



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 05:25 AM JST

PDB ID : 7VA9 / pdb_00007va9
EMDB ID : EMD-31835
Title : Rba sphaeroides PufY-KO RC-LH1 dimer type-1
Authors : Bracun, L.; Yamagata, A.; Liu, L.N.; Shirouzu, M.
Deposited on : 2021-08-27
Resolution : 3.08 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

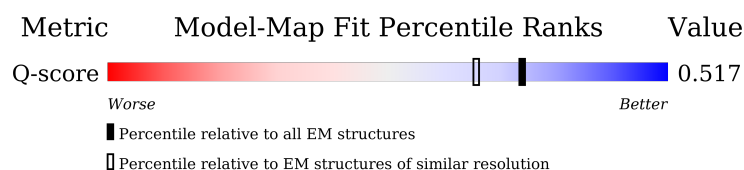
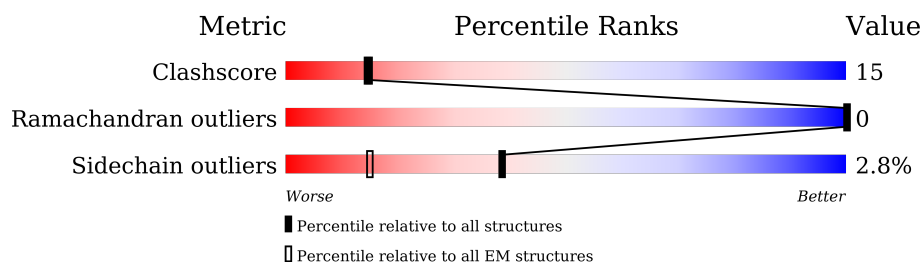
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.08 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14000 (2.58 - 3.58)

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

Mol	Chain	Length	Quality of chain
1	L	282	
1	l	282	
2	M	308	
2	m	308	

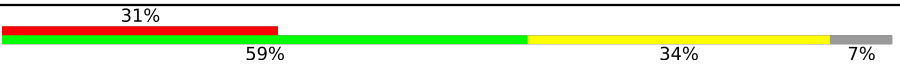
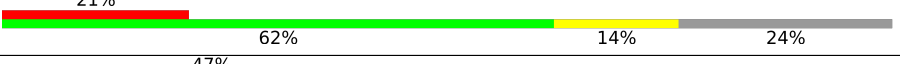
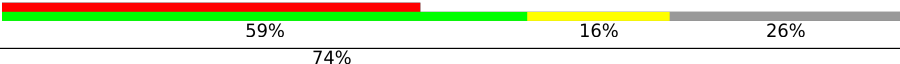
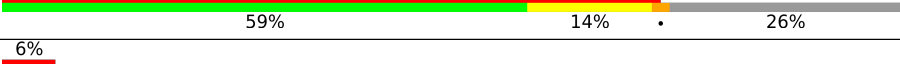
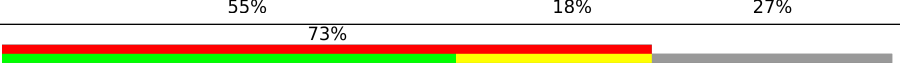
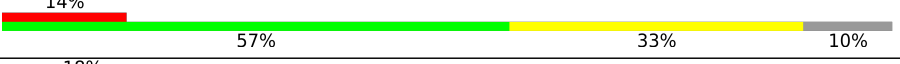
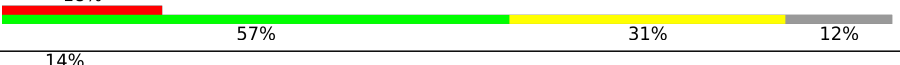
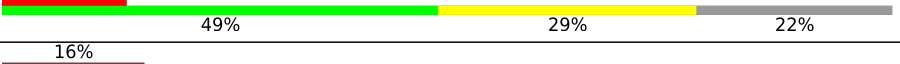
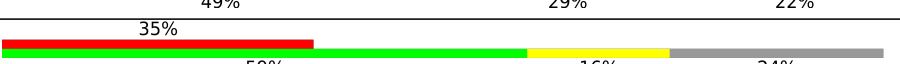
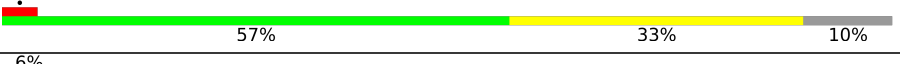
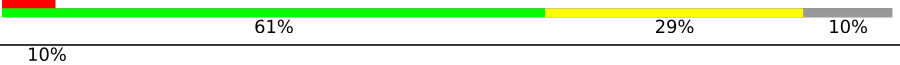
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Mol	Chain	Length	Quality of chain
3	H	260	
3	h	260	
4	1	58	
4	3	58	
4	5	58	
4	6	58	
4	7	58	
4	9	58	
4	A	58	
4	D	58	
4	F	58	
4	I	58	
4	K	58	
4	O	58	
4	Q	58	
4	S	58	
4	U	58	
4	W	58	
4	Y	58	
4	a	58	
4	d	58	
4	f	58	
4	i	58	
4	k	58	
4	o	58	

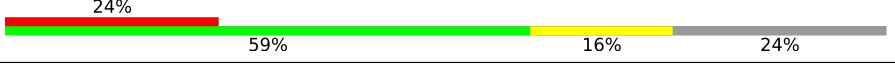
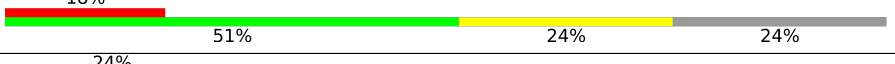
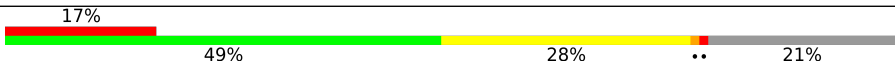
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Mol	Chain	Length	Quality of chain
4	q	58	
4	s	58	
4	u	58	
4	w	58	
4	y	58	
5	0	49	
5	2	49	
5	4	49	
5	8	49	
5	B	49	
5	E	49	
5	G	49	
5	J	49	
5	N	49	
5	P	49	
5	R	49	
5	T	49	
5	V	49	
5	X	49	
5	Z	49	
5	aa	49	
5	ab	49	
5	b	49	
5	e	49	
5	g	49	

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Mol	Chain	Length	Quality of chain
5	j	49	
5	n	49	
5	p	49	
5	r	49	
5	t	49	
5	v	49	
5	x	49	
5	z	49	
6	C	82	
6	c	82	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	SPO	0	102	-	X	-	-
12	SPO	3	101	-	X	-	-
12	SPO	3	103	-	X	-	-
12	SPO	8	101	-	X	-	-
12	SPO	9	102	-	X	-	-
12	SPO	A	102	-	X	-	-
12	SPO	B	102	-	X	-	-
12	SPO	B	103	-	X	-	-
12	SPO	D	102	-	X	-	-
12	SPO	F	102	-	X	-	-
12	SPO	G	102	-	X	-	-
12	SPO	G	103	-	X	-	-
12	SPO	I	102	-	X	-	-
12	SPO	K	102	-	X	-	-
12	SPO	M	1305	-	X	-	-
12	SPO	N	101	-	X	-	-
12	SPO	N	103	-	X	-	-
12	SPO	O	102	-	X	-	-
12	SPO	O	103	-	X	-	-
12	SPO	Q	102	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	SPO	R	102	-	X	-	-
12	SPO	S	102	-	X	-	-
12	SPO	T	102	-	X	-	-
12	SPO	U	102	-	X	-	-
12	SPO	a	104	-	X	-	-
12	SPO	aa	101	-	X	-	-
12	SPO	ab	102	-	X	-	-
12	SPO	d	103	-	X	-	-
12	SPO	e	101	-	X	-	-
12	SPO	e	103	-	X	-	-
12	SPO	g	102	-	X	-	-
12	SPO	i	102	-	X	-	-
12	SPO	j	101	-	X	-	-
12	SPO	j	103	-	X	-	-
12	SPO	k	102	-	X	-	-
12	SPO	m	1305	-	X	-	-
12	SPO	n	101	-	X	-	-
12	SPO	o	102	-	X	-	-
12	SPO	q	102	-	X	-	-
12	SPO	r	102	-	X	-	-
12	SPO	s	102	-	X	-	-
12	SPO	s	104	-	X	-	-
12	SPO	s	105	-	X	-	-
12	SPO	t	101	-	X	-	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 42176 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 Reaction center protein L chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L	281	Total	C	N	O	S	0	0
			2232	1507	355	362	8		
1	l	281	Total	C	N	O	S	0	0
			2232	1507	355	362	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	305	Total	C	N	O	S	0	0
			2431	1623	397	400	11		
2	m	305	Total	C	N	O	S	0	0
			2431	1623	397	400	11		

- Molecule 3 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	260	Total	C	N	O	S	0	0
			1972	1264	335	362	11		
3	h	260	Total	C	N	O	S	0	0
			1972	1264	335	362	11		

- Molecule 4 is a protein called Light-harvesting protein B-875 alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	D	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	F	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	I	54	Total	C	N	O	S	0	0
			455	310	73	69	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	O	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	Q	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	S	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	U	44	Total	C	N	O	S	0	0
			362	244	60	57	1		
4	W	43	Total	C	N	O	S	0	0
			351	235	59	56	1		
4	Y	43	Total	C	N	O	S	0	0
			351	235	59	56	1		
4	1	43	Total	C	N	O	S	0	0
			351	235	59	56	1		
4	7	46	Total	C	N	O	S	0	0
			392	271	60	58	3		
4	9	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	a	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	d	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	f	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	i	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	k	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	o	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	q	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	s	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	u	44	Total	C	N	O	S	0	0
			362	244	60	57	1		
4	w	43	Total	C	N	O	S	0	0
			351	235	59	56	1		
4	y	43	Total	C	N	O	S	0	0
			351	235	59	56	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	43	Total	C	N	O	S	0	0
			351	235	59	56	1		
4	6	46	Total	C	N	O	S	0	0
			392	271	60	58	3		
4	3	54	Total	C	N	O	S	0	0
			455	310	73	69	3		

- Molecule 5 is a protein called Light-harvesting protein B-875 beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	44	Total	C	N	O	S	0	0
			359	240	56	62	1		
5	E	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	G	44	Total	C	N	O	S	0	0
			359	240	56	62	1		
5	J	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	N	38	Total	C	N	O	S	0	0
			316	213	50	52	1		
5	P	38	Total	C	N	O	S	0	0
			316	213	50	52	1		
5	R	38	Total	C	N	O	S	0	0
			316	213	50	52	1		
5	T	38	Total	C	N	O	S	0	0
			316	213	50	52	1		
5	V	37	Total	C	N	O	S	0	0
			308	207	49	51	1		
5	X	37	Total	C	N	O	S	0	0
			308	207	49	51	1		
5	Z	37	Total	C	N	O	S	0	0
			308	207	49	51	1		
5	2	36	Total	C	N	O	S	0	0
			297	198	48	50	1		
5	8	44	Total	C	N	O	S	0	0
			359	240	56	62	1		
5	0	44	Total	C	N	O	S	0	0
			359	240	56	62	1		
5	b	44	Total	C	N	O	S	0	0
			359	240	56	62	1		
5	e	43	Total	C	N	O	S	0	0
			351	236	55	59	1		

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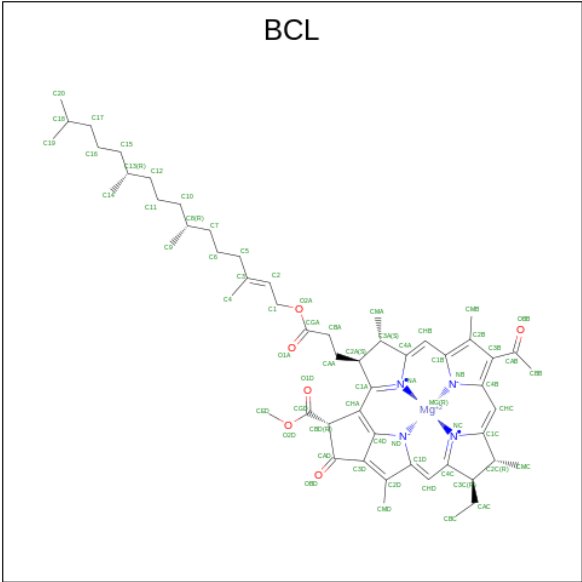
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Mol	Chain	Residues	Atoms					AltConf	Trace
5	g	44	Total	C	N	O	S	0	0
			359	240	56	62	1		
5	j	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	n	37	Total	C	N	O	S	0	0
			308	207	49	51	1		
5	p	37	Total	C	N	O	S	0	0
			308	207	49	51	1		
5	r	37	Total	C	N	O	S	0	0
			308	207	49	51	1		
5	t	37	Total	C	N	O	S	0	0
			308	207	49	51	1		
5	v	37	Total	C	N	O	S	0	0
			308	207	49	51	1		
5	x	37	Total	C	N	O	S	0	0
			308	207	49	51	1		
5	z	37	Total	C	N	O	S	0	0
			308	207	49	51	1		
5	4	36	Total	C	N	O	S	0	0
			297	198	48	50	1		
5	aa	44	Total	C	N	O	S	0	0
			359	240	56	62	1		
5	ab	44	Total	C	N	O	S	0	0
			359	240	56	62	1		

- Molecule 6 is a protein called Intrinsic membrane protein PufX.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	65	Total	C	N	O	S	0	0
			507	332	89	83	3		
6	c	65	Total	C	N	O	S	0	0
			507	332	89	83	3		

- Molecule 7 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
7	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	M	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	M	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	B	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	D	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	E	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	F	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	I	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	J	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	K	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	N	1	Total 66	C 55	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
7	O	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	P	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	R	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	S	1	Total 56	C 45	Mg 1	N 4	O 6	0
7	T	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	U	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	U	1	Total 46	C 35	Mg 1	N 4	O 6	0
7	W	1	Total 46	C 35	Mg 1	N 4	O 6	0
7	X	1	Total 46	C 35	Mg 1	N 4	O 6	0
7	Y	1	Total 46	C 35	Mg 1	N 4	O 6	0
7	Z	1	Total 46	C 35	Mg 1	N 4	O 6	0
7	1	1	Total 46	C 35	Mg 1	N 4	O 6	0
7	2	1	Total 46	C 35	Mg 1	N 4	O 6	0
7	7	1	Total 61	C 50	Mg 1	N 4	O 6	0
7	8	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	9	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	0	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	l	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	l	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	m	1	Total 66	C 55	Mg 1	N 4	O 6	0

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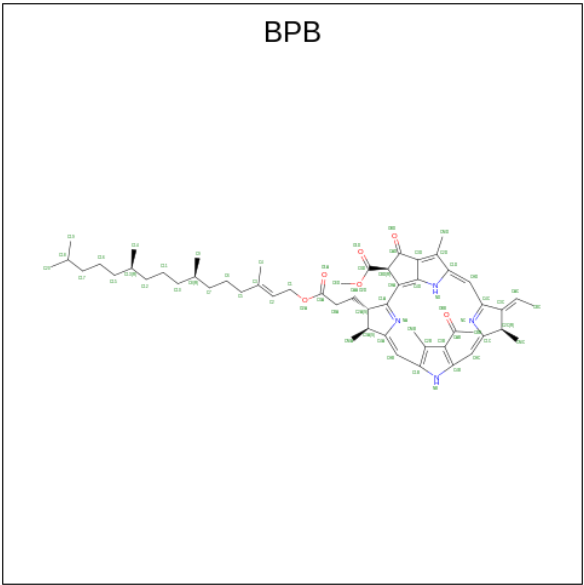
Mol	Chain	Residues	Atoms					AltConf
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7	a	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	b	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	d	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	e	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	f	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	g	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	i	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	j	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	k	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	k	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	o	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	p	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	q	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	r	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	s	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	s	1	Total 46	C 35	Mg 1	N 4	O 6	0
7	u	1	Total 51	C 40	Mg 1	N 4	O 6	0
7	v	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	w	1	Total 46	C 35	Mg 1	N 4	O 6	0
7	x	1	Total 46	C 35	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
7	y	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
7	z	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
7	5	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
7	5	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
7	aa	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	ab	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	c	1	Total	C	Mg	N	O	0
			61	50	1	4	6	

- Molecule 8 is BACTERIOPHEOPHYTIN B (CCD ID: BPB) (formula: C₅₅H₇₄N₄O₆) (labeled as "Ligand of Interest" by depositor).



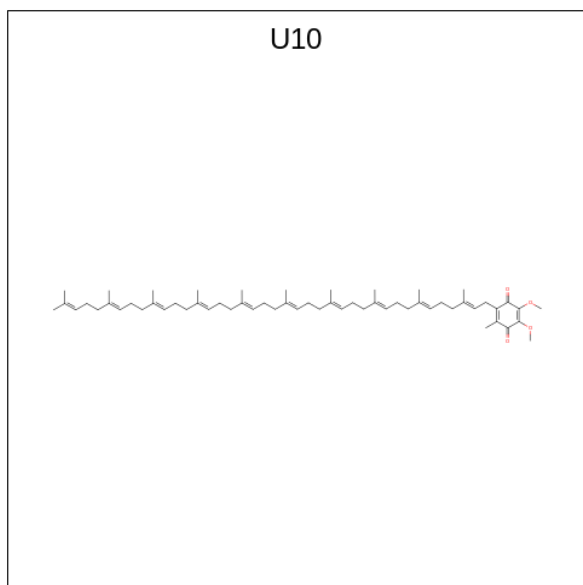
Mol	Chain	Residues	Atoms				AltConf
8	L	1	Total	C	N	O	0
			62	52	4	6	
8	L	1	Total	C	N	O	0
			55	45	4	6	
8	l	1	Total	C	N	O	0
			62	52	4	6	

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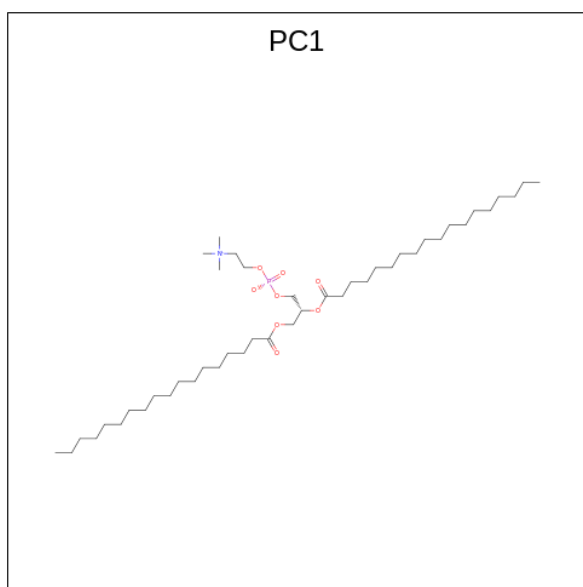
Mol	Chain	Residues	Atoms				AltConf
8	1	1	Total	C	N	O	0
			55	45	4	6	

- Molecule 9 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
9	L	1	Total	C	O	0
			43	39	4	
9	M	1	Total	C	O	0
			48	44	4	
9	l	1	Total	C	O	0
			63	59	4	
9	m	1	Total	C	O	0
			48	44	4	

- Molecule 10 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).

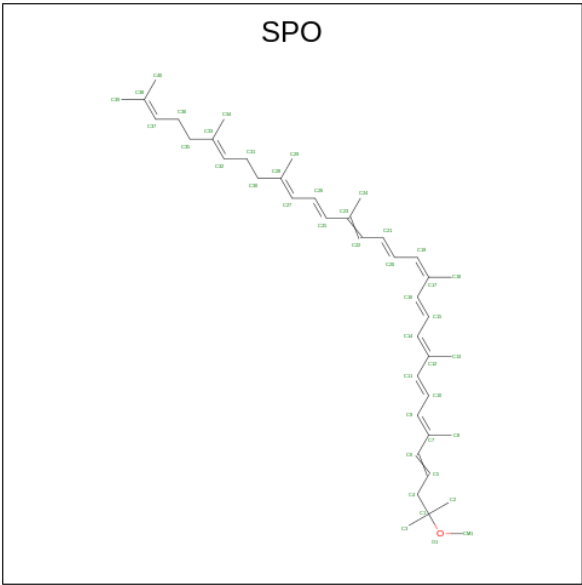


Mol	Chain	Residues	Atoms					AltConf
10	L	1	Total	C	N	O	P	0
			43	33	1	8	1	
10	M	1	Total	C	N	O	P	0
			53	43	1	8	1	
10	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
10	A	1	Total	C	N	O	P	0
			46	36	1	8	1	
10	C	1	Total	C	N	O	P	0
			54	44	1	8	1	
10	l	1	Total	C	N	O	P	0
			48	38	1	8	1	
10	h	1	Total	C	N	O	P	0
			48	38	1	8	1	
10	h	1	Total	C	N	O	P	0
			29	19	1	8	1	
10	a	1	Total	C	N	O	P	0
			40	30	1	8	1	
10	a	1	Total	C	N	O	P	0
			49	39	1	8	1	
10	d	1	Total	C	N	O	P	0
			41	31	1	8	1	

- Molecule 11 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 12 is SPHEROIDENE (CCD ID: SPO) (formula: C₄₁H₆₀O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
12	M	1	Total	C	O	0
			42	41	1	
12	A	1	Total	C	O	0
			42	41	1	
12	B	1	Total	C	O	0
			42	41	1	
12	B	1	Total	C	O	0
			42	41	1	
12	D	1	Total	C	O	0
			42	41	1	
12	F	1	Total	C	O	0
			42	41	1	
12	G	1	Total	C	O	0
			42	41	1	
12	G	1	Total	C	O	0
			42	41	1	
12	I	1	Total	C	O	0
			42	41	1	

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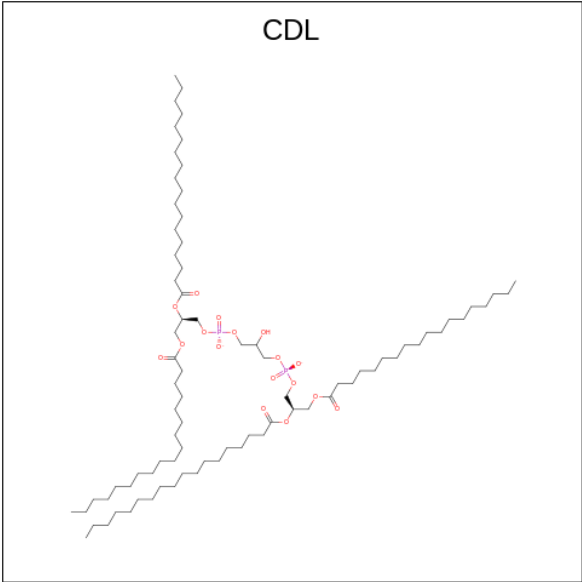
Mol	Chain	Residues	Atoms			AltConf
12	K	1	Total	C	O	0
			42	41	1	
12	N	1	Total	C	O	0
			42	41	1	
12	N	1	Total	C	O	0
			42	41	1	
12	O	1	Total	C	O	0
			42	41	1	
12	O	1	Total	C	O	0
			42	41	1	
12	Q	1	Total	C	O	0
			38	37	1	
12	R	1	Total	C	O	0
			42	41	1	
12	S	1	Total	C	O	0
			38	37	1	
12	T	1	Total	C	O	0
			42	41	1	
12	U	1	Total	C	O	0
			42	41	1	
12	8	1	Total	C	O	0
			42	41	1	
12	9	1	Total	C	O	0
			42	41	1	
12	0	1	Total	C	O	0
			42	41	1	
12	m	1	Total	C	O	0
			42	41	1	
12	a	1	Total	C	O	0
			42	41	1	
12	d	1	Total	C	O	0
			42	41	1	
12	e	1	Total	C	O	0
			42	41	1	
12	e	1	Total	C	O	0
			37	36	1	
12	g	1	Total	C	O	0
			42	41	1	
12	i	1	Total	C	O	0
			42	41	1	
12	j	1	Total	C	O	0
			42	41	1	

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Mol	Chain	Residues	Atoms			AltConf
12	j	1	Total	C	O	0
			42	41	1	
12	k	1	Total	C	O	0
			32	31	1	
12	n	1	Total	C	O	0
			42	41	1	
12	o	1	Total	C	O	0
			42	41	1	
12	q	1	Total	C	O	0
			42	41	1	
12	r	1	Total	C	O	0
			42	41	1	
12	s	1	Total	C	O	0
			42	41	1	
12	s	1	Total	C	O	0
			42	41	1	
12	s	1	Total	C	O	0
			42	41	1	
12	t	1	Total	C	O	0
			42	41	1	
12	aa	1	Total	C	O	0
			42	41	1	
12	3	1	Total	C	O	0
			42	41	1	
12	3	1	Total	C	O	0
			42	41	1	
12	ab	1	Total	C	O	0
			42	41	1	

- Molecule 13 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).

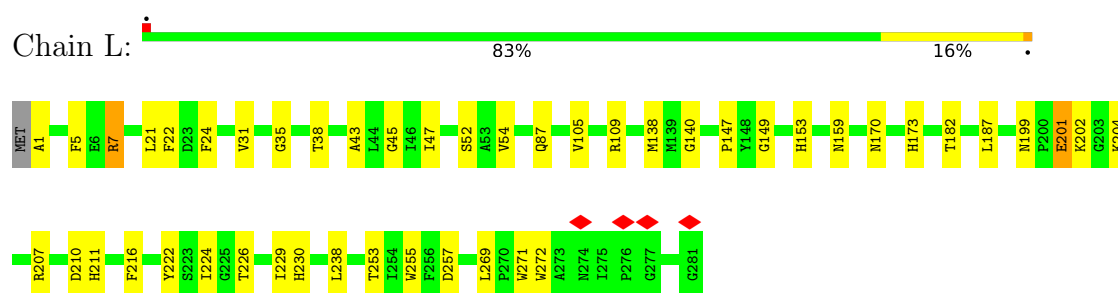


Mol	Chain	Residues	Atoms				AltConf
13	M	1	Total	C	O	P	0
			100	81	17	2	
13	m	1	Total	C	O	P	0
			100	81	17	2	

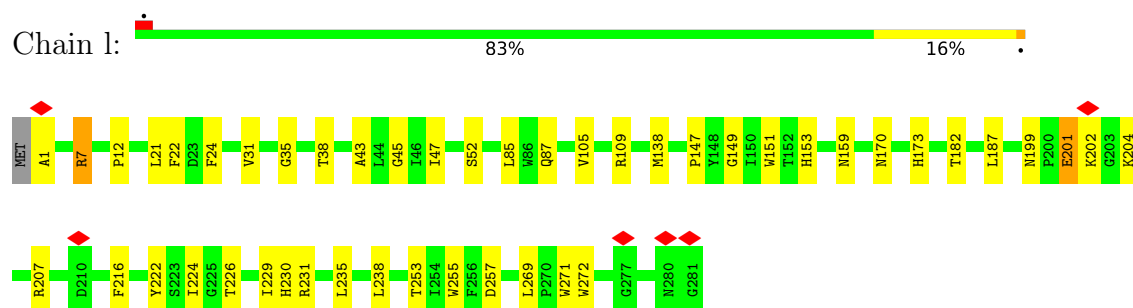
3 Residue-property plots [i](#)

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

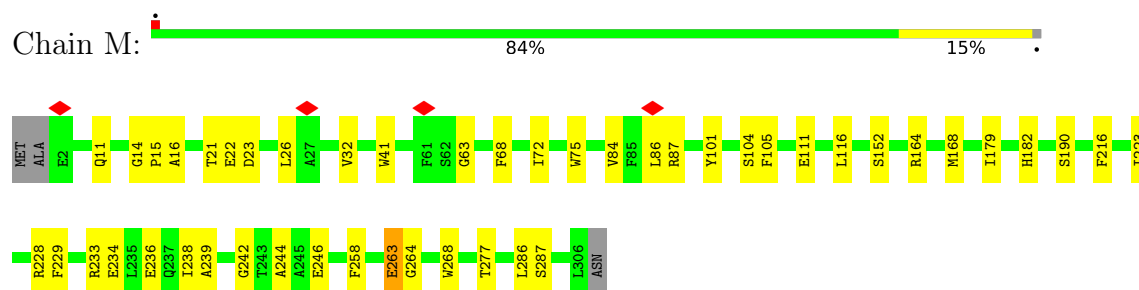
• Molecule 1: Reaction center protein L chain



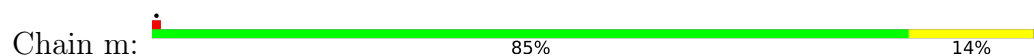
• Molecule 1: Reaction center protein L chain

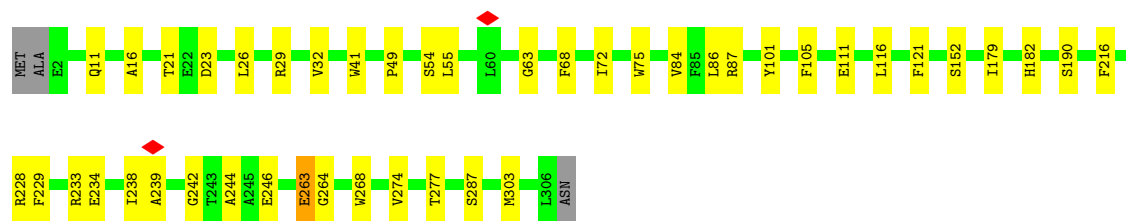


• Molecule 2: Reaction center protein M chain

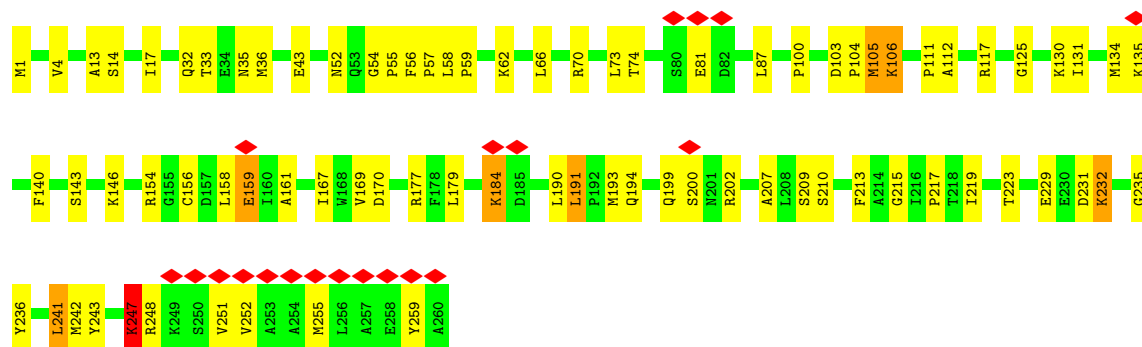


• Molecule 2: Reaction center protein M chain

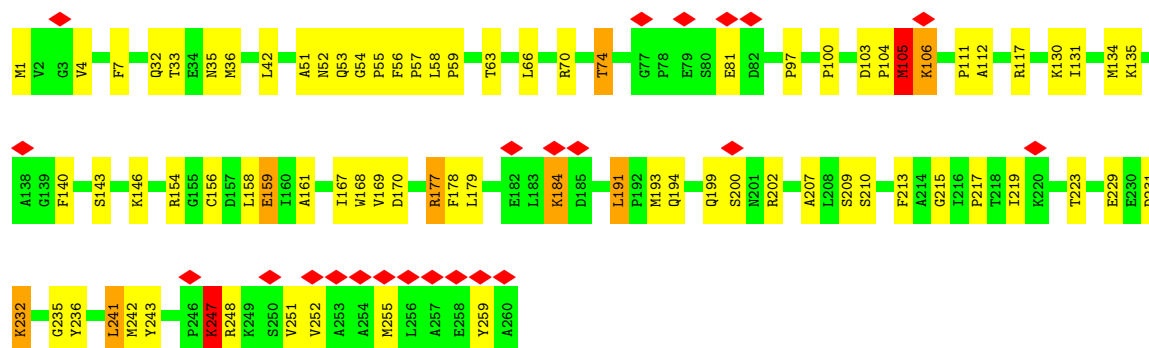




• Molecule 3: Reaction center protein H chain



• Molecule 3: Reaction center protein H chain



• Molecule 4: Light-harvesting protein B-875 alpha chain

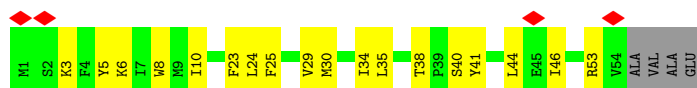


• Molecule 4: Light-harvesting protein B-875 alpha chain





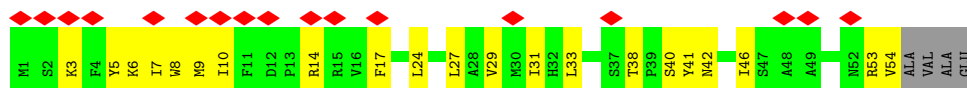
- Molecule 4: Light-harvesting protein B-875 alpha chain



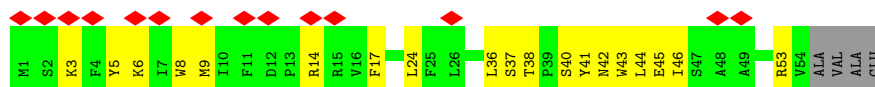
- Molecule 4: Light-harvesting protein B-875 alpha chain



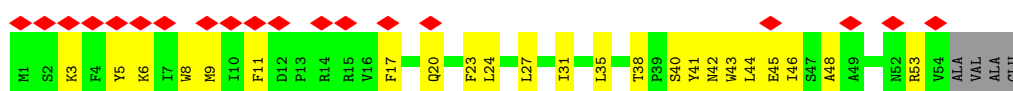
- Molecule 4: Light-harvesting protein B-875 alpha chain



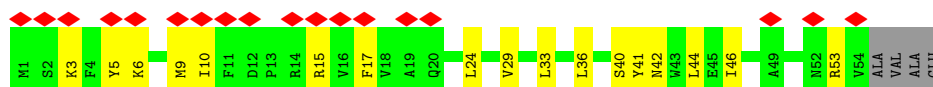
- Molecule 4: Light-harvesting protein B-875 alpha chain



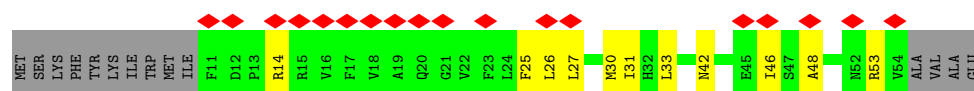
- Molecule 4: Light-harvesting protein B-875 alpha chain



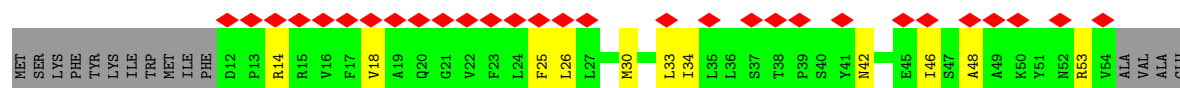
- Molecule 4: Light-harvesting protein B-875 alpha chain



- Molecule 4: Light-harvesting protein B-875 alpha chain



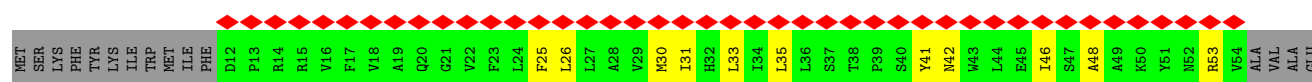
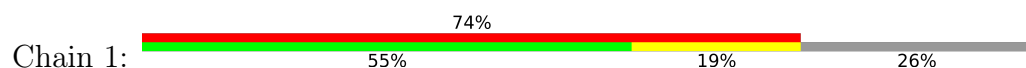
- Molecule 4: Light-harvesting protein B-875 alpha chain



- Molecule 4: Light-harvesting protein B-875 alpha chain



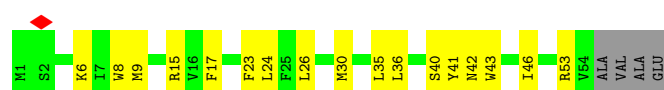
- Molecule 4: Light-harvesting protein B-875 alpha chain



- Molecule 4: Light-harvesting protein B-875 alpha chain



- Molecule 4: Light-harvesting protein B-875 alpha chain



- Molecule 4: Light-harvesting protein B-875 alpha chain



- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain d: 



- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain f: 



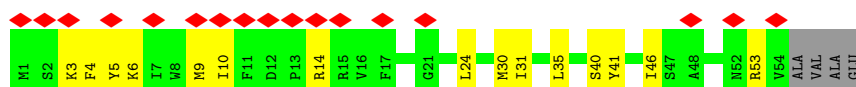
- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain i: 



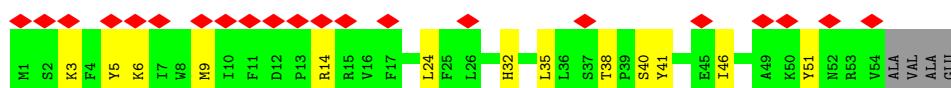
- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain k: 



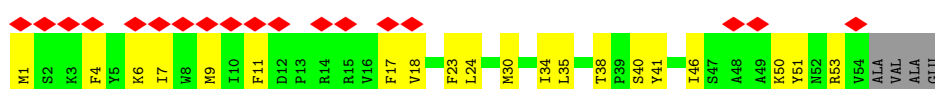
- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain o: 



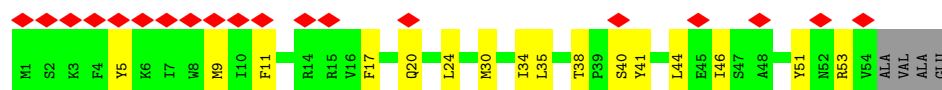
- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain q: 

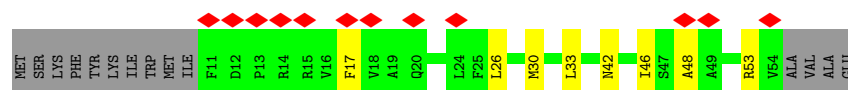


- Molecule 4: Light-harvesting protein B-875 alpha chain

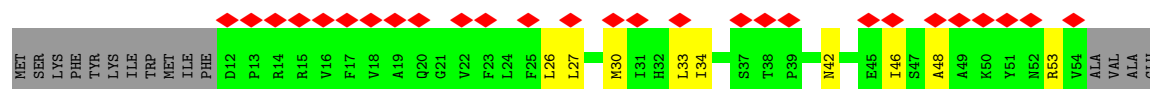
Chain s: 



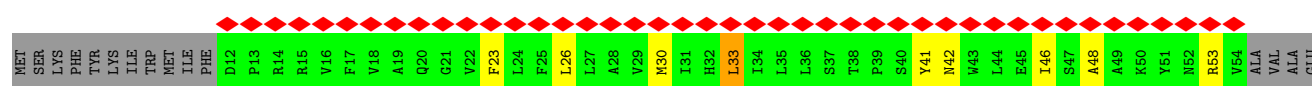
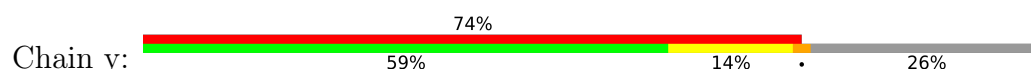
- Molecule 4: Light-harvesting protein B-875 alpha chain



- Molecule 4: Light-harvesting protein B-875 alpha chain



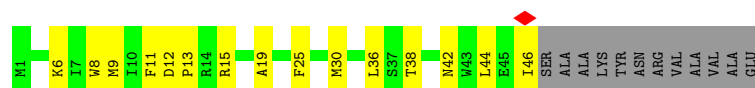
- Molecule 4: Light-harvesting protein B-875 alpha chain



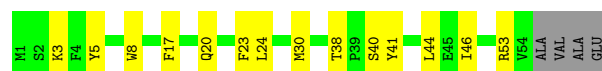
- Molecule 4: Light-harvesting protein B-875 alpha chain



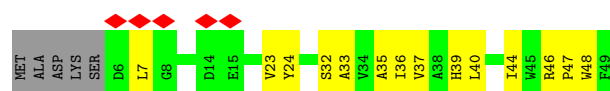
- Molecule 4: Light-harvesting protein B-875 alpha chain



- Molecule 4: Light-harvesting protein B-875 alpha chain



- Molecule 5: Light-harvesting protein B-875 beta chain



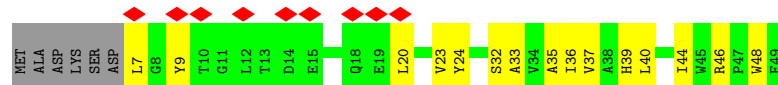
- Molecule 5: Light-harvesting protein B-875 beta chain



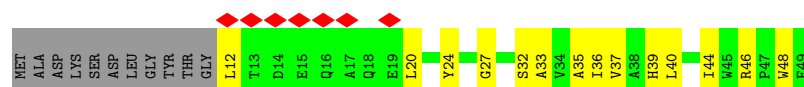
- Molecule 5: Light-harvesting protein B-875 beta chain



- Molecule 5: Light-harvesting protein B-875 beta chain



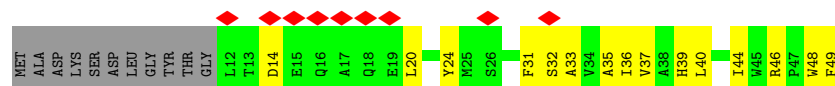
- Molecule 5: Light-harvesting protein B-875 beta chain



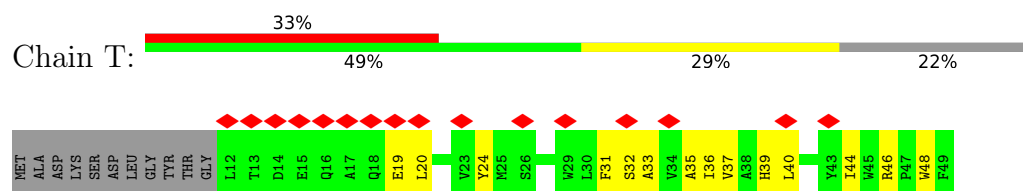
- Molecule 5: Light-harvesting protein B-875 beta chain



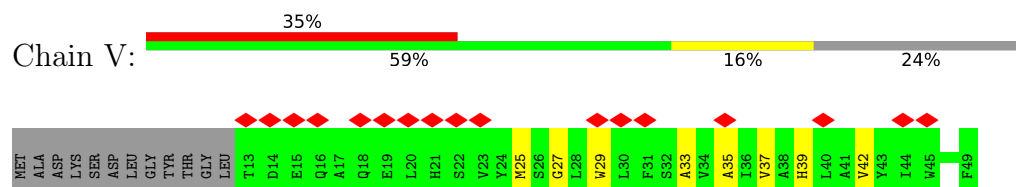
- Molecule 5: Light-harvesting protein B-875 beta chain



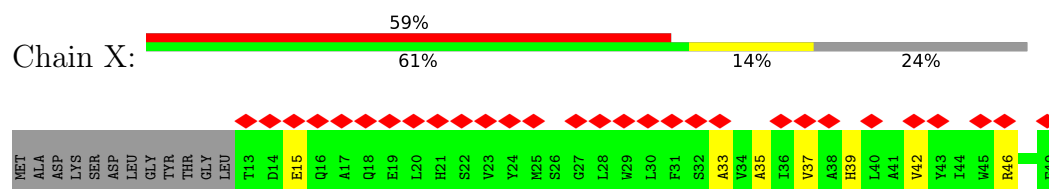
- Molecule 5: Light-harvesting protein B-875 beta chain



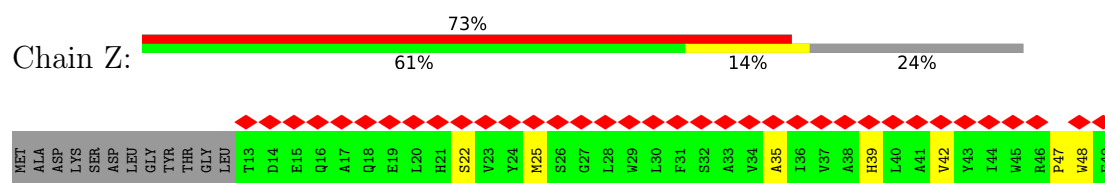
- Molecule 5: Light-harvesting protein B-875 beta chain



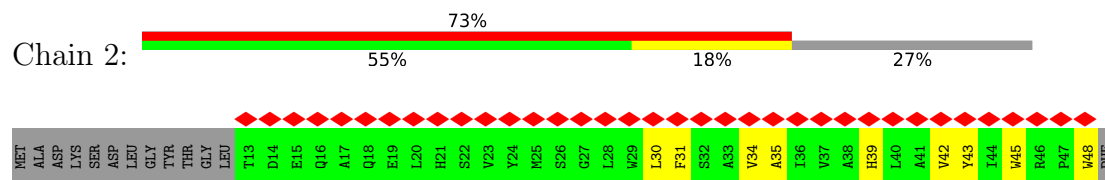
- Molecule 5: Light-harvesting protein B-875 beta chain



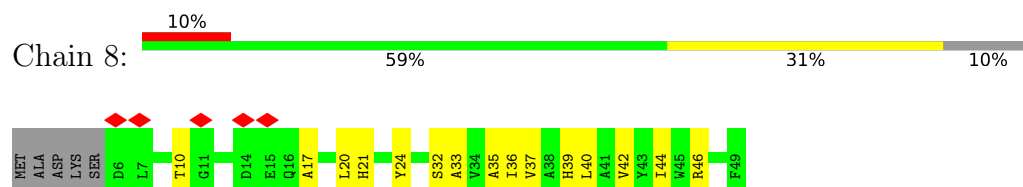
- Molecule 5: Light-harvesting protein B-875 beta chain



- Molecule 5: Light-harvesting protein B-875 beta chain

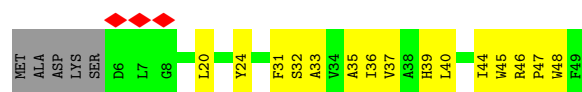


- Molecule 5: Light-harvesting protein B-875 beta chain

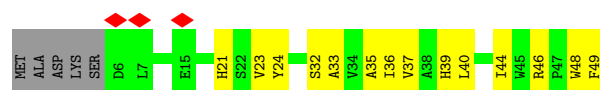


- Molecule 5: Light-harvesting protein B-875 beta chain

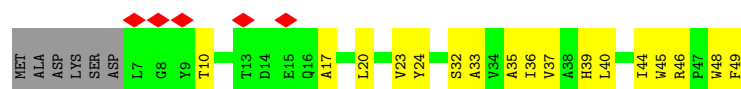




- Molecule 5: Light-harvesting protein B-875 beta chain



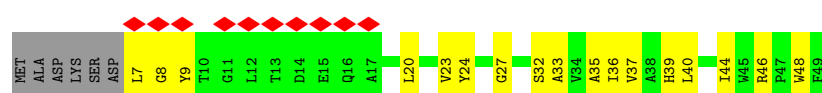
- Molecule 5: Light-harvesting protein B-875 beta chain



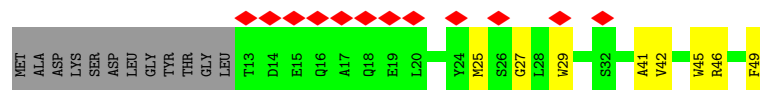
- Molecule 5: Light-harvesting protein B-875 beta chain



- Molecule 5: Light-harvesting protein B-875 beta chain



- Molecule 5: Light-harvesting protein B-875 beta chain



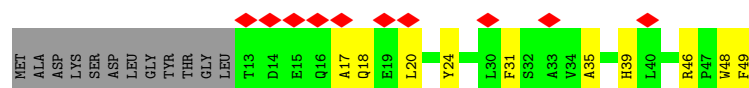
- Molecule 5: Light-harvesting protein B-875 beta chain



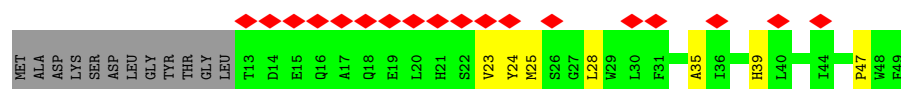
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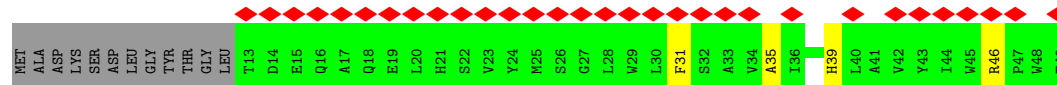
- Molecule 5: Light-harvesting protein B-875 beta chain



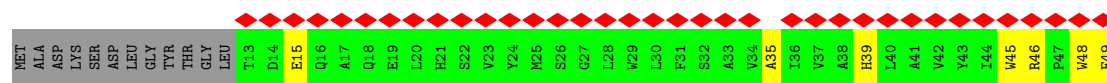
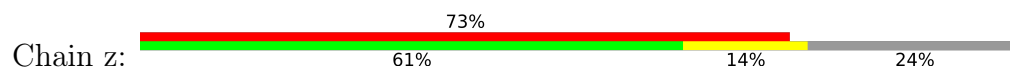
- Molecule 5: Light-harvesting protein B-875 beta chain



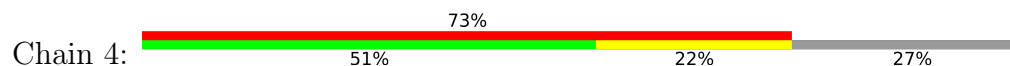
- Molecule 5: Light-harvesting protein B-875 beta chain



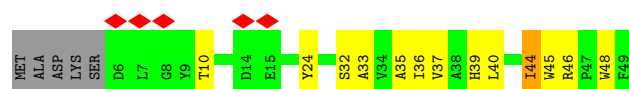
- Molecule 5: Light-harvesting protein B-875 beta chain



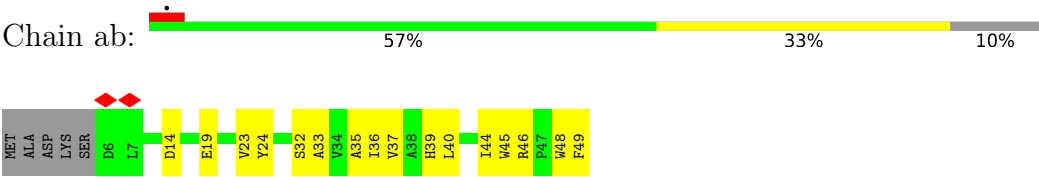
- Molecule 5: Light-harvesting protein B-875 beta chain



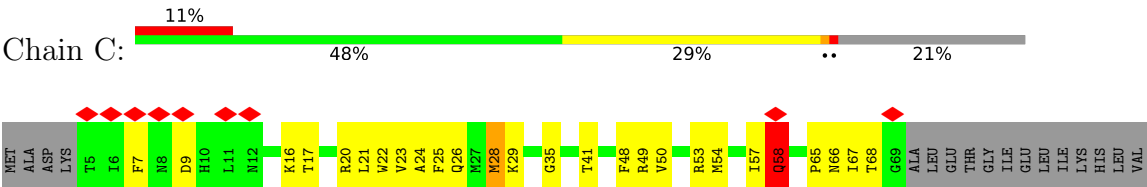
- Molecule 5: Light-harvesting protein B-875 beta chain



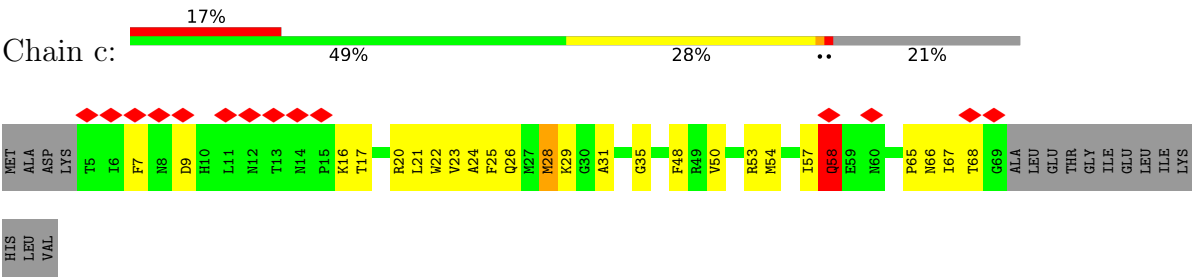
• Molecule 5: Light-harvesting protein B-875 beta chain



• Molecule 6: Intrinsic membrane protein PufX



• Molecule 6: Intrinsic membrane protein PufX



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	71027	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.868	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.217	Depositor
Minimum map value	-0.117	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0245	Depositor
Map size (Å)	289.97498, 289.97498, 289.97498	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8284999, 0.8284999, 0.8284999	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: CDL, BCL, SPO, FE2, PC1, U10, BPB

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	L	0.31	0/2320	0.46	0/3175
1	l	0.31	0/2320	0.46	0/3175
2	M	0.30	0/2524	0.48	0/3446
2	m	0.30	0/2524	0.47	0/3446
3	H	0.34	0/2023	0.67	2/2752 (0.1%)
3	h	0.34	0/2023	0.67	2/2752 (0.1%)
4	1	0.22	0/360	0.40	0/490
4	3	0.28	0/469	0.47	0/635
4	5	0.22	0/360	0.40	0/490
4	6	0.30	0/405	0.45	0/549
4	7	0.40	0/405	0.58	0/549
4	9	0.29	0/469	0.48	0/635
4	A	0.25	0/469	0.42	0/635
4	D	0.26	0/469	0.46	0/635
4	F	0.27	0/469	0.46	0/635
4	I	0.27	0/469	0.48	0/635
4	K	0.28	0/469	0.49	0/635
4	O	0.28	0/469	0.48	0/635
4	Q	0.24	0/469	0.47	0/635
4	S	0.26	0/469	0.47	0/635
4	U	0.22	0/372	0.40	0/506
4	W	0.22	0/360	0.40	0/490
4	Y	0.23	0/360	0.40	0/490
4	a	0.30	0/469	0.50	0/635
4	d	0.28	0/469	0.47	0/635
4	f	0.26	0/469	0.47	0/635
4	i	0.25	0/469	0.50	0/635
4	k	0.26	0/469	0.52	0/635
4	o	0.25	0/469	0.52	0/635
4	q	0.26	0/469	0.48	0/635
4	s	0.27	0/469	0.49	0/635
4	u	0.22	0/372	0.40	0/506

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	w	0.22	0/360	0.40	0/490
4	y	0.22	0/360	0.40	0/490
5	0	0.29	0/372	0.52	0/510
5	2	0.17	0/308	0.37	0/423
5	4	0.17	0/308	0.39	0/423
5	8	0.29	0/372	0.52	0/510
5	B	0.28	0/372	0.49	0/510
5	E	0.28	0/364	0.50	0/499
5	G	0.27	0/372	0.49	0/510
5	J	0.28	0/364	0.55	0/499
5	N	0.28	0/328	0.51	0/450
5	P	0.28	0/328	0.51	0/450
5	R	0.28	0/328	0.51	0/450
5	T	0.28	0/328	0.51	0/450
5	V	0.16	0/320	0.28	0/439
5	X	0.15	0/320	0.28	0/439
5	Z	0.18	0/320	0.49	0/439
5	aa	0.28	0/372	0.50	0/510
5	ab	0.28	0/372	0.52	0/510
5	b	0.28	0/372	0.49	0/510
5	e	0.28	0/364	0.50	0/499
5	g	0.28	0/372	0.51	0/510
5	j	0.28	0/364	0.52	0/499
5	n	0.22	0/320	0.35	0/439
5	p	0.24	0/320	0.38	0/439
5	r	0.18	0/320	0.34	0/439
5	t	0.31	0/320	0.45	0/439
5	v	0.15	0/320	0.30	0/439
5	x	0.15	0/320	0.27	0/439
5	z	0.17	0/320	0.35	0/439
6	C	0.31	0/521	0.66	1/707 (0.1%)
6	c	0.31	0/521	0.66	1/707 (0.1%)
All	All	0.28	0/36492	0.50	6/49752 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	1
1	l	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	H	0	3
3	h	0	3
All	All	0	8

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	h	177	ARG	CB-CG-CD	-7.23	94.67	111.30
3	H	177	ARG	CB-CG-CD	-7.18	94.78	111.30
3	H	247	LYS	CD-CE-NZ	5.95	130.95	111.90
3	h	247	LYS	CD-CE-NZ	5.94	130.90	111.90
6	C	58	GLN	CA-CB-CG	5.34	124.78	114.10
6	c	58	GLN	CA-CB-CG	5.33	124.77	114.10

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	105	MET	Peptide
3	H	106	LYS	Peptide
3	H	184	LYS	Peptide
1	L	201	GLU	Peptide
3	h	105	MET	Peptide
3	h	106	LYS	Peptide
3	h	184	LYS	Peptide
1	l	201	GLU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2232	0	2187	50	0
1	l	2232	0	2187	50	0
2	M	2431	0	2345	51	0
2	m	2431	0	2345	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	1972	0	1981	67	0
3	h	1972	0	1981	69	0
4	1	351	0	366	14	0
4	3	455	0	477	19	0
4	5	351	0	366	14	0
4	6	392	0	412	19	0
4	7	392	0	412	29	0
4	9	455	0	477	26	0
4	A	455	0	477	23	0
4	D	455	0	477	26	0
4	F	455	0	477	20	0
4	I	455	0	477	28	0
4	K	455	0	477	31	0
4	O	455	0	477	32	0
4	Q	455	0	477	30	0
4	S	455	0	477	24	0
4	U	362	0	375	9	0
4	W	351	0	366	5	0
4	Y	351	0	366	6	0
4	a	455	0	477	28	0
4	d	455	0	477	30	0
4	f	455	0	477	21	0
4	i	455	0	477	29	0
4	k	455	0	477	24	0
4	o	455	0	477	15	0
4	q	455	0	477	20	0
4	s	455	0	477	19	0
4	u	362	0	375	4	0
4	w	351	0	366	5	0
4	y	351	0	366	10	0
5	0	359	0	340	21	0
5	2	297	0	283	8	0
5	4	297	0	283	9	0
5	8	359	0	340	23	0
5	B	359	0	340	18	0
5	E	351	0	336	16	0
5	G	359	0	340	22	0
5	J	351	0	336	19	0
5	N	316	0	303	25	0
5	P	316	0	303	19	0
5	R	316	0	303	22	0
5	T	316	0	303	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	V	308	0	292	6	0
5	X	308	0	292	6	0
5	Z	308	0	292	6	0
5	aa	359	0	340	19	0
5	ab	359	0	340	21	0
5	b	359	0	340	22	0
5	e	351	0	336	26	0
5	g	359	0	340	25	0
5	j	351	0	336	26	0
5	n	308	0	292	10	0
5	p	308	0	292	11	0
5	r	308	0	292	7	0
5	t	308	0	292	14	0
5	v	308	0	292	6	0
5	x	308	0	292	3	0
5	z	308	0	292	14	0
6	C	507	0	511	27	0
6	c	507	0	511	27	0
7	0	66	0	74	3	0
7	1	46	0	35	7	0
7	2	46	0	35	6	0
7	3	66	0	74	4	0
7	5	92	0	70	5	0
7	7	61	0	61	2	0
7	8	66	0	74	2	0
7	9	66	0	74	6	0
7	A	66	0	74	7	0
7	B	66	0	74	3	0
7	D	66	0	74	7	0
7	E	66	0	74	5	0
7	F	66	0	74	9	0
7	G	66	0	74	3	0
7	I	66	0	74	2	0
7	J	66	0	74	5	0
7	K	66	0	74	8	0
7	L	132	0	148	2	0
7	M	132	0	148	4	0
7	N	66	0	74	5	0
7	O	66	0	74	3	0
7	P	66	0	74	2	0
7	Q	66	0	74	5	0
7	R	66	0	74	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	S	56	0	51	5	0
7	T	66	0	74	2	0
7	U	112	0	109	7	0
7	W	46	0	35	3	0
7	X	46	0	35	0	0
7	Y	46	0	35	2	0
7	Z	46	0	35	2	0
7	a	66	0	74	7	0
7	aa	66	0	74	2	0
7	ab	66	0	74	2	0
7	b	66	0	74	1	0
7	c	61	0	61	10	0
7	d	66	0	74	5	0
7	e	66	0	74	4	0
7	f	66	0	74	2	0
7	g	66	0	74	4	0
7	i	66	0	74	2	0
7	j	66	0	74	2	0
7	k	132	0	148	7	0
7	l	132	0	148	2	0
7	m	132	0	148	5	0
7	o	66	0	74	2	0
7	p	66	0	74	6	0
7	q	66	0	74	7	0
7	r	66	0	74	7	0
7	s	112	0	109	6	0
7	u	51	0	41	5	0
7	v	66	0	74	2	0
7	w	46	0	35	1	0
7	x	46	0	35	2	0
7	y	46	0	35	3	0
7	z	46	0	35	6	0
8	L	117	0	116	7	0
8	l	117	0	116	6	0
9	L	43	0	55	6	0
9	M	48	0	63	1	0
9	l	63	0	90	5	0
9	m	48	0	63	0	0
10	A	97	0	148	11	0
10	C	54	0	88	8	0
10	L	43	0	60	6	0
10	M	53	0	83	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	a	89	0	129	19	0
10	d	41	0	56	6	0
10	h	77	0	105	16	0
10	l	48	0	73	5	0
11	M	1	0	0	0	0
11	m	1	0	0	0	0
12	0	42	0	60	5	0
12	3	84	0	120	10	0
12	8	42	0	60	5	0
12	9	42	0	60	9	0
12	A	42	0	60	6	0
12	B	84	0	120	6	0
12	D	42	0	60	4	0
12	F	42	0	60	6	0
12	G	84	0	120	11	0
12	I	42	0	60	11	0
12	K	42	0	60	5	0
12	M	42	0	60	3	0
12	N	84	0	120	16	0
12	O	84	0	120	5	0
12	Q	38	0	51	9	0
12	R	42	0	60	3	0
12	S	38	0	51	5	0
12	T	42	0	60	3	0
12	U	42	0	60	4	0
12	a	42	0	60	2	0
12	aa	42	0	60	7	0
12	ab	42	0	60	4	0
12	d	42	0	60	15	0
12	e	79	0	109	18	0
12	g	42	0	60	5	0
12	i	42	0	60	4	0
12	j	84	0	120	18	0
12	k	32	0	41	5	0
12	m	42	0	60	3	0
12	n	42	0	60	2	0
12	o	42	0	60	5	0
12	q	42	0	60	6	0
12	r	42	0	60	3	0
12	s	126	0	180	18	0
12	t	42	0	60	6	0
13	M	100	0	156	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	m	100	0	156	4	0
All	All	42176	0	43423	1294	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 15.

All (1294) 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)
4:K:46:ILE:HD13	5:N:46:ARG:HH12	1.12	1.09
4:a:46:ILE:HG21	5:b:46:ARG:HH12	1.17	1.08
4:F:46:ILE:HD13	5:G:46:ARG:HH12	1.16	1.07
4:i:46:ILE:HD13	5:j:46:ARG:HH12	1.20	1.05
4:D:46:ILE:HD13	5:E:46:ARG:HH12	1.22	1.03
5:t:49:PHE:HB3	12:t:101:SPO:H82	1.41	1.02
2:m:233:ARG:HH12	3:h:131:ILE:HD11	1.25	1.00
4:S:46:ILE:HD13	5:T:46:ARG:HH12	1.28	0.95
4:3:46:ILE:HG21	5:ab:46:ARG:HH12	1.31	0.93
5:T:46:ARG:HH21	4:U:53:ARG:HG3	1.32	0.92
4:7:3:LYS:O	4:7:6:LYS:NZ	2.03	0.90
4:d:46:ILE:HD13	5:e:46:ARG:HH12	1.35	0.90
4:s:9:MET:HE3	5:t:17:ALA:HB2	1.55	0.89
4:F:46:ILE:HD13	5:G:46:ARG:NH1	1.89	0.87
5:J:46:ARG:HH21	4:K:53:ARG:HG2	1.36	0.87
4:i:46:ILE:HD13	5:j:46:ARG:NH1	1.91	0.85
4:K:46:ILE:HD13	5:N:46:ARG:NH1	1.90	0.85
4:a:46:ILE:HG21	5:b:46:ARG:NH1	1.90	0.84
2:M:264:GLY:HA3	3:H:35:ASN:OD1	1.78	0.82
3:h:54:GLY:HA3	10:h:301:PC1:H142	1.62	0.82
4:D:46:ILE:HD13	5:E:46:ARG:NH1	1.96	0.81
4:S:46:ILE:HD13	5:T:46:ARG:NH1	1.96	0.80
10:M:1307:PC1:H142	3:H:54:GLY:HA3	1.62	0.80
4:y:23:PHE:HE1	4:5:25:PHE:CZ	1.99	0.80
3:h:54:GLY:H	10:a:102:PC1:H131	1.45	0.80
4:O:42:ASN:ND2	4:O:45:GLU:HG2	1.96	0.80
12:F:102:SPO:H403	5:G:20:LEU:HD12	1.64	0.79
4:d:46:ILE:HD13	5:e:46:ARG:NH1	1.96	0.79
2:m:233:ARG:NH1	3:h:131:ILE:HD11	1.98	0.78
1:l:253:THR:HG23	6:c:57:ILE:HD11	1.65	0.78
4:K:38:THR:OG1	4:K:40:SER:O	1.99	0.78
5:G:46:ARG:HH21	4:I:53:ARG:CG	1.96	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:z:49:PHE:CE2	4:5:43:TRP:HB2	2.19	0.77
5:J:46:ARG:HH21	4:K:53:ARG:CG	1.97	0.77
12:d:103:SPO:H25	5:g:24:TYR:HE1	1.48	0.77
2:m:268:TRP:HE1	3:h:35:ASN:ND2	1.82	0.77
2:M:21:THR:HG23	2:M:26:LEU:HD11	1.67	0.76
2:M:236:GLU:OE1	3:H:117:ARG:NH2	2.18	0.76
5:r:35:ALA:O	5:r:39:HIS:ND1	2.19	0.76
4:3:46:ILE:HG21	5:ab:46:ARG:NH1	2.00	0.76
2:m:21:THR:HG23	2:m:26:LEU:HD11	1.67	0.75
4:7:8:TRP:HZ2	5:8:24:TYR:CD2	2.05	0.75
5:G:46:ARG:HH21	4:I:53:ARG:HG2	1.51	0.74
6:C:53:ARG:HE	10:C:1201:PC1:H153	1.52	0.74
5:z:35:ALA:O	5:z:39:HIS:ND1	2.18	0.74
4:d:46:ILE:HG21	5:e:46:ARG:HH12	1.53	0.74
5:t:35:ALA:O	5:t:39:HIS:ND1	2.17	0.74
1:l:1:ALA:HB2	10:a:103:PC1:H141	1.67	0.74
5:g:38:ALA:HA	12:g:102:SPO:H131	1.69	0.74
4:D:3:LYS:HB2	4:D:6:LYS:HE3	1.70	0.73
4:Q:46:ILE:HD13	5:R:46:ARG:NH1	2.03	0.73
2:m:228:ARG:HA	3:h:194:GLN:HE21	1.53	0.73
4:Q:6:LYS:NZ	5:T:19:GLU:OE2	2.17	0.73
10:A:103:PC1:H121	4:D:14:ARG:HB3	1.71	0.73
3:h:54:GLY:HA2	10:h:302:PC1:H131	1.71	0.72
1:l:47:ILE:HG21	4:3:30:MET:HE2	1.70	0.72
2:M:233:ARG:HH12	3:H:131:ILE:HD11	1.55	0.72
4:f:46:ILE:HG21	5:g:46:ARG:HH12	1.55	0.72
4:f:20:GLN:OE1	5:g:24:TYR:OH	2.06	0.72
4:s:20:GLN:OE1	5:t:24:TYR:OH	2.08	0.71
1:L:224:ILE:HB	9:L:303:U10:H103	1.72	0.71
4:A:46:ILE:HD13	5:B:46:ARG:NH1	2.05	0.71
4:9:46:ILE:HD13	5:0:46:ARG:NH1	2.06	0.71
5:N:46:ARG:HH21	4:O:53:ARG:CG	2.04	0.71
1:l:224:ILE:HB	9:l:303:U10:H103	1.72	0.70
12:s:105:SPO:H342	5:v:23:VAL:HB	1.72	0.70
3:h:51:ALA:HB3	4:a:15:ARG:HH12	1.56	0.70
4:3:46:ILE:HD13	5:ab:46:ARG:NH1	2.07	0.70
2:M:268:TRP:HE1	3:H:35:ASN:ND2	1.91	0.69
10:M:1307:PC1:H141	3:H:56:PHE:HB2	1.74	0.69
4:O:43:TRP:HA	4:O:46:ILE:HD12	1.72	0.69
5:8:24:TYR:HE1	12:8:101:SPO:H22	1.57	0.69
5:X:35:ALA:O	5:X:39:HIS:ND1	2.13	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:9:MET:SD	5:P:17:ALA:HB2	2.33	0.69
10:h:301:PC1:H3D1	10:h:301:PC1:H371	1.75	0.69
2:m:228:ARG:HA	3:h:194:GLN:HG3	1.73	0.69
4:F:6:LYS:HB3	12:I:102:SPO:H392	1.75	0.68
5:v:35:ALA:O	5:v:39:HIS:ND1	2.23	0.68
12:d:103:SPO:C28	5:g:27:GLY:HA3	2.24	0.68
4:Q:46:ILE:HD13	5:R:46:ARG:HH12	1.58	0.68
1:l:147:PRO:HD3	6:c:66:ASN:HD22	1.59	0.68
12:K:102:SPO:H19	4:O:24:LEU:HD21	1.76	0.68
12:T:102:SPO:H25	7:U:101:BCL:HED3	1.75	0.68
4:d:38:THR:OG1	4:d:40:SER:O	2.08	0.68
3:h:56:PHE:HB2	10:h:301:PC1:H141	1.74	0.68
1:l:199:ASN:HB3	13:m:1306:CDL:HB22	1.75	0.67
4:d:46:ILE:HG21	5:e:46:ARG:NH1	2.09	0.67
3:h:217:PRO:HD3	3:h:236:TYR:HD1	1.59	0.67
7:5:101:BCL:HH2	5:4:42:VAL:HG21	1.75	0.67
2:M:268:TRP:HH2	10:M:1307:PC1:H342	1.59	0.67
10:M:1307:PC1:H3D1	10:M:1307:PC1:H371	1.75	0.67
5:X:46:ARG:HG3	4:Y:53:ARG:NH1	2.08	0.67
5:e:46:ARG:HH21	4:f:53:ARG:HG3	1.59	0.67
4:o:6:LYS:NZ	5:r:19:GLU:OE2	2.23	0.67
6:c:58:GLN:O	6:c:58:GLN:NE2	2.27	0.67
4:F:24:LEU:HD21	12:F:102:SPO:H19	1.76	0.67
7:r:101:BCL:H102	7:r:101:BCL:H162	1.77	0.67
4:6:36:LEU:HD21	4:6:44:LEU:HG	1.77	0.67
4:i:24:LEU:HD21	12:j:101:SPO:H19	1.77	0.67
4:I:24:LEU:HD21	12:I:102:SPO:H19	1.77	0.66
4:d:7:ILE:HB	12:d:103:SPO:H343	1.77	0.66
1:L:147:PRO:HD3	6:C:66:ASN:HD22	1.60	0.66
10:M:1307:PC1:H151	3:H:56:PHE:HD2	1.60	0.66
4:D:24:LEU:HD21	12:D:102:SPO:H19	1.77	0.66
3:h:56:PHE:HD2	10:h:301:PC1:H151	1.60	0.66
1:l:201:GLU:O	1:l:204:LYS:HG2	1.96	0.66
4:a:24:LEU:HD21	12:3:101:SPO:H19	1.78	0.66
5:e:46:ARG:HH21	4:f:53:ARG:CG	2.07	0.66
4:o:38:THR:HG23	4:o:40:SER:O	1.95	0.66
5:V:35:ALA:O	5:V:39:HIS:ND1	2.21	0.66
6:C:58:GLN:O	6:C:58:GLN:NE2	2.27	0.66
5:4:17:ALA:O	5:4:21:HIS:HB2	1.95	0.66
1:L:204:LYS:HE2	1:L:207:ARG:NH2	2.11	0.66
12:d:103:SPO:H25	5:g:24:TYR:CE1	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:217:PRO:HD3	3:H:236:TYR:HD1	1.59	0.66
1:l:204:LYS:HE2	1:l:207:ARG:NH2	2.11	0.66
4:f:46:ILE:HG21	5:g:46:ARG:NH1	2.11	0.65
4:K:24:LEU:HD21	12:N:101:SPO:H19	1.78	0.65
4:9:24:LEU:HD21	12:9:102:SPO:H19	1.77	0.65
2:m:75:TRP:HE1	12:m:1305:SPO:HM12	1.61	0.65
5:2:42:VAL:HG21	7:2:101:BCL:HHD	1.79	0.65
4:3:24:LEU:HD21	12:3:103:SPO:H19	1.79	0.65
13:M:1306:CDL:H551	13:M:1306:CDL:H222	1.78	0.65
4:Q:24:LEU:HD21	12:Q:102:SPO:H19	1.79	0.65
2:m:229:PHE:HB2	2:m:244:ALA:HB2	1.78	0.65
7:v:101:BCL:H3A	7:v:101:BCL:H8	1.78	0.65
1:L:201:GLU:O	1:L:204:LYS:HG2	1.96	0.65
4:1:41:TYR:CE2	7:1:101:BCL:HMC1	2.32	0.65
13:m:1306:CDL:H551	13:m:1306:CDL:H222	1.78	0.65
12:s:102:SPO:H392	5:t:20:LEU:HA	1.77	0.64
4:3:38:THR:OG1	4:3:40:SER:O	2.12	0.64
2:M:75:TRP:HE1	12:M:1305:SPO:HM12	1.61	0.64
5:N:46:ARG:HH21	4:O:53:ARG:HG2	1.61	0.64
1:l:271:TRP:HB3	4:w:34:ILE:HG12	1.77	0.64
4:3:46:ILE:HD13	5:ab:46:ARG:HH12	1.62	0.64
4:k:3:LYS:HZ1	5:p:19:GLU:HG3	1.63	0.64
5:j:46:ARG:HH21	4:k:53:ARG:HD2	1.62	0.64
4:s:24:LEU:HD21	12:s:102:SPO:H19	1.79	0.64
1:L:199:ASN:HB3	13:M:1306:CDL:HB22	1.79	0.64
5:B:47:PRO:O	4:D:53:ARG:NH1	2.30	0.64
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.78	0.64
4:S:24:LEU:HD21	12:S:102:SPO:H19	1.79	0.64
4:1:35:LEU:HD11	7:1:101:BCL:CHD	2.28	0.64
2:m:268:TRP:HE1	3:h:35:ASN:HD21	1.46	0.64
3:h:57:PRO:HG3	10:d:102:PC1:H142	1.79	0.64
5:z:49:PHE:HD2	4:5:47:SER:HB3	1.63	0.64
5:G:35:ALA:O	5:G:39:HIS:ND1	2.26	0.63
4:Q:42:ASN:ND2	4:Q:45:GLU:HG2	2.13	0.63
4:k:3:LYS:NZ	5:p:19:GLU:HG3	2.13	0.63
4:o:24:LEU:HD21	12:o:102:SPO:H19	1.80	0.63
4:q:24:LEU:HD21	12:q:102:SPO:H19	1.79	0.63
1:L:216:PHE:CE2	9:L:303:U10:H102	2.34	0.63
4:A:24:LEU:HD21	12:A:102:SPO:H19	1.79	0.63
4:a:46:ILE:HD13	5:b:46:ARG:NH1	2.14	0.63
5:E:35:ALA:O	5:E:39:HIS:ND1	2.26	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:8:35:ALA:O	5:8:39:HIS:ND1	2.26	0.62
1:l:216:PHE:CE2	9:l:303:U10:H102	2.34	0.62
8:l:306:BPB:H55	8:l:306:BPB:HHD	1.80	0.62
3:H:159:GLU:OE1	3:H:159:GLU:HA	1.98	0.62
4:A:46:ILE:HD13	5:B:46:ARG:HH12	1.64	0.62
3:h:159:GLU:HA	3:h:159:GLU:OE1	1.98	0.62
4:d:24:LEU:HD21	12:e:101:SPO:H19	1.81	0.62
4:s:30:MET:O	4:s:34:ILE:HG12	1.99	0.62
7:5:102:BCL:HAA1	5:4:39:HIS:HE1	1.64	0.62
5:aa:35:ALA:O	5:aa:39:HIS:ND1	2.26	0.62
7:E:101:BCL:HMA1	7:F:101:BCL:HMA1	1.80	0.62
4:S:46:ILE:HG21	5:T:46:ARG:HH12	1.65	0.62
6:C:25:PHE:HB2	6:c:21:LEU:HD22	1.79	0.62
5:Z:48:TRP:CE2	7:Z:101:BCL:H2C	2.35	0.62
12:8:101:SPO:H37	6:C:20:ARG:HD3	1.80	0.62
1:l:151:TRP:CZ2	2:m:303:MET:HE3	2.34	0.62
2:m:239:ALA:HB1	3:h:66:LEU:HD11	1.81	0.62
4:O:46:ILE:HD13	5:P:46:ARG:NH1	2.14	0.62
4:k:6:LYS:HB3	12:o:102:SPO:H392	1.82	0.62
8:L:305:BPB:H55	8:L:305:BPB:HHD	1.80	0.62
12:j:103:SPO:H133	5:n:42:VAL:HG23	1.80	0.62
4:a:46:ILE:HD13	5:b:46:ARG:HH12	1.65	0.61
5:J:7:LEU:HD22	5:J:9:TYR:CZ	2.35	0.61
4:6:8:TRP:HZ2	5:aa:24:TYR:CD2	2.17	0.61
2:M:228:ARG:HA	3:H:194:GLN:HG3	1.82	0.61
4:A:43:TRP:HA	4:A:46:ILE:HD12	1.82	0.61
4:I:3:LYS:HA	4:I:5:TYR:CE1	2.35	0.61
4:Y:23:PHE:HE1	4:1:25:PHE:CZ	2.19	0.61
1:l:238:LEU:HD12	9:l:303:U10:H553	1.82	0.61
4:a:8:TRP:HZ2	5:b:24:TYR:CD2	2.19	0.61
5:g:35:ALA:O	5:g:39:HIS:ND1	2.26	0.61
4:k:31:ILE:HD11	12:k:102:SPO:H21A	1.82	0.61
4:3:5:TYR:OH	5:ab:14:ASP:OD1	2.16	0.61
5:R:46:ARG:HH21	4:S:53:ARG:CG	2.14	0.61
13:m:1306:CDL:H392	13:m:1306:CDL:H152	1.83	0.61
4:i:20:GLN:OE1	5:j:24:TYR:OH	2.13	0.61
6:c:28:MET:HB3	7:c:101:BCL:H93	1.82	0.60
5:R:46:ARG:HH21	4:S:53:ARG:HG2	1.66	0.60
4:s:5:TYR:CG	5:t:18:GLN:OE1	2.55	0.60
6:C:17:THR:O	6:C:21:LEU:HG	2.02	0.60
3:h:111:PRO:HG3	3:h:242:MET:HE3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:1306:CDL:H152	13:M:1306:CDL:H392	1.83	0.60
5:Z:35:ALA:O	5:Z:39:HIS:ND1	2.32	0.60
5:g:46:ARG:HH21	4:i:53:ARG:CG	2.13	0.60
5:B:46:ARG:HE	4:D:53:ARG:HD3	1.65	0.60
4:F:30:MET:HE3	4:F:34:ILE:HD11	1.84	0.60
12:F:102:SPO:H341	5:G:20:LEU:HG	1.82	0.60
5:g:38:ALA:HB1	12:g:102:SPO:H15	1.84	0.60
4:6:38:THR:HG21	4:3:44:LEU:HD13	1.82	0.60
5:P:46:ARG:HH21	4:Q:53:ARG:HD2	1.65	0.60
5:J:35:ALA:O	5:J:39:HIS:ND1	2.26	0.60
1:l:138:MET:HE3	6:c:48:PHE:HD1	1.66	0.60
5:B:35:ALA:O	5:B:39:HIS:ND1	2.26	0.59
1:L:138:MET:HE3	6:C:48:PHE:HD1	1.67	0.59
6:C:26:GLN:HA	6:C:29:LYS:HE2	1.84	0.59
5:p:32:SER:O	5:p:36:ILE:HG13	2.03	0.59
6:c:24:ALA:O	6:c:28:MET:HG3	2.02	0.59
3:H:111:PRO:HG3	3:H:242:MET:HE3	1.84	0.59
4:O:8:TRP:HZ2	5:P:24:TYR:CD2	2.19	0.59
12:Q:102:SPO:H341	5:R:20:LEU:HG	1.84	0.59
5:T:35:ALA:O	5:T:39:HIS:ND1	2.26	0.59
5:e:35:ALA:O	5:e:39:HIS:ND1	2.26	0.59
5:e:46:ARG:HG2	4:f:53:ARG:NH1	2.17	0.59
5:b:21:HIS:HE1	7:d:101:BCL:H191	1.66	0.59
4:i:10:ILE:HG23	4:k:14:ARG:HG2	1.83	0.59
4:9:35:LEU:HD11	7:0:101:BCL:HHD	1.84	0.59
5:r:49:PHE:O	4:s:51:TYR:OH	2.17	0.59
1:L:149:GLY:O	1:L:153:HIS:ND1	2.36	0.59
12:S:102:SPO:H341	5:T:20:LEU:HG	1.84	0.59
6:c:17:THR:O	6:c:21:LEU:HG	2.02	0.59
5:b:23:VAL:HB	4:3:3:LYS:HE2	1.85	0.59
10:d:102:PC1:H122	4:f:14:ARG:HB3	1.84	0.59
1:l:187:LEU:HD13	2:m:216:PHE:HB2	1.84	0.58
4:S:6:LYS:HD3	12:U:102:SPO:H37	1.85	0.58
4:S:46:ILE:HG21	5:T:46:ARG:NH1	2.18	0.58
7:U:103:BCL:HBC1	5:V:42:VAL:HG11	1.85	0.58
5:E:46:ARG:HH21	4:F:53:ARG:CG	2.16	0.58
4:O:42:ASN:HD22	4:O:45:GLU:HG2	1.66	0.58
6:C:24:ALA:O	6:C:28:MET:HG3	2.02	0.58
10:L:306:PC1:H2	10:A:104:PC1:H292	1.86	0.58
1:l:149:GLY:O	1:l:153:HIS:ND1	2.36	0.58
10:M:1307:PC1:H153	3:H:55:PRO:HD2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:y:101:BCL:HMD1	7:z:101:BCL:HAC2	1.86	0.58
5:ab:35:ALA:O	5:ab:39:HIS:ND1	2.26	0.58
1:L:87:GLN:HG2	10:C:1201:PC1:H2I1	1.86	0.58
10:L:306:PC1:H2A2	10:M:1307:PC1:H322	1.84	0.58
4:S:10:ILE:HG13	12:U:102:SPO:H341	1.86	0.58
4:d:4:PHE:HA	12:d:103:SPO:H352	1.85	0.58
12:3:103:SPO:H393	5:ab:23:VAL:HG11	1.85	0.58
6:c:26:GLN:HA	6:c:29:LYS:HE2	1.84	0.58
5:z:45:TRP:CD2	5:z:46:ARG:HG2	2.38	0.58
5:j:20:LEU:HD12	12:j:101:SPO:H393	1.86	0.58
1:L:47:ILE:HG21	4:9:30:MET:HE3	1.85	0.58
5:N:20:LEU:HD12	12:N:101:SPO:H403	1.86	0.58
5:0:35:ALA:O	5:0:39:HIS:ND1	2.26	0.58
1:l:269:LEU:HD23	1:l:272:TRP:CH2	2.39	0.58
3:h:199:GLN:OE1	3:h:202:ARG:NH2	2.36	0.58
4:d:7:ILE:HB	12:d:103:SPO:H361	1.85	0.58
5:ab:45:TRP:CD1	12:ab:102:SPO:H83	2.39	0.57
7:c:101:BCL:H112	7:c:101:BCL:H52	1.86	0.57
3:H:140:PHE:HD2	3:H:169:VAL:HG21	1.69	0.57
4:D:8:TRP:HZ2	5:E:24:TYR:CD2	2.21	0.57
10:a:102:PC1:H332	10:a:103:PC1:H391	1.87	0.57
5:e:23:VAL:HG13	12:e:101:SPO:H351	1.86	0.57
3:H:199:GLN:OE1	3:H:202:ARG:NH2	2.36	0.57
4:F:10:ILE:HD11	12:I:102:SPO:H393	1.86	0.57
5:G:46:ARG:HH21	4:I:53:ARG:HG3	1.67	0.57
4:7:30:MET:HE2	12:8:101:SPO:HM12	1.86	0.57
1:l:87:GLN:HG2	10:l:304:PC1:H2I1	1.86	0.57
2:m:228:ARG:HA	3:h:194:GLN:NE2	2.19	0.57
10:a:102:PC1:H112	4:d:18:VAL:HG21	1.86	0.57
5:P:35:ALA:O	5:P:39:HIS:ND1	2.26	0.57
3:h:54:GLY:N	10:a:102:PC1:H131	2.18	0.57
12:j:103:SPO:H23	5:n:45:TRP:HD1	1.70	0.57
4:7:3:LYS:HG3	4:7:6:LYS:HZ1	1.68	0.57
4:9:43:TRP:HA	4:9:46:ILE:HD12	1.86	0.57
10:h:301:PC1:H11	10:h:302:PC1:O11	2.05	0.57
5:j:20:LEU:HG	12:j:101:SPO:H341	1.84	0.57
1:L:269:LEU:HD23	1:L:272:TRP:CH2	2.39	0.57
3:h:63:THR:HG1	3:h:74:THR:HG1	1.52	0.57
5:e:20:LEU:HG	12:e:101:SPO:H341	1.86	0.57
3:h:55:PRO:HD2	10:h:301:PC1:H153	1.86	0.57
10:L:306:PC1:H231	3:H:55:PRO:HG3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:8:TRP:HZ2	5:J:24:TYR:CD2	2.23	0.57
6:C:21:LEU:HD22	6:c:25:PHE:HB2	1.84	0.57
5:e:24:TYR:CE1	12:e:101:SPO:H25	2.40	0.57
4:y:23:PHE:HE1	4:5:25:PHE:CE1	2.22	0.57
3:h:140:PHE:HD2	3:h:169:VAL:HG21	1.69	0.57
4:q:38:THR:HG21	4:s:44:LEU:HD13	1.86	0.57
4:9:46:ILE:HG21	5:0:46:ARG:NH1	2.19	0.56
12:j:101:SPO:H341	12:j:101:SPO:H37	1.87	0.56
2:M:14:GLY:HA3	3:H:140:PHE:CD1	2.39	0.56
5:G:46:ARG:HG2	4:I:53:ARG:NH1	2.20	0.56
4:U:48:ALA:HA	4:U:53:ARG:HH21	1.70	0.56
10:a:102:PC1:H2B2	10:a:103:PC1:H3D2	1.87	0.56
5:j:35:ALA:O	5:j:39:HIS:ND1	2.26	0.56
4:k:6:LYS:HA	4:k:9:MET:HE2	1.88	0.56
4:y:48:ALA:HA	4:y:53:ARG:HH21	1.71	0.56
4:6:30:MET:HE2	12:aa:101:SPO:HM12	1.86	0.56
4:D:6:LYS:HG2	4:D:9:MET:CE	2.35	0.56
5:N:35:ALA:O	5:N:39:HIS:ND1	2.26	0.56
12:Q:102:SPO:H25	5:R:24:TYR:CE1	2.40	0.56
7:r:101:BCL:H122	7:r:101:BCL:C2B	2.35	0.56
12:t:101:SPO:H25	7:u:101:BCL:HED3	1.87	0.56
4:w:48:ALA:HA	4:w:53:ARG:HH21	1.71	0.56
4:3:46:ILE:CG2	5:ab:46:ARG:HH12	2.11	0.56
2:M:233:ARG:NH1	3:H:131:ILE:HD11	2.20	0.56
5:j:24:TYR:CE1	12:j:101:SPO:H25	2.41	0.56
5:aa:24:TYR:HE1	12:aa:101:SPO:H22	1.70	0.56
4:F:38:THR:HG21	4:I:44:LEU:HD13	1.86	0.56
4:W:48:ALA:HA	4:W:53:ARG:HH21	1.71	0.56
4:5:48:ALA:HA	4:5:53:ARG:HH21	1.71	0.56
12:O:103:SPO:H302	12:O:103:SPO:H241	1.88	0.56
2:m:234:GLU:O	2:m:238:ILE:HG13	2.06	0.56
4:u:48:ALA:HA	4:u:53:ARG:HH21	1.70	0.56
5:G:34:VAL:HG11	12:G:102:SPO:H242	1.88	0.56
5:x:35:ALA:O	5:x:39:HIS:ND1	2.28	0.56
6:c:50:VAL:HG12	6:c:54:MET:HE2	1.88	0.56
2:M:234:GLU:O	2:M:238:ILE:HG13	2.06	0.56
4:1:48:ALA:HA	4:1:53:ARG:HH21	1.71	0.56
4:Q:20:GLN:OE1	5:R:24:TYR:OH	2.13	0.56
4:Q:43:TRP:HA	4:Q:46:ILE:HD12	1.87	0.55
4:7:3:LYS:HA	4:7:5:TYR:CE1	2.41	0.55
4:7:8:TRP:HZ2	5:8:24:TYR:HD2	1.52	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:6:36:LEU:HD23	4:6:42:ASN:OD1	2.05	0.55
3:H:134:MET:HG2	3:H:167:ILE:O	2.07	0.55
4:U:25:PHE:HB2	7:U:101:BCL:H51	1.88	0.55
4:Y:48:ALA:HA	4:Y:53:ARG:HH21	1.71	0.55
4:9:46:ILE:HD13	5:0:46:ARG:HH12	1.70	0.55
6:C:50:VAL:HG12	6:C:54:MET:HE2	1.88	0.55
2:m:268:TRP:NE1	3:h:35:ASN:HD21	2.04	0.55
4:q:23:PHE:CD2	7:s:101:BCL:H92	2.42	0.55
1:L:201:GLU:HB2	1:L:204:LYS:HD3	1.89	0.55
1:l:269:LEU:HD11	4:y:33:LEU:CD1	2.37	0.55
2:m:263:GLU:HG3	2:m:264:GLY:N	2.17	0.55
6:c:31:ALA:HB3	7:c:101:BCL:H51	1.87	0.55
3:H:146:LYS:HE3	3:H:200:SER:O	2.07	0.55
4:d:6:LYS:NZ	5:g:19:GLU:OE2	2.33	0.55
4:i:17:PHE:HZ	12:j:101:SPO:H342	1.72	0.55
4:y:23:PHE:CE1	4:5:25:PHE:CE1	2.95	0.55
1:L:271:TRP:HB3	4:W:34:ILE:HG12	1.89	0.55
7:Z:101:BCL:HMC3	7:2:101:BCL:OBB	2.06	0.55
7:p:101:BCL:H171	12:r:102:SPO:H14	1.88	0.55
4:A:38:THR:HG21	4:D:44:LEU:HD13	1.89	0.55
5:Z:22:SER:HA	5:Z:25:MET:SD	2.47	0.55
5:J:46:ARG:HG2	4:K:53:ARG:NH1	2.22	0.55
7:d:101:BCL:H171	12:e:103:SPO:H291	1.89	0.55
10:A:104:PC1:H32	4:9:15:ARG:HH21	1.71	0.54
4:q:1:MET:HA	4:q:4:PHE:CZ	2.42	0.54
4:7:8:TRP:CZ2	5:8:24:TYR:CD2	2.91	0.54
10:L:306:PC1:H391	10:M:1307:PC1:H2C1	1.90	0.54
5:N:46:ARG:HH21	4:O:53:ARG:HG3	1.72	0.54
5:R:35:ALA:O	5:R:39:HIS:ND1	2.26	0.54
12:U:102:SPO:H9	7:W:101:BCL:H3A	1.89	0.54
4:1:41:TYR:CE2	7:1:101:BCL:HBC2	2.41	0.54
3:h:134:MET:HG2	3:h:167:ILE:O	2.07	0.54
5:b:35:ALA:O	5:b:39:HIS:ND1	2.26	0.54
12:q:102:SPO:H341	12:q:102:SPO:H37	1.90	0.54
4:7:3:LYS:CG	4:7:6:LYS:HZ1	2.21	0.54
4:3:8:TRP:HZ2	5:ab:24:TYR:CD2	2.25	0.54
7:M:1301:BCL:C4A	7:M:1301:BCL:HBA2	2.38	0.54
4:F:25:PHE:O	4:F:29:VAL:HG23	2.07	0.54
1:l:159:ASN:ND2	6:c:65:PRO:O	2.32	0.54
7:A:101:BCL:H92	4:9:23:PHE:CD2	2.43	0.54
1:l:201:GLU:HB2	1:l:204:LYS:HD3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:q:6:LYS:HA	4:q:9:MET:HE2	1.89	0.54
3:h:146:LYS:HE3	3:h:200:SER:O	2.07	0.54
4:o:5:TYR:HE2	5:p:14:ASP:OD1	1.90	0.54
4:s:46:ILE:HD13	5:t:46:ARG:NH1	2.23	0.54
4:S:3:LYS:HA	4:S:5:TYR:CD1	2.43	0.54
5:T:46:ARG:HG2	4:U:53:ARG:HH11	1.72	0.54
5:aa:24:TYR:CE1	12:aa:101:SPO:H25	2.43	0.54
4:A:41:TYR:H	4:A:46:ILE:HD11	1.72	0.53
5:N:20:LEU:HD12	12:N:101:SPO:H392	1.90	0.53
1:l:1:ALA:H2	3:h:42:LEU:HD13	1.73	0.53
1:l:238:LEU:HD23	8:l:302:BPB:HBC	1.90	0.53
12:d:103:SPO:HM12	4:f:30:MET:HE2	1.89	0.53
5:t:46:ARG:HG3	4:u:53:ARG:NH1	2.24	0.53
1:L:138:MET:SD	1:L:253:THR:HG21	2.49	0.53
4:I:26:LEU:O	4:I:30:MET:HG2	2.08	0.53
10:a:103:PC1:H322	10:a:103:PC1:H361	1.90	0.53
4:6:8:TRP:HZ2	5:aa:24:TYR:HD2	1.56	0.53
1:L:272:TRP:HB2	2:M:87:ARG:HD3	1.91	0.53
5:z:48:TRP:CH2	7:z:101:BCL:H2C	2.43	0.53
2:M:15:PRO:HD2	3:H:140:PHE:HE1	1.73	0.53
4:a:14:ARG:CZ	10:a:103:PC1:H112	2.38	0.53
4:i:3:LYS:HA	4:i:5:TYR:CD1	2.44	0.53
12:n:101:SPO:H32A	5:p:45:TRP:HD1	1.73	0.53
1:L:170:ASN:HB3	1:L:173:HIS:HB2	1.91	0.53
12:F:102:SPO:H341	12:F:102:SPO:H37	1.90	0.53
3:h:255:MET:HE3	3:h:259:TYR:CE2	2.44	0.53
5:g:46:ARG:HH21	4:i:53:ARG:HG2	1.73	0.53
7:y:101:BCL:HED2	5:z:35:ALA:HB2	1.91	0.53
4:O:3:LYS:HA	4:O:5:TYR:CD1	2.44	0.53
10:C:1201:PC1:H12	10:C:1201:PC1:H122	1.91	0.53
12:d:103:SPO:HM11	4:i:33:LEU:HD21	1.90	0.53
4:6:8:TRP:CZ2	5:aa:24:TYR:CD2	2.96	0.53
1:L:21:LEU:HD22	4:7:15:ARG:HB2	1.91	0.53
12:I:102:SPO:H21A	7:K:101:BCL:HBB2	1.91	0.53
1:l:43:ALA:O	1:l:47:ILE:HG12	2.09	0.53
1:l:226:THR:O	1:l:230:HIS:ND1	2.41	0.53
10:l:304:PC1:H12	10:l:304:PC1:H122	1.91	0.53
5:g:21:HIS:HE1	7:i:101:BCL:H202	1.74	0.53
5:aa:46:ARG:HG2	4:3:53:ARG:NH1	2.24	0.53
1:L:238:LEU:HD23	8:L:302:BPB:HBC	1.90	0.53
5:8:46:ARG:HH21	4:9:53:ARG:CG	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:9:46:ILE:HG21	5:0:46:ARG:HH12	1.74	0.53
5:p:46:ARG:HG3	4:q:53:ARG:NH1	2.23	0.53
3:H:215:GLY:C	3:H:236:TYR:HE1	2.17	0.53
7:Y:201:BCL:HHD	5:Z:42:VAL:HG21	1.90	0.53
1:L:43:ALA:O	1:L:47:ILE:HG12	2.09	0.52
4:k:3:LYS:HA	4:k:5:TYR:CD1	2.44	0.52
1:L:210:ASP:OD2	3:H:125:GLY:N	2.41	0.52
7:m:1301:BCL:C4A	7:m:1301:BCL:HBA2	2.37	0.52
3:H:255:MET:HE3	3:H:259:TYR:CE2	2.44	0.52
1:l:138:MET:SD	1:l:253:THR:HG21	2.49	0.52
4:i:17:PHE:CZ	12:j:101:SPO:H342	2.44	0.52
7:1:101:BCL:HMD1	7:2:101:BCL:CAC	2.39	0.52
5:n:25:MET:O	5:n:29:TRP:CD1	2.63	0.52
2:M:263:GLU:HG3	2:M:264:GLY:N	2.17	0.52
3:H:156:CYS:HB2	3:H:248:ARG:HG3	1.92	0.52
4:O:38:THR:OG1	4:O:40:SER:O	2.22	0.52
5:j:20:LEU:HG	12:j:101:SPO:H37	1.92	0.52
1:L:7:ARG:NH1	3:H:87:LEU:HB2	2.25	0.52
4:Q:23:PHE:CD2	7:S:101:BCL:H92	2.45	0.52
1:l:269:LEU:HD11	4:y:33:LEU:HD13	1.92	0.52
4:i:29:VAL:O	4:i:33:LEU:HD23	2.10	0.52
4:o:35:LEU:HD11	7:p:101:BCL:HHD	1.91	0.52
5:x:31:PHE:HE2	7:x:101:BCL:HBA1	1.74	0.52
1:l:12:PRO:HG3	3:h:97:PRO:HB2	1.92	0.52
5:4:35:ALA:O	5:4:39:HIS:ND1	2.29	0.52
2:M:228:ARG:HA	3:H:194:GLN:HE21	1.74	0.52
4:9:41:TYR:H	4:9:46:ILE:HD11	1.74	0.52
1:l:170:ASN:HB3	1:l:173:HIS:HB2	1.91	0.52
3:H:219:ILE:HA	3:H:229:GLU:OE1	2.10	0.52
4:Q:3:LYS:HA	4:Q:5:TYR:CD1	2.45	0.52
5:T:46:ARG:NH2	4:U:53:ARG:HG3	2.13	0.52
10:l:304:PC1:H153	6:c:53:ARG:HE	1.75	0.52
3:h:7:PHE:CZ	4:f:34:ILE:HG12	2.45	0.52
4:3:8:TRP:HZ2	5:ab:24:TYR:HD2	1.58	0.52
3:h:215:GLY:C	3:h:236:TYR:HE1	2.17	0.51
9:M:1304:U10:H152	10:M:1307:PC1:H362	1.93	0.51
12:A:102:SPO:H393	5:B:23:VAL:HG11	1.92	0.51
4:S:3:LYS:HA	4:S:5:TYR:CE1	2.45	0.51
7:W:101:BCL:HHD	5:X:42:VAL:HG21	1.92	0.51
2:m:121:PHE:HZ	4:q:30:MET:HE2	1.75	0.51
4:i:35:LEU:HD11	7:j:102:BCL:HHD	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:t:101:SPO:H362	7:u:101:BCL:H41	1.93	0.51
4:6:11:PHE:C	5:aa:10:THR:HG21	2.34	0.51
12:F:102:SPO:H25	5:G:24:TYR:CE1	2.46	0.51
12:Q:102:SPO:HM11	4:S:33:LEU:HD11	1.92	0.51
4:a:8:TRP:HZ2	5:b:24:TYR:HD2	1.58	0.51
4:a:51:TYR:OH	5:ab:49:PHE:O	2.19	0.51
7:z:101:BCL:HAA2	7:z:101:BCL:HBD	1.90	0.51
7:5:102:BCL:HAC2	5:4:42:VAL:HG11	1.92	0.51
2:M:152:SER:HG	2:M:277:THR:HG1	1.57	0.51
4:a:53:ARG:HD2	5:ab:46:ARG:HE	1.75	0.51
5:r:33:ALA:O	5:r:37:VAL:HG23	2.10	0.51
1:L:159:ASN:ND2	6:C:65:PRO:O	2.33	0.51
10:A:103:PC1:H2B2	10:A:104:PC1:H291	1.91	0.51
5:R:49:PHE:HB3	12:R:102:SPO:H82	1.92	0.51
2:m:11:GLN:NE2	2:m:41:TRP:CD2	2.78	0.51
2:M:21:THR:CG2	2:M:26:LEU:HD11	2.39	0.51
4:7:8:TRP:CZ2	5:8:24:TYR:HD2	2.28	0.51
2:m:228:ARG:HA	3:h:194:GLN:CG	2.39	0.51
7:q:101:BCL:H41	12:r:102:SPO:H37	1.92	0.51
4:1:31:ILE:HD12	7:1:101:BCL:HED3	1.93	0.51
7:1:101:BCL:HMD1	7:2:101:BCL:HAC2	1.93	0.51
2:m:84:VAL:HA	2:m:87:ARG:HG2	1.92	0.51
4:Q:8:TRP:CZ2	5:R:24:TYR:HD2	2.29	0.51
12:R:102:SPO:H352	12:S:102:SPO:H241	1.92	0.51
2:M:11:GLN:NE2	2:M:41:TRP:CD2	2.78	0.51
2:M:268:TRP:CD1	3:H:35:ASN:HD21	2.29	0.51
3:H:209:SER:O	3:H:213:PHE:HD1	1.94	0.51
12:I:102:SPO:H11	7:J:101:BCL:HMA2	1.93	0.51
4:O:36:LEU:HD23	4:O:42:ASN:OD1	2.11	0.51
3:h:55:PRO:HB2	10:d:102:PC1:H272	1.91	0.51
3:h:209:SER:O	3:h:213:PHE:HD1	1.94	0.51
3:h:219:ILE:HA	3:h:229:GLU:OE1	2.10	0.51
2:M:84:VAL:HA	2:M:87:ARG:HG2	1.92	0.50
12:Q:102:SPO:HM11	4:S:33:LEU:CD1	2.41	0.50
5:X:46:ARG:HG3	4:Y:53:ARG:HH11	1.73	0.50
4:d:6:LYS:HA	4:d:9:MET:HE2	1.92	0.50
6:c:58:GLN:HE21	6:c:58:GLN:C	2.19	0.50
4:S:24:LEU:HB2	7:S:101:BCL:H42	1.92	0.50
5:8:46:ARG:HG2	4:9:53:ARG:NH1	2.26	0.50
4:i:3:LYS:HA	4:i:5:TYR:CE1	2.47	0.50
2:M:268:TRP:NE1	3:H:35:ASN:ND2	2.57	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:k:103:BCL:H161	12:n:101:SPO:H21	1.94	0.50
6:c:25:PHE:HA	6:c:28:MET:HE3	1.93	0.50
2:M:239:ALA:O	3:H:73:LEU:HD22	2.12	0.50
3:H:154:ARG:HD2	3:H:158:LEU:HA	1.94	0.50
5:j:20:LEU:HB2	12:j:101:SPO:H402	1.94	0.50
4:O:3:LYS:HA	4:O:5:TYR:CE1	2.46	0.50
4:7:3:LYS:HA	4:7:5:TYR:CD1	2.46	0.50
5:8:24:TYR:CE1	12:8:101:SPO:H22	2.44	0.50
5:8:46:ARG:HH12	4:6:46:ILE:C	2.20	0.50
3:h:156:CYS:HB2	3:h:248:ARG:HG3	1.92	0.50
1:L:204:LYS:HE2	1:L:207:ARG:HH21	1.77	0.50
4:Q:35:LEU:HD11	7:R:101:BCL:HHD	1.94	0.50
7:a:101:BCL:H92	4:3:23:PHE:CD2	2.47	0.50
12:k:102:SPO:H182	7:o:101:BCL:H91	1.93	0.50
2:M:268:TRP:HE1	3:H:35:ASN:HD22	1.57	0.50
4:D:23:PHE:CD2	7:F:101:BCL:H92	2.47	0.50
4:d:9:MET:SD	5:e:17:ALA:HB2	2.52	0.50
4:k:3:LYS:HA	4:k:5:TYR:CE1	2.47	0.50
4:3:8:TRP:CH2	4:3:17:PHE:HE1	2.30	0.50
6:c:7:PHE:CE2	6:c:9:ASP:HB3	2.47	0.50
4:D:38:THR:HG21	4:F:44:LEU:HD13	1.94	0.50
4:7:25:PHE:CZ	6:C:35:GLY:HA2	2.47	0.50
4:9:26:LEU:O	4:9:30:MET:HG3	2.12	0.50
12:d:103:SPO:H301	5:g:24:TYR:HA	1.93	0.50
4:F:35:LEU:HD11	7:G:101:BCL:HHD	1.93	0.50
1:l:204:LYS:HE2	1:l:207:ARG:HH21	1.77	0.50
4:a:3:LYS:HA	4:a:5:TYR:CE1	2.46	0.50
4:k:24:LEU:HB2	7:k:101:BCL:H42	1.93	0.50
4:o:41:TYR:H	4:o:46:ILE:HD11	1.76	0.50
4:s:38:THR:OG1	4:s:40:SER:O	2.20	0.49
7:3:102:BCL:C1D	12:ab:102:SPO:H181	2.41	0.49
4:A:8:TRP:HZ2	5:B:24:TYR:CD2	2.30	0.49
7:A:101:BCL:H161	5:0:24:TYR:HE2	1.77	0.49
12:N:101:SPO:H11	7:N:102:BCL:HMA2	1.93	0.49
4:a:18:VAL:HG22	10:a:103:PC1:H262	1.93	0.49
4:q:41:TYR:H	4:q:46:ILE:HD11	1.77	0.49
5:aa:39:HIS:CE1	7:c:101:BCL:OBD	2.64	0.49
4:I:8:TRP:CZ2	5:J:24:TYR:CD2	3.00	0.49
6:C:25:PHE:HA	6:C:28:MET:HE3	1.93	0.49
10:a:102:PC1:H231	7:d:101:BCL:H121	1.93	0.49
7:p:101:BCL:HHC	7:p:101:BCL:OBB	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:6:8:TRP:CZ2	5:aa:24:TYR:HD2	2.28	0.49
4:K:3:LYS:HA	4:K:5:TYR:CD1	2.46	0.49
4:f:32:HIS:CE1	7:g:101:BCL:HMD1	2.48	0.49
4:y:41:TYR:OH	4:5:47:SER:OG	2.02	0.49
4:D:46:ILE:HG21	5:E:46:ARG:HH12	1.78	0.49
4:F:3:LYS:NZ	4:F:5:TYR:OH	2.43	0.49
4:O:46:ILE:HD13	5:P:46:ARG:HH12	1.76	0.49
4:S:36:LEU:HD23	4:S:42:ASN:ND2	2.27	0.49
4:U:31:ILE:HD12	7:U:103:BCL:O1D	2.12	0.49
13:m:1306:CDL:H522	13:m:1306:CDL:H712	1.95	0.49
4:D:3:LYS:HA	4:D:5:TYR:CE1	2.48	0.49
4:Q:38:THR:HG21	4:S:44:LEU:HD13	1.94	0.49
1:L:253:THR:HG23	6:C:57:ILE:HD11	1.95	0.49
2:M:179:ILE:O	2:M:182:HIS:ND1	2.46	0.49
10:h:301:PC1:H121	10:h:302:PC1:C13	2.42	0.49
3:H:52:ASN:HD21	4:A:15:ARG:NE	2.11	0.49
4:7:11:PHE:C	5:8:10:THR:HG21	2.38	0.49
4:a:3:LYS:HA	4:a:5:TYR:CD1	2.47	0.49
12:B:103:SPO:H27	7:D:101:BCL:HED3	1.94	0.49
4:F:3:LYS:HA	4:F:5:TYR:CD1	2.48	0.49
5:N:46:ARG:HG2	4:O:53:ARG:NH1	2.28	0.49
4:9:41:TYR:OH	5:0:48:TRP:HB3	2.12	0.49
6:C:58:GLN:HE21	6:C:58:GLN:C	2.19	0.49
2:m:152:SER:HG	2:m:277:THR:HG1	1.56	0.49
4:k:30:MET:HE2	12:k:102:SPO:H22A	1.95	0.49
1:L:226:THR:O	1:L:230:HIS:ND1	2.41	0.49
7:F:101:BCL:HED1	5:G:31:PHE:CE1	2.48	0.49
4:Q:8:TRP:HZ2	5:R:24:TYR:CD2	2.31	0.49
4:1:46:ILE:HD11	5:2:45:TRP:CH2	2.48	0.49
3:h:36:MET:HE2	3:h:58:LEU:HD23	1.94	0.49
3:H:57:PRO:HB3	4:D:15:ARG:NH1	2.28	0.48
3:H:103:ASP:OD2	3:H:106:LYS:HB2	2.13	0.48
7:E:101:BCL:CBB	12:G:102:SPO:H15	2.43	0.48
4:K:3:LYS:HA	4:K:5:TYR:CE1	2.48	0.48
4:Q:24:LEU:HB2	7:Q:101:BCL:H42	1.95	0.48
1:l:105:VAL:O	1:l:109:ARG:HB2	2.14	0.48
2:m:21:THR:CG2	2:m:26:LEU:HD11	2.39	0.48
2:m:179:ILE:O	2:m:182:HIS:ND1	2.46	0.48
4:a:23:PHE:HD1	10:a:103:PC1:H3D1	1.78	0.48
12:D:102:SPO:H37	12:D:102:SPO:H341	1.95	0.48
4:Q:3:LYS:HA	4:Q:5:TYR:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:7:PHE:CE2	6:C:9:ASP:HB3	2.47	0.48
7:r:101:BCL:H92	7:r:101:BCL:H2	1.94	0.48
4:A:53:ARG:CG	5:0:46:ARG:HH21	2.26	0.48
4:A:53:ARG:NH1	5:0:46:ARG:HG2	2.28	0.48
4:K:38:THR:HG21	4:O:44:LEU:HD13	1.94	0.48
7:U:101:BCL:HHD	5:V:42:VAL:HG21	1.95	0.48
12:U:102:SPO:H27	5:V:27:GLY:HA3	1.94	0.48
1:L:105:VAL:O	1:L:109:ARG:HB2	2.14	0.48
12:K:102:SPO:H37	5:P:23:VAL:HG11	1.95	0.48
3:h:252:VAL:O	3:h:255:MET:HB3	2.14	0.48
12:t:101:SPO:H22	7:u:101:BCL:O1D	2.14	0.48
3:H:36:MET:HE2	3:H:58:LEU:HD23	1.94	0.48
12:K:102:SPO:H27	12:K:102:SPO:H311	1.65	0.48
5:Z:47:PRO:HD2	4:1:53:ARG:HH11	1.78	0.48
3:h:154:ARG:HD2	3:h:158:LEU:HA	1.94	0.48
4:i:10:ILE:HG23	4:k:14:ARG:CG	2.44	0.48
13:M:1306:CDL:H712	13:M:1306:CDL:H522	1.95	0.48
4:F:3:LYS:HA	4:F:5:TYR:CE1	2.48	0.48
12:I:102:SPO:H341	5:J:20:LEU:HG	1.96	0.48
7:m:1301:BCL:H72	7:m:1301:BCL:H111	1.66	0.48
3:h:103:ASP:OD2	3:h:106:LYS:HB2	2.13	0.48
4:Q:38:THR:OG1	4:Q:40:SER:O	2.20	0.48
5:2:35:ALA:O	5:2:39:HIS:ND1	2.28	0.48
5:E:46:ARG:HH21	4:F:53:ARG:HG2	1.77	0.48
4:I:3:LYS:HA	4:I:5:TYR:CD1	2.49	0.48
12:I:102:SPO:H27	12:I:102:SPO:H311	1.62	0.48
12:i:102:SPO:H183	12:i:102:SPO:H14	1.95	0.48
8:L:302:BPB:H14	7:M:1301:BCL:HBB3	1.96	0.48
5:V:33:ALA:O	5:V:37:VAL:HG23	2.14	0.48
8:l:302:BPB:H14	7:m:1301:BCL:HBB3	1.96	0.48
4:a:46:ILE:HD13	5:b:46:ARG:NH2	2.29	0.48
5:Z:47:PRO:HD2	4:1:53:ARG:NH1	2.29	0.48
1:l:21:LEU:HD11	4:6:11:PHE:CD1	2.49	0.48
5:b:46:ARG:HH21	4:d:53:ARG:CG	2.25	0.48
4:d:46:ILE:CG2	5:e:46:ARG:HH12	2.26	0.48
7:d:101:BCL:H91	12:3:101:SPO:H182	1.96	0.48
4:q:11:PHE:HZ	4:s:17:PHE:HB2	1.78	0.48
4:I:42:ASN:ND2	4:I:45:GLU:HG3	2.29	0.47
12:N:101:SPO:H11	7:N:102:BCL:CMA	2.44	0.47
4:7:8:TRP:CD2	5:8:20:LEU:CD2	2.97	0.47
4:k:41:TYR:H	4:k:46:ILE:HD11	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:q:101:BCL:H121	7:q:101:BCL:H162	1.56	0.47
7:F:101:BCL:H43	12:G:102:SPO:H32	1.96	0.47
1:l:272:TRP:HB2	2:m:87:ARG:HD3	1.96	0.47
3:h:104:PRO:HB2	3:h:243:TYR:CE2	2.49	0.47
4:d:35:LEU:HD11	7:e:102:BCL:HHD	1.96	0.47
3:H:241:LEU:HA	3:H:248:ARG:HH22	1.79	0.47
3:H:252:VAL:O	3:H:255:MET:HB3	2.14	0.47
4:I:8:TRP:CZ2	5:J:24:TYR:HD2	2.32	0.47
4:9:40:SER:O	4:9:41:TYR:HB2	2.14	0.47
6:C:41:THR:HG21	10:C:1201:PC1:H2B1	1.96	0.47
3:H:104:PRO:HB2	3:H:243:TYR:CE2	2.49	0.47
7:B:101:BCL:HMA1	7:D:101:BCL:HMA1	1.97	0.47
4:7:6:LYS:HB3	4:7:6:LYS:HE3	1.66	0.47
3:h:66:LEU:HB3	3:h:70:ARG:HB2	1.97	0.47
5:b:23:VAL:HG11	12:3:101:SPO:H393	1.95	0.47
4:d:3:LYS:HA	4:d:5:TYR:CD1	2.50	0.47
5:x:46:ARG:HG3	4:y:53:ARG:NH1	2.30	0.47
1:L:187:LEU:HD13	2:M:216:PHE:HB2	1.96	0.47
2:M:239:ALA:HB1	3:H:66:LEU:HD11	1.96	0.47
12:A:102:SPO:H37	12:A:102:SPO:H341	1.96	0.47
4:D:3:LYS:HA	4:D:5:TYR:CD1	2.49	0.47
12:I:102:SPO:H402	5:J:23:VAL:HG11	1.95	0.47
4:7:5:TYR:HA	5:8:21:HIS:CG	2.49	0.47
4:7:46:ILE:O	5:aa:46:ARG:NH1	2.48	0.47
10:h:301:PC1:C23	10:h:302:PC1:H231	2.45	0.47
7:a:101:BCL:O1D	12:a:104:SPO:H22	2.15	0.47
5:e:32:SER:O	5:e:36:ILE:HG13	2.15	0.47
4:s:41:TYR:H	4:s:46:ILE:HD11	1.80	0.47
12:t:101:SPO:H341	12:t:101:SPO:H361	1.76	0.47
3:H:66:LEU:HB3	3:H:70:ARG:HB2	1.97	0.47
5:B:32:SER:O	5:B:36:ILE:HG13	2.15	0.47
12:G:102:SPO:H343	12:G:102:SPO:H361	1.68	0.47
4:I:39:PRO:HB2	4:K:54:VAL:HG21	1.97	0.47
7:K:101:BCL:C4D	12:N:103:SPO:H181	2.44	0.47
5:N:32:SER:O	5:N:36:ILE:HG13	2.15	0.47
12:O:103:SPO:H19	7:Q:101:BCL:HMA3	1.97	0.47
5:X:15:GLU:OE1	5:X:15:GLU:N	2.47	0.47
4:7:8:TRP:CG	5:8:20:LEU:HD22	2.49	0.47
3:h:241:LEU:HA	3:h:248:ARG:HH22	1.79	0.47
4:f:6:LYS:HE2	4:f:9:MET:HE1	1.96	0.47
4:i:46:ILE:HG21	5:j:46:ARG:HH12	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:14:ASP:OD1	5:4:14:ASP:N	2.47	0.47
4:6:6:LYS:HG2	4:6:9:MET:HE2	1.96	0.47
5:ab:32:SER:O	5:ab:36:ILE:HG13	2.15	0.47
3:H:179:LEU:HG	3:H:193:MET:SD	2.55	0.47
5:E:24:TYR:C	5:E:24:TYR:CD1	2.93	0.47
5:G:32:SER:O	5:G:36:ILE:HG13	2.15	0.47
4:K:8:TRP:CZ2	5:N:24:TYR:CD2	3.03	0.47
5:8:32:SER:O	5:8:36:ILE:HG13	2.15	0.47
12:9:102:SPO:H341	5:0:20:LEU:HG	1.95	0.47
5:0:32:SER:O	5:0:36:ILE:HG13	2.15	0.47
3:h:179:LEU:HG	3:h:193:MET:SD	2.55	0.47
5:b:24:TYR:CD1	5:b:24:TYR:C	2.93	0.47
4:k:40:SER:O	4:k:41:TYR:HB2	2.15	0.47
4:q:35:LEU:HD11	7:r:101:BCL:HHD	1.97	0.47
5:E:32:SER:O	5:E:36:ILE:HG13	2.15	0.47
5:T:24:TYR:CD1	5:T:24:TYR:C	2.93	0.47
4:i:9:MET:HB3	5:j:8:GLY:H	1.80	0.47
2:M:15:PRO:HD2	3:H:140:PHE:CE1	2.50	0.47
3:H:54:GLY:H	10:A:103:PC1:H131	1.80	0.47
5:J:46:ARG:NH2	4:K:53:ARG:HG2	2.18	0.47
5:P:32:SER:O	5:P:36:ILE:HG13	2.15	0.47
4:1:41:TYR:OH	5:2:48:TRP:HB2	2.15	0.47
4:7:6:LYS:HG3	12:9:102:SPO:H361	1.96	0.47
1:l:226:THR:O	1:l:229:ILE:HG22	2.15	0.47
10:a:102:PC1:H291	10:a:103:PC1:H3D2	1.97	0.47
12:e:101:SPO:H182	7:f:101:BCL:H91	1.96	0.47
4:Q:8:TRP:CZ2	5:R:24:TYR:CD2	3.03	0.47
5:R:32:SER:O	5:R:36:ILE:HG13	2.15	0.47
1:l:21:LEU:HD11	4:6:11:PHE:HD1	1.80	0.47
4:d:24:LEU:HB2	7:d:101:BCL:H42	1.97	0.47
5:g:32:SER:O	5:g:36:ILE:HG13	2.15	0.47
5:j:32:SER:O	5:j:36:ILE:HG13	2.15	0.47
7:s:101:BCL:HED1	5:t:31:PHE:CE1	2.49	0.47
5:J:32:SER:O	5:J:36:ILE:HG13	2.15	0.46
1:l:31:VAL:O	1:l:35:GLY:HA3	2.15	0.46
4:d:3:LYS:HA	4:d:5:TYR:CE1	2.50	0.46
5:e:24:TYR:CD1	5:e:24:TYR:C	2.93	0.46
4:i:8:TRP:HZ2	5:j:24:TYR:CD2	2.33	0.46
5:aa:32:SER:O	5:aa:36:ILE:HG13	2.15	0.46
4:F:40:SER:O	4:F:41:TYR:HB2	2.15	0.46
5:G:24:TYR:CD1	5:G:24:TYR:C	2.93	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:24:TYR:CD1	5:J:24:TYR:C	2.93	0.46
5:N:24:TYR:CD1	5:N:24:TYR:C	2.93	0.46
5:T:32:SER:O	5:T:36:ILE:HG13	2.15	0.46
5:8:24:TYR:CD1	5:8:24:TYR:C	2.93	0.46
4:9:8:TRP:HZ2	5:0:24:TYR:CD2	2.34	0.46
3:h:54:GLY:CA	10:h:302:PC1:H131	2.41	0.46
3:h:117:ARG:HD2	3:h:231:ASP:OD2	2.16	0.46
4:a:19:ALA:HA	10:a:103:PC1:H362	1.97	0.46
12:d:103:SPO:H391	5:g:20:LEU:HD12	1.98	0.46
4:I:3:LYS:HG3	4:I:5:TYR:CE1	2.50	0.46
4:I:8:TRP:CH2	4:I:17:PHE:HE2	2.33	0.46
4:K:8:TRP:HZ2	5:N:24:TYR:CD2	2.33	0.46
4:O:9:MET:SD	5:P:17:ALA:CB	3.02	0.46
5:0:45:TRP:HB2	12:0:102:SPO:H10	1.96	0.46
5:b:32:SER:O	5:b:36:ILE:HG13	2.15	0.46
4:d:33:LEU:HG	12:3:101:SPO:HM11	1.96	0.46
12:t:101:SPO:H27	7:u:101:BCL:HED3	1.97	0.46
7:A:101:BCL:H93	7:A:101:BCL:H112	1.78	0.46
4:I:38:THR:OG1	4:I:40:SER:O	2.22	0.46
4:K:10:ILE:HG23	4:O:14:ARG:HG2	1.96	0.46
5:2:31:PHE:CE1	7:2:101:BCL:HED1	2.50	0.46
4:7:40:SER:O	4:7:41:TYR:HB2	2.15	0.46
5:8:24:TYR:CE1	12:8:101:SPO:H25	2.51	0.46
4:d:48:ALA:HA	4:d:53:ARG:HD3	1.97	0.46
12:j:103:SPO:H10	5:n:41:ALA:HB1	1.98	0.46
5:J:7:LEU:HD21	5:N:12:LEU:HD11	1.98	0.46
4:O:43:TRP:CE3	7:O:101:BCL:H2C	2.50	0.46
4:a:46:ILE:HD13	5:b:46:ARG:CZ	2.45	0.46
7:v:101:BCL:H161	7:v:101:BCL:HBB2	1.96	0.46
12:F:102:SPO:H37	5:G:20:LEU:HG	1.96	0.46
5:N:20:LEU:HB2	12:N:101:SPO:H392	1.97	0.46
4:f:38:THR:HG21	4:i:44:LEU:HD13	1.96	0.46
12:s:105:SPO:C34	5:v:23:VAL:HB	2.41	0.46
5:aa:24:TYR:CD1	5:aa:24:TYR:C	2.93	0.46
3:H:1:MET:O	3:H:1:MET:HG3	2.16	0.46
4:A:23:PHE:CD2	7:D:101:BCL:H92	2.50	0.46
10:C:1201:PC1:H362	5:aa:45:TRP:HB2	1.97	0.46
3:h:57:PRO:HG3	10:d:102:PC1:C14	2.44	0.46
12:e:103:SPO:H131	12:e:103:SPO:H15	1.43	0.46
4:i:4:PHE:HB3	7:k:101:BCL:H202	1.98	0.46
4:i:40:SER:O	4:i:41:TYR:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:117:ARG:HD2	3:H:231:ASP:OD2	2.16	0.46
4:9:36:LEU:HD23	4:9:42:ASN:OD1	2.14	0.46
1:l:45:GLY:HA3	8:l:302:BPB:H9B	1.98	0.46
12:e:103:SPO:H10	12:e:103:SPO:H81	1.60	0.46
5:g:24:TYR:CD1	5:g:24:TYR:C	2.93	0.46
4:5:28:ALA:HA	7:5:102:BCL:O1D	2.15	0.46
4:3:41:TYR:OH	5:ab:48:TRP:HB3	2.16	0.46
5:ab:24:TYR:CD1	5:ab:24:TYR:C	2.93	0.46
1:L:226:THR:O	1:L:229:ILE:HG22	2.15	0.46
12:O:103:SPO:H341	12:Q:102:SPO:H241	1.98	0.46
5:R:46:ARG:HG2	4:S:53:ARG:NH1	2.31	0.46
6:C:22:TRP:CE3	6:C:23:VAL:HG23	2.51	0.46
4:f:35:LEU:HD11	7:g:101:BCL:HHD	1.97	0.46
4:f:40:SER:O	4:f:41:TYR:HB2	2.16	0.46
5:j:23:VAL:HG13	12:j:101:SPO:H351	1.97	0.46
12:aa:101:SPO:H342	12:aa:101:SPO:C38	2.45	0.46
4:D:9:MET:O	5:E:8:GLY:HA2	2.16	0.46
4:k:46:ILE:HD13	5:n:46:ARG:NH1	2.30	0.46
12:k:102:SPO:H41	4:o:32:HIS:CG	2.51	0.46
4:6:12:ASP:HB3	4:6:15:ARG:HG2	1.98	0.46
6:c:22:TRP:CE3	6:c:23:VAL:HG23	2.51	0.46
1:L:31:VAL:O	1:L:35:GLY:HA3	2.15	0.45
10:M:1307:PC1:O32	3:H:32:GLN:NE2	2.48	0.45
4:K:29:VAL:O	4:K:33:LEU:HG	2.17	0.45
5:P:24:TYR:CD1	5:P:24:TYR:C	2.93	0.45
4:S:29:VAL:O	4:S:33:LEU:HD13	2.16	0.45
4:9:46:ILE:CG2	5:0:46:ARG:HH12	2.29	0.45
3:h:1:MET:O	3:h:1:MET:HG3	2.16	0.45
12:a:104:SPO:H362	12:a:104:SPO:H402	1.63	0.45
4:A:19:ALA:HB2	10:A:104:PC1:H261	1.98	0.45
5:B:24:TYR:CD1	5:B:24:TYR:C	2.93	0.45
12:B:103:SPO:H293	7:D:101:BCL:HMA2	1.97	0.45
5:R:24:TYR:CD1	5:R:24:TYR:C	2.93	0.45
2:m:105:PHE:HD1	2:m:116:LEU:HD13	1.81	0.45
4:s:17:PHE:HZ	12:s:102:SPO:H342	1.81	0.45
4:K:6:LYS:HG2	4:K:9:MET:CE	2.46	0.45
10:d:102:PC1:H112	10:d:102:PC1:H153	1.72	0.45
5:j:46:ARG:HG2	4:k:53:ARG:NH2	2.31	0.45
4:I:10:ILE:HG23	4:K:14:ARG:HG2	1.99	0.45
4:7:8:TRP:HZ2	5:8:24:TYR:CE2	2.34	0.45
4:7:9:MET:HG3	5:8:17:ALA:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:q:17:PHE:CZ	12:q:102:SPO:H342	2.51	0.45
12:s:105:SPO:H10	12:s:105:SPO:H81	1.59	0.45
5:4:21:HIS:O	5:4:25:MET:HG2	2.16	0.45
1:L:35:GLY:HA2	1:L:38:THR:HG22	1.97	0.45
4:I:8:TRP:HZ2	5:J:24:TYR:HD2	1.62	0.45
2:m:54:SER:HA	4:q:18:VAL:HG11	1.98	0.45
10:h:301:PC1:O21	10:h:302:PC1:H2	2.16	0.45
4:f:43:TRP:CD1	4:f:44:LEU:HD22	2.52	0.45
4:i:6:LYS:HE2	4:i:9:MET:HE1	1.97	0.45
8:L:305:BPB:H5A	2:M:63:GLY:HA3	1.98	0.45
2:M:105:PHE:HD1	2:M:116:LEU:HD13	1.81	0.45
5:E:33:ALA:O	5:E:37:VAL:HG23	2.17	0.45
5:0:33:ALA:O	5:0:37:VAL:HG23	2.17	0.45
6:C:7:PHE:CZ	6:C:9:ASP:HB3	2.51	0.45
10:C:1201:PC1:H3G2	7:c:101:BCL:HMA3	1.99	0.45
4:a:40:SER:O	4:a:41:TYR:HB2	2.16	0.45
5:e:33:ALA:O	5:e:37:VAL:HG23	2.17	0.45
7:e:102:BCL:H152	12:g:102:SPO:H181	1.99	0.45
12:e:103:SPO:H10	12:e:103:SPO:H132	1.67	0.45
5:j:24:TYR:HB2	12:j:101:SPO:H343	1.97	0.45
1:L:140:GLY:HA2	6:C:49:ARG:HH22	1.80	0.45
7:F:101:BCL:H18	7:F:101:BCL:H151	1.72	0.45
5:e:45:TRP:HB2	12:e:103:SPO:H42	1.99	0.45
4:f:4:PHE:HZ	5:j:27:GLY:HA2	1.81	0.45
5:g:33:ALA:O	5:g:37:VAL:HG23	2.17	0.45
5:j:24:TYR:CD1	5:j:24:TYR:C	2.93	0.45
5:4:34:VAL:O	5:4:37:VAL:HG22	2.17	0.45
1:L:22:PHE:HA	1:L:24:PHE:CE2	2.52	0.45
2:M:258:PHE:HB3	10:M:1307:PC1:H2	1.99	0.45
7:E:101:BCL:HBB2	12:G:102:SPO:H15	1.97	0.45
4:K:17:PHE:CZ	12:N:101:SPO:H342	2.51	0.45
5:N:20:LEU:HG	12:N:101:SPO:H341	1.99	0.45
4:O:46:ILE:CD1	5:P:46:ARG:HH12	2.29	0.45
1:l:35:GLY:HA2	1:l:38:THR:HG22	1.97	0.45
5:j:46:ARG:HH21	4:k:53:ARG:HB3	1.82	0.45
4:6:6:LYS:NZ	5:ab:19:GLU:OE2	2.49	0.45
4:A:14:ARG:NH1	10:A:104:PC1:H143	2.32	0.45
5:J:33:ALA:O	5:J:37:VAL:HG23	2.17	0.45
4:K:7:ILE:HG21	7:O:101:BCL:H172	1.97	0.45
12:R:102:SPO:H341	12:R:102:SPO:H362	1.77	0.45
4:q:30:MET:O	4:q:34:ILE:HG12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:s:41:TYR:OH	5:t:48:TRP:HB3	2.17	0.45
12:s:105:SPO:H351	12:s:105:SPO:H311	1.84	0.45
1:L:54:VAL:HG21	4:A:33:LEU:HD22	1.99	0.45
7:F:101:BCL:H2A	12:G:102:SPO:H22	1.98	0.45
4:S:40:SER:O	4:S:41:TYR:HB2	2.17	0.45
12:0:102:SPO:H362	12:0:102:SPO:H403	1.74	0.45
4:a:32:HIS:CG	12:3:103:SPO:H41	2.52	0.45
5:e:23:VAL:CG1	12:e:101:SPO:H351	2.46	0.45
4:i:46:ILE:HG21	5:j:46:ARG:NH1	2.31	0.45
12:j:103:SPO:H342	12:j:103:SPO:H312	1.67	0.45
4:k:4:PHE:CZ	12:o:102:SPO:H292	2.52	0.45
4:q:40:SER:O	4:q:41:TYR:HB2	2.15	0.45
4:6:25:PHE:CE2	6:c:35:GLY:HA2	2.52	0.45
6:c:22:TRP:NE1	6:c:26:GLN:HE21	2.15	0.45
1:L:47:ILE:CG2	4:9:30:MET:HE3	2.46	0.44
1:L:211:HIS:CD2	2:M:22:GLU:OE2	2.70	0.44
4:A:14:ARG:CZ	10:A:104:PC1:H111	2.47	0.44
7:J:101:BCL:HMA1	7:K:101:BCL:HMA1	1.98	0.44
4:Q:8:TRP:HZ2	5:R:24:TYR:HD2	1.63	0.44
5:T:33:ALA:O	5:T:37:VAL:HG23	2.17	0.44
8:l:306:BPB:H5A	2:m:63:GLY:HA3	1.98	0.44
2:m:68:PHE:O	2:m:72:ILE:HG12	2.17	0.44
3:h:32:GLN:NE2	10:h:301:PC1:O32	2.48	0.44
4:a:6:LYS:HG2	4:a:9:MET:CE	2.48	0.44
12:d:103:SPO:H392	5:g:23:VAL:HG11	1.99	0.44
12:s:105:SPO:H25	5:v:24:TYR:CD1	2.52	0.44
12:ab:102:SPO:H241	12:ab:102:SPO:H26	1.78	0.44
6:c:7:PHE:CZ	6:c:9:ASP:HB3	2.51	0.44
5:B:33:ALA:O	5:B:37:VAL:HG23	2.17	0.44
12:K:102:SPO:H182	7:Q:101:BCL:H91	1.99	0.44
5:2:43:TYR:HD1	5:2:48:TRP:CZ3	2.35	0.44
6:C:22:TRP:NE1	6:C:26:GLN:HE21	2.15	0.44
1:l:170:ASN:HB3	1:l:173:HIS:CB	2.47	0.44
10:a:103:PC1:H3A2	10:a:103:PC1:H372	1.65	0.44
4:d:8:TRP:HZ2	5:e:24:TYR:CD2	2.35	0.44
12:e:103:SPO:H82	12:e:103:SPO:H5	1.71	0.44
4:f:8:TRP:HZ2	5:g:24:TYR:CD2	2.35	0.44
5:aa:33:ALA:O	5:aa:37:VAL:HG23	2.17	0.44
5:G:49:PHE:CE1	12:G:103:SPO:H132	2.51	0.44
5:N:33:ALA:O	5:N:37:VAL:HG23	2.17	0.44
12:N:103:SPO:H15	12:N:103:SPO:H183	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1:46:ILE:HD11	5:2:45:TRP:HH2	1.82	0.44
4:9:24:LEU:HB2	7:9:101:BCL:H42	1.99	0.44
1:l:22:PHE:HA	1:l:24:PHE:CE2	2.52	0.44
7:l:305:BCL:OBB	7:l:305:BCL:HHC	2.18	0.44
3:H:232:LYS:HB3	3:H:232:LYS:HE3	1.74	0.44
4:A:40:SER:O	4:A:41:TYR:HB2	2.16	0.44
3:h:179:LEU:HB2	3:h:191:LEU:HB2	1.99	0.44
4:a:23:PHE:CD1	10:a:103:PC1:H3D1	2.52	0.44
5:j:7:LEU:O	5:j:7:LEU:HD23	2.17	0.44
4:o:41:TYR:HE1	5:p:46:ARG:HD3	1.82	0.44
7:o:101:BCL:OBB	7:o:101:BCL:HHC	2.17	0.44
2:M:14:GLY:HA3	3:H:140:PHE:CE1	2.52	0.44
4:I:35:LEU:HD11	7:J:101:BCL:HHD	1.99	0.44
4:O:8:TRP:CH2	4:O:17:PHE:HE1	2.34	0.44
4:S:6:LYS:HE2	4:S:9:MET:HE1	1.99	0.44
5:8:33:ALA:O	5:8:37:VAL:HG23	2.17	0.44
2:m:101:TYR:OH	2:m:111:GLU:OE2	2.27	0.44
4:a:15:ARG:NE	10:a:102:PC1:O12	2.50	0.44
5:g:46:ARG:HG2	4:i:53:ARG:NH1	2.32	0.44
7:s:101:BCL:OBB	7:s:101:BCL:HHC	2.18	0.44
12:s:105:SPO:H293	12:s:105:SPO:H26	1.71	0.44
5:v:25:MET:HE1	5:v:28:LEU:HD22	1.99	0.44
7:L:304:BCL:HHC	7:L:304:BCL:OBB	2.18	0.44
3:H:236:TYR:HD2	3:H:236:TYR:O	2.01	0.44
3:H:247:LYS:CB	3:H:247:LYS:NZ	2.81	0.44
12:A:102:SPO:H183	12:B:103:SPO:H343	1.99	0.44
4:D:41:TYR:H	4:D:46:ILE:HD11	1.82	0.44
4:K:17:PHE:HZ	12:N:101:SPO:H342	1.82	0.44
4:K:42:ASN:O	4:K:46:ILE:HG13	2.16	0.44
5:j:33:ALA:O	5:j:37:VAL:HG23	2.17	0.44
5:ab:33:ALA:O	5:ab:37:VAL:HG23	2.17	0.44
6:c:28:MET:HB3	7:c:101:BCL:C9	2.47	0.44
1:L:1:ALA:HB3	3:H:43:GLU:O	2.17	0.44
1:L:45:GLY:HA3	8:L:302:BPB:H9B	1.98	0.44
2:M:68:PHE:O	2:M:72:ILE:HG12	2.17	0.44
12:I:102:SPO:H42	7:K:101:BCL:C2B	2.48	0.44
4:Q:41:TYR:H	4:Q:46:ILE:HD11	1.82	0.44
10:C:1201:PC1:H2B2	10:C:1201:PC1:H2E2	1.80	0.44
4:i:4:PHE:HZ	5:n:27:GLY:HA2	1.83	0.44
2:M:268:TRP:NE1	3:H:35:ASN:HD21	2.16	0.44
3:H:161:ALA:HB2	3:H:210:SER:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:179:LEU:HB2	3:H:191:LEU:HB2	1.99	0.44
12:B:102:SPO:H343	12:B:102:SPO:H312	1.77	0.44
4:F:23:PHE:CD2	7:I:101:BCL:H92	2.53	0.44
4:K:17:PHE:HB3	12:N:103:SPO:H401	1.99	0.44
5:P:33:ALA:O	5:P:37:VAL:HG23	2.17	0.44
4:S:36:LEU:HD23	4:S:42:ASN:HD22	1.83	0.44
1:l:170:ASN:O	1:l:173:HIS:HB3	2.18	0.44
4:a:46:ILE:HD13	5:b:46:ARG:HH22	1.83	0.44
12:o:102:SPO:H27	12:o:102:SPO:H311	1.65	0.44
7:q:101:BCL:HAA2	7:q:101:BCL:HBD	2.00	0.44
1:L:170:ASN:O	1:L:173:HIS:HB3	2.18	0.44
4:D:40:SER:O	4:D:41:TYR:HB2	2.16	0.44
4:I:40:SER:O	4:I:41:TYR:HB2	2.16	0.44
12:N:103:SPO:H312	12:N:103:SPO:H351	1.84	0.44
4:7:3:LYS:CE	4:7:6:LYS:HZ1	2.31	0.44
3:h:236:TYR:HD2	3:h:236:TYR:O	2.01	0.44
5:b:33:ALA:O	5:b:37:VAL:HG23	2.17	0.44
4:q:50:LYS:NZ	4:q:51:TYR:CZ	2.84	0.44
4:s:17:PHE:CZ	12:s:102:SPO:H342	2.53	0.44
7:y:101:BCL:OBB	7:y:101:BCL:HHC	2.18	0.44
2:M:101:TYR:OH	2:M:111:GLU:OE2	2.27	0.43
2:M:286:LEU:HD13	3:H:13:ALA:HA	2.00	0.43
5:G:33:ALA:O	5:G:37:VAL:HG23	2.17	0.43
5:R:33:ALA:O	5:R:37:VAL:HG23	2.17	0.43
3:h:247:LYS:CB	3:h:247:LYS:NZ	2.81	0.43
4:d:40:SER:O	4:d:41:TYR:HB2	2.18	0.43
12:e:101:SPO:H27	12:e:101:SPO:H311	1.66	0.43
4:i:6:LYS:HG2	4:i:9:MET:CE	2.48	0.43
5:j:7:LEU:HD22	5:j:9:TYR:CE1	2.53	0.43
4:s:40:SER:O	4:s:41:TYR:HB2	2.18	0.43
1:L:170:ASN:HB3	1:L:173:HIS:CB	2.47	0.43
2:M:105:PHE:HE1	2:M:116:LEU:HD22	1.83	0.43
7:A:101:BCL:O1D	12:B:102:SPO:H22	2.18	0.43
12:I:102:SPO:C38	5:J:20:LEU:HD12	2.48	0.43
12:T:102:SPO:H312	12:T:102:SPO:H352	1.71	0.43
7:Y:201:BCL:OBB	7:Y:201:BCL:HHC	2.18	0.43
5:p:21:HIS:O	5:p:25:MET:HG2	2.18	0.43
5:p:48:TRP:HZ2	7:p:101:BCL:H141	1.82	0.43
2:M:75:TRP:HE1	12:M:1305:SPO:H22A	1.82	0.43
3:H:255:MET:HE3	3:H:259:TYR:HE2	1.83	0.43
5:B:7:LEU:HD23	5:B:7:LEU:HA	1.68	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:103:SPO:H362	12:B:103:SPO:H393	1.71	0.43
4:Q:40:SER:O	4:Q:41:TYR:HB2	2.18	0.43
4:Y:23:PHE:HE1	4:1:25:PHE:CE1	2.36	0.43
12:g:102:SPO:H403	12:g:102:SPO:H362	1.82	0.43
4:o:6:LYS:HE2	4:o:9:MET:HE1	1.99	0.43
7:3:102:BCL:H8	7:3:102:BCL:H52	1.82	0.43
4:D:8:TRP:HZ2	5:E:24:TYR:HD2	1.66	0.43
7:K:101:BCL:HHC	7:K:101:BCL:OBB	2.18	0.43
4:1:41:TYR:HE2	7:1:101:BCL:HBC2	1.81	0.43
4:7:12:ASP:HB3	4:7:15:ARG:HG2	2.00	0.43
4:9:6:LYS:HG2	4:9:9:MET:CE	2.47	0.43
3:h:161:ALA:HB2	3:h:210:SER:HA	2.00	0.43
5:b:46:ARG:HH21	4:d:53:ARG:HG2	1.83	0.43
7:f:101:BCL:HHC	7:f:101:BCL:OBB	2.19	0.43
4:o:40:SER:O	4:o:41:TYR:HB2	2.18	0.43
4:3:40:SER:O	4:3:41:TYR:HB2	2.18	0.43
7:F:101:BCL:H143	12:G:102:SPO:H37	1.99	0.43
12:I:102:SPO:H42	7:K:101:BCL:C3B	2.48	0.43
5:0:24:TYR:CD1	5:0:24:TYR:C	2.93	0.43
6:C:7:PHE:HZ	4:6:13:PRO:HG2	1.82	0.43
1:l:271:TRP:HZ3	4:y:33:LEU:HD21	1.81	0.43
12:q:102:SPO:H83	7:s:101:BCL:HAA1	2.01	0.43
5:z:48:TRP:C	4:5:51:TYR:HE2	2.27	0.43
1:L:138:MET:HE3	6:C:48:PHE:CD1	2.52	0.43
4:D:46:ILE:HG21	5:E:46:ARG:NH1	2.34	0.43
5:E:7:LEU:HB3	5:E:8:GLY:H	1.59	0.43
4:K:40:SER:O	4:K:41:TYR:HB2	2.18	0.43
12:Q:102:SPO:H83	7:S:101:BCL:HAA1	2.00	0.43
7:W:101:BCL:HHC	7:W:101:BCL:OBB	2.18	0.43
7:2:101:BCL:OBB	7:2:101:BCL:HHC	2.18	0.43
5:8:46:ARG:HH21	4:9:53:ARG:HG2	1.84	0.43
1:l:255:TRP:NE1	1:l:257:ASP:O	2.52	0.43
4:k:10:ILE:HG23	4:o:14:ARG:HG2	2.01	0.43
6:c:31:ALA:HB3	7:c:101:BCL:C7	2.48	0.43
2:M:11:GLN:NE2	2:M:41:TRP:CE2	2.86	0.43
7:A:101:BCL:H91	12:9:102:SPO:H182	2.01	0.43
4:F:41:TYR:H	4:F:46:ILE:HD11	1.83	0.43
4:I:7:ILE:HG21	7:K:101:BCL:H203	2.01	0.43
12:S:102:SPO:H311	12:S:102:SPO:H27	1.62	0.43
6:C:50:VAL:HG21	5:aa:44:ILE:HD13	1.99	0.43
10:l:304:PC1:H2E2	10:l:304:PC1:H2B2	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:h:232:LYS:HE3	3:h:232:LYS:HB3	1.74	0.43
3:h:255:MET:HE3	3:h:259:TYR:HE2	1.83	0.43
7:a:101:BCL:H93	7:a:101:BCL:H112	1.84	0.43
12:e:103:SPO:H21	12:e:103:SPO:H243	1.59	0.43
5:n:25:MET:O	5:n:29:TRP:HD1	2.01	0.43
4:s:5:TYR:CD2	5:t:18:GLN:OE1	2.72	0.43
7:s:103:BCL:HHC	7:s:103:BCL:OBB	2.18	0.43
4:O:6:LYS:HA	4:O:9:MET:HE2	2.00	0.43
4:O:6:LYS:HA	4:O:9:MET:CE	2.48	0.43
7:U:101:BCL:HHC	7:U:101:BCL:OBB	2.18	0.43
2:m:75:TRP:HE1	12:m:1305:SPO:H22A	1.82	0.43
5:z:48:TRP:CD1	5:z:49:PHE:CE2	3.07	0.43
12:3:103:SPO:H25	5:ab:24:TYR:CE1	2.53	0.43
10:L:306:PC1:H242	10:A:103:PC1:H332	2.00	0.43
10:L:306:PC1:H362	10:L:306:PC1:H392	1.84	0.43
2:M:105:PHE:CE1	2:M:116:LEU:HD22	2.54	0.43
5:B:46:ARG:HG2	4:D:53:ARG:NH2	2.33	0.43
4:I:4:PHE:HZ	5:N:27:GLY:HA2	1.84	0.43
7:I:101:BCL:HHC	7:I:101:BCL:OBB	2.18	0.43
7:S:101:BCL:HED1	5:T:31:PHE:CE1	2.54	0.43
2:m:55:LEU:HD23	2:m:55:LEU:HA	1.83	0.43
4:k:35:LEU:HD11	7:k:103:BCL:HHD	2.00	0.43
4:D:24:LEU:HB2	7:D:101:BCL:H42	2.01	0.43
4:K:8:TRP:CZ2	5:N:24:TYR:HD2	2.37	0.43
4:O:40:SER:O	4:O:41:TYR:HB2	2.17	0.43
12:O:102:SPO:H26	12:O:102:SPO:H292	1.80	0.43
7:7:101:BCL:HHD	5:8:42:VAL:HG21	2.01	0.43
7:8:102:BCL:H41	12:0:102:SPO:H26	2.01	0.43
7:9:101:BCL:HED1	5:0:31:PHE:CE1	2.53	0.43
6:C:16:LYS:O	6:C:20:ARG:HG3	2.19	0.43
5:b:49:PHE:O	4:d:51:TYR:OH	2.27	0.43
4:d:15:ARG:HD2	10:d:102:PC1:H11	2.00	0.43
5:e:46:ARG:HG2	4:f:53:ARG:HH11	1.82	0.43
4:q:17:PHE:HZ	12:q:102:SPO:H342	1.83	0.43
4:K:46:ILE:CD1	5:N:46:ARG:HH12	2.04	0.42
4:Q:46:ILE:HG21	5:R:46:ARG:NH1	2.34	0.42
1:l:47:ILE:CG2	4:3:30:MET:HE2	2.44	0.42
2:m:11:GLN:NE2	2:m:41:TRP:CE2	2.86	0.42
4:d:11:PHE:C	5:e:10:THR:HG21	2.44	0.42
4:q:41:TYR:HE1	5:r:46:ARG:HG2	1.82	0.42
12:s:102:SPO:H37	5:t:20:LEU:HG	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:216:PHE:HE2	1:L:222:TYR:O	2.01	0.42
2:M:104:SER:HA	4:O:37:SER:HB3	2.02	0.42
4:A:46:ILE:HG21	5:B:46:ARG:NH1	2.33	0.42
12:D:102:SPO:H27	12:D:102:SPO:H311	1.66	0.42
4:K:24:LEU:HB2	7:K:101:BCL:H42	2.00	0.42
12:N:101:SPO:H341	12:N:101:SPO:H37	2.01	0.42
7:7:101:BCL:HMC3	7:c:101:BCL:HBB1	2.01	0.42
7:l:305:BCL:H111	7:l:305:BCL:H3A	2.01	0.42
12:d:103:SPO:H27	12:d:103:SPO:H311	1.59	0.42
5:g:46:ARG:HH21	4:i:53:ARG:HG3	1.82	0.42
4:i:11:PHE:HB3	4:i:16:VAL:HG21	2.01	0.42
7:5:101:BCL:HHC	7:5:101:BCL:OBB	2.18	0.42
12:aa:101:SPO:H393	12:aa:101:SPO:H362	1.73	0.42
7:D:101:BCL:H141	7:D:101:BCL:H162	1.85	0.42
7:F:101:BCL:HHC	7:F:101:BCL:OBB	2.20	0.42
12:T:102:SPO:H22	7:U:101:BCL:O1D	2.19	0.42
3:h:207:ALA:HA	3:h:241:LEU:HD22	2.02	0.42
4:d:17:PHE:CZ	12:e:101:SPO:H342	2.54	0.42
4:o:3:LYS:HA	4:o:5:TYR:HD1	1.84	0.42
7:r:101:BCL:H143	7:r:101:BCL:H112	1.92	0.42
7:r:101:BCL:H192	7:r:101:BCL:H161	1.86	0.42
4:s:11:PHE:HZ	4:u:17:PHE:HB2	1.84	0.42
5:4:20:LEU:HA	5:4:23:VAL:HG12	2.00	0.42
8:L:305:BPB:H6	8:L:305:BPB:H4	1.83	0.42
4:A:27:LEU:O	4:A:31:ILE:HG13	2.20	0.42
7:D:101:BCL:H91	7:D:101:BCL:H112	1.77	0.42
4:O:46:ILE:CG1	5:P:46:ARG:HH12	2.32	0.42
10:C:1201:PC1:H371	10:C:1201:PC1:H3A1	1.69	0.42
2:m:105:PHE:HE1	2:m:116:LEU:HD22	1.83	0.42
12:o:102:SPO:H83	7:q:101:BCL:HAA1	2.00	0.42
12:s:105:SPO:H20	12:s:105:SPO:H181	1.75	0.42
5:z:39:HIS:CD2	7:z:101:BCL:HBC2	2.54	0.42
1:L:255:TRP:NE1	1:L:257:ASP:O	2.52	0.42
4:U:27:LEU:HD13	4:W:25:PHE:CE1	2.54	0.42
5:2:30:LEU:O	5:2:34:VAL:HG23	2.19	0.42
4:7:3:LYS:HE2	4:7:6:LYS:HZ1	1.84	0.42
4:7:10:ILE:HD11	12:9:102:SPO:H403	2.00	0.42
2:m:105:PHE:CE1	2:m:116:LEU:HD22	2.54	0.42
5:e:49:PHE:O	4:f:51:TYR:OH	2.28	0.42
4:q:9:MET:SD	5:r:17:ALA:HB2	2.59	0.42
4:Q:11:PHE:HZ	4:S:17:PHE:HB2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Q:101:BCL:HED1	5:R:31:PHE:CE1	2.55	0.42
7:S:101:BCL:HHC	7:S:101:BCL:OBB	2.19	0.42
7:9:101:BCL:OBB	7:9:101:BCL:HHC	2.19	0.42
12:9:102:SPO:H27	12:9:102:SPO:H311	1.66	0.42
8:l:306:BPB:H6	8:l:306:BPB:H4	1.83	0.42
3:h:100:PRO:HG2	3:h:104:PRO:HB3	2.01	0.42
3:h:236:TYR:CD2	3:h:236:TYR:C	2.97	0.42
10:h:301:PC1:H121	10:h:302:PC1:H132	2.02	0.42
7:q:101:BCL:H61	7:q:101:BCL:H101	1.50	0.42
5:r:38:ALA:HB1	12:r:102:SPO:H181	2.02	0.42
3:H:130:LYS:HG2	3:H:170:ASP:OD1	2.20	0.42
4:F:24:LEU:HB2	7:F:101:BCL:H42	2.01	0.42
4:K:40:SER:HA	4:K:46:ILE:HD11	2.02	0.42
7:O:101:BCL:OBB	7:O:101:BCL:HHC	2.19	0.42
4:S:6:LYS:HG2	4:S:9:MET:CE	2.49	0.42
1:l:216:PHE:HE2	1:l:222:TYR:O	2.01	0.42
7:a:101:BCL:H91	12:3:103:SPO:H182	2.00	0.42
5:e:24:TYR:HA	12:e:101:SPO:H311	2.02	0.42
12:3:103:SPO:H27	12:3:103:SPO:H311	1.63	0.42
2:M:242:GLY:O	2:M:246:GLU:HG3	2.20	0.42
7:A:101:BCL:HHC	7:A:101:BCL:OBB	2.20	0.42
5:B:47:PRO:HD2	4:D:53:ARG:HH12	1.85	0.42
7:Q:101:BCL:OBB	7:Q:101:BCL:HHC	2.20	0.42
4:7:38:THR:OG1	4:7:40:SER:O	2.21	0.42
1:l:229:ILE:HG21	9:l:303:U10:H3M2	2.01	0.42
10:l:304:PC1:H371	10:l:304:PC1:H3A1	1.69	0.42
4:a:41:TYR:OH	5:b:48:TRP:HB3	2.20	0.42
10:a:102:PC1:H111	10:a:102:PC1:H133	1.80	0.42
4:d:41:TYR:H	4:d:46:ILE:HD11	1.85	0.42
7:k:101:BCL:HHC	7:k:101:BCL:OBB	2.20	0.42
12:q:102:SPO:H27	12:q:102:SPO:H311	1.68	0.42
12:s:102:SPO:C34	5:t:24:TYR:HB2	2.49	0.42
7:w:101:BCL:HHC	7:w:101:BCL:OBB	2.18	0.42
4:5:44:LEU:O	4:5:47:SER:OG	2.37	0.42
4:6:19:ALA:HB1	7:3:102:BCL:H151	2.00	0.42
3:H:207:ALA:HA	3:H:241:LEU:HD22	2.02	0.42
4:A:53:ARG:HG3	5:0:46:ARG:HH21	1.85	0.42
4:q:7:ILE:HA	12:s:102:SPO:H362	2.01	0.42
7:u:101:BCL:HHC	7:u:101:BCL:OBB	2.18	0.42
3:H:190:LEU:HD23	3:H:190:LEU:HA	1.82	0.42
12:A:102:SPO:H27	12:A:102:SPO:H311	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:8:TRP:HZ2	5:G:24:TYR:CD2	2.38	0.42
5:G:46:ARG:NH2	4:I:53:ARG:HG2	2.27	0.42
4:I:27:LEU:O	4:I:31:ILE:HG13	2.20	0.42
12:K:102:SPO:H393	5:P:20:LEU:HD12	2.02	0.42
12:S:102:SPO:H25	5:T:24:TYR:CE1	2.55	0.42
3:h:112:ALA:HA	3:h:235:GLY:O	2.20	0.42
3:h:168:TRP:HB2	3:h:178:PHE:HB2	2.02	0.42
3:h:194:GLN:H	3:h:194:GLN:CD	2.26	0.42
12:e:103:SPO:H15	12:e:103:SPO:H182	1.65	0.42
12:i:102:SPO:H21A	12:i:102:SPO:H82	2.01	0.42
5:z:49:PHE:N	4:5:51:TYR:HE2	2.17	0.42
4:6:15:ARG:HD3	4:6:15:ARG:N	2.35	0.42
7:c:101:BCL:HHC	7:c:101:BCL:OBB	2.20	0.42
1:L:5:PHE:HB2	2:M:246:GLU:OE1	2.20	0.41
1:L:21:LEU:HD12	1:L:21:LEU:HA	1.88	0.41
8:L:302:BPB:H11A	8:L:302:BPB:H14A	1.77	0.41
5:B:48:TRP:HZ2	7:B:101:BCL:H141	1.86	0.41
4:D:17:PHE:CZ	12:D:102:SPO:H342	2.55	0.41
4:s:35:LEU:HD11	7:s:103:BCL:HHD	2.02	0.41
6:c:16:LYS:O	6:c:20:ARG:HG3	2.19	0.41
2:M:16:ALA:HB1	2:M:32:VAL:HG21	2.02	0.41
2:M:190:SER:HB2	7:M:1303:BCL:H3C	2.03	0.41
3:H:100:PRO:HG2	3:H:104:PRO:HB3	2.01	0.41
4:A:26:LEU:HD12	10:A:103:PC1:H2E2	2.03	0.41
7:9:101:BCL:H101	7:9:101:BCL:H52	2.01	0.41
2:m:105:PHE:HE1	12:m:1305:SPO:H403	1.85	0.41
2:m:233:ARG:NH1	3:h:177:ARG:HH21	2.17	0.41
7:a:101:BCL:HHC	7:a:101:BCL:OBB	2.20	0.41
4:k:41:TYR:HE1	5:n:46:ARG:CD	2.33	0.41
7:L:304:BCL:H111	7:L:304:BCL:H3A	2.01	0.41
5:G:48:TRP:HZ2	7:G:101:BCL:H141	1.86	0.41
4:I:29:VAL:O	4:I:33:LEU:HG	2.20	0.41
4:K:27:LEU:O	4:K:31:ILE:HG13	2.21	0.41
12:N:101:SPO:H27	12:N:101:SPO:H311	1.67	0.41
5:P:48:TRP:HZ2	7:P:101:BCL:H141	1.86	0.41
5:T:48:TRP:HZ2	7:T:101:BCL:H141	1.86	0.41
10:h:301:PC1:H231	10:h:302:PC1:H231	2.02	0.41
5:b:48:TRP:HZ2	7:b:101:BCL:H141	1.86	0.41
4:i:42:ASN:O	4:i:46:ILE:HG13	2.20	0.41
4:k:46:ILE:HD13	5:n:46:ARG:HH12	1.85	0.41
7:p:101:BCL:HMA1	7:q:101:BCL:HMA3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:s:102:SPO:H5	12:s:102:SPO:H23	1.90	0.41
1:L:21:LEU:HB2	4:7:15:ARG:HB3	2.02	0.41
1:L:182:THR:CG2	9:L:303:U10:H162	2.51	0.41
9:L:303:U10:H171	9:L:303:U10:H151	1.92	0.41
7:M:1301:BCL:H111	7:M:1301:BCL:H72	1.66	0.41
5:R:48:TRP:HZ2	7:R:101:BCL:H141	1.86	0.41
12:9:102:SPO:H25	5:0:24:TYR:CE1	2.55	0.41
3:h:52:ASN:ND2	10:h:302:PC1:H142	2.36	0.41
4:a:24:LEU:HB2	7:a:101:BCL:H42	2.03	0.41
5:p:36:ILE:O	5:p:40:LEU:HD23	2.20	0.41
1:L:216:PHE:HE2	9:L:303:U10:H102	1.82	0.41
3:H:236:TYR:C	3:H:236:TYR:CD2	2.97	0.41
4:A:53:ARG:NH1	5:0:47:PRO:O	2.47	0.41
12:A:102:SPO:H25	5:B:24:TYR:CE1	2.55	0.41
4:D:27:LEU:O	4:D:31:ILE:HG13	2.21	0.41
5:G:42:VAL:HG23	12:G:102:SPO:H14	2.00	0.41
4:Q:48:ALA:HA	4:Q:53:ARG:HG3	2.03	0.41
2:m:16:ALA:HB1	2:m:32:VAL:HG21	2.02	0.41
3:h:33:THR:HG22	3:h:59:PRO:HB3	2.03	0.41
4:f:10:ILE:HG22	4:f:11:PHE:CD1	2.56	0.41
5:j:48:TRP:HZ2	7:j:102:BCL:H141	1.86	0.41
12:k:102:SPO:H41	4:o:32:HIS:CD2	2.56	0.41
4:o:6:LYS:HG2	4:o:9:MET:CE	2.51	0.41
5:ab:48:TRP:HZ2	7:ab:101:BCL:H141	1.86	0.41
12:ab:102:SPO:H15	12:ab:102:SPO:H183	1.75	0.41
6:c:67:ILE:HG13	6:c:68:THR:N	2.36	0.41
1:L:7:ARG:O	1:L:7:ARG:HG2	2.20	0.41
2:M:23:ASP:N	2:M:23:ASP:OD1	2.53	0.41
4:7:23:PHE:CD2	7:9:101:BCL:H92	2.56	0.41
12:0:102:SPO:H341	12:0:102:SPO:H361	1.87	0.41
4:f:6:LYS:HG2	4:f:9:MET:CE	2.51	0.41
5:j:46:ARG:HG2	4:k:53:ARG:CZ	2.50	0.41
4:k:31:ILE:HD12	4:k:31:ILE:HG23	1.87	0.41
5:aa:48:TRP:HZ2	7:aa:102:BCL:H141	1.86	0.41
1:L:229:ILE:HG21	9:L:303:U10:H3M2	2.02	0.41
3:H:33:THR:HG22	3:H:59:PRO:HB3	2.03	0.41
4:A:46:ILE:CD1	5:B:46:ARG:HH12	2.33	0.41
12:G:102:SPO:H27	12:G:102:SPO:H311	1.80	0.41
5:P:32:SER:OG	7:P:101:BCL:H2	2.21	0.41
5:X:33:ALA:O	5:X:37:VAL:HG23	2.20	0.41
7:9:101:BCL:O1D	12:0:102:SPO:H22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:l:85:LEU:HD23	1:l:85:LEU:HA	1.93	0.41
2:m:190:SER:HB2	7:m:1303:BCL:H3C	2.02	0.41
3:h:52:ASN:HD21	4:a:15:ARG:NE	2.19	0.41
5:p:30:LEU:O	5:p:34:VAL:HG23	2.21	0.41
7:p:101:BCL:H161	7:p:101:BCL:H122	1.82	0.41
5:v:47:PRO:HD2	4:w:53:ARG:NH1	2.36	0.41
5:z:48:TRP:CH2	7:z:101:BCL:HBC3	2.56	0.41
4:5:42:ASN:O	4:5:46:ILE:HG12	2.21	0.41
2:M:105:PHE:HE1	12:M:1305:SPO:H403	1.85	0.41
2:M:223:ILE:HD13	2:M:223:ILE:HA	1.94	0.41
10:M:1307:PC1:H133	10:M:1307:PC1:O14	2.21	0.41
4:Q:9:MET:CE	5:R:14:ASP:HA	2.50	0.41
5:T:32:SER:OG	7:T:101:BCL:H2	2.21	0.41
4:W:42:ASN:O	4:W:46:ILE:HG12	2.21	0.41
1:l:7:ARG:O	1:l:7:ARG:HG2	2.20	0.41
4:a:8:TRP:CZ2	5:b:24:TYR:HD2	2.38	0.41
12:d:103:SPO:HM12	12:d:103:SPO:H22A	1.82	0.41
5:e:48:TRP:HZ2	7:e:102:BCL:H141	1.86	0.41
5:g:48:TRP:HZ2	7:g:101:BCL:H141	1.86	0.41
12:j:103:SPO:H32	7:k:101:BCL:H43	2.02	0.41
4:q:6:LYS:HA	4:q:9:MET:CE	2.51	0.41
12:s:102:SPO:H27	12:s:102:SPO:H311	1.62	0.41
12:s:102:SPO:H343	5:t:24:TYR:HB2	2.01	0.41
4:w:27:LEU:HD23	7:x:101:BCL:HED1	2.02	0.41
3:H:14:SER:HA	3:H:17:ILE:HG22	2.03	0.41
5:E:32:SER:OG	7:E:101:BCL:H2	2.21	0.41
5:E:48:TRP:HZ2	7:E:101:BCL:H141	1.85	0.41
4:I:48:ALA:HA	4:I:53:ARG:HD3	2.03	0.41
5:J:7:LEU:HD11	5:N:12:LEU:HD11	2.03	0.41
5:N:20:LEU:HD12	12:N:101:SPO:C40	2.51	0.41
5:N:48:TRP:HZ2	7:N:102:BCL:H141	1.86	0.41
4:Q:46:ILE:HG21	5:R:46:ARG:HH12	1.86	0.41
4:S:15:ARG:HH22	4:U:14:ARG:CZ	2.34	0.41
5:V:25:MET:HG3	5:V:29:TRP:NE1	2.35	0.41
5:8:32:SER:OG	7:8:102:BCL:H2	2.21	0.41
4:9:17:PHE:CZ	12:9:102:SPO:H342	2.56	0.41
2:m:23:ASP:N	2:m:23:ASP:OD1	2.53	0.41
2:m:152:SER:CB	2:m:274:VAL:HG13	2.51	0.41
2:m:242:GLY:O	2:m:246:GLU:HG3	2.20	0.41
3:h:130:LYS:HG2	3:h:170:ASP:OD1	2.20	0.41
12:d:103:SPO:H403	12:d:103:SPO:H362	1.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:32:SER:OG	7:e:102:BCL:H2	2.21	0.41
12:j:101:SPO:H27	12:j:101:SPO:H311	1.67	0.41
7:q:101:BCL:OBB	7:q:101:BCL:HHC	2.20	0.41
12:s:104:SPO:H343	12:s:104:SPO:H312	1.71	0.41
4:w:42:ASN:O	4:w:46:ILE:HG12	2.21	0.41
5:z:49:PHE:HE2	4:5:43:TRP:HB2	1.80	0.41
5:z:49:PHE:HA	4:5:50:LYS:HD3	2.03	0.41
7:z:101:BCL:O2A	7:z:101:BCL:HMA2	2.21	0.41
5:aa:24:TYR:HE1	12:aa:101:SPO:H25	1.85	0.41
5:aa:32:SER:OG	7:aa:102:BCL:H2	2.21	0.41
12:aa:101:SPO:H341	6:c:20:ARG:HB3	2.02	0.41
4:K:46:ILE:HG21	5:N:46:ARG:NH1	2.35	0.41
4:O:38:THR:HG21	4:Q:44:LEU:HD13	2.03	0.41
1:l:231:ARG:O	1:l:235:LEU:HD13	2.21	0.41
3:h:105:MET:HG3	3:h:243:TYR:HD2	1.86	0.41
12:d:103:SPO:H33	12:d:103:SPO:HM13	1.86	0.41
5:g:41:ALA:CB	12:g:102:SPO:H132	2.51	0.41
5:n:49:PHE:O	4:o:51:TYR:OH	2.21	0.41
7:r:101:BCL:H162	7:r:101:BCL:C10	2.48	0.41
4:y:42:ASN:O	4:y:46:ILE:HG12	2.21	0.41
1:L:199:ASN:OD1	3:H:62:LYS:NZ	2.43	0.40
2:M:164:ARG:O	2:M:168:MET:HG2	2.21	0.40
12:O:102:SPO:H392	12:O:102:SPO:H362	1.86	0.40
4:Y:42:ASN:O	4:Y:46:ILE:HG12	2.21	0.40
4:l:42:ASN:O	4:l:46:ILE:HG12	2.21	0.40
6:C:67:ILE:HG13	6:C:68:THR:N	2.36	0.40
3:h:52:ASN:O	3:h:53:GLN:NE2	2.54	0.40
4:d:41:TYR:OH	5:e:48:TRP:HB3	2.22	0.40
12:e:103:SPO:H5	12:e:103:SPO:H23	1.88	0.40
5:g:32:SER:OG	7:g:101:BCL:H2	2.21	0.40
12:i:102:SPO:H181	12:i:102:SPO:H20	1.46	0.40
7:3:102:BCL:H141	7:3:102:BCL:H162	1.92	0.40
5:ab:32:SER:OG	7:ab:101:BCL:H2	2.21	0.40
6:c:31:ALA:CB	7:c:101:BCL:H51	2.50	0.40
3:H:112:ALA:HA	3:H:235:GLY:O	2.20	0.40
7:A:101:BCL:HMA1	7:O:101:BCL:HMA1	2.02	0.40
4:O:8:TRP:HZ2	5:P:24:TYR:HD2	1.68	0.40
4:O:41:TYR:H	4:O:46:ILE:HD11	1.86	0.40
4:9:17:PHE:HZ	12:9:102:SPO:H342	1.86	0.40
10:h:301:PC1:O14	10:h:301:PC1:H133	2.21	0.40
7:k:101:BCL:H18	7:k:101:BCL:H151	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:263:GLU:CG	2:M:264:GLY:N	2.83	0.40
4:A:41:TYR:N	4:A:46:ILE:HD11	2.35	0.40
5:B:32:SER:OG	7:B:101:BCL:H2	2.21	0.40
5:J:48:TRP:HZ2	7:J:101:BCL:H141	1.86	0.40
5:N:32:SER:OG	7:N:102:BCL:H2	2.21	0.40
4:O:8:TRP:HZ2	5:P:24:TYR:CE2	2.39	0.40
4:Q:17:PHE:CZ	12:Q:102:SPO:H342	2.56	0.40
1:l:182:THR:CG2	9:l:303:U10:H162	2.51	0.40
2:m:29:ARG:HD3	2:m:49:PRO:HG2	2.03	0.40
7:m:1301:BCL:H161	7:m:1301:BCL:H122	1.91	0.40
7:a:101:BCL:H141	7:a:101:BCL:H162	1.93	0.40
7:i:101:BCL:HED3	12:i:102:SPO:H25	2.02	0.40
5:z:15:GLU:N	5:z:15:GLU:OE1	2.54	0.40
10:A:104:PC1:H321	4:9:15:ARG:HB3	2.03	0.40
4:I:31:ILE:HG21	7:J:101:BCL:C1D	2.51	0.40
5:0:32:SER:OG	7:0:101:BCL:H2	2.21	0.40
3:h:236:TYR:HD2	3:h:236:TYR:C	2.30	0.40
12:j:103:SPO:H131	12:j:103:SPO:H15	1.75	0.40
4:u:42:ASN:O	4:u:46:ILE:HG12	2.21	0.40
5:G:32:SER:OG	7:G:101:BCL:H2	2.21	0.40
12:G:102:SPO:H133	12:G:102:SPO:H10	1.64	0.40
4:K:31:ILE:HG21	7:N:102:BCL:C1D	2.51	0.40
4:O:8:TRP:CZ2	5:P:24:TYR:CD2	3.06	0.40
4:Q:17:PHE:HZ	12:Q:102:SPO:H342	1.85	0.40
4:Q:27:LEU:O	4:Q:31:ILE:HG13	2.22	0.40
4:U:42:ASN:O	4:U:46:ILE:HG12	2.21	0.40
4:W:14:ARG:O	4:W:18:VAL:HG23	2.22	0.40
1:l:151:TRP:CH2	2:m:303:MET:HE3	2.56	0.40
2:m:263:GLU:CG	2:m:264:GLY:N	2.84	0.40
10:a:102:PC1:H362	10:a:102:PC1:H392	1.89	0.40
10:a:103:PC1:H381	10:a:103:PC1:H352	1.45	0.40
4:s:51:TYR:HB2	4:s:53:ARG:NE	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	279/282 (99%)	271 (97%)	8 (3%)	0	100	100
1	l	279/282 (99%)	271 (97%)	8 (3%)	0	100	100
2	M	303/308 (98%)	298 (98%)	5 (2%)	0	100	100
2	m	303/308 (98%)	298 (98%)	5 (2%)	0	100	100
3	H	258/260 (99%)	252 (98%)	6 (2%)	0	100	100
3	h	258/260 (99%)	252 (98%)	6 (2%)	0	100	100
4	1	41/58 (71%)	40 (98%)	1 (2%)	0	100	100
4	3	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
4	5	41/58 (71%)	40 (98%)	1 (2%)	0	100	100
4	6	44/58 (76%)	44 (100%)	0	0	100	100
4	7	44/58 (76%)	44 (100%)	0	0	100	100
4	9	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
4	A	52/58 (90%)	52 (100%)	0	0	100	100
4	D	52/58 (90%)	52 (100%)	0	0	100	100
4	F	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
4	I	52/58 (90%)	50 (96%)	2 (4%)	0	100	100
4	K	52/58 (90%)	50 (96%)	2 (4%)	0	100	100
4	O	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
4	Q	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
4	S	52/58 (90%)	50 (96%)	2 (4%)	0	100	100
4	U	42/58 (72%)	41 (98%)	1 (2%)	0	100	100
4	W	41/58 (71%)	40 (98%)	1 (2%)	0	100	100
4	Y	41/58 (71%)	40 (98%)	1 (2%)	0	100	100
4	a	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
4	d	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
4	f	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
4	i	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
4	k	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
4	o	52/58 (90%)	51 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	q	52/58 (90%)	50 (96%)	2 (4%)	0	100	100
4	s	52/58 (90%)	49 (94%)	3 (6%)	0	100	100
4	u	42/58 (72%)	41 (98%)	1 (2%)	0	100	100
4	w	41/58 (71%)	40 (98%)	1 (2%)	0	100	100
4	y	41/58 (71%)	40 (98%)	1 (2%)	0	100	100
5	0	42/49 (86%)	41 (98%)	1 (2%)	0	100	100
5	2	34/49 (69%)	34 (100%)	0	0	100	100
5	4	34/49 (69%)	34 (100%)	0	0	100	100
5	8	42/49 (86%)	41 (98%)	1 (2%)	0	100	100
5	B	42/49 (86%)	41 (98%)	1 (2%)	0	100	100
5	E	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
5	G	42/49 (86%)	41 (98%)	1 (2%)	0	100	100
5	J	41/49 (84%)	39 (95%)	2 (5%)	0	100	100
5	N	36/49 (74%)	35 (97%)	1 (3%)	0	100	100
5	P	36/49 (74%)	35 (97%)	1 (3%)	0	100	100
5	R	36/49 (74%)	35 (97%)	1 (3%)	0	100	100
5	T	36/49 (74%)	35 (97%)	1 (3%)	0	100	100
5	V	35/49 (71%)	35 (100%)	0	0	100	100
5	X	35/49 (71%)	35 (100%)	0	0	100	100
5	Z	35/49 (71%)	34 (97%)	1 (3%)	0	100	100
5	aa	42/49 (86%)	41 (98%)	1 (2%)	0	100	100
5	ab	42/49 (86%)	40 (95%)	2 (5%)	0	100	100
5	b	42/49 (86%)	40 (95%)	2 (5%)	0	100	100
5	e	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
5	g	42/49 (86%)	41 (98%)	1 (2%)	0	100	100
5	j	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
5	n	35/49 (71%)	34 (97%)	1 (3%)	0	100	100
5	p	35/49 (71%)	34 (97%)	1 (3%)	0	100	100
5	r	35/49 (71%)	35 (100%)	0	0	100	100
5	t	35/49 (71%)	34 (97%)	1 (3%)	0	100	100
5	v	35/49 (71%)	35 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	x	35/49 (71%)	35 (100%)	0	0	100	100
5	z	35/49 (71%)	34 (97%)	1 (3%)	0	100	100
6	C	63/82 (77%)	61 (97%)	2 (3%)	0	100	100
6	c	63/82 (77%)	61 (97%)	2 (3%)	0	100	100
All	All	4222/4860 (87%)	4126 (98%)	96 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	220/221 (100%)	217 (99%)	3 (1%)	59	73
1	l	220/221 (100%)	217 (99%)	3 (1%)	59	73
2	M	239/241 (99%)	236 (99%)	3 (1%)	61	74
2	m	239/241 (99%)	236 (99%)	3 (1%)	61	74
3	H	208/208 (100%)	194 (93%)	14 (7%)	15	41
3	h	208/208 (100%)	194 (93%)	14 (7%)	15	41
4	1	38/51 (74%)	35 (92%)	3 (8%)	11	35
4	3	49/51 (96%)	48 (98%)	1 (2%)	48	69
4	5	38/51 (74%)	35 (92%)	3 (8%)	11	35
4	6	43/51 (84%)	43 (100%)	0	100	100
4	7	43/51 (84%)	43 (100%)	0	100	100
4	9	49/51 (96%)	49 (100%)	0	100	100
4	A	49/51 (96%)	49 (100%)	0	100	100
4	D	49/51 (96%)	49 (100%)	0	100	100
4	F	49/51 (96%)	49 (100%)	0	100	100
4	I	49/51 (96%)	49 (100%)	0	100	100
4	K	49/51 (96%)	49 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	O	49/51 (96%)	49 (100%)	0	100	100
4	Q	49/51 (96%)	49 (100%)	0	100	100
4	S	49/51 (96%)	49 (100%)	0	100	100
4	U	39/51 (76%)	36 (92%)	3 (8%)	12	36
4	W	38/51 (74%)	35 (92%)	3 (8%)	11	35
4	Y	38/51 (74%)	35 (92%)	3 (8%)	11	35
4	a	49/51 (96%)	49 (100%)	0	100	100
4	d	49/51 (96%)	49 (100%)	0	100	100
4	f	49/51 (96%)	49 (100%)	0	100	100
4	i	49/51 (96%)	49 (100%)	0	100	100
4	k	49/51 (96%)	49 (100%)	0	100	100
4	o	49/51 (96%)	49 (100%)	0	100	100
4	q	49/51 (96%)	49 (100%)	0	100	100
4	s	49/51 (96%)	49 (100%)	0	100	100
4	u	39/51 (76%)	36 (92%)	3 (8%)	12	36
4	w	38/51 (74%)	35 (92%)	3 (8%)	11	35
4	y	38/51 (74%)	35 (92%)	3 (8%)	11	35
5	0	36/40 (90%)	34 (94%)	2 (6%)	19	46
5	2	30/40 (75%)	30 (100%)	0	100	100
5	4	30/40 (75%)	30 (100%)	0	100	100
5	8	36/40 (90%)	34 (94%)	2 (6%)	19	46
5	B	36/40 (90%)	34 (94%)	2 (6%)	19	46
5	E	35/40 (88%)	33 (94%)	2 (6%)	18	46
5	G	36/40 (90%)	34 (94%)	2 (6%)	19	46
5	J	35/40 (88%)	33 (94%)	2 (6%)	18	46
5	N	32/40 (80%)	30 (94%)	2 (6%)	16	43
5	P	32/40 (80%)	30 (94%)	2 (6%)	16	43
5	R	32/40 (80%)	30 (94%)	2 (6%)	16	43
5	T	32/40 (80%)	30 (94%)	2 (6%)	16	43
5	V	31/40 (78%)	31 (100%)	0	100	100
5	X	31/40 (78%)	31 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	Z	31/40 (78%)	31 (100%)	0	100	100
5	aa	36/40 (90%)	34 (94%)	2 (6%)	19	46
5	ab	36/40 (90%)	34 (94%)	2 (6%)	19	46
5	b	36/40 (90%)	34 (94%)	2 (6%)	19	46
5	e	35/40 (88%)	33 (94%)	2 (6%)	18	46
5	g	36/40 (90%)	34 (94%)	2 (6%)	19	46
5	j	35/40 (88%)	33 (94%)	2 (6%)	18	46
5	n	31/40 (78%)	31 (100%)	0	100	100
5	p	31/40 (78%)	31 (100%)	0	100	100
5	r	31/40 (78%)	31 (100%)	0	100	100
5	t	31/40 (78%)	31 (100%)	0	100	100
5	v	31/40 (78%)	31 (100%)	0	100	100
5	x	31/40 (78%)	31 (100%)	0	100	100
5	z	31/40 (78%)	31 (100%)	0	100	100
6	C	52/66 (79%)	50 (96%)	2 (4%)	29	57
6	c	52/66 (79%)	50 (96%)	2 (4%)	29	57
All	All	3638/4020 (90%)	3537 (97%)	101 (3%)	38	63

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	7	ARG
1	L	52	SER
1	L	202	LYS
2	M	86	LEU
2	M	263	GLU
2	M	287	SER
3	H	4	VAL
3	H	74	THR
3	H	81	GLU
3	H	105	MET
3	H	135	LYS
3	H	143	SER
3	H	159	GLU
3	H	184	LYS
3	H	191	LEU

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Mol	Chain	Res	Type
3	H	223	THR
3	H	232	LYS
3	H	241	LEU
3	H	247	LYS
3	H	251	VAL
5	B	40	LEU
5	B	44	ILE
5	E	40	LEU
5	E	44	ILE
5	G	40	LEU
5	G	44	ILE
5	J	40	LEU
5	J	44	ILE
5	N	40	LEU
5	N	44	ILE
5	P	40	LEU
5	P	44	ILE
5	R	40	LEU
5	R	44	ILE
5	T	40	LEU
5	T	44	ILE
4	U	26	LEU
4	U	30	MET
4	U	33	LEU
4	W	26	LEU
4	W	30	MET
4	W	33	LEU
4	Y	26	LEU
4	Y	30	MET
4	Y	33	LEU
4	1	26	LEU
4	1	30	MET
4	1	33	LEU
5	8	40	LEU
5	8	44	ILE
5	0	40	LEU
5	0	44	ILE
6	C	28	MET
6	C	58	GLN
1	1	7	ARG
1	1	52	SER
1	1	202	LYS

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Mol	Chain	Res	Type
2	m	86	LEU
2	m	263	GLU
2	m	287	SER
3	h	4	VAL
3	h	74	THR
3	h	81	GLU
3	h	105	MET
3	h	135	LYS
3	h	143	SER
3	h	159	GLU
3	h	184	LYS
3	h	191	LEU
3	h	223	THR
3	h	232	LYS
3	h	241	LEU
3	h	247	LYS
3	h	251	VAL
5	b	40	LEU
5	b	44	ILE
5	e	40	LEU
5	e	44	ILE
5	g	40	LEU
5	g	44	ILE
5	j	40	LEU
5	j	44	ILE
4	u	26	LEU
4	u	30	MET
4	u	33	LEU
4	w	26	LEU
4	w	30	MET
4	w	33	LEU
4	y	26	LEU
4	y	30	MET
4	y	33	LEU
4	5	26	LEU
4	5	30	MET
4	5	33	LEU
5	aa	40	LEU
5	aa	44	ILE
4	3	20	GLN
5	ab	40	LEU
5	ab	44	ILE

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Mol	Chain	Res	Type
6	c	28	MET
6	c	58	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	280	ASN
3	H	204	HIS
5	E	16	GLN
5	G	16	GLN
4	I	42	ASN
5	Z	21	HIS
4	1	20	GLN
6	C	58	GLN
6	C	66	ASN
1	l	280	ASN
3	h	35	ASN
3	h	68	HIS
3	h	204	HIS
5	b	21	HIS
5	j	16	GLN
5	t	18	GLN
4	5	20	GLN
6	c	58	GLN
6	c	66	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 131 ligands modelled in this entry, 2 are monoatomic - leaving 129 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
7	BCL	i	101	-	69,74,74	1.14	5 (7%)	83,115,115	1.57	12 (14%)
7	BCL	c	101	-	64,69,74	1.21	7 (10%)	77,109,115	1.72	15 (19%)
8	BPB	l	302	-	54,67,70	1.58	5 (9%)	52,97,101	2.40	12 (23%)
12	SPO	n	101	-	40,41,41	5.72	17 (42%)	47,50,50	5.53	30 (63%)
7	BCL	5	101	-	49,54,74	1.28	5 (10%)	59,91,115	1.70	11 (18%)
7	BCL	u	101	-	54,59,74	1.26	5 (9%)	65,97,115	1.76	13 (20%)
7	BCL	j	102	5	69,74,74	1.09	5 (7%)	83,115,115	1.51	12 (14%)
10	PC1	L	306	-	42,42,53	1.14	2 (4%)	48,50,61	1.01	2 (4%)
12	SPO	U	102	-	40,41,41	5.54	17 (42%)	47,50,50	5.53	31 (65%)
7	BCL	K	101	-	69,74,74	1.11	7 (10%)	83,115,115	1.50	12 (14%)
7	BCL	8	102	5	69,74,74	1.10	5 (7%)	83,115,115	1.51	13 (15%)
12	SPO	B	102	-	40,41,41	5.60	17 (42%)	47,50,50	5.60	32 (68%)
9	U10	L	303	-	43,43,63	2.70	13 (30%)	52,55,79	1.66	13 (25%)
12	SPO	Q	102	-	36,37,41	5.84	16 (44%)	42,45,50	5.53	26 (61%)
7	BCL	Z	101	-	49,54,74	1.26	5 (10%)	59,91,115	1.48	6 (10%)
7	BCL	J	101	5	69,74,74	1.10	5 (7%)	83,115,115	1.51	13 (15%)
12	SPO	s	102	-	40,41,41	5.72	17 (42%)	47,50,50	5.24	29 (61%)
7	BCL	N	102	5	69,74,74	1.10	5 (7%)	83,115,115	1.51	13 (15%)
10	PC1	C	1201	-	53,53,53	1.12	3 (5%)	59,61,61	0.94	3 (5%)
12	SPO	A	102	-	40,41,41	5.68	17 (42%)	47,50,50	5.26	29 (61%)
12	SPO	M	1305	-	40,41,41	5.60	17 (42%)	47,50,50	5.30	31 (65%)
12	SPO	K	102	-	40,41,41	5.74	17 (42%)	47,50,50	5.26	28 (59%)
7	BCL	R	101	5	69,74,74	1.09	5 (7%)	83,115,115	1.51	13 (15%)
12	SPO	s	105	-	40,41,41	5.76	17 (42%)	47,50,50	5.41	30 (63%)
8	BPB	L	305	-	47,60,70	1.74	6 (12%)	44,89,101	2.33	10 (22%)
7	BCL	T	101	5	69,74,74	1.10	5 (7%)	83,115,115	1.50	12 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	PC1	d	102	-	40,40,53	1.17	3 (7%)	46,48,61	1.14	4 (8%)
12	SPO	e	101	-	40,41,41	5.69	17 (42%)	47,50,50	5.24	29 (61%)
7	BCL	x	101	5	49,54,74	1.29	4 (8%)	59,91,115	1.51	9 (15%)
12	SPO	g	102	-	40,41,41	5.62	17 (42%)	47,50,50	5.61	29 (61%)
12	SPO	k	102	-	30,31,41	5.01	15 (50%)	36,38,50	6.44	28 (77%)
12	SPO	a	104	-	40,41,41	5.51	17 (42%)	47,50,50	5.69	31 (65%)
7	BCL	o	101	-	69,74,74	1.14	6 (8%)	83,115,115	1.48	11 (13%)
7	BCL	Q	101	-	69,74,74	1.15	7 (10%)	83,115,115	1.51	13 (15%)
7	BCL	5	102	-	49,54,74	1.26	5 (10%)	59,91,115	1.59	13 (22%)
13	CDL	m	1306	-	99,99,99	1.07	7 (7%)	105,111,111	0.95	5 (4%)
7	BCL	a	101	-	69,74,74	1.15	8 (11%)	83,115,115	1.50	12 (14%)
7	BCL	9	101	-	69,74,74	1.17	8 (11%)	83,115,115	1.60	13 (15%)
7	BCL	D	101	-	69,74,74	1.15	7 (10%)	83,115,115	1.51	12 (14%)
7	BCL	l	305	2	69,74,74	1.16	7 (10%)	83,115,115	1.51	12 (14%)
12	SPO	O	103	-	40,41,41	5.72	17 (42%)	47,50,50	5.46	31 (65%)
12	SPO	s	104	-	40,41,41	5.69	17 (42%)	47,50,50	5.30	29 (61%)
12	SPO	0	102	-	40,41,41	5.47	17 (42%)	47,50,50	5.63	31 (65%)
7	BCL	aa	102	5	69,74,74	1.10	5 (7%)	83,115,115	1.51	13 (15%)
12	SPO	q	102	-	40,41,41	5.72	17 (42%)	47,50,50	5.26	29 (61%)
10	PC1	A	104	-	45,45,53	1.10	3 (6%)	51,53,61	1.03	4 (7%)
7	BCL	y	101	-	49,54,74	1.28	5 (10%)	59,91,115	1.70	11 (18%)
12	SPO	8	101	-	40,41,41	5.16	16 (40%)	47,50,50	5.96	34 (72%)
10	PC1	h	302	-	28,28,53	1.55	5 (17%)	34,36,61	1.30	3 (8%)
12	SPO	d	103	-	40,41,41	5.24	15 (37%)	47,50,50	6.17	31 (65%)
12	SPO	aa	101	-	40,41,41	5.16	17 (42%)	47,50,50	6.05	34 (72%)
7	BCL	F	101	-	69,74,74	1.14	7 (10%)	83,115,115	1.54	15 (18%)
8	BPB	l	306	-	47,60,70	1.73	6 (12%)	44,89,101	2.32	10 (22%)
12	SPO	e	103	-	35,36,41	5.52	16 (45%)	41,44,50	6.71	29 (70%)
12	SPO	i	102	-	40,41,41	5.41	17 (42%)	47,50,50	6.23	27 (57%)
12	SPO	G	103	-	40,41,41	5.61	17 (42%)	47,50,50	5.53	32 (68%)
13	CDL	M	1306	-	99,99,99	1.07	7 (7%)	105,111,111	0.95	5 (4%)
7	BCL	U	101	-	69,74,74	1.13	5 (7%)	83,115,115	1.56	14 (16%)
10	PC1	A	103	-	50,50,53	1.09	3 (6%)	56,58,61	0.97	3 (5%)
7	BCL	7	101	-	64,69,74	1.16	6 (9%)	77,109,115	1.68	11 (14%)
12	SPO	I	102	-	40,41,41	5.74	17 (42%)	47,50,50	5.27	28 (59%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	BCL	M	1301	1	69,74,74	1.15	7 (10%)	83,115,115	1.68	15 (18%)
9	U10	M	1304	-	48,48,63	2.67	14 (29%)	58,61,79	1.65	13 (22%)
7	BCL	p	101	5	69,74,74	1.08	6 (8%)	83,115,115	1.58	15 (18%)
10	PC1	h	301	-	47,47,53	1.13	3 (6%)	53,55,61	1.10	4 (7%)
12	SPO	t	101	-	40,41,41	5.26	17 (42%)	47,50,50	5.96	31 (65%)
7	BCL	S	101	-	59,64,74	1.22	7 (11%)	71,103,115	1.57	11 (15%)
7	BCL	P	101	5	69,74,74	1.10	5 (7%)	83,115,115	1.51	13 (15%)
7	BCL	d	101	-	69,74,74	1.17	7 (10%)	83,115,115	1.53	13 (15%)
7	BCL	s	101	-	69,74,74	1.12	5 (7%)	83,115,115	1.52	12 (14%)
7	BCL	r	101	5	69,74,74	1.08	5 (7%)	83,115,115	1.46	10 (12%)
7	BCL	2	101	-	49,54,74	1.28	5 (10%)	59,91,115	1.70	12 (20%)
12	SPO	N	101	-	40,41,41	5.74	17 (42%)	47,50,50	5.24	28 (59%)
7	BCL	A	101	-	69,74,74	1.15	6 (8%)	83,115,115	1.47	12 (14%)
12	SPO	m	1305	-	40,41,41	5.60	17 (42%)	47,50,50	5.30	31 (65%)
12	SPO	G	102	-	40,41,41	5.57	17 (42%)	47,50,50	5.91	31 (65%)
12	SPO	j	101	-	40,41,41	5.70	17 (42%)	47,50,50	5.18	28 (59%)
7	BCL	L	301	-	69,74,74	1.15	7 (10%)	83,115,115	1.46	11 (13%)
7	BCL	q	101	-	69,74,74	1.09	5 (7%)	83,115,115	1.56	12 (14%)
7	BCL	3	102	-	69,74,74	1.18	7 (10%)	83,115,115	1.54	12 (14%)
7	BCL	B	101	5	69,74,74	1.10	5 (7%)	83,115,115	1.51	13 (15%)
12	SPO	ab	102	-	40,41,41	5.56	17 (42%)	47,50,50	5.93	32 (68%)
7	BCL	m	1303	-	69,74,74	1.16	7 (10%)	83,115,115	1.51	11 (13%)
7	BCL	w	101	-	49,54,74	1.27	4 (8%)	59,91,115	1.70	12 (20%)
10	PC1	M	1307	-	52,52,53	1.08	3 (5%)	58,60,61	1.12	4 (6%)
12	SPO	3	101	-	40,41,41	5.70	17 (42%)	47,50,50	5.26	30 (63%)
12	SPO	F	102	-	40,41,41	5.67	17 (42%)	47,50,50	5.21	29 (61%)
12	SPO	9	102	-	40,41,41	5.69	17 (42%)	47,50,50	5.19	27 (57%)
7	BCL	1	101	-	49,54,74	1.20	5 (10%)	59,91,115	2.02	14 (23%)
7	BCL	L	304	2	69,74,74	1.16	7 (10%)	83,115,115	1.50	13 (15%)
7	BCL	m	1301	1	69,74,74	1.15	7 (10%)	83,115,115	1.68	15 (18%)
8	BPB	L	302	-	54,67,70	1.58	5 (9%)	52,97,101	2.40	12 (23%)
7	BCL	ab	101	5	69,74,74	1.10	5 (7%)	83,115,115	1.51	13 (15%)
7	BCL	U	103	5	49,54,74	1.27	5 (10%)	59,91,115	1.75	13 (22%)
7	BCL	W	101	-	49,54,74	1.28	5 (10%)	59,91,115	1.70	12 (20%)
7	BCL	e	102	5	69,74,74	1.10	5 (7%)	83,115,115	1.51	13 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	BCL	G	101	5	69,74,74	1.10	5 (7%)	83,115,115	1.51	13 (15%)
12	SPO	S	102	-	36,37,41	5.85	16 (44%)	42,45,50	5.60	26 (61%)
12	SPO	T	102	-	40,41,41	5.66	17 (42%)	47,50,50	5.52	31 (65%)
7	BCL	k	101	-	69,74,74	1.14	6 (8%)	83,115,115	1.58	12 (14%)
9	U10	l	303	-	63,63,63	2.71	17 (26%)	76,79,79	1.73	21 (27%)
9	U10	m	1304	-	48,48,63	2.67	14 (29%)	58,61,79	1.65	13 (22%)
12	SPO	D	102	-	40,41,41	5.70	17 (42%)	47,50,50	5.25	29 (61%)
10	PC1	a	103	-	48,48,53	1.14	3 (6%)	54,56,61	1.12	5 (9%)
12	SPO	r	102	-	40,41,41	5.61	17 (42%)	47,50,50	5.59	32 (68%)
10	PC1	l	304	-	47,47,53	1.17	3 (6%)	53,55,61	0.96	3 (5%)
7	BCL	Y	201	-	49,54,74	1.27	5 (10%)	59,91,115	1.70	12 (20%)
7	BCL	E	101	5	69,74,74	1.10	5 (7%)	83,115,115	1.51	13 (15%)
7	BCL	0	101	5	69,74,74	1.10	5 (7%)	83,115,115	1.51	13 (15%)
12	SPO	B	103	-	40,41,41	5.56	17 (42%)	47,50,50	5.45	30 (63%)
7	BCL	X	101	5	49,54,74	1.26	5 (10%)	59,91,115	1.62	8 (13%)
12	SPO	3	103	-	40,41,41	5.60	17 (42%)	47,50,50	5.46	31 (65%)
7	BCL	s	103	5	49,54,74	1.29	5 (10%)	59,91,115	1.66	11 (18%)
12	SPO	o	102	-	40,41,41	5.72	17 (42%)	47,50,50	5.30	28 (59%)
7	BCL	z	101	-	49,54,74	1.31	5 (10%)	59,91,115	1.69	10 (16%)
7	BCL	k	103	-	69,74,74	1.09	4 (5%)	83,115,115	1.66	15 (18%)
7	BCL	M	1303	-	69,74,74	1.15	7 (10%)	83,115,115	1.51	11 (13%)
7	BCL	v	101	5	69,74,74	1.10	4 (5%)	83,115,115	1.52	13 (15%)
7	BCL	O	101	-	69,74,74	1.14	7 (10%)	83,115,115	1.50	12 (14%)
7	BCL	I	101	-	69,74,74	1.14	7 (10%)	83,115,115	1.51	12 (14%)
7	BCL	l	301	-	69,74,74	1.15	7 (10%)	83,115,115	1.46	11 (13%)
7	BCL	f	101	-	69,74,74	1.16	7 (10%)	83,115,115	1.51	12 (14%)
12	SPO	N	103	-	40,41,41	5.63	17 (42%)	47,50,50	5.86	30 (63%)
10	PC1	a	102	-	39,39,53	1.23	3 (7%)	45,47,61	1.03	3 (6%)
12	SPO	R	102	-	40,41,41	5.69	17 (42%)	47,50,50	5.24	32 (68%)
7	BCL	b	101	5	69,74,74	1.10	5 (7%)	83,115,115	1.51	13 (15%)
12	SPO	O	102	-	40,41,41	5.53	17 (42%)	47,50,50	5.69	33 (70%)
12	SPO	j	103	-	40,41,41	5.60	17 (42%)	47,50,50	5.68	32 (68%)
7	BCL	g	101	5	69,74,74	1.10	6 (8%)	83,115,115	1.51	13 (15%)

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
7	BCL	i	101	-	-	11/41/137/137	-
7	BCL	c	101	-	-	9/35/131/137	-
8	BPB	l	302	-	-	9/34/102/105	0/5/6/6
12	SPO	n	101	-	-	28/47/47/47	-
7	BCL	5	101	-	-	0/17/113/137	-
7	BCL	u	101	-	-	1/23/119/137	-
7	BCL	j	102	5	-	4/41/137/137	-
10	PC1	L	306	-	-	11/46/46/57	-
12	SPO	U	102	-	-	20/47/47/47	-
7	BCL	K	101	-	-	6/41/137/137	-
7	BCL	8	102	5	-	4/41/137/137	-
12	SPO	B	102	-	-	19/47/47/47	-
9	U10	L	303	-	-	16/39/63/87	0/1/1/1
12	SPO	Q	102	-	-	21/43/43/47	-
7	BCL	Z	101	-	-	2/17/113/137	-
7	BCL	J	101	5	-	4/41/137/137	-
12	SPO	s	102	-	-	23/47/47/47	-
7	BCL	N	102	5	-	4/41/137/137	-
10	PC1	C	1201	-	-	25/57/57/57	-
12	SPO	A	102	-	-	23/47/47/47	-
12	SPO	M	1305	-	-	25/47/47/47	-
12	SPO	K	102	-	-	25/47/47/47	-
7	BCL	R	101	5	-	4/41/137/137	-
12	SPO	s	105	-	-	25/47/47/47	-
8	BPB	L	305	-	-	7/25/93/105	0/5/6/6
7	BCL	T	101	5	-	4/41/137/137	-
10	PC1	d	102	-	-	5/44/44/57	-
12	SPO	e	101	-	-	24/47/47/47	-
7	BCL	x	101	5	-	4/17/113/137	-
12	SPO	g	102	-	-	27/47/47/47	-
12	SPO	k	102	-	-	18/35/35/47	-
12	SPO	a	104	-	-	22/47/47/47	-
7	BCL	o	101	-	-	9/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BCL	Q	101	-	-	3/41/137/137	-
7	BCL	5	102	-	-	8/17/113/137	-
13	CDL	m	1306	-	-	44/110/110/110	-
7	BCL	a	101	-	-	7/41/137/137	-
7	BCL	9	101	-	-	7/41/137/137	-
7	BCL	D	101	-	-	7/41/137/137	-
7	BCL	l	305	2	-	6/41/137/137	-
12	SPO	O	103	-	-	26/47/47/47	-
12	SPO	s	104	-	-	20/47/47/47	-
12	SPO	0	102	-	-	16/47/47/47	-
7	BCL	aa	102	5	-	4/41/137/137	-
12	SPO	q	102	-	-	23/47/47/47	-
10	PC1	A	104	-	-	16/49/49/57	-
7	BCL	y	101	-	-	0/17/113/137	-
12	SPO	8	101	-	-	18/47/47/47	-
10	PC1	h	302	-	-	14/32/32/57	-
12	SPO	d	103	-	-	22/47/47/47	-
12	SPO	aa	101	-	-	16/47/47/47	-
7	BCL	F	101	-	-	6/41/137/137	-
8	BPB	l	306	-	-	7/25/93/105	0/5/6/6
12	SPO	e	103	-	-	18/41/41/47	-
12	SPO	i	102	-	-	18/47/47/47	-
12	SPO	G	103	-	-	21/47/47/47	-
13	CDL	M	1306	-	-	44/110/110/110	-
7	BCL	U	101	-	-	2/41/137/137	-
10	PC1	A	103	-	-	13/54/54/57	-
7	BCL	7	101	-	-	6/35/131/137	-
12	SPO	I	102	-	-	23/47/47/47	-
7	BCL	M	1301	1	-	11/41/137/137	-
9	U10	M	1304	-	-	5/45/69/87	0/1/1/1
7	BCL	p	101	5	-	6/41/137/137	-
10	PC1	h	301	-	-	23/51/51/57	-
12	SPO	t	101	-	-	18/47/47/47	-
7	BCL	S	101	-	-	3/29/125/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BCL	P	101	5	-	4/41/137/137	-
7	BCL	d	101	-	-	8/41/137/137	-
7	BCL	s	101	-	-	4/41/137/137	-
7	BCL	r	101	5	-	15/41/137/137	-
7	BCL	2	101	-	-	0/17/113/137	-
12	SPO	N	101	-	-	24/47/47/47	-
7	BCL	A	101	-	-	6/41/137/137	-
12	SPO	m	1305	-	-	25/47/47/47	-
12	SPO	G	102	-	-	22/47/47/47	-
12	SPO	j	101	-	-	25/47/47/47	-
7	BCL	L	301	-	-	5/41/137/137	-
7	BCL	q	101	-	-	12/41/137/137	-
7	BCL	3	102	-	-	8/41/137/137	-
7	BCL	B	101	5	-	4/41/137/137	-
12	SPO	ab	102	-	-	22/47/47/47	-
7	BCL	m	1303	-	-	1/41/137/137	-
7	BCL	w	101	-	-	0/17/113/137	-
10	PC1	M	1307	-	-	25/56/56/57	-
12	SPO	3	101	-	-	25/47/47/47	-
12	SPO	F	102	-	-	24/47/47/47	-
12	SPO	9	102	-	-	24/47/47/47	-
7	BCL	1	101	-	-	6/17/113/137	-
7	BCL	L	304	2	-	6/41/137/137	-
7	BCL	m	1301	1	-	11/41/137/137	-
8	BPB	L	302	-	-	8/34/102/105	0/5/6/6
7	BCL	ab	101	5	-	4/41/137/137	-
7	BCL	U	103	5	-	5/17/113/137	-
7	BCL	W	101	-	-	0/17/113/137	-
7	BCL	e	102	5	-	4/41/137/137	-
7	BCL	G	101	5	-	4/41/137/137	-
12	SPO	S	102	-	-	21/43/43/47	-
12	SPO	T	102	-	-	19/47/47/47	-
7	BCL	k	101	-	-	6/41/137/137	-
9	U10	l	303	-	-	24/63/87/87	0/1/1/1
9	U10	m	1304	-	-	5/45/69/87	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	SPO	D	102	-	-	23/47/47/47	-
10	PC1	a	103	-	-	26/52/52/57	-
12	SPO	r	102	-	-	20/47/47/47	-
10	PC1	l	304	-	-	23/51/51/57	-
7	BCL	Y	201	-	-	0/17/113/137	-
7	BCL	E	101	5	-	4/41/137/137	-
7	BCL	0	101	5	-	4/41/137/137	-
12	SPO	B	103	-	-	23/47/47/47	-
7	BCL	X	101	5	-	3/17/113/137	-
12	SPO	3	103	-	-	24/47/47/47	-
7	BCL	s	103	5	-	3/17/113/137	-
12	SPO	o	102	-	-	24/47/47/47	-
7	BCL	z	101	-	-	6/17/113/137	-
7	BCL	k	103	-	-	5/41/137/137	-
7	BCL	M	1303	-	-	2/41/137/137	-
7	BCL	v	101	5	-	15/41/137/137	-
7	BCL	O	101	-	-	6/41/137/137	-
7	BCL	I	101	-	-	3/41/137/137	-
7	BCL	l	301	-	-	5/41/137/137	-
7	BCL	f	101	-	-	5/41/137/137	-
12	SPO	N	103	-	-	25/47/47/47	-
10	PC1	a	102	-	-	20/43/43/57	-
12	SPO	R	102	-	-	21/47/47/47	-
7	BCL	b	101	5	-	4/41/137/137	-
12	SPO	O	102	-	-	19/47/47/47	-
12	SPO	j	103	-	-	26/47/47/47	-
7	BCL	g	101	5	-	4/41/137/137	-

All (1234) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	O	103	SPO	C27-C28	19.02	1.53	1.34
12	s	105	SPO	C27-C28	18.77	1.53	1.34
12	K	102	SPO	C27-C28	18.75	1.53	1.34
12	3	101	SPO	C27-C28	18.71	1.53	1.34
12	q	102	SPO	C27-C28	18.71	1.53	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	I	102	SPO	C27-C28	18.71	1.53	1.34
12	e	101	SPO	C27-C28	18.70	1.53	1.34
12	D	102	SPO	C27-C28	18.69	1.53	1.34
12	9	102	SPO	C27-C28	18.68	1.53	1.34
12	N	103	SPO	C27-C28	18.60	1.53	1.34
12	o	102	SPO	C27-C28	18.59	1.53	1.34
12	A	102	SPO	C27-C28	18.57	1.53	1.34
12	3	103	SPO	C27-C28	18.55	1.53	1.34
12	N	101	SPO	C27-C28	18.54	1.53	1.34
12	T	102	SPO	C27-C28	18.46	1.53	1.34
12	j	101	SPO	C27-C28	18.45	1.53	1.34
12	F	102	SPO	C27-C28	18.44	1.53	1.34
12	s	102	SPO	C27-C28	18.44	1.53	1.34
12	S	102	SPO	C27-C28	18.42	1.53	1.34
12	s	104	SPO	C27-C28	18.41	1.53	1.34
12	R	102	SPO	C27-C28	18.39	1.53	1.34
12	Q	102	SPO	C27-C28	18.35	1.53	1.34
12	B	102	SPO	C27-C28	18.35	1.53	1.34
12	ab	102	SPO	C27-C28	18.35	1.53	1.34
12	n	101	SPO	C27-C28	18.33	1.53	1.34
12	G	102	SPO	C27-C28	18.17	1.52	1.34
12	r	102	SPO	C27-C28	18.16	1.52	1.34
12	i	102	SPO	C27-C28	18.13	1.52	1.34
12	M	1305	SPO	C27-C28	18.07	1.52	1.34
12	O	102	SPO	C27-C28	18.07	1.52	1.34
12	j	103	SPO	C27-C28	18.05	1.52	1.34
12	m	1305	SPO	C27-C28	18.04	1.52	1.34
12	G	103	SPO	C27-C28	17.89	1.52	1.34
12	U	102	SPO	C27-C28	17.80	1.52	1.34
12	a	104	SPO	C27-C28	17.77	1.52	1.34
12	g	102	SPO	C27-C28	17.76	1.52	1.34
12	B	103	SPO	C27-C28	17.50	1.52	1.34
12	e	103	SPO	C27-C28	17.43	1.52	1.34
12	0	102	SPO	C27-C28	17.39	1.52	1.34
12	d	103	SPO	C27-C28	17.34	1.52	1.34
12	8	101	SPO	C27-C28	17.28	1.52	1.34
12	t	101	SPO	C27-C28	17.11	1.51	1.34
12	aa	101	SPO	C27-C28	17.05	1.51	1.34
12	s	102	SPO	C14-C12	13.92	1.54	1.35
12	F	102	SPO	C14-C12	13.89	1.54	1.35
12	Q	102	SPO	C14-C12	13.86	1.54	1.35
12	o	102	SPO	C14-C12	13.83	1.54	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	N	101	SPO	C14-C12	13.82	1.54	1.35
12	g	102	SPO	C14-C12	13.82	1.54	1.35
12	j	101	SPO	C14-C12	13.79	1.54	1.35
12	K	102	SPO	C14-C12	13.77	1.54	1.35
12	D	102	SPO	C14-C12	13.76	1.54	1.35
12	G	102	SPO	C14-C12	13.74	1.54	1.35
12	I	102	SPO	C14-C12	13.72	1.54	1.35
12	q	102	SPO	C14-C12	13.72	1.54	1.35
12	e	101	SPO	C14-C12	13.71	1.54	1.35
12	3	101	SPO	C14-C12	13.70	1.53	1.35
12	9	102	SPO	C14-C12	13.68	1.53	1.35
12	A	102	SPO	C14-C12	13.66	1.53	1.35
12	s	105	SPO	C14-C12	13.64	1.53	1.35
12	n	101	SPO	C14-C12	13.63	1.53	1.35
12	S	102	SPO	C14-C12	13.62	1.53	1.35
12	R	102	SPO	C14-C12	13.62	1.53	1.35
12	G	103	SPO	C14-C12	13.59	1.53	1.35
12	N	103	SPO	C14-C12	13.59	1.53	1.35
12	T	102	SPO	C14-C12	13.57	1.53	1.35
12	O	103	SPO	C14-C12	13.55	1.53	1.35
12	m	1305	SPO	C14-C12	13.49	1.53	1.35
12	j	103	SPO	C14-C12	13.48	1.53	1.35
12	M	1305	SPO	C14-C12	13.45	1.53	1.35
12	s	104	SPO	C14-C12	13.44	1.53	1.35
12	U	102	SPO	C14-C12	13.40	1.53	1.35
12	3	103	SPO	C14-C12	13.36	1.53	1.35
12	ab	102	SPO	C14-C12	13.35	1.53	1.35
12	B	102	SPO	C14-C12	13.32	1.53	1.35
12	n	101	SPO	C9-C7	13.31	1.53	1.35
12	B	103	SPO	C14-C12	13.30	1.53	1.35
12	r	102	SPO	C14-C12	13.26	1.53	1.35
12	0	102	SPO	C14-C12	13.26	1.53	1.35
12	O	102	SPO	C14-C12	13.23	1.53	1.35
12	a	104	SPO	C14-C12	13.19	1.53	1.35
12	N	101	SPO	C19-C17	13.17	1.53	1.35
12	e	103	SPO	C14-C12	13.16	1.53	1.35
12	R	102	SPO	C22-C23	13.10	1.53	1.35
12	B	103	SPO	C9-C7	13.10	1.53	1.35
12	s	105	SPO	C19-C17	13.07	1.53	1.35
12	G	103	SPO	C9-C7	13.06	1.53	1.35
12	T	102	SPO	C22-C23	13.05	1.53	1.35
12	s	105	SPO	C22-C23	13.04	1.53	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	r	102	SPO	C22-C23	13.02	1.53	1.35
12	a	104	SPO	C9-C7	13.02	1.53	1.35
12	K	102	SPO	C22-C23	13.01	1.53	1.35
12	K	102	SPO	C19-C17	13.00	1.53	1.35
12	N	103	SPO	C22-C23	13.00	1.53	1.35
12	o	102	SPO	C22-C23	13.00	1.53	1.35
12	N	101	SPO	C22-C23	12.98	1.53	1.35
12	e	101	SPO	C19-C17	12.98	1.53	1.35
12	3	101	SPO	C22-C23	12.98	1.53	1.35
12	s	102	SPO	C19-C17	12.97	1.53	1.35
12	S	102	SPO	C19-C17	12.95	1.53	1.35
12	I	102	SPO	C19-C17	12.94	1.52	1.35
12	9	102	SPO	C19-C17	12.93	1.52	1.35
12	g	102	SPO	C19-C17	12.93	1.52	1.35
12	q	102	SPO	C22-C23	12.92	1.52	1.35
12	Q	102	SPO	C19-C17	12.92	1.52	1.35
12	O	103	SPO	C19-C17	12.90	1.52	1.35
12	q	102	SPO	C19-C17	12.90	1.52	1.35
12	o	102	SPO	C19-C17	12.89	1.52	1.35
12	s	104	SPO	C22-C23	12.89	1.52	1.35
12	s	104	SPO	C9-C7	12.89	1.52	1.35
12	j	101	SPO	C19-C17	12.88	1.52	1.35
12	j	103	SPO	C9-C7	12.87	1.52	1.35
12	s	102	SPO	C22-C23	12.86	1.52	1.35
12	s	104	SPO	C19-C17	12.86	1.52	1.35
12	Q	102	SPO	C22-C23	12.85	1.52	1.35
12	n	101	SPO	C22-C23	12.85	1.52	1.35
12	m	1305	SPO	C22-C23	12.84	1.52	1.35
12	B	102	SPO	C9-C7	12.84	1.52	1.35
12	R	102	SPO	C19-C17	12.83	1.52	1.35
12	n	101	SPO	C19-C17	12.83	1.52	1.35
12	I	102	SPO	C22-C23	12.83	1.52	1.35
12	d	103	SPO	C14-C12	12.83	1.52	1.35
12	j	101	SPO	C22-C23	12.83	1.52	1.35
12	S	102	SPO	C22-C23	12.82	1.52	1.35
12	D	102	SPO	C22-C23	12.81	1.52	1.35
12	m	1305	SPO	C19-C17	12.81	1.52	1.35
12	9	102	SPO	C22-C23	12.80	1.52	1.35
12	s	102	SPO	C9-C7	12.80	1.52	1.35
12	M	1305	SPO	C22-C23	12.80	1.52	1.35
12	D	102	SPO	C19-C17	12.79	1.52	1.35
12	A	102	SPO	C19-C17	12.79	1.52	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	0	102	SPO	C9-C7	12.79	1.52	1.35
12	M	1305	SPO	C19-C17	12.77	1.52	1.35
12	B	103	SPO	C22-C23	12.77	1.52	1.35
12	k	102	SPO	C14-C12	12.77	1.52	1.35
12	U	102	SPO	C19-C17	12.76	1.52	1.35
12	e	101	SPO	C22-C23	12.76	1.52	1.35
12	O	103	SPO	C22-C23	12.76	1.52	1.35
12	A	102	SPO	C22-C23	12.75	1.52	1.35
12	I	102	SPO	C9-C7	12.75	1.52	1.35
12	j	101	SPO	C9-C7	12.75	1.52	1.35
12	g	102	SPO	C22-C23	12.73	1.52	1.35
12	i	102	SPO	C19-C17	12.72	1.52	1.35
12	q	102	SPO	C9-C7	12.71	1.52	1.35
12	3	101	SPO	C19-C17	12.70	1.52	1.35
12	F	102	SPO	C22-C23	12.70	1.52	1.35
12	F	102	SPO	C9-C7	12.69	1.52	1.35
12	F	102	SPO	C19-C17	12.69	1.52	1.35
12	T	102	SPO	C19-C17	12.68	1.52	1.35
12	U	102	SPO	C22-C23	12.66	1.52	1.35
12	K	102	SPO	C9-C7	12.66	1.52	1.35
12	R	102	SPO	C9-C7	12.65	1.52	1.35
12	j	103	SPO	C22-C23	12.64	1.52	1.35
12	G	102	SPO	C22-C23	12.62	1.52	1.35
12	G	102	SPO	C9-C7	12.62	1.52	1.35
12	G	103	SPO	C22-C23	12.61	1.52	1.35
12	N	101	SPO	C9-C7	12.61	1.52	1.35
12	M	1305	SPO	C9-C7	12.60	1.52	1.35
12	r	102	SPO	C19-C17	12.60	1.52	1.35
12	3	103	SPO	C22-C23	12.59	1.52	1.35
12	m	1305	SPO	C9-C7	12.58	1.52	1.35
12	S	102	SPO	C9-C7	12.58	1.52	1.35
12	O	103	SPO	C9-C7	12.57	1.52	1.35
12	D	102	SPO	C9-C7	12.56	1.52	1.35
12	s	105	SPO	C9-C7	12.56	1.52	1.35
12	T	102	SPO	C9-C7	12.54	1.52	1.35
12	B	103	SPO	C19-C17	12.54	1.52	1.35
12	B	102	SPO	C19-C17	12.54	1.52	1.35
12	r	102	SPO	C9-C7	12.52	1.52	1.35
12	o	102	SPO	C9-C7	12.52	1.52	1.35
12	3	101	SPO	C9-C7	12.51	1.52	1.35
12	O	102	SPO	C19-C17	12.50	1.52	1.35
12	t	101	SPO	C14-C12	12.49	1.52	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	3	103	SPO	C19-C17	12.49	1.52	1.35
12	A	102	SPO	C9-C7	12.49	1.52	1.35
12	g	102	SPO	C9-C7	12.46	1.52	1.35
12	O	102	SPO	C22-C23	12.46	1.52	1.35
12	G	103	SPO	C19-C17	12.45	1.52	1.35
12	ab	102	SPO	C9-C7	12.44	1.52	1.35
12	8	101	SPO	C14-C12	12.44	1.52	1.35
12	O	102	SPO	C9-C7	12.42	1.52	1.35
12	N	103	SPO	C9-C7	12.40	1.52	1.35
12	j	103	SPO	C19-C17	12.40	1.52	1.35
12	9	102	SPO	C9-C7	12.40	1.52	1.35
12	e	101	SPO	C9-C7	12.38	1.52	1.35
12	U	102	SPO	C9-C7	12.37	1.52	1.35
12	B	102	SPO	C22-C23	12.37	1.52	1.35
12	Q	102	SPO	C9-C7	12.36	1.52	1.35
12	ab	102	SPO	C22-C23	12.33	1.52	1.35
12	0	102	SPO	C19-C17	12.33	1.52	1.35
12	ab	102	SPO	C19-C17	12.31	1.52	1.35
12	N	103	SPO	C19-C17	12.31	1.52	1.35
12	k	102	SPO	C22-C23	12.28	1.52	1.35
12	0	102	SPO	C22-C23	12.25	1.52	1.35
12	a	104	SPO	C22-C23	12.24	1.52	1.35
12	i	102	SPO	C14-C12	12.19	1.51	1.35
12	e	103	SPO	C22-C23	12.16	1.51	1.35
12	G	102	SPO	C19-C17	12.16	1.51	1.35
12	a	104	SPO	C19-C17	12.13	1.51	1.35
12	aa	101	SPO	C14-C12	12.10	1.51	1.35
12	3	103	SPO	C9-C7	12.08	1.51	1.35
12	e	103	SPO	C9-C7	12.01	1.51	1.35
12	k	102	SPO	C19-C17	11.96	1.51	1.35
12	i	102	SPO	C22-C23	11.94	1.51	1.35
12	i	102	SPO	C9-C7	11.90	1.51	1.35
12	t	101	SPO	C22-C23	11.81	1.51	1.35
12	t	101	SPO	C9-C7	11.73	1.51	1.35
12	t	101	SPO	C19-C17	11.70	1.51	1.35
12	e	103	SPO	C19-C17	11.60	1.51	1.35
12	aa	101	SPO	C22-C23	11.56	1.51	1.35
12	d	103	SPO	C19-C17	11.55	1.51	1.35
12	k	102	SPO	C9-C7	11.54	1.51	1.35
12	8	101	SPO	C19-C17	11.46	1.51	1.35
12	d	103	SPO	C9-C7	11.36	1.50	1.35
12	aa	101	SPO	C19-C17	11.32	1.50	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	8	101	SPO	C22-C23	11.30	1.50	1.35
12	aa	101	SPO	C9-C7	11.24	1.50	1.35
12	d	103	SPO	C22-C23	11.21	1.50	1.35
12	8	101	SPO	C9-C7	11.20	1.50	1.35
12	s	105	SPO	C32-C33	9.13	1.54	1.33
12	d	103	SPO	C32-C33	8.96	1.54	1.33
12	N	101	SPO	C32-C33	8.90	1.54	1.33
12	I	102	SPO	C32-C33	8.88	1.54	1.33
12	S	102	SPO	C32-C33	8.82	1.54	1.33
12	A	102	SPO	C32-C33	8.81	1.54	1.33
12	K	102	SPO	C32-C33	8.80	1.54	1.33
12	Q	102	SPO	C32-C33	8.79	1.54	1.33
12	s	102	SPO	C32-C33	8.78	1.54	1.33
12	s	104	SPO	C32-C33	8.77	1.54	1.33
12	3	103	SPO	C32-C33	8.77	1.54	1.33
12	D	102	SPO	C32-C33	8.76	1.54	1.33
12	O	103	SPO	C32-C33	8.76	1.54	1.33
12	j	101	SPO	C32-C33	8.75	1.54	1.33
12	9	102	SPO	C32-C33	8.74	1.53	1.33
12	o	102	SPO	C32-C33	8.73	1.53	1.33
12	F	102	SPO	C32-C33	8.73	1.53	1.33
12	r	102	SPO	C32-C33	8.72	1.53	1.33
12	3	101	SPO	C32-C33	8.72	1.53	1.33
12	n	101	SPO	C32-C33	8.71	1.53	1.33
12	q	102	SPO	C32-C33	8.68	1.53	1.33
12	G	102	SPO	C32-C33	8.66	1.53	1.33
8	l	306	BPB	CAC-C3C	8.65	1.55	1.33
12	G	103	SPO	C32-C33	8.65	1.53	1.33
8	L	305	BPB	CAC-C3C	8.64	1.55	1.33
12	B	102	SPO	C32-C33	8.64	1.53	1.33
12	g	102	SPO	C32-C33	8.63	1.53	1.33
12	T	102	SPO	C32-C33	8.63	1.53	1.33
12	e	101	SPO	C32-C33	8.63	1.53	1.33
12	N	103	SPO	C32-C33	8.60	1.53	1.33
12	ab	102	SPO	C32-C33	8.60	1.53	1.33
12	R	102	SPO	C32-C33	8.59	1.53	1.33
12	M	1305	SPO	C32-C33	8.54	1.53	1.33
12	m	1305	SPO	C32-C33	8.53	1.53	1.33
12	O	102	SPO	C32-C33	8.51	1.53	1.33
12	j	103	SPO	C32-C33	8.50	1.53	1.33
12	aa	101	SPO	C32-C33	8.47	1.53	1.33
12	B	103	SPO	C32-C33	8.43	1.53	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	U	102	SPO	C32-C33	8.42	1.53	1.33
12	a	104	SPO	C32-C33	8.42	1.53	1.33
12	0	102	SPO	C32-C33	8.37	1.53	1.33
12	t	101	SPO	C32-C33	8.16	1.52	1.33
12	i	102	SPO	C32-C33	8.06	1.52	1.33
8	l	302	BPB	CAC-C3C	8.06	1.53	1.33
12	8	101	SPO	C32-C33	8.05	1.52	1.33
8	L	302	BPB	CAC-C3C	8.02	1.53	1.33
12	s	104	SPO	C37-C38	7.76	1.54	1.32
12	I	102	SPO	C37-C38	7.73	1.54	1.32
12	t	101	SPO	C37-C38	7.71	1.54	1.32
12	8	101	SPO	C37-C38	7.69	1.54	1.32
12	3	103	SPO	C37-C38	7.67	1.54	1.32
12	o	102	SPO	C37-C38	7.67	1.54	1.32
12	j	103	SPO	C37-C38	7.67	1.54	1.32
12	aa	101	SPO	C37-C38	7.67	1.54	1.32
12	n	101	SPO	C37-C38	7.66	1.54	1.32
12	9	102	SPO	C37-C38	7.65	1.54	1.32
12	B	102	SPO	C37-C38	7.65	1.54	1.32
12	G	103	SPO	C37-C38	7.59	1.54	1.32
12	ab	102	SPO	C37-C38	7.59	1.54	1.32
12	R	102	SPO	C37-C38	7.55	1.54	1.32
12	O	103	SPO	C37-C38	7.55	1.54	1.32
12	m	1305	SPO	C37-C38	7.54	1.54	1.32
12	3	101	SPO	C37-C38	7.54	1.54	1.32
12	M	1305	SPO	C37-C38	7.54	1.54	1.32
12	g	102	SPO	C37-C38	7.53	1.54	1.32
12	A	102	SPO	C37-C38	7.52	1.54	1.32
12	O	102	SPO	C37-C38	7.52	1.54	1.32
12	e	101	SPO	C37-C38	7.51	1.54	1.32
12	d	103	SPO	C37-C38	7.50	1.53	1.32
12	r	102	SPO	C37-C38	7.50	1.53	1.32
12	T	102	SPO	C37-C38	7.49	1.53	1.32
12	s	105	SPO	C37-C38	7.48	1.53	1.32
12	a	104	SPO	C37-C38	7.47	1.53	1.32
12	s	102	SPO	C37-C38	7.46	1.53	1.32
12	N	103	SPO	C37-C38	7.43	1.53	1.32
12	K	102	SPO	C37-C38	7.43	1.53	1.32
12	0	102	SPO	C37-C38	7.42	1.53	1.32
12	D	102	SPO	C37-C38	7.42	1.53	1.32
12	G	102	SPO	C37-C38	7.41	1.53	1.32
12	U	102	SPO	C37-C38	7.40	1.53	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	103	SPO	C37-C38	7.39	1.53	1.32
12	i	102	SPO	C37-C38	7.36	1.53	1.32
12	F	102	SPO	C37-C38	7.35	1.53	1.32
12	j	101	SPO	C37-C38	7.35	1.53	1.32
12	N	101	SPO	C37-C38	7.33	1.53	1.32
12	e	103	SPO	C32-C33	7.32	1.53	1.32
12	q	102	SPO	C37-C38	7.31	1.53	1.32
12	k	102	SPO	C27-C28	7.20	1.52	1.35
9	l	303	U10	C38-C39	6.29	1.48	1.33
9	l	303	U10	C43-C44	6.05	1.47	1.33
9	l	303	U10	C18-C19	6.04	1.47	1.33
9	L	303	U10	C18-C19	6.02	1.47	1.33
9	L	303	U10	C28-C29	5.99	1.47	1.33
9	l	303	U10	C23-C24	5.98	1.47	1.33
9	l	303	U10	C28-C29	5.97	1.47	1.33
9	L	303	U10	C23-C24	5.93	1.47	1.33
9	M	1304	U10	C28-C29	5.93	1.47	1.33
9	l	303	U10	C8-C9	5.92	1.47	1.33
9	L	303	U10	C8-C9	5.92	1.47	1.33
9	M	1304	U10	C33-C34	5.92	1.47	1.33
9	l	303	U10	C48-C49	5.91	1.47	1.33
9	l	303	U10	C33-C34	5.90	1.47	1.33
9	m	1304	U10	C28-C29	5.89	1.47	1.33
9	m	1304	U10	C33-C34	5.87	1.47	1.33
9	m	1304	U10	C8-C9	5.83	1.47	1.33
9	M	1304	U10	C13-C14	5.82	1.46	1.33
9	L	303	U10	C13-C14	5.82	1.46	1.33
9	M	1304	U10	C8-C9	5.82	1.46	1.33
9	l	303	U10	C13-C14	5.81	1.46	1.33
9	m	1304	U10	C13-C14	5.80	1.46	1.33
9	M	1304	U10	C18-C19	5.77	1.46	1.33
9	m	1304	U10	C18-C19	5.76	1.46	1.33
9	M	1304	U10	C23-C24	5.71	1.46	1.33
9	m	1304	U10	C23-C24	5.70	1.46	1.33
9	m	1304	U10	O3-C3	-5.58	1.23	1.36
9	M	1304	U10	O3-C3	-5.58	1.23	1.36
9	M	1304	U10	O4-C4	-5.56	1.23	1.36
9	m	1304	U10	O4-C4	-5.55	1.23	1.36
9	l	303	U10	O4-C4	-5.49	1.23	1.36
9	L	303	U10	O4-C4	-5.47	1.23	1.36
9	l	303	U10	O3-C3	-5.44	1.23	1.36
9	L	303	U10	O3-C3	-5.41	1.23	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	l	303	U10	C53-C54	5.31	1.47	1.32
9	m	1304	U10	C38-C39	5.15	1.47	1.32
9	L	303	U10	C33-C34	5.13	1.47	1.32
9	M	1304	U10	C38-C39	5.12	1.47	1.32
7	S	101	BCL	MG-NA	4.91	2.17	2.06
7	z	101	BCL	MG-NA	4.88	2.17	2.06
7	d	101	BCL	MG-NA	4.81	2.17	2.06
7	s	101	BCL	MG-NA	4.79	2.17	2.06
7	x	101	BCL	MG-NA	4.76	2.17	2.06
7	y	101	BCL	MG-NA	4.76	2.17	2.06
7	Q	101	BCL	MG-NA	4.76	2.17	2.06
7	5	101	BCL	MG-NA	4.75	2.17	2.06
7	s	103	BCL	MG-NA	4.75	2.17	2.06
7	W	101	BCL	MG-NA	4.74	2.17	2.06
7	Y	201	BCL	MG-NA	4.74	2.17	2.06
7	w	101	BCL	MG-NA	4.74	2.17	2.06
7	u	101	BCL	MG-NA	4.73	2.17	2.06
7	k	101	BCL	MG-NA	4.73	2.17	2.06
7	2	101	BCL	MG-NA	4.72	2.17	2.06
7	U	101	BCL	MG-NA	4.72	2.17	2.06
7	O	101	BCL	MG-NA	4.72	2.17	2.06
7	f	101	BCL	MG-NA	4.72	2.17	2.06
7	a	101	BCL	MG-NA	4.70	2.17	2.06
7	o	101	BCL	MG-NA	4.68	2.17	2.06
7	I	101	BCL	MG-NA	4.67	2.17	2.06
7	A	101	BCL	MG-NA	4.65	2.17	2.06
7	K	101	BCL	MG-NA	4.64	2.17	2.06
7	9	101	BCL	MG-NA	4.64	2.17	2.06
7	c	101	BCL	MG-NA	4.64	2.17	2.06
7	ab	101	BCL	MG-NA	4.63	2.17	2.06
7	B	101	BCL	MG-NA	4.63	2.17	2.06
7	J	101	BCL	MG-NA	4.62	2.17	2.06
7	v	101	BCL	MG-NA	4.62	2.17	2.06
7	E	101	BCL	MG-NA	4.62	2.17	2.06
7	aa	102	BCL	MG-NA	4.61	2.17	2.06
7	T	101	BCL	MG-NA	4.61	2.17	2.06
7	X	101	BCL	MG-NA	4.61	2.17	2.06
7	P	101	BCL	MG-NA	4.60	2.17	2.06
7	g	101	BCL	MG-NA	4.60	2.17	2.06
7	e	102	BCL	MG-NA	4.60	2.17	2.06
7	G	101	BCL	MG-NA	4.60	2.17	2.06
7	j	102	BCL	MG-NA	4.59	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	8	102	BCL	MG-NA	4.59	2.17	2.06
7	0	101	BCL	MG-NA	4.59	2.17	2.06
7	F	101	BCL	MG-NA	4.58	2.17	2.06
7	b	101	BCL	MG-NA	4.58	2.17	2.06
7	R	101	BCL	MG-NA	4.58	2.17	2.06
7	D	101	BCL	MG-NA	4.57	2.17	2.06
7	N	102	BCL	MG-NA	4.57	2.17	2.06
7	Z	101	BCL	MG-NA	4.52	2.17	2.06
7	5	102	BCL	MG-NA	4.50	2.17	2.06
7	U	103	BCL	MG-NA	4.49	2.16	2.06
7	p	101	BCL	MG-NA	4.48	2.16	2.06
7	q	101	BCL	MG-NA	4.40	2.16	2.06
7	l	301	BCL	MG-NA	4.37	2.16	2.06
7	i	101	BCL	MG-NA	4.37	2.16	2.06
7	L	301	BCL	MG-NA	4.36	2.16	2.06
7	k	103	BCL	MG-NA	4.35	2.16	2.06
7	l	305	BCL	MG-NA	4.34	2.16	2.06
7	L	304	BCL	MG-NA	4.31	2.16	2.06
7	m	1303	BCL	MG-NA	4.30	2.16	2.06
7	3	102	BCL	MG-NA	4.26	2.16	2.06
7	1	101	BCL	MG-NA	4.25	2.16	2.06
7	M	1303	BCL	MG-NA	4.24	2.16	2.06
7	M	1301	BCL	MG-NA	4.19	2.16	2.06
7	m	1301	BCL	MG-NA	4.17	2.16	2.06
7	r	101	BCL	MG-NA	4.10	2.16	2.06
12	g	102	SPO	C16-C17	4.10	1.54	1.45
8	L	305	BPB	CBD-CGD	-4.05	1.47	1.52
7	7	101	BCL	MG-NA	4.05	2.15	2.06
8	l	306	BPB	CBD-CGD	-4.01	1.47	1.52
12	n	101	SPO	C11-C12	4.00	1.54	1.45
12	O	103	SPO	C20-C19	3.99	1.55	1.43
12	N	101	SPO	C20-C19	3.98	1.55	1.43
12	n	101	SPO	C10-C9	3.98	1.55	1.43
12	N	101	SPO	C15-C14	3.97	1.55	1.43
12	Q	102	SPO	C20-C19	3.97	1.55	1.43
12	K	102	SPO	C20-C19	3.96	1.55	1.43
12	9	102	SPO	C20-C19	3.95	1.55	1.43
12	q	102	SPO	C20-C19	3.95	1.55	1.43
12	e	101	SPO	C15-C14	3.93	1.55	1.43
12	q	102	SPO	C15-C14	3.93	1.55	1.43
12	e	101	SPO	C20-C19	3.93	1.55	1.43
12	a	104	SPO	C6-C7	3.92	1.54	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	l	302	BPB	CBD-CGD	-3.92	1.47	1.52
12	S	102	SPO	C20-C19	3.92	1.55	1.43
12	I	102	SPO	C11-C12	3.92	1.54	1.45
12	K	102	SPO	C15-C14	3.91	1.55	1.43
12	j	101	SPO	C15-C14	3.91	1.55	1.43
8	L	302	BPB	CBD-CGD	-3.90	1.47	1.52
12	O	103	SPO	C15-C14	3.90	1.55	1.43
12	B	103	SPO	C10-C9	3.90	1.55	1.43
12	j	103	SPO	C20-C19	3.90	1.55	1.43
12	s	105	SPO	C11-C12	3.90	1.54	1.45
12	s	105	SPO	C6-C7	3.89	1.54	1.45
12	A	102	SPO	C20-C19	3.89	1.55	1.43
12	s	102	SPO	C20-C19	3.89	1.55	1.43
12	3	101	SPO	C20-C19	3.89	1.55	1.43
12	o	102	SPO	C15-C14	3.89	1.55	1.43
12	3	101	SPO	C15-C14	3.89	1.55	1.43
12	R	102	SPO	C20-C19	3.89	1.55	1.43
12	n	101	SPO	C20-C19	3.88	1.55	1.43
12	o	102	SPO	C20-C19	3.88	1.55	1.43
12	s	102	SPO	C15-C14	3.88	1.55	1.43
12	s	105	SPO	C10-C9	3.88	1.55	1.43
12	g	102	SPO	C15-C14	3.88	1.55	1.43
12	I	102	SPO	C15-C14	3.88	1.55	1.43
12	F	102	SPO	C15-C14	3.87	1.55	1.43
12	F	102	SPO	C11-C12	3.87	1.54	1.45
12	D	102	SPO	C15-C14	3.87	1.55	1.43
12	S	102	SPO	C15-C14	3.87	1.55	1.43
12	s	105	SPO	C20-C19	3.87	1.55	1.43
12	9	102	SPO	C15-C14	3.86	1.55	1.43
12	Q	102	SPO	C15-C14	3.85	1.55	1.43
12	I	102	SPO	C20-C19	3.85	1.55	1.43
12	D	102	SPO	C20-C19	3.85	1.55	1.43
12	s	102	SPO	C11-C12	3.85	1.54	1.45
12	n	101	SPO	C6-C7	3.85	1.54	1.45
12	q	102	SPO	C11-C12	3.84	1.54	1.45
12	T	102	SPO	C20-C19	3.84	1.55	1.43
12	B	103	SPO	C11-C12	3.84	1.54	1.45
12	i	102	SPO	C16-C17	3.84	1.54	1.45
12	e	101	SPO	C11-C12	3.83	1.54	1.45
12	F	102	SPO	C20-C19	3.83	1.55	1.43
12	j	101	SPO	C20-C19	3.83	1.55	1.43
12	A	102	SPO	C15-C14	3.83	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	R	102	SPO	C10-C9	3.83	1.55	1.43
12	R	102	SPO	C11-C12	3.82	1.54	1.45
12	R	102	SPO	C15-C14	3.82	1.55	1.43
12	s	102	SPO	C10-C9	3.82	1.55	1.43
12	S	102	SPO	C11-C12	3.82	1.54	1.45
12	e	101	SPO	C16-C17	3.81	1.54	1.45
12	s	104	SPO	C20-C19	3.81	1.55	1.43
12	M	1305	SPO	C20-C19	3.81	1.55	1.43
12	I	102	SPO	C21-C22	3.80	1.55	1.43
12	o	102	SPO	C10-C9	3.80	1.55	1.43
12	K	102	SPO	C21-C22	3.80	1.55	1.43
12	A	102	SPO	C11-C12	3.80	1.54	1.45
12	d	103	SPO	C15-C14	3.80	1.55	1.43
12	K	102	SPO	C11-C12	3.80	1.54	1.45
13	m	1306	CDL	OB6-CB5	3.80	1.45	1.34
12	D	102	SPO	C11-C12	3.79	1.54	1.45
12	I	102	SPO	C10-C9	3.79	1.55	1.43
12	N	101	SPO	C10-C9	3.79	1.55	1.43
12	i	102	SPO	C15-C14	3.79	1.55	1.43
12	s	105	SPO	C15-C14	3.79	1.55	1.43
12	s	104	SPO	C15-C14	3.79	1.55	1.43
12	o	102	SPO	C11-C12	3.78	1.54	1.45
12	s	102	SPO	C16-C17	3.78	1.54	1.45
12	3	103	SPO	C15-C14	3.78	1.55	1.43
12	Q	102	SPO	C16-C17	3.78	1.54	1.45
12	m	1305	SPO	C20-C19	3.78	1.55	1.43
12	a	104	SPO	C10-C9	3.78	1.55	1.43
12	K	102	SPO	C10-C9	3.78	1.55	1.43
12	B	103	SPO	C20-C19	3.78	1.55	1.43
12	B	103	SPO	C6-C7	3.78	1.54	1.45
12	N	101	SPO	C21-C22	3.78	1.55	1.43
13	M	1306	CDL	OB6-CB5	3.78	1.45	1.34
12	N	101	SPO	C16-C17	3.77	1.54	1.45
12	r	102	SPO	C20-C19	3.77	1.55	1.43
12	D	102	SPO	C21-C22	3.77	1.55	1.43
12	3	103	SPO	C20-C19	3.77	1.55	1.43
12	A	102	SPO	C10-C9	3.76	1.55	1.43
12	g	102	SPO	C20-C19	3.75	1.55	1.43
12	s	104	SPO	C10-C9	3.75	1.55	1.43
12	3	103	SPO	C11-C12	3.75	1.54	1.45
12	q	102	SPO	C10-C9	3.75	1.55	1.43
12	F	102	SPO	C10-C9	3.75	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	j	103	SPO	C21-C22	3.75	1.55	1.43
12	n	101	SPO	C15-C14	3.75	1.55	1.43
12	A	102	SPO	C21-C22	3.75	1.55	1.43
12	j	101	SPO	C11-C12	3.75	1.54	1.45
12	S	102	SPO	C10-C9	3.75	1.55	1.43
12	a	104	SPO	C11-C12	3.74	1.54	1.45
12	j	101	SPO	C10-C9	3.74	1.55	1.43
12	D	102	SPO	C10-C9	3.74	1.55	1.43
12	F	102	SPO	C16-C17	3.74	1.54	1.45
12	9	102	SPO	C16-C17	3.73	1.54	1.45
12	T	102	SPO	C15-C14	3.73	1.55	1.43
12	B	103	SPO	C15-C14	3.73	1.55	1.43
12	j	101	SPO	C16-C17	3.73	1.53	1.45
12	9	102	SPO	C21-C22	3.72	1.55	1.43
12	o	102	SPO	C21-C22	3.72	1.55	1.43
12	N	101	SPO	C11-C12	3.72	1.53	1.45
12	j	103	SPO	C11-C12	3.72	1.53	1.45
12	s	102	SPO	C21-C22	3.72	1.55	1.43
12	G	103	SPO	C15-C14	3.72	1.55	1.43
12	ab	102	SPO	C6-C7	3.72	1.53	1.45
12	3	101	SPO	C11-C12	3.72	1.53	1.45
12	3	101	SPO	C21-C22	3.72	1.55	1.43
12	Q	102	SPO	C21-C22	3.72	1.55	1.43
12	G	103	SPO	C20-C19	3.72	1.55	1.43
12	A	102	SPO	C16-C17	3.71	1.53	1.45
12	B	102	SPO	C15-C14	3.71	1.55	1.43
12	9	102	SPO	C10-C9	3.71	1.55	1.43
12	j	101	SPO	C21-C22	3.71	1.54	1.43
12	G	103	SPO	C11-C12	3.71	1.53	1.45
12	O	103	SPO	C21-C22	3.71	1.54	1.43
12	F	102	SPO	C21-C22	3.71	1.54	1.43
12	Q	102	SPO	C11-C12	3.71	1.53	1.45
12	ab	102	SPO	C11-C12	3.71	1.53	1.45
12	3	101	SPO	C16-C17	3.70	1.53	1.45
12	e	101	SPO	C21-C22	3.70	1.54	1.43
12	0	102	SPO	C10-C9	3.70	1.54	1.43
12	G	103	SPO	C10-C9	3.69	1.54	1.43
12	U	102	SPO	C15-C14	3.69	1.54	1.43
12	k	102	SPO	C15-C14	3.69	1.54	1.43
12	n	101	SPO	C21-C22	3.69	1.54	1.43
12	s	104	SPO	C11-C12	3.69	1.53	1.45
12	j	103	SPO	C15-C14	3.69	1.54	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	I	102	SPO	C16-C17	3.68	1.53	1.45
12	S	102	SPO	C16-C17	3.68	1.53	1.45
12	e	101	SPO	C10-C9	3.68	1.54	1.43
12	q	102	SPO	C21-C22	3.68	1.54	1.43
12	K	102	SPO	C16-C17	3.68	1.53	1.45
12	B	102	SPO	C20-C19	3.68	1.54	1.43
12	Q	102	SPO	C10-C9	3.68	1.54	1.43
12	j	103	SPO	C10-C9	3.67	1.54	1.43
12	ab	102	SPO	C20-C19	3.67	1.54	1.43
12	s	105	SPO	C21-C22	3.67	1.54	1.43
12	m	1305	SPO	C15-C14	3.67	1.54	1.43
12	O	103	SPO	C26-C27	3.67	1.54	1.43
12	U	102	SPO	C20-C19	3.67	1.54	1.43
12	o	102	SPO	C16-C17	3.67	1.53	1.45
12	G	102	SPO	C21-C22	3.67	1.54	1.43
12	M	1305	SPO	C15-C14	3.67	1.54	1.43
12	S	102	SPO	C21-C22	3.66	1.54	1.43
12	3	101	SPO	C10-C9	3.66	1.54	1.43
12	r	102	SPO	C15-C14	3.66	1.54	1.43
12	q	102	SPO	C16-C17	3.66	1.53	1.45
12	O	102	SPO	C15-C14	3.66	1.54	1.43
12	O	103	SPO	C16-C17	3.66	1.53	1.45
12	0	102	SPO	C20-C19	3.66	1.54	1.43
12	3	103	SPO	C10-C9	3.66	1.54	1.43
12	T	102	SPO	C21-C22	3.66	1.54	1.43
12	s	104	SPO	C21-C22	3.65	1.54	1.43
12	M	1305	SPO	C21-C22	3.64	1.54	1.43
12	3	103	SPO	C21-C22	3.64	1.54	1.43
12	g	102	SPO	C21-C22	3.64	1.54	1.43
12	ab	102	SPO	C10-C9	3.64	1.54	1.43
12	m	1305	SPO	C10-C9	3.64	1.54	1.43
12	N	103	SPO	C20-C19	3.63	1.54	1.43
12	T	102	SPO	C10-C9	3.63	1.54	1.43
12	D	102	SPO	C16-C17	3.63	1.53	1.45
12	0	102	SPO	C6-C7	3.63	1.53	1.45
12	N	103	SPO	C11-C12	3.63	1.53	1.45
12	M	1305	SPO	C10-C9	3.62	1.54	1.43
12	M	1305	SPO	C11-C12	3.62	1.53	1.45
12	R	102	SPO	C6-C7	3.62	1.53	1.45
12	U	102	SPO	C21-C22	3.62	1.54	1.43
12	G	102	SPO	C20-C19	3.62	1.54	1.43
12	a	104	SPO	C15-C14	3.62	1.54	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	r	102	SPO	C21-C22	3.62	1.54	1.43
12	T	102	SPO	C11-C12	3.61	1.53	1.45
12	U	102	SPO	C10-C9	3.61	1.54	1.43
12	g	102	SPO	C10-C9	3.61	1.54	1.43
12	0	102	SPO	C15-C14	3.61	1.54	1.43
12	m	1305	SPO	C21-C22	3.61	1.54	1.43
12	9	102	SPO	C11-C12	3.61	1.53	1.45
12	N	103	SPO	C15-C14	3.61	1.54	1.43
10	h	302	PC1	O31-C31	3.61	1.43	1.33
12	I	102	SPO	C6-C7	3.61	1.53	1.45
12	m	1305	SPO	C11-C12	3.60	1.53	1.45
12	j	103	SPO	C6-C7	3.60	1.53	1.45
12	O	102	SPO	C20-C19	3.60	1.54	1.43
12	R	102	SPO	C21-C22	3.60	1.54	1.43
12	k	102	SPO	C20-C19	3.59	1.54	1.43
12	O	102	SPO	C11-C12	3.59	1.53	1.45
12	e	103	SPO	C15-C14	3.59	1.54	1.43
12	B	102	SPO	C10-C9	3.59	1.54	1.43
12	s	105	SPO	C26-C27	3.59	1.54	1.43
12	i	102	SPO	C20-C19	3.59	1.54	1.43
12	O	103	SPO	C11-C12	3.59	1.53	1.45
12	G	103	SPO	C6-C7	3.59	1.53	1.45
12	3	103	SPO	C16-C17	3.58	1.53	1.45
12	O	102	SPO	C10-C9	3.58	1.54	1.43
12	R	102	SPO	C16-C17	3.58	1.53	1.45
12	s	104	SPO	C16-C17	3.58	1.53	1.45
12	O	103	SPO	C25-C23	3.58	1.53	1.45
12	d	103	SPO	C10-C9	3.58	1.54	1.43
12	j	101	SPO	C6-C7	3.56	1.53	1.45
12	N	101	SPO	C6-C7	3.56	1.53	1.45
12	g	102	SPO	C6-C7	3.56	1.53	1.45
12	r	102	SPO	C10-C9	3.56	1.54	1.43
12	N	103	SPO	C25-C23	3.56	1.53	1.45
12	G	102	SPO	C11-C12	3.56	1.53	1.45
12	g	102	SPO	C11-C12	3.56	1.53	1.45
12	s	104	SPO	C6-C7	3.56	1.53	1.45
12	k	102	SPO	C21-C22	3.55	1.54	1.43
12	s	105	SPO	C16-C17	3.55	1.53	1.45
12	B	102	SPO	C11-C12	3.55	1.53	1.45
12	N	103	SPO	C21-C22	3.55	1.54	1.43
12	e	103	SPO	C20-C19	3.55	1.54	1.43
12	k	102	SPO	C10-C9	3.55	1.54	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	t	101	SPO	C6-C7	3.55	1.53	1.45
12	O	103	SPO	C10-C9	3.55	1.54	1.43
12	N	103	SPO	C10-C9	3.55	1.54	1.43
12	N	103	SPO	C26-C27	3.54	1.54	1.43
12	G	102	SPO	C6-C7	3.54	1.53	1.45
12	o	102	SPO	C6-C7	3.53	1.53	1.45
12	D	102	SPO	C6-C7	3.53	1.53	1.45
12	q	102	SPO	C6-C7	3.53	1.53	1.45
12	B	103	SPO	C21-C22	3.53	1.54	1.43
12	G	103	SPO	C21-C22	3.53	1.54	1.43
9	m	1304	U10	C3-C2	-3.51	1.38	1.48
12	G	102	SPO	C10-C9	3.51	1.54	1.43
12	S	102	SPO	C6-C7	3.51	1.53	1.45
12	s	102	SPO	C6-C7	3.51	1.53	1.45
12	t	101	SPO	C10-C9	3.51	1.54	1.43
12	F	102	SPO	C6-C7	3.51	1.53	1.45
12	r	102	SPO	C26-C27	3.51	1.54	1.43
12	j	103	SPO	C16-C17	3.50	1.53	1.45
12	o	102	SPO	C25-C23	3.50	1.53	1.45
12	G	102	SPO	C15-C14	3.50	1.54	1.43
12	ab	102	SPO	C21-C22	3.50	1.54	1.43
12	a	104	SPO	C20-C19	3.50	1.54	1.43
12	0	102	SPO	C11-C12	3.50	1.53	1.45
12	A	102	SPO	C26-C27	3.49	1.54	1.43
12	k	102	SPO	C26-C27	3.49	1.54	1.43
9	M	1304	U10	C3-C2	-3.49	1.38	1.48
12	q	102	SPO	C25-C23	3.49	1.53	1.45
12	3	101	SPO	C6-C7	3.49	1.53	1.45
12	B	102	SPO	C6-C7	3.49	1.53	1.45
12	R	102	SPO	C26-C27	3.49	1.54	1.43
12	9	102	SPO	C6-C7	3.49	1.53	1.45
12	q	102	SPO	C26-C27	3.48	1.54	1.43
7	z	101	BCL	MG-NC	3.48	2.14	2.06
12	e	101	SPO	C26-C27	3.48	1.54	1.43
12	m	1305	SPO	C6-C7	3.48	1.53	1.45
12	ab	102	SPO	C15-C14	3.47	1.54	1.43
12	r	102	SPO	C11-C12	3.47	1.53	1.45
12	B	102	SPO	C26-C27	3.47	1.54	1.43
12	j	101	SPO	C26-C27	3.47	1.54	1.43
12	B	102	SPO	C21-C22	3.47	1.54	1.43
12	K	102	SPO	C6-C7	3.47	1.53	1.45
12	D	102	SPO	C25-C23	3.47	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	102	SPO	C6-C7	3.47	1.53	1.45
12	i	102	SPO	C6-C7	3.46	1.53	1.45
12	M	1305	SPO	C6-C7	3.46	1.53	1.45
12	D	102	SPO	C26-C27	3.46	1.54	1.43
12	O	102	SPO	C6-C7	3.46	1.53	1.45
12	i	102	SPO	C10-C9	3.46	1.54	1.43
9	m	1304	U10	C4-C5	-3.46	1.38	1.48
12	8	101	SPO	C15-C14	3.46	1.54	1.43
12	I	102	SPO	C26-C27	3.45	1.54	1.43
12	r	102	SPO	C6-C7	3.45	1.53	1.45
12	aa	101	SPO	C15-C14	3.45	1.54	1.43
12	O	103	SPO	C6-C7	3.45	1.53	1.45
12	U	102	SPO	C11-C12	3.45	1.53	1.45
12	K	102	SPO	C25-C23	3.45	1.53	1.45
12	8	101	SPO	C20-C19	3.45	1.54	1.43
12	i	102	SPO	C21-C22	3.45	1.54	1.43
12	N	103	SPO	C6-C7	3.45	1.53	1.45
12	3	103	SPO	C6-C7	3.44	1.53	1.45
12	r	102	SPO	C25-C23	3.44	1.53	1.45
12	9	102	SPO	C26-C27	3.44	1.54	1.43
12	o	102	SPO	C26-C27	3.44	1.54	1.43
12	T	102	SPO	C16-C17	3.44	1.53	1.45
12	K	102	SPO	C26-C27	3.44	1.54	1.43
12	N	101	SPO	C25-C23	3.44	1.53	1.45
12	n	101	SPO	C26-C27	3.44	1.54	1.43
9	M	1304	U10	C4-C5	-3.43	1.39	1.48
9	L	303	U10	C3-C2	-3.43	1.39	1.48
12	Q	102	SPO	C6-C7	3.43	1.53	1.45
12	3	103	SPO	C26-C27	3.43	1.54	1.43
12	n	101	SPO	C25-C23	3.42	1.53	1.45
9	l	303	U10	C3-C2	-3.42	1.39	1.48
12	T	102	SPO	C26-C27	3.42	1.54	1.43
12	t	101	SPO	C15-C14	3.42	1.54	1.43
12	s	104	SPO	C26-C27	3.42	1.54	1.43
12	O	102	SPO	C21-C22	3.41	1.54	1.43
12	3	101	SPO	C26-C27	3.41	1.54	1.43
12	B	102	SPO	C16-C17	3.41	1.53	1.45
12	I	102	SPO	C25-C23	3.41	1.53	1.45
12	t	101	SPO	C20-C19	3.41	1.54	1.43
12	T	102	SPO	C6-C7	3.40	1.53	1.45
12	j	101	SPO	C25-C23	3.40	1.53	1.45
12	N	101	SPO	C26-C27	3.40	1.54	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	S	102	SPO	C26-C27	3.40	1.54	1.43
12	e	101	SPO	C25-C23	3.40	1.53	1.45
12	Q	102	SPO	C26-C27	3.40	1.54	1.43
12	e	103	SPO	C10-C9	3.39	1.53	1.43
12	s	102	SPO	C26-C27	3.39	1.53	1.43
12	T	102	SPO	C25-C23	3.38	1.53	1.45
12	R	102	SPO	C25-C23	3.38	1.53	1.45
12	G	103	SPO	C26-C27	3.38	1.53	1.43
12	aa	101	SPO	C20-C19	3.38	1.53	1.43
12	G	103	SPO	C16-C17	3.37	1.53	1.45
12	a	104	SPO	C21-C22	3.37	1.53	1.43
12	e	101	SPO	C6-C7	3.37	1.53	1.45
12	S	102	SPO	C25-C23	3.37	1.53	1.45
12	m	1305	SPO	C16-C17	3.37	1.53	1.45
12	9	102	SPO	C25-C23	3.37	1.53	1.45
7	2	101	BCL	MG-NC	3.37	2.14	2.06
12	F	102	SPO	C26-C27	3.37	1.53	1.43
12	Q	102	SPO	C25-C23	3.36	1.53	1.45
7	W	101	BCL	MG-NC	3.36	2.14	2.06
12	F	102	SPO	C25-C23	3.35	1.53	1.45
12	M	1305	SPO	C16-C17	3.35	1.53	1.45
12	t	101	SPO	C26-C27	3.35	1.53	1.43
12	s	105	SPO	C25-C23	3.35	1.53	1.45
12	3	101	SPO	C25-C23	3.35	1.53	1.45
9	L	303	U10	C4-C5	-3.34	1.39	1.48
10	h	302	PC1	O21-C21	3.34	1.43	1.34
12	U	102	SPO	C16-C17	3.34	1.53	1.45
12	e	103	SPO	C21-C22	3.34	1.53	1.43
7	U	101	BCL	MG-NC	3.34	2.14	2.06
7	Y	201	BCL	MG-NC	3.34	2.14	2.06
12	r	102	SPO	C16-C17	3.33	1.53	1.45
7	u	101	BCL	MG-NC	3.33	2.14	2.06
7	x	101	BCL	MG-NC	3.33	2.14	2.06
7	5	101	BCL	MG-NC	3.33	2.14	2.06
7	w	101	BCL	MG-NC	3.33	2.14	2.06
12	A	102	SPO	C25-C23	3.32	1.53	1.45
12	d	103	SPO	C20-C19	3.32	1.53	1.43
9	l	303	U10	C4-C5	-3.32	1.39	1.48
12	s	102	SPO	C25-C23	3.32	1.53	1.45
12	O	102	SPO	C26-C27	3.31	1.53	1.43
12	U	102	SPO	C6-C7	3.31	1.53	1.45
7	y	101	BCL	MG-NC	3.31	2.14	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	a	104	SPO	C26-C27	3.31	1.53	1.43
12	m	1305	SPO	C26-C27	3.31	1.53	1.43
12	G	102	SPO	C26-C27	3.31	1.53	1.43
12	B	103	SPO	C16-C17	3.31	1.53	1.45
12	aa	101	SPO	C10-C9	3.30	1.53	1.43
12	ab	102	SPO	C26-C27	3.30	1.53	1.43
12	8	101	SPO	C10-C9	3.29	1.53	1.43
12	n	101	SPO	C16-C17	3.28	1.53	1.45
12	M	1305	SPO	C26-C27	3.27	1.53	1.43
12	0	102	SPO	C21-C22	3.27	1.53	1.43
12	B	102	SPO	C25-C23	3.27	1.53	1.45
12	G	102	SPO	C25-C23	3.26	1.53	1.45
12	k	102	SPO	C11-C12	3.26	1.53	1.45
12	3	103	SPO	C25-C23	3.26	1.53	1.45
7	Q	101	BCL	MG-NC	3.26	2.14	2.06
12	0	102	SPO	C16-C17	3.26	1.52	1.45
12	U	102	SPO	C26-C27	3.25	1.53	1.43
12	t	101	SPO	C21-C22	3.23	1.53	1.43
12	g	102	SPO	C25-C23	3.23	1.52	1.45
12	B	103	SPO	C26-C27	3.23	1.53	1.43
10	C	1201	PC1	O31-C31	3.22	1.42	1.33
10	l	304	PC1	O31-C31	3.22	1.42	1.33
7	S	101	BCL	MG-NC	3.21	2.13	2.06
10	a	102	PC1	O31-C31	3.21	1.42	1.33
12	j	103	SPO	C26-C27	3.21	1.53	1.43
12	g	102	SPO	C26-C27	3.21	1.53	1.43
12	s	104	SPO	C25-C23	3.20	1.52	1.45
12	N	103	SPO	C16-C17	3.19	1.52	1.45
12	m	1305	SPO	C25-C23	3.19	1.52	1.45
12	O	102	SPO	C16-C17	3.18	1.52	1.45
12	ab	102	SPO	C25-C23	3.17	1.52	1.45
12	M	1305	SPO	C25-C23	3.17	1.52	1.45
7	f	101	BCL	MG-NC	3.17	2.13	2.06
7	d	101	BCL	MG-NC	3.17	2.13	2.06
7	s	101	BCL	MG-NC	3.16	2.13	2.06
12	8	101	SPO	C26-C27	3.16	1.53	1.43
12	0	102	SPO	C26-C27	3.16	1.53	1.43
12	G	103	SPO	C25-C23	3.16	1.52	1.45
12	aa	101	SPO	C21-C22	3.16	1.53	1.43
12	d	103	SPO	C21-C22	3.15	1.53	1.43
12	8	101	SPO	C21-C22	3.15	1.53	1.43
12	aa	101	SPO	C26-C27	3.14	1.53	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	a	104	SPO	C16-C17	3.14	1.52	1.45
7	o	101	BCL	MG-NC	3.13	2.13	2.06
7	v	101	BCL	MG-NC	3.13	2.13	2.06
12	j	103	SPO	C25-C23	3.13	1.52	1.45
12	i	102	SPO	C26-C27	3.12	1.53	1.43
12	d	103	SPO	C26-C27	3.12	1.53	1.43
7	a	101	BCL	MG-NC	3.10	2.13	2.06
12	B	103	SPO	C25-C23	3.08	1.52	1.45
12	e	103	SPO	C11-C12	3.08	1.52	1.45
7	U	103	BCL	C3B-C4B	3.07	1.46	1.41
7	A	101	BCL	MG-NC	3.06	2.13	2.06
7	k	101	BCL	MG-NC	3.06	2.13	2.06
12	d	103	SPO	C11-C12	3.06	1.52	1.45
10	a	103	PC1	O31-C31	3.05	1.42	1.33
10	L	306	PC1	O21-C21	3.05	1.42	1.34
7	D	101	BCL	MG-NC	3.04	2.13	2.06
7	5	102	BCL	MG-NC	3.04	2.13	2.06
7	X	101	BCL	MG-NC	3.03	2.13	2.06
12	U	102	SPO	C25-C23	3.03	1.52	1.45
10	h	301	PC1	O21-C21	3.03	1.42	1.34
12	t	101	SPO	C11-C12	3.02	1.52	1.45
12	e	103	SPO	C26-C27	3.02	1.52	1.43
7	3	102	BCL	C3B-C4B	3.02	1.46	1.41
7	I	101	BCL	MG-NC	3.02	2.13	2.06
7	F	101	BCL	MG-NC	3.01	2.13	2.06
12	O	102	SPO	C25-C23	3.01	1.52	1.45
7	s	103	BCL	MG-NC	3.00	2.13	2.06
10	M	1307	PC1	O21-C21	3.00	1.42	1.34
7	O	101	BCL	MG-NC	2.99	2.13	2.06
7	d	101	BCL	C3B-C4B	2.99	1.46	1.41
12	e	103	SPO	C16-C17	2.98	1.52	1.45
12	e	103	SPO	C6-C7	2.98	1.52	1.45
7	i	101	BCL	C3B-C4B	2.98	1.46	1.41
7	c	101	BCL	MG-NC	2.97	2.13	2.06
7	Q	101	BCL	C3B-C4B	2.97	1.46	1.41
7	p	101	BCL	MG-NC	2.96	2.13	2.06
7	f	101	BCL	C3B-C4B	2.96	1.46	1.41
10	A	103	PC1	O31-C31	2.96	1.42	1.33
10	h	301	PC1	O31-C31	2.96	1.42	1.33
10	A	104	PC1	O31-C31	2.95	1.42	1.33
12	k	102	SPO	C16-C17	2.95	1.52	1.45
7	R	101	BCL	MG-NC	2.95	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	a	102	PC1	O21-C21	2.94	1.42	1.34
7	J	101	BCL	MG-NC	2.94	2.13	2.06
10	d	102	PC1	O21-C21	2.94	1.42	1.34
7	7	101	BCL	O2A-CGA	-2.93	1.24	1.33
7	K	101	BCL	MG-NC	2.93	2.13	2.06
10	M	1307	PC1	O31-C31	2.93	1.41	1.33
7	T	101	BCL	MG-NC	2.93	2.13	2.06
7	0	101	BCL	MG-NC	2.93	2.13	2.06
13	M	1306	CDL	OA6-CA4	-2.92	1.39	1.46
7	B	101	BCL	MG-NC	2.92	2.13	2.06
7	ab	101	BCL	MG-NC	2.92	2.13	2.06
7	l	301	BCL	O1A-CGA	-2.92	1.13	1.22
7	b	101	BCL	MG-NC	2.92	2.13	2.06
13	m	1306	CDL	OA6-CA4	-2.92	1.39	1.46
7	O	101	BCL	C3B-C4B	2.92	1.46	1.41
7	G	101	BCL	MG-NC	2.91	2.13	2.06
12	a	104	SPO	C25-C23	2.91	1.52	1.45
7	aa	102	BCL	MG-NC	2.91	2.13	2.06
7	Z	101	BCL	MG-NC	2.91	2.13	2.06
12	k	102	SPO	C6-C7	2.91	1.52	1.45
12	ab	102	SPO	C16-C17	2.91	1.52	1.45
7	8	102	BCL	MG-NC	2.91	2.13	2.06
7	P	101	BCL	MG-NC	2.90	2.13	2.06
7	9	101	BCL	MG-NC	2.90	2.13	2.06
7	e	102	BCL	MG-NC	2.90	2.13	2.06
7	L	301	BCL	O1A-CGA	-2.90	1.13	1.22
7	E	101	BCL	MG-NC	2.90	2.13	2.06
7	N	102	BCL	MG-NC	2.90	2.13	2.06
13	M	1306	CDL	OA8-CA7	2.89	1.41	1.33
7	L	304	BCL	MG-NC	2.89	2.13	2.06
13	m	1306	CDL	OB8-CB7	2.89	1.41	1.33
7	g	101	BCL	MG-NC	2.88	2.13	2.06
13	m	1306	CDL	OA8-CA7	2.88	1.41	1.33
12	i	102	SPO	C25-C23	2.88	1.52	1.45
12	aa	101	SPO	C6-C7	2.88	1.52	1.45
7	j	102	BCL	MG-NC	2.88	2.13	2.06
10	l	304	PC1	O21-C21	2.87	1.42	1.34
7	k	101	BCL	C3B-C4B	2.87	1.46	1.41
13	M	1306	CDL	OB8-CB7	2.87	1.41	1.33
10	C	1201	PC1	O21-C21	2.86	1.42	1.34
7	M	1303	BCL	C3B-C4B	2.86	1.46	1.41
7	F	101	BCL	C3B-C4B	2.86	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	l	302	BPB	C3D-CAD	-2.86	1.41	1.47
7	o	101	BCL	C3B-C4B	2.85	1.46	1.41
7	a	101	BCL	C3B-C4B	2.85	1.46	1.41
8	L	302	BPB	C3D-CAD	-2.85	1.41	1.47
12	d	103	SPO	C6-C7	2.85	1.52	1.45
7	m	1303	BCL	C3B-C4B	2.84	1.46	1.41
7	l	305	BCL	MG-NC	2.84	2.13	2.06
12	k	102	SPO	C25-C23	2.83	1.52	1.45
7	i	101	BCL	MG-NC	2.83	2.13	2.06
7	L	301	BCL	MG-NC	2.83	2.13	2.06
12	d	103	SPO	C16-C17	2.83	1.52	1.45
7	l	301	BCL	MG-NC	2.82	2.13	2.06
7	5	101	BCL	C3B-C4B	2.82	1.46	1.41
10	A	104	PC1	O21-C2	-2.82	1.39	1.46
12	G	102	SPO	C16-C17	2.82	1.52	1.45
12	8	101	SPO	C11-C12	2.81	1.52	1.45
10	d	102	PC1	O31-C31	2.81	1.41	1.33
12	0	102	SPO	C25-C23	2.81	1.52	1.45
10	A	103	PC1	O21-C21	2.81	1.42	1.34
7	u	101	BCL	C3B-C4B	2.81	1.46	1.41
7	S	101	BCL	C3B-C4B	2.79	1.46	1.41
7	W	101	BCL	C3B-C4B	2.79	1.46	1.41
7	U	103	BCL	MG-NC	2.79	2.12	2.06
7	l	101	BCL	C3B-C4B	2.78	1.46	1.41
10	a	103	PC1	O21-C21	2.78	1.42	1.34
7	y	101	BCL	C3B-C4B	2.78	1.46	1.41
12	s	105	SPO	C4-C5	2.77	1.54	1.50
10	L	306	PC1	O31-C31	2.77	1.41	1.33
9	l	303	U10	C6-C5	-2.77	1.38	1.46
7	U	101	BCL	C3B-C4B	2.76	1.46	1.41
7	5	102	BCL	C3B-C4B	2.76	1.46	1.41
8	L	305	BPB	C3D-CAD	-2.76	1.41	1.47
12	t	101	SPO	C25-C23	2.76	1.51	1.45
7	9	101	BCL	O1A-CGA	-2.76	1.14	1.22
7	A	101	BCL	C3B-C4B	2.75	1.46	1.41
12	i	102	SPO	C4-C5	2.75	1.54	1.50
9	L	303	U10	C6-C5	-2.75	1.38	1.46
7	w	101	BCL	C3B-C4B	2.75	1.46	1.41
7	Y	201	BCL	C3B-C4B	2.74	1.46	1.41
7	x	101	BCL	C3B-C4B	2.74	1.46	1.41
7	q	101	BCL	MG-NC	2.74	2.12	2.06
12	aa	101	SPO	C11-C12	2.74	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	s	101	BCL	C3B-C4B	2.74	1.46	1.41
7	2	101	BCL	C3B-C4B	2.73	1.46	1.41
8	l	306	BPB	C3D-CAD	-2.73	1.41	1.47
10	A	103	PC1	O21-C2	-2.73	1.39	1.46
7	l	301	BCL	C3B-C4B	2.72	1.46	1.41
7	L	301	BCL	C3B-C4B	2.71	1.46	1.41
12	g	102	SPO	C4-C5	2.71	1.54	1.50
12	n	101	SPO	C4-C5	2.71	1.54	1.50
10	h	302	PC1	P-O11	2.71	1.70	1.59
7	D	101	BCL	C3B-C4B	2.71	1.46	1.41
7	m	1301	BCL	O1A-CGA	-2.70	1.14	1.22
12	i	102	SPO	C11-C12	2.69	1.51	1.45
7	M	1303	BCL	MG-NC	2.68	2.12	2.06
12	B	103	SPO	C4-C5	2.68	1.54	1.50
7	9	101	BCL	C3B-C4B	2.68	1.46	1.41
7	l	305	BCL	O1A-CGA	-2.68	1.14	1.22
7	m	1301	BCL	MG-NC	2.68	2.12	2.06
7	L	304	BCL	O1A-CGA	-2.68	1.14	1.22
7	K	101	BCL	C3B-C4B	2.68	1.46	1.41
7	M	1301	BCL	O1A-CGA	-2.68	1.14	1.22
9	m	1304	U10	C6-C5	-2.68	1.39	1.46
7	M	1301	BCL	MG-NC	2.67	2.12	2.06
7	1	101	BCL	MG-NC	2.66	2.12	2.06
9	M	1304	U10	C6-C5	-2.66	1.39	1.46
10	C	1201	PC1	O21-C2	-2.66	1.40	1.46
7	l	305	BCL	C3B-C4B	2.65	1.46	1.41
7	3	102	BCL	O2A-CGA	-2.65	1.25	1.33
10	a	103	PC1	O21-C2	-2.65	1.40	1.46
7	m	1303	BCL	MG-NC	2.65	2.12	2.06
12	G	103	SPO	C4-C5	2.65	1.54	1.50
12	aa	101	SPO	C16-C17	2.65	1.51	1.45
12	a	104	SPO	C4-C5	2.64	1.54	1.50
12	t	101	SPO	C16-C17	2.64	1.51	1.45
7	U	103	BCL	CHD-C1D	2.64	1.43	1.38
7	I	101	BCL	C3B-C4B	2.64	1.46	1.41
10	l	304	PC1	O21-C2	-2.64	1.40	1.46
12	8	101	SPO	C16-C17	2.63	1.51	1.45
7	k	103	BCL	MG-NC	2.63	2.12	2.06
12	8	101	SPO	C6-C7	2.63	1.51	1.45
7	q	101	BCL	C3B-C4B	2.63	1.45	1.41
7	L	304	BCL	C3B-C4B	2.62	1.45	1.41
7	c	101	BCL	C3B-C4B	2.62	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	104	PC1	O21-C21	2.62	1.41	1.34
7	s	103	BCL	C3B-C4B	2.61	1.45	1.41
7	m	1301	BCL	C3B-C4B	2.61	1.45	1.41
12	0	102	SPO	C4-C5	2.59	1.54	1.50
7	r	101	BCL	C3C-C4C	-2.59	1.48	1.51
12	s	104	SPO	C4-C5	2.58	1.54	1.50
7	X	101	BCL	C3B-C4B	2.58	1.45	1.41
13	M	1306	CDL	OA6-CA5	2.58	1.41	1.34
13	m	1306	CDL	OA6-CA5	2.57	1.41	1.34
7	M	1301	BCL	C3B-C4B	2.57	1.45	1.41
7	1	101	BCL	CHD-C1D	2.56	1.43	1.38
7	m	1303	BCL	O1A-CGA	-2.55	1.15	1.22
12	t	101	SPO	C4-C5	2.55	1.54	1.50
7	M	1303	BCL	O1A-CGA	-2.53	1.15	1.22
7	D	101	BCL	O1A-CGA	-2.52	1.15	1.22
7	3	102	BCL	MG-NC	2.52	2.12	2.06
12	m	1305	SPO	C4-C5	2.51	1.54	1.50
10	a	102	PC1	O21-C2	-2.51	1.40	1.46
12	M	1305	SPO	C4-C5	2.51	1.54	1.50
7	7	101	BCL	C3B-C4B	2.50	1.45	1.41
12	I	102	SPO	C4-C5	2.50	1.54	1.50
8	L	302	BPB	C3B-C4B	2.50	1.45	1.41
12	O	102	SPO	C4-C5	2.49	1.54	1.50
7	5	102	BCL	CHD-C1D	2.49	1.43	1.38
8	l	302	BPB	C3B-C4B	2.48	1.45	1.41
7	f	101	BCL	O1A-CGA	-2.48	1.15	1.22
9	L	303	U10	C6-C1	2.46	1.39	1.35
12	R	102	SPO	C4-C5	2.46	1.54	1.50
9	l	303	U10	C6-C1	2.46	1.39	1.35
12	e	103	SPO	C25-C23	2.45	1.51	1.45
12	N	101	SPO	C4-C5	2.44	1.54	1.50
7	z	101	BCL	CHD-C1D	2.44	1.43	1.38
7	Z	101	BCL	C3B-C4B	2.43	1.45	1.41
12	aa	101	SPO	C25-C23	2.42	1.51	1.45
12	o	102	SPO	C4-C5	2.42	1.54	1.50
7	d	101	BCL	O1A-CGA	-2.41	1.15	1.22
12	U	102	SPO	C4-C5	2.41	1.54	1.50
7	c	101	BCL	C3D-C4D	-2.41	1.38	1.44
7	M	1303	BCL	C3D-C4D	-2.41	1.38	1.44
10	h	301	PC1	O21-C2	-2.40	1.40	1.46
12	ab	102	SPO	C4-C5	2.40	1.54	1.50
8	L	302	BPB	O1A-CGA	-2.40	1.15	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	l	302	BPB	O1A-CGA	-2.40	1.15	1.22
12	8	101	SPO	C25-C23	2.40	1.51	1.45
7	l	305	BCL	C1D-C2D	-2.40	1.40	1.45
7	7	101	BCL	MG-NC	2.40	2.12	2.06
7	m	1303	BCL	C3D-C4D	-2.39	1.38	1.44
7	3	102	BCL	O1A-CGA	-2.39	1.15	1.22
7	X	101	BCL	CHD-C1D	2.39	1.43	1.38
7	M	1301	BCL	C3D-C4D	-2.39	1.38	1.44
7	r	101	BCL	MG-NC	2.39	2.11	2.06
7	L	304	BCL	C1D-C2D	-2.38	1.40	1.45
7	A	101	BCL	O1A-CGA	-2.38	1.15	1.22
10	M	1307	PC1	O21-C2	-2.38	1.40	1.46
7	F	101	BCL	C1D-C2D	-2.37	1.40	1.45
9	m	1304	U10	C1-C2	-2.37	1.38	1.47
12	N	103	SPO	C4-C5	2.37	1.53	1.50
12	j	103	SPO	C4-C5	2.37	1.53	1.50
9	M	1304	U10	C1-C2	-2.37	1.38	1.47
12	9	102	SPO	C4-C5	2.37	1.53	1.50
7	v	101	BCL	CHD-C1D	2.36	1.43	1.38
7	p	101	BCL	C1D-C2D	-2.36	1.40	1.45
7	I	101	BCL	O1A-CGA	-2.36	1.15	1.22
9	m	1304	U10	C6-C1	2.35	1.39	1.35
7	m	1301	BCL	C3D-C4D	-2.35	1.38	1.44
7	s	103	BCL	CHD-C1D	2.35	1.42	1.38
12	O	103	SPO	C4-C5	2.34	1.53	1.50
7	N	102	BCL	C3B-C4B	2.34	1.45	1.41
9	M	1304	U10	C6-C1	2.34	1.39	1.35
7	l	305	BCL	C3D-C4D	-2.34	1.38	1.44
7	Q	101	BCL	O1A-CGA	-2.33	1.15	1.22
7	J	101	BCL	C3B-C4B	2.33	1.45	1.41
12	q	102	SPO	C4-C5	2.33	1.53	1.50
7	P	101	BCL	C3B-C4B	2.33	1.45	1.41
7	j	102	BCL	C3B-C4B	2.33	1.45	1.41
12	j	101	SPO	C4-C5	2.33	1.53	1.50
12	s	102	SPO	C4-C5	2.33	1.53	1.50
9	L	303	U10	C1-C2	-2.33	1.38	1.47
7	E	101	BCL	C3B-C4B	2.32	1.45	1.41
12	T	102	SPO	C4-C5	2.32	1.53	1.50
9	l	303	U10	C1-C2	-2.32	1.38	1.47
7	k	103	BCL	C3C-C4C	-2.32	1.48	1.51
7	5	101	BCL	CHD-C1D	2.32	1.42	1.38
13	M	1306	CDL	C51-CB5	2.31	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	0	101	BCL	C3B-C4B	2.31	1.45	1.41
12	3	101	SPO	C4-C5	2.31	1.53	1.50
7	2	101	BCL	CHD-C1D	2.31	1.42	1.38
7	T	101	BCL	C3B-C4B	2.31	1.45	1.41
7	ab	101	BCL	C3B-C4B	2.31	1.45	1.41
7	8	102	BCL	C3B-C4B	2.31	1.45	1.41
7	P	101	BCL	C3D-C4D	-2.30	1.39	1.44
7	L	304	BCL	C3D-C4D	-2.30	1.39	1.44
10	d	102	PC1	O21-C2	-2.30	1.40	1.46
7	e	102	BCL	C3B-C4B	2.30	1.45	1.41
7	R	101	BCL	C3B-C4B	2.30	1.45	1.41
7	u	101	BCL	CHD-C1D	2.29	1.42	1.38
7	B	101	BCL	C3B-C4B	2.29	1.45	1.41
7	aa	102	BCL	C3B-C4B	2.29	1.45	1.41
7	G	101	BCL	C3B-C4B	2.29	1.45	1.41
12	r	102	SPO	C4-C5	2.29	1.53	1.50
7	g	101	BCL	C3B-C4B	2.29	1.45	1.41
7	Y	201	BCL	CHD-C1D	2.29	1.42	1.38
7	U	101	BCL	CHD-C1D	2.29	1.42	1.38
7	b	101	BCL	C3B-C4B	2.28	1.45	1.41
13	m	1306	CDL	C51-CB5	2.28	1.57	1.50
7	J	101	BCL	C3D-C4D	-2.28	1.39	1.44
7	B	101	BCL	C3D-C4D	-2.28	1.39	1.44
7	0	101	BCL	C3D-C4D	-2.28	1.39	1.44
7	w	101	BCL	CHD-C1D	2.28	1.42	1.38
12	F	102	SPO	C4-C5	2.28	1.53	1.50
12	K	102	SPO	C4-C5	2.27	1.53	1.50
12	3	103	SPO	C4-C5	2.27	1.53	1.50
7	M	1301	BCL	CHD-C1D	2.27	1.42	1.38
7	G	101	BCL	C3D-C4D	-2.27	1.39	1.44
7	m	1301	BCL	CHD-C1D	2.27	1.42	1.38
7	L	304	BCL	CHD-C1D	2.27	1.42	1.38
12	aa	101	SPO	C4-C5	2.27	1.53	1.50
7	N	102	BCL	C3D-C4D	-2.26	1.39	1.44
7	8	102	BCL	C3D-C4D	-2.26	1.39	1.44
7	W	101	BCL	CHD-C1D	2.26	1.42	1.38
7	y	101	BCL	CHD-C1D	2.26	1.42	1.38
7	M	1301	BCL	C1D-C2D	-2.26	1.40	1.45
12	G	102	SPO	C4-C5	2.26	1.53	1.50
7	f	101	BCL	C1D-C2D	-2.26	1.40	1.45
7	b	101	BCL	C3D-C4D	-2.25	1.39	1.44
7	E	101	BCL	C3D-C4D	-2.25	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	h	302	PC1	O21-C2	-2.25	1.41	1.46
12	S	102	SPO	C4-C5	2.25	1.53	1.50
7	m	1301	BCL	C1D-C2D	-2.25	1.40	1.45
7	ab	101	BCL	C3D-C4D	-2.25	1.39	1.44
7	l	301	BCL	C3D-C4D	-2.24	1.39	1.44
7	aa	102	BCL	C3D-C4D	-2.24	1.39	1.44
7	j	102	BCL	C3D-C4D	-2.24	1.39	1.44
7	L	301	BCL	C1D-C2D	-2.24	1.40	1.45
7	f	101	BCL	C3D-C4D	-2.24	1.39	1.44
7	a	101	BCL	C3D-C4D	-2.23	1.39	1.44
7	L	301	BCL	C3D-C4D	-2.23	1.39	1.44
7	r	101	BCL	C1D-C2D	-2.23	1.40	1.45
7	v	101	BCL	C3B-C4B	2.23	1.45	1.41
7	T	101	BCL	C3D-C4D	-2.23	1.39	1.44
7	e	102	BCL	C3D-C4D	-2.22	1.39	1.44
7	R	101	BCL	C3D-C4D	-2.22	1.39	1.44
7	g	101	BCL	C3D-C4D	-2.22	1.39	1.44
7	z	101	BCL	C3B-C4B	2.22	1.45	1.41
7	K	101	BCL	C3D-C4D	-2.22	1.39	1.44
7	s	101	BCL	CHD-C1D	2.22	1.42	1.38
12	k	102	SPO	C4-C5	2.21	1.53	1.50
7	o	101	BCL	C1D-C2D	-2.21	1.41	1.45
7	9	101	BCL	O2A-CGA	-2.20	1.26	1.33
7	c	101	BCL	C1D-C2D	-2.20	1.41	1.45
7	O	101	BCL	O1A-CGA	-2.20	1.16	1.22
7	l	301	BCL	C1D-C2D	-2.20	1.41	1.45
7	s	103	BCL	C3D-C4D	-2.19	1.39	1.44
7	m	1303	BCL	CHD-C1D	2.19	1.42	1.38
7	l	305	BCL	CHD-C1D	2.19	1.42	1.38
7	A	101	BCL	C3D-C4D	-2.19	1.39	1.44
7	Q	101	BCL	CHD-C1D	2.19	1.42	1.38
8	L	305	BPB	C3A-C2A	-2.18	1.52	1.54
7	9	101	BCL	C3D-C4D	-2.18	1.39	1.44
12	Q	102	SPO	C4-C5	2.18	1.53	1.50
7	F	101	BCL	C3D-C4D	-2.18	1.39	1.44
7	M	1303	BCL	CHD-C1D	2.18	1.42	1.38
7	d	101	BCL	C3D-C4D	-2.17	1.39	1.44
12	B	102	SPO	C4-C5	2.17	1.53	1.50
7	c	101	BCL	O2A-CGA	-2.17	1.27	1.33
7	a	101	BCL	CHD-C1D	2.17	1.42	1.38
7	p	101	BCL	C3B-C4B	2.17	1.45	1.41
7	F	101	BCL	O1A-CGA	-2.16	1.16	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	101	BCL	C3D-C4D	-2.16	1.39	1.44
7	E	101	BCL	C1D-C2D	-2.16	1.41	1.45
7	ab	101	BCL	C1D-C2D	-2.16	1.41	1.45
7	p	101	BCL	C3D-C4D	-2.16	1.39	1.44
10	h	302	PC1	C22-C21	2.16	1.57	1.50
7	K	101	BCL	CHD-C1D	2.16	1.42	1.38
7	g	101	BCL	C1D-C2D	-2.16	1.41	1.45
7	aa	102	BCL	C1D-C2D	-2.16	1.41	1.45
7	a	101	BCL	C1D-C2D	-2.15	1.41	1.45
7	b	101	BCL	C1D-C2D	-2.15	1.41	1.45
12	e	101	SPO	C4-C5	2.15	1.53	1.50
7	x	101	BCL	CHD-C1D	2.14	1.42	1.38
7	U	103	BCL	C3D-C4D	-2.14	1.39	1.44
7	J	101	BCL	C1D-C2D	-2.14	1.41	1.45
7	N	102	BCL	C1D-C2D	-2.14	1.41	1.45
7	P	101	BCL	C1D-C2D	-2.14	1.41	1.45
7	e	102	BCL	C1D-C2D	-2.14	1.41	1.45
7	R	101	BCL	C1D-C2D	-2.14	1.41	1.45
8	L	305	BPB	C3B-C4B	2.14	1.45	1.41
8	l	306	BPB	C3A-C2A	-2.14	1.52	1.54
7	G	101	BCL	C1D-C2D	-2.14	1.41	1.45
7	0	101	BCL	C1D-C2D	-2.14	1.41	1.45
7	Q	101	BCL	C3D-C4D	-2.13	1.39	1.44
7	3	102	BCL	C1D-C2D	-2.13	1.41	1.45
7	c	101	BCL	CHD-C1D	2.13	1.42	1.38
8	l	306	BPB	C3B-C4B	2.13	1.45	1.41
12	D	102	SPO	C4-C5	2.13	1.53	1.50
7	L	301	BCL	CHD-C1D	2.13	1.42	1.38
7	T	101	BCL	C1D-C2D	-2.13	1.41	1.45
7	I	101	BCL	C3D-C4D	-2.13	1.39	1.44
7	8	102	BCL	C1D-C2D	-2.13	1.41	1.45
7	l	301	BCL	CHD-C1D	2.12	1.42	1.38
7	F	101	BCL	CHD-C1D	2.12	1.42	1.38
7	k	101	BCL	C1D-C2D	-2.11	1.41	1.45
7	i	101	BCL	CHD-C1D	2.11	1.42	1.38
13	M	1306	CDL	PA1-OA5	2.11	1.67	1.59
7	B	101	BCL	C1D-C2D	-2.11	1.41	1.45
13	m	1306	CDL	PA1-OA5	2.11	1.67	1.59
7	I	101	BCL	CHD-C1D	2.11	1.42	1.38
7	O	101	BCL	C3D-C4D	-2.11	1.39	1.44
7	z	101	BCL	C1D-ND	2.11	1.40	1.37
7	o	101	BCL	C3D-C4D	-2.11	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	102	SPO	C4-C5	2.11	1.53	1.50
7	r	101	BCL	C3D-C4D	-2.10	1.39	1.44
7	o	101	BCL	CHD-C1D	2.10	1.42	1.38
8	l	306	BPB	O1A-CGA	-2.10	1.16	1.22
7	5	102	BCL	C3D-C4D	-2.10	1.39	1.44
7	O	101	BCL	CHD-C1D	2.10	1.42	1.38
7	q	101	BCL	CHD-C1D	2.09	1.42	1.38
7	j	102	BCL	C1D-C2D	-2.09	1.41	1.45
7	s	101	BCL	C3D-C4D	-2.09	1.39	1.44
7	S	101	BCL	C3D-C4D	-2.09	1.39	1.44
7	K	101	BCL	O1A-CGA	-2.08	1.16	1.22
7	X	101	BCL	C3D-C4D	-2.08	1.39	1.44
7	k	101	BCL	C3D-C4D	-2.08	1.39	1.44
7	D	101	BCL	CHD-C1D	2.08	1.42	1.38
7	Z	101	BCL	C3D-C4D	-2.08	1.39	1.44
7	3	102	BCL	CHD-C1D	2.07	1.42	1.38
7	7	101	BCL	C1D-C2D	-2.07	1.41	1.45
7	9	101	BCL	CHD-C1D	2.07	1.42	1.38
7	Z	101	BCL	CHD-C1D	2.07	1.42	1.38
7	d	101	BCL	C1D-C2D	-2.07	1.41	1.45
7	7	101	BCL	CHD-C1D	2.07	1.42	1.38
7	D	101	BCL	C1D-C2D	-2.06	1.41	1.45
7	U	101	BCL	C3D-C4D	-2.06	1.39	1.44
7	S	101	BCL	C1D-C2D	-2.06	1.41	1.45
7	Q	101	BCL	C1D-C2D	-2.06	1.41	1.45
8	L	305	BPB	O1A-CGA	-2.05	1.16	1.22
7	1	101	BCL	C3D-C4D	-2.05	1.39	1.44
7	9	101	BCL	C1D-C2D	-2.05	1.41	1.45
7	i	101	BCL	C1D-C2D	-2.05	1.41	1.45
7	O	101	BCL	C1D-C2D	-2.05	1.41	1.45
7	d	101	BCL	CHD-C1D	2.05	1.42	1.38
7	p	101	BCL	CHD-C1D	2.05	1.42	1.38
7	K	101	BCL	C1D-C2D	-2.04	1.41	1.45
7	S	101	BCL	CHD-C1D	2.04	1.42	1.38
7	m	1303	BCL	C1D-C2D	-2.03	1.41	1.45
7	W	101	BCL	C3D-C4D	-2.03	1.39	1.44
7	a	101	BCL	O2A-CGA	-2.03	1.27	1.33
7	2	101	BCL	C3D-C4D	-2.03	1.39	1.44
7	q	101	BCL	C1D-C2D	-2.03	1.41	1.45
7	k	101	BCL	CHD-C1D	2.03	1.42	1.38
7	y	101	BCL	C3D-C4D	-2.03	1.39	1.44
7	A	101	BCL	CHD-C1D	2.03	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	g	101	BCL	CHD-C1D	2.02	1.42	1.38
7	Y	201	BCL	C3D-C4D	-2.02	1.39	1.44
7	M	1303	BCL	C1D-C2D	-2.02	1.41	1.45
7	a	101	BCL	O1A-CGA	-2.02	1.16	1.22
7	I	101	BCL	C1D-C2D	-2.02	1.41	1.45
7	S	101	BCL	O1A-CGA	-2.02	1.16	1.22
7	k	103	BCL	C3D-C4D	-2.01	1.39	1.44
7	5	101	BCL	C3D-C4D	-2.01	1.39	1.44
7	f	101	BCL	CHD-C1D	2.01	1.42	1.38
7	u	101	BCL	C3D-C4D	-2.00	1.39	1.44
12	e	103	SPO	C4-C5	2.00	1.53	1.50

All (2256) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	e	103	SPO	C15-C14-C12	-16.95	103.12	127.31
12	i	102	SPO	C10-C9-C7	-16.86	103.25	127.31
12	e	103	SPO	C10-C9-C7	-16.00	104.48	127.31
12	ab	102	SPO	C15-C14-C12	-14.99	105.91	127.31
12	N	103	SPO	C10-C9-C7	-14.36	106.82	127.31
12	G	102	SPO	C15-C14-C12	-14.33	106.86	127.31
12	n	101	SPO	C20-C19-C17	-14.14	107.12	127.31
12	G	102	SPO	C10-C9-C7	-14.12	107.16	127.31
12	e	103	SPO	C21-C22-C23	-13.97	107.37	127.31
12	s	105	SPO	C10-C9-C7	-13.90	107.47	127.31
12	i	102	SPO	C20-C19-C17	-13.79	107.63	127.31
12	ab	102	SPO	C10-C9-C7	-13.51	108.03	127.31
12	N	103	SPO	C15-C14-C12	-13.47	108.09	127.31
12	O	103	SPO	C10-C9-C7	-13.34	108.27	127.31
12	j	103	SPO	C15-C14-C12	-13.18	108.49	127.31
12	d	103	SPO	C18-C17-C19	-13.17	104.47	122.92
12	t	101	SPO	C15-C14-C12	-13.11	108.59	127.31
12	j	103	SPO	C10-C9-C7	-12.77	109.09	127.31
12	i	102	SPO	C8-C7-C9	-12.74	105.07	122.92
12	i	102	SPO	C18-C17-C19	-12.63	105.23	122.92
12	n	101	SPO	C13-C12-C14	-12.60	105.28	122.92
12	a	104	SPO	C10-C9-C7	-12.41	109.60	127.31
12	k	102	SPO	C13-C12-C14	-12.33	105.65	122.92
12	g	102	SPO	C10-C9-C7	-12.33	109.71	127.31
12	d	103	SPO	C13-C12-C14	-12.29	105.70	122.92
12	U	102	SPO	C20-C19-C17	-12.28	109.78	127.31
12	g	102	SPO	C18-C17-C19	-12.26	105.75	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	g	102	SPO	C21-C22-C23	-12.20	109.90	127.31
12	aa	101	SPO	C13-C12-C14	-12.03	106.08	122.92
12	G	103	SPO	C10-C9-C7	-11.98	110.21	127.31
12	d	103	SPO	C25-C23-C22	-11.97	100.57	118.94
12	O	102	SPO	C20-C19-C17	-11.95	110.26	127.31
12	G	102	SPO	C20-C19-C17	-11.92	110.30	127.31
12	T	102	SPO	C10-C9-C7	-11.90	110.32	127.31
12	ab	102	SPO	C20-C19-C17	-11.90	110.33	127.31
12	3	103	SPO	C20-C19-C17	-11.89	110.35	127.31
12	B	103	SPO	C21-C22-C23	-11.87	110.36	127.31
12	aa	101	SPO	C15-C14-C12	-11.80	110.47	127.31
12	N	103	SPO	C21-C22-C23	-11.77	110.51	127.31
12	B	102	SPO	C10-C9-C7	-11.76	110.52	127.31
12	G	103	SPO	C20-C19-C17	-11.75	110.54	127.31
12	r	102	SPO	C10-C9-C7	-11.75	110.54	127.31
12	k	102	SPO	C24-C23-C22	-11.70	106.54	122.92
12	8	101	SPO	C18-C17-C19	-11.67	106.57	122.92
12	k	102	SPO	C18-C17-C19	-11.62	106.64	122.92
12	B	102	SPO	C20-C19-C17	-11.60	110.75	127.31
12	B	102	SPO	C15-C14-C12	-11.56	110.81	127.31
12	t	101	SPO	C13-C12-C14	-11.55	106.75	122.92
12	O	102	SPO	C10-C9-C7	-11.50	110.90	127.31
12	s	104	SPO	C20-C19-C17	-11.44	110.98	127.31
12	aa	101	SPO	C18-C17-C19	-11.42	106.92	122.92
12	T	102	SPO	C15-C14-C12	-11.42	111.02	127.31
12	ab	102	SPO	C24-C23-C22	-11.36	107.01	122.92
12	e	103	SPO	C24-C23-C22	-11.35	107.02	122.92
12	r	102	SPO	C21-C22-C23	-11.34	111.12	127.31
8	L	302	BPB	C4D-CHA-CBD	-11.34	103.39	108.52
12	s	105	SPO	C20-C19-C17	-11.34	111.13	127.31
12	8	101	SPO	C13-C12-C14	-11.30	107.09	122.92
12	O	103	SPO	C24-C23-C22	-11.29	107.11	122.92
8	l	302	BPB	C4D-CHA-CBD	-11.25	103.43	108.52
12	F	102	SPO	C20-C19-C17	-11.24	111.27	127.31
12	ab	102	SPO	C8-C7-C9	-11.23	107.19	122.92
12	N	101	SPO	C20-C19-C17	-11.23	111.29	127.31
12	aa	101	SPO	C20-C19-C17	-11.19	111.34	127.31
12	r	102	SPO	C15-C14-C12	-11.16	111.38	127.31
12	d	103	SPO	C24-C23-C22	-11.16	107.29	122.92
12	e	103	SPO	C18-C17-C19	-11.15	107.30	122.92
12	t	101	SPO	C10-C9-C7	-11.15	111.40	127.31
12	S	102	SPO	C20-C19-C17	-11.13	111.42	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	102	SPO	C20-C19-C17	-11.13	111.43	127.31
12	k	102	SPO	C16-C17-C19	-11.11	101.89	118.94
12	q	102	SPO	C20-C19-C17	-11.08	111.49	127.31
12	3	103	SPO	C21-C22-C23	-11.08	111.49	127.31
12	Q	102	SPO	C20-C19-C17	-11.08	111.50	127.31
12	8	101	SPO	C24-C23-C22	-11.06	107.43	122.92
12	8	101	SPO	C15-C14-C12	-11.02	111.59	127.31
12	K	102	SPO	C20-C19-C17	-10.99	111.62	127.31
12	m	1305	SPO	C15-C14-C12	-10.99	111.63	127.31
12	n	101	SPO	C18-C17-C19	-10.98	107.54	122.92
12	M	1305	SPO	C15-C14-C12	-10.98	111.64	127.31
12	e	103	SPO	C8-C7-C9	-10.97	107.56	122.92
12	e	101	SPO	C20-C19-C17	-10.93	111.72	127.31
12	0	102	SPO	C20-C19-C17	-10.92	111.72	127.31
12	d	103	SPO	C20-C19-C17	-10.92	111.72	127.31
12	I	102	SPO	C20-C19-C17	-10.91	111.74	127.31
12	B	103	SPO	C13-C12-C14	-10.90	107.65	122.92
12	o	102	SPO	C20-C19-C17	-10.88	111.78	127.31
12	3	103	SPO	C8-C7-C9	-10.87	107.69	122.92
12	D	102	SPO	C20-C19-C17	-10.87	111.80	127.31
12	aa	101	SPO	C24-C23-C22	-10.85	107.72	122.92
12	i	102	SPO	C24-C23-C22	-10.83	107.75	122.92
12	3	101	SPO	C20-C19-C17	-10.81	111.88	127.31
12	j	101	SPO	C20-C19-C17	-10.81	111.88	127.31
12	9	102	SPO	C20-C19-C17	-10.81	111.88	127.31
12	N	103	SPO	C8-C7-C9	-10.81	107.78	122.92
8	L	305	BPB	C4D-CHA-CBD	-10.81	103.63	108.52
12	I	102	SPO	C21-C22-C23	-10.78	111.93	127.31
12	s	102	SPO	C20-C19-C17	-10.77	111.94	127.31
12	s	105	SPO	C8-C7-C9	-10.77	107.84	122.92
8	l	306	BPB	C4D-CHA-CBD	-10.75	103.65	108.52
12	i	102	SPO	C11-C12-C14	-10.75	102.45	118.94
12	j	103	SPO	C18-C17-C19	-10.72	107.91	122.92
12	S	102	SPO	C21-C22-C23	-10.70	112.03	127.31
12	8	101	SPO	C20-C19-C17	-10.69	112.05	127.31
12	O	103	SPO	C15-C14-C12	-10.68	112.07	127.31
12	0	102	SPO	C21-C22-C23	-10.67	112.08	127.31
12	3	103	SPO	C10-C9-C7	-10.67	112.09	127.31
12	N	103	SPO	C24-C23-C22	-10.66	107.99	122.92
12	R	102	SPO	C20-C19-C17	-10.66	112.10	127.31
12	d	103	SPO	C16-C17-C19	-10.66	102.59	118.94
12	G	103	SPO	C18-C17-C19	-10.65	108.00	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	aa	101	SPO	C10-C9-C7	-10.64	112.12	127.31
12	r	102	SPO	C20-C19-C17	-10.63	112.14	127.31
12	8	101	SPO	C25-C23-C22	-10.61	102.65	118.94
12	s	104	SPO	C10-C9-C7	-10.61	112.16	127.31
12	m	1305	SPO	C20-C19-C17	-10.59	112.20	127.31
12	M	1305	SPO	C20-C19-C17	-10.58	112.20	127.31
12	t	101	SPO	C24-C23-C22	-10.58	108.11	122.92
12	B	103	SPO	C8-C7-C9	-10.56	108.12	122.92
12	t	101	SPO	C20-C19-C17	-10.55	112.25	127.31
12	T	102	SPO	C20-C19-C17	-10.55	112.25	127.31
12	d	103	SPO	C11-C12-C14	-10.55	102.76	118.94
12	O	102	SPO	C15-C14-C12	-10.53	112.29	127.31
12	g	102	SPO	C8-C7-C9	-10.53	108.18	122.92
12	9	102	SPO	C8-C7-C9	-10.49	108.22	122.92
12	N	101	SPO	C21-C22-C23	-10.48	112.35	127.31
12	F	102	SPO	C21-C22-C23	-10.47	112.36	127.31
12	j	103	SPO	C13-C12-C14	-10.43	108.31	122.92
12	j	103	SPO	C20-C19-C17	-10.42	112.44	127.31
12	q	102	SPO	C21-C22-C23	-10.41	112.45	127.31
12	I	102	SPO	C8-C7-C9	-10.40	108.35	122.92
12	K	102	SPO	C21-C22-C23	-10.38	112.49	127.31
12	ab	102	SPO	C13-C12-C14	-10.38	108.38	122.92
12	N	103	SPO	C18-C17-C19	-10.38	108.39	122.92
12	G	102	SPO	C13-C12-C14	-10.38	108.39	122.92
12	U	102	SPO	C21-C22-C23	-10.34	112.55	127.31
12	8	101	SPO	C8-C7-C9	-10.33	108.45	122.92
12	i	102	SPO	C21-C22-C23	-10.30	112.60	127.31
12	aa	101	SPO	C25-C23-C22	-10.28	103.16	118.94
12	a	104	SPO	C13-C12-C14	-10.28	108.52	122.92
12	S	102	SPO	C24-C23-C22	-10.28	108.53	122.92
12	o	102	SPO	C21-C22-C23	-10.26	112.67	127.31
12	e	103	SPO	C13-C12-C14	-10.24	108.58	122.92
12	N	101	SPO	C8-C7-C9	-10.24	108.58	122.92
12	0	102	SPO	C15-C14-C12	-10.24	112.70	127.31
12	aa	101	SPO	C8-C7-C9	-10.23	108.59	122.92
12	a	104	SPO	C20-C19-C17	-10.23	112.72	127.31
12	A	102	SPO	C21-C22-C23	-10.21	112.73	127.31
12	O	102	SPO	C21-C22-C23	-10.21	112.74	127.31
12	9	102	SPO	C10-C9-C7	-10.21	112.74	127.31
12	Q	102	SPO	C21-C22-C23	-10.21	112.74	127.31
12	A	102	SPO	C8-C7-C9	-10.20	108.64	122.92
12	N	101	SPO	C10-C9-C7	-10.19	112.77	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	o	102	SPO	C10-C9-C7	-10.19	112.77	127.31
12	S	102	SPO	C10-C9-C7	-10.18	112.78	127.31
12	d	103	SPO	C21-C22-C23	-10.17	112.79	127.31
12	n	101	SPO	C21-C22-C23	-10.15	112.82	127.31
12	e	103	SPO	C20-C19-C17	-10.14	112.83	127.31
12	j	101	SPO	C10-C9-C7	-10.14	112.83	127.31
12	D	102	SPO	C21-C22-C23	-10.13	112.85	127.31
12	R	102	SPO	C21-C22-C23	-10.12	112.86	127.31
12	s	105	SPO	C15-C14-C12	-10.12	112.86	127.31
12	3	101	SPO	C21-C22-C23	-10.12	112.87	127.31
12	G	102	SPO	C18-C17-C19	-10.09	108.79	122.92
12	8	101	SPO	C10-C9-C7	-10.07	112.93	127.31
12	I	102	SPO	C10-C9-C7	-10.07	112.94	127.31
12	aa	101	SPO	C21-C22-C23	-10.07	112.94	127.31
12	B	102	SPO	C24-C23-C22	-10.06	108.83	122.92
12	s	102	SPO	C21-C22-C23	-10.05	112.97	127.31
12	A	102	SPO	C18-C17-C19	-10.01	108.90	122.92
12	K	102	SPO	C8-C7-C9	-10.01	108.90	122.92
12	r	102	SPO	C18-C17-C19	-10.01	108.90	122.92
12	Q	102	SPO	C10-C9-C7	-10.01	113.03	127.31
12	F	102	SPO	C8-C7-C9	-9.99	108.94	122.92
12	k	102	SPO	C15-C14-C12	-9.97	113.08	127.31
12	K	102	SPO	C10-C9-C7	-9.97	113.08	127.31
12	j	101	SPO	C21-C22-C23	-9.96	113.10	127.31
12	t	101	SPO	C18-C17-C19	-9.95	108.99	122.92
12	ab	102	SPO	C21-C22-C23	-9.94	113.12	127.31
12	o	102	SPO	C8-C7-C9	-9.92	109.03	122.92
12	j	101	SPO	C8-C7-C9	-9.91	109.04	122.92
12	0	102	SPO	C13-C12-C14	-9.90	109.06	122.92
12	A	102	SPO	C10-C9-C7	-9.90	113.19	127.31
12	O	102	SPO	C8-C7-C9	-9.89	109.07	122.92
12	m	1305	SPO	C21-C22-C23	-9.89	113.20	127.31
12	e	101	SPO	C8-C7-C9	-9.88	109.09	122.92
12	j	103	SPO	C21-C22-C23	-9.88	113.21	127.31
12	M	1305	SPO	C21-C22-C23	-9.88	113.22	127.31
12	O	102	SPO	C13-C12-C14	-9.86	109.12	122.92
12	s	102	SPO	C10-C9-C7	-9.83	113.28	127.31
12	3	101	SPO	C10-C9-C7	-9.82	113.29	127.31
12	Q	102	SPO	C18-C17-C19	-9.82	109.17	122.92
12	S	102	SPO	C8-C7-C9	-9.82	109.17	122.92
12	g	102	SPO	C24-C23-C22	-9.82	109.17	122.92
12	a	104	SPO	C21-C22-C23	-9.81	113.31	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	D	102	SPO	C8-C7-C9	-9.81	109.18	122.92
12	0	102	SPO	C18-C17-C19	-9.80	109.19	122.92
12	D	102	SPO	C10-C9-C7	-9.79	113.34	127.31
12	g	102	SPO	C15-C14-C12	-9.79	113.34	127.31
12	3	101	SPO	C8-C7-C9	-9.78	109.22	122.92
12	N	103	SPO	C20-C19-C17	-9.77	113.37	127.31
12	k	102	SPO	C20-C19-C17	-9.76	113.38	127.31
12	e	101	SPO	C10-C9-C7	-9.75	113.40	127.31
12	O	103	SPO	C20-C19-C17	-9.74	113.40	127.31
12	Q	102	SPO	C8-C7-C9	-9.74	109.27	122.92
12	9	102	SPO	C21-C22-C23	-9.73	113.42	127.31
12	3	103	SPO	C24-C23-C22	-9.73	109.30	122.92
12	a	104	SPO	C16-C17-C19	-9.72	104.03	118.94
12	e	101	SPO	C21-C22-C23	-9.72	113.44	127.31
12	I	102	SPO	C13-C12-C14	-9.70	109.34	122.92
12	q	102	SPO	C18-C17-C19	-9.69	109.35	122.92
12	a	104	SPO	C25-C23-C22	-9.69	104.07	118.94
12	U	102	SPO	C15-C14-C12	-9.69	113.49	127.31
12	g	102	SPO	C20-C19-C17	-9.67	113.51	127.31
12	3	103	SPO	C13-C12-C14	-9.67	109.38	122.92
12	R	102	SPO	C10-C9-C7	-9.66	113.53	127.31
12	O	103	SPO	C8-C7-C9	-9.65	109.40	122.92
12	q	102	SPO	C10-C9-C7	-9.65	113.54	127.31
12	O	103	SPO	C18-C17-C19	-9.65	109.41	122.92
12	n	101	SPO	C8-C7-C9	-9.64	109.42	122.92
12	T	102	SPO	C13-C12-C14	-9.64	109.42	122.92
12	Q	102	SPO	C24-C23-C22	-9.63	109.44	122.92
12	e	101	SPO	C18-C17-C19	-9.62	109.44	122.92
12	B	102	SPO	C13-C12-C14	-9.62	109.44	122.92
12	k	102	SPO	C25-C23-C22	-9.61	104.20	118.94
12	B	102	SPO	C18-C17-C19	-9.60	109.47	122.92
12	o	102	SPO	C18-C17-C19	-9.60	109.47	122.92
12	j	103	SPO	C8-C7-C9	-9.60	109.48	122.92
12	U	102	SPO	C18-C17-C19	-9.59	109.48	122.92
12	0	102	SPO	C8-C7-C9	-9.59	109.49	122.92
12	s	102	SPO	C24-C23-C22	-9.59	109.50	122.92
12	e	101	SPO	C24-C23-C22	-9.56	109.53	122.92
12	D	102	SPO	C18-C17-C19	-9.56	109.53	122.92
12	s	105	SPO	C13-C12-C14	-9.55	109.54	122.92
12	F	102	SPO	C18-C17-C19	-9.54	109.56	122.92
12	O	102	SPO	C18-C17-C19	-9.53	109.57	122.92
12	3	101	SPO	C18-C17-C19	-9.53	109.58	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	G	102	SPO	C8-C7-C9	-9.52	109.59	122.92
12	0	102	SPO	C10-C9-C7	-9.51	113.74	127.31
12	e	101	SPO	C13-C12-C14	-9.50	109.61	122.92
12	F	102	SPO	C10-C9-C7	-9.50	113.76	127.31
12	r	102	SPO	C24-C23-C22	-9.49	109.63	122.92
12	R	102	SPO	C18-C17-C19	-9.49	109.63	122.92
12	j	101	SPO	C24-C23-C22	-9.48	109.64	122.92
12	s	104	SPO	C13-C12-C14	-9.47	109.65	122.92
12	U	102	SPO	C8-C7-C9	-9.46	109.67	122.92
12	N	101	SPO	C18-C17-C19	-9.44	109.69	122.92
12	a	104	SPO	C24-C23-C22	-9.44	109.69	122.92
12	j	101	SPO	C18-C17-C19	-9.44	109.70	122.92
12	s	102	SPO	C8-C7-C9	-9.44	109.70	122.92
12	D	102	SPO	C24-C23-C22	-9.43	109.72	122.92
12	K	102	SPO	C18-C17-C19	-9.42	109.73	122.92
12	n	101	SPO	C24-C23-C22	-9.41	109.74	122.92
12	a	104	SPO	C18-C17-C19	-9.41	109.75	122.92
12	G	103	SPO	C24-C23-C22	-9.40	109.76	122.92
12	3	103	SPO	C18-C17-C19	-9.40	109.76	122.92
12	G	103	SPO	C15-C14-C12	-9.39	113.91	127.31
12	F	102	SPO	C24-C23-C22	-9.39	109.78	122.92
12	O	103	SPO	C13-C12-C14	-9.38	109.79	122.92
12	B	103	SPO	C18-C17-C19	-9.37	109.79	122.92
12	K	102	SPO	C24-C23-C22	-9.37	109.80	122.92
12	S	102	SPO	C18-C17-C19	-9.36	109.81	122.92
12	q	102	SPO	C24-C23-C22	-9.36	109.81	122.92
12	S	102	SPO	C13-C12-C14	-9.35	109.83	122.92
12	B	102	SPO	C21-C22-C23	-9.34	113.98	127.31
12	G	103	SPO	C21-C22-C23	-9.34	113.98	127.31
12	s	104	SPO	C8-C7-C9	-9.34	109.84	122.92
12	d	103	SPO	C8-C7-C9	-9.33	109.85	122.92
12	3	101	SPO	C24-C23-C22	-9.32	109.86	122.92
12	I	102	SPO	C24-C23-C22	-9.32	109.87	122.92
12	t	101	SPO	C16-C17-C19	-9.32	104.64	118.94
12	G	102	SPO	C21-C22-C23	-9.32	114.01	127.31
12	o	102	SPO	C24-C23-C22	-9.31	109.88	122.92
12	T	102	SPO	C21-C22-C23	-9.31	114.02	127.31
12	s	102	SPO	C18-C17-C19	-9.31	109.88	122.92
12	T	102	SPO	C18-C17-C19	-9.30	109.89	122.92
12	m	1305	SPO	C6-C7-C9	-9.26	104.73	118.94
12	N	101	SPO	C13-C12-C14	-9.25	109.96	122.92
12	M	1305	SPO	C6-C7-C9	-9.25	104.74	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	0	102	SPO	C24-C23-C22	-9.25	109.96	122.92
12	R	102	SPO	C8-C7-C9	-9.25	109.97	122.92
12	m	1305	SPO	C13-C12-C14	-9.24	109.99	122.92
12	G	103	SPO	C8-C7-C9	-9.23	110.00	122.92
12	K	102	SPO	C13-C12-C14	-9.23	110.00	122.92
12	s	104	SPO	C18-C17-C19	-9.22	110.00	122.92
12	k	102	SPO	C8-C7-C9	-9.22	110.00	122.92
12	T	102	SPO	C8-C7-C9	-9.22	110.01	122.92
12	I	102	SPO	C18-C17-C19	-9.21	110.02	122.92
12	M	1305	SPO	C13-C12-C14	-9.20	110.04	122.92
12	t	101	SPO	C8-C7-C9	-9.19	110.04	122.92
12	q	102	SPO	C13-C12-C14	-9.19	110.05	122.92
12	r	102	SPO	C13-C12-C14	-9.19	110.06	122.92
12	k	102	SPO	C6-C7-C9	-9.18	104.85	118.94
12	8	101	SPO	C21-C22-C23	-9.17	114.22	127.31
12	s	102	SPO	C13-C12-C14	-9.16	110.10	122.92
12	A	102	SPO	C24-C23-C22	-9.15	110.10	122.92
12	t	101	SPO	C21-C22-C23	-9.15	114.25	127.31
12	o	102	SPO	C13-C12-C14	-9.14	110.12	122.92
12	s	105	SPO	C18-C17-C19	-9.13	110.13	122.92
12	q	102	SPO	C8-C7-C9	-9.13	110.13	122.92
12	9	102	SPO	C13-C12-C14	-9.13	110.14	122.92
12	3	101	SPO	C13-C12-C14	-9.12	110.14	122.92
12	9	102	SPO	C18-C17-C19	-9.11	110.16	122.92
12	U	102	SPO	C13-C12-C14	-9.09	110.19	122.92
12	8	101	SPO	C16-C17-C19	-9.08	105.01	118.94
12	B	103	SPO	C20-C19-C17	-9.07	114.36	127.31
12	t	101	SPO	C25-C23-C22	-9.07	105.02	118.94
12	a	104	SPO	C8-C7-C9	-9.04	110.26	122.92
12	N	101	SPO	C24-C23-C22	-9.02	110.28	122.92
12	s	105	SPO	C21-C22-C23	-9.02	114.44	127.31
12	a	104	SPO	C11-C12-C14	-9.02	105.11	118.94
12	9	102	SPO	C24-C23-C22	-9.00	110.31	122.92
12	N	101	SPO	C15-C14-C12	-8.98	114.49	127.31
12	k	102	SPO	C11-C12-C14	-8.98	105.17	118.94
12	r	102	SPO	C8-C7-C9	-8.98	110.35	122.92
12	D	102	SPO	C13-C12-C14	-8.98	110.35	122.92
12	k	102	SPO	C21-C22-C23	-8.97	114.51	127.31
12	U	102	SPO	C10-C9-C7	-8.95	114.53	127.31
12	a	104	SPO	C15-C14-C12	-8.95	114.54	127.31
12	B	102	SPO	C8-C7-C9	-8.92	110.43	122.92
12	B	103	SPO	C15-C14-C12	-8.91	114.59	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	M	1305	SPO	C8-C7-C9	-8.91	110.44	122.92
12	9	102	SPO	C15-C14-C12	-8.90	114.61	127.31
12	m	1305	SPO	C8-C7-C9	-8.89	110.48	122.92
12	d	103	SPO	C15-C14-C12	-8.87	114.66	127.31
12	aa	101	SPO	C11-C12-C14	-8.87	105.34	118.94
12	N	103	SPO	C13-C12-C14	-8.86	110.52	122.92
12	i	102	SPO	C16-C17-C19	-8.85	105.36	118.94
12	8	101	SPO	C11-C12-C14	-8.85	105.36	118.94
12	3	103	SPO	C15-C14-C12	-8.84	114.69	127.31
12	s	105	SPO	C24-C23-C22	-8.84	110.55	122.92
12	0	102	SPO	C25-C23-C22	-8.79	105.45	118.94
12	A	102	SPO	C13-C12-C14	-8.78	110.63	122.92
12	B	103	SPO	C16-C17-C19	-8.77	105.48	118.94
12	aa	101	SPO	C16-C17-C19	-8.77	105.48	118.94
12	S	102	SPO	C15-C14-C12	-8.74	114.83	127.31
12	M	1305	SPO	C18-C17-C19	-8.73	110.70	122.92
12	s	104	SPO	C25-C23-C22	-8.72	105.56	118.94
12	K	102	SPO	C15-C14-C12	-8.72	114.87	127.31
12	G	103	SPO	C13-C12-C14	-8.71	110.72	122.92
12	G	102	SPO	C24-C23-C22	-8.71	110.73	122.92
12	O	102	SPO	C25-C23-C22	-8.70	105.59	118.94
12	F	102	SPO	C13-C12-C14	-8.70	110.74	122.92
12	m	1305	SPO	C18-C17-C19	-8.70	110.74	122.92
12	G	102	SPO	C18-C17-C16	-8.69	104.39	118.08
12	8	101	SPO	C6-C7-C9	-8.68	105.62	118.94
12	n	101	SPO	C10-C9-C7	-8.68	114.93	127.31
12	G	103	SPO	C25-C23-C22	-8.67	105.63	118.94
12	M	1305	SPO	C24-C23-C22	-8.66	110.79	122.92
12	I	102	SPO	C15-C14-C12	-8.65	114.96	127.31
12	Q	102	SPO	C13-C12-C14	-8.65	110.81	122.92
12	m	1305	SPO	C24-C23-C22	-8.65	110.81	122.92
12	O	103	SPO	C21-C22-C23	-8.62	115.00	127.31
12	T	102	SPO	C24-C23-C22	-8.62	110.85	122.92
12	B	102	SPO	C25-C23-C22	-8.61	105.73	118.94
12	R	102	SPO	C11-C12-C14	-8.61	105.73	118.94
12	j	101	SPO	C13-C12-C14	-8.58	110.90	122.92
12	q	102	SPO	C15-C14-C12	-8.58	115.06	127.31
12	d	103	SPO	C6-C7-C9	-8.58	105.78	118.94
12	D	102	SPO	C15-C14-C12	-8.57	115.08	127.31
12	U	102	SPO	C24-C23-C22	-8.56	110.93	122.92
12	Q	102	SPO	C15-C14-C12	-8.51	115.16	127.31
12	B	103	SPO	C24-C23-C22	-8.49	111.02	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	R	102	SPO	C24-C23-C22	-8.49	111.03	122.92
12	e	101	SPO	C15-C14-C12	-8.49	115.20	127.31
12	U	102	SPO	C11-C12-C14	-8.48	105.93	118.94
12	j	103	SPO	C24-C23-C22	-8.48	111.05	122.92
12	i	102	SPO	C15-C14-C12	-8.45	115.25	127.31
12	3	101	SPO	C15-C14-C12	-8.45	115.25	127.31
12	o	102	SPO	C15-C14-C12	-8.44	115.27	127.31
12	t	101	SPO	C11-C12-C14	-8.44	105.99	118.94
12	A	102	SPO	C15-C14-C12	-8.43	115.28	127.31
12	O	102	SPO	C24-C23-C22	-8.42	111.13	122.92
12	aa	101	SPO	C6-C7-C9	-8.41	106.03	118.94
12	U	102	SPO	C6-C7-C9	-8.40	106.04	118.94
12	g	102	SPO	C13-C12-C14	-8.40	111.15	122.92
12	s	102	SPO	C15-C14-C12	-8.40	115.33	127.31
12	R	102	SPO	C13-C12-C14	-8.39	111.17	122.92
12	s	104	SPO	C15-C14-C12	-8.34	115.41	127.31
12	s	104	SPO	C11-C12-C14	-8.28	106.24	118.94
12	F	102	SPO	C15-C14-C12	-8.27	115.51	127.31
12	0	102	SPO	C11-C12-C14	-8.26	106.26	118.94
12	s	104	SPO	C24-C23-C22	-8.26	111.36	122.92
12	j	101	SPO	C15-C14-C12	-8.25	115.53	127.31
12	B	103	SPO	C10-C9-C7	-8.24	115.55	127.31
7	1	101	BCL	CHD-C1D-ND	-8.24	116.88	124.45
12	s	104	SPO	C21-C22-C23	-8.22	115.58	127.31
12	k	102	SPO	C26-C27-C28	-8.21	115.53	127.30
12	ab	102	SPO	C18-C17-C19	-8.16	111.49	122.92
12	i	102	SPO	C13-C12-C14	-8.16	111.49	122.92
12	O	102	SPO	C16-C17-C19	-8.15	106.43	118.94
12	aa	101	SPO	C31-C32-C33	-8.11	108.13	127.66
12	ab	102	SPO	C18-C17-C16	-8.04	105.41	118.08
12	0	102	SPO	C16-C17-C19	-8.00	106.66	118.94
12	B	103	SPO	C11-C12-C14	-7.99	106.67	118.94
12	O	102	SPO	C11-C12-C14	-7.96	106.72	118.94
12	m	1305	SPO	C10-C9-C7	-7.90	116.03	127.31
12	R	102	SPO	C15-C14-C12	-7.88	116.06	127.31
12	o	102	SPO	C11-C12-C14	-7.87	106.86	118.94
12	S	102	SPO	C11-C12-C14	-7.87	106.86	118.94
12	M	1305	SPO	C10-C9-C7	-7.87	116.08	127.31
12	T	102	SPO	C25-C23-C22	-7.82	106.94	118.94
12	n	101	SPO	C15-C14-C12	-7.74	116.27	127.31
12	i	102	SPO	C6-C7-C9	-7.73	107.07	118.94
12	3	103	SPO	C11-C12-C14	-7.72	107.09	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	102	SPO	C11-C12-C14	-7.71	107.11	118.94
12	e	103	SPO	C25-C23-C22	-7.67	107.17	118.94
12	r	102	SPO	C11-C12-C14	-7.65	107.21	118.94
12	3	101	SPO	C11-C12-C14	-7.60	107.27	118.94
12	j	103	SPO	C25-C23-C22	-7.60	107.28	118.94
12	T	102	SPO	C16-C17-C19	-7.60	107.28	118.94
12	U	102	SPO	C31-C32-C33	-7.60	109.36	127.66
12	e	103	SPO	C5-C6-C7	-7.59	114.42	125.89
12	q	102	SPO	C11-C12-C14	-7.58	107.31	118.94
12	d	103	SPO	C10-C9-C7	-7.58	116.49	127.31
12	B	102	SPO	C6-C7-C9	-7.55	107.36	118.94
12	j	101	SPO	C11-C12-C14	-7.53	107.39	118.94
12	N	103	SPO	C25-C23-C22	-7.52	107.40	118.94
12	9	102	SPO	C11-C12-C14	-7.51	107.42	118.94
12	s	102	SPO	C11-C12-C14	-7.50	107.43	118.94
12	K	102	SPO	C11-C12-C14	-7.49	107.45	118.94
12	n	101	SPO	C18-C17-C16	-7.49	106.28	118.08
12	s	105	SPO	C25-C23-C22	-7.47	107.47	118.94
12	Q	102	SPO	C11-C12-C14	-7.46	107.50	118.94
12	d	103	SPO	C24-C23-C25	-7.42	106.39	118.08
12	r	102	SPO	C16-C17-C19	-7.41	107.56	118.94
12	N	103	SPO	C18-C17-C16	-7.41	106.40	118.08
12	e	101	SPO	C11-C12-C14	-7.39	107.60	118.94
12	i	102	SPO	C13-C12-C11	-7.38	106.45	118.08
12	D	102	SPO	C11-C12-C14	-7.37	107.64	118.94
12	O	102	SPO	C6-C7-C9	-7.36	107.65	118.94
12	m	1305	SPO	C11-C12-C14	-7.35	107.67	118.94
12	M	1305	SPO	C11-C12-C14	-7.34	107.68	118.94
12	I	102	SPO	C11-C12-C14	-7.33	107.69	118.94
12	U	102	SPO	C16-C17-C19	-7.32	107.71	118.94
12	d	103	SPO	C31-C32-C33	-7.32	110.04	127.66
12	n	101	SPO	C25-C23-C22	-7.31	107.72	118.94
12	R	102	SPO	C25-C23-C22	-7.30	107.74	118.94
12	t	101	SPO	C6-C7-C9	-7.29	107.75	118.94
12	F	102	SPO	C11-C12-C14	-7.20	107.89	118.94
12	N	101	SPO	C11-C12-C14	-7.20	107.89	118.94
12	s	104	SPO	C16-C17-C19	-7.19	107.91	118.94
12	t	101	SPO	C31-C32-C33	-7.16	110.42	127.66
12	S	102	SPO	C6-C7-C9	-7.16	107.95	118.94
12	K	102	SPO	C6-C7-C9	-7.15	107.97	118.94
12	B	102	SPO	C16-C17-C19	-7.15	107.97	118.94
12	G	102	SPO	C25-C23-C22	-7.14	107.98	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	U	102	SPO	C25-C23-C22	-7.14	107.98	118.94
12	t	101	SPO	C24-C23-C25	-7.13	106.84	118.08
12	Q	102	SPO	C6-C7-C9	-7.11	108.03	118.94
12	g	102	SPO	C16-C17-C19	-7.11	108.03	118.94
12	3	101	SPO	C6-C7-C9	-7.11	108.03	118.94
12	e	101	SPO	C6-C7-C9	-7.11	108.03	118.94
12	n	101	SPO	C31-C32-C33	-7.09	110.59	127.66
12	B	103	SPO	C25-C23-C22	-7.07	108.10	118.94
12	s	102	SPO	C6-C7-C9	-7.07	108.10	118.94
12	r	102	SPO	C25-C23-C22	-7.06	108.11	118.94
12	B	102	SPO	C31-C32-C33	-7.04	110.70	127.66
12	Q	102	SPO	C34-C33-C35	-7.02	107.95	115.98
12	8	101	SPO	C35-C33-C32	-7.02	106.91	121.12
12	0	102	SPO	C6-C7-C9	-7.02	108.17	118.94
12	e	101	SPO	C25-C23-C22	-6.99	108.22	118.94
12	s	105	SPO	C11-C12-C14	-6.98	108.23	118.94
12	m	1305	SPO	C25-C23-C22	-6.98	108.23	118.94
12	M	1305	SPO	C25-C23-C22	-6.98	108.23	118.94
12	T	102	SPO	C11-C12-C14	-6.97	108.24	118.94
12	D	102	SPO	C6-C7-C9	-6.96	108.26	118.94
12	S	102	SPO	C34-C33-C35	-6.94	108.05	115.98
12	B	103	SPO	C35-C33-C32	-6.94	107.08	121.12
12	3	103	SPO	C6-C7-C9	-6.92	108.32	118.94
12	r	102	SPO	C6-C7-C9	-6.91	108.34	118.94
12	T	102	SPO	C31-C32-C33	-6.89	111.07	127.66
12	0	102	SPO	C31-C32-C33	-6.88	111.08	127.66
12	i	102	SPO	C24-C23-C25	-6.87	107.25	118.08
12	s	102	SPO	C25-C23-C22	-6.86	108.41	118.94
12	g	102	SPO	C13-C12-C11	-6.86	107.27	118.08
12	j	101	SPO	C6-C7-C9	-6.83	108.46	118.94
12	M	1305	SPO	C16-C17-C19	-6.82	108.47	118.94
12	F	102	SPO	C25-C23-C22	-6.81	108.49	118.94
12	m	1305	SPO	C16-C17-C19	-6.81	108.49	118.94
12	G	103	SPO	C11-C12-C14	-6.80	108.50	118.94
12	q	102	SPO	C6-C7-C9	-6.80	108.51	118.94
12	A	102	SPO	C6-C7-C9	-6.78	108.53	118.94
12	F	102	SPO	C6-C7-C9	-6.77	108.55	118.94
12	m	1305	SPO	C31-C32-C33	-6.77	111.35	127.66
12	g	102	SPO	C6-C7-C9	-6.77	108.55	118.94
12	M	1305	SPO	C31-C32-C33	-6.76	111.37	127.66
12	T	102	SPO	C6-C7-C9	-6.73	108.62	118.94
12	k	102	SPO	C10-C9-C7	-6.73	117.71	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	O	103	SPO	C16-C17-C19	-6.72	108.62	118.94
12	G	103	SPO	C16-C17-C19	-6.72	108.63	118.94
12	G	103	SPO	C31-C32-C33	-6.72	111.49	127.66
12	I	102	SPO	C25-C23-C22	-6.71	108.64	118.94
12	i	102	SPO	C31-C32-C33	-6.71	111.50	127.66
12	o	102	SPO	C6-C7-C9	-6.70	108.67	118.94
12	a	104	SPO	C31-C32-C33	-6.69	111.55	127.66
12	B	103	SPO	C31-C32-C33	-6.68	111.56	127.66
12	s	105	SPO	C16-C17-C19	-6.68	108.69	118.94
12	F	102	SPO	C34-C33-C32	-6.68	106.55	123.68
12	N	103	SPO	C11-C12-C14	-6.64	108.75	118.94
12	q	102	SPO	C34-C33-C32	-6.63	106.68	123.68
12	R	102	SPO	C35-C33-C32	-6.62	107.71	121.12
12	O	102	SPO	C31-C32-C33	-6.61	111.75	127.66
12	q	102	SPO	C25-C23-C22	-6.59	108.82	118.94
12	a	104	SPO	C6-C7-C9	-6.59	108.83	118.94
12	t	101	SPO	C35-C33-C32	-6.58	107.80	121.12
12	A	102	SPO	C25-C23-C22	-6.57	108.86	118.94
12	o	102	SPO	C25-C23-C22	-6.56	108.87	118.94
12	G	102	SPO	C13-C12-C11	-6.56	107.75	118.08
12	8	101	SPO	C31-C32-C33	-6.53	111.94	127.66
12	S	102	SPO	C25-C23-C22	-6.52	108.94	118.94
12	N	101	SPO	C6-C7-C9	-6.51	108.94	118.94
12	3	101	SPO	C25-C23-C22	-6.51	108.95	118.94
12	R	102	SPO	C16-C17-C19	-6.51	108.95	118.94
12	T	102	SPO	C35-C33-C32	-6.49	107.99	121.12
12	U	102	SPO	C34-C33-C32	-6.48	107.05	123.68
12	D	102	SPO	C16-C17-C19	-6.48	109.00	118.94
12	N	101	SPO	C25-C23-C22	-6.47	109.02	118.94
12	9	102	SPO	C6-C7-C9	-6.46	109.03	118.94
12	s	104	SPO	C31-C32-C33	-6.44	112.15	127.66
12	3	103	SPO	C16-C17-C19	-6.43	109.07	118.94
12	D	102	SPO	C25-C23-C22	-6.43	109.08	118.94
12	O	103	SPO	C6-C7-C9	-6.42	109.08	118.94
12	Q	102	SPO	C25-C23-C22	-6.42	109.08	118.94
12	O	103	SPO	C31-C32-C33	-6.42	112.20	127.66
12	g	102	SPO	C31-C32-C33	-6.41	112.22	127.66
12	e	101	SPO	C34-C33-C32	-6.41	107.23	123.68
12	g	102	SPO	C11-C12-C14	-6.39	109.14	118.94
12	a	104	SPO	C35-C33-C32	-6.38	108.20	121.12
12	e	103	SPO	C13-C12-C11	-6.38	108.03	118.08
12	s	102	SPO	C16-C17-C19	-6.38	109.16	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	K	102	SPO	C25-C23-C22	-6.37	109.17	118.94
12	r	102	SPO	C31-C32-C33	-6.35	112.37	127.66
12	d	103	SPO	C5-C6-C7	-6.35	116.30	125.89
12	N	103	SPO	C31-C32-C33	-6.35	112.38	127.66
12	D	102	SPO	C34-C33-C32	-6.34	107.42	123.68
12	o	102	SPO	C16-C17-C19	-6.34	109.21	118.94
12	O	102	SPO	C35-C33-C32	-6.33	108.30	121.12
12	9	102	SPO	C34-C33-C32	-6.33	107.44	123.68
12	j	103	SPO	C31-C32-C33	-6.33	112.42	127.66
12	j	101	SPO	C25-C23-C22	-6.33	109.23	118.94
12	g	102	SPO	C35-C33-C32	-6.33	108.31	121.12
12	j	103	SPO	C35-C33-C32	-6.31	108.34	121.12
12	9	102	SPO	C25-C23-C22	-6.31	109.26	118.94
12	d	103	SPO	C8-C7-C6	-6.29	108.16	118.08
12	s	104	SPO	C6-C7-C9	-6.29	109.29	118.94
12	B	102	SPO	C11-C12-C14	-6.29	109.30	118.94
12	3	103	SPO	C34-C33-C32	-6.28	107.57	123.68
12	s	102	SPO	C34-C33-C32	-6.26	107.63	123.68
12	G	102	SPO	C5-C6-C7	-6.25	116.44	125.89
12	3	101	SPO	C34-C33-C32	-6.24	107.68	123.68
12	j	103	SPO	C16-C17-C19	-6.22	109.39	118.94
12	t	101	SPO	C18-C17-C16	-6.21	108.28	118.08
12	j	101	SPO	C16-C17-C19	-6.21	109.41	118.94
12	j	101	SPO	C34-C33-C32	-6.21	107.76	123.68
12	m	1305	SPO	C35-C33-C32	-6.20	108.58	121.12
12	9	102	SPO	C31-C32-C33	-6.18	112.79	127.66
12	M	1305	SPO	C35-C33-C32	-6.18	108.62	121.12
12	i	102	SPO	C36-C37-C38	-6.17	106.67	127.75
12	0	102	SPO	C35-C33-C32	-6.17	108.64	121.12
12	I	102	SPO	C16-C17-C19	-6.16	109.48	118.94
12	ab	102	SPO	C24-C23-C25	-6.16	108.37	118.08
7	M	1301	BCL	C1-C2-C3	6.15	136.68	126.04
12	R	102	SPO	C31-C32-C33	-6.15	112.86	127.66
7	m	1301	BCL	C1-C2-C3	6.14	136.67	126.04
12	G	102	SPO	C31-C32-C33	-6.13	112.90	127.66
12	q	102	SPO	C31-C32-C33	-6.12	112.92	127.66
12	aa	101	SPO	C34-C33-C32	-6.12	107.98	123.68
12	R	102	SPO	C6-C7-C9	-6.11	109.56	118.94
12	F	102	SPO	C16-C17-C19	-6.11	109.56	118.94
12	Q	102	SPO	C31-C32-C33	-6.11	112.94	127.66
12	e	103	SPO	C18-C17-C16	-6.11	108.45	118.08
12	A	102	SPO	C16-C17-C19	-6.11	109.56	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	3	101	SPO	C31-C32-C33	-6.11	112.95	127.66
12	3	103	SPO	C25-C23-C22	-6.11	109.57	118.94
12	I	102	SPO	C6-C7-C9	-6.10	109.58	118.94
12	N	101	SPO	C34-C33-C32	-6.10	108.02	123.68
12	G	102	SPO	C35-C33-C32	-6.10	108.77	121.12
12	n	101	SPO	C35-C33-C32	-6.10	108.78	121.12
12	o	102	SPO	C31-C32-C33	-6.09	113.01	127.66
12	K	102	SPO	C34-C33-C32	-6.08	108.08	123.68
12	ab	102	SPO	C34-C33-C32	-6.08	108.08	123.68
12	k	102	SPO	C8-C7-C6	-6.06	108.53	118.08
12	A	102	SPO	C34-C33-C32	-6.05	108.17	123.68
12	G	102	SPO	C16-C17-C19	-6.04	109.67	118.94
12	O	103	SPO	C25-C23-C22	-6.02	109.70	118.94
12	B	103	SPO	C6-C7-C9	-6.00	109.73	118.94
12	o	102	SPO	C35-C33-C32	-6.00	108.97	121.12
12	j	101	SPO	C13-C12-C11	-6.00	108.63	118.08
12	S	102	SPO	C31-C32-C33	-5.98	113.26	127.66
12	ab	102	SPO	C31-C32-C33	-5.97	113.28	127.66
7	U	103	BCL	CHD-C1D-ND	-5.97	118.97	124.45
12	9	102	SPO	C16-C17-C19	-5.97	109.79	118.94
12	D	102	SPO	C31-C32-C33	-5.96	113.30	127.66
12	G	103	SPO	C35-C33-C32	-5.95	109.07	121.12
12	I	102	SPO	C8-C7-C6	-5.95	108.70	118.08
12	s	104	SPO	C8-C7-C6	-5.94	108.71	118.08
12	o	102	SPO	C34-C33-C32	-5.94	108.44	123.68
12	R	102	SPO	C8-C7-C6	-5.94	108.72	118.08
12	I	102	SPO	C34-C33-C32	-5.93	108.46	123.68
12	G	103	SPO	C6-C7-C9	-5.90	109.89	118.94
12	N	103	SPO	C34-C33-C32	-5.90	108.55	123.68
12	r	102	SPO	C18-C17-C16	-5.88	108.81	118.08
12	g	102	SPO	C25-C23-C22	-5.88	109.92	118.94
12	3	101	SPO	C16-C17-C19	-5.88	109.92	118.94
12	s	105	SPO	C34-C33-C32	-5.88	108.60	123.68
12	q	102	SPO	C16-C17-C19	-5.87	109.93	118.94
12	I	102	SPO	C31-C32-C33	-5.87	113.53	127.66
12	A	102	SPO	C31-C32-C33	-5.86	113.56	127.66
12	S	102	SPO	C16-C17-C19	-5.86	109.96	118.94
12	e	103	SPO	C15-C16-C17	-5.83	110.04	126.42
12	s	102	SPO	C31-C32-C33	-5.83	113.63	127.66
12	K	102	SPO	C31-C32-C33	-5.82	113.66	127.66
12	j	101	SPO	C31-C32-C33	-5.80	113.69	127.66
12	ab	102	SPO	C35-C33-C32	-5.80	109.38	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	N	101	SPO	C16-C17-C19	-5.80	110.05	118.94
12	F	102	SPO	C8-C7-C6	-5.79	108.96	118.08
12	0	102	SPO	C8-C7-C6	-5.78	108.97	118.08
12	K	102	SPO	C16-C17-C19	-5.77	110.08	118.94
12	B	102	SPO	C13-C12-C11	-5.77	108.99	118.08
12	Q	102	SPO	C16-C17-C19	-5.77	110.09	118.94
12	d	103	SPO	C18-C17-C16	-5.76	108.99	118.08
12	j	103	SPO	C11-C12-C14	-5.76	110.10	118.94
12	N	103	SPO	C35-C33-C32	-5.76	109.45	121.12
12	M	1305	SPO	C18-C17-C16	-5.76	109.00	118.08
12	j	103	SPO	C18-C17-C16	-5.76	109.01	118.08
12	m	1305	SPO	C18-C17-C16	-5.75	109.02	118.08
12	r	102	SPO	C35-C33-C32	-5.75	109.49	121.12
12	8	101	SPO	C18-C17-C16	-5.74	109.04	118.08
12	t	101	SPO	C5-C6-C7	-5.74	117.22	125.89
12	R	102	SPO	C34-C33-C32	-5.74	108.96	123.68
12	8	101	SPO	C13-C12-C11	-5.73	109.05	118.08
12	aa	101	SPO	C13-C12-C11	-5.73	109.06	118.08
12	i	102	SPO	C35-C33-C32	-5.71	109.56	121.12
12	N	101	SPO	C31-C32-C33	-5.70	113.93	127.66
12	Q	102	SPO	C13-C12-C11	-5.69	109.11	118.08
12	j	103	SPO	C6-C7-C9	-5.68	110.23	118.94
12	d	103	SPO	C13-C12-C11	-5.68	109.13	118.08
12	N	101	SPO	C8-C7-C6	-5.67	109.15	118.08
12	0	102	SPO	C34-C33-C32	-5.66	109.16	123.68
12	j	103	SPO	C8-C7-C6	-5.66	109.17	118.08
12	N	103	SPO	C6-C7-C9	-5.65	110.27	118.94
12	U	102	SPO	C24-C23-C25	-5.65	109.17	118.08
12	3	103	SPO	C31-C32-C33	-5.65	114.05	127.66
12	t	101	SPO	C34-C33-C32	-5.65	109.20	123.68
12	O	103	SPO	C35-C33-C32	-5.64	109.70	121.12
12	F	102	SPO	C31-C32-C33	-5.64	114.08	127.66
12	e	101	SPO	C31-C32-C33	-5.63	114.09	127.66
12	B	102	SPO	C5-C6-C7	-5.63	117.38	125.89
12	q	102	SPO	C8-C7-C6	-5.62	109.22	118.08
12	0	102	SPO	C24-C23-C25	-5.61	109.23	118.08
12	aa	101	SPO	C36-C37-C38	-5.61	108.58	127.75
12	K	102	SPO	C8-C7-C6	-5.61	109.25	118.08
12	G	103	SPO	C13-C12-C11	-5.60	109.25	118.08
12	9	102	SPO	C35-C33-C32	-5.60	109.78	121.12
12	e	101	SPO	C8-C7-C6	-5.60	109.25	118.08
12	s	105	SPO	C18-C17-C16	-5.59	109.26	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	7	101	BCL	C4D-CHA-C1A	5.59	128.05	121.25
7	7	101	BCL	CHD-C1D-ND	-5.58	119.32	124.45
12	a	104	SPO	C34-C33-C32	-5.58	109.36	123.68
12	U	102	SPO	C8-C7-C6	-5.57	109.30	118.08
12	N	101	SPO	C13-C12-C11	-5.57	109.30	118.08
12	e	101	SPO	C16-C17-C19	-5.57	110.40	118.94
12	ab	102	SPO	C6-C7-C9	-5.56	110.40	118.94
12	s	102	SPO	C8-C7-C6	-5.56	109.31	118.08
12	M	1305	SPO	C34-C33-C32	-5.55	109.44	123.68
12	Q	102	SPO	C8-C7-C6	-5.55	109.33	118.08
12	m	1305	SPO	C34-C33-C32	-5.55	109.44	123.68
12	N	103	SPO	C16-C17-C19	-5.54	110.44	118.94
12	O	103	SPO	C34-C33-C32	-5.52	109.51	123.68
12	s	102	SPO	C13-C12-C11	-5.52	109.38	118.08
12	T	102	SPO	C8-C7-C6	-5.52	109.38	118.08
12	q	102	SPO	C35-C33-C32	-5.51	109.97	121.12
12	G	103	SPO	C8-C7-C6	-5.50	109.41	118.08
12	r	102	SPO	C34-C33-C32	-5.50	109.58	123.68
12	M	1305	SPO	C24-C23-C25	-5.50	109.42	118.08
12	U	102	SPO	C13-C12-C11	-5.49	109.42	118.08
12	0	102	SPO	C13-C12-C11	-5.49	109.42	118.08
7	c	101	BCL	C4D-CHA-C1A	5.49	127.93	121.25
12	m	1305	SPO	C24-C23-C25	-5.49	109.43	118.08
12	G	103	SPO	C29-C28-C27	-5.48	108.44	122.59
12	D	102	SPO	C13-C12-C11	-5.48	109.44	118.08
12	I	102	SPO	C35-C33-C32	-5.48	110.03	121.12
7	M	1303	BCL	C4D-CHA-C1A	5.48	127.92	121.25
8	l	302	BPB	CBC-CAC-C3C	-5.48	112.17	126.70
12	n	101	SPO	C6-C7-C9	-5.47	110.54	118.94
12	B	102	SPO	C34-C33-C32	-5.47	109.65	123.68
8	L	302	BPB	CBC-CAC-C3C	-5.47	112.20	126.70
12	e	103	SPO	C10-C11-C12	-5.46	111.06	126.42
12	s	104	SPO	C13-C12-C11	-5.46	109.47	118.08
12	s	104	SPO	C35-C33-C32	-5.46	110.06	121.12
12	8	101	SPO	C8-C7-C6	-5.46	109.47	118.08
12	o	102	SPO	C8-C7-C6	-5.46	109.48	118.08
12	3	101	SPO	C35-C33-C32	-5.46	110.07	121.12
12	0	102	SPO	C29-C28-C27	-5.45	108.52	122.59
12	t	101	SPO	C13-C12-C11	-5.45	109.48	118.08
12	A	102	SPO	C8-C7-C6	-5.45	109.49	118.08
12	aa	101	SPO	C18-C17-C16	-5.44	109.50	118.08
12	e	103	SPO	C21-C20-C19	-5.44	112.33	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	F	102	SPO	C13-C12-C11	-5.44	109.50	118.08
7	m	1301	BCL	CHD-C1D-ND	-5.44	119.46	124.45
7	m	1303	BCL	C4D-CHA-C1A	5.43	127.86	121.25
7	u	101	BCL	CHD-C1D-ND	-5.43	119.46	124.45
12	O	102	SPO	C34-C33-C32	-5.43	109.74	123.68
12	O	103	SPO	C13-C12-C11	-5.43	109.52	118.08
7	M	1301	BCL	CHD-C1D-ND	-5.43	119.47	124.45
12	N	101	SPO	C29-C28-C27	-5.42	108.60	122.59
7	X	101	BCL	C4D-CHA-C1A	5.42	127.84	121.25
12	B	102	SPO	C29-C28-C27	-5.42	108.61	122.59
12	j	103	SPO	C29-C28-C27	-5.42	108.61	122.59
12	k	102	SPO	C5-C6-C7	-5.42	117.71	125.89
7	l	305	BCL	CHD-C1D-ND	-5.41	119.48	124.45
12	3	101	SPO	C8-C7-C6	-5.41	109.55	118.08
12	o	102	SPO	C13-C12-C11	-5.41	109.56	118.08
7	L	304	BCL	CHD-C1D-ND	-5.41	119.49	124.45
12	j	101	SPO	C8-C7-C6	-5.40	109.56	118.08
12	g	102	SPO	C29-C28-C27	-5.40	108.66	122.59
12	ab	102	SPO	C25-C23-C22	-5.40	110.66	118.94
7	k	103	BCL	CHD-C1D-ND	-5.40	119.50	124.45
12	j	103	SPO	C34-C33-C32	-5.40	109.83	123.68
12	i	102	SPO	C34-C33-C32	-5.40	109.84	123.68
7	2	101	BCL	CHD-C1D-ND	-5.39	119.50	124.45
7	z	101	BCL	CHD-C1D-ND	-5.39	119.50	124.45
7	Y	201	BCL	CHD-C1D-ND	-5.39	119.50	124.45
12	D	102	SPO	C8-C7-C6	-5.39	109.59	118.08
12	T	102	SPO	C34-C33-C32	-5.39	109.86	123.68
12	G	102	SPO	C8-C7-C6	-5.39	109.59	118.08
7	5	101	BCL	CHD-C1D-ND	-5.38	119.51	124.45
7	c	101	BCL	CHD-C1D-ND	-5.38	119.51	124.45
7	3	102	BCL	C4D-CHA-C1A	5.37	127.78	121.25
12	9	102	SPO	C8-C7-C6	-5.37	109.62	118.08
12	n	101	SPO	C13-C12-C11	-5.36	109.63	118.08
12	Q	102	SPO	C34-C33-C32	-5.36	109.92	123.68
7	y	101	BCL	CHD-C1D-ND	-5.36	119.53	124.45
12	I	102	SPO	C13-C12-C11	-5.36	109.63	118.08
12	O	103	SPO	C11-C12-C14	-5.36	110.71	118.94
7	U	101	BCL	CHD-C1D-ND	-5.36	119.53	124.45
12	B	103	SPO	C34-C33-C32	-5.36	109.93	123.68
7	w	101	BCL	CHD-C1D-ND	-5.35	119.53	124.45
12	0	102	SPO	C18-C17-C16	-5.35	109.64	118.08
7	i	101	BCL	C4D-CHA-C1A	5.35	127.76	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	p	101	BCL	C4D-CHA-C1A	5.35	127.76	121.25
7	i	101	BCL	CHD-C1D-ND	-5.35	119.54	124.45
7	M	1303	BCL	CHD-C1D-ND	-5.35	119.54	124.45
12	B	103	SPO	C18-C17-C16	-5.35	109.66	118.08
12	j	101	SPO	C24-C23-C25	-5.34	109.66	118.08
7	W	101	BCL	CHD-C1D-ND	-5.34	119.55	124.45
12	q	102	SPO	C13-C12-C11	-5.34	109.67	118.08
12	n	101	SPO	C34-C33-C32	-5.33	110.00	123.68
12	G	103	SPO	C18-C17-C16	-5.33	109.68	118.08
12	e	101	SPO	C24-C23-C25	-5.32	109.69	118.08
12	K	102	SPO	C13-C12-C11	-5.32	109.69	118.08
12	O	102	SPO	C18-C17-C16	-5.32	109.69	118.08
12	B	102	SPO	C18-C17-C16	-5.32	109.70	118.08
12	G	102	SPO	C6-C7-C9	-5.32	110.78	118.94
12	9	102	SPO	C13-C12-C11	-5.31	109.70	118.08
7	m	1303	BCL	CHD-C1D-ND	-5.31	119.58	124.45
12	g	102	SPO	C34-C33-C32	-5.30	110.07	123.68
12	G	103	SPO	C34-C33-C32	-5.30	110.08	123.68
7	K	101	BCL	CHD-C1D-ND	-5.30	119.58	124.45
12	S	102	SPO	C34-C33-C32	-5.30	110.09	123.68
7	9	101	BCL	CHD-C1D-ND	-5.28	119.60	124.45
12	g	102	SPO	C24-C23-C25	-5.28	109.75	118.08
7	U	101	BCL	C4D-CHA-C1A	5.28	127.67	121.25
12	G	102	SPO	C24-C23-C25	-5.27	109.77	118.08
12	ab	102	SPO	C15-C16-C17	-5.27	111.61	126.42
12	d	103	SPO	C34-C33-C32	-5.27	110.16	123.68
12	T	102	SPO	C13-C12-C11	-5.27	109.78	118.08
12	a	104	SPO	C24-C23-C25	-5.26	109.78	118.08
12	r	102	SPO	C13-C12-C11	-5.26	109.79	118.08
7	u	101	BCL	C4D-CHA-C1A	5.26	127.65	121.25
12	3	101	SPO	C24-C23-C25	-5.25	109.80	118.08
12	N	101	SPO	C24-C23-C25	-5.25	109.80	118.08
7	q	101	BCL	C4D-CHA-C1A	5.25	127.64	121.25
7	s	103	BCL	C4D-CHA-C1A	5.25	127.64	121.25
12	e	101	SPO	C13-C12-C11	-5.25	109.81	118.08
12	n	101	SPO	C8-C7-C6	-5.24	109.81	118.08
12	O	102	SPO	C29-C28-C27	-5.24	109.06	122.59
7	2	101	BCL	C4D-CHA-C1A	5.24	127.63	121.25
7	y	101	BCL	C4D-CHA-C1A	5.24	127.63	121.25
12	Q	102	SPO	C24-C23-C25	-5.24	109.82	118.08
7	s	101	BCL	CHD-C1D-ND	-5.24	119.64	124.45
12	ab	102	SPO	C11-C12-C14	-5.23	110.91	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	w	101	BCL	C4D-CHA-C1A	5.23	127.62	121.25
12	N	103	SPO	C13-C12-C11	-5.23	109.83	118.08
12	I	102	SPO	C18-C17-C16	-5.23	109.84	118.08
7	W	101	BCL	C4D-CHA-C1A	5.23	127.61	121.25
7	q	101	BCL	CHD-C1D-ND	-5.23	119.65	124.45
7	I	101	BCL	CHD-C1D-ND	-5.23	119.65	124.45
12	U	102	SPO	C35-C33-C32	-5.23	110.54	121.12
12	q	102	SPO	C18-C17-C16	-5.22	109.85	118.08
7	3	102	BCL	CHD-C1D-ND	-5.22	119.65	124.45
12	r	102	SPO	C5-C6-C7	-5.22	118.00	125.89
7	k	101	BCL	C4D-CHA-C1A	5.22	127.60	121.25
12	K	102	SPO	C24-C23-C25	-5.22	109.85	118.08
7	Y	201	BCL	C4D-CHA-C1A	5.22	127.60	121.25
12	ab	102	SPO	C8-C7-C6	-5.22	109.85	118.08
12	S	102	SPO	C18-C17-C16	-5.22	109.86	118.08
12	a	104	SPO	C29-C28-C27	-5.21	109.14	122.59
12	s	105	SPO	C29-C28-C27	-5.21	109.15	122.59
7	k	103	BCL	C4D-CHA-C1A	5.21	127.59	121.25
12	ab	102	SPO	C29-C28-C27	-5.21	109.15	122.59
7	d	101	BCL	C4D-CHA-C1A	5.21	127.59	121.25
7	S	101	BCL	CHD-C1D-ND	-5.20	119.67	124.45
12	S	102	SPO	C13-C12-C11	-5.20	109.88	118.08
12	G	103	SPO	C24-C23-C25	-5.20	109.88	118.08
12	T	102	SPO	C18-C17-C16	-5.20	109.89	118.08
7	P	101	BCL	C4D-CHA-C1A	5.20	127.58	121.25
12	ab	102	SPO	C16-C17-C19	-5.19	110.97	118.94
7	5	101	BCL	C4D-CHA-C1A	5.19	127.56	121.25
12	3	101	SPO	C13-C12-C11	-5.19	109.90	118.08
7	J	101	BCL	C4D-CHA-C1A	5.19	127.56	121.25
7	D	101	BCL	CHD-C1D-ND	-5.18	119.69	124.45
12	B	103	SPO	C29-C28-C27	-5.18	109.23	122.59
7	0	101	BCL	C4D-CHA-C1A	5.18	127.55	121.25
7	O	101	BCL	CHD-C1D-ND	-5.18	119.70	124.45
7	9	101	BCL	C4D-CHA-C1A	5.18	127.55	121.25
7	ab	101	BCL	C4D-CHA-C1A	5.18	127.55	121.25
7	j	102	BCL	C4D-CHA-C1A	5.17	127.55	121.25
7	N	102	BCL	C4D-CHA-C1A	5.17	127.55	121.25
12	e	101	SPO	C35-C33-C32	-5.17	110.66	121.12
12	s	104	SPO	C34-C33-C32	-5.16	110.43	123.68
12	i	102	SPO	C26-C25-C23	-5.16	111.92	126.42
7	b	101	BCL	C4D-CHA-C1A	5.16	127.53	121.25
12	3	103	SPO	C24-C23-C25	-5.16	109.95	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	R	101	BCL	C4D-CHA-C1A	5.15	127.52	121.25
7	a	101	BCL	C4D-CHA-C1A	5.15	127.52	121.25
7	8	102	BCL	C4D-CHA-C1A	5.15	127.51	121.25
12	O	102	SPO	C13-C12-C11	-5.15	109.97	118.08
7	e	102	BCL	C4D-CHA-C1A	5.14	127.51	121.25
12	s	104	SPO	C24-C23-C25	-5.14	109.97	118.08
7	L	301	BCL	CHD-C1D-ND	-5.14	119.73	124.45
7	A	101	BCL	C4D-CHA-C1A	5.14	127.50	121.25
12	U	102	SPO	C29-C28-C27	-5.14	109.33	122.59
7	E	101	BCL	C4D-CHA-C1A	5.14	127.50	121.25
7	Q	101	BCL	CHD-C1D-ND	-5.14	119.73	124.45
12	K	102	SPO	C29-C28-C27	-5.13	109.34	122.59
7	v	101	BCL	C4D-CHA-C1A	5.13	127.50	121.25
12	B	103	SPO	C24-C23-C25	-5.13	109.99	118.08
12	S	102	SPO	C29-C28-C27	-5.13	109.34	122.59
12	j	101	SPO	C29-C28-C27	-5.13	109.36	122.59
12	D	102	SPO	C35-C33-C32	-5.13	110.74	121.12
7	B	101	BCL	C4D-CHA-C1A	5.13	127.49	121.25
7	F	101	BCL	CHD-C1D-ND	-5.13	119.74	124.45
12	R	102	SPO	C30-C28-C27	-5.13	106.46	121.98
12	o	102	SPO	C18-C17-C16	-5.13	110.00	118.08
7	G	101	BCL	C4D-CHA-C1A	5.12	127.48	121.25
12	Q	102	SPO	C29-C28-C27	-5.12	109.37	122.59
7	T	101	BCL	C4D-CHA-C1A	5.12	127.48	121.25
7	aa	102	BCL	C4D-CHA-C1A	5.12	127.48	121.25
7	f	101	BCL	C4D-CHA-C1A	5.12	127.48	121.25
12	3	101	SPO	C18-C17-C16	-5.12	110.01	118.08
7	g	101	BCL	C4D-CHA-C1A	5.12	127.48	121.25
7	O	101	BCL	C4D-CHA-C1A	5.12	127.48	121.25
7	a	101	BCL	CHD-C1D-ND	-5.12	119.75	124.45
12	A	102	SPO	C24-C23-C25	-5.12	110.01	118.08
12	s	102	SPO	C29-C28-C27	-5.12	109.39	122.59
7	U	103	BCL	C4D-CHA-C1A	5.12	127.48	121.25
7	L	304	BCL	C4D-CHA-C1A	5.12	127.47	121.25
12	e	103	SPO	C16-C17-C19	-5.11	111.09	118.94
12	e	103	SPO	C8-C7-C6	-5.11	110.02	118.08
12	q	102	SPO	C29-C28-C27	-5.11	109.40	122.59
7	f	101	BCL	CHD-C1D-ND	-5.11	119.76	124.45
7	X	101	BCL	CHD-C1D-ND	-5.11	119.76	124.45
12	3	103	SPO	C35-C33-C32	-5.11	110.78	121.12
7	k	101	BCL	CHD-C1D-ND	-5.11	119.76	124.45
7	l	301	BCL	CHD-C1D-ND	-5.10	119.77	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	K	101	BCL	C4D-CHA-C1A	5.10	127.46	121.25
7	l	101	BCL	C4D-CHA-C1A	5.10	127.45	121.25
7	s	103	BCL	CHD-C1D-ND	-5.10	119.77	124.45
12	s	102	SPO	C18-C17-C16	-5.10	110.05	118.08
12	G	102	SPO	C34-C33-C32	-5.10	110.61	123.68
7	d	101	BCL	CHD-C1D-ND	-5.09	119.78	124.45
12	j	101	SPO	C18-C17-C16	-5.09	110.06	118.08
12	I	102	SPO	C29-C28-C27	-5.09	109.47	122.59
12	A	102	SPO	C35-C33-C32	-5.08	110.83	121.12
12	r	102	SPO	C8-C7-C6	-5.08	110.07	118.08
12	s	104	SPO	C18-C17-C16	-5.08	110.07	118.08
12	O	102	SPO	C24-C23-C25	-5.08	110.08	118.08
12	k	102	SPO	C24-C23-C25	-5.08	110.08	118.08
12	S	102	SPO	C8-C7-C6	-5.07	110.08	118.08
12	o	102	SPO	C29-C28-C27	-5.07	109.51	122.59
7	l	301	BCL	C4D-CHA-C1A	5.07	127.42	121.25
12	s	102	SPO	C24-C23-C25	-5.07	110.09	118.08
7	L	301	BCL	C4D-CHA-C1A	5.07	127.42	121.25
7	l	305	BCL	C4D-CHA-C1A	5.07	127.42	121.25
7	S	101	BCL	C4D-CHA-C1A	5.06	127.41	121.25
7	o	101	BCL	C4D-CHA-C1A	5.06	127.41	121.25
12	0	102	SPO	C30-C28-C27	-5.06	106.65	121.98
12	e	103	SPO	C29-C28-C27	-5.06	109.53	122.59
12	D	102	SPO	C29-C28-C27	-5.06	109.54	122.59
12	O	103	SPO	C18-C17-C16	-5.06	110.11	118.08
12	3	103	SPO	C8-C7-C6	-5.06	110.11	118.08
7	Z	101	BCL	C4D-CHA-C1A	5.05	127.39	121.25
7	D	101	BCL	C4D-CHA-C1A	5.04	127.39	121.25
7	s	101	BCL	C4D-CHA-C1A	5.04	127.38	121.25
12	n	101	SPO	C24-C23-C25	-5.04	110.14	118.08
12	n	101	SPO	C29-C28-C27	-5.04	109.60	122.59
12	D	102	SPO	C24-C23-C25	-5.03	110.14	118.08
7	A	101	BCL	CHD-C1D-ND	-5.03	119.83	124.45
12	a	104	SPO	C18-C17-C16	-5.03	110.16	118.08
12	O	102	SPO	C8-C7-C6	-5.03	110.16	118.08
7	Q	101	BCL	C4D-CHA-C1A	5.03	127.36	121.25
12	R	102	SPO	C5-C6-C7	-5.01	118.32	125.89
12	8	101	SPO	C5-C6-C7	-5.01	118.32	125.89
12	q	102	SPO	C24-C23-C25	-5.01	110.19	118.08
12	G	102	SPO	C29-C28-C27	-5.00	109.68	122.59
7	o	101	BCL	CHD-C1D-ND	-5.00	119.86	124.45
12	T	102	SPO	C24-C23-C25	-5.00	110.20	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	n	101	SPO	C11-C12-C14	-5.00	111.27	118.94
12	R	102	SPO	C29-C28-C27	-4.99	109.71	122.59
12	S	102	SPO	C24-C23-C25	-4.99	110.22	118.08
12	e	103	SPO	C24-C23-C25	-4.98	110.22	118.08
12	s	105	SPO	C24-C23-C25	-4.98	110.22	118.08
12	N	101	SPO	C18-C17-C16	-4.98	110.23	118.08
12	K	102	SPO	C35-C33-C32	-4.98	111.04	121.12
7	r	101	BCL	CHD-C1D-ND	-4.98	119.88	124.45
12	d	103	SPO	C35-C33-C32	-4.98	111.05	121.12
7	I	101	BCL	C4D-CHA-C1A	4.97	127.30	121.25
12	Q	102	SPO	C18-C17-C16	-4.97	110.24	118.08
12	M	1305	SPO	C13-C12-C11	-4.97	110.24	118.08
12	aa	101	SPO	C29-C28-C27	-4.97	109.77	122.59
7	c	101	BCL	C11-C10-C8	4.97	131.98	115.92
12	m	1305	SPO	C13-C12-C11	-4.97	110.25	118.08
7	F	101	BCL	C4D-CHA-C1A	4.97	127.29	121.25
7	g	101	BCL	CHD-C1D-ND	-4.96	119.89	124.45
12	F	102	SPO	C29-C28-C27	-4.96	109.79	122.59
12	R	102	SPO	C18-C17-C16	-4.96	110.27	118.08
7	k	101	BCL	C11-C10-C8	4.96	131.94	115.92
7	M	1301	BCL	C4D-CHA-C1A	4.95	127.27	121.25
12	s	105	SPO	C34-C33-C35	-4.95	106.95	115.27
12	F	102	SPO	C29-C28-C30	-4.94	106.96	115.27
12	9	102	SPO	C29-C28-C27	-4.94	109.85	122.59
12	K	102	SPO	C18-C17-C16	-4.94	110.30	118.08
7	J	101	BCL	CHD-C1D-ND	-4.94	119.92	124.45
7	b	101	BCL	CHD-C1D-ND	-4.94	119.92	124.45
12	o	102	SPO	C24-C23-C25	-4.94	110.30	118.08
7	P	101	BCL	CHD-C1D-ND	-4.93	119.92	124.45
7	m	1301	BCL	C4D-CHA-C1A	4.93	127.25	121.25
7	E	101	BCL	CHD-C1D-ND	-4.93	119.93	124.45
12	t	101	SPO	C29-C28-C27	-4.92	109.90	122.59
12	s	105	SPO	C13-C12-C11	-4.92	110.33	118.08
12	aa	101	SPO	C24-C23-C25	-4.92	110.33	118.08
7	8	102	BCL	CHD-C1D-ND	-4.91	119.94	124.45
7	G	101	BCL	CHD-C1D-ND	-4.91	119.94	124.45
7	e	102	BCL	CHD-C1D-ND	-4.91	119.95	124.45
7	B	101	BCL	CHD-C1D-ND	-4.90	119.95	124.45
12	T	102	SPO	C5-C6-C7	-4.90	118.48	125.89
7	ab	101	BCL	CHD-C1D-ND	-4.90	119.95	124.45
12	A	102	SPO	C13-C12-C11	-4.90	110.36	118.08
7	0	101	BCL	CHD-C1D-ND	-4.89	119.96	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	102	BCL	CHD-C1D-ND	-4.89	119.96	124.45
7	Z	101	BCL	CHD-C1D-ND	-4.89	119.96	124.45
7	R	101	BCL	CHD-C1D-ND	-4.88	119.97	124.45
12	D	102	SPO	C18-C17-C16	-4.88	110.38	118.08
12	F	102	SPO	C18-C17-C16	-4.88	110.39	118.08
7	aa	102	BCL	CHD-C1D-ND	-4.88	119.97	124.45
12	3	101	SPO	C29-C28-C27	-4.88	110.01	122.59
7	j	102	BCL	CHD-C1D-ND	-4.87	119.98	124.45
12	U	102	SPO	C18-C17-C16	-4.87	110.40	118.08
7	T	101	BCL	CHD-C1D-ND	-4.86	119.98	124.45
12	3	103	SPO	C29-C28-C27	-4.85	110.07	122.59
12	g	102	SPO	C36-C37-C38	-4.85	111.18	127.75
12	j	103	SPO	C5-C6-C7	-4.85	118.57	125.89
12	a	104	SPO	C8-C7-C6	-4.84	110.44	118.08
7	p	101	BCL	CHD-C1D-ND	-4.84	120.01	124.45
12	B	103	SPO	C30-C28-C27	-4.82	107.38	121.98
12	B	103	SPO	C13-C12-C11	-4.82	110.48	118.08
7	5	102	BCL	CHD-C1D-ND	-4.81	120.03	124.45
12	i	102	SPO	C29-C28-C27	-4.81	110.18	122.59
12	3	103	SPO	C13-C12-C11	-4.80	110.52	118.08
12	r	102	SPO	C29-C28-C27	-4.80	110.22	122.59
12	9	102	SPO	C24-C23-C25	-4.79	110.54	118.08
12	A	102	SPO	C29-C28-C27	-4.78	110.26	122.59
12	m	1305	SPO	C8-C7-C6	-4.78	110.55	118.08
12	M	1305	SPO	C8-C7-C6	-4.78	110.55	118.08
7	v	101	BCL	CHD-C1D-ND	-4.77	120.07	124.45
12	s	102	SPO	C35-C33-C32	-4.77	111.46	121.12
12	U	102	SPO	C36-C37-C38	-4.77	111.45	127.75
12	I	102	SPO	C24-C23-C25	-4.77	110.56	118.08
12	N	101	SPO	C35-C33-C32	-4.77	111.47	121.12
12	8	101	SPO	C29-C28-C27	-4.77	110.30	122.59
12	M	1305	SPO	C29-C28-C27	-4.77	110.30	122.59
8	l	306	BPB	C4D-ND-C1D	-4.76	103.98	108.83
12	R	102	SPO	C24-C23-C25	-4.76	110.58	118.08
12	a	104	SPO	C13-C12-C11	-4.76	110.58	118.08
8	L	305	BPB	C4D-ND-C1D	-4.76	103.99	108.83
12	j	103	SPO	C13-C12-C11	-4.75	110.59	118.08
8	l	302	BPB	C11-C10-C8	-4.75	100.56	115.92
12	N	103	SPO	C29-C28-C27	-4.75	110.33	122.59
12	F	102	SPO	C24-C23-C25	-4.75	110.60	118.08
12	m	1305	SPO	C29-C28-C27	-4.75	110.34	122.59
12	ab	102	SPO	C13-C12-C11	-4.75	110.60	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	O	103	SPO	C5-C6-C7	-4.74	118.73	125.89
8	L	302	BPB	C11-C10-C8	-4.74	100.60	115.92
12	3	103	SPO	C5-C6-C7	-4.74	118.73	125.89
12	O	103	SPO	C29-C28-C27	-4.73	110.38	122.59
12	d	103	SPO	C29-C28-C27	-4.73	110.38	122.59
12	r	102	SPO	C30-C28-C27	-4.73	107.66	121.98
12	N	103	SPO	C8-C7-C6	-4.73	110.63	118.08
12	O	103	SPO	C24-C23-C25	-4.73	110.63	118.08
12	s	104	SPO	C29-C28-C27	-4.73	110.40	122.59
12	G	102	SPO	C36-C37-C38	-4.72	111.62	127.75
12	T	102	SPO	C29-C28-C27	-4.72	110.42	122.59
12	a	104	SPO	C36-C37-C38	-4.71	111.66	127.75
12	s	105	SPO	C8-C7-C6	-4.70	110.66	118.08
12	G	102	SPO	C11-C12-C14	-4.70	111.72	118.94
7	r	101	BCL	C4D-CHA-C1A	4.70	126.97	121.25
12	e	101	SPO	C18-C17-C16	-4.70	110.67	118.08
7	9	101	BCL	C11-C10-C8	4.68	131.04	115.92
12	A	102	SPO	C18-C17-C16	-4.66	110.74	118.08
12	O	103	SPO	C8-C7-C6	-4.66	110.74	118.08
12	3	103	SPO	C18-C17-C16	-4.66	110.74	118.08
12	B	103	SPO	C29-C28-C30	-4.65	107.45	115.27
12	9	102	SPO	C18-C17-C16	-4.64	110.77	118.08
12	i	102	SPO	C20-C21-C22	-4.64	113.97	123.47
12	B	102	SPO	C8-C7-C6	-4.63	110.78	118.08
7	x	101	BCL	CHD-C1D-ND	-4.63	120.20	124.45
12	j	101	SPO	C35-C33-C32	-4.63	111.75	121.12
12	B	102	SPO	C35-C33-C32	-4.62	111.76	121.12
10	a	103	PC1	O21-C21-C22	4.62	121.45	111.50
8	L	302	BPB	C4D-ND-C1D	-4.61	104.14	108.83
8	l	302	BPB	C4D-ND-C1D	-4.59	104.16	108.83
12	e	103	SPO	C6-C7-C9	-4.58	111.92	118.94
12	B	102	SPO	C24-C23-C25	-4.58	110.87	118.08
12	e	101	SPO	C29-C28-C27	-4.57	110.79	122.59
12	8	101	SPO	C24-C23-C25	-4.57	110.88	118.08
12	G	103	SPO	C5-C6-C7	-4.57	118.99	125.89
12	O	102	SPO	C29-C28-C30	-4.56	107.61	115.27
7	1	101	BCL	C4A-NA-C1A	4.54	108.75	106.71
12	s	104	SPO	C5-C6-C7	-4.53	119.04	125.89
12	i	102	SPO	C25-C23-C22	-4.53	111.99	118.94
12	d	103	SPO	C36-C37-C38	-4.53	112.26	127.75
12	B	103	SPO	C36-C37-C38	-4.53	112.27	127.75
12	a	104	SPO	C30-C28-C27	-4.52	108.30	121.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	j	103	SPO	C24-C23-C25	-4.50	110.99	118.08
12	3	103	SPO	C29-C28-C30	-4.49	107.72	115.27
12	O	103	SPO	C36-C37-C38	-4.49	112.41	127.75
12	B	103	SPO	C8-C7-C6	-4.49	111.01	118.08
12	o	102	SPO	C36-C37-C38	-4.48	112.44	127.75
7	k	103	BCL	C16-C15-C13	4.47	130.37	115.92
12	N	103	SPO	C5-C6-C7	-4.47	119.14	125.89
12	ab	102	SPO	C30-C28-C27	-4.47	108.45	121.98
12	e	103	SPO	C34-C33-C32	-4.46	109.77	122.65
7	u	101	BCL	C1-C2-C3	-4.45	119.55	126.75
12	t	101	SPO	C30-C28-C27	-4.45	108.51	121.98
12	e	103	SPO	C30-C28-C27	-4.45	108.52	121.98
7	7	101	BCL	C1-C2-C3	-4.45	118.35	126.04
12	ab	102	SPO	C5-C6-C7	-4.45	119.17	125.89
12	0	102	SPO	C36-C37-C38	-4.44	112.57	127.75
12	g	102	SPO	C8-C7-C6	-4.44	111.08	118.08
12	F	102	SPO	C35-C33-C32	-4.43	112.16	121.12
12	s	105	SPO	C36-C37-C38	-4.42	112.65	127.75
12	8	101	SPO	C36-C37-C38	-4.41	112.68	127.75
12	U	102	SPO	C30-C28-C27	-4.41	108.63	121.98
12	q	102	SPO	C5-C6-C7	-4.40	119.24	125.89
10	h	301	PC1	O21-C21-C22	4.38	120.93	111.50
12	R	102	SPO	C13-C12-C11	-4.37	111.19	118.08
12	r	102	SPO	C39-C38-C37	-4.37	110.02	122.65
12	T	102	SPO	C36-C37-C38	-4.37	112.81	127.75
12	g	102	SPO	C30-C28-C27	-4.37	108.75	121.98
12	R	102	SPO	C39-C38-C37	-4.37	110.02	122.65
12	N	103	SPO	C40-C38-C37	-4.37	110.03	122.65
12	s	102	SPO	C36-C37-C38	-4.36	112.84	127.75
12	O	102	SPO	C36-C37-C38	-4.36	112.84	127.75
10	M	1307	PC1	O21-C21-C22	4.35	120.88	111.50
12	A	102	SPO	C29-C28-C30	-4.35	107.95	115.27
12	G	103	SPO	C36-C37-C38	-4.34	112.90	127.75
12	ab	102	SPO	C40-C38-C37	-4.33	110.12	122.65
12	N	103	SPO	C15-C16-C17	-4.33	114.26	126.42
12	R	102	SPO	C36-C37-C38	-4.33	112.96	127.75
7	7	101	BCL	C4A-NA-C1A	4.33	108.65	106.71
12	B	102	SPO	C39-C38-C37	-4.32	110.17	122.65
12	0	102	SPO	C39-C38-C37	-4.30	110.21	122.65
12	A	102	SPO	C5-C6-C7	-4.30	119.40	125.89
12	T	102	SPO	C40-C38-C37	-4.29	110.25	122.65
12	G	102	SPO	C40-C38-C37	-4.28	110.27	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	r	102	SPO	C24-C23-C25	-4.28	111.33	118.08
12	N	103	SPO	C36-C37-C38	-4.27	113.14	127.75
12	T	102	SPO	C29-C28-C30	-4.27	108.09	115.27
12	s	104	SPO	C30-C28-C27	-4.26	109.09	121.98
12	9	102	SPO	C29-C28-C30	-4.26	108.11	115.27
12	j	103	SPO	C36-C37-C38	-4.26	113.20	127.75
12	a	104	SPO	C29-C28-C30	-4.25	108.11	115.27
7	x	101	BCL	C4D-CHA-C1A	4.25	126.42	121.25
12	B	103	SPO	C40-C38-C37	-4.23	110.41	122.65
12	3	101	SPO	C5-C6-C7	-4.23	119.49	125.89
12	aa	101	SPO	C5-C6-C7	-4.23	119.50	125.89
12	g	102	SPO	C39-C38-C37	-4.22	110.44	122.65
12	s	105	SPO	C29-C28-C30	-4.22	108.17	115.27
12	G	103	SPO	C30-C28-C27	-4.22	109.20	121.98
12	M	1305	SPO	C39-C38-C37	-4.22	110.45	122.65
12	m	1305	SPO	C39-C38-C37	-4.21	110.47	122.65
12	S	102	SPO	C35-C33-C32	-4.21	110.09	120.50
12	s	105	SPO	C40-C38-C37	-4.20	110.50	122.65
12	e	101	SPO	C5-C6-C7	-4.20	119.55	125.89
12	aa	101	SPO	C30-C28-C27	-4.18	109.33	121.98
12	G	102	SPO	C30-C28-C27	-4.18	109.33	121.98
12	G	103	SPO	C39-C38-C37	-4.17	110.58	122.65
12	K	102	SPO	C36-C37-C38	-4.17	113.49	127.75
12	0	102	SPO	C40-C38-C37	-4.16	110.63	122.65
12	O	102	SPO	C40-C38-C37	-4.16	110.63	122.65
12	j	103	SPO	C30-C28-C27	-4.15	109.40	121.98
12	j	103	SPO	C40-C38-C37	-4.15	110.64	122.65
7	i	101	BCL	C4A-NA-C1A	4.15	108.57	106.71
12	i	102	SPO	C30-C28-C27	-4.15	109.42	121.98
7	5	102	BCL	C4D-CHA-C1A	4.15	126.29	121.25
12	Q	102	SPO	C5-C6-C7	-4.13	119.64	125.89
12	A	102	SPO	C40-C38-C37	-4.13	110.72	122.65
7	z	101	BCL	C4D-CHA-C1A	4.12	126.27	121.25
7	q	101	BCL	C4A-NA-C1A	4.12	108.56	106.71
12	n	101	SPO	C29-C28-C30	-4.12	108.34	115.27
7	s	101	BCL	C4A-NA-C1A	4.12	108.56	106.71
12	s	104	SPO	C39-C38-C37	-4.12	110.75	122.65
7	a	101	BCL	C4A-NA-C1A	4.11	108.55	106.71
12	n	101	SPO	C36-C37-C38	-4.10	113.72	127.75
12	s	105	SPO	C31-C32-C33	-4.10	117.78	127.66
12	G	102	SPO	C39-C38-C37	-4.10	110.79	122.65
8	l	306	BPB	CBC-CAC-C3C	-4.10	115.83	126.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	e	101	SPO	C29-C28-C30	-4.09	108.38	115.27
8	L	305	BPB	CBC-CAC-C3C	-4.09	115.83	126.70
12	a	104	SPO	C40-C38-C37	-4.09	110.82	122.65
12	e	101	SPO	C36-C37-C38	-4.09	113.77	127.75
12	n	101	SPO	C30-C28-C27	-4.09	109.60	121.98
12	O	102	SPO	C30-C28-C27	-4.09	109.61	121.98
7	9	101	BCL	C4A-NA-C1A	4.08	108.54	106.71
12	e	103	SPO	C35-C33-C32	-4.08	110.85	122.65
12	M	1305	SPO	C30-C28-C27	-4.08	109.63	121.98
12	m	1305	SPO	C30-C28-C27	-4.08	109.63	121.98
12	D	102	SPO	C39-C38-C37	-4.07	110.87	122.65
12	r	102	SPO	C36-C37-C38	-4.07	113.83	127.75
7	M	1301	BCL	C1D-ND-C4D	-4.07	103.44	106.33
12	G	102	SPO	C10-C11-C12	-4.07	114.98	126.42
12	O	103	SPO	C39-C38-C37	-4.07	110.89	122.65
12	Q	102	SPO	C35-C33-C32	-4.07	110.44	120.50
12	j	101	SPO	C29-C28-C30	-4.07	108.43	115.27
12	s	102	SPO	C29-C28-C30	-4.06	108.44	115.27
7	k	103	BCL	C1D-ND-C4D	-4.06	103.45	106.33
12	N	103	SPO	C24-C23-C25	-4.06	111.69	118.08
12	B	103	SPO	C39-C38-C37	-4.05	110.93	122.65
12	k	102	SPO	C18-C17-C16	-4.05	111.69	118.08
12	3	101	SPO	C29-C28-C30	-4.05	108.46	115.27
12	T	102	SPO	C30-C28-C27	-4.05	109.72	121.98
12	g	102	SPO	C40-C38-C37	-4.05	110.94	122.65
12	G	102	SPO	C15-C16-C17	-4.05	115.04	126.42
7	c	101	BCL	C4A-NA-C1A	4.05	108.53	106.71
12	N	103	SPO	C30-C28-C27	-4.05	109.72	121.98
12	k	102	SPO	C13-C12-C11	-4.05	111.70	118.08
7	m	1301	BCL	C1D-ND-C4D	-4.05	103.46	106.33
12	a	104	SPO	C39-C38-C37	-4.04	110.96	122.65
12	I	102	SPO	C36-C37-C38	-4.04	113.94	127.75
7	O	101	BCL	C4A-NA-C1A	4.04	108.52	106.71
12	o	102	SPO	C5-C6-C7	-4.04	119.79	125.89
12	O	103	SPO	C30-C28-C27	-4.02	109.80	121.98
7	I	101	BCL	C4A-NA-C1A	4.02	108.52	106.71
12	a	104	SPO	C5-C6-C7	-4.02	119.82	125.89
12	D	102	SPO	C5-C6-C7	-4.01	119.83	125.89
7	A	101	BCL	C4A-NA-C1A	4.01	108.51	106.71
12	O	102	SPO	C5-C6-C7	-4.01	119.83	125.89
7	K	101	BCL	C4A-NA-C1A	4.01	108.51	106.71
12	9	102	SPO	C5-C6-C7	-4.01	119.84	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	r	101	BCL	C4A-NA-C1A	4.01	108.51	106.71
12	8	101	SPO	C34-C33-C32	-4.00	113.41	123.68
7	D	101	BCL	C4A-NA-C1A	4.00	108.50	106.71
12	d	103	SPO	C1-C4-C5	-3.99	102.47	113.06
13	M	1306	CDL	OB6-CB5-C51	3.99	120.11	111.50
13	m	1306	CDL	OB6-CB5-C51	3.98	120.08	111.50
12	N	103	SPO	C21-C20-C19	-3.98	115.32	123.47
12	m	1305	SPO	C36-C37-C38	-3.97	114.19	127.75
7	d	101	BCL	C4A-NA-C1A	3.96	108.49	106.71
12	I	102	SPO	C29-C28-C30	-3.96	108.61	115.27
12	t	101	SPO	C36-C37-C38	-3.95	114.23	127.75
12	aa	101	SPO	C35-C33-C32	-3.95	113.12	121.12
12	M	1305	SPO	C36-C37-C38	-3.95	114.24	127.75
7	k	101	BCL	C4A-NA-C1A	3.95	108.48	106.71
12	3	101	SPO	C36-C37-C38	-3.94	114.27	127.75
12	r	102	SPO	C40-C38-C37	-3.94	111.27	122.65
7	f	101	BCL	C4A-NA-C1A	3.93	108.47	106.71
10	C	1201	PC1	O21-C21-C22	3.93	119.97	111.50
10	a	102	PC1	O21-C21-C22	3.93	119.97	111.50
10	l	304	PC1	O21-C21-C22	3.93	119.96	111.50
12	3	103	SPO	C40-C38-C37	-3.92	111.31	122.65
12	s	105	SPO	C39-C38-C37	-3.92	111.33	122.65
12	n	101	SPO	C15-C16-C17	-3.91	115.42	126.42
12	O	103	SPO	C40-C38-C37	-3.91	111.34	122.65
12	aa	101	SPO	C8-C7-C6	-3.91	111.91	118.08
12	k	102	SPO	C2-C1-C4	-3.91	104.85	110.86
12	N	103	SPO	C39-C38-C37	-3.91	111.35	122.65
7	S	101	BCL	C4A-NA-C1A	3.90	108.46	106.71
12	q	102	SPO	C29-C28-C30	-3.89	108.72	115.27
7	F	101	BCL	C4A-NA-C1A	3.89	108.46	106.71
12	T	102	SPO	C39-C38-C37	-3.89	111.41	122.65
12	n	101	SPO	C40-C38-C37	-3.88	111.42	122.65
12	D	102	SPO	C29-C28-C30	-3.88	108.74	115.27
12	t	101	SPO	C29-C28-C30	-3.87	108.75	115.27
12	O	102	SPO	C39-C38-C37	-3.87	111.45	122.65
12	e	101	SPO	C39-C38-C37	-3.87	111.45	122.65
7	o	101	BCL	C4A-NA-C1A	3.87	108.45	106.71
12	n	101	SPO	C39-C38-C37	-3.87	111.46	122.65
12	s	102	SPO	C5-C6-C7	-3.87	120.04	125.89
12	S	102	SPO	C30-C28-C27	-3.86	110.30	121.98
12	B	103	SPO	C21-C20-C19	-3.85	115.58	123.47
12	0	102	SPO	C5-C6-C7	-3.85	120.07	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	101	BCL	C1D-ND-C4D	-3.85	103.60	106.33
12	e	103	SPO	C31-C32-C33	-3.84	114.63	127.75
12	U	102	SPO	C29-C28-C30	-3.84	108.81	115.27
12	k	102	SPO	C1-C4-C5	-3.84	102.89	113.06
7	W	101	BCL	C4A-NA-C1A	3.83	108.43	106.71
7	y	101	BCL	C4A-NA-C1A	3.83	108.43	106.71
12	t	101	SPO	C3-C1-C4	3.82	116.73	110.86
7	O	101	BCL	C1D-ND-C4D	-3.82	103.62	106.33
13	M	1306	CDL	OA6-CA5-C11	3.82	119.73	111.50
7	3	102	BCL	C4A-NA-C1A	3.82	108.42	106.71
12	i	102	SPO	C10-C11-C12	-3.81	115.70	126.42
12	s	102	SPO	C30-C28-C27	-3.81	110.46	121.98
7	K	101	BCL	C1D-ND-C4D	-3.80	103.63	106.33
12	A	102	SPO	C36-C37-C38	-3.80	114.76	127.75
13	m	1306	CDL	OA6-CA5-C11	3.80	119.69	111.50
12	O	103	SPO	C10-C11-C12	-3.80	115.75	126.42
12	G	103	SPO	C40-C38-C37	-3.79	111.69	122.65
7	m	1303	BCL	C4A-NA-C1A	3.79	108.41	106.71
7	s	101	BCL	C1D-ND-C4D	-3.79	103.64	106.33
12	9	102	SPO	C36-C37-C38	-3.79	114.81	127.75
12	B	102	SPO	C36-C37-C38	-3.79	114.81	127.75
12	I	102	SPO	C30-C28-C27	-3.77	110.56	121.98
7	5	101	BCL	C4A-NA-C1A	3.77	108.40	106.71
12	F	102	SPO	C30-C28-C27	-3.76	110.61	121.98
12	o	102	SPO	C30-C28-C27	-3.75	110.62	121.98
9	M	1304	U10	C22-C23-C24	-3.75	118.64	127.66
12	G	103	SPO	C34-C33-C35	-3.74	108.97	115.27
12	aa	101	SPO	C21-C20-C19	-3.74	115.82	123.47
7	M	1303	BCL	C4A-NA-C1A	3.74	108.39	106.71
12	3	103	SPO	C36-C37-C38	-3.73	114.99	127.75
9	m	1304	U10	C22-C23-C24	-3.73	118.67	127.66
7	Q	101	BCL	C4A-NA-C1A	3.73	108.38	106.71
12	q	102	SPO	C39-C38-C37	-3.73	111.87	122.65
12	q	102	SPO	C36-C37-C38	-3.73	115.00	127.75
12	S	102	SPO	C29-C28-C30	-3.72	109.00	115.27
12	3	101	SPO	C30-C28-C27	-3.72	110.72	121.98
7	F	101	BCL	C1D-ND-C4D	-3.72	103.69	106.33
12	K	102	SPO	C30-C28-C27	-3.72	110.73	121.98
7	p	101	BCL	CAB-C3B-C2B	3.72	133.91	128.34
7	L	304	BCL	C1D-ND-C4D	-3.71	103.70	106.33
12	B	102	SPO	C30-C28-C27	-3.71	110.74	121.98
12	j	101	SPO	C30-C28-C27	-3.71	110.74	121.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	s	105	SPO	C30-C28-C27	-3.71	110.76	121.98
7	l	305	BCL	C1D-ND-C4D	-3.70	103.70	106.33
7	S	101	BCL	C1D-ND-C4D	-3.70	103.71	106.33
7	k	101	BCL	C1D-ND-C4D	-3.70	103.71	106.33
12	ab	102	SPO	C26-C25-C23	-3.69	116.04	126.42
12	R	102	SPO	C40-C38-C37	-3.69	111.98	122.65
12	o	102	SPO	C29-C28-C30	-3.69	109.07	115.27
7	D	101	BCL	C1D-ND-C4D	-3.69	103.72	106.33
7	u	101	BCL	C4A-NA-C1A	3.69	108.36	106.71
12	3	101	SPO	C40-C38-C37	-3.68	112.00	122.65
12	Q	102	SPO	C29-C28-C30	-3.68	109.08	115.27
12	U	102	SPO	C39-C38-C37	-3.68	112.01	122.65
12	g	102	SPO	C21-C20-C19	-3.68	115.94	123.47
7	Y	201	BCL	C4A-NA-C1A	3.68	108.36	106.71
7	U	101	BCL	C4A-NA-C1A	3.67	108.36	106.71
12	9	102	SPO	C30-C28-C27	-3.67	110.87	121.98
12	t	101	SPO	C21-C20-C19	-3.67	115.95	123.47
7	9	101	BCL	C1D-ND-C4D	-3.67	103.73	106.33
12	U	102	SPO	C40-C38-C37	-3.67	112.05	122.65
12	K	102	SPO	C29-C28-C30	-3.66	109.11	115.27
12	K	102	SPO	C5-C6-C7	-3.66	120.36	125.89
7	2	101	BCL	C4A-NA-C1A	3.66	108.35	106.71
12	N	101	SPO	C30-C28-C27	-3.66	110.90	121.98
12	D	102	SPO	C36-C37-C38	-3.65	115.27	127.75
10	h	302	PC1	C11-C12-N	-3.65	103.59	115.78
7	f	101	BCL	C1D-ND-C4D	-3.65	103.74	106.33
12	n	101	SPO	C16-C17-C19	-3.65	113.34	118.94
12	Q	102	SPO	C30-C28-C27	-3.65	110.94	121.98
12	3	103	SPO	C30-C28-C27	-3.64	110.95	121.98
7	Q	101	BCL	C1D-ND-C4D	-3.64	103.75	106.33
12	D	102	SPO	C30-C28-C27	-3.64	110.97	121.98
12	g	102	SPO	C34-C33-C35	-3.63	109.16	115.27
12	K	102	SPO	C39-C38-C37	-3.63	112.17	122.65
12	8	101	SPO	C30-C28-C27	-3.62	111.02	121.98
12	s	102	SPO	C34-C33-C35	-3.62	109.19	115.27
7	k	103	BCL	C6-C7-C8	-3.62	104.23	115.92
12	N	101	SPO	C29-C28-C30	-3.61	109.20	115.27
7	U	103	BCL	C4A-NA-C1A	3.61	108.33	106.71
10	d	102	PC1	O21-C21-C22	3.61	119.28	111.50
7	z	101	BCL	C4A-NA-C1A	3.61	108.33	106.71
12	B	103	SPO	C34-C33-C35	-3.60	109.21	115.27
12	s	104	SPO	C34-C33-C35	-3.60	109.21	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	d	101	BCL	C1D-ND-C4D	-3.60	103.78	106.33
7	w	101	BCL	C4A-NA-C1A	3.60	108.32	106.71
9	l	303	U10	C35-C34-C36	3.60	121.32	115.27
12	S	102	SPO	C5-C6-C7	-3.59	120.47	125.89
7	a	101	BCL	C1D-ND-C4D	-3.58	103.79	106.33
7	u	101	BCL	C1D-ND-C4D	-3.58	103.79	106.33
12	A	102	SPO	C30-C28-C27	-3.58	111.15	121.98
12	F	102	SPO	C40-C38-C37	-3.58	112.31	122.65
12	a	104	SPO	C34-C33-C35	-3.58	109.26	115.27
7	2	101	BCL	C1D-ND-C4D	-3.57	103.80	106.33
12	j	103	SPO	C34-C33-C35	-3.57	109.27	115.27
12	o	102	SPO	C39-C38-C37	-3.57	112.34	122.65
12	q	102	SPO	C30-C28-C27	-3.57	111.18	121.98
7	y	101	BCL	C1D-ND-C4D	-3.56	103.81	106.33
7	o	101	BCL	C1D-ND-C4D	-3.56	103.81	106.33
12	8	101	SPO	C21-C20-C19	-3.56	116.19	123.47
12	ab	102	SPO	C36-C37-C38	-3.55	115.60	127.75
7	Z	101	BCL	CHA-C1A-NA	-3.55	118.27	126.40
7	Y	201	BCL	C1D-ND-C4D	-3.55	103.81	106.33
10	A	104	PC1	O21-C21-C22	3.55	119.14	111.50
12	M	1305	SPO	C40-C38-C37	-3.55	112.40	122.65
7	U	101	BCL	C1D-ND-C4D	-3.54	103.82	106.33
10	A	103	PC1	O21-C21-C22	3.54	119.14	111.50
12	m	1305	SPO	C40-C38-C37	-3.54	112.42	122.65
7	A	101	BCL	C1D-ND-C4D	-3.53	103.83	106.33
12	j	103	SPO	C26-C25-C23	-3.53	116.51	126.42
7	w	101	BCL	C1D-ND-C4D	-3.52	103.83	106.33
9	l	303	U10	C22-C23-C24	-3.52	119.19	127.66
12	j	103	SPO	C29-C28-C30	-3.52	109.35	115.27
12	j	103	SPO	C20-C21-C22	-3.52	116.27	123.47
7	U	101	BCL	C1-C2-C3	-3.51	119.97	126.04
12	3	103	SPO	C39-C38-C37	-3.51	112.50	122.65
12	N	103	SPO	C29-C28-C30	-3.51	109.37	115.27
12	m	1305	SPO	C34-C33-C35	-3.50	109.38	115.27
12	o	102	SPO	C40-C38-C37	-3.50	112.54	122.65
12	t	101	SPO	C8-C7-C6	-3.49	112.57	118.08
12	r	102	SPO	C29-C28-C30	-3.49	109.39	115.27
7	L	301	BCL	C1D-ND-C4D	-3.49	103.86	106.33
7	l	301	BCL	C1D-ND-C4D	-3.49	103.86	106.33
7	5	101	BCL	C1D-ND-C4D	-3.49	103.86	106.33
7	M	1303	BCL	C1D-ND-C4D	-3.49	103.86	106.33
9	L	303	U10	C22-C23-C24	-3.49	119.27	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	M	1305	SPO	C34-C33-C35	-3.48	109.41	115.27
7	W	101	BCL	C1D-ND-C4D	-3.48	103.86	106.33
12	aa	101	SPO	C29-C28-C30	-3.47	109.43	115.27
12	d	103	SPO	C9-C10-C11	-3.47	112.40	123.22
12	B	102	SPO	C10-C11-C12	-3.46	116.68	126.42
12	g	102	SPO	C5-C6-C7	-3.46	120.66	125.89
12	j	103	SPO	C21-C20-C19	-3.46	116.38	123.47
12	j	103	SPO	C39-C38-C37	-3.46	112.65	122.65
9	M	1304	U10	C25-C24-C26	3.45	121.08	115.27
7	k	103	BCL	C4A-NA-C1A	3.45	108.25	106.71
7	m	1303	BCL	C1D-ND-C4D	-3.44	103.89	106.33
9	l	303	U10	C32-C33-C34	-3.44	119.37	127.66
12	F	102	SPO	C36-C37-C38	-3.44	116.00	127.75
12	g	102	SPO	C29-C28-C30	-3.43	109.50	115.27
12	n	101	SPO	C5-C6-C7	-3.43	120.72	125.89
12	U	102	SPO	C34-C33-C35	-3.42	109.52	115.27
12	d	103	SPO	C20-C21-C22	-3.42	116.47	123.47
12	q	102	SPO	C40-C38-C37	-3.40	112.81	122.65
9	m	1304	U10	C25-C24-C26	3.40	120.99	115.27
12	B	102	SPO	C40-C38-C37	-3.40	112.83	122.65
9	l	303	U10	C50-C49-C51	3.40	120.98	115.27
12	a	104	SPO	C21-C20-C19	-3.40	116.52	123.47
7	c	101	BCL	C1D-ND-C4D	-3.39	103.92	106.33
7	s	103	BCL	C4A-NA-C1A	3.39	108.23	106.71
7	3	102	BCL	C1D-ND-C4D	-3.39	103.93	106.33
12	O	103	SPO	C34-C33-C35	-3.38	109.59	115.27
8	l	306	BPB	C3D-C4D-ND	3.38	112.32	107.72
12	8	101	SPO	C34-C33-C35	-3.37	109.60	115.27
7	p	101	BCL	C1D-ND-C4D	-3.37	103.94	106.33
12	M	1305	SPO	C29-C28-C30	-3.37	109.61	115.27
8	L	305	BPB	C3D-C4D-ND	3.37	112.31	107.72
12	m	1305	SPO	C29-C28-C30	-3.36	109.62	115.27
12	G	103	SPO	C10-C11-C12	-3.36	116.98	126.42
12	s	104	SPO	C29-C28-C30	-3.36	109.63	115.27
12	O	102	SPO	C20-C21-C22	-3.35	116.60	123.47
12	D	102	SPO	C40-C38-C37	-3.35	112.95	122.65
7	z	101	BCL	CHA-C1A-NA	-3.35	118.73	126.40
12	j	103	SPO	C15-C16-C17	-3.35	117.01	126.42
12	F	102	SPO	C5-C6-C7	-3.34	120.84	125.89
12	j	101	SPO	C5-C6-C7	-3.34	120.84	125.89
9	L	303	U10	C12-C13-C14	-3.34	119.61	127.66
12	s	105	SPO	C35-C33-C32	-3.34	114.36	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	l	101	BCL	CHD-C1D-C2D	3.34	132.49	125.48
12	k	102	SPO	C9-C10-C11	-3.34	112.80	123.22
12	s	104	SPO	C36-C37-C38	-3.34	116.35	127.75
7	r	101	BCL	C1D-ND-C4D	-3.33	103.97	106.33
7	z	101	BCL	C1D-ND-C4D	-3.33	103.97	106.33
8	L	302	BPB	C3D-C4D-ND	3.33	112.25	107.72
8	L	305	BPB	OBD-CAD-CBD	-3.33	120.94	125.82
12	O	102	SPO	C34-C33-C35	-3.32	109.68	115.27
12	N	103	SPO	C10-C11-C12	-3.32	117.09	126.42
7	g	101	BCL	C1D-ND-C4D	-3.32	103.98	106.33
9	l	303	U10	C12-C13-C14	-3.31	119.69	127.66
7	c	101	BCL	C6-C7-C8	-3.31	105.22	115.92
12	e	101	SPO	C30-C28-C27	-3.30	111.98	121.98
7	s	103	BCL	C1D-ND-C4D	-3.30	103.99	106.33
12	N	101	SPO	C34-C33-C35	-3.30	109.72	115.27
9	L	303	U10	C15-C14-C16	3.30	120.82	115.27
9	l	303	U10	C15-C14-C16	3.29	120.81	115.27
8	l	302	BPB	C3D-C4D-ND	3.29	112.21	107.72
12	3	101	SPO	C39-C38-C37	-3.29	113.14	122.65
7	aa	102	BCL	C1D-ND-C4D	-3.29	104.00	106.33
12	ab	102	SPO	C39-C38-C37	-3.29	113.15	122.65
12	d	103	SPO	C21-C20-C19	-3.28	116.75	123.47
7	P	101	BCL	C1D-ND-C4D	-3.28	104.00	106.33
12	U	102	SPO	C20-C21-C22	-3.28	116.75	123.47
7	B	101	BCL	C1D-ND-C4D	-3.28	104.00	106.33
12	0	102	SPO	C21-C20-C19	-3.27	116.77	123.47
7	N	102	BCL	C1D-ND-C4D	-3.27	104.01	106.33
7	p	101	BCL	O2A-C1-C2	-3.27	100.03	108.64
7	8	102	BCL	C1D-ND-C4D	-3.27	104.01	106.33
8	l	302	BPB	OBD-CAD-CBD	-3.27	121.02	125.82
7	5	102	BCL	CHA-C1A-NA	-3.27	118.91	126.40
7	J	101	BCL	C1D-ND-C4D	-3.27	104.01	106.33
7	T	101	BCL	C1D-ND-C4D	-3.27	104.01	106.33
7	R	101	BCL	C1D-ND-C4D	-3.26	104.02	106.33
8	L	302	BPB	OBD-CAD-CBD	-3.26	121.03	125.82
12	d	103	SPO	C30-C28-C27	-3.26	112.10	121.98
7	0	101	BCL	C1D-ND-C4D	-3.26	104.02	106.33
7	1	101	BCL	C1D-ND-C4D	-3.26	104.02	106.33
7	E	101	BCL	C1D-ND-C4D	-3.26	104.02	106.33
7	b	101	BCL	C1D-ND-C4D	-3.26	104.02	106.33
12	N	101	SPO	C5-C6-C7	-3.25	120.98	125.89
7	X	101	BCL	C1D-ND-C4D	-3.25	104.03	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	e	102	BCL	C1D-ND-C4D	-3.25	104.03	106.33
8	l	306	BPB	OBD-CAD-CBD	-3.25	121.05	125.82
7	G	101	BCL	C1D-ND-C4D	-3.24	104.03	106.33
7	1	101	BCL	CHD-C4C-NC	-3.24	121.48	125.08
12	N	101	SPO	C36-C37-C38	-3.24	116.68	127.75
12	B	102	SPO	C34-C33-C35	-3.24	109.83	115.27
12	8	101	SPO	C20-C21-C22	-3.23	116.85	123.47
12	B	102	SPO	C20-C21-C22	-3.23	116.85	123.47
12	8	101	SPO	C29-C28-C30	-3.23	109.84	115.27
7	j	102	BCL	C1D-ND-C4D	-3.22	104.04	106.33
7	p	101	BCL	C1-C2-C3	3.22	131.61	126.04
7	ab	101	BCL	C1D-ND-C4D	-3.22	104.05	106.33
7	q	101	BCL	C1D-ND-C4D	-3.21	104.05	106.33
12	O	103	SPO	C20-C21-C22	-3.21	116.89	123.47
12	aa	101	SPO	C20-C21-C22	-3.21	116.90	123.47
7	v	101	BCL	C1D-ND-C4D	-3.21	104.06	106.33
7	v	101	BCL	CAA-CBA-CGA	-3.21	103.89	113.25
9	m	1304	U10	C17-C18-C19	-3.19	119.97	127.66
12	ab	102	SPO	C20-C21-C22	-3.19	116.94	123.47
7	x	101	BCL	C1D-ND-C4D	-3.19	104.07	106.33
12	i	102	SPO	C34-C33-C35	-3.19	109.91	115.27
9	M	1304	U10	C17-C18-C19	-3.18	120.00	127.66
9	L	303	U10	C27-C28-C29	-3.18	120.01	127.66
9	l	303	U10	C27-C28-C29	-3.18	120.02	127.66
7	k	103	BCL	C17-C16-C15	3.17	127.82	113.24
7	v	101	BCL	CHA-C1A-NA	-3.17	119.14	126.40
12	0	102	SPO	C34-C33-C35	-3.16	109.95	115.27
9	l	303	U10	C17-C18-C19	-3.16	120.05	127.66
9	L	303	U10	C17-C18-C19	-3.16	120.06	127.66
12	j	103	SPO	C10-C11-C12	-3.15	117.56	126.42
7	s	103	BCL	CAB-C3B-C2B	3.15	133.06	128.34
12	G	102	SPO	C29-C28-C30	-3.15	109.97	115.27
12	U	102	SPO	C26-C25-C23	-3.15	117.57	126.42
7	7	101	BCL	C1D-ND-C4D	-3.14	104.10	106.33
7	U	103	BCL	C1D-ND-C4D	-3.14	104.10	106.33
7	x	101	BCL	CHA-C1A-NA	-3.14	119.22	126.40
12	aa	101	SPO	C9-C10-C11	-3.14	113.43	123.22
12	K	102	SPO	C40-C38-C37	-3.13	113.59	122.65
12	t	101	SPO	C15-C16-C17	-3.13	117.62	126.42
7	M	1303	BCL	CHA-C1A-NA	-3.13	119.24	126.40
7	m	1303	BCL	CHA-C1A-NA	-3.13	119.24	126.40
7	i	101	BCL	C1D-ND-C4D	-3.13	104.11	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	T	102	SPO	C34-C33-C35	-3.12	110.02	115.27
12	s	105	SPO	C20-C21-C22	-3.12	117.08	123.47
10	h	302	PC1	O21-C21-C22	3.12	118.22	111.50
7	z	101	BCL	CAC-C3C-C4C	3.11	119.48	112.58
12	j	101	SPO	C36-C37-C38	-3.10	117.14	127.75
7	L	304	BCL	CHA-C1A-NA	-3.10	119.29	126.40
12	t	101	SPO	C20-C21-C22	-3.10	117.12	123.47
12	s	104	SPO	C20-C21-C22	-3.10	117.12	123.47
9	M	1304	U10	C35-C34-C36	3.10	120.48	115.27
7	X	101	BCL	CHA-C1A-NA	-3.09	119.31	126.40
9	m	1304	U10	C35-C34-C36	3.09	120.47	115.27
12	D	102	SPO	C34-C33-C35	-3.09	110.08	115.27
12	N	101	SPO	C40-C38-C37	-3.09	113.73	122.65
12	K	102	SPO	C34-C33-C35	-3.08	110.09	115.27
7	ab	101	BCL	C4A-NA-C1A	3.08	108.09	106.71
12	d	103	SPO	C27-C26-C25	-3.06	113.67	123.22
7	3	102	BCL	CMB-C2B-C1B	-3.06	120.71	125.37
7	l	305	BCL	CHA-C1A-NA	-3.06	119.39	126.40
7	d	101	BCL	CHA-C1A-NA	-3.06	119.39	126.40
7	p	101	BCL	CHA-C1A-NA	-3.06	119.40	126.40
7	5	102	BCL	CHC-C4B-NB	-3.06	121.02	124.26
7	r	101	BCL	CHA-C1A-NA	-3.05	119.41	126.40
7	K	101	BCL	CAB-C3B-C2B	3.05	132.91	128.34
7	G	101	BCL	C4A-NA-C1A	3.05	108.08	106.71
12	8	101	SPO	C15-C16-C17	-3.04	117.86	126.42
12	G	102	SPO	C26-C25-C23	-3.04	117.87	126.42
9	l	303	U10	C45-C44-C46	3.04	120.39	115.27
8	L	302	BPB	CMB-C2B-C3B	3.04	130.37	124.68
7	3	102	BCL	CHC-C4B-NB	-3.04	121.04	124.26
7	Q	101	BCL	CHA-C1A-NA	-3.03	119.45	126.40
13	M	1306	CDL	OB8-CB7-C71	3.03	121.42	111.91
7	f	101	BCL	CHA-C1A-NA	-3.03	119.46	126.40
9	L	303	U10	C36-C34-C35	3.03	121.29	114.60
7	Z	101	BCL	C1D-ND-C4D	-3.03	104.18	106.33
12	8	101	SPO	C9-C10-C11	-3.03	113.77	123.22
8	l	302	BPB	CMB-C2B-C3B	3.03	130.34	124.68
7	E	101	BCL	C4A-NA-C1A	3.02	108.06	106.71
7	J	101	BCL	C4A-NA-C1A	3.02	108.06	106.71
7	8	102	BCL	CHA-C1A-NA	-3.02	119.48	126.40
12	e	101	SPO	C40-C38-C37	-3.02	113.91	122.65
7	c	101	BCL	CHA-C1A-NA	-3.02	119.48	126.40
7	q	101	BCL	CHA-C1A-NA	-3.02	119.48	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	e	102	BCL	CHA-C1A-NA	-3.02	119.49	126.40
7	o	101	BCL	CAB-C3B-C2B	3.02	132.86	128.34
13	m	1306	CDL	OB8-CB7-C71	3.02	121.38	111.91
7	J	101	BCL	CHA-C1A-NA	-3.02	119.49	126.40
7	b	101	BCL	CHA-C1A-NA	-3.01	119.50	126.40
7	E	101	BCL	CHA-C1A-NA	-3.01	119.50	126.40
7	g	101	BCL	CHA-C1A-NA	-3.01	119.50	126.40
7	N	102	BCL	CHA-C1A-NA	-3.01	119.50	126.40
7	S	101	BCL	CHA-C1A-NA	-3.01	119.50	126.40
7	j	102	BCL	CHA-C1A-NA	-3.01	119.50	126.40
7	l	101	BCL	CAB-C3B-C2B	3.01	132.84	128.34
7	aa	102	BCL	CHA-C1A-NA	-3.01	119.51	126.40
7	0	101	BCL	CHA-C1A-NA	-3.01	119.52	126.40
7	P	101	BCL	C4A-NA-C1A	3.01	108.06	106.71
7	o	101	BCL	CHA-C1A-NA	-3.00	119.52	126.40
7	R	101	BCL	CHA-C1A-NA	-3.00	119.52	126.40
7	P	101	BCL	CHA-C1A-NA	-3.00	119.53	126.40
12	ab	102	SPO	C29-C28-C30	-3.00	110.23	115.27
7	G	101	BCL	CHA-C1A-NA	-3.00	119.53	126.40
7	5	102	BCL	CAB-C3B-C2B	3.00	132.83	128.34
7	ab	101	BCL	CHA-C1A-NA	-3.00	119.54	126.40
7	B	101	BCL	C4A-NA-C1A	3.00	108.05	106.71
7	T	101	BCL	CHA-C1A-NA	-3.00	119.54	126.40
7	B	101	BCL	CHA-C1A-NA	-3.00	119.54	126.40
7	K	101	BCL	CHA-C1A-NA	-2.99	119.54	126.40
7	k	101	BCL	CHA-C1A-NA	-2.99	119.55	126.40
7	L	301	BCL	CHA-C1A-NA	-2.99	119.55	126.40
7	aa	102	BCL	C4A-NA-C1A	2.99	108.05	106.71
7	k	103	BCL	CHA-C1A-NA	-2.99	119.56	126.40
7	3	102	BCL	CHA-C1A-NA	-2.99	119.56	126.40
7	0	101	BCL	C4A-NA-C1A	2.99	108.05	106.71
7	i	101	BCL	CHA-C1A-NA	-2.98	119.57	126.40
12	A	102	SPO	C34-C33-C35	-2.98	110.26	115.27
7	O	101	BCL	CHA-C1A-NA	-2.98	119.57	126.40
7	l	101	BCL	CHA-C1A-NA	-2.98	119.57	126.40
12	aa	101	SPO	C15-C16-C17	-2.98	118.05	126.42
7	z	101	BCL	C2A-C1A-CHA	2.98	129.07	123.86
7	F	101	BCL	CHA-C1A-NA	-2.98	119.58	126.40
7	p	101	BCL	C4A-NA-C1A	2.98	108.04	106.71
9	m	1304	U10	C32-C33-C34	-2.97	120.50	127.66
9	M	1304	U10	C32-C33-C34	-2.97	120.50	127.66
7	I	101	BCL	CHA-C1A-NA	-2.97	119.59	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	T	101	BCL	C4A-NA-C1A	2.97	108.04	106.71
7	l	301	BCL	CHA-C1A-NA	-2.97	119.60	126.40
12	G	103	SPO	C29-C28-C30	-2.97	110.28	115.27
7	s	101	BCL	CHA-C1A-NA	-2.97	119.60	126.40
7	D	101	BCL	CHA-C1A-NA	-2.97	119.60	126.40
9	M	1304	U10	C10-C9-C11	2.97	120.26	115.27
12	ab	102	SPO	C34-C33-C35	-2.97	110.28	115.27
7	A	101	BCL	CHA-C1A-NA	-2.96	119.61	126.40
7	R	101	BCL	C4A-NA-C1A	2.96	108.04	106.71
7	P	101	BCL	C16-C15-C13	2.96	125.50	115.92
9	M	1304	U10	C27-C28-C29	-2.96	120.53	127.66
12	O	103	SPO	C29-C28-C30	-2.96	110.29	115.27
7	j	102	BCL	C4A-NA-C1A	2.96	108.04	106.71
12	g	102	SPO	C10-C11-C12	-2.96	118.11	126.42
7	5	101	BCL	CAB-C3B-C2B	2.96	132.77	128.34
7	0	101	BCL	C16-C15-C13	2.96	125.48	115.92
7	N	102	BCL	C16-C15-C13	2.96	125.48	115.92
7	j	102	BCL	C16-C15-C13	2.96	125.48	115.92
7	9	101	BCL	CHA-C1A-NA	-2.96	119.63	126.40
7	ab	101	BCL	C16-C15-C13	2.95	125.47	115.92
7	aa	102	BCL	C16-C15-C13	2.95	125.47	115.92
7	b	101	BCL	C16-C15-C13	2.95	125.46	115.92
7	u	101	BCL	CAB-C3B-C2B	2.95	132.76	128.34
7	R	101	BCL	C16-C15-C13	2.95	125.46	115.92
7	G	101	BCL	C16-C15-C13	2.95	125.46	115.92
7	x	101	BCL	CHC-C4B-NB	-2.95	121.13	124.26
7	E	101	BCL	C16-C15-C13	2.95	125.46	115.92
9	m	1304	U10	C10-C9-C11	2.95	120.23	115.27
7	l	305	BCL	CAB-C3B-C2B	2.95	132.76	128.34
7	J	101	BCL	C16-C15-C13	2.95	125.45	115.92
7	8	102	BCL	C16-C15-C13	2.95	125.45	115.92
7	B	101	BCL	C16-C15-C13	2.95	125.45	115.92
9	m	1304	U10	C27-C28-C29	-2.95	120.56	127.66
7	N	102	BCL	C4A-NA-C1A	2.95	108.03	106.71
7	e	102	BCL	C16-C15-C13	2.95	125.44	115.92
7	g	101	BCL	C16-C15-C13	2.95	125.44	115.92
7	M	1301	BCL	C4-C3-C5	-2.95	110.31	115.27
7	T	101	BCL	C16-C15-C13	2.94	125.43	115.92
7	e	102	BCL	C4A-NA-C1A	2.94	108.03	106.71
7	a	101	BCL	CHA-C1A-NA	-2.94	119.67	126.40
12	e	103	SPO	C11-C12-C14	-2.94	114.43	118.94
7	M	1301	BCL	CHA-C1A-NA	-2.94	119.67	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	s	101	BCL	CAB-C3B-C2B	2.93	132.73	128.34
7	m	1301	BCL	CHA-C1A-NA	-2.93	119.69	126.40
12	j	101	SPO	C39-C38-C37	-2.93	114.18	122.65
7	8	102	BCL	C4A-NA-C1A	2.93	108.02	106.71
7	W	101	BCL	CAB-C3B-C2B	2.92	132.72	128.34
7	7	101	BCL	CHA-C1A-NA	-2.92	119.71	126.40
7	U	101	BCL	CHA-C1A-NA	-2.92	119.72	126.40
7	m	1301	BCL	C4-C3-C5	-2.92	110.36	115.27
7	y	101	BCL	CAB-C3B-C2B	2.92	132.71	128.34
7	2	101	BCL	CAB-C3B-C2B	2.91	132.70	128.34
12	s	104	SPO	C40-C38-C37	-2.91	114.23	122.65
7	u	101	BCL	CHA-C1A-NA	-2.91	119.73	126.40
7	U	101	BCL	CAB-C3B-C2B	2.91	132.70	128.34
12	j	101	SPO	C34-C33-C35	-2.91	110.37	115.27
7	w	101	BCL	CHA-C1A-NA	-2.91	119.73	126.40
7	b	101	BCL	C4A-NA-C1A	2.91	108.01	106.71
7	w	101	BCL	CAB-C3B-C2B	2.91	132.69	128.34
12	ab	102	SPO	C10-C11-C12	-2.90	118.26	126.42
7	Y	201	BCL	CAB-C3B-C2B	2.90	132.69	128.34
7	L	304	BCL	CAB-C3B-C2B	2.90	132.69	128.34
7	Y	201	BCL	CHA-C1A-NA	-2.90	119.76	126.40
7	2	101	BCL	CHA-C1A-NA	-2.90	119.76	126.40
7	L	301	BCL	C2A-C1A-CHA	2.89	128.92	123.86
12	F	102	SPO	C39-C38-C37	-2.89	114.29	122.65
12	I	102	SPO	C5-C6-C7	-2.89	121.52	125.89
9	m	1304	U10	C12-C13-C14	-2.88	120.72	127.66
7	i	101	BCL	CHC-C4B-NB	-2.88	121.20	124.26
7	l	301	BCL	C2A-C1A-CHA	2.88	128.90	123.86
7	q	101	BCL	CMB-C2B-C1B	-2.88	120.98	125.37
9	M	1304	U10	C12-C13-C14	-2.88	120.72	127.66
7	g	101	BCL	C4A-NA-C1A	2.88	108.00	106.71
7	y	101	BCL	CHA-C1A-NA	-2.88	119.81	126.40
12	r	102	SPO	C10-C11-C12	-2.88	118.34	126.42
12	e	103	SPO	C26-C25-C23	-2.87	118.34	126.42
7	5	101	BCL	CHA-C1A-NA	-2.87	119.81	126.40
10	L	306	PC1	O21-C21-C22	2.87	117.69	111.50
7	I	101	BCL	CAB-C3B-C2B	2.87	132.65	128.34
7	W	101	BCL	CHA-C1A-NA	-2.87	119.82	126.40
12	3	101	SPO	C34-C33-C35	-2.87	110.44	115.27
12	o	102	SPO	C34-C33-C35	-2.86	110.46	115.27
12	s	102	SPO	C39-C38-C37	-2.85	114.41	122.65
7	L	304	BCL	C2A-C1A-CHA	2.84	128.83	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	l	306	BPB	CMB-C2B-C3B	2.84	130.00	124.68
9	l	303	U10	C25-C24-C26	2.84	120.04	115.27
7	v	101	BCL	O2A-C1-C2	-2.83	101.19	108.64
9	L	303	U10	C25-C24-C26	2.83	120.03	115.27
7	aa	102	BCL	C17-C16-C15	2.83	126.25	113.24
7	ab	101	BCL	C17-C16-C15	2.83	126.24	113.24
7	U	103	BCL	CHA-C1A-NA	-2.83	119.92	126.40
8	L	305	BPB	CMB-C2B-C3B	2.83	129.97	124.68
7	G	101	BCL	C17-C16-C15	2.83	126.23	113.24
7	j	102	BCL	C17-C16-C15	2.83	126.23	113.24
7	0	101	BCL	C17-C16-C15	2.83	126.22	113.24
7	s	103	BCL	CHA-C1A-NA	-2.83	119.93	126.40
7	N	102	BCL	C17-C16-C15	2.82	126.22	113.24
7	E	101	BCL	C17-C16-C15	2.82	126.21	113.24
7	e	102	BCL	C17-C16-C15	2.82	126.20	113.24
7	P	101	BCL	C17-C16-C15	2.82	126.20	113.24
7	b	101	BCL	C17-C16-C15	2.82	126.20	113.24
7	B	101	BCL	C17-C16-C15	2.82	126.20	113.24
7	8	102	BCL	C17-C16-C15	2.82	126.20	113.24
12	a	104	SPO	C14-C15-C16	-2.82	114.42	123.22
7	g	101	BCL	C17-C16-C15	2.82	126.19	113.24
7	T	101	BCL	C17-C16-C15	2.82	126.19	113.24
7	r	101	BCL	CAB-C3B-C2B	2.82	132.56	128.34
12	r	102	SPO	C21-C20-C19	-2.81	117.71	123.47
7	J	101	BCL	C17-C16-C15	2.81	126.17	113.24
12	r	102	SPO	C34-C33-C35	-2.81	110.54	115.27
7	l	305	BCL	C2A-C1A-CHA	2.81	128.78	123.86
7	R	101	BCL	C17-C16-C15	2.81	126.16	113.24
7	l	305	BCL	C4A-NA-C1A	2.81	107.97	106.71
12	G	102	SPO	C20-C21-C22	-2.81	117.72	123.47
9	l	303	U10	C40-C39-C41	2.80	119.99	115.27
7	r	101	BCL	C2A-C1A-CHA	2.80	128.75	123.86
12	a	104	SPO	C20-C21-C22	-2.80	117.74	123.47
12	e	103	SPO	C2-C1-C4	-2.80	106.56	110.86
7	q	101	BCL	CAB-C3B-C2B	2.79	132.51	128.34
7	7	101	BCL	CHC-C4B-NB	-2.78	121.31	124.26
9	L	303	U10	C30-C29-C31	2.78	119.95	115.27
12	I	102	SPO	C34-C33-C35	-2.78	110.60	115.27
7	q	101	BCL	CHC-C4B-NB	-2.78	121.32	124.26
12	m	1305	SPO	C15-C16-C17	-2.78	118.62	126.42
12	k	102	SPO	C30-C28-C27	-2.77	107.94	122.73
12	M	1305	SPO	C15-C16-C17	-2.77	118.64	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	O	101	BCL	CAB-C3B-C2B	2.77	132.48	128.34
13	M	1306	CDL	OA8-CA7-C31	2.76	120.57	111.91
13	m	1306	CDL	OA8-CA7-C31	2.76	120.56	111.91
7	F	101	BCL	C15-C13-C12	-2.76	97.63	112.13
9	l	303	U10	C47-C48-C49	-2.76	121.02	127.66
8	l	306	BPB	C2D-C1D-ND	2.76	111.43	109.53
7	q	101	BCL	C2A-C1A-CHA	2.75	128.68	123.86
7	i	101	BCL	C2A-C1A-CHA	2.75	128.67	123.86
7	S	101	BCL	CAB-C3B-C2B	2.75	132.46	128.34
7	v	101	BCL	C2A-C1A-CHA	2.75	128.67	123.86
10	d	102	PC1	C13-N-C12	2.75	121.17	109.92
10	h	302	PC1	O31-C31-C32	2.75	120.54	111.91
7	F	101	BCL	CAB-C3B-C2B	2.75	132.46	128.34
9	l	303	U10	C30-C29-C31	2.74	119.88	115.27
12	t	101	SPO	C2-C1-C4	-2.74	106.65	110.86
7	i	101	BCL	C6-C7-C8	-2.74	107.06	115.92
7	M	1303	BCL	CHC-C4B-NB	-2.74	121.36	124.26
7	k	101	BCL	CAB-C3B-C2B	2.73	132.43	128.34
12	n	101	SPO	C20-C21-C22	-2.73	117.89	123.47
10	l	304	PC1	O31-C31-C32	2.72	120.46	111.91
12	R	102	SPO	C34-C33-C35	-2.72	110.69	115.27
7	f	101	BCL	CAB-C3B-C2B	2.72	132.41	128.34
12	n	101	SPO	C34-C33-C35	-2.72	110.70	115.27
8	l	302	BPB	C11-C12-C13	-2.72	107.13	115.92
12	3	103	SPO	C40-C38-C39	-2.72	108.60	114.60
12	B	103	SPO	C14-C15-C16	-2.72	114.74	123.22
7	z	101	BCL	CHC-C4B-NB	-2.72	121.38	124.26
7	i	101	BCL	CMB-C2B-C1B	-2.72	121.23	125.37
8	L	305	BPB	C2D-C1D-ND	2.72	111.40	109.53
7	v	101	BCL	CAB-C3B-C2B	2.71	132.41	128.34
12	U	102	SPO	C5-C6-C7	-2.71	121.79	125.89
10	C	1201	PC1	O31-C31-C32	2.71	120.42	111.91
8	L	302	BPB	C11-C12-C13	-2.71	107.16	115.92
12	k	102	SPO	C27-C26-C25	-2.71	114.76	123.22
12	O	102	SPO	C26-C25-C23	-2.71	118.81	126.42
7	Q	101	BCL	CAB-C3B-C2B	2.71	132.40	128.34
7	m	1303	BCL	CHC-C4B-NB	-2.71	121.39	124.26
10	a	102	PC1	O31-C31-C32	2.71	120.40	111.91
7	k	103	BCL	O2A-C1-C2	-2.70	101.54	108.64
7	r	101	BCL	CAC-C3C-C4C	-2.70	106.60	112.58
7	3	102	BCL	C2A-C1A-CHA	2.69	128.56	123.86
7	L	301	BCL	CAB-C3B-C2B	2.69	132.37	128.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	9	101	BCL	CAB-C3B-C2B	2.69	132.37	128.34
12	N	101	SPO	C39-C38-C37	-2.68	114.89	122.65
7	M	1301	BCL	C2A-C1A-CHA	2.68	128.55	123.86
7	l	301	BCL	CAB-C3B-C2B	2.68	132.35	128.34
7	m	1301	BCL	C2A-C1A-CHA	2.68	128.54	123.86
7	a	101	BCL	C2A-C1A-CHA	2.68	128.54	123.86
12	q	102	SPO	C34-C33-C35	-2.67	110.77	115.27
12	k	102	SPO	C30-C28-C29	-2.67	108.70	114.60
7	J	101	BCL	C2A-C1A-CHA	2.66	128.51	123.86
7	7	101	BCL	C2A-C1A-CHA	2.66	128.51	123.86
8	l	302	BPB	C2D-C1D-ND	2.66	111.36	109.53
7	M	1303	BCL	C2A-C1A-CHA	2.66	128.51	123.86
10	a	103	PC1	O31-C31-C32	2.66	120.25	111.91
7	0	101	BCL	C2A-C1A-CHA	2.65	128.50	123.86
7	m	1303	BCL	C2A-C1A-CHA	2.65	128.50	123.86
7	E	101	BCL	C2A-C1A-CHA	2.65	128.49	123.86
7	P	101	BCL	C2A-C1A-CHA	2.65	128.49	123.86
7	d	101	BCL	C2A-C1A-CHA	2.65	128.49	123.86
7	L	304	BCL	C4A-NA-C1A	2.64	107.89	106.71
7	j	102	BCL	C2A-C1A-CHA	2.64	128.48	123.86
7	ab	101	BCL	C2A-C1A-CHA	2.64	128.48	123.86
7	8	102	BCL	C2A-C1A-CHA	2.64	128.48	123.86
7	N	102	BCL	C2A-C1A-CHA	2.64	128.48	123.86
7	5	102	BCL	C4A-NA-C1A	2.64	107.89	106.71
7	M	1303	BCL	CAB-C3B-C2B	2.64	132.29	128.34
7	B	101	BCL	C2A-C1A-CHA	2.64	128.47	123.86
7	e	102	BCL	C2A-C1A-CHA	2.63	128.47	123.86
7	b	101	BCL	C2A-C1A-CHA	2.63	128.46	123.86
12	O	103	SPO	C21-C20-C19	-2.63	118.08	123.47
9	M	1304	U10	C15-C14-C16	2.63	119.70	115.27
7	R	101	BCL	C2A-C1A-CHA	2.63	128.46	123.86
7	g	101	BCL	C2A-C1A-CHA	2.63	128.45	123.86
7	G	101	BCL	C2A-C1A-CHA	2.63	128.45	123.86
7	c	101	BCL	CMB-C2B-C1B	-2.63	121.37	125.37
7	aa	102	BCL	C2A-C1A-CHA	2.63	128.45	123.86
9	l	303	U10	C20-C19-C21	2.63	119.69	115.27
7	T	101	BCL	C2A-C1A-CHA	2.62	128.45	123.86
12	m	1305	SPO	C26-C25-C23	-2.62	119.05	126.42
9	m	1304	U10	C15-C14-C16	2.62	119.68	115.27
12	G	102	SPO	C34-C33-C35	-2.62	110.87	115.27
7	O	101	BCL	C2A-C1A-CHA	2.62	128.43	123.86
7	X	101	BCL	CAB-C3B-C2B	2.61	132.25	128.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	d	103	SPO	C34-C33-C35	-2.61	110.88	115.27
12	M	1305	SPO	C26-C25-C23	-2.61	119.08	126.42
9	L	303	U10	C20-C19-C21	2.61	119.66	115.27
9	l	303	U10	C42-C43-C44	-2.61	121.38	127.66
7	m	1303	BCL	CAB-C3B-C2B	2.61	132.25	128.34
8	L	302	BPB	O2D-CGD-CBD	2.61	114.30	111.00
10	M	1307	PC1	O31-C31-C32	2.61	120.09	111.91
7	D	101	BCL	CAB-C3B-C2B	2.61	132.24	128.34
10	h	301	PC1	O31-C31-C32	2.60	120.08	111.91
7	f	101	BCL	C2A-C1A-CHA	2.60	128.41	123.86
12	G	103	SPO	C21-C20-C19	-2.60	118.14	123.47
7	A	101	BCL	C2A-C1A-CHA	2.60	128.41	123.86
7	D	101	BCL	CMB-C2B-C1B	-2.60	121.41	125.37
7	c	101	BCL	C2A-C1A-CHA	2.59	128.39	123.86
10	A	103	PC1	C13-N-C12	2.59	120.52	109.92
8	L	302	BPB	C2D-C1D-ND	2.59	111.31	109.53
7	U	103	BCL	CHC-C4B-NB	-2.58	121.52	124.26
12	i	102	SPO	C40-C38-C39	2.58	120.31	114.60
7	M	1303	BCL	CMB-C2B-C1B	-2.58	121.44	125.37
12	O	102	SPO	C10-C11-C12	-2.58	119.18	126.42
7	5	102	BCL	C1D-ND-C4D	-2.58	104.50	106.33
7	D	101	BCL	CHC-C4B-NB	-2.58	121.53	124.26
7	M	1301	BCL	CAB-C3B-C2B	2.58	132.20	128.34
7	m	1303	BCL	CMB-C2B-C1B	-2.57	121.45	125.37
12	t	101	SPO	C9-C10-C11	-2.57	115.20	123.22
12	I	102	SPO	C40-C38-C37	-2.57	115.22	122.65
12	g	102	SPO	C26-C25-C23	-2.56	119.23	126.42
7	p	101	BCL	C11-C10-C8	-2.56	107.65	115.92
8	l	302	BPB	O2D-CGD-CBD	2.56	114.23	111.00
7	a	101	BCL	CAB-C3B-C2B	2.56	132.17	128.34
7	m	1301	BCL	CAB-C3B-C2B	2.56	132.17	128.34
7	l	305	BCL	CMB-C2B-C1B	-2.55	121.48	125.37
12	T	102	SPO	C10-C11-C12	-2.55	119.26	126.42
7	i	101	BCL	CAB-C3B-C2B	2.55	132.15	128.34
7	u	101	BCL	C1-O2A-CGA	-2.54	109.77	116.44
7	Q	101	BCL	C2A-C1A-CHA	2.54	128.30	123.86
7	Z	101	BCL	CHC-C4B-NB	-2.53	121.58	124.26
12	s	102	SPO	C40-C38-C37	-2.53	115.33	122.65
7	X	101	BCL	C4A-NA-C1A	2.53	107.84	106.71
7	A	101	BCL	CHC-C4B-NB	-2.53	121.58	124.26
7	D	101	BCL	C2A-C1A-CHA	2.53	128.28	123.86
7	L	301	BCL	CHC-C4B-NB	-2.53	121.58	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	l	301	BCL	CHC-C4B-NB	-2.53	121.58	124.26
7	U	101	BCL	C2A-C1A-CHA	2.52	128.27	123.86
12	0	102	SPO	C29-C28-C30	-2.52	111.03	115.27
7	L	304	BCL	CMB-C2B-C1B	-2.52	121.53	125.37
12	e	103	SPO	C27-C26-C25	-2.52	115.35	123.22
7	1	101	BCL	CHC-C4B-NB	-2.52	121.59	124.26
12	N	103	SPO	C34-C33-C35	-2.51	111.04	115.27
7	A	101	BCL	CAB-C3B-C2B	2.51	132.10	128.34
7	9	101	BCL	CHC-C4B-NB	-2.51	121.60	124.26
7	y	101	BCL	C2A-C1A-CHA	2.51	128.25	123.86
7	3	102	BCL	C4B-C3B-C2B	-2.51	104.32	108.36
7	o	101	BCL	C2A-C1A-CHA	2.51	128.25	123.86
7	u	101	BCL	C2A-C1A-CHA	2.51	128.25	123.86
10	d	102	PC1	C3-C2-C1	-2.51	105.86	111.79
9	M	1304	U10	C20-C19-C21	2.51	119.49	115.27
7	I	101	BCL	CHC-C4B-NB	-2.51	121.60	124.26
10	L	306	PC1	C13-N-C12	2.51	120.17	109.92
7	W	101	BCL	C2A-C1A-CHA	2.51	128.24	123.86
7	a	101	BCL	CHC-C4B-NB	-2.50	121.61	124.26
7	Y	201	BCL	C2A-C1A-CHA	2.50	128.24	123.86
7	5	102	BCL	C1C-NC-C4C	2.50	107.83	106.71
7	I	101	BCL	CMB-C2B-C1B	-2.50	121.56	125.37
7	2	101	BCL	C2A-C1A-CHA	2.50	128.22	123.86
7	w	101	BCL	C2A-C1A-CHA	2.50	128.22	123.86
7	s	101	BCL	CHC-C4B-NB	-2.50	121.61	124.26
7	q	101	BCL	C4B-C3B-C2B	-2.50	104.34	108.36
7	s	101	BCL	C2A-C1A-CHA	2.49	128.22	123.86
7	d	101	BCL	CHC-C4B-NB	-2.49	121.62	124.26
12	k	102	SPO	C21-C20-C19	-2.49	118.37	123.47
12	aa	101	SPO	C27-C26-C25	-2.49	115.44	123.22
7	I	101	BCL	C2A-C1A-CHA	2.49	128.21	123.86
12	A	102	SPO	C40-C38-C39	-2.49	109.11	114.60
12	T	102	SPO	C21-C20-C19	-2.49	118.38	123.47
12	R	102	SPO	C29-C28-C30	-2.48	111.09	115.27
10	M	1307	PC1	C13-N-C12	2.48	120.07	109.92
7	k	101	BCL	C2A-C1A-CHA	2.48	128.20	123.86
9	M	1304	U10	C30-C29-C31	2.48	119.44	115.27
7	F	101	BCL	CHC-C4B-NB	-2.48	121.64	124.26
7	f	101	BCL	CHC-C4B-NB	-2.48	121.64	124.26
7	U	103	BCL	C2A-C1A-CHA	2.48	128.19	123.86
10	h	301	PC1	C13-N-C12	2.48	120.04	109.92
9	l	303	U10	C52-C53-C54	-2.47	119.29	127.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	5	101	BCL	C2A-C1A-CHA	2.47	128.18	123.86
10	a	103	PC1	C2-O21-C21	-2.47	111.71	117.79
7	S	101	BCL	C2A-C1A-CHA	2.47	128.18	123.86
9	m	1304	U10	C20-C19-C21	2.47	119.43	115.27
12	B	102	SPO	C29-C28-C30	-2.47	111.12	115.27
12	s	104	SPO	C14-C15-C16	-2.47	115.52	123.22
7	c	101	BCL	CAB-C3B-C2B	2.47	132.03	128.34
7	9	101	BCL	C2A-C1A-CHA	2.47	128.17	123.86
7	k	101	BCL	CHC-C4B-NB	-2.46	121.65	124.26
10	a	102	PC1	C11-C12-N	-2.46	107.58	115.78
10	l	304	PC1	C13-N-C12	2.46	119.96	109.92
7	M	1301	BCL	C1-O2A-CGA	2.45	122.87	116.44
7	e	102	BCL	CAB-C3B-C2B	2.45	132.01	128.34
10	C	1201	PC1	C13-N-C12	2.45	119.93	109.92
7	K	101	BCL	CHC-C4B-NB	-2.45	121.67	124.26
7	O	101	BCL	CHC-C4B-NB	-2.44	121.67	124.26
7	k	101	BCL	CMB-C2B-C1B	-2.44	121.65	125.37
7	U	103	BCL	CAB-C3B-C2B	2.44	132.00	128.34
12	3	101	SPO	C40-C38-C39	-2.44	109.21	114.60
9	m	1304	U10	C30-C29-C31	2.44	119.38	115.27
12	U	102	SPO	C9-C10-C11	-2.44	115.60	123.22
12	9	102	SPO	C34-C33-C35	-2.44	111.17	115.27
7	U	103	BCL	CMB-C2B-C1B	-2.44	121.66	125.37
9	L	303	U10	C32-C33-C34	-2.44	119.42	127.75
7	Q	101	BCL	CHC-C4B-NB	-2.44	121.68	124.26
12	O	103	SPO	C15-C16-C17	-2.43	119.58	126.42
7	R	101	BCL	CAB-C3B-C2B	2.43	131.98	128.34
7	J	101	BCL	CAB-C3B-C2B	2.43	131.98	128.34
7	m	1301	BCL	C1-O2A-CGA	2.43	122.82	116.44
7	8	102	BCL	CAB-C3B-C2B	2.43	131.98	128.34
12	s	102	SPO	C20-C21-C22	-2.43	118.50	123.47
12	A	102	SPO	C39-C38-C37	-2.43	115.63	122.65
7	F	101	BCL	C2A-C1A-CHA	2.43	128.10	123.86
7	1	101	BCL	CHB-C1B-NB	-2.43	121.69	124.26
7	j	102	BCL	CAB-C3B-C2B	2.42	131.97	128.34
12	s	105	SPO	C6-C7-C9	-2.42	115.22	118.94
7	G	101	BCL	CAB-C3B-C2B	2.42	131.97	128.34
7	E	101	BCL	CAB-C3B-C2B	2.42	131.97	128.34
7	s	101	BCL	CMB-C2B-C1B	-2.42	121.68	125.37
7	a	101	BCL	CMB-C2B-C1B	-2.42	121.68	125.37
8	L	302	BPB	CMD-C2D-C3D	2.42	129.20	124.68
7	aa	102	BCL	CAB-C3B-C2B	2.42	131.96	128.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	ab	101	BCL	CAB-C3B-C2B	2.42	131.96	128.34
7	N	102	BCL	CAB-C3B-C2B	2.42	131.96	128.34
7	P	101	BCL	CAB-C3B-C2B	2.42	131.96	128.34
7	0	101	BCL	CAB-C3B-C2B	2.41	131.96	128.34
7	L	304	BCL	CHC-C4B-NB	-2.41	121.70	124.26
7	M	1301	BCL	C4A-NA-C1A	2.41	107.79	106.71
7	A	101	BCL	CMB-C2B-C1B	-2.41	121.69	125.37
7	g	101	BCL	CAB-C3B-C2B	2.41	131.95	128.34
7	M	1301	BCL	CHC-C4B-NB	-2.41	121.70	124.26
8	l	302	BPB	CMD-C2D-C3D	2.41	129.19	124.68
7	b	101	BCL	CAB-C3B-C2B	2.41	131.95	128.34
12	B	102	SPO	C15-C16-C17	-2.41	119.64	126.42
12	aa	101	SPO	C2-C1-C4	-2.41	107.16	110.86
12	F	102	SPO	C34-C33-C35	-2.41	111.22	115.27
7	B	101	BCL	CAB-C3B-C2B	2.41	131.95	128.34
7	m	1303	BCL	OBB-CAB-CBB	-2.41	114.39	119.73
7	p	101	BCL	OBB-CAB-CBB	-2.41	114.39	119.73
7	d	101	BCL	CAB-C3B-C2B	2.40	131.94	128.34
7	T	101	BCL	CAB-C3B-C2B	2.40	131.94	128.34
7	K	101	BCL	C2A-C1A-CHA	2.40	128.06	123.86
7	m	1301	BCL	CHC-C4B-NB	-2.40	121.72	124.26
7	o	101	BCL	CHC-C4B-NB	-2.40	121.72	124.26
7	m	1301	BCL	C4A-NA-C1A	2.40	107.78	106.71
7	l	305	BCL	CHC-C4B-NB	-2.40	121.72	124.26
12	d	103	SPO	C2-C1-C4	-2.39	107.18	110.86
7	R	101	BCL	C1C-NC-C4C	2.39	107.78	106.71
7	U	103	BCL	C1C-NC-C4C	2.39	107.78	106.71
7	x	101	BCL	CHC-C1C-NC	-2.39	121.21	124.51
7	M	1303	BCL	OBB-CAB-CBB	-2.39	114.44	119.73
8	l	306	BPB	CMD-C2D-C3D	2.39	129.15	124.68
8	L	305	BPB	O2D-CGD-CBD	2.39	114.02	111.00
7	F	101	BCL	CMB-C2B-C1B	-2.39	121.74	125.37
7	K	101	BCL	CMB-C2B-C1B	-2.39	121.74	125.37
8	L	305	BPB	CMD-C2D-C3D	2.38	129.14	124.68
7	i	101	BCL	C4B-C3B-C2B	-2.38	104.53	108.36
12	0	102	SPO	C20-C21-C22	-2.38	118.61	123.47
7	Q	101	BCL	CMB-C2B-C1B	-2.37	121.76	125.37
7	s	103	BCL	C2A-C1A-CHA	2.37	128.00	123.86
7	s	103	BCL	CHC-C4B-NB	-2.37	121.75	124.26
8	L	302	BPB	OBB-CAB-CBB	-2.37	114.84	120.17
7	2	101	BCL	CHC-C4B-NB	-2.37	121.75	124.26
7	S	101	BCL	CHC-C4B-NB	-2.36	121.75	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	l	301	BCL	C4A-NA-C1A	2.36	107.77	106.71
10	M	1307	PC1	C3-C2-C1	-2.36	106.20	111.79
7	x	101	BCL	C2A-C1A-CHA	2.36	127.99	123.86
7	Y	201	BCL	CHC-C4B-NB	-2.36	121.76	124.26
7	c	101	BCL	CHC-C4B-NB	-2.35	121.77	124.26
7	D	101	BCL	C4B-C3B-C2B	-2.35	104.57	108.36
7	K	101	BCL	C4B-C3B-C2B	-2.35	104.58	108.36
7	K	101	BCL	OBB-CAB-CBB	-2.35	114.52	119.73
10	h	301	PC1	C3-C2-C1	-2.35	106.23	111.79
7	L	301	BCL	CMB-C2B-C1B	-2.35	121.79	125.37
12	aa	101	SPO	C1-C4-C5	-2.35	106.83	113.06
7	M	1303	BCL	C4B-C3B-C2B	-2.35	104.58	108.36
7	J	101	BCL	C1C-NC-C4C	2.35	107.76	106.71
7	w	101	BCL	CHC-C4B-NB	-2.35	121.77	124.26
12	R	102	SPO	C27-C26-C25	-2.35	115.90	123.22
7	s	101	BCL	C4B-C3B-C2B	-2.34	104.59	108.36
7	X	101	BCL	CHC-C4B-NB	-2.34	121.78	124.26
7	d	101	BCL	C1C-NC-C4C	2.34	107.76	106.71
12	S	102	SPO	C20-C21-C22	-2.34	118.67	123.47
7	I	101	BCL	C4B-C3B-C2B	-2.34	104.59	108.36
12	D	102	SPO	C20-C21-C22	-2.34	118.68	123.47
7	d	101	BCL	OBB-CAB-CBB	-2.34	114.54	119.73
7	7	101	BCL	C2D-C1D-ND	2.34	111.83	110.10
7	v	101	BCL	CHC-C4B-NB	-2.34	121.78	124.26
7	9	101	BCL	CMB-C2B-C1B	-2.34	121.81	125.37
12	T	102	SPO	C15-C16-C17	-2.34	119.86	126.42
12	G	103	SPO	C20-C21-C22	-2.33	118.69	123.47
7	c	101	BCL	C1C-NC-C4C	2.33	107.75	106.71
7	k	103	BCL	C2A-C1A-CHA	2.33	127.94	123.86
7	y	101	BCL	CHC-C4B-NB	-2.33	121.79	124.26
7	m	1303	BCL	C4B-C3B-C2B	-2.33	104.61	108.36
8	l	302	BPB	OBB-CAB-CBB	-2.33	114.92	120.17
12	0	102	SPO	C15-C16-C17	-2.33	119.87	126.42
7	Q	101	BCL	C11-C10-C8	-2.33	108.39	115.92
7	5	102	BCL	C4B-C3B-C2B	-2.33	104.62	108.36
8	l	306	BPB	O2D-CGD-CBD	2.33	113.94	111.00
7	W	101	BCL	CHC-C4B-NB	-2.33	121.80	124.26
7	5	101	BCL	CHC-C4B-NB	-2.33	121.80	124.26
7	l	301	BCL	CMB-C2B-C1B	-2.32	121.83	125.37
7	U	103	BCL	C4B-C3B-C2B	-2.32	104.62	108.36
9	M	1304	U10	C41-C39-C40	2.32	119.73	114.60
7	D	101	BCL	OBB-CAB-CBB	-2.32	114.59	119.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	u	101	BCL	CHC-C4B-NB	-2.32	121.80	124.26
10	A	103	PC1	O31-C31-C32	2.32	119.18	111.91
7	l	101	BCL	CMD-C2D-C1D	2.32	128.80	124.71
7	o	101	BCL	OBB-CAB-CBB	-2.32	114.60	119.73
7	k	101	BCL	C4B-C3B-C2B	-2.32	104.63	108.36
7	s	101	BCL	OBB-CAB-CBB	-2.31	114.60	119.73
7	ab	101	BCL	C1C-NC-C4C	2.31	107.75	106.71
12	B	102	SPO	C1-C4-C5	-2.31	106.93	113.06
7	B	101	BCL	C1C-NC-C4C	2.31	107.75	106.71
7	d	101	BCL	C4B-C3B-C2B	-2.31	104.64	108.36
7	m	1301	BCL	C11-C10-C8	-2.31	108.46	115.92
7	aa	102	BCL	C1C-NC-C4C	2.31	107.74	106.71
7	F	101	BCL	C4B-C3B-C2B	-2.31	104.65	108.36
7	f	101	BCL	CMB-C2B-C1B	-2.31	121.86	125.37
7	Q	101	BCL	C4B-C3B-C2B	-2.31	104.65	108.36
12	k	102	SPO	C29-C28-C27	-2.30	110.45	122.73
9	m	1304	U10	C41-C39-C40	2.30	119.69	114.60
7	U	101	BCL	CHC-C4B-NB	-2.30	121.82	124.26
7	D	101	BCL	C1C-NC-C4C	2.30	107.74	106.71
7	T	101	BCL	C1C-NC-C4C	2.30	107.74	106.71
12	8	101	SPO	C27-C26-C25	-2.30	116.04	123.22
12	R	102	SPO	C14-C15-C16	-2.30	116.05	123.22
7	a	101	BCL	C4B-C3B-C2B	-2.30	104.66	108.36
7	g	101	BCL	CHC-C4B-NB	-2.30	121.83	124.26
12	s	105	SPO	C15-C16-C17	-2.30	119.97	126.42
7	p	101	BCL	C2A-C1A-CHA	2.30	127.87	123.86
12	8	101	SPO	C14-C15-C16	-2.29	116.06	123.22
12	m	1305	SPO	C9-C10-C11	-2.29	116.06	123.22
7	F	101	BCL	OBB-CAB-CBB	-2.29	114.65	119.73
7	G	101	BCL	CHC-C4B-NB	-2.29	121.83	124.26
7	Z	101	BCL	C2A-C1A-CHA	2.29	127.87	123.86
7	G	101	BCL	C1C-NC-C4C	2.29	107.74	106.71
12	8	101	SPO	C2-C1-C4	-2.29	107.34	110.86
7	S	101	BCL	C4B-C3B-C2B	-2.29	104.68	108.36
7	R	101	BCL	CHC-C4B-NB	-2.29	121.83	124.26
7	r	101	BCL	CHC-C4B-NB	-2.29	121.83	124.26
7	L	301	BCL	C4B-C3B-C2B	-2.29	104.68	108.36
12	s	105	SPO	C10-C11-C12	-2.29	119.99	126.42
7	0	101	BCL	C1C-NC-C4C	2.28	107.73	106.71
12	M	1305	SPO	C9-C10-C11	-2.28	116.09	123.22
7	M	1301	BCL	C11-C10-C8	-2.28	108.54	115.92
7	l	301	BCL	C4B-C3B-C2B	-2.28	104.69	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	j	102	BCL	CHC-C4B-NB	-2.28	121.84	124.26
12	a	104	SPO	C27-C26-C25	-2.28	116.11	123.22
10	d	102	PC1	C14-N-C13	-2.28	103.12	108.97
7	d	101	BCL	C17-C16-C15	-2.28	102.78	113.24
12	3	103	SPO	C34-C33-C35	-2.28	111.44	115.27
7	l	305	BCL	OBB-CAB-CBB	-2.28	114.69	119.73
7	b	101	BCL	CHC-C4B-NB	-2.27	121.85	124.26
7	P	101	BCL	C1C-NC-C4C	2.27	107.73	106.71
12	8	101	SPO	C40-C38-C39	2.27	119.62	114.60
12	3	103	SPO	C20-C21-C22	-2.27	118.82	123.47
7	ab	101	BCL	CHC-C4B-NB	-2.27	121.85	124.26
12	s	102	SPO	C26-C25-C23	-2.27	120.04	126.42
7	O	101	BCL	C4B-C3B-C2B	-2.27	104.71	108.36
7	aa	102	BCL	CHC-C4B-NB	-2.27	121.86	124.26
7	d	101	BCL	CMB-C2B-C1B	-2.27	121.91	125.37
7	L	301	BCL	OBB-CAB-CBB	-2.27	114.71	119.73
7	9	101	BCL	C4B-C3B-C2B	-2.27	104.72	108.36
7	e	102	BCL	CHC-C4B-NB	-2.27	121.86	124.26
12	3	103	SPO	C14-C15-C16	-2.26	116.15	123.22
7	9	101	BCL	OBB-CAB-CBB	-2.26	114.72	119.73
12	aa	101	SPO	C39-C38-C37	-2.26	116.11	122.65
7	L	304	BCL	OBB-CAB-CBB	-2.26	114.72	119.73
10	A	104	PC1	C3-C2-C1	-2.26	106.44	111.79
7	M	1301	BCL	CMB-C2B-C1B	-2.26	121.93	125.37
12	0	102	SPO	C27-C26-C25	-2.26	116.17	123.22
7	B	101	BCL	CHC-C4B-NB	-2.26	121.87	124.26
7	a	101	BCL	OBB-CAB-CBB	-2.26	114.73	119.73
7	5	101	BCL	CMB-C2B-C1B	-2.26	121.93	125.37
7	l	301	BCL	OBB-CAB-CBB	-2.26	114.73	119.73
7	1	101	BCL	C4B-C3B-C2B	-2.25	104.73	108.36
7	f	101	BCL	OBB-CAB-CBB	-2.25	114.74	119.73
7	k	101	BCL	OBB-CAB-CBB	-2.25	114.74	119.73
10	A	104	PC1	C13-N-C12	2.25	119.13	109.92
7	m	1301	BCL	CMB-C2B-C1B	-2.25	121.94	125.37
7	8	102	BCL	CHC-C4B-NB	-2.25	121.88	124.26
7	j	102	BCL	C1C-NC-C4C	2.25	107.72	106.71
7	W	101	BCL	CMB-C2B-C1B	-2.25	121.94	125.37
7	x	101	BCL	CAB-C3B-C2B	2.25	131.71	128.34
7	Q	101	BCL	OBB-CAB-CBB	-2.25	114.75	119.73
7	l	305	BCL	C4B-C3B-C2B	-2.25	104.75	108.36
7	8	102	BCL	C1C-NC-C4C	2.24	107.72	106.71
7	A	101	BCL	C4B-C3B-C2B	-2.24	104.75	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	9	101	BCL	C1C-NC-C4C	2.24	107.71	106.71
7	I	101	BCL	OBB-CAB-CBB	-2.24	114.76	119.73
7	E	101	BCL	C1C-NC-C4C	2.24	107.71	106.71
7	2	101	BCL	CMB-C2B-C1B	-2.24	121.97	125.37
7	A	101	BCL	OBB-CAB-CBB	-2.23	114.78	119.73
7	y	101	BCL	CMB-C2B-C1B	-2.23	121.97	125.37
7	0	101	BCL	CHC-C4B-NB	-2.23	121.89	124.26
7	y	101	BCL	C4B-C3B-C2B	-2.23	104.77	108.36
12	aa	101	SPO	C14-C15-C16	-2.23	116.25	123.22
7	u	101	BCL	C4B-C3B-C2B	-2.23	104.77	108.36
7	5	101	BCL	C4B-C3B-C2B	-2.23	104.77	108.36
7	U	101	BCL	C4B-C3B-C2B	-2.23	104.77	108.36
7	s	103	BCL	OBB-CAB-CBB	-2.23	114.79	119.73
12	9	102	SPO	C26-C25-C23	-2.23	120.15	126.42
7	f	101	BCL	C4B-C3B-C2B	-2.23	104.77	108.36
12	r	102	SPO	C27-C26-C25	-2.23	116.26	123.22
7	g	101	BCL	C1C-NC-C4C	2.23	107.71	106.71
7	S	101	BCL	CMB-C2B-C1B	-2.23	121.98	125.37
7	O	101	BCL	OBB-CAB-CBB	-2.23	114.80	119.73
12	A	102	SPO	C26-C25-C23	-2.23	120.17	126.42
7	w	101	BCL	CMB-C2B-C1B	-2.22	121.98	125.37
7	S	101	BCL	OBB-CAB-CBB	-2.22	114.81	119.73
7	W	101	BCL	C4B-C3B-C2B	-2.22	104.79	108.36
7	e	102	BCL	C1C-NC-C4C	2.22	107.70	106.71
7	M	1301	BCL	OBB-CAB-CBB	-2.22	114.81	119.73
7	u	101	BCL	CMB-C2B-C1B	-2.22	121.99	125.37
7	w	101	BCL	C4B-C3B-C2B	-2.22	104.79	108.36
12	j	101	SPO	C20-C21-C22	-2.22	118.94	123.47
7	I	101	BCL	C1C-NC-C4C	2.22	107.70	106.71
7	P	101	BCL	CHC-C4B-NB	-2.22	121.91	124.26
7	Y	201	BCL	C4B-C3B-C2B	-2.21	104.80	108.36
7	N	102	BCL	C1C-NC-C4C	2.21	107.70	106.71
7	E	101	BCL	CHC-C4B-NB	-2.21	121.92	124.26
12	F	102	SPO	C26-C25-C23	-2.21	120.21	126.42
7	U	101	BCL	CMB-C2B-C1B	-2.21	122.01	125.37
7	k	103	BCL	C2D-C1D-ND	2.21	111.73	110.10
7	2	101	BCL	C4B-C3B-C2B	-2.21	104.81	108.36
7	F	101	BCL	O2D-CGD-O1D	-2.21	119.52	123.84
12	9	102	SPO	C40-C38-C37	-2.21	116.27	122.65
7	m	1301	BCL	OBB-CAB-CBB	-2.21	114.84	119.73
7	O	101	BCL	CMB-C2B-C1B	-2.20	122.01	125.37
7	b	101	BCL	C1C-NC-C4C	2.20	107.70	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	102	BCL	CHC-C4B-NB	-2.20	121.92	124.26
7	s	103	BCL	C4B-C3B-C2B	-2.20	104.81	108.36
12	m	1305	SPO	C20-C21-C22	-2.20	118.96	123.47
7	L	301	BCL	C4A-NA-C1A	2.20	107.70	106.71
12	D	102	SPO	C26-C25-C23	-2.20	120.23	126.42
12	S	102	SPO	C26-C25-C23	-2.20	120.24	126.42
12	3	103	SPO	C26-C25-C23	-2.20	120.24	126.42
7	Y	201	BCL	CMB-C2B-C1B	-2.20	122.02	125.37
7	T	101	BCL	CHC-C4B-NB	-2.20	121.93	124.26
12	B	102	SPO	C40-C38-C39	-2.19	109.76	114.60
10	a	103	PC1	C13-N-C12	2.19	118.89	109.92
12	O	102	SPO	C14-C15-C16	-2.19	116.37	123.22
12	K	102	SPO	C26-C25-C23	-2.19	120.26	126.42
7	L	304	BCL	C4B-C3B-C2B	-2.19	104.84	108.36
7	a	101	BCL	C1C-NC-C4C	2.19	107.69	106.71
7	p	101	BCL	CHC-C4B-NB	-2.18	121.94	124.26
7	J	101	BCL	CHC-C4B-NB	-2.18	121.94	124.26
7	m	1301	BCL	C4B-C3B-C2B	-2.18	104.85	108.36
12	M	1305	SPO	C20-C21-C22	-2.18	119.00	123.47
7	U	103	BCL	OBB-CAB-CBB	-2.18	114.90	119.73
7	s	101	BCL	C1C-NC-C4C	2.18	107.69	106.71
12	i	102	SPO	C8-C7-C6	-2.18	114.64	118.08
12	B	103	SPO	C27-C26-C25	-2.18	116.42	123.22
12	O	102	SPO	C15-C16-C17	-2.18	120.30	126.42
7	w	101	BCL	OBB-CAB-CBB	-2.18	114.91	119.73
12	I	102	SPO	C26-C25-C23	-2.17	120.31	126.42
7	o	101	BCL	C4B-C3B-C2B	-2.17	104.86	108.36
9	l	303	U10	C7-C8-C9	-2.17	123.17	126.79
7	M	1301	BCL	C4B-C3B-C2B	-2.17	104.87	108.36
7	U	101	BCL	OBB-CAB-CBB	-2.17	114.92	119.73
12	t	101	SPO	C14-C15-C16	-2.17	116.45	123.22
9	L	303	U10	C7-C8-C9	-2.17	123.18	126.79
7	7	101	BCL	C11-C10-C8	-2.17	108.92	115.92
7	c	101	BCL	OBB-CAB-CBB	-2.17	114.93	119.73
12	N	101	SPO	C26-C25-C23	-2.16	120.34	126.42
12	e	101	SPO	C20-C21-C22	-2.16	119.04	123.47
7	f	101	BCL	C1C-NC-C4C	2.16	107.68	106.71
7	5	101	BCL	OBB-CAB-CBB	-2.16	114.94	119.73
12	I	102	SPO	C39-C38-C37	-2.16	116.40	122.65
7	v	101	BCL	O2D-CGD-O1D	-2.16	119.62	123.84
7	r	101	BCL	C1C-NC-C4C	2.16	107.68	106.71
7	3	102	BCL	OBB-CAB-CBB	-2.16	114.95	119.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	Y	201	BCL	OBB-CAB-CBB	-2.16	114.95	119.73
12	G	103	SPO	C15-C16-C17	-2.16	120.36	126.42
12	R	102	SPO	C20-C21-C22	-2.15	119.06	123.47
7	u	101	BCL	OBB-CAB-CBB	-2.15	114.96	119.73
7	o	101	BCL	CMB-C2B-C1B	-2.15	122.09	125.37
7	y	101	BCL	OBB-CAB-CBB	-2.15	114.96	119.73
12	O	102	SPO	C21-C20-C19	-2.15	119.06	123.47
12	ab	102	SPO	C40-C38-C39	-2.15	109.85	114.60
7	p	101	BCL	CMB-C2B-C1B	-2.15	122.09	125.37
12	k	102	SPO	C20-C21-C22	-2.15	119.07	123.47
7	W	101	BCL	OBB-CAB-CBB	-2.15	114.97	119.73
12	3	101	SPO	C26-C25-C23	-2.15	120.38	126.42
7	5	102	BCL	CHC-C1C-NC	-2.15	121.54	124.51
7	2	101	BCL	OBB-CAB-CBB	-2.15	114.97	119.73
7	5	102	BCL	OBB-CAB-CBB	-2.14	114.98	119.73
7	U	101	BCL	O2A-C1-C2	-2.14	103.00	108.64
7	1	101	BCL	C2A-C1A-CHA	2.14	127.60	123.86
7	1	101	BCL	C1C-NC-C4C	2.14	107.67	106.71
9	l	303	U10	C35-C34-C33	-2.14	118.19	123.68
7	2	101	BCL	C1C-NC-C4C	2.13	107.67	106.71
7	p	101	BCL	C4B-C3B-C2B	-2.13	104.93	108.36
7	k	103	BCL	CAB-C3B-C2B	2.13	131.53	128.34
9	L	303	U10	O5-C5-C6	-2.13	117.82	121.55
12	k	102	SPO	C14-C15-C16	-2.13	116.58	123.22
12	d	103	SPO	C14-C15-C16	-2.13	116.58	123.22
12	8	101	SPO	C10-C11-C12	-2.12	120.45	126.42
12	i	102	SPO	C1-C4-C5	-2.12	107.44	113.06
9	l	303	U10	C56-C54-C55	2.12	119.28	114.60
7	7	101	BCL	C4B-C3B-C2B	-2.12	104.95	108.36
7	k	103	BCL	CAA-CBA-CGA	-2.12	107.07	113.25
12	q	102	SPO	C26-C25-C23	-2.11	120.48	126.42
12	Q	102	SPO	C20-C21-C22	-2.11	119.15	123.47
7	c	101	BCL	C4B-C3B-C2B	-2.11	104.97	108.36
12	o	102	SPO	C26-C25-C23	-2.11	120.50	126.42
8	l	306	BPB	OBB-CAB-CBB	-2.10	115.43	120.17
7	k	103	BCL	CAC-C3C-C4C	-2.10	107.91	112.58
7	X	101	BCL	C4B-C3B-C2B	-2.10	104.97	108.36
12	T	102	SPO	C20-C21-C22	-2.10	119.16	123.47
7	x	101	BCL	C4B-C3B-C2B	-2.10	104.98	108.36
12	R	102	SPO	C21-C20-C19	-2.10	119.17	123.47
7	Y	201	BCL	C1C-NC-C4C	2.10	107.65	106.71
7	3	102	BCL	CMB-C2B-C3B	2.10	131.59	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	101	BCL	C1C-NC-C4C	2.10	107.65	106.71
7	s	103	BCL	CMB-C2B-C1B	-2.09	122.18	125.37
7	q	101	BCL	OBB-CAB-CBB	-2.09	115.09	119.73
7	W	101	BCL	C1C-NC-C4C	2.09	107.65	106.71
7	q	101	BCL	C2D-C1D-ND	2.09	111.64	110.10
9	l	303	U10	O5-C5-C6	-2.09	117.89	121.55
10	A	104	PC1	O31-C31-C32	2.09	118.45	111.91
12	r	102	SPO	C15-C16-C17	-2.08	120.56	126.42
12	M	1305	SPO	C21-C20-C19	-2.08	119.21	123.47
12	m	1305	SPO	C21-C20-C19	-2.08	119.21	123.47
7	3	102	BCL	C2D-C1D-ND	2.08	111.64	110.10
12	e	101	SPO	C34-C33-C35	-2.08	111.77	115.27
8	L	305	BPB	OBB-CAB-CBB	-2.08	115.49	120.17
12	Q	102	SPO	C26-C25-C23	-2.08	120.58	126.42
7	O	101	BCL	C1C-NC-C4C	2.08	107.64	106.71
12	U	102	SPO	C14-C15-C16	-2.07	116.76	123.22
12	3	101	SPO	C20-C21-C22	-2.07	119.24	123.47
12	F	102	SPO	C20-C21-C22	-2.07	119.24	123.47
12	e	101	SPO	C40-C38-C39	-2.07	110.04	114.60
9	L	303	U10	C10-C9-C11	2.07	118.75	115.27
12	j	101	SPO	C26-C25-C23	-2.06	120.61	126.42
7	z	101	BCL	CAA-CBA-CGA	2.06	117.99	112.51
7	L	304	BCL	C2D-C1D-ND	2.06	111.62	110.10
12	G	103	SPO	C14-C15-C16	-2.06	116.79	123.22
9	l	303	U10	C10-C9-C11	2.06	118.73	115.27
7	8	102	BCL	C4B-C3B-C2B	-2.05	105.06	108.36
7	v	101	BCL	C4A-NA-C1A	2.05	107.63	106.71
7	v	101	BCL	C1C-NC-C4C	2.05	107.63	106.71
7	F	101	BCL	C16-C15-C13	2.05	122.55	115.92
7	z	101	BCL	CAB-C3B-C2B	2.05	131.41	128.34
12	aa	101	SPO	C10-C11-C12	-2.05	120.65	126.42
7	e	102	BCL	C4B-C3B-C2B	-2.05	105.06	108.36
7	v	101	BCL	C4B-C3B-C2B	-2.05	105.06	108.36
12	q	102	SPO	C20-C21-C22	-2.05	119.28	123.47
7	U	103	BCL	CHD-C1D-C2D	2.05	129.77	125.48
7	5	102	BCL	C2A-C1A-CHA	2.05	127.44	123.86
10	a	103	PC1	O21-C21-O22	-2.04	118.76	123.70
12	r	102	SPO	C40-C38-C39	-2.04	110.09	114.60
7	J	101	BCL	C4B-C3B-C2B	-2.04	105.07	108.36
7	U	101	BCL	C1C-NC-C4C	2.04	107.62	106.71
13	M	1306	CDL	OA8-CA7-OA9	-2.04	118.45	123.59
12	B	103	SPO	C5-C6-C7	-2.04	122.81	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	aa	102	BCL	CMB-C2B-C1B	-2.04	122.26	125.37
7	c	101	BCL	O2A-C1-C2	-2.04	103.28	108.64
12	R	102	SPO	C9-C10-C11	-2.04	116.86	123.22
9	m	1304	U10	C37-C38-C39	-2.03	120.80	127.75
7	E	101	BCL	C4B-C3B-C2B	-2.03	105.09	108.36
7	5	102	BCL	CMB-C2B-C1B	-2.03	122.27	125.37
7	P	101	BCL	C4B-C3B-C2B	-2.03	105.09	108.36
9	M	1304	U10	C37-C38-C39	-2.03	120.81	127.75
7	e	102	BCL	CMB-C2B-C1B	-2.03	122.28	125.37
7	N	102	BCL	C4B-C3B-C2B	-2.03	105.10	108.36
7	ab	101	BCL	CMB-C2B-C1B	-2.03	122.28	125.37
13	m	1306	CDL	OA8-CA7-OA9	-2.03	118.47	123.59
7	w	101	BCL	C1C-NC-C4C	2.03	107.62	106.71
7	b	101	BCL	C4B-C3B-C2B	-2.03	105.10	108.36
7	ab	101	BCL	C4B-C3B-C2B	-2.03	105.10	108.36
7	k	103	BCL	CHC-C4B-NB	-2.02	122.12	124.26
7	G	101	BCL	C4B-C3B-C2B	-2.02	105.11	108.36
7	R	101	BCL	CMB-C2B-C1B	-2.02	122.29	125.37
7	8	102	BCL	CMB-C2B-C1B	-2.02	122.29	125.37
7	J	101	BCL	CMB-C2B-C1B	-2.02	122.30	125.37
7	B	101	BCL	CMB-C2B-C1B	-2.02	122.30	125.37
7	G	101	BCL	CMB-C2B-C1B	-2.02	122.30	125.37
7	g	101	BCL	CMB-C2B-C1B	-2.02	122.30	125.37
7	E	101	BCL	CMB-C2B-C1B	-2.02	122.30	125.37
7	K	101	BCL	C1C-NC-C4C	2.02	107.61	106.71
7	p	101	BCL	C5-C3-C2	-2.02	117.04	121.12
7	0	101	BCL	CMB-C2B-C1B	-2.02	122.30	125.37
7	N	102	BCL	CMB-C2B-C1B	-2.01	122.30	125.37
7	R	101	BCL	C4B-C3B-C2B	-2.01	105.12	108.36
7	j	102	BCL	C4B-C3B-C2B	-2.01	105.12	108.36
7	L	304	BCL	C15-C13-C12	-2.01	101.54	112.13
7	0	101	BCL	C4B-C3B-C2B	-2.01	105.12	108.36
7	l	305	BCL	C15-C13-C12	-2.01	101.54	112.13
7	g	101	BCL	C4B-C3B-C2B	-2.01	105.12	108.36
7	B	101	BCL	C4B-C3B-C2B	-2.01	105.13	108.36
7	Q	101	BCL	C2D-C1D-ND	2.01	111.58	110.10
7	aa	102	BCL	C4B-C3B-C2B	-2.01	105.13	108.36
7	i	101	BCL	OBB-CAB-CBB	-2.01	115.28	119.73
12	s	105	SPO	C1-C4-C5	2.00	118.37	113.06
7	b	101	BCL	CMB-C2B-C1B	-2.00	122.32	125.37
7	T	101	BCL	C4B-C3B-C2B	-2.00	105.14	108.36
12	n	101	SPO	C40-C38-C39	-2.00	110.18	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	e	103	SPO	C1-C4-C5	-2.00	107.75	113.06
7	P	101	BCL	CMB-C2B-C1B	-2.00	122.32	125.37
7	F	101	BCL	C1C-NC-C4C	2.00	107.61	106.71

There are no chirality outliers.

All (1669) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	M	1301	BCL	C1A-C2A-CAA-CBA
7	M	1301	BCL	C2A-CAA-CBA-CGA
7	M	1301	BCL	O2A-C1-C2-C3
7	B	101	BCL	O2A-C1-C2-C3
7	E	101	BCL	O2A-C1-C2-C3
7	G	101	BCL	O2A-C1-C2-C3
7	J	101	BCL	O2A-C1-C2-C3
7	N	102	BCL	O2A-C1-C2-C3
7	P	101	BCL	O2A-C1-C2-C3
7	R	101	BCL	O2A-C1-C2-C3
7	T	101	BCL	O2A-C1-C2-C3
7	U	103	BCL	C2C-C3C-CAC-CBC
7	U	103	BCL	C4C-C3C-CAC-CBC
7	U	103	BCL	CHA-CBD-CGD-O1D
7	U	103	BCL	CHA-CBD-CGD-O2D
7	X	101	BCL	C1A-C2A-CAA-CBA
7	Z	101	BCL	CHA-CBD-CGD-O1D
7	Z	101	BCL	CHA-CBD-CGD-O2D
7	1	101	BCL	C2C-C3C-CAC-CBC
7	1	101	BCL	C4C-C3C-CAC-CBC
7	1	101	BCL	CHA-CBD-CGD-O1D
7	1	101	BCL	CHA-CBD-CGD-O2D
7	7	101	BCL	C2C-C3C-CAC-CBC
7	7	101	BCL	C4C-C3C-CAC-CBC
7	8	102	BCL	O2A-C1-C2-C3
7	0	101	BCL	O2A-C1-C2-C3
7	m	1301	BCL	C1A-C2A-CAA-CBA
7	m	1301	BCL	C2A-CAA-CBA-CGA
7	m	1301	BCL	O2A-C1-C2-C3
7	b	101	BCL	O2A-C1-C2-C3
7	e	102	BCL	O2A-C1-C2-C3
7	g	101	BCL	O2A-C1-C2-C3
7	i	101	BCL	C2C-C3C-CAC-CBC
7	i	101	BCL	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
7	j	102	BCL	O2A-C1-C2-C3
7	q	101	BCL	C2C-C3C-CAC-CBC
7	q	101	BCL	C4C-C3C-CAC-CBC
7	q	101	BCL	C11-C10-C8-C9
7	s	103	BCL	C2C-C3C-CAC-CBC
7	s	103	BCL	C4C-C3C-CAC-CBC
7	z	101	BCL	C2C-C3C-CAC-CBC
7	z	101	BCL	C4C-C3C-CAC-CBC
7	5	102	BCL	C2C-C3C-CAC-CBC
7	5	102	BCL	C4C-C3C-CAC-CBC
7	5	102	BCL	CHA-CBD-CGD-O1D
7	5	102	BCL	CHA-CBD-CGD-O2D
7	aa	102	BCL	O2A-C1-C2-C3
7	ab	101	BCL	O2A-C1-C2-C3
8	L	302	BPB	C2C-C3C-CAC-CBC
8	L	302	BPB	C4C-C3C-CAC-CBC
8	L	305	BPB	C2-C3-C5-C6
8	L	305	BPB	C4-C3-C5-C6
8	L	305	BPB	C4C-C3C-CAC-CBC
8	l	302	BPB	C2C-C3C-CAC-CBC
8	l	302	BPB	C4C-C3C-CAC-CBC
8	l	306	BPB	C2-C3-C5-C6
8	l	306	BPB	C4-C3-C5-C6
8	l	306	BPB	C4C-C3C-CAC-CBC
9	L	303	U10	C12-C13-C14-C15
9	L	303	U10	C12-C13-C14-C16
9	l	303	U10	C12-C13-C14-C15
9	l	303	U10	C12-C13-C14-C16
10	L	306	PC1	C11-O13-P-O12
10	L	306	PC1	O13-C11-C12-N
10	A	103	PC1	C1-O11-P-O14
10	A	103	PC1	C1-O11-P-O13
10	A	104	PC1	O13-C11-C12-N
10	A	104	PC1	O22-C21-O21-C2
10	A	104	PC1	C22-C21-O21-C2
10	h	302	PC1	C1-O11-P-O12
10	h	302	PC1	C1-O11-P-O14
10	h	302	PC1	C1-O11-P-O13
10	a	102	PC1	C11-O13-P-O14
10	a	102	PC1	C22-C21-O21-C2
10	a	103	PC1	C1-O11-P-O13
10	d	102	PC1	C12-C11-O13-P

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Mol	Chain	Res	Type	Atoms
12	M	1305	SPO	C5-C6-C7-C8
12	M	1305	SPO	C8-C7-C9-C10
12	M	1305	SPO	C10-C11-C12-C13
12	M	1305	SPO	C13-C12-C14-C15
12	M	1305	SPO	C18-C17-C19-C20
12	M	1305	SPO	C21-C22-C23-C24
12	M	1305	SPO	C26-C27-C28-C29
12	A	102	SPO	C1-C4-C5-C6
12	A	102	SPO	C8-C7-C9-C10
12	A	102	SPO	C13-C12-C14-C15
12	A	102	SPO	C18-C17-C19-C20
12	A	102	SPO	C17-C19-C20-C21
12	A	102	SPO	C21-C22-C23-C24
12	A	102	SPO	C25-C26-C27-C28
12	A	102	SPO	C26-C27-C28-C29
12	A	102	SPO	C28-C30-C31-C32
12	A	102	SPO	C31-C32-C33-C34
12	A	102	SPO	C31-C32-C33-C35
12	B	102	SPO	C8-C7-C9-C10
12	B	102	SPO	C10-C11-C12-C13
12	B	102	SPO	C13-C12-C14-C15
12	B	102	SPO	C18-C17-C19-C20
12	B	102	SPO	C21-C22-C23-C24
12	B	102	SPO	C26-C27-C28-C29
12	B	102	SPO	C29-C28-C30-C31
12	B	103	SPO	C5-C6-C7-C8
12	B	103	SPO	C8-C7-C9-C10
12	B	103	SPO	C13-C12-C14-C15
12	B	103	SPO	C15-C16-C17-C18
12	B	103	SPO	C18-C17-C19-C20
12	B	103	SPO	C21-C22-C23-C24
12	B	103	SPO	C22-C23-C25-C26
12	B	103	SPO	C26-C27-C28-C29
12	B	103	SPO	C27-C28-C30-C31
12	D	102	SPO	C1-C4-C5-C6
12	D	102	SPO	C8-C7-C9-C10
12	D	102	SPO	C13-C12-C14-C15
12	D	102	SPO	C18-C17-C19-C20
12	D	102	SPO	C17-C19-C20-C21
12	D	102	SPO	C21-C22-C23-C24
12	D	102	SPO	C25-C26-C27-C28
12	D	102	SPO	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
12	D	102	SPO	C28-C30-C31-C32
12	D	102	SPO	C31-C32-C33-C34
12	D	102	SPO	C31-C32-C33-C35
12	D	102	SPO	C36-C37-C38-C39
12	D	102	SPO	C36-C37-C38-C40
12	F	102	SPO	C1-C4-C5-C6
12	F	102	SPO	C8-C7-C9-C10
12	F	102	SPO	C13-C12-C14-C15
12	F	102	SPO	C18-C17-C19-C20
12	F	102	SPO	C17-C19-C20-C21
12	F	102	SPO	C20-C21-C22-C23
12	F	102	SPO	C21-C22-C23-C24
12	F	102	SPO	C25-C26-C27-C28
12	F	102	SPO	C26-C27-C28-C29
12	F	102	SPO	C28-C30-C31-C32
12	F	102	SPO	C31-C32-C33-C34
12	F	102	SPO	C31-C32-C33-C35
12	F	102	SPO	C36-C37-C38-C39
12	F	102	SPO	C36-C37-C38-C40
12	G	102	SPO	C1-C4-C5-C6
12	G	102	SPO	C5-C6-C7-C8
12	G	102	SPO	C8-C7-C9-C10
12	G	102	SPO	C10-C11-C12-C14
12	G	102	SPO	C13-C12-C14-C15
12	G	102	SPO	C16-C17-C19-C20
12	G	102	SPO	C18-C17-C19-C20
12	G	102	SPO	C21-C22-C23-C25
12	G	102	SPO	C26-C27-C28-C29
12	G	102	SPO	C31-C32-C33-C34
12	G	102	SPO	C34-C33-C35-C36
12	G	102	SPO	C33-C35-C36-C37
12	G	102	SPO	C36-C37-C38-C39
12	G	103	SPO	C5-C6-C7-C8
12	G	103	SPO	C8-C7-C9-C10
12	G	103	SPO	C10-C11-C12-C13
12	G	103	SPO	C13-C12-C14-C15
12	G	103	SPO	C12-C14-C15-C16
12	G	103	SPO	C18-C17-C19-C20
12	G	103	SPO	C21-C22-C23-C24
12	G	103	SPO	C24-C23-C25-C26
12	G	103	SPO	C26-C27-C28-C29
12	G	103	SPO	C29-C28-C30-C31

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Mol	Chain	Res	Type	Atoms
12	G	103	SPO	C31-C32-C33-C34
12	I	102	SPO	C1-C4-C5-C6
12	I	102	SPO	C8-C7-C9-C10
12	I	102	SPO	C13-C12-C14-C15
12	I	102	SPO	C18-C17-C19-C20
12	I	102	SPO	C17-C19-C20-C21
12	I	102	SPO	C20-C21-C22-C23
12	I	102	SPO	C21-C22-C23-C24
12	I	102	SPO	C25-C26-C27-C28
12	I	102	SPO	C26-C27-C28-C29
12	I	102	SPO	C28-C30-C31-C32
12	I	102	SPO	C31-C32-C33-C34
12	I	102	SPO	C31-C32-C33-C35
12	I	102	SPO	C32-C33-C35-C36
12	K	102	SPO	C1-C4-C5-C6
12	K	102	SPO	C8-C7-C9-C10
12	K	102	SPO	C13-C12-C14-C15
12	K	102	SPO	C18-C17-C19-C20
12	K	102	SPO	C17-C19-C20-C21
12	K	102	SPO	C21-C22-C23-C24
12	K	102	SPO	C25-C26-C27-C28
12	K	102	SPO	C26-C27-C28-C29
12	K	102	SPO	C28-C30-C31-C32
12	K	102	SPO	C31-C32-C33-C34
12	K	102	SPO	C31-C32-C33-C35
12	N	101	SPO	C1-C4-C5-C6
12	N	101	SPO	C8-C7-C9-C10
12	N	101	SPO	C13-C12-C14-C15
12	N	101	SPO	C18-C17-C19-C20
12	N	101	SPO	C17-C19-C20-C21
12	N	101	SPO	C21-C22-C23-C24
12	N	101	SPO	C25-C26-C27-C28
12	N	101	SPO	C26-C27-C28-C29
12	N	101	SPO	C28-C30-C31-C32
12	N	101	SPO	C31-C32-C33-C34
12	N	101	SPO	C31-C32-C33-C35
12	N	101	SPO	C36-C37-C38-C40
12	N	103	SPO	C8-C7-C9-C10
12	N	103	SPO	C10-C11-C12-C13
12	N	103	SPO	C13-C12-C14-C15
12	N	103	SPO	C15-C16-C17-C18
12	N	103	SPO	C16-C17-C19-C20

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Mol	Chain	Res	Type	Atoms
12	N	103	SPO	C21-C22-C23-C25
12	N	103	SPO	C25-C26-C27-C28
12	N	103	SPO	C26-C27-C28-C29
12	N	103	SPO	C26-C27-C28-C30
12	N	103	SPO	C31-C32-C33-C35
12	N	103	SPO	C33-C35-C36-C37
12	O	102	SPO	C8-C7-C9-C10
12	O	102	SPO	C13-C12-C14-C15
12	O	102	SPO	C15-C16-C17-C18
12	O	102	SPO	C15-C16-C17-C19
12	O	102	SPO	C18-C17-C19-C20
12	O	102	SPO	C21-C22-C23-C24
12	O	102	SPO	C26-C27-C28-C29
12	O	102	SPO	C26-C27-C28-C30
12	O	102	SPO	C27-C28-C30-C31
12	O	102	SPO	C31-C32-C33-C34
12	O	103	SPO	C5-C6-C7-C8
12	O	103	SPO	C8-C7-C9-C10
12	O	103	SPO	C10-C11-C12-C13
12	O	103	SPO	C15-C16-C17-C18
12	O	103	SPO	C15-C16-C17-C19
12	O	103	SPO	C18-C17-C19-C20
12	O	103	SPO	C21-C22-C23-C25
12	O	103	SPO	C24-C23-C25-C26
12	O	103	SPO	C26-C27-C28-C30
12	O	103	SPO	C27-C28-C30-C31
12	Q	102	SPO	C1-C4-C5-C6
12	Q	102	SPO	C8-C7-C9-C10
12	Q	102	SPO	C13-C12-C14-C15
12	Q	102	SPO	C18-C17-C19-C20
12	Q	102	SPO	C17-C19-C20-C21
12	Q	102	SPO	C21-C22-C23-C24
12	Q	102	SPO	C25-C26-C27-C28
12	Q	102	SPO	C26-C27-C28-C29
12	Q	102	SPO	C28-C30-C31-C32
12	Q	102	SPO	C31-C32-C33-C34
12	Q	102	SPO	C31-C32-C33-C35
12	Q	102	SPO	C32-C33-C35-C36
12	R	102	SPO	C5-C6-C7-C8
12	R	102	SPO	C8-C7-C9-C10
12	R	102	SPO	C13-C12-C14-C15
12	R	102	SPO	C18-C17-C19-C20

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Mol	Chain	Res	Type	Atoms
12	R	102	SPO	C21-C22-C23-C24
12	R	102	SPO	C22-C23-C25-C26
12	R	102	SPO	C26-C27-C28-C29
12	R	102	SPO	C29-C28-C30-C31
12	R	102	SPO	C34-C33-C35-C36
12	R	102	SPO	C33-C35-C36-C37
12	R	102	SPO	C36-C37-C38-C39
12	S	102	SPO	C1-C4-C5-C6
12	S	102	SPO	C8-C7-C9-C10
12	S	102	SPO	C13-C12-C14-C15
12	S	102	SPO	C18-C17-C19-C20
12	S	102	SPO	C17-C19-C20-C21
12	S	102	SPO	C20-C21-C22-C23
12	S	102	SPO	C21-C22-C23-C24
12	S	102	SPO	C25-C26-C27-C28
12	S	102	SPO	C26-C27-C28-C29
12	S	102	SPO	C28-C30-C31-C32
12	S	102	SPO	C31-C32-C33-C34
12	S	102	SPO	C31-C32-C33-C35
12	S	102	SPO	C32-C33-C35-C36
12	T	102	SPO	C8-C7-C9-C10
12	T	102	SPO	C11-C10-C9-C7
12	T	102	SPO	C10-C11-C12-C14
12	T	102	SPO	C13-C12-C14-C15
12	T	102	SPO	C15-C16-C17-C18
12	T	102	SPO	C15-C16-C17-C19
12	T	102	SPO	C18-C17-C19-C20
12	T	102	SPO	C21-C22-C23-C24
12	T	102	SPO	C22-C23-C25-C26
12	T	102	SPO	C24-C23-C25-C26
12	T	102	SPO	C26-C27-C28-C30
12	T	102	SPO	C27-C28-C30-C31
12	T	102	SPO	C31-C32-C33-C35
12	T	102	SPO	C32-C33-C35-C36
12	U	102	SPO	C8-C7-C9-C10
12	U	102	SPO	C13-C12-C14-C15
12	U	102	SPO	C15-C16-C17-C18
12	U	102	SPO	C15-C16-C17-C19
12	U	102	SPO	C18-C17-C19-C20
12	U	102	SPO	C21-C22-C23-C24
12	U	102	SPO	C22-C23-C25-C26
12	U	102	SPO	C24-C23-C25-C26

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Mol	Chain	Res	Type	Atoms
12	U	102	SPO	C26-C27-C28-C29
12	U	102	SPO	C28-C30-C31-C32
12	U	102	SPO	C31-C32-C33-C34
12	U	102	SPO	C32-C33-C35-C36
12	8	101	SPO	C8-C7-C9-C10
12	8	101	SPO	C13-C12-C14-C15
12	8	101	SPO	C18-C17-C19-C20
12	8	101	SPO	C21-C22-C23-C24
12	8	101	SPO	C24-C23-C25-C26
12	8	101	SPO	C26-C27-C28-C29
12	8	101	SPO	C31-C32-C33-C34
12	9	102	SPO	C1-C4-C5-C6
12	9	102	SPO	C8-C7-C9-C10
12	9	102	SPO	C13-C12-C14-C15
12	9	102	SPO	C18-C17-C19-C20
12	9	102	SPO	C17-C19-C20-C21
12	9	102	SPO	C21-C22-C23-C24
12	9	102	SPO	C26-C27-C28-C29
12	9	102	SPO	C28-C30-C31-C32
12	9	102	SPO	C31-C32-C33-C34
12	9	102	SPO	C31-C32-C33-C35
12	9	102	SPO	C36-C37-C38-C40
12	0	102	SPO	C8-C7-C9-C10
12	0	102	SPO	C10-C11-C12-C13
12	0	102	SPO	C13-C12-C14-C15
12	0	102	SPO	C15-C16-C17-C18
12	0	102	SPO	C18-C17-C19-C20
12	0	102	SPO	C21-C22-C23-C24
12	0	102	SPO	C26-C27-C28-C29
12	0	102	SPO	C29-C28-C30-C31
12	m	1305	SPO	C5-C6-C7-C8
12	m	1305	SPO	C8-C7-C9-C10
12	m	1305	SPO	C10-C11-C12-C13
12	m	1305	SPO	C13-C12-C14-C15
12	m	1305	SPO	C18-C17-C19-C20
12	m	1305	SPO	C21-C22-C23-C24
12	m	1305	SPO	C26-C27-C28-C29
12	a	104	SPO	C6-C7-C9-C10
12	a	104	SPO	C10-C11-C12-C13
12	a	104	SPO	C13-C12-C14-C15
12	a	104	SPO	C18-C17-C19-C20
12	a	104	SPO	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
12	a	104	SPO	C26-C27-C28-C29
12	a	104	SPO	C26-C27-C28-C30
12	d	103	SPO	C5-C6-C7-C8
12	d	103	SPO	C5-C6-C7-C9
12	d	103	SPO	C8-C7-C9-C10
12	d	103	SPO	C10-C11-C12-C13
12	d	103	SPO	C10-C11-C12-C14
12	d	103	SPO	C13-C12-C14-C15
12	d	103	SPO	C18-C17-C19-C20
12	d	103	SPO	C21-C22-C23-C24
12	d	103	SPO	C26-C27-C28-C29
12	d	103	SPO	C30-C31-C32-C33
12	d	103	SPO	C31-C32-C33-C35
12	e	101	SPO	C1-C4-C5-C6
12	e	101	SPO	C8-C7-C9-C10
12	e	101	SPO	C13-C12-C14-C15
12	e	101	SPO	C15-C16-C17-C19
12	e	101	SPO	C18-C17-C19-C20
12	e	101	SPO	C20-C21-C22-C23
12	e	101	SPO	C21-C22-C23-C24
12	e	101	SPO	C26-C27-C28-C29
12	e	101	SPO	C28-C30-C31-C32
12	e	101	SPO	C31-C32-C33-C34
12	e	101	SPO	C31-C32-C33-C35
12	e	103	SPO	C1-C4-C5-C6
12	e	103	SPO	C5-C6-C7-C8
12	e	103	SPO	C5-C6-C7-C9
12	e	103	SPO	C8-C7-C9-C10
12	e	103	SPO	C10-C11-C12-C13
12	e	103	SPO	C13-C12-C14-C15
12	e	103	SPO	C15-C16-C17-C18
12	e	103	SPO	C16-C17-C19-C20
12	e	103	SPO	C21-C22-C23-C24
12	e	103	SPO	C22-C23-C25-C26
12	e	103	SPO	C26-C27-C28-C29
12	g	102	SPO	O1-C1-C4-C5
12	g	102	SPO	C2-C1-C4-C5
12	g	102	SPO	C3-C1-C4-C5
12	g	102	SPO	C8-C7-C9-C10
12	g	102	SPO	C10-C11-C12-C13
12	g	102	SPO	C11-C12-C14-C15
12	g	102	SPO	C16-C17-C19-C20

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Mol	Chain	Res	Type	Atoms
12	g	102	SPO	C21-C22-C23-C24
12	g	102	SPO	C26-C27-C28-C29
12	i	102	SPO	C8-C7-C9-C10
12	i	102	SPO	C13-C12-C14-C15
12	i	102	SPO	C15-C16-C17-C18
12	i	102	SPO	C18-C17-C19-C20
12	i	102	SPO	C21-C22-C23-C25
12	i	102	SPO	C26-C27-C28-C29
12	j	101	SPO	C2-C1-O1-CM1
12	j	101	SPO	C1-C4-C5-C6
12	j	101	SPO	C8-C7-C9-C10
12	j	101	SPO	C13-C12-C14-C15
12	j	101	SPO	C18-C17-C19-C20
12	j	101	SPO	C17-C19-C20-C21
12	j	101	SPO	C21-C22-C23-C24
12	j	101	SPO	C25-C26-C27-C28
12	j	101	SPO	C26-C27-C28-C29
12	j	101	SPO	C28-C30-C31-C32
12	j	101	SPO	C31-C32-C33-C34
12	j	101	SPO	C31-C32-C33-C35
12	j	103	SPO	C2-C1-C4-C5
12	j	103	SPO	C3-C1-C4-C5
12	j	103	SPO	C5-C6-C7-C8
12	j	103	SPO	C8-C7-C9-C10
12	j	103	SPO	C11-C10-C9-C7
12	j	103	SPO	C10-C11-C12-C13
12	j	103	SPO	C13-C12-C14-C15
12	j	103	SPO	C16-C17-C19-C20
12	j	103	SPO	C22-C23-C25-C26
12	j	103	SPO	C24-C23-C25-C26
12	j	103	SPO	C25-C26-C27-C28
12	j	103	SPO	C26-C27-C28-C29
12	j	103	SPO	C31-C32-C33-C34
12	k	102	SPO	C5-C6-C7-C8
12	k	102	SPO	C8-C7-C9-C10
12	k	102	SPO	C10-C11-C12-C14
12	k	102	SPO	C13-C12-C14-C15
12	k	102	SPO	C15-C16-C17-C18
12	k	102	SPO	C15-C16-C17-C19
12	k	102	SPO	C18-C17-C19-C20
12	k	102	SPO	C21-C22-C23-C24
12	k	102	SPO	C22-C23-C25-C26

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Mol	Chain	Res	Type	Atoms
12	k	102	SPO	C24-C23-C25-C26
12	k	102	SPO	C26-C27-C28-C30
12	n	101	SPO	C5-C6-C7-C8
12	n	101	SPO	C5-C6-C7-C9
12	n	101	SPO	C6-C7-C9-C10
12	n	101	SPO	C8-C7-C9-C10
12	n	101	SPO	C10-C11-C12-C13
12	n	101	SPO	C11-C12-C14-C15
12	n	101	SPO	C18-C17-C19-C20
12	n	101	SPO	C21-C22-C23-C24
12	n	101	SPO	C24-C23-C25-C26
12	n	101	SPO	C26-C27-C28-C29
12	n	101	SPO	C26-C27-C28-C30
12	n	101	SPO	C31-C32-C33-C35
12	n	101	SPO	C33-C35-C36-C37
12	o	102	SPO	C1-C4-C5-C6
12	o	102	SPO	C8-C7-C9-C10
12	o	102	SPO	C13-C12-C14-C15
12	o	102	SPO	C18-C17-C19-C20
12	o	102	SPO	C17-C19-C20-C21
12	o	102	SPO	C20-C21-C22-C23
12	o	102	SPO	C21-C22-C23-C24
12	o	102	SPO	C25-C26-C27-C28
12	o	102	SPO	C26-C27-C28-C29
12	o	102	SPO	C28-C30-C31-C32
12	o	102	SPO	C31-C32-C33-C34
12	o	102	SPO	C31-C32-C33-C35
12	o	102	SPO	C32-C33-C35-C36
12	o	102	SPO	C36-C37-C38-C39
12	q	102	SPO	C1-C4-C5-C6
12	q	102	SPO	C8-C7-C9-C10
12	q	102	SPO	C13-C12-C14-C15
12	q	102	SPO	C18-C17-C19-C20
12	q	102	SPO	C17-C19-C20-C21
12	q	102	SPO	C20-C21-C22-C23
12	q	102	SPO	C21-C22-C23-C24
12	q	102	SPO	C25-C26-C27-C28
12	q	102	SPO	C26-C27-C28-C29
12	q	102	SPO	C28-C30-C31-C32
12	q	102	SPO	C31-C32-C33-C34
12	q	102	SPO	C31-C32-C33-C35
12	q	102	SPO	C32-C33-C35-C36

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Mol	Chain	Res	Type	Atoms
12	r	102	SPO	C8-C7-C9-C10
12	r	102	SPO	C10-C11-C12-C13
12	r	102	SPO	C13-C12-C14-C15
12	r	102	SPO	C18-C17-C19-C20
12	r	102	SPO	C21-C22-C23-C24
12	r	102	SPO	C22-C23-C25-C26
12	r	102	SPO	C24-C23-C25-C26
12	r	102	SPO	C26-C27-C28-C29
12	r	102	SPO	C31-C32-C33-C34
12	r	102	SPO	C34-C33-C35-C36
12	s	102	SPO	C1-C4-C5-C6
12	s	102	SPO	C8-C7-C9-C10
12	s	102	SPO	C13-C12-C14-C15
12	s	102	SPO	C18-C17-C19-C20
12	s	102	SPO	C17-C19-C20-C21
12	s	102	SPO	C20-C21-C22-C23
12	s	102	SPO	C21-C22-C23-C24
12	s	102	SPO	C25-C26-C27-C28
12	s	102	SPO	C26-C27-C28-C29
12	s	102	SPO	C28-C30-C31-C32
12	s	102	SPO	C31-C32-C33-C34
12	s	102	SPO	C31-C32-C33-C35
12	s	104	SPO	C8-C7-C9-C10
12	s	104	SPO	C10-C11-C12-C13
12	s	104	SPO	C10-C11-C12-C14
12	s	104	SPO	C13-C12-C14-C15
12	s	104	SPO	C18-C17-C19-C20
12	s	104	SPO	C21-C22-C23-C24
12	s	104	SPO	C26-C27-C28-C29
12	s	104	SPO	C26-C27-C28-C30
12	s	104	SPO	C31-C32-C33-C34
12	s	104	SPO	C36-C37-C38-C39
12	s	105	SPO	C2-C1-O1-CM1
12	s	105	SPO	C4-C1-O1-CM1
12	s	105	SPO	O1-C1-C4-C5
12	s	105	SPO	C2-C1-C4-C5
12	s	105	SPO	C3-C1-C4-C5
12	s	105	SPO	C8-C7-C9-C10
12	s	105	SPO	C10-C11-C12-C14
12	s	105	SPO	C13-C12-C14-C15
12	s	105	SPO	C18-C17-C19-C20
12	s	105	SPO	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
12	s	105	SPO	C24-C23-C25-C26
12	s	105	SPO	C26-C27-C28-C29
12	s	105	SPO	C26-C27-C28-C30
12	s	105	SPO	C31-C32-C33-C34
12	s	105	SPO	C32-C33-C35-C36
12	t	101	SPO	C5-C6-C7-C8
12	t	101	SPO	C5-C6-C7-C9
12	t	101	SPO	C8-C7-C9-C10
12	t	101	SPO	C13-C12-C14-C15
12	t	101	SPO	C18-C17-C19-C20
12	t	101	SPO	C21-C22-C23-C24
12	t	101	SPO	C26-C27-C28-C29
12	t	101	SPO	C26-C27-C28-C30
12	t	101	SPO	C27-C28-C30-C31
12	t	101	SPO	C28-C30-C31-C32
12	t	101	SPO	C31-C32-C33-C34
12	t	101	SPO	C34-C33-C35-C36
12	aa	101	SPO	C5-C6-C7-C8
12	aa	101	SPO	C8-C7-C9-C10
12	aa	101	SPO	C13-C12-C14-C15
12	aa	101	SPO	C18-C17-C19-C20
12	aa	101	SPO	C21-C22-C23-C24
12	aa	101	SPO	C26-C27-C28-C29
12	aa	101	SPO	C27-C28-C30-C31
12	3	101	SPO	C2-C1-O1-CM1
12	3	101	SPO	C1-C4-C5-C6
12	3	101	SPO	C8-C7-C9-C10
12	3	101	SPO	C13-C12-C14-C15
12	3	101	SPO	C18-C17-C19-C20
12	3	101	SPO	C17-C19-C20-C21
12	3	101	SPO	C21-C22-C23-C24
12	3	101	SPO	C25-C26-C27-C28
12	3	101	SPO	C26-C27-C28-C29
12	3	101	SPO	C28-C30-C31-C32
12	3	101	SPO	C31-C32-C33-C34
12	3	101	SPO	C31-C32-C33-C35
12	3	101	SPO	C36-C37-C38-C39
12	3	101	SPO	C36-C37-C38-C40
12	3	103	SPO	C1-C4-C5-C6
12	3	103	SPO	C8-C7-C9-C10
12	3	103	SPO	C13-C12-C14-C15
12	3	103	SPO	C18-C17-C19-C20

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Mol	Chain	Res	Type	Atoms
12	3	103	SPO	C21-C22-C23-C24
12	3	103	SPO	C25-C26-C27-C28
12	3	103	SPO	C26-C27-C28-C29
12	3	103	SPO	C28-C30-C31-C32
12	3	103	SPO	C31-C32-C33-C34
12	3	103	SPO	C31-C32-C33-C35
12	ab	102	SPO	C8-C7-C9-C10
12	ab	102	SPO	C13-C12-C14-C15
12	ab	102	SPO	C16-C17-C19-C20
12	ab	102	SPO	C21-C22-C23-C25
12	ab	102	SPO	C24-C23-C25-C26
12	ab	102	SPO	C26-C27-C28-C29
12	ab	102	SPO	C26-C27-C28-C30
12	ab	102	SPO	C31-C32-C33-C35
13	M	1306	CDL	CA2-OA2-PA1-OA3
13	M	1306	CDL	CA2-OA2-PA1-OA4
13	M	1306	CDL	OA6-CA4-CA6-OA8
13	m	1306	CDL	CA2-OA2-PA1-OA3
13	m	1306	CDL	CA2-OA2-PA1-OA4
13	m	1306	CDL	OA6-CA4-CA6-OA8
12	M	1305	SPO	C36-C37-C38-C39
12	A	102	SPO	C36-C37-C38-C39
12	A	102	SPO	C36-C37-C38-C40
12	I	102	SPO	C36-C37-C38-C39
12	K	102	SPO	C36-C37-C38-C39
12	9	102	SPO	C36-C37-C38-C39
12	m	1305	SPO	C36-C37-C38-C39
12	e	101	SPO	C36-C37-C38-C39
12	e	101	SPO	C36-C37-C38-C40
12	j	101	SPO	C36-C37-C38-C39
12	q	102	SPO	C36-C37-C38-C40
12	s	102	SPO	C36-C37-C38-C39
12	s	102	SPO	C36-C37-C38-C40
12	s	105	SPO	C36-C37-C38-C40
12	3	103	SPO	C36-C37-C38-C39
12	3	103	SPO	C36-C37-C38-C40
10	a	102	PC1	O22-C21-O21-C2
12	G	103	SPO	C36-C37-C38-C39
12	r	102	SPO	C36-C37-C38-C40
12	ab	102	SPO	C36-C37-C38-C40
7	7	101	BCL	C4-C3-C5-C6
9	l	303	U10	C40-C39-C41-C42

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Mol	Chain	Res	Type	Atoms
9	l	303	U10	C38-C39-C41-C42
12	M	1305	SPO	C32-C33-C35-C36
12	m	1305	SPO	C32-C33-C35-C36
7	r	101	BCL	C2A-CAA-CBA-CGA
12	M	1305	SPO	C31-C32-C33-C34
12	B	102	SPO	C31-C32-C33-C34
12	B	103	SPO	C31-C32-C33-C34
12	O	103	SPO	C31-C32-C33-C34
12	R	102	SPO	C31-C32-C33-C34
12	0	102	SPO	C31-C32-C33-C34
12	m	1305	SPO	C31-C32-C33-C34
12	a	104	SPO	C31-C32-C33-C34
12	g	102	SPO	C31-C32-C33-C34
12	i	102	SPO	C31-C32-C33-C34
12	aa	101	SPO	C31-C32-C33-C34
10	C	1201	PC1	C37-C38-C39-C3A
10	l	304	PC1	C37-C38-C39-C3A
12	A	102	SPO	C20-C21-C22-C23
12	D	102	SPO	C20-C21-C22-C23
12	G	103	SPO	C25-C26-C27-C28
12	K	102	SPO	C20-C21-C22-C23
12	N	101	SPO	C20-C21-C22-C23
12	Q	102	SPO	C20-C21-C22-C23
12	9	102	SPO	C20-C21-C22-C23
12	9	102	SPO	C25-C26-C27-C28
12	e	101	SPO	C17-C19-C20-C21
12	e	101	SPO	C25-C26-C27-C28
12	g	102	SPO	C25-C26-C27-C28
12	j	101	SPO	C20-C21-C22-C23
12	j	103	SPO	C20-C21-C22-C23
12	n	101	SPO	C11-C10-C9-C7
12	3	101	SPO	C20-C21-C22-C23
12	3	103	SPO	C20-C21-C22-C23
10	M	1307	PC1	C22-C21-O21-C2
10	h	301	PC1	C22-C21-O21-C2
12	N	103	SPO	C36-C37-C38-C39
12	O	103	SPO	C36-C37-C38-C40
12	0	102	SPO	C36-C37-C38-C40
12	n	101	SPO	C36-C37-C38-C40
10	a	103	PC1	C37-C38-C39-C3A
10	a	103	PC1	C35-C36-C37-C38
10	a	102	PC1	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
13	M	1306	CDL	C38-C39-C40-C41
13	m	1306	CDL	C38-C39-C40-C41
12	B	102	SPO	C36-C37-C38-C40
12	T	102	SPO	C36-C37-C38-C39
12	U	102	SPO	C36-C37-C38-C39
12	a	104	SPO	C36-C37-C38-C40
12	e	103	SPO	C31-C32-C33-C35
12	g	102	SPO	C36-C37-C38-C40
12	j	101	SPO	C36-C37-C38-C40
12	j	103	SPO	C36-C37-C38-C40
12	q	102	SPO	C36-C37-C38-C39
12	N	103	SPO	C34-C33-C35-C36
12	e	103	SPO	C29-C28-C30-C31
12	i	102	SPO	C29-C28-C30-C31
12	O	103	SPO	C32-C33-C35-C36
12	U	102	SPO	C27-C28-C30-C31
12	0	102	SPO	C32-C33-C35-C36
12	a	104	SPO	C27-C28-C30-C31
12	n	101	SPO	C27-C28-C30-C31
12	ab	102	SPO	C27-C28-C30-C31
12	ab	102	SPO	C32-C33-C35-C36
12	M	1305	SPO	C28-C30-C31-C32
12	M	1305	SPO	C33-C35-C36-C37
12	B	102	SPO	C33-C35-C36-C37
12	B	103	SPO	C28-C30-C31-C32
12	B	103	SPO	C33-C35-C36-C37
12	O	102	SPO	C28-C30-C31-C32
12	O	102	SPO	C33-C35-C36-C37
12	m	1305	SPO	C28-C30-C31-C32
12	m	1305	SPO	C33-C35-C36-C37
12	a	104	SPO	C28-C30-C31-C32
12	g	102	SPO	C33-C35-C36-C37
12	s	104	SPO	C33-C35-C36-C37
12	s	105	SPO	C28-C30-C31-C32
12	ab	102	SPO	C33-C35-C36-C37
12	G	102	SPO	C35-C36-C37-C38
12	B	103	SPO	C36-C37-C38-C39
12	O	102	SPO	C36-C37-C38-C39
12	aa	101	SPO	C36-C37-C38-C39
9	l	303	U10	C37-C38-C39-C40
10	M	1307	PC1	O22-C21-O21-C2
10	h	301	PC1	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
9	l	303	U10	C37-C38-C39-C41
10	a	102	PC1	C32-C31-O31-C3
7	l	301	BCL	C13-C15-C16-C17
10	M	1307	PC1	C32-C33-C34-C35
10	h	301	PC1	C32-C33-C34-C35
12	B	102	SPO	C12-C14-C15-C16
12	B	103	SPO	C20-C21-C22-C23
12	R	102	SPO	C17-C19-C20-C21
7	L	301	BCL	C13-C15-C16-C17
10	C	1201	PC1	O21-C2-C3-O31
10	l	304	PC1	O21-C2-C3-O31
10	a	103	PC1	O21-C2-C3-O31
10	a	102	PC1	O32-C31-O31-C3
12	O	103	SPO	C29-C28-C30-C31
7	7	101	BCL	C2-C3-C5-C6
7	L	304	BCL	C6-C7-C8-C9
7	A	101	BCL	C11-C10-C8-C9
7	D	101	BCL	C11-C10-C8-C9
7	K	101	BCL	C11-C10-C8-C9
7	O	101	BCL	C11-C10-C8-C9
7	l	305	BCL	C6-C7-C8-C9
7	a	101	BCL	C11-C10-C8-C9
7	d	101	BCL	C11-C10-C8-C9
7	d	101	BCL	C14-C13-C15-C16
7	o	101	BCL	C11-C12-C13-C14
7	q	101	BCL	C11-C12-C13-C14
7	r	101	BCL	C11-C12-C13-C14
10	A	104	PC1	C24-C25-C26-C27
12	M	1305	SPO	C15-C16-C17-C18
12	M	1305	SPO	C24-C23-C25-C26
12	A	102	SPO	C10-C11-C12-C13
12	B	102	SPO	C5-C6-C7-C8
12	B	102	SPO	C24-C23-C25-C26
12	B	103	SPO	C10-C11-C12-C13
12	D	102	SPO	C10-C11-C12-C13
12	F	102	SPO	C10-C11-C12-C13
12	G	102	SPO	C15-C16-C17-C18
12	I	102	SPO	C10-C11-C12-C13
12	K	102	SPO	C10-C11-C12-C13
12	N	101	SPO	C10-C11-C12-C13
12	N	103	SPO	C24-C23-C25-C26
12	Q	102	SPO	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
12	S	102	SPO	C10-C11-C12-C13
12	T	102	SPO	C5-C6-C7-C8
12	U	102	SPO	C5-C6-C7-C8
12	8	101	SPO	C5-C6-C7-C8
12	8	101	SPO	C10-C11-C12-C13
12	8	101	SPO	C15-C16-C17-C18
12	9	102	SPO	C10-C11-C12-C13
12	0	102	SPO	C24-C23-C25-C26
12	m	1305	SPO	C15-C16-C17-C18
12	m	1305	SPO	C24-C23-C25-C26
12	a	104	SPO	C15-C16-C17-C18
12	a	104	SPO	C24-C23-C25-C26
12	d	103	SPO	C24-C23-C25-C26
12	e	101	SPO	C10-C11-C12-C13
12	g	102	SPO	C5-C6-C7-C8
12	g	102	SPO	C15-C16-C17-C18
12	i	102	SPO	C5-C6-C7-C8
12	i	102	SPO	C10-C11-C12-C13
12	i	102	SPO	C24-C23-C25-C26
12	j	101	SPO	C10-C11-C12-C13
12	o	102	SPO	C10-C11-C12-C13
12	q	102	SPO	C10-C11-C12-C13
12	r	102	SPO	C5-C6-C7-C8
12	s	102	SPO	C10-C11-C12-C13
12	s	104	SPO	C15-C16-C17-C18
12	s	105	SPO	C5-C6-C7-C8
12	s	105	SPO	C15-C16-C17-C18
12	t	101	SPO	C10-C11-C12-C13
12	t	101	SPO	C15-C16-C17-C18
12	t	101	SPO	C24-C23-C25-C26
12	aa	101	SPO	C15-C16-C17-C18
12	aa	101	SPO	C24-C23-C25-C26
12	3	101	SPO	C10-C11-C12-C13
12	3	103	SPO	C10-C11-C12-C13
12	ab	102	SPO	C5-C6-C7-C8
12	ab	102	SPO	C15-C16-C17-C18
12	A	102	SPO	C5-C6-C7-C9
12	A	102	SPO	C15-C16-C17-C19
12	A	102	SPO	C22-C23-C25-C26
12	D	102	SPO	C5-C6-C7-C9
12	D	102	SPO	C15-C16-C17-C19
12	D	102	SPO	C22-C23-C25-C26

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Mol	Chain	Res	Type	Atoms
12	F	102	SPO	C5-C6-C7-C9
12	F	102	SPO	C15-C16-C17-C19
12	F	102	SPO	C22-C23-C25-C26
12	G	102	SPO	C5-C6-C7-C9
12	G	102	SPO	C22-C23-C25-C26
12	G	103	SPO	C5-C6-C7-C9
12	G	103	SPO	C10-C11-C12-C14
12	G	103	SPO	C15-C16-C17-C19
12	I	102	SPO	C5-C6-C7-C9
12	I	102	SPO	C15-C16-C17-C19
12	I	102	SPO	C22-C23-C25-C26
12	K	102	SPO	C5-C6-C7-C9
12	K	102	SPO	C15-C16-C17-C19
12	K	102	SPO	C22-C23-C25-C26
12	N	101	SPO	C5-C6-C7-C9
12	N	101	SPO	C15-C16-C17-C19
12	N	101	SPO	C22-C23-C25-C26
12	N	103	SPO	C5-C6-C7-C9
12	O	102	SPO	C10-C11-C12-C14
12	Q	102	SPO	C5-C6-C7-C9
12	Q	102	SPO	C15-C16-C17-C19
12	Q	102	SPO	C22-C23-C25-C26
12	R	102	SPO	C5-C6-C7-C9
12	S	102	SPO	C15-C16-C17-C19
12	S	102	SPO	C22-C23-C25-C26
12	9	102	SPO	C5-C6-C7-C9
12	9	102	SPO	C15-C16-C17-C19
12	9	102	SPO	C22-C23-C25-C26
12	e	101	SPO	C22-C23-C25-C26
12	g	102	SPO	C10-C11-C12-C14
12	j	101	SPO	C5-C6-C7-C9
12	j	101	SPO	C15-C16-C17-C19
12	j	101	SPO	C22-C23-C25-C26
12	j	103	SPO	C15-C16-C17-C19
12	o	102	SPO	C5-C6-C7-C9
12	o	102	SPO	C15-C16-C17-C19
12	o	102	SPO	C22-C23-C25-C26
12	q	102	SPO	C15-C16-C17-C19
12	q	102	SPO	C22-C23-C25-C26
12	r	102	SPO	C15-C16-C17-C19
12	s	102	SPO	C5-C6-C7-C9
12	s	102	SPO	C15-C16-C17-C19

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Mol	Chain	Res	Type	Atoms
12	s	102	SPO	C22-C23-C25-C26
12	3	101	SPO	C15-C16-C17-C19
12	3	101	SPO	C22-C23-C25-C26
12	3	103	SPO	C5-C6-C7-C9
12	3	103	SPO	C15-C16-C17-C19
12	3	103	SPO	C22-C23-C25-C26
10	h	302	PC1	C21-C22-C23-C24
10	a	102	PC1	C21-C22-C23-C24
7	F	101	BCL	C8-C10-C11-C12
7	r	101	BCL	C10-C11-C12-C13
9	M	1304	U10	C37-C38-C39-C40
9	m	1304	U10	C37-C38-C39-C40
12	B	102	SPO	C36-C37-C38-C39
12	O	102	SPO	C36-C37-C38-C40
10	C	1201	PC1	C31-C32-C33-C34
10	l	304	PC1	C31-C32-C33-C34
7	o	101	BCL	C10-C11-C12-C13
7	q	101	BCL	C15-C16-C17-C18
10	A	103	PC1	C33-C34-C35-C36
10	a	103	PC1	C11-C12-N-C15
12	j	103	SPO	C36-C37-C38-C39
7	d	101	BCL	C11-C10-C8-C7
12	M	1305	SPO	C25-C26-C27-C28
12	G	102	SPO	C12-C14-C15-C16
12	m	1305	SPO	C25-C26-C27-C28
12	i	102	SPO	C12-C14-C15-C16
12	j	103	SPO	C12-C14-C15-C16
12	s	104	SPO	C17-C19-C20-C21
12	3	103	SPO	C17-C19-C20-C21
12	ab	102	SPO	C11-C10-C9-C7
7	1	101	BCL	C2A-CAA-CBA-CGA
7	k	101	BCL	C10-C11-C12-C13
9	M	1304	U10	C34-C36-C37-C38
9	m	1304	U10	C34-C36-C37-C38
12	G	103	SPO	C33-C35-C36-C37
12	I	102	SPO	C33-C35-C36-C37
12	R	102	SPO	C28-C30-C31-C32
12	i	102	SPO	C33-C35-C36-C37
12	t	101	SPO	C33-C35-C36-C37
13	M	1306	CDL	C63-C64-C65-C66
13	m	1306	CDL	C63-C64-C65-C66
12	a	104	SPO	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
12	s	105	SPO	C36-C37-C38-C39
7	M	1301	BCL	C13-C15-C16-C17
7	m	1301	BCL	C13-C15-C16-C17
7	M	1301	BCL	C5-C6-C7-C8
7	m	1301	BCL	C5-C6-C7-C8
7	c	101	BCL	C5-C6-C7-C8
10	L	306	PC1	C11-O13-P-O11
10	L	306	PC1	C1-O11-P-O13
10	a	102	PC1	C1-O11-P-O13
13	M	1306	CDL	CA2-OA2-PA1-OA5
13	M	1306	CDL	CB2-OB2-PB2-OB5
13	m	1306	CDL	CA2-OA2-PA1-OA5
13	m	1306	CDL	CB2-OB2-PB2-OB5
10	M	1307	PC1	C21-C22-C23-C24
10	h	301	PC1	C21-C22-C23-C24
10	A	103	PC1	C2A-C2B-C2C-C2D
10	a	103	PC1	C3B-C3C-C3D-C3E
7	O	101	BCL	C15-C16-C17-C18
10	C	1201	PC1	C11-C12-N-C13
10	C	1201	PC1	C11-C12-N-C14
10	C	1201	PC1	C11-C12-N-C15
10	l	304	PC1	C11-C12-N-C13
10	l	304	PC1	C11-C12-N-C14
10	l	304	PC1	C11-C12-N-C15
12	N	103	SPO	C12-C14-C15-C16
12	O	103	SPO	C25-C26-C27-C28
12	R	102	SPO	C11-C10-C9-C7
12	g	102	SPO	C12-C14-C15-C16
12	n	101	SPO	C12-C14-C15-C16
12	r	102	SPO	C20-C21-C22-C23
12	N	103	SPO	C21-C22-C23-C24
12	O	103	SPO	C13-C12-C14-C15
12	O	103	SPO	C21-C22-C23-C24
12	e	103	SPO	C18-C17-C19-C20
12	g	102	SPO	C13-C12-C14-C15
12	g	102	SPO	C18-C17-C19-C20
12	i	102	SPO	C21-C22-C23-C24
12	j	103	SPO	C21-C22-C23-C24
10	a	102	PC1	C24-C25-C26-C27
9	M	1304	U10	C37-C38-C39-C41
9	m	1304	U10	C37-C38-C39-C41
10	h	301	PC1	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
13	M	1306	CDL	C43-C44-C45-C46
10	M	1307	PC1	C34-C35-C36-C37
13	m	1306	CDL	C43-C44-C45-C46
13	M	1306	CDL	O1-C1-CA2-OA2
13	m	1306	CDL	O1-C1-CA2-OA2
10	M	1307	PC1	C3D-C3E-C3F-C3G
12	A	102	SPO	C16-C17-C19-C20
12	D	102	SPO	C16-C17-C19-C20
12	F	102	SPO	C16-C17-C19-C20
12	G	102	SPO	C11-C12-C14-C15
12	I	102	SPO	C16-C17-C19-C20
12	K	102	SPO	C16-C17-C19-C20
12	N	101	SPO	C16-C17-C19-C20
12	N	103	SPO	C11-C12-C14-C15
12	O	103	SPO	C11-C12-C14-C15
12	Q	102	SPO	C16-C17-C19-C20
12	S	102	SPO	C16-C17-C19-C20
12	U	102	SPO	C21-C22-C23-C25
12	9	102	SPO	C16-C17-C19-C20
12	d	103	SPO	C6-C7-C9-C10
12	d	103	SPO	C11-C12-C14-C15
12	i	102	SPO	C16-C17-C19-C20
12	j	101	SPO	C16-C17-C19-C20
12	j	103	SPO	C11-C12-C14-C15
12	j	103	SPO	C21-C22-C23-C25
12	k	102	SPO	C6-C7-C9-C10
12	o	102	SPO	C16-C17-C19-C20
12	q	102	SPO	C16-C17-C19-C20
12	r	102	SPO	C16-C17-C19-C20
12	r	102	SPO	C21-C22-C23-C25
12	s	104	SPO	C21-C22-C23-C25
12	s	105	SPO	C16-C17-C19-C20
12	t	101	SPO	C6-C7-C9-C10
12	3	101	SPO	C16-C17-C19-C20
12	3	103	SPO	C16-C17-C19-C20
10	h	301	PC1	C3D-C3E-C3F-C3G
7	d	101	BCL	C10-C11-C12-C13
7	v	101	BCL	C16-C17-C18-C19
7	c	101	BCL	C11-C12-C13-C15
12	g	102	SPO	C34-C33-C35-C36
12	N	103	SPO	C27-C28-C30-C31
7	A	101	BCL	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
7	9	101	BCL	C11-C12-C13-C14
7	d	101	BCL	C6-C7-C8-C9
7	f	101	BCL	C6-C7-C8-C9
7	i	101	BCL	C6-C7-C8-C9
7	k	101	BCL	C6-C7-C8-C9
7	o	101	BCL	C6-C7-C8-C9
7	k	103	BCL	C2A-CAA-CBA-CGA
12	O	102	SPO	C5-C6-C7-C8
12	O	102	SPO	C24-C23-C25-C26
12	R	102	SPO	C10-C11-C12-C13
12	U	102	SPO	C10-C11-C12-C13
12	0	102	SPO	C5-C6-C7-C8
12	d	103	SPO	C15-C16-C17-C18
12	n	101	SPO	C15-C16-C17-C18
12	s	104	SPO	C5-C6-C7-C8
12	s	104	SPO	C24-C23-C25-C26
12	aa	101	SPO	C10-C11-C12-C13
13	M	1306	CDL	C18-C19-C20-C21
13	m	1306	CDL	C18-C19-C20-C21
12	M	1305	SPO	C10-C11-C12-C14
12	B	102	SPO	C5-C6-C7-C9
12	B	102	SPO	C15-C16-C17-C19
12	O	103	SPO	C10-C11-C12-C14
12	R	102	SPO	C15-C16-C17-C19
12	S	102	SPO	C5-C6-C7-C9
12	m	1305	SPO	C10-C11-C12-C14
12	a	104	SPO	C5-C6-C7-C9
12	e	101	SPO	C5-C6-C7-C9
12	g	102	SPO	C22-C23-C25-C26
12	q	102	SPO	C5-C6-C7-C9
12	3	101	SPO	C5-C6-C7-C9
12	ab	102	SPO	C10-C11-C12-C14
10	A	103	PC1	O22-C21-O21-C2
10	A	103	PC1	C22-C21-O21-C2
10	A	103	PC1	C21-C22-C23-C24
13	M	1306	CDL	CB5-C51-C52-C53
13	m	1306	CDL	CB5-C51-C52-C53
7	c	101	BCL	C11-C12-C13-C14
7	i	101	BCL	C8-C10-C11-C12
10	M	1307	PC1	C37-C38-C39-C3A
10	C	1201	PC1	C2D-C2E-C2F-C2G
10	l	304	PC1	C2D-C2E-C2F-C2G

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Mol	Chain	Res	Type	Atoms
10	h	301	PC1	C37-C38-C39-C3A
7	D	101	BCL	C8-C10-C11-C12
7	i	101	BCL	C5-C6-C7-C8
13	M	1306	CDL	C31-CA7-OA8-CA6
13	m	1306	CDL	C31-CA7-OA8-CA6
7	X	101	BCL	C3A-C2A-CAA-CBA
7	v	101	BCL	C3A-C2A-CAA-CBA
13	M	1306	CDL	C34-C35-C36-C37
13	m	1306	CDL	C34-C35-C36-C37
7	f	101	BCL	C8-C10-C11-C12
9	l	303	U10	C50-C49-C51-C52
9	l	303	U10	C48-C49-C51-C52
12	o	102	SPO	C27-C28-C30-C31
10	M	1307	PC1	C38-C39-C3A-C3B
10	h	301	PC1	C38-C39-C3A-C3B
12	e	103	SPO	C31-C32-C33-C34
12	K	102	SPO	C36-C37-C38-C40
7	r	101	BCL	C3-C5-C6-C7
10	l	304	PC1	C32-C31-O31-C3
7	i	101	BCL	C10-C11-C12-C13
7	p	101	BCL	C15-C16-C17-C18
10	M	1307	PC1	C2B-C2C-C2D-C2E
10	M	1307	PC1	C3A-C3B-C3C-C3D
10	h	301	PC1	C3A-C3B-C3C-C3D
12	8	101	SPO	C36-C37-C38-C40
12	g	102	SPO	C36-C37-C38-C39
7	3	102	BCL	C4-C3-C5-C6
9	L	303	U10	C15-C14-C16-C17
9	l	303	U10	C15-C14-C16-C17
7	A	101	BCL	C6-C7-C8-C10
7	O	101	BCL	C11-C10-C8-C7
7	a	101	BCL	C6-C7-C8-C10
7	d	101	BCL	C6-C7-C8-C10
7	o	101	BCL	C6-C7-C8-C10
7	q	101	BCL	C11-C12-C13-C15
7	q	101	BCL	C12-C13-C15-C16
7	r	101	BCL	C11-C10-C8-C7
7	r	101	BCL	C11-C12-C13-C15
7	3	102	BCL	C2-C3-C5-C6
8	L	302	BPB	C2-C3-C5-C6
8	l	302	BPB	C2-C3-C5-C6
12	B	102	SPO	C32-C33-C35-C36

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Mol	Chain	Res	Type	Atoms
12	9	102	SPO	C27-C28-C30-C31
12	d	103	SPO	C27-C28-C30-C31
13	M	1306	CDL	OA9-CA7-OA8-CA6
13	m	1306	CDL	OA9-CA7-OA8-CA6
12	B	102	SPO	C11-C10-C9-C7
12	G	102	SPO	C17-C19-C20-C21
12	U	102	SPO	C25-C26-C27-C28
12	d	103	SPO	C25-C26-C27-C28
7	B	101	BCL	C16-C17-C18-C19
7	E	101	BCL	C16-C17-C18-C19
7	G	101	BCL	C16-C17-C18-C19
7	J	101	BCL	C16-C17-C18-C19
7	N	102	BCL	C16-C17-C18-C19
7	P	101	BCL	C16-C17-C18-C19
7	R	101	BCL	C16-C17-C18-C19
7	T	101	BCL	C16-C17-C18-C19
7	8	102	BCL	C16-C17-C18-C19
7	0	101	BCL	C16-C17-C18-C19
7	b	101	BCL	C16-C17-C18-C19
7	e	102	BCL	C16-C17-C18-C19
7	g	101	BCL	C16-C17-C18-C19
7	j	102	BCL	C16-C17-C18-C19
7	v	101	BCL	C16-C17-C18-C20
7	aa	102	BCL	C16-C17-C18-C19
7	ab	101	BCL	C16-C17-C18-C19
10	C	1201	PC1	C32-C31-O31-C3
10	C	1201	PC1	C3B-C3C-C3D-C3E
12	o	102	SPO	C33-C35-C36-C37
10	d	102	PC1	C33-C34-C35-C36
10	a	102	PC1	C31-C32-C33-C34
10	a	102	PC1	O11-C1-C2-O21
10	h	302	PC1	O22-C21-O21-C2
13	M	1306	CDL	OB6-CB4-CB6-OB8
13	m	1306	CDL	OB6-CB4-CB6-OB8
7	o	101	BCL	C16-C17-C18-C19
7	i	101	BCL	C15-C16-C17-C18
8	L	302	BPB	C4-C3-C5-C6
8	l	302	BPB	C4-C3-C5-C6
12	A	102	SPO	C27-C28-C30-C31
12	D	102	SPO	C27-C28-C30-C31
12	F	102	SPO	C32-C33-C35-C36
12	N	101	SPO	C32-C33-C35-C36

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Mol	Chain	Res	Type	Atoms
12	R	102	SPO	C32-C33-C35-C36
12	9	102	SPO	C32-C33-C35-C36
12	j	101	SPO	C32-C33-C35-C36
7	K	101	BCL	C6-C7-C8-C9
7	r	101	BCL	C11-C10-C8-C9
7	v	101	BCL	C6-C7-C8-C9
12	B	103	SPO	C36-C37-C38-C40
12	a	104	SPO	C5-C6-C7-C8
12	r	102	SPO	C10-C11-C12-C14
7	v	101	BCL	C1A-C2A-CAA-CBA
7	5	102	BCL	C1A-C2A-CAA-CBA
7	M	1301	BCL	C16-C17-C18-C20
7	B	101	BCL	C16-C17-C18-C20
7	E	101	BCL	C16-C17-C18-C20
7	J	101	BCL	C16-C17-C18-C20
7	N	102	BCL	C16-C17-C18-C20
7	P	101	BCL	C16-C17-C18-C20
7	R	101	BCL	C16-C17-C18-C20
7	T	101	BCL	C16-C17-C18-C20
7	8	102	BCL	C16-C17-C18-C20
7	0	101	BCL	C16-C17-C18-C20
7	m	1301	BCL	C16-C17-C18-C20
7	b	101	BCL	C16-C17-C18-C20
7	e	102	BCL	C16-C17-C18-C20
7	g	101	BCL	C16-C17-C18-C20
7	j	102	BCL	C16-C17-C18-C20
7	aa	102	BCL	C16-C17-C18-C20
7	ab	101	BCL	C16-C17-C18-C20
10	a	103	PC1	C25-C26-C27-C28
10	a	103	PC1	C32-C33-C34-C35
12	M	1305	SPO	C20-C21-C22-C23
12	m	1305	SPO	C20-C21-C22-C23
12	r	102	SPO	C17-C19-C20-C21
10	A	103	PC1	C28-C29-C2A-C2B
10	M	1307	PC1	O11-C1-C2-C3
10	h	301	PC1	O11-C1-C2-C3
7	G	101	BCL	C16-C17-C18-C20
10	a	102	PC1	C22-C23-C24-C25
13	m	1306	CDL	C62-C63-C64-C65
13	M	1306	CDL	CB2-C1-CA2-OA2
13	m	1306	CDL	CB2-C1-CA2-OA2
12	j	101	SPO	C29-C28-C30-C31

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Mol	Chain	Res	Type	Atoms
12	o	102	SPO	C29-C28-C30-C31
12	S	102	SPO	C27-C28-C30-C31
12	8	101	SPO	C27-C28-C30-C31
12	3	101	SPO	C27-C28-C30-C31
13	M	1306	CDL	C62-C63-C64-C65
7	9	101	BCL	C8-C10-C11-C12
10	a	102	PC1	C23-C24-C25-C26
10	C	1201	PC1	O32-C31-O31-C3
10	l	304	PC1	O32-C31-O31-C3
10	a	103	PC1	C11-C12-N-C14
10	A	104	PC1	C1-C2-C3-O31
10	C	1201	PC1	C1-C2-C3-O31
10	l	304	PC1	C1-C2-C3-O31
10	a	103	PC1	C1-C2-C3-O31
13	M	1306	CDL	CA3-CA4-CA6-OA8
13	m	1306	CDL	CA3-CA4-CA6-OA8
7	r	101	BCL	C15-C16-C17-C18
10	A	103	PC1	C25-C26-C27-C28
10	C	1201	PC1	C27-C28-C29-C2A
10	l	304	PC1	C27-C28-C29-C2A
10	a	103	PC1	C36-C37-C38-C39
12	g	102	SPO	C28-C30-C31-C32
12	aa	101	SPO	C33-C35-C36-C37
10	h	302	PC1	C22-C21-O21-C2
7	r	101	BCL	C4-C3-C5-C6
12	A	102	SPO	C29-C28-C30-C31
12	D	102	SPO	C29-C28-C30-C31
12	K	102	SPO	C29-C28-C30-C31
12	N	101	SPO	C29-C28-C30-C31
12	O	102	SPO	C34-C33-C35-C36
12	S	102	SPO	C29-C28-C30-C31
12	9	102	SPO	C29-C28-C30-C31
12	s	102	SPO	C29-C28-C30-C31
12	3	101	SPO	C29-C28-C30-C31
12	g	102	SPO	C32-C33-C35-C36
12	j	101	SPO	C27-C28-C30-C31
10	A	104	PC1	C32-C31-O31-C3
10	L	306	PC1	C34-C35-C36-C37
10	a	103	PC1	C23-C24-C25-C26
10	a	103	PC1	C11-C12-N-C13
7	o	101	BCL	C16-C17-C18-C20
10	C	1201	PC1	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
10	l	304	PC1	C24-C25-C26-C27
12	B	103	SPO	C16-C17-C19-C20
12	9	102	SPO	C21-C22-C23-C25
12	e	101	SPO	C16-C17-C19-C20
12	j	101	SPO	C3-C1-O1-CM1
12	k	102	SPO	C2-C1-O1-CM1
12	s	102	SPO	C16-C17-C19-C20
12	s	105	SPO	C3-C1-O1-CM1
12	3	101	SPO	C3-C1-O1-CM1
10	M	1307	PC1	C39-C3A-C3B-C3C
12	M	1305	SPO	C2-C1-C4-C5
12	M	1305	SPO	C3-C1-C4-C5
12	m	1305	SPO	C2-C1-C4-C5
12	m	1305	SPO	C3-C1-C4-C5
12	n	101	SPO	C2-C1-C4-C5
12	n	101	SPO	C3-C1-C4-C5
10	h	301	PC1	C39-C3A-C3B-C3C
10	h	301	PC1	C3E-C3F-C3G-C3H
12	F	102	SPO	C29-C28-C30-C31
12	I	102	SPO	C29-C28-C30-C31
12	Q	102	SPO	C29-C28-C30-C31
12	e	101	SPO	C29-C28-C30-C31
12	q	102	SPO	C29-C28-C30-C31
12	3	103	SPO	C29-C28-C30-C31
7	A	101	BCL	C11-C10-C8-C7
7	K	101	BCL	C6-C7-C8-C10
7	K	101	BCL	C11-C10-C8-C7
7	U	101	BCL	C12-C13-C15-C16
7	a	101	BCL	C11-C10-C8-C7
7	v	101	BCL	C6-C7-C8-C10
7	v	101	BCL	C11-C10-C8-C7
7	3	102	BCL	C11-C12-C13-C15
12	M	1305	SPO	C27-C28-C30-C31
12	m	1305	SPO	C27-C28-C30-C31
12	s	104	SPO	C32-C33-C35-C36
7	v	101	BCL	C11-C10-C8-C9
7	3	102	BCL	C11-C12-C13-C14
12	A	102	SPO	C5-C6-C7-C8
12	D	102	SPO	C5-C6-C7-C8
12	F	102	SPO	C5-C6-C7-C8
12	I	102	SPO	C5-C6-C7-C8
12	K	102	SPO	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
12	N	101	SPO	C5-C6-C7-C8
12	Q	102	SPO	C5-C6-C7-C8
12	R	102	SPO	C24-C23-C25-C26
12	S	102	SPO	C5-C6-C7-C8
12	9	102	SPO	C5-C6-C7-C8
12	e	101	SPO	C5-C6-C7-C8
12	j	101	SPO	C5-C6-C7-C8
12	o	102	SPO	C5-C6-C7-C8
12	q	102	SPO	C5-C6-C7-C8
12	s	102	SPO	C5-C6-C7-C8
12	3	101	SPO	C5-C6-C7-C8
12	3	103	SPO	C5-C6-C7-C8
12	N	103	SPO	C15-C16-C17-C19
12	O	103	SPO	C22-C23-C25-C26
12	ab	102	SPO	C22-C23-C25-C26
13	M	1306	CDL	C51-CB5-OB6-CB4
13	m	1306	CDL	C51-CB5-OB6-CB4
10	C	1201	PC1	O11-C1-C2-C3
10	l	304	PC1	O11-C1-C2-C3
10	a	102	PC1	O11-C1-C2-C3
13	M	1306	CDL	C74-C75-C76-C77
7	p	101	BCL	C4-C3-C5-C6
9	L	303	U10	C12-C11-C9-C10
9	l	303	U10	C12-C11-C9-C10
12	8	101	SPO	C34-C33-C35-C36
12	A	102	SPO	C32-C33-C35-C36
12	G	102	SPO	C27-C28-C30-C31
12	e	101	SPO	C32-C33-C35-C36
12	j	103	SPO	C27-C28-C30-C31
12	aa	101	SPO	C32-C33-C35-C36
13	m	1306	CDL	C74-C75-C76-C77
7	f	101	BCL	C5-C6-C7-C8
7	M	1301	BCL	C3A-C2A-CAA-CBA
7	m	1301	BCL	C3A-C2A-CAA-CBA
7	O	101	BCL	C5-C6-C7-C8
10	C	1201	PC1	C3C-C3D-C3E-C3F
12	T	102	SPO	C12-C14-C15-C16
12	0	102	SPO	C25-C26-C27-C28
13	M	1306	CDL	C84-C85-C86-C87
13	m	1306	CDL	C84-C85-C86-C87
10	a	103	PC1	C32-C31-O31-C3
13	M	1306	CDL	CB3-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
13	m	1306	CDL	CB3-CB4-CB6-OB8
10	C	1201	PC1	C33-C34-C35-C36
10	l	304	PC1	C33-C34-C35-C36
12	ab	102	SPO	C36-C37-C38-C39
7	p	101	BCL	C2-C3-C5-C6
9	L	303	U10	C13-C14-C16-C17
9	l	303	U10	C13-C14-C16-C17
12	D	102	SPO	C32-C33-C35-C36
12	d	103	SPO	C32-C33-C35-C36
12	s	102	SPO	C32-C33-C35-C36
10	a	102	PC1	C33-C34-C35-C36
13	M	1306	CDL	C54-C55-C56-C57
13	m	1306	CDL	C54-C55-C56-C57
10	a	102	PC1	C34-C35-C36-C37
10	A	104	PC1	O32-C31-O31-C3
12	N	101	SPO	C36-C37-C38-C39
7	v	101	BCL	C2A-CAA-CBA-CGA
10	M	1307	PC1	O11-C1-C2-O21
10	h	301	PC1	O11-C1-C2-O21
13	M	1306	CDL	OA5-CA3-CA4-OA6
13	m	1306	CDL	OA5-CA3-CA4-OA6
13	m	1306	CDL	C36-C37-C38-C39
9	L	303	U10	C7-C8-C9-C10
9	l	303	U10	C7-C8-C9-C10
13	M	1306	CDL	C36-C37-C38-C39
10	a	102	PC1	C29-C2A-C2B-C2C
7	9	101	BCL	C5-C6-C7-C8
7	m	1301	BCL	C15-C16-C17-C18
7	M	1301	BCL	C16-C17-C18-C19
7	m	1301	BCL	C16-C17-C18-C19
7	M	1301	BCL	C15-C16-C17-C18
7	p	101	BCL	C10-C11-C12-C13
12	O	103	SPO	C33-C35-C36-C37
7	u	101	BCL	C2-C1-O2A-CGA
9	L	303	U10	C12-C11-C9-C8
9	l	303	U10	C12-C11-C9-C8
7	I	101	BCL	C6-C7-C8-C9
7	a	101	BCL	C6-C7-C8-C9
10	M	1307	PC1	C29-C2A-C2B-C2C
10	h	301	PC1	C3F-C3G-C3H-C3I
10	a	103	PC1	C2-C1-O11-P
8	L	305	BPB	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
8	l	306	BPB	C6-C7-C8-C9
13	m	1306	CDL	C21-C22-C23-C24
12	G	103	SPO	C36-C37-C38-C40
13	M	1306	CDL	C21-C22-C23-C24
12	M	1305	SPO	C5-C6-C7-C9
12	O	103	SPO	C5-C6-C7-C9
12	m	1305	SPO	C5-C6-C7-C9
12	i	102	SPO	C15-C16-C17-C19
12	k	102	SPO	C26-C27-C28-C29
13	M	1306	CDL	OB7-CB5-OB6-CB4
13	m	1306	CDL	OB7-CB5-OB6-CB4
10	a	103	PC1	C22-C23-C24-C25
13	M	1306	CDL	CA7-C31-C32-C33
13	m	1306	CDL	CA7-C31-C32-C33
7	d	101	BCL	C5-C6-C7-C8
7	f	101	BCL	C10-C11-C12-C13
7	I	101	BCL	C6-C7-C8-C10
7	7	101	BCL	C11-C10-C8-C7
7	f	101	BCL	C6-C7-C8-C10
7	q	101	BCL	C11-C10-C8-C7
7	r	101	BCL	C2-C3-C5-C6
12	F	102	SPO	C27-C28-C30-C31
12	Q	102	SPO	C27-C28-C30-C31
12	q	102	SPO	C27-C28-C30-C31
12	M	1305	SPO	C17-C19-C20-C21
12	B	102	SPO	C25-C26-C27-C28
12	G	103	SPO	C11-C10-C9-C7
12	8	101	SPO	C17-C19-C20-C21
12	m	1305	SPO	C17-C19-C20-C21
12	s	104	SPO	C11-C10-C9-C7
10	C	1201	PC1	C2C-C2D-C2E-C2F
10	l	304	PC1	C2C-C2D-C2E-C2F
10	h	302	PC1	C23-C24-C25-C26
7	v	101	BCL	C5-C6-C7-C8
10	a	103	PC1	C3C-C3D-C3E-C3F
7	Q	101	BCL	C5-C6-C7-C8
8	L	305	BPB	C6-C7-C8-C10
8	l	306	BPB	C6-C7-C8-C10
7	L	304	BCL	CAD-CBD-CGD-O2D
7	l	305	BCL	CAD-CBD-CGD-O2D
8	L	305	BPB	CAD-CBD-CGD-O2D
8	l	306	BPB	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
7	A	101	BCL	C5-C6-C7-C8
12	B	103	SPO	C34-C33-C35-C36
12	G	103	SPO	C34-C33-C35-C36
12	s	105	SPO	C34-C33-C35-C36
7	F	101	BCL	C5-C6-C7-C8
9	M	1304	U10	C5-C4-O4-C4M
9	m	1304	U10	C5-C4-O4-C4M
9	L	303	U10	C9-C11-C12-C13
10	C	1201	PC1	O11-C1-C2-O21
10	l	304	PC1	O11-C1-C2-O21
10	a	103	PC1	O32-C31-O31-C3
12	T	102	SPO	C36-C37-C38-C40
7	x	101	BCL	CHA-CBD-CGD-O1D
7	x	101	BCL	CHA-CBD-CGD-O2D
12	ab	102	SPO	C12-C14-C15-C16
12	M	1305	SPO	C21-C22-C23-C25
12	m	1305	SPO	C21-C22-C23-C25
12	s	104	SPO	C6-C7-C9-C10
7	a	101	BCL	C5-C6-C7-C8
7	o	101	BCL	C5-C6-C7-C8
10	A	104	PC1	C11-C12-N-C13
12	g	102	SPO	C29-C28-C30-C31
10	A	104	PC1	C35-C36-C37-C38
10	C	1201	PC1	C26-C27-C28-C29
10	l	304	PC1	C26-C27-C28-C29
12	3	103	SPO	C27-C28-C30-C31
7	O	101	BCL	C6-C7-C8-C9
7	7	101	BCL	C11-C10-C8-C9
7	c	101	BCL	C6-C7-C8-C9
7	S	101	BCL	C5-C6-C7-C8
7	o	101	BCL	C8-C10-C11-C12
7	U	103	BCL	C2A-CAA-CBA-CGA
12	G	102	SPO	C24-C23-C25-C26
12	e	101	SPO	C15-C16-C17-C18
13	M	1306	CDL	C55-C56-C57-C58
13	m	1306	CDL	C55-C56-C57-C58
12	j	103	SPO	C10-C11-C12-C14
12	s	105	SPO	C5-C6-C7-C9
7	x	101	BCL	C1A-C2A-CAA-CBA
7	I	101	BCL	C5-C6-C7-C8
12	B	103	SPO	C12-C14-C15-C16
12	O	102	SPO	C12-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
12	a	104	SPO	C11-C10-C9-C7
12	aa	101	SPO	C12-C14-C15-C16
12	I	102	SPO	C27-C28-C30-C31
12	N	101	SPO	C27-C28-C30-C31
10	L	306	PC1	C11-O13-P-O14
10	L	306	PC1	C1-O11-P-O14
10	a	102	PC1	C1-O11-P-O12
13	M	1306	CDL	CA3-OA5-PA1-OA3
13	M	1306	CDL	CB2-OB2-PB2-OB3
13	m	1306	CDL	CA3-OA5-PA1-OA3
13	m	1306	CDL	CB2-OB2-PB2-OB3
7	k	101	BCL	C16-C17-C18-C19
7	A	101	BCL	C10-C11-C12-C13
9	l	303	U10	C9-C11-C12-C13
7	p	101	BCL	C2A-CAA-CBA-CGA
10	M	1307	PC1	C3E-C3F-C3G-C3H
7	D	101	BCL	C5-C6-C7-C8
9	L	303	U10	C2-C3-O3-C3M
9	l	303	U10	C2-C3-O3-C3M
7	v	101	BCL	CAD-CBD-CGD-O1D
7	s	101	BCL	C8-C10-C11-C12
12	d	103	SPO	C1-C4-C5-C6
12	g	102	SPO	C1-C4-C5-C6
7	r	101	BCL	C5-C6-C7-C8
10	a	102	PC1	C27-C28-C29-C2A
7	L	304	BCL	C6-C7-C8-C10
7	D	101	BCL	C11-C10-C8-C7
7	l	305	BCL	C6-C7-C8-C10
7	d	101	BCL	C12-C13-C15-C16
7	3	102	BCL	C2C-C3C-CAC-CBC
12	M	1305	SPO	C12-C14-C15-C16
12	N	103	SPO	C20-C21-C22-C23
12	O	103	SPO	C17-C19-C20-C21
12	m	1305	SPO	C12-C14-C15-C16
7	v	101	BCL	C8-C10-C11-C12
7	B	101	BCL	C2A-CAA-CBA-CGA
7	E	101	BCL	C2A-CAA-CBA-CGA
7	G	101	BCL	C2A-CAA-CBA-CGA
7	J	101	BCL	C2A-CAA-CBA-CGA
7	N	102	BCL	C2A-CAA-CBA-CGA
7	P	101	BCL	C2A-CAA-CBA-CGA
7	R	101	BCL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
7	T	101	BCL	C2A-CAA-CBA-CGA
7	8	102	BCL	C2A-CAA-CBA-CGA
7	0	101	BCL	C2A-CAA-CBA-CGA
7	b	101	BCL	C2A-CAA-CBA-CGA
7	e	102	BCL	C2A-CAA-CBA-CGA
7	g	101	BCL	C2A-CAA-CBA-CGA
7	j	102	BCL	C2A-CAA-CBA-CGA
7	aa	102	BCL	C2A-CAA-CBA-CGA
7	ab	101	BCL	C2A-CAA-CBA-CGA
10	M	1307	PC1	C24-C25-C26-C27
10	M	1307	PC1	C2E-C2F-C2G-C2H
10	h	301	PC1	C24-C25-C26-C27
10	h	302	PC1	O13-C11-C12-N
10	A	104	PC1	O21-C2-C3-O31
7	q	101	BCL	C8-C10-C11-C12
7	s	101	BCL	C5-C6-C7-C8
10	A	103	PC1	O21-C21-C22-C23
12	K	102	SPO	C27-C28-C30-C31
10	M	1307	PC1	C25-C26-C27-C28
7	k	101	BCL	C5-C6-C7-C8
7	L	304	BCL	C11-C10-C8-C9
7	D	101	BCL	C6-C7-C8-C9
7	F	101	BCL	C11-C10-C8-C9
7	l	305	BCL	C11-C10-C8-C9
10	h	301	PC1	C25-C26-C27-C28
7	U	101	BCL	C13-C15-C16-C17
12	8	101	SPO	C33-C35-C36-C37
12	N	103	SPO	C23-C25-C26-C27
12	O	103	SPO	C14-C15-C16-C17
12	O	103	SPO	C23-C25-C26-C27
12	a	104	SPO	C9-C10-C11-C12
12	g	102	SPO	C14-C15-C16-C17
12	i	102	SPO	C14-C15-C16-C17
12	n	101	SPO	C9-C10-C11-C12
12	0	102	SPO	C12-C14-C15-C16
10	A	104	PC1	C3A-C3B-C3C-C3D
9	L	303	U10	C5-C4-O4-C4M
9	l	303	U10	C5-C4-O4-C4M
12	3	101	SPO	C32-C33-C35-C36
10	C	1201	PC1	C28-C29-C2A-C2B
10	l	304	PC1	C28-C29-C2A-C2B
10	A	104	PC1	C1-C2-O21-C21

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Mol	Chain	Res	Type	Atoms
13	M	1306	CDL	OA5-CA3-CA4-CA6
13	m	1306	CDL	OA5-CA3-CA4-CA6
7	L	301	BCL	C2A-CAA-CBA-CGA
7	l	301	BCL	C2A-CAA-CBA-CGA
13	m	1306	CDL	C12-C13-C14-C15
7	L	304	BCL	C2-C1-O2A-CGA
7	l	305	BCL	C2-C1-O2A-CGA
8	L	305	BPB	C2-C1-O2A-CGA
8	l	306	BPB	C2-C1-O2A-CGA
10	A	103	PC1	C2F-C2G-C2H-C2I
13	M	1306	CDL	C12-C13-C14-C15
12	d	103	SPO	C31-C32-C33-C34
10	M	1307	PC1	C2-C1-O11-P
10	h	301	PC1	C2-C1-O11-P
10	A	103	PC1	C26-C27-C28-C29
10	C	1201	PC1	C22-C23-C24-C25
10	l	304	PC1	C22-C23-C24-C25
10	A	104	PC1	C11-C12-N-C15
12	K	102	SPO	C21-C22-C23-C25
12	k	102	SPO	C3-C1-O1-CM1
12	3	103	SPO	C21-C22-C23-C25
10	M	1307	PC1	C11-O13-P-O11
10	A	104	PC1	C11-O13-P-O11
10	h	301	PC1	C11-O13-P-O11
13	M	1306	CDL	CB3-OB5-PB2-OB2
13	m	1306	CDL	CB3-OB5-PB2-OB2
12	B	103	SPO	C3-C1-C4-C5
10	h	301	PC1	C29-C2A-C2B-C2C
9	l	303	U10	C45-C44-C46-C47
7	L	304	BCL	C11-C10-C8-C7
7	D	101	BCL	C6-C7-C8-C10
7	F	101	BCL	C6-C7-C8-C10
7	O	101	BCL	C6-C7-C8-C10
7	Q	101	BCL	C6-C7-C8-C10
7	l	305	BCL	C11-C10-C8-C7
7	i	101	BCL	C6-C7-C8-C10
7	q	101	BCL	C6-C7-C8-C10
7	r	101	BCL	C6-C7-C8-C10
7	s	101	BCL	C6-C7-C8-C10
12	s	102	SPO	C27-C28-C30-C31
12	U	102	SPO	C36-C37-C38-C40
7	Q	101	BCL	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
7	i	101	BCL	C14-C13-C15-C16
7	K	101	BCL	C5-C6-C7-C8
12	d	103	SPO	C17-C19-C20-C21
7	k	101	BCL	C16-C17-C18-C20
7	3	102	BCL	C16-C17-C18-C20
12	M	1305	SPO	O1-C1-C4-C5
12	m	1305	SPO	O1-C1-C4-C5
12	s	104	SPO	C29-C28-C30-C31
12	n	101	SPO	C30-C31-C32-C33
12	e	101	SPO	C27-C28-C30-C31
7	X	101	BCL	C2A-CAA-CBA-CGA
12	N	103	SPO	C17-C19-C20-C21
12	U	102	SPO	C12-C14-C15-C16
12	e	103	SPO	C20-C21-C22-C23
12	j	103	SPO	C17-C19-C20-C21
12	k	102	SPO	C17-C19-C20-C21
12	n	101	SPO	C20-C21-C22-C23
12	n	101	SPO	C25-C26-C27-C28
12	r	102	SPO	C28-C30-C31-C32
10	a	103	PC1	C39-C3A-C3B-C3C
7	L	301	BCL	C16-C17-C18-C19
7	l	301	BCL	C16-C17-C18-C19
7	c	101	BCL	C2-C3-C5-C6
7	c	101	BCL	C8-C10-C11-C12
13	M	1306	CDL	C53-C54-C55-C56
13	m	1306	CDL	C53-C54-C55-C56
7	5	102	BCL	C3A-C2A-CAA-CBA
10	A	104	PC1	C11-C12-N-C14
12	T	102	SPO	C17-C19-C20-C21
12	8	101	SPO	C12-C14-C15-C16
7	5	102	BCL	CAA-CBA-CGA-O1A
7	c	101	BCL	C4-C3-C5-C6
10	A	103	PC1	C2E-C2F-C2G-C2H
7	M	1303	BCL	C14-C13-C15-C16
7	m	1303	BCL	C14-C13-C15-C16
12	N	103	SPO	C18-C17-C19-C20
12	j	103	SPO	C18-C17-C19-C20
12	ab	102	SPO	C18-C17-C19-C20
12	ab	102	SPO	C21-C22-C23-C24
7	L	301	BCL	C16-C17-C18-C20
7	S	101	BCL	C6-C7-C8-C10
7	l	301	BCL	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
7	v	101	BCL	O2A-C1-C2-C3
12	e	103	SPO	C24-C23-C25-C26
12	d	103	SPO	C28-C30-C31-C32
12	n	101	SPO	C22-C23-C25-C26
10	L	306	PC1	C3-C2-O21-C21
7	i	101	BCL	C4-C3-C5-C6
7	z	101	BCL	C1A-C2A-CAA-CBA
7	k	101	BCL	C6-C7-C8-C10
10	a	103	PC1	C34-C35-C36-C37
7	z	101	BCL	CAA-CBA-CGA-O1A
7	5	102	BCL	CAA-CBA-CGA-O2A
12	r	102	SPO	C29-C28-C30-C31
7	a	101	BCL	C10-C11-C12-C13
10	C	1201	PC1	O22-C21-O21-C2
10	l	304	PC1	O22-C21-O21-C2
10	M	1307	PC1	C2D-C2E-C2F-C2G
12	B	103	SPO	C6-C7-C9-C10
12	o	102	SPO	C21-C22-C23-C25
12	B	103	SPO	C25-C26-C27-C28
12	ab	102	SPO	C17-C19-C20-C21
13	m	1306	CDL	C42-C43-C44-C45
12	a	104	SPO	C1-C4-C5-C6
7	S	101	BCL	C6-C7-C8-C9
13	M	1306	CDL	C42-C43-C44-C45
9	L	303	U10	C25-C24-C26-C27
9	l	303	U10	C25-C24-C26-C27
12	a	104	SPO	C34-C33-C35-C36
7	i	101	BCL	C2-C3-C5-C6
7	F	101	BCL	C6-C7-C8-C9
7	9	101	BCL	C6-C7-C8-C9
7	s	101	BCL	C6-C7-C8-C9
7	c	101	BCL	C11-C10-C8-C9
7	z	101	BCL	CAA-CBA-CGA-O2A
7	r	101	BCL	C8-C10-C11-C12
7	3	102	BCL	C15-C16-C17-C18
12	O	103	SPO	C36-C37-C38-C39
12	G	103	SPO	C20-C21-C22-C23
12	aa	101	SPO	C17-C19-C20-C21
12	a	104	SPO	C10-C11-C12-C14
12	n	101	SPO	C10-C11-C12-C14
9	l	303	U10	C43-C44-C46-C47
12	n	101	SPO	C32-C33-C35-C36

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Mol	Chain	Res	Type	Atoms
10	C	1201	PC1	C2A-C2B-C2C-C2D
10	l	304	PC1	C2A-C2B-C2C-C2D
10	A	104	PC1	C27-C28-C29-C2A
10	h	302	PC1	C11-C12-N-C13
10	L	306	PC1	O11-C1-C2-C3
12	k	102	SPO	C4-C1-O1-CM1
7	9	101	BCL	C11-C12-C13-C15
7	o	101	BCL	C11-C12-C13-C15
12	3	103	SPO	C32-C33-C35-C36
13	m	1306	CDL	C61-C62-C63-C64
13	M	1306	CDL	C61-C62-C63-C64
12	a	104	SPO	C8-C7-C9-C10
12	n	101	SPO	C13-C12-C14-C15
7	L	301	BCL	C4-C3-C5-C6
7	l	301	BCL	C4-C3-C5-C6
7	k	103	BCL	C4-C3-C5-C6
7	q	101	BCL	C4-C3-C5-C6
7	v	101	BCL	C4-C3-C5-C6
9	L	303	U10	C30-C29-C31-C32
9	l	303	U10	C30-C29-C31-C32
7	K	101	BCL	C8-C10-C11-C12
10	a	102	PC1	C11-O13-P-O11
12	K	102	SPO	C32-C33-C35-C36
12	s	105	SPO	C27-C28-C30-C31
13	M	1306	CDL	C12-C11-CA5-OA6
7	F	101	BCL	C11-C12-C13-C14
7	9	101	BCL	C11-C10-C8-C9
7	q	101	BCL	C14-C13-C15-C16
7	r	101	BCL	C6-C7-C8-C9
7	v	101	BCL	C14-C13-C15-C16
7	x	101	BCL	C3A-C2A-CAA-CBA
7	M	1301	BCL	CAD-CBD-CGD-O2D
7	m	1301	BCL	CAD-CBD-CGD-O2D
7	3	102	BCL	C16-C17-C18-C19
12	t	101	SPO	C12-C14-C15-C16
10	d	102	PC1	C22-C23-C24-C25
13	m	1306	CDL	C12-C11-CA5-OA6
10	h	301	PC1	C27-C28-C29-C2A
10	M	1307	PC1	C27-C28-C29-C2A
12	0	102	SPO	C36-C37-C38-C39
10	h	302	PC1	O31-C31-C32-C33
7	k	103	BCL	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
8	L	302	BPB	O2A-C1-C2-C3
8	l	302	BPB	O2A-C1-C2-C3
7	r	101	BCL	CHA-CBD-CGD-O2D
12	j	103	SPO	C34-C33-C35-C36
9	L	303	U10	C28-C29-C31-C32
9	l	303	U10	C28-C29-C31-C32
10	a	103	PC1	C29-C2A-C2B-C2C
12	F	102	SPO	C21-C22-C23-C25
10	a	103	PC1	O21-C21-C22-C23
10	M	1307	PC1	O21-C2-C3-O31
10	h	301	PC1	O21-C2-C3-O31
10	h	302	PC1	C11-C12-N-C14
8	L	302	BPB	CHA-CBD-CGD-O1D
8	l	302	BPB	CHA-CBD-CGD-O1D
8	l	302	BPB	CHA-CBD-CGD-O2D
10	l	304	PC1	C2B-C2C-C2D-C2E
10	h	302	PC1	O21-C21-C22-C23
7	9	101	BCL	C6-C7-C8-C10
7	a	101	BCL	C11-C12-C13-C15
7	k	103	BCL	C2-C3-C5-C6
7	D	101	BCL	C15-C16-C17-C18
10	C	1201	PC1	C2B-C2C-C2D-C2E
8	L	302	BPB	C11-C10-C8-C9
8	l	302	BPB	C11-C10-C8-C9
9	L	303	U10	C24-C26-C27-C28
9	l	303	U10	C24-C26-C27-C28
12	N	103	SPO	C28-C30-C31-C32
12	k	102	SPO	C12-C14-C15-C16
10	a	103	PC1	C3E-C3F-C3G-C3H
10	C	1201	PC1	C22-C21-O21-C2
10	l	304	PC1	C22-C21-O21-C2
7	z	101	BCL	C2A-CAA-CBA-CGA
12	N	101	SPO	C35-C36-C37-C38
10	L	306	PC1	C38-C39-C3A-C3B
13	m	1306	CDL	C39-C40-C41-C42
13	M	1306	CDL	C39-C40-C41-C42
13	m	1306	CDL	C12-C11-CA5-OA7
7	l	101	BCL	C1A-C2A-CAA-CBA
7	p	101	BCL	C1A-C2A-CAA-CBA
7	s	103	BCL	C1A-C2A-CAA-CBA
10	h	302	PC1	O32-C31-C32-C33
13	M	1306	CDL	C12-C11-CA5-OA7

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Mol	Chain	Res	Type	Atoms
12	8	101	SPO	C36-C37-C38-C39
10	M	1307	PC1	O21-C21-C22-C23
10	h	301	PC1	O21-C21-C22-C23
10	M	1307	PC1	C11-O13-P-O14
10	h	301	PC1	C11-O13-P-O14
10	a	103	PC1	C11-O13-P-O14
10	h	302	PC1	O22-C21-C22-C23
10	d	102	PC1	O11-C1-C2-C3
10	a	103	PC1	C38-C39-C3A-C3B
9	M	1304	U10	C35-C34-C36-C37
12	R	102	SPO	C25-C26-C27-C28
13	m	1306	CDL	C32-C33-C34-C35
9	L	303	U10	C23-C24-C26-C27
9	l	303	U10	C23-C24-C26-C27
7	k	103	BCL	CAD-CBD-CGD-O1D
13	M	1306	CDL	C32-C33-C34-C35
7	M	1301	BCL	C10-C11-C12-C13
13	M	1306	CDL	C33-C34-C35-C36
13	m	1306	CDL	C33-C34-C35-C36
7	m	1301	BCL	C10-C11-C12-C13
10	d	102	PC1	C29-C2A-C2B-C2C
9	m	1304	U10	C35-C34-C36-C37
12	K	102	SPO	C34-C33-C35-C36
12	i	102	SPO	C34-C33-C35-C36
13	M	1306	CDL	C23-C24-C25-C26
7	c	101	BCL	C11-C10-C8-C7
8	L	302	BPB	C11-C10-C8-C7
8	l	302	BPB	C11-C10-C8-C7
10	L	306	PC1	O11-C1-C2-O21
10	a	103	PC1	O22-C21-C22-C23
13	m	1306	CDL	C23-C24-C25-C26
13	M	1306	CDL	C44-C45-C46-C47
12	B	103	SPO	C5-C6-C7-C9
13	m	1306	CDL	C44-C45-C46-C47
9	L	303	U10	C3-C4-O4-C4M
9	l	303	U10	C3-C4-O4-C4M
12	8	101	SPO	C28-C30-C31-C32
12	e	103	SPO	C28-C30-C31-C32
7	M	1303	BCL	C16-C17-C18-C19

There are no ring outliers.

125 monomers are involved in 528 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	i	101	BCL	2	0
7	c	101	BCL	10	0
8	l	302	BPB	3	0
12	n	101	SPO	2	0
7	5	101	BCL	2	0
7	u	101	BCL	5	0
7	j	102	BCL	2	0
10	L	306	PC1	6	0
12	U	102	SPO	4	0
7	K	101	BCL	8	0
7	8	102	BCL	2	0
12	B	102	SPO	2	0
9	L	303	U10	6	0
12	Q	102	SPO	9	0
7	Z	101	BCL	2	0
7	J	101	BCL	5	0
12	s	102	SPO	10	0
7	N	102	BCL	5	0
10	C	1201	PC1	8	0
12	A	102	SPO	6	0
12	M	1305	SPO	3	0
12	K	102	SPO	5	0
7	R	101	BCL	2	0
12	s	105	SPO	7	0
8	L	305	BPB	3	0
7	T	101	BCL	2	0
10	d	102	PC1	6	0
12	e	101	SPO	9	0
7	x	101	BCL	2	0
12	g	102	SPO	5	0
12	k	102	SPO	5	0
12	a	104	SPO	2	0
7	o	101	BCL	2	0
7	Q	101	BCL	5	0
7	5	102	BCL	3	0
13	m	1306	CDL	4	0
7	a	101	BCL	7	0
7	9	101	BCL	6	0
7	D	101	BCL	7	0
7	l	305	BCL	2	0
12	O	103	SPO	3	0
12	s	104	SPO	1	0
12	0	102	SPO	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	aa	102	BCL	2	0
12	q	102	SPO	6	0
10	A	104	PC1	7	0
7	y	101	BCL	3	0
12	8	101	SPO	5	0
10	h	302	PC1	9	0
12	d	103	SPO	15	0
12	aa	101	SPO	7	0
7	F	101	BCL	9	0
8	l	306	BPB	3	0
12	e	103	SPO	9	0
12	i	102	SPO	4	0
12	G	103	SPO	1	0
13	M	1306	CDL	4	0
7	U	101	BCL	5	0
10	A	103	PC1	5	0
7	7	101	BCL	2	0
12	I	102	SPO	11	0
7	M	1301	BCL	3	0
9	M	1304	U10	1	0
7	p	101	BCL	6	0
10	h	301	PC1	13	0
12	t	101	SPO	6	0
7	S	101	BCL	5	0
7	P	101	BCL	2	0
7	d	101	BCL	5	0
7	s	101	BCL	4	0
7	r	101	BCL	7	0
7	2	101	BCL	6	0
12	N	101	SPO	12	0
7	A	101	BCL	7	0
12	m	1305	SPO	3	0
12	G	102	SPO	10	0
12	j	101	SPO	12	0
7	q	101	BCL	7	0
7	3	102	BCL	4	0
7	B	101	BCL	3	0
12	ab	102	SPO	4	0
7	m	1303	BCL	1	0
7	w	101	BCL	1	0
10	M	1307	PC1	12	0
12	3	101	SPO	4	0

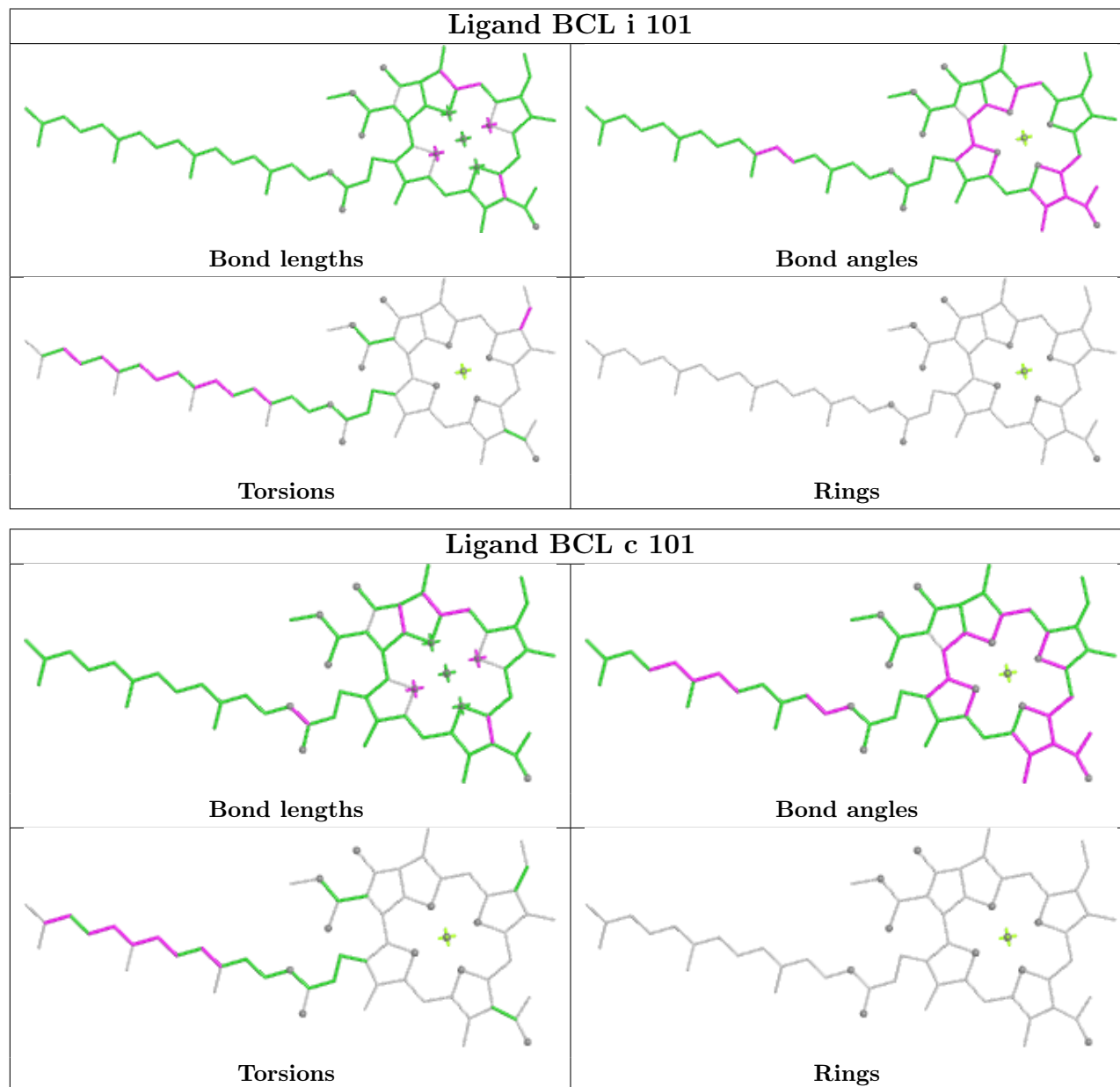
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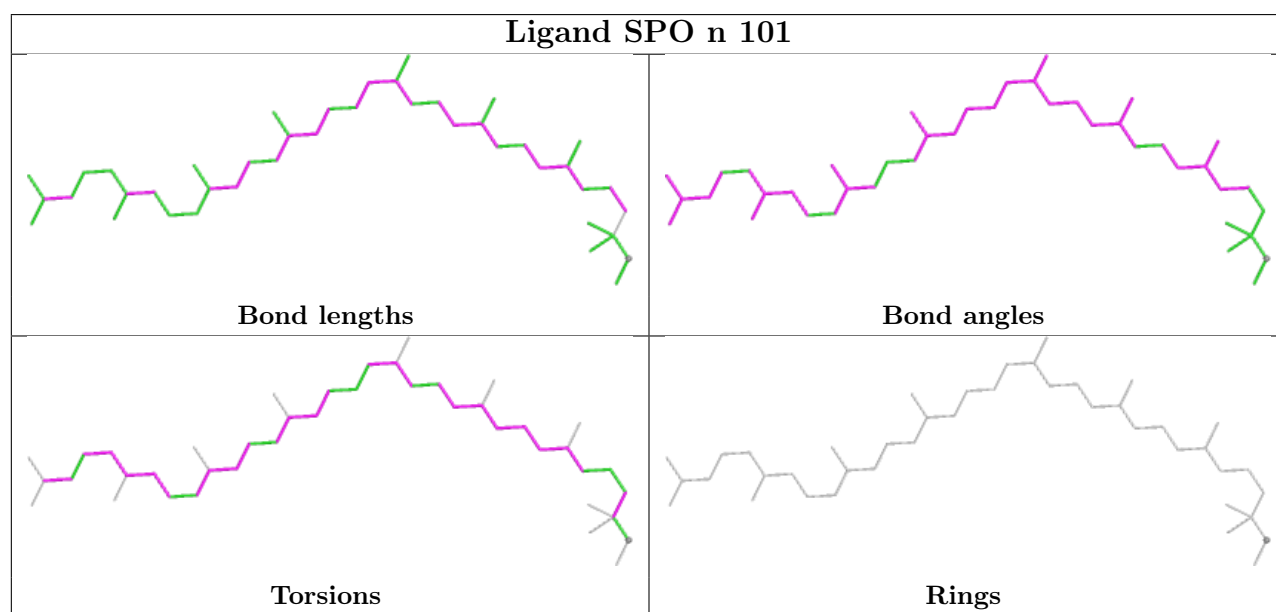
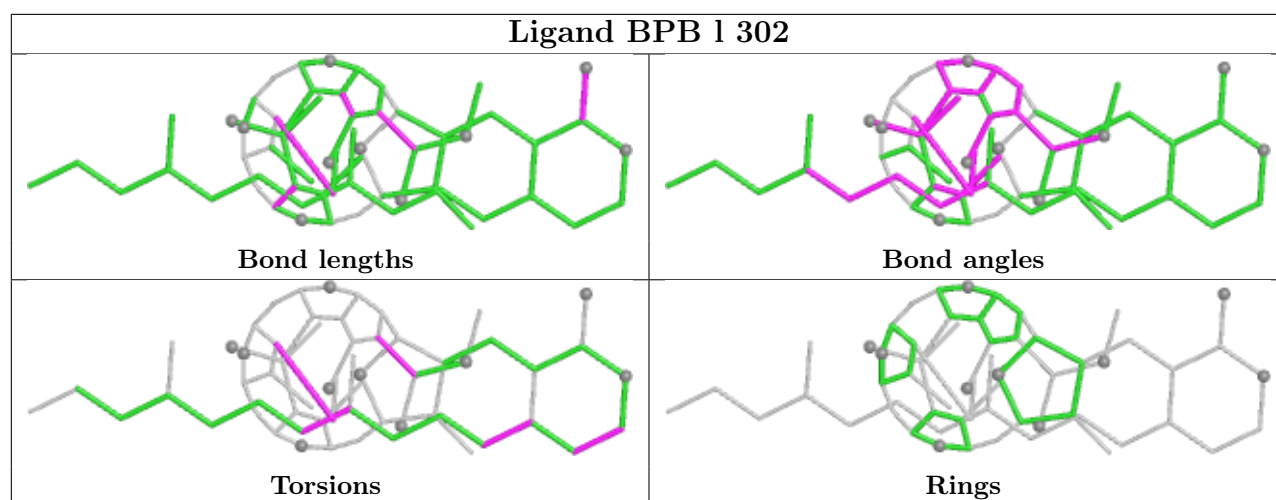
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	F	102	SPO	6	0
12	9	102	SPO	9	0
7	1	101	BCL	7	0
7	L	304	BCL	2	0
7	m	1301	BCL	4	0
8	L	302	BPB	4	0
7	ab	101	BCL	2	0
7	U	103	BCL	2	0
7	W	101	BCL	3	0
7	e	102	BCL	4	0
7	G	101	BCL	3	0
12	S	102	SPO	5	0
12	T	102	SPO	3	0
7	k	101	BCL	5	0
9	l	303	U10	5	0
12	D	102	SPO	4	0
10	a	103	PC1	12	0
12	r	102	SPO	3	0
10	l	304	PC1	5	0
7	Y	201	BCL	2	0
7	E	101	BCL	5	0
7	0	101	BCL	3	0
12	B	103	SPO	4	0
12	3	103	SPO	6	0
7	s	103	BCL	2	0
12	o	102	SPO	5	0
7	z	101	BCL	6	0
7	k	103	BCL	2	0
7	M	1303	BCL	1	0
7	v	101	BCL	2	0
7	O	101	BCL	3	0
7	I	101	BCL	2	0
7	f	101	BCL	2	0
12	N	103	SPO	4	0
10	a	102	PC1	10	0
12	R	102	SPO	3	0
7	b	101	BCL	1	0
12	O	102	SPO	2	0
12	j	103	SPO	6	0
7	g	101	BCL	4	0

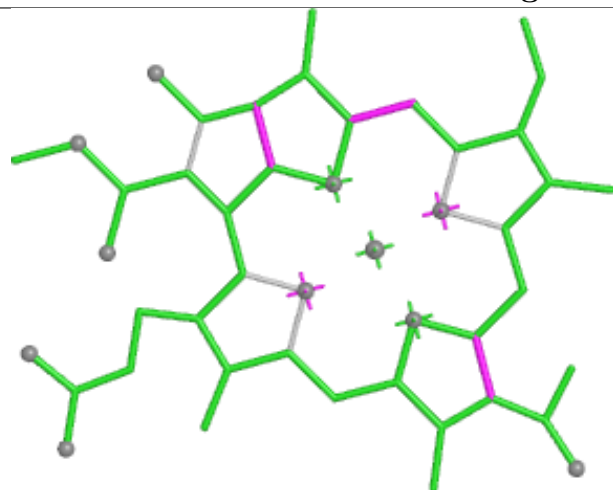
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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

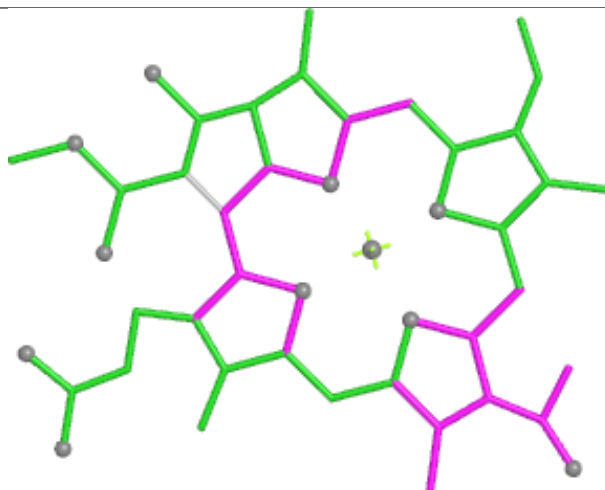




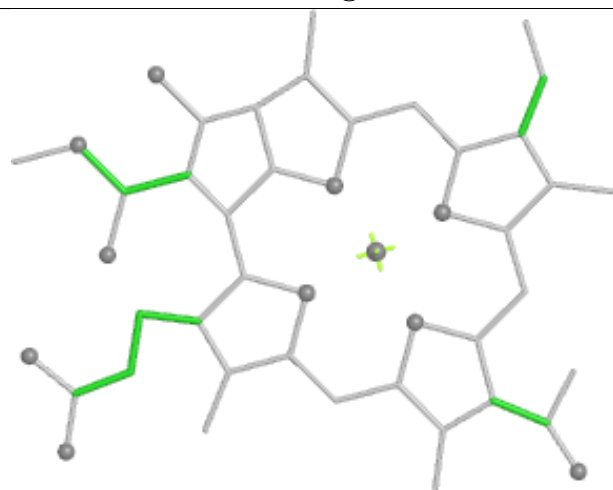
Ligand BCL 5 101



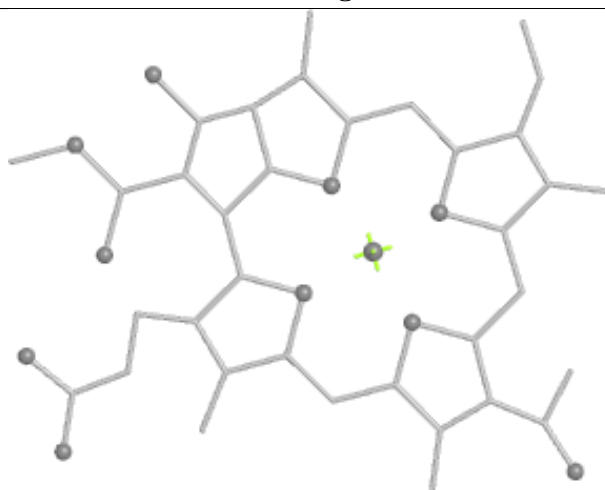
Bond lengths



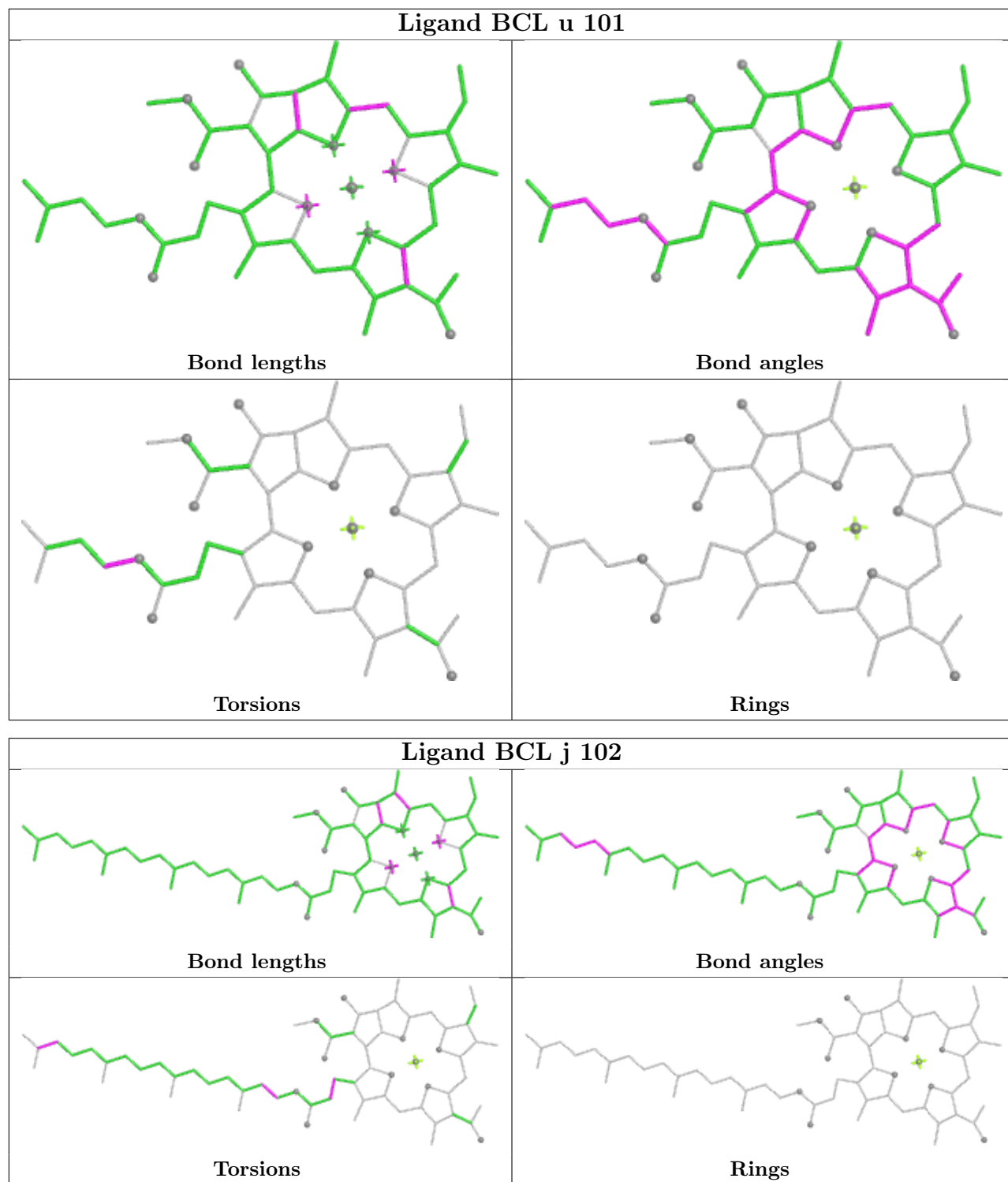
Bond angles

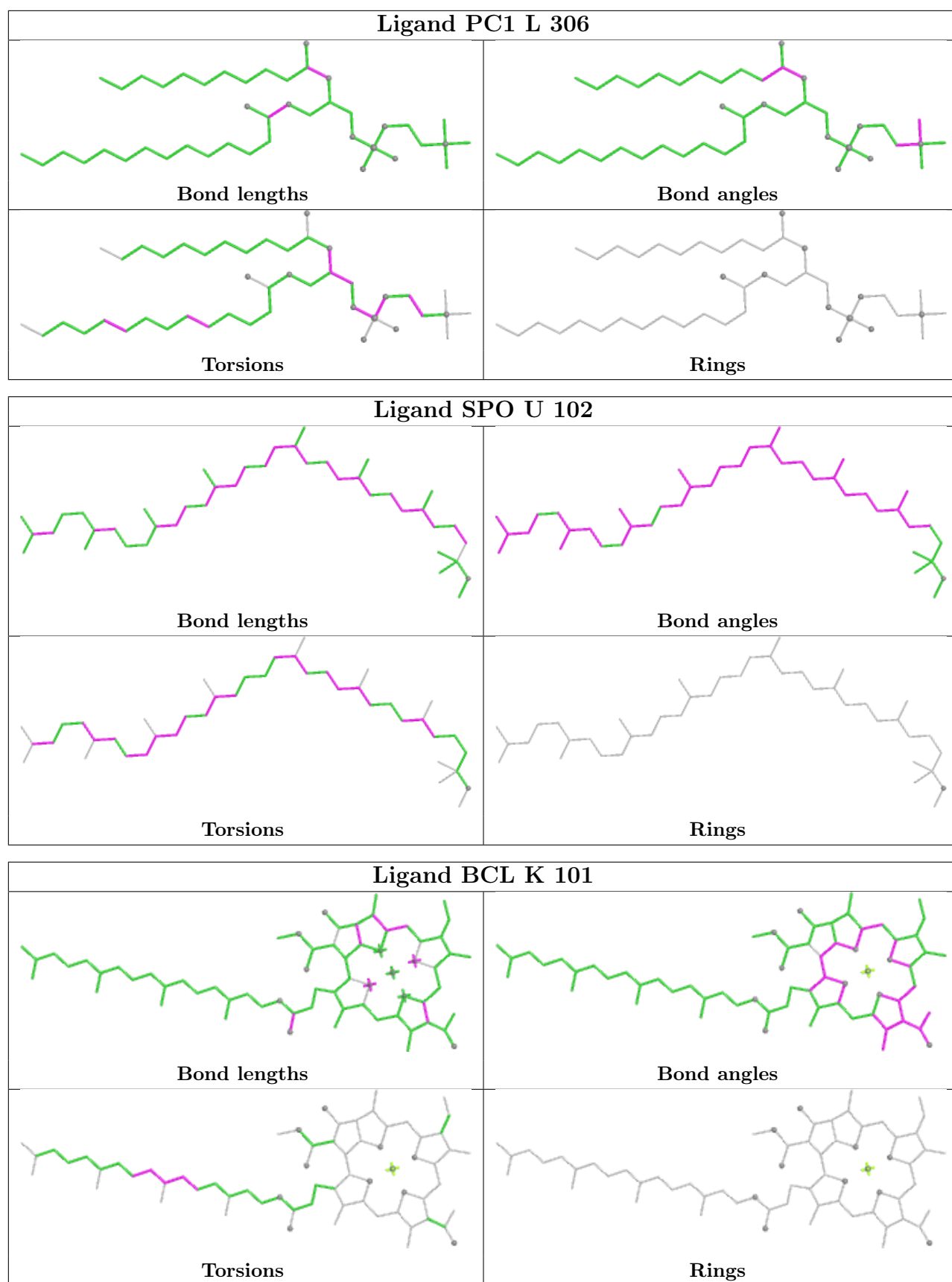


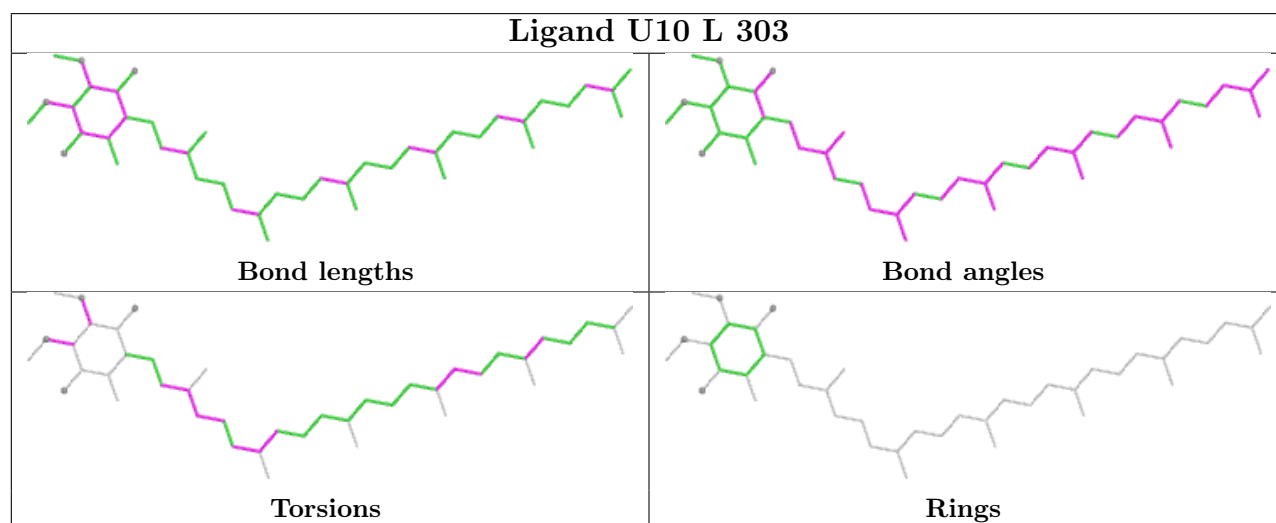
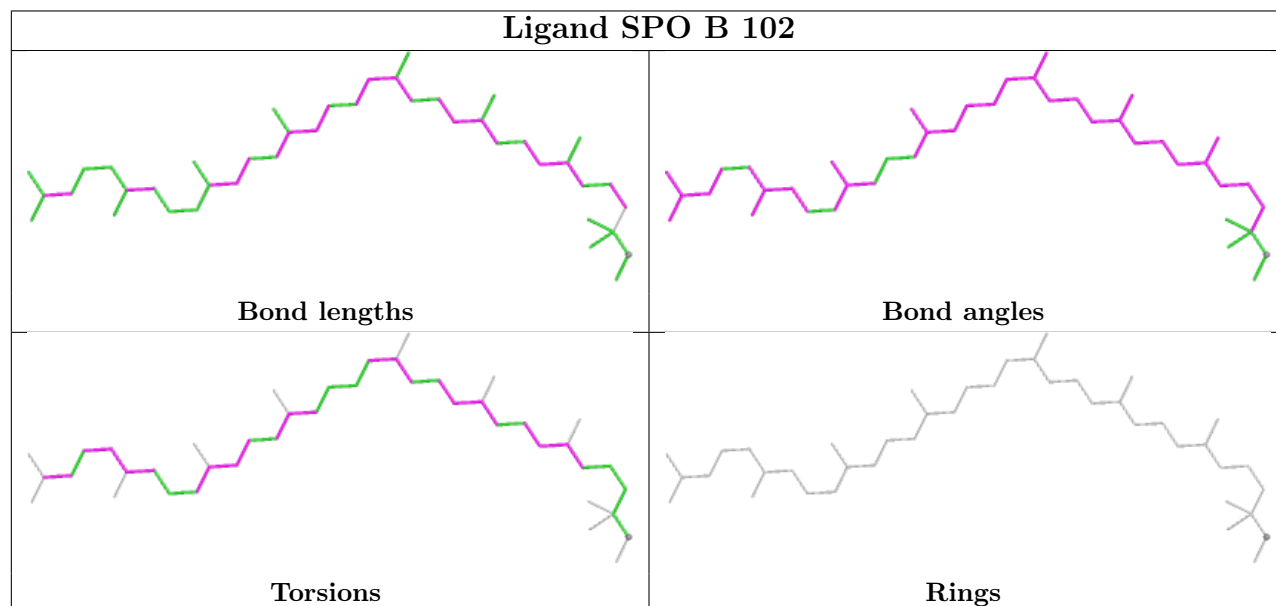
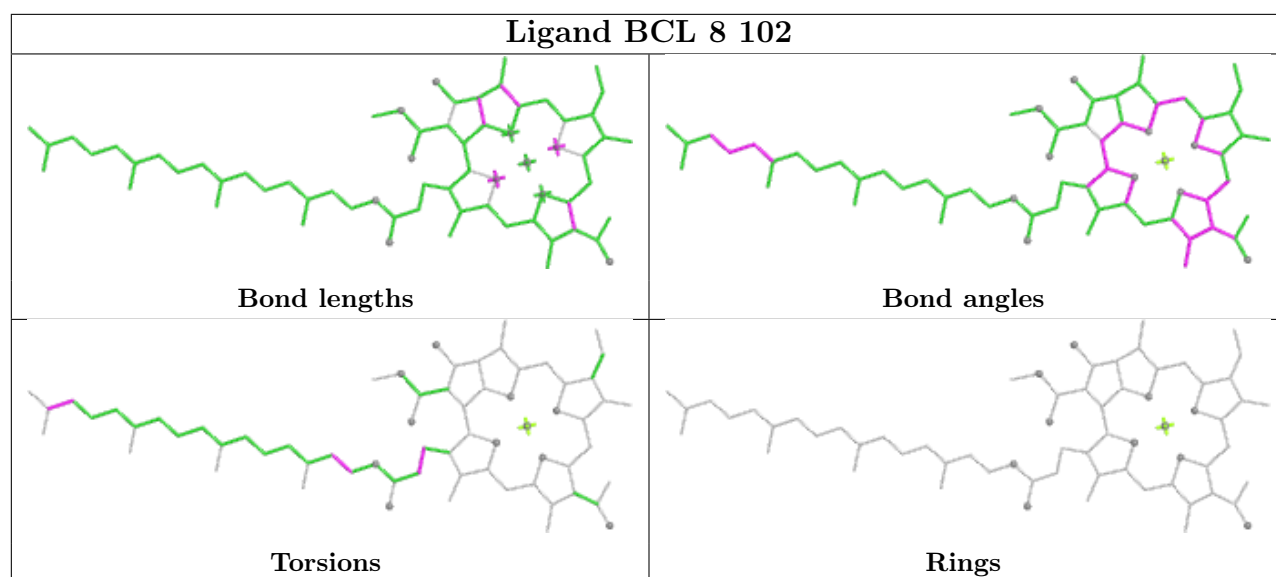
Torsions

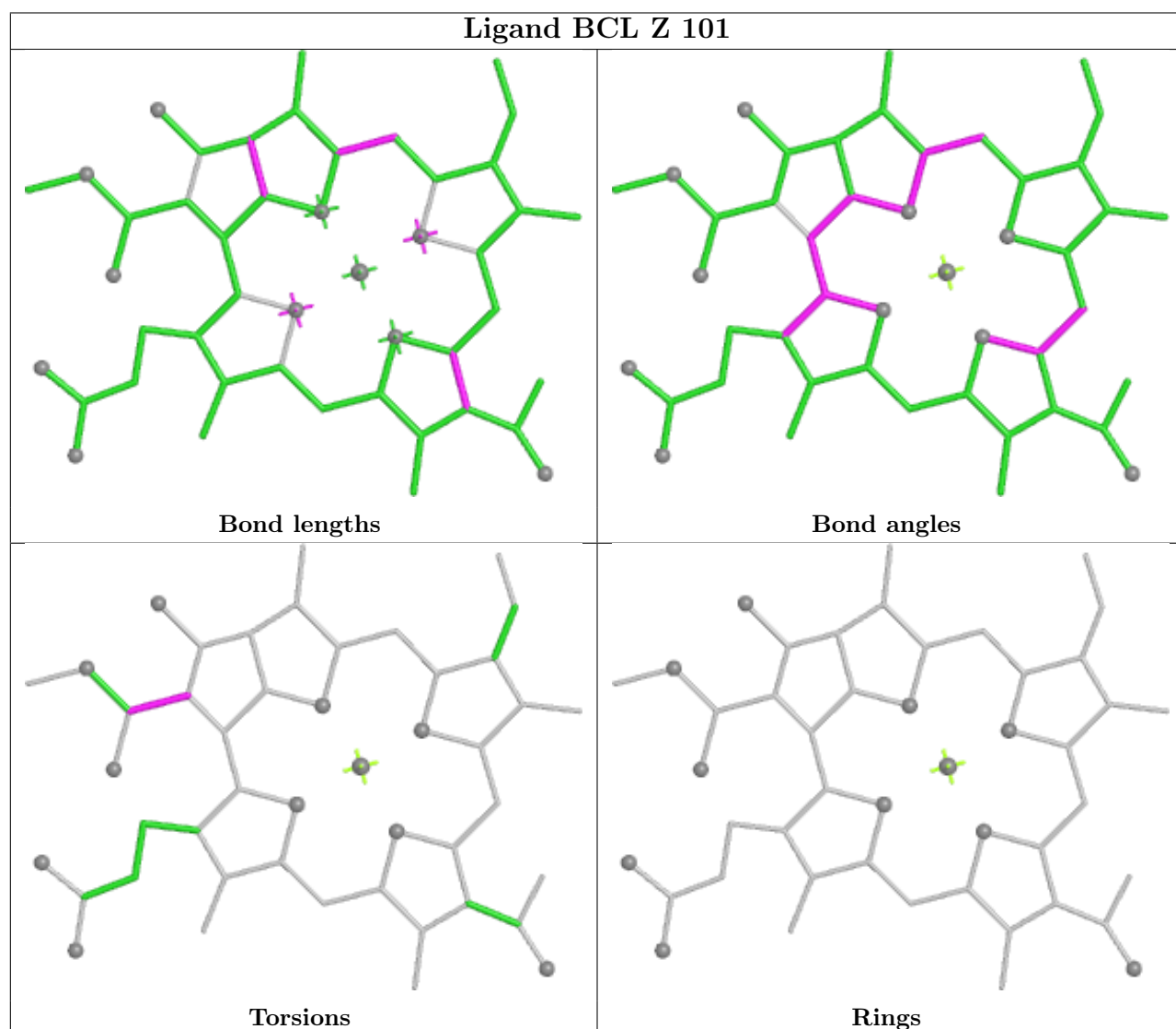
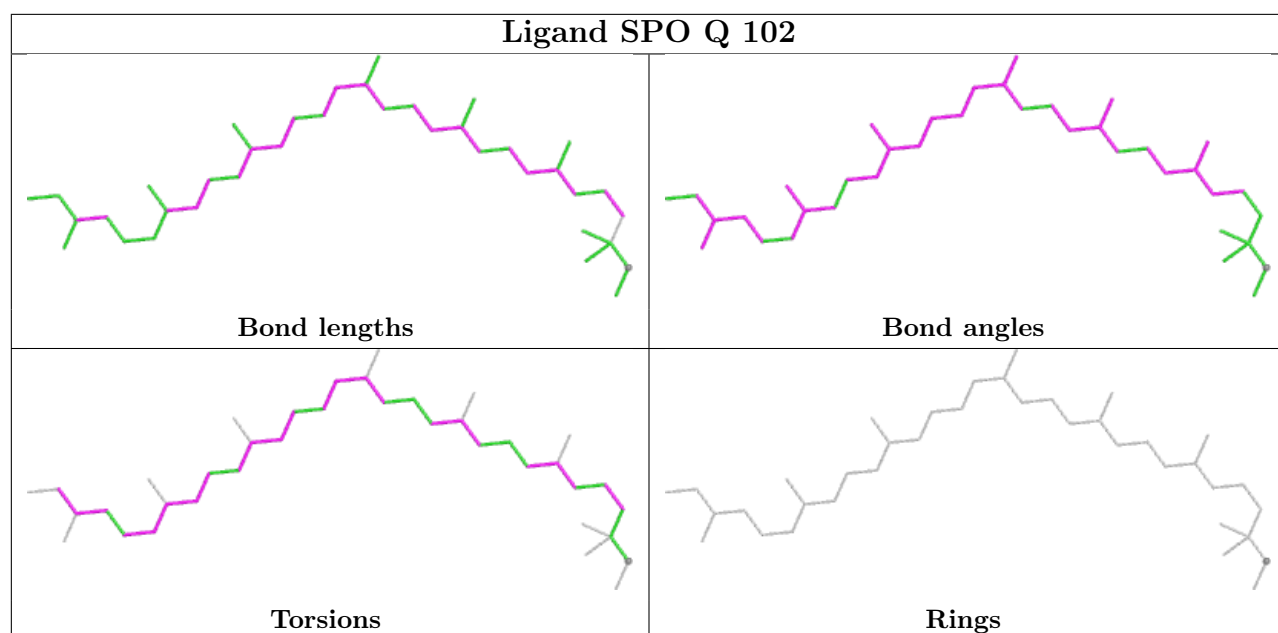


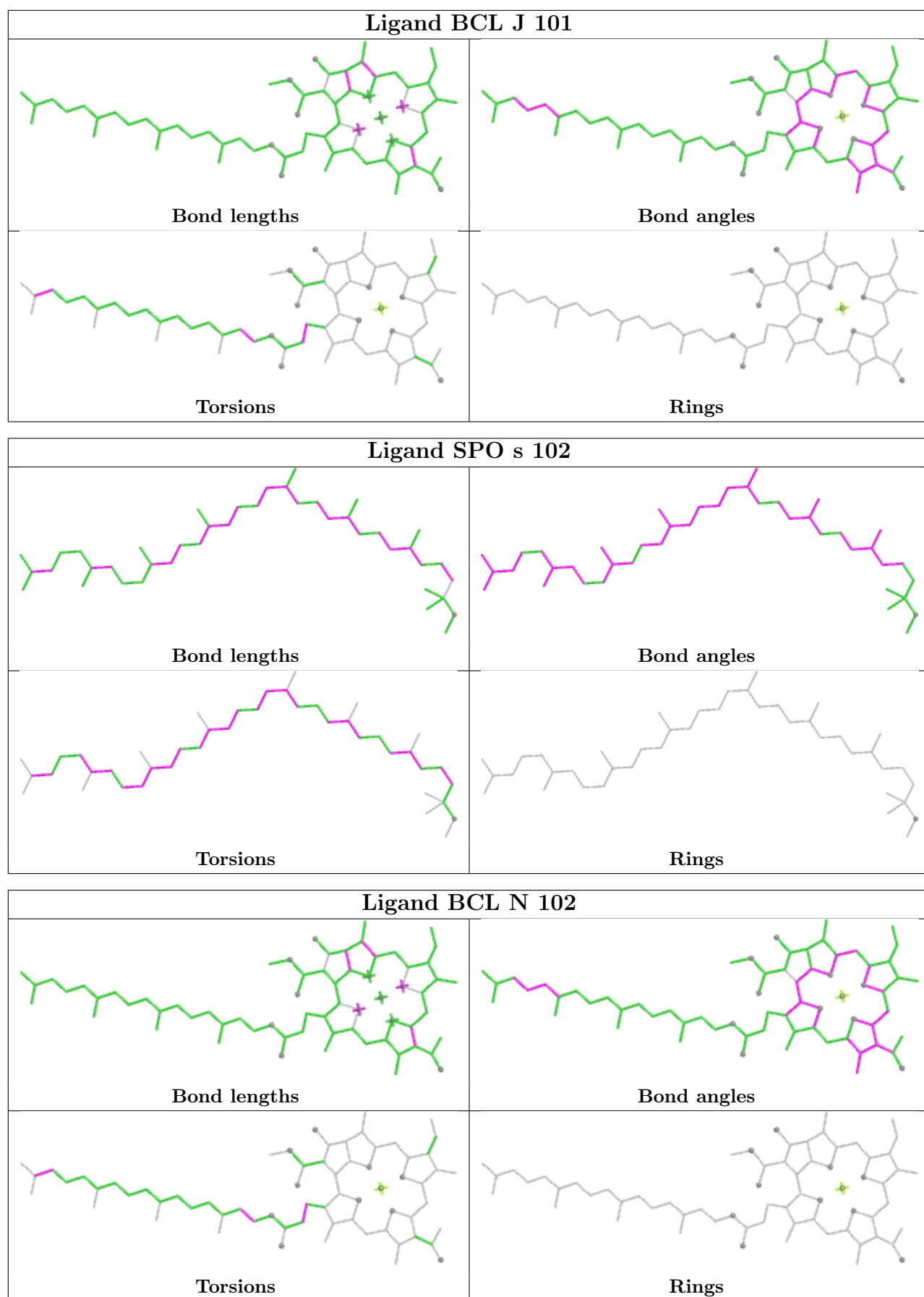
Rings

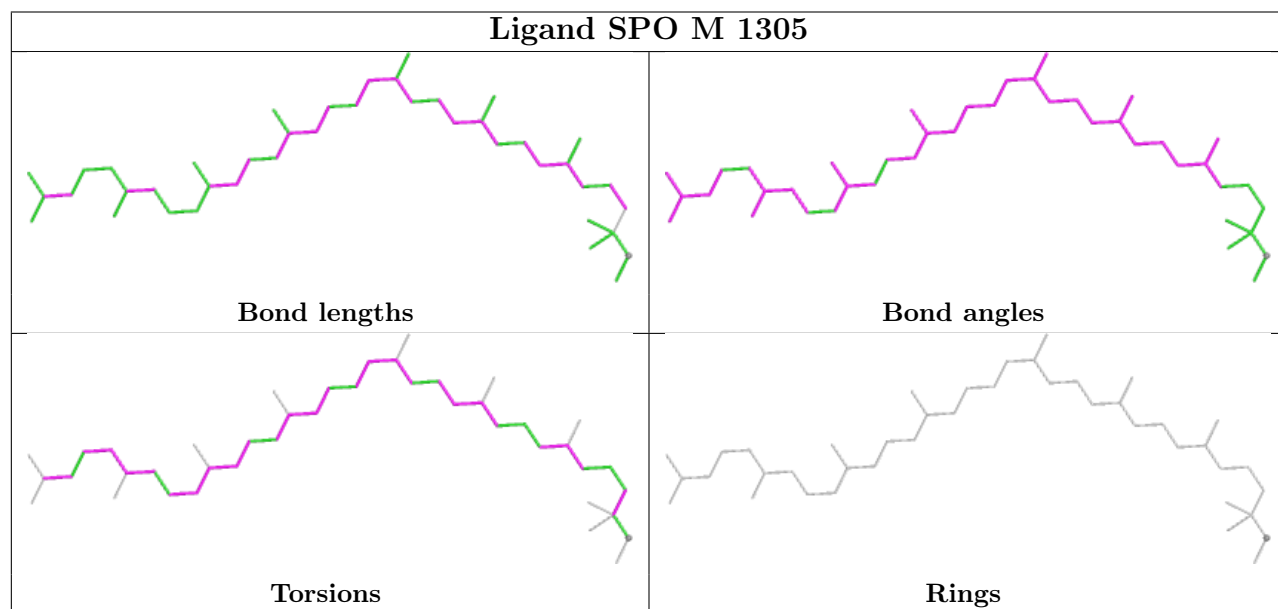
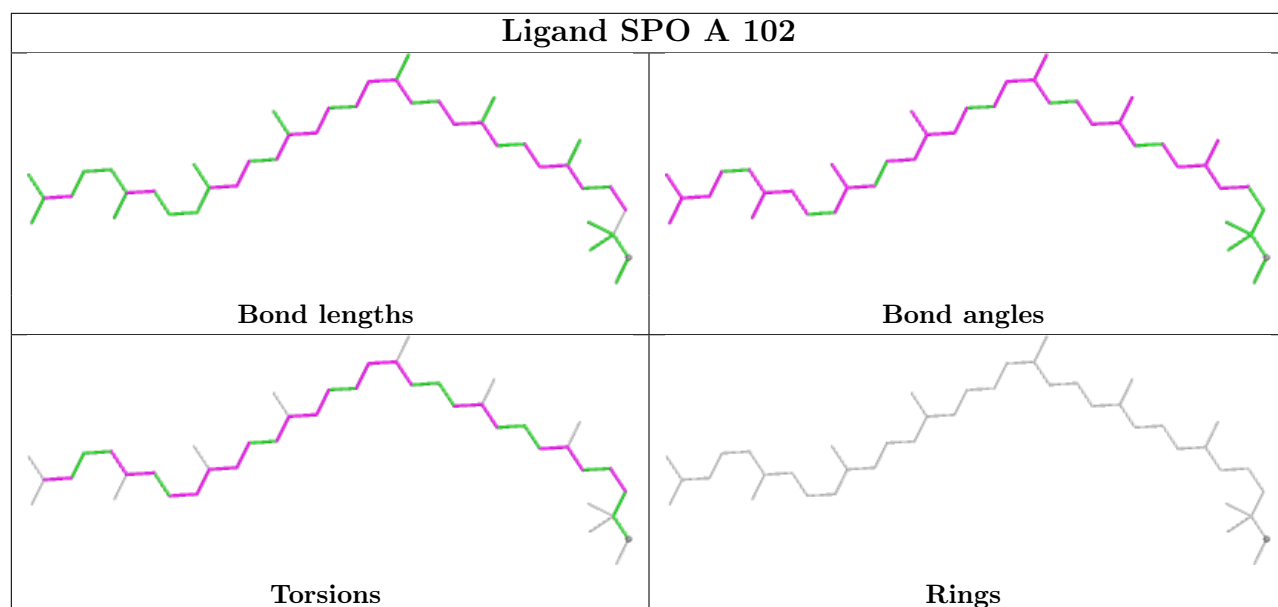
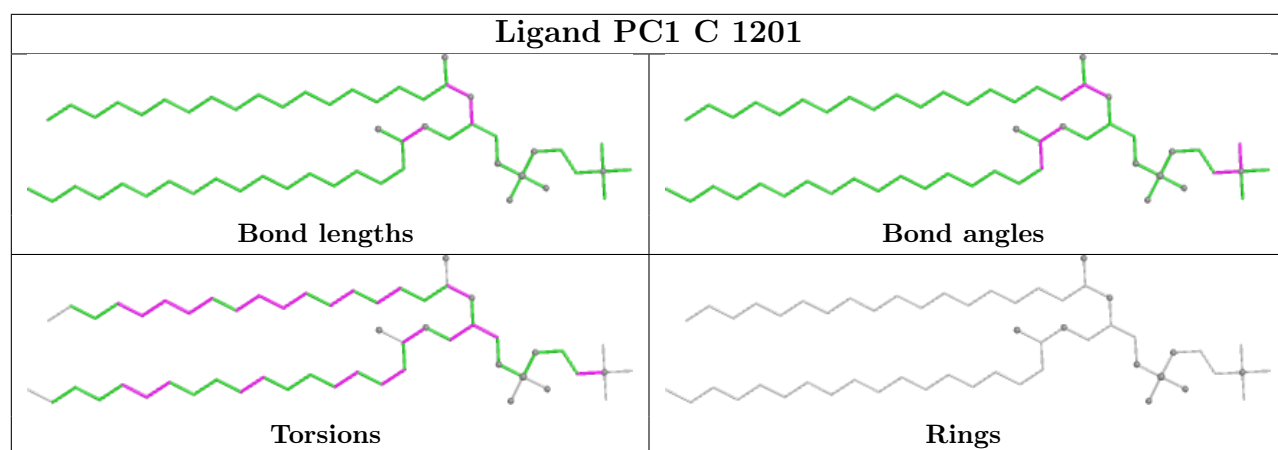


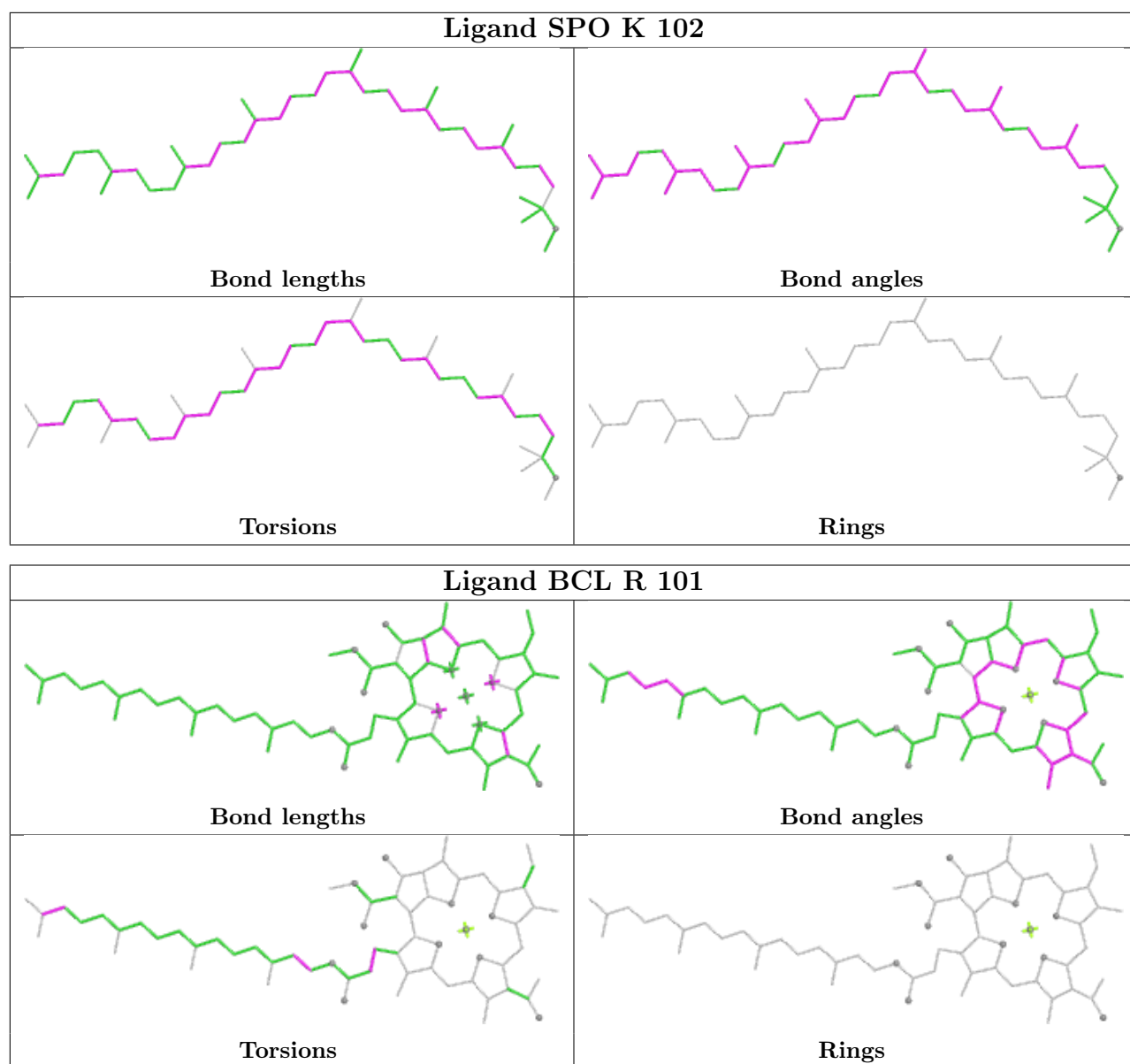


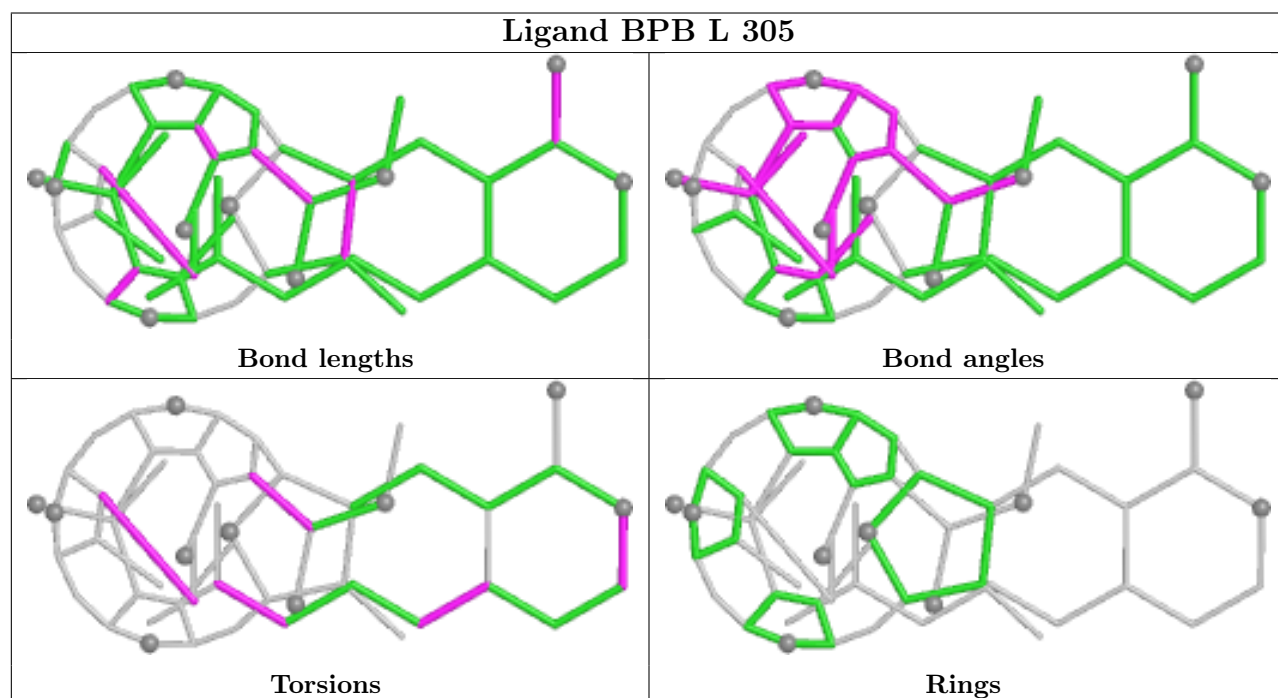
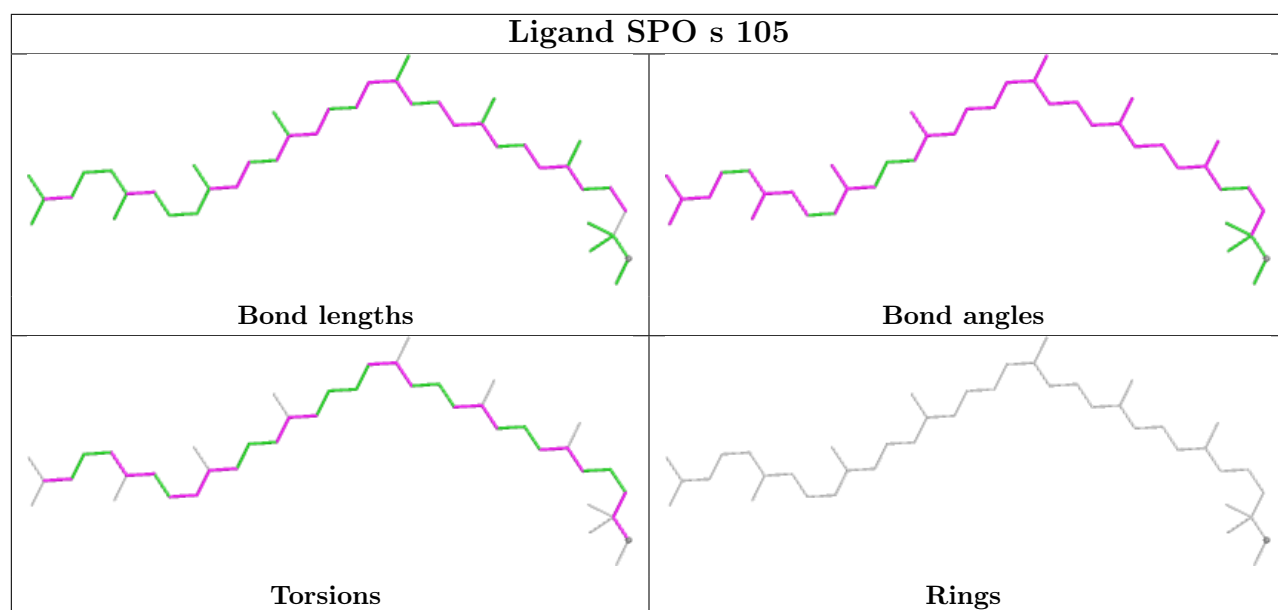


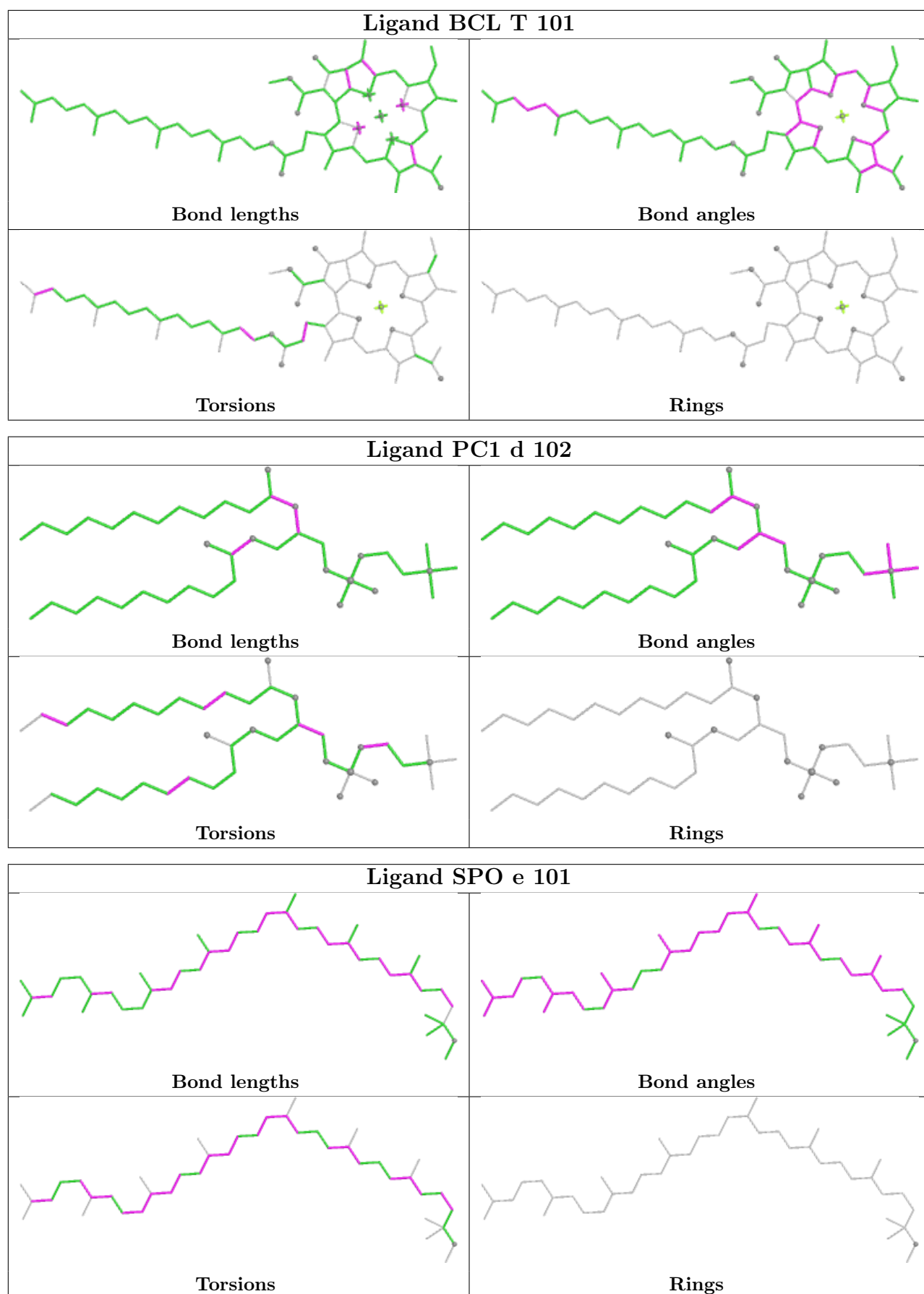


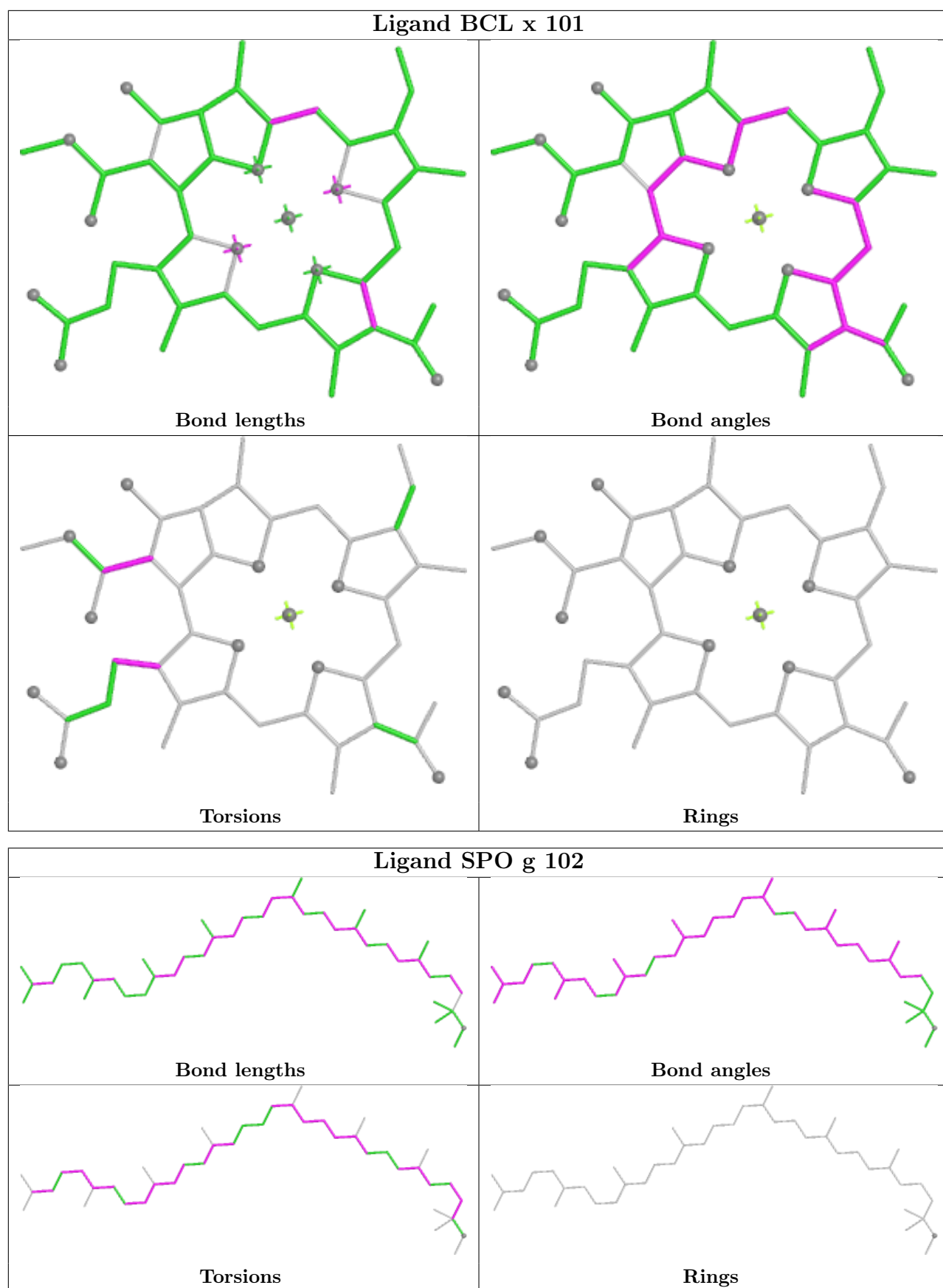


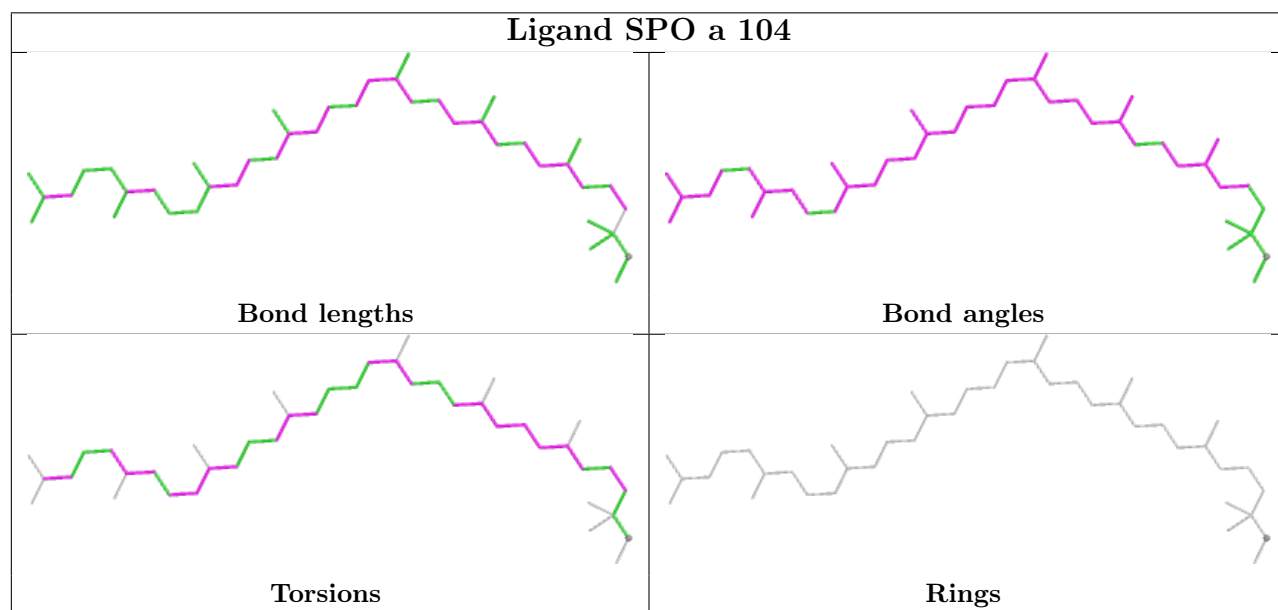
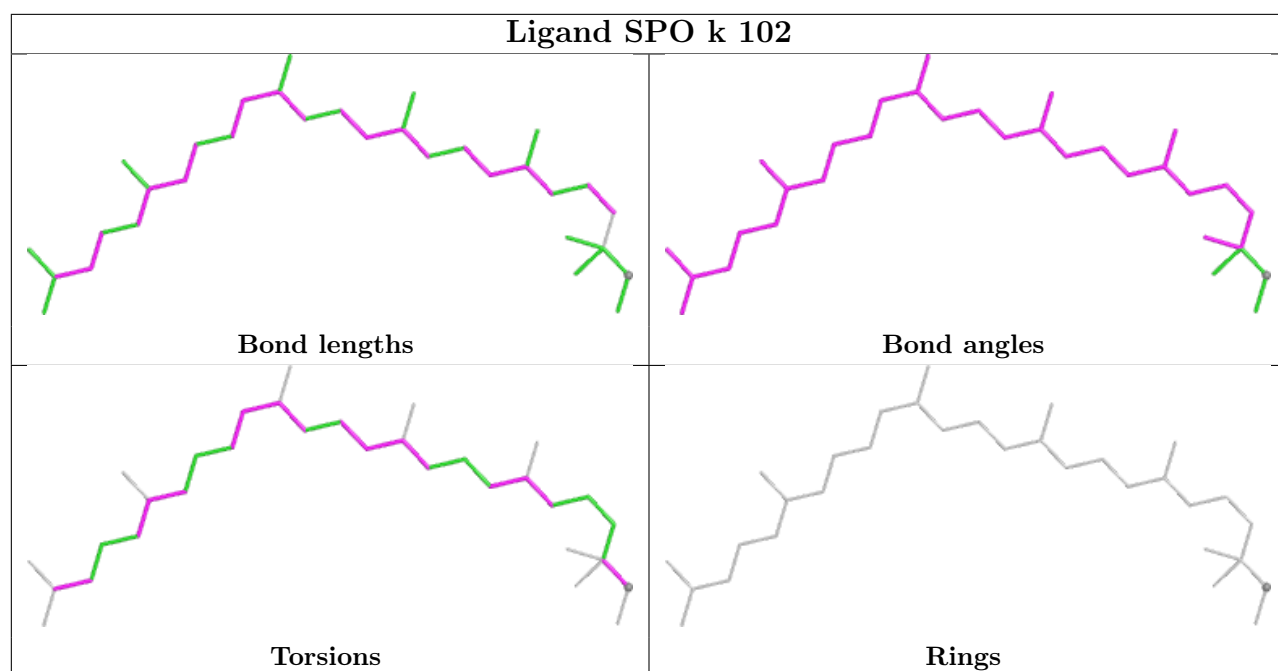


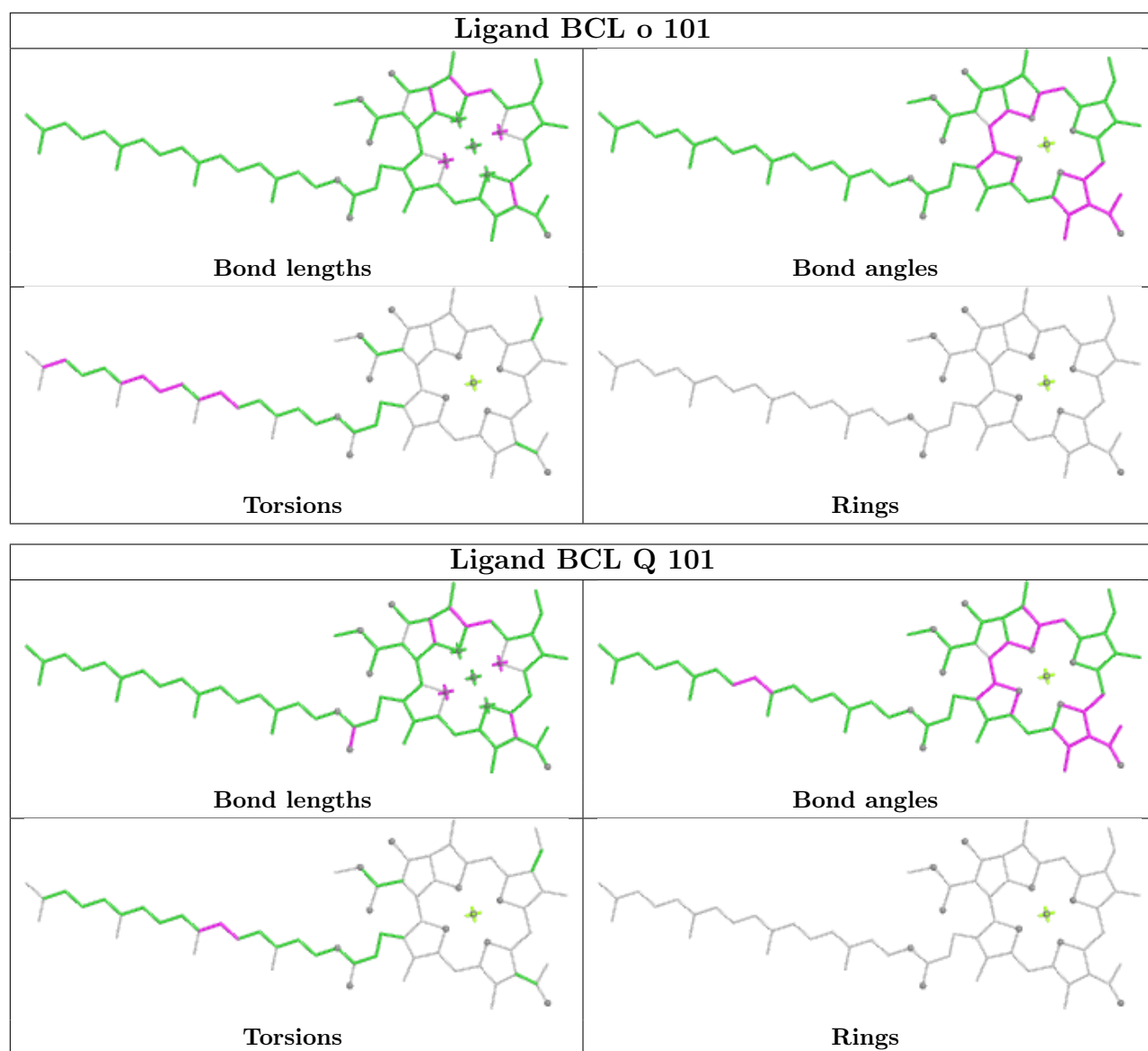




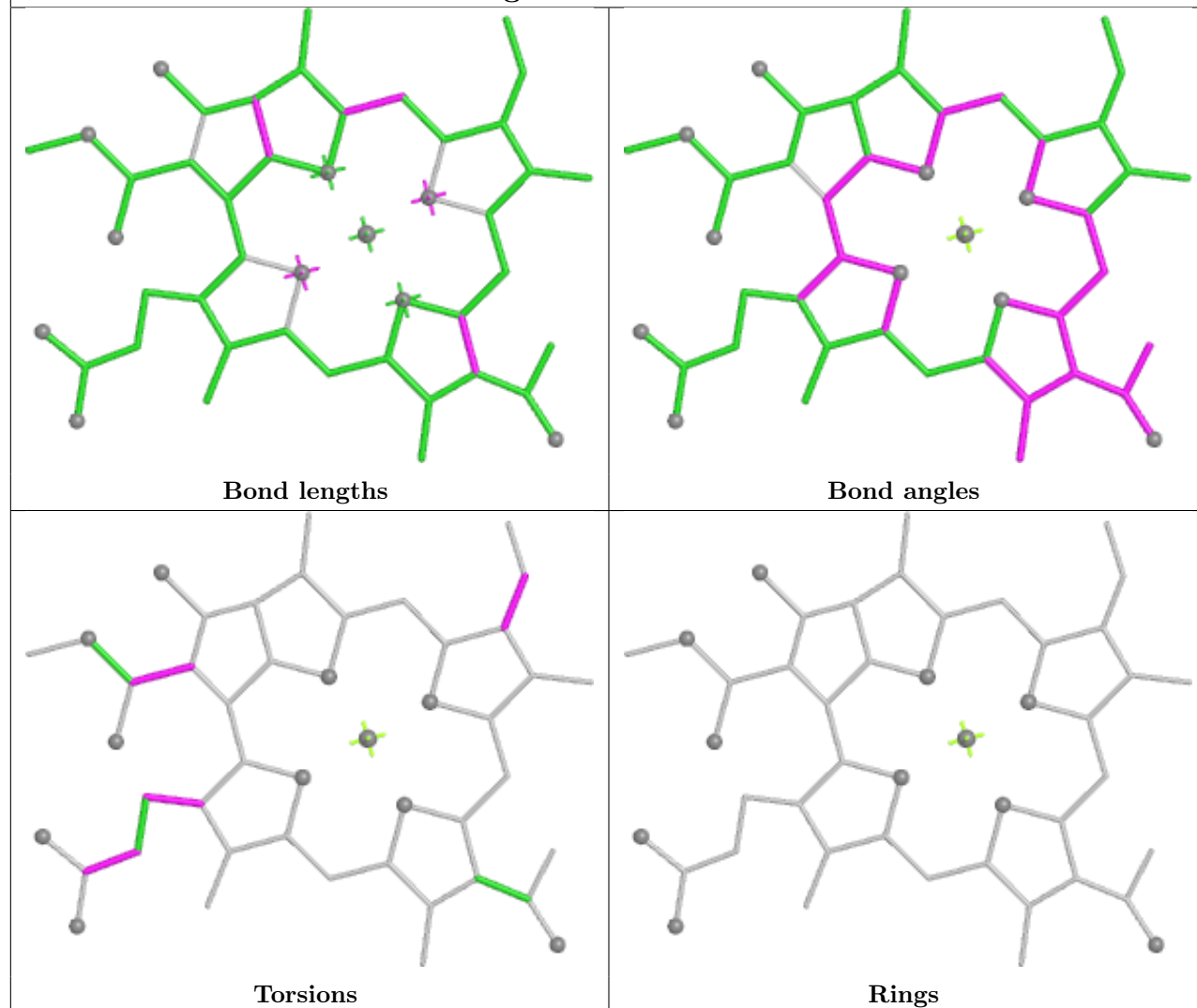




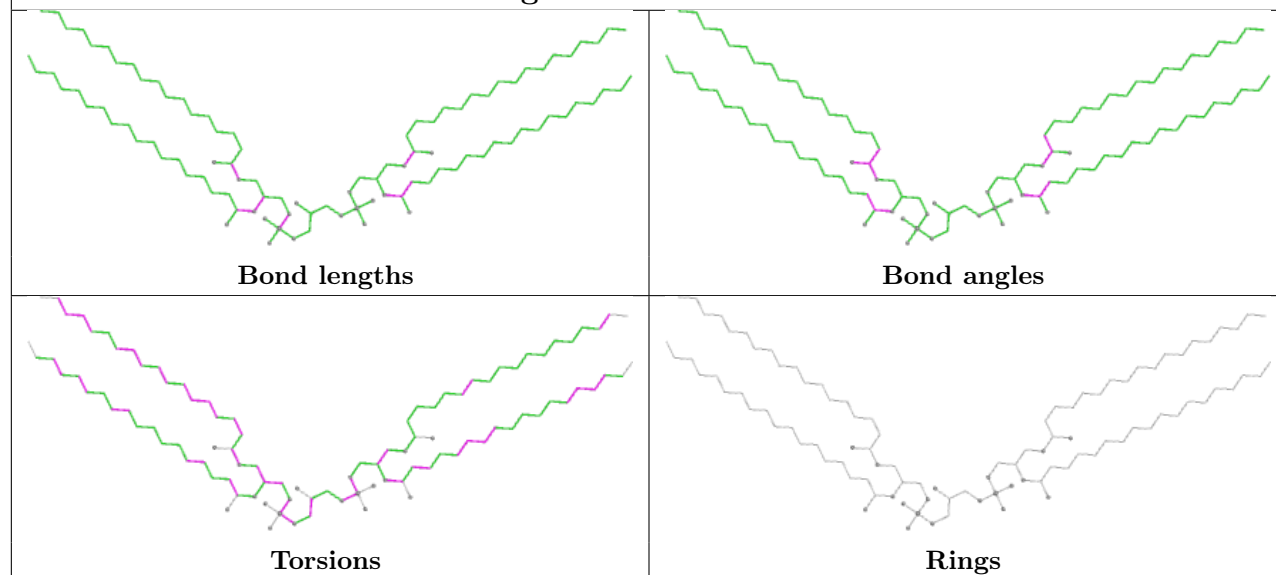


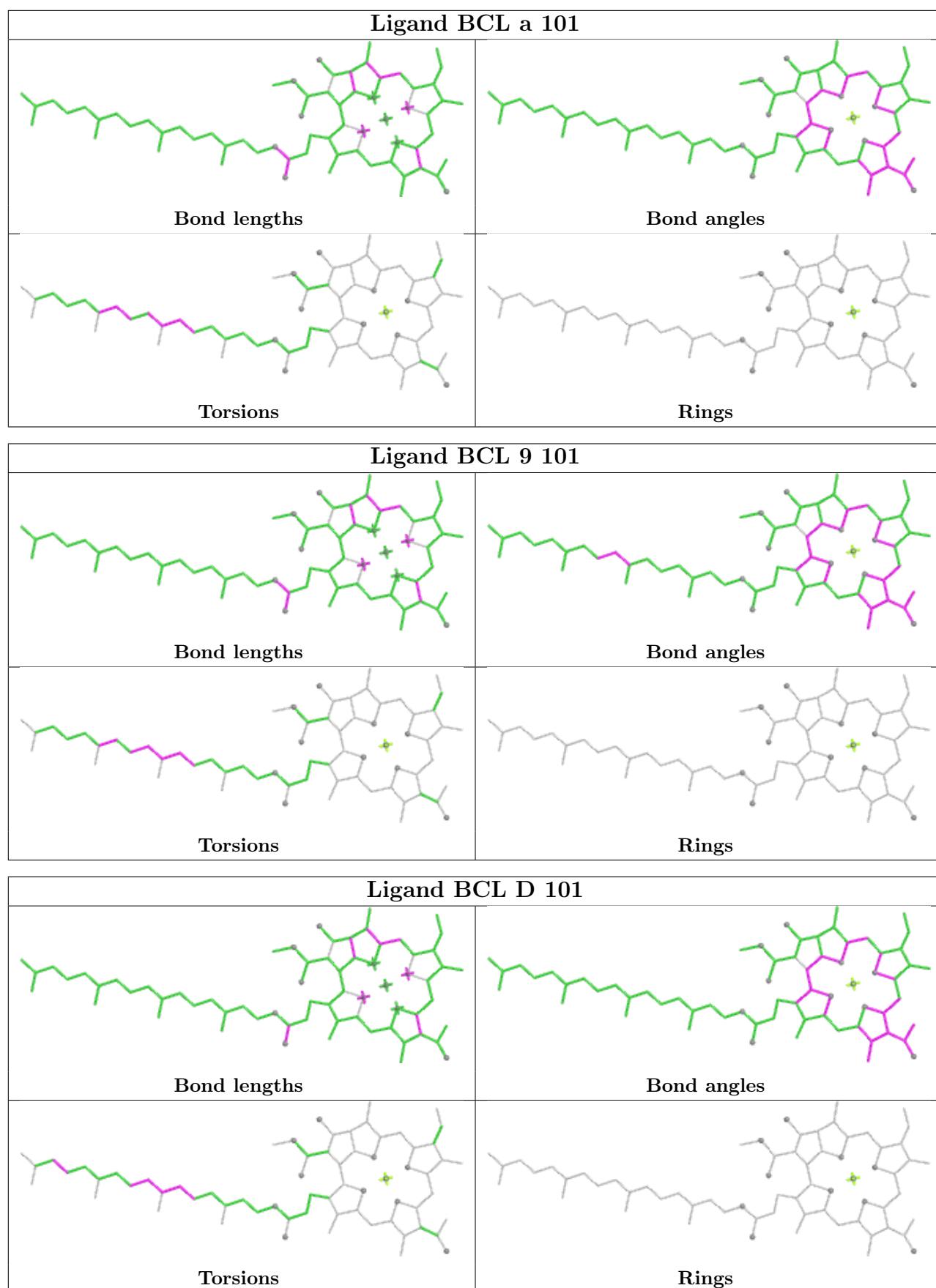


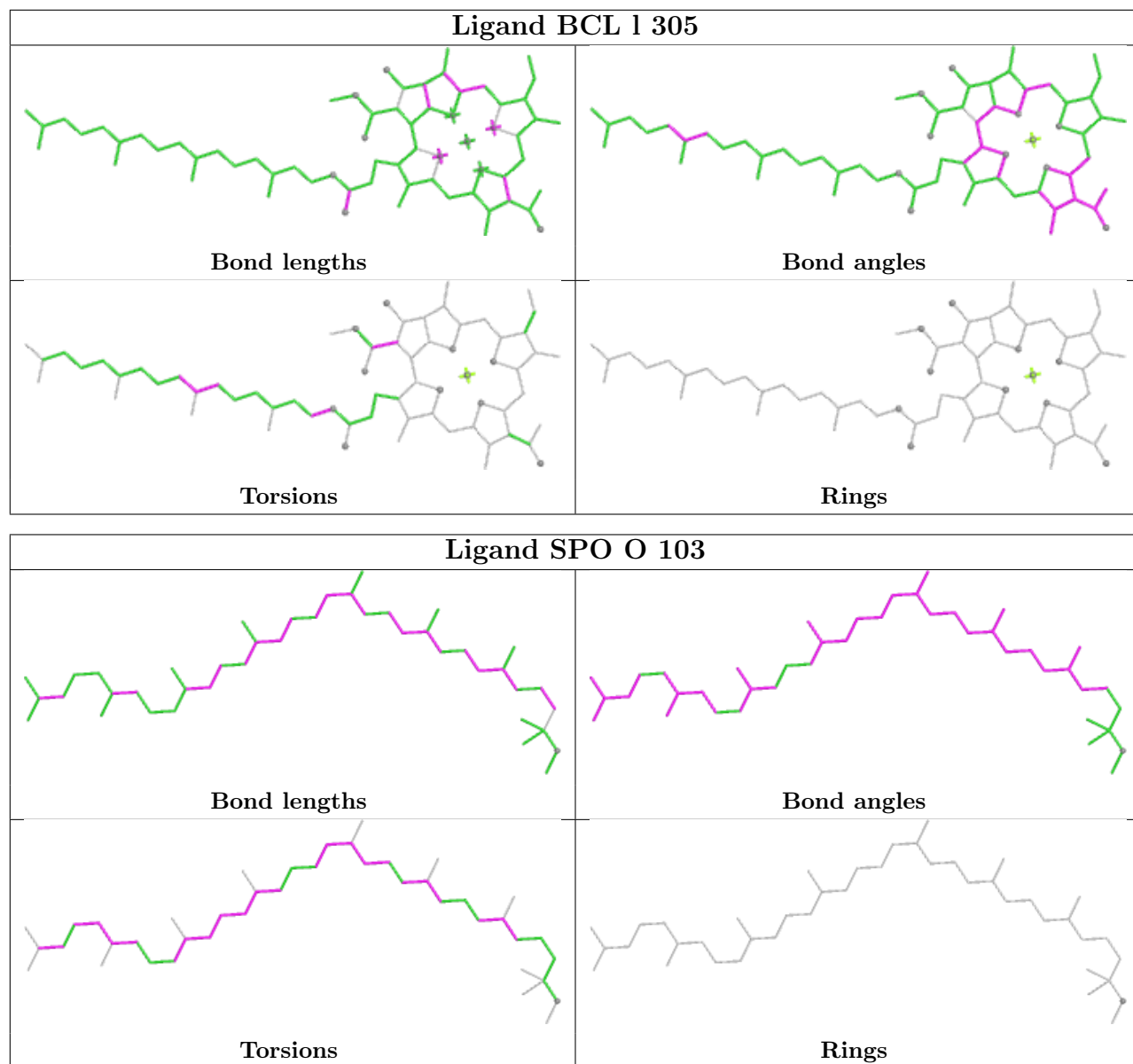
Ligand BCL 5 102

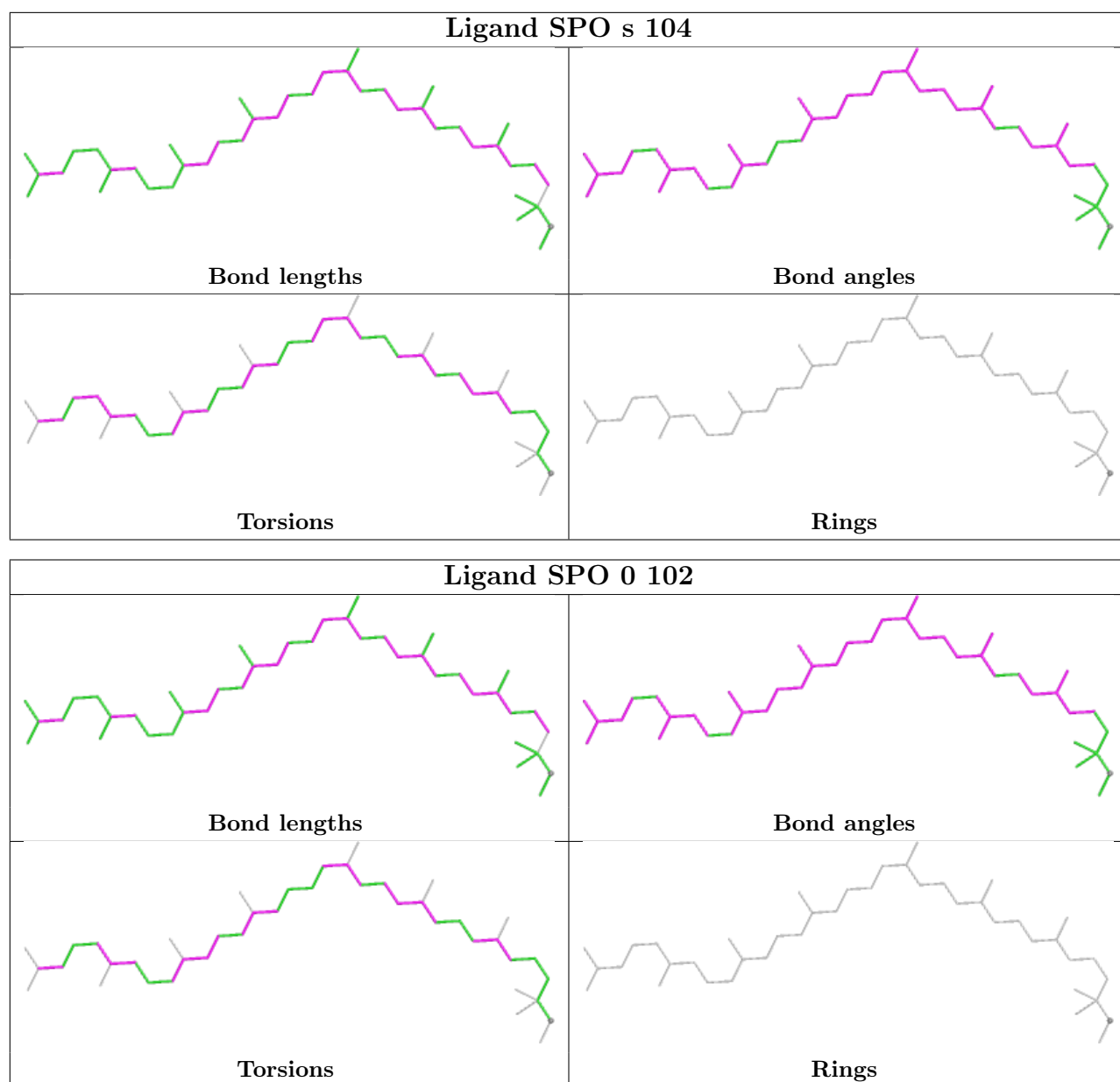


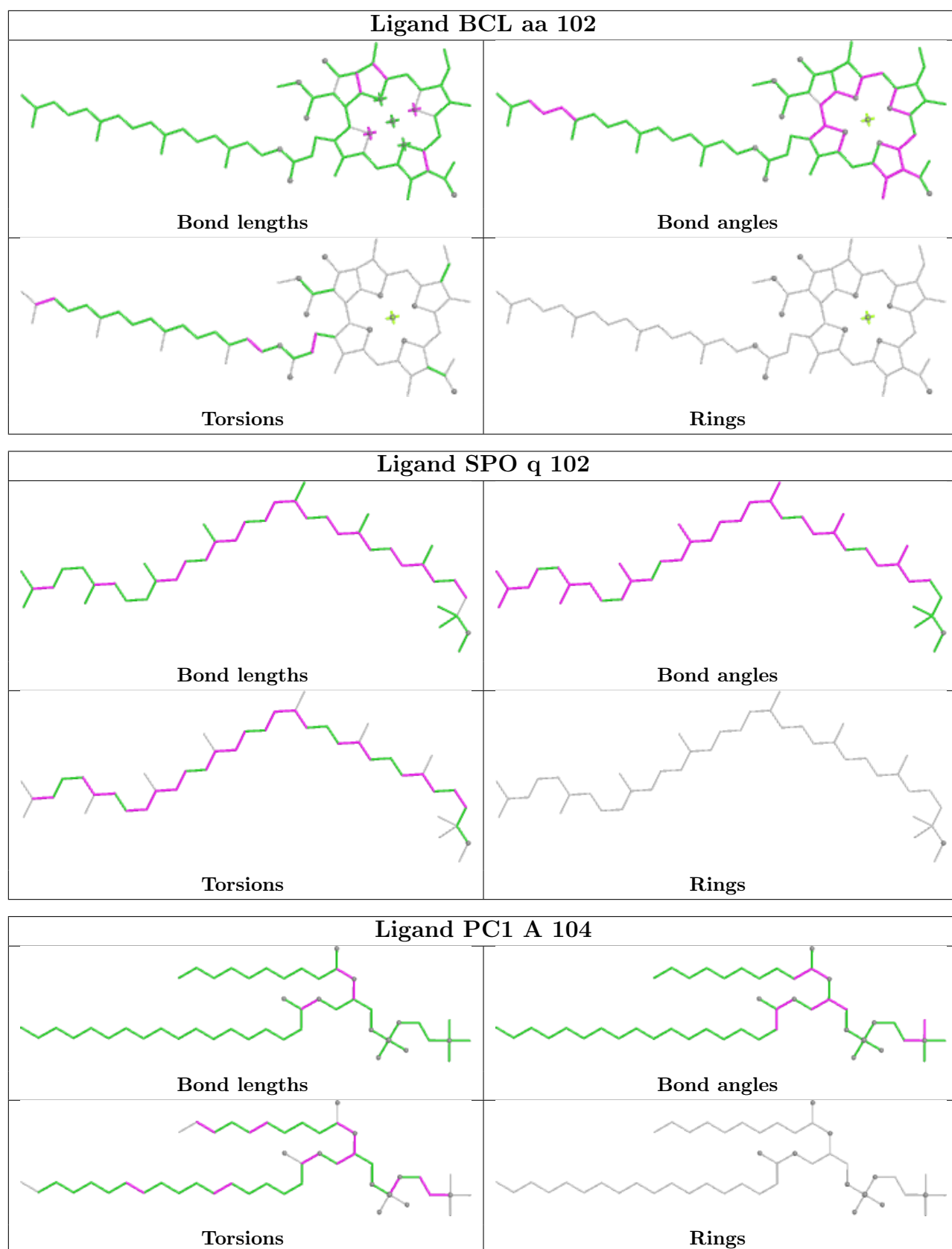
Ligand CDL m 1306



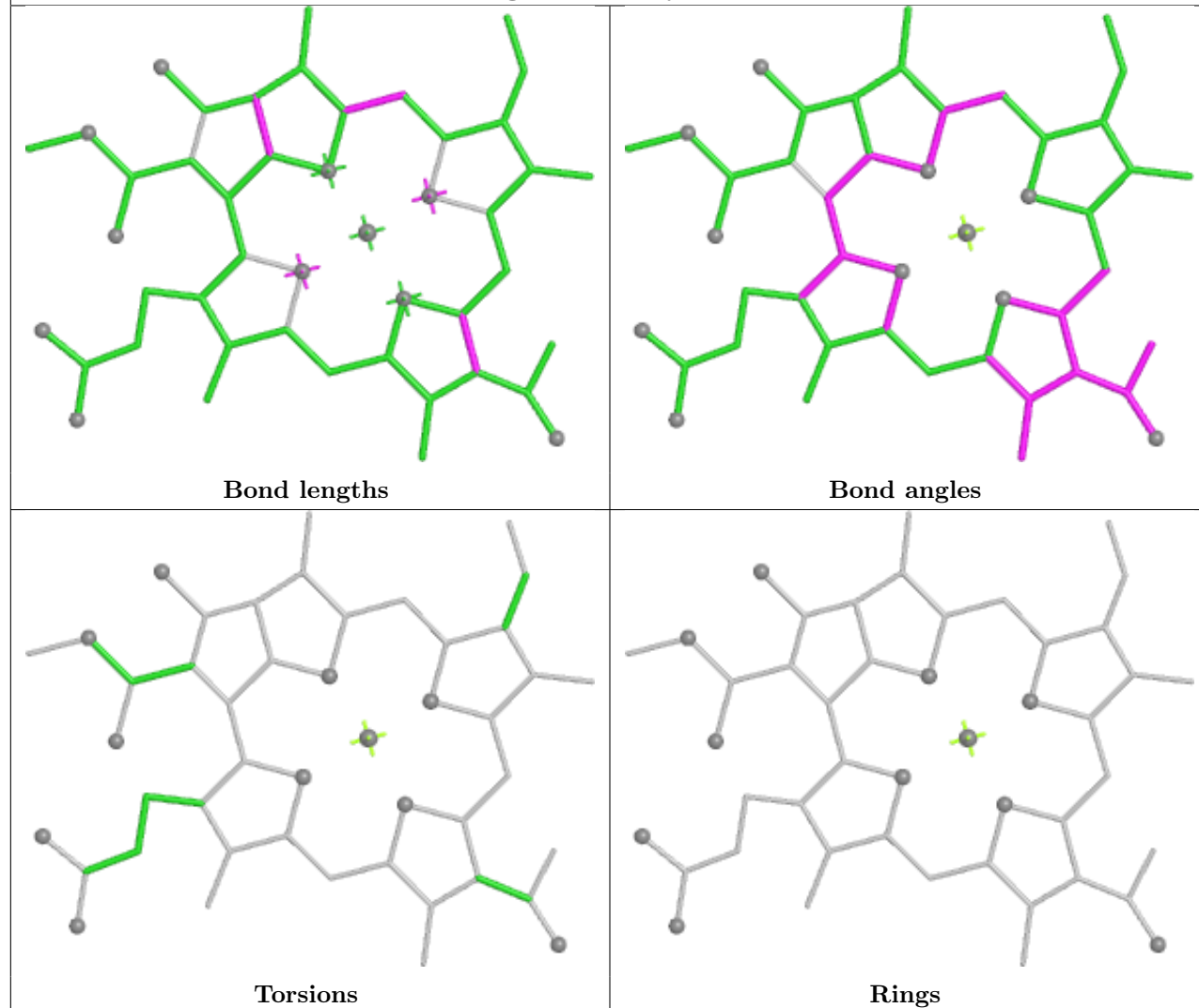




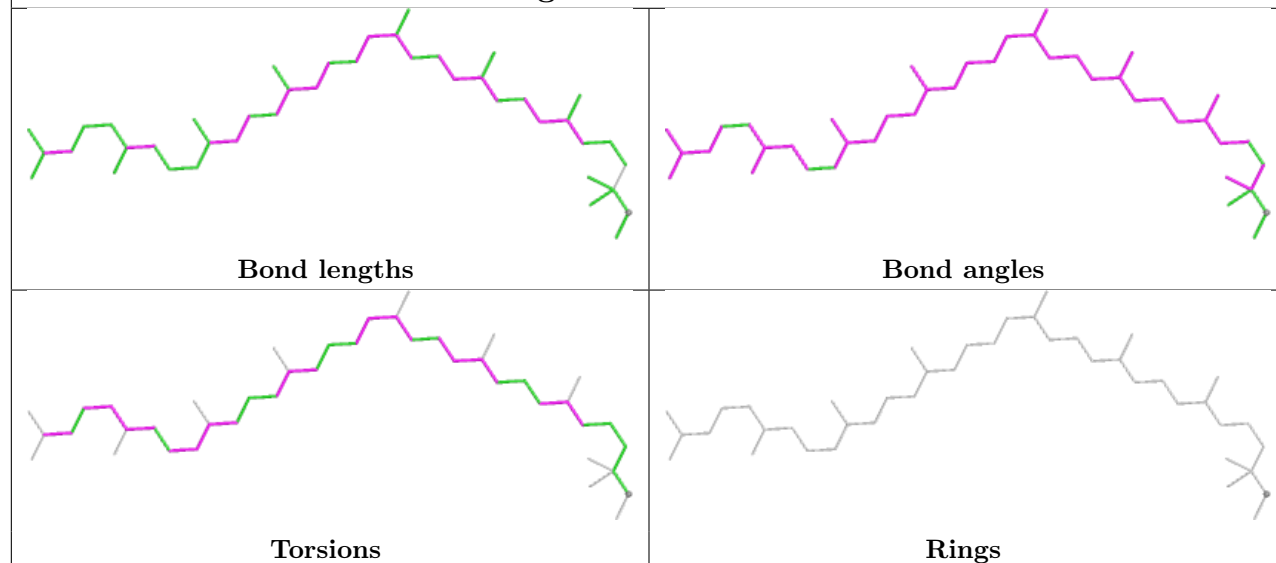


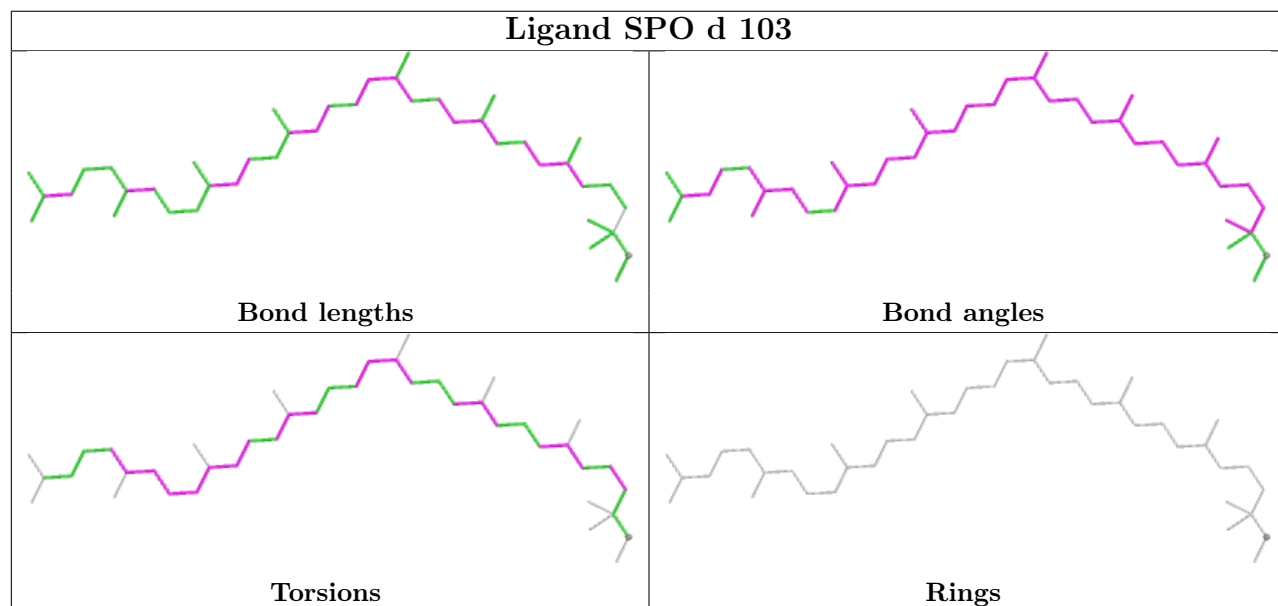
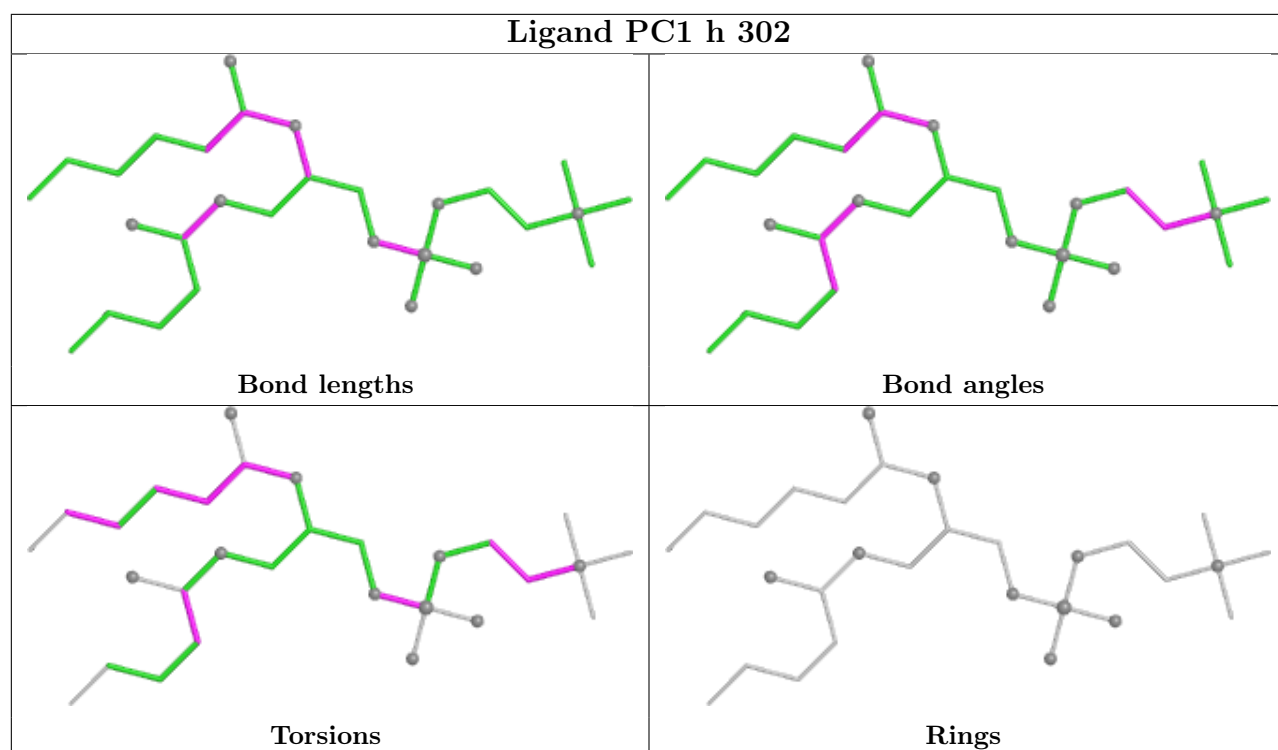


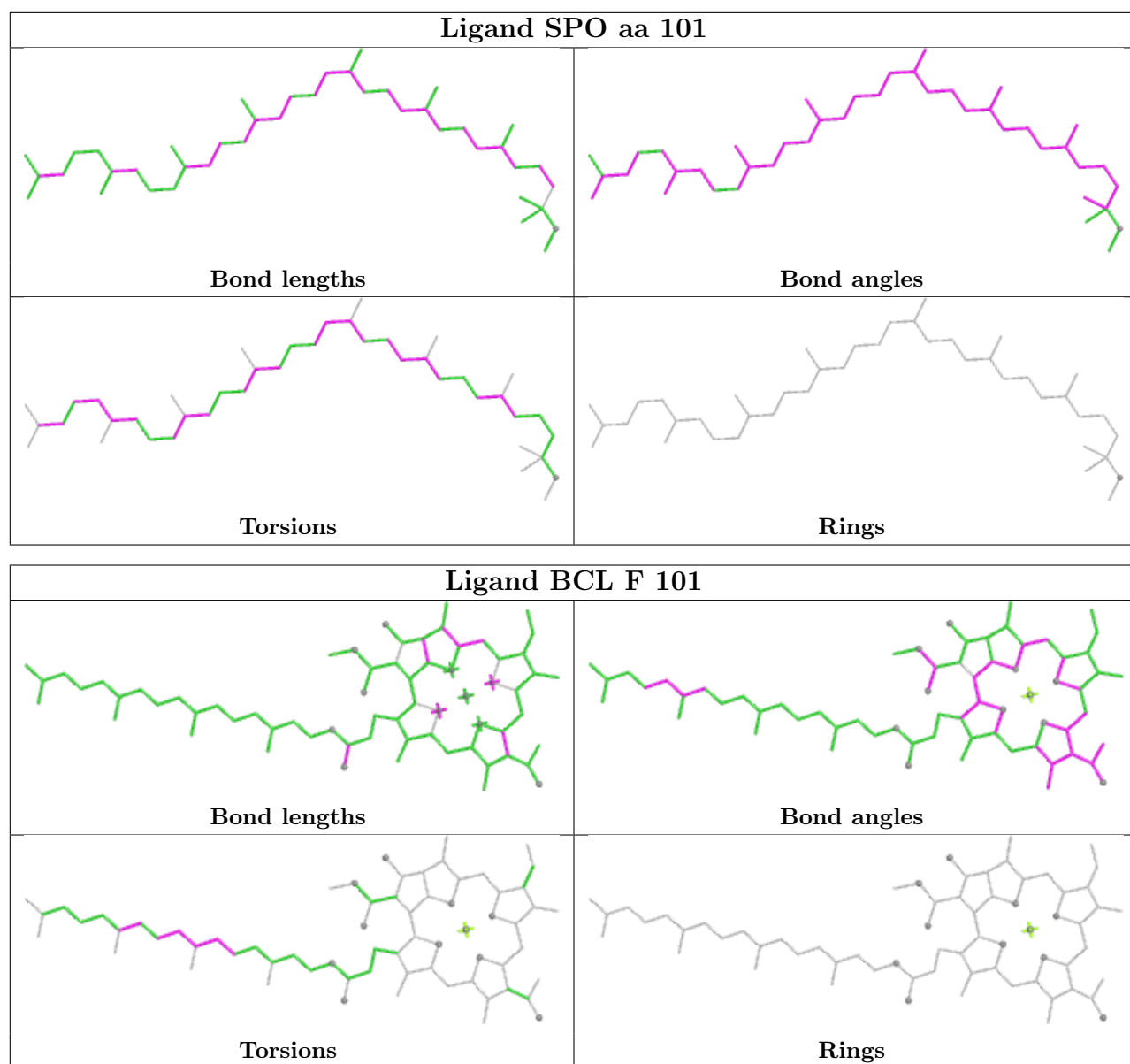
Ligand BCL y 101

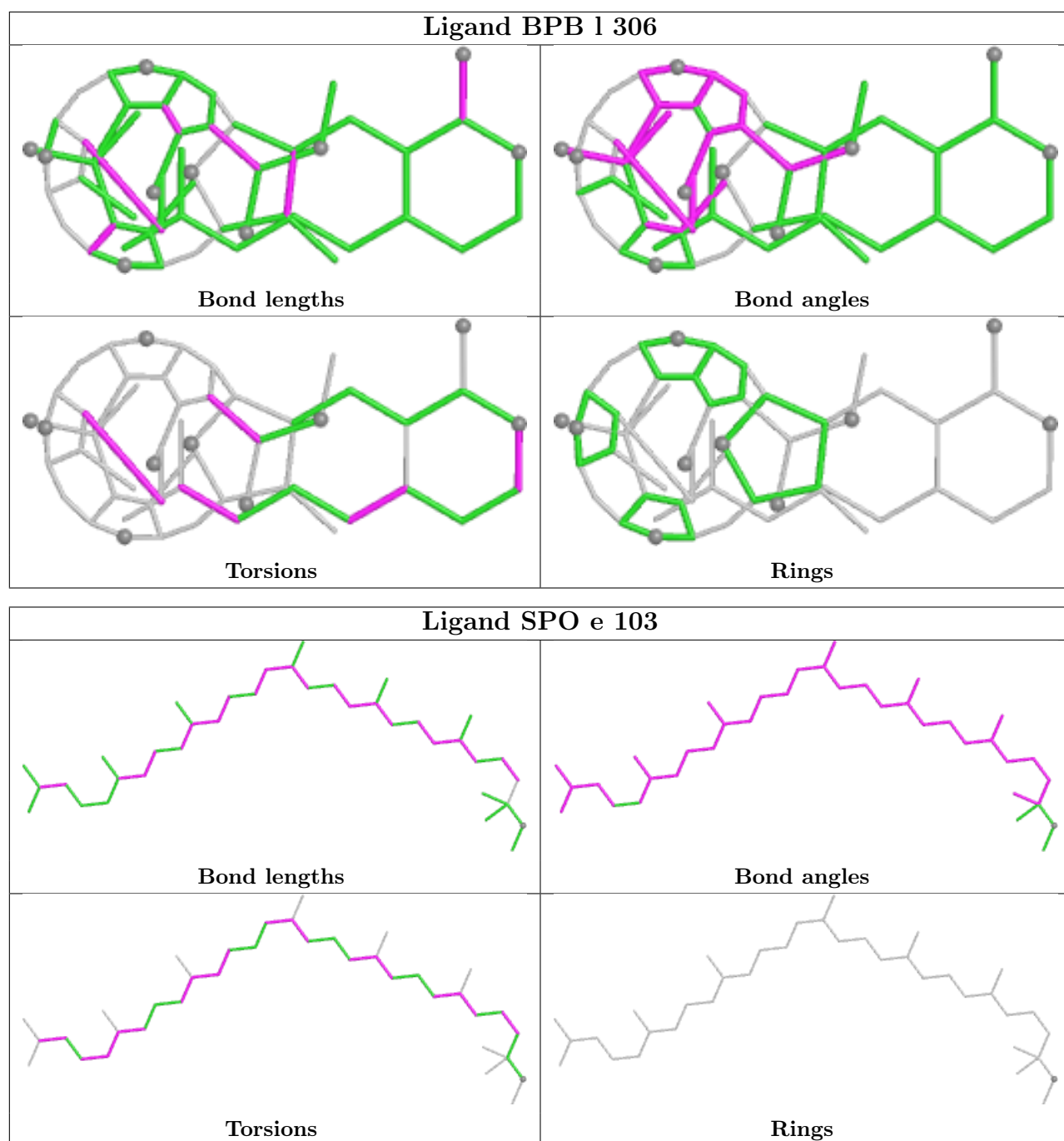


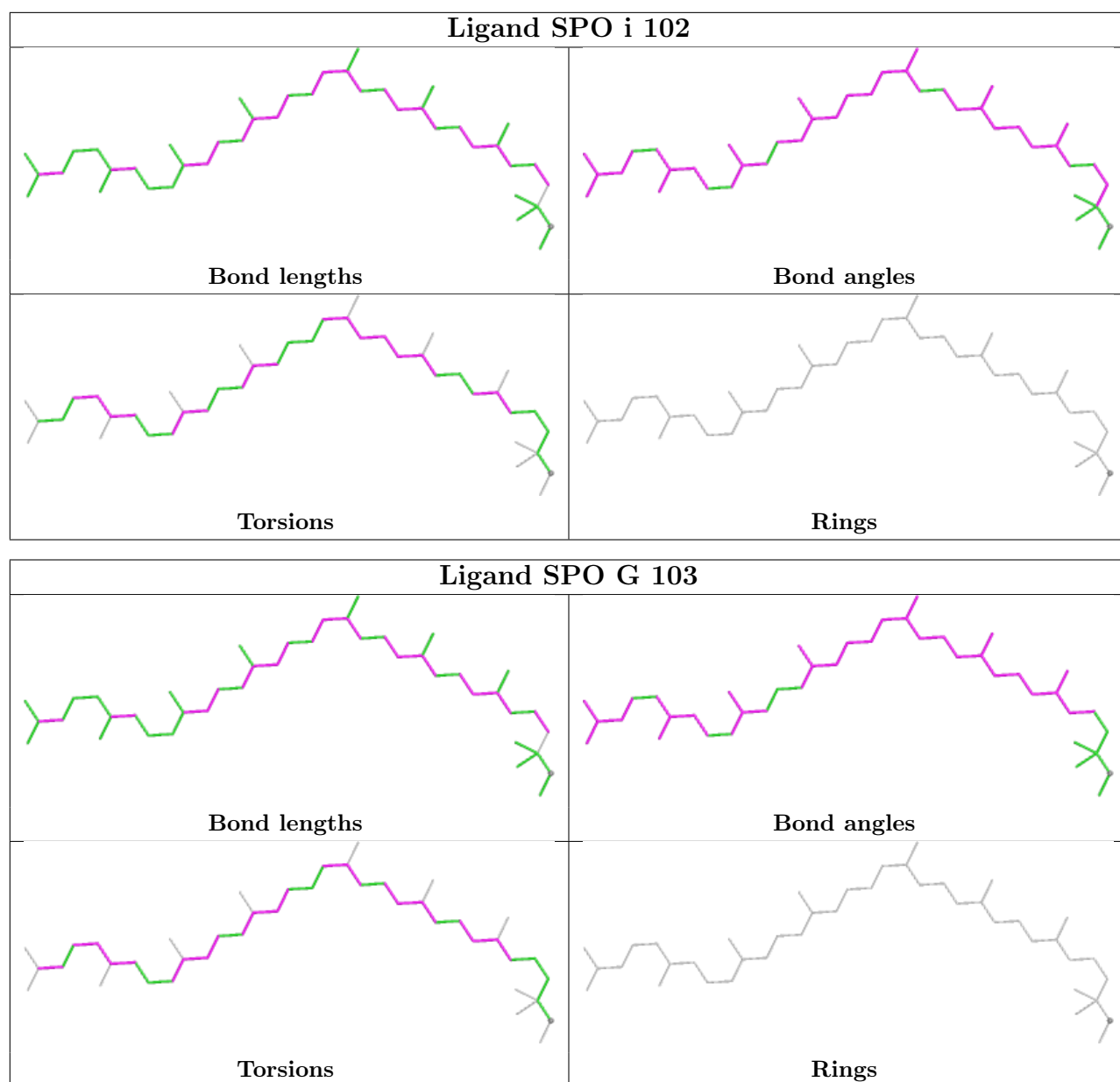
Ligand SPO 8 101

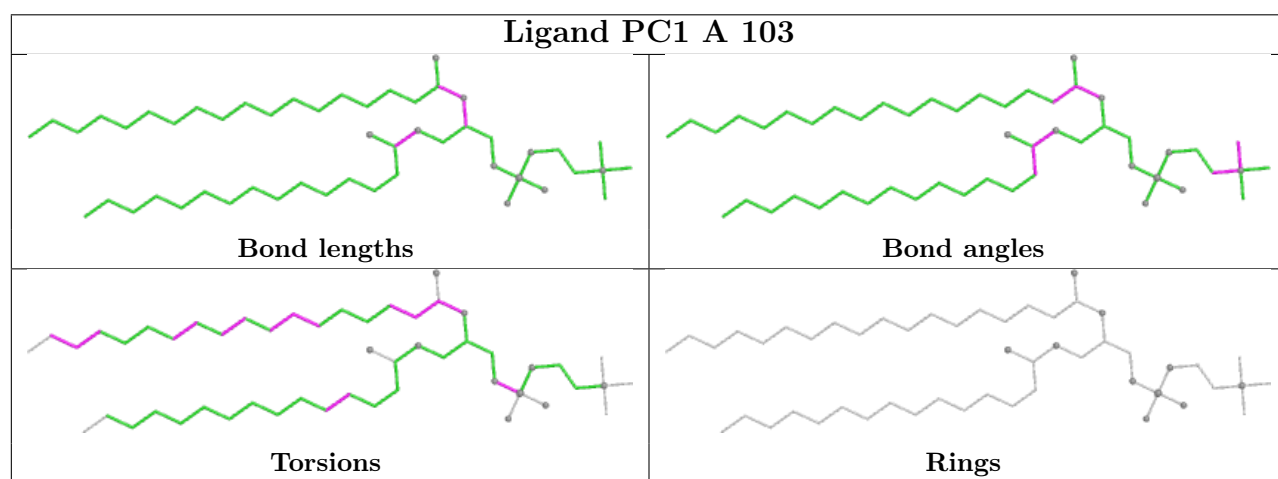
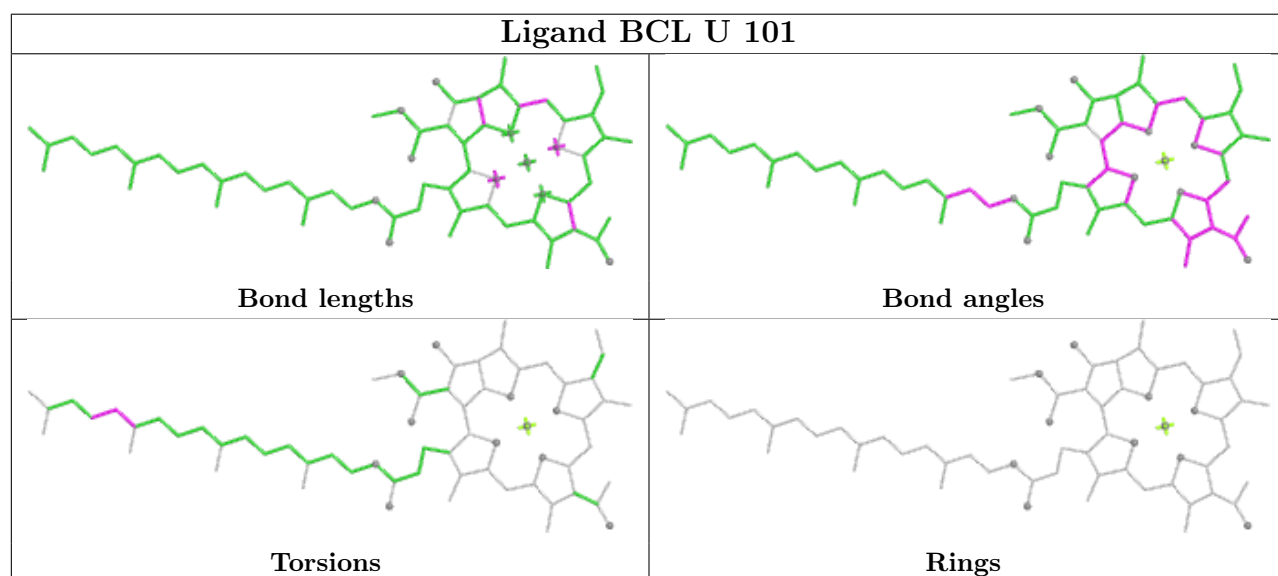
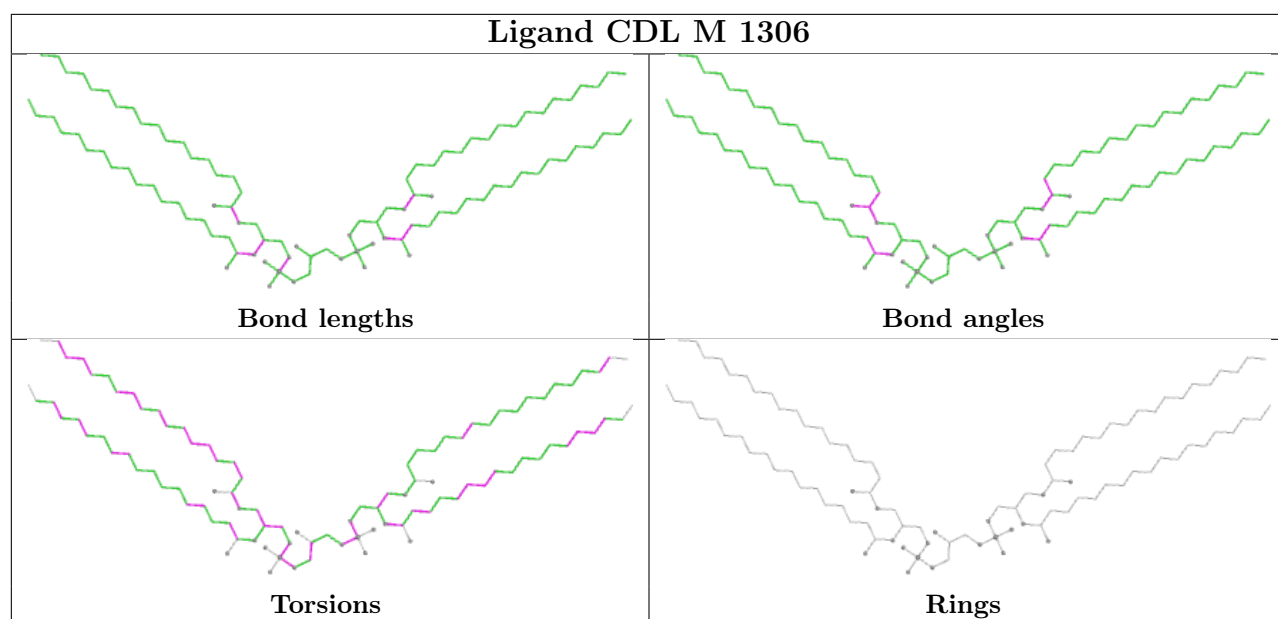


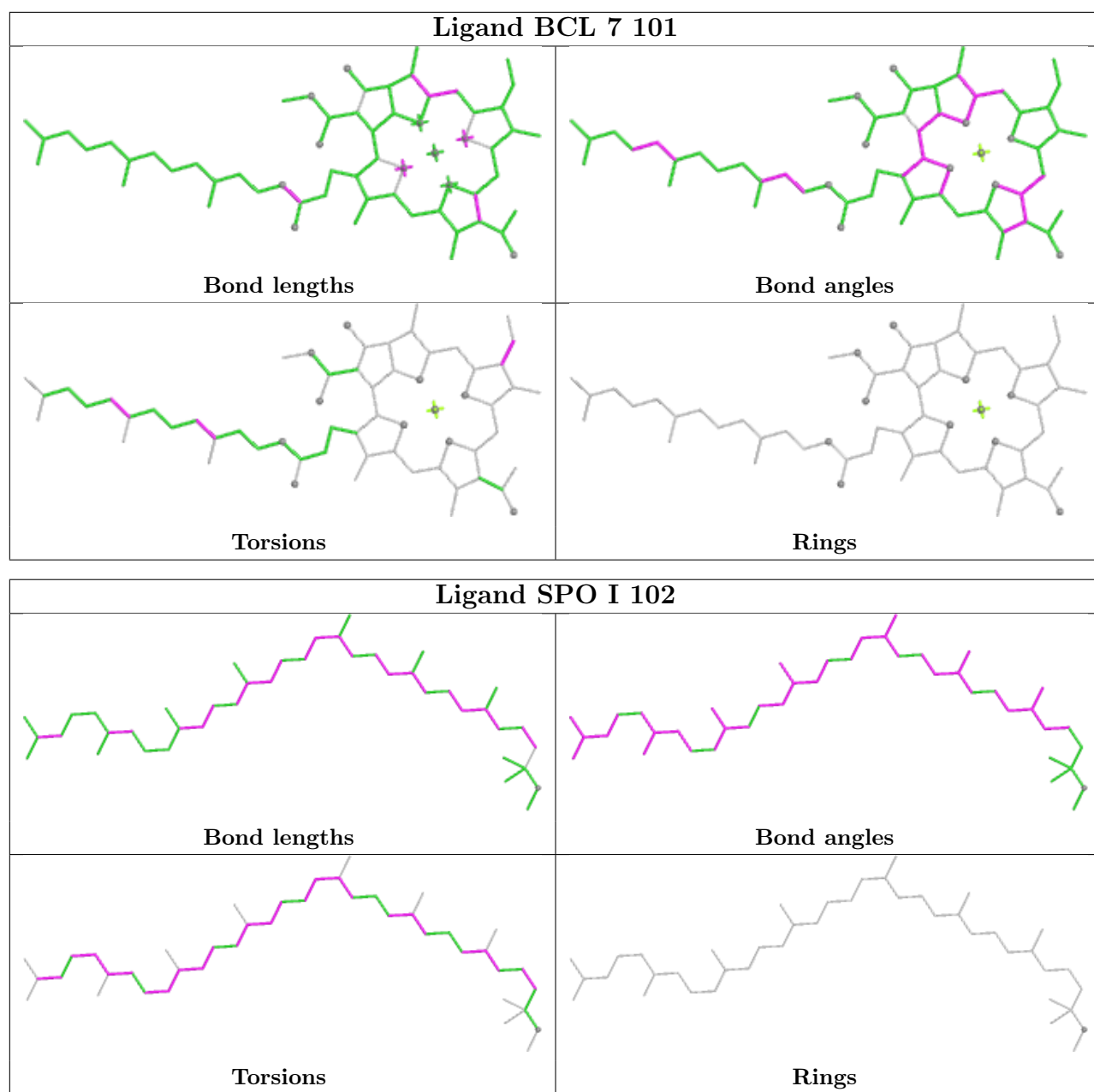


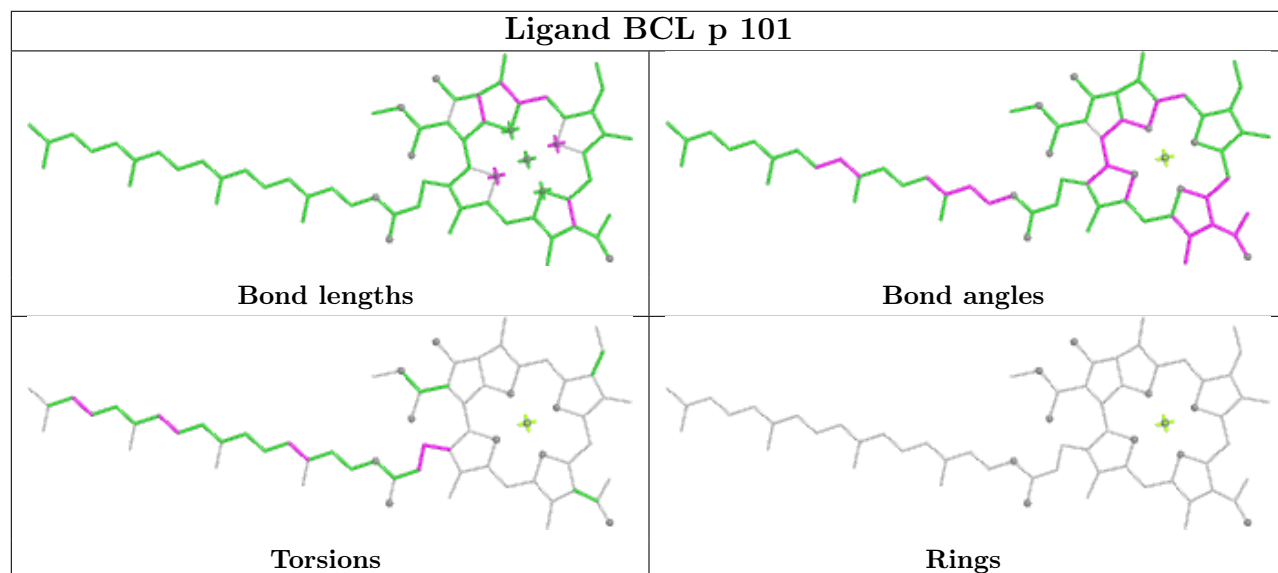
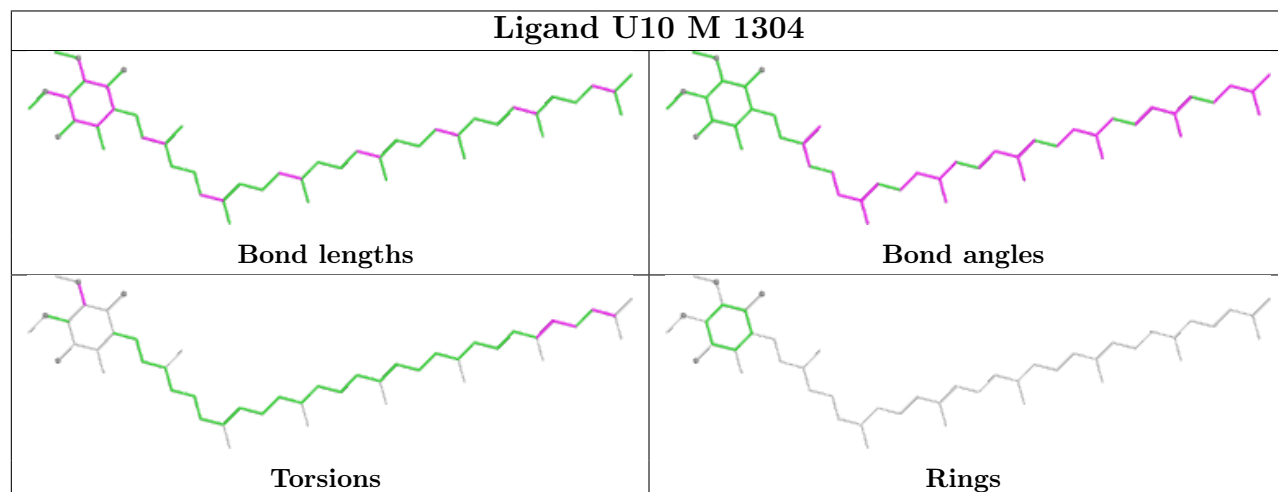
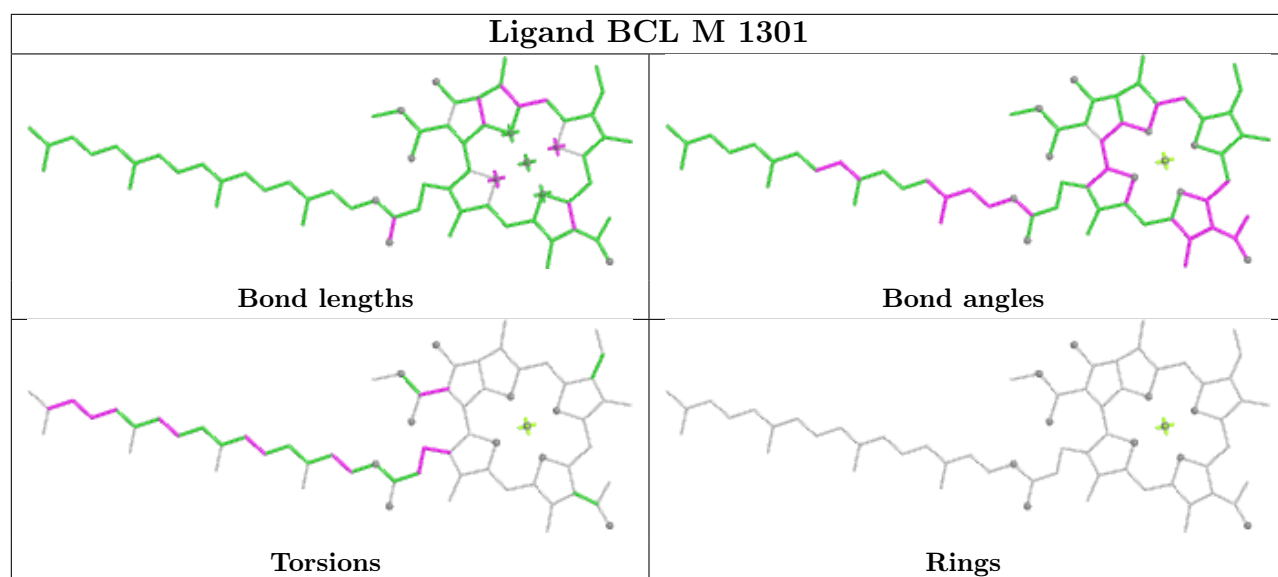


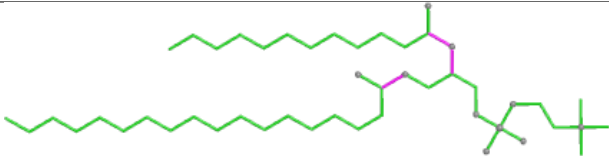
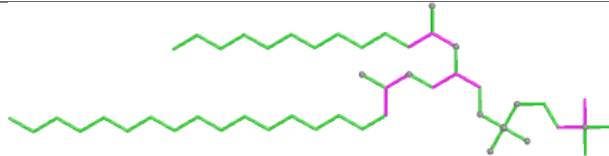
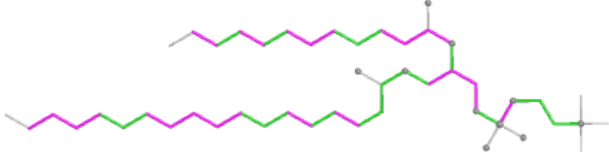
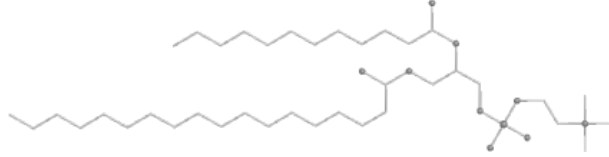
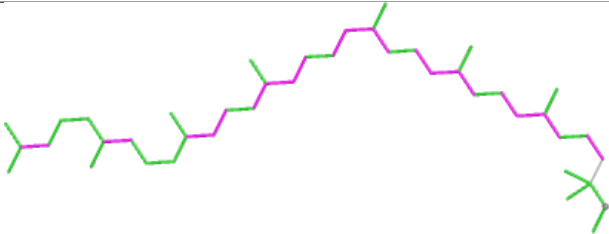
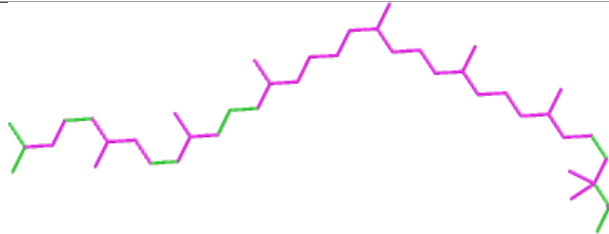
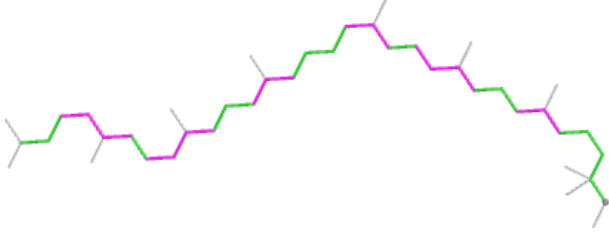
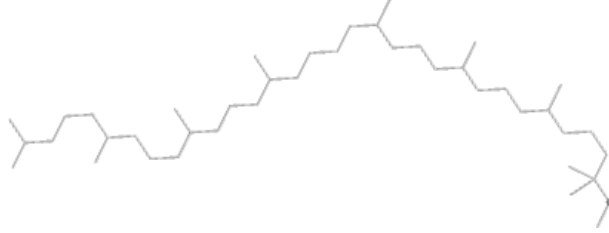


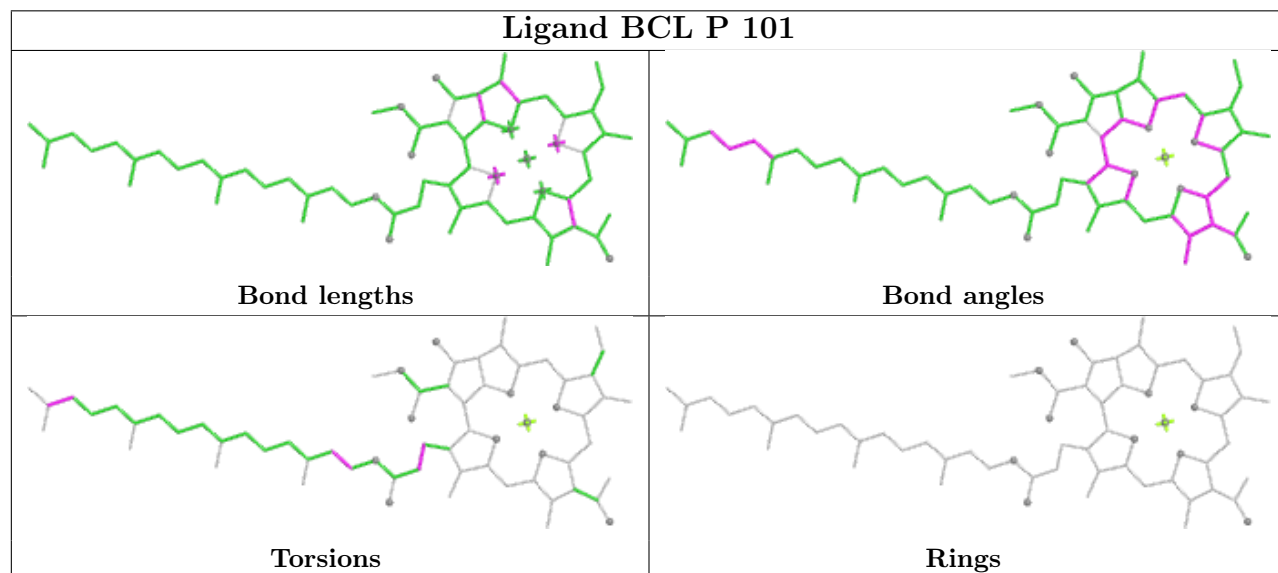
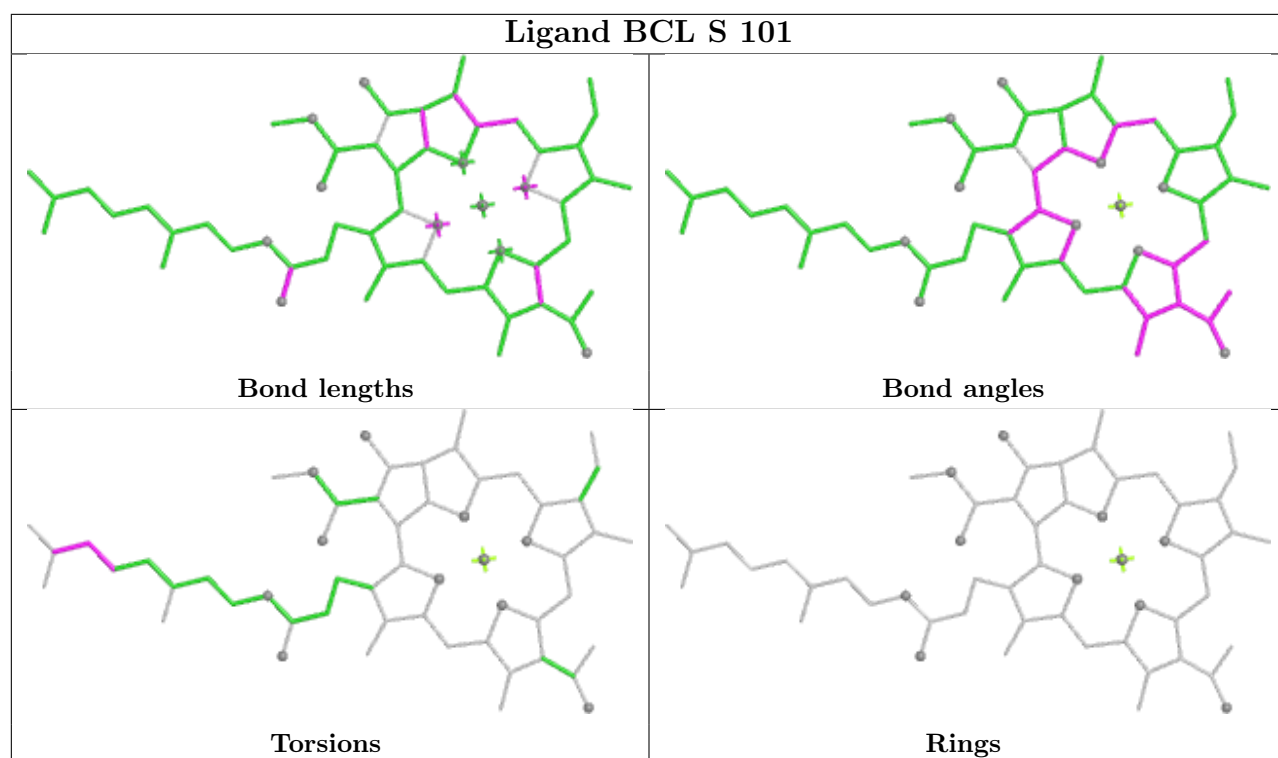


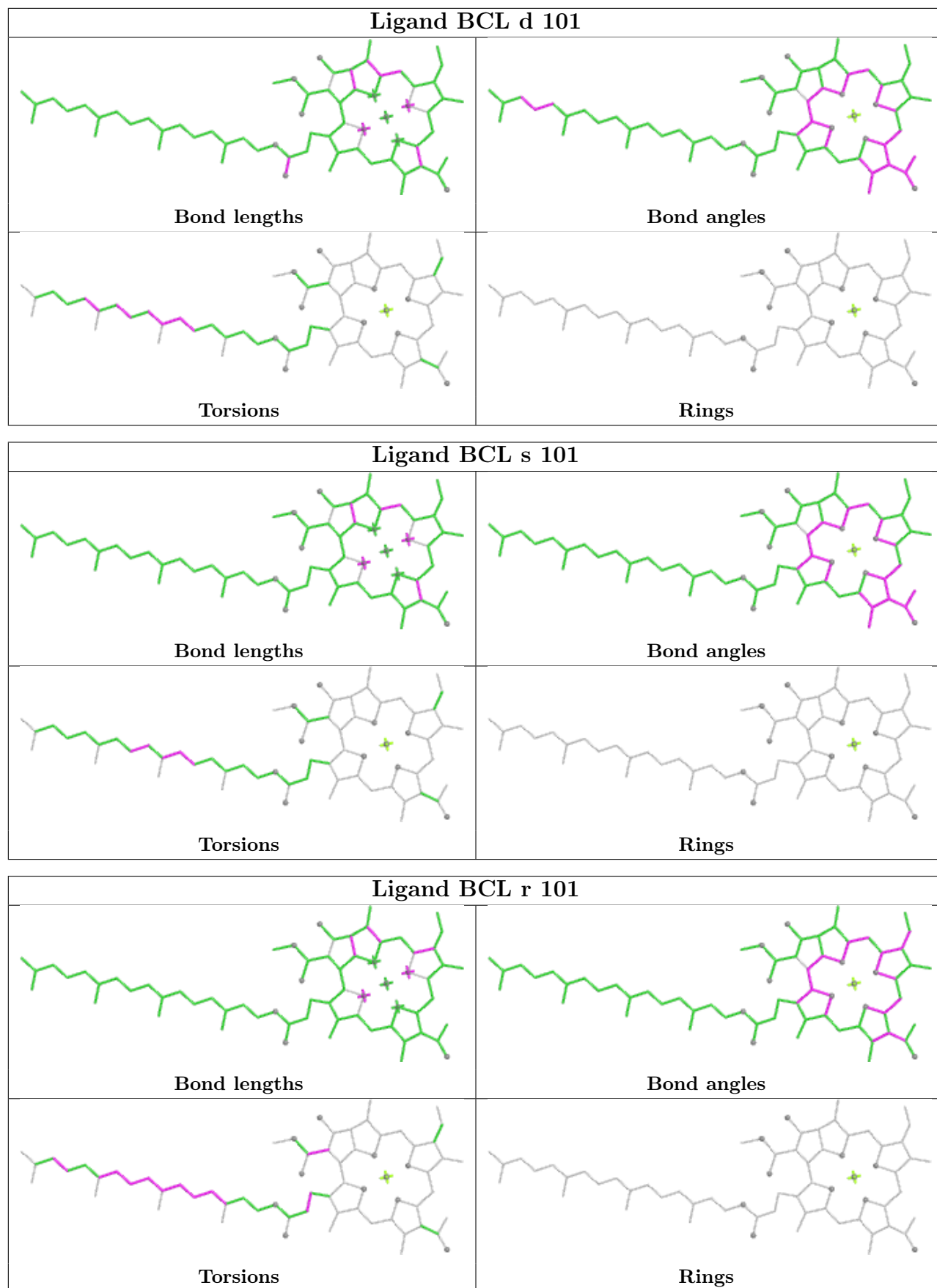




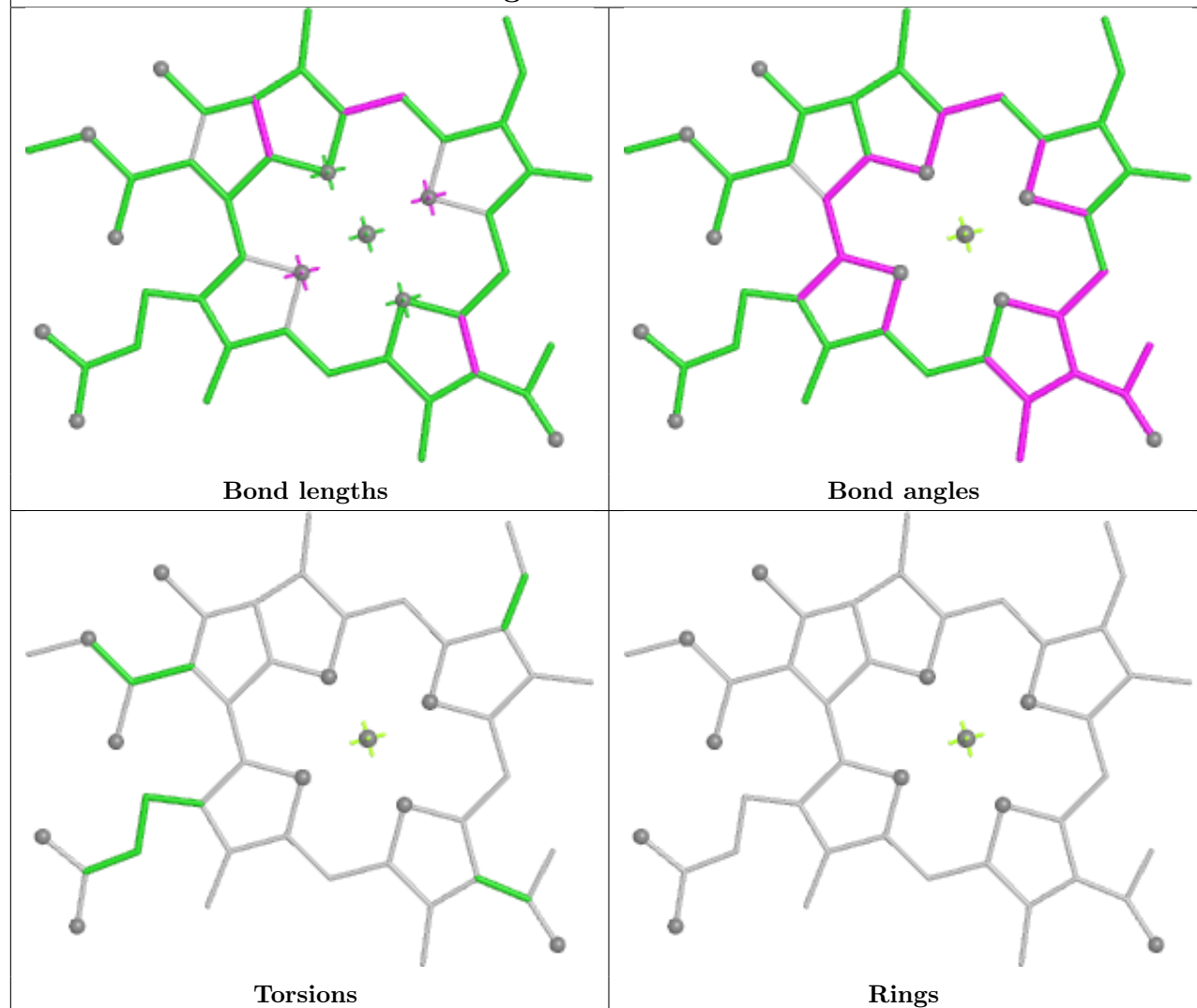


Ligand PC1 h 301	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand SPO t 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

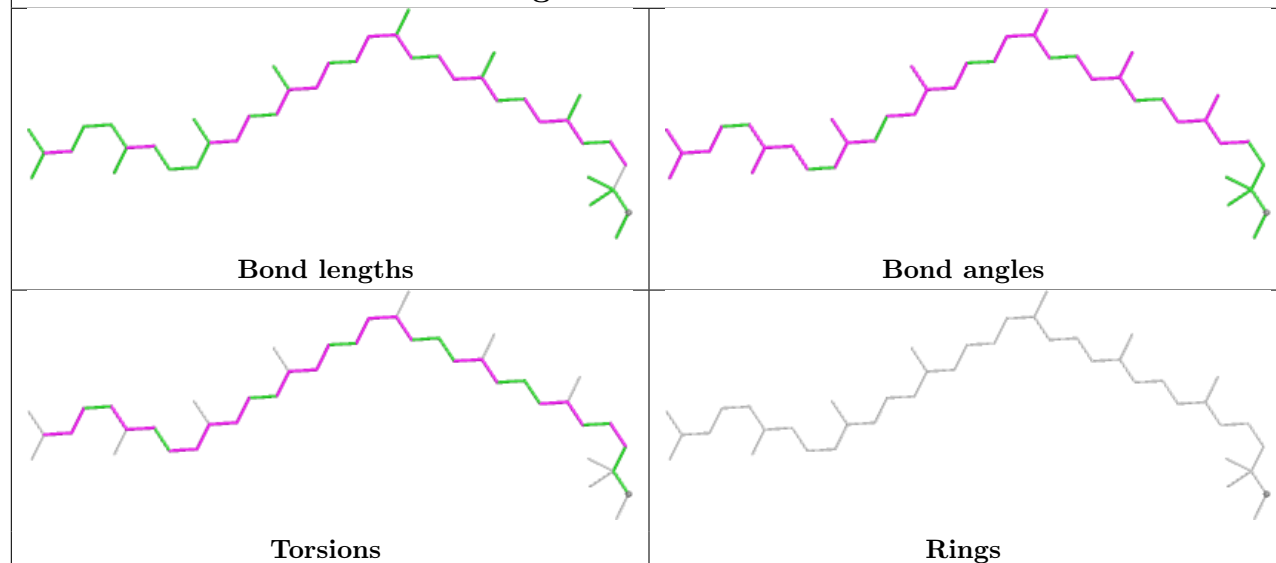


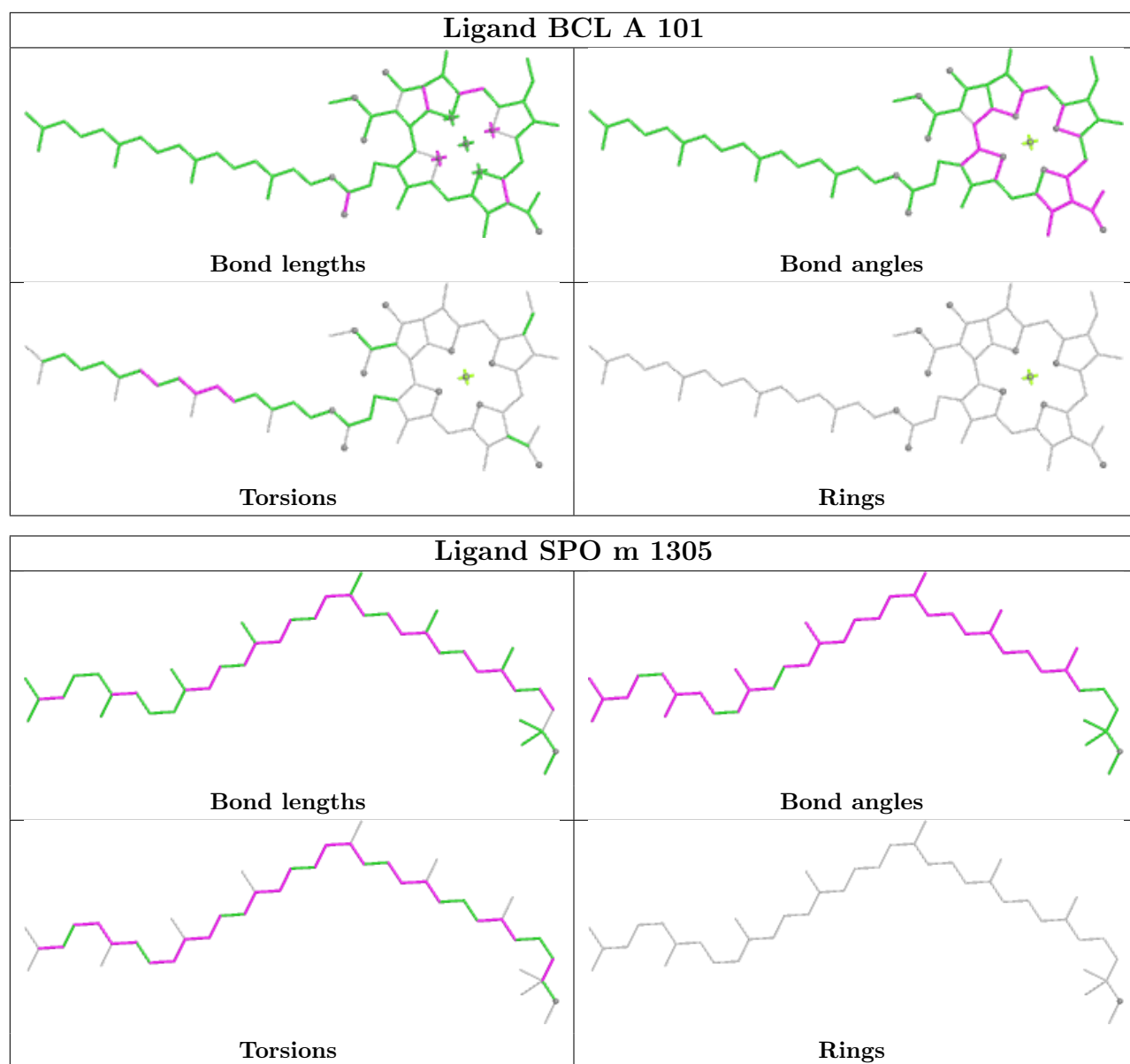


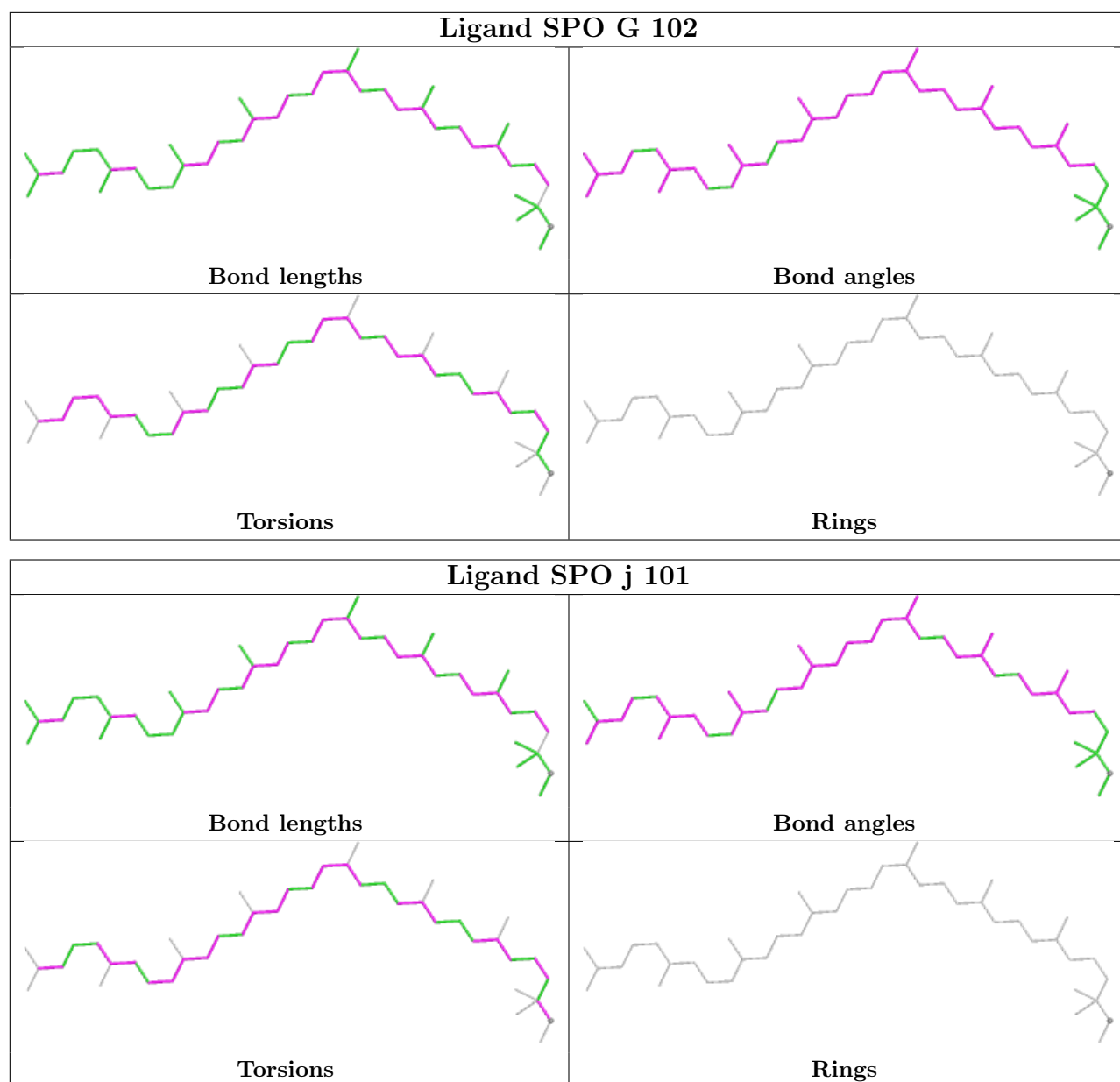
Ligand BCL 2 101

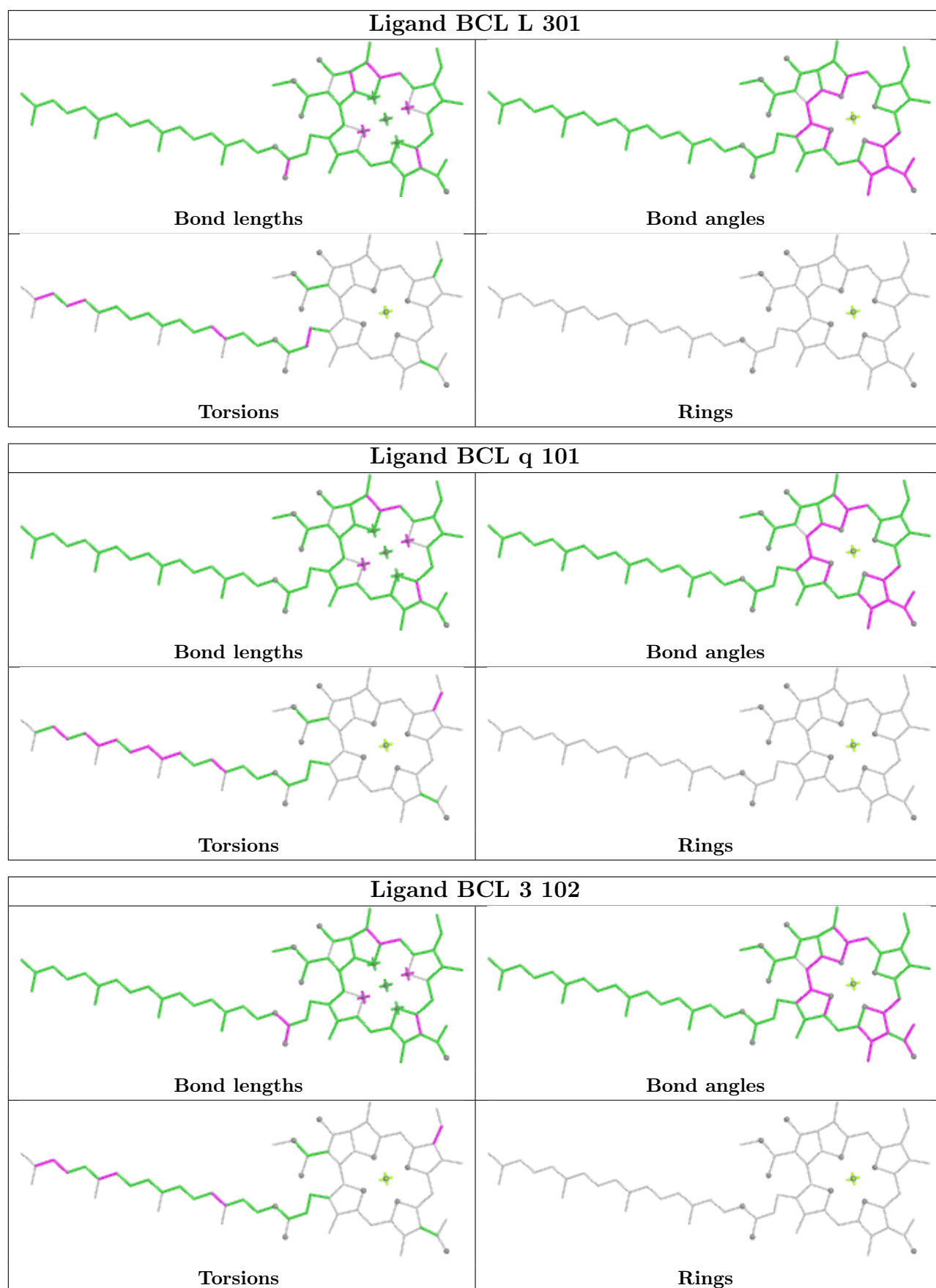


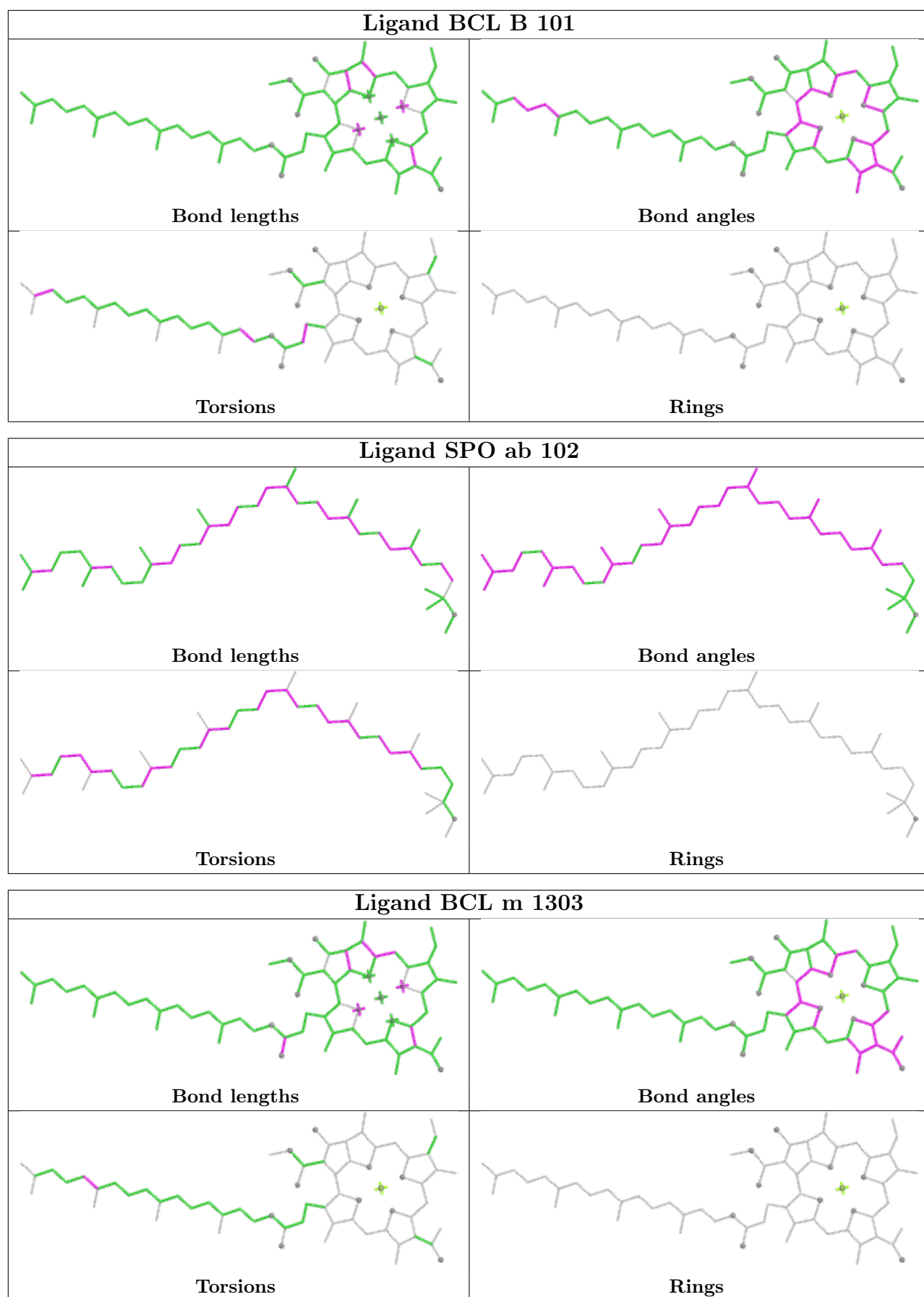
Ligand SPO N 101

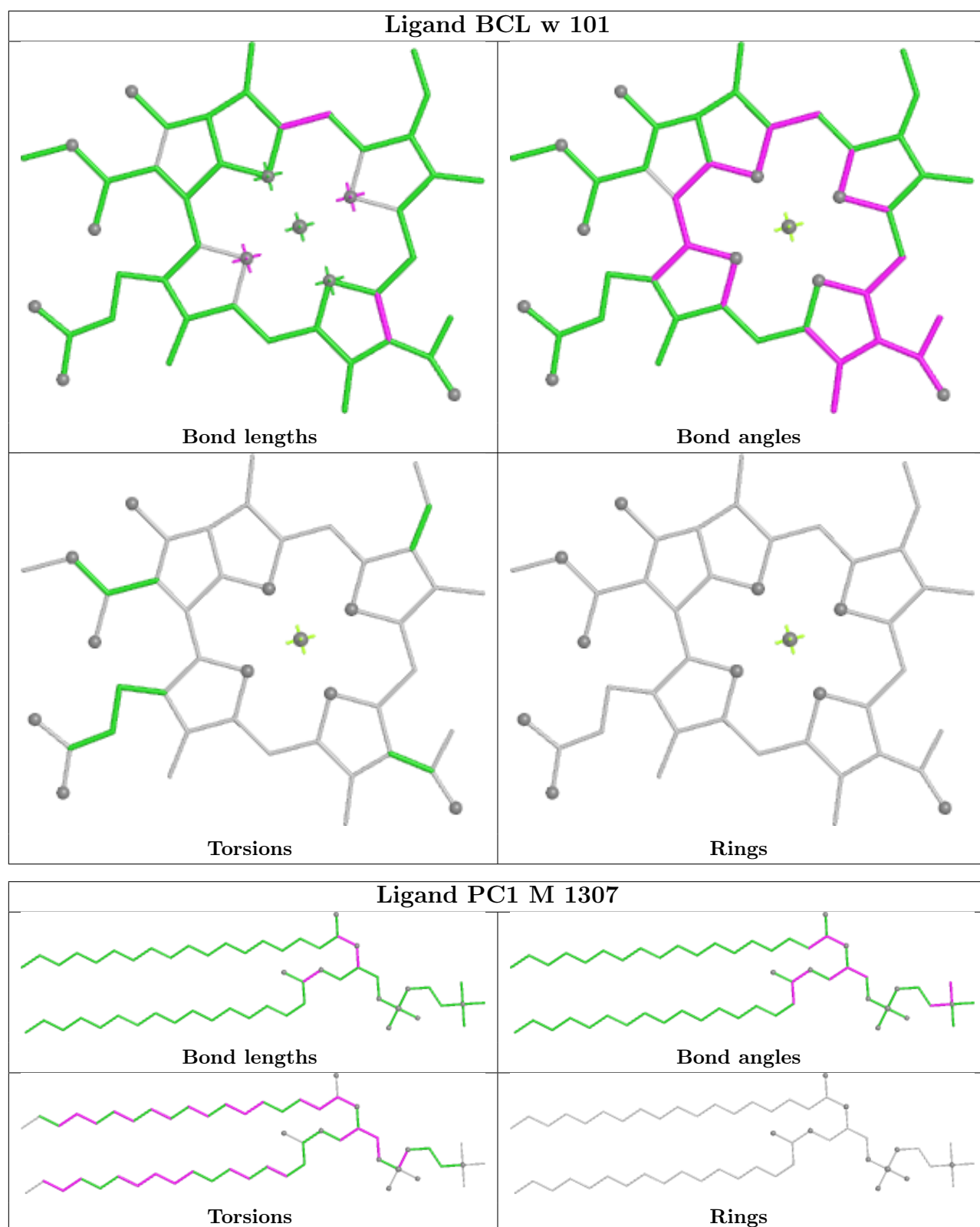


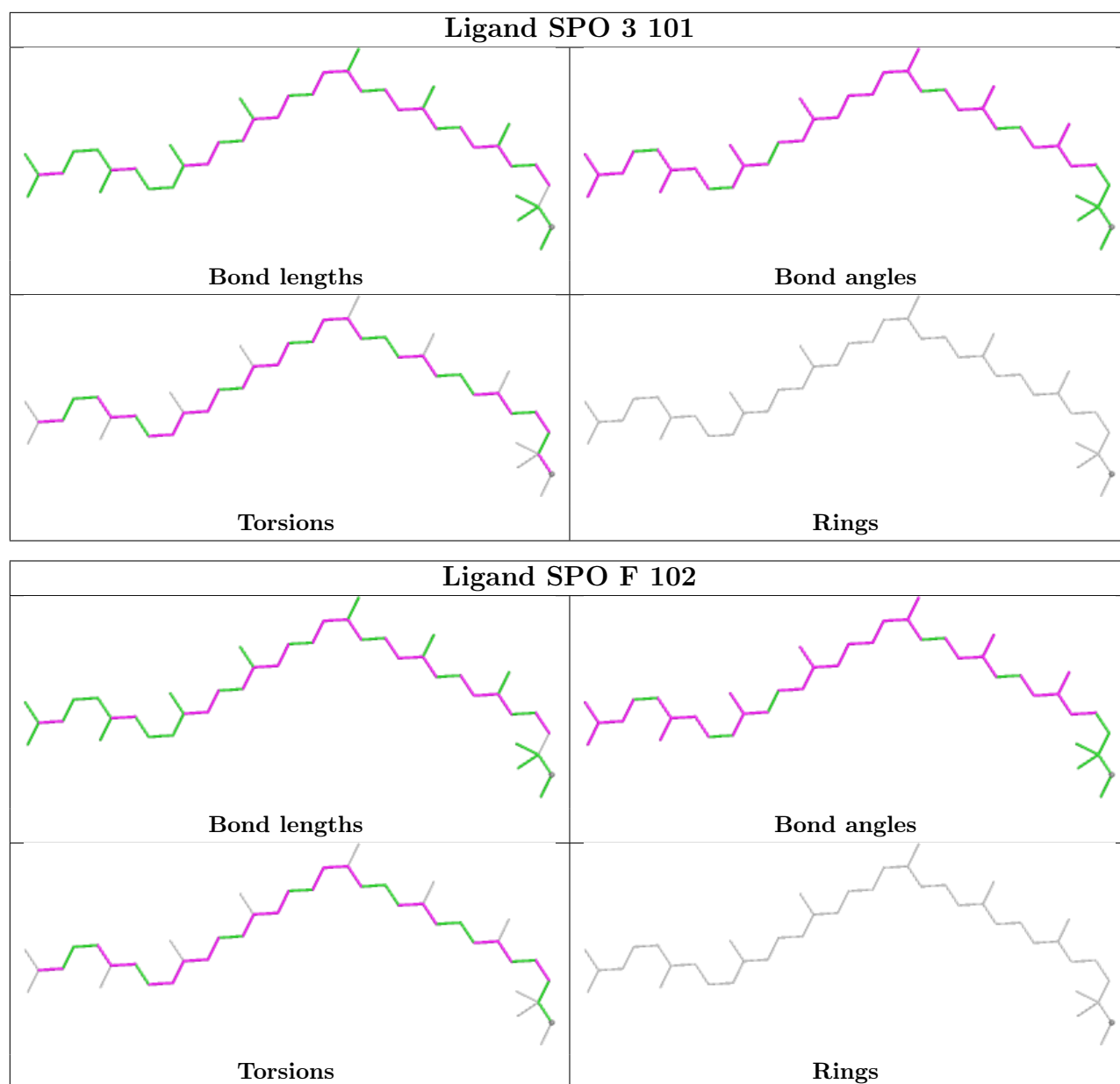


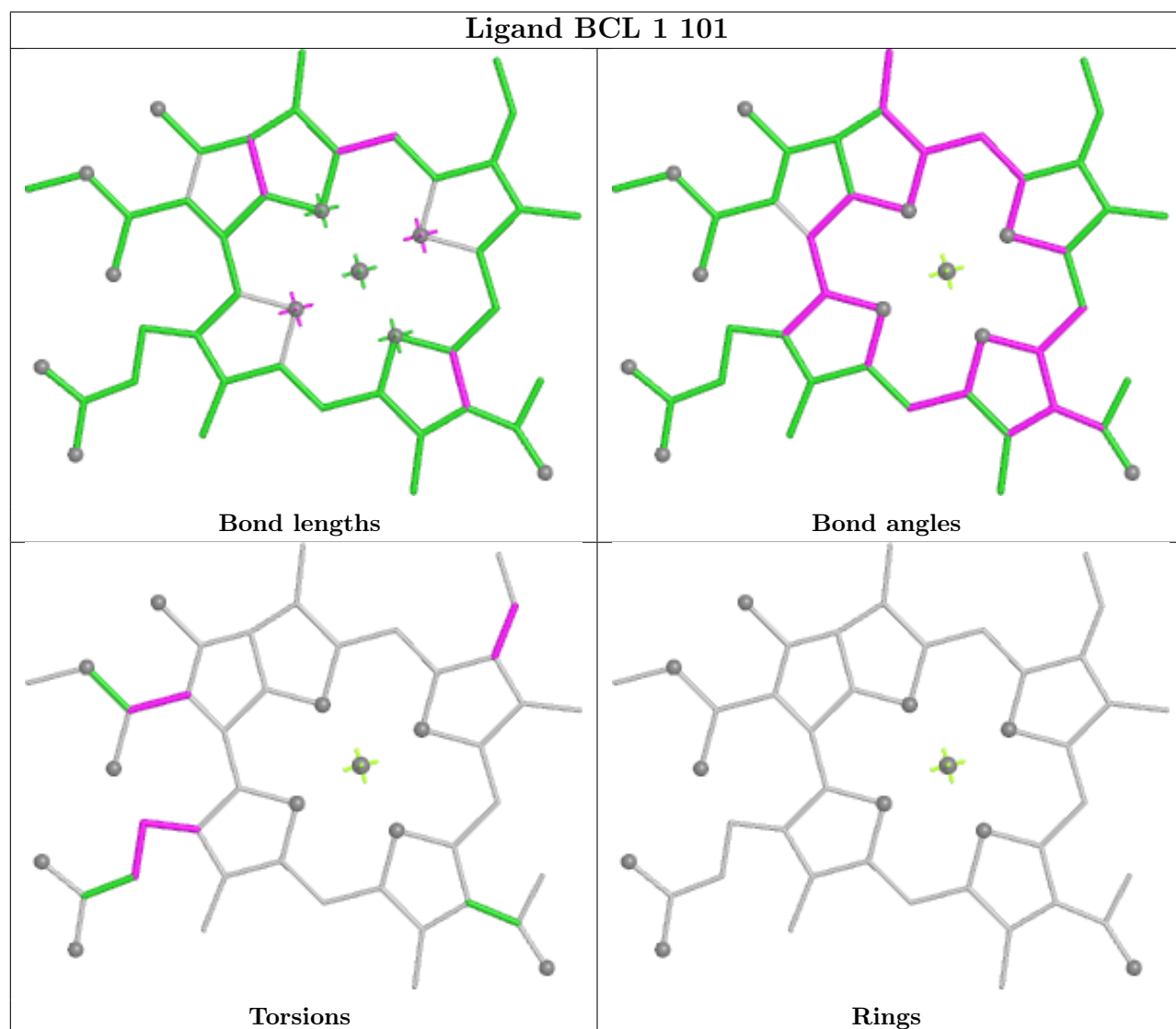
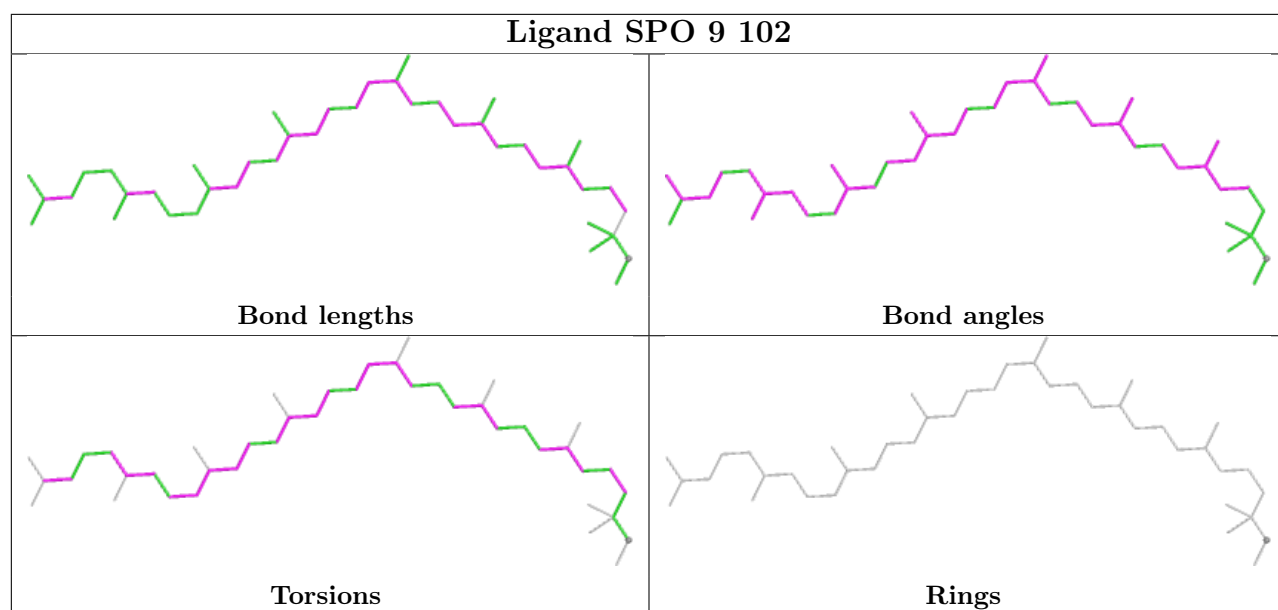


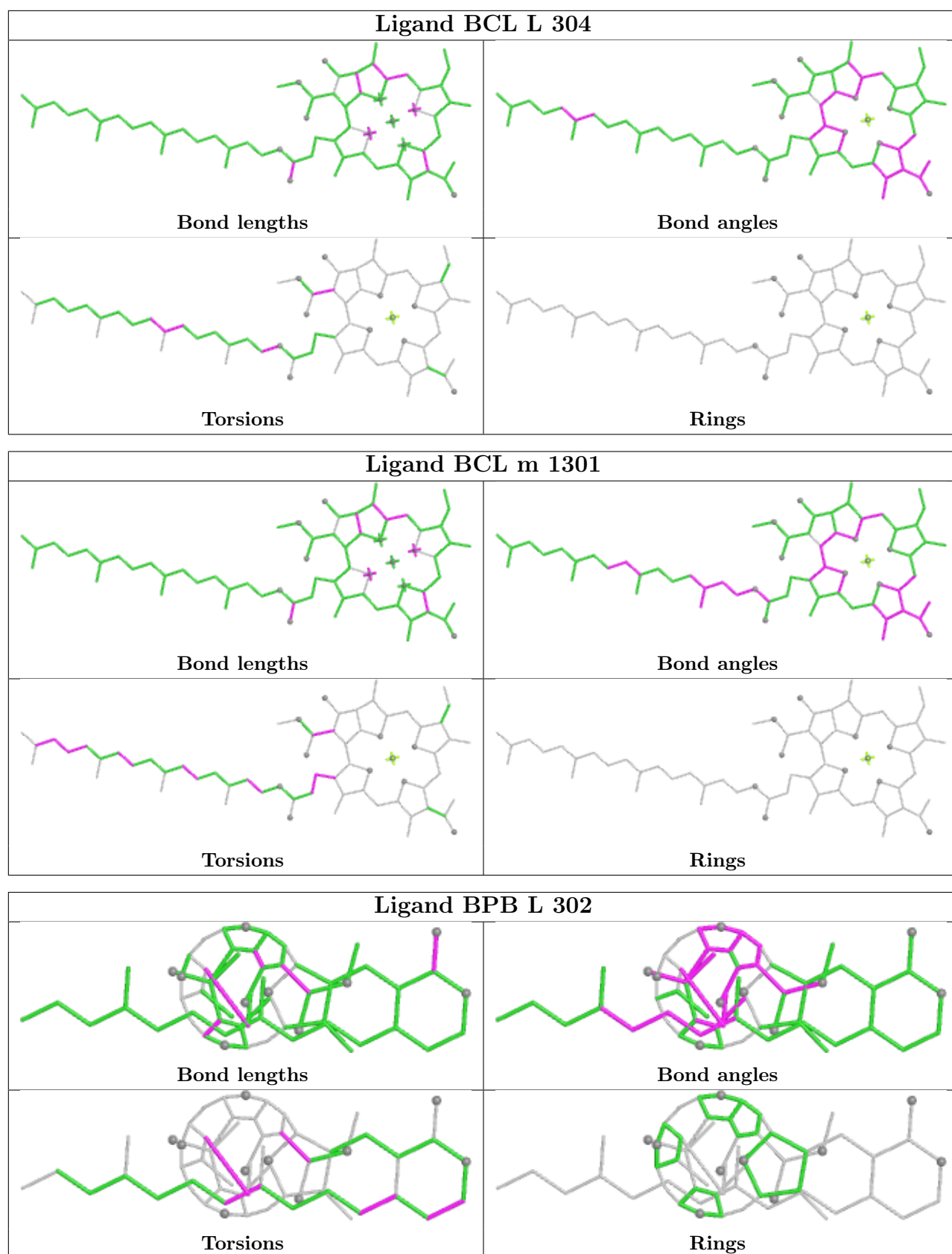


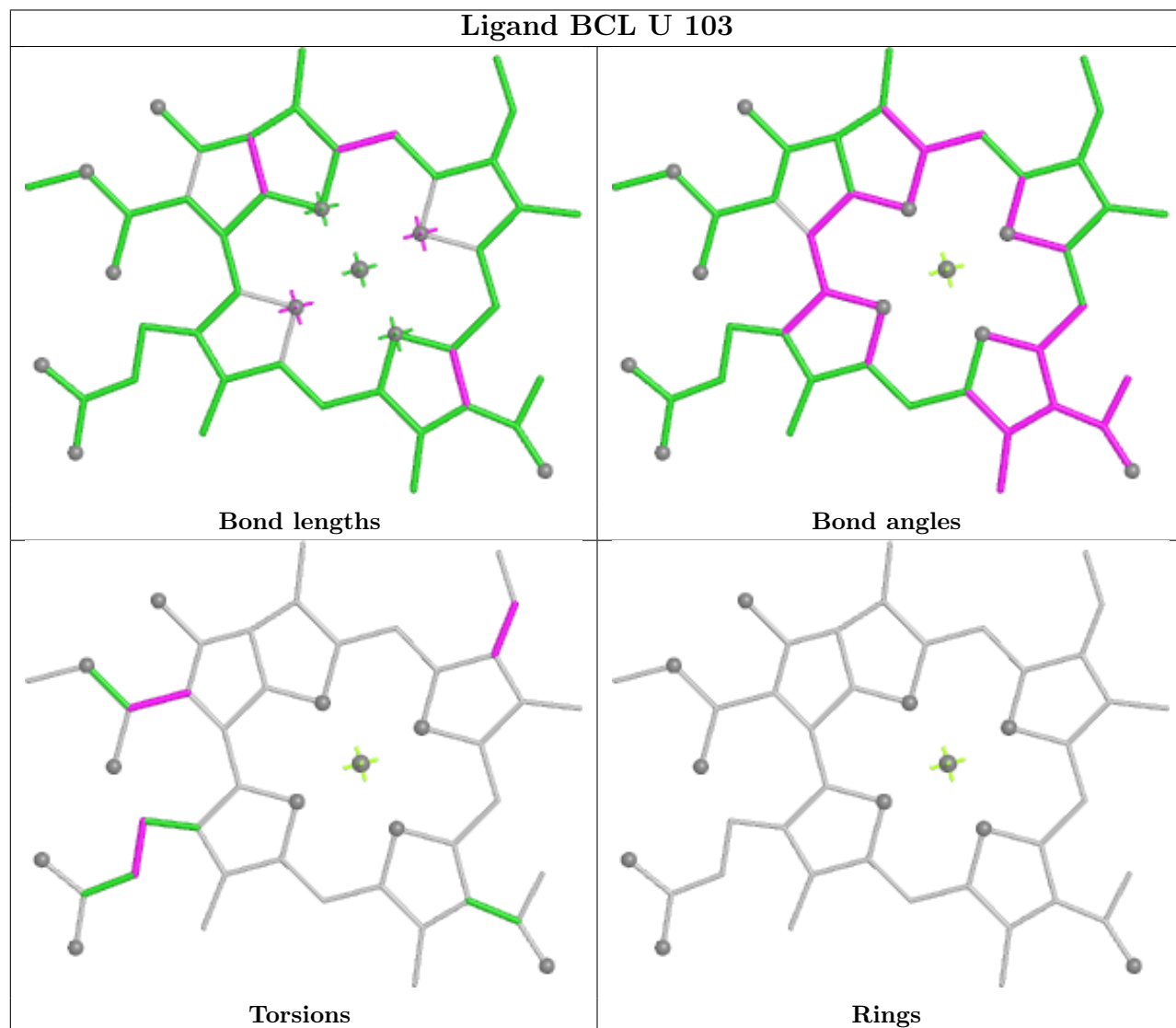
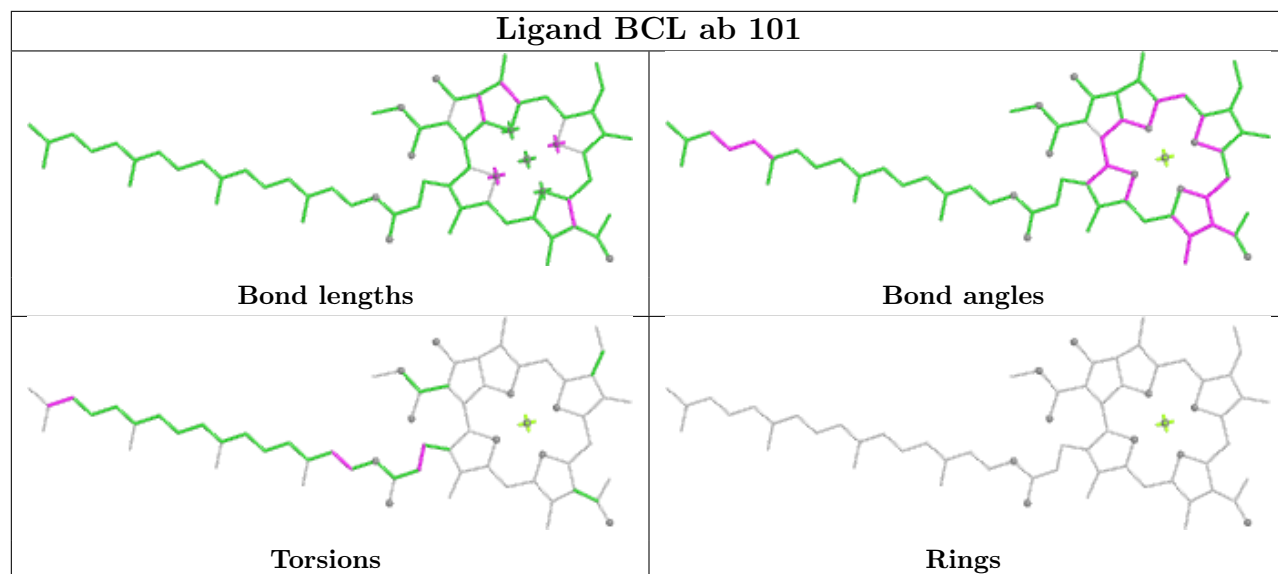


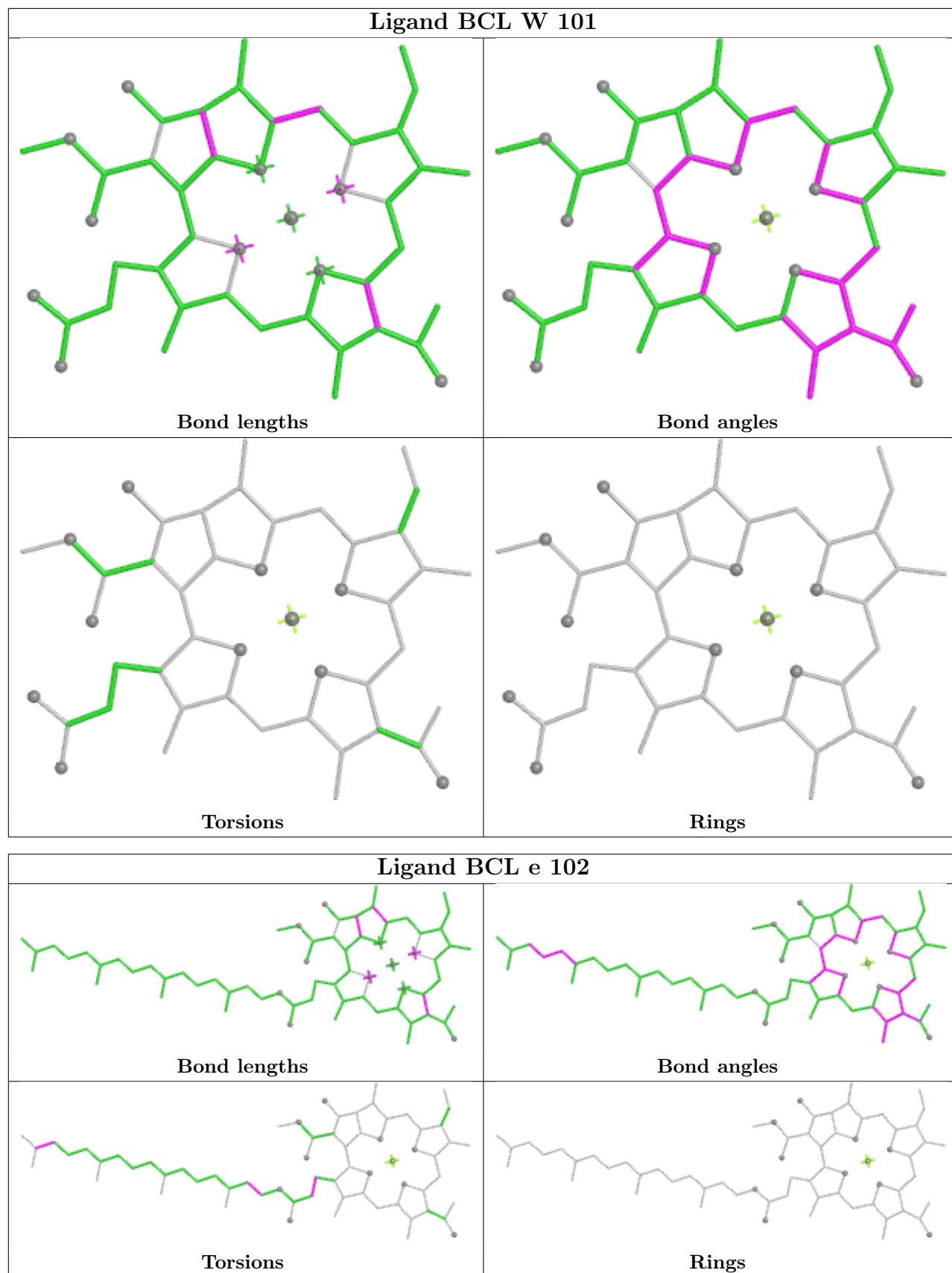


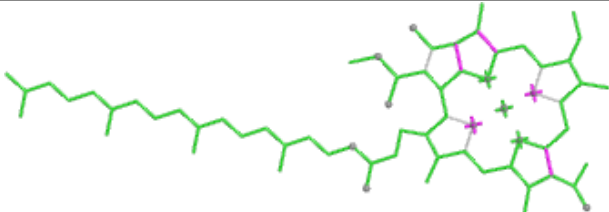
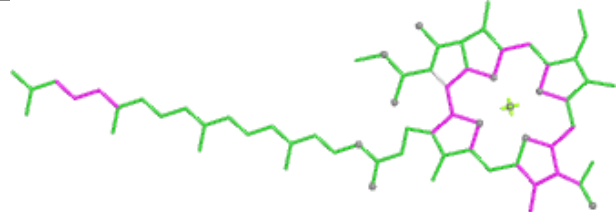
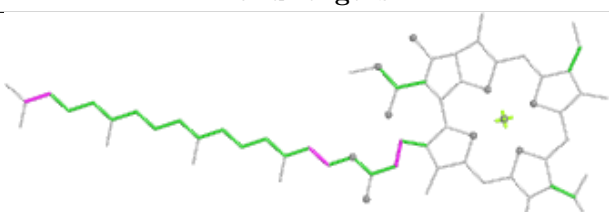
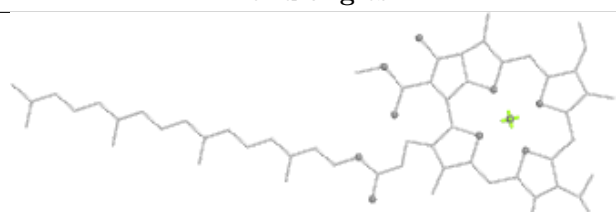
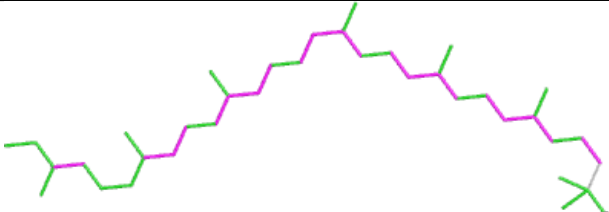
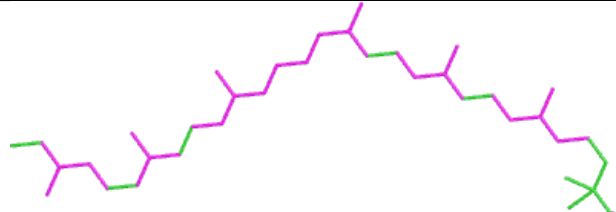
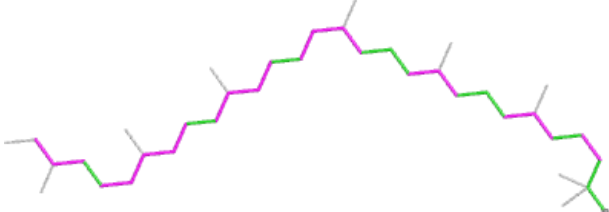
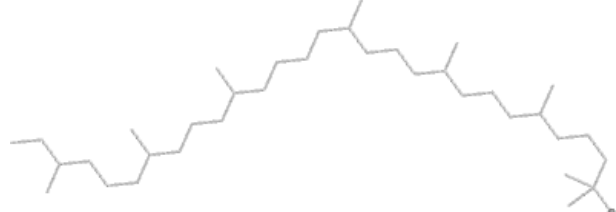


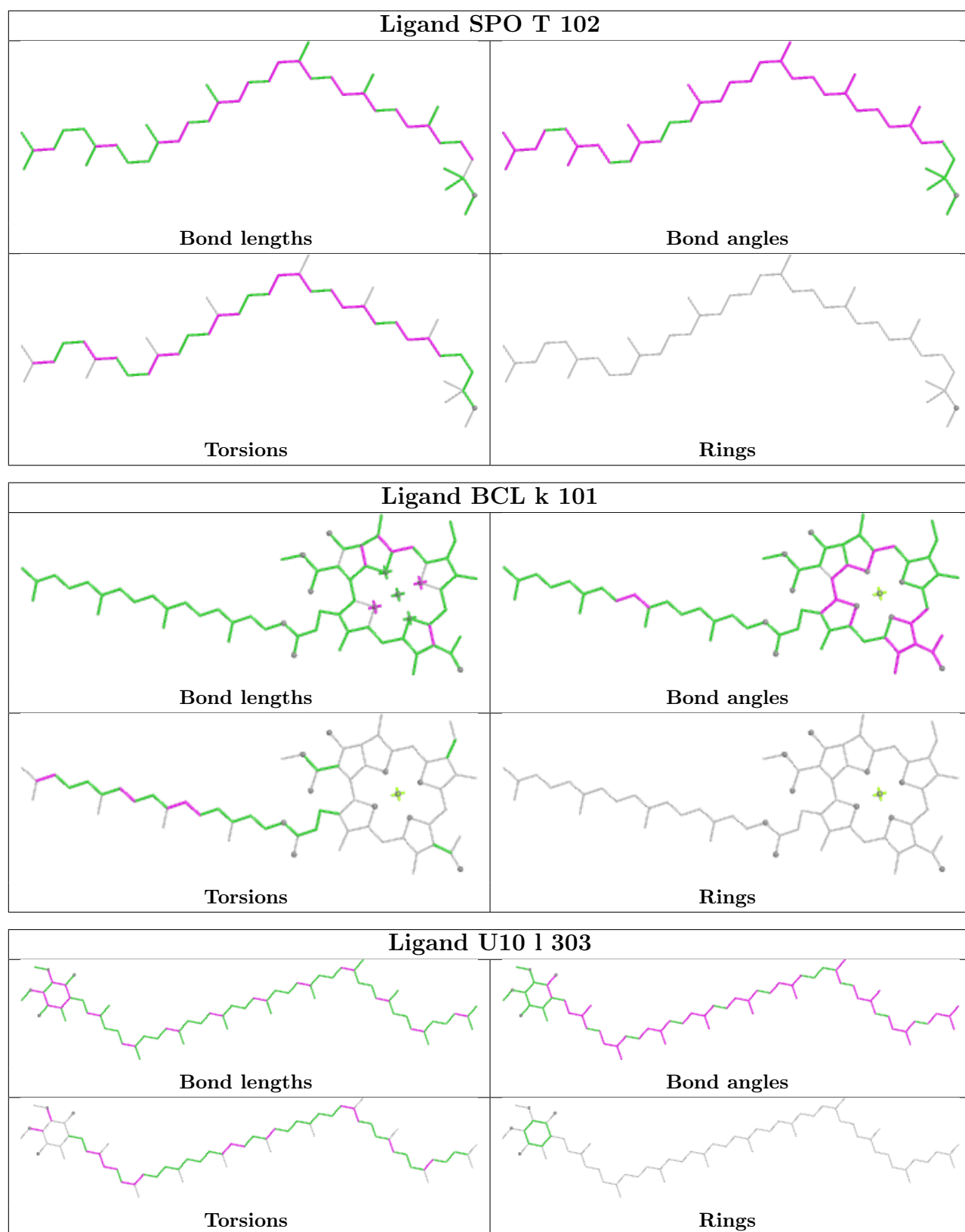


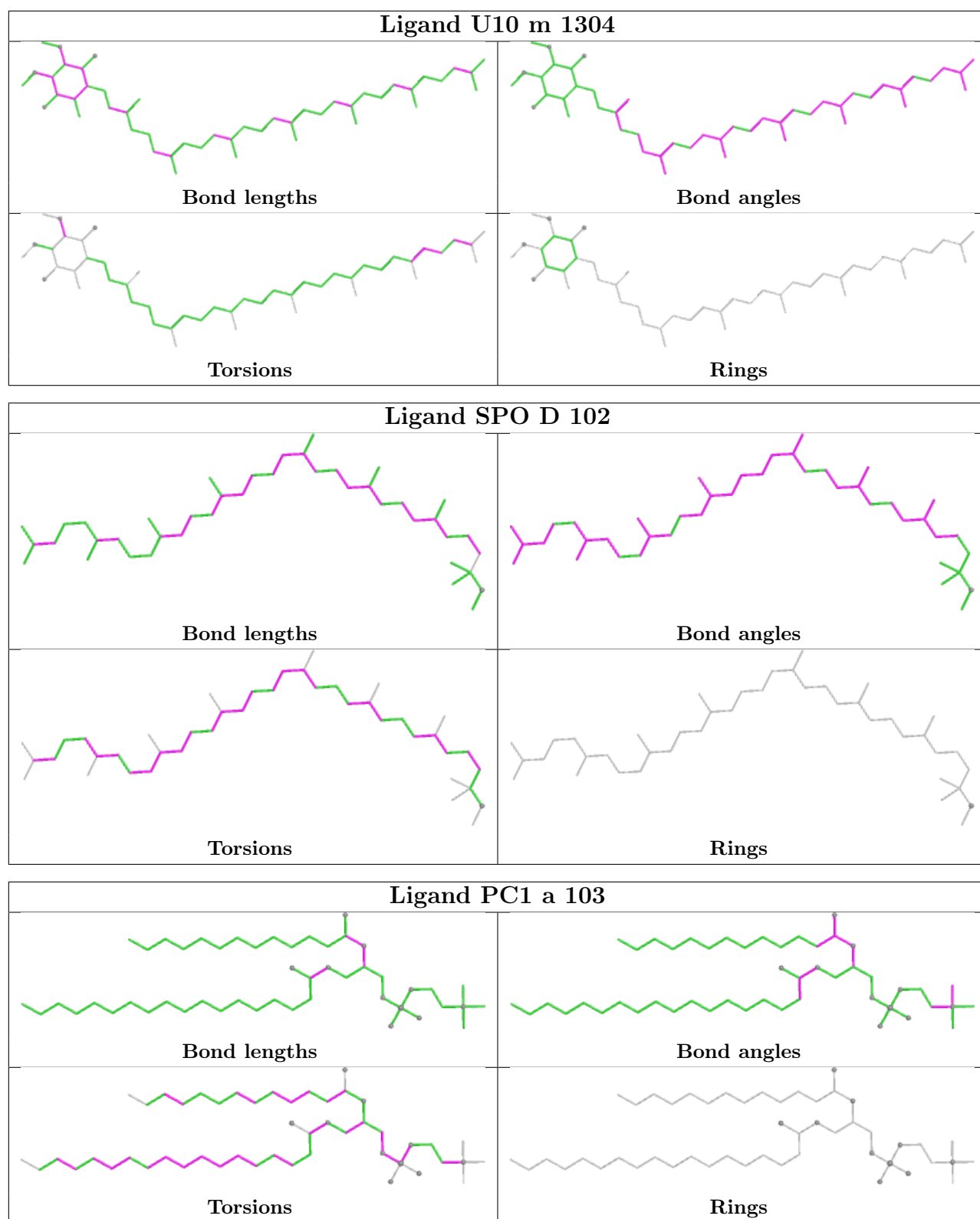


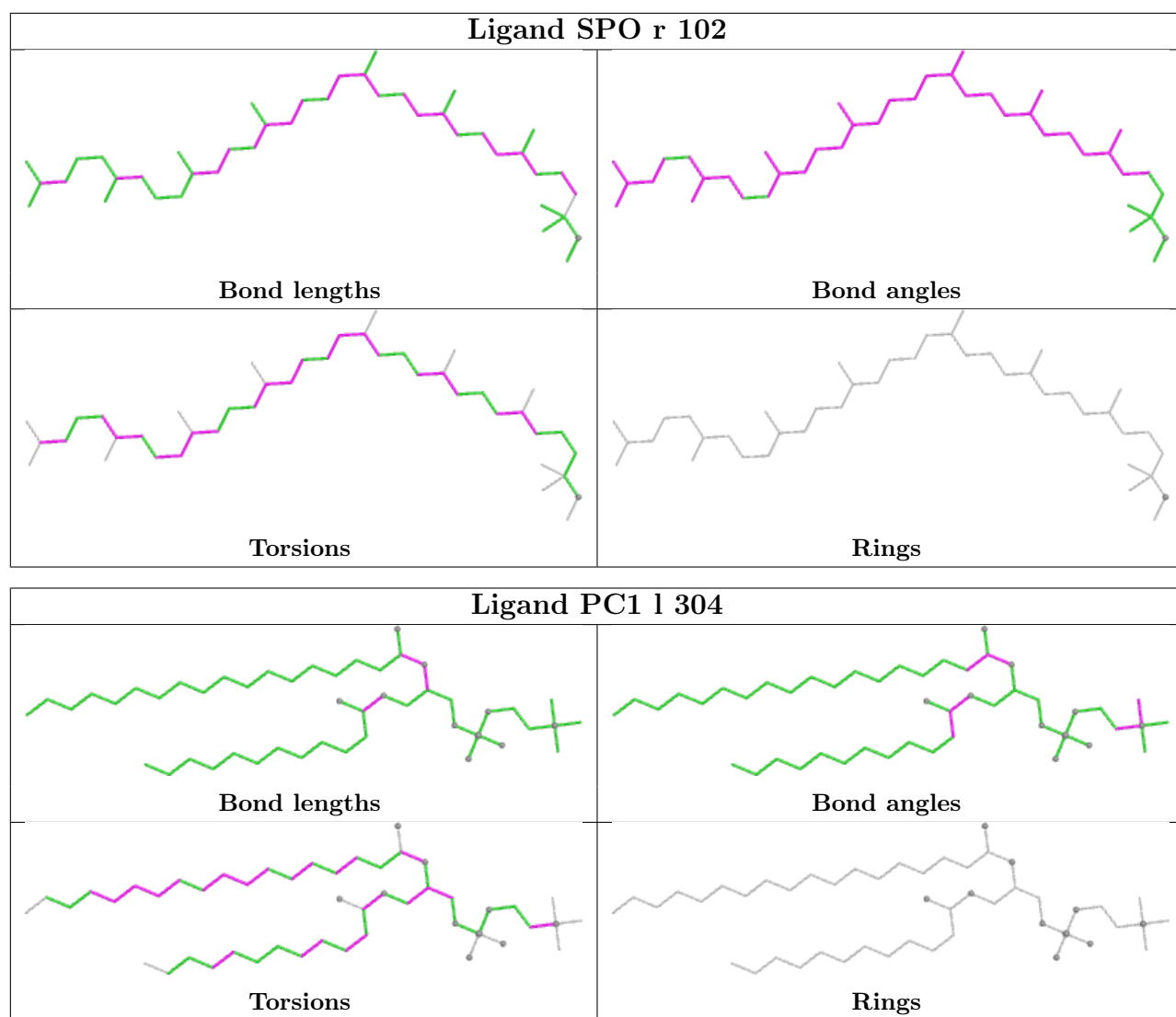


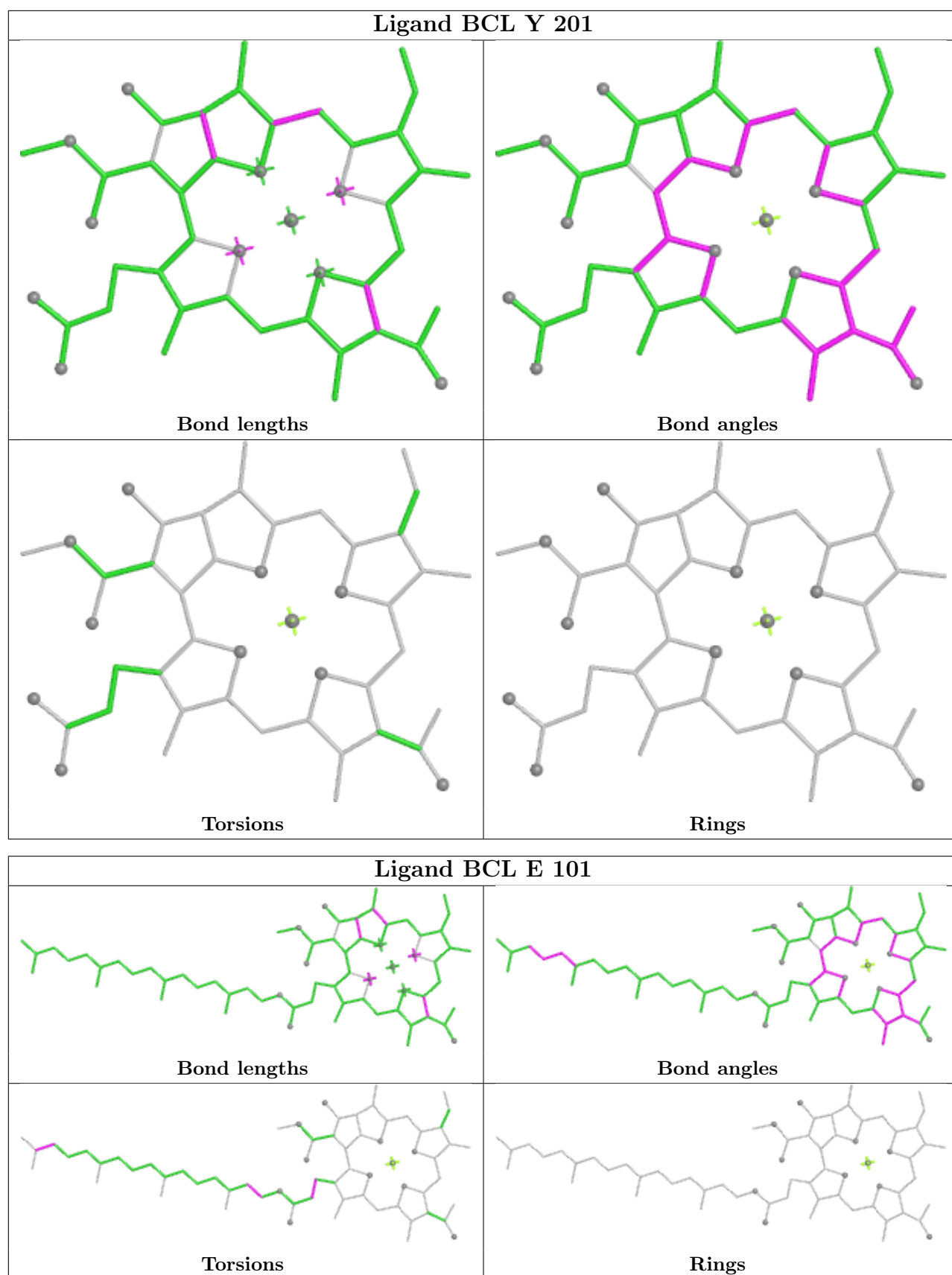


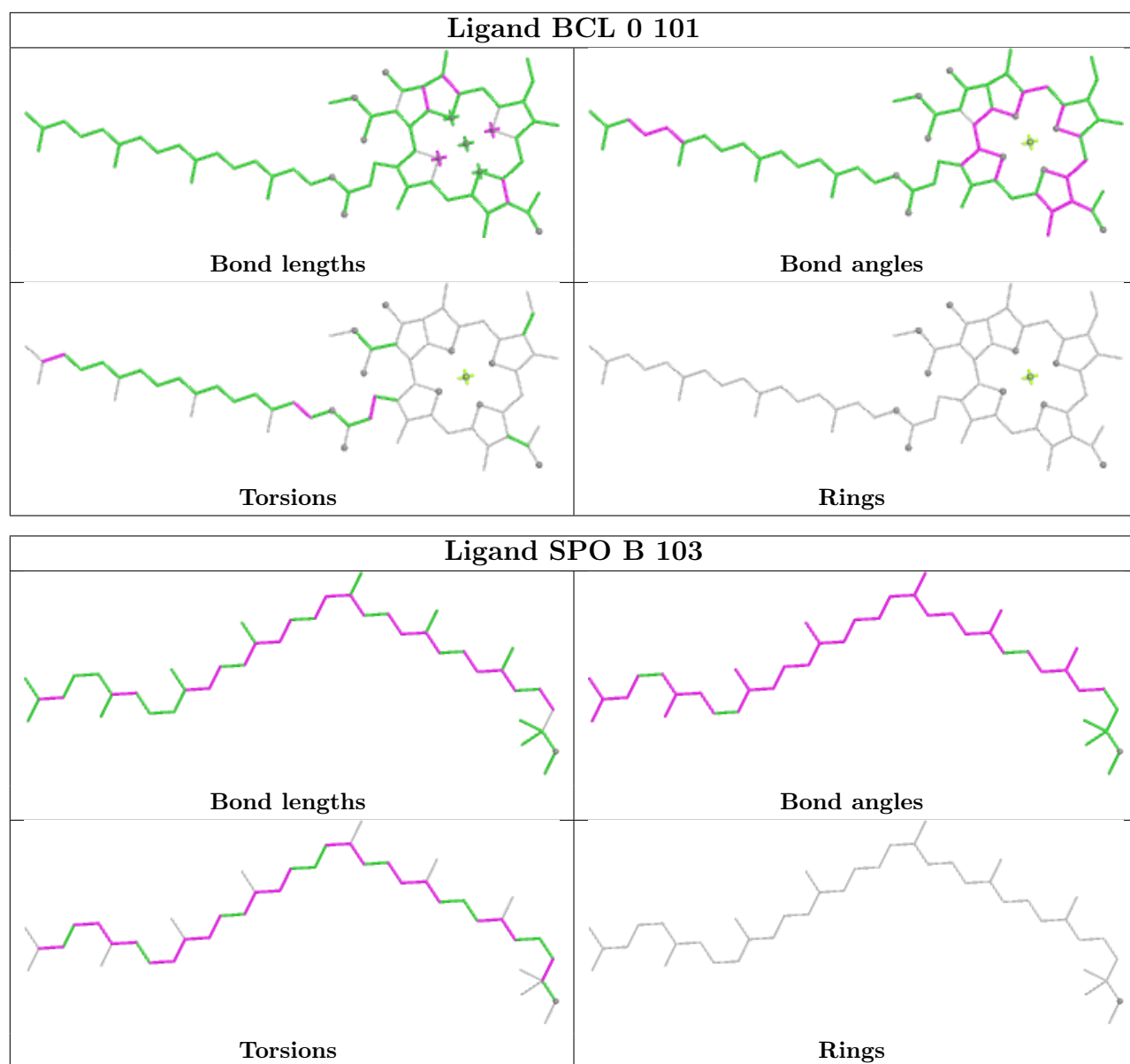
Ligand BCL G 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand SPO S 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

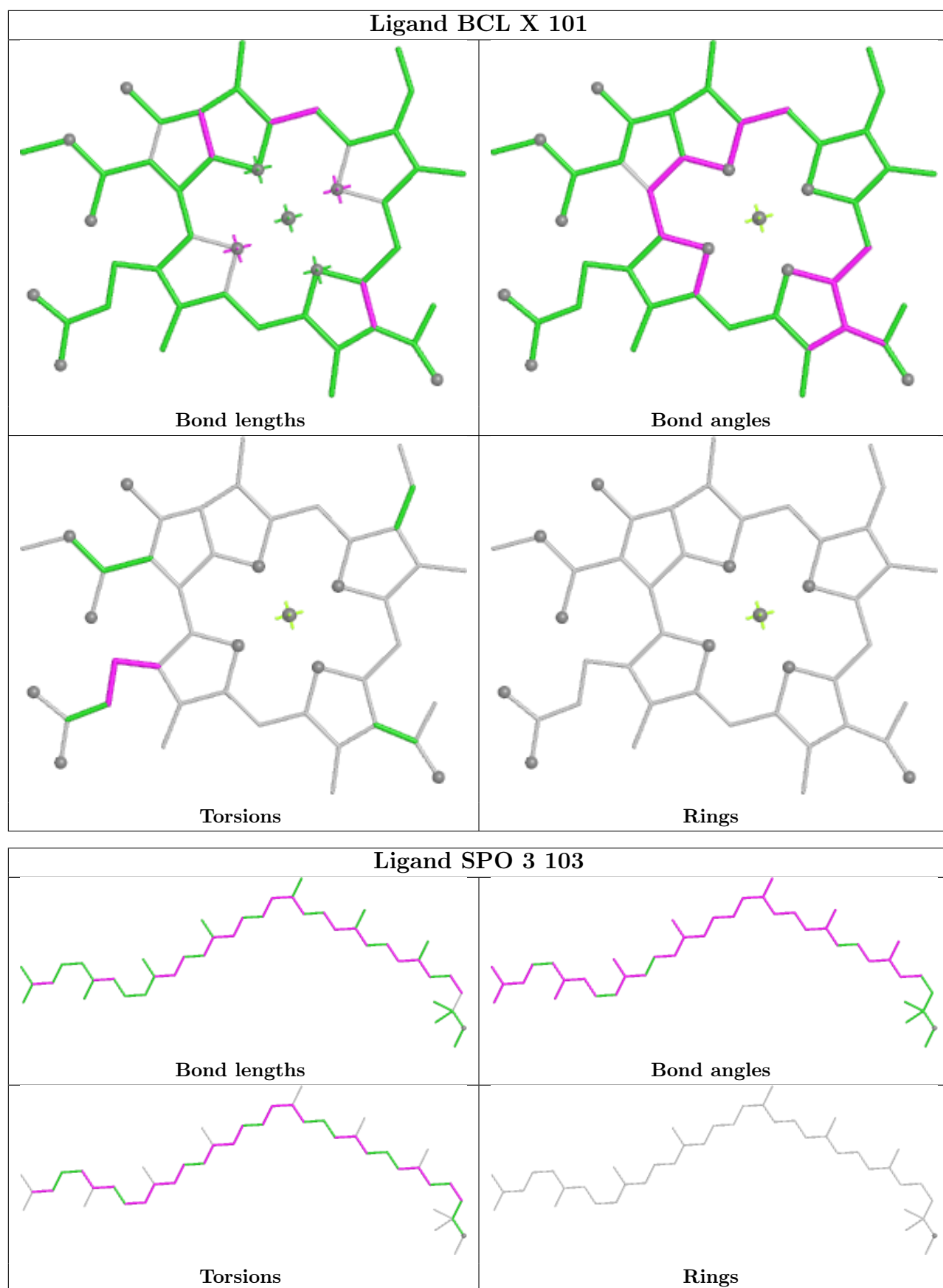




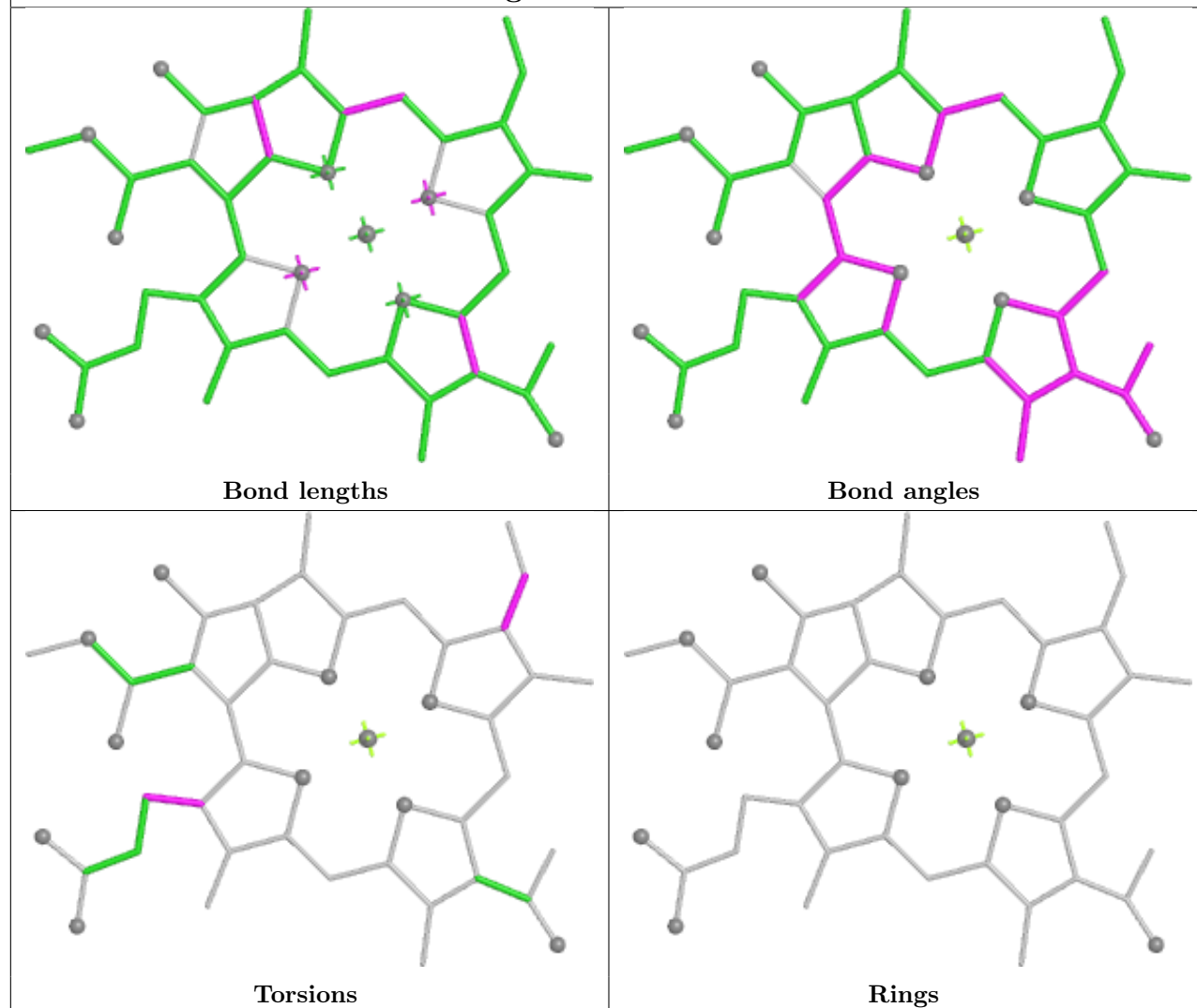




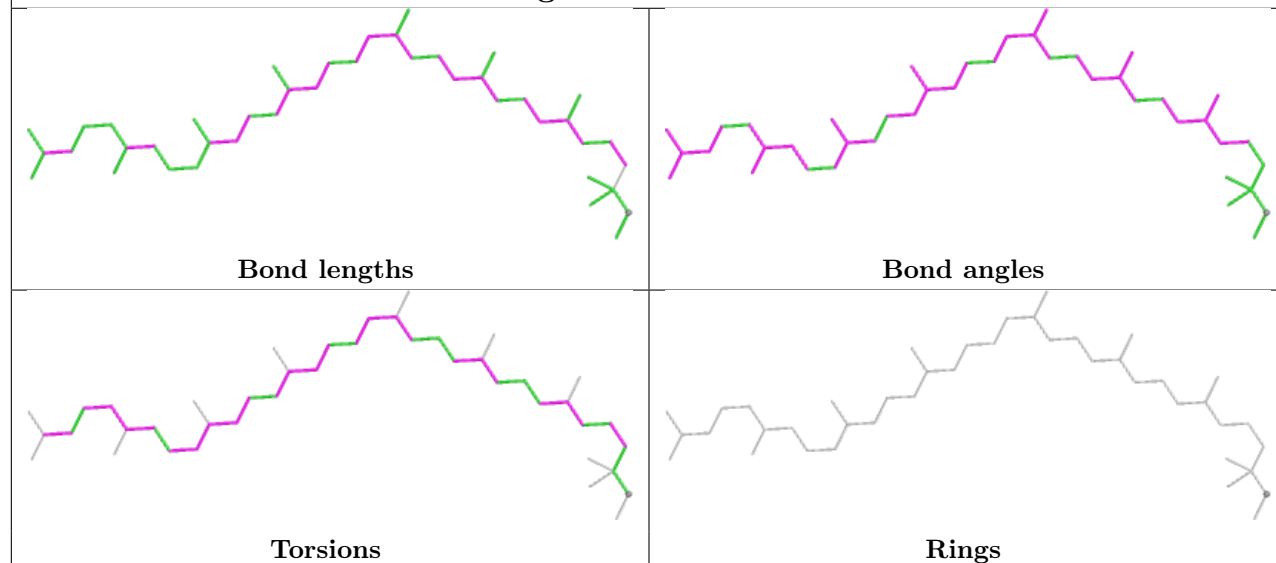




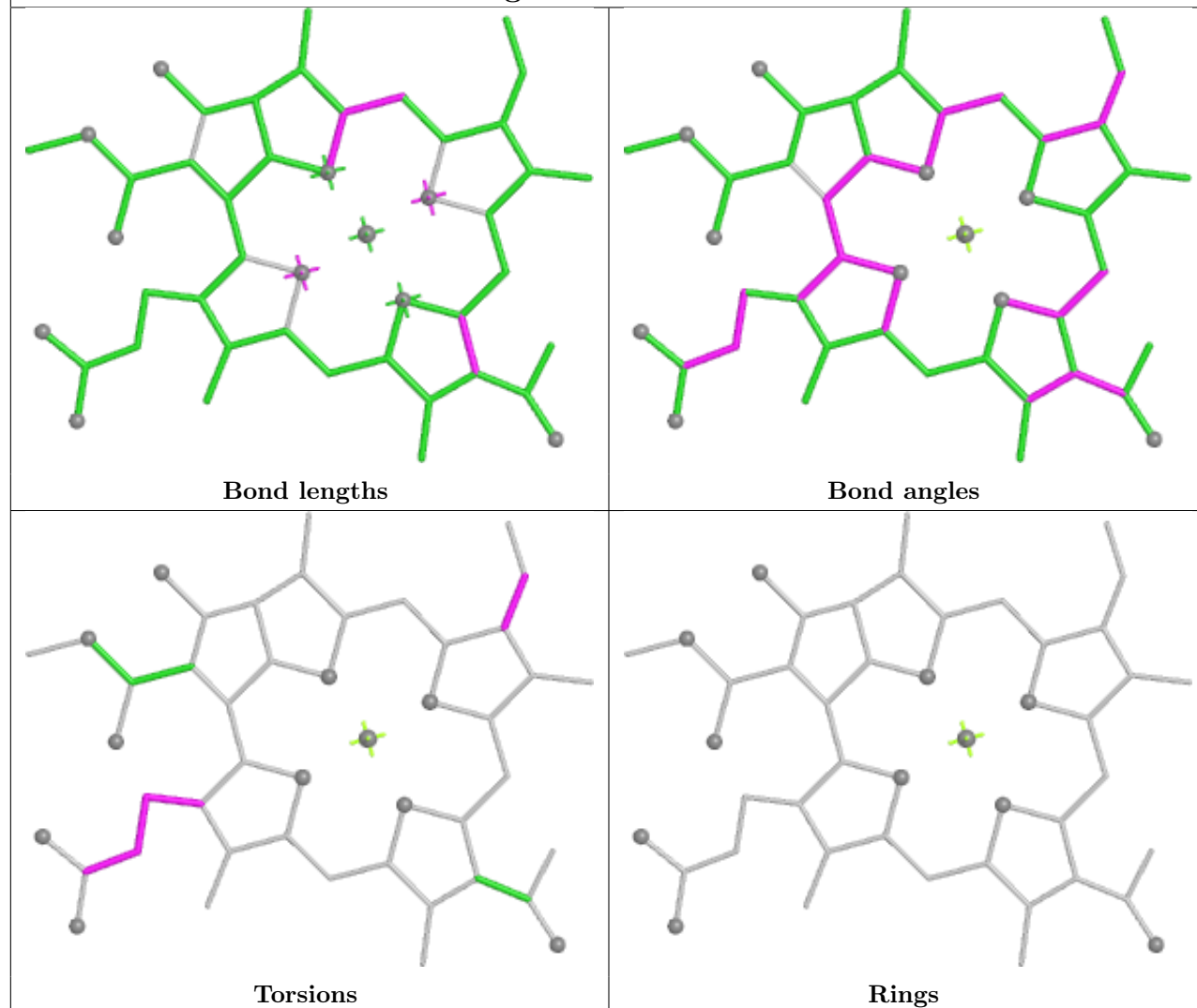
Ligand BCL s 103



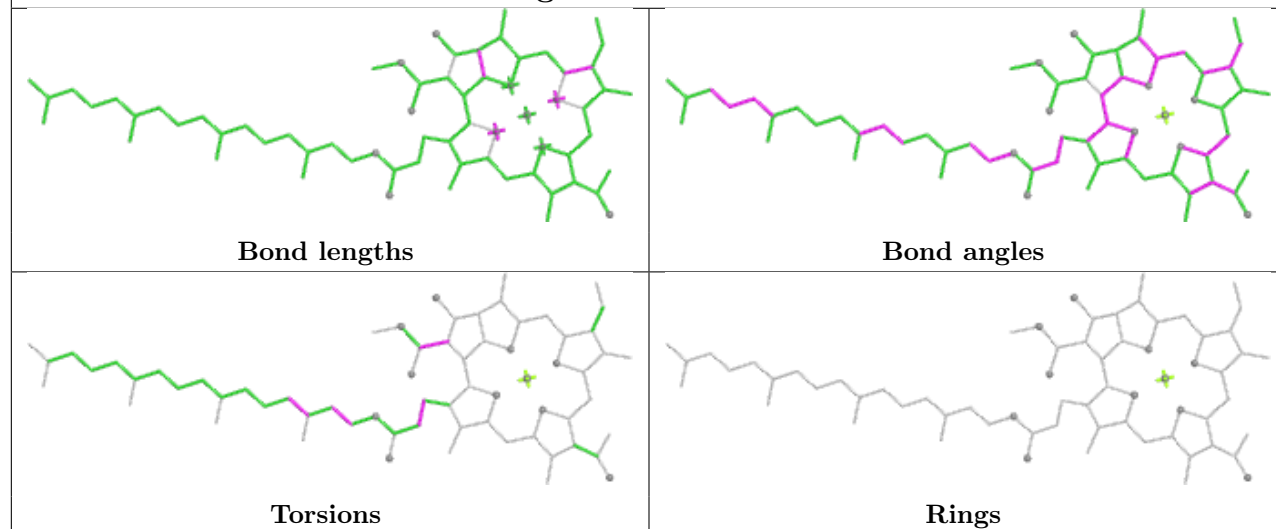
Ligand SPO o 102

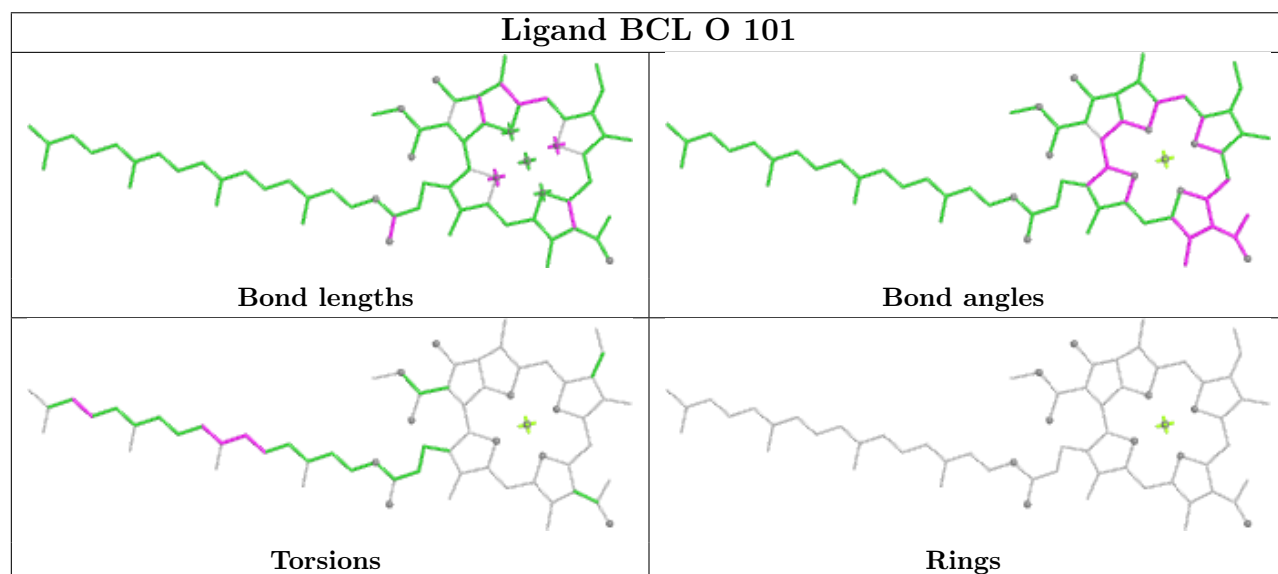
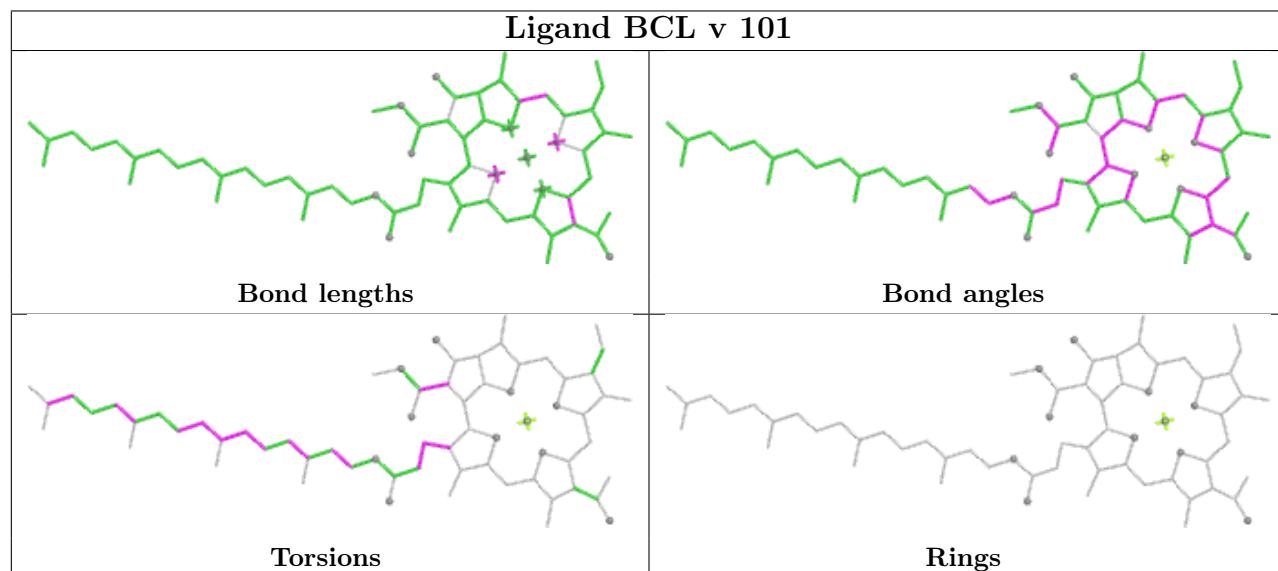
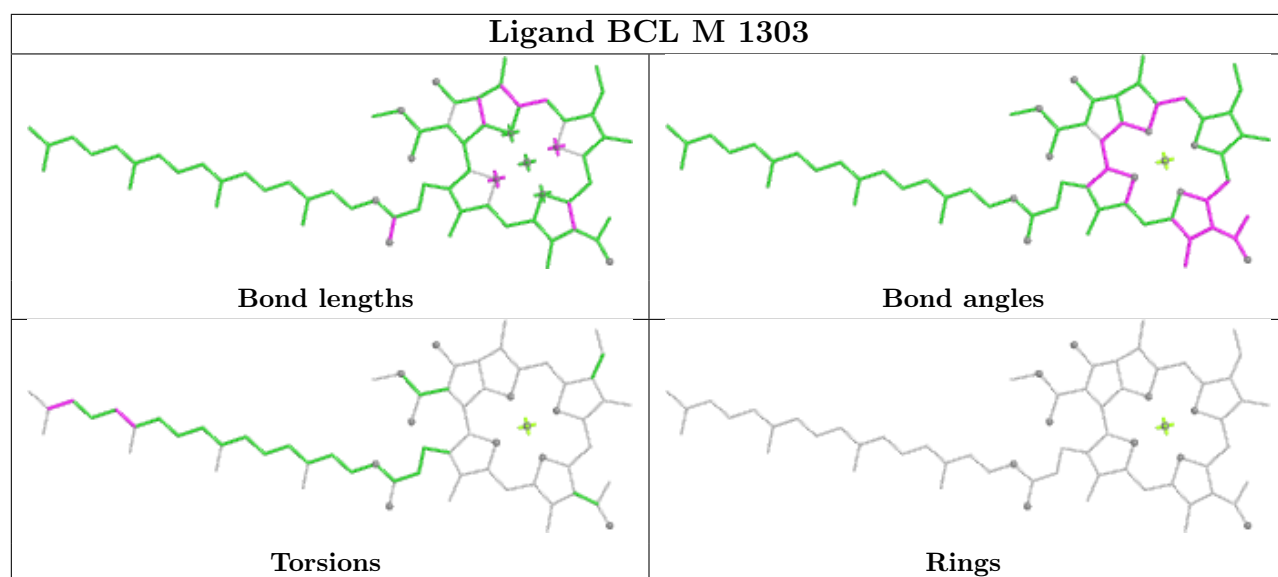


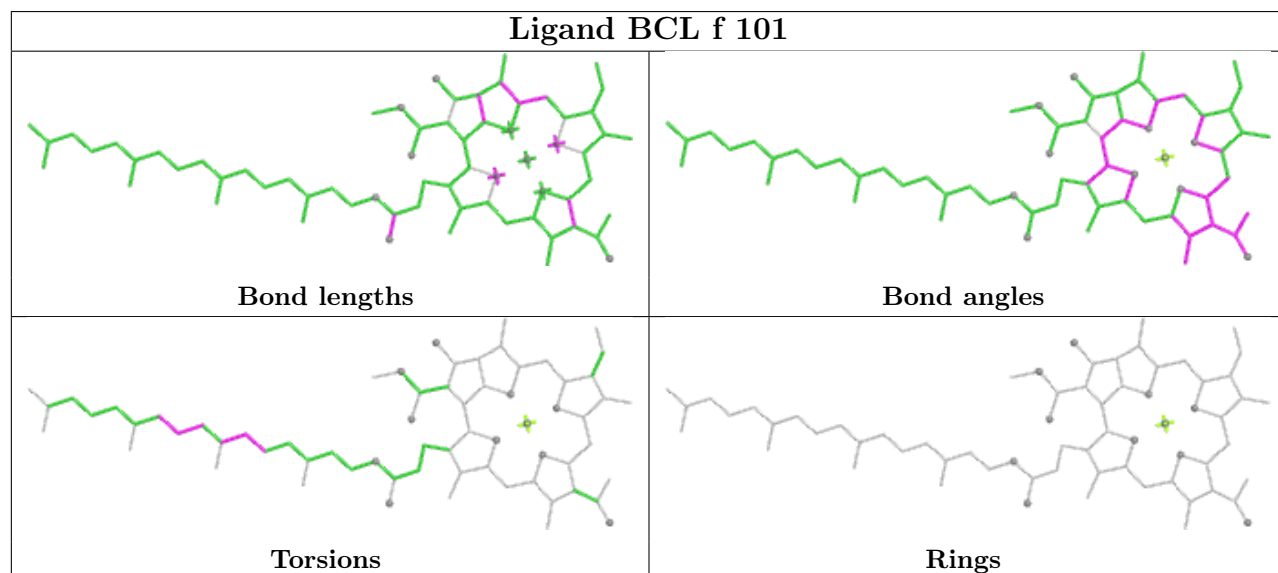
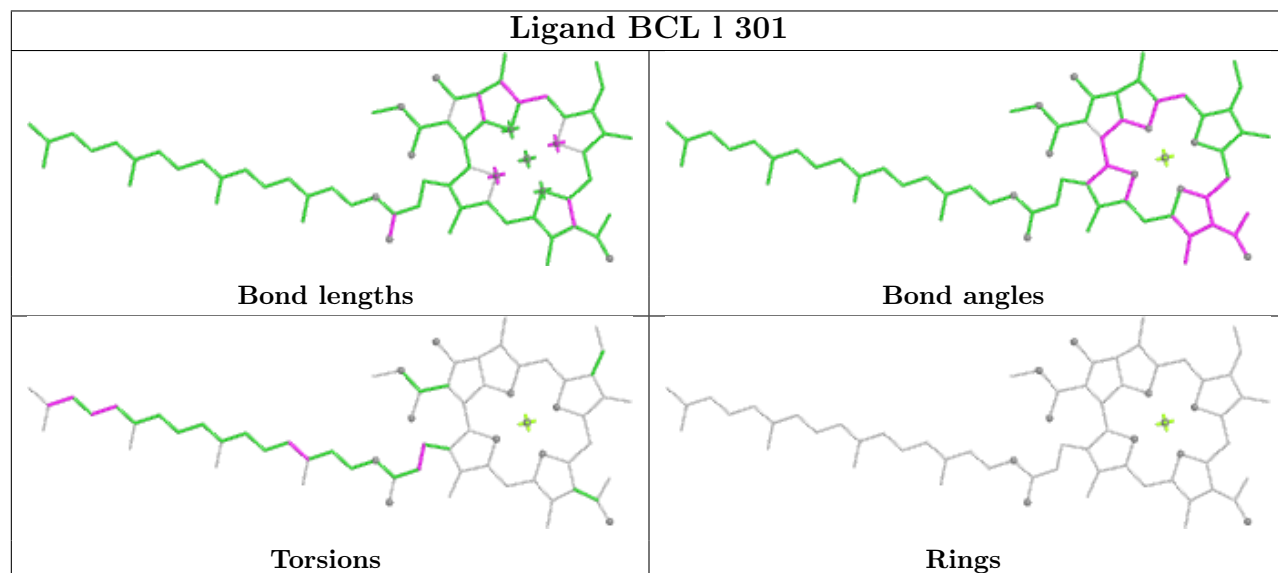
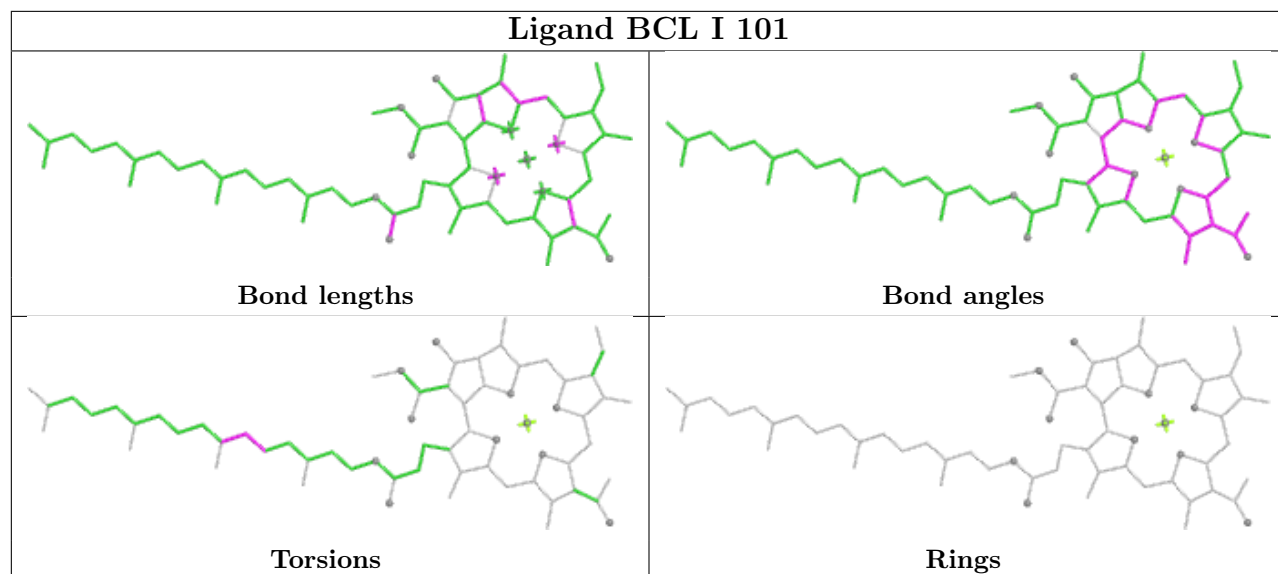
Ligand BCL z 101

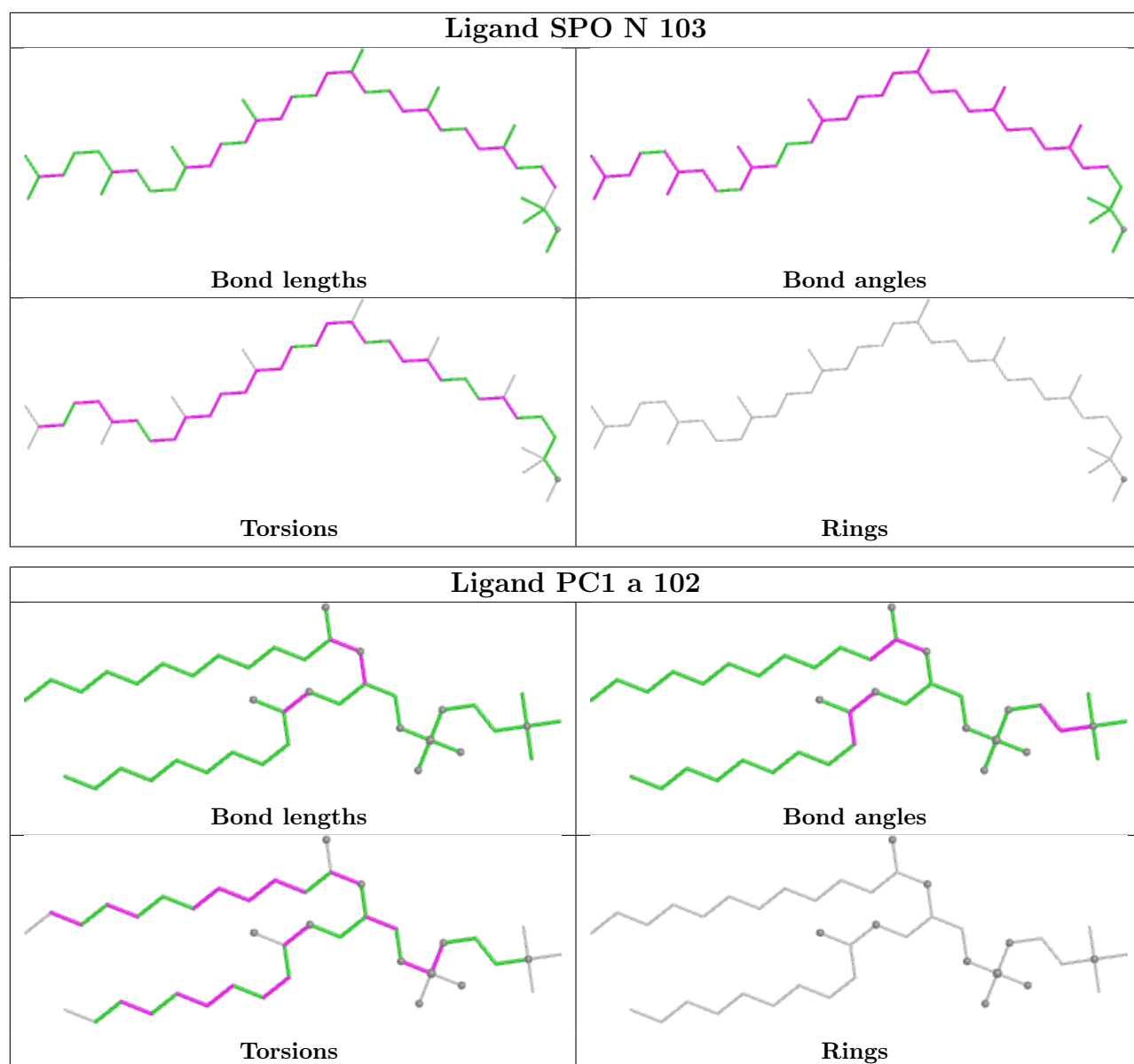


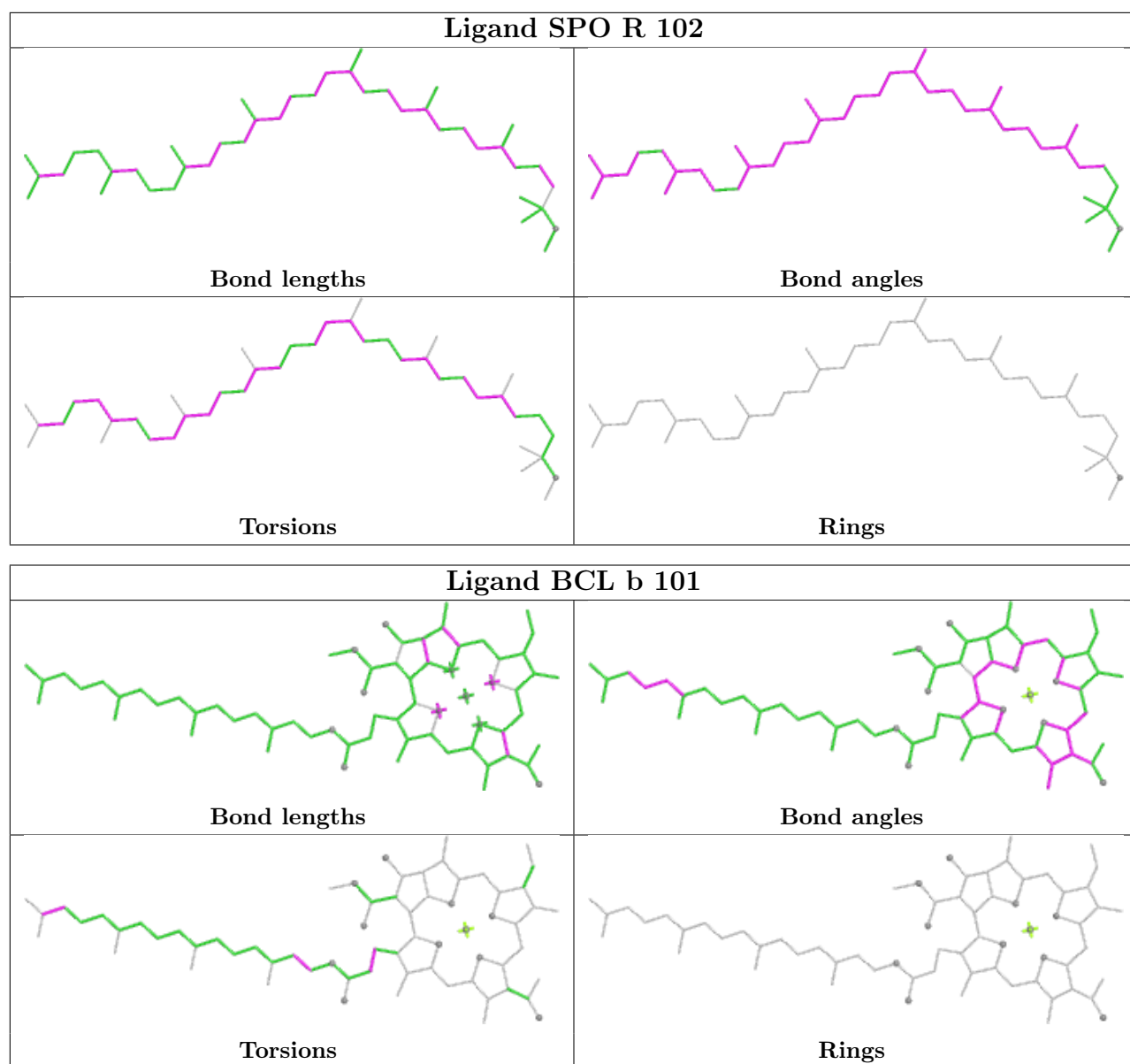
Ligand BCL k 103

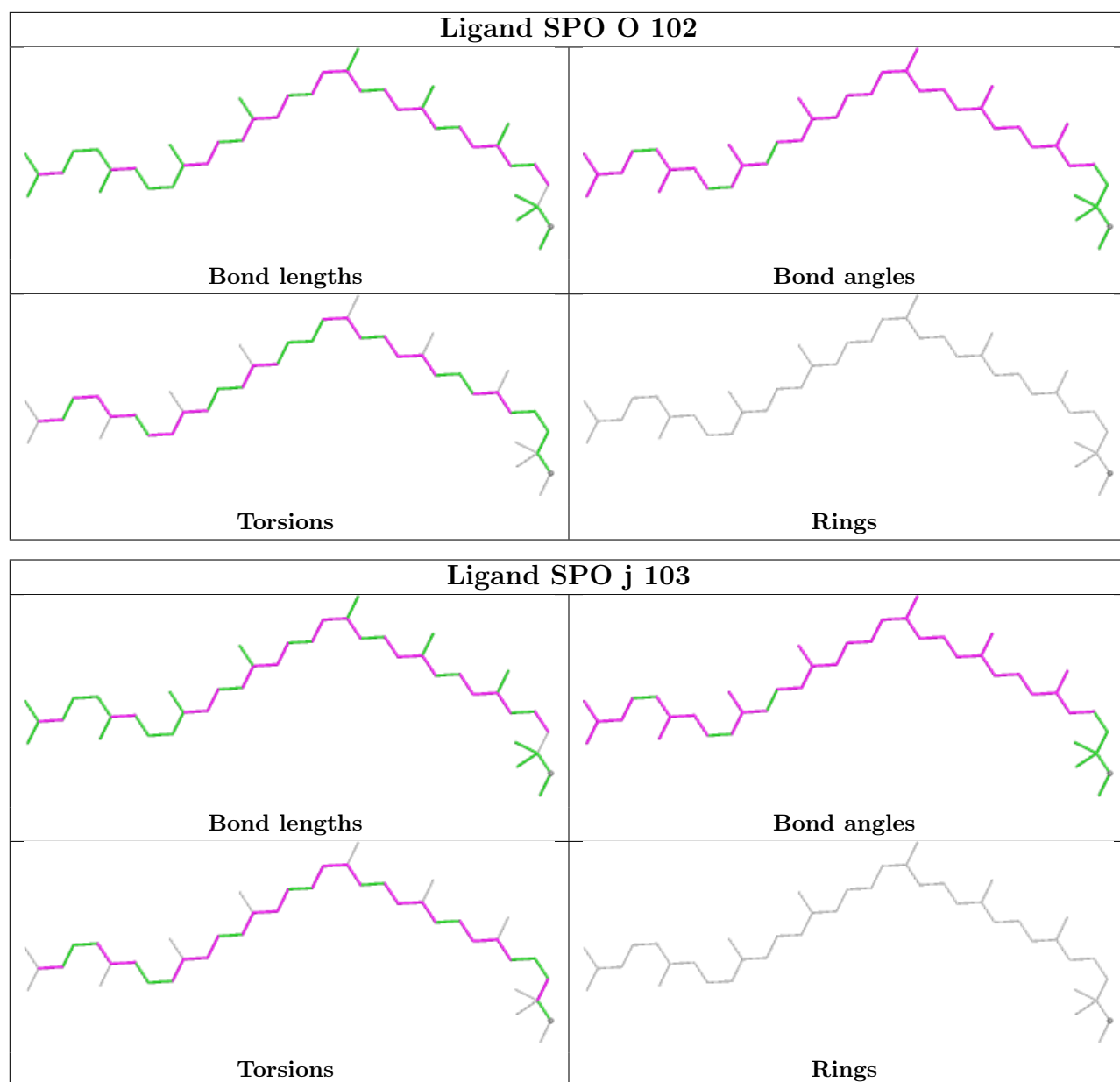


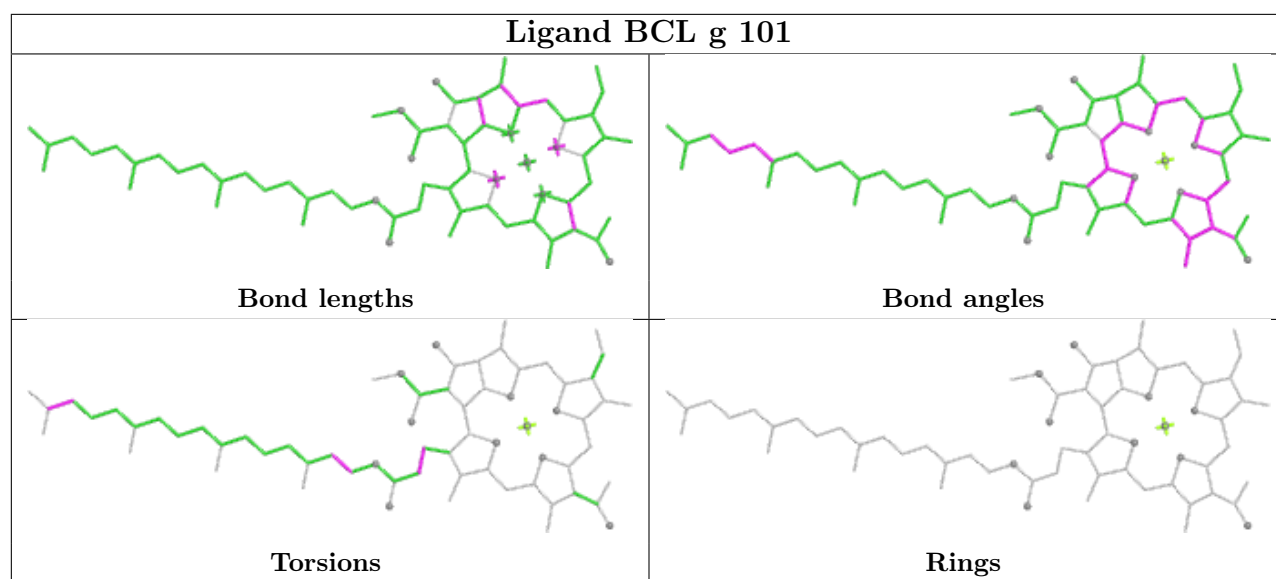












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

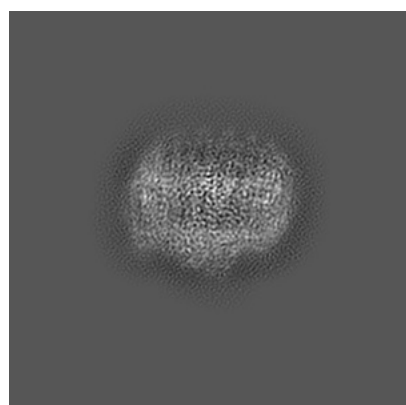
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31835. These allow visual inspection of the internal detail of the map and identification of artifacts.

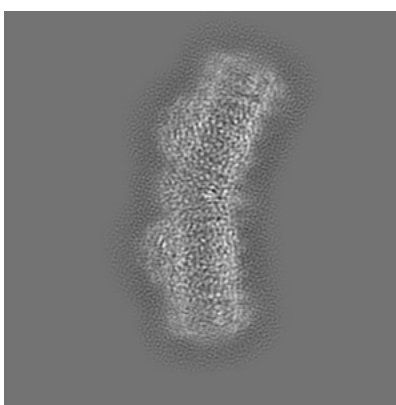
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

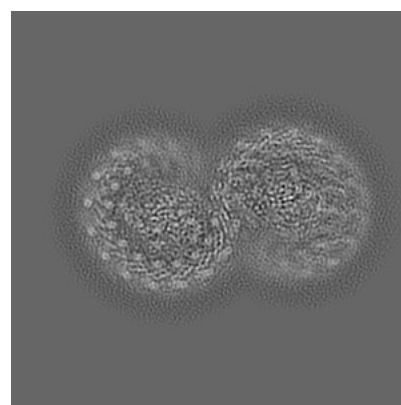
6.1.1 Primary map



X



Y

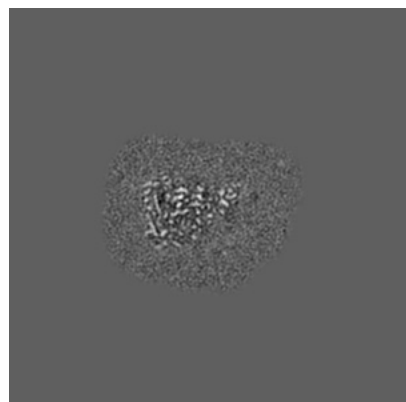


Z

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

6.2 Central slices [i](#)

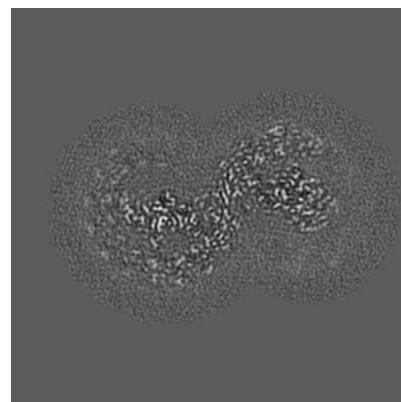
6.2.1 Primary map



X Index: 175



Y Index: 175

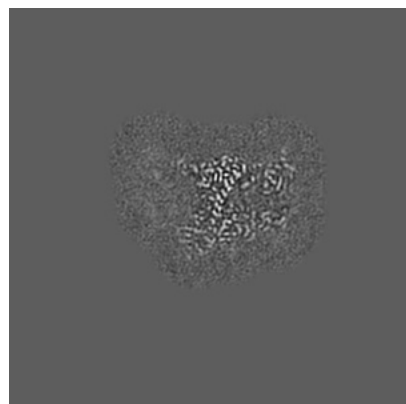


Z Index: 175

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

6.3 Largest variance slices [i](#)

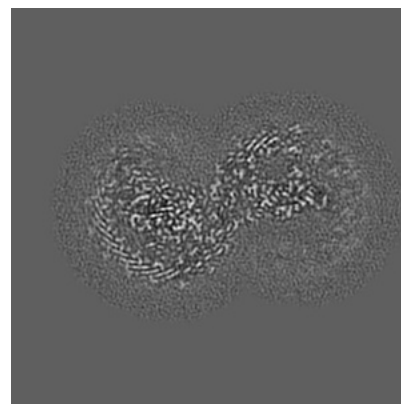
6.3.1 Primary map



X Index: 240



Y Index: 179

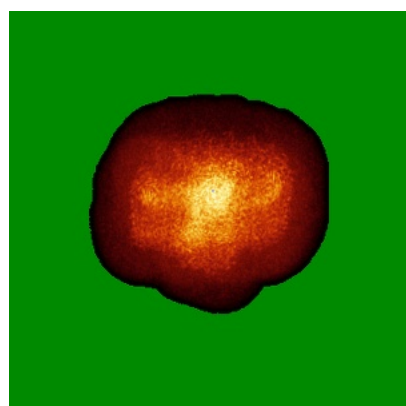


Z Index: 189

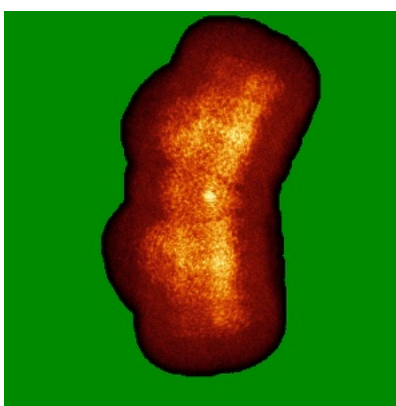
The images above show the largest variance slices of the map in three orthogonal directions.

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

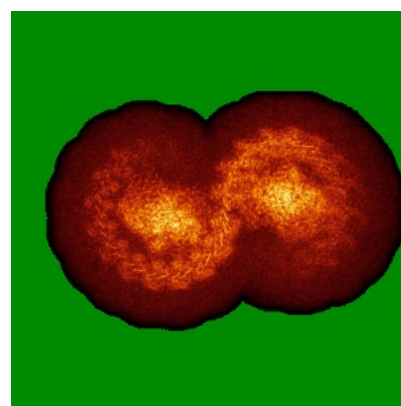
6.4.1 Primary map



X



Y

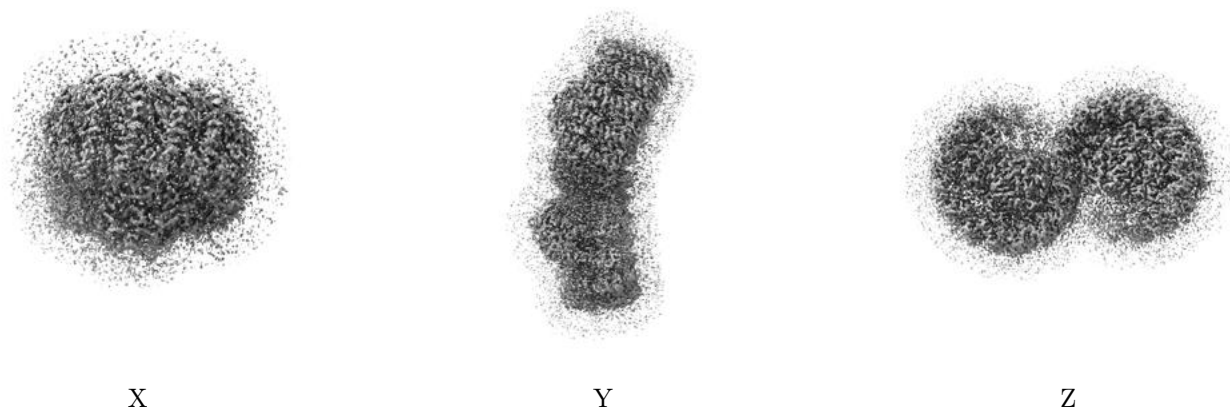


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0245. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

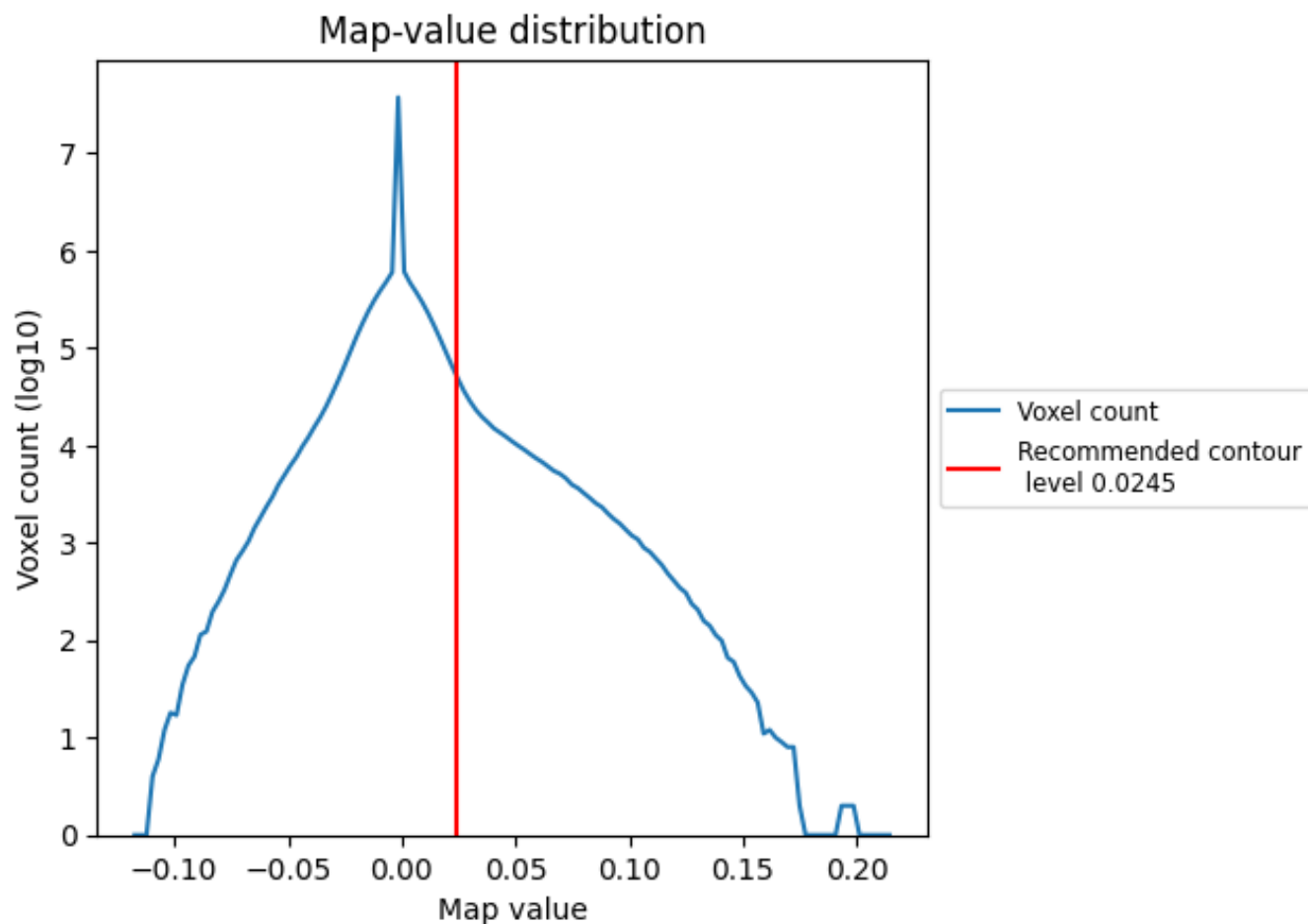
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

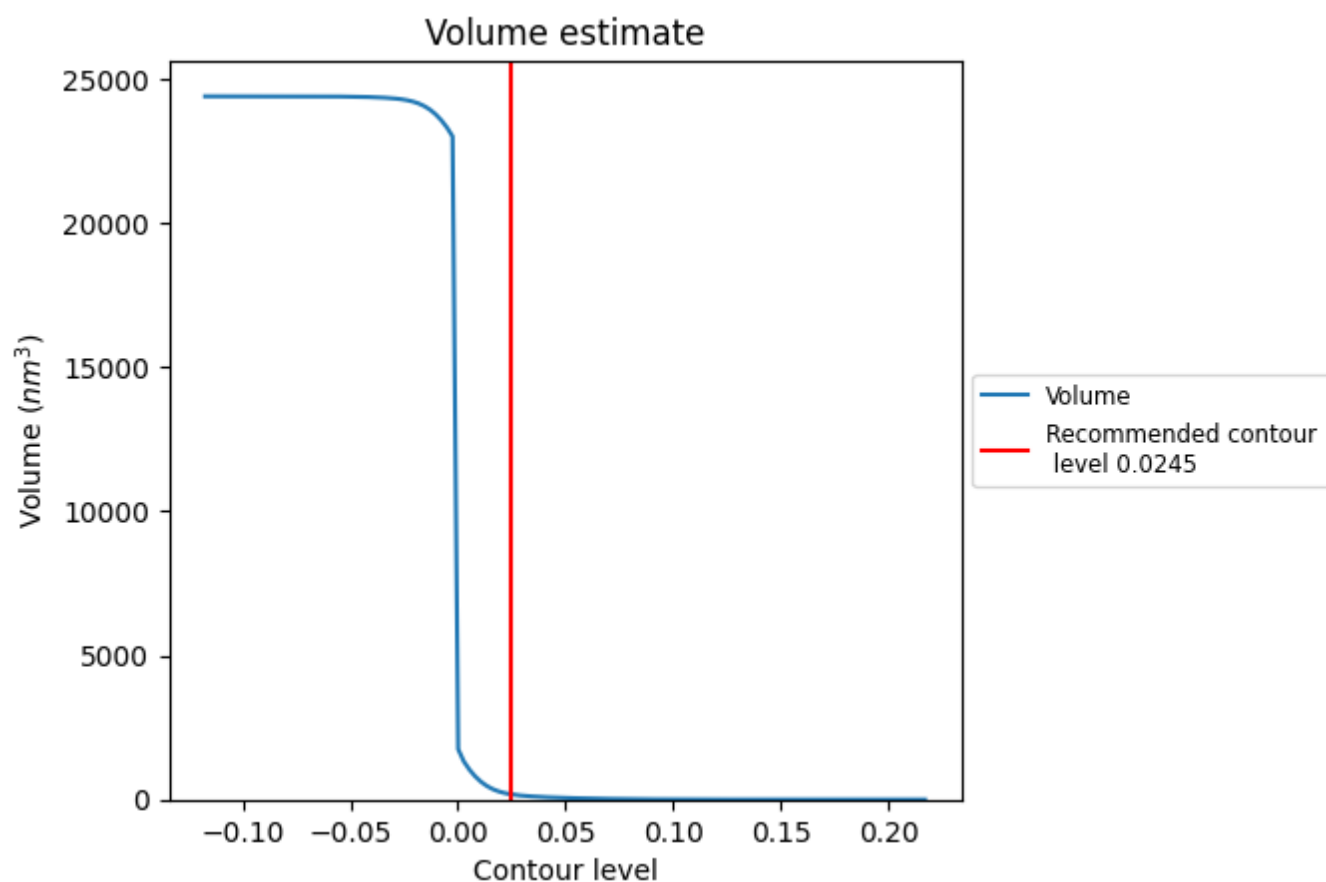
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

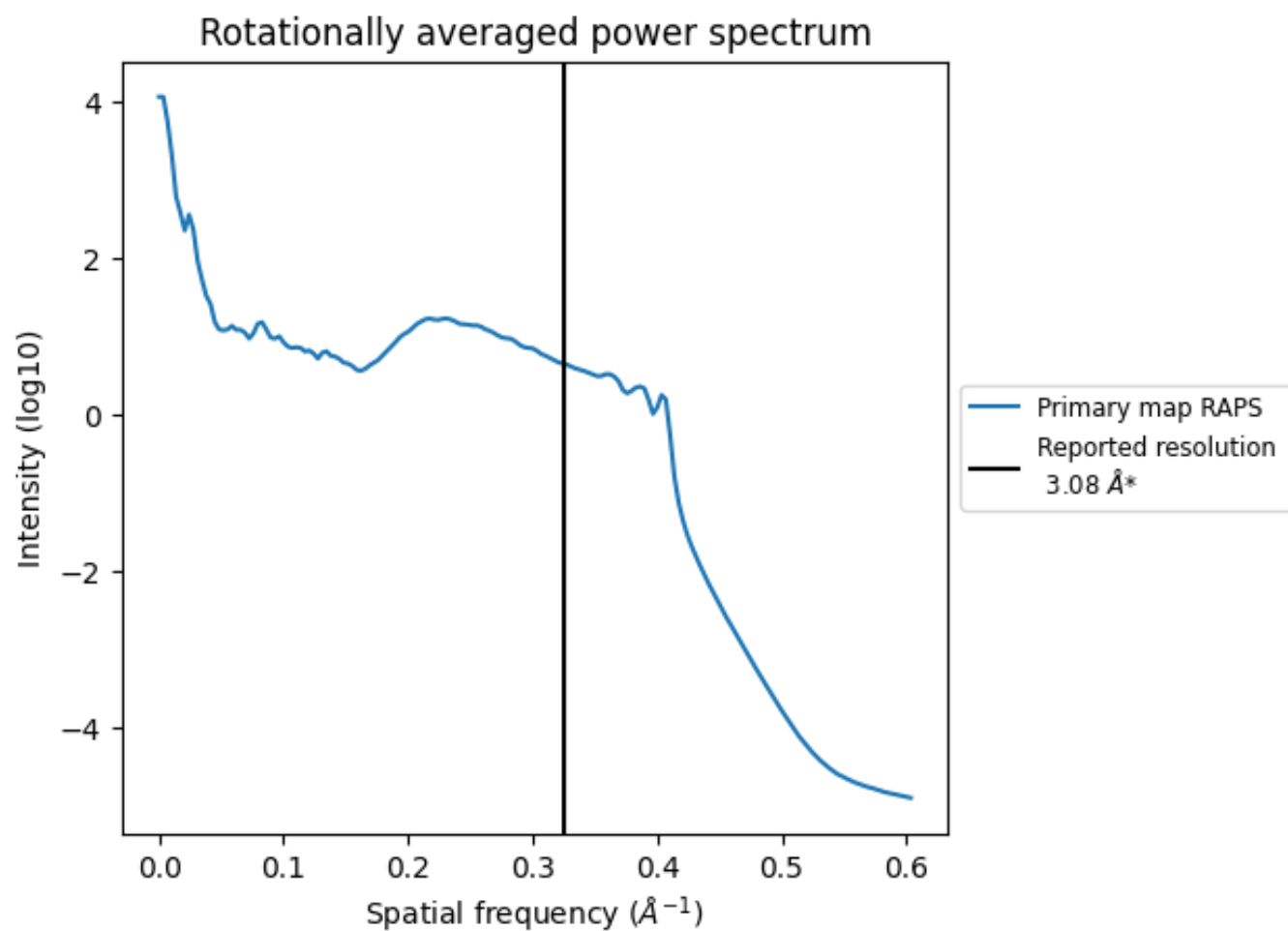
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 186 nm³; this corresponds to an approximate mass of 168 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

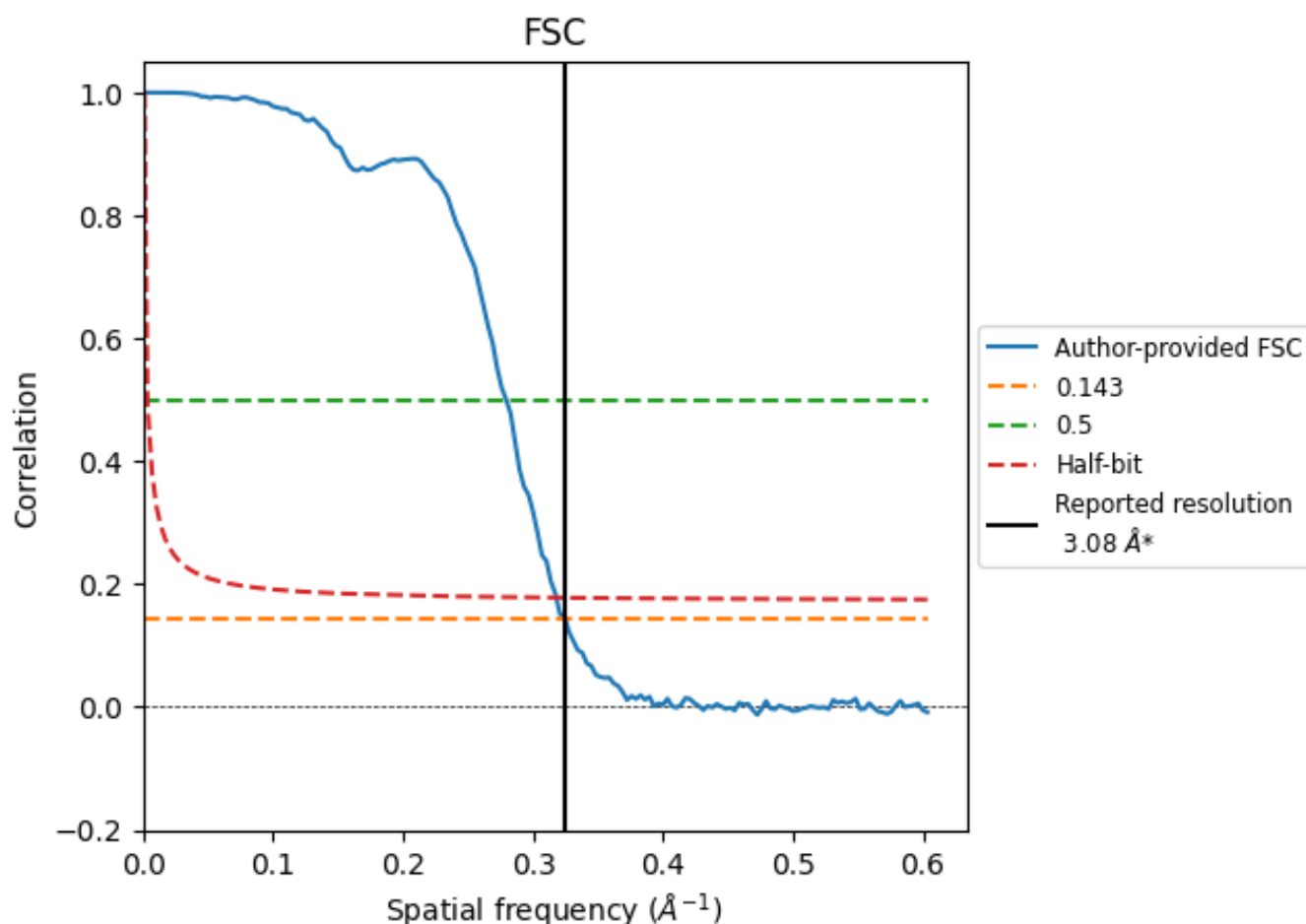


*Reported resolution corresponds to spatial frequency of 0.325 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.325 Å⁻¹

8.2 Resolution estimates [i](#)

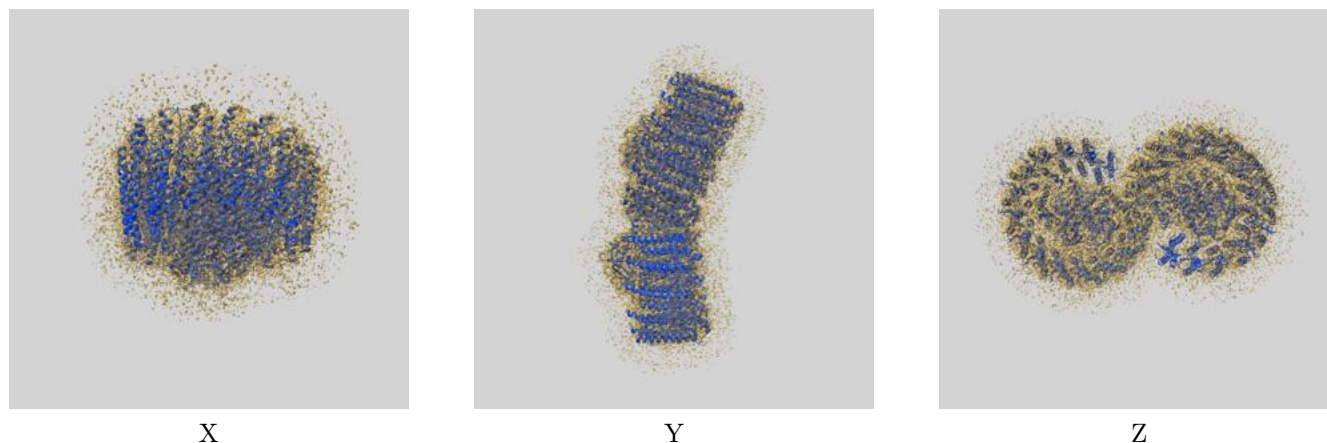
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.08	-	-
Author-provided FSC curve	3.08	3.58	3.15
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

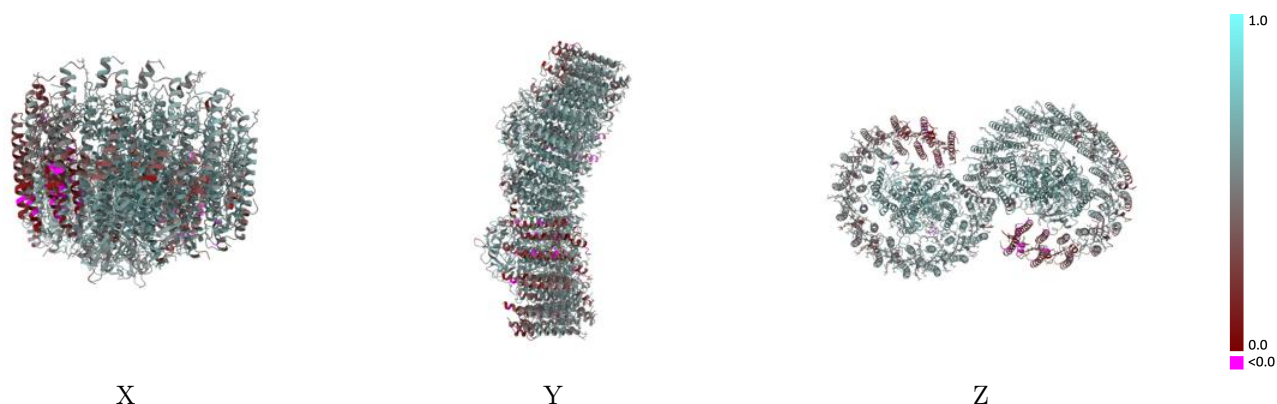
This section contains information regarding the fit between EMDB map EMD-31835 and PDB model 7VA9. Per-residue inclusion information can be found in section [3](#) on page [21](#).

9.1 Map-model overlay [i](#)



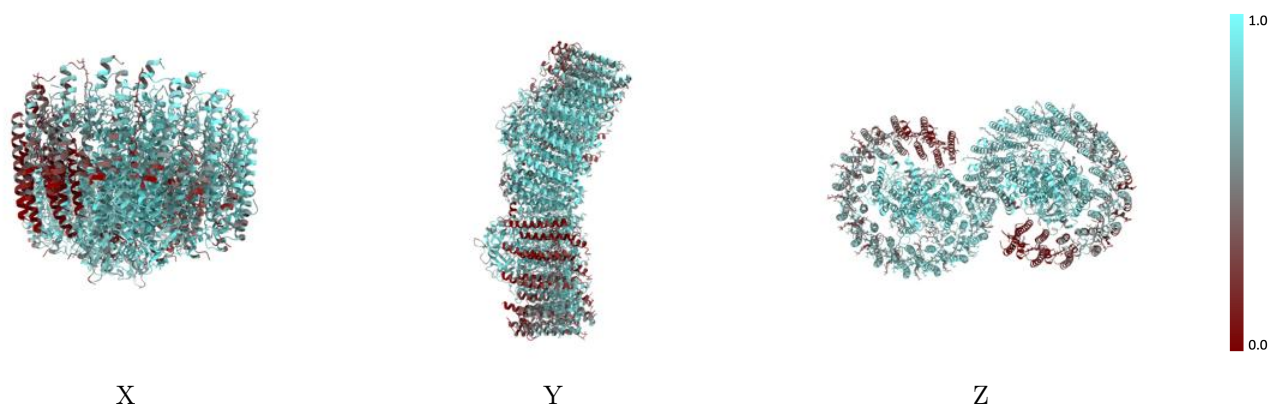
The images above show the 3D surface view of the map at the recommended contour level 0.0245 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



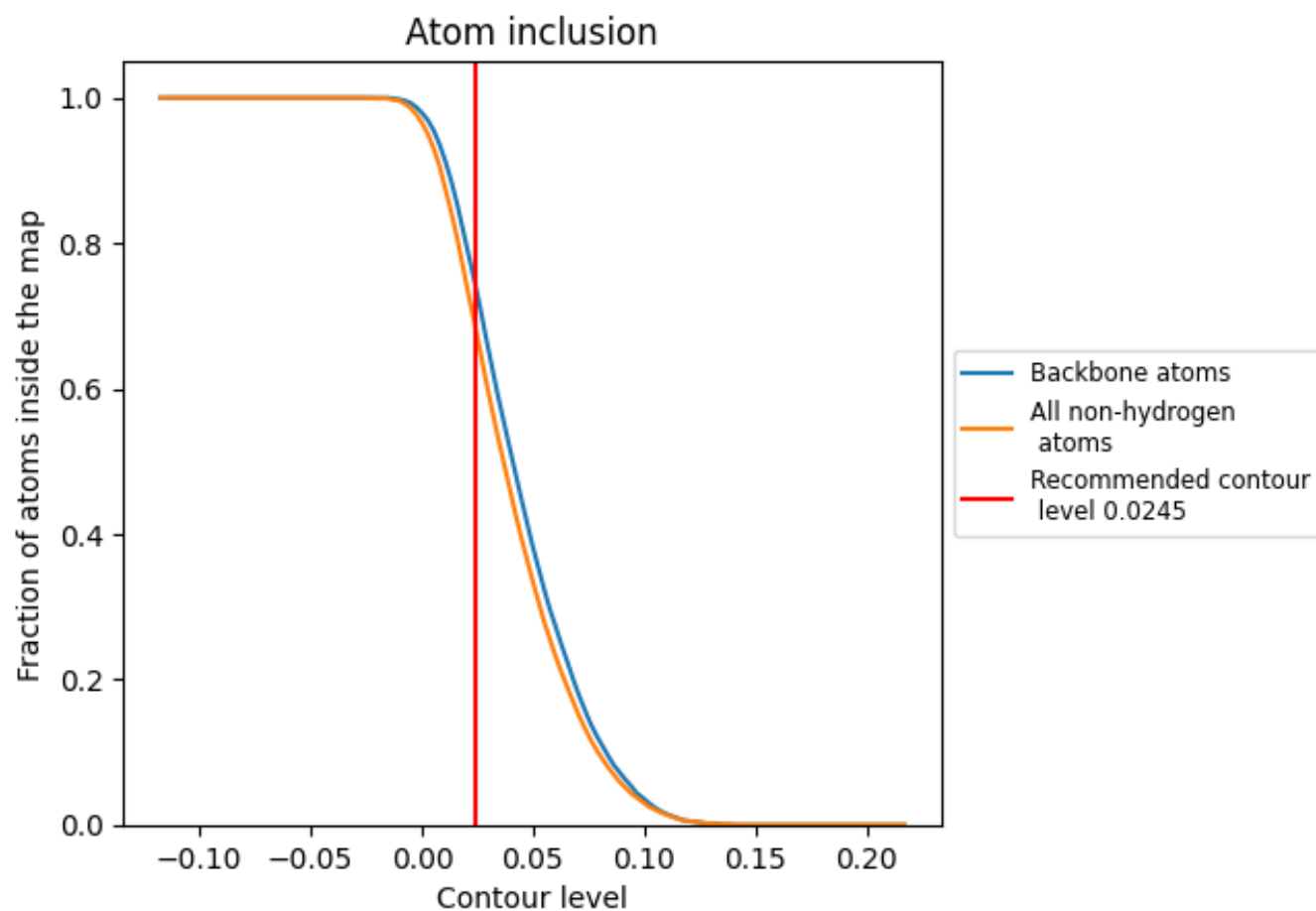
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0245).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0245) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6780	 0.5170
0	 0.7980	 0.5760
1	 0.0340	 0.1340
2	 0.0630	 0.1850
3	 0.8800	 0.6020
4	 0.0790	 0.2420
5	 0.0630	 0.1710
6	 0.8460	 0.5700
7	 0.7980	 0.5400
8	 0.7910	 0.5620
9	 0.8800	 0.5950
A	 0.8270	 0.5800
B	 0.7770	 0.5520
C	 0.7150	 0.5470
D	 0.8470	 0.5910
E	 0.7780	 0.5630
F	 0.7960	 0.5760
G	 0.6820	 0.5150
H	 0.7330	 0.5370
I	 0.6920	 0.5420
J	 0.6520	 0.4930
K	 0.6220	 0.4960
L	 0.8980	 0.6320
M	 0.8800	 0.6260
N	 0.5960	 0.4830
O	 0.5610	 0.4750
P	 0.6010	 0.4650
Q	 0.5850	 0.4960
R	 0.5400	 0.4580
S	 0.5600	 0.4770
T	 0.4650	 0.4200
U	 0.5070	 0.4630
V	 0.4090	 0.3920
W	 0.3390	 0.3590
X	 0.2390	 0.3080



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Chain	Atom inclusion	Q-score
Y	 0.1540	 0.2220
Z	 0.1020	 0.2080
a	 0.8220	 0.5790
aa	 0.7800	 0.5530
ab	 0.7540	 0.5440
b	 0.7840	 0.5470
c	 0.6910	 0.5260
d	 0.7720	 0.5810
e	 0.7500	 0.5430
f	 0.7490	 0.5570
g	 0.6750	 0.5100
h	 0.7220	 0.5370
i	 0.6310	 0.4930
j	 0.5580	 0.4710
k	 0.5870	 0.4830
l	 0.9040	 0.6310
m	 0.8800	 0.6220
n	 0.4980	 0.4250
o	 0.5550	 0.4640
p	 0.5760	 0.4730
q	 0.5530	 0.4770
r	 0.5090	 0.4710
s	 0.5210	 0.4810
t	 0.4810	 0.4400
u	 0.5370	 0.4730
v	 0.4240	 0.3990
w	 0.3850	 0.3830
x	 0.2160	 0.2590
y	 0.1380	 0.2310
z	 0.1460	 0.1940