



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 07:15 AM UTC

PDB ID : 9J2F / pdb_00009j2f
EMDB ID : EMD-61095
Title : Structure of photosynthetic LH1-RC complex from the purple bacterium *Blas-tochloris tepida*
Authors : Kimura, Y.; Kanno, R.; Mori, K.; Matsuda, Y.; Seto, R.; Takenaka, S.; Mino, H.; Ohkubo, T.; Honda, M.; Sasaki, Y.C.; Kishikawa, J.; Mitsuoka, K.; Mio, K.; Hall, M.; Purba, E.R.; Mochizuki, T.; Mizoguchi, A.; Humbel, B.M.; Madigan, M.T.; Wang-Otomo, Z.-Y.; Tani, K.
Deposited on : 2024-08-06
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

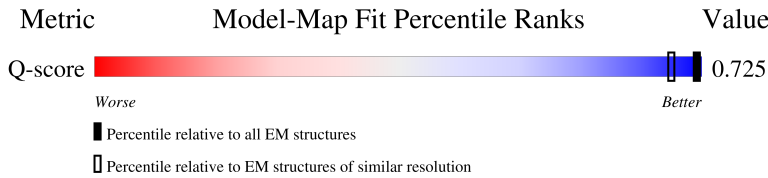
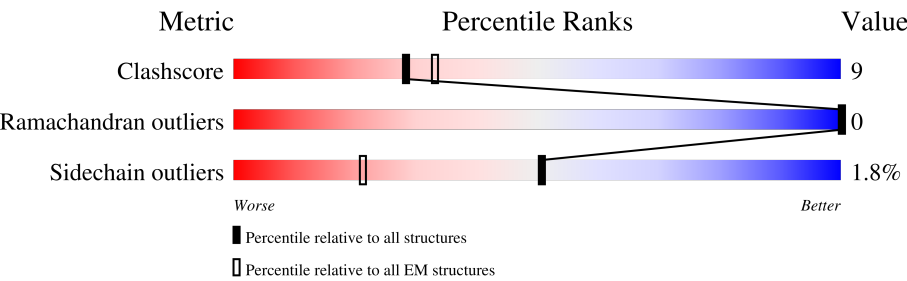
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.20 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	3184 (1.71 - 2.70)

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	C	354	
2	L	274	
3	M	332	

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Mol	Chain	Length	Quality of chain
4	H	260	
5	3	69	
5	6	69	
5	9	69	
5	A	69	
5	D	69	
5	I	69	
5	N	69	
5	Q	69	
5	T	69	
5	W	69	
5	Z	69	
5	b	69	
5	e	69	
5	h	69	
5	k	69	
5	n	69	
5	q	69	
6	0	69	
6	1	69	
6	4	69	
6	7	69	
6	B	69	
6	E	69	
6	J	69	

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Mol	Chain	Length	Quality of chain
6	O	69	
6	R	69	
6	U	69	
6	X	69	
6	c	69	
6	f	69	
6	i	69	
6	l	69	
6	o	69	
6	r	69	
7	G	56	
8	2	57	
8	5	57	
8	8	57	
8	F	57	
8	K	57	
8	P	57	
8	S	57	
8	V	57	
8	Y	57	
8	a	57	
8	d	57	
8	g	57	
8	j	57	
8	m	57	

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Mol	Chain	Length	Quality of chain
8	p	57	

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
13	BCB	0	102	X	-	-	-
13	BCB	1	101	X	-	-	-
13	BCB	3	101	X	-	-	-
13	BCB	4	101	X	-	-	-
13	BCB	6	101	X	-	-	-
13	BCB	7	102	X	-	-	-
13	BCB	9	101	X	-	-	-
13	BCB	A	102	X	-	-	-
13	BCB	B	202	X	-	-	-
13	BCB	D	101	X	-	-	-
13	BCB	E	101	X	-	-	-
13	BCB	I	101	X	-	-	-
13	BCB	J	101	X	-	-	-
13	BCB	L	302	X	-	-	-
13	BCB	L	303	X	-	-	-
13	BCB	M	402	X	-	-	-
13	BCB	M	403	X	-	-	-
13	BCB	N	101	X	-	-	-
13	BCB	O	102	X	-	-	-
13	BCB	Q	402	X	-	-	-
13	BCB	R	102	X	-	-	-
13	BCB	T	101	X	-	-	-
13	BCB	U	102	X	-	-	-
13	BCB	W	302	X	-	-	-
13	BCB	X	102	X	-	-	-
13	BCB	Z	101	X	-	-	-
13	BCB	b	101	X	-	-	-
13	BCB	c	101	X	-	-	-
13	BCB	e	101	X	-	-	-
13	BCB	f	101	X	-	-	-
13	BCB	h	102	X	-	-	-
13	BCB	i	101	X	-	-	-
13	BCB	k	102	X	-	-	-
13	BCB	l	102	X	-	-	-
13	BCB	n	101	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	BCB	o	102	X	-	-	-
13	BCB	q	101	X	-	-	-
13	BCB	r	101	X	-	-	-

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 32918 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 Photosynthetic reaction center cytochrome c subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	331	Total	C	N	O	S	0	0
			2585	1637	455	471	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	273	Total	C	N	O	S	0	0
			2159	1454	347	352	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	331	Total	C	N	O	S	0	0
			2621	1746	433	427	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	260	Total	C	N	O	S	0	0
			2041	1313	343	382	3		

- Molecule 5 is a protein called Antenna complex alpha/beta subunit domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	A	50	Total	C	N	O	0	0
			424	288	72	64		
5	D	50	Total	C	N	O	0	0
			424	288	72	64		
5	I	50	Total	C	N	O	0	0
			424	288	72	64		
5	N	50	Total	C	N	O	0	0
			424	288	72	64		

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Mol	Chain	Residues	Atoms				AltConf	Trace
5	Q	50	Total	C	N	O	0	0
			424	288	72	64		
5	T	50	Total	C	N	O	0	0
			424	288	72	64		
5	W	50	Total	C	N	O	0	0
			424	288	72	64		
5	Z	50	Total	C	N	O	0	0
			424	288	72	64		
5	3	50	Total	C	N	O	0	0
			424	288	72	64		
5	6	50	Total	C	N	O	0	0
			424	288	72	64		
5	9	50	Total	C	N	O	0	0
			424	288	72	64		
5	b	50	Total	C	N	O	0	0
			424	288	72	64		
5	e	50	Total	C	N	O	0	0
			424	288	72	64		
5	h	50	Total	C	N	O	0	0
			424	288	72	64		
5	k	50	Total	C	N	O	0	0
			424	288	72	64		
5	n	50	Total	C	N	O	0	0
			424	288	72	64		
5	q	50	Total	C	N	O	0	0
			424	288	72	64		

- Molecule 6 is a protein called Antenna complex alpha/beta subunit domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	51	Total	C	N	O	S	0	0
			407	274	63	69	1		
6	E	51	Total	C	N	O	S	0	0
			407	274	63	69	1		
6	J	48	Total	C	N	O	S	0	0
			386	260	60	65	1		
6	O	51	Total	C	N	O	S	0	0
			407	274	63	69	1		
6	R	50	Total	C	N	O	S	0	0
			400	269	62	68	1		
6	U	50	Total	C	N	O	S	0	0
			400	269	62	68	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	X	50	Total 400	C 269	N 62	O 68	S 1	0	0
6	1	50	Total 400	C 269	N 62	O 68	S 1	0	0
6	4	50	Total 400	C 269	N 62	O 68	S 1	0	0
6	7	50	Total 400	C 269	N 62	O 68	S 1	0	0
6	0	50	Total 400	C 269	N 62	O 68	S 1	0	0
6	c	50	Total 400	C 269	N 62	O 68	S 1	0	0
6	f	50	Total 400	C 269	N 62	O 68	S 1	0	0
6	i	50	Total 400	C 269	N 62	O 68	S 1	0	0
6	l	50	Total 400	C 269	N 62	O 68	S 1	0	0
6	o	50	Total 400	C 269	N 62	O 68	S 1	0	0
6	r	50	Total 400	C 269	N 62	O 68	S 1	0	0

- Molecule 7 is a protein called Light-harvesting protein gamma1.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	28	Total 232	C 159	N 36	O 37	0	0

- Molecule 8 is a protein called Light-harvesting protein B-1015 gamma chain.

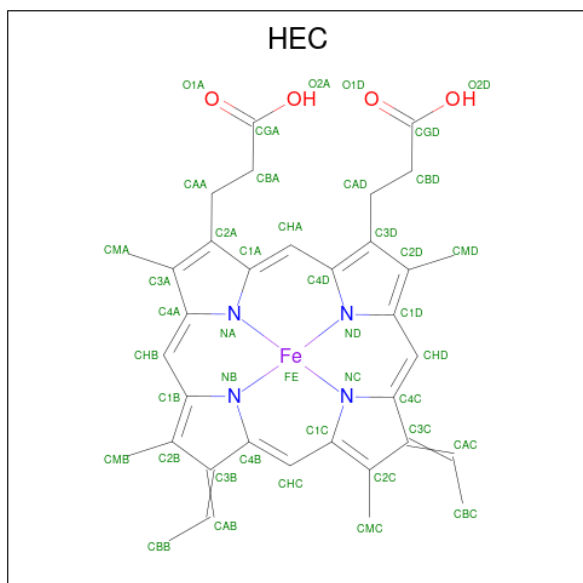
Mol	Chain	Residues	Atoms				AltConf	Trace
8	F	36	Total 279	C 189	N 42	O 48	0	0
8	K	36	Total 279	C 189	N 42	O 48	0	0
8	P	36	Total 279	C 189	N 42	O 48	0	0
8	S	36	Total 279	C 189	N 42	O 48	0	0
8	V	36	Total 279	C 189	N 42	O 48	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
8	Y	36	Total	C	N	O	0	0
			279	189	42	48		
8	2	36	Total	C	N	O	0	0
			279	189	42	48		
8	5	36	Total	C	N	O	0	0
			279	189	42	48		
8	8	36	Total	C	N	O	0	0
			279	189	42	48		
8	a	36	Total	C	N	O	0	0
			279	189	42	48		
8	d	36	Total	C	N	O	0	0
			279	189	42	48		
8	g	36	Total	C	N	O	0	0
			279	189	42	48		
8	j	36	Total	C	N	O	0	0
			279	189	42	48		
8	m	36	Total	C	N	O	0	0
			279	189	42	48		
8	p	36	Total	C	N	O	0	0
			279	189	42	48		

- Molecule 9 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

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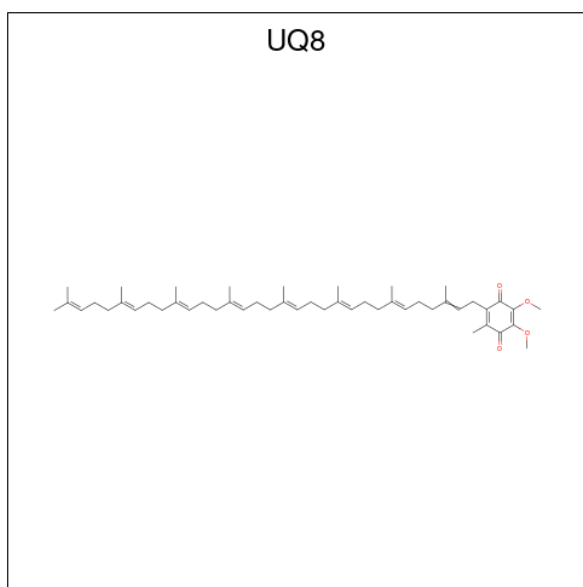
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Mol	Chain	Residues	Atoms					AltConf
9	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
9	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
9	C	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

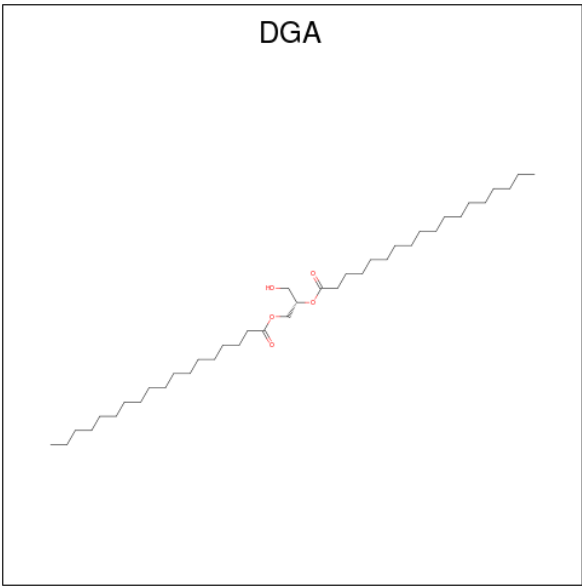
Mol	Chain	Residues	Atoms		AltConf
10	C	1	Total	Mg	0
			1	1	

- Molecule 11 is Ubiquinone-8 (CCD ID: UQ8) (formula: C₄₉H₇₄O₄).



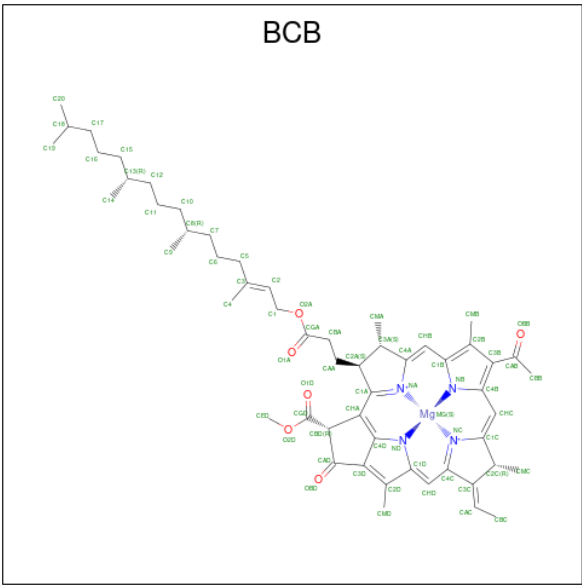
Mol	Chain	Residues	Atoms			AltConf
11	C	1	Total	C	O	0
			15	11	4	
11	L	1	Total	C	O	0
			31	27	4	
11	M	1	Total	C	O	0
			25	21	4	
11	M	1	Total	C	O	0
			53	49	4	
11	A	1	Total	C	O	0
			53	49	4	

- Molecule 12 is DIACYL GLYCEROL (CCD ID: DGA) (formula: C₃₉H₇₆O₅).



Mol	Chain	Residues	Atoms			AltConf
12	L	1	Total	C	O	0
			23	19	4	

- Molecule 13 is BACTERIOCHLOROPHYLL B (CCD ID: BCB) (formula: C₅₅H₇₂MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



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

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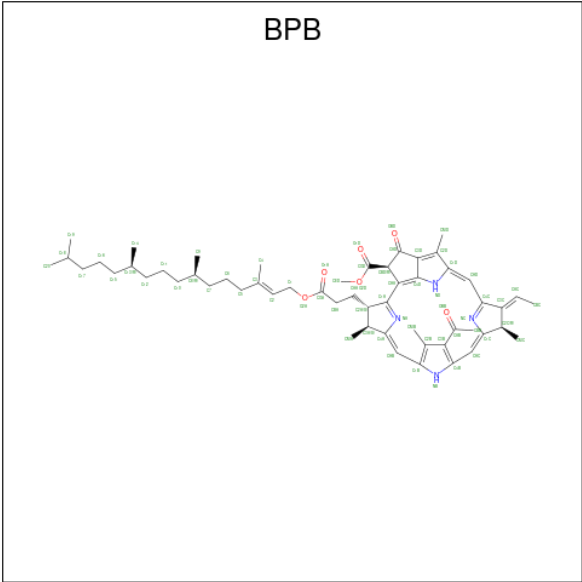
Mol	Chain	Residues	Atoms					AltConf
13	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	M	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	M	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	B	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	D	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	E	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	I	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	J	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	O	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	R	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	T	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	U	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	W	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	X	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	Z	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	1	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	3	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	4	1	Total 66	C 55	Mg 1	N 4	O 6	0

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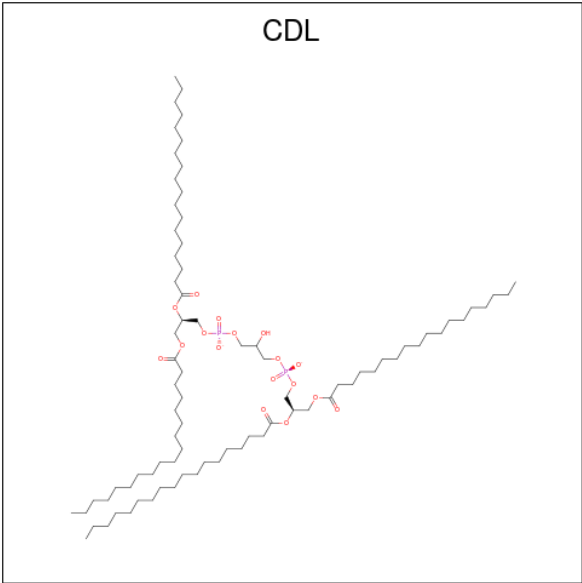
Mol	Chain	Residues	Atoms					AltConf
13	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	9	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	0	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	b	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	c	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	e	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	f	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	h	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	i	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	k	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	l	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	o	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	q	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	r	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 14 is BACTERIOPHEOPHYTIN B (CCD ID: BPB) (formula: $C_{55}H_{74}N_4O_6$).



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

- Molecule 15 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



Mol	Chain	Residues	Atoms				AltConf
15	L	1	Total	C	O	P	0
			75	56	17	2	
15	M	1	Total	C	O	P	0
			85	66	17	2	

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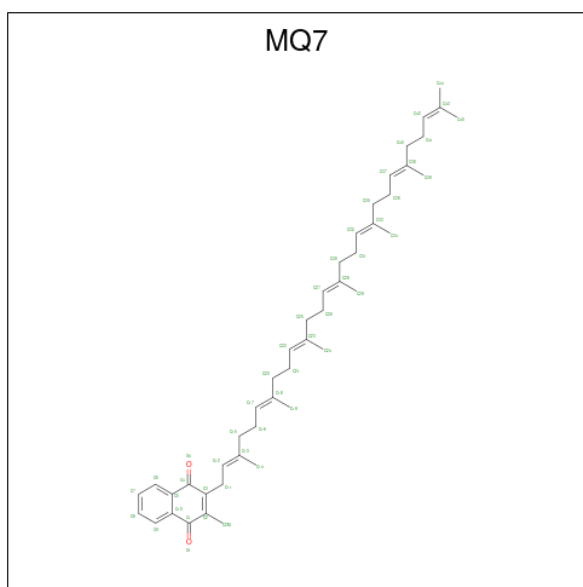
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Mol	Chain	Residues	Atoms				AltConf
15	H	1	Total	C	O	P	0
			98	79	17	2	
15	H	1	Total	C	O	P	0
			72	53	17	2	
15	r	1	Total	C	O	P	0
			68	49	17	2	

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

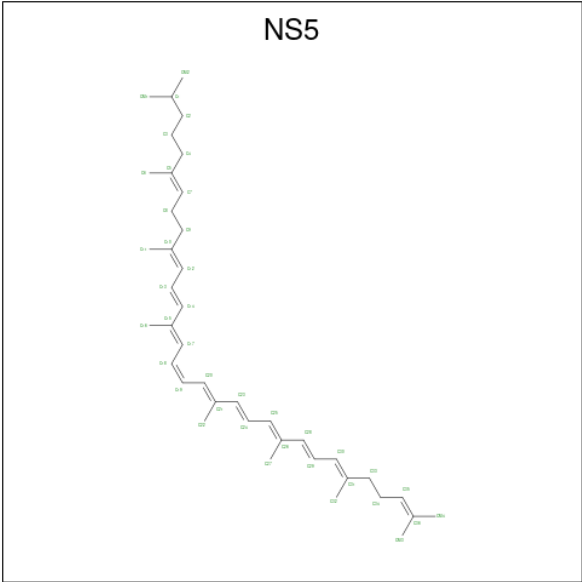
Mol	Chain	Residues	Atoms		AltConf
16	M	1	Total	Fe	0
			1	1	

- Molecule 17 is MENAQUINONE-7 (CCD ID: MQ7) (formula: C₄₆H₆₄O₂).



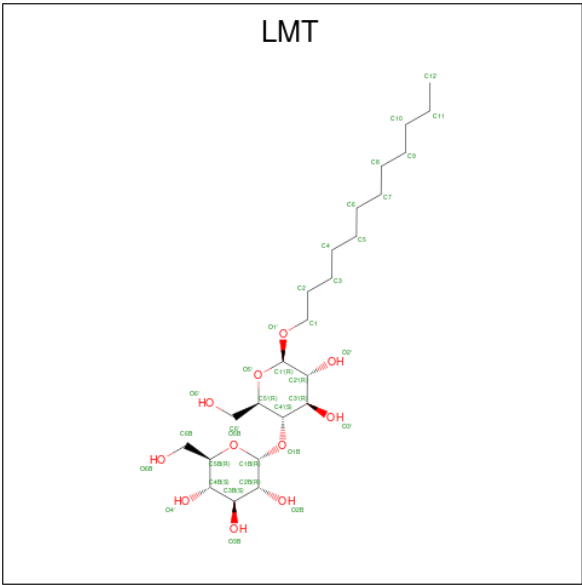
Mol	Chain	Residues	Atoms			AltConf
17	M	1	Total	C	O	0
			48	46	2	

- Molecule 18 is 15-cis-1,2-dihydroneurosporene (CCD ID: NS5) (formula: C₄₀H₆₀).



Mol	Chain	Residues	Atoms			AltConf
18	M	1	Total	C		0
			40	40		

- Molecule 19 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



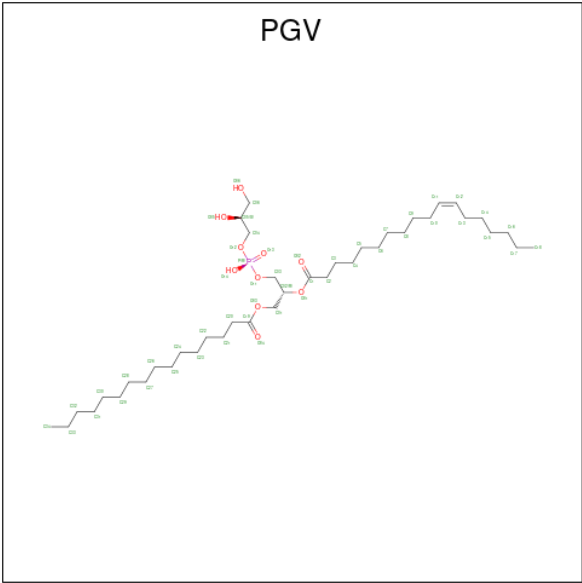
Mol	Chain	Residues	Atoms			AltConf
19	M	1	Total	C	O	0
			25	19	6	
19	B	1	Total	C	O	0
			15	13	2	
19	T	1	Total	C	O	0
			26	19	7	

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Mol	Chain	Residues	Atoms			AltConf
19	b	1	Total	C	O	0
			35	24	11	
19	b	1	Total	C	O	0
			35	24	11	
19	h	1	Total	C	O	0
			35	24	11	
19	k	1	Total	C	O	0
			35	24	11	
19	n	1	Total	C	O	0
			35	24	11	

- Molecule 20 is (1R)-2-{{[[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P).



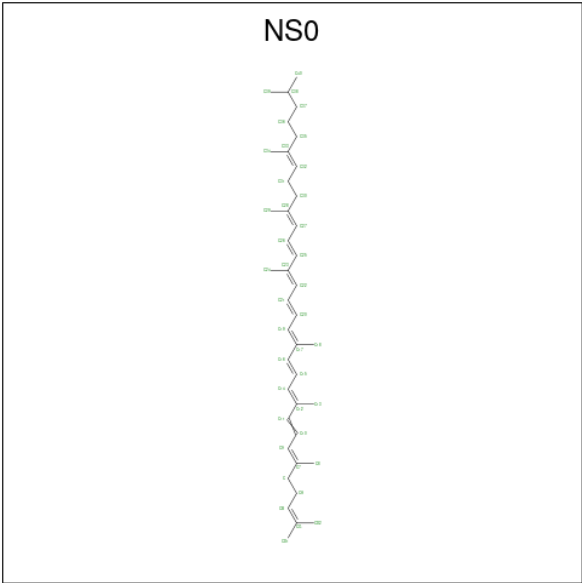
Mol	Chain	Residues	Atoms				AltConf
20	M	1	Total	C	O	P	0
			45	34	10	1	
20	D	1	Total	C	O	P	0
			47	36	10	1	
20	I	1	Total	C	O	P	0
			51	40	10	1	
20	N	1	Total	C	O	P	0
			38	27	10	1	
20	Q	1	Total	C	O	P	0
			49	39	9	1	

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Mol	Chain	Residues	Atoms				AltConf
20	W	1	Total	C	O	P	0
			48	37	10	1	

- Molecule 21 is all-trans-1,2-dihydroneurosporene (CCD ID: NS0) (formula: C₄₀H₆₀).



Mol	Chain	Residues	Atoms		AltConf
21	A	1	Total	C	0
			40	40	
21	D	1	Total	C	0
			40	40	
21	O	1	Total	C	0
			40	40	
21	R	1	Total	C	0
			40	40	
21	U	1	Total	C	0
			40	40	
21	W	1	Total	C	0
			40	40	
21	X	1	Total	C	0
			40	40	
21	2	1	Total	C	0
			40	40	
21	7	1	Total	C	0
			40	40	
21	9	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
21	0	1	Total C 40 40	0
21	h	1	Total C 40 40	0
21	k	1	Total C 40 40	0
21	l	1	Total C 40 40	0
21	o	1	Total C 40 40	0
21	q	1	Total C 40 40	0

- Molecule 22 is water.

Mol	Chain	Residues	Atoms	AltConf
22	C	98	Total O 98 98	0
22	L	59	Total O 59 59	0
22	M	75	Total O 75 75	0
22	H	22	Total O 22 22	0
22	A	6	Total O 6 6	0
22	B	2	Total O 2 2	0
22	D	6	Total O 6 6	0
22	E	3	Total O 3 3	0
22	I	7	Total O 7 7	0
22	J	3	Total O 3 3	0
22	K	2	Total O 2 2	0
22	N	6	Total O 6 6	0
22	O	3	Total O 3 3	0

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Mol	Chain	Residues	Atoms	AltConf
22	Q	6	Total O 6 6	0
22	R	5	Total O 5 5	0
22	S	1	Total O 1 1	0
22	T	6	Total O 6 6	0
22	U	5	Total O 5 5	0
22	V	2	Total O 2 2	0
22	W	3	Total O 3 3	0
22	X	5	Total O 5 5	0
22	Y	2	Total O 2 2	0
22	Z	4	Total O 4 4	0
22	1	3	Total O 3 3	0
22	2	3	Total O 3 3	0
22	3	5	Total O 5 5	0
22	4	7	Total O 7 7	0
22	5	5	Total O 5 5	0
22	6	10	Total O 10 10	0
22	7	4	Total O 4 4	0
22	8	1	Total O 1 1	0
22	9	6	Total O 6 6	0
22	0	1	Total O 1 1	0
22	b	10	Total O 10 10	0

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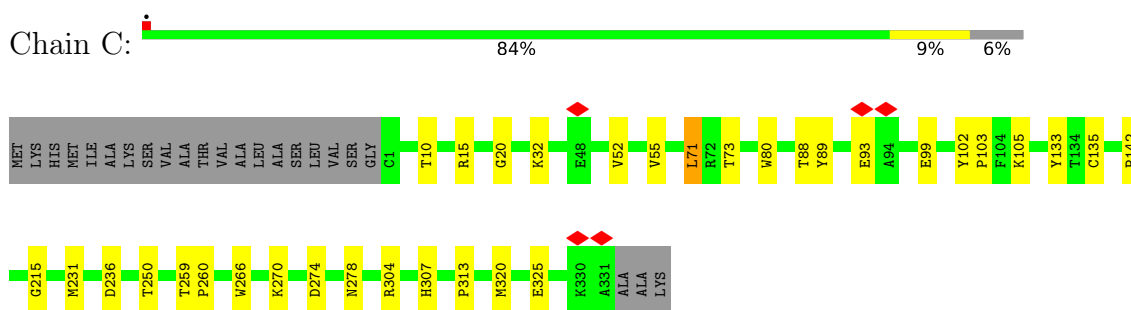
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
22	c	4	Total 4	O 4	0
22	e	9	Total 9	O 9	0
22	f	2	Total 2	O 2	0
22	g	1	Total 1	O 1	0
22	h	4	Total 4	O 4	0
22	i	1	Total 1	O 1	0
22	j	2	Total 2	O 2	0
22	k	5	Total 5	O 5	0
22	l	1	Total 1	O 1	0
22	n	4	Total 4	O 4	0
22	o	1	Total 1	O 1	0
22	p	1	Total 1	O 1	0
22	q	2	Total 2	O 2	0

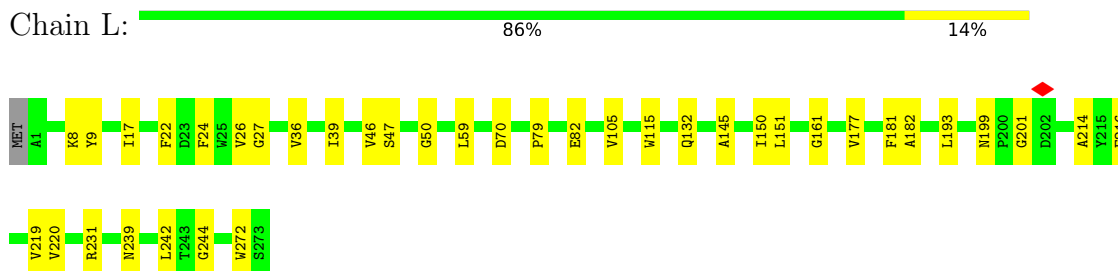
3 Residue-property plots

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.

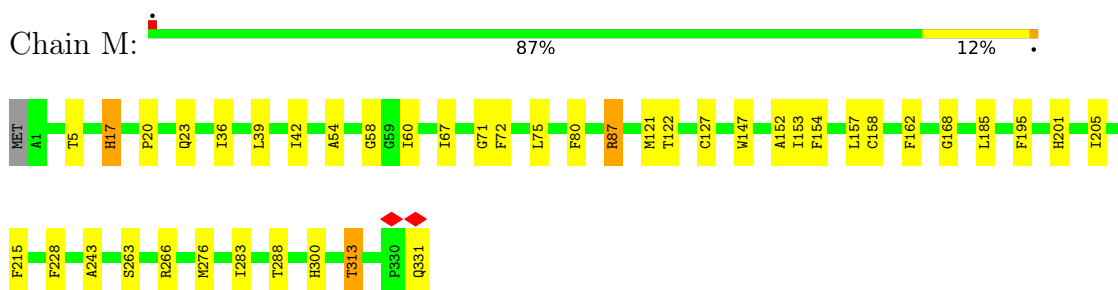
- Molecule 1: Photosynthetic reaction center cytochrome c subunit



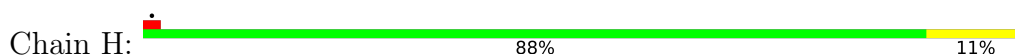
- Molecule 2: Reaction center protein L chain

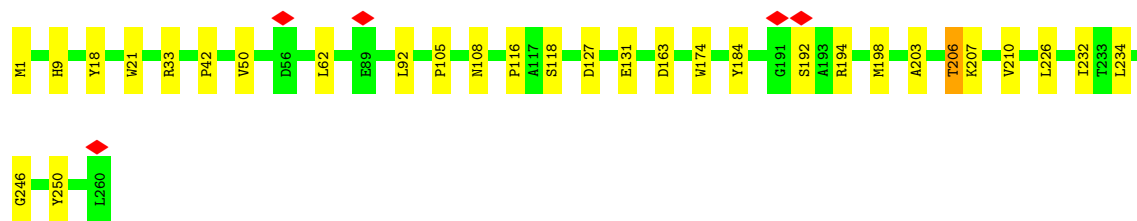


- Molecule 3: Reaction center protein M chain



- Molecule 4: Photosynthetic reaction center subunit H

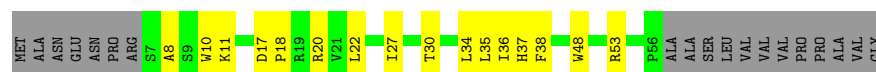




- Molecule 5: Antenna complex alpha/beta subunit domain-containing protein



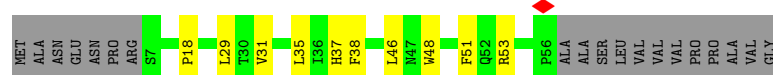
- Molecule 5: Antenna complex alpha/beta subunit domain-containing protein



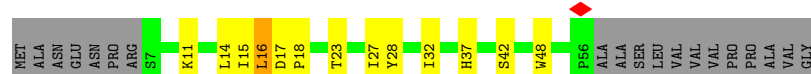
- Molecule 5: Antenna complex alpha/beta subunit domain-containing protein



- Molecule 5: Antenna complex alpha/beta subunit domain-containing protein



- Molecule 5: Antenna complex alpha/beta subunit domain-containing protein

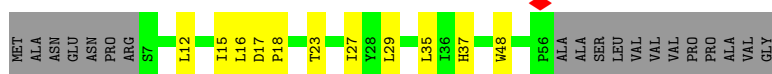


- Molecule 5: Antenna complex alpha/beta subunit domain-containing protein





- Molecule 5: Antenna complex alpha/beta subunit domain-containing protein



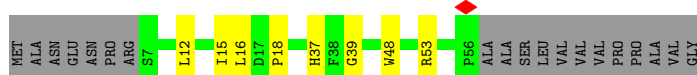
- Molecule 5: Antenna complex alpha/beta subunit domain-containing protein



- Molecule 5: Antenna complex alpha/beta subunit domain-containing protein



- Molecule 5: Antenna complex alpha/beta subunit domain-containing protein



- Molecule 5: Antenna complex alpha/beta subunit domain-containing protein



- Molecule 5: Antenna complex alpha/beta subunit domain-containing protein



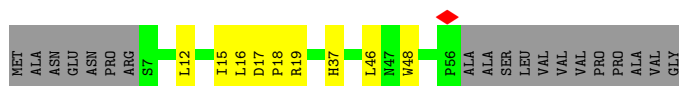
- Molecule 5: Antenna complex alpha/beta subunit domain-containing protein

Chain e:  64% 9% 28%



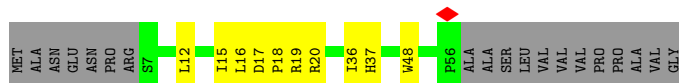
- Molecule 5: Antenna complex alpha/beta subunit domain-containing protein

Chain h:  59% 13% 28%



- Molecule 5: Antenna complex alpha/beta subunit domain-containing protein

Chain k:  58% 14% 28%



- Molecule 5: Antenna complex alpha/beta subunit domain-containing protein

Chain n:  59% 13% 28%



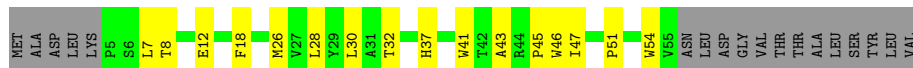
- Molecule 5: Antenna complex alpha/beta subunit domain-containing protein

Chain q:  59% 12% 28%



- Molecule 6: Antenna complex alpha/beta subunit domain-containing protein

Chain B:  51% 23% 26%



- Molecule 6: Antenna complex alpha/beta subunit domain-containing protein

Chain E:  59% 13% 26%



- Molecule 6: Antenna complex alpha/beta subunit domain-containing protein

Chain J: 



- Molecule 6: Antenna complex alpha/beta subunit domain-containing protein

Chain O: 



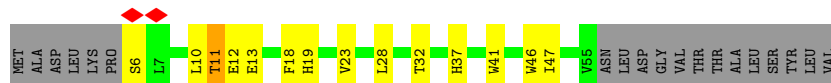
- Molecule 6: Antenna complex alpha/beta subunit domain-containing protein

Chain R: 



- Molecule 6: Antenna complex alpha/beta subunit domain-containing protein

Chain U: 



- Molecule 6: Antenna complex alpha/beta subunit domain-containing protein

Chain X: 



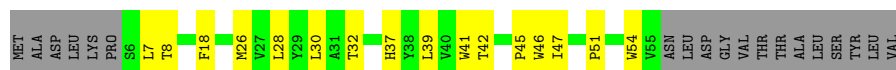
- Molecule 6: Antenna complex alpha/beta subunit domain-containing protein

Chain 1: 



- Molecule 6: Antenna complex alpha/beta subunit domain-containing protein

Chain 4: 



- Molecule 6: Antenna complex alpha/beta subunit domain-containing protein

Chain 7: 



- Molecule 6: Antenna complex alpha/beta subunit domain-containing protein

Chain 0: 



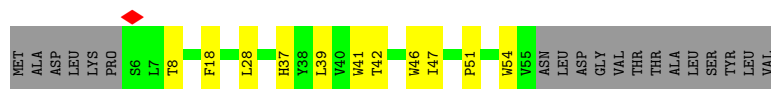
- Molecule 6: Antenna complex alpha/beta subunit domain-containing protein

Chain c: 



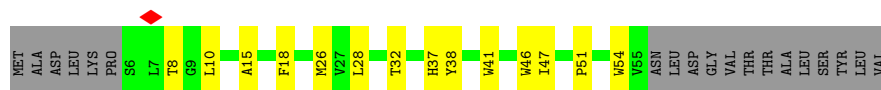
- Molecule 6: Antenna complex alpha/beta subunit domain-containing protein

Chain f: 



- Molecule 6: Antenna complex alpha/beta subunit domain-containing protein

Chain i: 



- Molecule 6: Antenna complex alpha/beta subunit domain-containing protein

Chain l: 



- Molecule 6: Antenna complex alpha/beta subunit domain-containing protein

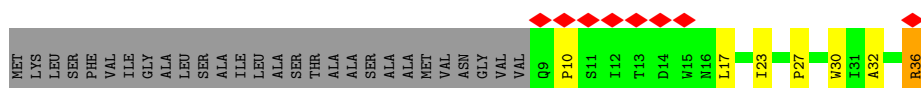
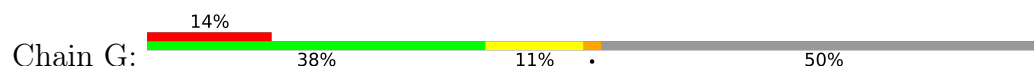
Chain o: 



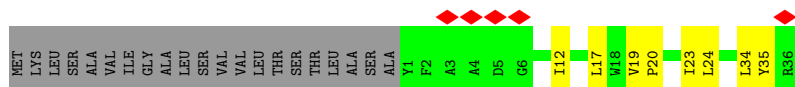
- Molecule 6: Antenna complex alpha/beta subunit domain-containing protein



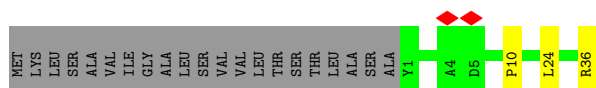
- Molecule 7: Light-harvesting protein gammal



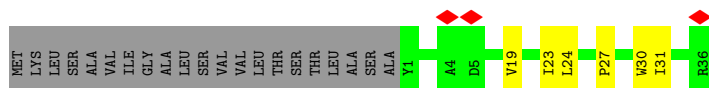
- Molecule 8: Light-harvesting protein B-1015 gamma chain



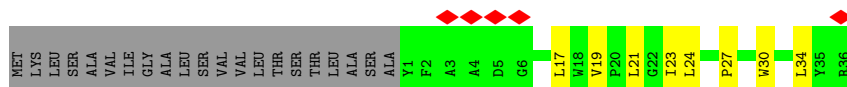
- Molecule 8: Light-harvesting protein B-1015 gamma chain



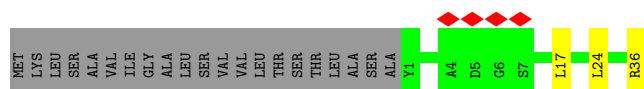
- Molecule 8: Light-harvesting protein B-1015 gamma chain



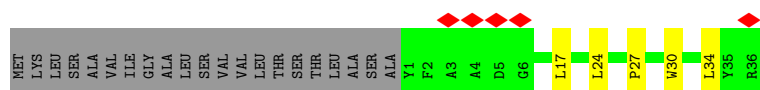
- Molecule 8: Light-harvesting protein B-1015 gamma chain



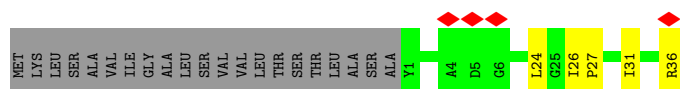
- Molecule 8: Light-harvesting protein B-1015 gamma chain



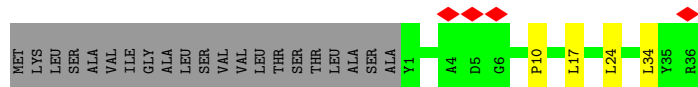
- Molecule 8: Light-harvesting protein B-1015 gamma chain



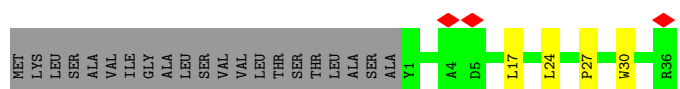
- Molecule 8: Light-harvesting protein B-1015 gamma chain



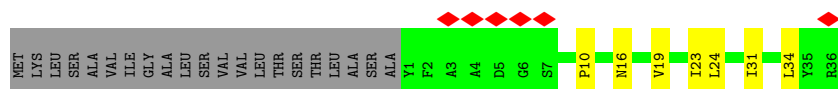
- Molecule 8: Light-harvesting protein B-1015 gamma chain



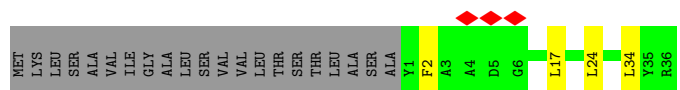
- Molecule 8: Light-harvesting protein B-1015 gamma chain



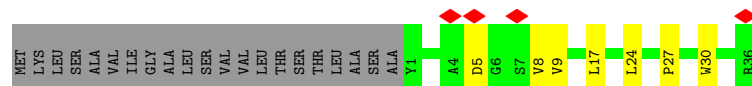
- Molecule 8: Light-harvesting protein B-1015 gamma chain



- Molecule 8: Light-harvesting protein B-1015 gamma chain



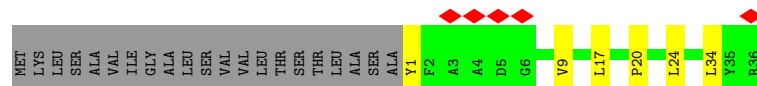
- Molecule 8: Light-harvesting protein B-1015 gamma chain



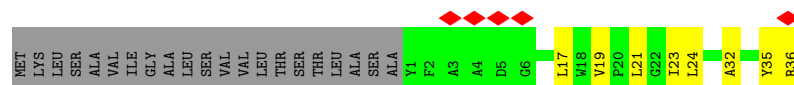
- Molecule 8: Light-harvesting protein B-1015 gamma chain



- Molecule 8: Light-harvesting protein B-1015 gamma chain



- Molecule 8: Light-harvesting protein B-1015 gamma chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	294012	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.434	Depositor
Minimum map value	-0.179	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.045	Depositor
Map size ($\text{\AA}$)	328.0, 328.0, 328.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.82, 0.82, 0.82	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MQ7, NS5, LMT, FME, MG, PGV, DGA, HEC, BPB, FE, UQ8, CDL, BCB, NS0

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	C	0.20	0/2657	0.38	0/3614
2	L	0.21	0/2246	0.40	0/3062
3	M	0.22	0/2725	0.38	0/3718
4	H	0.18	0/2087	0.36	0/2848
5	3	0.22	0/438	0.39	0/599
5	6	0.20	0/438	0.38	0/599
5	9	0.20	0/438	0.35	0/599
5	A	0.20	0/438	0.37	0/599
5	D	0.20	0/438	0.37	0/599
5	I	0.21	0/438	0.37	0/599
5	N	0.18	0/438	0.36	0/599
5	Q	0.19	0/438	0.35	0/599
5	T	0.18	0/438	0.35	0/599
5	W	0.18	0/438	0.37	0/599
5	Z	0.21	0/438	0.39	0/599
5	b	0.19	0/438	0.36	0/599
5	e	0.19	0/438	0.37	0/599
5	h	0.18	0/438	0.34	0/599
5	k	0.20	0/438	0.33	0/599
5	n	0.18	0/438	0.34	0/599
5	q	0.18	0/438	0.36	0/599
6	0	0.20	0/414	0.36	0/569
6	1	0.20	0/414	0.34	0/569
6	4	0.20	0/414	0.35	0/569
6	7	0.20	0/414	0.34	0/569
6	B	0.18	0/422	0.37	0/580
6	E	0.21	0/422	0.34	0/580
6	J	0.20	0/400	0.33	0/550
6	O	0.20	0/422	0.35	0/580
6	R	0.19	0/414	0.34	0/569
6	U	0.22	0/414	0.45	0/569
6	X	0.20	0/414	0.39	0/569

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	c	0.20	0/414	0.37	0/569
6	f	0.19	0/414	0.33	0/569
6	i	0.20	0/414	0.41	0/569
6	l	0.19	0/414	0.41	0/569
6	o	0.20	0/414	0.36	0/569
6	r	0.19	0/414	0.36	0/569
7	G	0.18	0/241	0.45	0/333
8	2	0.18	0/288	0.47	0/397
8	5	0.19	0/288	0.43	0/397
8	8	0.19	0/288	0.42	0/397
8	F	0.18	0/288	0.42	0/397
8	K	0.18	0/288	0.41	0/397
8	P	0.17	0/288	0.43	0/397
8	S	0.18	0/288	0.45	0/397
8	V	0.18	0/288	0.47	0/397
8	Y	0.19	0/288	0.46	0/397
8	a	0.17	0/288	0.40	0/397
8	d	0.19	0/288	0.45	0/397
8	g	0.18	0/288	0.41	0/397
8	j	0.20	0/288	0.46	0/397
8	m	0.18	0/288	0.43	0/397
8	p	0.17	0/288	0.40	0/397
All	All	0.20	0/28770	0.38	0/39400

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2585	0	2550	23	0
2	L	2159	0	2087	35	0
3	M	2621	0	2526	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	2041	0	2004	20	0
5	3	424	0	442	10	0
5	6	424	0	442	9	0
5	9	424	0	442	14	0
5	A	424	0	442	18	0
5	D	424	0	442	18	0
5	I	424	0	442	13	0
5	N	424	0	442	12	0
5	Q	424	0	442	12	0
5	T	424	0	442	13	0
5	W	424	0	442	12	0
5	Z	424	0	442	15	0
5	b	424	0	442	13	0
5	e	424	0	442	8	0
5	h	424	0	442	11	0
5	k	424	0	442	10	0
5	n	424	0	442	10	0
5	q	424	0	442	10	0
6	0	400	0	402	13	0
6	1	400	0	402	11	0
6	4	400	0	402	15	0
6	7	400	0	402	11	0
6	B	407	0	410	17	0
6	E	407	0	410	12	0
6	J	386	0	386	13	0
6	O	407	0	410	9	0
6	R	400	0	402	11	0
6	U	400	0	402	16	0
6	X	400	0	402	10	0
6	c	400	0	402	17	0
6	f	400	0	402	11	0
6	i	400	0	402	15	0
6	l	400	0	402	10	0
6	o	400	0	402	11	0
6	r	400	0	402	11	0
7	G	232	0	239	7	0
8	2	279	0	287	3	0
8	5	279	0	287	4	0
8	8	279	0	287	4	0
8	F	279	0	287	6	0
8	K	279	0	287	4	0
8	P	279	0	287	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	S	279	0	287	7	0
8	V	279	0	287	3	0
8	Y	279	0	287	4	0
8	a	279	0	287	7	0
8	d	279	0	287	6	0
8	g	279	0	287	5	0
8	j	279	0	287	9	0
8	m	279	0	287	5	0
8	p	279	0	287	6	0
9	C	172	0	121	6	0
10	C	1	0	0	0	0
11	A	53	0	74	11	0
11	C	15	0	11	0	0
11	L	31	0	36	2	0
11	M	78	0	101	17	0
12	L	23	0	27	0	0
13	0	66	0	72	11	0
13	1	66	0	72	7	0
13	3	66	0	72	6	0
13	4	66	0	72	8	0
13	6	66	0	72	7	0
13	7	66	0	72	7	0
13	9	66	0	72	7	0
13	A	66	0	72	6	0
13	B	66	0	72	8	0
13	D	66	0	72	9	0
13	E	66	0	72	8	0
13	I	66	0	72	7	0
13	J	66	0	72	7	0
13	L	132	0	144	11	0
13	M	132	0	144	10	0
13	N	66	0	72	5	0
13	O	66	0	72	16	0
13	Q	66	0	72	7	0
13	R	66	0	72	8	0
13	T	66	0	72	5	0
13	U	66	0	72	6	0
13	W	66	0	72	7	0
13	X	66	0	72	7	0
13	Z	66	0	72	8	0
13	b	66	0	72	7	0
13	c	66	0	72	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	e	66	0	72	4	0
13	f	66	0	72	7	0
13	h	66	0	72	6	0
13	i	66	0	72	10	0
13	k	66	0	72	5	0
13	l	66	0	72	7	0
13	n	66	0	72	5	0
13	o	66	0	72	12	0
13	q	66	0	72	4	0
13	r	66	0	72	7	0
14	L	65	0	74	4	0
14	M	65	0	74	5	0
15	H	170	0	237	14	0
15	L	75	0	94	4	0
15	M	85	0	117	10	0
15	r	68	0	80	7	0
16	M	1	0	0	0	0
17	M	48	0	64	1	0
18	M	40	0	60	1	0
19	B	15	0	19	0	0
19	M	25	0	35	3	0
19	T	26	0	35	2	0
19	b	70	0	92	6	0
19	h	35	0	46	2	0
19	k	35	0	46	0	0
19	n	35	0	46	2	0
20	D	47	0	65	6	0
20	I	51	0	76	4	0
20	M	45	0	58	1	0
20	N	38	0	44	2	0
20	Q	49	0	72	5	0
20	W	48	0	67	1	0
21	0	40	0	0	0	0
21	2	40	0	0	0	0
21	7	40	0	0	0	0
21	9	40	0	0	0	0
21	A	40	0	0	0	0
21	D	40	0	0	0	0
21	O	40	0	0	0	0
21	R	40	0	0	0	0
21	U	40	0	0	0	0
21	W	40	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	X	40	0	0	0	0
21	h	40	0	0	0	0
21	k	40	0	0	0	0
21	l	40	0	0	0	0
21	o	40	0	0	1	0
21	q	40	0	0	0	0
22	0	1	0	0	0	0
22	1	3	0	0	0	0
22	2	3	0	0	0	0
22	3	5	0	0	0	0
22	4	7	0	0	0	0
22	5	5	0	0	0	0
22	6	10	0	0	0	0
22	7	4	0	0	0	0
22	8	1	0	0	0	0
22	9	6	0	0	0	0
22	A	6	0	0	0	0
22	B	2	0	0	0	0
22	C	98	0	0	0	0
22	D	6	0	0	0	0
22	E	3	0	0	0	0
22	H	22	0	0	0	0
22	I	7	0	0	0	0
22	J	3	0	0	0	0
22	K	2	0	0	0	0
22	L	59	0	0	0	0
22	M	75	0	0	0	0
22	N	6	0	0	0	0
22	O	3	0	0	0	0
22	Q	6	0	0	0	0
22	R	5	0	0	0	0
22	S	1	0	0	0	0
22	T	6	0	0	1	0
22	U	5	0	0	0	0
22	V	2	0	0	0	0
22	W	3	0	0	0	0
22	X	5	0	0	0	0
22	Y	2	0	0	0	0
22	Z	4	0	0	0	0
22	b	10	0	0	0	0
22	c	4	0	0	0	0
22	e	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	f	2	0	0	0	0
22	g	1	0	0	0	0
22	h	4	0	0	0	0
22	i	1	0	0	1	0
22	j	2	0	0	0	0
22	k	5	0	0	0	0
22	l	1	0	0	0	0
22	n	4	0	0	0	0
22	o	1	0	0	0	0
22	p	1	0	0	0	0
22	q	2	0	0	0	0
All	All	32918	0	32674	616	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 9.

All (616) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:CYS:SG	9:C:402:HEC:CAC	2.11	1.38
1:C:135:CYS:SG	9:C:402:HEC:HAC	1.67	1.32
13:L:302:BCB:H2C	13:M:403:BCB:H2C	1.50	0.94
6:r:34:VAL:HG13	15:r:102:CDL:H381	1.57	0.85
6:J:26:MET:HE1	13:J:101:BCB:H172	1.60	0.84
6:4:45:PRO:HG3	8:5:10:PRO:HB3	1.65	0.79
5:Z:37:HIS:CE1	13:1:101:BCB:HMD1	2.18	0.78
5:h:37:HIS:CE1	13:i:101:BCB:HMD1	2.18	0.78
5:3:37:HIS:CE1	13:4:101:BCB:HMD1	2.20	0.77
5:I:37:HIS:CE1	13:J:101:BCB:HMD1	2.20	0.77
5:6:37:HIS:CE1	13:7:102:BCB:HMD1	2.20	0.77
5:T:37:HIS:CE1	13:U:102:BCB:HMD1	2.21	0.76
6:i:26:MET:HE1	13:i:101:BCB:H172	1.68	0.76
5:N:37:HIS:CE1	13:O:102:BCB:HMD1	2.20	0.75
5:k:37:HIS:CE1	13:l:102:BCB:HMD1	2.21	0.75
3:M:122:THR:HG22	11:M:408:UQ8:H15	1.69	0.75
6:O:46:TRP:CD2	13:O:102:BCB:H2C	2.22	0.74
5:9:37:HIS:CE1	13:0:102:BCB:HMD1	2.23	0.74
5:A:37:HIS:CE1	13:B:202:BCB:HMD1	2.23	0.73
6:0:46:TRP:CD2	13:0:102:BCB:H2C	2.23	0.73
13:L:302:BCB:H11	13:L:303:BCB:H2C	1.70	0.73
6:7:46:TRP:CD2	13:7:102:BCB:H2C	2.24	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:n:37:HIS:CE1	13:o:102:BCB:HMD1	2.22	0.73
6:R:46:TRP:CD2	13:R:102:BCB:H2C	2.23	0.72
5:e:37:HIS:CE1	13:f:101:BCB:HMD1	2.25	0.72
5:Q:37:HIS:CE1	13:R:102:BCB:HMD1	2.25	0.71
5:q:37:HIS:CE1	13:r:101:BCB:HMD1	2.25	0.71
1:C:135:CYS:SG	9:C:402:HEC:C3C	2.78	0.71
6:c:46:TRP:CD2	13:c:101:BCB:H2C	2.25	0.71
5:b:37:HIS:CE1	13:c:101:BCB:HMD1	2.24	0.71
4:H:9:HIS:O	4:H:9:HIS:ND1	2.23	0.71
6:E:46:TRP:CD2	13:E:101:BCB:H2C	2.26	0.71
6:X:46:TRP:CD2	13:X:102:BCB:H2C	2.26	0.70
6:U:46:TRP:CD2	13:U:102:BCB:H2C	2.26	0.70
6:f:46:TRP:CD2	13:f:101:BCB:H2C	2.26	0.70
5:W:37:HIS:CE1	13:X:102:BCB:HMD1	2.26	0.70
13:R:102:BCB:H111	13:T:101:BCB:H51	1.73	0.70
13:O:102:BCB:H71	8:P:31:ILE:HD11	1.75	0.69
13:O:102:BCB:HHB	8:P:24:LEU:HD21	1.75	0.69
6:O:45:PRO:HG3	8:a:10:PRO:HG3	1.73	0.69
6:i:46:TRP:CD2	13:i:101:BCB:H2C	2.28	0.69
3:M:263:SER:HA	3:M:266:ARG:HG3	1.75	0.69
11:M:408:UQ8:H16A	5:Z:31:VAL:HG22	1.73	0.69
6:r:46:TRP:CD2	13:r:101:BCB:H2C	2.28	0.69
5:A:38:PHE:HE2	20:D:102:PGV:H41	1.58	0.69
6:l:46:TRP:CD2	13:l:102:BCB:H2C	2.29	0.68
13:i:101:BCB:HHB	8:j:24:LEU:HD21	1.76	0.68
6:B:43:ALA:HB2	15:r:102:CDL:HB62	1.76	0.68
5:D:37:HIS:CE1	13:E:101:BCB:HMD1	2.28	0.68
5:9:37:HIS:NE2	13:9:101:BCB:NB	2.42	0.68
5:k:37:HIS:NE2	13:k:102:BCB:NB	2.40	0.68
3:M:158:CYS:HA	3:M:162:PHE:HB2	1.76	0.67
6:4:46:TRP:CD2	13:4:101:BCB:H2C	2.30	0.67
6:1:46:TRP:CD2	13:1:101:BCB:H2C	2.29	0.67
13:1:101:BCB:HHB	8:2:24:LEU:HD21	1.76	0.67
6:o:46:TRP:CD2	13:o:102:BCB:H2C	2.29	0.67
13:f:101:BCB:HHB	8:g:24:LEU:HD21	1.77	0.66
13:f:101:BCB:H192	13:h:102:BCB:H142	1.77	0.66
4:H:174:TRP:HB2	4:H:184:TYR:HB2	1.77	0.66
6:l:37:HIS:NE2	13:l:102:BCB:NB	2.43	0.66
1:C:236:ASP:OD2	1:C:304:ARG:NH2	2.27	0.66
2:L:46:VAL:HG22	13:L:303:BCB:H201	1.76	0.66
2:L:115:TRP:H	15:L:306:CDL:HB62	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:9:HIS:NE2	15:H:301:CDL:OA4	2.29	0.65
5:D:48:TRP:CE2	13:D:101:BCB:H2C	2.32	0.65
13:U:102:BCB:HHB	8:V:24:LEU:HD21	1.77	0.65
15:H:302:CDL:HB62	20:I:102:PGV:H211	1.79	0.65
5:q:17:ASP:H	6:r:8:THR:HG21	1.62	0.65
5:A:48:TRP:CE2	13:A:102:BCB:H2C	2.32	0.65
3:M:67:ILE:HG21	14:M:404:BPB:H15	1.78	0.64
6:J:46:TRP:CD2	13:J:101:BCB:H2C	2.32	0.64
5:Z:17:ASP:H	6:1:8:THR:HG21	1.62	0.64
13:E:101:BCB:HHB	8:F:24:LEU:HD21	1.78	0.64
13:o:102:BCB:HHB	8:p:24:LEU:HD21	1.79	0.64
5:Q:37:HIS:NE2	13:Q:402:BCB:NB	2.46	0.64
5:N:37:HIS:NE2	13:N:101:BCB:NB	2.45	0.64
13:r:101:BCB:H142	15:r:102:CDL:H731	1.79	0.64
15:H:301:CDL:H831	5:N:31:VAL:HG22	1.80	0.64
4:H:50:VAL:HG11	5:I:17:ASP:H	1.61	0.64
5:3:37:HIS:NE2	13:3:101:BCB:NB	2.46	0.63
5:b:20:ARG:HB2	19:b:102:LMT:H6D	1.80	0.63
6:B:46:TRP:CD2	13:B:202:BCB:H2C	2.34	0.63
5:9:20:ARG:NH2	19:b:102:LMT:O2'	2.30	0.63
5:I:22:LEU:HD13	13:I:101:BCB:H142	1.79	0.63
5:Z:37:HIS:NE2	13:Z:101:BCB:NB	2.47	0.62
3:M:300:HIS:HA	15:H:301:CDL:OA4	1.99	0.62
5:W:12:LEU:HD11	5:W:16:LEU:HD22	1.82	0.62
6:0:46:TRP:CD1	6:0:47:ILE:HG13	2.35	0.62
13:l:102:BCB:HHB	8:m:24:LEU:HD21	1.82	0.62
5:T:14:LEU:HD22	6:U:6:SER:HB2	1.82	0.61
5:e:37:HIS:NE2	13:e:101:BCB:NB	2.48	0.61
5:q:18:PRO:HB3	6:r:18:PHE:CZ	2.36	0.61
5:W:16:LEU:HD21	13:Z:101:BCB:H143	1.82	0.60
6:7:46:TRP:CD1	6:7:47:ILE:HG13	2.37	0.60
6:l:46:TRP:CD1	6:l:47:ILE:HG13	2.36	0.60
4:H:116:PRO:HB2	4:H:246:GLY:HA2	1.83	0.60
5:W:17:ASP:H	6:X:8:THR:HG21	1.66	0.60
1:C:274:ASP:OD1	1:C:278:ASN:ND2	2.34	0.60
5:9:12:LEU:HD11	5:9:16:LEU:HD12	1.83	0.60
13:O:102:BCB:H141	13:O:102:BCB:H203	1.84	0.59
13:r:101:BCB:H43	13:r:101:BCB:H3A	1.83	0.59
5:Q:15:ILE:HG22	6:R:7:LEU:HD12	1.84	0.59
2:L:199:ASN:HB3	15:M:409:CDL:HA21	1.84	0.59
5:W:37:HIS:NE2	13:W:302:BCB:NB	2.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:M:408:UQ8:H3M	15:M:409:CDL:H771	1.84	0.59
5:e:48:TRP:CE2	13:e:101:BCB:H2C	2.38	0.59
6:B:51:PRO:HG2	6:B:54:TRP:HB2	1.85	0.59
5:I:48:TRP:CE2	13:I:101:BCB:H2C	2.36	0.59
2:L:79:PRO:HG2	2:L:82:GLU:HB2	1.85	0.59
3:M:228:PHE:HB2	3:M:243:ALA:HB2	1.85	0.59
6:J:28:LEU:O	6:J:32:THR:HG22	2.03	0.59
5:b:37:HIS:NE2	13:b:101:BCB:NB	2.51	0.59
5:W:48:TRP:CE2	13:W:302:BCB:H2C	2.37	0.59
5:6:48:TRP:CE2	13:6:101:BCB:H2C	2.37	0.59
5:n:17:ASP:H	6:o:8:THR:HG21	1.67	0.59
1:C:142:PRO:HD2	9:C:402:HEC:HBD2	1.85	0.59
5:Z:17:ASP:OD2	5:Z:20:ARG:NE	2.30	0.58
2:L:214:ALA:HB2	3:M:20:PRO:HD2	1.85	0.58
11:M:408:UQ8:H46	5:Z:24:ALA:HB2	1.85	0.58
5:e:17:ASP:H	6:f:8:THR:HG21	1.67	0.58
11:M:408:UQ8:C6	11:M:408:UQ8:H10	2.34	0.58
6:f:51:PRO:HG2	6:f:54:TRP:HB2	1.86	0.58
5:n:20:ARG:NH2	19:n:102:LMT:O6'	2.35	0.58
5:3:48:TRP:CE2	13:3:101:BCB:H2C	2.38	0.58
14:L:304:BPB:CBB	14:L:304:BPB:HHC	2.33	0.58
13:Q:402:BCB:HMD1	6:R:37:HIS:CE1	2.39	0.58
13:A:102:BCB:H8	13:A:102:BCB:H41	1.86	0.57
5:3:17:ASP:H	6:4:8:THR:HG21	1.69	0.57
6:c:28:LEU:O	6:c:32:THR:HG22	2.03	0.57
2:L:36:VAL:HG13	5:D:27:ILE:HD11	1.86	0.57
13:M:403:BCB:HAA2	13:M:403:BCB:HBD	1.86	0.57
6:U:37:HIS:NE2	13:U:102:BCB:NB	2.52	0.57
5:e:18:PRO:HB3	6:f:18:PHE:CZ	2.40	0.57
5:I:18:PRO:HB3	6:J:18:PHE:CZ	2.40	0.57
6:c:51:PRO:HG2	6:c:54:TRP:HB2	1.85	0.57
13:6:101:BCB:HMD1	6:7:37:HIS:CE1	2.40	0.57
2:L:201:GLY:HA2	15:M:409:CDL:HB21	1.86	0.56
19:M:410:LMT:H121	19:T:102:LMT:H61	1.87	0.56
13:I:101:BCB:HMD1	6:J:37:HIS:CE1	2.40	0.56
13:e:101:BCB:HMD1	6:f:37:HIS:CE1	2.40	0.56
5:h:19:ARG:HH21	19:h:103:LMT:H2B	1.70	0.56
6:7:28:LEU:O	6:7:32:THR:HG22	2.04	0.56
6:f:46:TRP:CD1	6:f:47:ILE:HG13	2.41	0.56
20:M:411:PGV:H311	20:M:411:PGV:H92	1.88	0.56
5:D:30:THR:HG23	20:D:102:PGV:H302	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Z:22:LEU:HB3	13:Z:101:BCB:H142	1.87	0.56
5:n:18:PRO:HB3	6:o:18:PHE:CZ	2.39	0.56
2:L:181:PHE:HB3	14:M:404:BPB:HBBA	1.87	0.56
6:J:16:LYS:O	8:K:36:ARG:NH2	2.39	0.56
5:h:18:PRO:HB3	6:i:18:PHE:CZ	2.40	0.56
5:6:37:HIS:NE2	13:6:101:BCB:NB	2.54	0.56
6:i:51:PRO:HG2	6:i:54:TRP:HB2	1.86	0.56
6:R:46:TRP:CD1	6:R:47:ILE:HG13	2.40	0.56
6:o:26:MET:HE1	13:o:102:BCB:H172	1.88	0.56
1:C:259:THR:C	3:M:313:THR:HG21	2.31	0.56
6:c:46:TRP:CE2	13:c:101:BCB:H2C	2.41	0.56
13:J:101:BCB:HBB	8:K:24:LEU:HD21	1.87	0.56
15:M:409:CDL:H342	15:M:409:CDL:H152	1.88	0.56
5:A:18:PRO:HB3	6:B:18:PHE:CZ	2.41	0.56
5:N:48:TRP:CE2	13:N:101:BCB:H2C	2.40	0.56
13:b:101:BCB:HMD1	6:c:37:HIS:CE1	2.41	0.55
6:c:46:TRP:CD1	6:c:47:ILE:HG13	2.41	0.55
6:J:20:SER:HB2	8:K:36:ARG:HH21	1.71	0.55
5:b:48:TRP:CE2	13:b:101:BCB:H2C	2.41	0.55
5:n:48:TRP:CE2	13:n:101:BCB:H2C	2.40	0.55
5:6:12:LEU:HD11	5:6:16:LEU:HD22	1.88	0.55
14:M:404:BPB:CBB	14:M:404:BPB:HHC	2.37	0.55
5:h:37:HIS:NE2	13:h:102:BCB:NB	2.55	0.55
5:q:37:HIS:NE2	13:q:101:BCB:NB	2.53	0.55
5:I:19:ARG:HH22	20:I:102:PGV:H05	1.71	0.55
5:Q:11:LYS:HG3	5:Q:14:LEU:HD12	1.88	0.55
5:Q:48:TRP:CE2	13:Q:402:BCB:H2C	2.42	0.55
5:b:12:LEU:HD11	5:b:16:LEU:HD22	1.88	0.55
5:A:48:TRP:CD2	13:A:102:BCB:H2C	2.42	0.55
6:O:28:LEU:O	6:O:32:THR:HG22	2.06	0.55
13:N:101:BCB:HMD1	6:O:37:HIS:CE1	2.42	0.55
13:Z:101:BCB:HMD1	6:l:37:HIS:CE1	2.41	0.55
5:n:37:HIS:NE2	13:n:101:BCB:NB	2.55	0.55
13:n:101:BCB:HMD1	6:o:37:HIS:CE1	2.41	0.54
2:L:8:LYS:HD2	4:H:118:SER:HB3	1.88	0.54
14:M:404:BPB:HHC	14:M:404:BPB:HBBB	1.88	0.54
13:O:102:BCB:HBB	8:a:24:LEU:HD21	1.90	0.54
5:T:37:HIS:NE2	13:T:101:BCB:NB	2.56	0.54
5:T:48:TRP:CE2	13:T:101:BCB:H2C	2.42	0.54
5:T:53:ARG:NH2	22:T:201:HOH:O	2.27	0.54
15:H:301:CDL:H591	5:N:35:LEU:HD21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:46:TRP:CE2	13:7:102:BCB:H2C	2.42	0.54
6:i:46:TRP:CD1	6:i:47:ILE:HG13	2.43	0.54
5:D:8:ALA:HB1	5:D:11:LYS:HD2	1.88	0.54
5:Z:48:TRP:CE2	13:Z:101:BCB:H2C	2.43	0.54
6:f:46:TRP:CE2	13:f:101:BCB:H2C	2.43	0.54
5:k:15:ILE:HG22	6:l:7:LEU:HD13	1.89	0.54
3:M:54:ALA:HB3	11:M:408:UQ8:H41A	1.89	0.53
13:W:302:BCB:HMD1	6:X:37:HIS:CE1	2.43	0.53
13:X:102:BCB:HHB	8:Y:24:LEU:HD21	1.90	0.53
5:b:17:ASP:H	6:c:8:THR:HG21	1.73	0.53
6:r:37:HIS:CG	15:r:102:CDL:H611	2.43	0.53
2:L:39:ILE:HG13	17:M:405:MQ7:H411	1.90	0.53
13:D:101:BCB:HMD1	6:E:37:HIS:CE1	2.43	0.53
6:O:46:TRP:CD1	6:O:47:ILE:HG13	2.43	0.53
13:T:101:BCB:HMD1	6:U:37:HIS:CE1	2.42	0.53
5:9:17:ASP:H	6:0:8:THR:HG21	1.73	0.53
6:4:39:LEU:O	6:4:42:THR:OG1	2.26	0.53
5:Q:17:ASP:H	6:R:8:THR:HG21	1.73	0.53
6:R:46:TRP:CE2	13:R:102:BCB:H2C	2.43	0.53
13:R:102:BCB:HHB	8:S:24:LEU:HD21	1.89	0.53
13:4:101:BCB:HHB	8:5:24:LEU:HD21	1.89	0.53
5:9:18:PRO:HB3	6:0:18:PHE:CZ	2.43	0.53
13:h:102:BCB:HMD1	6:i:37:HIS:CE1	2.43	0.53
3:M:154:PHE:HB2	11:M:408:UQ8:H4M	1.90	0.53
6:X:46:TRP:CD1	6:X:47:ILE:HG13	2.44	0.53
4:H:198:MET:HE3	4:H:203:ALA:HB2	1.91	0.53
5:k:18:PRO:HB3	6:l:18:PHE:CZ	2.43	0.53
13:k:102:BCB:HMD1	6:l:37:HIS:CE1	2.44	0.53
13:B:202:BCB:H43	13:B:202:BCB:HMA2	1.91	0.52
8:P:27:PRO:HA	8:P:30:TRP:NE1	2.24	0.52
13:3:101:BCB:HMD1	6:4:37:HIS:CE1	2.44	0.52
5:b:18:PRO:HB3	6:c:18:PHE:CZ	2.44	0.52
6:J:46:TRP:CD1	6:J:47:ILE:HG13	2.44	0.52
13:L:302:BCB:HBB3	13:L:302:BCB:HMB1	1.91	0.52
5:T:13:TRP:HD1	6:U:19:HIS:HB2	1.74	0.52
5:T:14:LEU:HD21	6:U:12:GLU:HA	1.91	0.52
6:4:46:TRP:CD1	6:4:47:ILE:HG13	2.45	0.52
2:L:231:ARG:HD3	3:M:5:THR:O	2.09	0.52
5:D:48:TRP:CD2	13:D:101:BCB:H2C	2.45	0.52
6:4:51:PRO:HG2	6:4:54:TRP:HB2	1.91	0.52
6:E:46:TRP:CE2	13:E:101:BCB:H2C	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:c:101:BCB:HHB	8:d:24:LEU:HD21	1.91	0.52
6:l:41:TRP:CG	8:m:17:LEU:HD13	2.45	0.52
8:m:1:TYR:N	8:m:9:VAL:O	2.42	0.52
5:n:16:LEU:HD13	5:q:19:ARG:HG2	1.92	0.52
6:i:10:LEU:HD23	6:i:15:ALA:HA	1.92	0.52
5:T:13:TRP:CD1	6:U:19:HIS:HB2	2.45	0.52
8:m:34:LEU:HD22	6:o:28:LEU:HD12	1.91	0.52
4:H:127:ASP:HB2	4:H:234:LEU:HD21	1.93	0.51
6:i:46:TRP:CE2	13:i:101:BCB:H2C	2.44	0.51
1:C:93:GLU:H	1:C:93:GLU:CD	2.17	0.51
5:A:17:ASP:H	6:B:8:THR:HG21	1.75	0.51
5:3:18:PRO:HB3	6:4:18:PHE:CZ	2.46	0.51
6:7:51:PRO:HG2	6:7:54:TRP:HB2	1.92	0.51
13:L:303:BCB:HMA2	15:H:301:CDL:H452	1.93	0.51
11:A:101:UQ8:H41A	5:q:39:GLY:HA2	1.92	0.51
5:I:12:LEU:HD11	5:I:16:LEU:HD22	1.92	0.51
5:3:48:TRP:CD2	13:3:101:BCB:H2C	2.46	0.51
13:O:102:BCB:H142	8:P:31:ILE:HG12	1.93	0.51
13:0:102:BCB:H122	13:b:101:BCB:H72	1.92	0.51
5:A:31:VAL:HG21	11:A:101:UQ8:H10B	1.91	0.51
6:X:46:TRP:CE2	13:X:102:BCB:H2C	2.46	0.51
6:4:46:TRP:CE2	13:4:101:BCB:H2C	2.44	0.51
13:r:101:BCB:H171	15:r:102:CDL:H532	1.93	0.51
6:o:46:TRP:CD1	6:o:47:ILE:HG13	2.45	0.51
1:C:102:TYR:CD2	1:C:103:PRO:HD3	2.46	0.51
3:M:23:GLN:HG3	19:M:410:LMT:H3'	1.93	0.51
4:H:42:PRO:HD3	4:H:62:LEU:HD11	1.93	0.50
5:N:51:PHE:O	5:N:53:ARG:HD3	2.12	0.50
2:L:272:TRP:CD1	3:M:87:ARG:HD3	2.47	0.50
13:M:402:BCB:HHC	13:M:402:BCB:HBB2	1.93	0.50
5:b:48:TRP:CD2	13:b:101:BCB:H2C	2.47	0.50
6:0:28:LEU:O	6:0:32:THR:HG22	2.12	0.50
3:M:157:LEU:HD11	11:M:408:UQ8:H11	1.94	0.50
4:H:33:ARG:HH21	15:H:302:CDL:HA31	1.75	0.50
5:3:15:ILE:HG22	6:4:7:LEU:HD12	1.94	0.50
6:U:11:THR:C	6:U:13:GLU:H	2.20	0.50
6:7:41:TRP:CG	8:8:17:LEU:HD13	2.47	0.50
2:L:193:LEU:HD22	2:L:216:PHE:CE2	2.47	0.50
3:M:23:GLN:OE1	5:Z:19:ARG:NH2	2.42	0.50
6:l:28:LEU:O	6:l:32:THR:HG22	2.10	0.50
5:N:18:PRO:HB3	6:O:18:PHE:CZ	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:38:PHE:HB3	20:N:102:PGV:H012	1.94	0.50
6:O:46:TRP:NE1	13:O:102:BCB:HHC	2.27	0.50
6:U:23:VAL:HG11	8:V:36:ARG:HB3	1.93	0.50
5:9:48:TRP:CE2	13:9:101:BCB:H2C	2.47	0.50
6:i:41:TRP:CG	8:j:17:LEU:HD13	2.47	0.50
6:R:28:LEU:O	6:R:32:THR:HG22	2.12	0.49
6:r:28:LEU:O	6:r:32:THR:HG22	2.12	0.49
13:r:101:BCB:H143	15:r:102:CDL:H561	1.94	0.49
6:U:46:TRP:CE2	13:U:102:BCB:H2C	2.46	0.49
3:M:122:THR:HG23	3:M:157:LEU:HD21	1.93	0.49
5:I:37:HIS:NE2	13:I:101:BCB:NB	2.60	0.49
6:J:46:TRP:CE2	13:J:101:BCB:H2C	2.48	0.49
6:O:46:TRP:CE2	13:O:102:BCB:H2C	2.48	0.49
13:O:102:BCB:HMA1	13:Q:402:BCB:HMA1	1.94	0.49
2:L:182:ALA:HA	13:M:402:BCB:H43	1.95	0.49
6:O:26:MET:HE1	13:O:102:BCB:H143	1.94	0.49
5:9:15:ILE:O	5:b:19:ARG:HD3	2.13	0.49
3:M:60:ILE:HD13	14:M:404:BPB:H5A	1.94	0.49
6:4:37:HIS:NE2	13:4:101:BCB:NB	2.61	0.49
13:q:101:BCB:HMD1	6:r:37:HIS:CE1	2.48	0.49
5:h:17:ASP:H	6:i:8:THR:HG21	1.78	0.49
15:H:301:CDL:OA9	15:H:301:CDL:H131	2.13	0.49
4:H:18:TYR:OH	15:H:301:CDL:HA61	2.13	0.49
13:9:101:BCB:HMD1	6:0:37:HIS:CE1	2.47	0.49
6:X:41:TRP:CG	8:Y:17:LEU:HD13	2.48	0.49
8:Y:27:PRO:HA	8:Y:30:TRP:NE1	2.27	0.49
5:h:17:ASP:OD2	19:h:103:LMT:O6'	2.31	0.49
3:M:185:LEU:HD21	13:M:402:BCB:CAC	2.42	0.48
11:A:101:UQ8:H25B	20:D:102:PGV:H132	1.96	0.48
5:T:51:PHE:O	5:T:53:ARG:HD3	2.13	0.48
6:X:37:HIS:NE2	13:X:102:BCB:NB	2.61	0.48
5:6:48:TRP:CD2	13:6:101:BCB:H2C	2.49	0.48
6:f:39:LEU:O	6:f:42:THR:OG1	2.25	0.48
1:C:99:GLU:O	1:C:105:LYS:NZ	2.36	0.48
5:k:17:ASP:H	6:l:8:THR:HG21	1.78	0.48
5:k:20:ARG:NH2	19:n:102:LMT:O2'	2.47	0.48
5:A:52:GLN:HG2	6:r:51:PRO:HG3	1.94	0.48
5:b:18:PRO:HG2	6:c:10:LEU:HD11	1.96	0.48
5:h:48:TRP:CE2	13:h:102:BCB:H2C	2.48	0.48
6:l:46:TRP:CE2	13:l:102:BCB:H2C	2.48	0.48
3:M:67:ILE:HD11	13:M:403:BCB:H18	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:3:21:VAL:HG22	13:6:101:BCB:H171	1.95	0.48
5:3:29:LEU:HD22	13:4:101:BCB:HED1	1.95	0.48
2:L:8:LYS:HE3	2:L:9:TYR:CE2	2.49	0.48
2:L:193:LEU:HD22	2:L:216:PHE:HE2	1.78	0.48
19:b:103:LMT:H51	5:e:24:ALA:HA	1.96	0.48
5:k:12:LEU:HD11	5:k:16:LEU:HD22	1.96	0.48
5:I:48:TRP:CD2	13:I:101:BCB:H2C	2.48	0.48
6:o:46:TRP:CE2	13:o:102:BCB:H2C	2.48	0.48
6:0:26:MET:HE2	8:a:31:ILE:HD13	1.96	0.48
6:B:28:LEU:O	6:B:32:THR:HG22	2.13	0.48
6:E:37:HIS:NE2	13:E:101:BCB:NB	2.62	0.47
2:L:115:TRP:CD1	15:L:306:CDL:HB32	2.50	0.47
13:N:101:BCB:H112	13:N:101:BCB:H152	1.56	0.47
8:S:19:VAL:O	8:S:23:ILE:HG13	2.13	0.47
6:7:37:HIS:NE2	13:7:102:BCB:NB	2.62	0.47
13:7:102:BCB:H43	8:8:24:LEU:HD23	1.95	0.47
6:1:28:LEU:O	6:1:32:THR:HG22	2.13	0.47
13:o:102:BCB:H141	8:p:35:TYR:CE2	2.50	0.47
15:M:409:CDL:OB9	19:T:102:LMT:O2'	2.25	0.47
13:A:102:BCB:HMD1	6:B:37:HIS:CE1	2.49	0.47
6:E:41:TRP:CG	8:F:17:LEU:HD13	2.49	0.47
13:7:102:BCB:H122	13:7:102:BCB:H8	1.64	0.47
3:M:58:GLY:HA2	5:3:27:ILE:HG21	1.96	0.47
3:M:147:TRP:CD1	15:M:409:CDL:HB61	2.49	0.47
4:H:9:HIS:O	5:Q:42:SER:HB3	2.15	0.47
6:B:46:TRP:CD1	6:B:47:ILE:HG13	2.48	0.47
13:J:101:BCB:H112	13:J:101:BCB:H93	1.79	0.47
3:M:71:GLY:HA3	18:M:406:NS5:H31	1.96	0.47
5:Q:18:PRO:HB3	6:R:18:PHE:CZ	2.50	0.47
5:n:15:ILE:O	5:q:19:ARG:HD3	2.14	0.47
2:L:24:PHE:CE1	5:D:20:ARG:HG2	2.50	0.47
11:M:408:UQ8:H32	11:M:408:UQ8:H35	1.66	0.47
5:A:22:LEU:HB3	13:A:102:BCB:H121	1.96	0.47
7:G:27:PRO:HA	7:G:30:TRP:NE1	2.29	0.47
5:D:17:ASP:H	6:E:8:THR:CG2	2.28	0.47
5:W:18:PRO:HB3	6:X:18:PHE:CZ	2.49	0.47
13:X:102:BCB:H42	13:Z:101:BCB:HMA2	1.95	0.47
5:q:48:TRP:CE2	13:q:101:BCB:H2C	2.48	0.47
3:M:39:LEU:HD12	3:M:42:ILE:HD11	1.96	0.47
2:L:47:SER:HB3	5:D:35:LEU:HD22	1.96	0.47
11:A:101:UQ8:H37	11:A:101:UQ8:H40	1.74	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:c:101:BCB:H141	13:c:101:BCB:H162	1.80	0.47
13:9:101:BCB:H152	13:9:101:BCB:H112	1.61	0.47
8:g:27:PRO:HA	8:g:30:TRP:NE1	2.31	0.46
6:E:28:LEU:O	6:E:32:THR:HG22	2.14	0.46
5:6:18:PRO:HB3	6:7:18:PHE:CZ	2.50	0.46
11:A:101:UQ8:H10	11:A:101:UQ8:H7A	1.57	0.46
6:c:39:LEU:O	6:c:42:THR:OG1	2.30	0.46
6:E:46:TRP:CD1	6:E:47:ILE:HG13	2.50	0.46
2:L:26:VAL:HG22	5:D:20:ARG:HD2	1.98	0.46
6:B:41:TRP:CD2	7:G:17:LEU:HD13	2.50	0.46
5:9:36:ILE:HD12	13:0:102:BCB:O1D	2.16	0.46
6:0:46:TRP:CE2	13:0:102:BCB:H2C	2.49	0.46
6:U:41:TRP:CG	8:V:17:LEU:HD13	2.51	0.46
6:f:37:HIS:NE2	13:f:101:BCB:NB	2.64	0.46
5:n:48:TRP:CD2	13:n:101:BCB:H2C	2.51	0.46
2:L:105:VAL:HG21	15:L:306:CDL:H341	1.97	0.46
3:M:17:HIS:O	3:M:17:HIS:ND1	2.49	0.46
3:M:153:ILE:HG21	11:M:408:UQ8:H11A	1.98	0.46
13:O:102:BCB:CHB	8:P:24:LEU:HD21	2.46	0.46
13:o:102:BCB:CHB	8:p:24:LEU:HD21	2.46	0.46
15:H:301:CDL:H802	15:H:301:CDL:H771	1.78	0.46
13:E:101:BCB:H61	13:E:101:BCB:H102	1.52	0.46
8:S:27:PRO:HA	8:S:30:TRP:NE1	2.31	0.46
6:4:28:LEU:O	6:4:32:THR:HG22	2.15	0.46
1:C:89:TYR:OH	9:C:402:HEC:O2A	2.30	0.46
13:f:101:BCB:H62	13:f:101:BCB:H102	1.68	0.46
5:h:12:LEU:HD11	5:h:16:LEU:HD22	1.97	0.46
5:k:48:TRP:CE2	13:k:102:BCB:H2C	2.51	0.46
1:C:80:TRP:CD1	1:C:133:TYR:HB2	2.51	0.46
13:c:101:BCB:H93	13:c:101:BCB:H112	1.85	0.46
5:A:37:HIS:NE2	13:A:102:BCB:NB	2.64	0.45
6:B:45:PRO:HB3	7:G:10:PRO:HB3	1.98	0.45
5:D:37:HIS:NE2	13:D:101:BCB:NB	2.64	0.45
6:1:46:TRP:CD1	6:1:47:ILE:HG13	2.51	0.45
6:1:46:TRP:CE2	13:1:101:BCB:H2C	2.51	0.45
6:4:41:TRP:CG	8:5:17:LEU:HD13	2.50	0.45
8:j:19:VAL:O	8:j:23:ILE:HG13	2.16	0.45
19:M:410:LMT:H123	13:Z:101:BCB:H191	1.96	0.45
5:W:29:LEU:HD22	13:X:102:BCB:HED1	1.98	0.45
6:o:50:ILE:HG23	6:o:54:TRP:HB3	1.97	0.45
14:L:304:BPB:HHC	14:L:304:BPB:HBBB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:101:UQ8:H25	11:A:101:UQ8:H22	1.67	0.45
8:F:34:LEU:HD23	8:F:35:TYR:CZ	2.51	0.45
13:0:102:BCB:HMA1	13:b:101:BCB:HMA1	1.97	0.45
6:i:28:LEU:O	6:i:32:THR:HG22	2.17	0.45
5:A:12:LEU:O	5:A:15:ILE:HG12	2.16	0.45
11:A:101:UQ8:H18	11:A:101:UQ8:H22A	1.65	0.45
5:Q:28:TYR:O	5:Q:32:ILE:HG12	2.16	0.45
13:6:101:BCB:H202	13:6:101:BCB:H162	1.73	0.45
1:C:73:THR:OG1	1:C:325:GLU:OE2	2.33	0.45
2:L:272:TRP:CG	3:M:87:ARG:HD3	2.52	0.45
6:B:26:MET:HE1	13:B:202:BCB:H202	1.98	0.45
5:Q:48:TRP:CD2	13:Q:402:BCB:H2C	2.52	0.45
5:W:15:ILE:HG22	6:X:7:LEU:HD12	1.99	0.45
5:9:26:PHE:CD1	13:9:101:BCB:H41	2.52	0.45
1:C:215:GLY:HA2	3:M:168:GLY:O	2.17	0.45
2:L:132:GLN:OE1	2:L:145:ALA:HB1	2.17	0.45
5:A:19:ARG:O	5:A:23:THR:HG22	2.17	0.45
6:r:41:TRP:CD1	15:r:102:CDL:H311	2.51	0.45
8:a:34:LEU:HD22	6:c:28:LEU:HD12	1.99	0.45
5:A:46:LEU:HD13	13:B:202:BCB:HBC3	2.00	0.44
8:S:34:LEU:HD22	6:U:28:LEU:HD12	1.99	0.44
5:T:52:GLN:NE2	5:T:53:ARG:O	2.47	0.44
5:h:46:LEU:HD13	13:i:101:BCB:HBC3	1.98	0.44
11:A:101:UQ8:H46	11:A:101:UQ8:H42A	1.69	0.44
6:c:37:HIS:NE2	13:c:101:BCB:NB	2.66	0.44
1:C:102:TYR:CG	1:C:103:PRO:HD3	2.52	0.44
15:M:409:CDL:H362	15:M:409:CDL:H172	1.99	0.44
5:N:48:TRP:CD2	13:N:101:BCB:H2C	2.52	0.44
13:9:101:BCB:H111	13:9:101:BCB:H72	1.62	0.44
8:d:34:LEU:HD22	6:f:28:LEU:HD12	1.99	0.44
3:M:72:PHE:HZ	5:6:39:GLY:HA2	1.81	0.44
5:A:36:ILE:HD12	13:B:202:BCB:O1D	2.18	0.44
3:M:283:ILE:HD11	13:M:403:BCB:OBD	2.17	0.44
5:Z:17:ASP:H	6:l:8:THR:CG2	2.29	0.44
3:M:121:MET:HG3	13:M:403:BCB:H202	2.00	0.44
3:M:152:ALA:HA	3:M:276:MET:SD	2.58	0.44
11:M:407:UQ8:H12	11:M:407:UQ8:H15	1.65	0.44
5:Z:48:TRP:CD2	13:Z:101:BCB:H2C	2.53	0.44
6:R:41:TRP:CG	8:S:17:LEU:HD13	2.53	0.44
5:q:12:LEU:O	5:q:16:LEU:HB2	2.17	0.44
5:6:16:LEU:HD12	5:9:19:ARG:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:i:37:HIS:NE2	13:i:101:BCB:NB	2.65	0.44
13:i:101:BCB:H141	8:j:35:TYR:OH	2.18	0.44
6:E:7:LEU:HD11	6:J:8:THR:HB	1.99	0.44
8:P:19:VAL:O	8:P:23:ILE:HG13	2.18	0.44
6:R:46:TRP:NE1	13:R:102:BCB:HHC	2.33	0.44
5:e:48:TRP:CD2	13:e:101:BCB:H2C	2.53	0.44
5:D:36:ILE:HD12	13:E:101:BCB:O1D	2.18	0.43
5:T:18:PRO:HB3	6:U:18:PHE:CE2	2.52	0.43
6:U:28:LEU:O	6:U:32:THR:HG22	2.17	0.43
5:Z:18:PRO:HB3	6:l:18:PHE:CZ	2.53	0.43
5:6:15:ILE:O	5:9:19:ARG:HD3	2.17	0.43
6:0:47:ILE:HG22	8:a:16:ASN:ND2	2.33	0.43
8:p:32:ALA:O	8:p:36:ARG:HB2	2.18	0.43
5:q:48:TRP:CD2	13:q:101:BCB:H2C	2.53	0.43
3:M:283:ILE:HD13	3:M:283:ILE:HA	1.89	0.43
11:M:407:UQ8:H7	11:M:407:UQ8:H10	1.75	0.43
13:O:102:BCB:H152	13:Q:402:BCB:H122	2.00	0.43
13:l:101:BCB:H62	13:l:101:BCB:H102	1.76	0.43
6:i:46:TRP:CZ2	8:j:20:PRO:HG3	2.53	0.43
8:p:19:VAL:O	8:p:23:ILE:HG13	2.18	0.43
1:C:231:MET:HB3	9:C:403:HEC:C4B	2.49	0.43
13:M:403:BCB:HAA2	13:M:403:BCB:CBD	2.46	0.43
5:I:55:LEU:HD13	5:N:51:PHE:CZ	2.53	0.43
5:Q:23:THR:O	5:Q:27:ILE:HG12	2.19	0.43
6:U:11:THR:O	6:U:13:GLU:N	2.49	0.43
5:W:48:TRP:CD2	13:W:302:BCB:H2C	2.53	0.43
13:3:101:BCB:H62	13:3:101:BCB:H41	1.69	0.43
6:c:49:PRO:HG2	8:d:2:PHE:CE2	2.54	0.43
8:F:19:VAL:O	8:F:23:ILE:HG13	2.18	0.43
13:4:101:BCB:H121	13:6:101:BCB:H71	2.00	0.43
13:c:101:BCB:H43	8:d:24:LEU:HD23	2.00	0.43
1:C:15:ARG:HB3	2:L:70:ASP:OD1	2.17	0.43
5:Z:27:ILE:O	5:Z:31:VAL:HG23	2.18	0.43
2:L:150:ILE:HD13	14:L:304:BPB:H20B	2.01	0.43
7:G:27:PRO:HA	7:G:30:TRP:CE2	2.53	0.43
6:c:41:TRP:CG	8:d:17:LEU:HD13	2.53	0.43
13:L:302:BCB:H151	14:L:304:BPB:H5A	1.99	0.43
6:B:46:TRP:CE2	13:B:202:BCB:H2C	2.54	0.43
7:G:23:ILE:HG23	13:D:101:BCB:O1D	2.19	0.43
20:Q:401:PGV:H131	20:Q:401:PGV:H102	1.75	0.43
13:Q:402:BCB:HMB1	13:Q:402:BCB:HBB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:27:GLY:HA2	20:I:102:PGV:O13	2.19	0.43
4:H:163:ASP:OD1	4:H:163:ASP:N	2.50	0.43
5:D:17:ASP:H	6:E:8:THR:HG22	1.84	0.43
5:W:18:PRO:HB3	6:X:18:PHE:CE2	2.54	0.43
5:b:20:ARG:NH1	19:b:103:LMT:O2'	2.51	0.43
5:b:37:HIS:NE2	13:c:101:BCB:HMD1	2.34	0.43
11:L:305:UQ8:H7	11:L:305:UQ8:H10	1.65	0.43
4:H:9:HIS:O	4:H:9:HIS:CG	2.71	0.43
7:G:32:ALA:O	7:G:36:ARG:HD2	2.19	0.43
13:D:101:BCB:H62	13:D:101:BCB:H41	1.76	0.43
5:N:29:LEU:HD22	13:O:102:BCB:HED1	2.00	0.43
8:2:26:ILE:HB	8:2:27:PRO:HD3	2.01	0.43
4:H:18:TYR:HB3	20:Q:401:PGV:H102	2.01	0.43
6:c:49:PRO:HG2	8:d:2:PHE:CZ	2.54	0.43
13:L:303:BCB:HMD2	13:M:403:BCB:CAB	2.48	0.42
11:L:305:UQ8:H12	11:L:305:UQ8:H15	1.74	0.42
20:D:102:PGV:H131	20:D:102:PGV:H102	1.67	0.42
8:Y:34:LEU:HD22	6:1:28:LEU:HD12	2.00	0.42
2:L:244:GLY:O	13:L:302:BCB:HED3	2.18	0.42
3:M:127:CYS:SG	11:M:408:UQ8:H23	2.59	0.42
15:H:301:CDL:H382	15:H:301:CDL:H352	1.81	0.42
6:B:26:MET:O	6:B:30:LEU:HG	2.19	0.42
6:O:37:HIS:NE2	13:O:102:BCB:NB	2.67	0.42
13:4:101:BCB:H143	13:4:101:BCB:H112	1.80	0.42
5:h:48:TRP:CD2	13:h:102:BCB:H2C	2.54	0.42
11:M:408:UQ8:H30	11:M:408:UQ8:H27	1.61	0.42
5:A:28:TYR:CZ	11:A:101:UQ8:H4MB	2.53	0.42
13:R:102:BCB:CHB	8:S:24:LEU:HD21	2.49	0.42
13:3:101:BCB:H192	13:3:101:BCB:H161	1.64	0.42
5:9:43:THR:O	5:9:47:ASN:HB2	2.19	0.42
3:M:147:TRP:CZ3	15:M:409:CDL:H742	2.54	0.42
4:H:116:PRO:HD2	4:H:250:TYR:CE2	2.54	0.42
8:F:23:ILE:HG23	13:I:101:BCB:O1D	2.19	0.42
5:I:37:HIS:NE2	13:J:101:BCB:HMD1	2.33	0.42
8:a:19:VAL:O	8:a:23:ILE:HG13	2.19	0.42
5:n:29:LEU:HD22	13:o:102:BCB:HED1	2.01	0.42
20:I:102:PGV:H182	20:I:102:PGV:H312	2.01	0.42
13:o:102:BCB:H142	13:o:102:BCB:H111	1.75	0.42
13:o:102:BCB:H203	13:o:102:BCB:H161	1.93	0.42
15:L:306:CDL:H112	15:L:306:CDL:H141	1.77	0.42
3:M:75:LEU:HG	3:M:80:PHE:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:D:101:BCB:H161	13:D:101:BCB:H121	1.84	0.42
6:f:41:TRP:CG	8:g:17:LEU:HD13	2.54	0.42
13:h:102:BCB:H112	13:h:102:BCB:H152	1.88	0.42
6:o:41:TRP:CG	8:p:17:LEU:HD13	2.54	0.42
13:W:302:BCB:H193	13:W:302:BCB:H161	1.80	0.42
5:Z:37:HIS:NE2	13:1:101:BCB:HMD1	2.34	0.42
5:9:48:TRP:CD2	13:9:101:BCB:H2C	2.54	0.42
6:B:45:PRO:HD3	7:G:10:PRO:HG3	2.00	0.42
6:1:54:TRP:CZ3	6:4:45:PRO:HD2	2.55	0.42
6:r:46:TRP:CE2	13:r:101:BCB:H2C	2.55	0.42
2:L:161:GLY:HA3	13:L:302:BCB:HAC1	2.02	0.42
1:C:260:PRO:N	3:M:313:THR:HG21	2.35	0.42
8:g:27:PRO:HA	8:g:30:TRP:CD1	2.55	0.42
8:j:27:PRO:HA	8:j:30:TRP:NE1	2.34	0.42
1:C:71:LEU:HD12	1:C:71:LEU:HA	1.91	0.41
1:C:307:HIS:CE1	1:C:313:PRO:HD3	2.55	0.41
2:L:50:GLY:HA2	20:N:102:PGV:H11	2.01	0.41
3:M:122:THR:HG22	11:M:408:UQ8:H12	2.01	0.41
11:A:101:UQ8:H31A	11:A:101:UQ8:H35	2.02	0.41
20:Q:401:PGV:H281	20:Q:401:PGV:H252	1.83	0.41
6:1:39:LEU:O	6:1:42:THR:OG1	2.36	0.41
8:5:34:LEU:HD22	6:7:28:LEU:HD12	2.02	0.41
2:L:22:PHE:CZ	13:D:101:BCB:H191	2.56	0.41
2:L:239:ASN:HA	2:L:242:LEU:HB2	2.02	0.41
3:M:201:HIS:CE1	3:M:205:ILE:HD11	2.55	0.41
13:R:102:BCB:H203	13:R:102:BCB:H161	1.91	0.41
5:W:23:THR:O	5:W:27:ILE:HG12	2.18	0.41
6:0:37:HIS:NE2	13:0:102:BCB:NB	2.68	0.41
13:0:102:BCB:CHB	8:a:24:LEU:HD21	2.49	0.41
13:o:102:BCB:H93	13:o:102:BCB:H62	1.78	0.41
5:A:18:PRO:HB3	6:B:18:PHE:CE2	2.55	0.41
5:A:25:LEU:HD12	5:A:25:LEU:HA	1.89	0.41
6:U:46:TRP:CD1	6:U:47:ILE:HG13	2.54	0.41
6:4:26:MET:O	6:4:30:LEU:HG	2.20	0.41
6:i:47:ILE:O	22:i:201:HOH:O	2.21	0.41
11:M:408:UQ8:H4M	15:M:409:CDL:H601	2.01	0.41
5:D:18:PRO:HB3	6:E:18:PHE:CZ	2.55	0.41
5:D:38:PHE:CE1	20:D:102:PGV:H201	2.54	0.41
5:I:18:PRO:HB3	6:J:18:PHE:CE2	2.55	0.41
13:I:101:BCB:H171	13:I:101:BCB:H13	1.94	0.41
13:1:101:BCB:H121	8:2:31:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:59:LEU:HD13	2:L:59:LEU:HA	1.94	0.41
2:L:151:LEU:HD11	15:H:301:CDL:H362	2.03	0.41
4:H:226:LEU:HD11	4:H:232:ILE:HD12	2.01	0.41
5:D:22:LEU:HD22	13:D:101:BCB:H101	2.02	0.41
13:L:303:BCB:H203	13:L:303:BCB:H161	1.73	0.41
4:H:206:THR:HG22	4:H:207:LYS:H	1.85	0.41
6:R:34:VAL:HG13	8:S:21:LEU:HD22	2.02	0.41
13:W:302:BCB:H61	13:W:302:BCB:H92	1.78	0.41
13:i:101:BCB:H93	13:i:101:BCB:H111	1.85	0.41
2:L:219:VAL:HG12	2:L:220:VAL:HG13	2.03	0.41
5:D:34:LEU:HD23	20:D:102:PGV:H252	2.03	0.41
4:H:21:TRP:CG	20:Q:401:PGV:H322	2.56	0.41
13:O:102:BCB:H143	13:O:102:BCB:H112	1.85	0.41
13:W:302:BCB:H143	13:W:302:BCB:H162	1.76	0.41
11:M:408:UQ8:H17	11:M:408:UQ8:H20	1.71	0.41
5:N:46:LEU:HD13	13:O:102:BCB:HBC3	2.03	0.41
5:T:36:ILE:HD12	13:U:102:BCB:O1D	2.21	0.41
20:W:301:PGV:H302	20:W:301:PGV:H272	1.93	0.41
13:O:102:BCB:H101	13:O:102:BCB:H62	1.75	0.41
13:b:101:BCB:HMB1	13:b:101:BCB:HBB3	2.03	0.41
6:c:38:TYR:O	6:c:42:THR:HG23	2.21	0.41
13:i:101:BCB:HBA1	13:i:101:BCB:H3A	1.91	0.41
8:j:12:ILE:H	8:j:12:ILE:HG13	1.57	0.41
13:k:102:BCB:H161	13:k:102:BCB:H143	1.72	0.41
13:k:102:BCB:H203	13:k:102:BCB:H162	1.88	0.41
1:C:10:THR:O	1:C:20:GLY:HA3	2.21	0.41
2:L:177:VAL:HG13	13:L:302:BCB:HMB3	2.02	0.41
4:H:92:LEU:HD23	4:H:105:PRO:HA	2.03	0.41
6:B:37:HIS:NE2	13:B:202:BCB:NB	2.69	0.41
13:n:101:BCB:H141	13:n:101:BCB:H161	1.78	0.41
13:E:101:BCB:HBB2	8:F:20:PRO:HA	2.03	0.40
6:J:45:PRO:HD3	8:K:10:PRO:HG3	2.01	0.40
6:c:30:LEU:O	6:c:34:VAL:HG23	2.21	0.40
6:r:38:TYR:O	6:r:42:THR:HG23	2.21	0.40
1:C:32:LYS:HE3	1:C:32:LYS:HB2	1.88	0.40
5:D:10:TRP:CZ3	6:E:12:GLU:HG3	2.56	0.40
5:I:55:LEU:HD12	5:I:55:LEU:HA	1.91	0.40
5:T:48:TRP:CD2	13:T:101:BCB:H2C	2.56	0.40
8:j:12:ILE:HA	8:j:17:LEU:HD23	2.04	0.40
15:H:301:CDL:H642	20:Q:401:PGV:H62	2.03	0.40
5:Z:12:LEU:HD11	5:Z:16:LEU:HD12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:0:26:MET:HE1	13:0:102:BCB:H151	2.02	0.40
8:g:5:ASP:OD1	8:g:5:ASP:N	2.53	0.40
6:o:51:PRO:HG2	6:o:54:TRP:HB2	2.04	0.40
15:M:409:CDL:H321	15:M:409:CDL:H351	1.92	0.40
5:A:14:LEU:HD11	6:B:12:GLU:HG2	2.03	0.40
11:A:101:UQ8:H27	11:A:101:UQ8:H30	1.87	0.40
5:Q:16:LEU:HD23	5:Q:16:LEU:HA	1.79	0.40
6:7:54:TRP:CZ3	6:0:45:PRO:HD2	2.56	0.40
5:b:28:TYR:CD1	19:b:102:LMT:H101	2.56	0.40
19:b:103:LMT:H102	5:e:28:TYR:HD1	1.86	0.40
5:h:15:ILE:HB	5:k:19:ARG:HD2	2.03	0.40
6:i:38:TYR:CE1	8:j:12:ILE:HG23	2.56	0.40
21:o:101:NS0:C16	13:o:102:BCB:H2	2.52	0.40
1:C:266:TRP:NE1	1:C:270:LYS:HD2	2.36	0.40
15:H:301:CDL:HB4	15:H:301:CDL:OA3	2.21	0.40
6:J:26:MET:O	6:J:30:LEU:HG	2.22	0.40
13:7:102:BCB:HBB	8:8:24:LEU:HD21	2.02	0.40
8:8:27:PRO:HA	8:8:30:TRP:NE1	2.36	0.40
5:k:36:ILE:HD12	13:l:102:BCB:O1D	2.21	0.40
13:l:102:BCB:HBB2	8:m:20:PRO:HA	2.02	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	C	329/354 (93%)	323 (98%)	6 (2%)	0	100	100
2	L	271/274 (99%)	262 (97%)	9 (3%)	0	100	100
3	M	329/332 (99%)	320 (97%)	9 (3%)	0	100	100
4	H	258/260 (99%)	251 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	3	48/69 (70%)	46 (96%)	2 (4%)	0	100	100
5	6	48/69 (70%)	45 (94%)	3 (6%)	0	100	100
5	9	48/69 (70%)	46 (96%)	2 (4%)	0	100	100
5	A	48/69 (70%)	47 (98%)	1 (2%)	0	100	100
5	D	48/69 (70%)	45 (94%)	3 (6%)	0	100	100
5	I	48/69 (70%)	45 (94%)	3 (6%)	0	100	100
5	N	48/69 (70%)	46 (96%)	2 (4%)	0	100	100
5	Q	48/69 (70%)	47 (98%)	1 (2%)	0	100	100
5	T	48/69 (70%)	46 (96%)	2 (4%)	0	100	100
5	W	48/69 (70%)	47 (98%)	1 (2%)	0	100	100
5	Z	48/69 (70%)	47 (98%)	1 (2%)	0	100	100
5	b	48/69 (70%)	46 (96%)	2 (4%)	0	100	100
5	e	48/69 (70%)	46 (96%)	2 (4%)	0	100	100
5	h	48/69 (70%)	47 (98%)	1 (2%)	0	100	100
5	k	48/69 (70%)	46 (96%)	2 (4%)	0	100	100
5	n	48/69 (70%)	45 (94%)	3 (6%)	0	100	100
5	q	48/69 (70%)	46 (96%)	2 (4%)	0	100	100
6	0	48/69 (70%)	46 (96%)	2 (4%)	0	100	100
6	1	48/69 (70%)	47 (98%)	1 (2%)	0	100	100
6	4	48/69 (70%)	46 (96%)	2 (4%)	0	100	100
6	7	48/69 (70%)	46 (96%)	2 (4%)	0	100	100
6	B	49/69 (71%)	47 (96%)	2 (4%)	0	100	100
6	E	49/69 (71%)	48 (98%)	1 (2%)	0	100	100
6	J	46/69 (67%)	45 (98%)	1 (2%)	0	100	100
6	O	49/69 (71%)	48 (98%)	1 (2%)	0	100	100
6	R	48/69 (70%)	47 (98%)	1 (2%)	0	100	100
6	U	48/69 (70%)	44 (92%)	4 (8%)	0	100	100
6	X	48/69 (70%)	45 (94%)	3 (6%)	0	100	100
6	c	48/69 (70%)	47 (98%)	1 (2%)	0	100	100
6	f	48/69 (70%)	47 (98%)	1 (2%)	0	100	100
6	i	48/69 (70%)	45 (94%)	3 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	l	48/69 (70%)	43 (90%)	5 (10%)	0	100	100
6	o	48/69 (70%)	46 (96%)	2 (4%)	0	100	100
6	r	48/69 (70%)	44 (92%)	4 (8%)	0	100	100
7	G	26/56 (46%)	26 (100%)	0	0	100	100
8	2	34/57 (60%)	33 (97%)	1 (3%)	0	100	100
8	5	34/57 (60%)	34 (100%)	0	0	100	100
8	8	34/57 (60%)	33 (97%)	1 (3%)	0	100	100
8	F	34/57 (60%)	33 (97%)	1 (3%)	0	100	100
8	K	34/57 (60%)	34 (100%)	0	0	100	100
8	P	34/57 (60%)	34 (100%)	0	0	100	100
8	S	34/57 (60%)	34 (100%)	0	0	100	100
8	V	34/57 (60%)	33 (97%)	1 (3%)	0	100	100
8	Y	34/57 (60%)	33 (97%)	1 (3%)	0	100	100
8	a	34/57 (60%)	34 (100%)	0	0	100	100
8	d	34/57 (60%)	34 (100%)	0	0	100	100
8	g	34/57 (60%)	34 (100%)	0	0	100	100
8	j	34/57 (60%)	34 (100%)	0	0	100	100
8	m	34/57 (60%)	33 (97%)	1 (3%)	0	100	100
8	p	34/57 (60%)	34 (100%)	0	0	100	100
All	All	3356/4477 (75%)	3250 (97%)	106 (3%)	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	C	279/295 (95%)	273 (98%)	6 (2%)	45	61
2	L	213/214 (100%)	212 (100%)	1 (0%)	81	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	M	257/258 (100%)	249 (97%)	8 (3%)	35	48
4	H	209/209 (100%)	203 (97%)	6 (3%)	37	51
5	3	45/59 (76%)	45 (100%)	0	100	100
5	6	45/59 (76%)	44 (98%)	1 (2%)	45	61
5	9	45/59 (76%)	44 (98%)	1 (2%)	45	61
5	A	45/59 (76%)	43 (96%)	2 (4%)	25	34
5	D	45/59 (76%)	44 (98%)	1 (2%)	45	61
5	I	45/59 (76%)	45 (100%)	0	100	100
5	N	45/59 (76%)	45 (100%)	0	100	100
5	Q	45/59 (76%)	44 (98%)	1 (2%)	45	61
5	T	45/59 (76%)	42 (93%)	3 (7%)	15	17
5	W	45/59 (76%)	44 (98%)	1 (2%)	45	61
5	Z	45/59 (76%)	45 (100%)	0	100	100
5	b	45/59 (76%)	45 (100%)	0	100	100
5	e	45/59 (76%)	45 (100%)	0	100	100
5	h	45/59 (76%)	45 (100%)	0	100	100
5	k	45/59 (76%)	45 (100%)	0	100	100
5	n	45/59 (76%)	44 (98%)	1 (2%)	45	61
5	q	45/59 (76%)	43 (96%)	2 (4%)	25	34
6	0	43/59 (73%)	42 (98%)	1 (2%)	44	59
6	1	43/59 (73%)	43 (100%)	0	100	100
6	4	43/59 (73%)	43 (100%)	0	100	100
6	7	43/59 (73%)	42 (98%)	1 (2%)	44	59
6	B	44/59 (75%)	43 (98%)	1 (2%)	44	59
6	E	44/59 (75%)	43 (98%)	1 (2%)	44	59
6	J	41/59 (70%)	41 (100%)	0	100	100
6	O	44/59 (75%)	43 (98%)	1 (2%)	44	59
6	R	43/59 (73%)	43 (100%)	0	100	100
6	U	43/59 (73%)	41 (95%)	2 (5%)	23	31
6	X	43/59 (73%)	42 (98%)	1 (2%)	44	59
6	c	43/59 (73%)	43 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	f	43/59 (73%)	43 (100%)	0	100	100
6	i	43/59 (73%)	43 (100%)	0	100	100
6	l	43/59 (73%)	42 (98%)	1 (2%)	44	59
6	o	43/59 (73%)	42 (98%)	1 (2%)	44	59
6	r	43/59 (73%)	41 (95%)	2 (5%)	23	31
7	G	25/44 (57%)	24 (96%)	1 (4%)	28	38
8	2	29/45 (64%)	28 (97%)	1 (3%)	32	44
8	5	29/45 (64%)	29 (100%)	0	100	100
8	8	29/45 (64%)	29 (100%)	0	100	100
8	F	29/45 (64%)	28 (97%)	1 (3%)	32	44
8	K	29/45 (64%)	29 (100%)	0	100	100
8	P	29/45 (64%)	29 (100%)	0	100	100
8	S	29/45 (64%)	29 (100%)	0	100	100
8	V	29/45 (64%)	29 (100%)	0	100	100
8	Y	29/45 (64%)	29 (100%)	0	100	100
8	a	29/45 (64%)	29 (100%)	0	100	100
8	d	29/45 (64%)	29 (100%)	0	100	100
8	g	29/45 (64%)	27 (93%)	2 (7%)	14	16
8	j	29/45 (64%)	28 (97%)	1 (3%)	32	44
8	m	29/45 (64%)	29 (100%)	0	100	100
8	p	29/45 (64%)	28 (97%)	1 (3%)	32	44
All	All	2915/3701 (79%)	2862 (98%)	53 (2%)	51	68

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	52	VAL
1	C	55	VAL
1	C	71	LEU
1	C	88	THR
1	C	250	THR
1	C	320	MET
2	L	17	ILE
3	M	17	HIS
3	M	36	ILE

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Mol	Chain	Res	Type
3	M	87	ARG
3	M	195	PHE
3	M	215	PHE
3	M	288	THR
3	M	313	THR
3	M	331	GLN
4	H	108	ASN
4	H	131	GLU
4	H	192	SER
4	H	194	ARG
4	H	206	THR
4	H	210	VAL
5	A	23	THR
5	A	25	LEU
6	B	7	LEU
7	G	36	ARG
5	D	53	ARG
6	E	12	GLU
8	F	12	ILE
6	O	30	LEU
5	Q	16	LEU
5	T	16	LEU
5	T	19	ARG
5	T	53	ARG
6	U	10	LEU
6	U	11	THR
5	W	35	LEU
6	X	30	LEU
8	2	36	ARG
5	6	53	ARG
6	7	12	GLU
5	9	16	LEU
6	0	12	GLU
8	g	8	VAL
8	g	9	VAL
8	j	12	ILE
6	l	10	LEU
5	n	9	SER
6	o	13	GLU
8	p	21	LEU
5	q	16	LEU
5	q	35	LEU

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Mol	Chain	Res	Type
6	r	27	VAL
6	r	50	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	170	HIS
1	C	184	ASN
1	C	295	GLN
2	L	158	ASN
3	M	109	ASN
7	G	16	ASN
5	W	44	ASN
5	W	52	GLN
5	Z	52	GLN
5	3	44	ASN
5	9	52	GLN
5	b	44	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	FME	H	1	4	8,9,10	0.50	0	8,9,11	1.18	2 (25%)

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
4	FME	H	1	4	-	3/7/9/11	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1	FME	O-C-CA	-2.56	118.19	124.77
4	H	1	FME	CA-N-CN	-2.09	119.61	122.82

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	1	FME	O1-CN-N-CA
4	H	1	FME	CB-CA-N-CN
4	H	1	FME	CA-CB-CG-SD

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 89 ligands modelled in this entry, 2 are monoatomic - leaving 87 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
13	BCB	R	102	-	60,74,74	2.98	18 (30%)	59,115,115	2.32	16 (27%)
13	BCB	q	101	-	60,74,74	3.10	18 (30%)	59,115,115	2.27	15 (25%)
12	DGA	L	301	1	22,22,43	1.37	3 (13%)	24,24,45	1.76	5 (20%)
19	LMT	b	102	-	36,36,36	0.45	0	47,47,47	0.79	0
17	MQ7	M	405	-	49,49,49	1.39	2 (4%)	61,63,63	1.47	14 (22%)
11	UQ8	L	305	-	31,31,53	1.62	2 (6%)	39,40,67	1.46	7 (17%)
21	NS0	7	101	-	39,39,39	1.17	3 (7%)	46,46,46	1.26	6 (13%)
13	BCB	B	202	-	60,74,74	3.02	17 (28%)	59,115,115	2.24	14 (23%)
13	BCB	6	101	-	60,74,74	3.11	18 (30%)	59,115,115	2.26	15 (25%)
21	NS0	2	101	-	39,39,39	1.18	3 (7%)	46,46,46	1.16	9 (19%)
15	CDL	H	301	-	97,97,99	0.92	4 (4%)	103,109,111	1.07	6 (5%)
11	UQ8	M	408	-	53,53,53	1.28	2 (3%)	66,67,67	1.56	15 (22%)
9	HEC	C	403	1	46,50,50	1.77	9 (19%)	58,82,82	1.55	11 (18%)
11	UQ8	C	406	-	15,15,53	2.23	2 (13%)	20,21,67	1.44	2 (10%)
13	BCB	f	101	-	60,74,74	2.97	18 (30%)	59,115,115	2.20	15 (25%)
20	PGV	W	301	-	47,47,50	0.95	2 (4%)	50,53,56	1.09	4 (8%)
13	BCB	D	101	-	60,74,74	3.08	18 (30%)	59,115,115	2.30	14 (23%)
21	NS0	k	101	-	39,39,39	1.15	4 (10%)	46,46,46	1.29	9 (19%)
13	BCB	c	101	-	60,74,74	2.97	18 (30%)	59,115,115	2.30	15 (25%)
13	BCB	W	302	-	60,74,74	3.07	18 (30%)	59,115,115	2.31	14 (23%)
20	PGV	I	102	-	50,50,50	0.89	2 (4%)	53,56,56	1.04	3 (5%)
21	NS0	o	101	-	39,39,39	1.15	3 (7%)	46,46,46	1.20	6 (13%)
9	HEC	C	402	1	46,50,50	1.77	11 (23%)	58,82,82	1.55	11 (18%)
20	PGV	Q	401	-	48,48,50	0.96	2 (4%)	51,53,56	1.00	2 (3%)
21	NS0	X	101	-	39,39,39	1.15	3 (7%)	46,46,46	1.22	8 (17%)
13	BCB	0	102	-	60,74,74	2.96	17 (28%)	59,115,115	2.28	14 (23%)
13	BCB	k	102	-	60,74,74	3.10	18 (30%)	59,115,115	2.13	15 (25%)
13	BCB	M	403	-	60,74,74	3.12	18 (30%)	59,115,115	2.37	19 (32%)
15	CDL	H	302	-	71,71,99	1.10	4 (5%)	77,83,111	1.10	5 (6%)
13	BCB	b	101	-	60,74,74	3.03	18 (30%)	59,115,115	2.31	18 (30%)
13	BCB	J	101	-	60,74,74	2.98	17 (28%)	59,115,115	2.23	14 (23%)
13	BCB	n	101	-	60,74,74	3.08	18 (30%)	59,115,115	2.23	16 (27%)
15	CDL	M	409	-	84,84,99	0.99	4 (4%)	90,96,111	1.12	9 (10%)
13	BCB	r	101	-	60,74,74	3.00	17 (28%)	59,115,115	2.19	14 (23%)
21	NS0	R	101	-	39,39,39	1.16	3 (7%)	46,46,46	1.26	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	BCB	h	102	-	60,74,74	3.08	18 (30%)	59,115,115	2.26	16 (27%)
19	LMT	h	103	-	36,36,36	0.36	0	47,47,47	0.71	1 (2%)
11	UQ8	A	101	-	53,53,53	1.25	2 (3%)	66,67,67	1.59	14 (21%)
19	LMT	k	103	-	36,36,36	0.44	0	47,47,47	0.88	1 (2%)
20	PGV	D	102	-	46,46,50	0.95	2 (4%)	49,52,56	1.08	3 (6%)
14	BPB	L	304	-	57,70,70	0.90	6 (10%)	55,101,101	0.94	3 (5%)
13	BCB	O	102	-	60,74,74	2.95	18 (30%)	59,115,115	2.31	13 (22%)
20	PGV	N	102	-	37,37,50	1.08	2 (5%)	40,43,56	1.06	3 (7%)
13	BCB	I	101	-	60,74,74	3.10	18 (30%)	59,115,115	2.26	16 (27%)
19	LMT	M	410	-	25,25,36	0.42	0	30,30,47	0.64	0
15	CDL	r	102	-	67,67,99	1.11	4 (5%)	73,79,111	1.15	5 (6%)
13	BCB	l	102	-	60,74,74	2.98	18 (30%)	59,115,115	2.22	15 (25%)
13	BCB	M	402	-	60,74,74	3.03	18 (30%)	59,115,115	2.41	13 (22%)
13	BCB	o	102	-	60,74,74	2.95	18 (30%)	59,115,115	2.28	14 (23%)
9	HEC	C	401	1	46,50,50	1.74	9 (19%)	58,82,82	1.65	14 (24%)
21	NS0	D	103	-	39,39,39	1.18	3 (7%)	46,46,46	1.15	6 (13%)
11	UQ8	M	407	-	25,25,53	1.76	2 (8%)	31,33,67	1.47	7 (22%)
13	BCB	3	101	-	60,74,74	3.06	18 (30%)	59,115,115	2.35	16 (27%)
13	BCB	1	101	-	60,74,74	2.95	18 (30%)	59,115,115	2.22	15 (25%)
13	BCB	T	101	-	60,74,74	3.11	18 (30%)	59,115,115	2.19	15 (25%)
15	CDL	L	306	-	74,74,99	1.06	4 (5%)	80,86,111	1.19	8 (10%)
21	NS0	A	103	-	39,39,39	1.16	4 (10%)	46,46,46	1.17	8 (17%)
13	BCB	7	102	-	60,74,74	2.97	17 (28%)	59,115,115	2.14	15 (25%)
9	HEC	C	404	1	46,50,50	1.78	11 (23%)	58,82,82	1.59	11 (18%)
13	BCB	9	101	-	60,74,74	3.08	18 (30%)	59,115,115	2.38	16 (27%)
21	NS0	l	101	-	39,39,39	1.14	3 (7%)	46,46,46	1.23	9 (19%)
19	LMT	B	201	-	14,14,36	0.70	0	14,14,47	0.58	0
14	BPB	M	404	-	57,70,70	0.87	3 (5%)	55,101,101	0.93	3 (5%)
21	NS0	W	303	-	39,39,39	1.17	3 (7%)	46,46,46	1.30	7 (15%)
13	BCB	E	101	-	60,74,74	2.98	17 (28%)	59,115,115	2.20	15 (25%)
13	BCB	X	102	-	60,74,74	2.97	17 (28%)	59,115,115	2.18	16 (27%)
13	BCB	i	101	-	60,74,74	2.97	17 (28%)	59,115,115	2.31	15 (25%)
21	NS0	O	101	-	39,39,39	1.14	3 (7%)	46,46,46	1.20	7 (15%)
21	NS0	0	101	-	39,39,39	1.17	3 (7%)	46,46,46	1.16	7 (15%)
13	BCB	L	302	-	60,74,74	3.05	18 (30%)	59,115,115	2.34	15 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	BCB	Z	101	-	60,74,74	3.07	18 (30%)	59,115,115	2.28	16 (27%)
21	NS0	9	102	-	39,39,39	1.17	4 (10%)	46,46,46	1.27	8 (17%)
21	NS0	U	101	-	39,39,39	1.15	3 (7%)	46,46,46	1.22	8 (17%)
19	LMT	T	102	-	26,26,36	0.41	0	31,31,47	1.04	2 (6%)
18	NS5	M	406	-	39,39,39	1.14	5 (12%)	46,46,46	1.20	6 (13%)
19	LMT	n	102	-	36,36,36	0.40	0	47,47,47	0.79	1 (2%)
13	BCB	A	102	-	60,74,74	3.10	18 (30%)	59,115,115	2.38	17 (28%)
13	BCB	e	101	-	60,74,74	3.09	18 (30%)	59,115,115	2.26	16 (27%)
19	LMT	b	103	-	36,36,36	0.41	0	47,47,47	0.94	2 (4%)
13	BCB	Q	402	-	60,74,74	3.10	18 (30%)	59,115,115	2.26	14 (23%)
13	BCB	L	303	-	60,74,74	3.05	18 (30%)	59,115,115	2.51	16 (27%)
20	PGV	M	411	-	44,44,50	0.97	2 (4%)	47,50,56	0.96	3 (6%)
13	BCB	U	102	-	60,74,74	2.96	18 (30%)	59,115,115	2.27	16 (27%)
21	NS0	h	101	-	39,39,39	1.16	4 (10%)	46,46,46	1.15	6 (13%)
13	BCB	N	101	-	60,74,74	3.08	18 (30%)	59,115,115	2.24	15 (25%)
21	NS0	q	102	-	39,39,39	1.16	3 (7%)	46,46,46	1.19	7 (15%)
13	BCB	4	101	-	60,74,74	2.91	17 (28%)	59,115,115	2.22	13 (22%)

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
13	BCB	R	102	-	2/2/21/26	6/37/137/137	-
13	BCB	q	101	-	2/2/21/26	16/37/137/137	-
12	DGA	L	301	1	-	12/23/23/45	-
19	LMT	b	102	-	-	11/21/61/61	0/2/2/2
17	MQ7	M	405	-	-	0/41/61/61	0/2/2/2
11	UQ8	L	305	-	-	7/25/49/75	0/1/1/1
21	NS0	7	101	-	-	6/43/43/43	-
13	BCB	B	202	-	2/2/21/26	6/37/137/137	-
13	BCB	6	101	-	2/2/21/26	8/37/137/137	-
21	NS0	2	101	-	-	6/43/43/43	-
15	CDL	H	301	-	-	41/108/108/110	-
11	UQ8	M	408	-	-	11/51/75/75	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	HEC	C	403	1	-	4/14/54/54	-
11	UQ8	C	406	-	-	0/6/30/75	0/1/1/1
13	BCB	f	101	-	2/2/21/26	13/37/137/137	-
20	PGV	W	301	-	-	16/52/52/55	-
13	BCB	D	101	-	2/2/21/26	10/37/137/137	-
21	NS0	k	101	-	-	4/43/43/43	-
13	BCB	c	101	-	2/2/21/26	11/37/137/137	-
13	BCB	W	302	-	2/2/21/26	10/37/137/137	-
20	PGV	I	102	-	-	16/55/55/55	-
21	NS0	o	101	-	-	5/43/43/43	-
9	HEC	C	402	1	-	7/14/54/54	-
20	PGV	Q	401	-	-	17/52/52/55	-
21	NS0	X	101	-	-	4/43/43/43	-
13	BCB	0	102	-	2/2/21/26	10/37/137/137	-
13	BCB	k	102	-	2/2/21/26	11/37/137/137	-
13	BCB	M	403	-	2/2/21/26	8/37/137/137	-
15	CDL	H	302	-	-	37/82/82/110	-
13	BCB	b	101	-	2/2/21/26	12/37/137/137	-
13	BCB	J	101	-	2/2/21/26	11/37/137/137	-
13	BCB	n	101	-	2/2/21/26	4/37/137/137	-
15	CDL	M	409	-	-	36/95/95/110	-
13	BCB	r	101	-	2/2/21/26	12/37/137/137	-
21	NS0	R	101	-	-	6/43/43/43	-
13	BCB	h	102	-	2/2/21/26	5/37/137/137	-
19	LMT	h	103	-	-	4/21/61/61	0/2/2/2
11	UQ8	A	101	-	-	14/51/75/75	0/1/1/1
19	LMT	k	103	-	-	3/21/61/61	0/2/2/2
20	PGV	D	102	-	-	13/51/51/55	-
14	BPB	L	304	-	-	2/37/105/105	0/5/6/6
13	BCB	O	102	-	2/2/21/26	15/37/137/137	-
20	PGV	N	102	-	-	11/42/42/55	-
13	BCB	I	101	-	2/2/21/26	6/37/137/137	-
19	LMT	M	410	-	-	6/17/37/61	0/1/1/2
15	CDL	r	102	-	-	39/78/78/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	BCB	l	102	-	2/2/21/26	4/37/137/137	-
13	BCB	M	402	-	2/2/21/26	7/37/137/137	-
13	BCB	o	102	-	2/2/21/26	16/37/137/137	-
9	HEC	C	401	1	-	6/14/54/54	-
21	NS0	D	103	-	-	3/43/43/43	-
11	UQ8	M	407	-	-	0/18/42/75	0/1/1/1
13	BCB	3	101	-	2/2/21/26	14/37/137/137	-
13	BCB	1	101	-	2/2/21/26	12/37/137/137	-
13	BCB	T	101	-	2/2/21/26	11/37/137/137	-
15	CDL	L	306	-	-	27/85/85/110	-
21	NS0	A	103	-	-	2/43/43/43	-
13	BCB	7	102	-	2/2/21/26	18/37/137/137	-
9	HEC	C	404	1	-	7/14/54/54	-
13	BCB	9	101	-	2/2/21/26	14/37/137/137	-
21	NS0	l	101	-	-	5/43/43/43	-
19	LMT	B	201	-	-	6/13/13/61	-
14	BPB	M	404	-	-	4/37/105/105	0/5/6/6
21	NS0	W	303	-	-	7/43/43/43	-
13	BCB	E	101	-	2/2/21/26	11/37/137/137	-
13	BCB	X	102	-	2/2/21/26	18/37/137/137	-
13	BCB	i	101	-	2/2/21/26	10/37/137/137	-
21	NS0	O	101	-	-	8/43/43/43	-
21	NS0	0	101	-	-	4/43/43/43	-
13	BCB	L	302	-	2/2/21/26	4/37/137/137	-
13	BCB	Z	101	-	2/2/21/26	7/37/137/137	-
21	NS0	9	102	-	-	5/43/43/43	-
21	NS0	U	101	-	-	6/43/43/43	-
19	LMT	T	102	-	-	1/17/38/61	0/1/1/2
18	NS5	M	406	-	-	2/43/43/43	-
19	LMT	n	102	-	-	4/21/61/61	0/2/2/2
13	BCB	A	102	-	2/2/21/26	18/37/137/137	-
13	BCB	e	101	-	2/2/21/26	10/37/137/137	-
19	LMT	b	103	-	-	6/21/61/61	0/2/2/2
13	BCB	Q	402	-	2/2/21/26	8/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	BCB	L	303	-	2/2/21/26	3/37/137/137	-
20	PGV	M	411	-	-	13/49/49/55	-
13	BCB	U	102	-	2/2/21/26	7/37/137/137	-
21	NS0	h	101	-	-	1/43/43/43	-
13	BCB	N	101	-	2/2/21/26	16/37/137/137	-
21	NS0	q	102	-	-	6/43/43/43	-
13	BCB	4	101	-	2/2/21/26	8/37/137/137	-

All (828) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	402	BCB	C1D-C2D	9.24	1.50	1.39
13	9	101	BCB	C1D-C2D	9.04	1.49	1.39
13	L	303	BCB	C1D-C2D	8.95	1.49	1.39
13	M	403	BCB	C1A-CHA	8.82	1.50	1.40
13	k	102	BCB	C1A-CHA	8.81	1.50	1.40
13	6	101	BCB	C1A-CHA	8.78	1.50	1.40
13	I	101	BCB	C1D-C2D	8.75	1.49	1.39
13	e	101	BCB	C1A-CHA	8.72	1.49	1.40
13	A	102	BCB	C1D-C2D	8.70	1.49	1.39
13	T	101	BCB	C1A-CHA	8.70	1.49	1.40
13	L	302	BCB	C1A-CHA	8.66	1.49	1.40
13	D	101	BCB	C1D-C2D	8.66	1.49	1.39
13	k	102	BCB	C1D-C2D	8.65	1.49	1.39
13	W	302	BCB	C1A-CHA	8.63	1.49	1.40
13	T	101	BCB	C1D-C2D	8.60	1.49	1.39
13	M	403	BCB	C1D-C2D	8.58	1.49	1.39
13	Z	101	BCB	C1A-CHA	8.58	1.49	1.40
13	h	102	BCB	C1A-CHA	8.57	1.49	1.40
13	N	101	BCB	C1A-CHA	8.57	1.49	1.40
13	q	101	BCB	C1D-C2D	8.54	1.49	1.39
13	n	101	BCB	C1A-CHA	8.54	1.49	1.40
13	b	101	BCB	C1A-CHA	8.52	1.49	1.40
13	Q	402	BCB	C1D-C2D	8.50	1.49	1.39
13	3	101	BCB	C1D-C2D	8.49	1.49	1.39
13	J	101	BCB	C1B-C2B	8.47	1.49	1.39
13	L	302	BCB	C1B-C2B	8.46	1.49	1.39
13	I	101	BCB	C1A-CHA	8.46	1.49	1.40
13	N	101	BCB	C1D-C2D	8.42	1.49	1.39
13	e	101	BCB	C1D-C2D	8.41	1.49	1.39
13	b	101	BCB	C1B-C2B	8.38	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	3	101	BCB	C1A-CHA	8.38	1.49	1.40
13	c	101	BCB	C1B-C2B	8.37	1.49	1.39
13	Q	402	BCB	C1A-CHA	8.37	1.49	1.40
13	6	101	BCB	C1B-C2B	8.37	1.49	1.39
13	L	302	BCB	C1D-C2D	8.35	1.49	1.39
13	i	101	BCB	C1B-C2B	8.35	1.49	1.39
13	h	102	BCB	C1D-C2D	8.31	1.49	1.39
13	M	402	BCB	C1B-C2B	8.30	1.49	1.39
13	n	101	BCB	C1D-C2D	8.30	1.49	1.39
13	6	101	BCB	C1D-C2D	8.30	1.49	1.39
13	e	101	BCB	C1B-C2B	8.28	1.49	1.39
13	Z	101	BCB	C1D-C2D	8.26	1.49	1.39
13	W	302	BCB	C1D-C2D	8.26	1.49	1.39
13	r	101	BCB	C1B-C2B	8.25	1.48	1.39
13	A	102	BCB	C1B-C2B	8.25	1.48	1.39
13	0	102	BCB	C1B-C2B	8.25	1.48	1.39
13	D	101	BCB	C1B-C2B	8.23	1.48	1.39
13	q	101	BCB	C1A-CHA	8.19	1.49	1.40
13	M	403	BCB	C1B-C2B	8.19	1.48	1.39
13	9	101	BCB	C1A-CHA	8.17	1.49	1.40
13	o	102	BCB	C1B-C2B	8.16	1.48	1.39
13	k	102	BCB	C1B-C2B	8.16	1.48	1.39
13	Q	402	BCB	C1B-C2B	8.15	1.48	1.39
13	O	102	BCB	C1B-C2B	8.12	1.48	1.39
13	A	102	BCB	C1A-CHA	8.12	1.49	1.40
13	Z	101	BCB	C1B-C2B	8.09	1.48	1.39
13	D	101	BCB	C1A-CHA	8.09	1.49	1.40
13	B	202	BCB	C1D-C2D	8.09	1.48	1.39
13	E	101	BCB	C1B-C2B	8.09	1.48	1.39
13	O	102	BCB	C1A-CHA	8.04	1.49	1.40
13	L	303	BCB	C1B-C2B	8.04	1.48	1.39
13	3	101	BCB	C1B-C2B	8.03	1.48	1.39
13	W	302	BCB	C1B-C2B	8.01	1.48	1.39
13	6	101	BCB	CHC-C1C	8.01	1.48	1.38
13	h	102	BCB	C1B-C2B	7.99	1.48	1.39
11	M	408	UQ8	C6-C1	7.98	1.49	1.35
13	X	102	BCB	C1D-C2D	7.97	1.48	1.39
13	q	101	BCB	C1B-C2B	7.97	1.48	1.39
13	B	202	BCB	C1B-C2B	7.97	1.48	1.39
13	U	102	BCB	C1B-C2B	7.97	1.48	1.39
13	R	102	BCB	C1B-C2B	7.96	1.48	1.39
13	T	101	BCB	C1B-C2B	7.93	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	9	101	BCB	C1B-C2B	7.93	1.48	1.39
13	I	101	BCB	C1B-C2B	7.93	1.48	1.39
13	7	102	BCB	C1B-C2B	7.89	1.48	1.39
13	4	101	BCB	C1B-C2B	7.88	1.48	1.39
13	b	101	BCB	C1D-C2D	7.87	1.48	1.39
13	X	102	BCB	C1A-CHA	7.86	1.48	1.40
13	n	101	BCB	C1B-C2B	7.85	1.48	1.39
13	f	101	BCB	C1B-C2B	7.82	1.48	1.39
17	M	405	MQ7	C3-C2	7.80	1.49	1.35
13	1	101	BCB	C1B-C2B	7.80	1.48	1.39
13	l	102	BCB	C1B-C2B	7.80	1.48	1.39
13	E	101	BCB	C1D-C2D	7.79	1.48	1.39
13	N	101	BCB	C1B-C2B	7.78	1.48	1.39
11	M	407	UQ8	C6-C1	7.78	1.49	1.35
13	4	101	BCB	C1A-CHA	7.78	1.48	1.40
13	U	102	BCB	CHC-C1C	7.77	1.48	1.38
13	D	101	BCB	CHC-C1C	7.76	1.48	1.38
13	N	101	BCB	CHC-C1C	7.76	1.48	1.38
13	Q	402	BCB	CHC-C1C	7.75	1.48	1.38
13	I	101	BCB	CHC-C1C	7.73	1.48	1.38
13	T	101	BCB	CHC-C1C	7.73	1.48	1.38
11	L	305	UQ8	C6-C1	7.73	1.49	1.35
13	M	403	BCB	CHC-C1C	7.72	1.48	1.38
13	J	101	BCB	C1D-C2D	7.70	1.48	1.39
13	Z	101	BCB	CHC-C1C	7.69	1.48	1.38
13	f	101	BCB	C1D-C2D	7.68	1.48	1.39
13	7	102	BCB	C1D-C2D	7.66	1.48	1.39
13	L	303	BCB	CHC-C1C	7.66	1.48	1.38
13	e	101	BCB	CHC-C1C	7.66	1.48	1.38
11	C	406	UQ8	C6-C1	7.64	1.48	1.35
13	c	101	BCB	C1A-CHA	7.63	1.48	1.40
13	A	102	BCB	CHC-C1C	7.63	1.47	1.38
13	h	102	BCB	CHC-C1C	7.63	1.47	1.38
13	0	102	BCB	CHC-C1C	7.62	1.47	1.38
13	R	102	BCB	C1D-C2D	7.62	1.48	1.39
13	9	101	BCB	CHC-C1C	7.61	1.47	1.38
13	k	102	BCB	CHC-C1C	7.61	1.47	1.38
13	r	101	BCB	C1D-C2D	7.60	1.48	1.39
13	X	102	BCB	C1B-C2B	7.60	1.48	1.39
13	q	101	BCB	CHC-C1C	7.60	1.47	1.38
13	l	102	BCB	C1A-CHA	7.60	1.48	1.40
11	A	101	UQ8	C6-C1	7.57	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	E	101	BCB	C1A-CHA	7.56	1.48	1.40
13	r	101	BCB	CHC-C1C	7.56	1.47	1.38
13	J	101	BCB	C1A-CHA	7.56	1.48	1.40
13	B	202	BCB	C1A-CHA	7.55	1.48	1.40
13	B	202	BCB	CHC-C1C	7.55	1.47	1.38
13	l	102	BCB	C1D-C2D	7.55	1.48	1.39
13	i	101	BCB	CHC-C1C	7.55	1.47	1.38
13	c	101	BCB	CHC-C1C	7.54	1.47	1.38
13	W	302	BCB	CHC-C1C	7.53	1.47	1.38
13	7	102	BCB	C1A-CHA	7.51	1.48	1.40
13	R	102	BCB	CHC-C1C	7.50	1.47	1.38
13	3	101	BCB	CHC-C1C	7.49	1.47	1.38
13	0	102	BCB	C1D-C2D	7.49	1.48	1.39
13	i	101	BCB	C1A-CHA	7.48	1.48	1.40
13	J	101	BCB	CHC-C1C	7.48	1.47	1.38
13	r	101	BCB	C1A-CHA	7.47	1.48	1.40
13	X	102	BCB	CHC-C1C	7.46	1.47	1.38
13	f	101	BCB	C1A-CHA	7.45	1.48	1.40
13	o	102	BCB	C1A-CHA	7.44	1.48	1.40
13	i	101	BCB	C1D-C2D	7.44	1.48	1.39
13	n	101	BCB	CHC-C1C	7.43	1.47	1.38
13	7	102	BCB	CHC-C1C	7.42	1.47	1.38
13	R	102	BCB	C1A-CHA	7.41	1.48	1.40
13	E	101	BCB	CHC-C1C	7.40	1.47	1.38
13	o	102	BCB	CHC-C1C	7.40	1.47	1.38
13	l	101	BCB	CHC-C1C	7.38	1.47	1.38
13	f	101	BCB	CHC-C1C	7.34	1.47	1.38
13	O	102	BCB	C1D-C2D	7.34	1.47	1.39
13	M	402	BCB	C1A-CHA	7.31	1.48	1.40
13	l	102	BCB	CHC-C1C	7.30	1.47	1.38
13	b	101	BCB	CHC-C1C	7.29	1.47	1.38
13	U	102	BCB	C1D-C2D	7.26	1.47	1.39
13	1	101	BCB	C1D-C2D	7.26	1.47	1.39
13	M	402	BCB	CHC-C1C	7.19	1.47	1.38
13	4	101	BCB	CHC-C1C	7.19	1.47	1.38
13	0	102	BCB	C1A-CHA	7.17	1.48	1.40
13	1	101	BCB	C1A-CHA	7.17	1.48	1.40
13	L	302	BCB	CHC-C1C	7.14	1.47	1.38
13	U	102	BCB	C1A-CHA	7.12	1.48	1.40
13	o	102	BCB	C1D-C2D	7.10	1.47	1.39
13	4	101	BCB	C1D-C2D	7.06	1.47	1.39
13	O	102	BCB	CHC-C1C	7.05	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	c	101	BCB	C1D-C2D	6.88	1.47	1.39
13	L	303	BCB	C1A-CHA	6.82	1.47	1.40
13	3	101	BCB	C3B-C2B	6.56	1.50	1.39
13	I	101	BCB	C3B-C2B	6.53	1.50	1.39
13	M	403	BCB	C3B-C2B	6.49	1.50	1.39
13	R	102	BCB	C3B-C2B	6.48	1.50	1.39
13	b	101	BCB	C3B-C2B	6.47	1.50	1.39
13	D	101	BCB	C3B-C2B	6.47	1.50	1.39
13	T	101	BCB	C3B-C2B	6.46	1.50	1.39
13	W	302	BCB	C3B-C2B	6.46	1.50	1.39
13	N	101	BCB	C3B-C2B	6.43	1.50	1.39
13	k	102	BCB	C3B-C2B	6.40	1.50	1.39
13	n	101	BCB	C3B-C2B	6.39	1.50	1.39
13	L	303	BCB	C3B-C2B	6.38	1.50	1.39
13	1	101	BCB	C3B-C2B	6.36	1.50	1.39
13	q	101	BCB	C3B-C2B	6.36	1.50	1.39
13	c	101	BCB	C3B-C2B	6.36	1.50	1.39
13	6	101	BCB	C3B-C2B	6.36	1.50	1.39
13	o	102	BCB	C3B-C2B	6.35	1.50	1.39
13	h	102	BCB	C3B-C2B	6.35	1.50	1.39
13	l	102	BCB	C3B-C2B	6.34	1.50	1.39
13	A	102	BCB	C3B-C2B	6.34	1.50	1.39
13	f	101	BCB	C3B-C2B	6.31	1.50	1.39
13	B	202	BCB	C3B-C2B	6.31	1.50	1.39
13	e	101	BCB	C3B-C2B	6.30	1.50	1.39
13	Q	402	BCB	C3B-C2B	6.30	1.50	1.39
13	U	102	BCB	C3B-C2B	6.30	1.50	1.39
13	7	102	BCB	C3B-C2B	6.29	1.50	1.39
13	9	101	BCB	C3B-C2B	6.28	1.50	1.39
13	L	302	BCB	C3B-C2B	6.27	1.50	1.39
13	4	101	BCB	C3B-C2B	6.26	1.50	1.39
13	i	101	BCB	C3B-C2B	6.23	1.50	1.39
13	O	102	BCB	C3B-C2B	6.22	1.50	1.39
13	E	101	BCB	C3B-C2B	6.21	1.50	1.39
13	0	102	BCB	C3B-C2B	6.21	1.50	1.39
13	X	102	BCB	C3B-C2B	6.14	1.50	1.39
13	r	101	BCB	C3B-C2B	6.13	1.50	1.39
13	Z	101	BCB	C3B-C2B	6.13	1.50	1.39
13	J	101	BCB	C3B-C2B	6.08	1.50	1.39
13	M	403	BCB	C3D-C4D	-5.49	1.33	1.41
13	6	101	BCB	C3B-C4B	5.43	1.50	1.41
13	L	303	BCB	C3D-C4D	-5.42	1.33	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	T	101	BCB	C3B-C4B	5.41	1.50	1.41
13	l	102	BCB	C3D-C2D	5.38	1.48	1.39
13	M	403	BCB	C3B-C4B	5.37	1.50	1.41
13	R	102	BCB	C3D-C4D	-5.36	1.33	1.41
13	D	101	BCB	CHC-C4B	5.35	1.48	1.39
13	1	101	BCB	C3D-C4D	-5.33	1.33	1.41
13	c	101	BCB	C3D-C4D	-5.33	1.33	1.41
13	Q	402	BCB	CHC-C4B	5.31	1.48	1.39
13	0	102	BCB	C3D-C4D	-5.31	1.33	1.41
13	6	101	BCB	CHC-C4B	5.30	1.48	1.39
13	n	101	BCB	C3D-C2D	5.29	1.48	1.39
13	r	101	BCB	C3D-C2D	5.29	1.48	1.39
13	A	102	BCB	CHC-C4B	5.28	1.48	1.39
13	B	202	BCB	C3D-C4D	-5.28	1.33	1.41
13	Q	402	BCB	C3D-C2D	5.27	1.48	1.39
13	A	102	BCB	C3B-C4B	5.27	1.50	1.41
13	E	101	BCB	C3D-C4D	-5.26	1.33	1.41
13	M	402	BCB	C3B-C2B	5.25	1.48	1.39
13	M	403	BCB	CHC-C4B	5.25	1.48	1.39
13	T	101	BCB	CHC-C4B	5.25	1.48	1.39
13	N	101	BCB	C3B-C4B	5.23	1.49	1.41
13	7	102	BCB	C3D-C4D	-5.23	1.33	1.41
13	M	402	BCB	C3D-C4D	-5.22	1.33	1.41
13	f	101	BCB	C3D-C2D	5.21	1.48	1.39
13	N	101	BCB	CHC-C4B	5.21	1.48	1.39
13	q	101	BCB	CHC-C4B	5.21	1.48	1.39
13	0	102	BCB	C3B-C4B	5.20	1.49	1.41
13	o	102	BCB	C3D-C4D	-5.20	1.33	1.41
13	i	101	BCB	C3D-C4D	-5.20	1.33	1.41
13	D	101	BCB	C3B-C4B	5.20	1.49	1.41
13	o	102	BCB	C3D-C2D	5.19	1.48	1.39
13	f	101	BCB	C3D-C4D	-5.19	1.33	1.41
13	Z	101	BCB	C3B-C4B	5.19	1.49	1.41
13	U	102	BCB	C3D-C4D	-5.18	1.33	1.41
13	O	102	BCB	C3D-C2D	5.18	1.48	1.39
13	T	101	BCB	C3D-C2D	5.17	1.48	1.39
13	h	102	BCB	CHC-C4B	5.17	1.48	1.39
13	Q	402	BCB	C3B-C4B	5.17	1.49	1.41
13	L	303	BCB	CHC-C4B	5.17	1.48	1.39
13	k	102	BCB	C3D-C2D	5.16	1.48	1.39
13	n	101	BCB	CHC-C4B	5.16	1.48	1.39
13	e	101	BCB	C3D-C2D	5.16	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	N	101	BCB	C3D-C2D	5.15	1.48	1.39
13	I	101	BCB	CHC-C4B	5.15	1.48	1.39
13	3	101	BCB	CHC-C4B	5.14	1.47	1.39
13	0	102	BCB	C3D-C2D	5.13	1.48	1.39
13	U	102	BCB	C3B-C4B	5.13	1.49	1.41
13	l	102	BCB	C3D-C4D	-5.13	1.33	1.41
13	A	102	BCB	C3D-C4D	-5.13	1.33	1.41
13	L	303	BCB	C3B-C4B	5.12	1.49	1.41
13	J	101	BCB	C3D-C2D	5.12	1.48	1.39
13	r	101	BCB	C3D-C4D	-5.12	1.33	1.41
13	q	101	BCB	C3B-C4B	5.12	1.49	1.41
13	q	101	BCB	C3D-C2D	5.12	1.48	1.39
13	h	102	BCB	C3B-C4B	5.12	1.49	1.41
13	W	302	BCB	C3B-C4B	5.11	1.49	1.41
13	Z	101	BCB	CHC-C4B	5.11	1.47	1.39
13	Z	101	BCB	C3D-C2D	5.10	1.48	1.39
13	M	402	BCB	C3B-C4B	5.10	1.49	1.41
13	9	101	BCB	C3B-C4B	5.10	1.49	1.41
13	k	102	BCB	C3B-C4B	5.10	1.49	1.41
13	n	101	BCB	O2D-CGD	5.09	1.45	1.33
13	R	102	BCB	C3B-C4B	5.09	1.49	1.41
13	I	101	BCB	C3D-C4D	-5.09	1.33	1.41
13	4	101	BCB	C3D-C2D	5.08	1.48	1.39
13	W	302	BCB	C3D-C2D	5.08	1.48	1.39
13	U	102	BCB	C3D-C2D	5.07	1.48	1.39
13	7	102	BCB	C3D-C2D	5.07	1.48	1.39
13	X	102	BCB	C3D-C2D	5.07	1.48	1.39
13	L	302	BCB	O2D-CGD	5.06	1.45	1.33
13	e	101	BCB	O2D-CGD	5.06	1.45	1.33
13	4	101	BCB	C3D-C4D	-5.06	1.33	1.41
13	b	101	BCB	C3D-C4D	-5.06	1.33	1.41
13	X	102	BCB	C3D-C4D	-5.06	1.33	1.41
13	n	101	BCB	C3B-C4B	5.05	1.49	1.41
13	I	101	BCB	C3B-C4B	5.05	1.49	1.41
13	1	101	BCB	C3B-C4B	5.05	1.49	1.41
13	3	101	BCB	C3B-C4B	5.05	1.49	1.41
13	7	102	BCB	C3B-C4B	5.05	1.49	1.41
13	B	202	BCB	C3D-C2D	5.04	1.48	1.39
13	e	101	BCB	C3B-C4B	5.04	1.49	1.41
13	c	101	BCB	C3B-C4B	5.04	1.49	1.41
13	e	101	BCB	CHC-C4B	5.03	1.47	1.39
13	A	102	BCB	C3D-C2D	5.03	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	L	302	BCB	C3D-C4D	-5.02	1.33	1.41
13	D	101	BCB	C3D-C4D	-5.02	1.33	1.41
13	c	101	BCB	CHC-C4B	5.02	1.47	1.39
13	c	101	BCB	C3D-C2D	5.02	1.48	1.39
13	E	101	BCB	C3B-C4B	5.02	1.49	1.41
13	b	101	BCB	CHC-C4B	5.01	1.47	1.39
13	l	101	BCB	O2D-CGD	5.01	1.45	1.33
13	R	102	BCB	O2D-CGD	5.01	1.45	1.33
13	9	101	BCB	C3D-C4D	-5.00	1.33	1.41
13	q	101	BCB	C3D-C4D	-5.00	1.33	1.41
13	M	402	BCB	C3D-C2D	5.00	1.48	1.39
17	M	405	MQ7	C10-C5	4.99	1.48	1.40
13	J	101	BCB	C3B-C4B	4.99	1.49	1.41
13	6	101	BCB	C3D-C2D	4.98	1.48	1.39
13	B	202	BCB	C3B-C4B	4.98	1.49	1.41
13	f	101	BCB	O2D-CGD	4.98	1.45	1.33
13	l	101	BCB	C3D-C2D	4.98	1.48	1.39
13	q	101	BCB	C3A-C2A	-4.98	1.50	1.54
13	h	102	BCB	O2D-CGD	4.98	1.45	1.33
13	W	302	BCB	CHC-C4B	4.97	1.47	1.39
13	h	102	BCB	C3D-C2D	4.97	1.48	1.39
13	J	101	BCB	C3D-C4D	-4.97	1.33	1.41
13	9	101	BCB	O2D-CGD	4.97	1.45	1.33
13	I	101	BCB	C3D-C2D	4.97	1.48	1.39
13	U	102	BCB	CHC-C4B	4.97	1.47	1.39
13	E	101	BCB	C3D-C2D	4.97	1.48	1.39
13	X	102	BCB	O2D-CGD	4.96	1.45	1.33
13	i	101	BCB	O2D-CGD	4.96	1.45	1.33
13	Z	101	BCB	C3D-C4D	-4.96	1.34	1.41
13	R	102	BCB	CHC-C4B	4.95	1.47	1.39
13	9	101	BCB	CHC-C4B	4.95	1.47	1.39
13	9	101	BCB	C3D-C2D	4.95	1.48	1.39
13	W	302	BCB	O2D-CGD	4.95	1.45	1.33
13	M	402	BCB	CHC-C4B	4.94	1.47	1.39
13	i	101	BCB	C3D-C2D	4.94	1.48	1.39
13	l	102	BCB	C3B-C4B	4.94	1.49	1.41
13	r	101	BCB	CHC-C4B	4.94	1.47	1.39
13	O	102	BCB	C3D-C4D	-4.94	1.34	1.41
13	U	102	BCB	O2D-CGD	4.93	1.45	1.33
13	Q	402	BCB	C3D-C4D	-4.93	1.34	1.41
13	k	102	BCB	CHC-C4B	4.93	1.47	1.39
13	0	102	BCB	O2D-CGD	4.92	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	h	102	BCB	C3D-C4D	-4.92	1.34	1.41
13	l	102	BCB	CHC-C4B	4.92	1.47	1.39
13	r	101	BCB	C3B-C4B	4.91	1.49	1.41
13	6	101	BCB	O2D-CGD	4.91	1.45	1.33
13	k	102	BCB	O2D-CGD	4.91	1.45	1.33
13	l	102	BCB	O2D-CGD	4.91	1.45	1.33
13	W	302	BCB	C3D-C4D	-4.90	1.34	1.41
13	3	101	BCB	O2D-CGD	4.90	1.45	1.33
13	7	102	BCB	O2D-CGD	4.89	1.45	1.33
13	B	202	BCB	O2D-CGD	4.89	1.45	1.33
13	b	101	BCB	O2D-CGD	4.89	1.45	1.33
13	c	101	BCB	O2D-CGD	4.89	1.45	1.33
13	3	101	BCB	C3D-C2D	4.89	1.48	1.39
13	B	202	BCB	CHC-C4B	4.89	1.47	1.39
13	b	101	BCB	C3B-C4B	4.88	1.49	1.41
13	D	101	BCB	C3D-C2D	4.88	1.48	1.39
13	E	101	BCB	O2D-CGD	4.87	1.45	1.33
13	e	101	BCB	C3D-C4D	-4.87	1.34	1.41
13	R	102	BCB	C3D-C2D	4.87	1.47	1.39
13	M	403	BCB	O2D-CGD	4.87	1.45	1.33
13	b	101	BCB	C3D-C2D	4.86	1.47	1.39
13	o	102	BCB	O2D-CGD	4.86	1.45	1.33
13	4	101	BCB	CHC-C4B	4.86	1.47	1.39
13	f	101	BCB	C3B-C4B	4.86	1.49	1.41
13	Z	101	BCB	O2D-CGD	4.85	1.45	1.33
13	k	102	BCB	C3D-C4D	-4.85	1.34	1.41
13	E	101	BCB	CHC-C4B	4.85	1.47	1.39
13	r	101	BCB	O2D-CGD	4.85	1.45	1.33
13	M	403	BCB	C3D-C2D	4.85	1.47	1.39
13	D	101	BCB	O2D-CGD	4.85	1.45	1.33
13	q	101	BCB	O2D-CGD	4.84	1.45	1.33
13	X	102	BCB	CHC-C4B	4.84	1.47	1.39
13	f	101	BCB	CHC-C4B	4.84	1.47	1.39
13	0	102	BCB	CHC-C4B	4.83	1.47	1.39
13	4	101	BCB	O2D-CGD	4.83	1.45	1.33
13	L	302	BCB	CHC-C4B	4.83	1.47	1.39
13	A	102	BCB	O2D-CGD	4.83	1.45	1.33
13	T	101	BCB	O2D-CGD	4.82	1.45	1.33
13	n	101	BCB	C3D-C4D	-4.82	1.34	1.41
13	J	101	BCB	O2D-CGD	4.82	1.45	1.33
13	1	101	BCB	CHC-C4B	4.81	1.47	1.39
13	J	101	BCB	CHC-C4B	4.81	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	X	102	BCB	C3B-C4B	4.81	1.49	1.41
13	O	102	BCB	C3B-C4B	4.80	1.49	1.41
13	Q	402	BCB	O2D-CGD	4.80	1.45	1.33
13	o	102	BCB	C3B-C4B	4.80	1.49	1.41
13	I	101	BCB	O2D-CGD	4.79	1.45	1.33
13	N	101	BCB	C3D-C4D	-4.78	1.34	1.41
13	7	102	BCB	CHC-C4B	4.78	1.47	1.39
13	3	101	BCB	C3D-C4D	-4.78	1.34	1.41
13	i	101	BCB	C3B-C4B	4.78	1.49	1.41
13	6	101	BCB	C3D-C4D	-4.75	1.34	1.41
13	o	102	BCB	CHC-C4B	4.75	1.47	1.39
13	N	101	BCB	O2D-CGD	4.74	1.44	1.33
13	O	102	BCB	O2D-CGD	4.72	1.44	1.33
13	L	303	BCB	C3D-C2D	4.72	1.47	1.39
13	L	303	BCB	CHB-C4A	-4.71	1.32	1.38
13	q	101	BCB	OBD-CAD	4.71	1.28	1.22
13	B	202	BCB	C3A-C2A	-4.71	1.50	1.54
13	n	101	BCB	OBD-CAD	4.70	1.28	1.22
13	L	303	BCB	O2D-CGD	4.69	1.44	1.33
13	T	101	BCB	C3D-C4D	-4.68	1.34	1.41
13	Q	402	BCB	CHB-C4A	-4.67	1.33	1.38
13	M	402	BCB	O2D-CGD	4.67	1.44	1.33
13	h	102	BCB	OBD-CAD	4.67	1.28	1.22
13	4	101	BCB	C3B-C4B	4.65	1.48	1.41
13	M	402	BCB	CHB-C4A	-4.65	1.33	1.38
13	i	101	BCB	CHC-C4B	4.64	1.47	1.39
13	L	302	BCB	C3D-C2D	4.64	1.47	1.39
13	O	102	BCB	CHC-C4B	4.63	1.47	1.39
13	e	101	BCB	OBD-CAD	4.63	1.28	1.22
13	D	101	BCB	OBD-CAD	4.62	1.28	1.22
13	r	101	BCB	OBD-CAD	4.61	1.28	1.22
13	A	102	BCB	OBD-CAD	4.60	1.28	1.22
13	T	101	BCB	OBD-CAD	4.60	1.28	1.22
13	W	302	BCB	C3A-C2A	-4.60	1.50	1.54
13	9	101	BCB	OBD-CAD	4.60	1.28	1.22
13	k	102	BCB	OBD-CAD	4.59	1.28	1.22
13	c	101	BCB	CHB-C1B	4.59	1.47	1.39
13	L	302	BCB	C3B-C4B	4.58	1.48	1.41
13	o	102	BCB	OBD-CAD	4.57	1.28	1.22
13	Q	402	BCB	C3A-C2A	-4.55	1.50	1.54
13	6	101	BCB	C3A-C2A	-4.55	1.50	1.54
13	O	102	BCB	OBD-CAD	4.55	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	L	303	BCB	OBD-CAD	4.54	1.28	1.22
13	b	101	BCB	CHB-C1B	4.52	1.46	1.39
13	i	101	BCB	CHB-C1B	4.51	1.46	1.39
13	o	102	BCB	CHB-C1B	4.51	1.46	1.39
13	I	101	BCB	C3A-C2A	-4.50	1.50	1.54
13	J	101	BCB	CHB-C1B	4.50	1.46	1.39
13	R	102	BCB	CHB-C1B	4.50	1.46	1.39
13	L	302	BCB	OBD-CAD	4.49	1.28	1.22
9	C	403	HEC	CBB-CAB	-4.49	1.32	1.49
9	C	402	HEC	CBC-CAC	-4.49	1.32	1.49
13	B	202	BCB	OBD-CAD	4.48	1.28	1.22
13	Z	101	BCB	OBD-CAD	4.48	1.28	1.22
13	W	302	BCB	OBD-CAD	4.47	1.28	1.22
13	U	102	BCB	CHB-C1B	4.47	1.46	1.39
13	3	101	BCB	OBD-CAD	4.47	1.28	1.22
13	I	101	BCB	OBD-CAD	4.47	1.28	1.22
13	6	101	BCB	OBD-CAD	4.46	1.28	1.22
13	h	102	BCB	C3A-C2A	-4.45	1.50	1.54
13	M	402	BCB	OBD-CAD	4.45	1.28	1.22
13	n	101	BCB	CHB-C4A	-4.44	1.33	1.38
9	C	404	HEC	CBC-CAC	-4.44	1.33	1.49
15	H	302	CDL	OA8-CA7	4.44	1.46	1.33
13	N	101	BCB	C3A-C2A	-4.43	1.50	1.54
13	O	102	BCB	CHB-C1B	4.43	1.46	1.39
13	M	403	BCB	CHB-C1B	4.42	1.46	1.39
13	I	101	BCB	CHB-C4A	-4.42	1.33	1.38
13	l	102	BCB	OBD-CAD	4.42	1.28	1.22
13	l	102	BCB	CHB-C1B	4.42	1.46	1.39
13	Q	402	BCB	OBD-CAD	4.41	1.28	1.22
13	B	202	BCB	CHB-C1B	4.41	1.46	1.39
13	X	102	BCB	OBD-CAD	4.41	1.28	1.22
13	A	102	BCB	CHB-C4A	-4.41	1.33	1.38
13	E	101	BCB	CHB-C1B	4.40	1.46	1.39
13	E	101	BCB	OBD-CAD	4.40	1.28	1.22
13	1	101	BCB	OBD-CAD	4.40	1.28	1.22
9	C	401	HEC	CBB-CAB	-4.39	1.33	1.49
13	3	101	BCB	CHB-C1B	4.39	1.46	1.39
13	N	101	BCB	OBD-CAD	4.39	1.28	1.22
13	4	101	BCB	CHB-C1B	4.38	1.46	1.39
13	c	101	BCB	O2A-CGA	4.38	1.46	1.33
13	q	101	BCB	CHB-C4A	-4.38	1.33	1.38
13	n	101	BCB	C3A-C2A	-4.37	1.50	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	f	101	BCB	O2A-CGA	4.37	1.46	1.33
13	J	101	BCB	O2A-CGA	4.37	1.46	1.33
13	f	101	BCB	CHB-C1B	4.37	1.46	1.39
13	J	101	BCB	OBD-CAD	4.36	1.28	1.22
13	T	101	BCB	C3A-C2A	-4.36	1.50	1.54
13	f	101	BCB	CHB-C4A	-4.36	1.33	1.38
15	H	301	CDL	OA8-CA7	4.35	1.46	1.33
13	L	303	BCB	O2A-CGA	4.35	1.46	1.33
13	e	101	BCB	CHB-C1B	4.34	1.46	1.39
13	Z	101	BCB	CHB-C1B	4.34	1.46	1.39
13	B	202	BCB	CHB-C4A	-4.34	1.33	1.38
20	Q	401	PGV	O03-C19	4.34	1.46	1.33
13	6	101	BCB	CHB-C1B	4.34	1.46	1.39
9	C	404	HEC	CBB-CAB	-4.33	1.33	1.49
20	D	102	PGV	O01-C1	4.33	1.46	1.34
13	W	302	BCB	CHB-C1B	4.33	1.46	1.39
13	1	101	BCB	O2A-CGA	4.33	1.46	1.33
13	X	102	BCB	O2A-CGA	4.33	1.46	1.33
9	C	403	HEC	CBC-CAC	-4.33	1.33	1.49
15	H	302	CDL	OA6-CA5	4.33	1.46	1.34
13	h	102	BCB	CHB-C1B	4.33	1.46	1.39
13	c	101	BCB	OBD-CAD	4.33	1.28	1.22
13	3	101	BCB	C3A-C2A	-4.33	1.51	1.54
13	R	102	BCB	OBD-CAD	4.32	1.28	1.22
13	D	101	BCB	O2A-CGA	4.32	1.45	1.33
20	W	301	PGV	O03-C19	4.32	1.45	1.33
13	r	101	BCB	O2A-CGA	4.32	1.45	1.33
20	N	102	PGV	O03-C19	4.32	1.45	1.33
13	7	102	BCB	CHB-C4A	-4.31	1.33	1.38
13	T	101	BCB	CHB-C4A	-4.31	1.33	1.38
13	f	101	BCB	OBD-CAD	4.31	1.27	1.22
9	C	401	HEC	CBC-CAC	-4.31	1.33	1.49
13	T	101	BCB	CHB-C1B	4.30	1.46	1.39
13	D	101	BCB	CHB-C1B	4.30	1.46	1.39
13	4	101	BCB	O2A-CGA	4.30	1.45	1.33
13	A	102	BCB	C3A-C2A	-4.30	1.51	1.54
13	B	202	BCB	O2A-CGA	4.30	1.45	1.33
13	U	102	BCB	OBD-CAD	4.30	1.27	1.22
13	r	101	BCB	CHB-C4A	-4.30	1.33	1.38
13	N	101	BCB	CHB-C1B	4.30	1.46	1.39
20	N	102	PGV	O01-C1	4.30	1.46	1.34
13	i	101	BCB	O2A-CGA	4.30	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	Z	101	BCB	CHB-C4A	-4.29	1.33	1.38
13	b	101	BCB	OBD-CAD	4.29	1.27	1.22
13	U	102	BCB	CHB-C4A	-4.29	1.33	1.38
13	T	101	BCB	O2A-CGA	4.29	1.45	1.33
13	q	101	BCB	CHB-C1B	4.29	1.46	1.39
13	0	102	BCB	OBD-CAD	4.28	1.27	1.22
13	4	101	BCB	CHB-C4A	-4.28	1.33	1.38
13	1	101	BCB	CHB-C4A	-4.28	1.33	1.38
13	3	101	BCB	O2A-CGA	4.28	1.45	1.33
13	Z	101	BCB	C3A-C2A	-4.27	1.51	1.54
15	r	102	CDL	OA6-CA5	4.27	1.46	1.34
15	L	306	CDL	OA8-CA7	4.27	1.45	1.33
15	r	102	CDL	OB6-CB5	4.27	1.46	1.34
13	L	303	BCB	CHB-C1B	4.27	1.46	1.39
13	M	403	BCB	O2A-CGA	4.27	1.45	1.33
13	E	101	BCB	O2A-CGA	4.27	1.45	1.33
9	C	402	HEC	CBB-CAB	-4.27	1.33	1.49
13	l	102	BCB	O2A-CGA	4.27	1.45	1.33
13	Z	101	BCB	O2A-CGA	4.27	1.45	1.33
13	l	102	BCB	C3A-C2A	-4.27	1.51	1.54
13	r	101	BCB	C3A-C2A	-4.27	1.51	1.54
13	k	102	BCB	CHB-C1B	4.26	1.46	1.39
13	h	102	BCB	CHB-C4A	-4.26	1.33	1.38
13	7	102	BCB	OBD-CAD	4.26	1.27	1.22
13	W	302	BCB	O2A-CGA	4.26	1.45	1.33
13	O	102	BCB	O2A-CGA	4.25	1.45	1.33
15	H	302	CDL	OB8-CB7	4.25	1.45	1.33
13	9	101	BCB	CHB-C1B	4.25	1.46	1.39
13	N	101	BCB	CHB-C4A	-4.25	1.33	1.38
13	4	101	BCB	OBD-CAD	4.24	1.27	1.22
13	L	302	BCB	C3A-C2A	-4.24	1.51	1.54
13	E	101	BCB	CHB-C4A	-4.23	1.33	1.38
13	0	102	BCB	O2A-CGA	4.23	1.45	1.33
13	X	102	BCB	CHB-C1B	4.23	1.46	1.39
15	H	301	CDL	OA6-CA5	4.22	1.46	1.34
13	N	101	BCB	O2A-CGA	4.22	1.45	1.33
13	o	102	BCB	O2A-CGA	4.22	1.45	1.33
13	i	101	BCB	CHB-C4A	-4.22	1.33	1.38
13	R	102	BCB	O2A-CGA	4.22	1.45	1.33
13	9	101	BCB	CHB-C4A	-4.21	1.33	1.38
13	1	101	BCB	CHB-C1B	4.21	1.46	1.39
13	i	101	BCB	OBD-CAD	4.20	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	7	102	BCB	CHB-C1B	4.20	1.46	1.39
13	n	101	BCB	CHB-C1B	4.20	1.46	1.39
15	M	409	CDL	OA8-CA7	4.20	1.45	1.33
13	e	101	BCB	O2A-CGA	4.19	1.45	1.33
13	b	101	BCB	O2A-CGA	4.19	1.45	1.33
20	Q	401	PGV	O01-C1	4.19	1.46	1.34
13	U	102	BCB	O2A-CGA	4.18	1.45	1.33
13	7	102	BCB	O2A-CGA	4.18	1.45	1.33
13	k	102	BCB	CHB-C4A	-4.18	1.33	1.38
20	I	102	PGV	O03-C19	4.16	1.45	1.33
13	k	102	BCB	C3A-C2A	-4.16	1.51	1.54
13	l	101	BCB	C3A-C2A	-4.16	1.51	1.54
15	r	102	CDL	OA8-CA7	4.16	1.45	1.33
13	n	101	BCB	O2A-CGA	4.15	1.45	1.33
13	A	102	BCB	O2A-CGA	4.14	1.45	1.33
13	A	102	BCB	CHB-C1B	4.14	1.46	1.39
13	O	102	BCB	CHB-C4A	-4.14	1.33	1.38
13	D	101	BCB	CHB-C4A	-4.14	1.33	1.38
13	r	101	BCB	CHB-C1B	4.13	1.46	1.39
13	0	102	BCB	CHB-C1B	4.13	1.46	1.39
13	X	102	BCB	CHB-C4A	-4.13	1.33	1.38
13	L	302	BCB	CHB-C1B	4.12	1.46	1.39
12	L	301	DGA	OG1-CA1	4.12	1.45	1.33
13	R	102	BCB	C3A-C2A	-4.12	1.51	1.54
15	r	102	CDL	OB8-CB7	4.12	1.45	1.33
20	D	102	PGV	O03-C19	4.11	1.45	1.33
13	q	101	BCB	O2A-CGA	4.11	1.45	1.33
9	C	403	HEC	CAC-C3C	4.11	1.48	1.35
13	9	101	BCB	O2A-CGA	4.10	1.45	1.33
13	M	402	BCB	O2A-CGA	4.10	1.45	1.33
13	l	102	BCB	CHB-C4A	-4.10	1.33	1.38
20	M	411	PGV	O03-C19	4.10	1.45	1.33
13	0	102	BCB	C3A-C2A	-4.09	1.51	1.54
13	Q	402	BCB	CHB-C1B	4.09	1.46	1.39
13	I	101	BCB	O2A-CGA	4.09	1.45	1.33
13	o	102	BCB	CHB-C4A	-4.09	1.33	1.38
13	R	102	BCB	CHB-C4A	-4.09	1.33	1.38
13	9	101	BCB	C3A-C2A	-4.08	1.51	1.54
13	L	302	BCB	CHB-C4A	-4.08	1.33	1.38
15	L	306	CDL	OB6-CB5	4.08	1.45	1.34
15	L	306	CDL	OB8-CB7	4.07	1.45	1.33
13	6	101	BCB	O2A-CGA	4.07	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	402	HEC	CAB-C3B	4.06	1.48	1.35
13	h	102	BCB	O2A-CGA	4.06	1.45	1.33
13	k	102	BCB	O2A-CGA	4.06	1.45	1.33
13	I	101	BCB	CHB-C1B	4.05	1.46	1.39
13	M	403	BCB	CHD-C4C	4.05	1.47	1.39
15	M	409	CDL	OA6-CA5	4.05	1.45	1.34
9	C	402	HEC	CAC-C3C	4.05	1.48	1.35
15	M	409	CDL	OB6-CB5	4.05	1.45	1.34
13	Q	402	BCB	O2A-CGA	4.04	1.45	1.33
20	M	411	PGV	O01-C1	4.04	1.45	1.34
9	C	401	HEC	CAC-C3C	4.04	1.48	1.35
13	b	101	BCB	C3A-C2A	-4.04	1.51	1.54
15	L	306	CDL	OA6-CA5	4.03	1.45	1.34
13	e	101	BCB	C3A-C2A	-4.02	1.51	1.54
13	M	403	BCB	CHB-C4A	-4.01	1.33	1.38
13	W	302	BCB	CHB-C4A	-4.01	1.33	1.38
15	M	409	CDL	OB8-CB7	3.98	1.45	1.33
20	I	102	PGV	O01-C1	3.98	1.45	1.34
13	L	303	BCB	C3A-C2A	-3.98	1.51	1.54
15	H	301	CDL	OB6-CB5	3.97	1.45	1.34
13	3	101	BCB	CHB-C4A	-3.97	1.33	1.38
13	M	402	BCB	CHB-C1B	3.97	1.46	1.39
13	k	102	BCB	CHD-C4C	3.95	1.47	1.39
13	0	102	BCB	CHB-C4A	-3.95	1.33	1.38
13	b	101	BCB	CHB-C4A	-3.94	1.33	1.38
13	M	402	BCB	C3A-C2A	-3.94	1.51	1.54
9	C	404	HEC	CAC-C3C	3.93	1.47	1.35
13	D	101	BCB	C3A-C2A	-3.93	1.51	1.54
13	f	101	BCB	C3A-C2A	-3.93	1.51	1.54
13	e	101	BCB	CHB-C4A	-3.92	1.33	1.38
13	6	101	BCB	CHB-C4A	-3.91	1.33	1.38
13	J	101	BCB	CHB-C4A	-3.90	1.33	1.38
13	i	101	BCB	C3A-C2A	-3.90	1.51	1.54
15	H	302	CDL	OB6-CB5	3.89	1.45	1.34
20	W	301	PGV	O01-C1	3.89	1.45	1.34
13	X	102	BCB	C3A-C2A	-3.89	1.51	1.54
13	M	403	BCB	OBD-CAD	3.89	1.27	1.22
13	9	101	BCB	CHD-C4C	3.88	1.46	1.39
12	L	301	DGA	OG2-CB1	3.88	1.45	1.34
9	C	404	HEC	CAB-C3B	3.88	1.47	1.35
13	A	102	BCB	CHD-C4C	3.87	1.46	1.39
13	O	102	BCB	C3A-C2A	-3.87	1.51	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	402	BCB	CHD-C4C	3.86	1.46	1.39
13	c	101	BCB	CHB-C4A	-3.85	1.34	1.38
13	J	101	BCB	C3A-C2A	-3.82	1.51	1.54
13	7	102	BCB	C3A-C2A	-3.81	1.51	1.54
13	L	302	BCB	O2A-CGA	3.79	1.44	1.33
13	M	402	BCB	CHD-C1D	3.78	1.45	1.39
13	e	101	BCB	CHD-C1D	3.77	1.45	1.39
15	H	301	CDL	OB8-CB7	3.76	1.44	1.33
9	C	403	HEC	CAB-C3B	3.76	1.47	1.35
13	L	303	BCB	CHD-C4C	3.76	1.46	1.39
13	c	101	BCB	C3A-C2A	-3.74	1.51	1.54
13	E	101	BCB	CHD-C4C	3.74	1.46	1.39
11	A	101	UQ8	C4-C3	3.73	1.49	1.36
9	C	401	HEC	CAB-C3B	3.72	1.47	1.35
13	E	101	BCB	C3A-C2A	-3.71	1.51	1.54
13	I	101	BCB	CHD-C4C	3.71	1.46	1.39
13	o	102	BCB	C3A-C2A	-3.71	1.51	1.54
13	Q	402	BCB	CHD-C4C	3.70	1.46	1.39
13	T	101	BCB	CHD-C4C	3.68	1.46	1.39
13	A	102	BCB	CHD-C1D	3.68	1.45	1.39
13	L	303	BCB	CHD-C1D	3.67	1.45	1.39
13	9	101	BCB	CHD-C1D	3.67	1.45	1.39
13	n	101	BCB	CHD-C4C	3.66	1.46	1.39
13	3	101	BCB	CHD-C4C	3.64	1.46	1.39
13	I	101	BCB	CHD-C1D	3.64	1.45	1.39
13	D	101	BCB	CHD-C4C	3.63	1.46	1.39
13	L	302	BCB	CHD-C4C	3.63	1.46	1.39
13	Z	101	BCB	CHD-C4C	3.62	1.46	1.39
13	k	102	BCB	CHD-C1D	3.61	1.45	1.39
13	J	101	BCB	CHD-C4C	3.61	1.46	1.39
13	e	101	BCB	CHD-C4C	3.60	1.46	1.39
13	q	101	BCB	CHD-C4C	3.60	1.46	1.39
13	M	403	BCB	CHD-C1D	3.60	1.45	1.39
13	7	102	BCB	CHD-C4C	3.60	1.46	1.39
13	r	101	BCB	CHD-C4C	3.60	1.46	1.39
13	q	101	BCB	CHD-C1D	3.60	1.45	1.39
13	X	102	BCB	CHD-C1D	3.60	1.45	1.39
13	h	102	BCB	CHD-C4C	3.59	1.46	1.39
13	i	101	BCB	CHD-C4C	3.58	1.46	1.39
13	n	101	BCB	CHD-C1D	3.58	1.45	1.39
13	U	102	BCB	CHD-C4C	3.57	1.46	1.39
13	N	101	BCB	CHD-C4C	3.57	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	7	102	BCB	CHD-C1D	3.57	1.45	1.39
13	B	202	BCB	CHD-C4C	3.56	1.46	1.39
13	6	101	BCB	CHD-C4C	3.55	1.46	1.39
13	l	102	BCB	CHD-C1D	3.55	1.45	1.39
13	l	102	BCB	CHD-C4C	3.54	1.46	1.39
13	L	302	BCB	CHD-C1D	3.54	1.45	1.39
13	W	302	BCB	CHD-C4C	3.54	1.46	1.39
11	L	305	UQ8	C4-C3	3.53	1.49	1.36
13	U	102	BCB	C3A-C2A	-3.53	1.51	1.54
13	i	101	BCB	CHD-C1D	3.53	1.45	1.39
13	X	102	BCB	CHD-C4C	3.53	1.46	1.39
13	E	101	BCB	CHD-C1D	3.52	1.45	1.39
13	Q	402	BCB	CHD-C1D	3.51	1.45	1.39
13	1	101	BCB	CHD-C4C	3.51	1.46	1.39
13	f	101	BCB	CHD-C1D	3.51	1.45	1.39
13	M	403	BCB	C3A-C2A	-3.51	1.51	1.54
13	b	101	BCB	CHD-C4C	3.50	1.46	1.39
13	N	101	BCB	CHD-C1D	3.49	1.45	1.39
13	0	102	BCB	CHD-C4C	3.48	1.46	1.39
13	R	102	BCB	CHD-C4C	3.47	1.46	1.39
13	f	101	BCB	CHD-C4C	3.46	1.46	1.39
13	T	101	BCB	CHD-C1D	3.46	1.45	1.39
13	B	202	BCB	CHD-C1D	3.43	1.45	1.39
13	h	102	BCB	CHD-C1D	3.42	1.45	1.39
13	J	101	BCB	CHD-C1D	3.40	1.45	1.39
13	W	302	BCB	CHD-C1D	3.40	1.45	1.39
13	o	102	BCB	CHD-C4C	3.39	1.45	1.39
13	4	101	BCB	CHD-C1D	3.38	1.45	1.39
13	3	101	BCB	CHD-C1D	3.38	1.45	1.39
13	R	102	BCB	CHD-C1D	3.38	1.45	1.39
13	0	102	BCB	CHD-C1D	3.38	1.45	1.39
13	1	101	BCB	CHD-C1D	3.37	1.45	1.39
13	4	101	BCB	CHD-C4C	3.37	1.45	1.39
13	O	102	BCB	CHD-C4C	3.37	1.45	1.39
13	r	101	BCB	CHD-C1D	3.37	1.45	1.39
13	D	101	BCB	CHD-C1D	3.35	1.45	1.39
13	U	102	BCB	CHD-C1D	3.35	1.45	1.39
11	C	406	UQ8	C4-C3	3.34	1.48	1.36
13	4	101	BCB	C3A-C2A	-3.32	1.51	1.54
11	M	407	UQ8	C4-C3	3.32	1.48	1.36
13	O	102	BCB	CHD-C1D	3.31	1.45	1.39
13	c	101	BCB	CHD-C4C	3.28	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	Z	101	BCB	CHD-C1D	3.26	1.44	1.39
13	o	102	BCB	CHD-C1D	3.26	1.44	1.39
13	6	101	BCB	CHD-C1D	3.21	1.44	1.39
11	M	408	UQ8	C4-C3	3.18	1.47	1.36
13	b	101	BCB	CHD-C1D	3.16	1.44	1.39
13	c	101	BCB	CHD-C1D	3.12	1.44	1.39
21	2	101	NS0	C16-C17	-3.10	1.39	1.46
9	C	404	HEC	C1B-NB	-3.04	1.33	1.39
21	W	303	NS0	C16-C17	-2.99	1.39	1.46
21	9	102	NS0	C16-C17	-2.95	1.39	1.46
9	C	403	HEC	C4B-NB	-2.93	1.34	1.39
13	L	302	BCB	CBD-CGD	-2.92	1.48	1.52
14	M	404	BPB	C4D-CHA	2.92	1.43	1.39
9	C	403	HEC	C1B-NB	-2.91	1.34	1.39
21	7	101	NS0	C16-C17	-2.88	1.39	1.46
21	D	103	NS0	C11-C12	-2.88	1.39	1.46
9	C	401	HEC	C4B-NB	-2.87	1.34	1.39
14	L	304	BPB	C4D-CHA	2.84	1.43	1.39
9	C	404	HEC	C4B-NB	-2.83	1.34	1.39
21	0	101	NS0	C16-C17	-2.83	1.39	1.46
21	D	103	NS0	C16-C17	-2.80	1.40	1.46
9	C	403	HEC	C4D-ND	-2.79	1.34	1.39
21	O	101	NS0	C16-C17	-2.79	1.40	1.46
13	h	102	BCB	CBD-CGD	-2.79	1.49	1.52
21	R	101	NS0	C16-C17	-2.78	1.40	1.46
21	q	102	NS0	C16-C17	-2.77	1.40	1.46
9	C	402	HEC	C1B-NB	-2.77	1.34	1.39
21	W	303	NS0	C25-C23	-2.77	1.40	1.46
13	b	101	BCB	CBD-CGD	-2.77	1.49	1.52
21	h	101	NS0	C16-C17	-2.77	1.40	1.46
9	C	402	HEC	C1D-ND	-2.75	1.34	1.39
21	A	103	NS0	C16-C17	-2.74	1.40	1.46
9	C	403	HEC	C1D-ND	-2.74	1.34	1.39
9	C	401	HEC	C1B-NB	-2.72	1.34	1.39
21	U	101	NS0	C16-C17	-2.71	1.40	1.46
21	o	101	NS0	C16-C17	-2.71	1.40	1.46
21	2	101	NS0	C11-C12	-2.70	1.40	1.46
9	C	404	HEC	C4D-ND	-2.69	1.34	1.39
21	7	101	NS0	C11-C12	-2.69	1.40	1.46
21	R	101	NS0	C11-C12	-2.68	1.40	1.46
21	0	101	NS0	C25-C23	-2.68	1.40	1.46
13	N	101	BCB	CBD-CGD	-2.68	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	k	101	NS0	C16-C17	-2.67	1.40	1.46
21	9	102	NS0	C11-C12	-2.65	1.40	1.46
21	X	101	NS0	C16-C17	-2.64	1.40	1.46
21	2	101	NS0	C25-C23	-2.64	1.40	1.46
21	X	101	NS0	C11-C12	-2.63	1.40	1.46
21	D	103	NS0	C25-C23	-2.63	1.40	1.46
21	o	101	NS0	C11-C12	-2.62	1.40	1.46
13	W	302	BCB	CBD-CGD	-2.62	1.49	1.52
13	T	101	BCB	CBD-CGD	-2.62	1.49	1.52
21	l	101	NS0	C16-C17	-2.62	1.40	1.46
14	L	304	BPB	C4C-C3C	-2.61	1.36	1.45
21	l	101	NS0	C11-C12	-2.61	1.40	1.46
9	C	401	HEC	C1D-ND	-2.61	1.34	1.39
21	A	103	NS0	C25-C23	-2.61	1.40	1.46
21	W	303	NS0	C11-C12	-2.61	1.40	1.46
21	q	102	NS0	C11-C12	-2.61	1.40	1.46
21	0	101	NS0	C11-C12	-2.60	1.40	1.46
9	C	402	HEC	C4D-ND	-2.60	1.34	1.39
9	C	404	HEC	C1D-ND	-2.60	1.34	1.39
18	M	406	NS5	C14-C15	-2.59	1.40	1.46
13	3	101	BCB	CBD-CGD	-2.58	1.49	1.52
12	L	301	DGA	OG2-CG2	-2.57	1.42	1.47
21	q	102	NS0	C25-C23	-2.56	1.40	1.46
13	L	303	BCB	CBD-CGD	-2.54	1.49	1.52
21	7	101	NS0	C25-C23	-2.54	1.40	1.46
9	C	402	HEC	C4B-NB	-2.53	1.34	1.39
21	O	101	NS0	C11-C12	-2.53	1.40	1.46
21	h	101	NS0	C11-C12	-2.53	1.40	1.46
21	A	103	NS0	C11-C12	-2.53	1.40	1.46
21	U	101	NS0	C11-C12	-2.52	1.40	1.46
21	U	101	NS0	C25-C23	-2.52	1.40	1.46
21	X	101	NS0	C25-C23	-2.52	1.40	1.46
21	k	101	NS0	C25-C23	-2.52	1.40	1.46
13	I	101	BCB	CBD-CGD	-2.51	1.49	1.52
21	9	102	NS0	C25-C23	-2.51	1.40	1.46
21	k	101	NS0	C11-C12	-2.50	1.40	1.46
21	O	101	NS0	C25-C23	-2.50	1.40	1.46
13	Z	101	BCB	CBD-CGD	-2.50	1.49	1.52
21	l	101	NS0	C25-C23	-2.49	1.40	1.46
9	C	401	HEC	C4A-C3A	-2.48	1.40	1.45
21	h	101	NS0	C25-C23	-2.46	1.40	1.46
14	M	404	BPB	C4C-C3C	-2.45	1.36	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	401	HEC	C4D-ND	-2.45	1.35	1.39
13	Q	402	BCB	CBD-CGD	-2.45	1.49	1.52
18	M	406	NS5	C28-C26	-2.44	1.40	1.46
14	M	404	BPB	C3A-C2A	-2.42	1.52	1.54
21	R	101	NS0	C25-C23	-2.42	1.40	1.46
21	o	101	NS0	C25-C23	-2.42	1.40	1.46
13	n	101	BCB	CBD-CGD	-2.41	1.49	1.52
13	M	402	BCB	CBD-CGD	-2.41	1.49	1.52
14	L	304	BPB	C1B-C2B	2.40	1.42	1.39
18	M	406	NS5	C23-C21	-2.40	1.40	1.46
13	q	101	BCB	CBD-CGD	-2.40	1.49	1.52
9	C	402	HEC	C4A-C3A	-2.39	1.40	1.45
13	6	101	BCB	CBD-CGD	-2.33	1.49	1.52
13	1	101	BCB	CBD-CGD	-2.29	1.49	1.52
14	L	304	BPB	C3A-C2A	-2.27	1.52	1.54
13	e	101	BCB	CBD-CGD	-2.26	1.49	1.52
9	C	403	HEC	C1A-C2A	-2.25	1.41	1.45
13	c	101	BCB	CBD-CGD	-2.25	1.49	1.52
18	M	406	NS5	C25-C26	2.24	1.41	1.35
13	9	101	BCB	CBD-CGD	-2.23	1.49	1.52
9	C	404	HEC	C1A-C2A	-2.22	1.41	1.45
13	k	102	BCB	CBD-CGD	-2.21	1.49	1.52
13	l	102	BCB	CBD-CGD	-2.21	1.49	1.52
9	C	404	HEC	C3C-C4C	-2.21	1.42	1.46
13	o	102	BCB	CBD-CGD	-2.20	1.49	1.52
9	C	402	HEC	C1A-C2A	-2.19	1.41	1.45
14	L	304	BPB	C4D-ND	-2.17	1.35	1.38
9	C	404	HEC	C4A-C3A	-2.15	1.41	1.45
13	M	403	BCB	C1C-C2C	-2.15	1.46	1.51
9	C	402	HEC	C3C-C4C	-2.14	1.42	1.46
13	U	102	BCB	CBD-CGD	-2.14	1.49	1.52
13	A	102	BCB	CBD-CGD	-2.11	1.49	1.52
21	k	101	NS0	C19-C17	2.10	1.40	1.35
21	9	102	NS0	C19-C17	2.10	1.40	1.35
14	L	304	BPB	CBD-CGD	-2.09	1.49	1.52
13	O	102	BCB	CBD-CGD	-2.07	1.49	1.52
18	M	406	NS5	C20-C21	2.07	1.40	1.35
13	f	101	BCB	CBD-CGD	-2.06	1.49	1.52
13	R	102	BCB	CBD-CGD	-2.04	1.49	1.52
21	h	101	NS0	C22-C23	2.03	1.40	1.35
21	A	103	NS0	C19-C17	2.01	1.40	1.35
13	D	101	BCB	CBD-CGD	-2.00	1.50	1.52

All (875) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	L	303	BCB	O2D-CGD-CBD	9.74	121.65	110.95
13	q	101	BCB	C4B-CHC-C1C	8.87	127.03	121.32
13	M	402	BCB	O2D-CGD-CBD	8.76	120.58	110.95
13	A	102	BCB	C4B-CHC-C1C	8.55	126.82	121.32
13	M	403	BCB	O2D-CGD-CBD	8.48	120.26	110.95
13	N	101	BCB	C4B-CHC-C1C	8.27	126.64	121.32
13	6	101	BCB	C4B-CHC-C1C	8.14	126.56	121.32
13	D	101	BCB	C4B-CHC-C1C	8.11	126.54	121.32
13	A	102	BCB	O2D-CGD-CBD	8.05	119.79	110.95
13	3	101	BCB	C4B-CHC-C1C	8.03	126.49	121.32
13	L	302	BCB	C1B-CHB-C4A	8.00	126.47	121.32
13	b	101	BCB	C4B-CHC-C1C	7.92	126.42	121.32
13	Z	101	BCB	C4B-CHC-C1C	7.90	126.41	121.32
13	L	303	BCB	C4B-CHC-C1C	7.75	126.31	121.32
13	T	101	BCB	C4B-CHC-C1C	7.66	126.25	121.32
13	I	101	BCB	C4B-CHC-C1C	7.65	126.24	121.32
13	O	102	BCB	O2D-CGD-CBD	7.63	119.33	110.95
13	i	101	BCB	O2D-CGD-CBD	7.60	119.29	110.95
13	W	302	BCB	C4B-CHC-C1C	7.57	126.19	121.32
13	R	102	BCB	O2D-CGD-CBD	7.54	119.23	110.95
13	9	101	BCB	C4B-CHC-C1C	7.47	126.13	121.32
13	i	101	BCB	C4B-CHC-C1C	7.40	126.08	121.32
13	O	102	BCB	C4B-CHC-C1C	7.37	126.06	121.32
13	l	102	BCB	C4B-CHC-C1C	7.33	126.04	121.32
13	c	101	BCB	O2D-CGD-CBD	7.32	118.99	110.95
13	o	102	BCB	O2D-CGD-CBD	7.22	118.89	110.95
13	k	102	BCB	C4B-CHC-C1C	7.21	125.96	121.32
13	B	202	BCB	O2D-CGD-CBD	7.16	118.82	110.95
13	J	101	BCB	C4B-CHC-C1C	7.15	125.92	121.32
13	f	101	BCB	O2D-CGD-CBD	7.11	118.75	110.95
13	Q	402	BCB	C4B-CHC-C1C	7.09	125.88	121.32
13	U	102	BCB	O2D-CGD-CBD	7.09	118.74	110.95
13	U	102	BCB	C4B-CHC-C1C	7.09	125.88	121.32
13	n	101	BCB	C4B-CHC-C1C	7.08	125.88	121.32
13	l	102	BCB	O2D-CGD-CBD	7.07	118.72	110.95
13	1	101	BCB	C4B-CHC-C1C	7.07	125.87	121.32
13	h	102	BCB	C4B-CHC-C1C	7.06	125.87	121.32
13	9	101	BCB	O2D-CGD-CBD	7.05	118.69	110.95
13	c	101	BCB	C1B-CHB-C4A	7.04	125.85	121.32
13	R	102	BCB	C4B-CHC-C1C	7.02	125.84	121.32
13	0	102	BCB	O2D-CGD-CBD	6.99	118.62	110.95
13	I	101	BCB	O2D-CGD-CBD	6.92	118.55	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	o	102	BCB	C4B-CHC-C1C	6.92	125.77	121.32
13	r	101	BCB	O2D-CGD-CBD	6.87	118.50	110.95
13	e	101	BCB	O2D-CGD-CBD	6.86	118.48	110.95
13	M	402	BCB	C4B-CHC-C1C	6.84	125.72	121.32
13	c	101	BCB	C4B-CHC-C1C	6.83	125.72	121.32
13	4	101	BCB	O2D-CGD-CBD	6.81	118.42	110.95
13	7	102	BCB	O2D-CGD-CBD	6.80	118.42	110.95
13	e	101	BCB	C4B-CHC-C1C	6.78	125.69	121.32
13	f	101	BCB	C4B-CHC-C1C	6.77	125.68	121.32
13	4	101	BCB	C4B-CHC-C1C	6.76	125.67	121.32
13	O	102	BCB	C1B-CHB-C4A	6.72	125.65	121.32
13	0	102	BCB	C1B-CHB-C4A	6.72	125.64	121.32
13	E	101	BCB	O2D-CGD-CBD	6.71	118.32	110.95
13	7	102	BCB	C4B-CHC-C1C	6.71	125.64	121.32
13	Z	101	BCB	O2D-CGD-CBD	6.68	118.28	110.95
13	Q	402	BCB	O2D-CGD-CBD	6.66	118.26	110.95
13	9	101	BCB	C1B-CHB-C4A	6.64	125.59	121.32
13	X	102	BCB	O2D-CGD-CBD	6.61	118.20	110.95
13	R	102	BCB	C1B-CHB-C4A	6.61	125.57	121.32
13	N	101	BCB	O2D-CGD-CBD	6.60	118.20	110.95
13	L	302	BCB	O2D-CGD-CBD	6.60	118.19	110.95
13	M	403	BCB	C1B-CHB-C4A	6.58	125.56	121.32
13	D	101	BCB	O2D-CGD-CBD	6.58	118.17	110.95
13	L	302	BCB	C4B-CHC-C1C	6.57	125.55	121.32
13	B	202	BCB	C1B-CHB-C4A	6.57	125.55	121.32
13	J	101	BCB	C1B-CHB-C4A	6.55	125.54	121.32
13	Q	402	BCB	C1B-CHB-C4A	6.54	125.53	121.32
13	1	101	BCB	O2D-CGD-CBD	6.52	118.11	110.95
13	0	102	BCB	C4B-CHC-C1C	6.50	125.50	121.32
13	W	302	BCB	O2D-CGD-CBD	6.47	118.05	110.95
13	n	101	BCB	O2D-CGD-CBD	6.46	118.04	110.95
13	3	101	BCB	O2D-CGD-CBD	6.43	118.01	110.95
13	h	102	BCB	O2D-CGD-CBD	6.42	118.00	110.95
13	W	302	BCB	C1B-CHB-C4A	6.42	125.45	121.32
13	E	101	BCB	C4B-CHC-C1C	6.40	125.44	121.32
13	X	102	BCB	C4B-CHC-C1C	6.38	125.43	121.32
13	M	402	BCB	C1B-CHB-C4A	6.36	125.42	121.32
13	b	101	BCB	O2D-CGD-CBD	6.36	117.93	110.95
13	h	102	BCB	C1B-CHB-C4A	6.35	125.41	121.32
13	J	101	BCB	O2D-CGD-CBD	6.32	117.89	110.95
13	4	101	BCB	C1B-CHB-C4A	6.29	125.37	121.32
13	B	202	BCB	C4B-CHC-C1C	6.28	125.36	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	e	101	BCB	C1B-CHB-C4A	6.26	125.35	121.32
13	9	101	BCB	CHA-C1A-C2A	-6.25	118.62	133.31
13	o	102	BCB	C1B-CHB-C4A	6.25	125.34	121.32
13	6	101	BCB	O2D-CGD-CBD	6.22	117.78	110.95
13	3	101	BCB	C1B-CHB-C4A	6.22	125.32	121.32
13	E	101	BCB	C1B-CHB-C4A	6.21	125.32	121.32
13	0	102	BCB	CHA-C1A-C2A	-6.18	118.81	133.31
13	q	101	BCB	O2D-CGD-CBD	6.16	117.72	110.95
13	r	101	BCB	C4B-CHC-C1C	6.15	125.28	121.32
13	D	101	BCB	CHA-C1A-C2A	-6.12	118.95	133.31
13	M	402	BCB	CHA-C1A-C2A	-6.08	119.04	133.31
13	L	303	BCB	C1B-CHB-C4A	6.05	125.21	121.32
13	U	102	BCB	CHA-C1A-C2A	-6.04	119.12	133.31
13	R	102	BCB	CHA-C1A-C2A	-6.04	119.13	133.31
13	U	102	BCB	C1B-CHB-C4A	6.01	125.19	121.32
13	T	101	BCB	O2D-CGD-CBD	6.01	117.55	110.95
13	q	101	BCB	CHA-C1A-C2A	-6.00	119.21	133.31
13	B	202	BCB	CHA-C1A-C2A	-5.98	119.27	133.31
13	A	102	BCB	CHA-C1A-C2A	-5.97	119.29	133.31
13	r	101	BCB	C1B-CHB-C4A	5.95	125.15	121.32
13	L	303	BCB	CHA-C1A-C2A	-5.94	119.36	133.31
13	i	101	BCB	CHA-C1A-C2A	-5.92	119.40	133.31
13	b	101	BCB	C1B-CHB-C4A	5.89	125.11	121.32
13	X	102	BCB	C1B-CHB-C4A	5.89	125.11	121.32
13	6	101	BCB	C1B-CHB-C4A	5.87	125.10	121.32
13	k	102	BCB	O2D-CGD-CBD	5.79	117.31	110.95
13	M	403	BCB	CHA-C1A-C2A	-5.79	119.72	133.31
13	X	102	BCB	CHA-C1A-C2A	-5.78	119.74	133.31
13	r	101	BCB	CHA-C1A-C2A	-5.77	119.76	133.31
13	1	101	BCB	CHA-C1A-C2A	-5.75	119.80	133.31
13	o	102	BCB	CHA-C1A-C2A	-5.75	119.81	133.31
13	f	101	BCB	CHA-C1A-C2A	-5.74	119.82	133.31
13	1	101	BCB	C1B-CHB-C4A	5.73	125.01	121.32
13	3	101	BCB	CHA-C1A-C2A	-5.71	119.89	133.31
13	J	101	BCB	CHA-C1A-C2A	-5.71	119.89	133.31
13	7	102	BCB	CHA-C1A-C2A	-5.71	119.91	133.31
13	l	102	BCB	CHA-C1A-C2A	-5.68	119.97	133.31
13	c	101	BCB	CHA-C1A-C2A	-5.68	119.97	133.31
13	h	102	BCB	CHA-C1A-C2A	-5.66	120.02	133.31
13	b	101	BCB	CHA-C1A-C2A	-5.66	120.03	133.31
13	6	101	BCB	CHA-C1A-C2A	-5.64	120.08	133.31
13	O	102	BCB	CHA-C1A-C2A	-5.62	120.11	133.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	i	101	BCB	C1B-CHB-C4A	5.61	124.93	121.32
13	4	101	BCB	CHA-C1A-C2A	-5.60	120.16	133.31
13	E	101	BCB	CHA-C1A-C2A	-5.58	120.21	133.31
13	W	302	BCB	CHA-C1A-C2A	-5.55	120.28	133.31
13	Z	101	BCB	C1B-CHB-C4A	5.54	124.88	121.32
13	n	101	BCB	CHA-C1A-C2A	-5.53	120.32	133.31
13	Z	101	BCB	CHA-C1A-C2A	-5.51	120.38	133.31
13	e	101	BCB	CHA-C1A-C2A	-5.50	120.40	133.31
13	D	101	BCB	C1B-CHB-C4A	5.49	124.85	121.32
13	Q	402	BCB	CHA-C1A-C2A	-5.48	120.44	133.31
13	N	101	BCB	CHA-C1A-C2A	-5.48	120.45	133.31
13	k	102	BCB	CHA-C1A-C2A	-5.47	120.47	133.31
13	I	101	BCB	C1B-CHB-C4A	5.43	124.82	121.32
13	n	101	BCB	C1B-CHB-C4A	5.42	124.81	121.32
13	T	101	BCB	CHA-C1A-C2A	-5.37	120.69	133.31
13	f	101	BCB	C1B-CHB-C4A	5.37	124.78	121.32
13	I	101	BCB	CHA-C1A-C2A	-5.33	120.80	133.31
13	M	403	BCB	C4B-CHC-C1C	5.10	124.61	121.32
9	C	401	HEC	CHC-C4B-NB	5.08	129.98	124.45
13	7	102	BCB	C1B-CHB-C4A	5.07	124.58	121.32
13	L	302	BCB	CHA-C1A-C2A	-5.02	121.51	133.31
12	L	301	DGA	CG2-OG2-CB1	-4.96	110.62	117.78
9	C	404	HEC	CHC-C4B-NB	4.91	129.80	124.45
13	k	102	BCB	C1B-CHB-C4A	4.84	124.44	121.32
13	T	101	BCB	C1B-CHB-C4A	4.84	124.44	121.32
9	C	403	HEC	CHC-C4B-NB	4.71	129.58	124.45
9	C	402	HEC	CHC-C4B-NB	4.71	129.58	124.45
12	L	301	DGA	OG2-CB1-CB2	4.65	121.54	111.48
13	A	102	BCB	C1B-CHB-C4A	4.64	124.31	121.32
13	3	101	BCB	C1-C2-C3	-4.56	118.72	126.20
15	r	102	CDL	OB6-CB5-C51	4.55	121.33	111.48
13	q	101	BCB	C1B-CHB-C4A	4.51	124.22	121.32
13	J	101	BCB	C4D-ND-C1D	-4.43	101.86	105.22
13	N	101	BCB	C1B-CHB-C4A	4.42	124.16	121.32
13	e	101	BCB	C1-C2-C3	-4.42	118.96	126.20
13	Q	402	BCB	C1-C2-C3	-4.41	118.97	126.20
9	C	403	HEC	CBB-CAB-C3B	-4.39	118.66	127.43
13	l	102	BCB	C1B-CHB-C4A	4.35	124.12	121.32
13	M	402	BCB	C4D-ND-C1D	-4.34	101.93	105.22
13	Z	101	BCB	C1-C2-C3	-4.33	119.09	126.20
15	H	301	CDL	OA6-CA5-C11	4.33	120.86	111.48
15	H	302	CDL	OA6-CA5-C11	4.25	120.68	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	I	101	BCB	C1-C2-C3	-4.20	119.31	126.20
13	M	403	BCB	C1-C2-C3	-4.20	119.31	126.20
21	R	101	NS0	C21-C20-C19	4.19	132.10	123.52
15	M	409	CDL	OA6-CA5-C11	4.18	120.52	111.48
20	I	102	PGV	O01-C1-C2	4.17	120.51	111.48
11	A	101	UQ8	C7-C8-C9	-4.16	119.66	126.83
13	n	101	BCB	C1-C2-C3	-4.16	119.39	126.20
15	M	409	CDL	OB6-CB5-C51	4.15	120.46	111.48
13	M	402	BCB	CHC-C1C-C2C	-4.14	111.61	122.69
13	L	302	BCB	C1-C2-C3	-4.09	119.50	126.20
13	c	101	BCB	C4D-ND-C1D	-4.07	102.13	105.22
13	N	101	BCB	CMB-C2B-C3B	4.07	132.81	124.68
15	L	306	CDL	OB6-CB5-C51	4.07	120.28	111.48
13	L	303	BCB	C4D-ND-C1D	-4.06	102.14	105.22
13	W	302	BCB	C1-C2-C3	-4.06	119.54	126.20
13	A	102	BCB	C1-C2-C3	-4.06	119.55	126.20
13	f	101	BCB	C4D-ND-C1D	-4.05	102.14	105.22
15	r	102	CDL	OA6-CA5-C11	4.04	120.23	111.48
15	H	301	CDL	OB6-CB5-C51	4.03	120.21	111.48
13	L	302	BCB	CHC-C1C-C2C	-4.03	111.91	122.69
13	N	101	BCB	C1-C2-C3	-4.00	119.64	126.20
9	C	401	HEC	CBB-CAB-C3B	-4.00	119.44	127.43
20	W	301	PGV	O01-C1-C2	3.99	120.11	111.48
13	M	403	BCB	CHC-C1C-C2C	-3.98	112.03	122.69
13	k	102	BCB	CHC-C1C-C2C	-3.97	112.05	122.69
13	l	101	BCB	C4D-ND-C1D	-3.96	102.22	105.22
13	1	101	BCB	CMB-C2B-C3B	3.95	132.57	124.68
13	i	101	BCB	C4D-ND-C1D	-3.95	102.22	105.22
21	X	101	NS0	C21-C20-C19	3.94	131.58	123.52
13	4	101	BCB	CHC-C1C-C2C	-3.93	112.16	122.69
13	0	102	BCB	C4D-ND-C1D	-3.93	102.24	105.22
13	f	101	BCB	CHC-C1C-C2C	-3.92	112.18	122.69
13	L	303	BCB	CMB-C2B-C3B	3.92	132.52	124.68
13	O	102	BCB	CHC-C1C-C2C	-3.92	112.20	122.69
13	U	102	BCB	C4D-ND-C1D	-3.91	102.25	105.22
9	C	404	HEC	CBB-CAB-C3B	-3.89	119.65	127.43
13	L	303	BCB	CHC-C1C-C2C	-3.89	112.26	122.69
13	4	101	BCB	C4D-ND-C1D	-3.88	102.27	105.22
13	7	102	BCB	CHC-C1C-C2C	-3.88	112.30	122.69
13	h	102	BCB	CHC-C1C-C2C	-3.88	112.31	122.69
13	e	101	BCB	CHC-C1C-C2C	-3.88	112.31	122.69
13	M	402	BCB	C1-C2-C3	-3.88	119.84	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	l	101	BCB	CHC-C1C-C2C	-3.87	112.33	122.69
13	l	102	BCB	CMB-C2B-C3B	3.86	132.39	124.68
13	o	102	BCB	C4D-ND-C1D	-3.85	102.30	105.22
21	W	303	NS0	C10-C9-C7	-3.84	122.29	127.69
13	q	101	BCB	CMB-C2B-C3B	3.84	132.36	124.68
13	n	101	BCB	CHC-C1C-C2C	-3.84	112.41	122.69
13	9	101	BCB	CHC-C1C-C2C	-3.83	112.42	122.69
13	J	101	BCB	CHC-C1C-C2C	-3.83	112.43	122.69
13	o	102	BCB	CHC-C1C-C2C	-3.82	112.45	122.69
13	k	102	BCB	CMB-C2B-C3B	3.82	132.32	124.68
13	E	101	BCB	CHC-C1C-C2C	-3.82	112.47	122.69
13	9	101	BCB	C1-C2-C3	-3.82	119.94	126.20
13	I	101	BCB	CHC-C1C-C2C	-3.80	112.50	122.69
13	b	101	BCB	CHC-C1C-C2C	-3.80	112.52	122.69
13	D	101	BCB	CMB-C2B-C3B	3.80	132.27	124.68
13	I	101	BCB	CMB-C2B-C3B	3.80	132.27	124.68
13	0	102	BCB	CMB-C2B-C3B	3.78	132.23	124.68
13	A	102	BCB	CHC-C1C-C2C	-3.77	112.61	122.69
13	0	102	BCB	CHC-C1C-C2C	-3.76	112.61	122.69
13	O	102	BCB	C4D-ND-C1D	-3.76	102.36	105.22
21	W	303	NS0	C21-C20-C19	3.76	131.21	123.52
13	b	101	BCB	C1-C2-C3	-3.76	120.04	126.20
13	R	102	BCB	CHC-C1C-C2C	-3.75	112.64	122.69
13	B	202	BCB	CHC-C1C-C2C	-3.75	112.65	122.69
13	B	202	BCB	C4D-ND-C1D	-3.74	102.38	105.22
14	L	304	BPB	C4D-CHA-CBD	-3.74	106.66	108.45
13	X	102	BCB	CHC-C1C-C2C	-3.74	112.67	122.69
13	7	102	BCB	CMB-C2B-C3B	3.74	132.15	124.68
13	R	102	BCB	CMB-C2B-C3B	3.73	132.14	124.68
13	E	101	BCB	C4D-ND-C1D	-3.73	102.39	105.22
11	M	408	UQ8	C17-C18-C19	-3.73	119.09	127.62
13	W	302	BCB	CMB-C2B-C3B	3.73	132.13	124.68
13	9	101	BCB	C4D-ND-C1D	-3.73	102.39	105.22
11	A	101	UQ8	C7-C6-C1	-3.72	118.51	124.89
13	c	101	BCB	CHC-C1C-C2C	-3.71	112.77	122.69
21	9	102	NS0	C21-C20-C19	3.70	131.09	123.52
13	D	101	BCB	C4D-ND-C1D	-3.70	102.41	105.22
13	i	101	BCB	CHC-C1C-C2C	-3.69	112.80	122.69
13	r	101	BCB	CHC-C1C-C2C	-3.69	112.80	122.69
13	Q	402	BCB	CMB-C2B-C3B	3.69	132.06	124.68
13	T	101	BCB	CHC-C1C-C2C	-3.69	112.81	122.69
13	3	101	BCB	CHC-C1C-C2C	-3.68	112.82	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	D	101	BCB	CHC-C1C-C2C	-3.68	112.85	122.69
13	U	102	BCB	CMB-C2B-C3B	3.67	132.03	124.68
13	o	102	BCB	CMB-C2B-C3B	3.67	132.02	124.68
13	4	101	BCB	CMB-C2B-C3B	3.67	132.01	124.68
13	U	102	BCB	CHC-C1C-C2C	-3.66	112.89	122.69
13	h	102	BCB	CMB-C2B-C3B	3.66	132.00	124.68
13	l	102	BCB	CHC-C1C-C2C	-3.65	112.91	122.69
13	h	102	BCB	C1-C2-C3	-3.65	120.22	126.20
13	k	102	BCB	C1-C2-C3	-3.65	120.22	126.20
13	B	202	BCB	CMB-C2B-C3B	3.63	131.94	124.68
13	X	102	BCB	C4D-ND-C1D	-3.63	102.46	105.22
13	X	102	BCB	CMB-C2B-C3B	3.63	131.94	124.68
13	M	403	BCB	C4D-ND-C1D	-3.63	102.47	105.22
13	T	101	BCB	C1-C2-C3	-3.63	120.26	126.20
13	Q	402	BCB	CHC-C1C-C2C	-3.62	112.99	122.69
13	b	101	BCB	CMB-C2B-C3B	3.62	131.91	124.68
13	T	101	BCB	CMB-C2B-C3B	3.61	131.89	124.68
13	W	302	BCB	CHC-C1C-C2C	-3.60	113.04	122.69
15	H	302	CDL	OB6-CB5-C51	3.60	119.27	111.48
20	Q	401	PGV	O01-C1-C2	3.60	119.27	111.48
15	L	306	CDL	OA6-CA5-C11	3.60	119.27	111.48
13	q	101	BCB	CHC-C1C-C2C	-3.60	113.06	122.69
13	6	101	BCB	CHC-C1C-C2C	-3.59	113.06	122.69
13	R	102	BCB	C4D-ND-C1D	-3.58	102.50	105.22
13	Z	101	BCB	CHC-C1C-C2C	-3.58	113.11	122.69
13	A	102	BCB	CMB-C2B-C3B	3.57	131.81	124.68
13	N	101	BCB	CHC-C1C-C2C	-3.54	113.21	122.69
13	L	302	BCB	C4-C3-C5	3.54	121.36	115.23
14	M	404	BPB	C4D-CHA-CBD	-3.53	106.76	108.45
20	D	102	PGV	O01-C1-C2	3.53	119.12	111.48
13	O	102	BCB	CMB-C2B-C3B	3.53	131.74	124.68
13	M	403	BCB	CMB-C2B-C3B	3.53	131.73	124.68
13	n	101	BCB	CMB-C2B-C3B	3.52	131.72	124.68
13	L	303	BCB	O1D-CGD-CBD	-3.52	119.39	124.72
13	f	101	BCB	CMB-C2B-C3B	3.52	131.71	124.68
13	9	101	BCB	CMB-C2B-C3B	3.51	131.69	124.68
21	o	101	NS0	C21-C20-C19	3.49	130.67	123.52
21	q	102	NS0	C21-C20-C19	3.49	130.66	123.52
21	7	101	NS0	C10-C9-C7	-3.48	122.80	127.69
20	M	411	PGV	O01-C1-C2	3.47	118.99	111.48
21	l	101	NS0	C21-C20-C19	3.47	130.61	123.52
21	k	101	NS0	C21-C20-C19	3.45	130.57	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	l	102	BCB	C4D-ND-C1D	-3.44	102.61	105.22
15	L	306	CDL	CA4-OA6-CA5	-3.44	109.56	117.80
9	C	401	HEC	CBC-CAC-C3C	-3.43	120.57	127.43
13	3	101	BCB	CMB-C2B-C3B	3.43	131.54	124.68
21	U	101	NS0	C21-C20-C19	3.42	130.51	123.52
13	Z	101	BCB	CMB-C2B-C3B	3.40	131.48	124.68
13	L	302	BCB	C4D-ND-C1D	-3.40	102.64	105.22
13	e	101	BCB	CMB-C2B-C3B	3.40	131.47	124.68
11	M	408	UQ8	C25-C24-C26	3.39	121.10	115.23
13	6	101	BCB	C1-C2-C3	-3.38	120.66	126.20
21	h	101	NS0	C21-C20-C19	3.37	130.41	123.52
11	L	305	UQ8	C7-C8-C9	-3.37	121.03	126.83
13	L	303	BCB	C1-C2-C3	-3.36	120.69	126.20
13	E	101	BCB	CMB-C2B-C3B	3.36	131.40	124.68
20	D	102	PGV	O03-C19-C20	3.36	122.07	111.83
21	7	101	NS0	C21-C20-C19	3.34	130.35	123.52
13	r	101	BCB	C4D-ND-C1D	-3.33	102.69	105.22
13	r	101	BCB	CMB-C2B-C3B	3.32	131.32	124.68
13	M	402	BCB	C4-C3-C5	3.32	120.99	115.23
13	c	101	BCB	CMB-C2B-C3B	3.32	131.32	124.68
13	6	101	BCB	CMB-C2B-C3B	3.31	131.31	124.68
21	9	102	NS0	C10-C9-C7	-3.29	123.07	127.69
13	7	102	BCB	C4D-ND-C1D	-3.29	102.73	105.22
13	J	101	BCB	CMB-C2B-C3B	3.28	131.25	124.68
13	q	101	BCB	C4D-ND-C1D	-3.28	102.73	105.22
21	2	101	NS0	C21-C20-C19	3.28	130.23	123.52
19	k	103	LMT	C1B-O1B-C4'	-3.28	110.21	117.98
13	L	302	BCB	CMB-C2B-C3B	3.28	131.23	124.68
13	W	302	BCB	O2A-CGA-CBA	3.25	121.75	111.83
21	D	103	NS0	C21-C20-C19	3.23	130.13	123.52
13	T	101	BCB	C6-C5-C3	-3.23	105.61	113.47
13	6	101	BCB	C4D-ND-C1D	-3.22	102.77	105.22
13	A	102	BCB	C4D-ND-C1D	-3.22	102.78	105.22
17	M	405	MQ7	C39-C38-C40	3.20	120.79	115.23
11	M	408	UQ8	C27-C28-C29	-3.18	120.35	127.62
13	M	403	BCB	C3D-C4D-CHA	3.18	113.37	108.54
13	h	102	BCB	C4D-ND-C1D	-3.17	102.81	105.22
13	b	101	BCB	C4D-ND-C1D	-3.17	102.81	105.22
13	c	101	BCB	O2A-CGA-CBA	3.17	121.49	111.83
13	i	101	BCB	CMB-C2B-C3B	3.17	131.01	124.68
13	M	402	BCB	O1D-CGD-CBD	-3.16	119.93	124.72
21	A	103	NS0	C21-C20-C19	3.16	129.97	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	101	UQ8	C22-C23-C24	-3.11	120.51	127.62
11	C	406	UQ8	C7-C6-C1	-3.11	119.55	124.23
9	C	402	HEC	CBC-CAC-C3C	-3.10	121.24	127.43
9	C	402	HEC	CBB-CAB-C3B	-3.10	121.24	127.43
13	R	102	BCB	C4-C3-C5	3.09	120.60	115.23
13	l	102	BCB	C1-C2-C3	-3.08	121.14	126.20
11	A	101	UQ8	C17-C18-C19	-3.07	120.59	127.62
21	O	101	NS0	C21-C20-C19	3.07	129.80	123.52
13	r	101	BCB	C1-C2-C3	-3.07	121.17	126.20
13	O	102	BCB	C3D-C4D-CHA	3.07	113.21	108.54
13	E	101	BCB	O2A-CGA-CBA	3.07	121.19	111.83
11	A	101	UQ8	C40-C39-C41	3.06	120.54	115.23
11	M	408	UQ8	C35-C34-C36	3.05	120.52	115.23
13	W	302	BCB	C3D-C4D-CHA	3.05	113.17	108.54
13	q	101	BCB	C1-C2-C3	-3.04	121.21	126.20
13	0	102	BCB	O2A-CGA-CBA	3.04	121.11	111.83
13	T	101	BCB	O2A-CGA-CBA	3.04	121.11	111.83
15	L	306	CDL	OA8-CA7-C31	3.03	121.07	111.83
13	N	101	BCB	O2A-CGA-CBA	3.03	121.06	111.83
13	9	101	BCB	C4-C3-C5	3.02	120.48	115.23
11	A	101	UQ8	C25-C24-C26	3.02	120.47	115.23
15	H	302	CDL	OA8-CA7-C31	3.02	121.04	111.83
13	n	101	BCB	C3D-C4D-CHA	3.01	113.12	108.54
21	k	101	NS0	C20-C21-C22	3.01	129.67	123.52
13	r	101	BCB	O2A-CGA-CBA	3.00	120.99	111.83
11	M	407	UQ8	C12-C13-C14	-3.00	120.77	127.62
13	b	101	BCB	C3D-C4D-CHA	2.99	113.09	108.54
13	k	102	BCB	C3D-C4D-CHA	2.99	113.09	108.54
13	7	102	BCB	C1-C2-C3	-2.99	121.29	126.20
13	X	102	BCB	C1-C2-C3	-2.99	121.30	126.20
13	3	101	BCB	C4D-ND-C1D	-2.99	102.95	105.22
13	N	101	BCB	C3D-C4D-CHA	2.99	113.08	108.54
13	o	102	BCB	O2A-CGA-CBA	2.99	120.94	111.83
17	M	405	MQ7	C34-C33-C35	2.98	120.41	115.23
19	n	102	LMT	C1B-O1B-C4'	-2.98	110.92	117.98
13	T	101	BCB	C3D-C4D-CHA	2.97	113.06	108.54
13	U	102	BCB	O2A-CGA-CBA	2.97	120.90	111.83
11	A	101	UQ8	C10-C9-C11	2.97	120.38	115.23
13	J	101	BCB	O2A-CGA-CBA	2.96	120.86	111.83
13	W	302	BCB	C4D-ND-C1D	-2.96	102.97	105.22
11	M	408	UQ8	C30-C29-C31	2.95	120.36	115.23
21	0	101	NS0	C21-C20-C19	2.95	129.55	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	301	DGA	OG1-CA1-CA2	2.95	120.83	111.83
9	C	403	HEC	CBC-CAC-C3C	-2.94	121.55	127.43
20	W	301	PGV	C02-O01-C1	-2.94	110.76	117.80
19	T	102	LMT	C1-O1'-C1'	-2.94	108.66	113.68
9	C	402	HEC	CHD-C1D-ND	2.94	129.19	123.86
13	M	403	BCB	O2A-CGA-CBA	2.93	120.78	111.83
13	6	101	BCB	C3D-C4D-CHA	2.93	112.99	108.54
13	e	101	BCB	O2A-CGA-CBA	2.92	120.74	111.83
13	X	102	BCB	O2A-CGA-CBA	2.92	120.74	111.83
13	4	101	BCB	O2A-CGA-CBA	2.92	120.74	111.83
13	h	102	BCB	C4-C3-C5	2.92	120.29	115.23
9	C	404	HEC	CBC-CAC-C3C	-2.92	121.61	127.43
13	Z	101	BCB	C3D-C4D-CHA	2.90	112.95	108.54
14	L	304	BPB	C2B-C1B-NB	-2.89	107.34	109.43
17	M	405	MQ7	C26-C27-C28	-2.89	121.01	127.62
18	M	406	NS5	C22-C21-C20	-2.89	118.13	122.82
13	D	101	BCB	C3D-C4D-CHA	2.89	112.93	108.54
11	M	408	UQ8	C20-C19-C21	2.89	120.24	115.23
13	i	101	BCB	O2A-CGA-CBA	2.89	120.63	111.83
13	J	101	BCB	C3D-C4D-CHA	2.88	112.92	108.54
13	b	101	BCB	C4-C3-C5	2.88	120.23	115.23
13	E	101	BCB	C1-C2-C3	-2.88	121.47	126.20
13	I	101	BCB	C6-C5-C3	-2.88	106.46	113.47
11	M	407	UQ8	C10-C9-C11	2.87	120.21	115.23
13	L	302	BCB	CED-O2D-CGD	2.86	122.41	115.92
9	C	404	HEC	CHD-C4C-NC	2.86	127.57	124.45
13	1	101	BCB	O2A-CGA-CBA	2.86	120.56	111.83
13	l	102	BCB	O2A-CGA-CBA	2.86	120.56	111.83
18	M	406	NS5	C18-C19-C20	2.86	129.37	123.52
13	T	101	BCB	CHD-C4C-C3C	-2.86	121.50	130.04
13	6	101	BCB	C4-C3-C5	2.85	120.18	115.23
13	c	101	BCB	CHD-C4C-C3C	-2.85	121.51	130.04
13	3	101	BCB	C3D-C4D-CHA	2.85	112.88	108.54
13	O	102	BCB	O2A-CGA-CBA	2.85	120.53	111.83
13	h	102	BCB	C3D-C4D-CHA	2.85	112.87	108.54
13	3	101	BCB	C6-C5-C3	-2.85	106.53	113.47
11	M	408	UQ8	C15-C14-C16	2.85	120.17	115.23
20	W	301	PGV	O03-C19-C20	2.85	120.52	111.83
13	Q	402	BCB	C4-C3-C5	2.84	120.16	115.23
13	e	101	BCB	C4D-ND-C1D	-2.84	103.06	105.22
11	M	408	UQ8	C7-C8-C9	2.84	131.72	126.83
13	L	302	BCB	C3D-C4D-CHA	2.84	112.85	108.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	D	101	BCB	O2A-CGA-CBA	2.83	120.47	111.83
9	C	404	HEC	CHA-C1A-NA	2.83	127.53	124.45
13	Z	101	BCB	CHD-C4C-C3C	-2.83	121.60	130.04
13	M	403	BCB	O2D-CGD-O1D	-2.83	118.35	123.85
13	I	101	BCB	C3D-C4D-CHA	2.82	112.82	108.54
13	Z	101	BCB	O2A-CGA-CBA	2.82	120.43	111.83
13	e	101	BCB	C3D-C4D-CHA	2.82	112.82	108.54
13	q	101	BCB	C3D-C4D-CHA	2.80	112.80	108.54
9	C	403	HEC	CHD-C1D-ND	2.80	128.94	123.86
13	W	302	BCB	CHD-C4C-C3C	-2.80	121.67	130.04
13	f	101	BCB	O2A-CGA-CBA	2.80	120.38	111.83
13	7	102	BCB	O2A-CGA-CBA	2.80	120.36	111.83
13	Q	402	BCB	C3D-C4D-CHA	2.79	112.78	108.54
13	i	101	BCB	C4-C3-C5	2.79	120.07	115.23
13	N	101	BCB	CHD-C4C-C3C	-2.79	121.70	130.04
13	E	101	BCB	C3D-C4D-CHA	2.79	112.78	108.54
13	o	102	BCB	C4-C3-C5	2.79	120.07	115.23
11	L	305	UQ8	C17-C18-C19	-2.78	121.25	127.62
19	b	103	LMT	C1-O1'-C1'	-2.78	108.93	113.68
13	Z	101	BCB	C4D-ND-C1D	-2.78	103.11	105.22
13	O	102	BCB	C4-C3-C5	2.77	120.04	115.23
13	o	102	BCB	C1-C2-C3	-2.77	121.66	126.20
13	0	102	BCB	C1-C2-C3	-2.77	121.66	126.20
13	D	101	BCB	C1-C2-C3	-2.76	121.67	126.20
13	X	102	BCB	C3D-C4D-CHA	2.76	112.74	108.54
13	3	101	BCB	O2A-CGA-CBA	2.76	120.26	111.83
13	Q	402	BCB	CHD-C4C-C3C	-2.76	121.80	130.04
17	M	405	MQ7	C36-C37-C38	-2.76	121.31	127.62
13	3	101	BCB	CHD-C4C-C3C	-2.75	121.82	130.04
20	N	102	PGV	O03-C19-C20	2.75	120.22	111.83
13	B	202	BCB	C4-C3-C5	2.75	120.00	115.23
13	b	101	BCB	O2A-CGA-CBA	2.74	120.20	111.83
13	r	101	BCB	C3D-C4D-CHA	2.74	112.71	108.54
13	6	101	BCB	CHD-C4C-C3C	-2.74	121.86	130.04
9	C	404	HEC	CHD-C1D-ND	2.74	128.82	123.86
13	o	102	BCB	C3D-C4D-CHA	2.74	112.70	108.54
13	c	101	BCB	C3D-C4D-CHA	2.73	112.69	108.54
9	C	401	HEC	CHD-C1D-ND	2.73	128.82	123.86
15	L	306	CDL	OB8-CB7-C71	2.73	120.16	111.83
13	4	101	BCB	C4-C3-C5	2.73	119.97	115.23
13	A	102	BCB	O1D-CGD-CBD	-2.73	120.59	124.72
15	M	409	CDL	OA8-CA7-C31	2.73	120.15	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	L	302	BCB	O2A-CGA-CBA	2.73	120.15	111.83
13	k	102	BCB	C4-C3-C5	2.72	119.95	115.23
13	I	101	BCB	O2A-CGA-CBA	2.72	120.14	111.83
13	q	101	BCB	CHD-C4C-C3C	-2.72	121.91	130.04
13	n	101	BCB	CAA-CBA-CGA	-2.72	105.48	113.21
13	A	102	BCB	C3D-C4D-CHA	2.72	112.67	108.54
13	l	102	BCB	C3D-C4D-CHA	2.72	112.67	108.54
11	A	101	UQ8	C37-C38-C39	-2.72	121.40	127.62
13	4	101	BCB	C3D-C4D-CHA	2.72	112.67	108.54
21	0	101	NS0	C10-C9-C7	-2.71	123.87	127.69
13	D	101	BCB	C6-C5-C3	-2.71	106.86	113.47
21	O	101	NS0	C13-C12-C14	-2.71	118.42	122.82
9	C	402	HEC	CHA-C4D-ND	2.71	128.77	123.86
11	L	305	UQ8	C1M-C1-C6	-2.71	120.00	124.45
15	L	306	CDL	CB4-OB6-CB5	-2.71	111.32	117.80
13	n	101	BCB	O2A-CGA-CBA	2.71	120.08	111.83
13	W	302	BCB	C6-C5-C3	-2.70	106.89	113.47
17	M	405	MQ7	C29-C28-C30	2.70	119.92	115.23
13	h	102	BCB	CAA-CBA-CGA	-2.70	105.56	113.21
20	N	102	PGV	O01-C1-C2	2.69	117.31	111.48
13	O	102	BCB	CHD-C4C-C3C	-2.69	122.00	130.04
13	R	102	BCB	O2A-CGA-CBA	2.69	120.04	111.83
21	X	101	NS0	C18-C17-C19	-2.69	118.46	122.82
12	L	301	DGA	OG2-CB1-OB1	-2.69	117.42	123.70
13	b	101	BCB	CHD-C4C-C3C	-2.69	122.01	130.04
18	M	406	NS5	C23-C21-C20	2.68	123.23	119.01
13	D	101	BCB	CHD-C4C-C3C	-2.68	122.03	130.04
13	L	303	BCB	C4-C3-C5	2.68	119.88	115.23
13	1	101	BCB	C3D-C4D-CHA	2.68	112.61	108.54
13	U	102	BCB	C4-C3-C5	2.68	119.88	115.23
13	B	202	BCB	CHD-C4C-C3C	-2.68	122.03	130.04
13	f	101	BCB	C3D-C4D-CHA	2.68	112.61	108.54
13	B	202	BCB	C1-C2-C3	-2.67	121.82	126.20
13	6	101	BCB	O2A-CGA-CBA	2.67	119.99	111.83
21	U	101	NS0	C24-C23-C22	-2.67	118.49	122.82
13	7	102	BCB	C3D-C4D-CHA	2.67	112.60	108.54
21	D	103	NS0	C20-C21-C22	2.67	128.98	123.52
21	q	102	NS0	C13-C12-C14	-2.67	118.50	122.82
11	M	407	UQ8	C8-C7-C6	-2.67	105.51	112.08
13	R	102	BCB	CHD-C4C-C3C	-2.67	122.08	130.04
13	Q	402	BCB	O2A-CGA-CBA	2.66	119.96	111.83
20	M	411	PGV	O03-C19-C20	2.66	119.96	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	I	101	BCB	CHD-C4C-C3C	-2.66	122.09	130.04
13	h	102	BCB	CHD-C4C-C3C	-2.66	122.09	130.04
13	0	102	BCB	C4-C3-C5	2.66	119.84	115.23
13	B	202	BCB	O2A-CGA-CBA	2.66	119.94	111.83
13	J	101	BCB	C4-C3-C5	2.66	119.84	115.23
13	q	101	BCB	C4-C3-C5	2.65	119.83	115.23
19	b	103	LMT	O1'-C1'-C2'	2.65	112.30	108.27
13	9	101	BCB	C3D-C4D-CHA	2.65	112.56	108.54
19	T	102	LMT	O1'-C1'-C2'	2.65	112.29	108.27
21	k	101	NS0	C24-C23-C22	-2.64	118.53	122.82
15	H	301	CDL	OA8-CA7-C31	2.64	119.89	111.83
9	C	401	HEC	CHA-C4D-ND	2.64	128.64	123.86
13	o	102	BCB	CHD-C4C-C3C	-2.64	122.16	130.04
18	M	406	NS5	C28-C26-C25	2.63	123.15	119.01
13	Z	101	BCB	CAA-CBA-CGA	-2.63	105.73	113.21
13	6	101	BCB	CAA-CBA-CGA	-2.63	105.74	113.21
21	2	101	NS0	C24-C23-C22	-2.63	118.56	122.82
13	0	102	BCB	O2D-CGD-O1D	-2.63	118.73	123.85
20	Q	401	PGV	O03-C19-C20	2.63	119.85	111.83
21	k	101	NS0	C13-C12-C14	-2.63	118.56	122.82
11	M	408	UQ8	C16-C14-C13	-2.63	115.27	121.17
13	q	101	BCB	O2A-CGA-CBA	2.63	119.84	111.83
21	U	101	NS0	C13-C12-C14	-2.62	118.57	122.82
13	l	102	BCB	C4-C3-C5	2.62	119.77	115.23
15	M	409	CDL	OB8-CB7-C71	2.61	119.80	111.83
18	M	406	NS5	C27-C26-C25	-2.61	118.58	122.82
13	L	303	BCB	CHD-C4C-C3C	-2.61	122.25	130.04
13	Q	402	BCB	C4D-ND-C1D	-2.61	103.24	105.22
13	M	402	BCB	C3D-C4D-CHA	2.61	112.50	108.54
9	C	404	HEC	CAD-CBD-CGD	-2.61	106.75	113.67
13	U	102	BCB	CHD-C4C-C3C	-2.60	122.26	130.04
11	L	305	UQ8	C10-C9-C11	2.60	119.74	115.23
13	O	102	BCB	O2D-CGD-O1D	-2.60	118.79	123.85
21	k	101	NS0	C18-C17-C19	-2.60	118.61	122.82
13	9	101	BCB	CHD-C4C-C3C	-2.60	122.28	130.04
21	W	303	NS0	C13-C12-C14	-2.60	118.61	122.82
9	C	401	HEC	CHB-C1B-NB	2.59	128.56	123.86
13	A	102	BCB	CHD-C4C-C3C	-2.59	122.30	130.04
17	M	405	MQ7	C21-C22-C23	-2.59	121.70	127.62
21	R	101	NS0	C18-C17-C19	-2.59	118.63	122.82
21	l	101	NS0	C24-C23-C22	-2.59	118.63	122.82
13	i	101	BCB	CHD-C4C-C3C	-2.58	122.32	130.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	R	102	BCB	C3D-C4D-CHA	2.58	112.47	108.54
21	2	101	NS0	C13-C12-C14	-2.58	118.63	122.82
13	q	101	BCB	CAA-CBA-CGA	-2.58	105.88	113.21
21	A	103	NS0	C20-C21-C22	2.57	128.78	123.52
21	l	101	NS0	C13-C12-C14	-2.57	118.65	122.82
13	R	102	BCB	C1-C2-C3	-2.57	121.98	126.20
13	n	101	BCB	C4D-ND-C1D	-2.57	103.27	105.22
21	l	101	NS0	C18-C17-C19	-2.57	118.66	122.82
11	M	407	UQ8	C1M-C1-C6	-2.57	120.23	124.45
21	D	103	NS0	C18-C17-C19	-2.56	118.66	122.82
13	e	101	BCB	CHD-C4C-C3C	-2.56	122.38	130.04
14	L	304	BPB	CMA-C3A-C4A	-2.56	109.09	114.61
13	U	102	BCB	C3D-C4D-CHA	2.56	112.43	108.54
11	C	406	UQ8	C1M-C1-C6	-2.56	120.24	124.45
21	q	102	NS0	C18-C17-C19	-2.56	118.67	122.82
21	U	101	NS0	C20-C21-C22	2.56	128.75	123.52
13	0	102	BCB	C3D-C4D-CHA	2.56	112.42	108.54
13	X	102	BCB	CHD-C4C-C3C	-2.55	122.41	130.04
13	r	101	BCB	C4-C3-C5	2.55	119.66	115.23
13	B	202	BCB	C3D-C4D-CHA	2.55	112.42	108.54
21	h	101	NS0	C20-C21-C22	2.55	128.74	123.52
13	A	102	BCB	CMA-C3A-C4A	-2.55	109.12	114.61
14	M	404	BPB	C2B-C1B-NB	-2.55	107.59	109.43
20	N	102	PGV	C03-C02-C01	-2.55	105.85	111.78
13	c	101	BCB	C4-C3-C5	2.55	119.65	115.23
11	L	305	UQ8	C12-C13-C14	-2.55	121.80	127.62
13	L	303	BCB	O2D-CGD-O1D	-2.53	118.92	123.85
13	r	101	BCB	CHD-C4C-C3C	-2.53	122.47	130.04
15	H	302	CDL	CB4-OB6-CB5	-2.53	111.74	117.80
20	I	102	PGV	C02-O01-C1	-2.53	111.74	117.80
13	l	102	BCB	CHD-C4C-C3C	-2.53	122.49	130.04
13	0	102	BCB	CHD-C4C-C3C	-2.53	122.50	130.04
14	M	404	BPB	CMA-C3A-C4A	-2.52	109.17	114.61
13	I	101	BCB	C4D-ND-C1D	-2.52	103.31	105.22
13	k	102	BCB	O2A-CGA-CBA	2.51	119.50	111.83
9	C	403	HEC	CHA-C1A-NA	2.51	127.19	124.45
13	N	101	BCB	CAA-CBA-CGA	-2.51	106.07	113.21
13	M	402	BCB	CHD-C4C-C3C	-2.51	122.54	130.04
13	n	101	BCB	CHD-C4C-C3C	-2.51	122.54	130.04
13	B	202	BCB	O2D-CGD-O1D	-2.51	118.97	123.85
21	7	101	NS0	C24-C23-C22	-2.50	118.76	122.82
13	T	101	BCB	C4D-ND-C1D	-2.50	103.32	105.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	R	101	NS0	C13-C12-C14	-2.50	118.77	122.82
13	k	102	BCB	CHD-C4C-C3C	-2.50	122.57	130.04
13	n	101	BCB	CED-O2D-CGD	2.50	121.58	115.92
9	C	402	HEC	CHD-C4C-NC	2.50	127.17	124.45
21	R	101	NS0	C16-C17-C19	2.50	122.94	119.01
13	i	101	BCB	C1-C2-C3	-2.49	122.11	126.20
21	O	101	NS0	C10-C9-C7	-2.49	124.18	127.69
21	W	303	NS0	C18-C17-C19	-2.49	118.78	122.82
9	C	402	HEC	CHA-C1A-NA	2.49	127.17	124.45
21	7	101	NS0	C20-C21-C22	2.49	128.62	123.52
13	W	302	BCB	CAA-CBA-CGA	-2.49	106.14	113.21
21	X	101	NS0	C24-C23-C22	-2.49	118.78	122.82
13	h	102	BCB	O2A-CGA-CBA	2.49	119.42	111.83
21	9	102	NS0	C13-C12-C14	-2.48	118.79	122.82
13	A	102	BCB	O2A-CGA-CBA	2.48	119.39	111.83
21	W	303	NS0	C24-C23-C22	-2.48	118.80	122.82
9	C	403	HEC	CHB-C1B-NB	2.48	128.35	123.86
13	i	101	BCB	C3D-C4D-CHA	2.47	112.30	108.54
13	J	101	BCB	CHD-C4C-C3C	-2.47	122.65	130.04
13	i	101	BCB	C1-O2A-CGA	2.47	122.64	116.65
21	0	101	NS0	C13-C12-C14	-2.47	118.81	122.82
21	U	101	NS0	C18-C17-C19	-2.47	118.82	122.82
13	f	101	BCB	C4-C3-C5	2.47	119.51	115.23
21	R	101	NS0	C24-C23-C22	-2.46	118.83	122.82
13	L	303	BCB	O2A-CGA-CBA	2.46	119.33	111.83
13	U	102	BCB	C1-C2-C3	-2.46	122.17	126.20
13	9	101	BCB	O2A-CGA-CBA	2.45	119.31	111.83
13	N	101	BCB	C4D-ND-C1D	-2.45	103.36	105.22
13	L	302	BCB	CHD-C4C-C3C	-2.45	122.72	130.04
21	D	103	NS0	C24-C23-C22	-2.45	118.85	122.82
13	1	101	BCB	CED-O2D-CGD	2.45	121.47	115.92
11	A	101	UQ8	C15-C14-C16	2.45	119.47	115.23
21	A	103	NS0	C18-C17-C19	-2.44	118.86	122.82
13	1	101	BCB	CHD-C4C-C3C	-2.44	122.75	130.04
21	h	101	NS0	C24-C23-C22	-2.44	118.87	122.82
21	q	102	NS0	C16-C17-C19	2.43	122.84	119.01
21	q	102	NS0	C20-C21-C22	2.43	128.49	123.52
20	I	102	PGV	O03-C19-C20	2.43	119.24	111.83
13	7	102	BCB	CHD-C4C-C3C	-2.43	122.79	130.04
13	r	101	BCB	O2D-CGD-O1D	-2.42	119.14	123.85
11	L	305	UQ8	C7-C6-C1	-2.42	120.74	124.89
21	A	103	NS0	C24-C23-C22	-2.42	118.90	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	3	101	BCB	O1D-CGD-CBD	-2.42	121.06	124.72
13	4	101	BCB	CHD-C4C-C3C	-2.41	122.83	130.04
15	H	301	CDL	OB8-CB7-C71	2.41	119.19	111.83
21	l	101	NS0	C20-C21-C22	2.41	128.45	123.52
13	1	101	BCB	C4-C3-C5	2.41	119.41	115.23
11	A	101	UQ8	C30-C29-C31	2.41	119.41	115.23
11	M	407	UQ8	C7-C6-C1	-2.41	120.76	124.89
21	0	101	NS0	C18-C17-C19	-2.41	118.92	122.82
21	k	101	NS0	C10-C9-C7	-2.41	124.30	127.69
13	4	101	BCB	O2D-CGD-O1D	-2.41	119.16	123.85
9	C	401	HEC	CBD-CAD-C3D	-2.40	105.89	112.53
21	7	101	NS0	C13-C12-C14	-2.40	118.92	122.82
9	C	402	HEC	CHB-C1B-NB	2.40	128.22	123.86
21	k	101	NS0	C11-C12-C14	2.40	122.78	119.01
21	9	102	NS0	C24-C23-C22	-2.39	118.94	122.82
21	o	101	NS0	C18-C17-C19	-2.39	118.94	122.82
13	E	101	BCB	CHD-C4C-C3C	-2.39	122.90	130.04
15	M	409	CDL	CA4-OA6-CA5	-2.39	112.08	117.80
21	h	101	NS0	C18-C17-C19	-2.39	118.95	122.82
21	q	102	NS0	C24-C23-C22	-2.39	118.95	122.82
13	E	101	BCB	C4-C3-C5	2.39	119.37	115.23
21	k	101	NS0	C16-C17-C19	2.39	122.76	119.01
11	M	407	UQ8	C15-C14-C16	2.39	119.37	115.23
13	L	302	BCB	O1D-CGD-CBD	-2.38	121.11	124.72
13	E	101	BCB	O2D-CGD-O1D	-2.38	119.21	123.85
21	9	102	NS0	C18-C17-C19	-2.38	118.96	122.82
13	4	101	BCB	C1-C2-C3	-2.37	122.31	126.20
21	2	101	NS0	C18-C17-C19	-2.37	118.97	122.82
21	o	101	NS0	C13-C12-C14	-2.37	118.97	122.82
13	f	101	BCB	CHD-C4C-C3C	-2.37	122.97	130.04
13	i	101	BCB	O2D-CGD-O1D	-2.37	119.24	123.85
13	Q	402	BCB	CAA-CBA-CGA	-2.36	106.50	113.21
13	R	102	BCB	O2D-CGD-O1D	-2.36	119.25	123.85
21	k	101	NS0	C25-C23-C22	2.36	122.72	119.01
13	r	101	BCB	CMA-C3A-C4A	-2.36	109.53	114.61
9	C	401	HEC	C2A-C1A-NA	-2.36	108.05	110.32
13	k	102	BCB	C4D-ND-C1D	-2.36	103.43	105.22
13	c	101	BCB	C1-C2-C3	-2.35	122.34	126.20
13	9	101	BCB	O1D-CGD-CBD	-2.35	121.16	124.72
13	D	101	BCB	O2D-CGD-O1D	-2.35	119.27	123.85
21	O	101	NS0	C24-C23-C22	-2.35	119.02	122.82
9	C	404	HEC	CHB-C1B-NB	2.34	128.11	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	7	102	BCB	O2D-CGD-O1D	-2.34	119.29	123.85
21	h	101	NS0	C13-C12-C14	-2.34	119.02	122.82
13	e	101	BCB	O1D-CGD-CBD	-2.34	121.17	124.72
17	M	405	MQ7	C2M-C2-C3	-2.34	120.61	124.45
17	M	405	MQ7	C31-C32-C33	-2.34	122.27	127.62
21	X	101	NS0	C13-C12-C14	-2.34	119.03	122.82
17	M	405	MQ7	C45-C43-C44	2.34	119.97	114.59
9	C	401	HEC	CHD-C4C-NC	2.34	127.00	124.45
9	C	403	HEC	CHA-C4D-ND	2.33	128.09	123.86
13	n	101	BCB	C6-C5-C3	-2.33	107.80	113.47
21	X	101	NS0	C16-C17-C19	2.33	122.67	119.01
21	D	103	NS0	C16-C17-C19	2.32	122.67	119.01
13	k	102	BCB	CAA-CBA-CGA	-2.32	106.61	113.21
13	E	101	BCB	OBd-CAD-C3D	-2.32	124.27	127.89
9	C	403	HEC	O2D-CGD-CBD	2.32	121.33	114.00
21	O	101	NS0	C18-C17-C19	-2.32	119.06	122.82
13	M	403	BCB	CMC-C2C-C1C	-2.31	102.94	113.58
13	f	101	BCB	C1-C2-C3	-2.31	122.41	126.20
13	k	102	BCB	C4D-CHA-CBD	-2.31	106.64	108.97
21	A	103	NS0	C15-C14-C12	2.31	130.51	127.28
11	A	101	UQ8	C1M-C1-C6	-2.31	120.66	124.45
17	M	405	MQ7	C19-C18-C20	2.31	119.23	115.23
13	T	101	BCB	C4D-CHA-CBD	-2.30	106.64	108.97
21	2	101	NS0	C25-C23-C22	2.30	122.63	119.01
13	e	101	BCB	C6-C5-C3	-2.30	107.86	113.47
15	M	409	CDL	OB6-CB5-OB7	-2.30	118.33	123.70
13	k	102	BCB	CED-O2D-CGD	2.30	121.13	115.92
13	M	403	BCB	CED-O2D-CGD	2.30	121.12	115.92
13	M	403	BCB	C1-O2A-CGA	2.30	122.21	116.65
13	N	101	BCB	C6-C5-C3	-2.30	107.88	113.47
21	o	101	NS0	C24-C23-C22	-2.29	119.10	122.82
21	7	101	NS0	C18-C17-C19	-2.29	119.11	122.82
13	e	101	BCB	CAA-CBA-CGA	-2.28	106.72	113.21
11	A	101	UQ8	C7-C6-C5	2.28	121.16	118.52
13	L	302	BCB	O2A-CGA-O1A	-2.27	117.95	123.63
11	M	408	UQ8	C32-C33-C34	-2.27	122.43	127.62
13	U	102	BCB	CED-O2D-CGD	2.27	121.06	115.92
19	h	103	LMT	C1B-O1B-C4'	-2.27	112.60	117.98
21	q	102	NS0	C11-C12-C14	2.27	122.58	119.01
13	b	101	BCB	O1D-CGD-CBD	-2.27	121.29	124.72
9	C	401	HEC	O2D-CGD-CBD	2.26	121.15	114.00
11	M	408	UQ8	C7-C6-C1	-2.26	121.01	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	b	101	BCB	CAA-CBA-CGA	-2.26	106.78	113.21
9	C	402	HEC	CAD-CBD-CGD	-2.26	107.66	113.67
13	M	402	BCB	O2D-CGD-O1D	-2.26	119.45	123.85
13	L	303	BCB	C3D-C4D-CHA	2.26	111.97	108.54
9	C	404	HEC	CHD-C1D-C2D	-2.26	120.87	127.43
11	A	101	UQ8	C12-C13-C14	-2.25	122.47	127.62
15	H	301	CDL	CB4-OB6-CB5	-2.25	112.41	117.80
13	T	101	BCB	CAA-CBA-CGA	-2.25	106.82	113.21
17	M	405	MQ7	C24-C23-C25	2.25	119.13	115.23
13	o	102	BCB	O2D-CGD-O1D	-2.25	119.47	123.85
13	W	302	BCB	C4D-CHA-CBD	-2.25	106.70	108.97
9	C	403	HEC	C2A-C1A-NA	-2.25	108.16	110.32
21	A	103	NS0	C16-C17-C19	2.24	122.54	119.01
11	M	408	UQ8	C1M-C1-C6	-2.24	120.77	124.45
9	C	404	HEC	CHA-C4D-ND	2.24	127.92	123.86
21	l	101	NS0	C11-C12-C14	2.24	122.53	119.01
9	C	401	HEC	CHB-C1B-C2B	-2.24	120.94	127.43
21	U	101	NS0	C25-C23-C22	2.23	122.52	119.01
21	0	101	NS0	C24-C23-C22	-2.23	119.20	122.82
21	O	101	NS0	C11-C12-C14	2.23	122.52	119.01
13	X	102	BCB	C4-C3-C5	2.23	119.10	115.23
15	H	302	CDL	OB8-CB7-C71	2.23	118.64	111.83
13	E	101	BCB	O2A-CGA-O1A	-2.23	118.06	123.63
9	C	403	HEC	C4B-NB-C1B	2.22	109.45	105.82
13	0	102	BCB	O2A-CGA-O1A	-2.22	118.07	123.63
13	Q	402	BCB	O1D-CGD-CBD	-2.22	121.36	124.72
13	c	101	BCB	O1D-CGD-CBD	-2.22	121.36	124.72
13	M	403	BCB	CHD-C4C-C3C	-2.22	123.41	130.04
12	L	301	DGA	OG1-CA1-OA1	-2.22	118.08	123.63
13	e	101	BCB	CED-O2D-CGD	2.22	120.95	115.92
9	C	402	HEC	CHD-C1D-C2D	-2.21	121.00	127.43
21	U	101	NS0	C11-C12-C14	2.21	122.49	119.01
13	L	303	BCB	CMA-C3A-C4A	-2.21	109.84	114.61
13	Z	101	BCB	C4-C3-C5	2.21	119.06	115.23
13	n	101	BCB	C4-C3-C5	2.21	119.06	115.23
21	l	101	NS0	C16-C17-C19	2.21	122.48	119.01
13	R	102	BCB	OBD-CAD-C3D	-2.21	124.45	127.89
13	M	403	BCB	O1D-CGD-CBD	-2.21	121.38	124.72
20	W	301	PGV	O01-C1-O02	-2.21	118.55	123.70
18	M	406	NS5	C18-C17-C15	2.20	130.37	127.28
11	L	305	UQ8	C20-C19-C21	2.20	119.05	115.23
13	1	101	BCB	C1-C2-C3	-2.20	122.60	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	X	102	BCB	C6-C5-C3	-2.19	108.14	113.47
13	I	101	BCB	CAA-CBA-CGA	-2.19	107.00	113.21
13	A	102	BCB	O2D-CGD-O1D	-2.19	119.59	123.85
11	M	408	UQ8	C46-C44-C45	2.18	119.61	114.59
13	M	403	BCB	C4-C3-C5	2.18	119.02	115.23
13	n	101	BCB	O1D-CGD-CBD	-2.18	121.42	124.72
13	6	101	BCB	C4D-CHA-CBD	-2.18	106.77	108.97
21	9	102	NS0	C20-C21-C22	2.17	127.97	123.52
11	M	408	UQ8	C22-C23-C24	-2.17	122.65	127.62
13	L	303	BCB	C1-O2A-CGA	2.17	121.91	116.65
17	M	405	MQ7	C14-C13-C15	2.17	119.00	115.23
21	R	101	NS0	C11-C12-C14	2.17	122.42	119.01
21	l	101	NS0	C25-C23-C22	2.16	122.41	119.01
13	B	202	BCB	O2A-CGA-O1A	-2.16	118.22	123.63
13	U	102	BCB	O2D-CGD-O1D	-2.16	119.64	123.85
13	f	101	BCB	O2D-CGD-O1D	-2.16	119.64	123.85
11	M	407	UQ8	C7-C8-C9	-2.15	123.12	126.83
13	X	102	BCB	O2D-CGD-O1D	-2.15	119.65	123.85
13	c	101	BCB	O2D-CGD-O1D	-2.15	119.66	123.85
13	3	101	BCB	C4D-CHA-CBD	-2.15	106.80	108.97
13	b	101	BCB	C4D-CHA-CBD	-2.15	106.80	108.97
21	R	101	NS0	C10-C9-C7	-2.15	124.66	127.69
17	M	405	MQ7	C16-C17-C18	-2.15	122.70	127.62
13	i	101	BCB	O1D-CGD-CBD	-2.15	121.46	124.72
11	M	408	UQ8	C37-C38-C39	-2.15	122.71	127.62
15	r	102	CDL	OB6-CB5-OB7	-2.15	118.69	123.70
13	M	403	BCB	C4D-CHA-CBD	-2.14	106.81	108.97
13	h	102	BCB	C4D-CHA-CBD	-2.14	106.81	108.97
15	M	409	CDL	OA6-CA5-OA7	-2.14	118.70	123.70
21	0	101	NS0	C20-C21-C22	2.14	127.89	123.52
21	2	101	NS0	C11-C12-C14	2.14	122.37	119.01
13	7	102	BCB	C4-C3-C5	2.13	118.93	115.23
9	C	404	HEC	C2A-C1A-NA	-2.13	108.26	110.32
15	L	306	CDL	OA8-CA7-OA9	-2.13	118.29	123.63
21	W	303	NS0	C16-C17-C19	2.13	122.36	119.01
13	b	101	BCB	C16-C15-C13	-2.13	108.90	115.97
21	9	102	NS0	C16-C17-C19	2.13	122.35	119.01
21	o	101	NS0	C15-C14-C12	2.12	130.26	127.28
13	X	102	BCB	CED-O2D-CGD	2.12	120.73	115.92
21	U	101	NS0	C16-C17-C19	2.12	122.35	119.01
13	l	102	BCB	O1D-CGD-CBD	-2.12	121.51	124.72
13	R	102	BCB	CED-O2D-CGD	2.12	120.71	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	r	102	CDL	OB8-CB7-C71	2.11	118.28	111.83
13	R	102	BCB	O1D-CGD-CBD	-2.11	121.52	124.72
13	Z	101	BCB	C4D-CHA-CBD	-2.11	106.84	108.97
9	C	403	HEC	CHD-C1D-C2D	-2.11	121.30	127.43
13	h	102	BCB	O1D-CGD-CBD	-2.11	121.52	124.72
13	e	101	BCB	C4-C3-C5	2.11	118.89	115.23
21	A	103	NS0	C13-C12-C14	-2.11	119.40	122.82
9	C	401	HEC	CHA-C1A-NA	2.11	126.75	124.45
21	l	101	NS0	C10-C9-C7	-2.10	124.73	127.69
21	D	103	NS0	C13-C12-C14	-2.10	119.41	122.82
13	7	102	BCB	O2A-CGA-O1A	-2.10	118.37	123.63
9	C	401	HEC	CHD-C1D-C2D	-2.10	121.33	127.43
13	l	102	BCB	O2D-CGD-O1D	-2.10	119.77	123.85
20	M	411	PGV	O03-C19-O04	-2.09	118.39	123.63
13	9	101	BCB	C11-C10-C8	-2.09	109.01	115.97
13	O	102	BCB	C1-C2-C3	-2.09	122.77	126.20
21	X	101	NS0	C20-C21-C22	2.09	127.80	123.52
13	9	101	BCB	CED-O2D-CGD	2.09	120.65	115.92
21	2	101	NS0	C10-C9-C7	-2.09	124.75	127.69
13	M	402	BCB	CMA-C3A-C4A	-2.08	110.12	114.61
13	I	101	BCB	O2D-CGD-O1D	-2.08	119.80	123.85
13	J	101	BCB	CED-O2D-CGD	2.08	120.64	115.92
13	h	102	BCB	CED-O2D-CGD	2.08	120.63	115.92
21	O	101	NS0	C20-C21-C22	2.08	127.77	123.52
21	h	101	NS0	C16-C17-C19	2.08	122.28	119.01
15	L	306	CDL	OB6-CB5-OB7	-2.07	118.86	123.70
13	6	101	BCB	CED-O2D-CGD	2.07	120.61	115.92
21	X	101	NS0	C25-C23-C22	2.06	122.25	119.01
13	9	101	BCB	C6-C5-C3	-2.06	108.44	113.47
13	U	102	BCB	CAA-CBA-CGA	-2.06	107.35	113.21
13	3	101	BCB	CED-O2D-CGD	2.06	120.59	115.92
13	f	101	BCB	O1D-CGD-CBD	-2.06	121.60	124.72
13	U	102	BCB	O1D-CGD-CBD	-2.05	121.61	124.72
13	D	101	BCB	C4-C3-C5	2.05	118.79	115.23
21	9	102	NS0	C11-C12-C14	2.05	122.24	119.01
13	c	101	BCB	OBD-CAD-C3D	-2.05	124.69	127.89
13	b	101	BCB	OBD-CAD-C3D	-2.05	124.70	127.89
13	N	101	BCB	C4D-CHA-CBD	-2.05	106.90	108.97
21	2	101	NS0	C16-C17-C19	2.05	122.23	119.01
13	7	102	BCB	CED-O2D-CGD	2.05	120.56	115.92
13	T	101	BCB	O1D-CGD-CBD	-2.05	121.62	124.72
15	r	102	CDL	OA8-CA7-C31	2.04	118.07	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	W	303	NS0	C25-C23-C22	2.04	122.22	119.01
13	A	102	BCB	C4-C3-C5	2.04	118.77	115.23
21	0	101	NS0	C16-C17-C19	2.04	122.22	119.01
21	A	103	NS0	C25-C23-C22	2.04	122.22	119.01
11	A	101	UQ8	C46-C44-C45	2.04	119.28	114.59
13	3	101	BCB	C11-C10-C8	-2.04	109.19	115.97
13	f	101	BCB	CED-O2D-CGD	2.04	120.54	115.92
13	o	102	BCB	O1D-CGD-CBD	-2.04	121.63	124.72
13	Z	101	BCB	CED-O2D-CGD	2.04	120.54	115.92
15	M	409	CDL	CB6-CB4-CB3	-2.04	107.04	111.78
13	A	102	BCB	CBA-CAA-C2A	-2.04	107.78	113.78
15	M	409	CDL	CB4-OB6-CB5	-2.04	112.92	117.80
13	I	101	BCB	O1D-CGD-CBD	-2.03	121.64	124.72
13	q	101	BCB	CED-O2D-CGD	2.03	120.53	115.92
15	H	301	CDL	CA4-OA6-CA5	-2.03	112.93	117.80
13	M	403	BCB	CAA-CBA-CGA	-2.03	107.44	113.21
20	D	102	PGV	O03-C19-O04	-2.03	118.55	123.63
13	J	101	BCB	O2D-CGD-O1D	-2.03	119.89	123.85
9	C	402	HEC	O2D-CGD-CBD	2.03	120.41	114.00
13	J	101	BCB	C1-O2A-CGA	2.03	121.56	116.65
21	2	101	NS0	C20-C21-C22	2.03	127.67	123.52
9	C	401	HEC	CHB-C4A-NA	2.03	126.66	124.45
13	1	101	BCB	O1D-CGD-CBD	-2.03	121.65	124.72
13	N	101	BCB	O1D-CGD-CBD	-2.03	121.65	124.72
13	1	101	BCB	C1-O2A-CGA	2.02	121.54	116.65
21	X	101	NS0	C10-C9-C7	-2.02	124.85	127.69
13	Z	101	BCB	O1D-CGD-CBD	-2.02	121.66	124.72
13	A	102	BCB	C6-C5-C3	-2.02	108.55	113.47
13	b	101	BCB	C1-O2A-CGA	2.01	121.52	116.65
13	I	101	BCB	C4D-CHA-CBD	-2.01	106.94	108.97
21	o	101	NS0	C10-C9-C7	-2.01	124.87	127.69
17	M	405	MQ7	C41-C42-C43	-2.00	120.96	127.64
13	q	101	BCB	O1D-CGD-CBD	-2.00	121.69	124.72
13	l	102	BCB	CED-O2D-CGD	2.00	120.45	115.92
13	X	102	BCB	O2A-CGA-O1A	-2.00	118.62	123.63

All (76) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	L	302	BCB	NA
13	L	302	BCB	NC
13	L	303	BCB	NA

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Mol	Chain	Res	Type	Atom
13	L	303	BCB	NC
13	M	402	BCB	NA
13	M	402	BCB	NC
13	M	403	BCB	NA
13	M	403	BCB	NC
13	A	102	BCB	NA
13	A	102	BCB	NC
13	B	202	BCB	NA
13	B	202	BCB	NC
13	D	101	BCB	NA
13	D	101	BCB	NC
13	E	101	BCB	NA
13	E	101	BCB	NC
13	I	101	BCB	NA
13	I	101	BCB	NC
13	J	101	BCB	NA
13	J	101	BCB	NC
13	N	101	BCB	NA
13	N	101	BCB	NC
13	O	102	BCB	NA
13	O	102	BCB	NC
13	Q	402	BCB	NA
13	Q	402	BCB	NC
13	R	102	BCB	NA
13	R	102	BCB	NC
13	T	101	BCB	NA
13	T	101	BCB	NC
13	U	102	BCB	NA
13	U	102	BCB	NC
13	W	302	BCB	NA
13	W	302	BCB	NC
13	X	102	BCB	NA
13	X	102	BCB	NC
13	Z	101	BCB	NA
13	Z	101	BCB	NC
13	1	101	BCB	NA
13	1	101	BCB	NC
13	3	101	BCB	NA
13	3	101	BCB	NC
13	4	101	BCB	NA
13	4	101	BCB	NC
13	6	101	BCB	NA

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Mol	Chain	Res	Type	Atom
13	6	101	BCB	NC
13	7	102	BCB	NA
13	7	102	BCB	NC
13	9	101	BCB	NA
13	9	101	BCB	NC
13	0	102	BCB	NA
13	0	102	BCB	NC
13	b	101	BCB	NA
13	b	101	BCB	NC
13	c	101	BCB	NA
13	c	101	BCB	NC
13	e	101	BCB	NA
13	e	101	BCB	NC
13	f	101	BCB	NA
13	f	101	BCB	NC
13	h	102	BCB	NA
13	h	102	BCB	NC
13	i	101	BCB	NA
13	i	101	BCB	NC
13	k	102	BCB	NA
13	k	102	BCB	NC
13	l	102	BCB	NA
13	l	102	BCB	NC
13	n	101	BCB	NA
13	n	101	BCB	NC
13	o	102	BCB	NA
13	o	102	BCB	NC
13	q	101	BCB	NA
13	q	101	BCB	NC
13	r	101	BCB	NA
13	r	101	BCB	NC

All (851) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	401	HEC	C2B-C3B-CAB-CBB
9	C	401	HEC	C2C-C3C-CAC-CBC
9	C	401	HEC	C4C-C3C-CAC-CBC
9	C	402	HEC	C2B-C3B-CAB-CBB
9	C	402	HEC	C4B-C3B-CAB-CBB
9	C	402	HEC	C2C-C3C-CAC-CBC
9	C	402	HEC	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
9	C	403	HEC	C2B-C3B-CAB-CBB
9	C	403	HEC	C2C-C3C-CAC-CBC
9	C	403	HEC	C4C-C3C-CAC-CBC
9	C	404	HEC	C2B-C3B-CAB-CBB
9	C	404	HEC	C4B-C3B-CAB-CBB
9	C	404	HEC	C2C-C3C-CAC-CBC
9	C	404	HEC	C4C-C3C-CAC-CBC
11	M	408	UQ8	C6-C7-C8-C9
11	A	101	UQ8	C34-C36-C37-C38
11	A	101	UQ8	C25-C24-C26-C27
11	A	101	UQ8	C23-C24-C26-C27
12	L	301	DGA	CB2-CB1-OG2-CG2
13	M	403	BCB	CAD-CBD-CGD-O1D
13	M	403	BCB	CAD-CBD-CGD-O2D
13	E	101	BCB	C14-C13-C15-C16
13	Q	402	BCB	CBD-CGD-O2D-CED
13	Q	402	BCB	C14-C13-C15-C16
13	W	302	BCB	CHA-CBD-CGD-O1D
13	W	302	BCB	CBD-CGD-O2D-CED
13	Z	101	BCB	CHA-CBD-CGD-O1D
13	Z	101	BCB	CBD-CGD-O2D-CED
13	3	101	BCB	CHA-CBD-CGD-O1D
13	3	101	BCB	CBD-CGD-O2D-CED
13	b	101	BCB	CBD-CGD-O2D-CED
13	h	102	BCB	CHA-CBD-CGD-O2D
13	h	102	BCB	CBD-CGD-O2D-CED
13	i	101	BCB	CBA-CGA-O2A-C1
13	i	101	BCB	O1A-CGA-O2A-C1
13	i	101	BCB	C11-C12-C13-C14
13	k	102	BCB	CBD-CGD-O2D-CED
13	q	101	BCB	C1A-C2A-CAA-CBA
13	q	101	BCB	C3A-C2A-CAA-CBA
15	L	306	CDL	O1-C1-CB2-OB2
15	M	409	CDL	CA2-OA2-PA1-OA5
15	H	301	CDL	CA2-OA2-PA1-OA3
15	H	301	CDL	CA3-OA5-PA1-OA2
15	H	301	CDL	CB2-OB2-PB2-OB3
15	H	301	CDL	CB2-OB2-PB2-OB4
15	H	301	CDL	CB2-OB2-PB2-OB5
15	H	301	CDL	CB3-OB5-PB2-OB2
15	H	301	CDL	CB3-OB5-PB2-OB3
15	H	301	CDL	CB3-OB5-PB2-OB4

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Mol	Chain	Res	Type	Atoms
15	H	302	CDL	CA2-OA2-PA1-OA4
15	H	302	CDL	CA2-OA2-PA1-OA5
15	H	302	CDL	CA3-OA5-PA1-OA2
15	H	302	CDL	CB2-OB2-PB2-OB3
15	H	302	CDL	CB2-OB2-PB2-OB4
15	H	302	CDL	CB2-OB2-PB2-OB5
15	H	302	CDL	CB3-OB5-PB2-OB2
15	H	302	CDL	CB3-OB5-PB2-OB4
15	r	102	CDL	CA3-OA5-PA1-OA4
15	r	102	CDL	CB2-OB2-PB2-OB4
15	r	102	CDL	CB2-OB2-PB2-OB5
15	r	102	CDL	CB3-OB5-PB2-OB2
15	r	102	CDL	CB3-OB5-PB2-OB4
15	r	102	CDL	OB5-CB3-CB4-OB6
15	r	102	CDL	OB7-CB5-OB6-CB4
15	r	102	CDL	C51-CB5-OB6-CB4
19	b	102	LMT	O5'-C1'-O1'-C1
19	k	103	LMT	O5'-C1'-O1'-C1
20	M	411	PGV	C03-O11-P-O12
20	M	411	PGV	C03-O11-P-O14
20	M	411	PGV	C04-O12-P-O11
20	M	411	PGV	C04-O12-P-O13
20	M	411	PGV	C04-O12-P-O14
20	D	102	PGV	C04-O12-P-O11
20	I	102	PGV	C03-O11-P-O12
20	I	102	PGV	C04-O12-P-O11
20	I	102	PGV	C04-O12-P-O13
20	I	102	PGV	C04-O12-P-O14
20	N	102	PGV	C04-O12-P-O11
20	N	102	PGV	C04-O12-P-O14
20	Q	401	PGV	C04-O12-P-O13
20	W	301	PGV	C04-O12-P-O11
20	W	301	PGV	C04-O12-P-O14
13	A	102	BCB	CBD-CGD-O2D-CED
13	T	101	BCB	CBD-CGD-O2D-CED
13	6	101	BCB	CBD-CGD-O2D-CED
13	9	101	BCB	CBD-CGD-O2D-CED
13	e	101	BCB	CBD-CGD-O2D-CED
13	q	101	BCB	CBD-CGD-O2D-CED
13	Z	101	BCB	O1D-CGD-O2D-CED
13	3	101	BCB	O1D-CGD-O2D-CED
13	h	102	BCB	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	Q	402	BCB	O1D-CGD-O2D-CED
13	n	101	BCB	CBD-CGD-O2D-CED
12	L	301	DGA	OB1-CB1-OG2-CG2
15	H	302	CDL	OA7-CA5-OA6-CA4
13	A	102	BCB	C3-C5-C6-C7
13	q	101	BCB	C3-C5-C6-C7
13	W	302	BCB	O1D-CGD-O2D-CED
13	D	101	BCB	CBD-CGD-O2D-CED
13	I	101	BCB	CBD-CGD-O2D-CED
13	N	101	BCB	CBD-CGD-O2D-CED
15	H	302	CDL	C11-CA5-OA6-CA4
13	k	102	BCB	O1D-CGD-O2D-CED
13	b	101	BCB	C4-C3-C5-C6
21	R	101	NS0	C29-C28-C30-C31
13	b	101	BCB	C2-C3-C5-C6
21	R	101	NS0	C27-C28-C30-C31
13	b	101	BCB	O1D-CGD-O2D-CED
12	L	301	DGA	OA1-CA1-OG1-CG1
19	b	103	LMT	O5'-C5'-C6'-O6'
19	n	102	LMT	O5B-C5B-C6B-O6B
13	i	101	BCB	C3-C5-C6-C7
13	r	101	BCB	C3-C5-C6-C7
15	M	409	CDL	O1-C1-CA2-OA2
15	M	409	CDL	O1-C1-CB2-OB2
15	H	302	CDL	O1-C1-CB2-OB2
15	r	102	CDL	O1-C1-CB2-OB2
13	T	101	BCB	O1D-CGD-O2D-CED
13	9	101	BCB	O1D-CGD-O2D-CED
13	6	101	BCB	O1D-CGD-O2D-CED
13	J	101	BCB	CBD-CGD-O2D-CED
13	o	102	BCB	CBD-CGD-O2D-CED
20	Q	401	PGV	C2-C1-O01-C02
13	e	101	BCB	O1D-CGD-O2D-CED
12	L	301	DGA	CA2-CA1-OG1-CG1
18	M	406	NS5	C11-C10-C9-C8
18	M	406	NS5	C12-C10-C9-C8
21	q	102	NS0	C27-C28-C30-C31
20	Q	401	PGV	O02-C1-O01-C02
19	M	410	LMT	O5'-C5'-C6'-O6'
11	L	305	UQ8	C14-C16-C17-C18
11	M	408	UQ8	C39-C41-C42-C43
11	M	408	UQ8	C29-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
11	A	101	UQ8	C19-C21-C22-C23
9	C	402	HEC	C3D-CAD-CBD-CGD
13	q	101	BCB	O1D-CGD-O2D-CED
19	n	102	LMT	C4B-C5B-C6B-O6B
15	r	102	CDL	C31-CA7-OA8-CA6
13	q	101	BCB	C8-C10-C11-C12
15	r	102	CDL	OA9-CA7-OA8-CA6
13	X	102	BCB	CBD-CGD-O2D-CED
15	L	306	CDL	CA2-C1-CB2-OB2
15	M	409	CDL	CA2-C1-CB2-OB2
15	H	302	CDL	CA2-C1-CB2-OB2
20	I	102	PGV	O12-C04-C05-C06
20	D	102	PGV	C20-C19-O03-C01
13	r	101	BCB	CBD-CGD-O2D-CED
13	A	102	BCB	O1D-CGD-O2D-CED
13	n	101	BCB	O1D-CGD-O2D-CED
13	L	303	BCB	C13-C15-C16-C17
13	L	302	BCB	C4-C3-C5-C6
21	q	102	NS0	C29-C28-C30-C31
13	L	302	BCB	C2-C3-C5-C6
13	A	102	BCB	C11-C12-C13-C14
13	J	101	BCB	C6-C7-C8-C9
13	O	102	BCB	C11-C12-C13-C14
13	U	102	BCB	C14-C13-C15-C16
13	X	102	BCB	C11-C12-C13-C14
13	X	102	BCB	C14-C13-C15-C16
13	4	101	BCB	C11-C10-C8-C9
13	7	102	BCB	C11-C12-C13-C14
13	0	102	BCB	C11-C12-C13-C14
13	c	101	BCB	C11-C10-C8-C9
13	e	101	BCB	C14-C13-C15-C16
13	o	102	BCB	C6-C7-C8-C9
13	o	102	BCB	C11-C12-C13-C14
13	r	101	BCB	C11-C10-C8-C9
15	L	306	CDL	O1-C1-CA2-OA2
20	I	102	PGV	O12-C04-C05-O05
20	D	102	PGV	O04-C19-O03-C01
13	I	101	BCB	O1D-CGD-O2D-CED
13	6	101	BCB	C15-C16-C17-C18
19	b	103	LMT	C4'-C5'-C6'-O6'
15	M	409	CDL	C11-CA5-OA6-CA4
13	9	101	BCB	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
13	N	101	BCB	O1D-CGD-O2D-CED
13	D	101	BCB	C15-C16-C17-C18
13	E	101	BCB	C10-C11-C12-C13
13	n	101	BCB	C13-C15-C16-C17
15	r	102	CDL	C71-CB7-OB8-CB6
19	b	102	LMT	O5B-C5B-C6B-O6B
13	X	102	BCB	C13-C15-C16-C17
15	L	306	CDL	CA5-C11-C12-C13
20	Q	401	PGV	C19-C20-C21-C22
11	M	408	UQ8	C19-C21-C22-C23
21	0	101	NS0	C33-C35-C36-C37
15	r	102	CDL	CA7-C31-C32-C33
15	r	102	CDL	C11-CA5-OA6-CA4
13	A	102	BCB	C5-C6-C7-C8
13	D	101	BCB	C13-C15-C16-C17
13	J	101	BCB	C8-C10-C11-C12
13	r	101	BCB	C13-C15-C16-C17
13	M	403	BCB	C2A-CAA-CBA-CGA
13	A	102	BCB	C15-C16-C17-C18
13	Q	402	BCB	C13-C15-C16-C17
13	Q	402	BCB	C15-C16-C17-C18
13	T	101	BCB	C10-C11-C12-C13
13	W	302	BCB	C10-C11-C12-C13
13	Z	101	BCB	C8-C10-C11-C12
13	1	101	BCB	C10-C11-C12-C13
13	3	101	BCB	C10-C11-C12-C13
13	E	101	BCB	C8-C10-C11-C12
13	I	101	BCB	C13-C15-C16-C17
13	e	101	BCB	C5-C6-C7-C8
13	r	101	BCB	C8-C10-C11-C12
15	H	301	CDL	O1-C1-CA2-OA2
15	H	302	CDL	O1-C1-CA2-OA2
13	D	101	BCB	O1D-CGD-O2D-CED
13	k	102	BCB	C13-C15-C16-C17
15	H	301	CDL	CB5-C51-C52-C53
19	B	201	LMT	O1'-C1-C2-C3
13	M	402	BCB	C15-C16-C17-C18
13	R	102	BCB	C10-C11-C12-C13
13	E	101	BCB	C13-C15-C16-C17
20	W	301	PGV	C27-C28-C29-C30
15	M	409	CDL	OA7-CA5-OA6-CA4
15	r	102	CDL	OA7-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
15	M	409	CDL	CB2-C1-CA2-OA2
15	H	301	CDL	CB2-C1-CA2-OA2
15	H	302	CDL	CB2-C1-CA2-OA2
13	A	102	BCB	CBA-CGA-O2A-C1
13	D	101	BCB	C8-C10-C11-C12
13	R	102	BCB	C8-C10-C11-C12
13	W	302	BCB	C5-C6-C7-C8
13	X	102	BCB	C15-C16-C17-C18
13	1	101	BCB	C8-C10-C11-C12
13	4	101	BCB	C10-C11-C12-C13
13	7	102	BCB	C5-C6-C7-C8
13	9	101	BCB	C10-C11-C12-C13
13	Z	101	BCB	C5-C6-C7-C8
13	1	101	BCB	C15-C16-C17-C18
13	3	101	BCB	C5-C6-C7-C8
13	r	101	BCB	C10-C11-C12-C13
13	J	101	BCB	O1D-CGD-O2D-CED
20	W	301	PGV	C2-C1-O01-C02
21	O	101	NS0	C31-C32-C33-C34
11	A	101	UQ8	C14-C16-C17-C18
15	r	102	CDL	O1-C1-CA2-OA2
20	M	411	PGV	C1-C2-C3-C4
21	O	101	NS0	C10-C11-C12-C13
21	O	101	NS0	C10-C11-C12-C14
20	N	102	PGV	C04-C05-C06-O06
20	W	301	PGV	C04-C05-C06-O06
13	M	402	BCB	C16-C17-C18-C20
13	o	102	BCB	O1D-CGD-O2D-CED
15	r	102	CDL	OB9-CB7-OB8-CB6
19	M	410	LMT	C4'-C5'-C6'-O6'
13	M	403	BCB	C2-C1-O2A-CGA
13	N	101	BCB	C16-C17-C18-C19
13	O	102	BCB	C16-C17-C18-C19
13	f	101	BCB	C16-C17-C18-C20
13	A	102	BCB	O1A-CGA-O2A-C1
13	X	102	BCB	C10-C11-C12-C13
13	c	101	BCB	C8-C10-C11-C12
15	L	306	CDL	C79-C80-C81-C82
15	r	102	CDL	C53-C54-C55-C56
15	H	301	CDL	C53-C54-C55-C56
15	M	409	CDL	C13-C14-C15-C16
20	W	301	PGV	O02-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
19	b	102	LMT	C2-C1-O1'-C1'
15	H	302	CDL	CB5-C51-C52-C53
19	B	201	LMT	C1-C2-C3-C4
13	N	101	BCB	C16-C17-C18-C20
13	O	102	BCB	C16-C17-C18-C20
13	9	101	BCB	C16-C17-C18-C20
15	L	306	CDL	C51-CB5-OB6-CB4
15	H	301	CDL	C51-CB5-OB6-CB4
13	N	101	BCB	C11-C12-C13-C15
13	7	102	BCB	C6-C7-C8-C10
13	c	101	BCB	C6-C7-C8-C10
15	H	301	CDL	C13-C14-C15-C16
13	O	102	BCB	C3A-C2A-CAA-CBA
13	R	102	BCB	C3A-C2A-CAA-CBA
13	X	102	BCB	C3A-C2A-CAA-CBA
13	7	102	BCB	C3A-C2A-CAA-CBA
13	9	101	BCB	C3A-C2A-CAA-CBA
13	0	102	BCB	C3A-C2A-CAA-CBA
13	f	101	BCB	C3A-C2A-CAA-CBA
13	l	102	BCB	C3A-C2A-CAA-CBA
13	o	102	BCB	C3A-C2A-CAA-CBA
13	r	101	BCB	C3A-C2A-CAA-CBA
13	7	102	BCB	CBD-CGD-O2D-CED
13	i	101	BCB	C13-C15-C16-C17
13	M	402	BCB	C16-C17-C18-C19
13	f	101	BCB	C16-C17-C18-C19
13	9	101	BCB	CBA-CGA-O2A-C1
15	H	301	CDL	C32-C33-C34-C35
12	L	301	DGA	CA2-CA3-CA4-CA5
15	L	306	CDL	C11-C12-C13-C14
13	W	302	BCB	C13-C15-C16-C17
20	Q	401	PGV	C5-C6-C7-C8
15	M	409	CDL	C51-CB5-OB6-CB4
19	b	102	LMT	C1-C2-C3-C4
12	L	301	DGA	CB2-CB3-CB4-CB5
15	M	409	CDL	OB7-CB5-OB6-CB4
20	M	411	PGV	C3-C4-C5-C6
19	M	410	LMT	C3-C4-C5-C6
19	b	102	LMT	C7-C8-C9-C10
13	k	102	BCB	C10-C11-C12-C13
20	Q	401	PGV	C6-C7-C8-C9
20	M	411	PGV	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
15	H	301	CDL	C33-C34-C35-C36
20	N	102	PGV	C6-C7-C8-C9
13	1	101	BCB	C16-C17-C18-C19
15	L	306	CDL	C11-CA5-OA6-CA4
15	H	301	CDL	C11-CA5-OA6-CA4
20	I	102	PGV	C2-C1-O01-C02
13	N	101	BCB	C13-C15-C16-C17
15	L	306	CDL	OA7-CA5-OA6-CA4
15	L	306	CDL	OB7-CB5-OB6-CB4
15	H	301	CDL	OA7-CA5-OA6-CA4
15	H	301	CDL	OB7-CB5-OB6-CB4
20	I	102	PGV	O02-C1-O01-C02
13	3	101	BCB	C15-C16-C17-C18
15	H	301	CDL	CA5-C11-C12-C13
13	T	101	BCB	C3-C5-C6-C7
13	9	101	BCB	C16-C17-C18-C19
13	7	102	BCB	C4-C3-C5-C6
13	7	102	BCB	C2-C3-C5-C6
13	9	101	BCB	O1A-CGA-O2A-C1
13	N	101	BCB	C3-C5-C6-C7
13	o	102	BCB	C13-C15-C16-C17
20	D	102	PGV	C1-C2-C3-C4
20	D	102	PGV	C28-C29-C30-C31
19	T	102	LMT	O5'-C5'-C6'-O6'
13	N	101	BCB	C5-C6-C7-C8
13	1	101	BCB	C13-C15-C16-C17
19	B	201	LMT	C4-C5-C6-C7
19	b	103	LMT	C1-C2-C3-C4
15	M	409	CDL	OB6-CB4-CB6-OB8
13	E	101	BCB	C5-C6-C7-C8
13	U	102	BCB	C10-C11-C12-C13
13	X	102	BCB	O1D-CGD-O2D-CED
19	n	102	LMT	C6-C7-C8-C9
15	r	102	CDL	CA2-C1-CB2-OB2
19	B	201	LMT	C2-C3-C4-C5
15	H	302	CDL	C59-C60-C61-C62
13	J	101	BCB	C15-C16-C17-C18
15	L	306	CDL	C32-C33-C34-C35
15	H	301	CDL	C51-C52-C53-C54
20	W	301	PGV	O05-C05-C06-O06
20	N	102	PGV	C5-C6-C7-C8
15	r	102	CDL	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
20	W	301	PGV	C26-C27-C28-C29
15	M	409	CDL	C12-C13-C14-C15
15	H	302	CDL	C35-C36-C37-C38
19	M	410	LMT	C4-C5-C6-C7
15	L	306	CDL	OA5-CA3-CA4-CA6
15	r	102	CDL	OB5-CB3-CB4-CB6
13	E	101	BCB	C6-C7-C8-C10
13	E	101	BCB	C12-C13-C15-C16
13	I	101	BCB	C12-C13-C15-C16
13	N	101	BCB	C11-C10-C8-C7
13	N	101	BCB	C12-C13-C15-C16
13	O	102	BCB	C11-C12-C13-C15
13	O	102	BCB	C12-C13-C15-C16
13	3	101	BCB	C11-C10-C8-C7
13	c	101	BCB	C11-C10-C8-C7
13	i	101	BCB	C12-C13-C15-C16
13	o	102	BCB	C6-C7-C8-C10
13	r	101	BCB	C11-C10-C8-C7
14	M	404	BPB	C11-C10-C8-C7
13	E	101	BCB	C15-C16-C17-C18
21	W	303	NS0	CA-CB-CG-CD1
13	I	101	BCB	C14-C13-C15-C16
13	N	101	BCB	C11-C10-C8-C9
13	N	101	BCB	C14-C13-C15-C16
13	O	102	BCB	C14-C13-C15-C16
13	3	101	BCB	C11-C10-C8-C9
13	e	101	BCB	C11-C10-C8-C9
19	M	410	LMT	C2-C3-C4-C5
15	H	301	CDL	C71-CB7-OB8-CB6
13	f	101	BCB	C15-C16-C17-C18
21	U	101	NS0	C31-C32-C33-C34
15	M	409	CDL	CB3-CB4-CB6-OB8
15	H	302	CDL	CA3-CA4-CA6-OA8
13	7	102	BCB	CBA-CGA-O2A-C1
15	M	409	CDL	C31-CA7-OA8-CA6
15	H	302	CDL	C58-C59-C60-C61
15	r	102	CDL	C12-C13-C14-C15
13	D	101	BCB	CHA-CBD-CGD-O1D
13	Q	402	BCB	CHA-CBD-CGD-O1D
13	T	101	BCB	CHA-CBD-CGD-O1D
13	W	302	BCB	CHA-CBD-CGD-O2D
13	Z	101	BCB	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
13	3	101	BCB	CHA-CBD-CGD-O2D
13	6	101	BCB	CHA-CBD-CGD-O1D
13	6	101	BCB	CHA-CBD-CGD-O2D
13	9	101	BCB	CHA-CBD-CGD-O1D
13	b	101	BCB	CHA-CBD-CGD-O1D
13	k	102	BCB	CHA-CBD-CGD-O1D
13	q	101	BCB	CHA-CBD-CGD-O1D
13	q	101	BCB	CHA-CBD-CGD-O2D
13	l	102	BCB	C8-C10-C11-C12
15	H	302	CDL	C51-C52-C53-C54
13	c	101	BCB	C5-C6-C7-C8
19	b	102	LMT	C11-C10-C9-C8
13	1	101	BCB	C16-C17-C18-C20
21	q	102	NS0	C36-C37-C38-C39
13	U	102	BCB	C13-C15-C16-C17
13	3	101	BCB	C13-C15-C16-C17
12	L	301	DGA	CB3-CB4-CB5-CB6
14	L	304	BPB	O2A-C1-C2-C3
13	e	101	BCB	C13-C15-C16-C17
13	f	101	BCB	C13-C15-C16-C17
13	n	101	BCB	C15-C16-C17-C18
20	W	301	PGV	C20-C21-C22-C23
15	M	409	CDL	C71-CB7-OB8-CB6
13	3	101	BCB	C4-C3-C5-C6
11	A	101	UQ8	C31-C32-C33-C34
20	D	102	PGV	C20-C21-C22-C23
20	W	301	PGV	C2-C3-C4-C5
15	M	409	CDL	C40-C41-C42-C43
15	H	302	CDL	C53-C54-C55-C56
15	L	306	CDL	C41-C42-C43-C44
15	H	301	CDL	C22-C23-C24-C25
13	R	102	BCB	C13-C15-C16-C17
13	6	101	BCB	C8-C10-C11-C12
13	r	101	BCB	O1D-CGD-O2D-CED
20	Q	401	PGV	C15-C16-C17-C18
19	k	103	LMT	C5-C6-C7-C8
20	N	102	PGV	O05-C05-C06-O06
13	M	403	BCB	C14-C13-C15-C16
13	W	302	BCB	C14-C13-C15-C16
13	7	102	BCB	C11-C10-C8-C9
13	i	101	BCB	C14-C13-C15-C16
13	k	102	BCB	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
14	M	404	BPB	C11-C10-C8-C9
13	l	102	BCB	C13-C15-C16-C17
20	M	411	PGV	C26-C27-C28-C29
12	L	301	DGA	CA5-CA6-CA7-CA8
13	O	102	BCB	C13-C15-C16-C17
13	M	403	BCB	C12-C13-C15-C16
13	Q	402	BCB	C12-C13-C15-C16
13	7	102	BCB	C11-C10-C8-C7
13	e	101	BCB	C11-C10-C8-C7
13	k	102	BCB	C11-C10-C8-C7
13	o	102	BCB	C11-C12-C13-C15
13	q	101	BCB	C11-C10-C8-C7
15	M	409	CDL	OA9-CA7-OA8-CA6
15	L	306	CDL	C53-C54-C55-C56
19	h	103	LMT	O1'-C1-C2-C3
21	U	101	NS0	CA-C-C7-C8
21	X	101	NS0	C34-C33-C35-C36
13	O	102	BCB	C15-C16-C17-C18
13	7	102	BCB	O1A-CGA-O2A-C1
13	c	101	BCB	CBA-CGA-O2A-C1
13	7	102	BCB	C8-C10-C11-C12
15	r	102	CDL	CB2-C1-CA2-OA2
13	A	102	BCB	C10-C11-C12-C13
15	H	302	CDL	CB3-CB4-CB6-OB8
20	I	102	PGV	O03-C01-C02-C03
13	b	101	BCB	C16-C17-C18-C20
13	O	102	BCB	C1A-C2A-CAA-CBA
13	7	102	BCB	C1A-C2A-CAA-CBA
13	0	102	BCB	C1A-C2A-CAA-CBA
13	o	102	BCB	C1A-C2A-CAA-CBA
13	r	101	BCB	C1A-C2A-CAA-CBA
11	M	408	UQ8	C15-C14-C16-C17
21	R	101	NS0	CA-C-C7-C8
15	L	306	CDL	C72-C73-C74-C75
15	L	306	CDL	OA5-CA3-CA4-OA6
21	A	103	NS0	C26-C27-C28-C29
21	U	101	NS0	C8-C7-C9-C10
21	W	303	NS0	C26-C27-C28-C29
21	2	101	NS0	C26-C27-C28-C29
21	7	101	NS0	C26-C27-C28-C29
21	9	102	NS0	C26-C27-C28-C29
21	l	101	NS0	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
21	o	101	NS0	C26-C27-C28-C29
15	H	301	CDL	OB9-CB7-OB8-CB6
13	N	101	BCB	C8-C10-C11-C12
15	L	306	CDL	C52-C53-C54-C55
21	W	303	NS0	CA-CB-CG-CD2
15	H	301	CDL	OA6-CA4-CA6-OA8
15	H	302	CDL	OB6-CB4-CB6-OB8
20	D	102	PGV	O03-C01-C02-O01
20	I	102	PGV	O03-C01-C02-O01
15	r	102	CDL	C34-C35-C36-C37
13	4	101	BCB	C15-C16-C17-C18
11	M	408	UQ8	C13-C14-C16-C17
21	R	101	NS0	CA-C-C7-C9
21	U	101	NS0	CA-C-C7-C9
21	X	101	NS0	C32-C33-C35-C36
15	H	301	CDL	C54-C55-C56-C57
13	X	102	BCB	C16-C17-C18-C20
13	6	101	BCB	C16-C17-C18-C19
21	q	102	NS0	C36-C37-C38-C40
19	k	103	LMT	C1-C2-C3-C4
13	B	202	BCB	C14-C13-C15-C16
13	q	101	BCB	C11-C10-C8-C9
15	M	409	CDL	C77-C78-C79-C80
19	B	201	LMT	C5-C6-C7-C8
20	D	102	PGV	O12-C04-C05-C06
15	H	302	CDL	CA7-C31-C32-C33
20	M	411	PGV	C23-C24-C25-C26
20	N	102	PGV	C01-C02-C03-O11
13	L	302	BCB	C12-C13-C15-C16
13	A	102	BCB	C11-C12-C13-C15
13	B	202	BCB	C12-C13-C15-C16
13	o	102	BCB	C12-C13-C15-C16
15	H	302	CDL	C11-C12-C13-C14
20	Q	401	PGV	C27-C28-C29-C30
15	r	102	CDL	C32-C33-C34-C35
15	H	301	CDL	C40-C41-C42-C43
11	M	408	UQ8	C30-C29-C31-C32
21	R	101	NS0	C34-C33-C35-C36
21	0	101	NS0	CA-C-C7-C8
15	M	409	CDL	OB9-CB7-OB8-CB6
14	M	404	BPB	C13-C15-C16-C17
15	H	302	CDL	CA6-CA4-OA6-CA5

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Mol	Chain	Res	Type	Atoms
15	r	102	CDL	CA6-CA4-OA6-CA5
15	r	102	CDL	C36-C37-C38-C39
15	H	301	CDL	C34-C35-C36-C37
20	Q	401	PGV	C26-C27-C28-C29
13	Z	101	BCB	C10-C11-C12-C13
15	H	302	CDL	OB5-CB3-CB4-OB6
20	N	102	PGV	O01-C02-C03-O11
13	U	102	BCB	C15-C16-C17-C18
21	9	102	NS0	CA-C-C7-C8
21	o	101	NS0	C34-C33-C35-C36
21	9	102	NS0	CA-C-C7-C9
13	q	101	BCB	O1A-CGA-O2A-C1
15	H	302	CDL	OA6-CA4-CA6-OA8
13	A	102	BCB	C14-C13-C15-C16
13	c	101	BCB	O1A-CGA-O2A-C1
13	T	101	BCB	C13-C15-C16-C17
13	7	102	BCB	O1D-CGD-O2D-CED
13	6	101	BCB	C16-C17-C18-C20
13	J	101	BCB	C13-C15-C16-C17
15	M	409	CDL	C16-C17-C18-C19
21	U	101	NS0	C34-C33-C35-C36
21	2	101	NS0	CA-C-C7-C8
21	7	101	NS0	C34-C33-C35-C36
21	0	101	NS0	CA-C-C7-C9
13	q	101	BCB	CBA-CGA-O2A-C1
19	h	103	LMT	C7-C8-C9-C10
21	X	101	NS0	CA-C-C7-C8
21	7	101	NS0	CA-C-C7-C8
21	l	101	NS0	C34-C33-C35-C36
21	R	101	NS0	C32-C33-C35-C36
15	M	409	CDL	C60-C61-C62-C63
13	0	102	BCB	C10-C11-C12-C13
13	U	102	BCB	C12-C13-C15-C16
13	X	102	BCB	C11-C12-C13-C15
13	1	101	BCB	C12-C13-C15-C16
13	7	102	BCB	C11-C12-C13-C15
13	7	102	BCB	C12-C13-C15-C16
13	b	101	BCB	C11-C12-C13-C15
13	e	101	BCB	C12-C13-C15-C16
13	f	101	BCB	C12-C13-C15-C16
13	b	101	BCB	C16-C17-C18-C19
13	e	101	BCB	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
15	M	409	CDL	C73-C74-C75-C76
13	o	102	BCB	CBA-CGA-O2A-C1
15	H	302	CDL	C12-C13-C14-C15
15	r	102	CDL	C1-CA2-OA2-PA1
15	r	102	CDL	C1-CB2-OB2-PB2
19	b	103	LMT	O1'-C1-C2-C3
9	C	401	HEC	C4B-C3B-CAB-CBB
9	C	403	HEC	C4B-C3B-CAB-CBB
11	A	101	UQ8	C30-C29-C31-C32
21	O	101	NS0	C34-C33-C35-C36
21	o	101	NS0	CA-C-C7-C8
21	q	102	NS0	CA-C-C7-C8
19	b	102	LMT	C4B-C5B-C6B-O6B
19	b	103	LMT	C2-C3-C4-C5
15	r	102	CDL	C13-C14-C15-C16
15	M	409	CDL	OA5-CA3-CA4-OA6
13	L	302	BCB	C14-C13-C15-C16
15	M	409	CDL	C35-C36-C37-C38
20	W	301	PGV	C25-C26-C27-C28
19	h	103	LMT	C2-C3-C4-C5
15	H	301	CDL	C44-C45-C46-C47
19	n	102	LMT	C5-C6-C7-C8
15	r	102	CDL	C54-C55-C56-C57
13	o	102	BCB	O1A-CGA-O2A-C1
15	L	306	CDL	OB6-CB4-CB6-OB8
21	O	101	NS0	CA-C-C7-C8
21	l	101	NS0	CA-C-C7-C8
21	7	101	NS0	C32-C33-C35-C36
21	o	101	NS0	C32-C33-C35-C36
20	Q	401	PGV	C28-C29-C30-C31
15	r	102	CDL	C11-C12-C13-C14
15	H	301	CDL	C18-C19-C20-C21
13	D	101	BCB	CHA-CBD-CGD-O2D
13	Q	402	BCB	CHA-CBD-CGD-O2D
13	T	101	BCB	CHA-CBD-CGD-O2D
13	9	101	BCB	CHA-CBD-CGD-O2D
13	b	101	BCB	CHA-CBD-CGD-O2D
13	h	102	BCB	CHA-CBD-CGD-O1D
13	k	102	BCB	CHA-CBD-CGD-O2D
15	M	409	CDL	CA2-OA2-PA1-OA3
15	H	301	CDL	CA3-OA5-PA1-OA3
15	H	302	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
15	H	302	CDL	CB3-OB5-PB2-OB3
15	r	102	CDL	CA3-OA5-PA1-OA2
15	r	102	CDL	CB2-OB2-PB2-OB3
20	D	102	PGV	C04-O12-P-O13
20	I	102	PGV	C03-O11-P-O13
20	Q	401	PGV	C04-O12-P-O11
20	Q	401	PGV	C04-O12-P-O14
20	W	301	PGV	C03-O11-P-O12
20	W	301	PGV	C03-O11-P-O14
21	2	101	NS0	C26-C27-C28-C30
21	7	101	NS0	C26-C27-C28-C30
13	I	101	BCB	C3-C5-C6-C7
15	H	302	CDL	C57-C58-C59-C60
13	N	101	BCB	C15-C16-C17-C18
21	k	101	NS0	CA-C-C7-C8
11	M	408	UQ8	C28-C29-C31-C32
15	L	306	CDL	C1-CB2-OB2-PB2
20	N	102	PGV	C19-C20-C21-C22
19	M	410	LMT	C9-C10-C11-C12
13	4	101	BCB	C13-C15-C16-C17
15	H	301	CDL	C21-C22-C23-C24
20	D	102	PGV	C03-C02-O01-C1
21	2	101	NS0	CA-C-C7-C9
15	M	409	CDL	OA5-CA3-CA4-CA6
13	X	102	BCB	C8-C10-C11-C12
13	T	101	BCB	C14-C13-C15-C16
13	f	101	BCB	C11-C12-C13-C14
13	o	102	BCB	C14-C13-C15-C16
13	J	101	BCB	C6-C7-C8-C10
20	I	102	PGV	C2-C3-C4-C5
13	3	101	BCB	C2-C3-C5-C6
11	L	305	UQ8	C5-C4-O4-C4M
13	X	102	BCB	C16-C17-C18-C19
15	L	306	CDL	C81-C82-C83-C84
21	D	103	NS0	C34-C33-C35-C36
20	W	301	PGV	C11-C10-C9-C8
13	O	102	BCB	C10-C11-C12-C13
19	B	201	LMT	C3-C4-C5-C6
21	O	101	NS0	C31-C32-C33-C35
13	A	102	BCB	C4-C3-C5-C6
21	2	101	NS0	C34-C33-C35-C36
21	9	102	NS0	C34-C33-C35-C36

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Mol	Chain	Res	Type	Atoms
21	k	101	NS0	C34-C33-C35-C36
21	U	101	NS0	C32-C33-C35-C36
21	7	101	NS0	CA-C-C7-C9
21	q	102	NS0	CA-C-C7-C9
20	W	301	PGV	O12-C04-C05-C06
13	b	101	BCB	C11-C12-C13-C14
13	f	101	BCB	C14-C13-C15-C16
13	E	101	BCB	C4-C3-C5-C6
21	X	101	NS0	CA-C-C7-C9
21	9	102	NS0	C32-C33-C35-C36
21	l	101	NS0	C32-C33-C35-C36
13	A	102	BCB	C12-C13-C15-C16
19	h	103	LMT	C9-C10-C11-C12
13	E	101	BCB	C3A-C2A-CAA-CBA
13	J	101	BCB	C3A-C2A-CAA-CBA
13	1	101	BCB	C3A-C2A-CAA-CBA
21	W	303	NS0	CA-C-C7-C8
21	D	103	NS0	C32-C33-C35-C36
21	O	101	NS0	CA-C-C7-C9
21	2	101	NS0	C32-C33-C35-C36
15	H	302	CDL	C32-C33-C34-C35
13	M	403	BCB	C15-C16-C17-C18
13	f	101	BCB	C8-C10-C11-C12
21	h	101	NS0	C35-C36-C37-C38
15	M	409	CDL	C62-C63-C64-C65
19	b	102	LMT	C6-C7-C8-C9
11	L	305	UQ8	C20-C19-C21-C22
11	A	101	UQ8	C28-C29-C31-C32
21	O	101	NS0	C32-C33-C35-C36
21	k	101	NS0	CA-C-C7-C9
21	l	101	NS0	CA-C-C7-C9
21	o	101	NS0	CA-C-C7-C9
19	b	102	LMT	C5'-C4'-O1B-C1B
15	H	301	CDL	CB3-CB4-CB6-OB8
15	r	102	CDL	CB3-CB4-CB6-OB8
20	M	411	PGV	C25-C26-C27-C28
9	C	402	HEC	CAA-CBA-CGA-O1A
13	J	101	BCB	C11-C10-C8-C9
13	N	101	BCB	C11-C12-C13-C14
13	W	302	BCB	C6-C7-C8-C9
13	4	101	BCB	C6-C7-C8-C9
13	k	102	BCB	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
13	R	102	BCB	C1A-C2A-CAA-CBA
13	X	102	BCB	C1A-C2A-CAA-CBA
13	9	101	BCB	C1A-C2A-CAA-CBA
13	f	101	BCB	C1A-C2A-CAA-CBA
20	W	301	PGV	C22-C23-C24-C25
9	C	402	HEC	CAA-CBA-CGA-O2A
13	X	102	BCB	CBA-CGA-O2A-C1
11	L	305	UQ8	C3-C4-O4-C4M
20	Q	401	PGV	C14-C15-C16-C17
19	b	102	LMT	C3'-C4'-O1B-C1B
13	f	101	BCB	CBA-CGA-O2A-C1
11	L	305	UQ8	C12-C11-C9-C10
11	M	408	UQ8	C40-C39-C41-C42
20	D	102	PGV	C29-C30-C31-C32
20	Q	401	PGV	C29-C30-C31-C32
13	E	101	BCB	C2-C3-C5-C6
21	D	103	NS0	C-CA-CB-CG
20	D	102	PGV	C3-C4-C5-C6
9	C	401	HEC	CAA-CBA-CGA-O1A
13	q	101	BCB	C5-C6-C7-C8
15	M	409	CDL	C63-C64-C65-C66
13	O	102	BCB	C11-C10-C8-C7
13	X	102	BCB	C11-C10-C8-C7
15	H	301	CDL	C61-C62-C63-C64
20	N	102	PGV	C1-C2-C3-C4
13	O	102	BCB	C3-C5-C6-C7
11	A	101	UQ8	C5-C4-O4-C4M
20	I	102	PGV	C20-C21-C22-C23
13	B	202	BCB	C13-C15-C16-C17
20	I	102	PGV	C1-C2-C3-C4
9	C	401	HEC	CAA-CBA-CGA-O2A
13	c	101	BCB	C4-C3-C5-C6
21	0	101	NS0	C34-C33-C35-C36
13	0	102	BCB	C5-C6-C7-C8
11	M	408	UQ8	C38-C39-C41-C42
13	i	101	BCB	C2-C3-C5-C6
21	W	303	NS0	CA-C-C7-C9
21	k	101	NS0	C32-C33-C35-C36
13	L	303	BCB	C14-C13-C15-C16
13	M	402	BCB	C11-C10-C8-C9
15	L	306	CDL	C80-C81-C82-C83
13	J	101	BCB	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
20	M	411	PGV	C6-C7-C8-C9
11	M	408	UQ8	C12-C11-C9-C10
11	A	101	UQ8	C40-C39-C41-C42
13	D	101	BCB	C4-C3-C5-C6
13	i	101	BCB	C4-C3-C5-C6
13	f	101	BCB	O1A-CGA-O2A-C1
9	C	404	HEC	C3D-CAD-CBD-CGD
15	r	102	CDL	C14-C15-C16-C17
19	b	103	LMT	C3-C4-C5-C6
13	D	101	BCB	C5-C6-C7-C8
13	X	102	BCB	O1A-CGA-O2A-C1
13	0	102	BCB	O1A-CGA-O2A-C1
11	A	101	UQ8	C2-C3-O3-C3M
13	0	102	BCB	CBA-CGA-O2A-C1
13	M	403	BCB	CHA-CBD-CGD-O2D
13	A	102	BCB	CHA-CBD-CGD-O1D
13	A	102	BCB	CHA-CBD-CGD-O2D
13	B	202	BCB	CHA-CBD-CGD-O1D
13	B	202	BCB	CHA-CBD-CGD-O2D
15	H	302	CDL	OB5-CB3-CB4-CB6
20	I	102	PGV	C01-C02-C03-O11
13	B	202	BCB	C4-C3-C5-C6
13	o	102	BCB	C5-C6-C7-C8
13	o	102	BCB	C10-C11-C12-C13
13	0	102	BCB	C11-C12-C13-C15
12	L	301	DGA	CA3-CA4-CA5-CA6
20	D	102	PGV	O12-C04-C05-O05
13	M	402	BCB	C14-C13-C15-C16
13	1	101	BCB	C14-C13-C15-C16
13	D	101	BCB	C2-C1-O2A-CGA
13	W	302	BCB	C2-C1-O2A-CGA
13	4	101	BCB	C3A-C2A-CAA-CBA
13	c	101	BCB	C3A-C2A-CAA-CBA
13	c	101	BCB	C2-C3-C5-C6
20	Q	401	PGV	C13-C14-C15-C16
20	N	102	PGV	C03-C02-O01-C1
13	A	102	BCB	C13-C15-C16-C17
15	M	409	CDL	C39-C40-C41-C42
15	L	306	CDL	CB2-C1-CA2-OA2
13	O	102	BCB	CBA-CGA-O2A-C1
11	A	101	UQ8	C39-C41-C42-C43
15	H	301	CDL	CA3-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
13	3	101	BCB	C16-C17-C18-C19
13	9	101	BCB	CAA-CBA-CGA-O2A
21	W	303	NS0	C11-C10-C9-C7
13	0	102	BCB	C8-C10-C11-C12
15	L	306	CDL	C32-C31-CA7-OA8
15	M	409	CDL	C80-C81-C82-C83
13	c	101	BCB	C6-C7-C8-C9
15	H	302	CDL	C31-C32-C33-C34
20	Q	401	PGV	O03-C19-C20-C21
15	M	409	CDL	C61-C62-C63-C64
13	O	102	BCB	O1A-CGA-O2A-C1
13	4	101	BCB	C16-C17-C18-C20
11	L	305	UQ8	C12-C11-C9-C8
11	A	101	UQ8	C38-C39-C41-C42
13	L	303	BCB	C12-C13-C15-C16
13	M	402	BCB	C11-C10-C8-C7
13	M	402	BCB	C12-C13-C15-C16
13	A	102	BCB	C11-C10-C8-C7
13	X	102	BCB	C12-C13-C15-C16
13	4	101	BCB	C11-C10-C8-C7
13	i	101	BCB	C11-C12-C13-C15
13	N	101	BCB	C2-C1-O2A-CGA
13	T	101	BCB	C2-C1-O2A-CGA
13	7	102	BCB	C2-C1-O2A-CGA
15	L	306	CDL	C40-C41-C42-C43
15	M	409	CDL	C59-C60-C61-C62
15	H	301	CDL	C55-C56-C57-C58
13	r	101	BCB	O1A-CGA-O2A-C1
13	1	101	BCB	CBA-CGA-O2A-C1
12	L	301	DGA	OG2-CB1-CB2-CB3
15	M	409	CDL	C12-C11-CA5-OA6
15	H	301	CDL	C20-C21-C22-C23
15	H	301	CDL	C71-C72-C73-C74
20	I	102	PGV	C31-C32-C33-C34
15	L	306	CDL	C12-C11-CA5-OA6
13	A	102	BCB	C2-C3-C5-C6
15	L	306	CDL	C82-C83-C84-C85
13	T	101	BCB	CAA-CBA-CGA-O2A
13	U	102	BCB	CAA-CBA-CGA-O2A
13	b	101	BCB	CAA-CBA-CGA-O2A
11	A	101	UQ8	C24-C26-C27-C28
13	U	102	BCB	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
9	C	404	HEC	CAD-CBD-CGD-O1D
15	M	409	CDL	C36-C37-C38-C39
14	L	304	BPB	C8-C10-C11-C12
14	M	404	BPB	C15-C16-C17-C18
13	X	102	BCB	C3-C5-C6-C7
13	e	101	BCB	C2-C1-O2A-CGA
13	q	101	BCB	C2-C1-O2A-CGA
13	0	102	BCB	C12-C13-C15-C16
20	M	411	PGV	C11-C12-C13-C14
15	M	409	CDL	C52-C53-C54-C55
13	h	102	BCB	C13-C15-C16-C17
21	W	303	NS0	C35-C36-C37-C38
13	q	101	BCB	CAA-CBA-CGA-O2A
20	Q	401	PGV	O04-C19-C20-C21
19	b	102	LMT	C9-C10-C11-C12
12	L	301	DGA	OB1-CB1-CB2-CB3
13	1	101	BCB	O1A-CGA-O2A-C1
11	L	305	UQ8	C18-C19-C21-C22
12	L	301	DGA	OG1-CG1-CG2-CG3
13	R	102	BCB	CBA-CGA-O2A-C1
13	r	101	BCB	CBA-CGA-O2A-C1
13	7	102	BCB	C14-C13-C15-C16
15	r	102	CDL	C52-C51-CB5-OB6
13	9	101	BCB	CAA-CBA-CGA-O1A
15	H	301	CDL	C16-C17-C18-C19
9	C	404	HEC	CAD-CBD-CGD-O2D
13	k	102	BCB	C8-C10-C11-C12
21	A	103	NS0	C35-C36-C37-C38
15	H	302	CDL	OB7-CB5-OB6-CB4
13	b	101	BCB	CAA-CBA-CGA-O1A
15	L	306	CDL	C32-C31-CA7-OA9
13	k	102	BCB	CAA-CBA-CGA-O2A
15	H	301	CDL	C12-C11-CA5-OA6
13	T	101	BCB	CAA-CBA-CGA-O1A
15	M	409	CDL	C12-C11-CA5-OA7
13	f	101	BCB	C10-C11-C12-C13
13	o	102	BCB	C15-C16-C17-C18
13	3	101	BCB	C2-C1-O2A-CGA
13	q	101	BCB	CAA-CBA-CGA-O1A
15	r	102	CDL	C32-C31-CA7-OA8
13	J	101	BCB	C1A-C2A-CAA-CBA
13	1	101	BCB	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
13	l	102	BCB	C1A-C2A-CAA-CBA
15	H	302	CDL	C51-CB5-OB6-CB4
15	r	102	CDL	C52-C51-CB5-OB7
15	H	301	CDL	C12-C11-CA5-OA7

There are no ring outliers.

66 monomers are involved in 364 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	R	102	BCB	8	0
13	q	101	BCB	4	0
19	b	102	LMT	3	0
17	M	405	MQ7	1	0
11	L	305	UQ8	2	0
13	B	202	BCB	8	0
13	6	101	BCB	7	0
15	H	301	CDL	12	0
11	M	408	UQ8	15	0
9	C	403	HEC	1	0
13	f	101	BCB	7	0
20	W	301	PGV	1	0
13	D	101	BCB	9	0
13	c	101	BCB	9	0
13	W	302	BCB	7	0
20	I	102	PGV	4	0
21	o	101	NS0	1	0
9	C	402	HEC	5	0
20	Q	401	PGV	5	0
13	0	102	BCB	11	0
13	k	102	BCB	5	0
13	M	403	BCB	7	0
15	H	302	CDL	2	0
13	b	101	BCB	7	0
13	J	101	BCB	7	0
13	n	101	BCB	5	0
15	M	409	CDL	10	0
13	r	101	BCB	7	0
13	h	102	BCB	6	0
19	h	103	LMT	2	0
11	A	101	UQ8	11	0
20	D	102	PGV	6	0
14	L	304	BPB	4	0

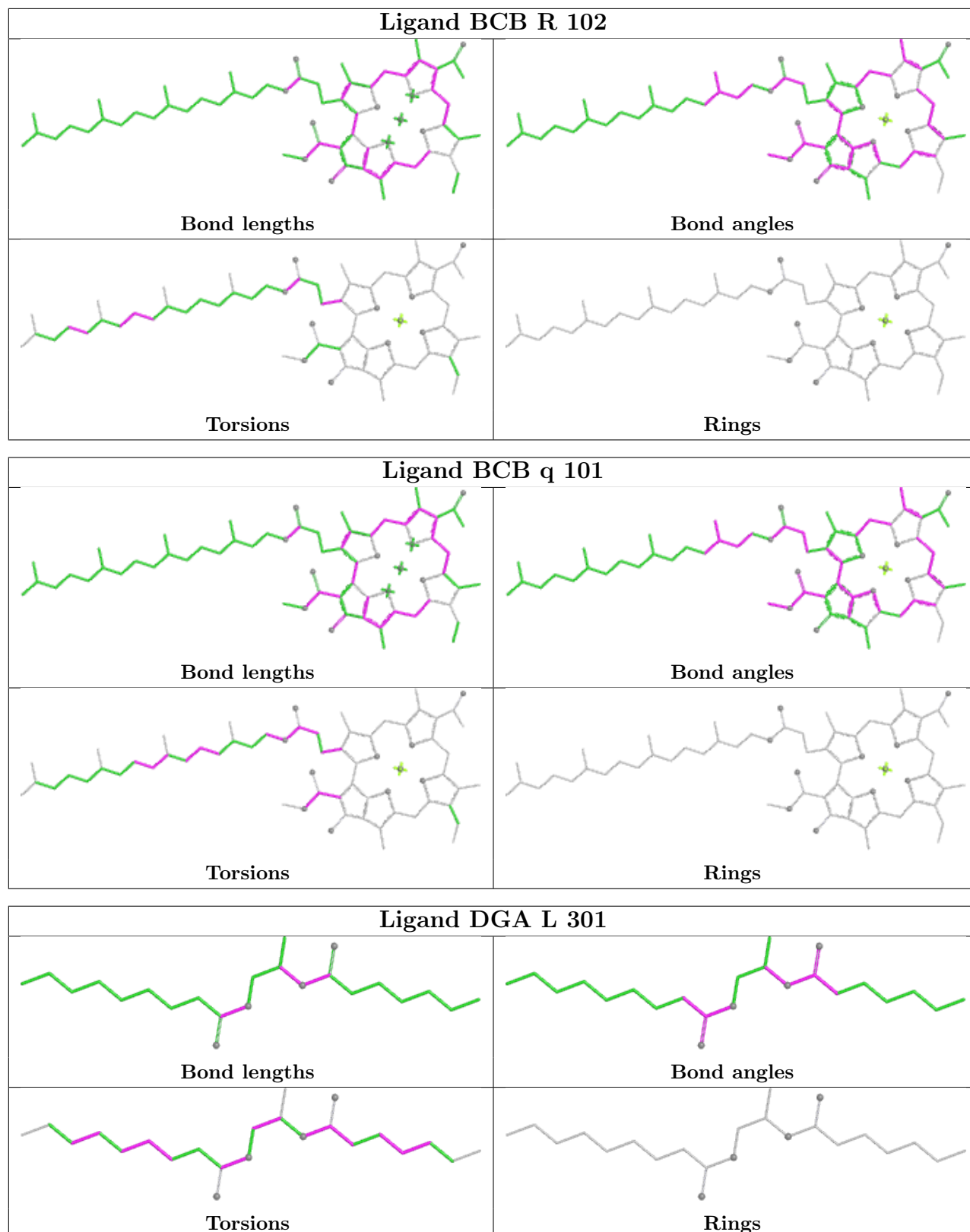
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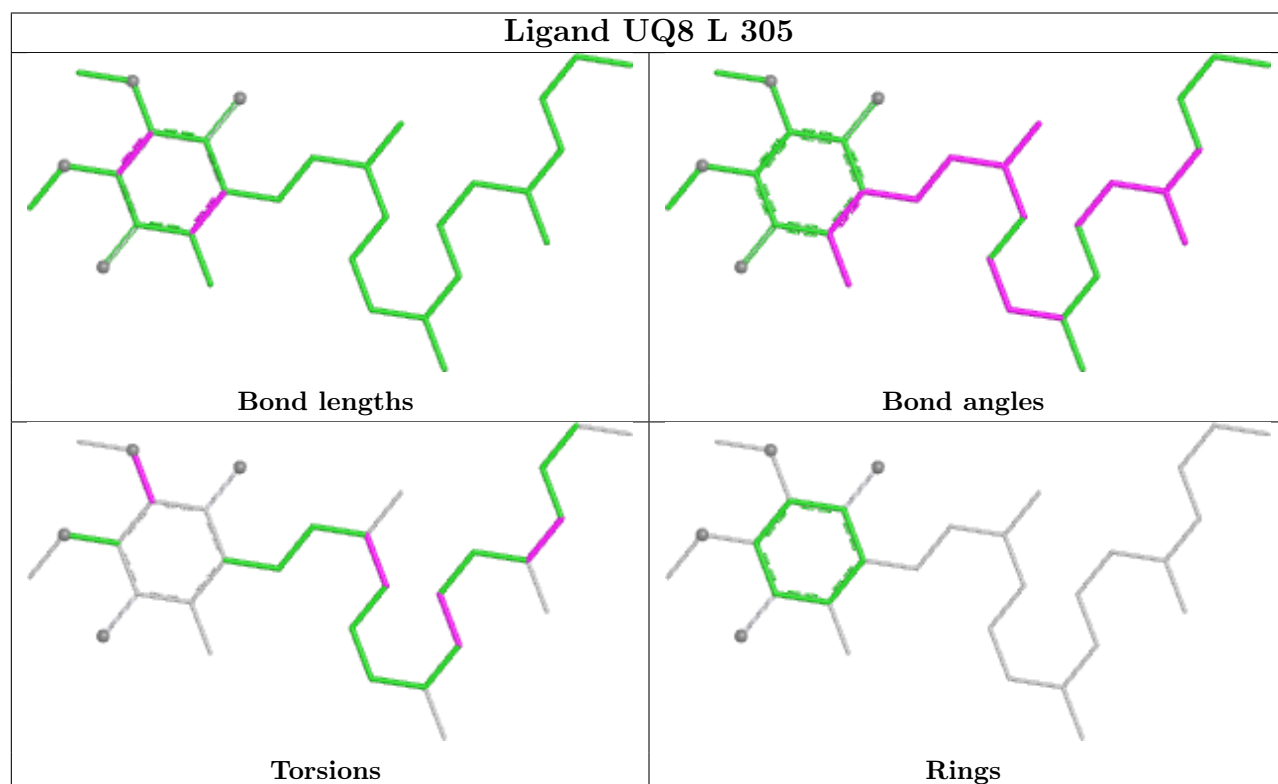
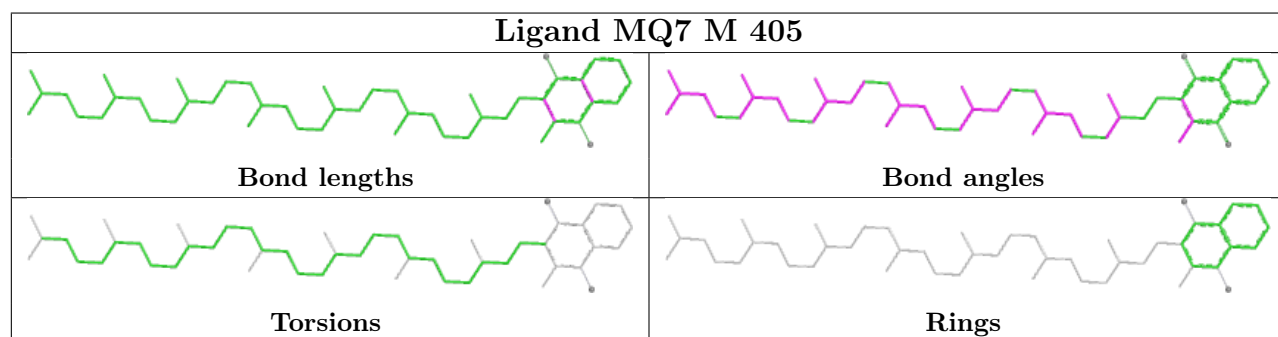
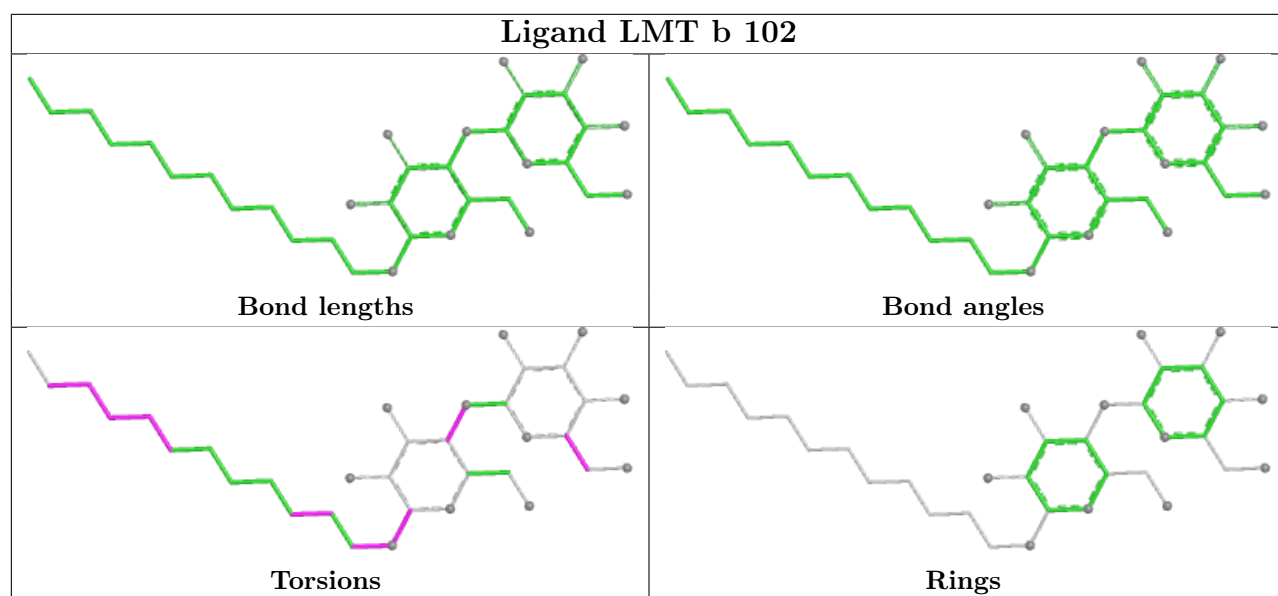
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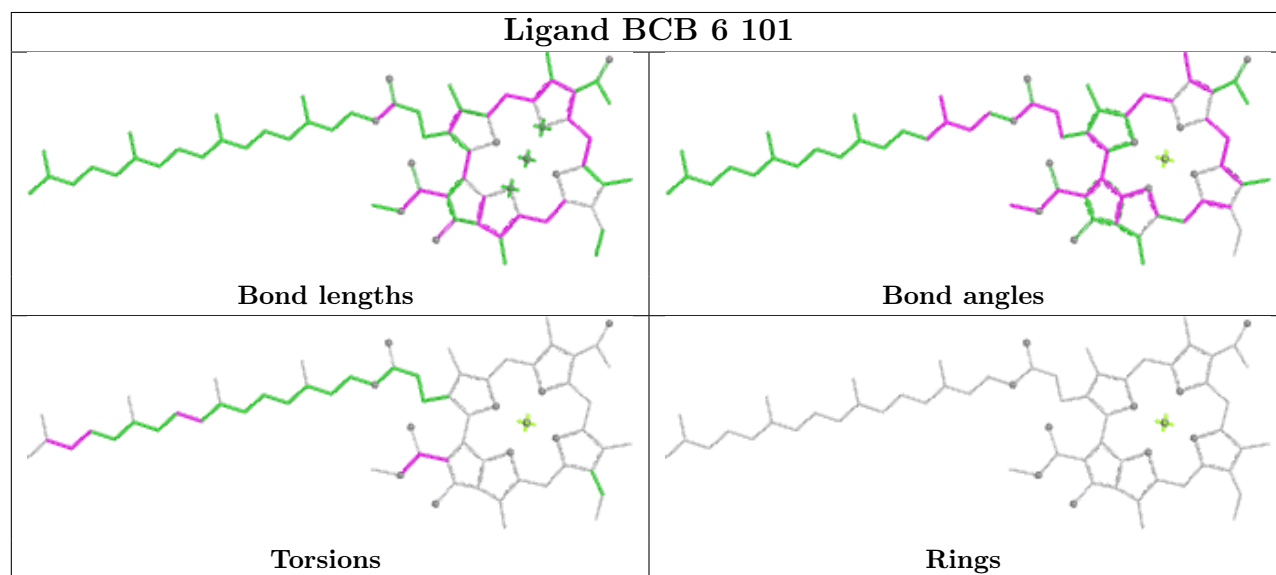
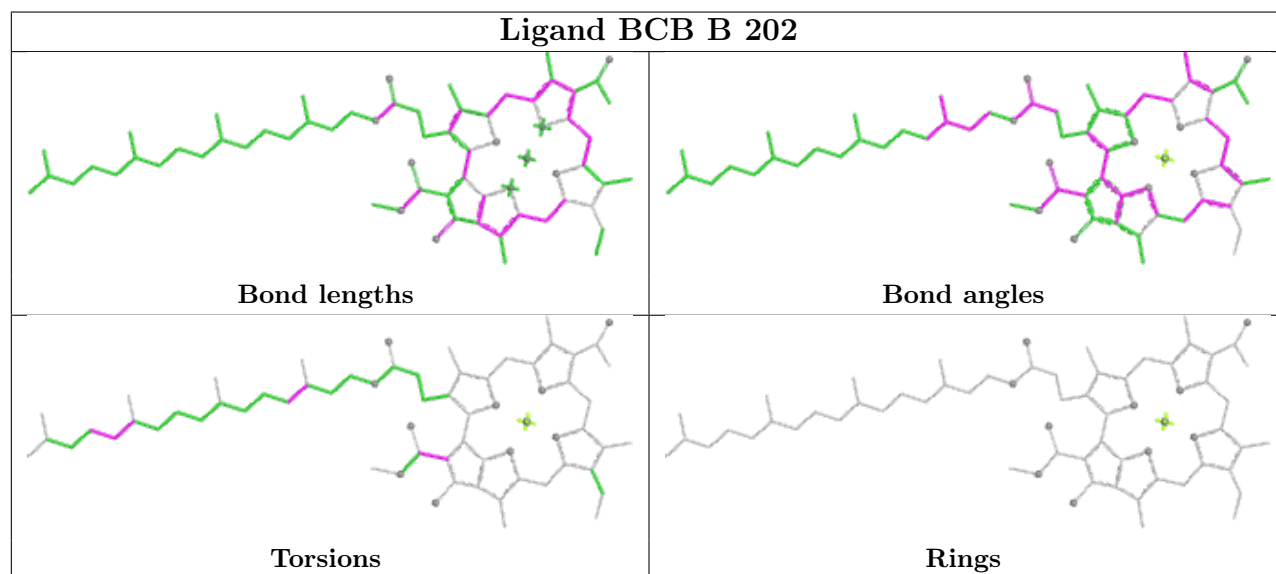
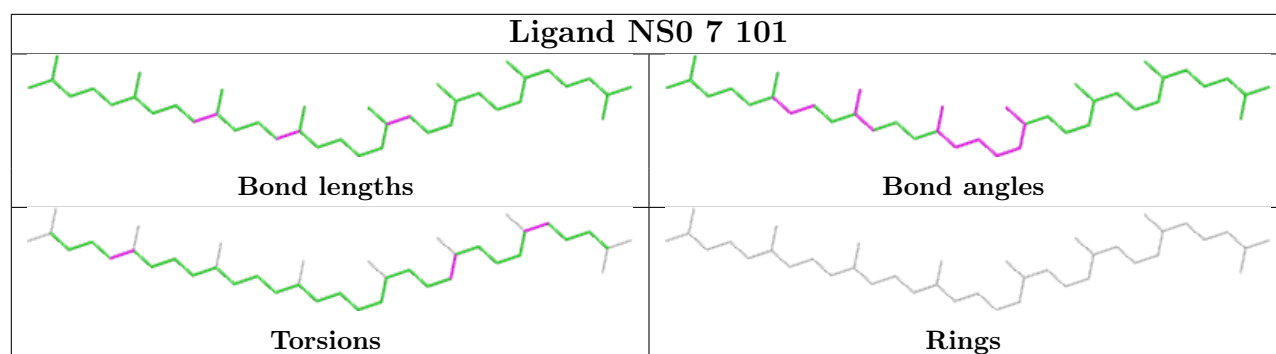
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	O	102	BCB	16	0
20	N	102	PGV	2	0
13	I	101	BCB	7	0
19	M	410	LMT	3	0
15	r	102	CDL	7	0
13	l	102	BCB	7	0
13	M	402	BCB	3	0
13	o	102	BCB	12	0
11	M	407	UQ8	2	0
13	3	101	BCB	6	0
13	1	101	BCB	7	0
13	T	101	BCB	5	0
15	L	306	CDL	4	0
13	7	102	BCB	7	0
13	9	101	BCB	7	0
14	M	404	BPB	5	0
13	E	101	BCB	8	0
13	X	102	BCB	7	0
13	i	101	BCB	10	0
13	L	302	BCB	7	0
13	Z	101	BCB	8	0
19	T	102	LMT	2	0
18	M	406	NS5	1	0
19	n	102	LMT	2	0
13	A	102	BCB	6	0
13	e	101	BCB	4	0
19	b	103	LMT	3	0
13	Q	402	BCB	7	0
13	L	303	BCB	5	0
20	M	411	PGV	1	0
13	U	102	BCB	6	0
13	N	101	BCB	5	0
13	4	101	BCB	8	0

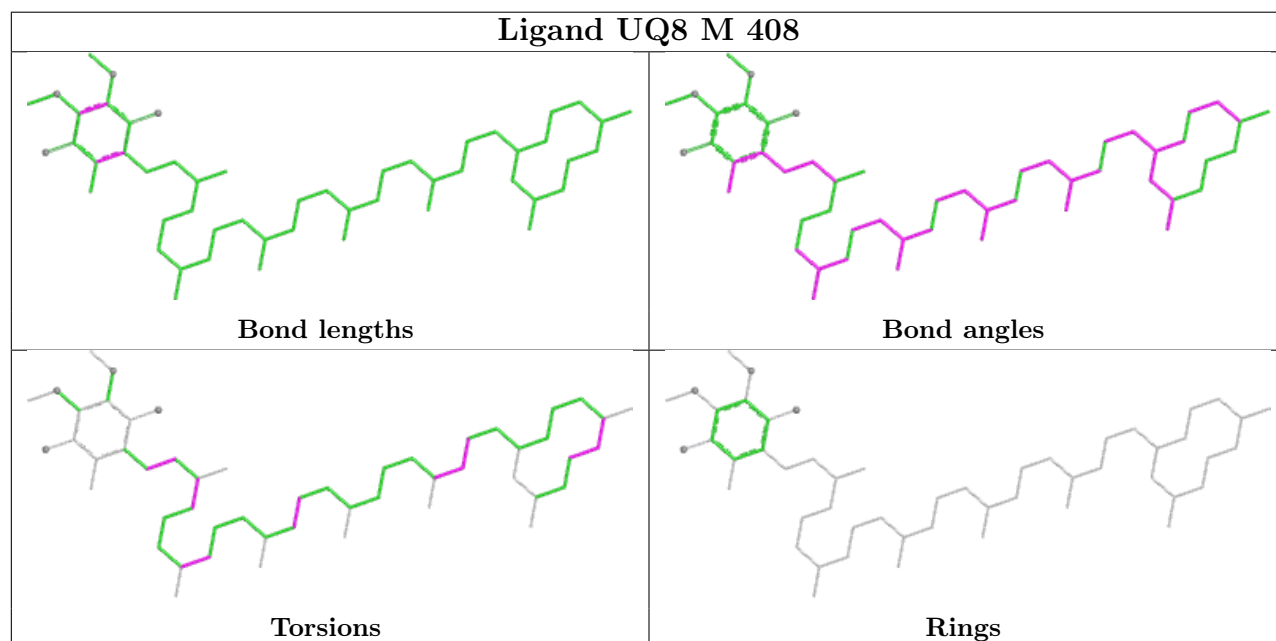
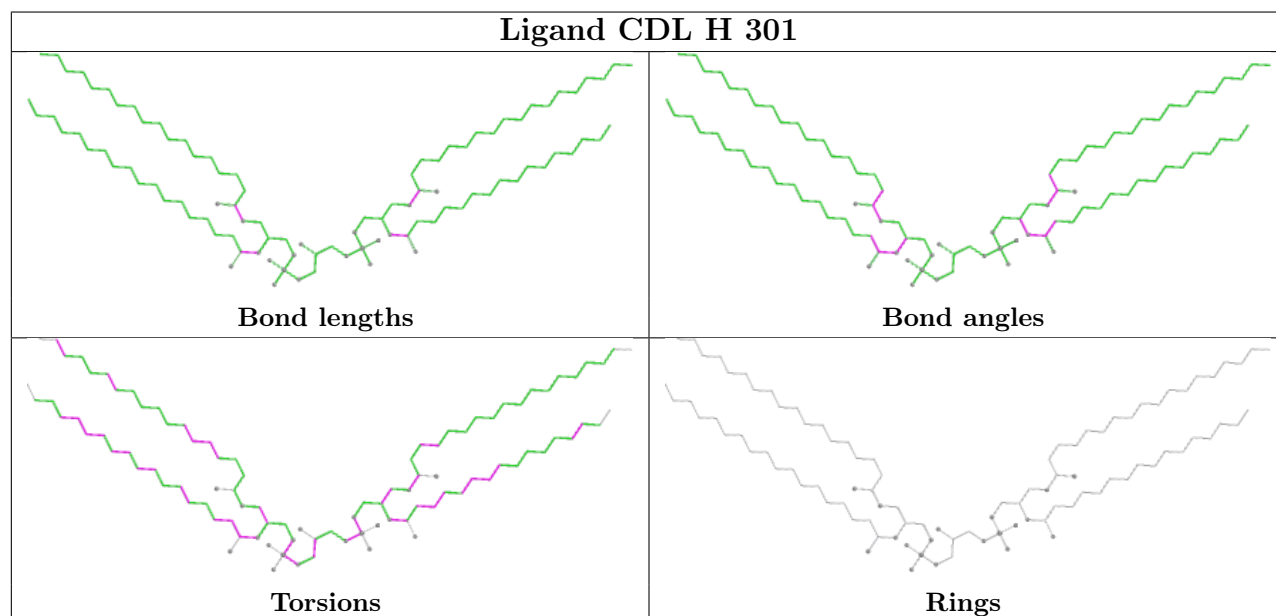
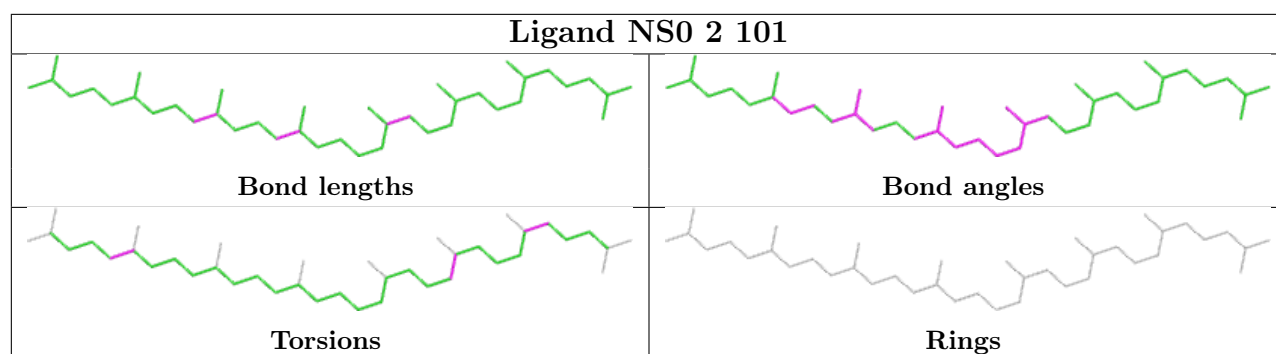
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

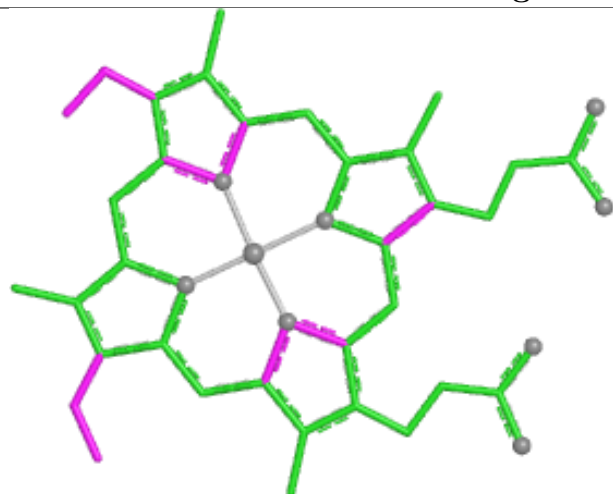




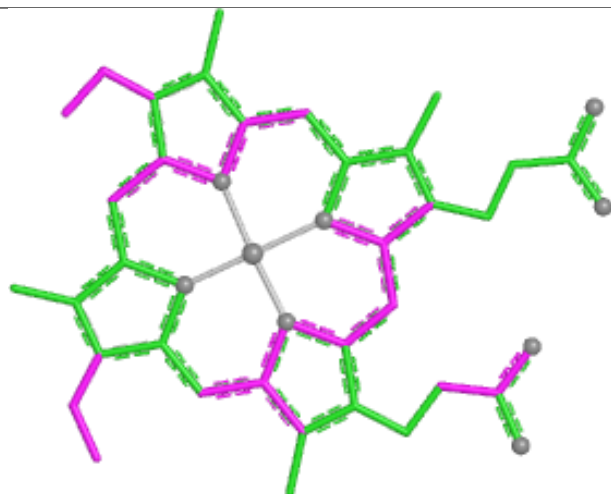




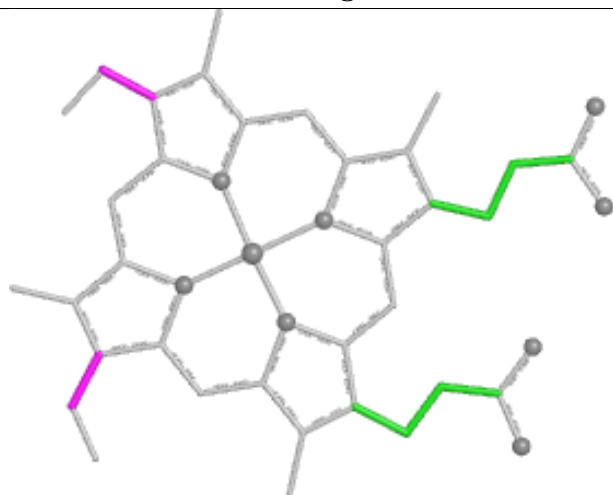
Ligand HEC C 403



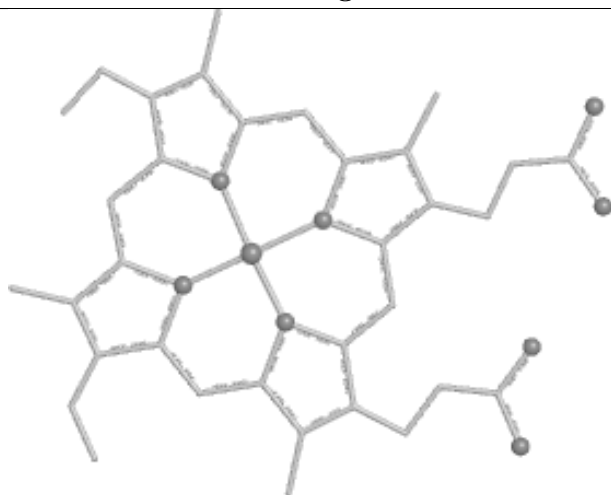
Bond lengths



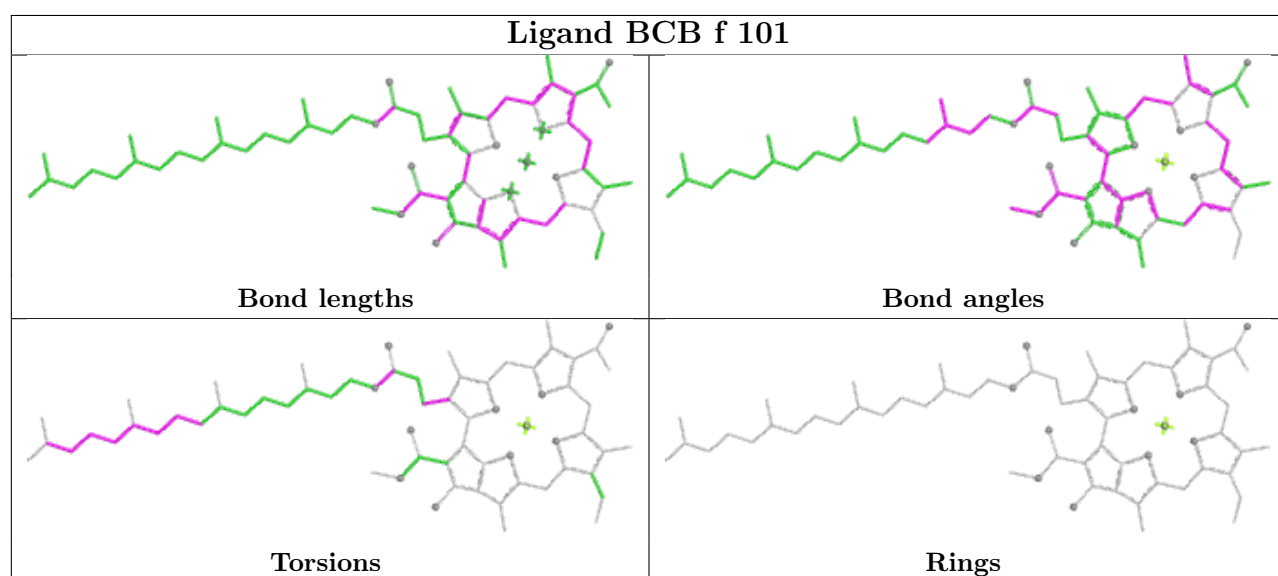
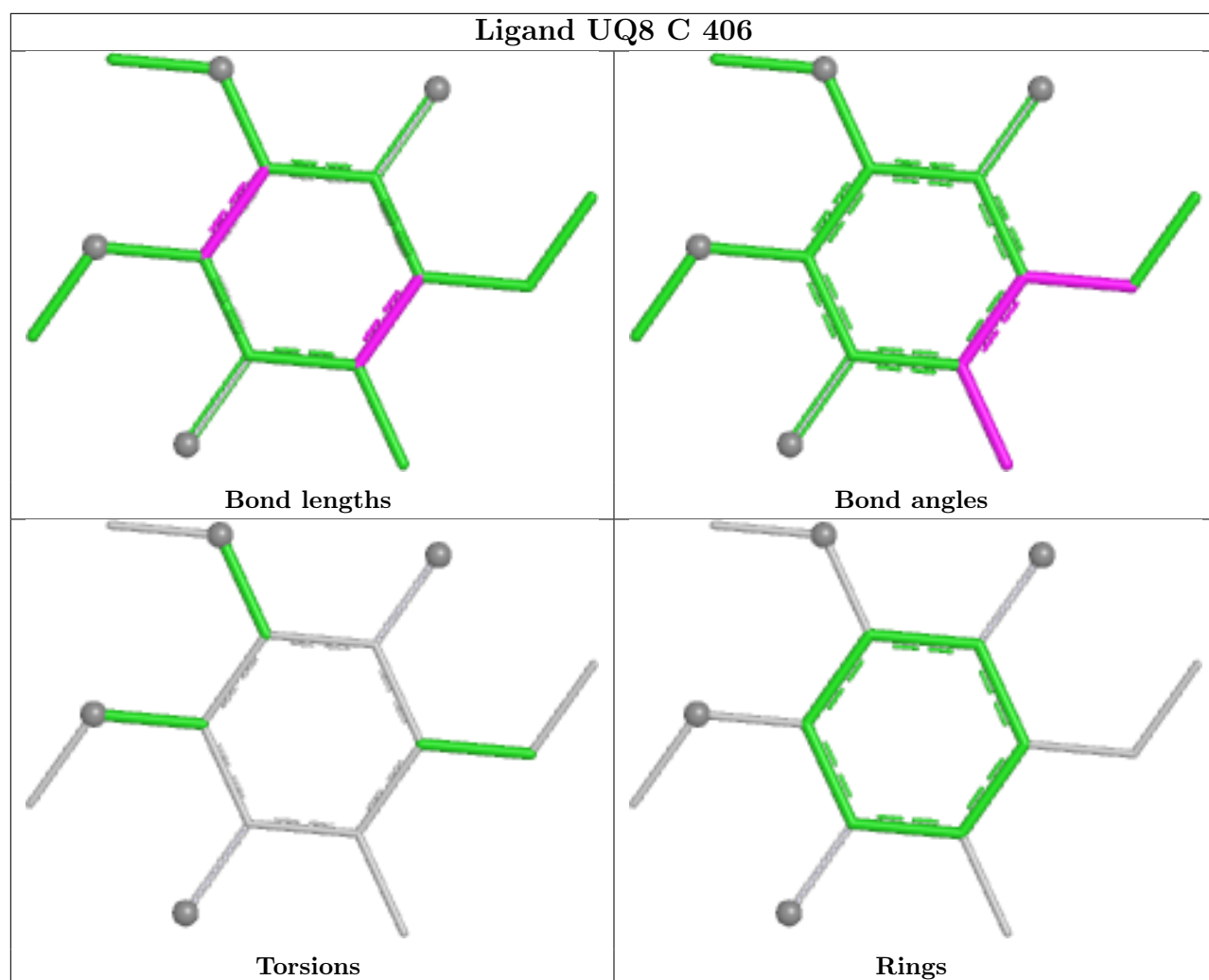
Bond angles

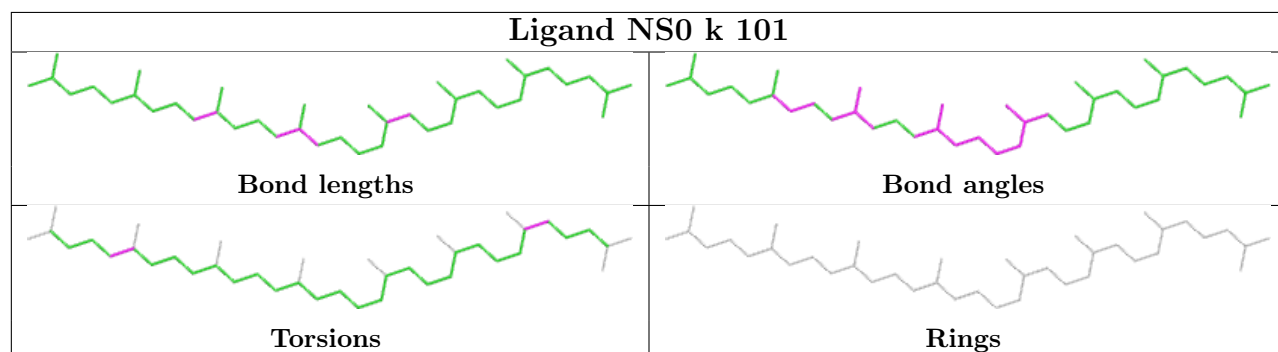
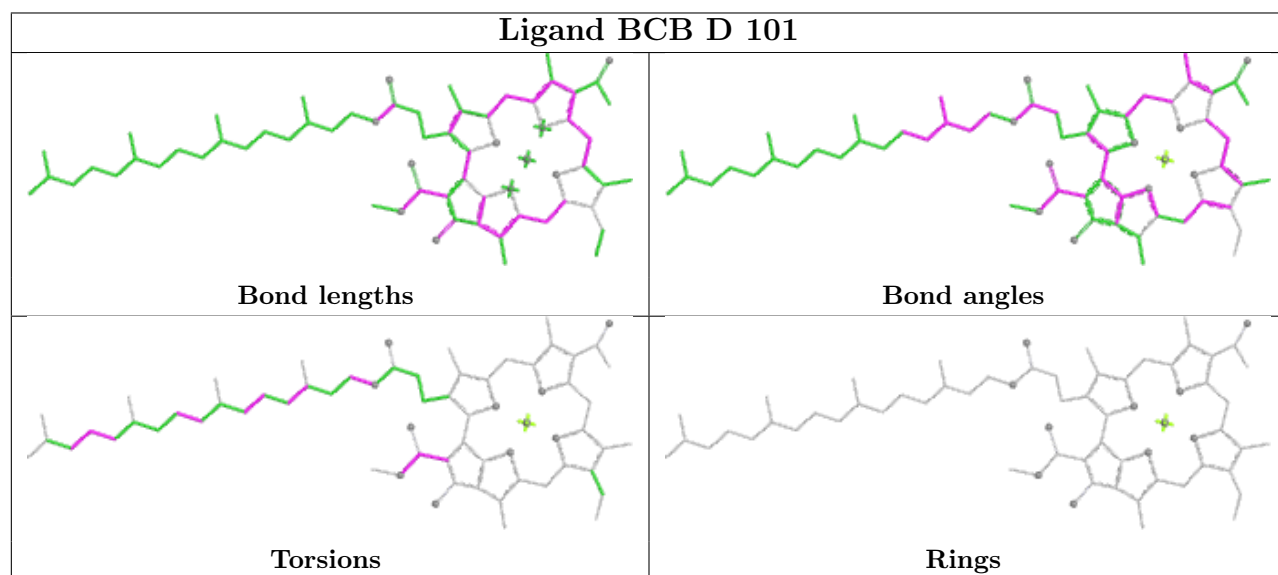
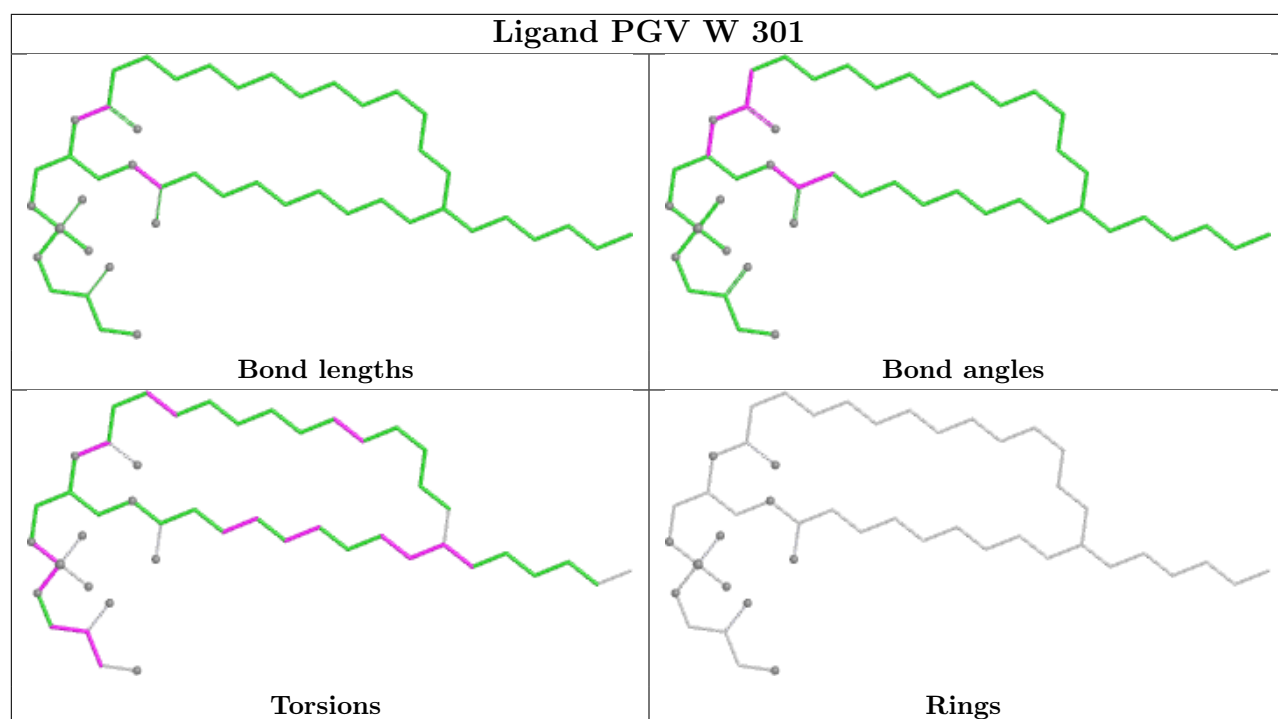


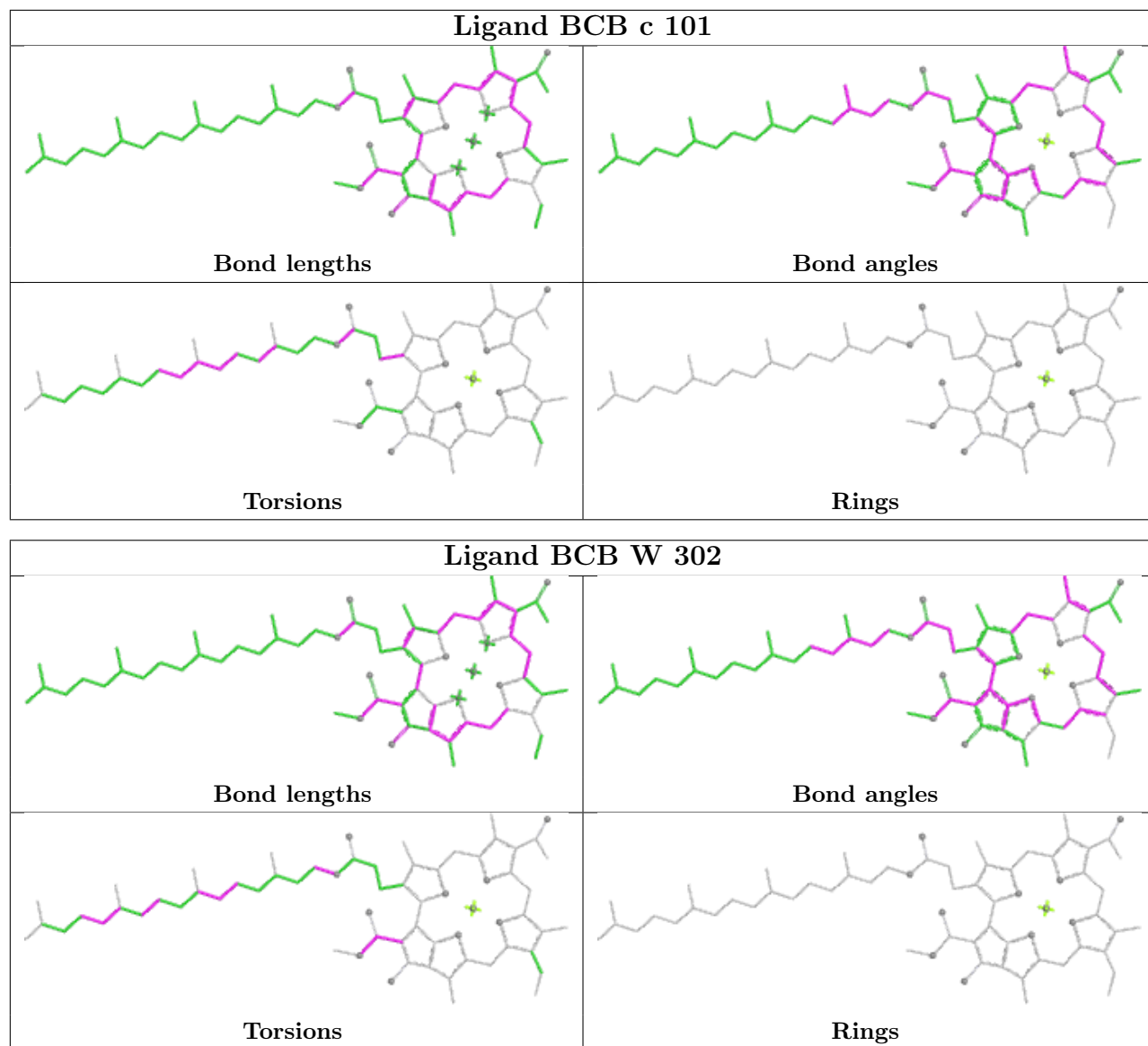
Torsions

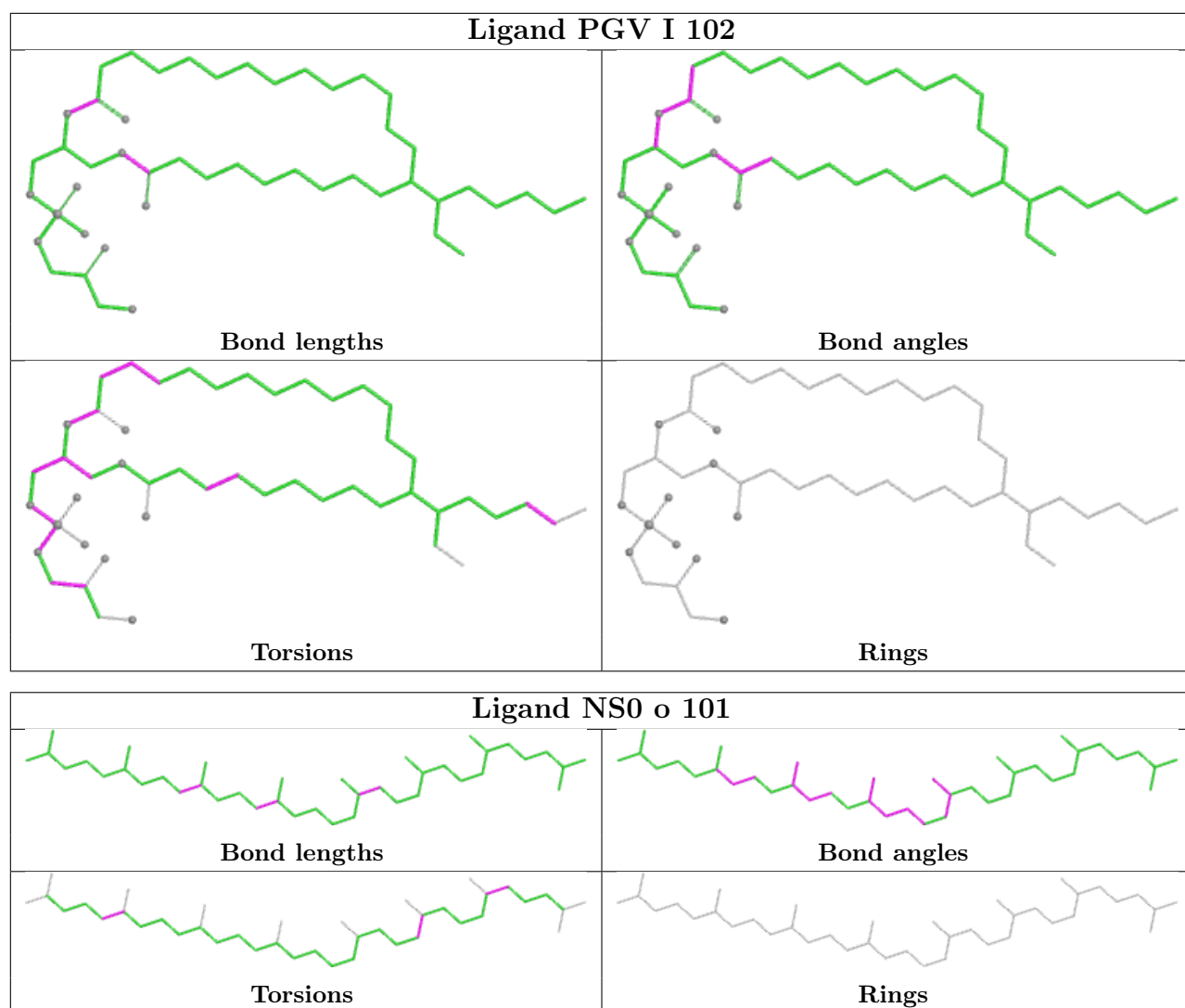


Rings

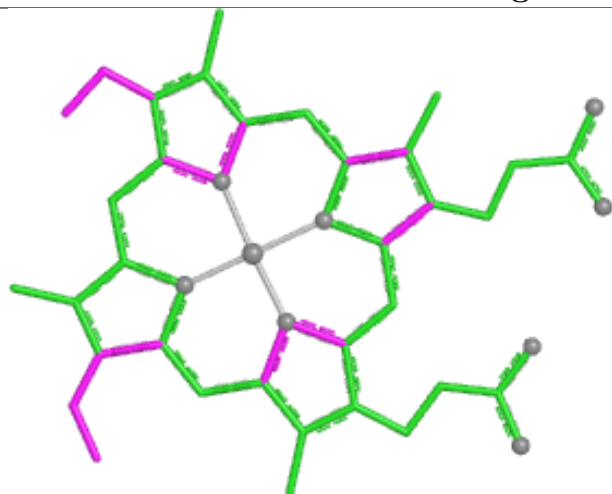




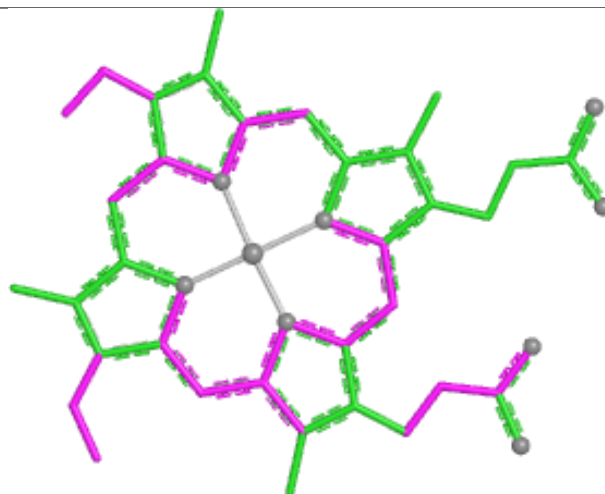




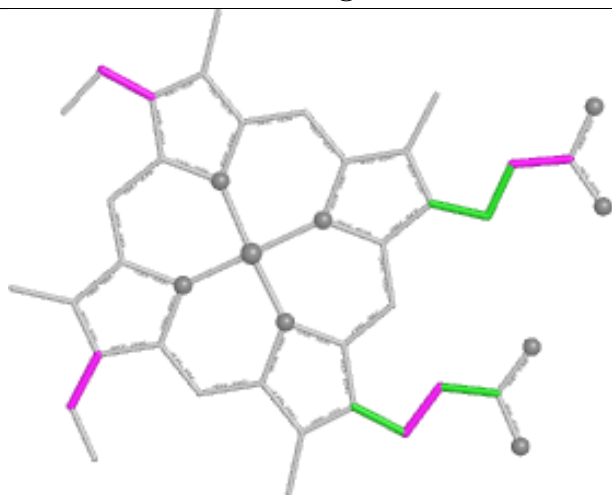
Ligand HEC C 402



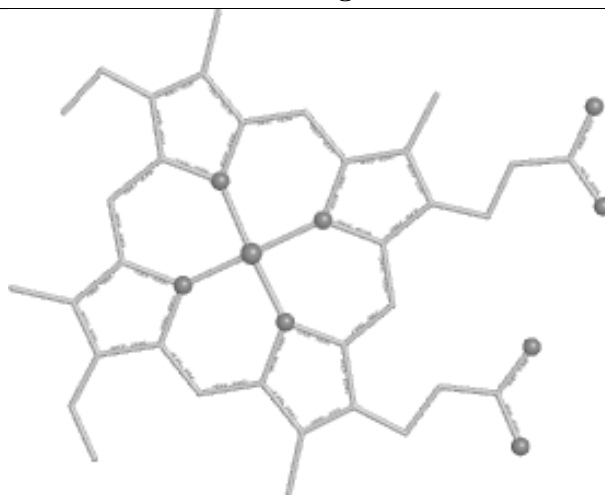
Bond lengths



Bond angles

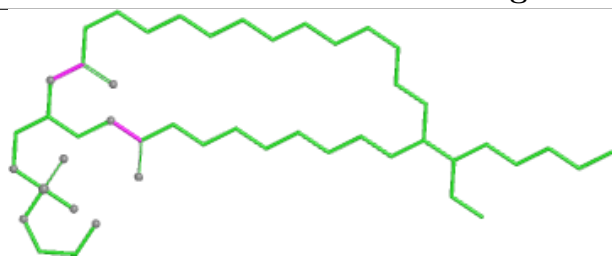


Torsions

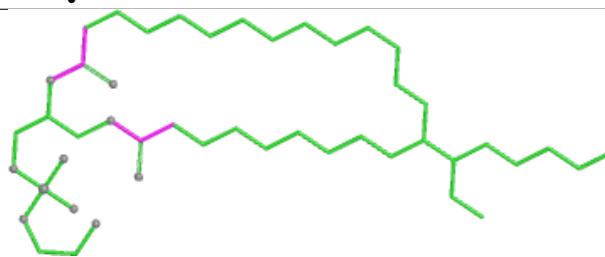


Rings

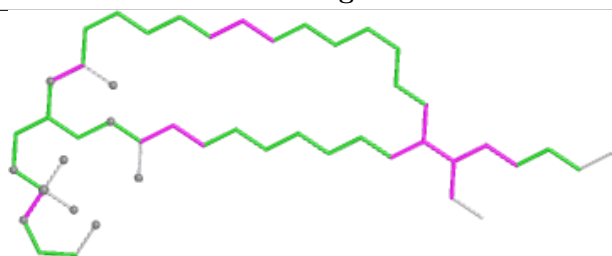
Ligand PGV Q 401



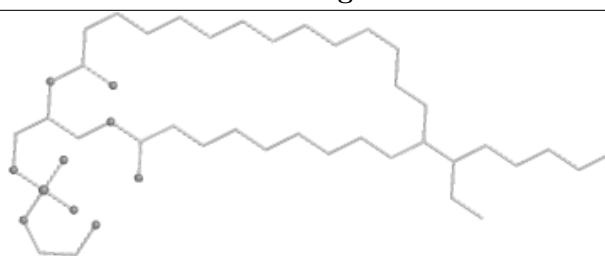
Bond lengths



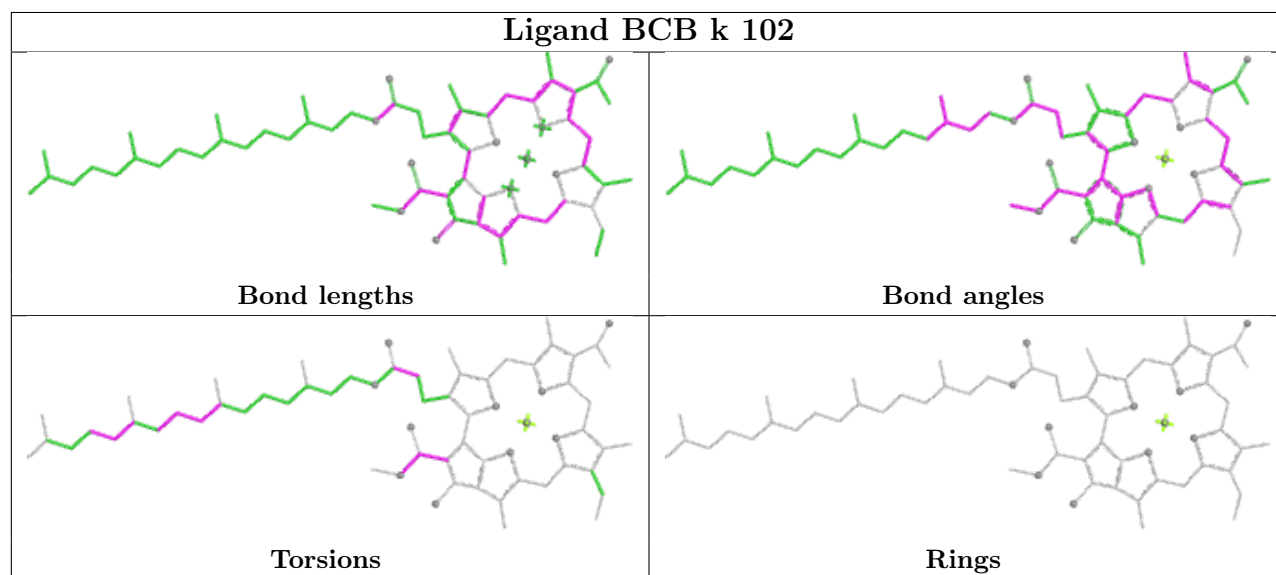
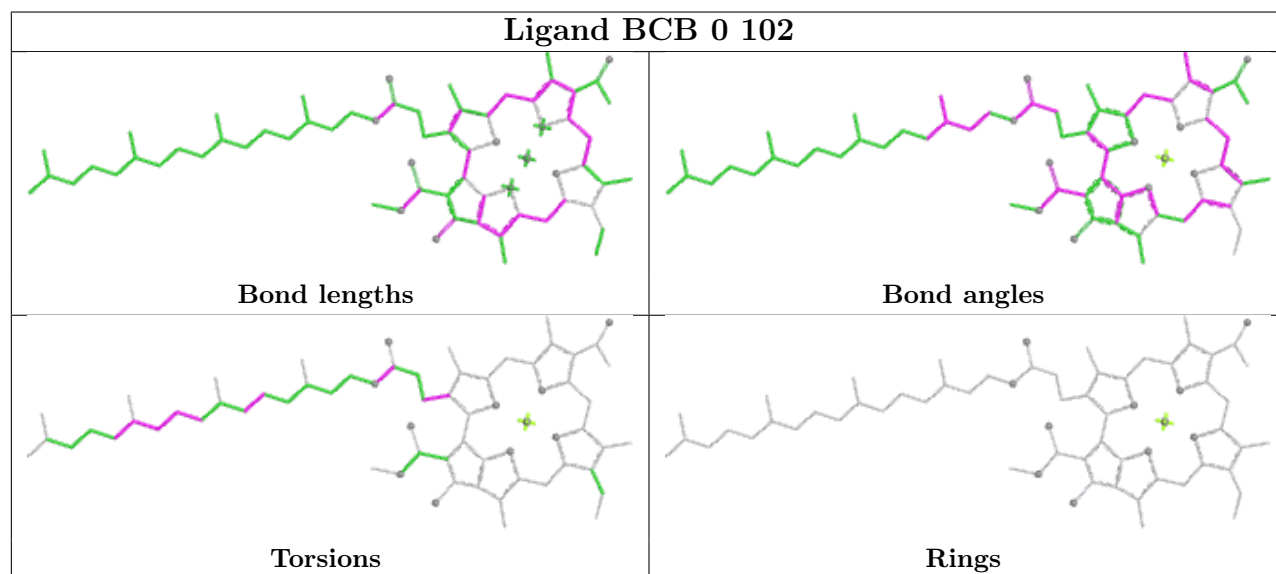
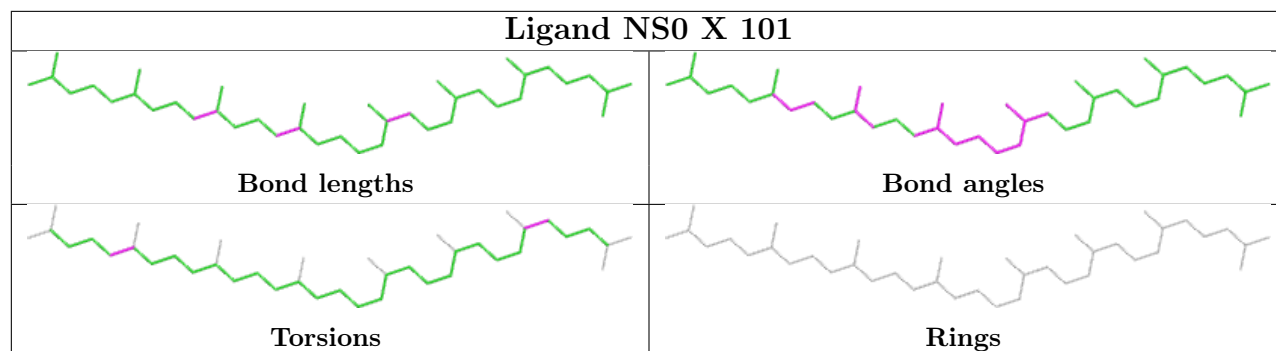
Bond angles

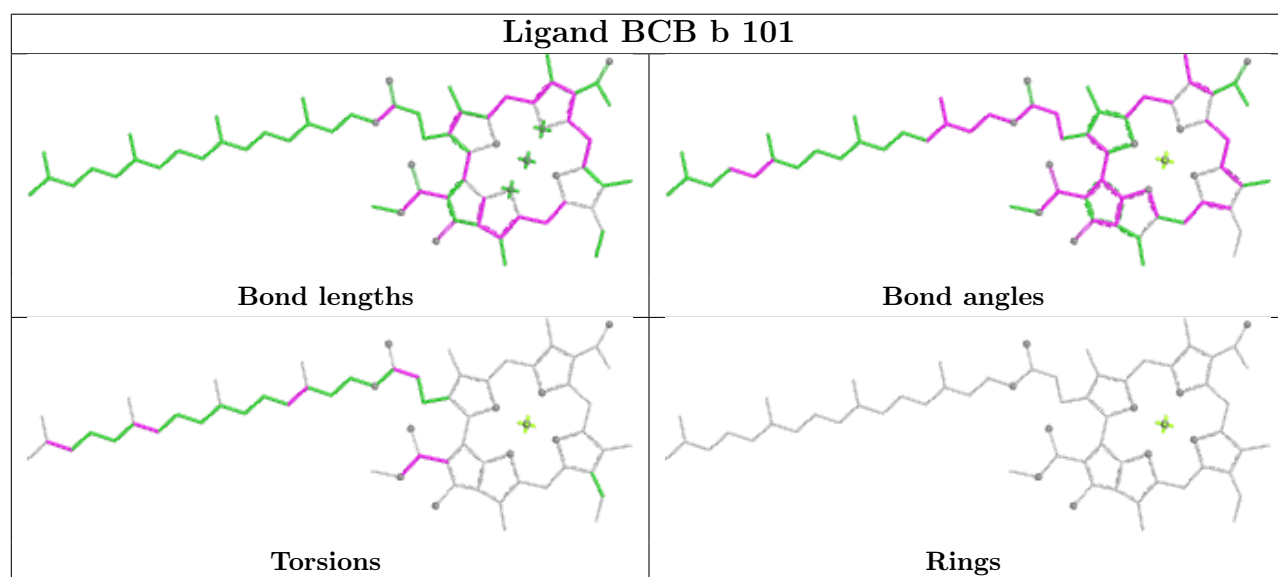
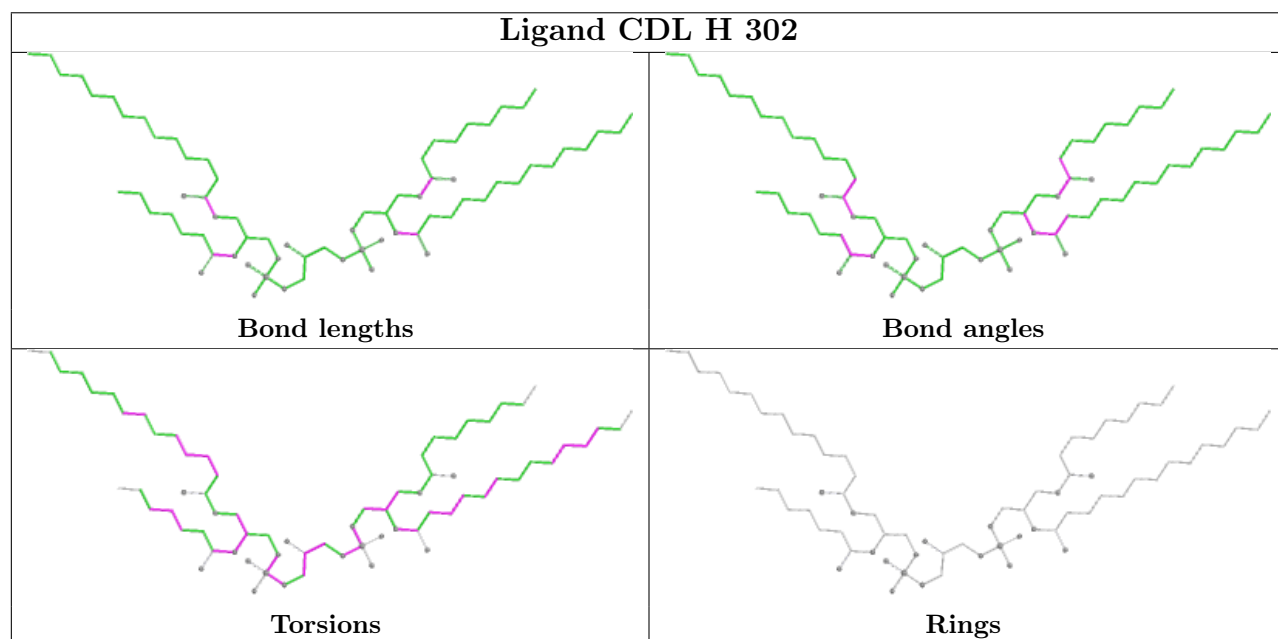
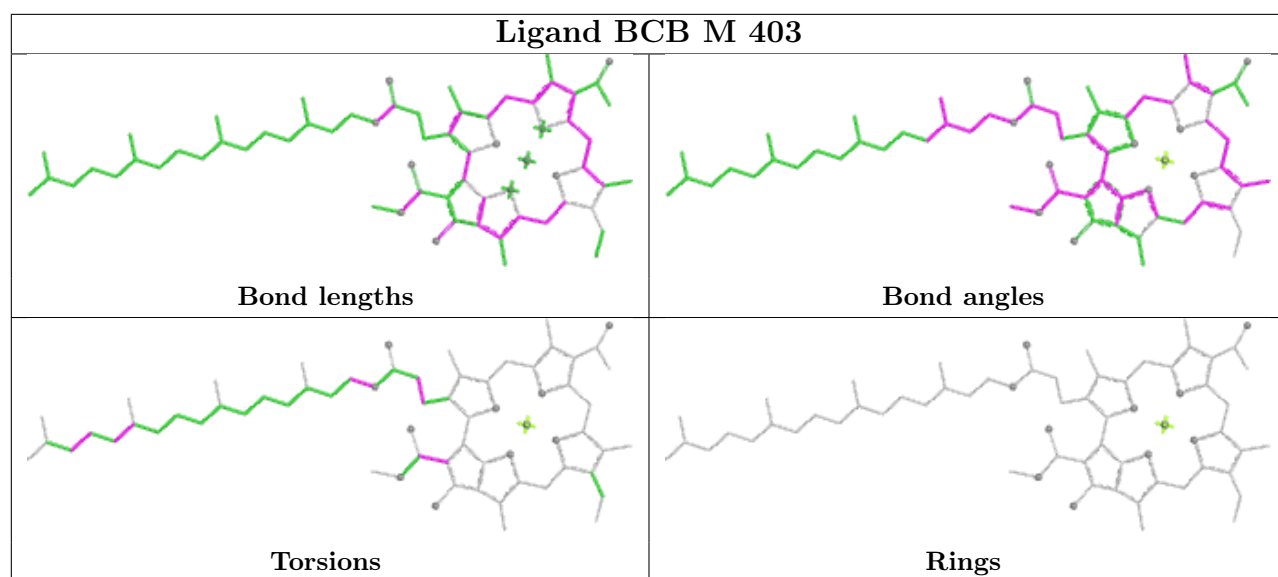


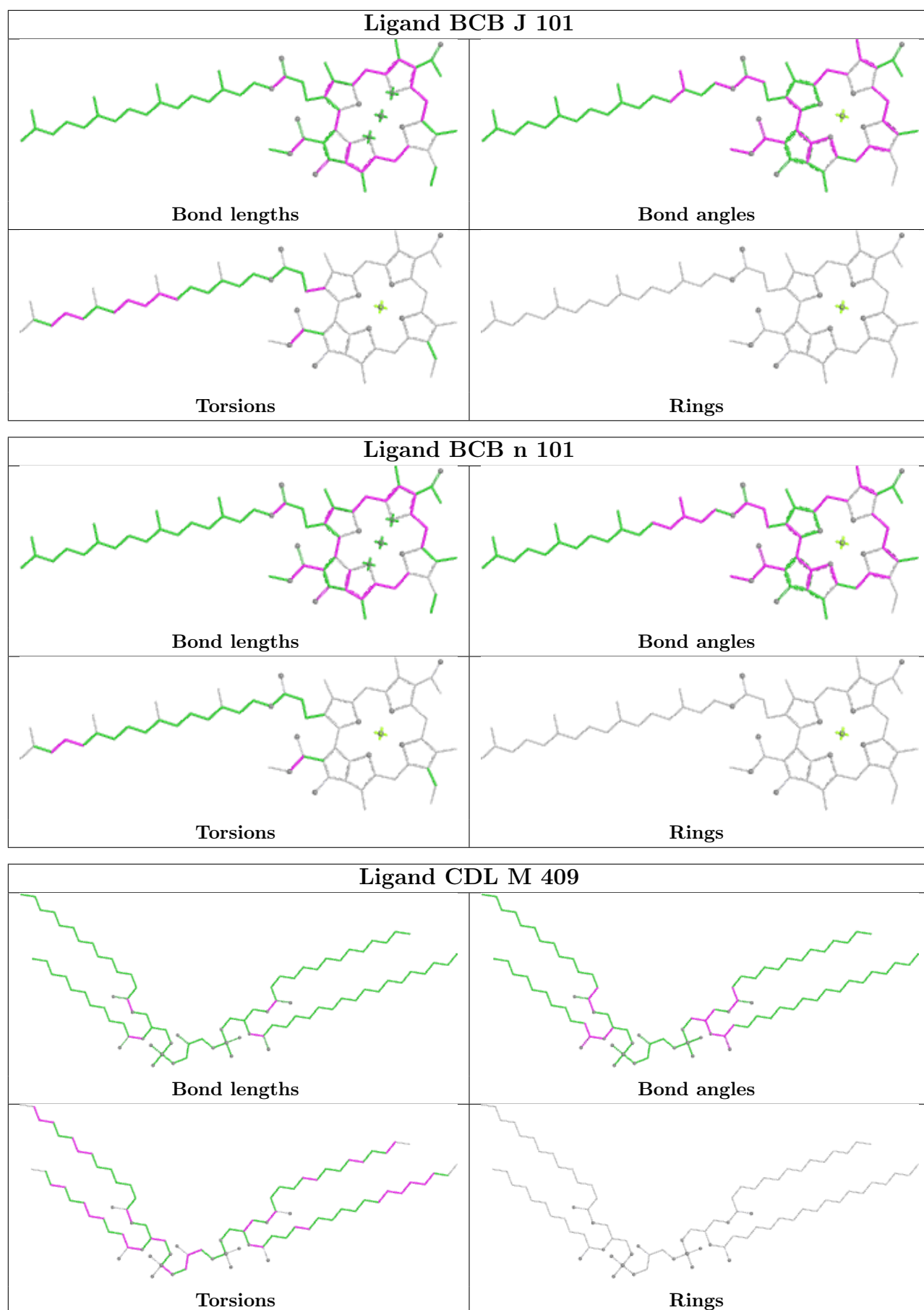
Torsions

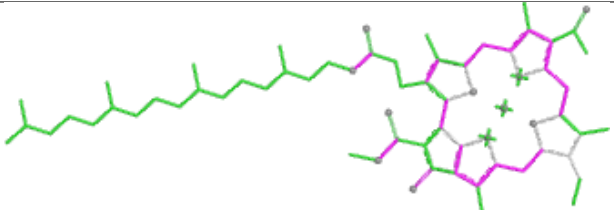
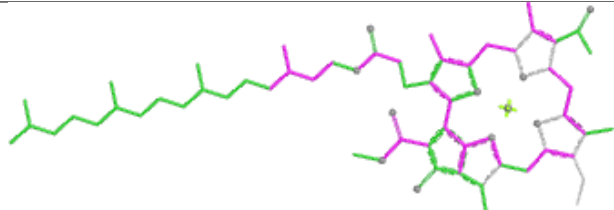
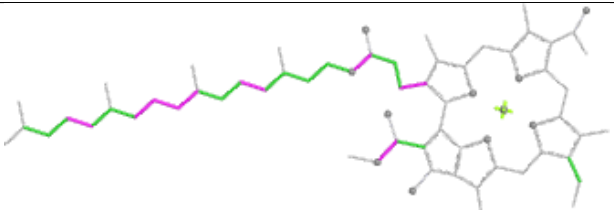
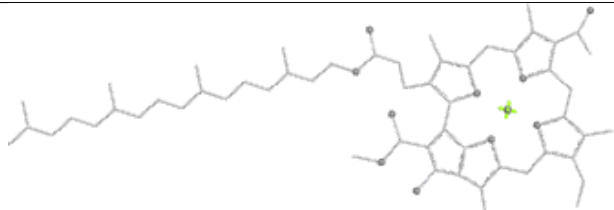


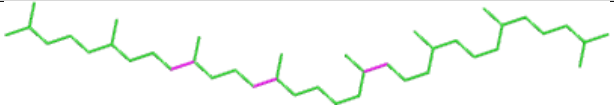
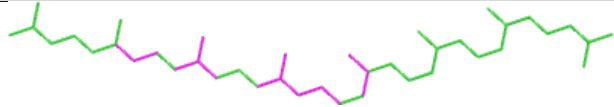
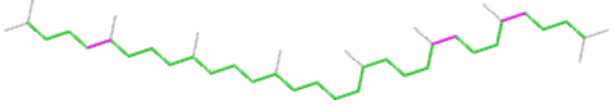
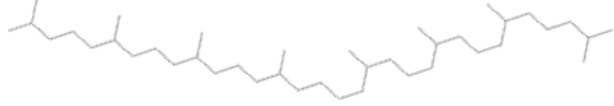
Rings

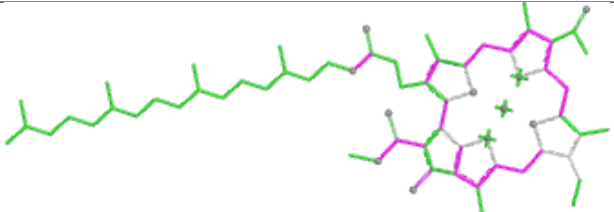
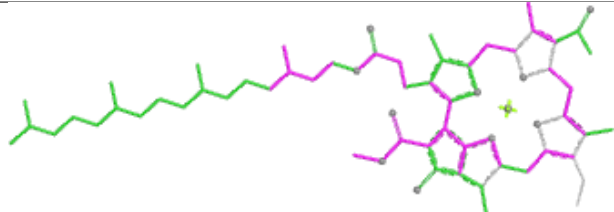
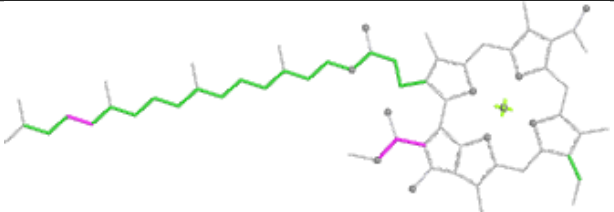
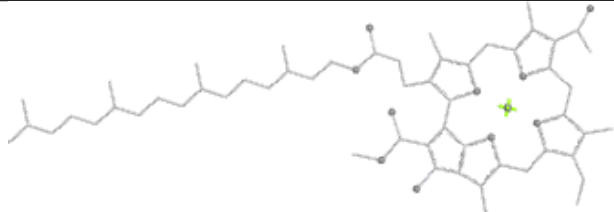


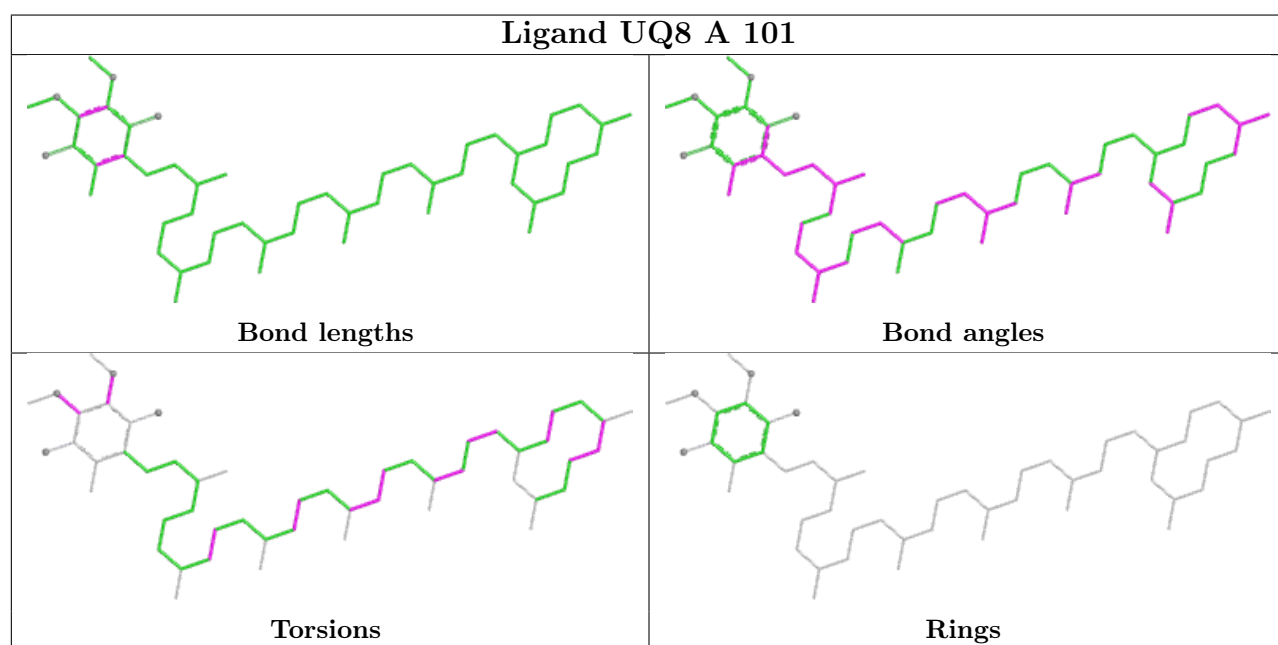
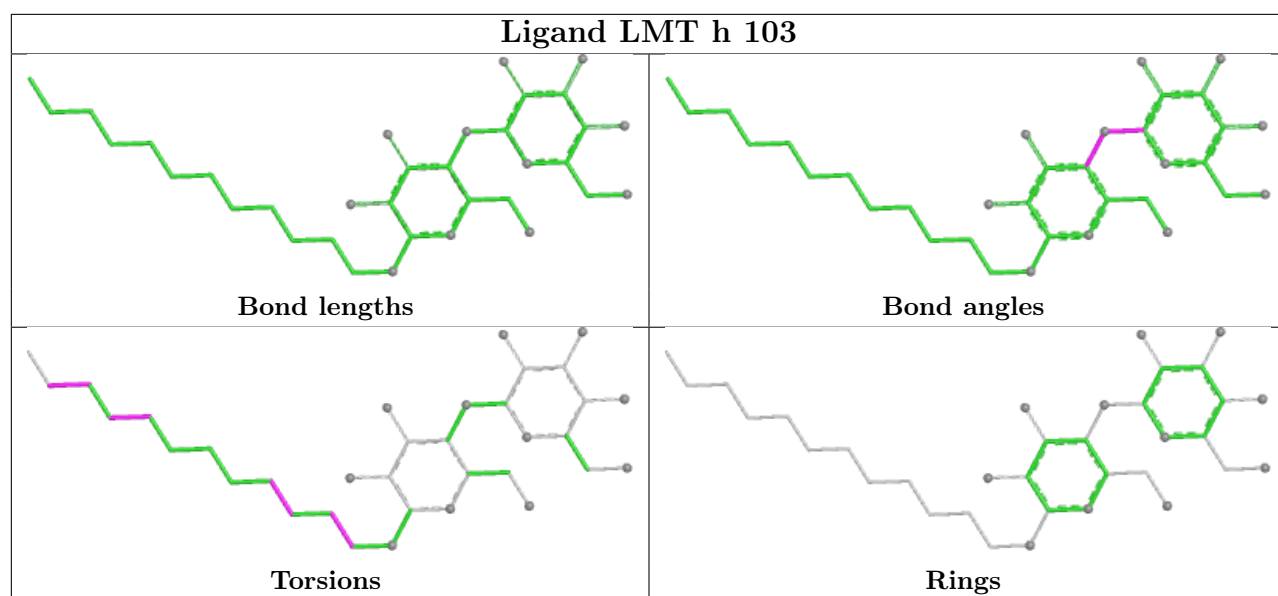


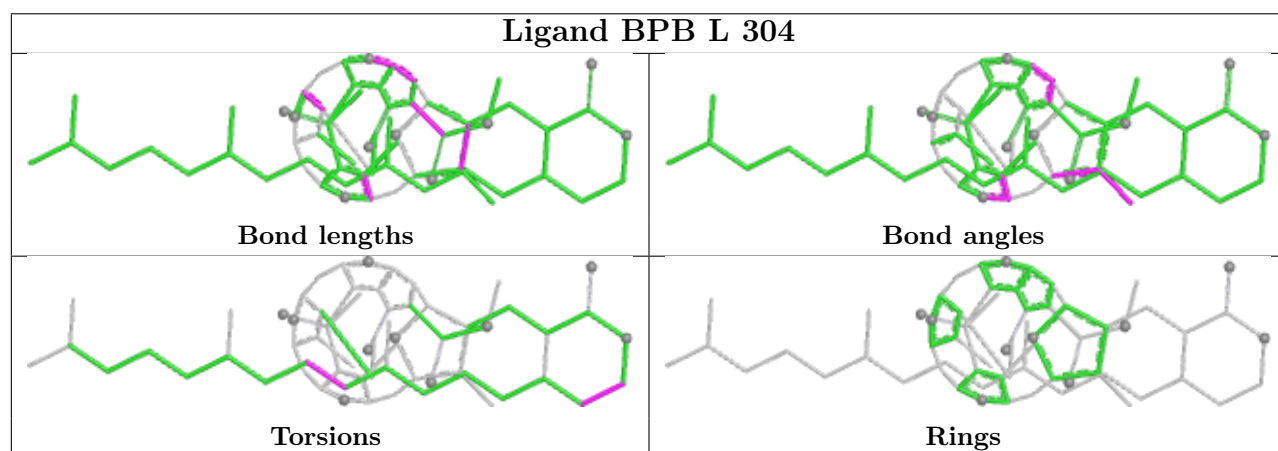
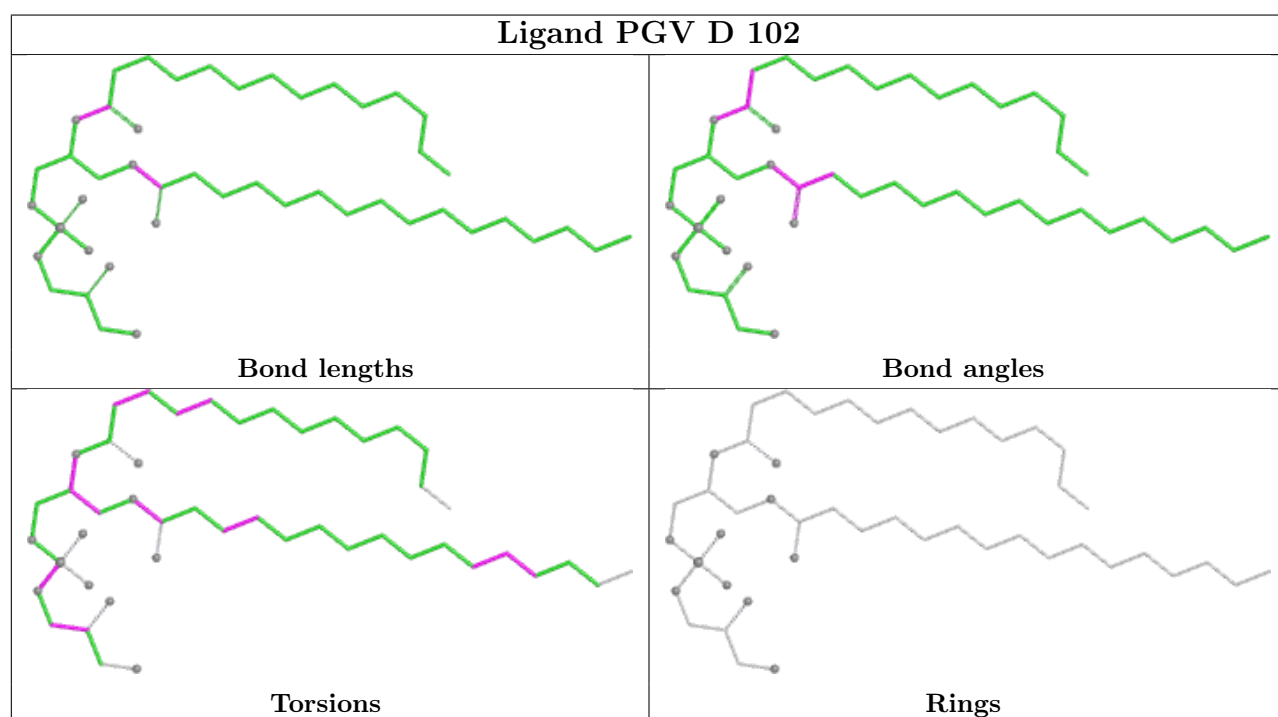
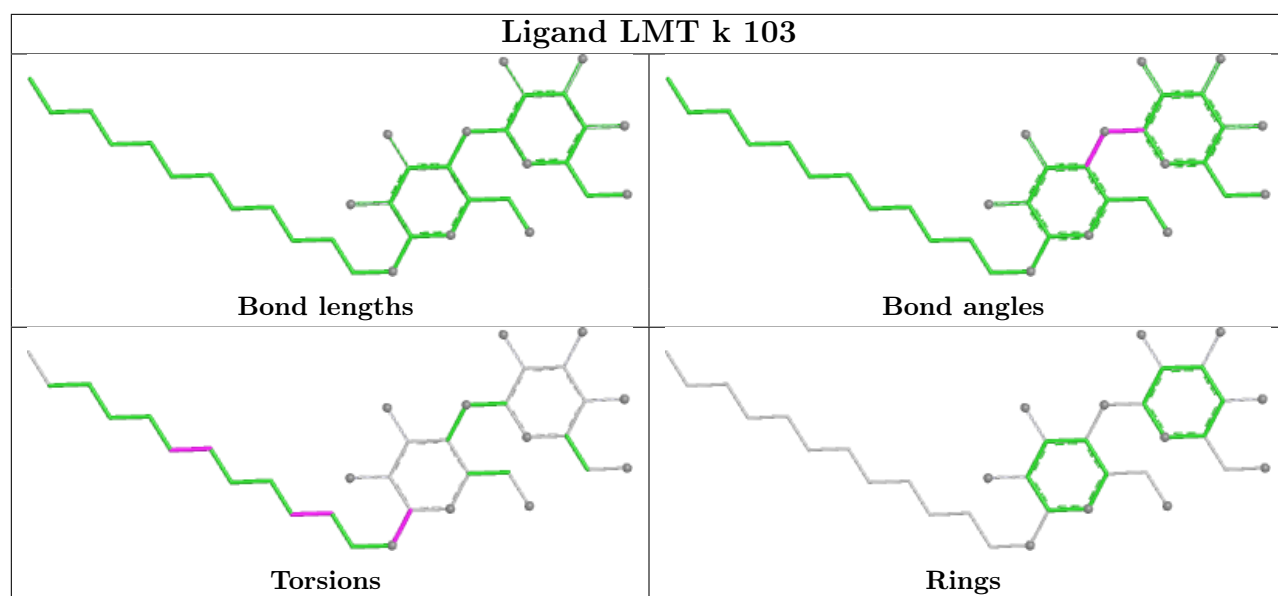


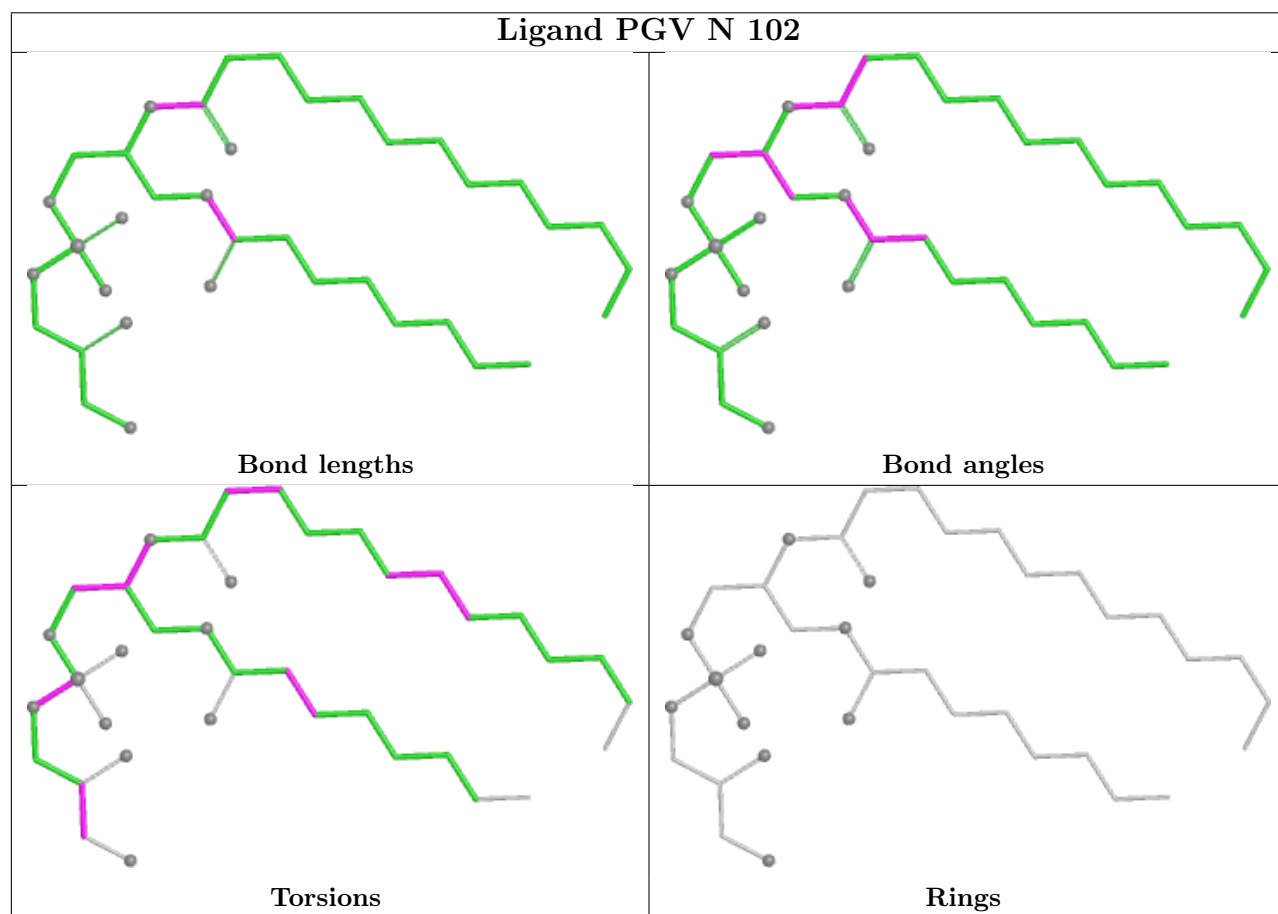
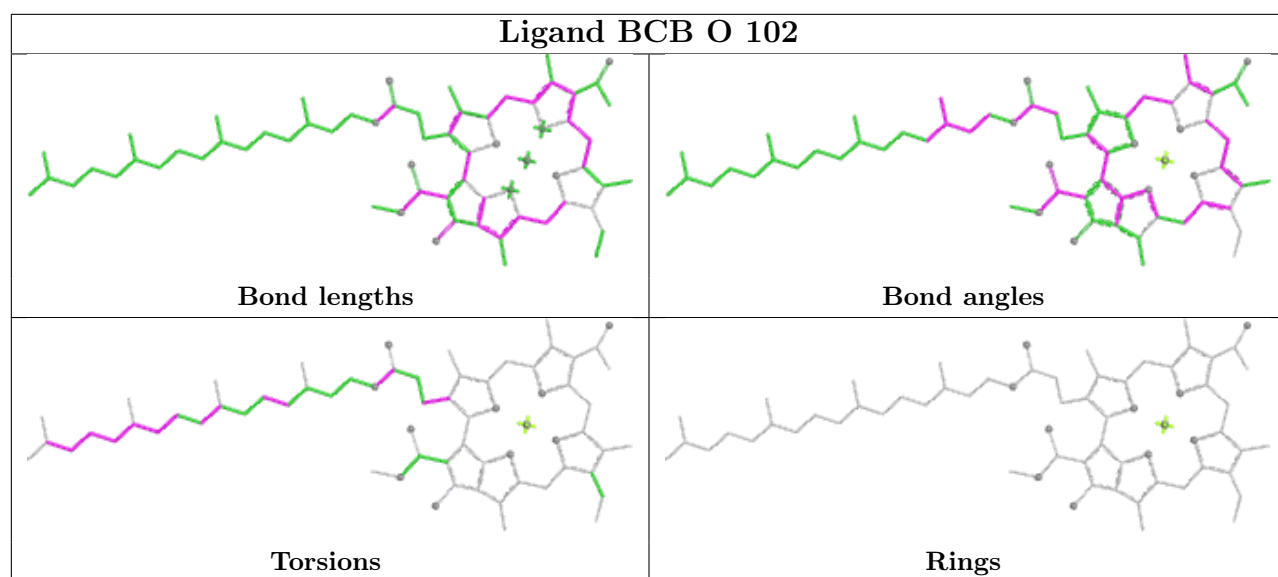
Ligand BCB r 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

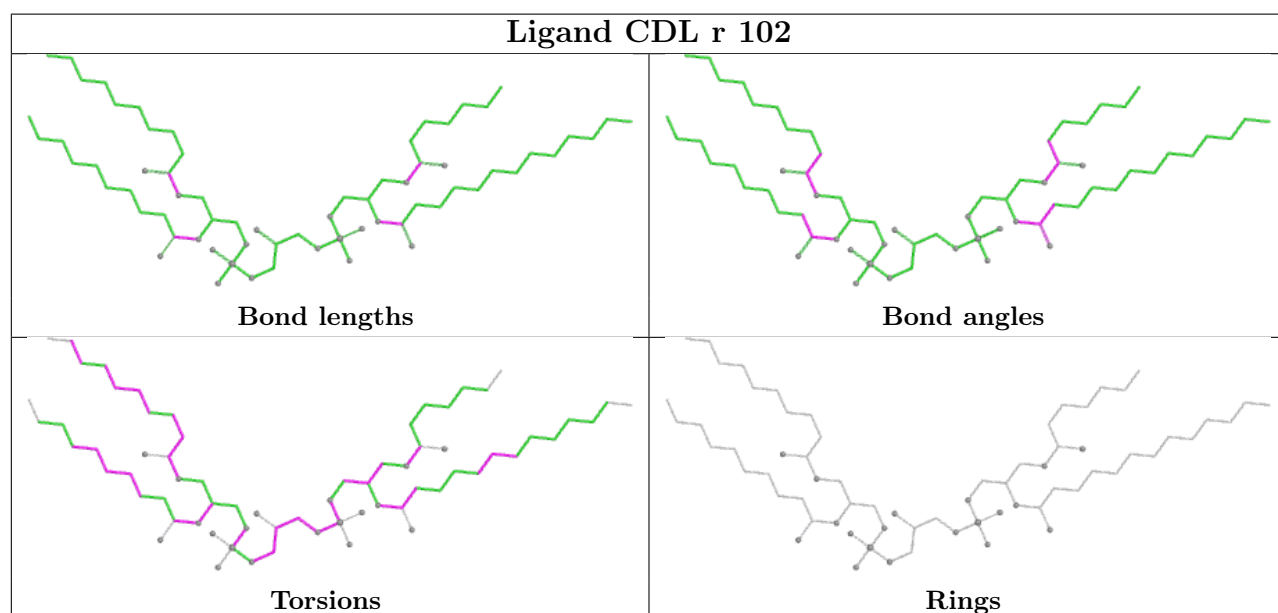
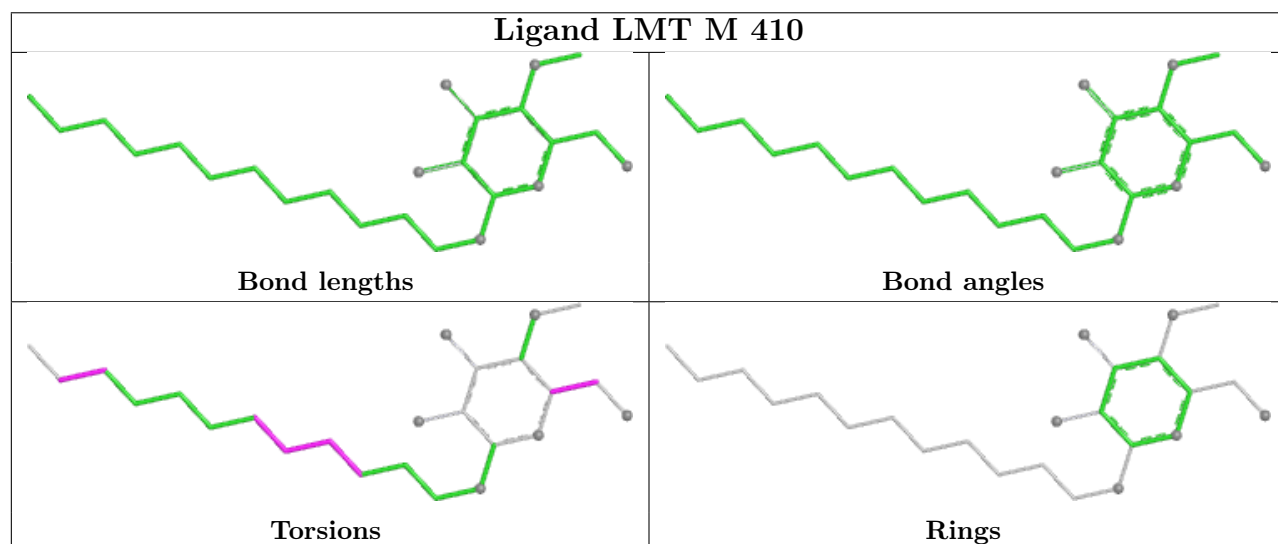
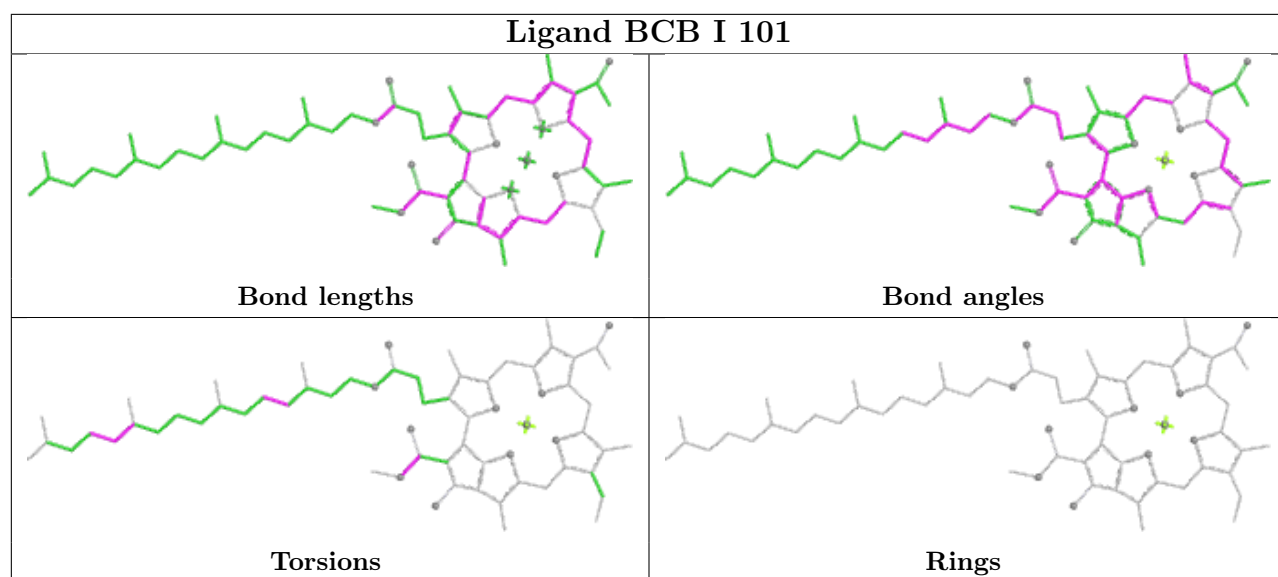
Ligand NS0 R 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

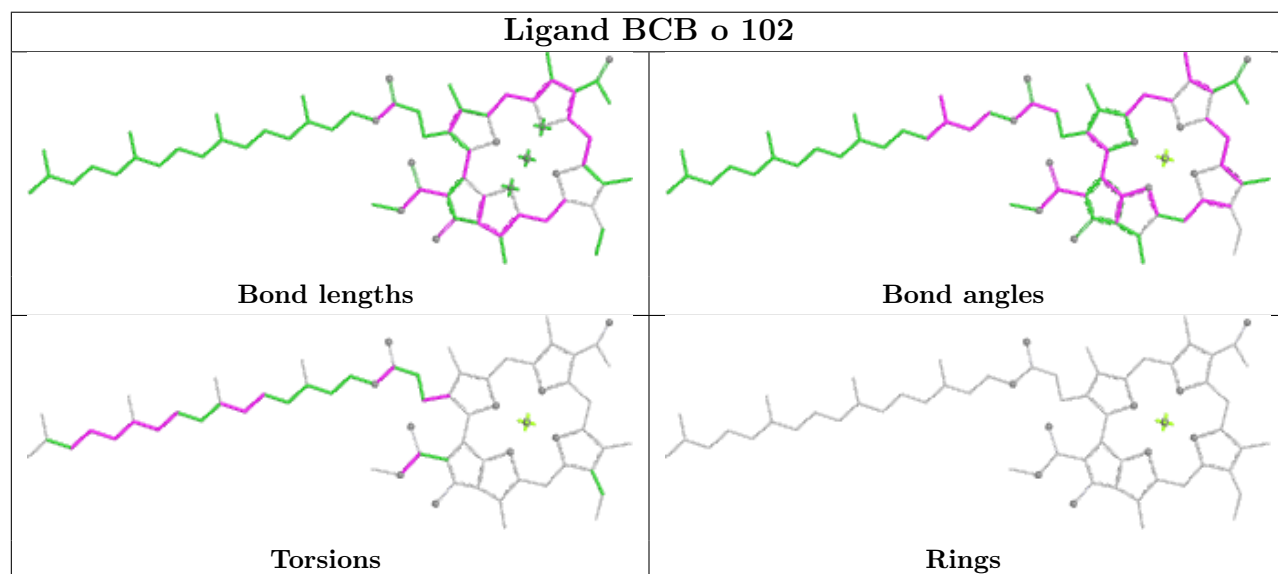
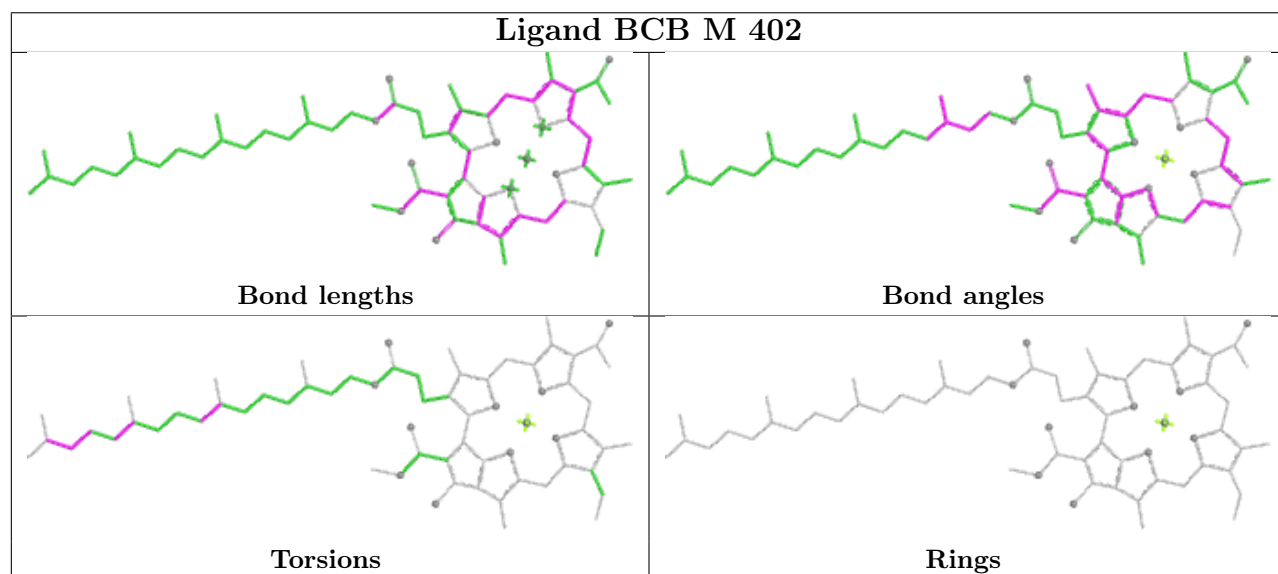
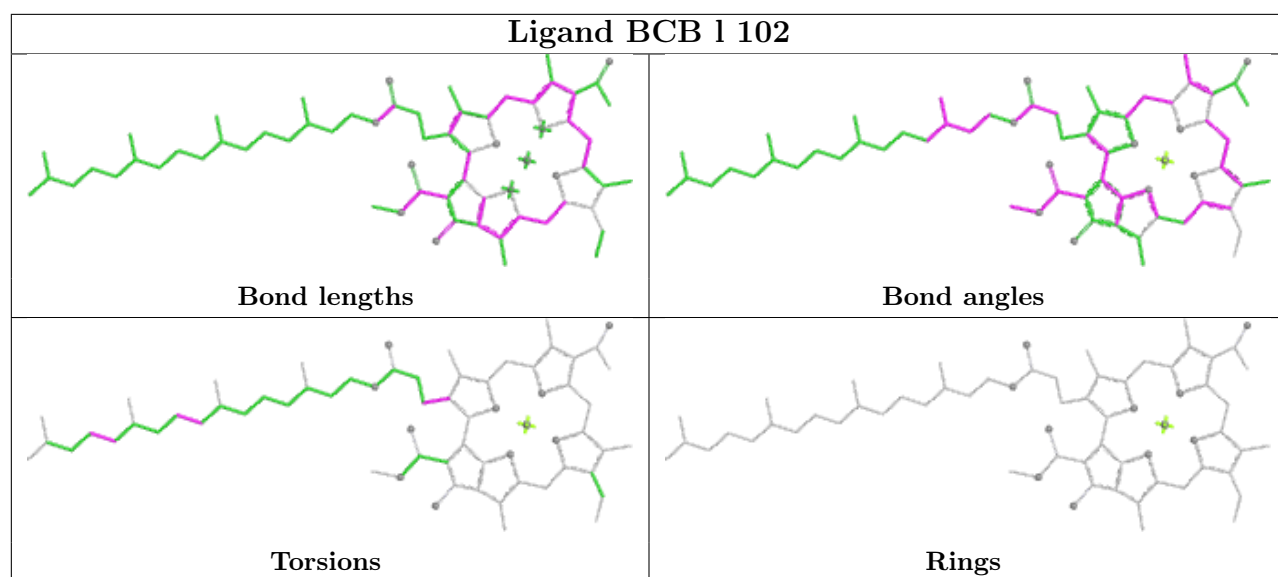
Ligand BCB h 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

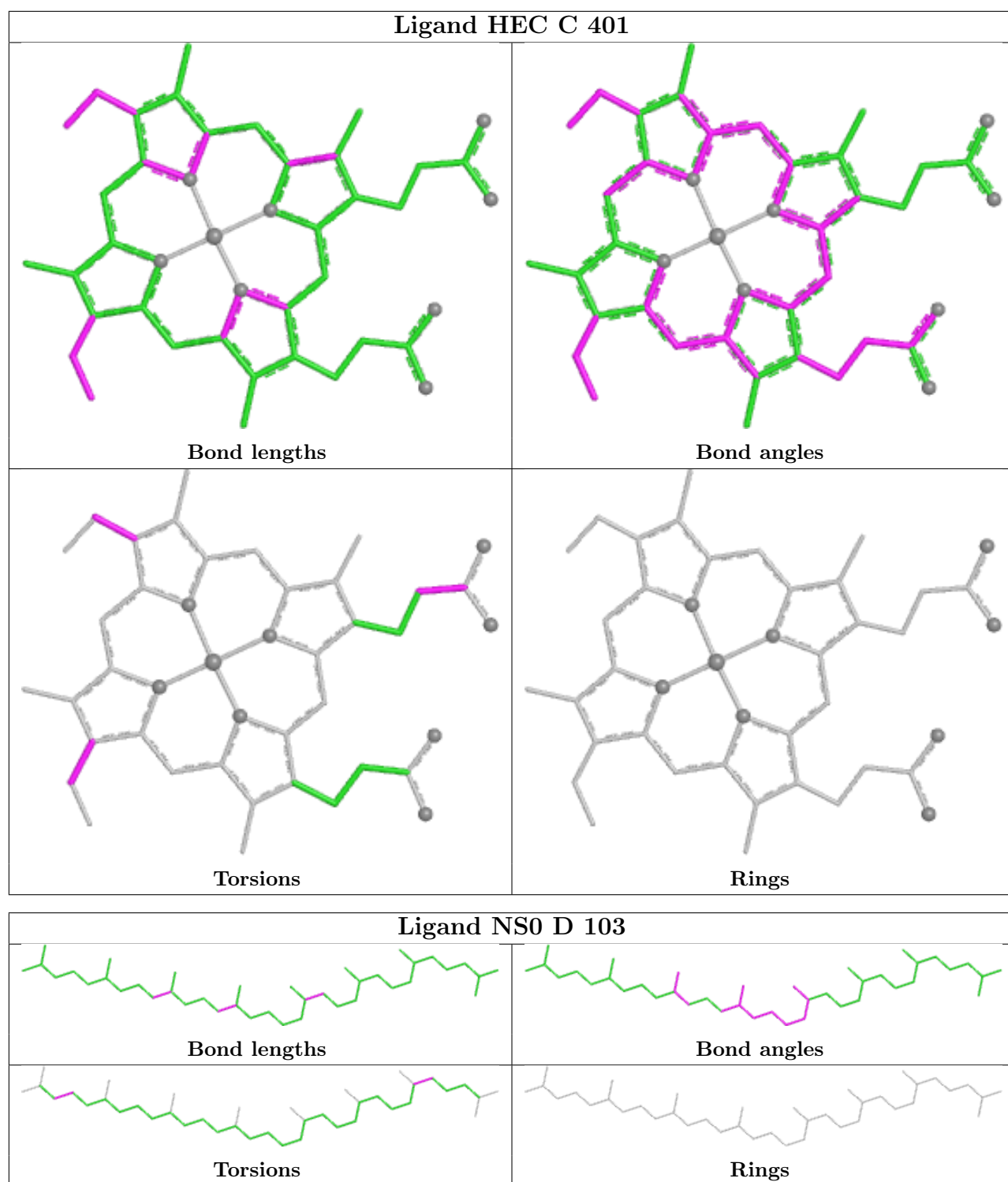


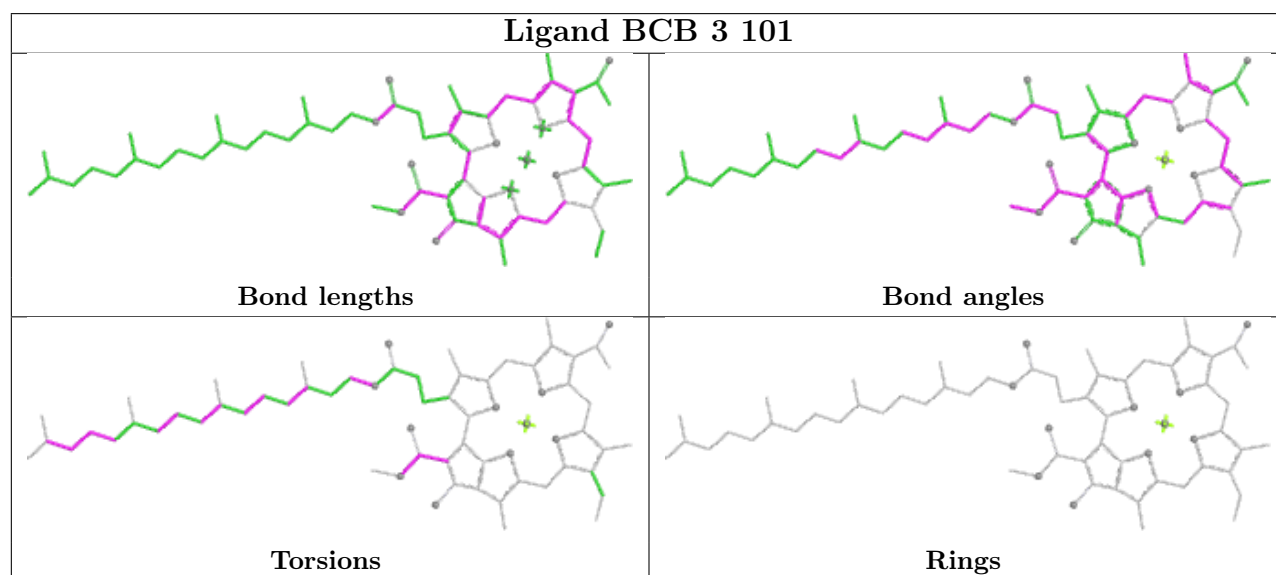
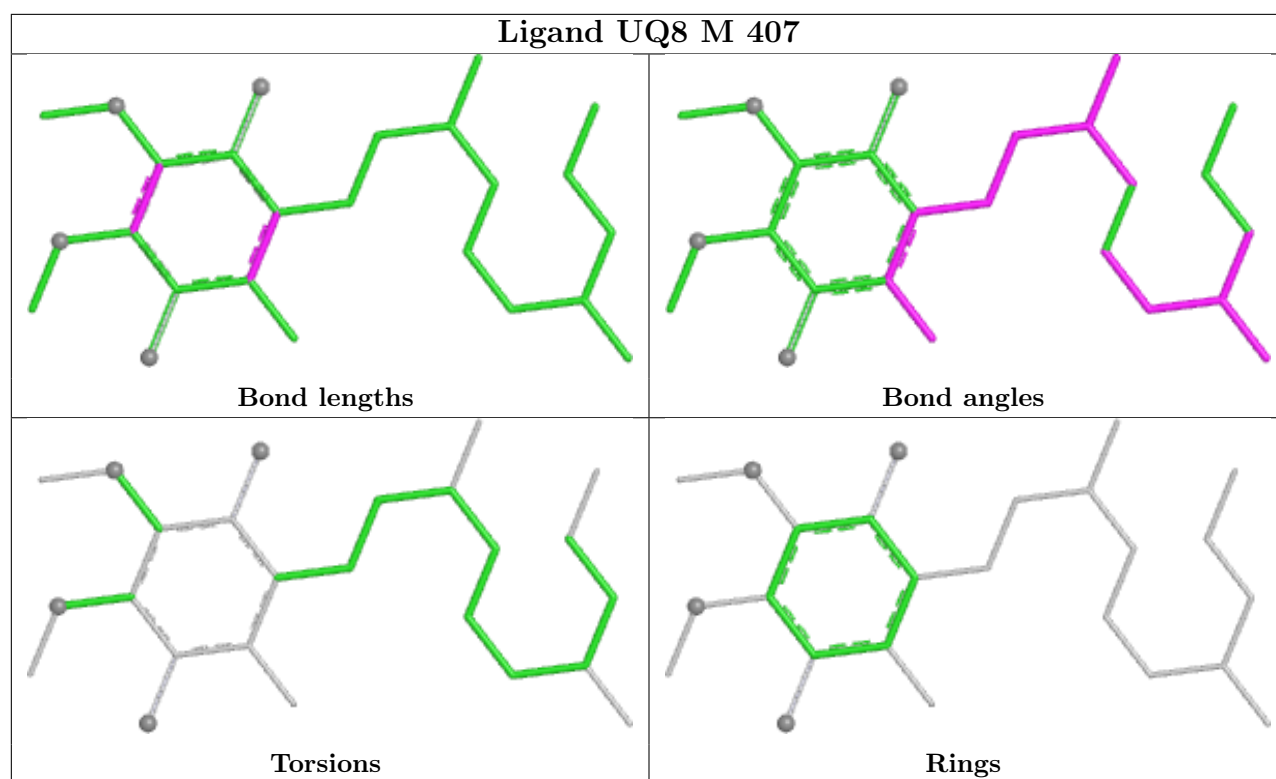


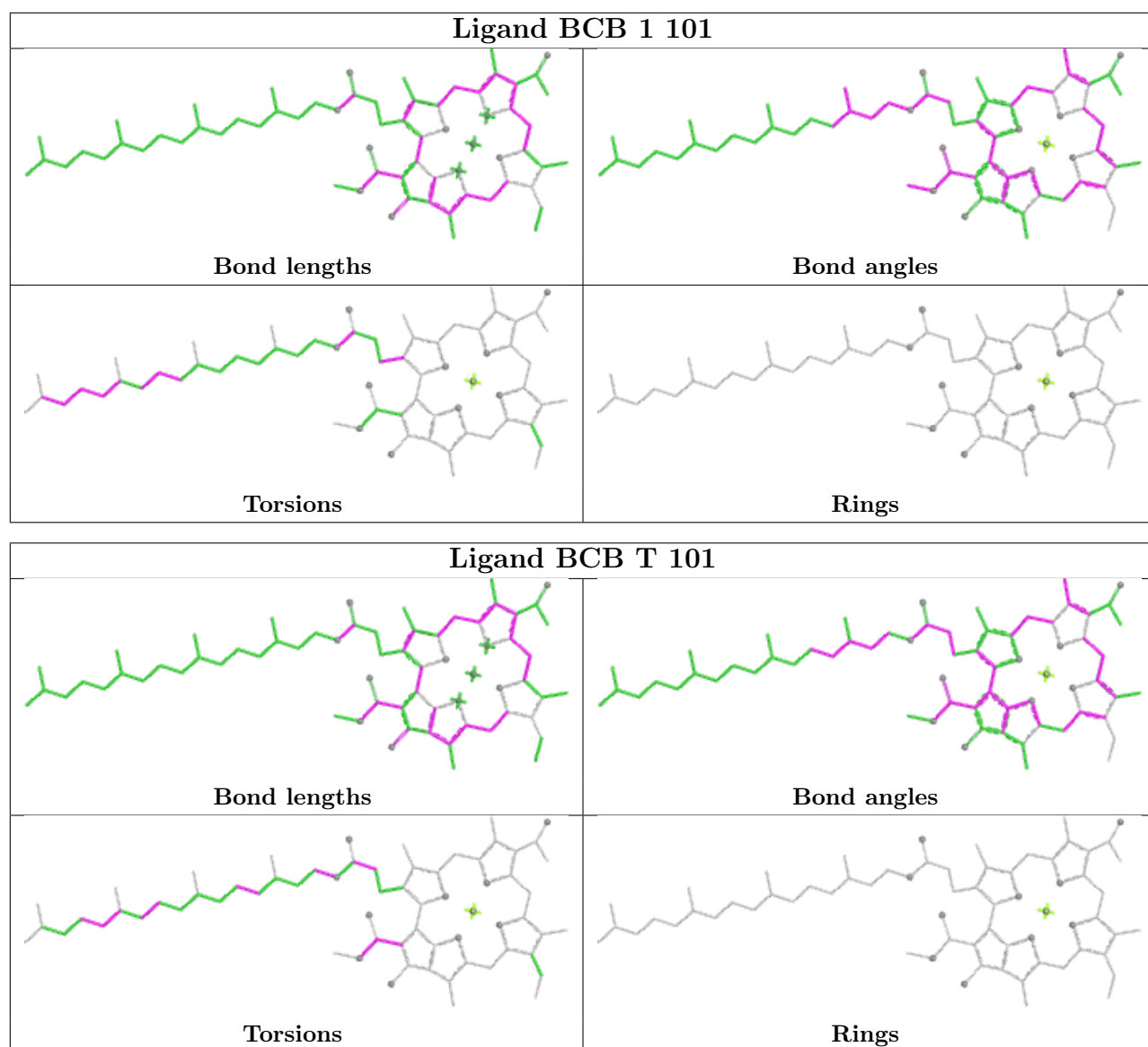


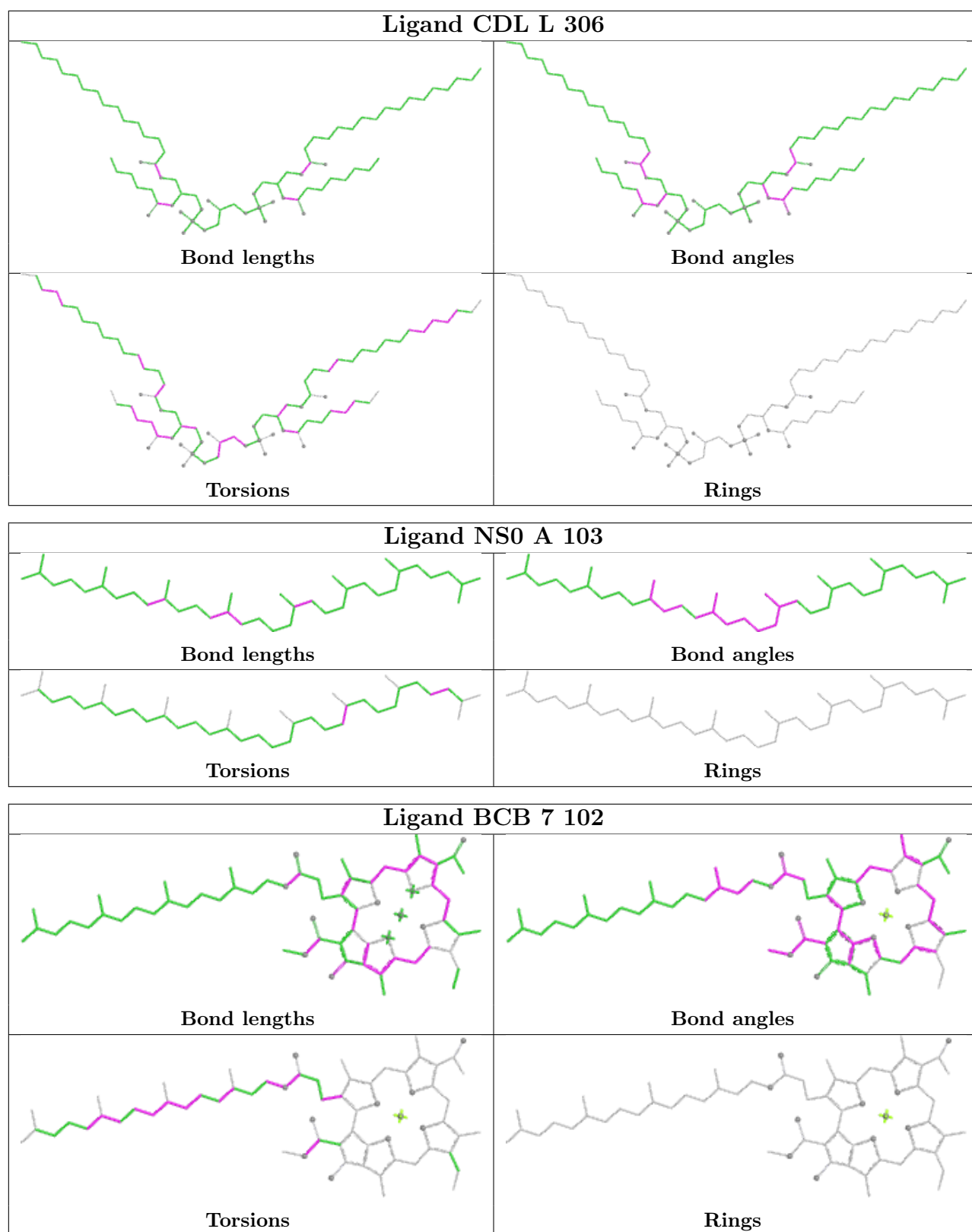




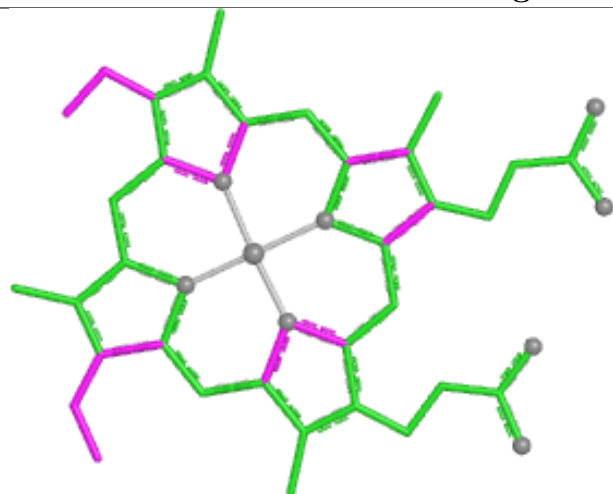




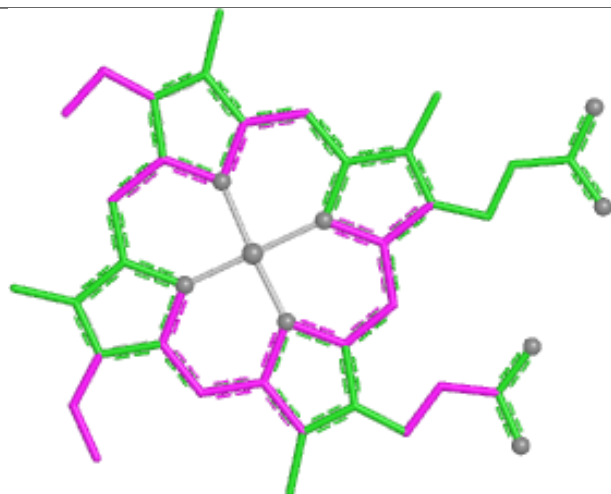




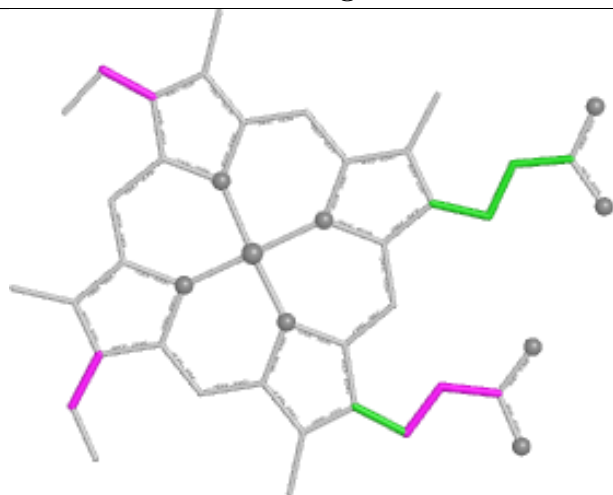
Ligand HEC C 404



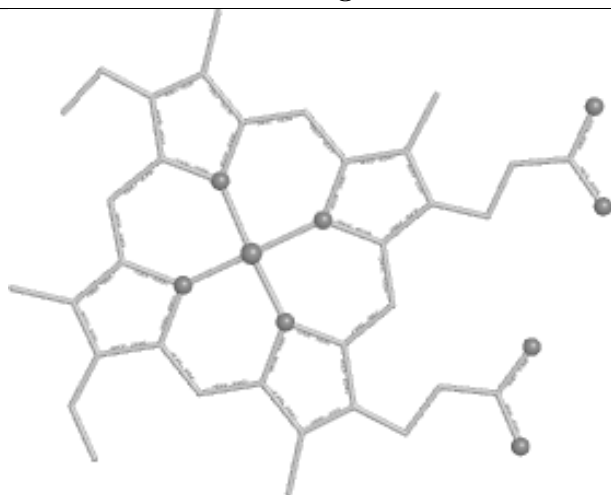
Bond lengths



Bond angles

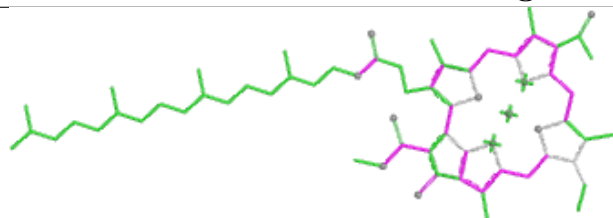


Torsions

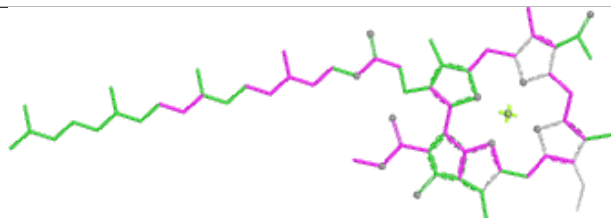


Rings

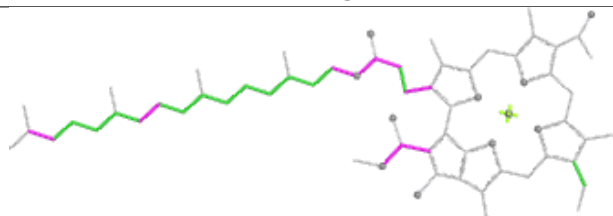
Ligand BCB 9 101



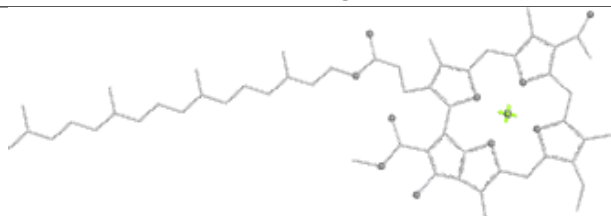
Bond lengths



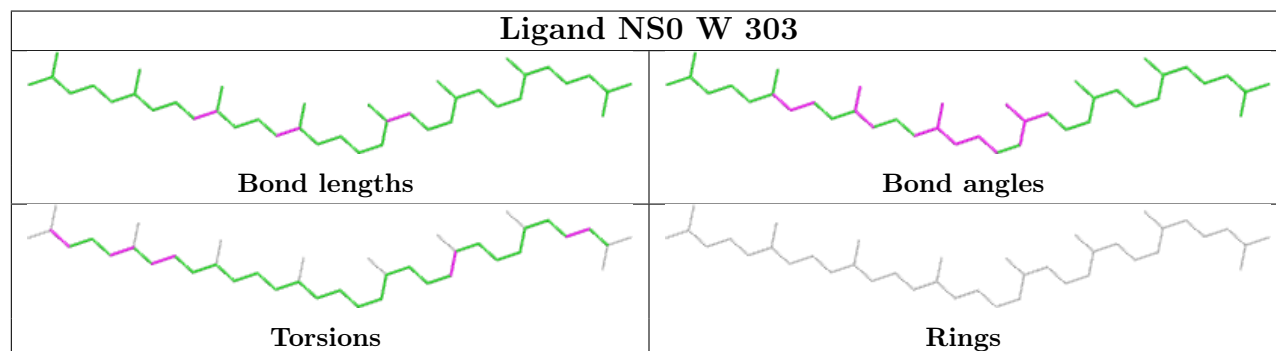
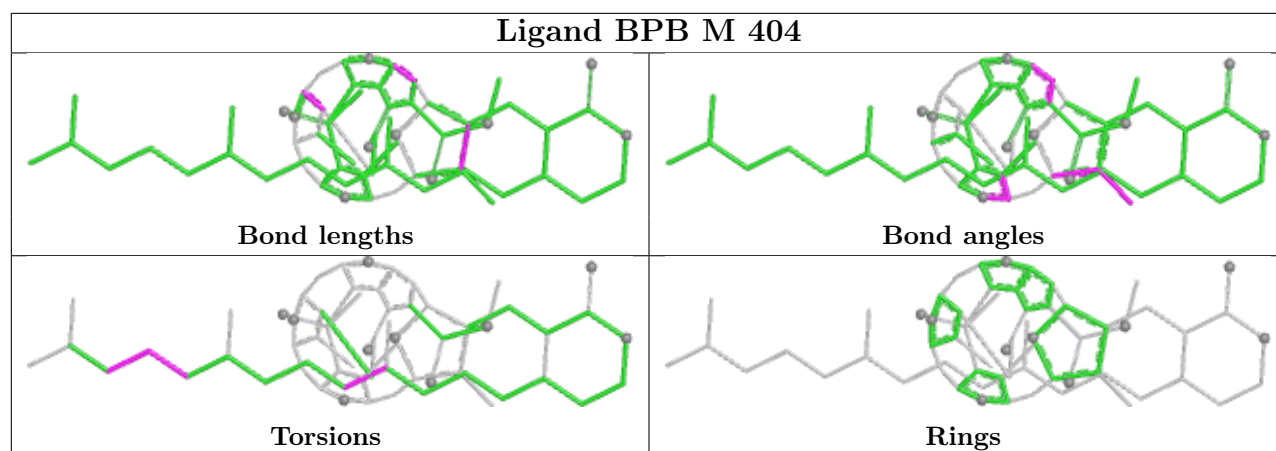
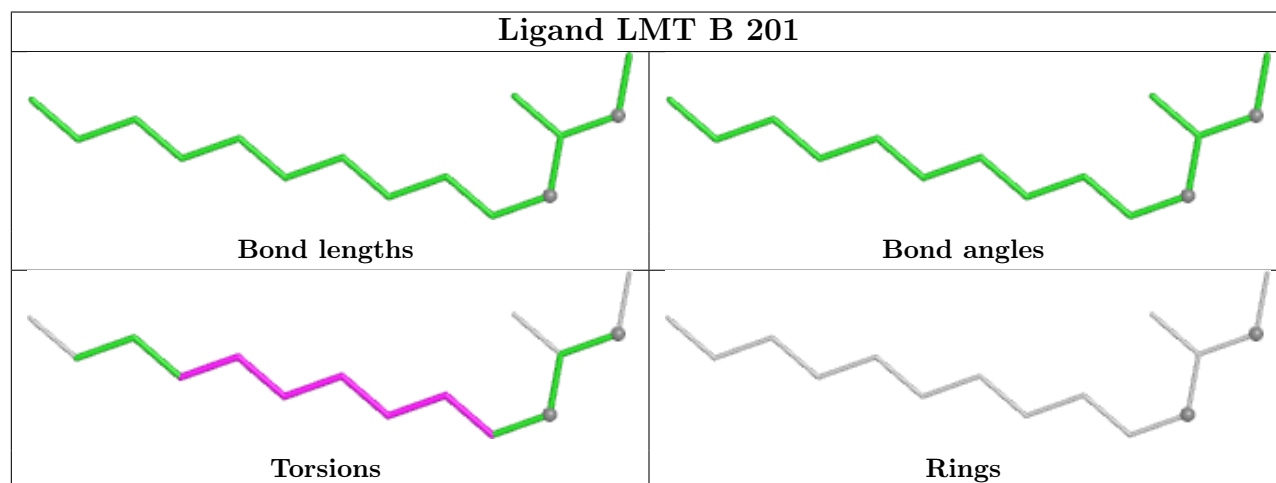
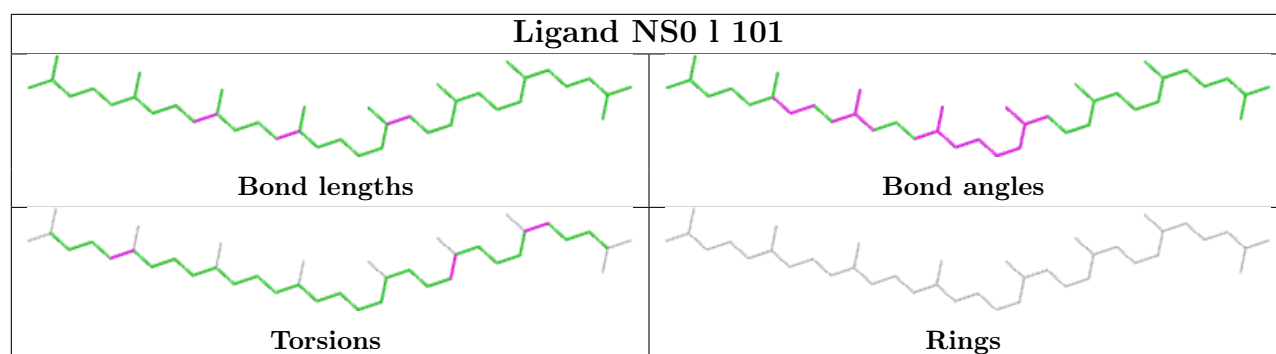
Bond angles

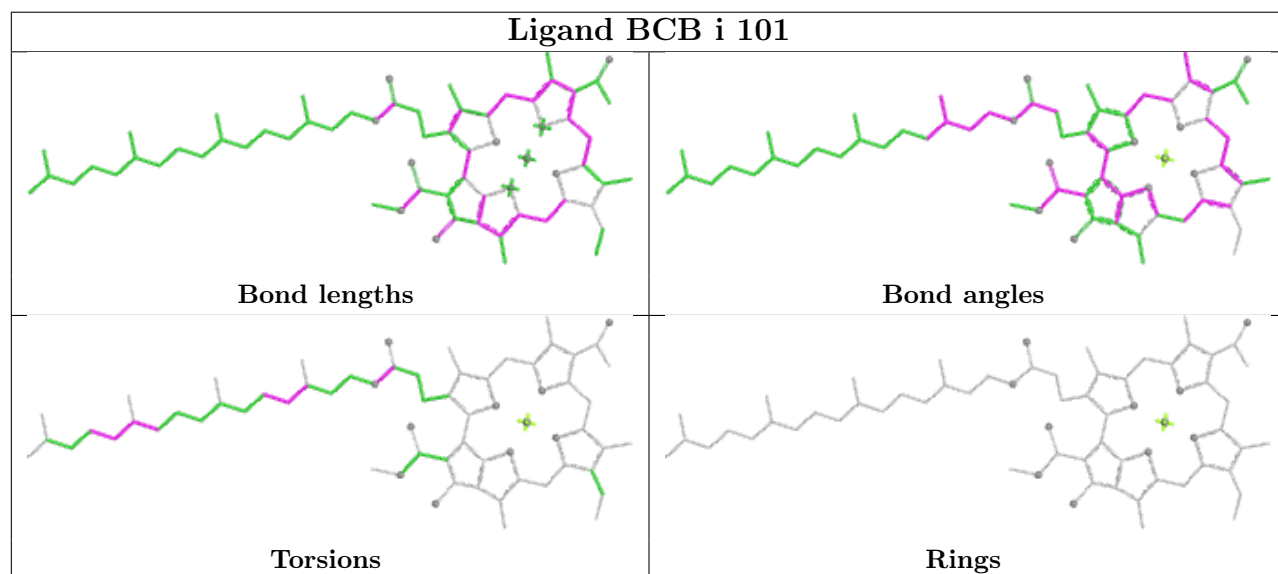
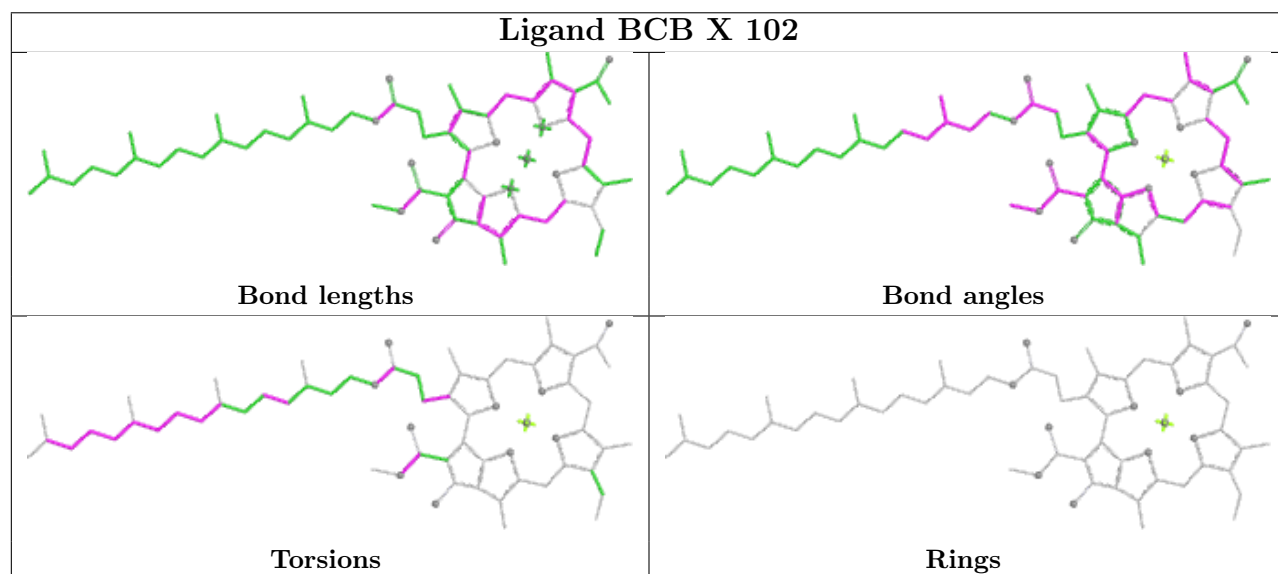
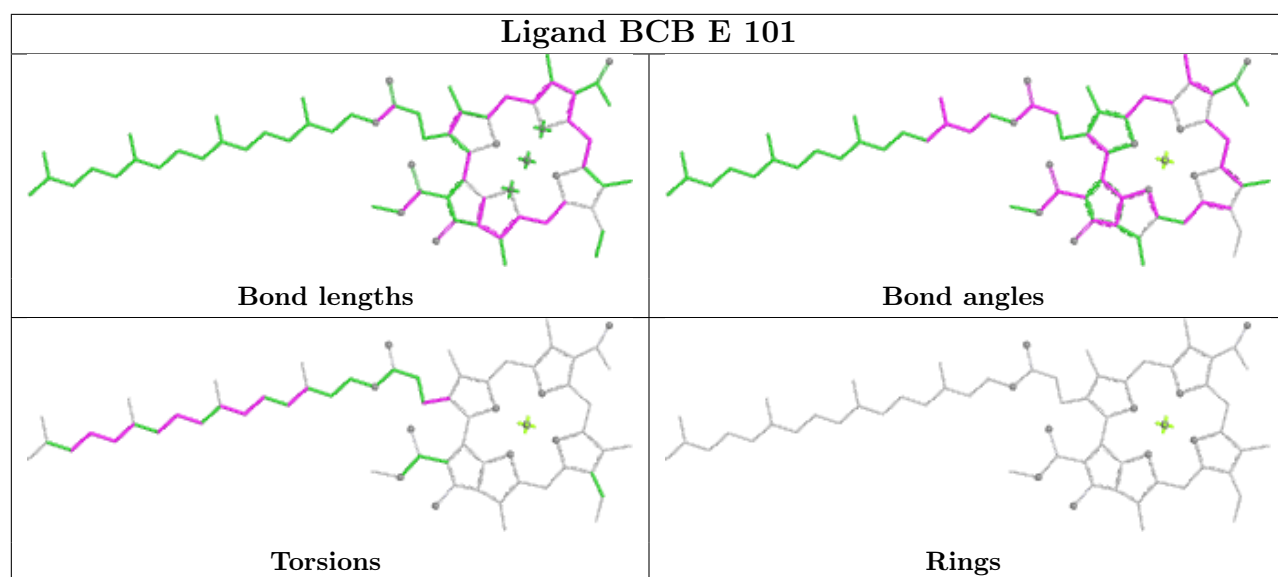


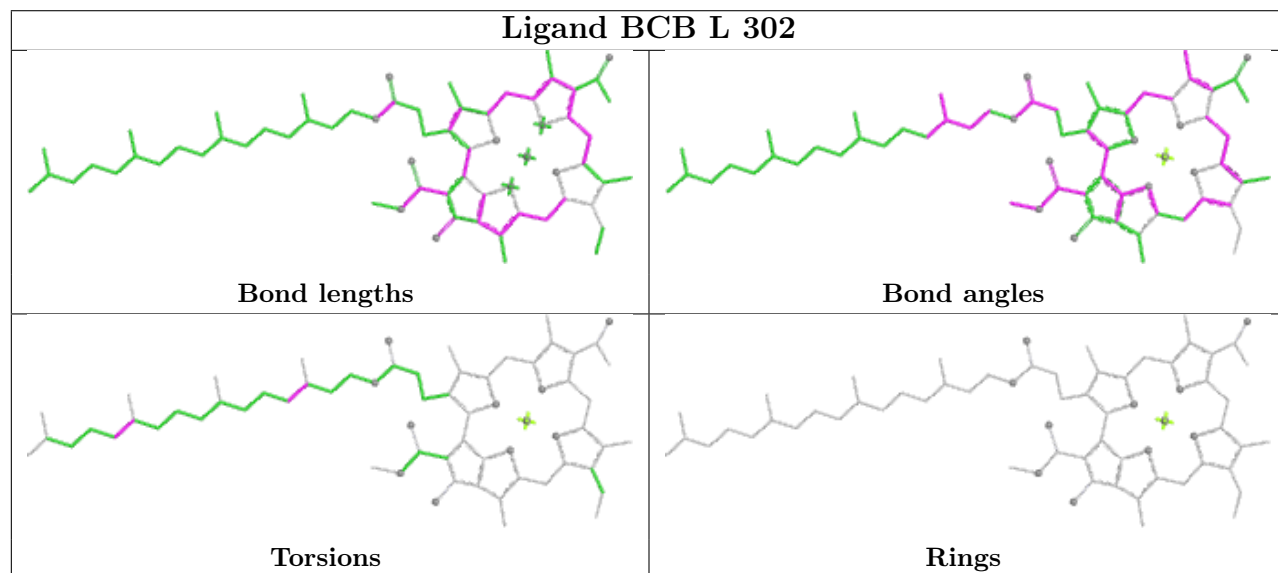
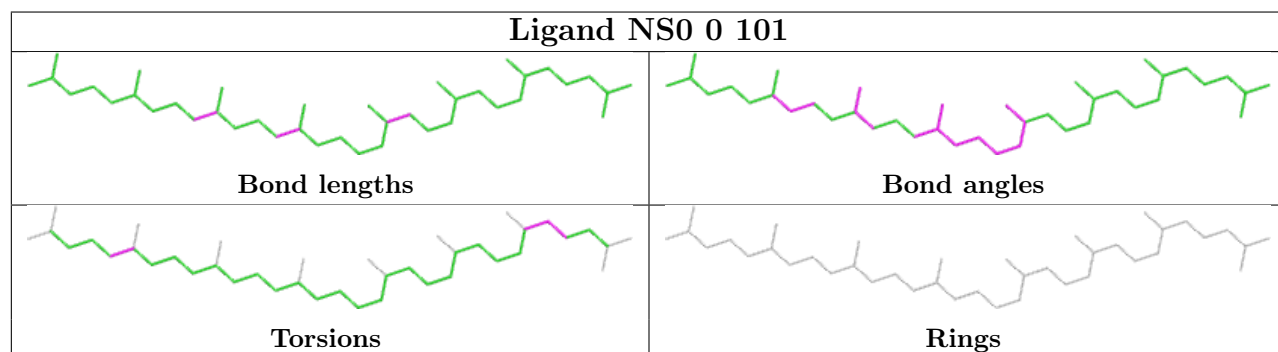
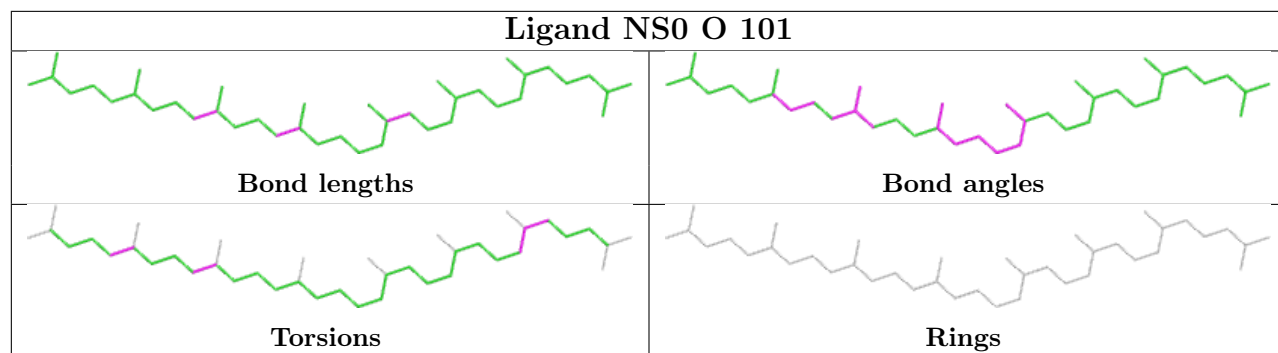
Torsions

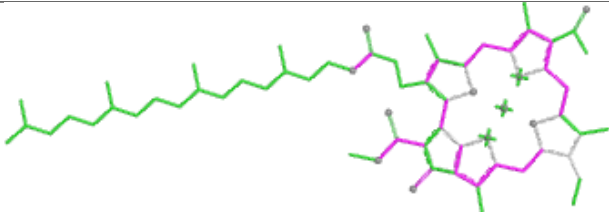
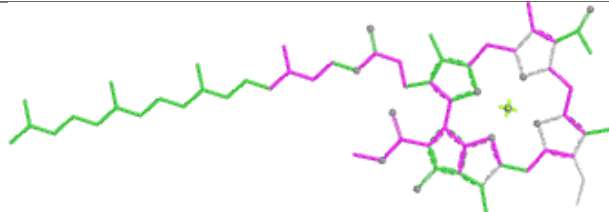
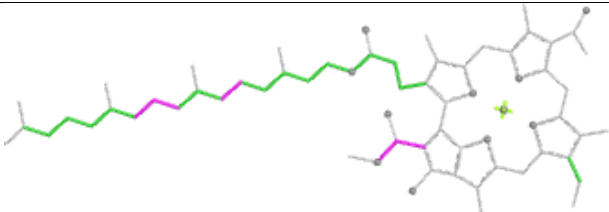
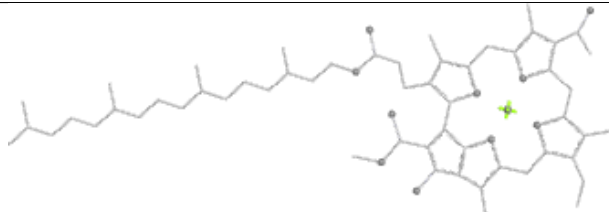


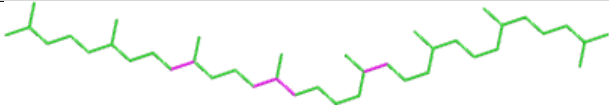
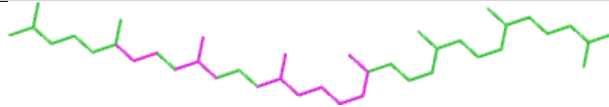
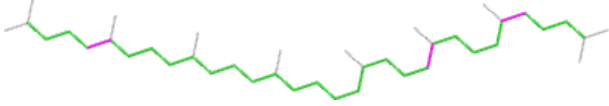
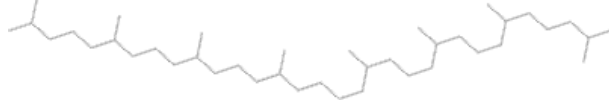
Rings

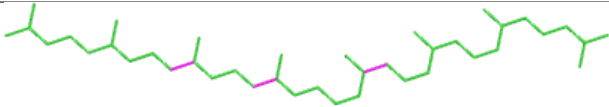
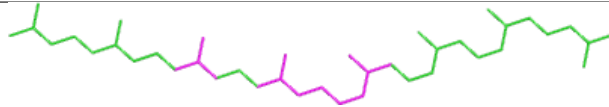
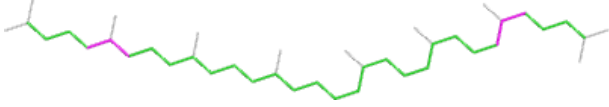
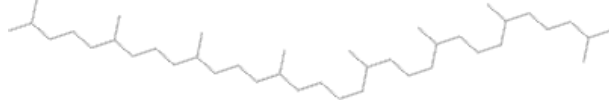


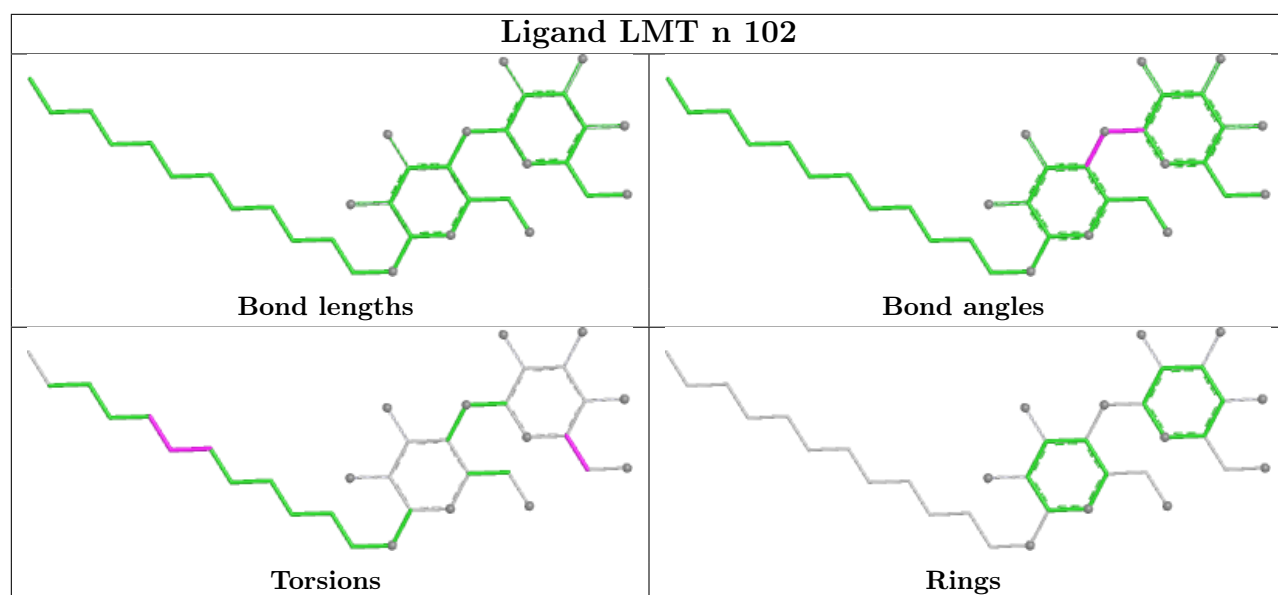
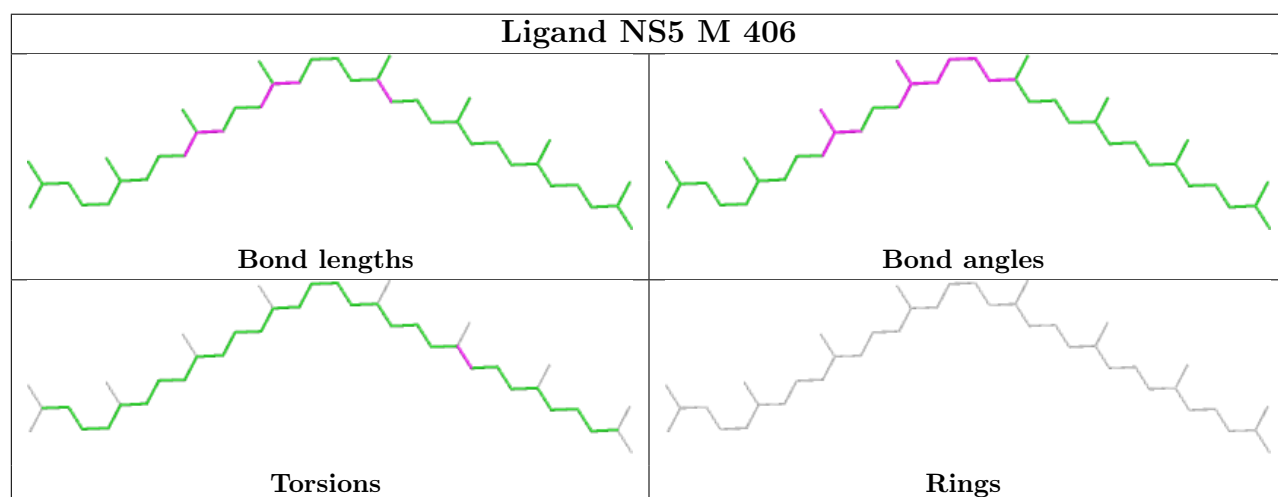
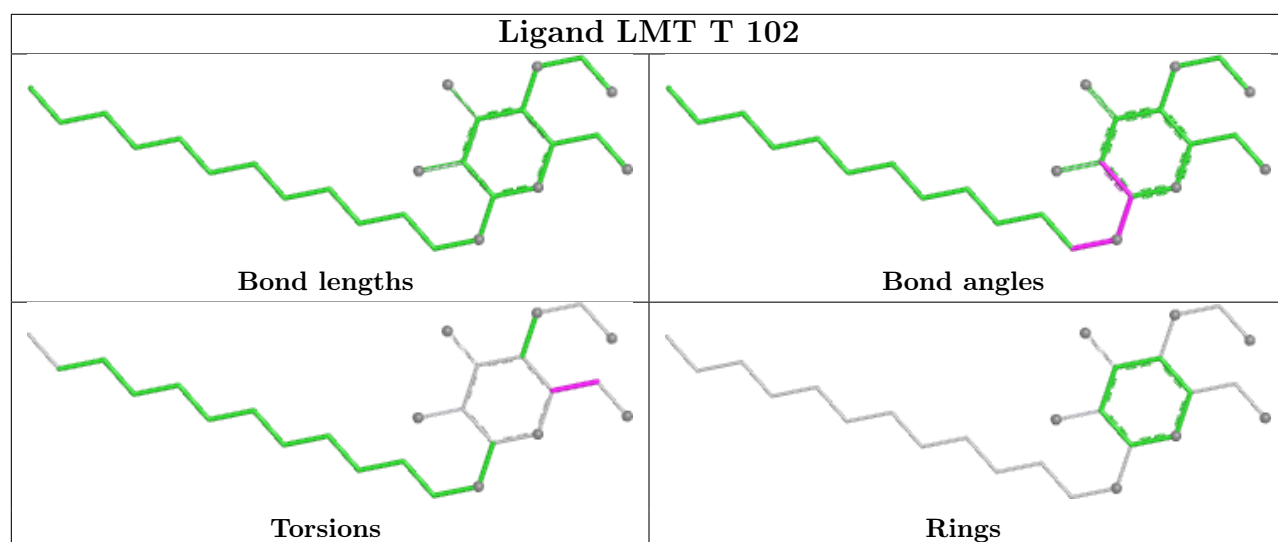


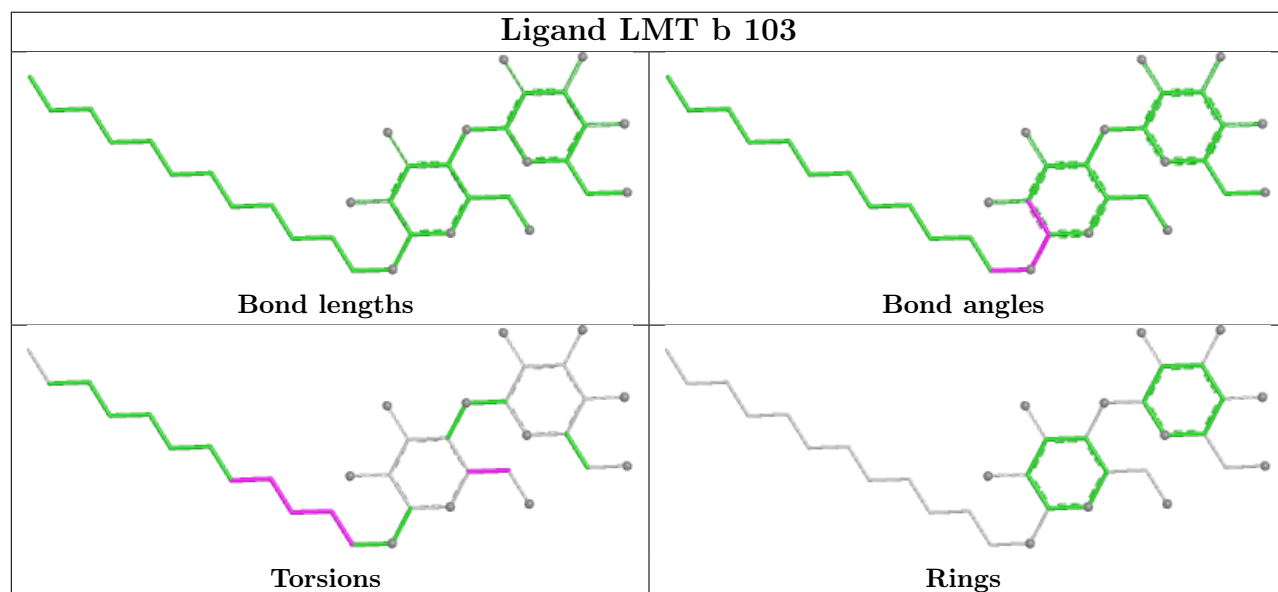
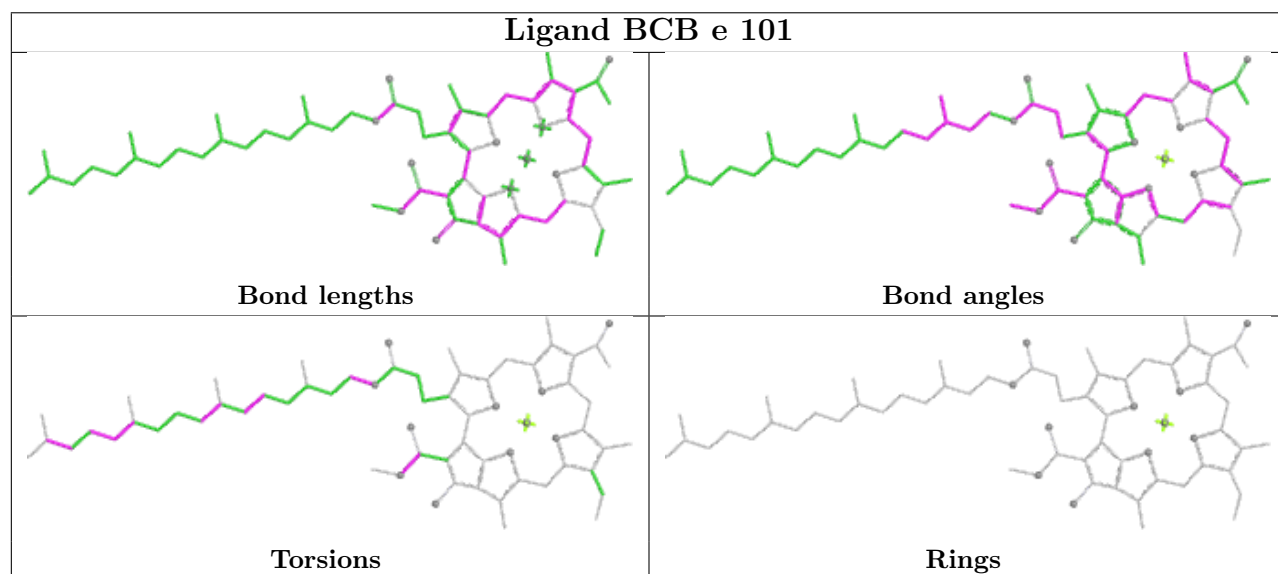
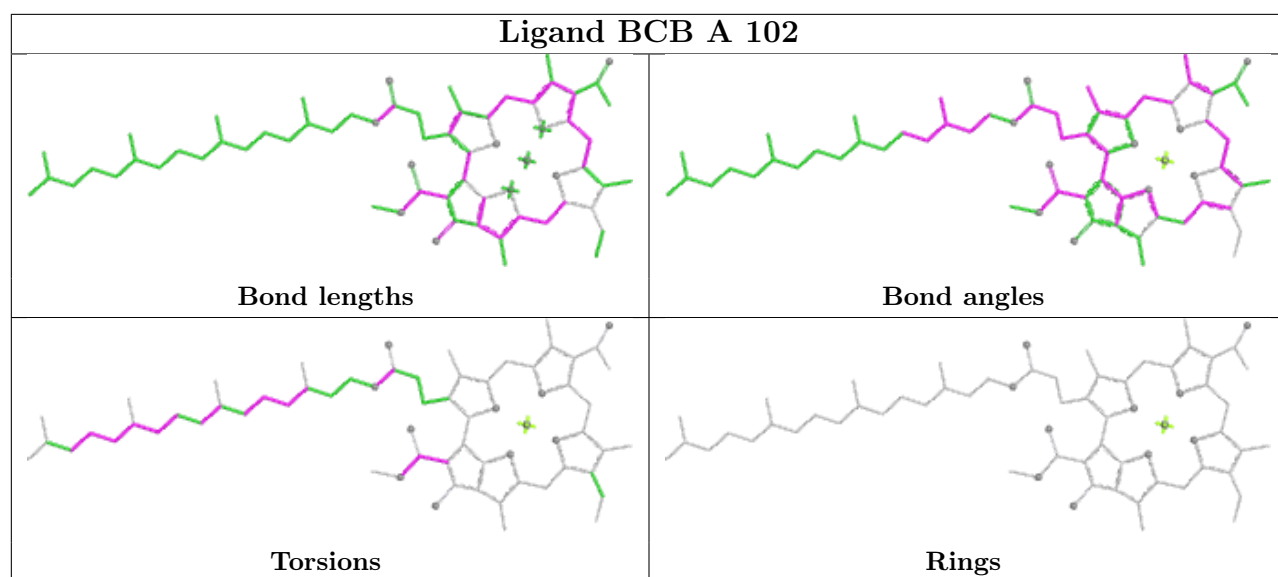


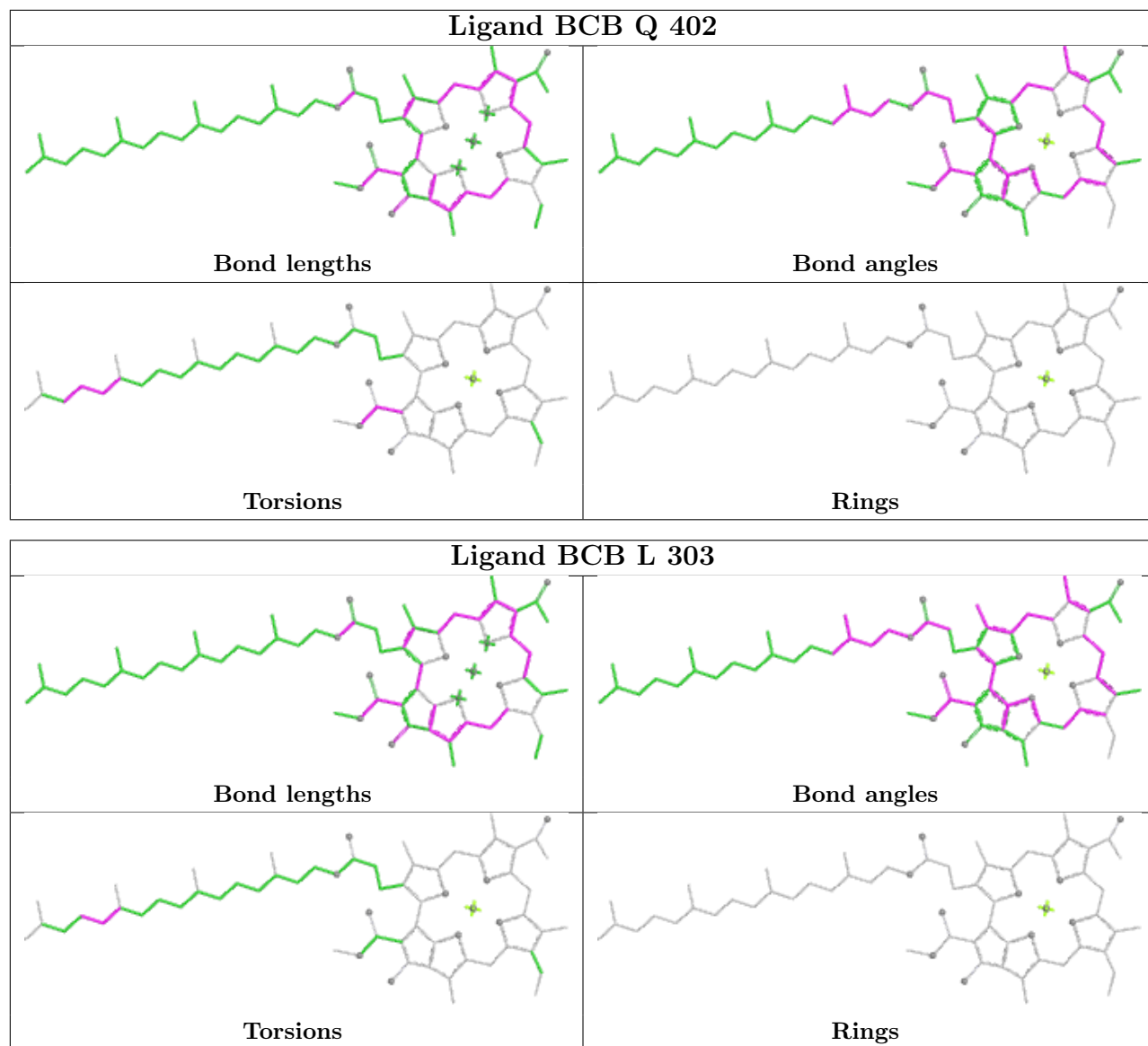
Ligand BCB Z 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

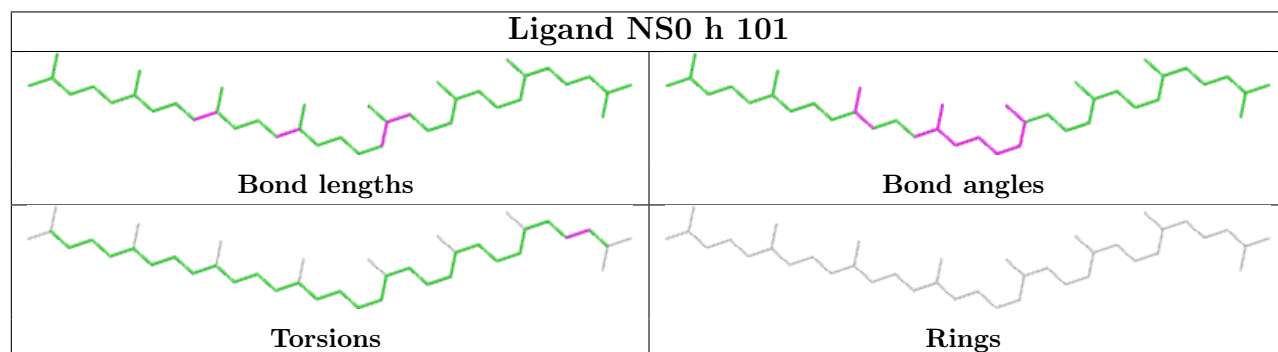
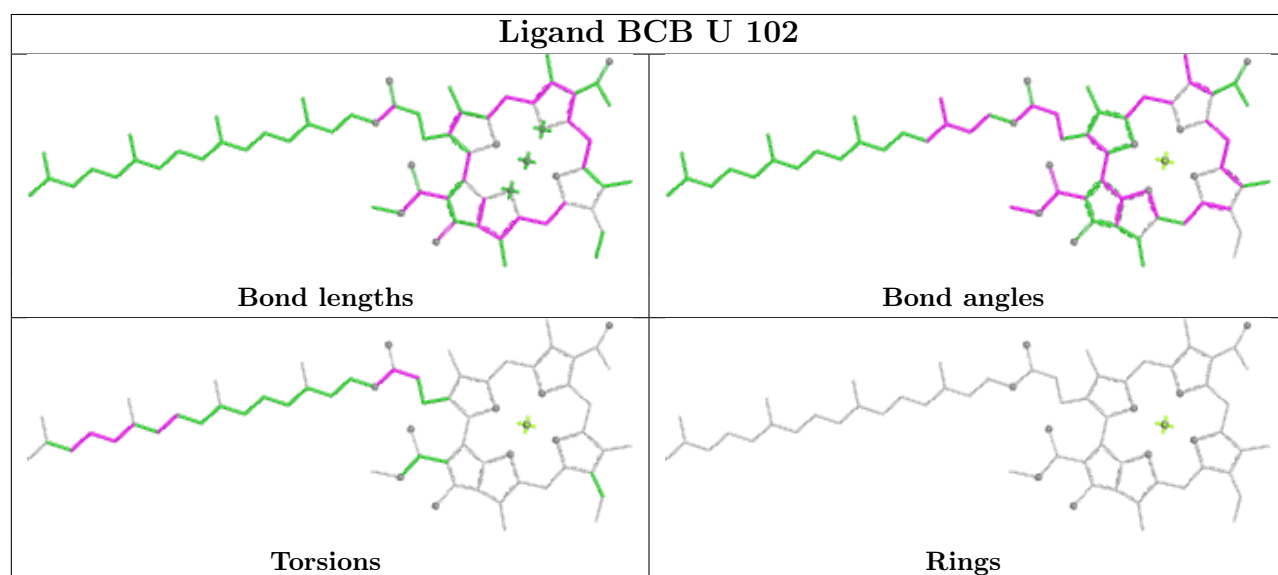
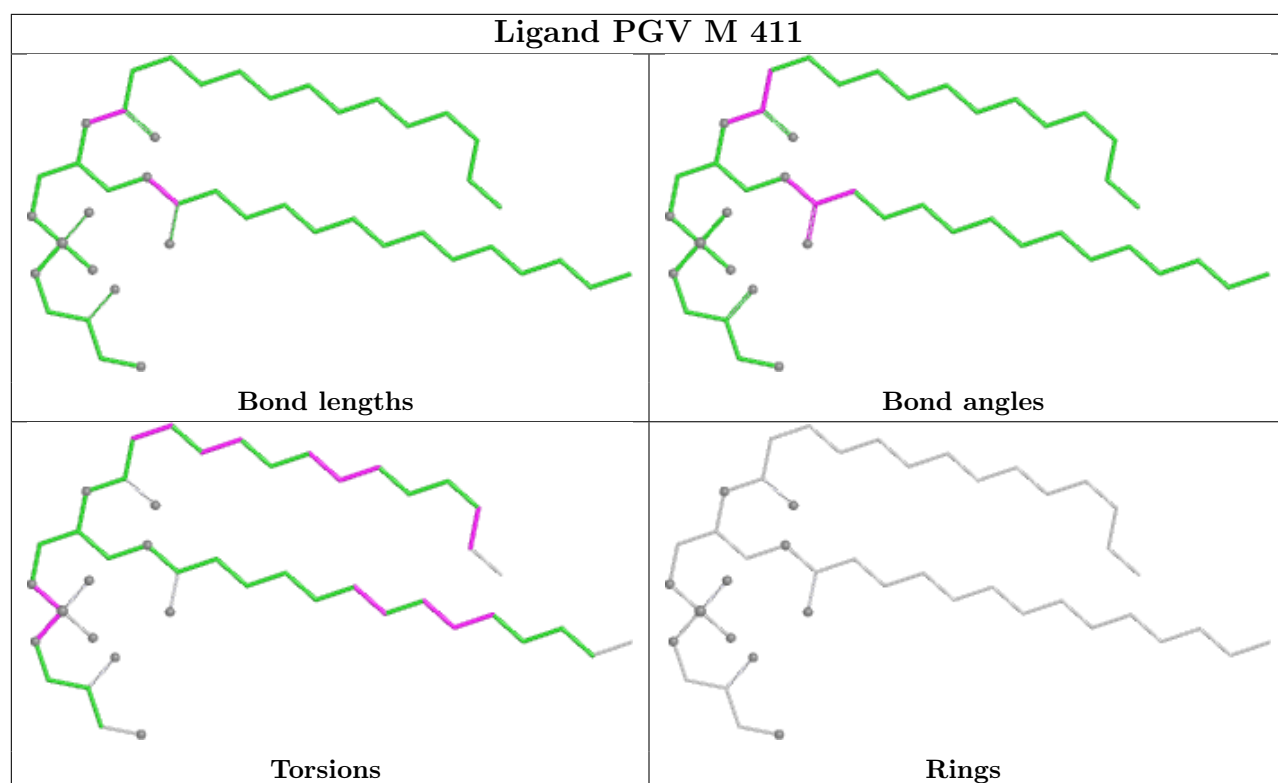
Ligand NS0 9 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

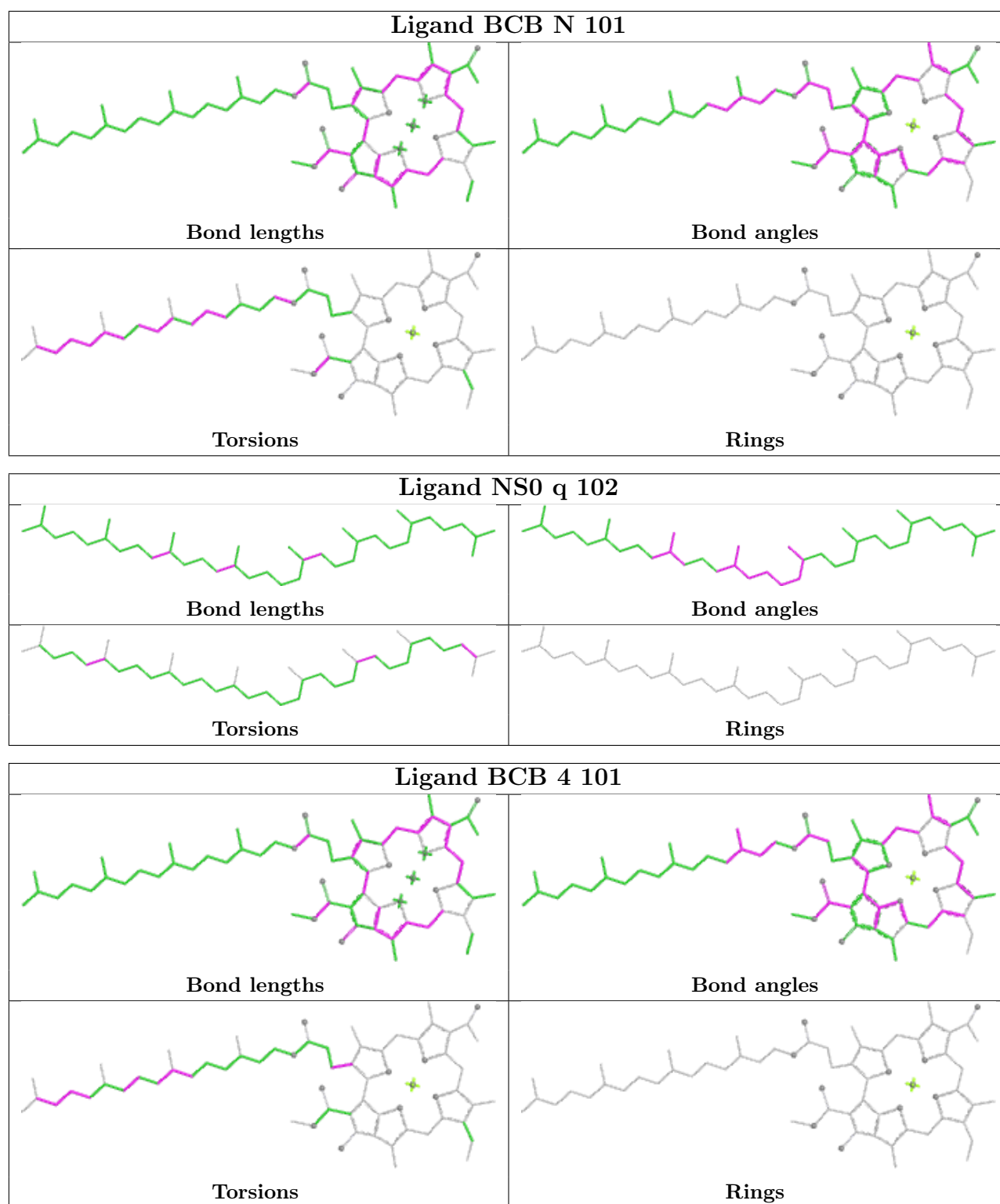
Ligand NS0 U 101	
	
Bond lengths	Bond angles
	
Torsions	Rings











5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

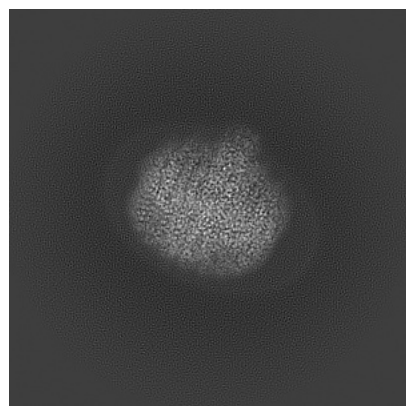
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61095. These allow visual inspection of the internal detail of the map and identification of artifacts.

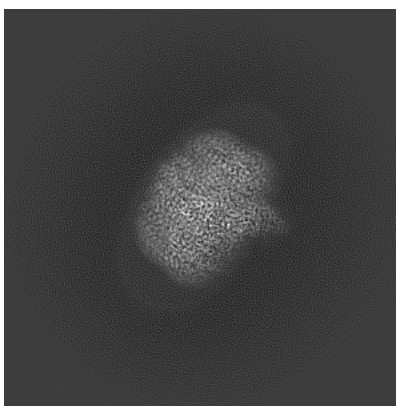
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

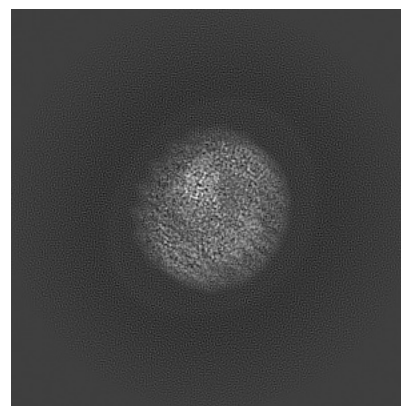
6.1.1 Primary map



X

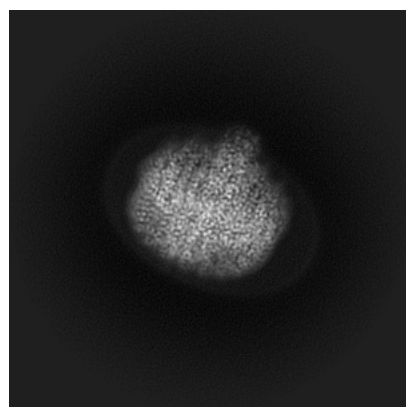


Y

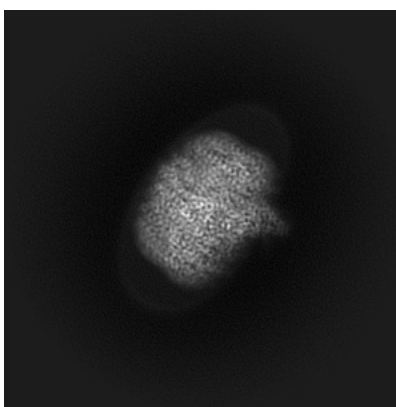


Z

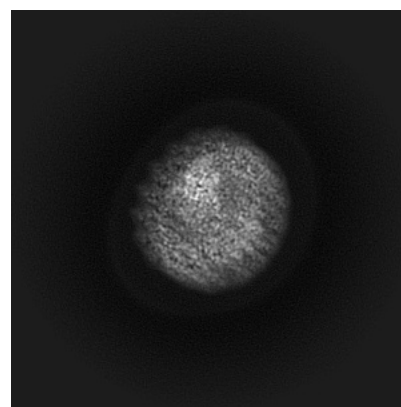
6.1.2 Raw map



X



Y

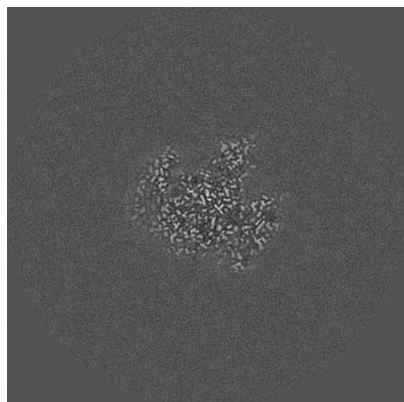


Z

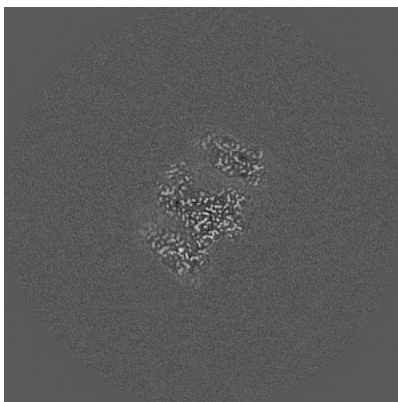
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

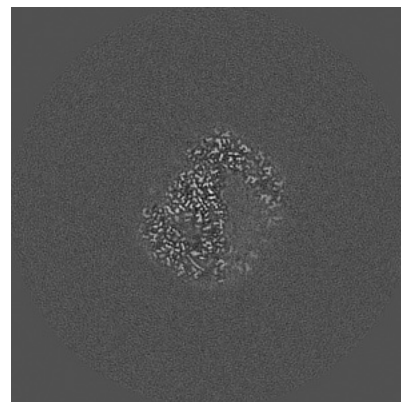
6.2.1 Primary map



X Index: 200

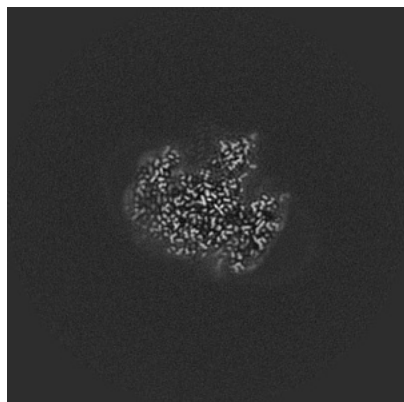


Y Index: 200

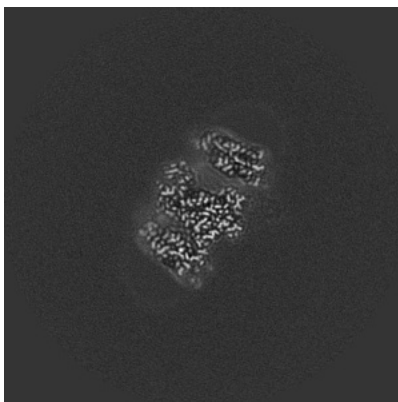


Z Index: 200

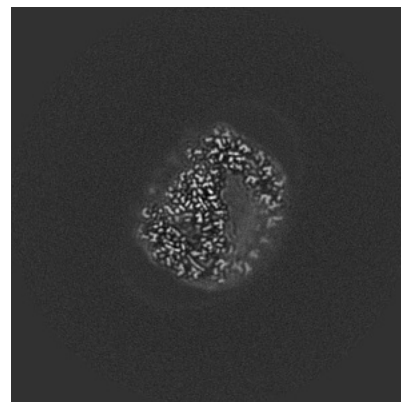
6.2.2 Raw map



X Index: 200



Y Index: 200

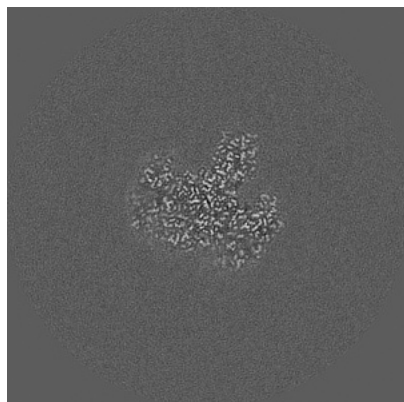


Z Index: 200

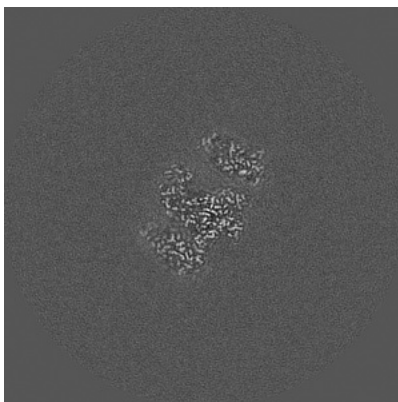
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

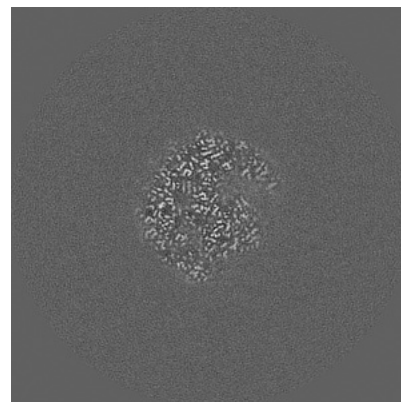
6.3.1 Primary map



X Index: 194

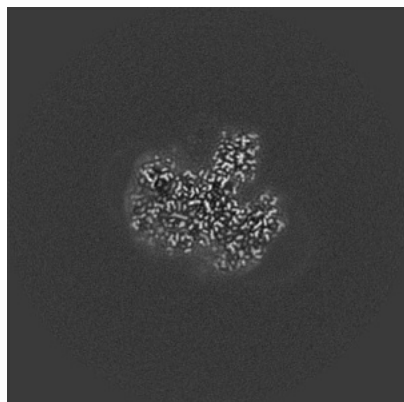


Y Index: 201

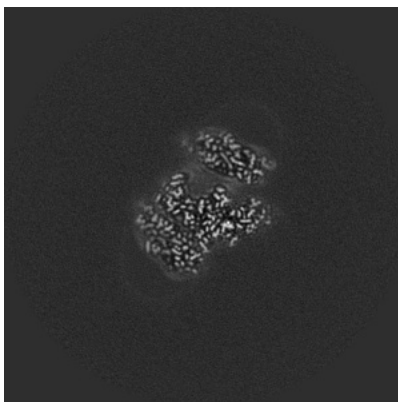


Z Index: 183

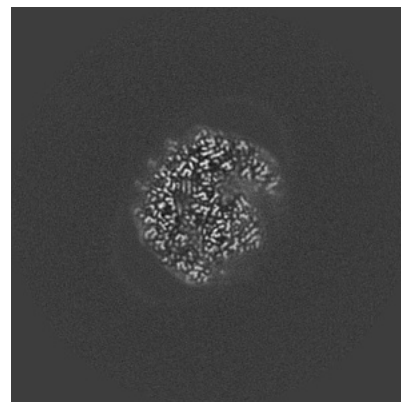
6.3.2 Raw map



X Index: 193



Y Index: 212

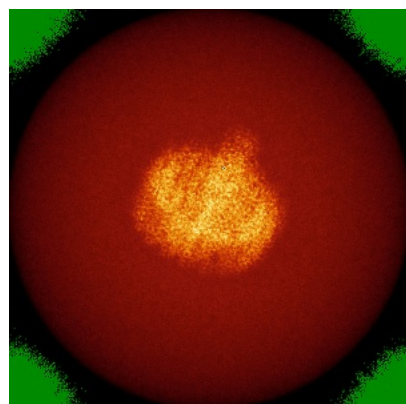


Z Index: 183

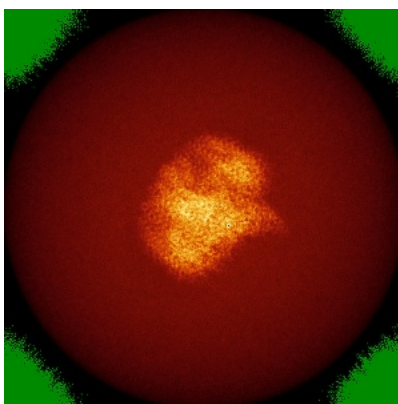
The images above show the largest variance slices of the map in three orthogonal directions.

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

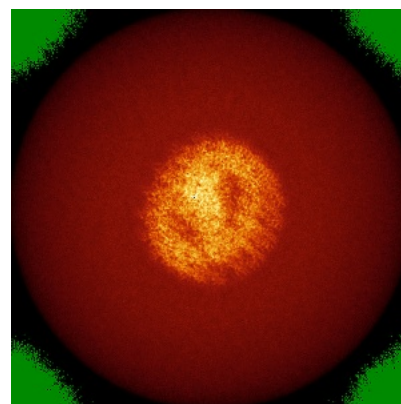
6.4.1 Primary map



X

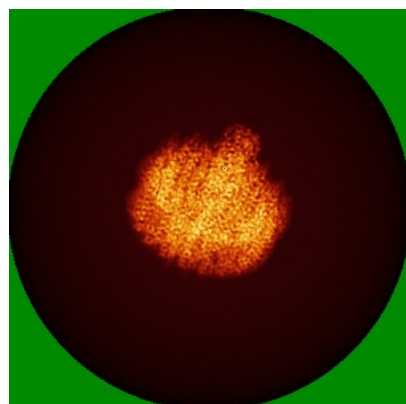


Y

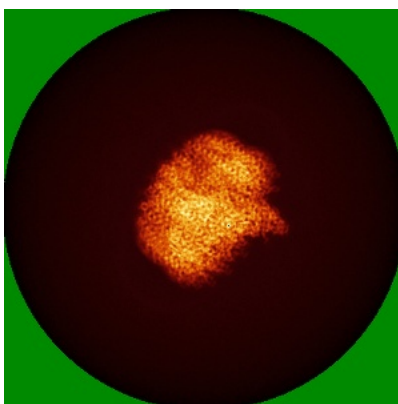


Z

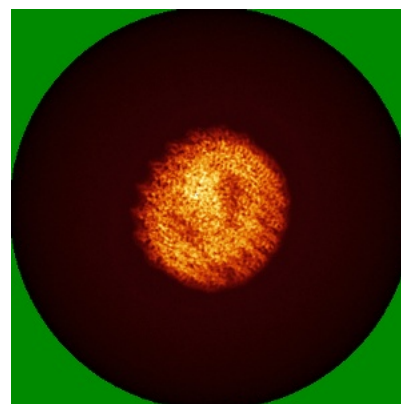
6.4.2 Raw map



X



Y

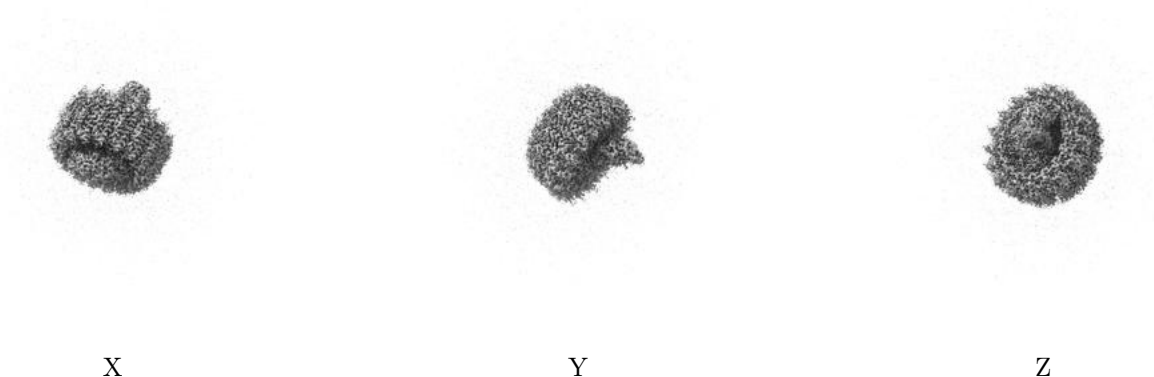


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

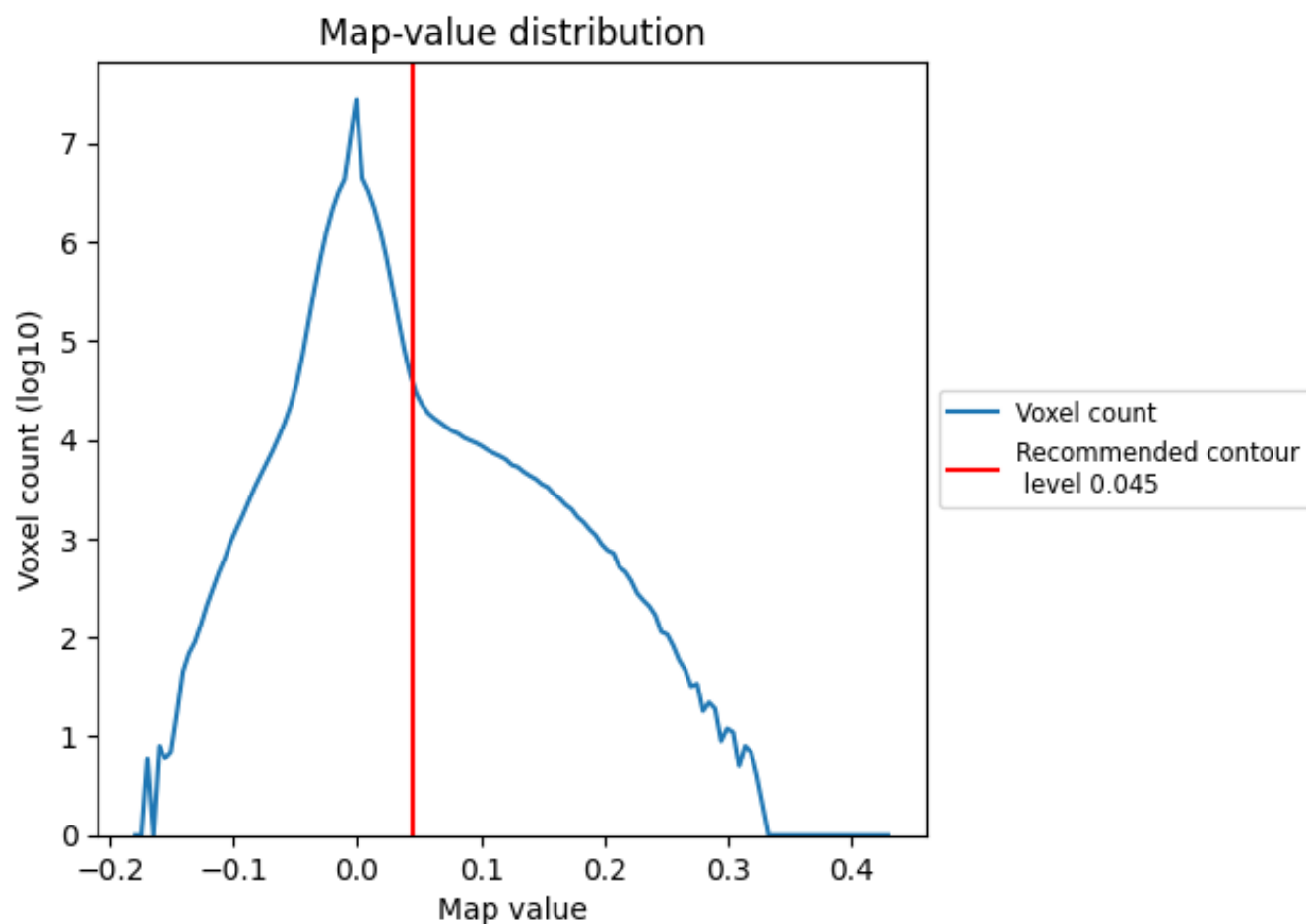
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

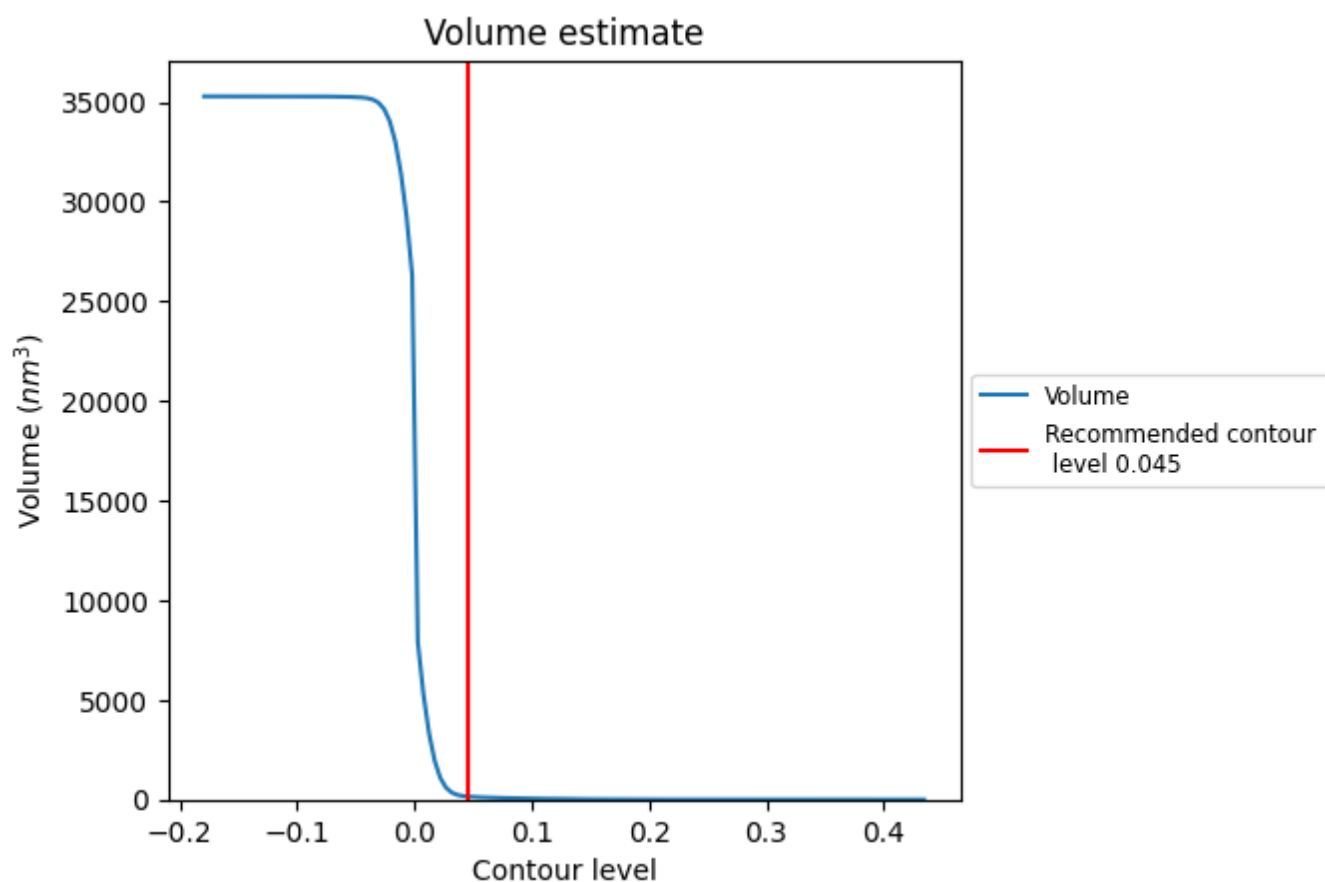
This section contains the results of statistical analysis of the map.

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.

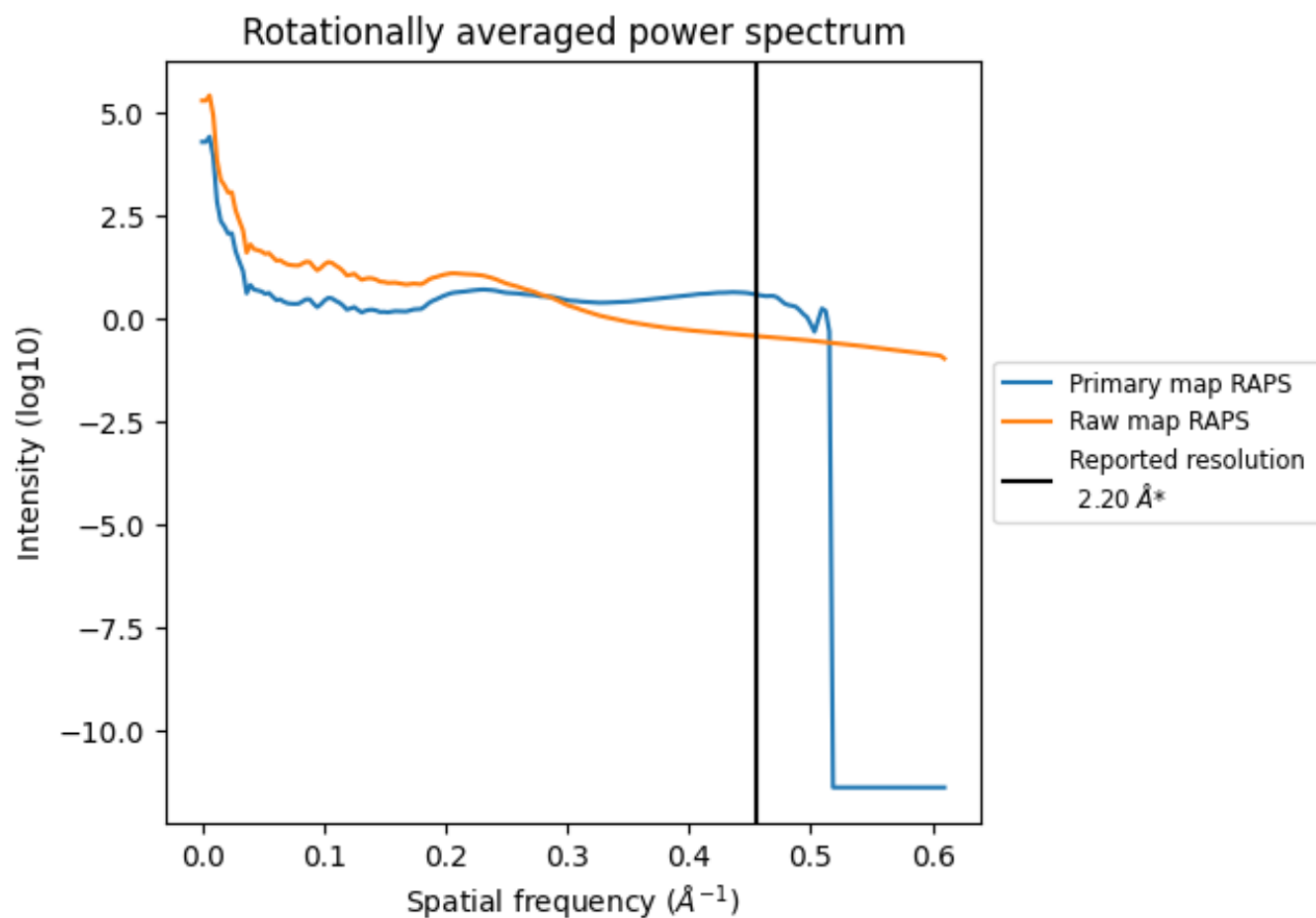
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 155 nm³; this corresponds to an approximate mass of 140 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 ⓘ

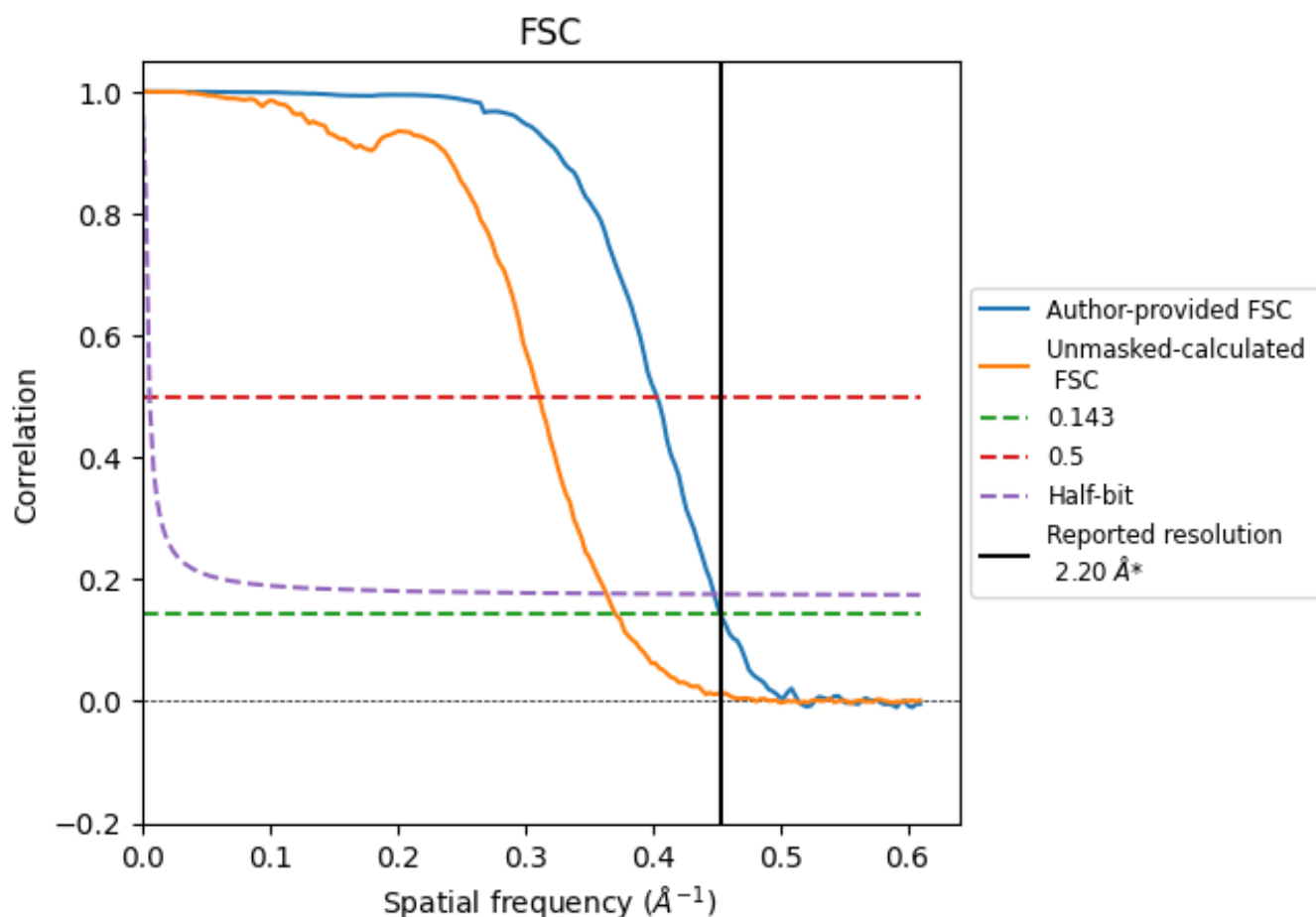


*Reported resolution corresponds to spatial frequency of 0.455 Å⁻¹

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 0.455 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

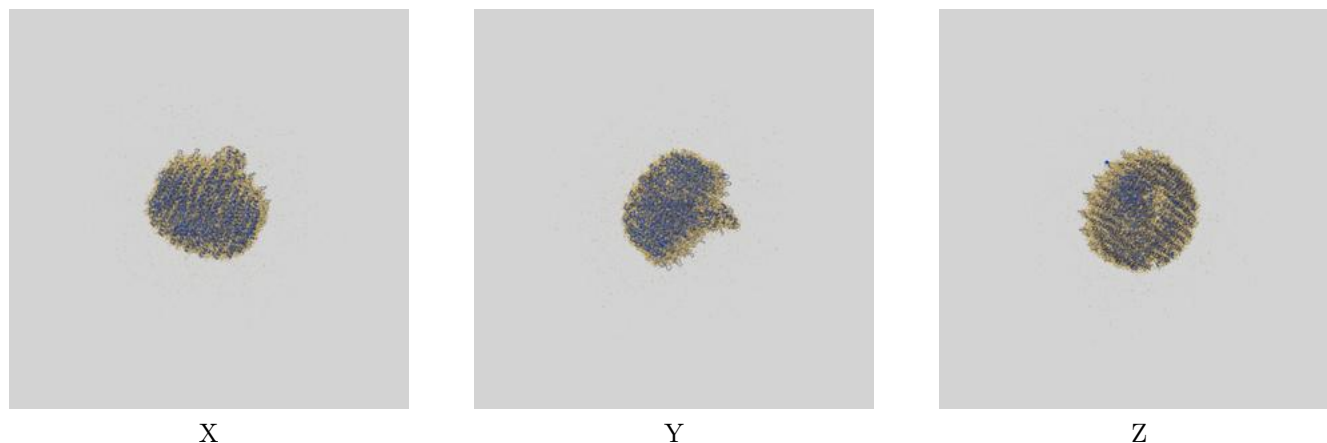
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.20	-	-
Author-provided FSC curve	2.21	2.48	2.23
Unmasked-calculated*	2.69	3.21	2.75

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.69 differs from the reported value 2.2 by more than 10 %

9 Map-model fit [i](#)

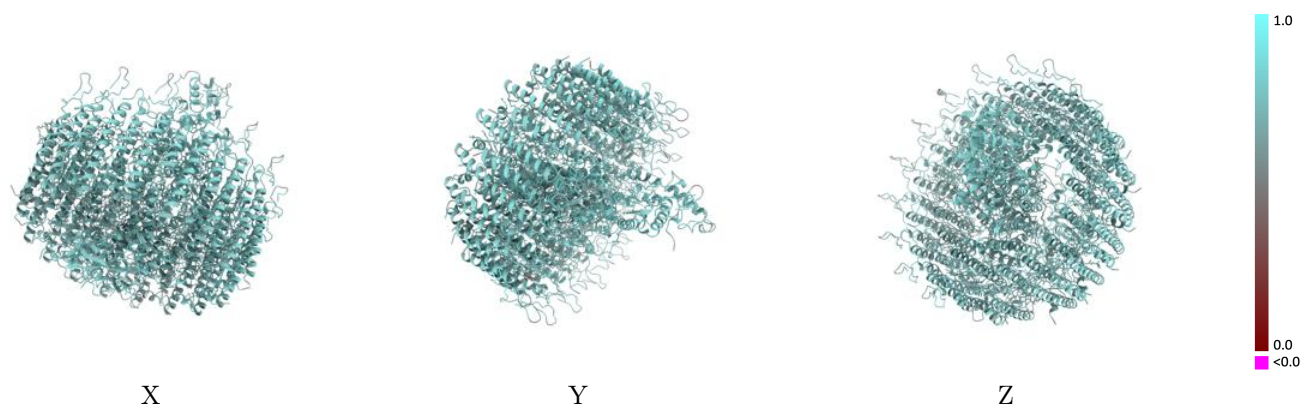
This section contains information regarding the fit between EMDB map EMD-61095 and PDB model 9J2F. Per-residue inclusion information can be found in section 3 on page 23.

9.1 Map-model overlay [i](#)



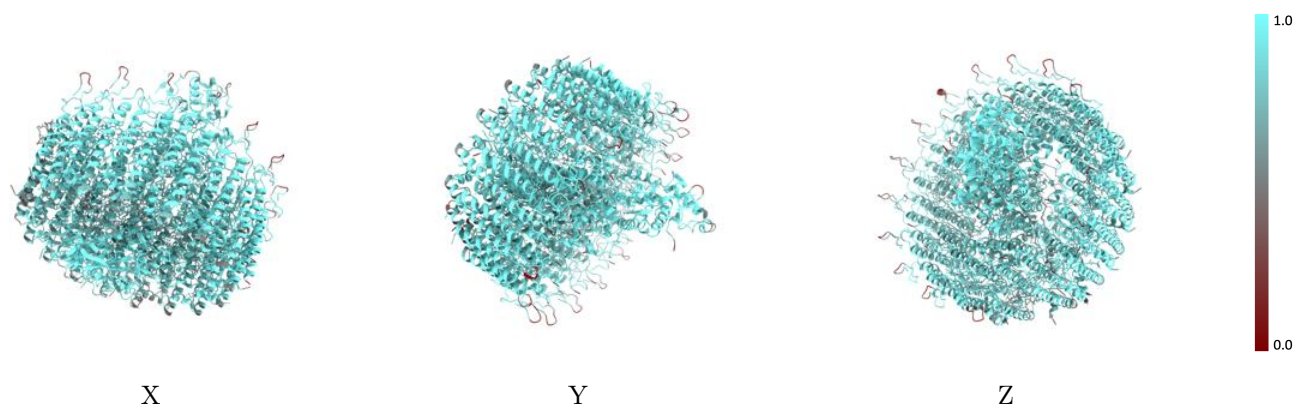
The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



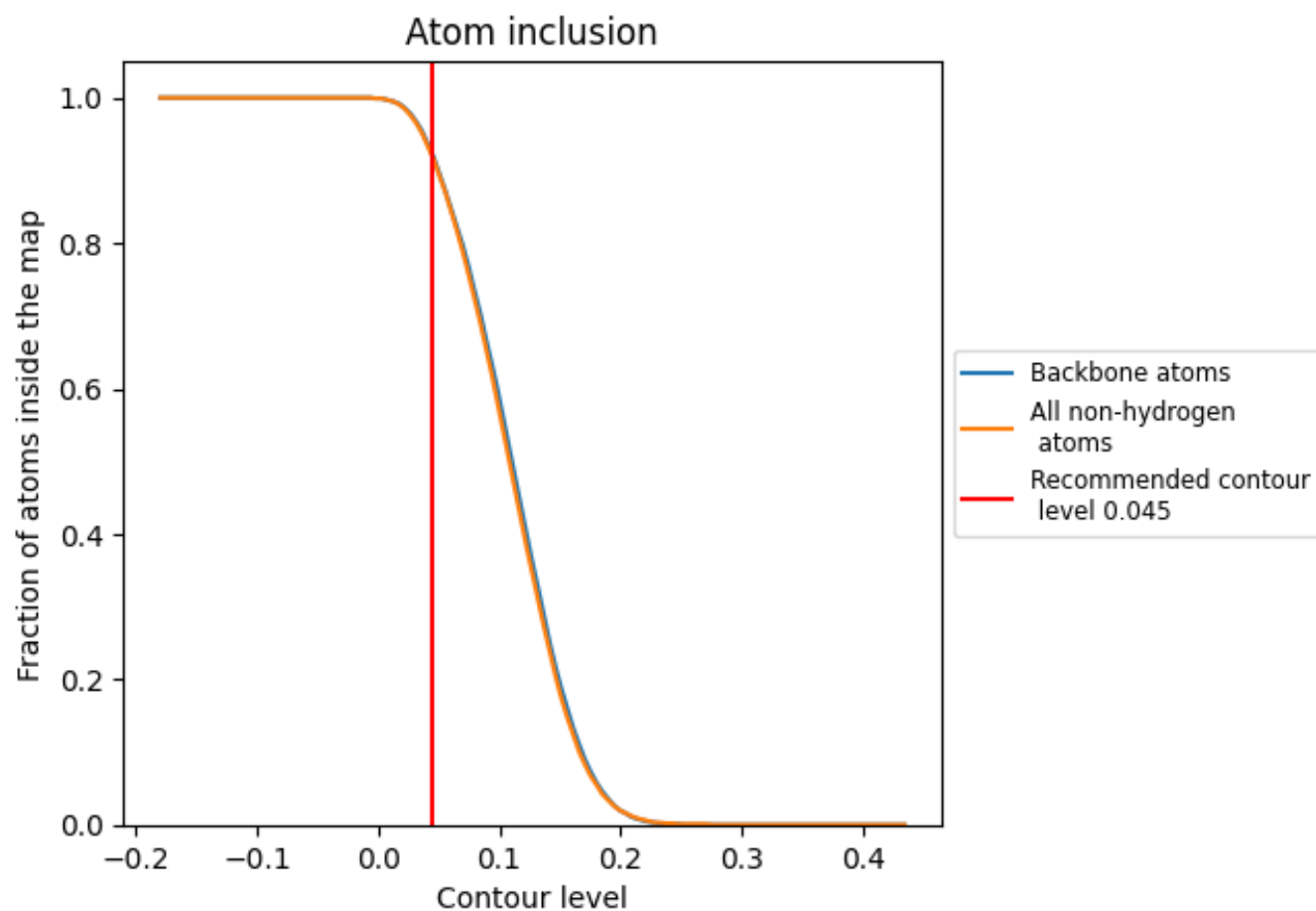
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.045).

9.4 Atom inclusion ⓘ



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

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9190	 0.7250
0	 0.9210	 0.7210
1	 0.9600	 0.7460
2	 0.9010	 0.7020
3	 0.9640	 0.7430
4	 0.9320	 0.7340
5	 0.8750	 0.7030
6	 0.9470	 0.7320
7	 0.9310	 0.7340
8	 0.8860	 0.7010
9	 0.9490	 0.7350
A	 0.9050	 0.7200
B	 0.8600	 0.6930
C	 0.9540	 0.7460
D	 0.9410	 0.7300
E	 0.9460	 0.7350
F	 0.8320	 0.7000
G	 0.6060	 0.6270
H	 0.9160	 0.7160
I	 0.9370	 0.7240
J	 0.9520	 0.7380
K	 0.9010	 0.7070
L	 0.9720	 0.7600
M	 0.9580	 0.7480
N	 0.9310	 0.7270
O	 0.9460	 0.7270
P	 0.8540	 0.6930
Q	 0.9270	 0.7230
R	 0.9210	 0.7220
S	 0.8460	 0.6950
T	 0.8700	 0.6950
U	 0.8870	 0.7000
V	 0.8170	 0.6830
W	 0.9300	 0.7230
X	 0.9050	 0.7210



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Chain	Atom inclusion	Q-score
Y	 0.8650	 0.6920
Z	 0.9490	 0.7400
a	 0.7870	 0.6870
b	 0.8930	 0.7150
c	 0.9190	 0.7290
d	 0.8320	 0.6880
e	 0.9600	 0.7360
f	 0.9390	 0.7290
g	 0.8860	 0.7030
h	 0.9200	 0.7200
i	 0.9080	 0.7130
j	 0.9010	 0.6970
k	 0.9270	 0.7180
l	 0.9230	 0.7200
m	 0.8830	 0.6970
n	 0.8900	 0.7140
o	 0.9210	 0.7170
p	 0.8390	 0.6920
q	 0.8830	 0.7010
r	 0.7900	 0.6730