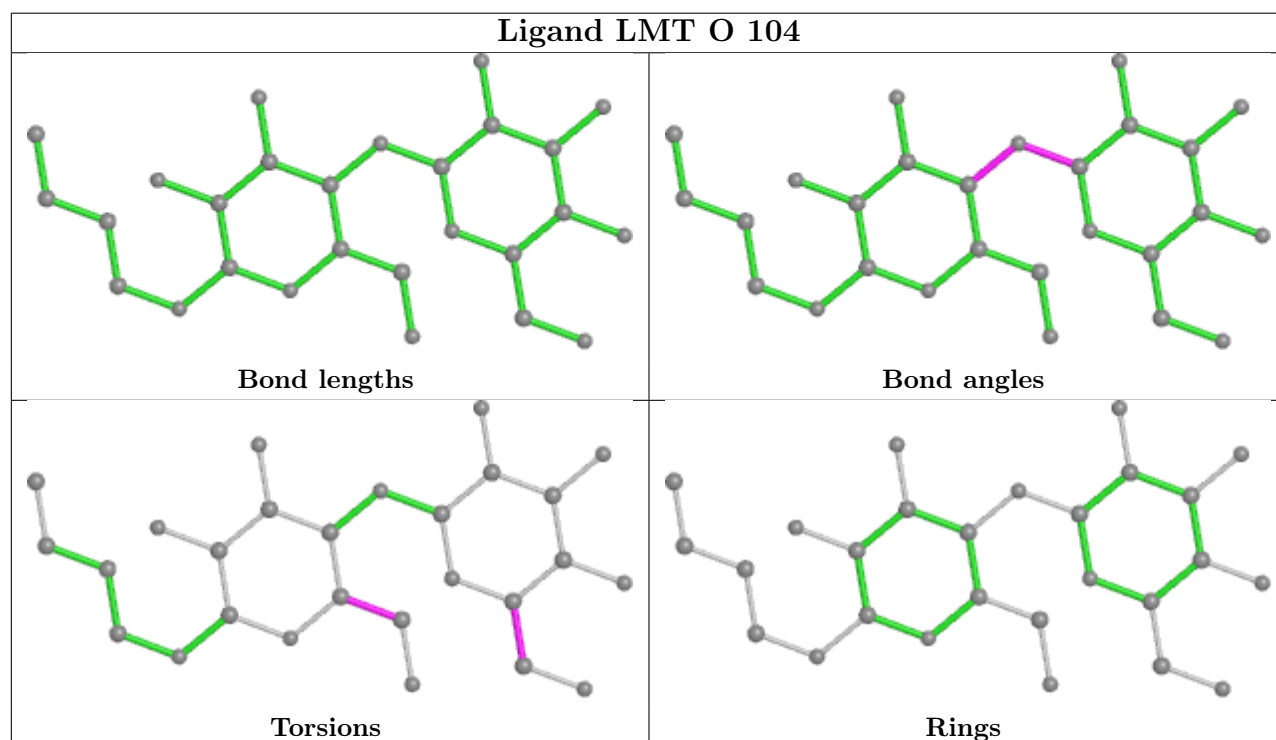
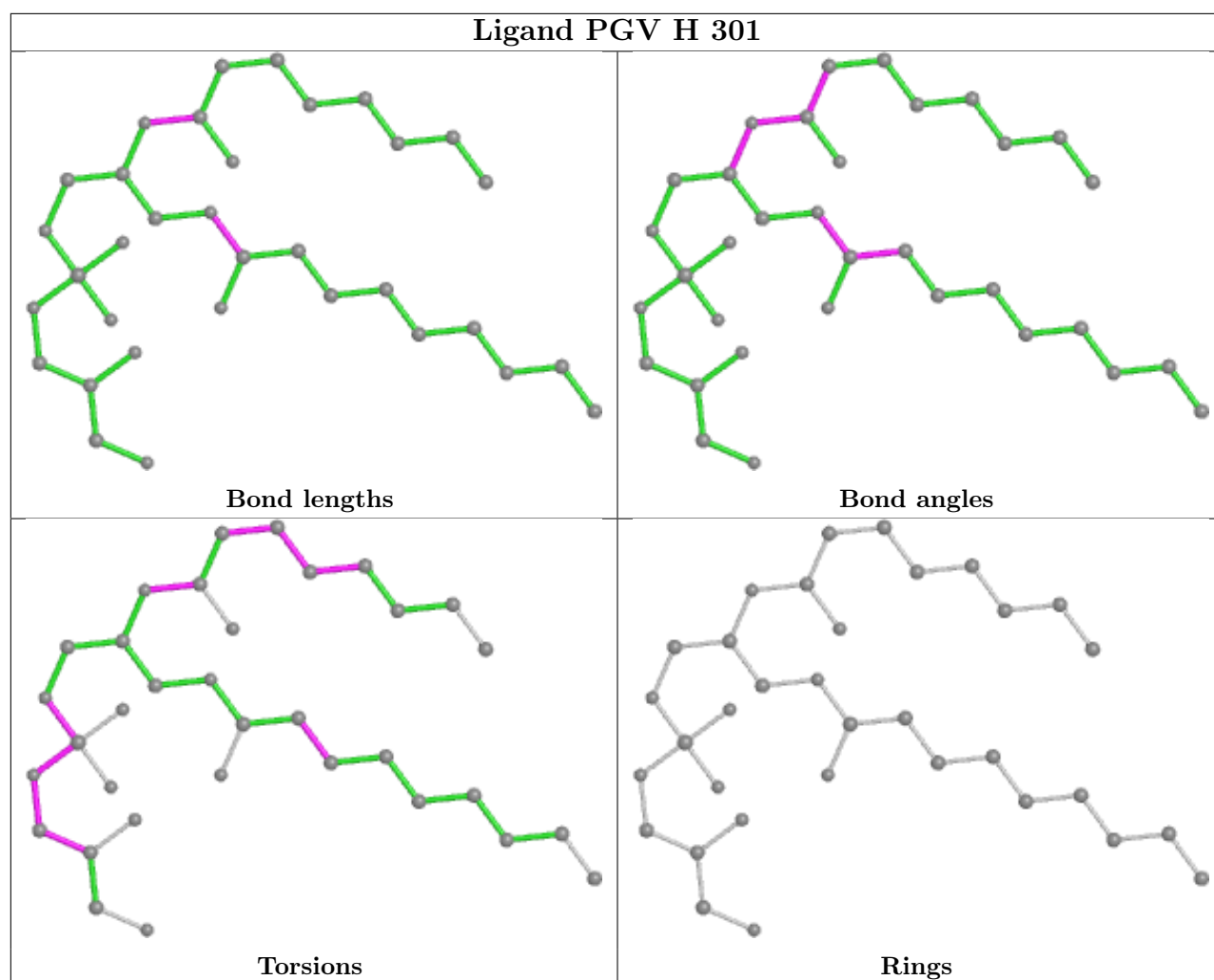


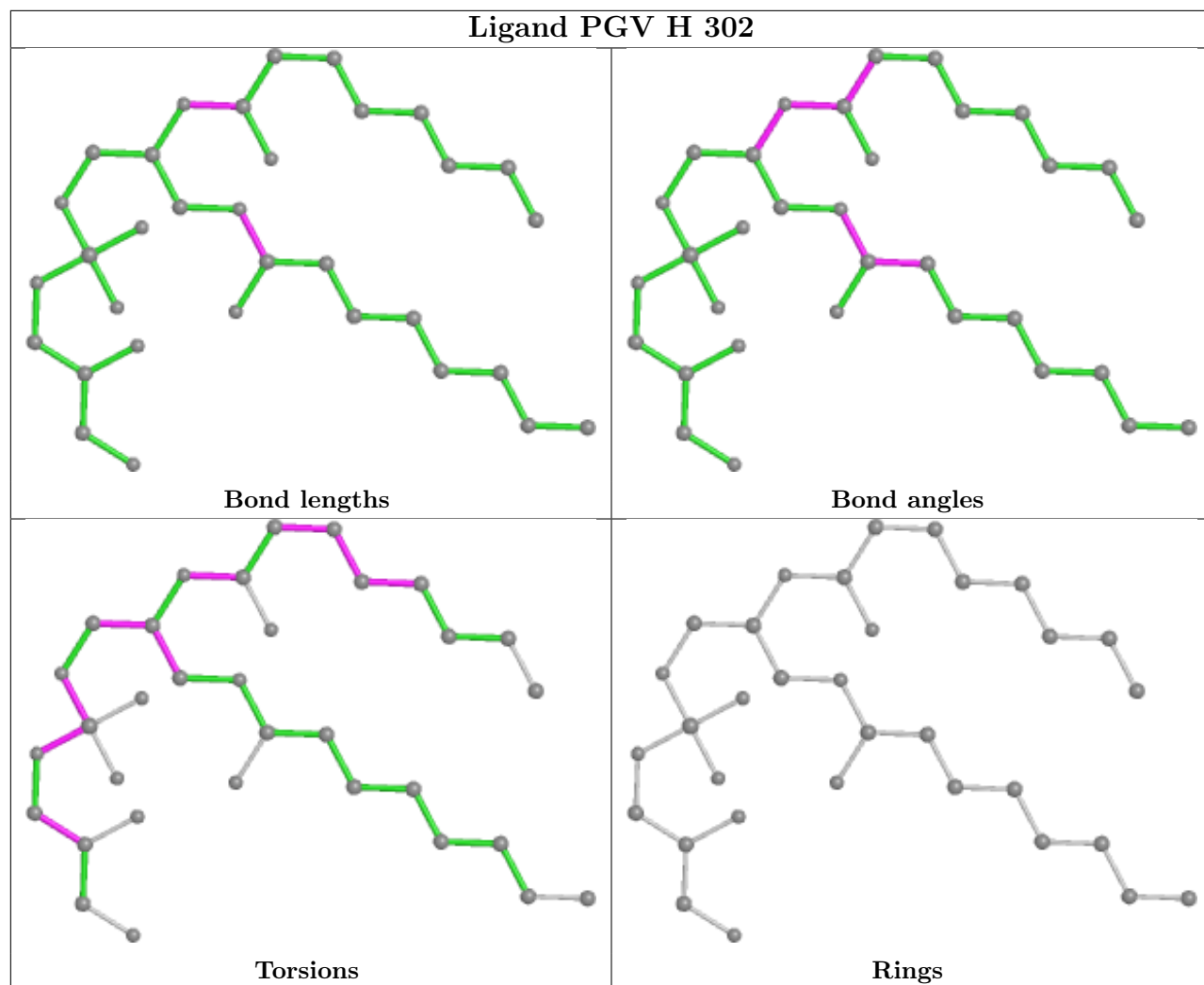
Ligand LMT 7 104

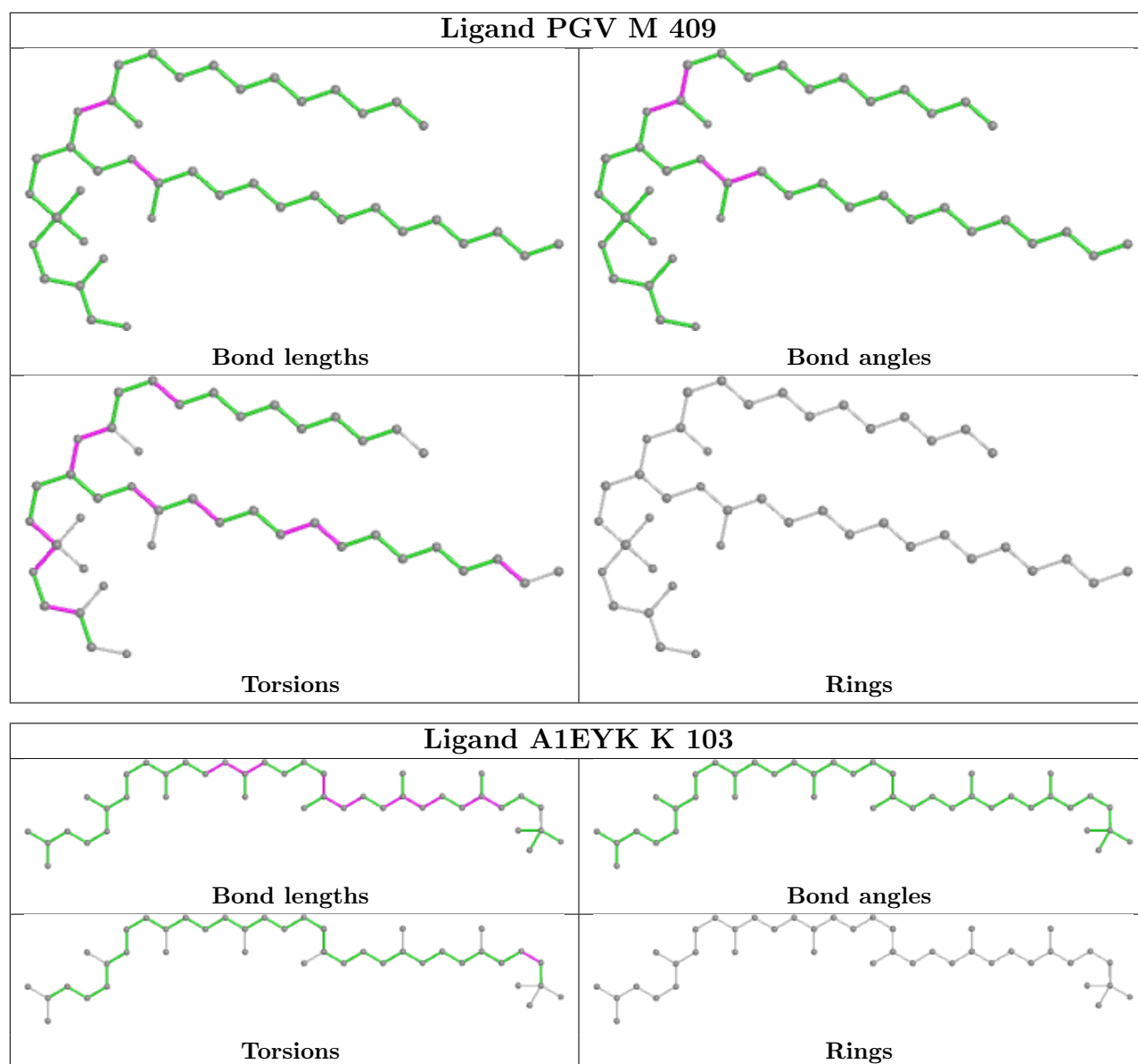


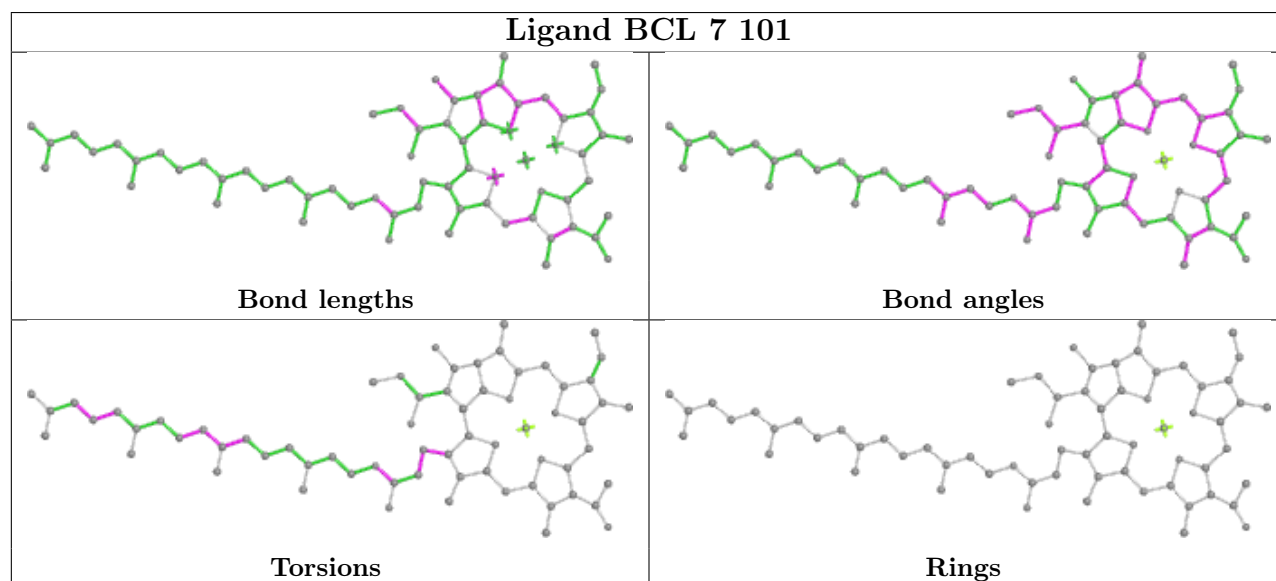
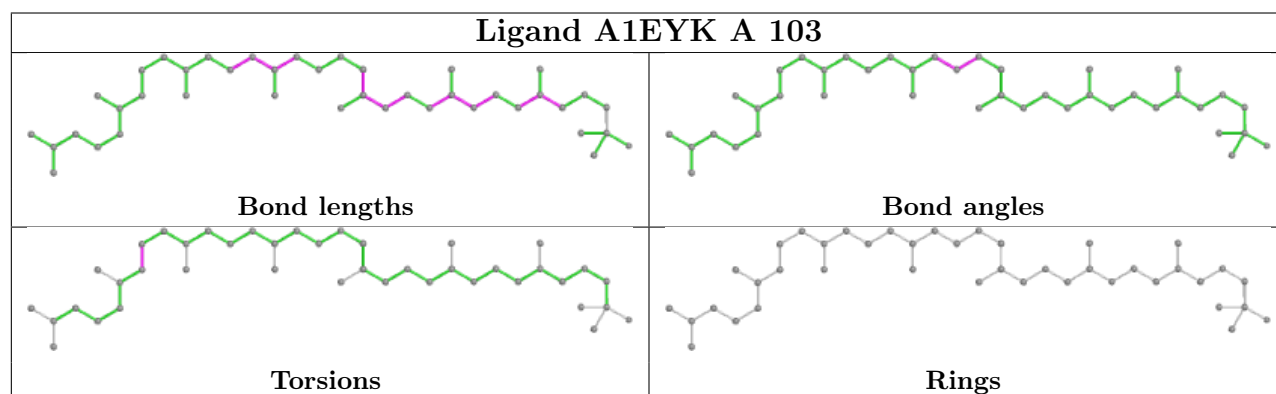
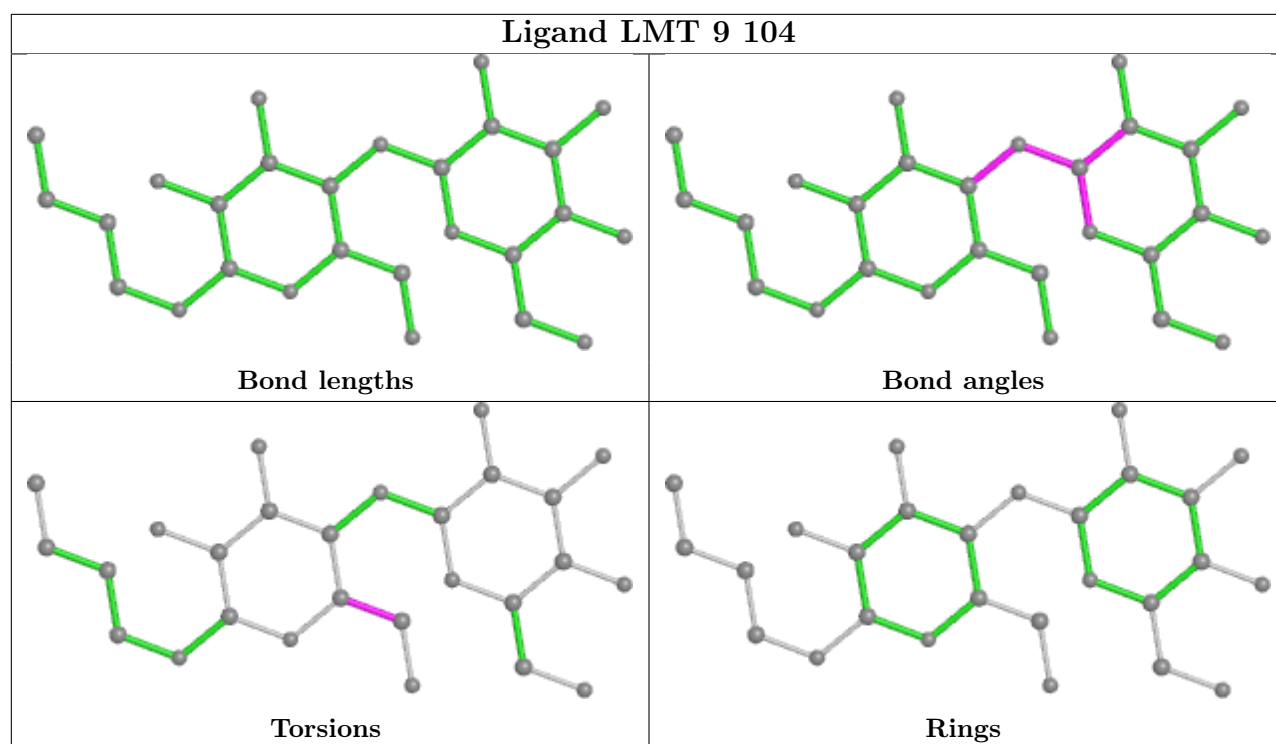
Ligand BCL V 101

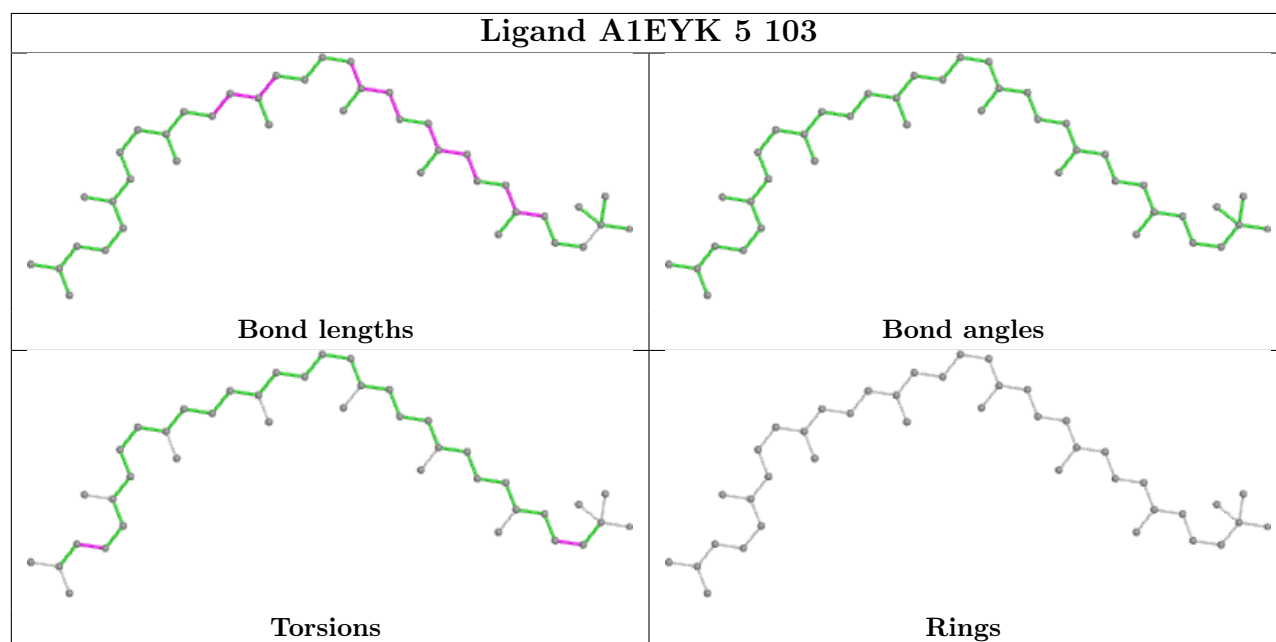
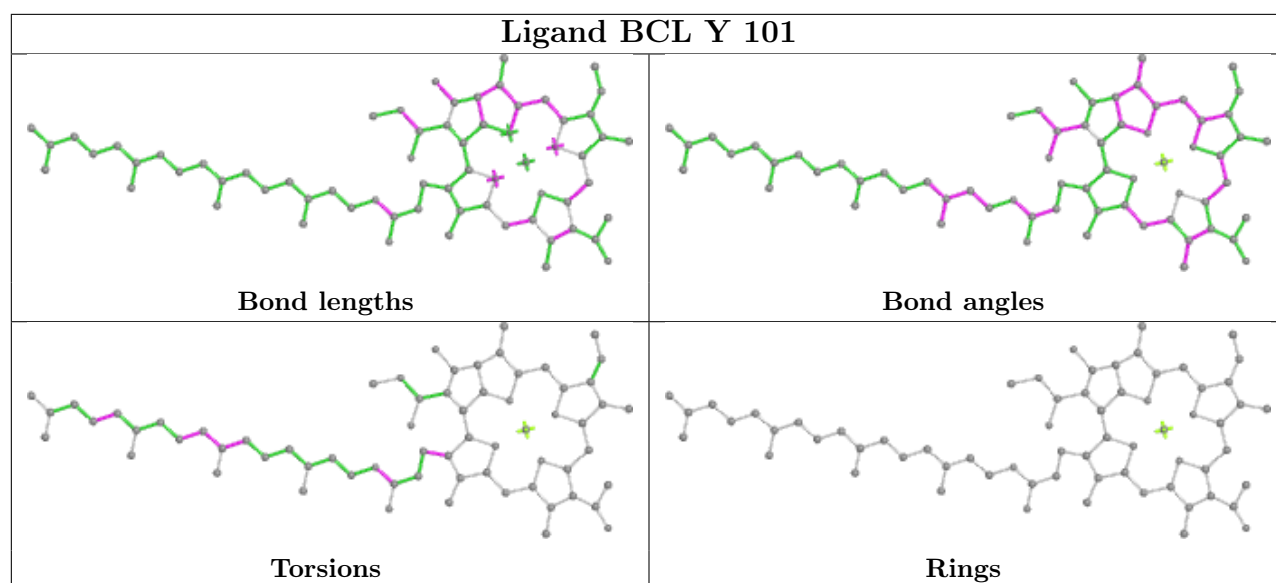


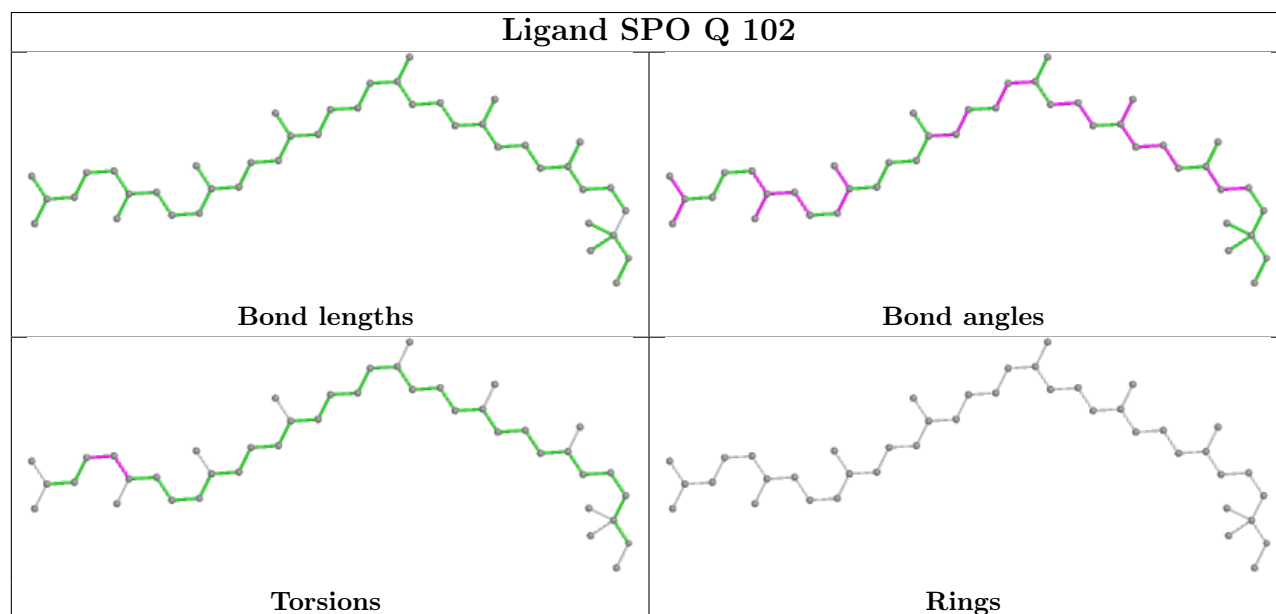
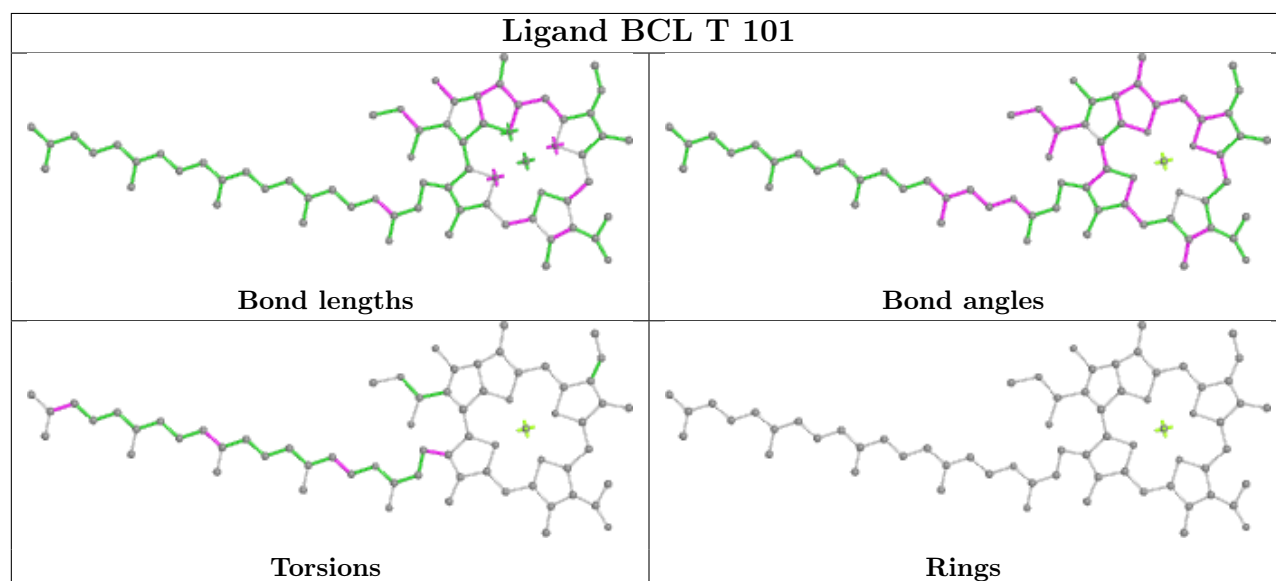
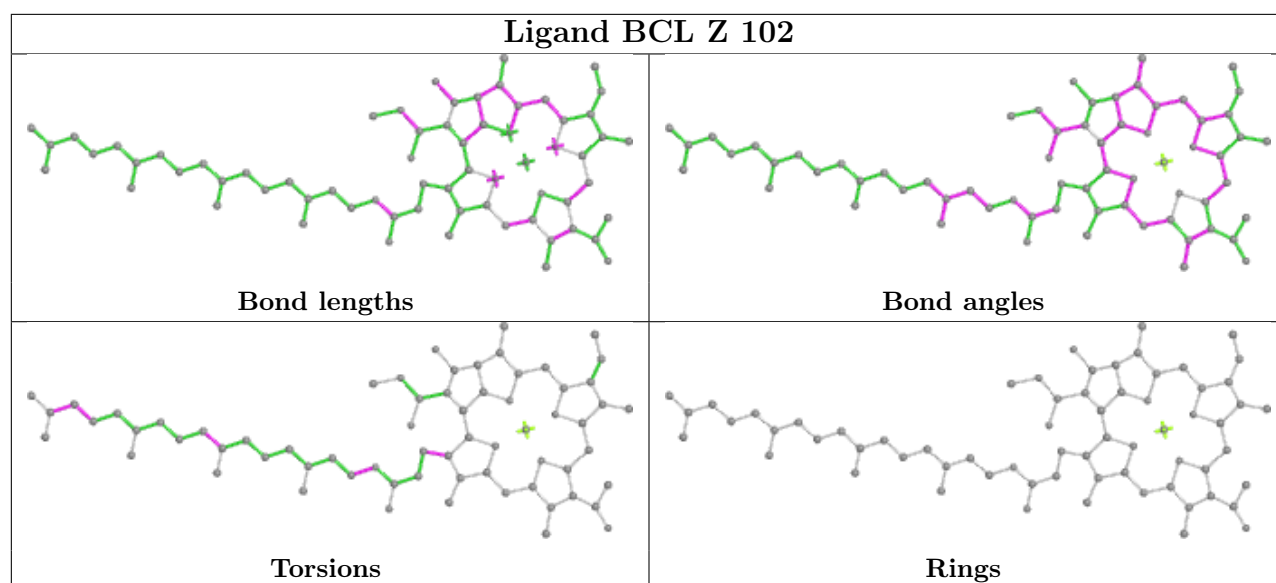




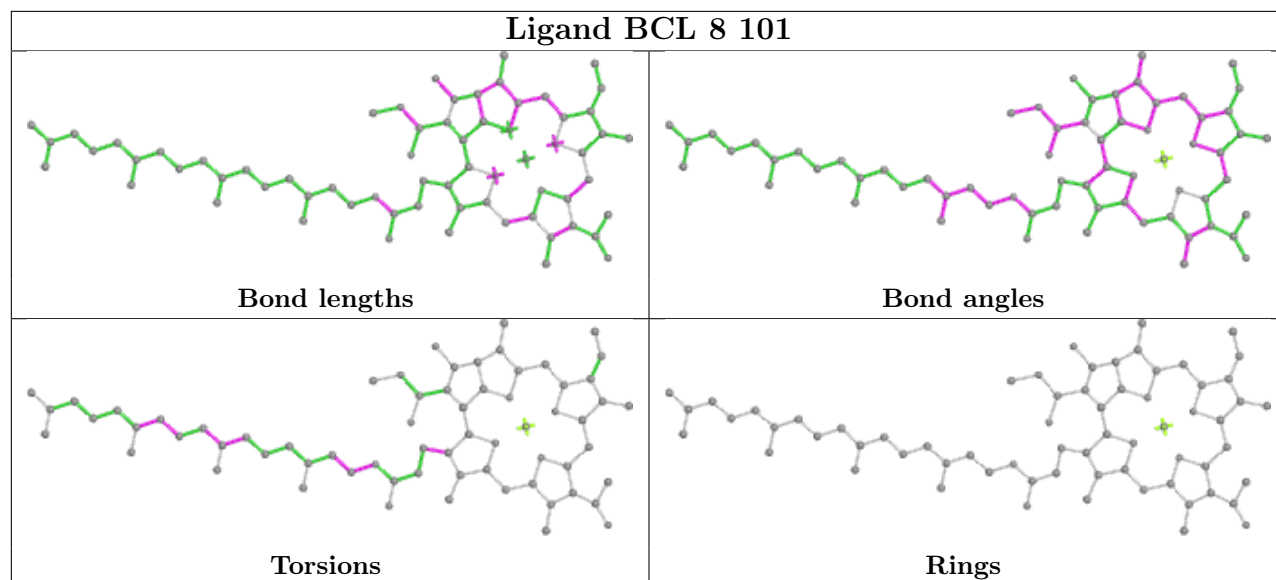




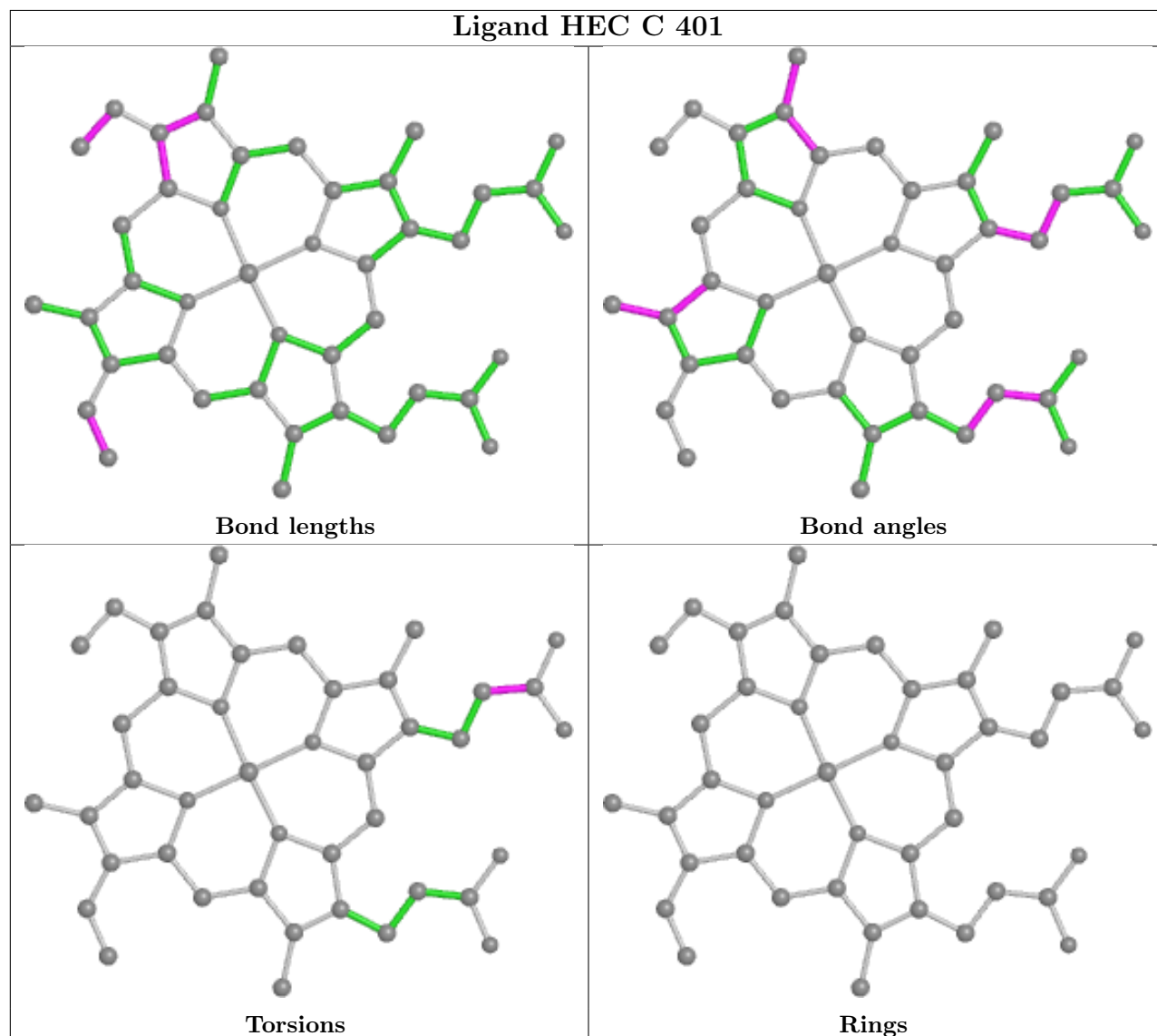


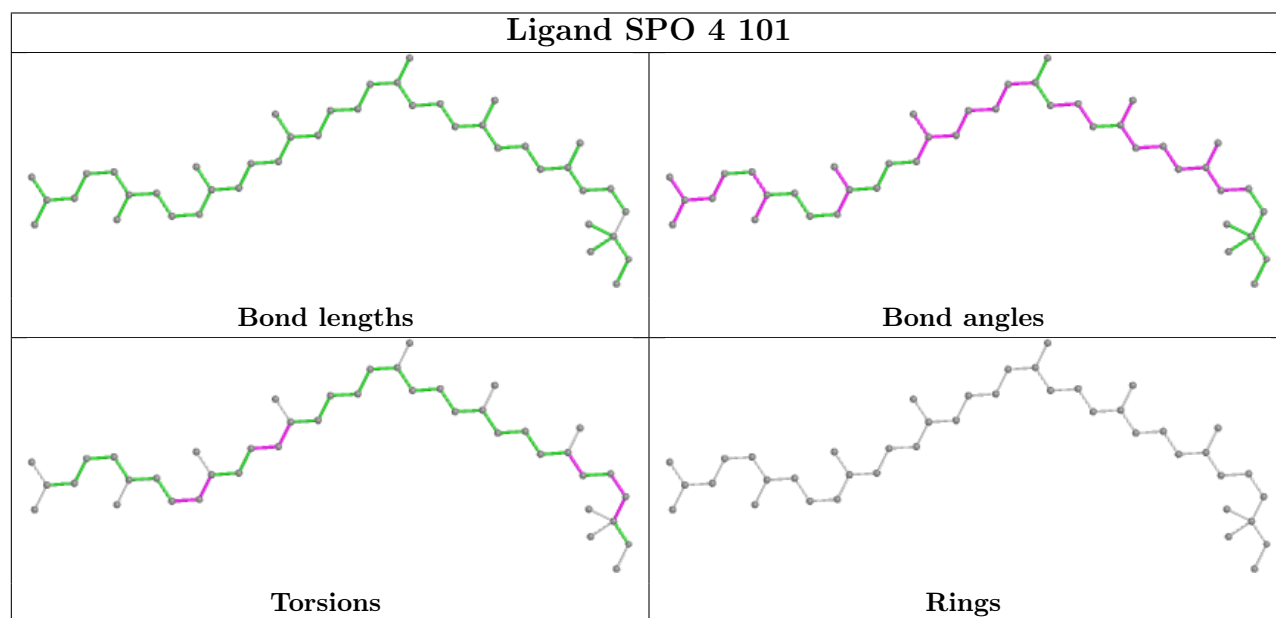
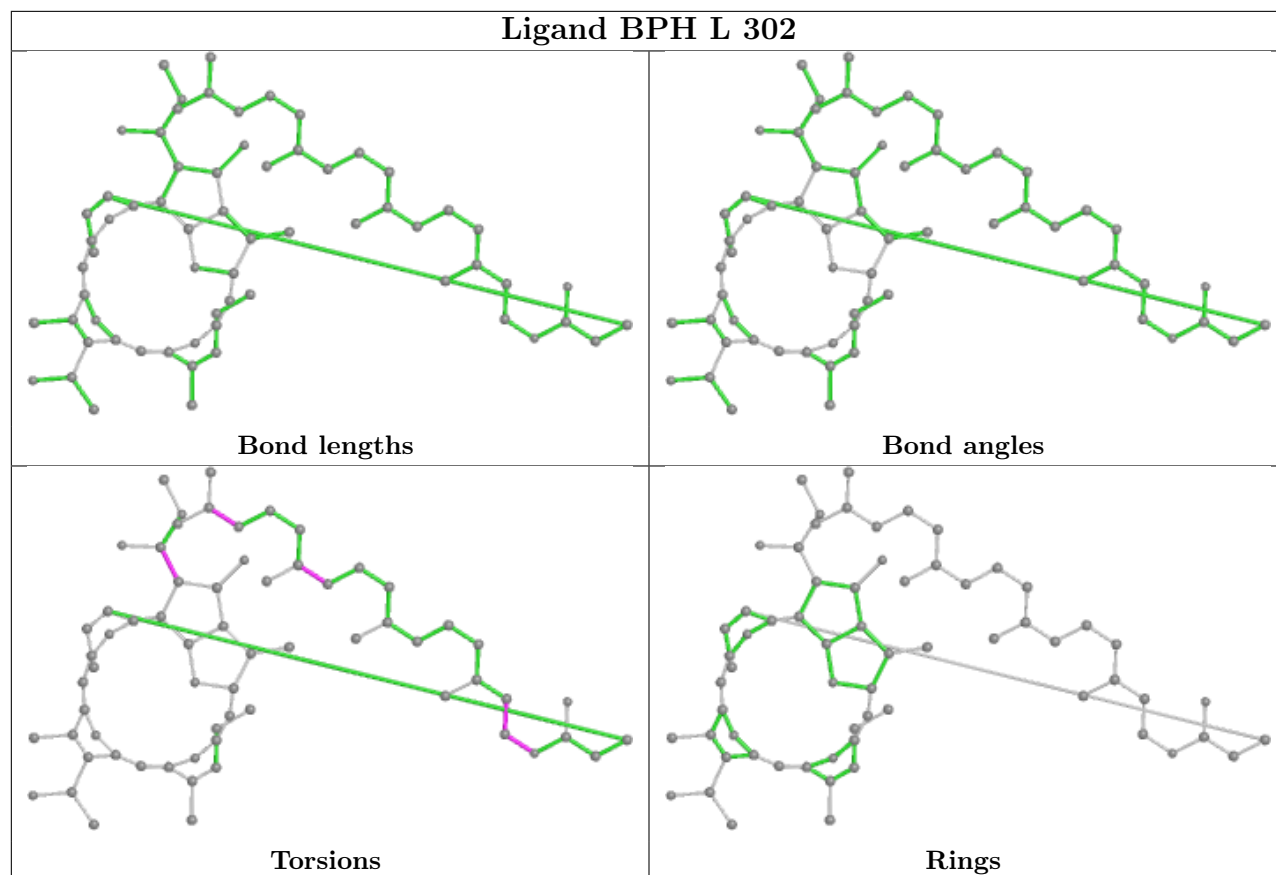


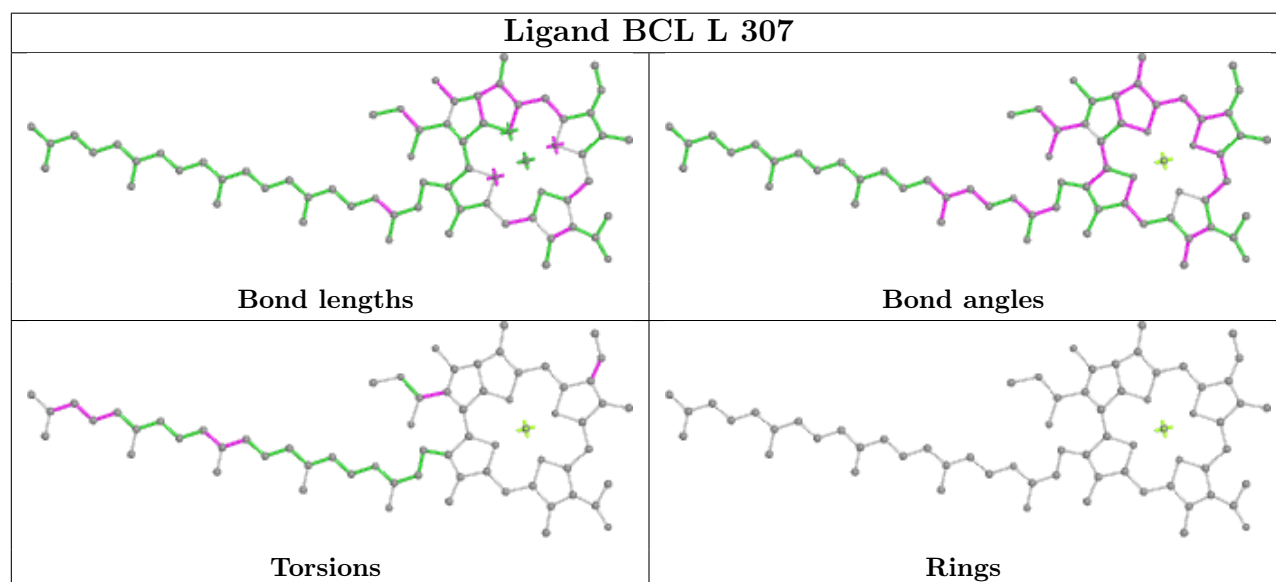
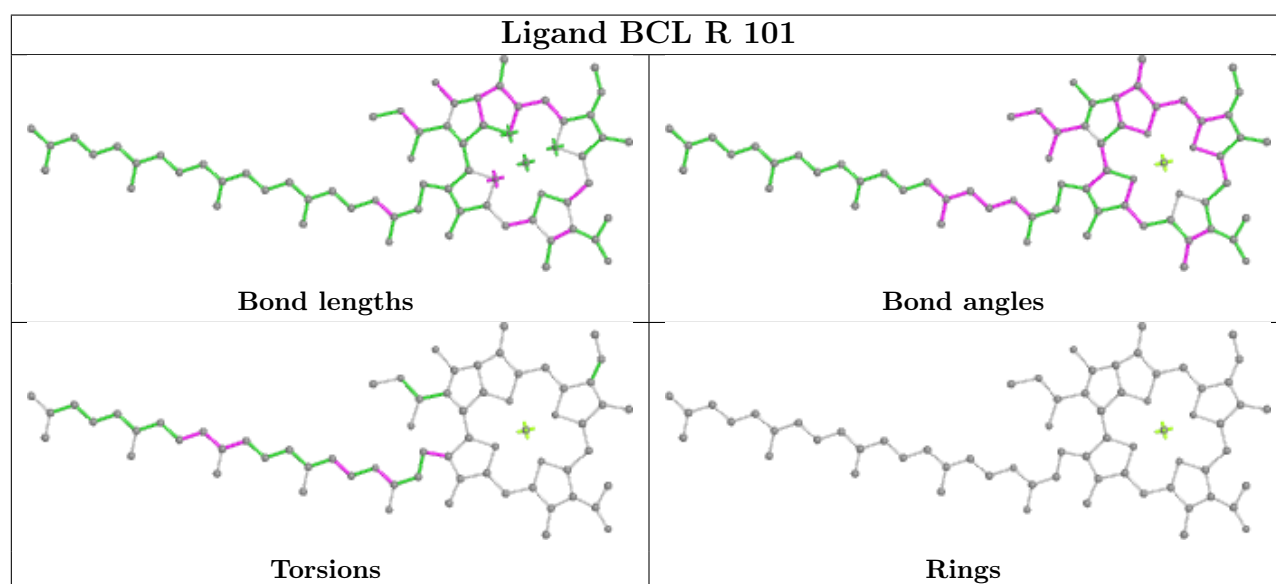
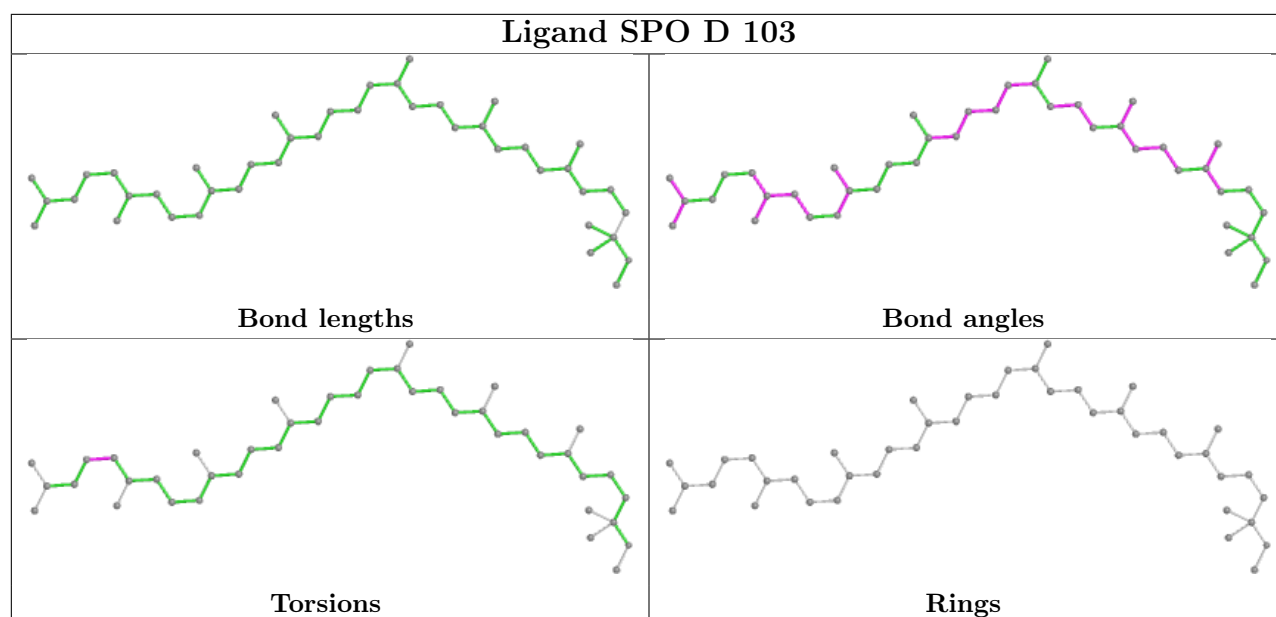
Ligand BCL 8 101

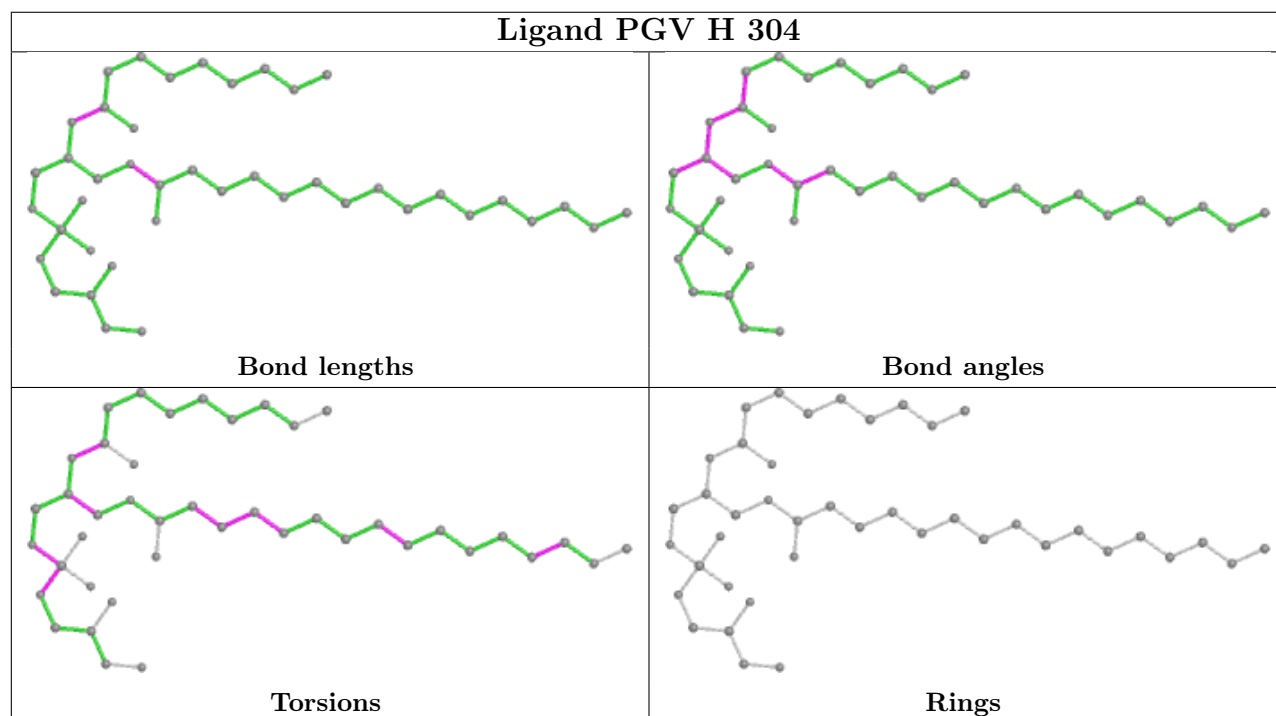
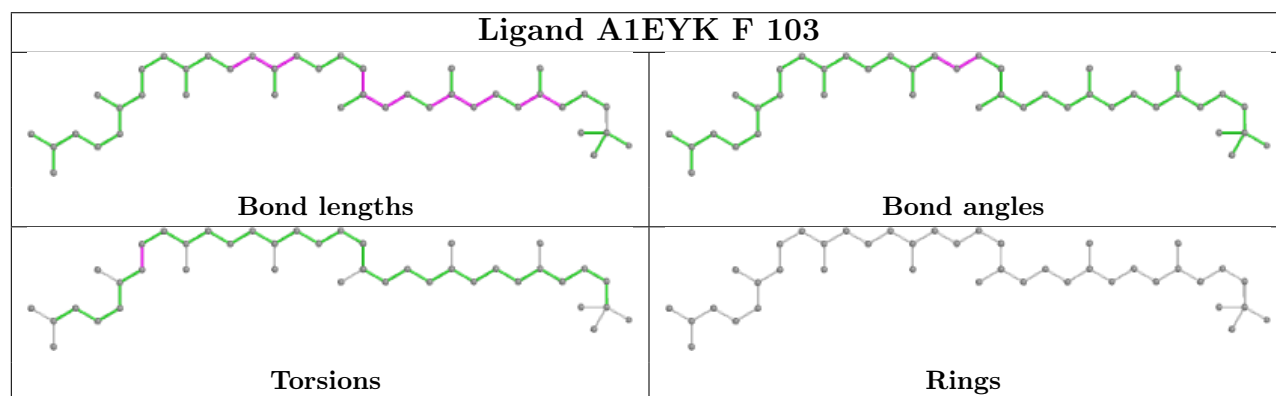
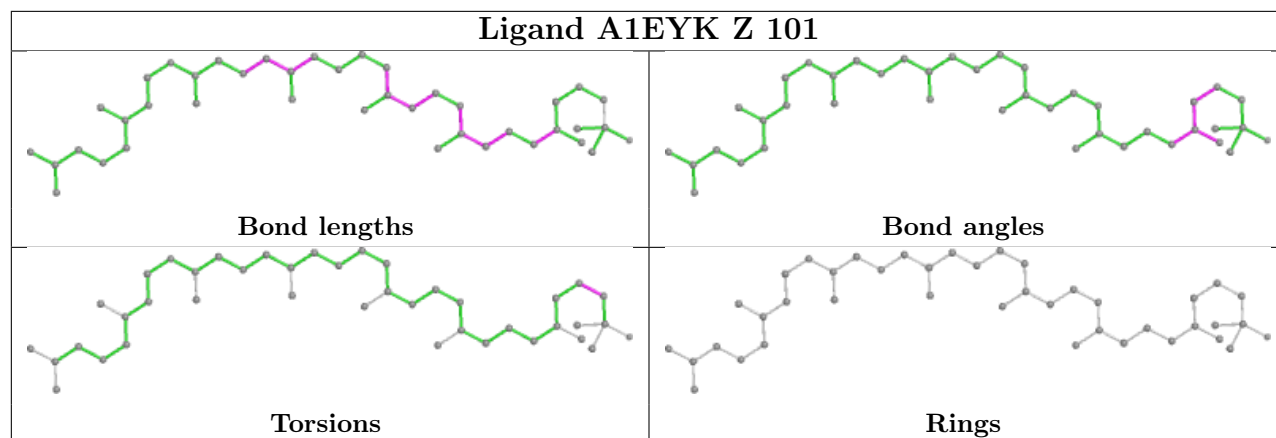


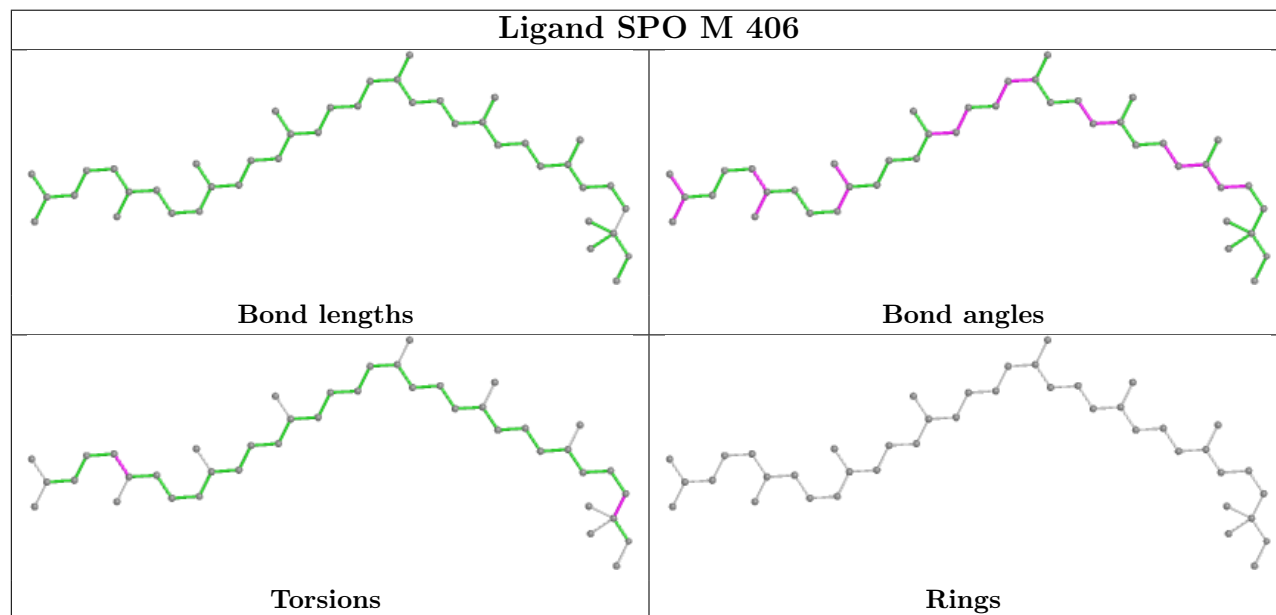
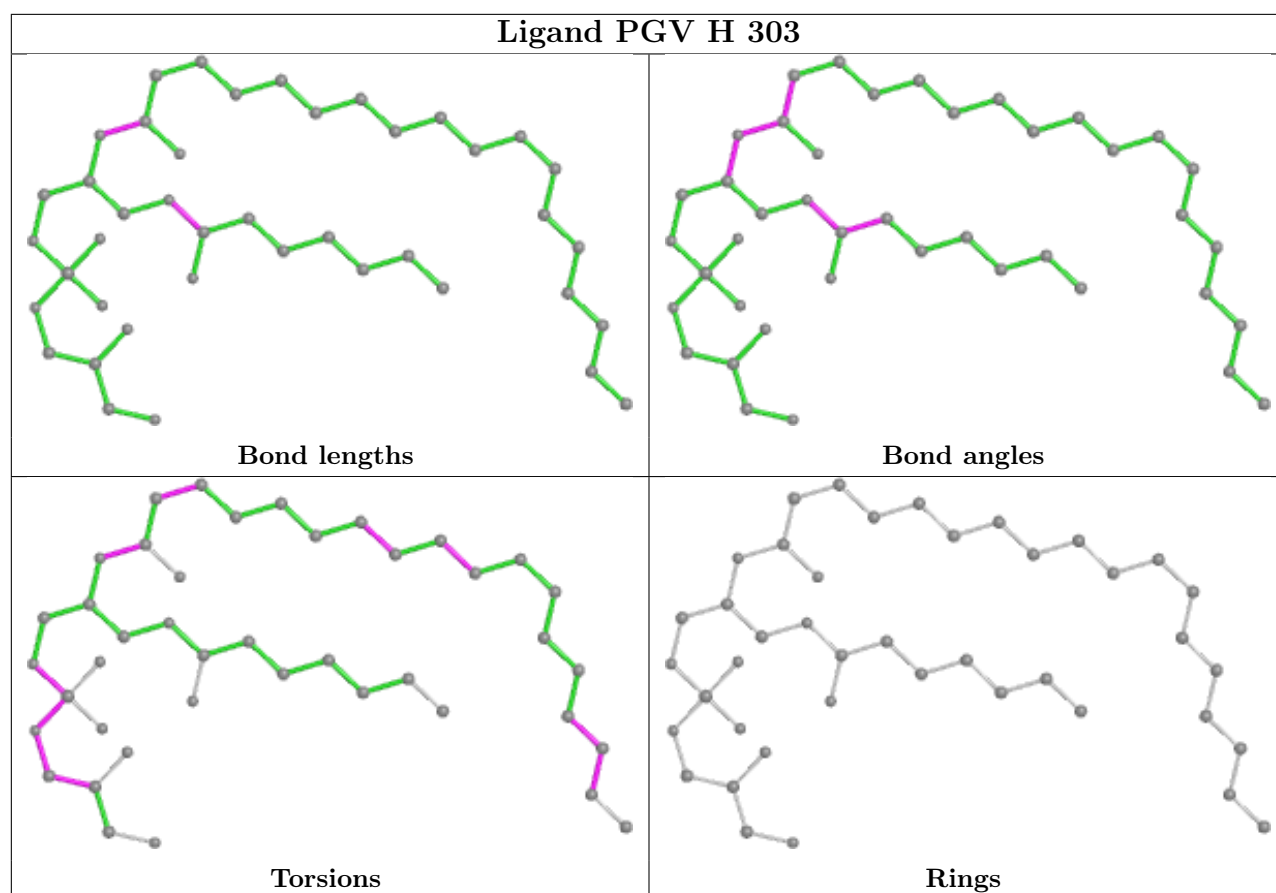
Ligand HEC C 401

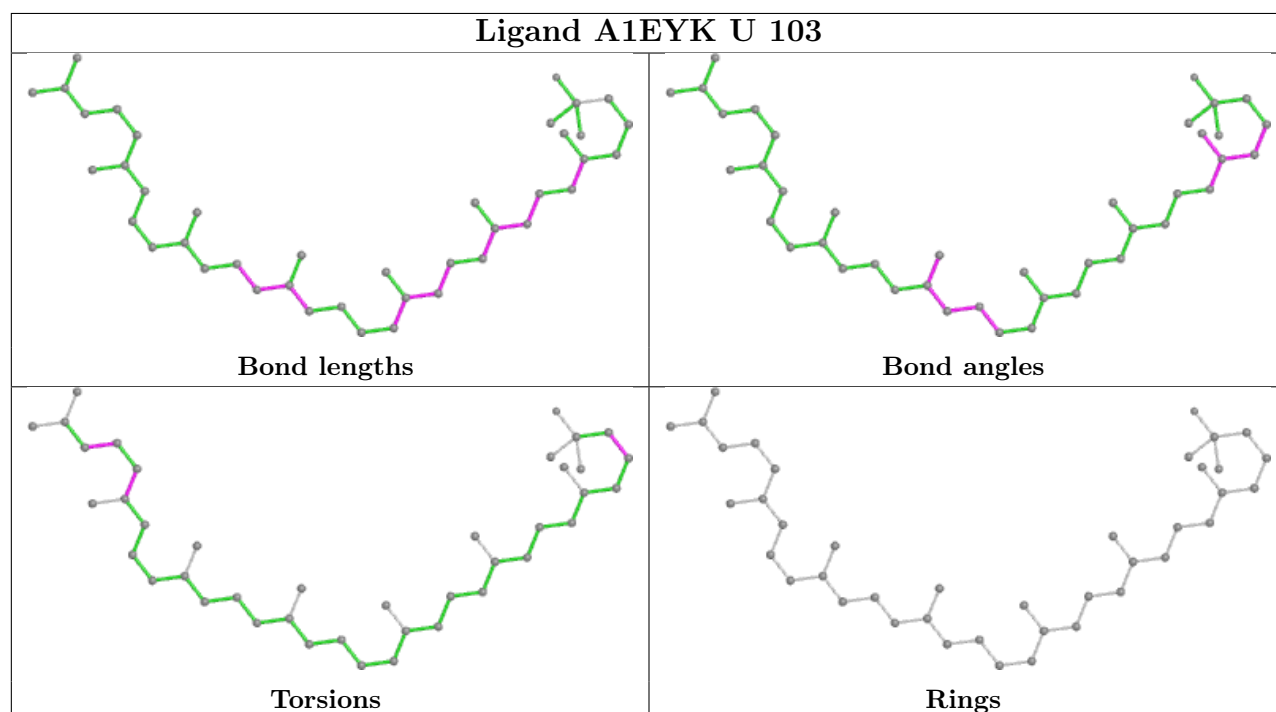
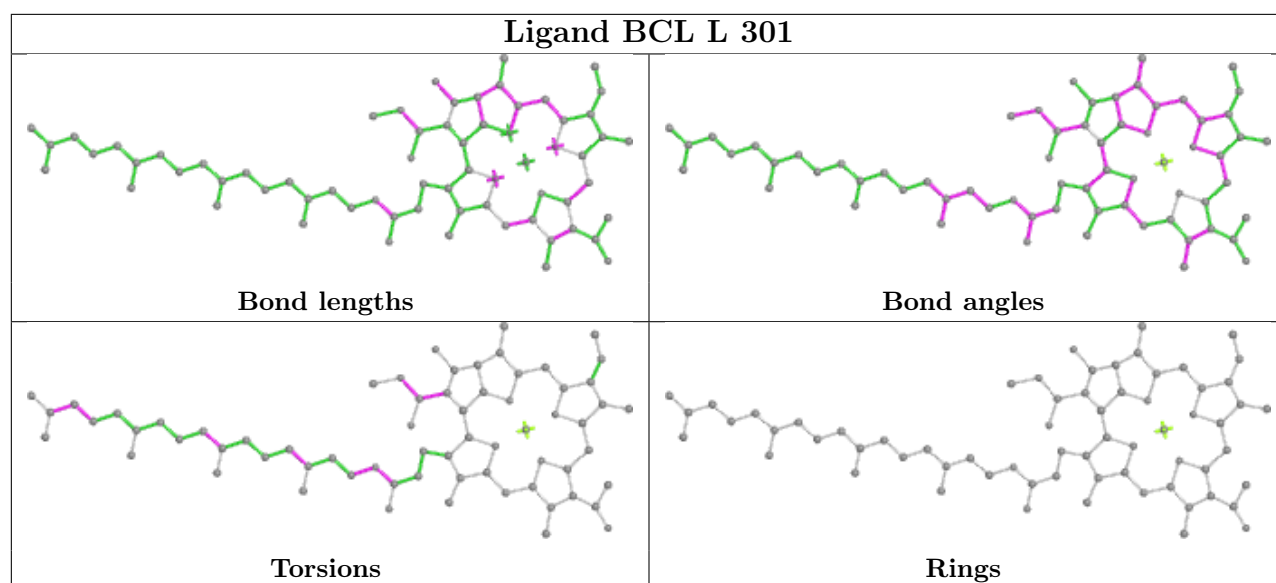




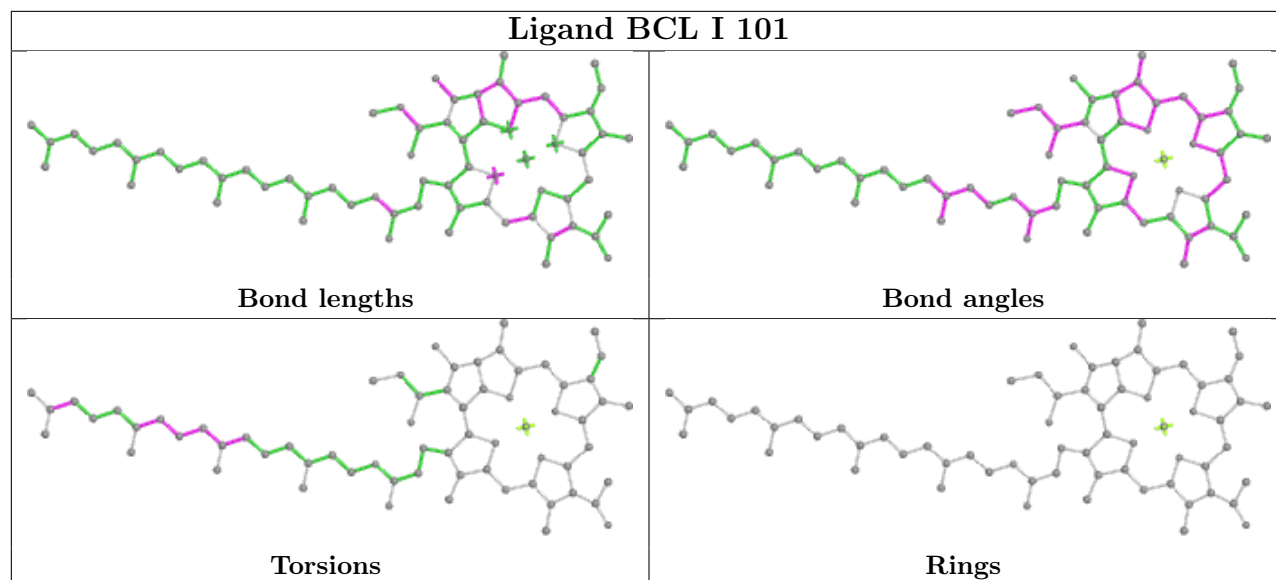




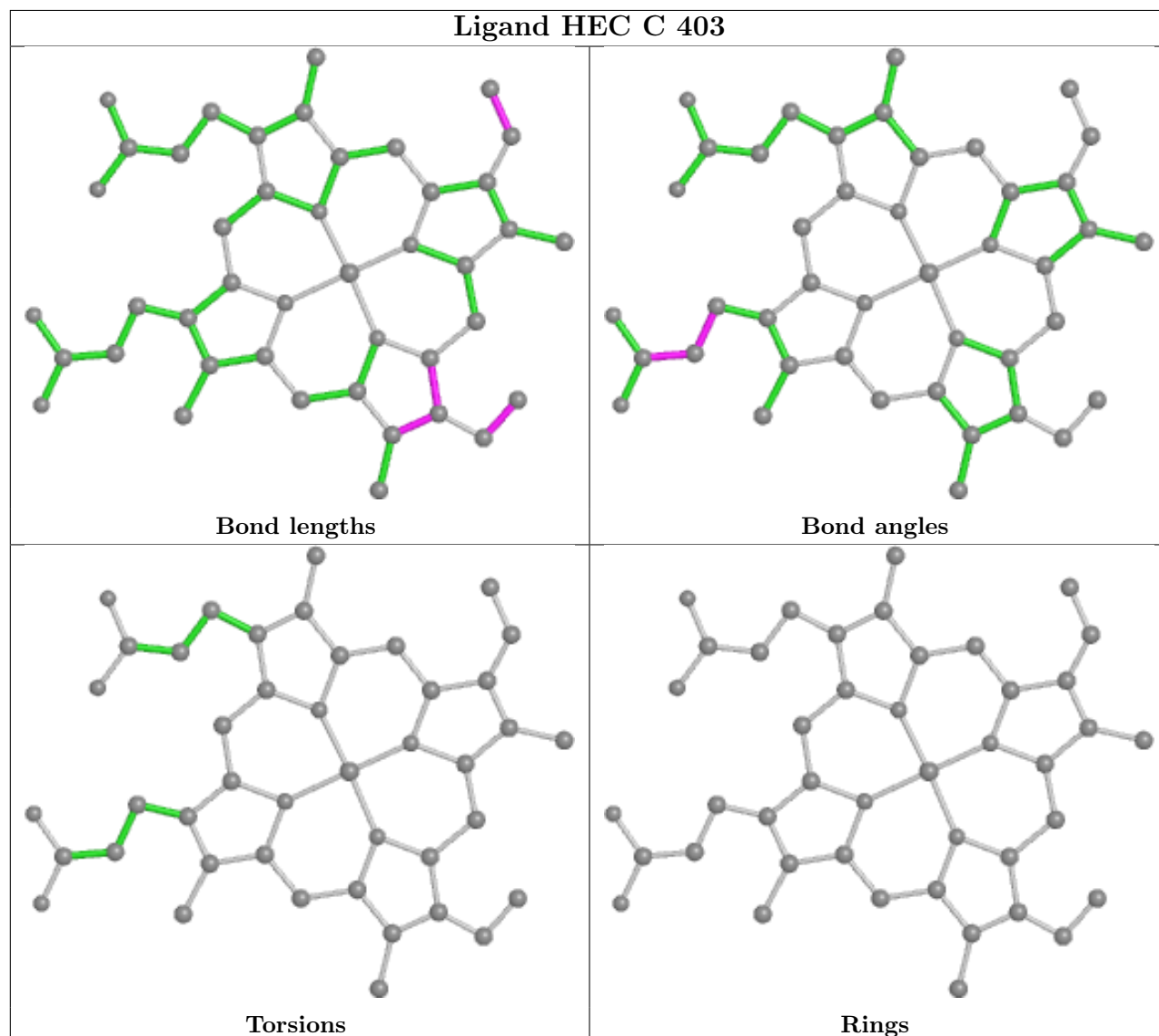


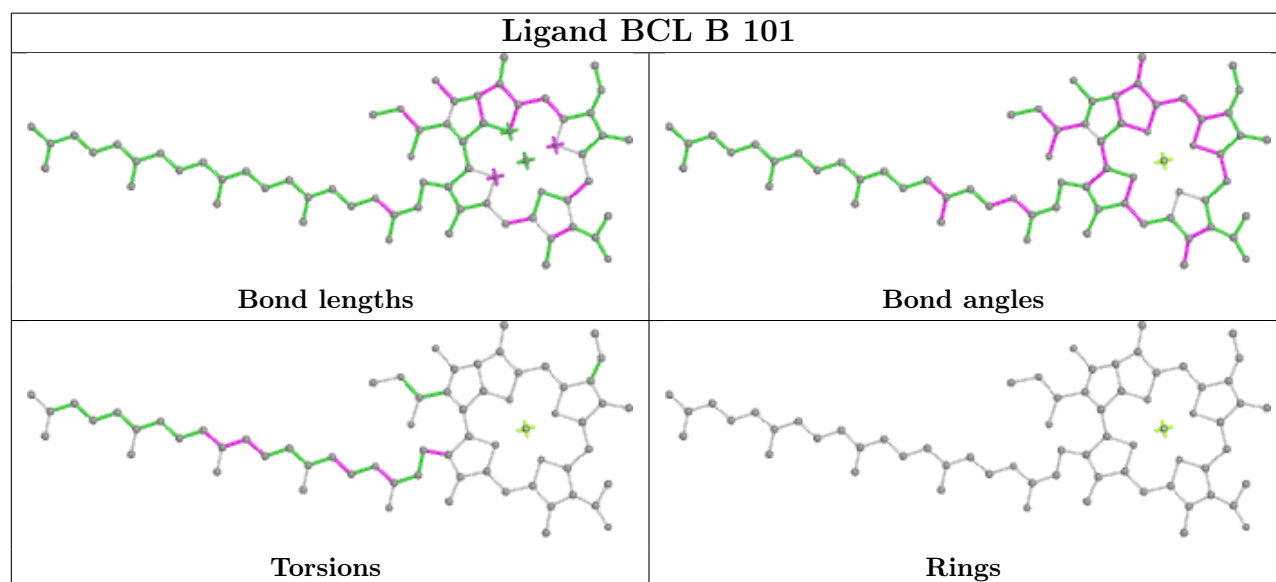
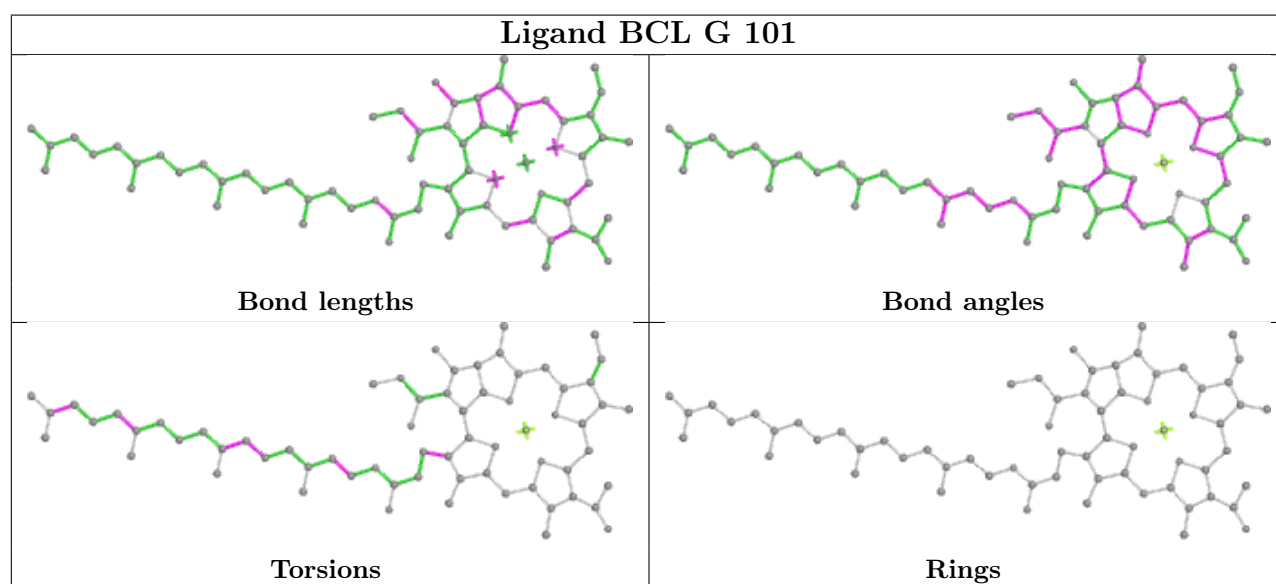
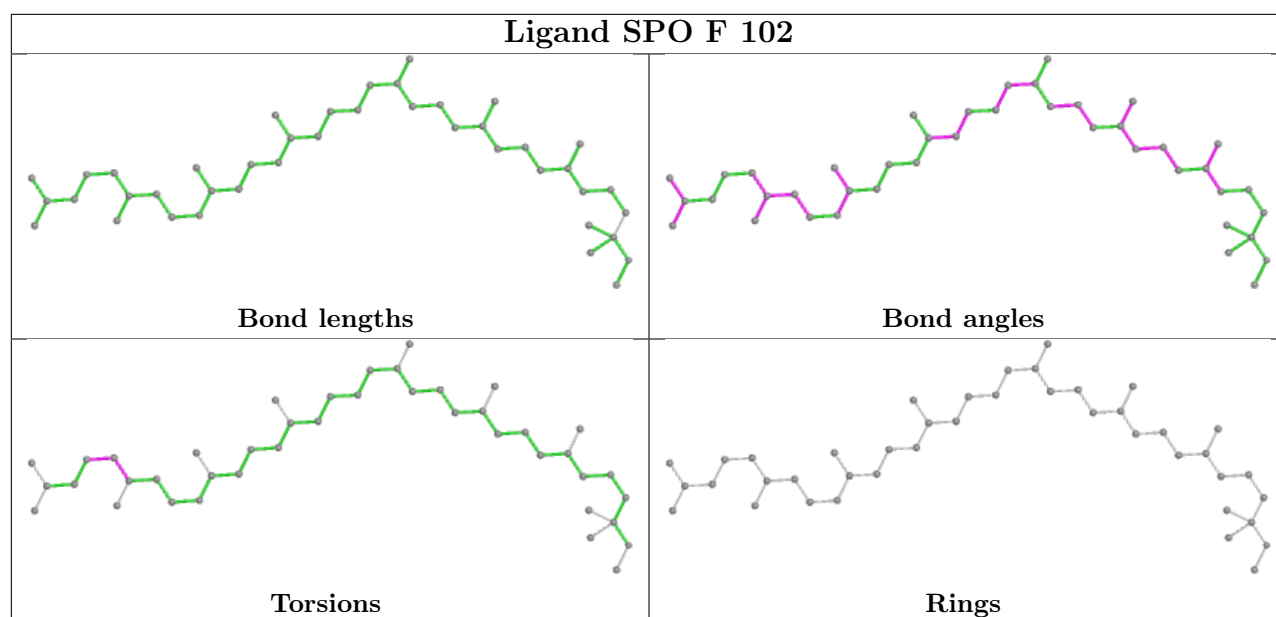


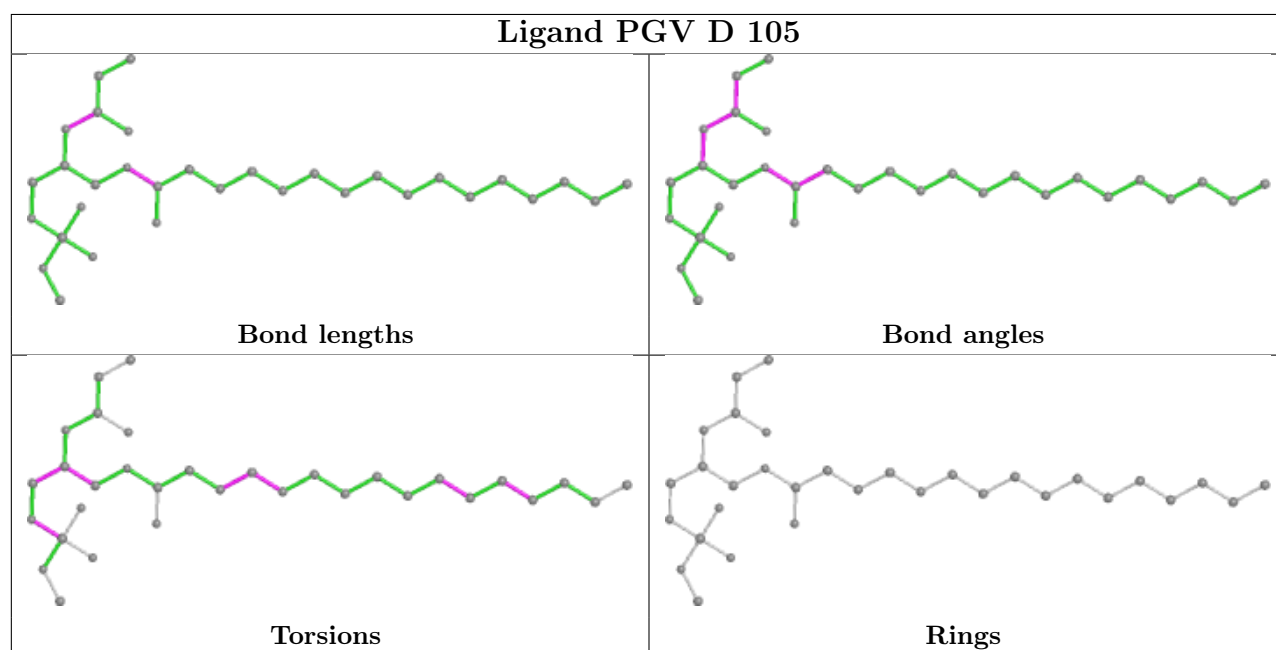
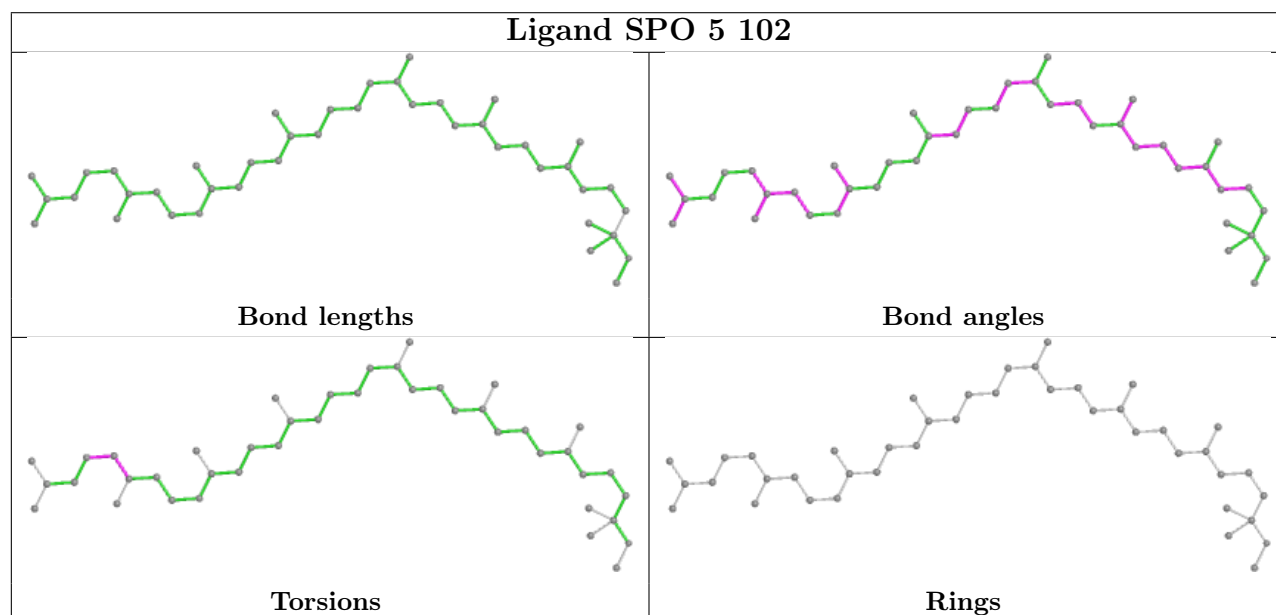
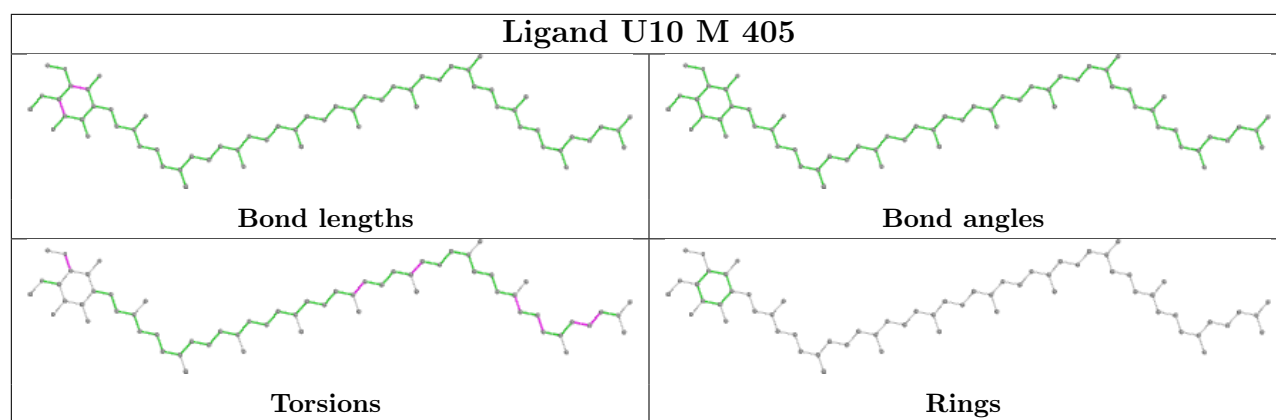
Ligand BCL I 101

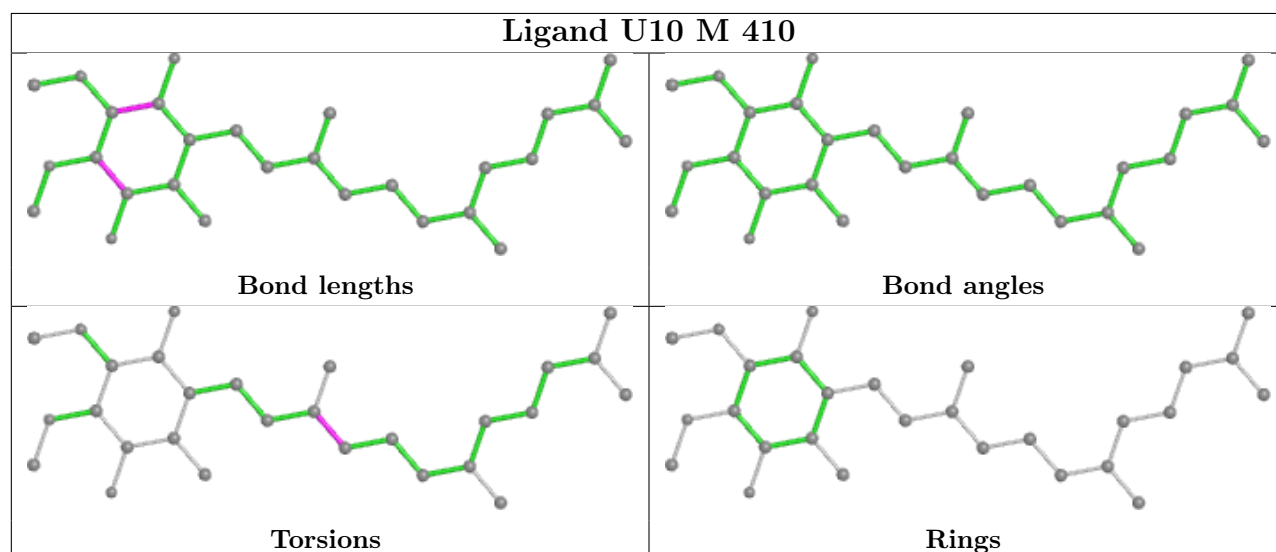
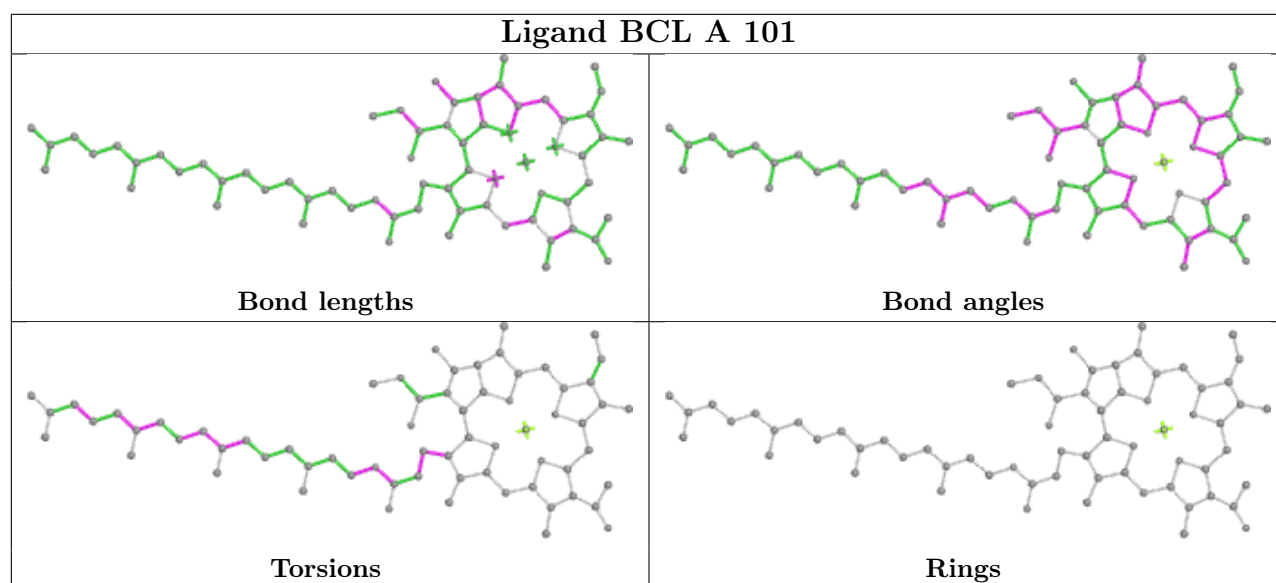


Ligand HEC C 403

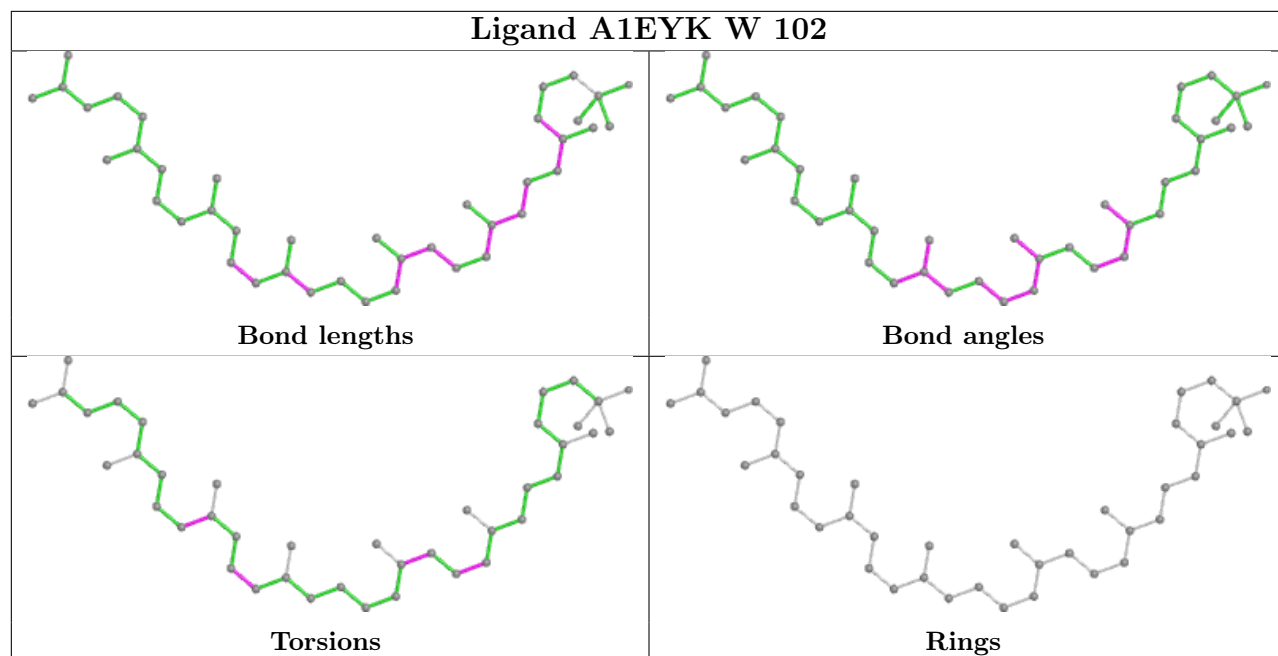




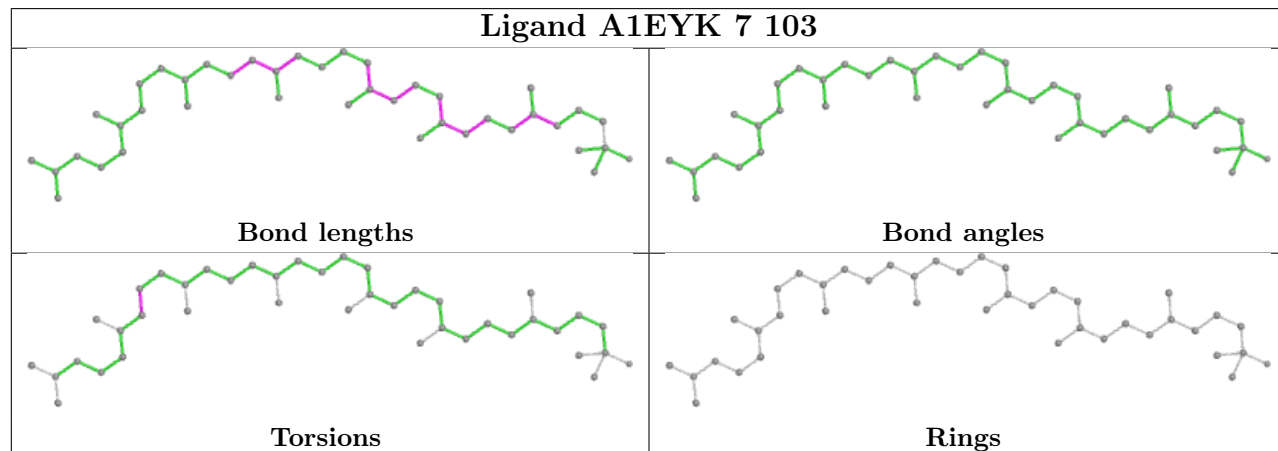




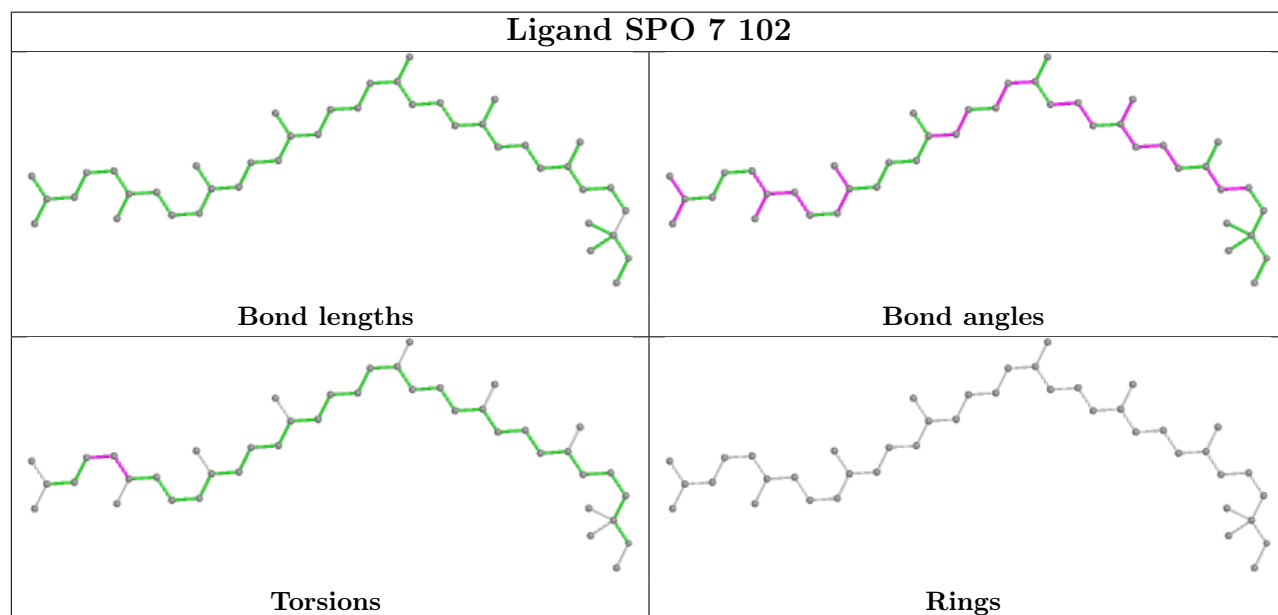
Ligand A1EYK W 102



Ligand A1EYK 7 103



Ligand SPO 7 102



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.