Full wwPDB EM Validation Report ⓘ

Dec 11, 2024 – 08:30 PM JST

PDB ID	:	9J2F
EMDB ID	:	EMD-61095
Title	:	Structure of photosynthetic LH1-RC complex from the purple bacterium Blastochloris 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:

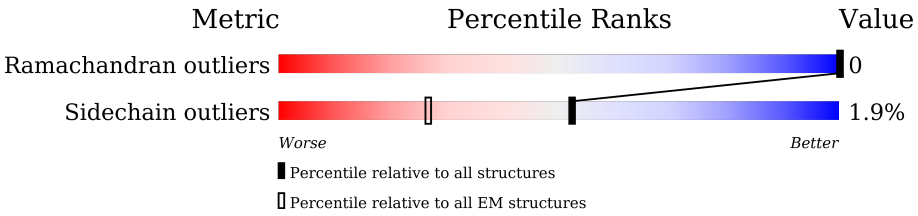
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance

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

The reported resolution of this entry is 2.20 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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	91% · 6%
2	L	274	99% ·
3	M	332	98% ·
4	H	260	98% ·
5	3	69	72% 28%
5	6	69	71% · 28%
5	9	69	71% · 28%
5	A	69	70% · 28%
5	D	69	71% · 28%

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Mol	Chain	Length	Quality of chain
5	I	69	72% 28%
5	N	69	71% 28%
5	Q	69	71% 28%
5	T	69	70% 28%
5	W	69	71% 28%
5	Z	69	72% 28%
5	b	69	72% 28%
5	e	69	72% 28%
5	h	69	71% 28%
5	k	69	71% 28%
5	n	69	72% 28%
5	q	69	71% 28%
6	0	69	71% 28%
6	1	69	72% 28%
6	4	69	71% 28%
6	7	69	71% 28%
6	B	69	72% 26%
6	E	69	72% 26%
6	J	69	70% 30%
6	O	69	72% 26%
6	R	69	72% 28%
6	U	69	70% 28%
6	X	69	71% 28%
6	c	69	72% 28%
6	f	69	72% 28%

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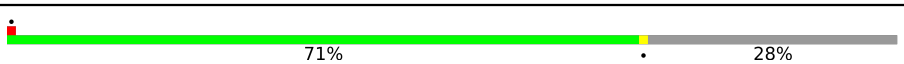
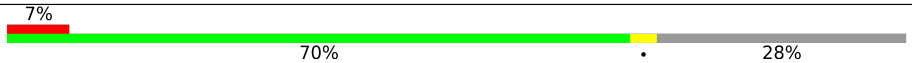
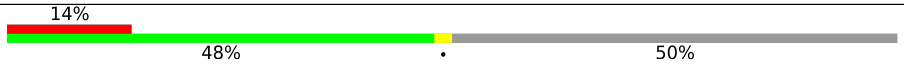
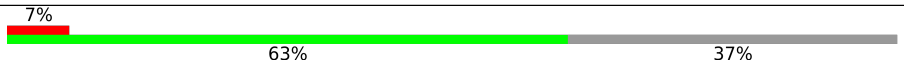
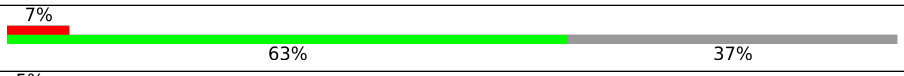
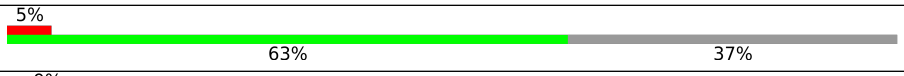
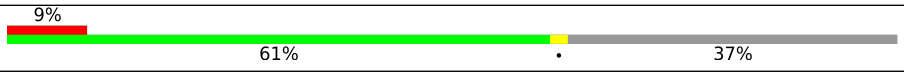
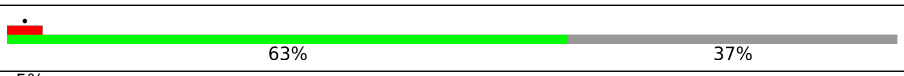
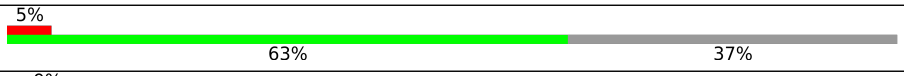
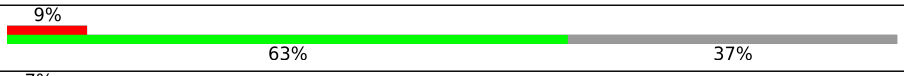
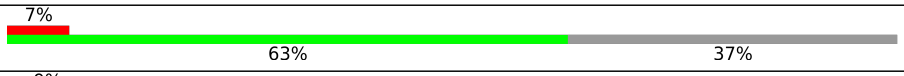
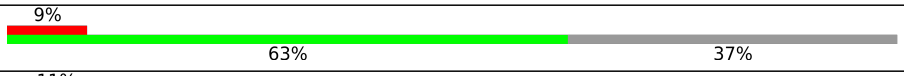
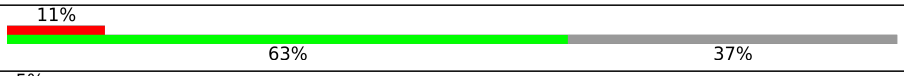
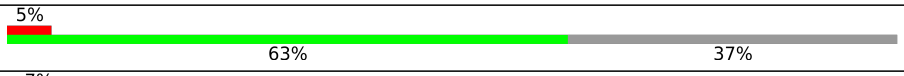
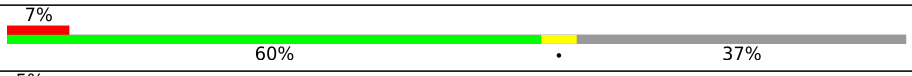
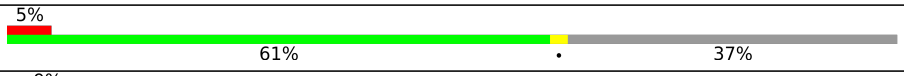
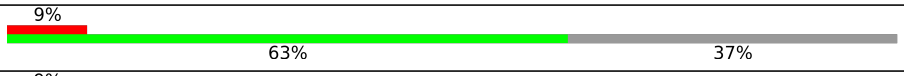
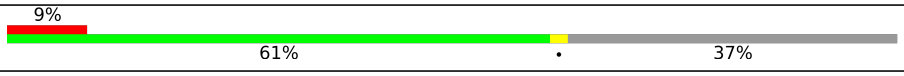
Mol	Chain	Length	Quality of chain
6	i	69	
6	l	69	
6	o	69	
6	r	69	
7	G	56	
8	2	57	
8	5	57	
8	8	57	
8	F	57	
8	K	57	
8	P	57	
8	S	57	
8	V	57	
8	Y	57	
8	a	57	
8	d	57	
8	g	57	
8	j	57	
8	m	57	
8	p	57	

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	-	-	-

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

2 Entry composition (i)

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 424	C 288	N 72	O 64	0	0
5	T	50	Total 424	C 288	N 72	O 64	0	0
5	W	50	Total 424	C 288	N 72	O 64	0	0
5	Z	50	Total 424	C 288	N 72	O 64	0	0
5	3	50	Total 424	C 288	N 72	O 64	0	0
5	6	50	Total 424	C 288	N 72	O 64	0	0
5	9	50	Total 424	C 288	N 72	O 64	0	0
5	b	50	Total 424	C 288	N 72	O 64	0	0
5	e	50	Total 424	C 288	N 72	O 64	0	0
5	h	50	Total 424	C 288	N 72	O 64	0	0
5	k	50	Total 424	C 288	N 72	O 64	0	0
5	n	50	Total 424	C 288	N 72	O 64	0	0
5	q	50	Total 424	C 288	N 72	O 64	0	0

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

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

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

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

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

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

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

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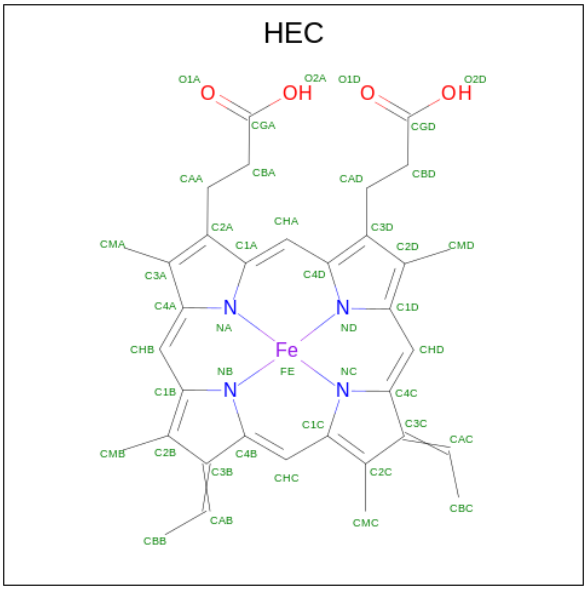
Mol	Chain	Residues	Atoms				AltConf	Trace
8	Y	36	Total	C	N	O	0	0
			279	189	42	48		
8	2	36	Total	C	N	O	0	0
			279	189	42	48		
8	5	36	Total	C	N	O	0	0
			279	189	42	48		
8	8	36	Total	C	N	O	0	0
			279	189	42	48		
8	a	36	Total	C	N	O	0	0
			279	189	42	48		
8	d	36	Total	C	N	O	0	0
			279	189	42	48		
8	g	36	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 (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

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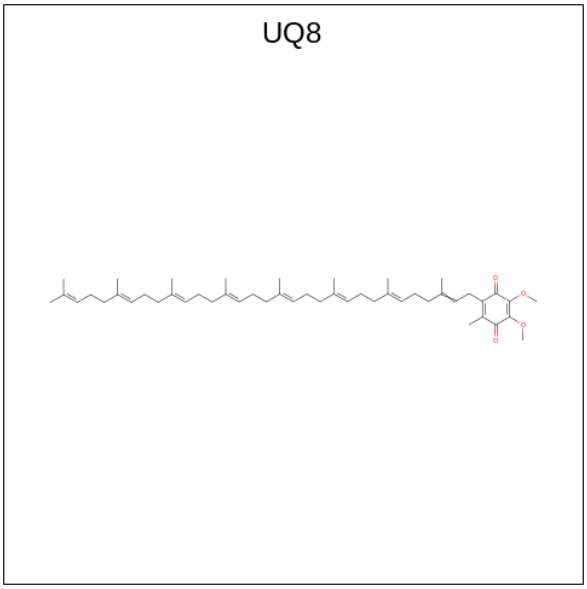
Mol	Chain	Residues	Atoms					AltConf
9	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
9	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
9	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

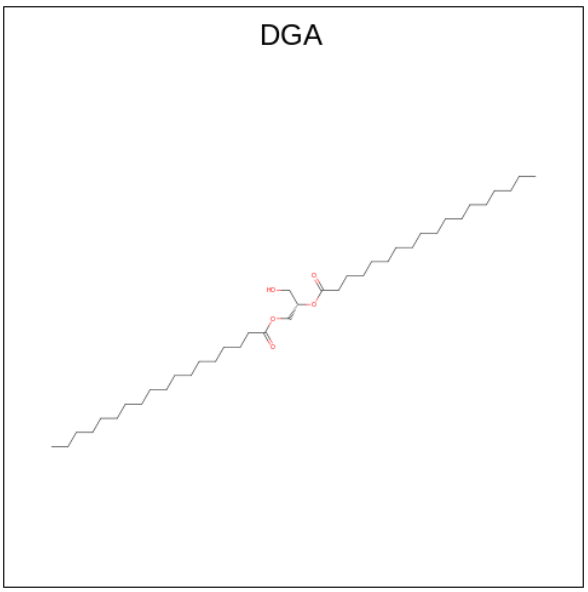
Mol	Chain	Residues	Atoms		AltConf
10	C	1	Total	Mg	0
			1	1	

- Molecule 11 is Ubiquinone-8 (three-letter code: UQ8) (formula: $C_{49}H_{74}O_4$).



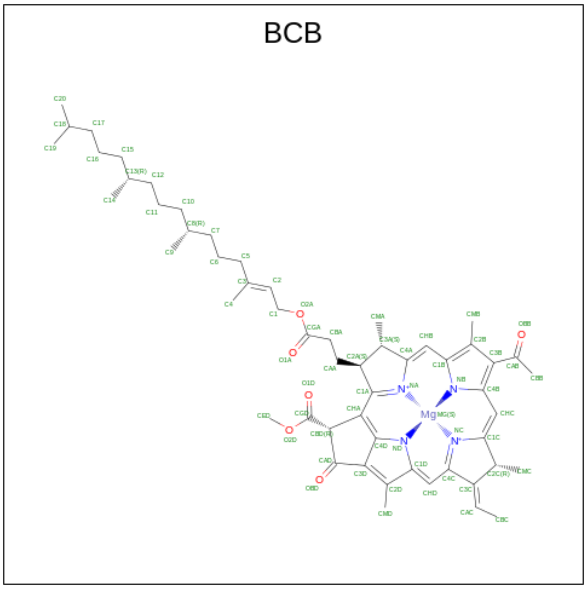
Mol	Chain	Residues	Atoms			AltConf
11	C	1	Total	C	O	0
			15	11	4	
11	L	1	Total	C	O	0
			31	27	4	
11	M	1	Total	C	O	0
			25	21	4	
11	M	1	Total	C	O	0
			53	49	4	
11	A	1	Total	C	O	0
			53	49	4	

- Molecule 12 is DIACYL GLYCEROL (three-letter code: DGA) (formula: $C_{39}H_{76}O_5$).



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

- Molecule 13 is BACTERIOCHLOROPHYLL B (three-letter code: BCB) (formula: $C_{55}H_{72}MgN_4O_6$) (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	C	Mg	N	O	0
			66	55	1	4	6	
13	M	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	M	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	A	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	D	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	I	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	J	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	
13	T	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	U	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	X	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	Z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	4	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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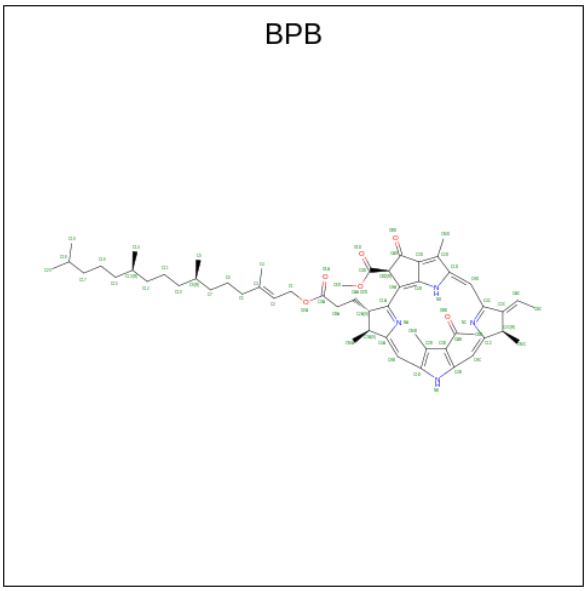
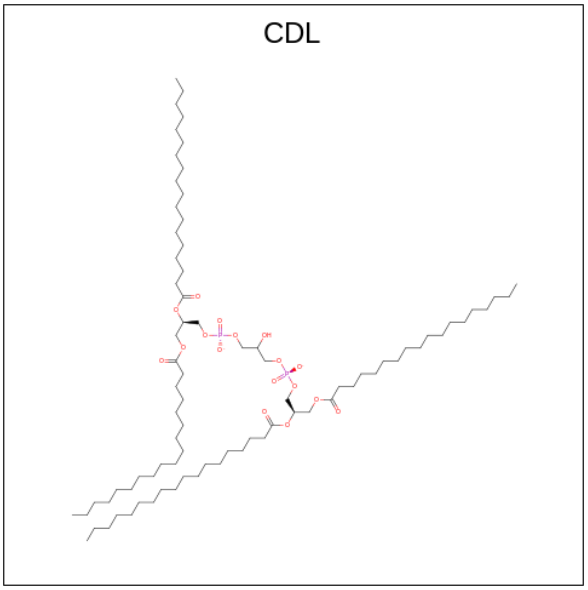
Mol	Chain	Residues	Atoms					AltConf
13	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	9	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	0	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	b	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	c	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	e	1	Total	C	Mg	N	O	0
			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 (three-letter code: 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 (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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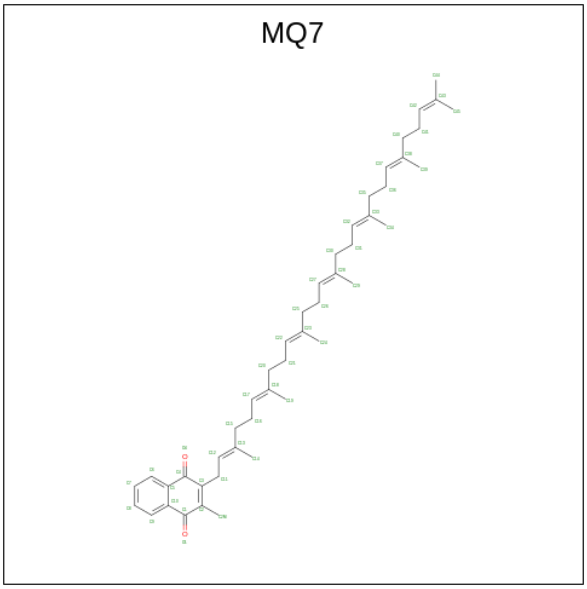
Mol	Chain	Residues	Atoms				AltConf
15	H	1	Total	C	O	P	0
			98	79	17	2	
15	H	1	Total	C	O	P	0
			72	53	17	2	
15	r	1	Total	C	O	P	0
			68	49	17	2	

- Molecule 16 is FE (III) ION (three-letter code: FE) (formula: Fe).

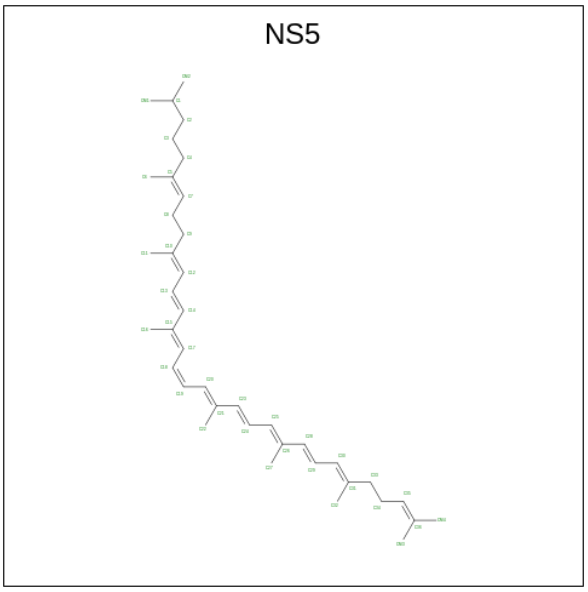
Mol	Chain	Residues	Atoms		AltConf
16	M	1	Total	Fe	0
			1	1	

- Molecule 17 is MENAQUINONE-7 (three-letter code: MQ7) (formula: $C_{46}H_{64}O_2$).



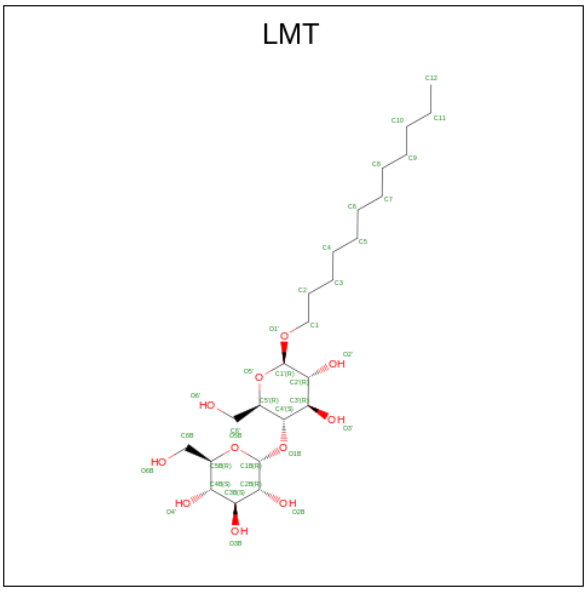
Mol	Chain	Residues	Atoms			AltConf
17	M	1	Total	C	O	0
			48	46	2	

- Molecule 18 is 15-cis-1,2-dihydroneurosporene (three-letter code: NS5) (formula: $C_{40}H_{60}$).



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

- Molecule 19 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



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

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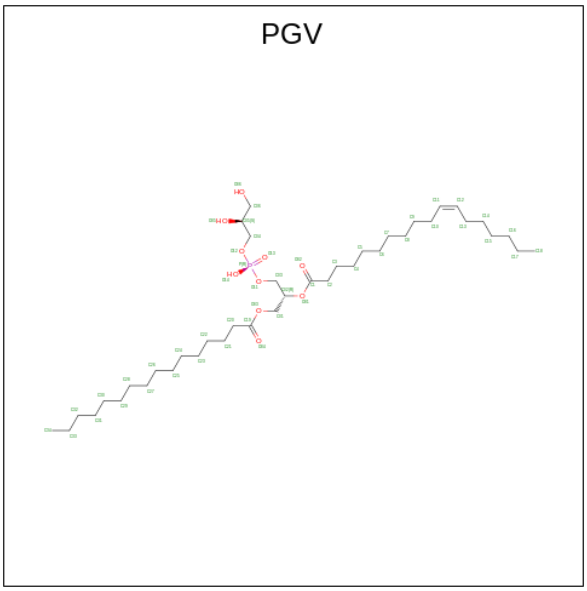
Mol	Chain	Residues	Atoms	AltConf
19	T	1	Total C O 26 19 7	0
19	b	1	Total C O 35 24 11	0
19	b	1	Total C O 35 24 11	0
19	h	1	Total C O 35 24 11	0
19	k	1	Total C O 35 24 11	0
19	n	1	Total C O 35 24 11	0

- Molecule 20 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: $C_{40}H_{77}O_{10}P$).



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

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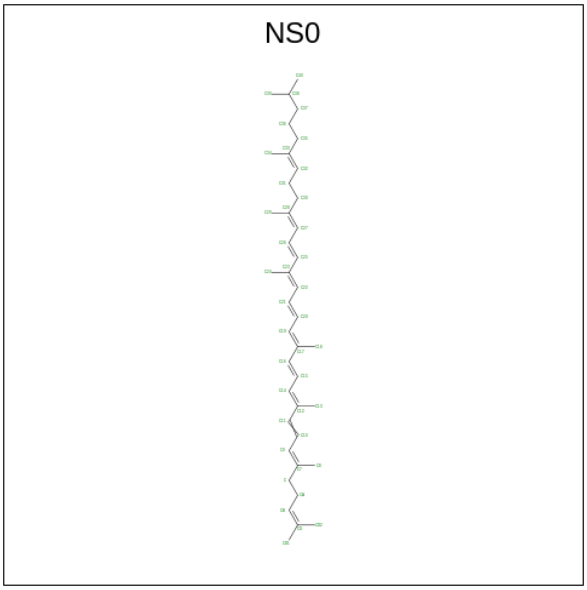
Mol	Chain	Residues	Atoms	AltConf
20	Q	1	Total C O P 49 39 9 1	0
20	W	1	Total C O P 48 37 10 1	0

- Molecule 21 is all-trans-1,2-dihydroneurosporene (three-letter code: NS0) (formula: $C_{40}H_{60}$).



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

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Mol	Chain	Residues	Atoms	AltConf
21	9	1	Total C 40 40	0
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

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Mol	Chain	Residues	Atoms	AltConf
22	O	3	Total O 3 3	0
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

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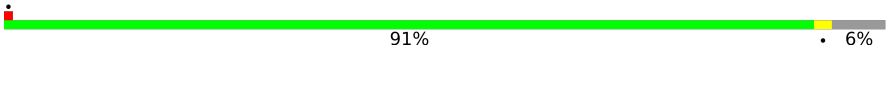
Mol	Chain	Residues	Atoms	AltConf
22	b	10	Total O 10 10	0
22	c	4	Total O 4 4	0
22	e	9	Total O 9 9	0
22	f	2	Total O 2 2	0
22	g	1	Total O 1 1	0
22	h	4	Total O 4 4	0
22	i	1	Total O 1 1	0
22	j	2	Total O 2 2	0
22	k	5	Total O 5 5	0
22	l	1	Total O 1 1	0
22	n	4	Total O 4 4	0
22	o	1	Total O 1 1	0
22	p	1	Total O 1 1	0
22	q	2	Total O 2 2	0

3 Residue-property plots (i)

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

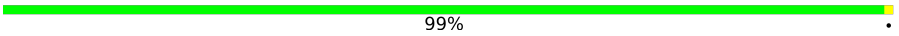
• Molecule 1: Photosynthetic reaction center cytochrome c subunit

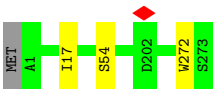
Chain C:



• Molecule 2: Reaction center protein L chain

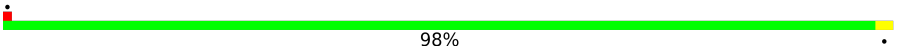
Chain L:





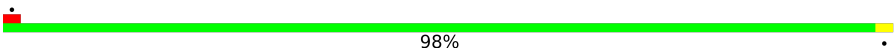
• Molecule 3: Reaction center protein M chain

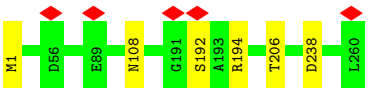
Chain M:



• Molecule 4: Photosynthetic reaction center subunit H

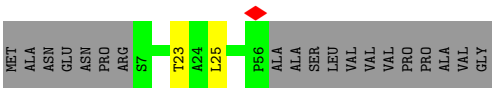
Chain H:





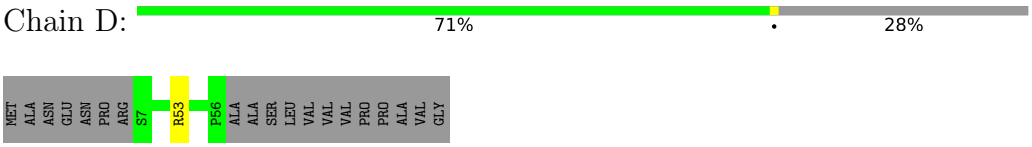
• Molecule 5: Antenna complex alpha/beta subunit domain-containing protein

Chain A:



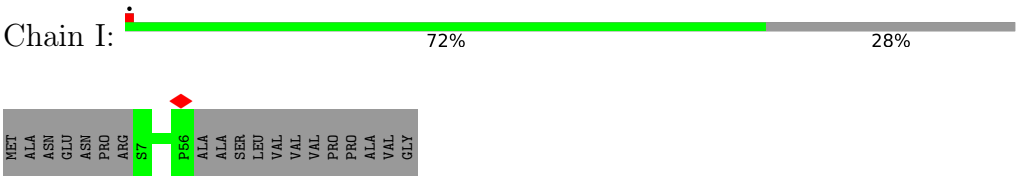
• Molecule 5: Antenna complex alpha/beta subunit domain-containing protein

Chain D:



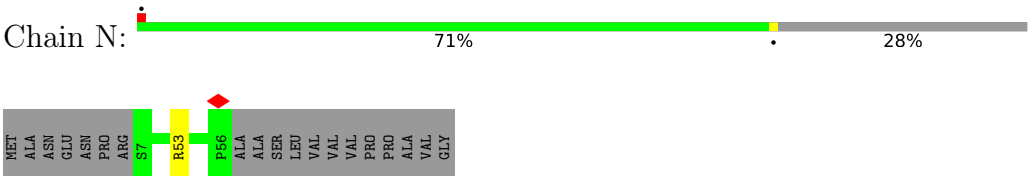
• Molecule 5: Antenna complex alpha/beta subunit domain-containing protein

Chain I:



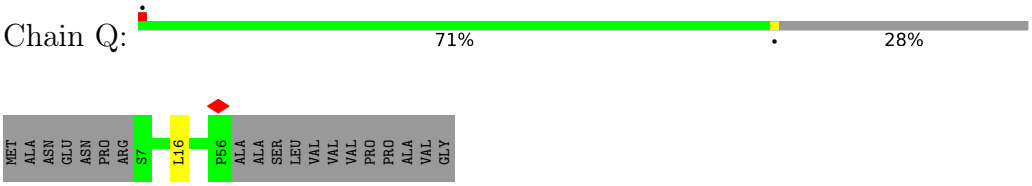
• Molecule 5: Antenna complex alpha/beta subunit domain-containing protein

Chain N:



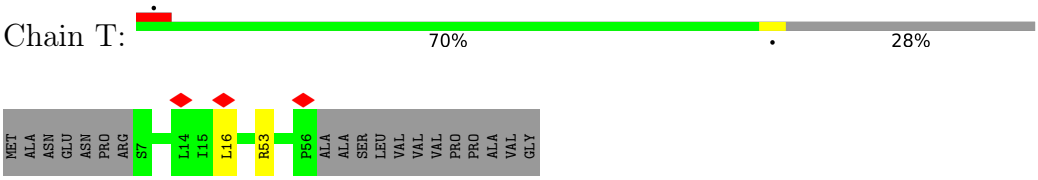
• Molecule 5: Antenna complex alpha/beta subunit domain-containing protein

Chain Q:



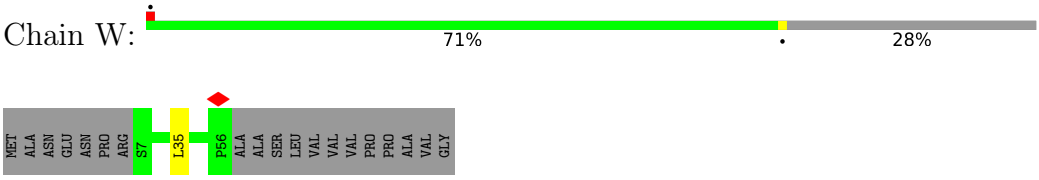
• Molecule 5: Antenna complex alpha/beta subunit domain-containing protein

Chain T:



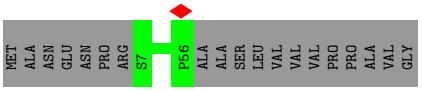
• Molecule 5: Antenna complex alpha/beta subunit domain-containing protein

Chain W:



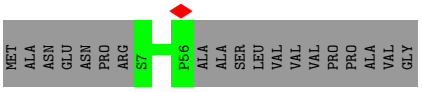
• Molecule 5: Antenna complex alpha/beta subunit domain-containing protein

Chain Z:



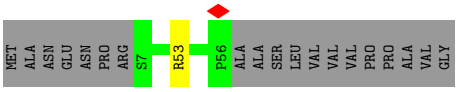
• Molecule 5: Antenna complex alpha/beta subunit domain-containing protein

Chain 3:



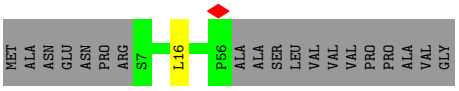
• Molecule 5: Antenna complex alpha/beta subunit domain-containing protein

Chain 6:



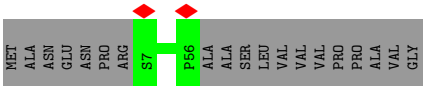
• Molecule 5: Antenna complex alpha/beta subunit domain-containing protein

Chain 9:



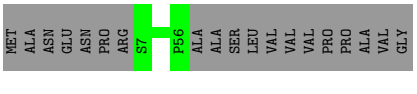
• Molecule 5: Antenna complex alpha/beta subunit domain-containing protein

Chain b:



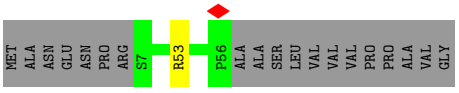
• Molecule 5: Antenna complex alpha/beta subunit domain-containing protein

Chain e:



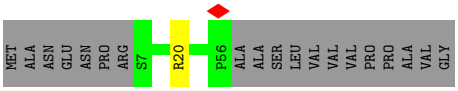
• Molecule 5: Antenna complex alpha/beta subunit domain-containing protein

Chain h:



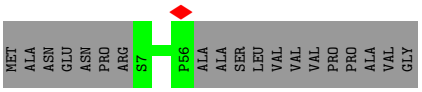
• Molecule 5: Antenna complex alpha/beta subunit domain-containing protein

Chain k:



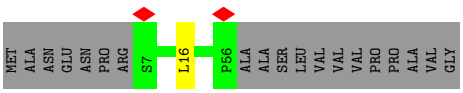
• Molecule 5: Antenna complex alpha/beta subunit domain-containing protein

Chain n:



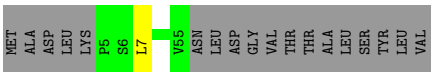
• Molecule 5: Antenna complex alpha/beta subunit domain-containing protein

Chain q:



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

Chain B:

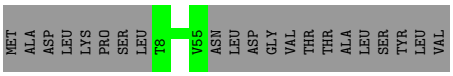


• Molecule 6: Antenna complex alpha/beta subunit domain-containing protein

Chain E:

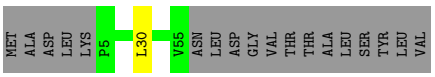
• Molecule 6: Antenna complex alpha/beta subunit domain-containing protein

Chain J:



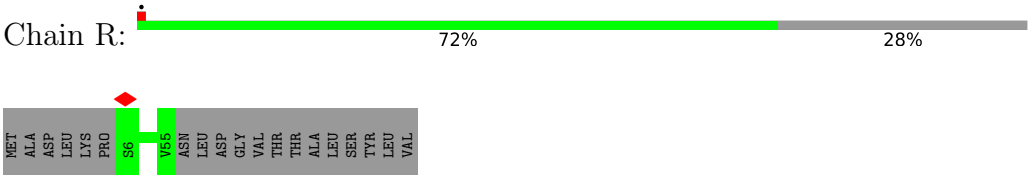
• Molecule 6: Antenna complex alpha/beta subunit domain-containing protein

Chain O:



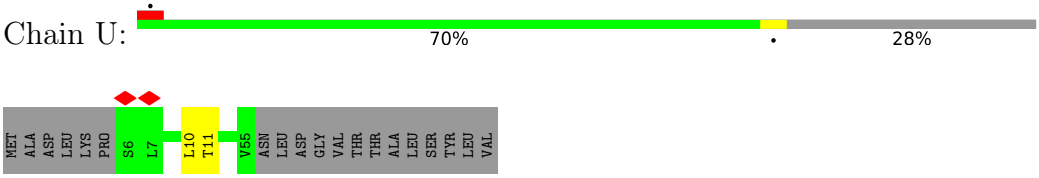
• Molecule 6: Antenna complex alpha/beta subunit domain-containing protein

Chain R:



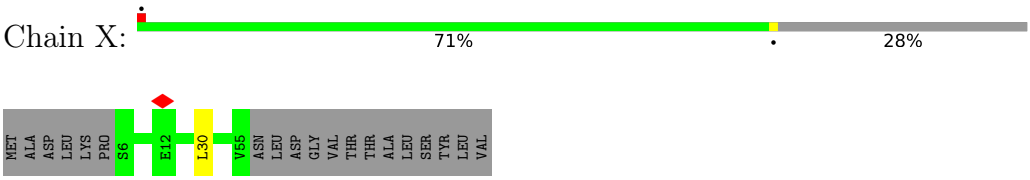
• Molecule 6: Antenna complex alpha/beta subunit domain-containing protein

Chain U:



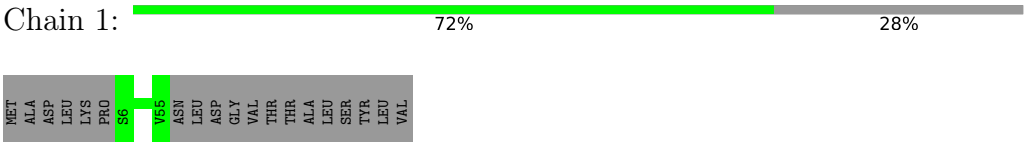
• Molecule 6: Antenna complex alpha/beta subunit domain-containing protein

Chain X:



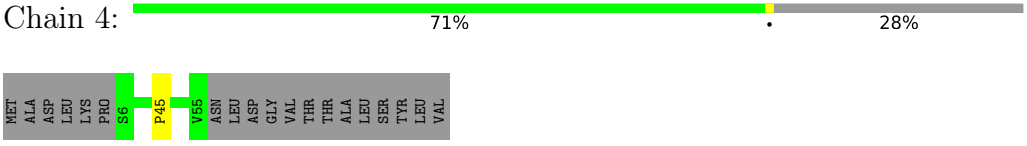
• Molecule 6: Antenna complex alpha/beta subunit domain-containing protein

Chain 1:



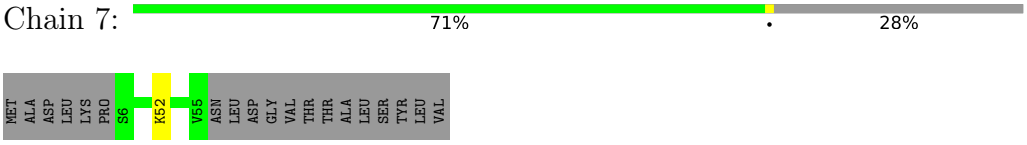
• Molecule 6: Antenna complex alpha/beta subunit domain-containing protein

Chain 4:



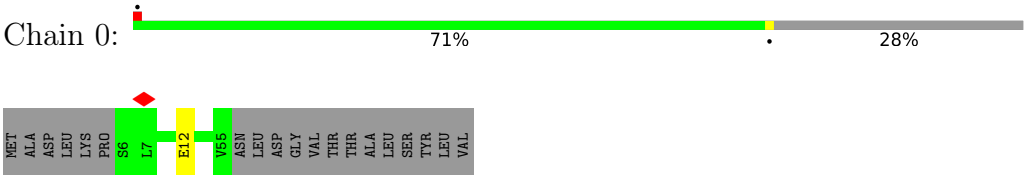
• Molecule 6: Antenna complex alpha/beta subunit domain-containing protein

Chain 7:



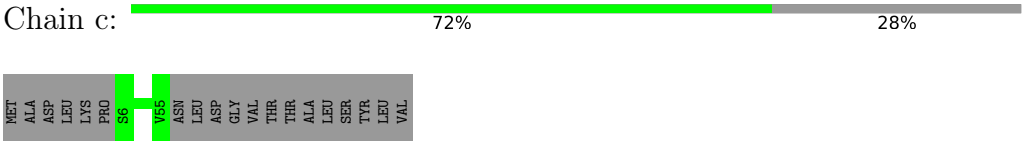
• Molecule 6: Antenna complex alpha/beta subunit domain-containing protein

Chain 0:



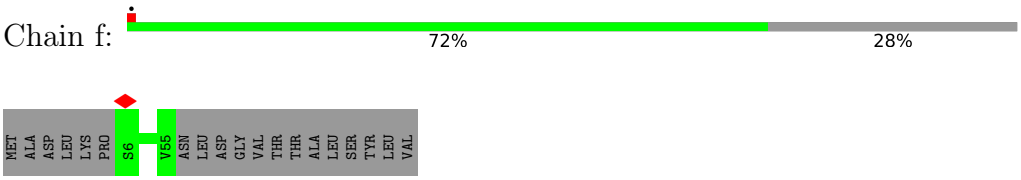
• Molecule 6: Antenna complex alpha/beta subunit domain-containing protein

Chain c:



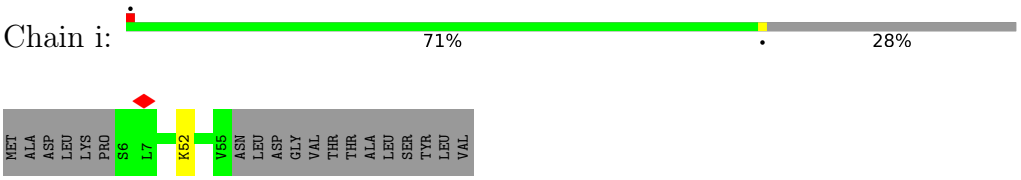
• Molecule 6: Antenna complex alpha/beta subunit domain-containing protein

Chain f:



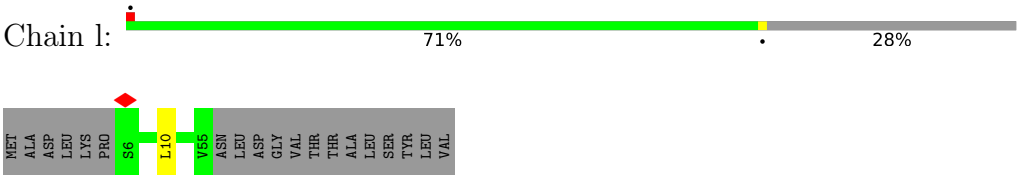
• Molecule 6: Antenna complex alpha/beta subunit domain-containing protein

Chain i:



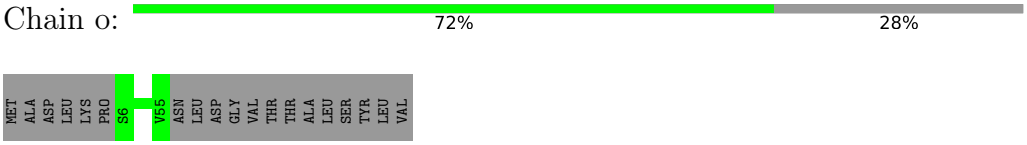
• Molecule 6: Antenna complex alpha/beta subunit domain-containing protein

Chain l:



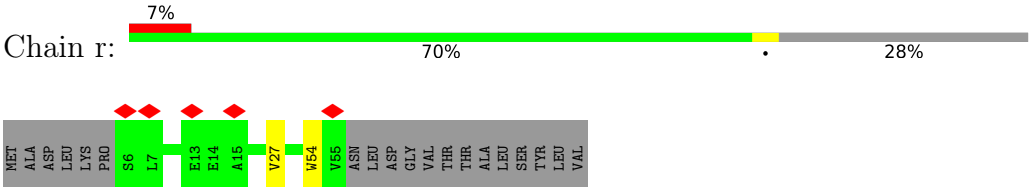
• Molecule 6: Antenna complex alpha/beta subunit domain-containing protein

Chain o:



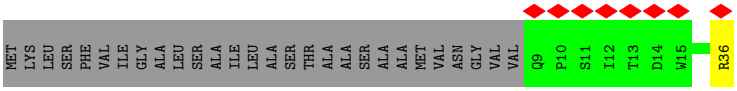
• Molecule 6: Antenna complex alpha/beta subunit domain-containing protein

Chain r:

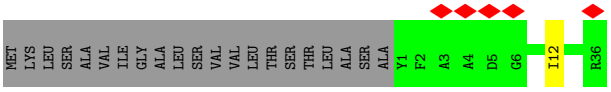


• Molecule 7: Light-harvesting protein gamma1

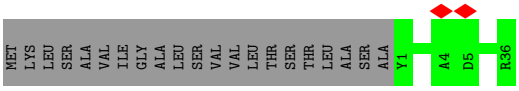
Chain G:



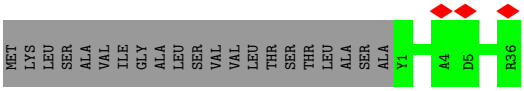
• Molecule 8: Light-harvesting protein B-1015 gamma chain



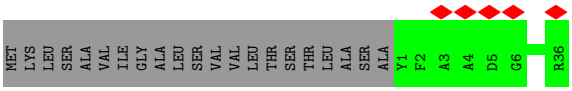
• Molecule 8: Light-harvesting protein B-1015 gamma chain



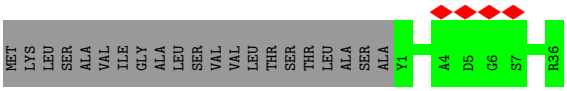
• Molecule 8: Light-harvesting protein B-1015 gamma chain



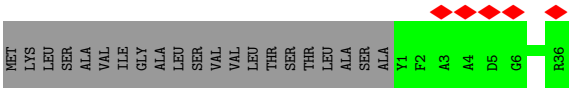
• Molecule 8: Light-harvesting protein B-1015 gamma chain



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

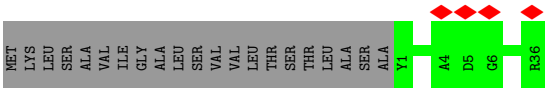


• Molecule 8: Light-harvesting protein B-1015 gamma chain



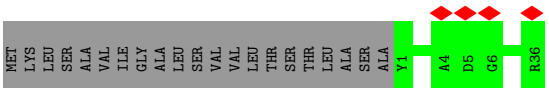
• Molecule 8: Light-harvesting protein B-1015 gamma chain

Chain 2:



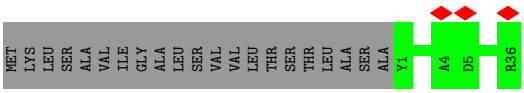
• Molecule 8: Light-harvesting protein B-1015 gamma chain

Chain 5:



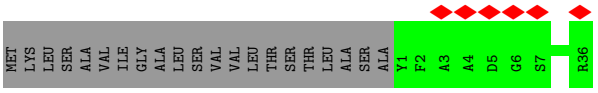
• Molecule 8: Light-harvesting protein B-1015 gamma chain

Chain 8:



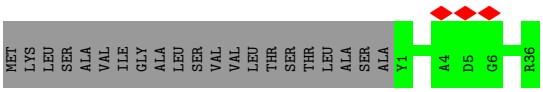
• Molecule 8: Light-harvesting protein B-1015 gamma chain

Chain a:



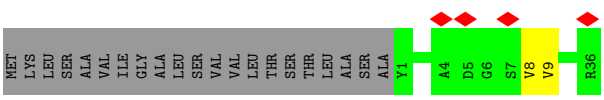
• Molecule 8: Light-harvesting protein B-1015 gamma chain

Chain d:



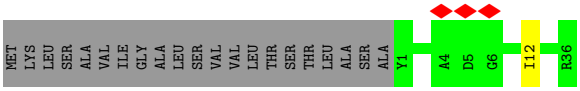
• Molecule 8: Light-harvesting protein B-1015 gamma chain

Chain g:

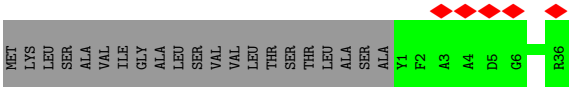


• Molecule 8: Light-harvesting protein B-1015 gamma chain

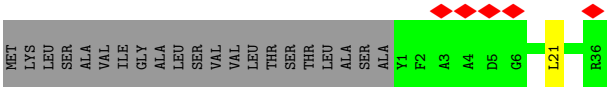
Chain j:



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



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



4 Experimental information (i)

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 ($e^-/Å^2$)	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 (Å)	328.0, 328.0, 328.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.31	0/2657	0.53	0/3614
2	L	0.31	0/2246	0.48	0/3062
3	M	0.31	0/2725	0.50	0/3718
4	H	0.30	0/2087	0.54	0/2848
5	3	0.28	0/438	0.51	0/599
5	6	0.28	0/438	0.52	0/599
5	9	0.28	0/438	0.51	0/599
5	A	0.29	0/438	0.51	0/599
5	D	0.28	0/438	0.49	0/599
5	I	0.28	0/438	0.49	0/599
5	N	0.27	0/438	0.49	0/599
5	Q	0.26	0/438	0.49	0/599
5	T	0.26	0/438	0.51	0/599
5	W	0.26	0/438	0.50	0/599
5	Z	0.28	0/438	0.52	0/599
5	b	0.27	0/438	0.49	0/599
5	e	0.26	0/438	0.49	0/599
5	h	0.25	0/438	0.51	0/599
5	k	0.28	0/438	0.50	0/599
5	n	0.26	0/438	0.51	0/599
5	q	0.26	0/438	0.50	0/599
6	0	0.29	0/414	0.45	0/569
6	1	0.31	0/414	0.43	0/569
6	4	0.30	0/414	0.44	0/569
6	7	0.30	0/414	0.44	0/569
6	B	0.28	0/422	0.44	0/580
6	E	0.30	0/422	0.44	0/580
6	J	0.30	0/400	0.43	0/550
6	O	0.29	0/422	0.45	0/580
6	R	0.29	0/414	0.45	0/569
6	U	0.29	0/414	0.50	0/569
6	X	0.29	0/414	0.46	0/569

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
6	c	0.29	0/414	0.46	0/569
6	f	0.30	0/414	0.43	0/569
6	i	0.28	0/414	0.46	0/569
6	l	0.28	0/414	0.44	0/569
6	o	0.28	0/414	0.43	0/569
6	r	0.29	0/414	0.45	0/569
7	G	0.27	0/241	0.52	0/333
8	2	0.28	0/288	0.53	0/397
8	5	0.29	0/288	0.52	0/397
8	8	0.29	0/288	0.50	0/397
8	F	0.28	0/288	0.50	0/397
8	K	0.27	0/288	0.51	0/397
8	P	0.28	0/288	0.49	0/397
8	S	0.28	0/288	0.53	0/397
8	V	0.29	0/288	0.51	0/397
8	Y	0.27	0/288	0.51	0/397
8	a	0.27	0/288	0.50	0/397
8	d	0.29	0/288	0.52	0/397
8	g	0.29	0/288	0.50	0/397
8	j	0.30	0/288	0.50	0/397
8	m	0.28	0/288	0.49	0/397
8	p	0.28	0/288	0.50	0/397
All	All	0.29	0/28770	0.49	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

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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 (i)

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%)	271 (97%)	8 (3%)	37	50
2	L	213/214 (100%)	210 (99%)	3 (1%)	62	77
3	M	257/258 (100%)	250 (97%)	7 (3%)	40	53
4	H	209/209 (100%)	204 (98%)	5 (2%)	44	57
5	3	45/59 (76%)	45 (100%)	0	100	100
5	6	45/59 (76%)	44 (98%)	1 (2%)	47	61
5	9	45/59 (76%)	44 (98%)	1 (2%)	47	61
5	A	45/59 (76%)	43 (96%)	2 (4%)	24	31
5	D	45/59 (76%)	44 (98%)	1 (2%)	47	61
5	I	45/59 (76%)	45 (100%)	0	100	100
5	N	45/59 (76%)	44 (98%)	1 (2%)	47	61
5	Q	45/59 (76%)	44 (98%)	1 (2%)	47	61
5	T	45/59 (76%)	43 (96%)	2 (4%)	24	31
5	W	45/59 (76%)	44 (98%)	1 (2%)	47	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%)	44 (98%)	1 (2%)	47	61
5	k	45/59 (76%)	44 (98%)	1 (2%)	47	61
5	n	45/59 (76%)	45 (100%)	0	100	100
5	q	45/59 (76%)	44 (98%)	1 (2%)	47	61
6	0	43/59 (73%)	42 (98%)	1 (2%)	45	59
6	1	43/59 (73%)	43 (100%)	0	100	100
6	4	43/59 (73%)	42 (98%)	1 (2%)	45	59
6	7	43/59 (73%)	42 (98%)	1 (2%)	45	59
6	B	44/59 (75%)	43 (98%)	1 (2%)	45	59
6	E	44/59 (75%)	43 (98%)	1 (2%)	45	59
6	J	41/59 (70%)	41 (100%)	0	100	100
6	O	44/59 (75%)	43 (98%)	1 (2%)	45	59
6	R	43/59 (73%)	43 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	U	43/59 (73%)	41 (95%)	2 (5%)	22 29
6	X	43/59 (73%)	42 (98%)	1 (2%)	45 59
6	c	43/59 (73%)	43 (100%)	0	100 100
6	f	43/59 (73%)	43 (100%)	0	100 100
6	i	43/59 (73%)	42 (98%)	1 (2%)	45 59
6	l	43/59 (73%)	42 (98%)	1 (2%)	45 59
6	o	43/59 (73%)	43 (100%)	0	100 100
6	r	43/59 (73%)	41 (95%)	2 (5%)	22 29
7	G	25/44 (57%)	24 (96%)	1 (4%)	27 35
8	2	29/45 (64%)	29 (100%)	0	100 100
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 42
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%)	13 14
8	j	29/45 (64%)	28 (97%)	1 (3%)	32 42
8	m	29/45 (64%)	29 (100%)	0	100 100
8	p	29/45 (64%)	28 (97%)	1 (3%)	32 42
All	All	2915/3701 (79%)	2860 (98%)	55 (2%)	52 67

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	38	TYR
1	C	52	VAL
1	C	55	VAL
1	C	71	LEU
1	C	88	THR

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Mol	Chain	Res	Type
1	C	115	ARG
1	C	250	THR
1	C	320	MET
2	L	17	ILE
2	L	54	SER
2	L	272	TRP
3	M	17	HIS
3	M	36	ILE
3	M	87	ARG
3	M	195	PHE
3	M	215	PHE
3	M	288	THR
3	M	313	THR
4	H	108	ASN
4	H	192	SER
4	H	194	ARG
4	H	206	THR
4	H	238	ASP
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
5	N	53	ARG
6	O	30	LEU
5	Q	16	LEU
5	T	16	LEU
5	T	53	ARG
6	U	10	LEU
6	U	11	THR
5	W	35	LEU
6	X	30	LEU
6	4	45	PRO
5	6	53	ARG
6	7	52	LYS
5	9	16	LEU
6	0	12	GLU
8	g	8	VAL
8	g	9	VAL
5	h	53	ARG

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Mol	Chain	Res	Type
6	i	52	LYS
8	j	12	ILE
5	k	20	ARG
6	l	10	LEU
8	p	21	LEU
5	q	16	LEU
6	r	27	VAL
6	r	54	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	267	GLN
1	C	295	GLN
4	H	94	GLN
4	H	108	ASN
7	G	16	ASN
5	D	44	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	0.46	0	7,9,11	1.24	2 (28%)

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(^{o})	Ideal(^{o})
4	H	1	FME	O-C-CA	-2.52	118.19	124.78
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	$\#\|Z\|>2$
21	NS0	h	101	-	39,39,39	1.42	6 (15%)	44,46,46	1.25	7 (15%)
14	BPB	L	304	-	49,70,70	0.58	1 (2%)	47,101,101	0.77	1 (2%)
20	PGV	N	102	-	37,37,50	1.08	2 (5%)	40,43,56	1.04	3 (7%)
13	BCB	4	101	-	63,74,74	2.97	15 (23%)	74,115,115	2.85	21 (28%)
13	BCB	E	101	-	63,74,74	2.97	15 (23%)	74,115,115	2.82	22 (29%)
13	BCB	c	101	-	63,74,74	3.00	15 (23%)	74,115,115	2.86	21 (28%)
9	HEC	C	403	1	32,50,50	1.64	5 (15%)	24,82,82	1.37	3 (12%)
21	NS0	R	101	-	39,39,39	1.41	6 (15%)	44,46,46	1.32	6 (13%)
13	BCB	U	102	-	63,74,74	3.00	15 (23%)	74,115,115	2.83	24 (32%)
19	LMT	h	103	-	36,36,36	0.36	0	47,47,47	0.70	1 (2%)
19	LMT	b	103	-	36,36,36	0.40	0	47,47,47	0.94	2 (4%)
21	NS0	l	101	-	39,39,39	1.38	6 (15%)	44,46,46	1.30	8 (18%)
13	BCB	B	202	-	63,74,74	3.00	15 (23%)	74,115,115	2.88	23 (31%)
20	PGV	Q	401	-	48,48,50	0.96	2 (4%)	51,53,56	0.99	2 (3%)
13	BCB	6	101	-	63,74,74	2.98	15 (23%)	74,115,115	2.81	22 (29%)
15	CDL	H	301	-	97,97,99	0.92	4 (4%)	103,109,111	1.06	5 (4%)
20	PGV	I	102	-	50,50,50	0.89	2 (4%)	53,56,56	1.03	3 (5%)
21	NS0	0	101	-	39,39,39	1.41	6 (15%)	44,46,46	1.20	6 (13%)
15	CDL	L	306	-	74,74,99	1.05	4 (5%)	80,86,111	1.17	8 (10%)
13	BCB	3	101	-	63,74,74	2.92	15 (23%)	74,115,115	2.95	24 (32%)
13	BCB	h	102	-	63,74,74	2.99	15 (23%)	74,115,115	2.94	23 (31%)
11	UQ8	M	407	-	25,25,53	1.70	2 (8%)	30,33,67	1.53	7 (23%)
19	LMT	B	201	-	14,14,36	0.69	0	14,14,47	0.59	0
9	HEC	C	402	1	32,50,50	1.56	4 (12%)	24,82,82	1.43	3 (12%)
21	NS0	9	102	-	39,39,39	1.42	6 (15%)	44,46,46	1.27	8 (18%)
13	BCB	Q	402	-	63,74,74	2.96	14 (22%)	74,115,115	2.87	21 (28%)
19	LMT	k	103	-	36,36,36	0.43	0	47,47,47	0.86	1 (2%)
9	HEC	C	401	1	32,50,50	1.61	4 (12%)	24,82,82	1.51	3 (12%)
13	BCB	0	102	-	63,74,74	2.98	14 (22%)	74,115,115	2.80	22 (29%)
13	BCB	J	101	-	63,74,74	2.99	15 (23%)	74,115,115	2.81	22 (29%)
13	BCB	b	101	-	63,74,74	2.93	15 (23%)	74,115,115	2.93	23 (31%)
13	BCB	T	101	-	63,74,74	3.00	16 (25%)	74,115,115	2.85	20 (27%)
21	NS0	X	101	-	39,39,39	1.39	6 (15%)	44,46,46	1.30	7 (15%)
13	BCB	L	303	-	63,74,74	2.96	15 (23%)	74,115,115	2.97	24 (32%)
21	NS0	2	101	-	39,39,39	1.41	6 (15%)	44,46,46	1.24	8 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	BCB	A	102	-	63,74,74	2.98	15 (23%)	74,115,115	2.91	22 (29%)
19	LMT	n	102	-	36,36,36	0.40	0	47,47,47	0.78	1 (2%)
13	BCB	D	101	-	63,74,74	2.96	16 (25%)	74,115,115	2.87	23 (31%)
14	BPB	M	404	-	49,70,70	0.56	1 (2%)	47,101,101	0.81	2 (4%)
13	BCB	Z	101	-	63,74,74	2.94	15 (23%)	74,115,115	2.90	21 (28%)
13	BCB	N	101	-	63,74,74	2.94	15 (23%)	74,115,115	2.87	20 (27%)
21	NS0	7	101	-	39,39,39	1.41	6 (15%)	44,46,46	1.25	6 (13%)
12	DGA	L	301	1	22,22,43	1.37	3 (13%)	24,24,45	1.83	5 (20%)
21	NS0	k	101	-	39,39,39	1.41	6 (15%)	44,46,46	1.36	8 (18%)
15	CDL	r	102	-	67,67,99	1.11	4 (5%)	73,79,111	1.14	4 (5%)
15	CDL	H	302	-	71,71,99	1.10	4 (5%)	77,83,111	1.09	5 (6%)
13	BCB	X	102	-	63,74,74	3.00	14 (22%)	74,115,115	2.82	23 (31%)
11	UQ8	L	305	-	31,31,53	1.56	2 (6%)	37,40,67	1.43	6 (16%)
21	NS0	W	303	-	39,39,39	1.38	8 (20%)	44,46,46	1.28	7 (15%)
13	BCB	M	403	-	63,74,74	2.98	16 (25%)	74,115,115	2.88	21 (28%)
13	BCB	r	101	-	63,74,74	3.02	14 (22%)	74,115,115	2.80	22 (29%)
13	BCB	o	102	-	63,74,74	3.01	15 (23%)	74,115,115	2.84	21 (28%)
13	BCB	f	101	-	63,74,74	2.98	15 (23%)	74,115,115	2.85	23 (31%)
11	UQ8	A	101	-	53,53,53	1.21	2 (3%)	64,67,67	1.59	15 (23%)
20	PGV	D	102	-	46,46,50	0.95	2 (4%)	48,52,56	1.07	2 (4%)
21	NS0	o	101	-	39,39,39	1.40	6 (15%)	44,46,46	1.26	7 (15%)
13	BCB	q	101	-	63,74,74	2.97	16 (25%)	74,115,115	2.87	22 (29%)
19	LMT	M	410	-	25,25,36	0.42	0	30,30,47	0.63	0
19	LMT	T	102	-	26,26,36	0.41	0	31,31,47	1.05	2 (6%)
18	NS5	M	406	-	39,39,39	1.43	6 (15%)	44,46,46	1.28	7 (15%)
9	HEC	C	404	1	32,50,50	1.62	5 (15%)	24,82,82	1.30	1 (4%)
21	NS0	q	102	-	39,39,39	1.40	6 (15%)	44,46,46	1.29	7 (15%)
20	PGV	M	411	-	44,44,50	0.96	2 (4%)	46,50,56	0.95	3 (6%)
15	CDL	M	409	-	84,84,99	0.99	4 (4%)	90,96,111	1.11	8 (8%)
13	BCB	e	101	-	63,74,74	2.99	15 (23%)	74,115,115	2.88	22 (29%)
11	UQ8	C	406	-	15,15,53	2.16	2 (13%)	19,21,67	1.42	2 (10%)
13	BCB	L	302	-	63,74,74	2.92	14 (22%)	74,115,115	2.92	20 (27%)
13	BCB	k	102	-	63,74,74	2.97	15 (23%)	74,115,115	2.81	21 (28%)
11	UQ8	M	408	-	53,53,53	1.25	2 (3%)	64,67,67	1.61	17 (26%)
13	BCB	l	102	-	63,74,74	3.01	15 (23%)	74,115,115	2.89	22 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	NS0	O	101	-	39,39,39	1.38	6 (15%)	44,46,46	1.24	6 (13%)
13	BCB	1	101	-	63,74,74	2.98	14 (22%)	74,115,115	2.89	22 (29%)
13	BCB	n	101	-	63,74,74	3.01	14 (22%)	74,115,115	2.85	23 (31%)
21	NS0	U	101	-	39,39,39	1.39	6 (15%)	44,46,46	1.31	8 (18%)
13	BCB	O	102	-	63,74,74	2.94	15 (23%)	74,115,115	2.87	20 (27%)
13	BCB	I	101	-	63,74,74	2.96	15 (23%)	74,115,115	2.88	20 (27%)
21	NS0	D	103	-	39,39,39	1.43	6 (15%)	44,46,46	1.25	7 (15%)
17	MQ7	M	405	-	49,49,49	1.36	2 (4%)	60,63,63	1.48	13 (21%)
13	BCB	M	402	-	63,74,74	2.98	15 (23%)	74,115,115	2.91	20 (27%)
20	PGV	W	301	-	47,47,50	0.95	2 (4%)	50,53,56	1.07	4 (8%)
13	BCB	R	102	-	63,74,74	3.01	15 (23%)	74,115,115	2.90	22 (29%)
13	BCB	W	302	-	63,74,74	2.98	15 (23%)	74,115,115	2.90	21 (28%)
13	BCB	9	101	-	63,74,74	2.97	15 (23%)	74,115,115	2.87	23 (31%)
21	NS0	A	103	-	39,39,39	1.41	6 (15%)	44,46,46	1.26	8 (18%)
19	LMT	b	102	-	36,36,36	0.44	0	47,47,47	0.78	0
13	BCB	7	102	-	63,74,74	2.99	14 (22%)	74,115,115	2.80	23 (31%)
13	BCB	i	101	-	63,74,74	2.96	15 (23%)	74,115,115	2.86	25 (33%)

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
21	NS0	h	101	-	-	1/43/43/43	-
14	BPB	L	304	-	-	3/37/105/105	0/5/6/6
20	PGV	N	102	-	-	11/42/42/55	-
13	BCB	4	101	-	2/2/21/26	12/37/137/137	-
13	BCB	E	101	-	2/2/21/26	14/37/137/137	-
13	BCB	c	101	-	2/2/21/26	14/37/137/137	-
9	HEC	C	403	1	-	0/10/54/54	-
21	NS0	R	101	-	-	6/43/43/43	-
13	BCB	U	102	-	2/2/21/26	11/37/137/137	-
19	LMT	h	103	-	-	4/21/61/61	0/2/2/2
19	LMT	b	103	-	-	6/21/61/61	0/2/2/2
21	NS0	l	101	-	-	7/43/43/43	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	BCB	B	202	-	2/2/21/26	4/37/137/137	-
20	PGV	Q	401	-	-	17/52/52/55	-
13	BCB	6	101	-	2/2/21/26	6/37/137/137	-
15	CDL	H	301	-	-	41/108/108/110	-
20	PGV	I	102	-	-	16/55/55/55	-
21	NS0	0	101	-	-	4/43/43/43	-
15	CDL	L	306	-	-	31/85/85/110	-
13	BCB	3	101	-	2/2/21/26	12/37/137/137	-
13	BCB	h	102	-	2/2/21/26	4/37/137/137	-
11	UQ8	M	407	-	-	0/18/42/75	0/1/1/1
19	LMT	B	201	-	-	6/13/13/61	-
9	HEC	C	402	1	-	3/10/54/54	-
21	NS0	9	102	-	-	6/43/43/43	-
13	BCB	Q	402	-	2/2/21/26	6/37/137/137	-
19	LMT	k	103	-	-	3/21/61/61	0/2/2/2
9	HEC	C	401	1	-	2/10/54/54	-
13	BCB	0	102	-	2/2/21/26	13/37/137/137	-
13	BCB	J	101	-	2/2/21/26	13/37/137/137	-
13	BCB	b	101	-	2/2/21/26	10/37/137/137	-
13	BCB	T	101	-	2/2/21/26	10/37/137/137	-
21	NS0	X	101	-	-	4/43/43/43	-
13	BCB	L	303	-	2/2/21/26	3/37/137/137	-
21	NS0	2	101	-	-	6/43/43/43	-
13	BCB	A	102	-	2/2/21/26	17/37/137/137	-
19	LMT	n	102	-	-	4/21/61/61	0/2/2/2
13	BCB	D	101	-	2/2/21/26	10/37/137/137	-
14	BPB	M	404	-	-	5/37/105/105	0/5/6/6
13	BCB	Z	101	-	2/2/21/26	6/37/137/137	-
13	BCB	N	101	-	2/2/21/26	17/37/137/137	-
21	NS0	7	101	-	-	6/43/43/43	-
12	DGA	L	301	1	-	13/23/23/45	-
21	NS0	k	101	-	-	4/43/43/43	-
15	CDL	r	102	-	-	42/78/78/110	-
15	CDL	H	302	-	-	36/82/82/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	BCB	X	102	-	2/2/21/26	19/37/137/137	-
11	UQ8	L	305	-	-	6/25/49/75	0/1/1/1
21	NS0	W	303	-	-	7/43/43/43	-
13	BCB	M	403	-	2/2/21/26	8/37/137/137	-
13	BCB	r	101	-	2/2/21/26	14/37/137/137	-
13	BCB	o	102	-	2/2/21/26	18/37/137/137	-
13	BCB	f	101	-	2/2/21/26	17/37/137/137	-
11	UQ8	A	101	-	-	14/51/75/75	0/1/1/1
20	PGV	D	102	-	-	14/51/51/55	-
21	NS0	o	101	-	-	6/43/43/43	-
13	BCB	q	101	-	2/2/21/26	14/37/137/137	-
19	LMT	M	410	-	-	6/17/37/61	0/1/1/2
19	LMT	T	102	-	-	1/17/38/61	0/1/1/2
18	NS5	M	406	-	-	2/43/43/43	-
9	HEC	C	404	1	-	3/10/54/54	-
21	NS0	q	102	-	-	7/43/43/43	-
20	PGV	M	411	-	-	13/49/49/55	-
15	CDL	M	409	-	-	38/95/95/110	-
13	BCB	e	101	-	2/2/21/26	10/37/137/137	-
11	UQ8	C	406	-	-	0/6/30/75	0/1/1/1
13	BCB	L	302	-	2/2/21/26	5/37/137/137	-
13	BCB	k	102	-	2/2/21/26	11/37/137/137	-
11	UQ8	M	408	-	-	12/51/75/75	0/1/1/1
13	BCB	l	102	-	2/2/21/26	6/37/137/137	-
21	NS0	O	101	-	-	8/43/43/43	-
13	BCB	1	101	-	2/2/21/26	14/37/137/137	-
13	BCB	n	101	-	2/2/21/26	4/37/137/137	-
21	NS0	U	101	-	-	6/43/43/43	-
13	BCB	O	102	-	2/2/21/26	17/37/137/137	-
13	BCB	I	101	-	2/2/21/26	8/37/137/137	-
21	NS0	D	103	-	-	3/43/43/43	-
17	MQ7	M	405	-	-	0/41/61/61	0/2/2/2
13	BCB	M	402	-	2/2/21/26	8/37/137/137	-
20	PGV	W	301	-	-	16/52/52/55	-
13	BCB	R	102	-	2/2/21/26	10/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	BCB	W	302	-	2/2/21/26	10/37/137/137	-
13	BCB	9	101	-	2/2/21/26	12/37/137/137	-
21	NS0	A	103	-	-	2/43/43/43	-
19	LMT	b	102	-	-	11/21/61/61	0/2/2/2
13	BCB	7	102	-	2/2/21/26	21/37/137/137	-
13	BCB	i	101	-	2/2/21/26	14/37/137/137	-

All (737) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	R	102	BCB	C4B-NB	12.73	1.46	1.35
13	J	101	BCB	C4B-NB	12.71	1.46	1.35
13	o	102	BCB	C4B-NB	12.65	1.46	1.35
13	B	202	BCB	C4B-NB	12.59	1.46	1.35
13	c	101	BCB	C4B-NB	12.58	1.46	1.35
13	X	102	BCB	C4B-NB	12.51	1.46	1.35
13	0	102	BCB	C4B-NB	12.44	1.46	1.35
13	7	102	BCB	C4B-NB	12.42	1.46	1.35
13	4	101	BCB	C4B-NB	12.42	1.46	1.35
13	U	102	BCB	C4B-NB	12.38	1.46	1.35
13	n	101	BCB	C4B-NB	12.37	1.46	1.35
13	6	101	BCB	C4B-NB	12.33	1.46	1.35
13	l	102	BCB	C4B-NB	12.31	1.46	1.35
13	e	101	BCB	C4B-NB	12.30	1.46	1.35
13	W	302	BCB	C4B-NB	12.29	1.46	1.35
13	f	101	BCB	C4B-NB	12.26	1.46	1.35
13	h	102	BCB	C4B-NB	12.23	1.46	1.35
13	i	101	BCB	C4B-NB	12.23	1.46	1.35
13	T	101	BCB	C4B-NB	12.18	1.46	1.35
13	k	102	BCB	C4B-NB	12.15	1.46	1.35
13	Q	402	BCB	C4B-NB	12.14	1.46	1.35
13	E	101	BCB	C4B-NB	12.11	1.46	1.35
13	9	101	BCB	C4B-NB	12.10	1.46	1.35
13	r	101	BCB	C4B-NB	12.10	1.46	1.35
13	O	102	BCB	C4B-NB	12.09	1.46	1.35
13	1	101	BCB	C4B-NB	12.08	1.46	1.35
13	M	402	BCB	C4B-NB	12.03	1.45	1.35
13	Z	101	BCB	C4B-NB	12.02	1.45	1.35
13	L	303	BCB	C4B-NB	11.88	1.45	1.35
13	b	101	BCB	C4B-NB	11.88	1.45	1.35
13	I	101	BCB	C4B-NB	11.88	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	r	101	BCB	C1B-NB	11.84	1.45	1.35
13	N	101	BCB	C4B-NB	11.79	1.45	1.35
13	D	101	BCB	C4B-NB	11.59	1.45	1.35
13	A	102	BCB	C4B-NB	11.58	1.45	1.35
13	3	101	BCB	C4B-NB	11.58	1.45	1.35
13	q	101	BCB	C4B-NB	11.54	1.45	1.35
13	M	403	BCB	C4B-NB	11.52	1.45	1.35
13	M	402	BCB	C1B-NB	11.40	1.45	1.35
13	U	102	BCB	C1B-NB	11.32	1.45	1.35
13	L	302	BCB	C4B-NB	11.31	1.45	1.35
13	l	102	BCB	C1B-NB	11.28	1.45	1.35
13	J	101	BCB	C1B-NB	11.14	1.45	1.35
13	T	101	BCB	C1B-NB	11.14	1.45	1.35
13	o	102	BCB	C1B-NB	11.14	1.45	1.35
13	1	101	BCB	C1B-NB	11.12	1.45	1.35
13	q	101	BCB	C1B-NB	11.12	1.45	1.35
13	X	102	BCB	C1B-NB	11.06	1.45	1.35
13	A	102	BCB	C1B-NB	10.99	1.45	1.35
13	0	102	BCB	C1B-NB	10.97	1.45	1.35
13	L	303	BCB	C1B-NB	10.96	1.45	1.35
13	n	101	BCB	C1B-NB	10.95	1.45	1.35
13	E	101	BCB	C1B-NB	10.95	1.45	1.35
13	B	202	BCB	C1B-NB	10.94	1.45	1.35
13	f	101	BCB	C1B-NB	10.93	1.45	1.35
13	h	102	BCB	C1B-NB	10.91	1.44	1.35
13	L	302	BCB	C1B-NB	10.91	1.44	1.35
13	c	101	BCB	C1B-NB	10.88	1.44	1.35
13	D	101	BCB	C1B-NB	10.88	1.44	1.35
13	7	102	BCB	C1B-NB	10.84	1.44	1.35
13	4	101	BCB	C1B-NB	10.84	1.44	1.35
13	i	101	BCB	C1B-NB	10.83	1.44	1.35
13	6	101	BCB	C1B-NB	10.82	1.44	1.35
13	R	102	BCB	C1B-NB	10.79	1.44	1.35
13	Q	402	BCB	C1B-NB	10.78	1.44	1.35
13	k	102	BCB	C1B-NB	10.76	1.44	1.35
13	Z	101	BCB	C1B-NB	10.74	1.44	1.35
13	O	102	BCB	C1B-NB	10.73	1.44	1.35
13	N	101	BCB	C1B-NB	10.69	1.44	1.35
13	e	101	BCB	C1B-NB	10.68	1.44	1.35
13	9	101	BCB	C1B-NB	10.66	1.44	1.35
13	M	403	BCB	C1B-NB	10.65	1.44	1.35
13	W	302	BCB	C1B-NB	10.59	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	3	101	BCB	C1B-NB	10.54	1.44	1.35
13	I	101	BCB	C1B-NB	10.51	1.44	1.35
13	b	101	BCB	C1B-NB	10.33	1.44	1.35
11	M	408	UQ8	C6-C1	7.83	1.49	1.35
13	M	403	BCB	C1D-ND	7.69	1.47	1.37
17	M	405	MQ7	C3-C2	7.66	1.49	1.35
11	M	407	UQ8	C6-C1	7.64	1.49	1.35
13	A	102	BCB	C1D-ND	7.62	1.47	1.37
11	L	305	UQ8	C6-C1	7.58	1.49	1.35
13	9	101	BCB	C1D-ND	7.51	1.47	1.37
11	C	406	UQ8	C6-C1	7.49	1.48	1.35
11	A	101	UQ8	C6-C1	7.43	1.48	1.35
13	D	101	BCB	C1D-ND	7.42	1.46	1.37
13	b	101	BCB	C1D-ND	7.41	1.46	1.37
13	T	101	BCB	C1D-ND	7.40	1.46	1.37
13	n	101	BCB	C1D-ND	7.39	1.46	1.37
13	I	101	BCB	C1D-ND	7.38	1.46	1.37
13	L	302	BCB	C1D-ND	7.38	1.46	1.37
13	q	101	BCB	C1D-ND	7.37	1.46	1.37
13	e	101	BCB	C1D-ND	7.35	1.46	1.37
13	h	102	BCB	C1D-ND	7.31	1.46	1.37
13	W	302	BCB	C1D-ND	7.28	1.46	1.37
13	6	101	BCB	C1D-ND	7.27	1.46	1.37
13	M	402	BCB	C1D-ND	7.25	1.46	1.37
13	3	101	BCB	C1D-ND	7.25	1.46	1.37
13	L	303	BCB	C1D-ND	7.17	1.46	1.37
13	k	102	BCB	C1D-ND	7.14	1.46	1.37
13	Q	402	BCB	C1D-ND	7.10	1.46	1.37
13	Z	101	BCB	C1D-ND	7.09	1.46	1.37
13	N	101	BCB	C1D-ND	7.07	1.46	1.37
13	o	102	BCB	C1D-ND	7.07	1.46	1.37
13	7	102	BCB	C1D-ND	6.99	1.46	1.37
13	X	102	BCB	C1D-ND	6.92	1.46	1.37
13	r	101	BCB	C1D-ND	6.91	1.46	1.37
13	B	202	BCB	C1D-ND	6.90	1.46	1.37
13	O	102	BCB	C1D-ND	6.90	1.46	1.37
13	E	101	BCB	C1D-ND	6.83	1.46	1.37
13	4	101	BCB	C1D-ND	6.81	1.46	1.37
13	R	102	BCB	C1D-ND	6.75	1.46	1.37
13	f	101	BCB	C1D-ND	6.71	1.46	1.37
13	c	101	BCB	C1D-ND	6.69	1.46	1.37
13	i	101	BCB	C1D-ND	6.69	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	0	102	BCB	C1D-ND	6.65	1.46	1.37
13	U	102	BCB	C1D-ND	6.64	1.45	1.37
13	J	101	BCB	C1D-ND	6.62	1.45	1.37
13	l	102	BCB	C1D-ND	6.60	1.45	1.37
13	1	101	BCB	C1D-ND	6.57	1.45	1.37
13	3	101	BCB	C3B-C2B	6.36	1.50	1.39
13	I	101	BCB	C3B-C2B	6.33	1.50	1.39
13	M	403	BCB	C3B-C2B	6.29	1.50	1.39
13	R	102	BCB	C3B-C2B	6.29	1.50	1.39
13	b	101	BCB	C3B-C2B	6.28	1.50	1.39
13	D	101	BCB	C3B-C2B	6.27	1.50	1.39
13	T	101	BCB	C3B-C2B	6.26	1.50	1.39
13	W	302	BCB	C3B-C2B	6.26	1.50	1.39
13	N	101	BCB	C3B-C2B	6.24	1.50	1.39
13	k	102	BCB	C3B-C2B	6.21	1.50	1.39
13	n	101	BCB	C3B-C2B	6.20	1.50	1.39
13	L	303	BCB	C3B-C2B	6.19	1.50	1.39
13	1	101	BCB	C3B-C2B	6.18	1.50	1.39
13	q	101	BCB	C3B-C2B	6.18	1.50	1.39
13	c	101	BCB	C3B-C2B	6.17	1.50	1.39
13	6	101	BCB	C3B-C2B	6.17	1.50	1.39
13	o	102	BCB	C3B-C2B	6.17	1.50	1.39
13	h	102	BCB	C3B-C2B	6.16	1.50	1.39
13	l	102	BCB	C3B-C2B	6.15	1.50	1.39
13	A	102	BCB	C3B-C2B	6.15	1.50	1.39
13	f	101	BCB	C3B-C2B	6.13	1.50	1.39
13	B	202	BCB	C3B-C2B	6.13	1.50	1.39
13	e	101	BCB	C3B-C2B	6.12	1.50	1.39
13	Q	402	BCB	C3B-C2B	6.12	1.50	1.39
13	U	102	BCB	C3B-C2B	6.11	1.50	1.39
13	7	102	BCB	C3B-C2B	6.11	1.50	1.39
13	9	101	BCB	C3B-C2B	6.10	1.50	1.39
13	M	403	BCB	C2C-C3C	-6.09	1.43	1.51
13	L	302	BCB	C3B-C2B	6.09	1.50	1.39
13	4	101	BCB	C3B-C2B	6.08	1.50	1.39
13	i	101	BCB	C3B-C2B	6.04	1.50	1.39
13	O	102	BCB	C3B-C2B	6.04	1.50	1.39
13	E	101	BCB	C3B-C2B	6.03	1.50	1.39
13	0	102	BCB	C3B-C2B	6.03	1.50	1.39
13	c	101	BCB	C2C-C3C	-6.01	1.43	1.51
13	X	102	BCB	C3B-C2B	5.96	1.50	1.39
13	r	101	BCB	C3B-C2B	5.96	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	Z	101	BCB	C3B-C2B	5.95	1.50	1.39
13	J	101	BCB	C3B-C2B	5.91	1.50	1.39
13	e	101	BCB	CAC-C3C	5.90	1.49	1.33
13	I	101	BCB	CAC-C3C	5.89	1.49	1.33
13	Q	402	BCB	CAC-C3C	5.88	1.49	1.33
13	l	102	BCB	CAC-C3C	5.88	1.49	1.33
13	B	202	BCB	CAC-C3C	5.87	1.49	1.33
13	n	101	BCB	CAC-C3C	5.87	1.49	1.33
13	R	102	BCB	C2C-C3C	-5.86	1.44	1.51
13	U	102	BCB	CAC-C3C	5.86	1.49	1.33
13	Z	101	BCB	CAC-C3C	5.85	1.49	1.33
13	h	102	BCB	CAC-C3C	5.85	1.49	1.33
13	T	101	BCB	CAC-C3C	5.85	1.49	1.33
13	6	101	BCB	CAC-C3C	5.85	1.49	1.33
13	b	101	BCB	CAC-C3C	5.84	1.49	1.33
13	c	101	BCB	CAC-C3C	5.83	1.49	1.33
13	0	102	BCB	CAC-C3C	5.83	1.49	1.33
13	E	101	BCB	CAC-C3C	5.83	1.49	1.33
13	k	102	BCB	CAC-C3C	5.82	1.49	1.33
13	L	302	BCB	CAC-C3C	5.82	1.49	1.33
13	1	101	BCB	C2C-C3C	-5.81	1.44	1.51
13	q	101	BCB	CAC-C3C	5.81	1.49	1.33
13	W	302	BCB	CAC-C3C	5.80	1.49	1.33
13	A	102	BCB	C2C-C3C	-5.80	1.44	1.51
13	r	101	BCB	CAC-C3C	5.80	1.49	1.33
13	O	102	BCB	C2C-C3C	-5.79	1.44	1.51
13	3	101	BCB	CAC-C3C	5.79	1.49	1.33
13	1	101	BCB	CAC-C3C	5.78	1.49	1.33
13	N	101	BCB	CAC-C3C	5.78	1.49	1.33
13	9	101	BCB	CAC-C3C	5.78	1.49	1.33
13	4	101	BCB	CAC-C3C	5.78	1.49	1.33
13	D	101	BCB	CAC-C3C	5.77	1.49	1.33
13	7	102	BCB	CAC-C3C	5.77	1.49	1.33
13	o	102	BCB	CAC-C3C	5.76	1.49	1.33
13	A	102	BCB	CAC-C3C	5.75	1.49	1.33
13	M	403	BCB	CAC-C3C	5.75	1.49	1.33
13	L	303	BCB	CAC-C3C	5.74	1.49	1.33
13	i	101	BCB	CAC-C3C	5.74	1.49	1.33
13	X	102	BCB	CAC-C3C	5.72	1.49	1.33
13	J	101	BCB	CAC-C3C	5.72	1.49	1.33
13	O	102	BCB	CAC-C3C	5.71	1.49	1.33
13	l	102	BCB	C2C-C3C	-5.71	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	R	102	BCB	CAC-C3C	5.71	1.49	1.33
13	f	101	BCB	C2C-C3C	-5.70	1.44	1.51
13	4	101	BCB	C2C-C3C	-5.70	1.44	1.51
13	M	402	BCB	C2C-C3C	-5.70	1.44	1.51
13	f	101	BCB	CAC-C3C	5.69	1.49	1.33
13	7	102	BCB	C2C-C3C	-5.69	1.44	1.51
13	M	402	BCB	CAC-C3C	5.68	1.49	1.33
13	E	101	BCB	C2C-C3C	-5.68	1.44	1.51
13	X	102	BCB	C2C-C3C	-5.68	1.44	1.51
13	U	102	BCB	C2C-C3C	-5.61	1.44	1.51
13	r	101	BCB	C2C-C3C	-5.56	1.44	1.51
13	0	102	BCB	C2C-C3C	-5.56	1.44	1.51
13	i	101	BCB	C2C-C3C	-5.55	1.44	1.51
13	o	102	BCB	C2C-C3C	-5.54	1.44	1.51
13	6	101	BCB	C2C-C3C	-5.53	1.44	1.51
13	D	101	BCB	C2C-C3C	-5.50	1.44	1.51
13	W	302	BCB	C2C-C3C	-5.50	1.44	1.51
13	I	101	BCB	C2C-C3C	-5.48	1.44	1.51
13	b	101	BCB	C2C-C3C	-5.47	1.44	1.51
13	N	101	BCB	C2C-C3C	-5.45	1.44	1.51
13	L	302	BCB	C2C-C3C	-5.41	1.44	1.51
13	h	102	BCB	C2C-C3C	-5.41	1.44	1.51
13	3	101	BCB	C2C-C3C	-5.38	1.44	1.51
13	B	202	BCB	C2C-C3C	-5.36	1.44	1.51
13	e	101	BCB	C2C-C3C	-5.31	1.44	1.51
13	J	101	BCB	C2C-C3C	-5.31	1.44	1.51
13	n	101	BCB	C2C-C3C	-5.31	1.44	1.51
13	Q	402	BCB	C2C-C3C	-5.24	1.44	1.51
13	L	303	BCB	C2C-C3C	-5.21	1.45	1.51
13	Z	101	BCB	C2C-C3C	-5.19	1.45	1.51
13	9	101	BCB	C2C-C3C	-5.16	1.45	1.51
13	q	101	BCB	C2C-C3C	-5.15	1.45	1.51
13	n	101	BCB	O2D-CGD	5.14	1.45	1.33
13	L	302	BCB	O2D-CGD	5.11	1.45	1.33
13	M	402	BCB	C3B-C2B	5.11	1.48	1.39
13	e	101	BCB	O2D-CGD	5.11	1.45	1.33
13	1	101	BCB	O2D-CGD	5.06	1.45	1.33
13	k	102	BCB	C2C-C3C	-5.06	1.45	1.51
13	R	102	BCB	O2D-CGD	5.06	1.45	1.33
13	f	101	BCB	O2D-CGD	5.03	1.45	1.33
13	h	102	BCB	O2D-CGD	5.03	1.45	1.33
13	T	101	BCB	C2C-C3C	-5.02	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	9	101	BCB	O2D-CGD	5.02	1.45	1.33
13	X	102	BCB	O2D-CGD	5.01	1.45	1.33
13	i	101	BCB	O2D-CGD	5.01	1.45	1.33
13	W	302	BCB	O2D-CGD	5.00	1.45	1.33
13	U	102	BCB	O2D-CGD	4.98	1.45	1.33
13	0	102	BCB	O2D-CGD	4.97	1.45	1.33
13	6	101	BCB	O2D-CGD	4.96	1.45	1.33
13	k	102	BCB	O2D-CGD	4.96	1.45	1.33
13	l	102	BCB	O2D-CGD	4.96	1.45	1.33
13	3	101	BCB	O2D-CGD	4.95	1.45	1.33
13	7	102	BCB	O2D-CGD	4.94	1.45	1.33
13	B	202	BCB	O2D-CGD	4.94	1.45	1.33
13	b	101	BCB	O2D-CGD	4.94	1.45	1.33
13	c	101	BCB	O2D-CGD	4.94	1.45	1.33
13	E	101	BCB	O2D-CGD	4.92	1.45	1.33
13	M	403	BCB	O2D-CGD	4.92	1.45	1.33
13	o	102	BCB	O2D-CGD	4.91	1.45	1.33
13	Z	101	BCB	O2D-CGD	4.90	1.45	1.33
17	M	405	MQ7	C10-C5	4.90	1.48	1.40
13	r	101	BCB	O2D-CGD	4.90	1.45	1.33
13	D	101	BCB	O2D-CGD	4.90	1.45	1.33
13	q	101	BCB	O2D-CGD	4.89	1.45	1.33
13	M	403	BCB	C3D-C4D	-4.89	1.33	1.44
13	4	101	BCB	O2D-CGD	4.88	1.45	1.33
13	A	102	BCB	O2D-CGD	4.87	1.45	1.33
13	T	101	BCB	O2D-CGD	4.87	1.45	1.33
13	J	101	BCB	O2D-CGD	4.86	1.45	1.33
13	Q	402	BCB	O2D-CGD	4.85	1.45	1.33
13	L	303	BCB	C3D-C4D	-4.84	1.33	1.44
13	I	101	BCB	O2D-CGD	4.84	1.45	1.33
13	R	102	BCB	C3D-C4D	-4.79	1.33	1.44
13	N	101	BCB	O2D-CGD	4.79	1.44	1.33
13	1	101	BCB	C3D-C4D	-4.78	1.33	1.44
13	c	101	BCB	C3D-C4D	-4.78	1.33	1.44
13	O	102	BCB	O2D-CGD	4.77	1.44	1.33
13	0	102	BCB	C3D-C4D	-4.76	1.33	1.44
13	B	202	BCB	C3D-C4D	-4.74	1.33	1.44
13	L	303	BCB	O2D-CGD	4.74	1.44	1.33
9	C	403	HEC	C2B-C3B	-4.73	1.35	1.40
13	E	101	BCB	C3D-C4D	-4.73	1.33	1.44
13	M	402	BCB	O2D-CGD	4.71	1.44	1.33
13	7	102	BCB	C3D-C4D	-4.71	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	402	BCB	C3D-C4D	-4.70	1.33	1.44
13	o	102	BCB	C3D-C4D	-4.69	1.33	1.44
13	i	101	BCB	C3D-C4D	-4.69	1.33	1.44
13	f	101	BCB	C3D-C4D	-4.68	1.33	1.44
13	U	102	BCB	C3D-C4D	-4.68	1.33	1.44
13	l	102	BCB	C3D-C4D	-4.64	1.33	1.44
13	A	102	BCB	C3D-C4D	-4.64	1.33	1.44
13	r	101	BCB	C3D-C4D	-4.64	1.33	1.44
9	C	401	HEC	C2B-C3B	-4.62	1.35	1.40
13	I	101	BCB	C3D-C4D	-4.61	1.33	1.44
13	4	101	BCB	C3D-C4D	-4.59	1.33	1.44
13	b	101	BCB	C3D-C4D	-4.59	1.33	1.44
13	X	102	BCB	C3D-C4D	-4.59	1.33	1.44
13	L	302	BCB	C3D-C4D	-4.57	1.33	1.44
13	D	101	BCB	C3D-C4D	-4.57	1.33	1.44
13	9	101	BCB	C3D-C4D	-4.56	1.33	1.44
13	q	101	BCB	C3D-C4D	-4.56	1.33	1.44
13	J	101	BCB	C3D-C4D	-4.53	1.33	1.44
13	Z	101	BCB	C3D-C4D	-4.52	1.34	1.44
13	O	102	BCB	C3D-C4D	-4.51	1.34	1.44
13	Q	402	BCB	C3D-C4D	-4.51	1.34	1.44
13	h	102	BCB	C3D-C4D	-4.50	1.34	1.44
13	W	302	BCB	C3D-C4D	-4.49	1.34	1.44
13	e	101	BCB	C3D-C4D	-4.47	1.34	1.44
13	k	102	BCB	C3D-C4D	-4.45	1.34	1.44
13	n	101	BCB	C3D-C4D	-4.43	1.34	1.44
15	H	302	CDL	OA8-CA7	4.43	1.46	1.33
9	C	404	HEC	C2B-C3B	-4.43	1.36	1.40
9	C	403	HEC	CBB-CAB	-4.42	1.32	1.49
9	C	402	HEC	CBC-CAC	-4.42	1.32	1.49
13	N	101	BCB	C3D-C4D	-4.41	1.34	1.44
13	3	101	BCB	C3D-C4D	-4.40	1.34	1.44
13	6	101	BCB	C3D-C4D	-4.38	1.34	1.44
9	C	404	HEC	CBC-CAC	-4.37	1.33	1.49
13	c	101	BCB	O2A-CGA	4.37	1.46	1.33
13	f	101	BCB	O2A-CGA	4.37	1.46	1.33
13	J	101	BCB	O2A-CGA	4.36	1.46	1.33
15	H	301	CDL	OA8-CA7	4.34	1.46	1.33
13	L	303	BCB	O2A-CGA	4.34	1.46	1.33
13	T	101	BCB	C3D-C4D	-4.34	1.34	1.44
20	D	102	PGV	O01-C1	4.33	1.46	1.34
20	Q	401	PGV	O03-C19	4.33	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	401	HEC	CBB-CAB	-4.33	1.33	1.49
15	H	302	CDL	OA6-CA5	4.33	1.46	1.34
13	1	101	BCB	O2A-CGA	4.32	1.46	1.33
13	X	102	BCB	O2A-CGA	4.32	1.46	1.33
13	D	101	BCB	O2A-CGA	4.31	1.45	1.33
20	W	301	PGV	O03-C19	4.31	1.45	1.33
13	r	101	BCB	O2A-CGA	4.31	1.45	1.33
20	N	102	PGV	O03-C19	4.31	1.45	1.33
20	N	102	PGV	O01-C1	4.29	1.46	1.34
13	4	101	BCB	O2A-CGA	4.29	1.45	1.33
13	B	202	BCB	O2A-CGA	4.29	1.45	1.33
13	i	101	BCB	O2A-CGA	4.29	1.45	1.33
13	T	101	BCB	O2A-CGA	4.28	1.45	1.33
9	C	404	HEC	CBB-CAB	-4.27	1.33	1.49
15	r	102	CDL	OA6-CA5	4.27	1.46	1.34
15	r	102	CDL	OB6-CB5	4.27	1.46	1.34
9	C	403	HEC	CBC-CAC	-4.27	1.33	1.49
13	3	101	BCB	O2A-CGA	4.27	1.45	1.33
15	L	306	CDL	OA8-CA7	4.26	1.45	1.33
13	M	403	BCB	O2A-CGA	4.26	1.45	1.33
13	E	101	BCB	O2A-CGA	4.26	1.45	1.33
13	l	102	BCB	O2A-CGA	4.26	1.45	1.33
13	Z	101	BCB	O2A-CGA	4.26	1.45	1.33
13	W	302	BCB	O2A-CGA	4.25	1.45	1.33
9	C	401	HEC	CBC-CAC	-4.25	1.33	1.49
13	O	102	BCB	O2A-CGA	4.25	1.45	1.33
15	H	302	CDL	OB8-CB7	4.24	1.45	1.33
13	0	102	BCB	O2A-CGA	4.22	1.45	1.33
15	H	301	CDL	OA6-CA5	4.22	1.46	1.34
9	C	402	HEC	CBB-CAB	-4.21	1.33	1.49
13	N	101	BCB	O2A-CGA	4.21	1.45	1.33
13	o	102	BCB	O2A-CGA	4.21	1.45	1.33
13	R	102	BCB	O2A-CGA	4.21	1.45	1.33
15	M	409	CDL	OA8-CA7	4.19	1.45	1.33
13	e	101	BCB	O2A-CGA	4.19	1.45	1.33
20	Q	401	PGV	O01-C1	4.18	1.46	1.34
13	b	101	BCB	O2A-CGA	4.18	1.45	1.33
13	U	102	BCB	O2A-CGA	4.17	1.45	1.33
13	7	102	BCB	O2A-CGA	4.17	1.45	1.33
20	I	102	PGV	O03-C19	4.16	1.45	1.33
15	r	102	CDL	OA8-CA7	4.15	1.45	1.33
13	n	101	BCB	O2A-CGA	4.14	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	102	BCB	O2A-CGA	4.14	1.45	1.33
12	L	301	DGA	OG1-CA1	4.11	1.45	1.33
15	r	102	CDL	OB8-CB7	4.11	1.45	1.33
20	D	102	PGV	O03-C19	4.11	1.45	1.33
13	q	101	BCB	O2A-CGA	4.10	1.45	1.33
13	9	101	BCB	O2A-CGA	4.09	1.45	1.33
13	M	402	BCB	O2A-CGA	4.09	1.45	1.33
20	M	411	PGV	O03-C19	4.09	1.45	1.33
13	I	101	BCB	O2A-CGA	4.08	1.45	1.33
15	L	306	CDL	OB6-CB5	4.08	1.45	1.34
15	L	306	CDL	OB8-CB7	4.06	1.45	1.33
13	6	101	BCB	O2A-CGA	4.06	1.45	1.33
15	M	409	CDL	OA6-CA5	4.05	1.45	1.34
13	h	102	BCB	O2A-CGA	4.05	1.45	1.33
13	k	102	BCB	O2A-CGA	4.05	1.45	1.33
15	M	409	CDL	OB6-CB5	4.04	1.45	1.34
20	M	411	PGV	O01-C1	4.04	1.45	1.34
13	Q	402	BCB	O2A-CGA	4.03	1.45	1.33
15	L	306	CDL	OA6-CA5	4.02	1.45	1.34
20	I	102	PGV	O01-C1	3.98	1.45	1.34
15	M	409	CDL	OB8-CB7	3.98	1.45	1.33
15	H	301	CDL	OB6-CB5	3.97	1.45	1.34
18	M	406	NS5	C25-C26	3.93	1.41	1.35
15	H	302	CDL	OB6-CB5	3.89	1.45	1.34
20	W	301	PGV	O01-C1	3.89	1.45	1.34
12	L	301	DGA	OG2-CB1	3.88	1.45	1.34
9	C	402	HEC	C2B-C3B	-3.86	1.36	1.40
13	M	402	BCB	CHD-C1D	3.79	1.45	1.38
13	e	101	BCB	CHD-C1D	3.78	1.45	1.38
13	L	302	BCB	O2A-CGA	3.78	1.44	1.33
15	H	301	CDL	OB8-CB7	3.75	1.44	1.33
13	A	102	BCB	CHD-C1D	3.70	1.45	1.38
13	L	303	BCB	CHD-C1D	3.70	1.45	1.38
13	9	101	BCB	CHD-C1D	3.69	1.45	1.38
21	k	101	NS0	C19-C17	3.68	1.40	1.35
21	9	102	NS0	C19-C17	3.67	1.40	1.35
13	I	101	BCB	CHD-C1D	3.67	1.45	1.38
13	k	102	BCB	CHD-C1D	3.65	1.45	1.38
13	M	403	BCB	CHD-C1D	3.64	1.45	1.38
13	q	101	BCB	CHD-C1D	3.64	1.45	1.38
13	X	102	BCB	CHD-C1D	3.64	1.45	1.38
13	n	101	BCB	CHD-C1D	3.62	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	M	406	NS5	C20-C21	3.62	1.40	1.35
13	7	102	BCB	CHD-C1D	3.61	1.45	1.38
13	l	102	BCB	CHD-C1D	3.60	1.45	1.38
13	L	302	BCB	CHD-C1D	3.59	1.45	1.38
13	i	101	BCB	CHD-C1D	3.58	1.45	1.38
13	E	101	BCB	CHD-C1D	3.58	1.45	1.38
13	Q	402	BCB	CHD-C1D	3.57	1.45	1.38
13	f	101	BCB	CHD-C1D	3.56	1.45	1.38
13	l	102	BCB	C3D-C2D	3.55	1.48	1.39
21	h	101	NS0	C22-C23	3.55	1.40	1.35
13	N	101	BCB	CHD-C1D	3.55	1.45	1.38
13	T	101	BCB	CHD-C1D	3.52	1.45	1.38
21	A	103	NS0	C19-C17	3.52	1.40	1.35
13	n	101	BCB	C3D-C2D	3.50	1.48	1.39
13	r	101	BCB	C3D-C2D	3.50	1.48	1.39
13	B	202	BCB	CHD-C1D	3.50	1.45	1.38
21	D	103	NS0	C22-C23	3.50	1.40	1.35
21	R	101	NS0	C22-C23	3.49	1.40	1.35
21	R	101	NS0	C19-C17	3.49	1.40	1.35
13	h	102	BCB	CHD-C1D	3.49	1.45	1.38
13	Q	402	BCB	C3D-C2D	3.49	1.48	1.39
13	q	101	BCB	OBD-CAD	3.48	1.28	1.22
13	J	101	BCB	CHD-C1D	3.48	1.45	1.38
13	n	101	BCB	OBD-CAD	3.47	1.28	1.22
13	W	302	BCB	CHD-C1D	3.47	1.45	1.38
13	M	403	BCB	CHD-C4C	3.47	1.47	1.39
21	h	101	NS0	C19-C17	3.46	1.40	1.35
13	4	101	BCB	CHD-C1D	3.46	1.45	1.38
21	q	102	NS0	C19-C17	3.46	1.40	1.35
13	3	101	BCB	CHD-C1D	3.46	1.45	1.38
13	R	102	BCB	CHD-C1D	3.45	1.45	1.38
13	0	102	BCB	CHD-C1D	3.45	1.45	1.38
13	1	101	BCB	CHD-C1D	3.45	1.45	1.38
13	f	101	BCB	C3D-C2D	3.45	1.48	1.39
13	h	102	BCB	OBD-CAD	3.45	1.28	1.22
13	r	101	BCB	CHD-C1D	3.44	1.45	1.38
13	D	101	BCB	CHD-C1D	3.43	1.45	1.38
13	o	102	BCB	C3D-C2D	3.43	1.48	1.39
13	O	102	BCB	C3D-C2D	3.43	1.48	1.39
13	U	102	BCB	CHD-C1D	3.43	1.45	1.38
13	T	101	BCB	C3D-C2D	3.42	1.48	1.39
13	e	101	BCB	OBD-CAD	3.42	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	k	102	BCB	C3D-C2D	3.42	1.48	1.39
13	D	101	BCB	OBD-CAD	3.41	1.28	1.22
21	o	101	NS0	C19-C17	3.41	1.40	1.35
13	e	101	BCB	C3D-C2D	3.41	1.48	1.39
21	9	102	NS0	C22-C23	3.41	1.40	1.35
13	N	101	BCB	C3D-C2D	3.41	1.48	1.39
13	r	101	BCB	OBD-CAD	3.41	1.28	1.22
13	0	102	BCB	C3D-C2D	3.40	1.48	1.39
13	A	102	BCB	OBD-CAD	3.40	1.28	1.22
13	T	101	BCB	OBD-CAD	3.40	1.28	1.22
13	O	102	BCB	CHD-C1D	3.40	1.45	1.38
13	9	101	BCB	OBD-CAD	3.40	1.28	1.22
13	J	101	BCB	C3D-C2D	3.39	1.48	1.39
13	k	102	BCB	OBD-CAD	3.39	1.28	1.22
13	q	101	BCB	C3D-C2D	3.39	1.48	1.39
21	U	101	NS0	C19-C17	3.39	1.40	1.35
21	0	101	NS0	C19-C17	3.39	1.40	1.35
13	k	102	BCB	CHD-C4C	3.38	1.47	1.39
13	Z	101	BCB	C3D-C2D	3.38	1.48	1.39
21	o	101	NS0	C22-C23	3.38	1.40	1.35
21	X	101	NS0	C14-C12	3.38	1.40	1.35
13	o	102	BCB	OBD-CAD	3.37	1.28	1.22
21	q	102	NS0	C22-C23	3.37	1.40	1.35
13	4	101	BCB	C3D-C2D	3.36	1.48	1.39
13	W	302	BCB	C3D-C2D	3.36	1.48	1.39
13	U	102	BCB	C3D-C2D	3.36	1.48	1.39
13	7	102	BCB	C3D-C2D	3.36	1.48	1.39
13	Z	101	BCB	CHD-C1D	3.36	1.44	1.38
13	X	102	BCB	C3D-C2D	3.36	1.48	1.39
13	O	102	BCB	OBD-CAD	3.36	1.28	1.22
13	o	102	BCB	CHD-C1D	3.36	1.44	1.38
21	D	103	NS0	C19-C17	3.36	1.40	1.35
21	7	101	NS0	C19-C17	3.35	1.40	1.35
13	L	303	BCB	OBD-CAD	3.35	1.28	1.22
21	U	101	NS0	C22-C23	3.35	1.40	1.35
21	7	101	NS0	C22-C23	3.35	1.40	1.35
13	B	202	BCB	C3D-C2D	3.34	1.48	1.39
13	A	102	BCB	C3D-C2D	3.33	1.48	1.39
21	k	101	NS0	C22-C23	3.33	1.40	1.35
13	c	101	BCB	C3D-C2D	3.33	1.48	1.39
21	2	101	NS0	C19-C17	3.32	1.40	1.35
13	9	101	BCB	CHD-C4C	3.32	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	103	NS0	C22-C23	3.32	1.40	1.35
13	M	402	BCB	C3D-C2D	3.32	1.48	1.39
13	L	302	BCB	OBD-CAD	3.32	1.28	1.22
13	6	101	BCB	CHD-C1D	3.31	1.44	1.38
13	A	102	BCB	CHD-C4C	3.31	1.46	1.39
11	A	101	UQ8	C4-C3	3.31	1.49	1.36
13	6	101	BCB	C3D-C2D	3.31	1.48	1.39
21	l	101	NS0	C22-C23	3.30	1.40	1.35
13	M	402	BCB	CHD-C4C	3.30	1.46	1.39
13	B	202	BCB	OBD-CAD	3.30	1.28	1.22
13	1	101	BCB	C3D-C2D	3.30	1.48	1.39
13	Z	101	BCB	OBD-CAD	3.30	1.28	1.22
13	h	102	BCB	C3D-C2D	3.30	1.48	1.39
13	W	302	BCB	OBD-CAD	3.30	1.28	1.22
13	3	101	BCB	OBD-CAD	3.30	1.28	1.22
13	I	101	BCB	C3D-C2D	3.30	1.48	1.39
13	E	101	BCB	C3D-C2D	3.29	1.48	1.39
13	I	101	BCB	OBD-CAD	3.29	1.28	1.22
13	6	101	BCB	OBD-CAD	3.29	1.28	1.22
21	O	101	NS0	C19-C17	3.28	1.40	1.35
13	9	101	BCB	C3D-C2D	3.28	1.48	1.39
13	i	101	BCB	C3D-C2D	3.28	1.48	1.39
13	M	402	BCB	OBD-CAD	3.28	1.28	1.22
21	h	101	NS0	C14-C12	3.28	1.40	1.35
21	0	101	NS0	C22-C23	3.28	1.40	1.35
13	b	101	BCB	CHD-C1D	3.28	1.44	1.38
13	l	102	BCB	OBD-CAD	3.26	1.28	1.22
13	Q	402	BCB	OBD-CAD	3.25	1.28	1.22
21	X	101	NS0	C19-C17	3.25	1.40	1.35
13	X	102	BCB	OBD-CAD	3.25	1.28	1.22
13	3	101	BCB	C3D-C2D	3.25	1.48	1.39
13	c	101	BCB	CHD-C1D	3.24	1.44	1.38
13	E	101	BCB	OBD-CAD	3.24	1.28	1.22
13	1	101	BCB	OBD-CAD	3.24	1.28	1.22
13	D	101	BCB	C3D-C2D	3.24	1.48	1.39
13	N	101	BCB	OBD-CAD	3.23	1.28	1.22
13	R	102	BCB	C3D-C2D	3.23	1.47	1.39
13	b	101	BCB	C3D-C2D	3.23	1.47	1.39
21	A	103	NS0	C14-C12	3.22	1.40	1.35
13	M	403	BCB	C3D-C2D	3.22	1.47	1.39
13	L	303	BCB	CHD-C4C	3.22	1.46	1.39
21	l	101	NS0	C19-C17	3.21	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	J	101	BCB	OBD-CAD	3.21	1.28	1.22
13	E	101	BCB	CHD-C4C	3.20	1.46	1.39
13	c	101	BCB	OBD-CAD	3.19	1.28	1.22
21	k	101	NS0	C14-C12	3.19	1.40	1.35
13	R	102	BCB	OBD-CAD	3.19	1.28	1.22
21	o	101	NS0	C14-C12	3.18	1.40	1.35
13	I	101	BCB	CHD-C4C	3.18	1.46	1.39
13	f	101	BCB	OBD-CAD	3.17	1.27	1.22
13	U	102	BCB	OBD-CAD	3.17	1.27	1.22
13	Q	402	BCB	CHD-C4C	3.16	1.46	1.39
13	b	101	BCB	OBD-CAD	3.16	1.27	1.22
18	M	406	NS5	C17-C15	3.16	1.40	1.35
13	0	102	BCB	OBD-CAD	3.15	1.27	1.22
13	T	101	BCB	CHD-C4C	3.15	1.46	1.39
13	L	303	BCB	C3D-C2D	3.14	1.47	1.39
13	7	102	BCB	OBD-CAD	3.14	1.27	1.22
11	L	305	UQ8	C4-C3	3.13	1.49	1.36
13	n	101	BCB	CHD-C4C	3.13	1.46	1.39
21	2	101	NS0	C22-C23	3.12	1.39	1.35
13	4	101	BCB	OBD-CAD	3.12	1.27	1.22
13	3	101	BCB	CHD-C4C	3.12	1.46	1.39
13	D	101	BCB	CHD-C4C	3.11	1.46	1.39
13	L	302	BCB	CHD-C4C	3.10	1.46	1.39
13	Z	101	BCB	CHD-C4C	3.10	1.46	1.39
21	O	101	NS0	C22-C23	3.10	1.39	1.35
21	X	101	NS0	C22-C23	3.10	1.39	1.35
21	O	101	NS0	C14-C12	3.10	1.39	1.35
13	i	101	BCB	OBD-CAD	3.09	1.27	1.22
13	L	302	BCB	C3D-C2D	3.09	1.47	1.39
13	J	101	BCB	CHD-C4C	3.09	1.46	1.39
21	2	101	NS0	C16-C17	-3.09	1.39	1.45
13	e	101	BCB	CHD-C4C	3.08	1.46	1.39
13	q	101	BCB	CHD-C4C	3.08	1.46	1.39
13	7	102	BCB	CHD-C4C	3.08	1.46	1.39
13	r	101	BCB	CHD-C4C	3.08	1.46	1.39
13	h	102	BCB	CHD-C4C	3.07	1.46	1.39
13	i	101	BCB	CHD-C4C	3.07	1.46	1.39
21	D	103	NS0	C14-C12	3.07	1.39	1.35
21	0	101	NS0	C14-C12	3.07	1.39	1.35
13	U	102	BCB	CHD-C4C	3.06	1.46	1.39
21	W	303	NS0	C19-C17	3.06	1.39	1.35
21	l	101	NS0	C14-C12	3.06	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	N	101	BCB	CHD-C4C	3.05	1.46	1.39
21	q	102	NS0	C14-C12	3.05	1.39	1.35
13	B	202	BCB	CHD-C4C	3.05	1.46	1.39
21	U	101	NS0	C14-C12	3.05	1.39	1.35
13	6	101	BCB	CHD-C4C	3.04	1.46	1.39
13	l	102	BCB	CHD-C4C	3.04	1.46	1.39
13	W	302	BCB	CHD-C4C	3.03	1.46	1.39
13	X	102	BCB	CHD-C4C	3.02	1.46	1.39
21	2	101	NS0	C14-C12	3.01	1.39	1.35
13	1	101	BCB	CHD-C4C	3.00	1.46	1.39
13	b	101	BCB	CHD-C4C	2.99	1.46	1.39
13	0	102	BCB	CHD-C4C	2.98	1.46	1.39
21	R	101	NS0	C14-C12	2.98	1.39	1.35
13	R	102	BCB	CHD-C4C	2.98	1.46	1.39
21	W	303	NS0	C16-C17	-2.97	1.39	1.45
11	C	406	UQ8	C4-C3	2.97	1.48	1.36
13	f	101	BCB	CHD-C4C	2.97	1.46	1.39
11	M	407	UQ8	C4-C3	2.94	1.48	1.36
21	7	101	NS0	C14-C12	2.94	1.39	1.35
21	9	102	NS0	C16-C17	-2.93	1.39	1.45
13	o	102	BCB	CHD-C4C	2.90	1.45	1.39
13	4	101	BCB	CHD-C4C	2.89	1.45	1.39
13	O	102	BCB	CHD-C4C	2.89	1.45	1.39
9	C	402	HEC	C4B-C3B	2.87	1.48	1.43
21	7	101	NS0	C16-C17	-2.86	1.39	1.45
21	D	103	NS0	C11-C12	-2.86	1.39	1.45
21	W	303	NS0	C14-C12	2.85	1.39	1.35
13	M	403	BCB	OBD-CAD	2.85	1.27	1.22
11	M	408	UQ8	C4-C3	2.82	1.47	1.36
21	9	102	NS0	C14-C12	2.82	1.39	1.35
21	0	101	NS0	C16-C17	-2.81	1.39	1.45
13	c	101	BCB	CHD-C4C	2.81	1.45	1.39
21	W	303	NS0	C22-C23	2.81	1.39	1.35
21	D	103	NS0	C16-C17	-2.79	1.40	1.45
21	O	101	NS0	C16-C17	-2.78	1.40	1.45
21	R	101	NS0	C16-C17	-2.77	1.40	1.45
21	q	102	NS0	C16-C17	-2.76	1.40	1.45
21	W	303	NS0	C25-C23	-2.76	1.40	1.45
21	h	101	NS0	C16-C17	-2.75	1.40	1.45
21	A	103	NS0	C16-C17	-2.73	1.40	1.45
21	U	101	NS0	C16-C17	-2.70	1.40	1.45
21	o	101	NS0	C16-C17	-2.69	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	401	HEC	C4B-C3B	2.69	1.47	1.43
21	2	101	NS0	C11-C12	-2.68	1.40	1.45
21	7	101	NS0	C11-C12	-2.67	1.40	1.45
21	R	101	NS0	C11-C12	-2.67	1.40	1.45
21	0	101	NS0	C25-C23	-2.67	1.40	1.45
21	k	101	NS0	C16-C17	-2.66	1.40	1.45
21	9	102	NS0	C11-C12	-2.63	1.40	1.45
21	X	101	NS0	C16-C17	-2.63	1.40	1.45
21	2	101	NS0	C25-C23	-2.62	1.40	1.45
13	D	101	BCB	C4B-CHC	2.62	1.48	1.41
21	X	101	NS0	C11-C12	-2.62	1.40	1.45
21	D	103	NS0	C25-C23	-2.61	1.40	1.45
21	o	101	NS0	C11-C12	-2.61	1.40	1.45
9	C	404	HEC	C4B-C3B	2.61	1.47	1.43
21	l	101	NS0	C16-C17	-2.60	1.40	1.45
13	Q	402	BCB	C4B-CHC	2.60	1.48	1.41
21	l	101	NS0	C11-C12	-2.60	1.40	1.45
13	6	101	BCB	C4B-CHC	2.59	1.48	1.41
21	A	103	NS0	C25-C23	-2.59	1.40	1.45
21	W	303	NS0	C11-C12	-2.59	1.40	1.45
21	q	102	NS0	C11-C12	-2.59	1.40	1.45
13	A	102	BCB	C4B-CHC	2.58	1.48	1.41
21	0	101	NS0	C11-C12	-2.58	1.40	1.45
18	M	406	NS5	C14-C15	-2.58	1.40	1.45
13	M	403	BCB	C4B-CHC	2.56	1.48	1.41
13	T	101	BCB	C4B-CHC	2.56	1.48	1.41
12	L	301	DGA	OG2-CG2	-2.56	1.42	1.47
21	q	102	NS0	C25-C23	-2.55	1.40	1.45
13	N	101	BCB	C4B-CHC	2.54	1.48	1.41
13	q	101	BCB	C4B-CHC	2.54	1.48	1.41
21	7	101	NS0	C25-C23	-2.53	1.40	1.45
13	h	102	BCB	C4B-CHC	2.52	1.48	1.41
13	L	303	BCB	C4B-CHC	2.52	1.48	1.41
21	O	101	NS0	C11-C12	-2.51	1.40	1.45
21	h	101	NS0	C11-C12	-2.51	1.40	1.45
13	n	101	BCB	C4B-CHC	2.51	1.48	1.41
21	A	103	NS0	C11-C12	-2.51	1.40	1.45
21	U	101	NS0	C11-C12	-2.51	1.40	1.45
21	U	101	NS0	C25-C23	-2.51	1.40	1.45
21	X	101	NS0	C25-C23	-2.51	1.40	1.45
9	C	403	HEC	C4B-C3B	2.51	1.47	1.43
21	k	101	NS0	C25-C23	-2.51	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	I	101	BCB	C4B-CHC	2.51	1.48	1.41
13	3	101	BCB	C4B-CHC	2.50	1.47	1.41
21	9	102	NS0	C25-C23	-2.49	1.40	1.45
21	k	101	NS0	C11-C12	-2.49	1.40	1.45
21	O	101	NS0	C25-C23	-2.49	1.40	1.45
13	Z	101	BCB	C4B-CHC	2.48	1.47	1.41
21	l	101	NS0	C25-C23	-2.48	1.40	1.45
21	h	101	NS0	C25-C23	-2.45	1.40	1.45
13	e	101	BCB	C4B-CHC	2.44	1.47	1.41
13	c	101	BCB	C4B-CHC	2.43	1.47	1.41
18	M	406	NS5	C28-C26	-2.43	1.40	1.45
13	b	101	BCB	C4B-CHC	2.43	1.47	1.41
13	M	402	BCB	C1D-C2D	2.41	1.50	1.45
21	R	101	NS0	C25-C23	-2.41	1.40	1.45
13	W	302	BCB	C4B-CHC	2.40	1.47	1.41
21	o	101	NS0	C25-C23	-2.40	1.40	1.45
13	U	102	BCB	C4B-CHC	2.40	1.47	1.41
13	R	102	BCB	C4B-CHC	2.39	1.47	1.41
13	9	101	BCB	C4B-CHC	2.39	1.47	1.41
13	M	402	BCB	C4B-CHC	2.39	1.47	1.41
13	r	101	BCB	C4B-CHC	2.39	1.47	1.41
18	M	406	NS5	C23-C21	-2.38	1.40	1.45
13	k	102	BCB	C4B-CHC	2.38	1.47	1.41
13	l	102	BCB	C4B-CHC	2.37	1.47	1.41
13	B	202	BCB	C4B-CHC	2.35	1.47	1.41
13	4	101	BCB	C4B-CHC	2.34	1.47	1.41
13	E	101	BCB	C4B-CHC	2.33	1.47	1.41
13	X	102	BCB	C4B-CHC	2.33	1.47	1.41
13	f	101	BCB	C4B-CHC	2.33	1.47	1.41
13	0	102	BCB	C4B-CHC	2.32	1.47	1.41
13	L	302	BCB	C4B-CHC	2.32	1.47	1.41
13	1	101	BCB	C4B-CHC	2.31	1.47	1.41
13	J	101	BCB	C4B-CHC	2.31	1.47	1.41
13	9	101	BCB	C1D-C2D	2.29	1.49	1.45
13	7	102	BCB	C4B-CHC	2.29	1.47	1.41
14	M	404	BPB	C3A-C2A	-2.28	1.52	1.54
13	o	102	BCB	C4B-CHC	2.27	1.47	1.41
9	C	403	HEC	C3C-C2C	-2.26	1.38	1.40
13	L	303	BCB	C1D-C2D	2.24	1.49	1.45
13	i	101	BCB	C4B-CHC	2.21	1.47	1.41
13	O	102	BCB	C4B-CHC	2.21	1.47	1.41
13	c	101	BCB	C1B-CHB	2.18	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	404	HEC	C3C-C2C	-2.17	1.38	1.40
13	b	101	BCB	C1B-CHB	2.14	1.46	1.41
14	L	304	BPB	C3A-C2A	-2.14	1.52	1.54
13	i	101	BCB	C1B-CHB	2.13	1.46	1.41
13	o	102	BCB	C1B-CHB	2.13	1.46	1.41
13	J	101	BCB	C1B-CHB	2.13	1.46	1.41
13	R	102	BCB	C1B-CHB	2.13	1.46	1.41
13	I	101	BCB	C1D-C2D	2.12	1.49	1.45
13	U	102	BCB	C1B-CHB	2.11	1.46	1.41
13	A	102	BCB	C1D-C2D	2.09	1.49	1.45
13	O	102	BCB	C1B-CHB	2.09	1.46	1.41
13	M	403	BCB	C1B-CHB	2.08	1.46	1.41
13	l	102	BCB	C1B-CHB	2.08	1.46	1.41
13	B	202	BCB	C1B-CHB	2.08	1.46	1.41
13	D	101	BCB	C1D-C2D	2.07	1.49	1.45
13	E	101	BCB	C1B-CHB	2.07	1.46	1.41
13	k	102	BCB	C1D-C2D	2.07	1.49	1.45
13	3	101	BCB	C1B-CHB	2.07	1.46	1.41
13	4	101	BCB	C1B-CHB	2.06	1.46	1.41
13	f	101	BCB	C1B-CHB	2.05	1.46	1.41
13	e	101	BCB	C1B-CHB	2.04	1.46	1.41
13	Z	101	BCB	C1B-CHB	2.04	1.46	1.41
13	T	101	BCB	C1D-C2D	2.04	1.49	1.45
13	6	101	BCB	C1B-CHB	2.03	1.46	1.41
13	W	302	BCB	C1B-CHB	2.03	1.46	1.41
13	h	102	BCB	C1B-CHB	2.03	1.46	1.41
21	W	303	NS0	C21-C22	-2.03	1.37	1.43
13	M	403	BCB	C1D-C2D	2.03	1.49	1.45
13	T	101	BCB	C1B-CHB	2.02	1.46	1.41
13	D	101	BCB	C1B-CHB	2.01	1.46	1.41
21	W	303	NS0	C20-C19	-2.01	1.37	1.43
13	N	101	BCB	C1B-CHB	2.01	1.46	1.41
13	q	101	BCB	C1B-CHB	2.01	1.46	1.41
13	q	101	BCB	C1D-C2D	2.00	1.49	1.45

All (1087) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	h	102	BCB	C1C-NC-C4C	-18.83	98.24	106.71
13	3	101	BCB	C1C-NC-C4C	-18.76	98.27	106.71
13	O	102	BCB	C1C-NC-C4C	-18.72	98.29	106.71
13	l	102	BCB	C1C-NC-C4C	-18.68	98.31	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	1	101	BCB	C1C-NC-C4C	-18.61	98.34	106.71
13	4	101	BCB	C1C-NC-C4C	-18.59	98.35	106.71
13	R	102	BCB	C1C-NC-C4C	-18.52	98.38	106.71
13	b	101	BCB	C1C-NC-C4C	-18.44	98.42	106.71
13	f	101	BCB	C1C-NC-C4C	-18.40	98.43	106.71
13	B	202	BCB	C1C-NC-C4C	-18.39	98.44	106.71
13	c	101	BCB	C1C-NC-C4C	-18.38	98.44	106.71
13	Z	101	BCB	C1C-NC-C4C	-18.36	98.45	106.71
13	Q	402	BCB	C1C-NC-C4C	-18.20	98.52	106.71
13	i	101	BCB	C1C-NC-C4C	-18.19	98.53	106.71
13	W	302	BCB	C1C-NC-C4C	-18.18	98.53	106.71
13	L	302	BCB	C1C-NC-C4C	-18.16	98.54	106.71
13	o	102	BCB	C1C-NC-C4C	-18.14	98.55	106.71
13	U	102	BCB	C1C-NC-C4C	-18.03	98.60	106.71
13	7	102	BCB	C1C-NC-C4C	-18.02	98.61	106.71
13	N	101	BCB	C1C-NC-C4C	-18.01	98.61	106.71
13	e	101	BCB	C1C-NC-C4C	-17.98	98.62	106.71
13	I	101	BCB	C1C-NC-C4C	-17.95	98.63	106.71
13	T	101	BCB	C1C-NC-C4C	-17.95	98.64	106.71
13	n	101	BCB	C1C-NC-C4C	-17.94	98.64	106.71
13	r	101	BCB	C1C-NC-C4C	-17.89	98.66	106.71
13	E	101	BCB	C1C-NC-C4C	-17.88	98.67	106.71
13	X	102	BCB	C1C-NC-C4C	-17.87	98.67	106.71
13	J	101	BCB	C1C-NC-C4C	-17.85	98.68	106.71
13	q	101	BCB	C1C-NC-C4C	-17.85	98.68	106.71
13	A	102	BCB	C1C-NC-C4C	-17.82	98.69	106.71
13	k	102	BCB	C1C-NC-C4C	-17.70	98.75	106.71
13	L	303	BCB	C1C-NC-C4C	-17.66	98.77	106.71
13	D	101	BCB	C1C-NC-C4C	-17.45	98.86	106.71
13	0	102	BCB	C1C-NC-C4C	-17.40	98.88	106.71
13	M	402	BCB	C1C-NC-C4C	-17.35	98.91	106.71
13	6	101	BCB	C1C-NC-C4C	-17.32	98.92	106.71
13	9	101	BCB	C1C-NC-C4C	-17.04	99.05	106.71
13	M	403	BCB	C1C-NC-C4C	-16.24	99.41	106.71
13	M	403	BCB	CMD-C2D-C1D	7.06	137.15	124.71
13	L	303	BCB	CMD-C2D-C1D	6.91	136.88	124.71
13	M	402	BCB	CMD-C2D-C1D	6.78	136.66	124.71
13	9	101	BCB	CMD-C2D-C1D	6.75	136.61	124.71
13	A	102	BCB	CMD-C2D-C1D	6.66	136.45	124.71
13	D	101	BCB	CMD-C2D-C1D	6.58	136.30	124.71
13	I	101	BCB	CMD-C2D-C1D	6.56	136.27	124.71
13	L	302	BCB	CMD-C2D-C1D	6.55	136.25	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	q	101	BCB	CMD-C2D-C1D	6.42	136.03	124.71
13	b	101	BCB	CMD-C2D-C1D	6.38	135.96	124.71
13	3	101	BCB	CMD-C2D-C1D	6.30	135.82	124.71
13	J	101	BCB	C1D-ND-C4D	-6.30	101.86	106.33
13	6	101	BCB	CMD-C2D-C1D	6.29	135.79	124.71
13	M	402	BCB	C1D-ND-C4D	-6.21	101.93	106.33
13	e	101	BCB	CMD-C2D-C1D	6.19	135.62	124.71
13	k	102	BCB	CMD-C2D-C1D	6.17	135.58	124.71
13	T	101	BCB	CMD-C2D-C1D	6.16	135.58	124.71
13	N	101	BCB	CMD-C2D-C1D	6.06	135.39	124.71
13	h	102	BCB	CMD-C2D-C1D	6.06	135.39	124.71
13	W	302	BCB	CMD-C2D-C1D	6.03	135.34	124.71
13	Q	402	BCB	CMD-C2D-C1D	6.02	135.31	124.71
13	c	101	BCB	C1D-ND-C4D	-5.92	102.13	106.33
13	n	101	BCB	CMD-C2D-C1D	5.92	135.14	124.71
13	L	303	BCB	C1D-ND-C4D	-5.91	102.14	106.33
13	f	101	BCB	C1D-ND-C4D	-5.90	102.14	106.33
13	L	303	BCB	O2D-CGD-CBD	5.84	121.65	111.27
13	Z	101	BCB	CMD-C2D-C1D	5.82	134.96	124.71
13	1	101	BCB	C1D-ND-C4D	-5.80	102.22	106.33
13	i	101	BCB	C1D-ND-C4D	-5.79	102.22	106.33
13	0	102	BCB	C1D-ND-C4D	-5.77	102.24	106.33
13	U	102	BCB	C1D-ND-C4D	-5.74	102.25	106.33
13	4	101	BCB	C1D-ND-C4D	-5.72	102.27	106.33
13	o	102	BCB	C1D-ND-C4D	-5.69	102.30	106.33
12	L	301	DGA	CG2-OG2-CB1	-5.64	110.62	117.88
13	O	102	BCB	C1D-ND-C4D	-5.59	102.36	106.33
13	B	202	BCB	C1D-ND-C4D	-5.57	102.38	106.33
13	E	101	BCB	C1D-ND-C4D	-5.56	102.39	106.33
13	9	101	BCB	C1D-ND-C4D	-5.55	102.39	106.33
13	D	101	BCB	C1D-ND-C4D	-5.52	102.41	106.33
13	X	102	BCB	C1D-ND-C4D	-5.45	102.46	106.33
13	M	403	BCB	C1D-ND-C4D	-5.45	102.47	106.33
13	R	102	BCB	C1D-ND-C4D	-5.39	102.50	106.33
13	M	402	BCB	CHD-C1D-ND	-5.35	119.53	124.45
13	l	102	BCB	C1D-ND-C4D	-5.25	102.61	106.33
13	M	402	BCB	O2D-CGD-CBD	5.24	120.58	111.27
13	E	101	BCB	CMD-C2D-C1D	5.20	133.88	124.71
13	L	302	BCB	C1D-ND-C4D	-5.20	102.64	106.33
13	B	202	BCB	CMD-C2D-C1D	5.17	133.83	124.71
13	r	101	BCB	C1D-ND-C4D	-5.13	102.69	106.33
13	X	102	BCB	CMD-C2D-C1D	5.11	133.72	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	M	402	BCB	C2C-C1C-CHC	-5.11	111.61	123.64
13	R	102	BCB	CMD-C2D-C1D	5.09	133.68	124.71
13	7	102	BCB	C1D-ND-C4D	-5.08	102.73	106.33
13	q	101	BCB	C1D-ND-C4D	-5.08	102.73	106.33
13	M	403	BCB	O2D-CGD-CBD	5.06	120.26	111.27
13	6	101	BCB	C1D-ND-C4D	-5.01	102.77	106.33
13	A	102	BCB	C1D-ND-C4D	-5.01	102.78	106.33
13	L	302	BCB	C2C-C1C-CHC	-4.98	111.91	123.64
13	h	102	BCB	C1D-ND-C4D	-4.96	102.81	106.33
13	b	101	BCB	C1D-ND-C4D	-4.96	102.81	106.33
13	M	403	BCB	C2C-C1C-CHC	-4.93	112.03	123.64
13	k	102	BCB	C2C-C1C-CHC	-4.92	112.05	123.64
13	M	403	BCB	CHD-C1D-ND	-4.89	119.96	124.45
13	4	101	BCB	C2C-C1C-CHC	-4.88	112.16	123.64
13	f	101	BCB	C2C-C1C-CHC	-4.87	112.18	123.64
13	O	102	BCB	C2C-C1C-CHC	-4.86	112.20	123.64
13	L	303	BCB	C2C-C1C-CHC	-4.83	112.26	123.64
13	7	102	BCB	C2C-C1C-CHC	-4.82	112.30	123.64
13	h	102	BCB	C2C-C1C-CHC	-4.81	112.31	123.64
13	e	101	BCB	C2C-C1C-CHC	-4.81	112.31	123.64
13	0	102	BCB	CMD-C2D-C1D	4.80	133.18	124.71
13	1	101	BCB	C2C-C1C-CHC	-4.80	112.33	123.64
13	A	102	BCB	O2D-CGD-CBD	4.80	119.79	111.27
13	n	101	BCB	C2C-C1C-CHC	-4.77	112.41	123.64
13	3	101	BCB	C1D-ND-C4D	-4.76	102.95	106.33
13	9	101	BCB	C2C-C1C-CHC	-4.76	112.42	123.64
13	J	101	BCB	C2C-C1C-CHC	-4.76	112.43	123.64
13	o	102	BCB	C2C-C1C-CHC	-4.75	112.45	123.64
13	E	101	BCB	C2C-C1C-CHC	-4.75	112.47	123.64
13	W	302	BCB	C1D-ND-C4D	-4.73	102.97	106.33
13	r	101	BCB	CMD-C2D-C1D	4.73	133.05	124.71
13	I	101	BCB	C2C-C1C-CHC	-4.73	112.50	123.64
13	b	101	BCB	C2C-C1C-CHC	-4.72	112.52	123.64
13	A	102	BCB	C2C-C1C-CHC	-4.69	112.61	123.64
13	0	102	BCB	C2C-C1C-CHC	-4.68	112.61	123.64
13	1	101	BCB	CMD-C2D-C1D	4.68	132.96	124.71
13	R	102	BCB	C2C-C1C-CHC	-4.67	112.64	123.64
13	B	202	BCB	C2C-C1C-CHC	-4.67	112.65	123.64
12	L	301	DGA	OG2-CB1-CB2	4.66	121.54	111.50
13	X	102	BCB	C2C-C1C-CHC	-4.66	112.67	123.64
13	c	101	BCB	C2C-C1C-CHC	-4.62	112.77	123.64
13	e	101	BCB	C1D-ND-C4D	-4.61	103.06	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	i	101	BCB	C2C-C1C-CHC	-4.60	112.80	123.64
13	r	101	BCB	C2C-C1C-CHC	-4.60	112.80	123.64
13	T	101	BCB	C2C-C1C-CHC	-4.60	112.81	123.64
13	3	101	BCB	C2C-C1C-CHC	-4.59	112.82	123.64
13	D	101	BCB	C2C-C1C-CHC	-4.58	112.85	123.64
13	M	403	BCB	C3D-C2D-C1D	-4.58	99.58	105.83
13	7	102	BCB	CMD-C2D-C1D	4.57	132.77	124.71
13	U	102	BCB	C2C-C1C-CHC	-4.57	112.89	123.64
15	r	102	CDL	OB6-CB5-C51	4.56	121.33	111.50
13	l	102	BCB	C2C-C1C-CHC	-4.56	112.91	123.64
13	O	102	BCB	O2D-CGD-CBD	4.54	119.33	111.27
13	Z	101	BCB	C1D-ND-C4D	-4.54	103.11	106.33
13	o	102	BCB	CMD-C2D-C1D	4.53	132.69	124.71
13	Q	402	BCB	C2C-C1C-CHC	-4.52	112.99	123.64
13	i	101	BCB	O2D-CGD-CBD	4.52	119.29	111.27
13	J	101	BCB	CMD-C2D-C1D	4.51	132.66	124.71
13	W	302	BCB	C2C-C1C-CHC	-4.50	113.04	123.64
13	q	101	BCB	C2C-C1C-CHC	-4.49	113.06	123.64
13	6	101	BCB	C2C-C1C-CHC	-4.49	113.06	123.64
13	R	102	BCB	O2D-CGD-CBD	4.48	119.23	111.27
13	Z	101	BCB	C2C-C1C-CHC	-4.47	113.11	123.64
13	O	102	BCB	CMD-C2D-C1D	4.46	132.57	124.71
13	N	101	BCB	C2C-C1C-CHC	-4.43	113.21	123.64
13	i	101	BCB	CMD-C2D-C1D	4.38	132.44	124.71
13	Q	402	BCB	C1D-ND-C4D	-4.36	103.24	106.33
13	N	101	BCB	CMB-C2B-C3B	4.35	132.81	124.68
13	c	101	BCB	O2D-CGD-CBD	4.35	118.99	111.27
15	H	301	CDL	OA6-CA5-C11	4.34	120.86	111.50
13	n	101	BCB	C1D-ND-C4D	-4.32	103.27	106.33
13	D	101	BCB	C3D-C2D-C1D	-4.31	99.94	105.83
13	f	101	BCB	CMD-C2D-C1D	4.29	132.27	124.71
13	o	102	BCB	O2D-CGD-CBD	4.29	118.89	111.27
11	A	101	UQ8	C7-C8-C9	-4.28	119.66	126.79
13	I	101	BCB	C1D-ND-C4D	-4.27	103.31	106.33
15	H	302	CDL	OA6-CA5-C11	4.26	120.68	111.50
13	B	202	BCB	O2D-CGD-CBD	4.25	118.82	111.27
13	T	101	BCB	C1D-ND-C4D	-4.24	103.32	106.33
13	U	102	BCB	CMD-C2D-C1D	4.24	132.18	124.71
13	3	101	BCB	C1-C2-C3	-4.23	118.72	126.04
13	c	101	BCB	CMD-C2D-C1D	4.22	132.15	124.71
13	1	101	BCB	CMB-C2B-C3B	4.22	132.57	124.68
13	f	101	BCB	O2D-CGD-CBD	4.21	118.75	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	R	101	NS0	C21-C20-C19	4.21	132.10	123.47
13	L	303	BCB	CHD-C1D-ND	-4.21	120.58	124.45
13	U	102	BCB	O2D-CGD-CBD	4.20	118.74	111.27
13	6	101	BCB	C3D-C2D-C1D	-4.20	100.11	105.83
13	l	102	BCB	O2D-CGD-CBD	4.19	118.72	111.27
13	L	303	BCB	CMB-C2B-C3B	4.19	132.52	124.68
13	N	101	BCB	C1D-ND-C4D	-4.19	103.36	106.33
15	M	409	CDL	OA6-CA5-C11	4.19	120.52	111.50
20	I	102	PGV	O01-C1-C2	4.18	120.51	111.50
13	9	101	BCB	O2D-CGD-CBD	4.18	118.69	111.27
13	b	101	BCB	C3D-C2D-C1D	-4.18	100.13	105.83
15	M	409	CDL	OB6-CB5-C51	4.16	120.46	111.50
13	0	102	BCB	O2D-CGD-CBD	4.14	118.62	111.27
13	l	102	BCB	CMB-C2B-C3B	4.12	132.39	124.68
13	q	101	BCB	CMB-C2B-C3B	4.10	132.36	124.68
13	I	101	BCB	O2D-CGD-CBD	4.10	118.55	111.27
13	e	101	BCB	C1-C2-C3	-4.09	118.96	126.04
13	Q	402	BCB	C1-C2-C3	-4.09	118.97	126.04
13	k	102	BCB	C1D-ND-C4D	-4.09	103.43	106.33
13	k	102	BCB	CMB-C2B-C3B	4.08	132.32	124.68
13	M	402	BCB	C3D-C2D-C1D	-4.08	100.27	105.83
15	L	306	CDL	OB6-CB5-C51	4.07	120.28	111.50
13	r	101	BCB	O2D-CGD-CBD	4.07	118.50	111.27
13	L	302	BCB	C3D-C2D-C1D	-4.07	100.28	105.83
13	W	302	BCB	C3D-C2D-C1D	-4.07	100.28	105.83
13	3	101	BCB	C3D-C2D-C1D	-4.06	100.29	105.83
13	q	101	BCB	C3D-C2D-C1D	-4.06	100.29	105.83
13	e	101	BCB	O2D-CGD-CBD	4.06	118.48	111.27
13	D	101	BCB	CMB-C2B-C3B	4.06	132.27	124.68
13	I	101	BCB	CMB-C2B-C3B	4.06	132.27	124.68
13	Z	101	BCB	C3D-C2D-C1D	-4.05	100.30	105.83
15	r	102	CDL	OA6-CA5-C11	4.05	120.23	111.50
15	H	301	CDL	OB6-CB5-C51	4.04	120.21	111.50
13	N	101	BCB	C3D-C2D-C1D	-4.04	100.32	105.83
13	0	102	BCB	CMB-C2B-C3B	4.04	132.23	124.68
13	4	101	BCB	O2D-CGD-CBD	4.03	118.42	111.27
13	7	102	BCB	O2D-CGD-CBD	4.03	118.42	111.27
13	Z	101	BCB	C1-C2-C3	-4.02	119.09	126.04
13	e	101	BCB	C3D-C2D-C1D	-4.01	100.36	105.83
13	A	102	BCB	C3D-C2D-C1D	-4.00	100.37	105.83
20	W	301	PGV	O01-C1-C2	3.99	120.11	111.50
13	7	102	BCB	CMB-C2B-C3B	3.99	132.15	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	R	102	BCB	CMB-C2B-C3B	3.99	132.14	124.68
13	W	302	BCB	CMB-C2B-C3B	3.98	132.13	124.68
13	9	101	BCB	CHD-C1D-ND	-3.97	120.81	124.45
13	E	101	BCB	O2D-CGD-CBD	3.97	118.32	111.27
13	T	101	BCB	C3D-C2D-C1D	-3.96	100.43	105.83
21	X	101	NS0	C21-C20-C19	3.96	131.58	123.47
13	9	101	BCB	C3D-C2D-C1D	-3.95	100.44	105.83
13	h	102	BCB	C3D-C2D-C1D	-3.95	100.44	105.83
13	Z	101	BCB	O2D-CGD-CBD	3.95	118.28	111.27
9	C	401	HEC	CBD-CAD-C3D	-3.95	105.89	112.62
13	Q	402	BCB	CMB-C2B-C3B	3.95	132.06	124.68
13	Q	402	BCB	O2D-CGD-CBD	3.94	118.26	111.27
13	l	102	BCB	CMD-C2D-C1D	3.93	131.64	124.71
13	U	102	BCB	CMB-C2B-C3B	3.93	132.03	124.68
13	o	102	BCB	CMB-C2B-C3B	3.92	132.02	124.68
13	4	101	BCB	CMB-C2B-C3B	3.92	132.01	124.68
13	h	102	BCB	CMB-C2B-C3B	3.91	132.00	124.68
13	X	102	BCB	O2D-CGD-CBD	3.90	118.20	111.27
13	N	101	BCB	O2D-CGD-CBD	3.90	118.20	111.27
13	L	302	BCB	O2D-CGD-CBD	3.90	118.19	111.27
13	I	101	BCB	C1-C2-C3	-3.89	119.31	126.04
13	M	403	BCB	C1-C2-C3	-3.89	119.31	126.04
13	4	101	BCB	CMD-C2D-C1D	3.89	131.57	124.71
13	D	101	BCB	O2D-CGD-CBD	3.89	118.17	111.27
13	B	202	BCB	CMB-C2B-C3B	3.88	131.94	124.68
13	I	101	BCB	C3D-C2D-C1D	-3.88	100.53	105.83
13	X	102	BCB	CMB-C2B-C3B	3.88	131.94	124.68
13	Q	402	BCB	C3D-C2D-C1D	-3.88	100.54	105.83
13	b	101	BCB	CMB-C2B-C3B	3.87	131.91	124.68
13	T	101	BCB	CMB-C2B-C3B	3.86	131.89	124.68
13	1	101	BCB	O2D-CGD-CBD	3.85	118.11	111.27
13	n	101	BCB	C1-C2-C3	-3.85	119.39	126.04
13	k	102	BCB	C3D-C2D-C1D	-3.83	100.60	105.83
13	n	101	BCB	C3D-C2D-C1D	-3.82	100.61	105.83
13	W	302	BCB	O2D-CGD-CBD	3.82	118.05	111.27
13	A	102	BCB	CMB-C2B-C3B	3.81	131.81	124.68
13	n	101	BCB	O2D-CGD-CBD	3.81	118.04	111.27
13	3	101	BCB	O2D-CGD-CBD	3.80	118.01	111.27
13	A	102	BCB	CHD-C1D-ND	-3.79	120.97	124.45
13	h	102	BCB	O2D-CGD-CBD	3.79	118.00	111.27
13	L	302	BCB	C1-C2-C3	-3.78	119.50	126.04
21	W	303	NS0	C21-C20-C19	3.78	131.21	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	O	102	BCB	CMB-C2B-C3B	3.77	131.74	124.68
13	M	403	BCB	CMB-C2B-C3B	3.77	131.73	124.68
13	n	101	BCB	CMB-C2B-C3B	3.76	131.72	124.68
13	f	101	BCB	CMB-C2B-C3B	3.76	131.71	124.68
13	W	302	BCB	C1-C2-C3	-3.76	119.54	126.04
13	A	102	BCB	C1-C2-C3	-3.76	119.55	126.04
13	b	101	BCB	O2D-CGD-CBD	3.75	117.93	111.27
13	9	101	BCB	CMB-C2B-C3B	3.75	131.69	124.68
13	J	101	BCB	O2D-CGD-CBD	3.73	117.89	111.27
21	9	102	NS0	C21-C20-C19	3.72	131.09	123.47
13	L	303	BCB	C3D-C2D-C1D	-3.72	100.76	105.83
13	N	101	BCB	C1-C2-C3	-3.70	119.64	126.04
13	r	101	BCB	CHB-C4A-NA	3.67	129.59	124.51
13	3	101	BCB	CMB-C2B-C3B	3.67	131.54	124.68
13	6	101	BCB	O2D-CGD-CBD	3.67	117.78	111.27
13	Z	101	BCB	CMB-C2B-C3B	3.64	131.48	124.68
13	e	101	BCB	CMB-C2B-C3B	3.63	131.47	124.68
13	q	101	BCB	O2D-CGD-CBD	3.63	117.72	111.27
13	L	302	BCB	C4-C3-C5	3.62	121.36	115.27
15	H	302	CDL	OB6-CB5-C51	3.61	119.27	111.50
20	Q	401	PGV	O01-C1-C2	3.60	119.27	111.50
15	L	306	CDL	OA6-CA5-C11	3.60	119.27	111.50
13	E	101	BCB	CMB-C2B-C3B	3.59	131.40	124.68
13	M	402	BCB	C1-C2-C3	-3.58	119.84	126.04
11	M	408	UQ8	C17-C18-C19	-3.56	119.09	127.66
13	i	101	BCB	C4D-CHA-C1A	-3.56	116.92	121.25
13	r	101	BCB	CMB-C2B-C3B	3.55	131.32	124.68
13	c	101	BCB	CMB-C2B-C3B	3.55	131.32	124.68
13	D	101	BCB	CHD-C1D-ND	-3.55	121.20	124.45
13	J	101	BCB	C3D-C4D-ND	3.54	115.97	110.24
13	6	101	BCB	CMB-C2B-C3B	3.54	131.31	124.68
13	T	101	BCB	O2D-CGD-CBD	3.54	117.55	111.27
20	D	102	PGV	O01-C1-C2	3.53	119.12	111.50
13	9	101	BCB	C1-C2-C3	-3.53	119.94	126.04
13	O	102	BCB	C3D-C2D-C1D	-3.52	101.02	105.83
13	J	101	BCB	CHD-C1D-ND	-3.52	121.22	124.45
13	E	101	BCB	C3D-C2D-C1D	-3.51	101.03	105.83
13	N	101	BCB	CMB-C2B-C1B	-3.51	123.07	128.46
21	o	101	NS0	C21-C20-C19	3.51	130.67	123.47
13	J	101	BCB	CMB-C2B-C3B	3.51	131.25	124.68
13	T	101	BCB	CHD-C4C-C3C	-3.51	121.50	125.89
21	q	102	NS0	C21-C20-C19	3.51	130.66	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	L	303	BCB	C3D-C4D-ND	3.51	115.91	110.24
13	J	101	BCB	C3D-C2D-C1D	-3.50	101.05	105.83
13	L	302	BCB	CMB-C2B-C3B	3.50	131.23	124.68
13	c	101	BCB	CHD-C4C-C3C	-3.50	121.51	125.89
13	o	102	BCB	C3D-C2D-C1D	-3.49	101.06	105.83
21	l	101	NS0	C21-C20-C19	3.48	130.61	123.47
20	M	411	PGV	O01-C1-C2	3.47	118.99	111.50
13	b	101	BCB	C1-C2-C3	-3.47	120.04	126.04
11	M	408	UQ8	C25-C24-C26	3.47	121.10	115.27
21	k	101	NS0	C21-C20-C19	3.46	130.57	123.47
11	L	305	UQ8	C7-C8-C9	-3.46	121.03	126.79
13	M	402	BCB	C3D-C4D-ND	3.45	115.82	110.24
21	U	101	NS0	C21-C20-C19	3.44	130.51	123.47
13	Q	402	BCB	CHD-C1D-ND	-3.43	121.30	124.45
13	Z	101	BCB	CHD-C4C-C3C	-3.43	121.60	125.89
13	B	202	BCB	C3D-C2D-C1D	-3.42	101.16	105.83
13	L	302	BCB	CHD-C1D-ND	-3.42	121.31	124.45
18	M	406	NS5	C22-C21-C20	-3.42	118.13	122.92
13	c	101	BCB	C3D-C2D-C1D	-3.41	101.17	105.83
13	f	101	BCB	C3D-C4D-ND	3.41	115.75	110.24
13	M	402	BCB	C4-C3-C5	3.40	120.99	115.27
13	k	102	BCB	O2D-CGD-CBD	3.40	117.31	111.27
13	1	101	BCB	C3D-C2D-C1D	-3.40	101.20	105.83
13	0	102	BCB	C3D-C4D-ND	3.39	115.73	110.24
13	R	102	BCB	CMB-C2B-C1B	-3.39	123.25	128.46
13	E	101	BCB	CHD-C1D-ND	-3.39	121.34	124.45
21	h	101	NS0	C21-C20-C19	3.39	130.41	123.47
13	i	101	BCB	CMB-C2B-C3B	3.38	131.01	124.68
13	M	403	BCB	C1D-CHD-C4C	-3.38	118.77	126.06
13	r	101	BCB	C3D-C2D-C1D	-3.38	101.22	105.83
13	W	302	BCB	CHD-C4C-C3C	-3.38	121.67	125.89
13	f	101	BCB	C3D-C2D-C1D	-3.37	101.23	105.83
13	h	102	BCB	C1-C2-C3	-3.37	120.22	126.04
13	k	102	BCB	C1-C2-C3	-3.37	120.22	126.04
13	W	302	BCB	CHD-C1D-ND	-3.36	121.36	124.45
21	7	101	NS0	C21-C20-C19	3.36	130.35	123.47
13	X	102	BCB	CHD-C1D-ND	-3.36	121.37	124.45
13	e	101	BCB	C4D-CHA-C1A	-3.36	117.17	121.25
13	W	302	BCB	CMB-C2B-C1B	-3.35	123.31	128.46
11	M	407	UQ8	C17-C16-C14	-3.35	109.14	114.62
13	q	101	BCB	CHD-C1D-ND	-3.35	121.38	124.45
13	T	101	BCB	C1-C2-C3	-3.35	120.26	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	N	101	BCB	CHD-C4C-C3C	-3.35	121.70	125.89
15	L	306	CDL	CA4-OA6-CA5	-3.34	109.56	117.79
13	U	102	BCB	C3D-C2D-C1D	-3.34	101.28	105.83
13	i	101	BCB	C3D-C4D-ND	3.33	115.63	110.24
13	R	102	BCB	C3D-C2D-C1D	-3.33	101.29	105.83
13	l	102	BCB	CMB-C2B-C1B	-3.32	123.36	128.46
13	7	102	BCB	CMB-C2B-C1B	-3.32	123.36	128.46
13	l	102	BCB	C3D-C2D-C1D	-3.32	101.31	105.83
21	2	101	NS0	C21-C20-C19	3.30	130.23	123.47
13	6	101	BCB	CHD-C1D-ND	-3.29	121.43	124.45
13	0	102	BCB	C4D-CHA-C1A	-3.28	117.25	121.25
13	1	101	BCB	C3D-C4D-ND	3.28	115.55	110.24
17	M	405	MQ7	C39-C38-C40	3.28	120.79	115.27
13	k	102	BCB	CMB-C2B-C1B	-3.28	123.43	128.46
13	Q	402	BCB	CHD-C4C-C3C	-3.27	121.80	125.89
13	3	101	BCB	CHD-C4C-C3C	-3.26	121.82	125.89
21	D	103	NS0	C21-C20-C19	3.25	130.13	123.47
13	4	101	BCB	C4D-CHA-C1A	-3.25	117.30	121.25
13	X	102	BCB	C3D-C4D-ND	3.25	115.49	110.24
20	D	102	PGV	O03-C19-C20	3.24	122.07	111.91
13	R	102	BCB	C4D-CHA-C1A	-3.24	117.31	121.25
13	U	102	BCB	C3D-C4D-ND	3.23	115.46	110.24
13	7	102	BCB	C4D-CHA-C1A	-3.23	117.32	121.25
13	n	101	BCB	CHD-C1D-ND	-3.22	121.49	124.45
13	6	101	BCB	CHD-C4C-C3C	-3.22	121.86	125.89
21	O	101	NS0	C13-C12-C14	-3.21	118.42	122.92
13	c	101	BCB	C3D-C4D-ND	3.21	115.43	110.24
13	4	101	BCB	C3D-C4D-ND	3.20	115.41	110.24
13	B	202	BCB	C3D-C4D-ND	3.19	115.40	110.24
13	U	102	BCB	C4D-CHA-C1A	-3.19	117.37	121.25
13	X	102	BCB	C3D-C2D-C1D	-3.19	101.48	105.83
21	X	101	NS0	C18-C17-C19	-3.19	118.46	122.92
13	B	202	BCB	CMB-C2B-C1B	-3.19	123.56	128.46
13	0	102	BCB	CHB-C4A-NA	3.18	128.91	124.51
13	q	101	BCB	CHD-C4C-C3C	-3.18	121.91	125.89
13	e	101	BCB	CHD-C1D-ND	-3.18	121.53	124.45
13	1	101	BCB	CMB-C2B-C1B	-3.18	123.58	128.46
21	A	103	NS0	C21-C20-C19	3.17	129.97	123.47
13	4	101	BCB	C3D-C2D-C1D	-3.17	101.50	105.83
13	4	101	BCB	CMB-C2B-C1B	-3.17	123.59	128.46
13	R	102	BCB	C4-C3-C5	3.17	120.60	115.27
13	7	102	BCB	C3D-C4D-ND	3.17	115.36	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	U	101	NS0	C24-C23-C22	-3.16	118.49	122.92
13	B	202	BCB	CHD-C1D-ND	-3.16	121.55	124.45
21	q	102	NS0	C13-C12-C14	-3.16	118.50	122.92
13	B	202	BCB	C4D-CHA-C1A	-3.16	117.40	121.25
13	A	102	BCB	CHB-C4A-NA	3.15	128.87	124.51
13	0	102	BCB	CHD-C1D-ND	-3.15	121.56	124.45
13	L	303	BCB	CMB-C2B-C1B	-3.15	123.62	128.46
13	7	102	BCB	C3D-C2D-C1D	-3.15	101.54	105.83
13	o	102	BCB	CMB-C2B-C1B	-3.14	123.63	128.46
13	L	302	BCB	CHB-C4A-NA	3.14	128.85	124.51
13	c	101	BCB	C4D-CHA-C1A	-3.14	117.43	121.25
13	W	302	BCB	O2A-CGA-CBA	3.14	121.75	111.91
21	k	101	NS0	C24-C23-C22	-3.13	118.53	122.92
11	A	101	UQ8	C40-C39-C41	3.13	120.54	115.27
13	0	102	BCB	C3D-C2D-C1D	-3.13	101.55	105.83
19	k	103	LMT	C1B-O1B-C4'	-3.13	110.21	117.96
19	T	102	LMT	C1-O1'-C1'	-3.12	108.66	113.84
13	b	101	BCB	CMB-C2B-C1B	-3.12	123.67	128.46
11	M	408	UQ8	C35-C34-C36	3.12	120.52	115.27
13	l	102	BCB	C3D-C4D-ND	3.12	115.28	110.24
21	2	101	NS0	C24-C23-C22	-3.12	118.56	122.92
21	k	101	NS0	C13-C12-C14	-3.12	118.56	122.92
13	0	102	BCB	CMB-C2B-C1B	-3.11	123.68	128.46
13	O	102	BCB	CHD-C4C-C3C	-3.11	122.00	125.89
13	6	101	BCB	C1-C2-C3	-3.11	120.66	126.04
21	U	101	NS0	C13-C12-C14	-3.11	118.57	122.92
13	b	101	BCB	CHD-C4C-C3C	-3.10	122.01	125.89
13	L	303	BCB	C1-C2-C3	-3.10	120.69	126.04
18	M	406	NS5	C27-C26-C25	-3.10	118.58	122.92
13	9	101	BCB	C4-C3-C5	3.10	120.48	115.27
13	X	102	BCB	CMB-C2B-C1B	-3.09	123.71	128.46
11	A	101	UQ8	C25-C24-C26	3.09	120.47	115.27
21	O	101	NS0	C21-C20-C19	3.09	129.80	123.47
13	D	101	BCB	CHD-C4C-C3C	-3.09	122.03	125.89
13	6	101	BCB	C4D-CHA-C1A	-3.08	117.50	121.25
13	B	202	BCB	CHD-C4C-C3C	-3.08	122.03	125.89
13	O	102	BCB	C3D-C4D-ND	3.08	115.22	110.24
21	k	101	NS0	C18-C17-C19	-3.08	118.61	122.92
13	E	101	BCB	C3D-C4D-ND	3.08	115.22	110.24
21	W	303	NS0	C13-C12-C14	-3.08	118.61	122.92
13	f	101	BCB	C4D-CHA-C1A	-3.08	117.51	121.25
13	E	101	BCB	C4D-CHA-C1A	-3.07	117.52	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	R	101	NS0	C18-C17-C19	-3.07	118.63	122.92
21	l	101	NS0	C24-C23-C22	-3.07	118.63	122.92
13	h	102	BCB	CMB-C2B-C1B	-3.06	123.76	128.46
21	2	101	NS0	C13-C12-C14	-3.06	118.63	122.92
13	T	101	BCB	CMB-C2B-C1B	-3.06	123.76	128.46
17	M	405	MQ7	C34-C33-C35	3.05	120.41	115.27
13	c	101	BCB	O2A-CGA-CBA	3.05	121.49	111.91
21	l	101	NS0	C13-C12-C14	-3.05	118.65	122.92
13	I	101	BCB	CMB-C2B-C1B	-3.05	123.77	128.46
13	R	102	BCB	CHD-C4C-C3C	-3.05	122.08	125.89
13	R	102	BCB	C3D-C4D-ND	3.05	115.17	110.24
21	l	101	NS0	C18-C17-C19	-3.05	118.66	122.92
13	U	102	BCB	CMB-C2B-C1B	-3.05	123.78	128.46
13	i	101	BCB	C3D-C2D-C1D	-3.05	101.67	105.83
21	D	103	NS0	C18-C17-C19	-3.04	118.66	122.92
13	r	101	BCB	C4D-CHA-C1A	-3.04	117.55	121.25
13	Z	101	BCB	C4D-CHA-C1A	-3.04	117.55	121.25
21	q	102	NS0	C18-C17-C19	-3.04	118.67	122.92
11	M	408	UQ8	C27-C28-C29	-3.04	120.35	127.66
13	I	101	BCB	CHD-C4C-C3C	-3.03	122.09	125.89
13	h	102	BCB	CHD-C4C-C3C	-3.03	122.09	125.89
11	A	101	UQ8	C10-C9-C11	3.03	120.38	115.27
13	o	102	BCB	C3D-C4D-ND	3.03	115.14	110.24
13	R	102	BCB	CHB-C4A-NA	3.03	128.70	124.51
13	l	102	BCB	C1B-CHB-C4A	-3.03	124.12	130.12
21	k	101	NS0	C20-C21-C22	3.02	129.67	123.47
11	M	408	UQ8	C30-C29-C31	3.02	120.36	115.27
13	L	303	BCB	CHB-C4A-NA	3.02	128.69	124.51
13	D	101	BCB	CHB-C4A-NA	3.02	128.69	124.51
13	c	101	BCB	CHB-C4A-NA	3.01	128.67	124.51
13	N	101	BCB	C1B-CHB-C4A	-3.01	124.16	130.12
13	B	202	BCB	CHB-C4A-NA	3.00	128.67	124.51
13	q	101	BCB	CMB-C2B-C1B	-3.00	123.86	128.46
13	9	101	BCB	C2A-C1A-CHA	-2.99	118.62	123.86
13	T	101	BCB	C6-C5-C3	-2.99	105.61	113.45
13	h	102	BCB	C4-C3-C5	2.98	120.29	115.27
13	1	101	BCB	CHD-C1D-ND	-2.98	121.72	124.45
13	o	102	BCB	CHD-C4C-C3C	-2.98	122.16	125.89
13	f	101	BCB	CHD-C1D-ND	-2.98	121.72	124.45
13	q	101	BCB	C1B-CHB-C4A	-2.98	124.22	130.12
13	h	102	BCB	CHD-C1D-ND	-2.97	121.72	124.45
13	r	101	BCB	CHD-C1D-ND	-2.97	121.72	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	7	101	NS0	C24-C23-C22	-2.97	118.76	122.92
13	f	101	BCB	CMB-C2B-C1B	-2.97	123.90	128.46
13	9	101	BCB	C4D-CHA-C1A	-2.97	117.64	121.25
13	l	102	BCB	CHD-C1D-ND	-2.97	121.72	124.45
21	R	101	NS0	C13-C12-C14	-2.97	118.77	122.92
11	A	101	UQ8	C22-C23-C24	-2.97	120.51	127.66
21	0	101	NS0	C21-C20-C19	2.97	129.55	123.47
13	l	102	BCB	C4D-CHA-C1A	-2.96	117.64	121.25
19	b	103	LMT	C1-O1'-C1'	-2.96	108.93	113.84
13	4	101	BCB	CHB-C4A-NA	2.96	128.60	124.51
21	W	303	NS0	C18-C17-C19	-2.96	118.78	122.92
11	M	408	UQ8	C7-C8-C9	2.96	131.72	126.79
13	E	101	BCB	O2A-CGA-CBA	2.96	121.19	111.91
13	I	101	BCB	CHD-C1D-ND	-2.96	121.74	124.45
21	X	101	NS0	C24-C23-C22	-2.96	118.78	122.92
13	k	102	BCB	CHD-C1D-ND	-2.96	121.74	124.45
11	M	408	UQ8	C20-C19-C21	2.95	120.24	115.27
13	b	101	BCB	C4-C3-C5	2.95	120.23	115.27
13	r	101	BCB	C3D-C4D-ND	2.95	115.01	110.24
13	J	101	BCB	CHB-C4A-NA	2.95	128.59	124.51
21	9	102	NS0	C13-C12-C14	-2.95	118.79	122.92
13	9	101	BCB	CMB-C2B-C1B	-2.95	123.94	128.46
13	X	102	BCB	C4D-CHA-C1A	-2.95	117.66	121.25
13	e	101	BCB	CMB-C2B-C1B	-2.94	123.94	128.46
21	W	303	NS0	C24-C23-C22	-2.94	118.80	122.92
11	M	407	UQ8	C10-C9-C11	2.94	120.21	115.27
11	A	101	UQ8	C17-C18-C19	-2.93	120.59	127.66
13	A	102	BCB	C1B-CHB-C4A	-2.93	124.31	130.12
21	0	101	NS0	C13-C12-C14	-2.93	118.81	122.92
13	0	102	BCB	O2A-CGA-CBA	2.93	121.11	111.91
13	T	101	BCB	O2A-CGA-CBA	2.93	121.11	111.91
13	N	101	BCB	CHD-C1D-ND	-2.93	121.76	124.45
21	U	101	NS0	C18-C17-C19	-2.93	118.82	122.92
13	n	101	BCB	CMB-C2B-C1B	-2.93	123.97	128.46
21	R	101	NS0	C24-C23-C22	-2.92	118.83	122.92
15	L	306	CDL	OA8-CA7-C31	2.92	121.07	111.91
13	6	101	BCB	C4-C3-C5	2.92	120.18	115.27
13	3	101	BCB	CHD-C1D-ND	-2.92	121.77	124.45
13	N	101	BCB	O2A-CGA-CBA	2.92	121.06	111.91
13	X	102	BCB	CHB-C4A-NA	2.91	128.54	124.51
11	M	408	UQ8	C15-C14-C16	2.91	120.17	115.27
13	D	101	BCB	CMB-C2B-C1B	-2.91	123.99	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	H	302	CDL	OA8-CA7-C31	2.91	121.04	111.91
13	L	303	BCB	CHD-C4C-C3C	-2.91	122.25	125.89
13	Q	402	BCB	C4-C3-C5	2.91	120.16	115.27
21	D	103	NS0	C24-C23-C22	-2.91	118.85	122.92
13	i	101	BCB	CHB-C4A-NA	2.91	128.53	124.51
13	c	101	BCB	C1D-CHD-C4C	-2.91	119.79	126.06
21	A	103	NS0	C18-C17-C19	-2.90	118.86	122.92
13	9	101	BCB	CHB-C4A-NA	2.90	128.53	124.51
13	O	102	BCB	C1D-CHD-C4C	-2.90	119.80	126.06
13	b	101	BCB	CHD-C1D-ND	-2.90	121.79	124.45
13	U	102	BCB	CHD-C4C-C3C	-2.90	122.26	125.89
13	r	101	BCB	O2A-CGA-CBA	2.90	120.99	111.91
21	h	101	NS0	C24-C23-C22	-2.89	118.87	122.92
11	M	408	UQ8	C16-C14-C13	-2.89	115.27	121.12
13	0	102	BCB	C2A-C1A-CHA	-2.89	118.81	123.86
13	9	101	BCB	CHD-C4C-C3C	-2.88	122.28	125.89
18	M	406	NS5	C18-C19-C20	2.88	129.37	123.47
13	o	102	BCB	O2A-CGA-CBA	2.88	120.94	111.91
13	1	101	BCB	C4D-CHA-C1A	-2.87	117.75	121.25
21	A	103	NS0	C24-C23-C22	-2.87	118.90	122.92
13	A	102	BCB	CHD-C4C-C3C	-2.87	122.30	125.89
13	T	101	BCB	C1B-CHB-C4A	-2.87	124.44	130.12
13	k	102	BCB	C1B-CHB-C4A	-2.87	124.44	130.12
13	f	101	BCB	CHB-C4A-NA	2.87	128.48	124.51
13	U	102	BCB	O2A-CGA-CBA	2.86	120.90	111.91
13	L	302	BCB	CED-O2D-CGD	2.86	122.41	115.94
11	M	407	UQ8	C12-C13-C14	-2.86	120.77	127.66
21	0	101	NS0	C18-C17-C19	-2.86	118.92	122.92
13	O	102	BCB	CHB-C4A-NA	2.86	128.47	124.51
20	W	301	PGV	C02-O01-C1	-2.86	110.76	117.79
21	7	101	NS0	C13-C12-C14	-2.86	118.92	122.92
13	i	101	BCB	C4-C3-C5	2.85	120.07	115.27
13	J	101	BCB	O2A-CGA-CBA	2.85	120.86	111.91
13	o	102	BCB	C4-C3-C5	2.85	120.07	115.27
13	i	101	BCB	CHD-C4C-C3C	-2.85	122.32	125.89
19	n	102	LMT	C1B-O1B-C4'	-2.85	110.92	117.96
21	9	102	NS0	C24-C23-C22	-2.85	118.94	122.92
21	o	101	NS0	C18-C17-C19	-2.84	118.94	122.92
12	L	301	DGA	OG1-CA1-CA2	2.84	120.83	111.91
13	9	101	BCB	C3D-C4D-ND	2.84	114.83	110.24
13	Q	402	BCB	C4D-CHA-C1A	-2.84	117.80	121.25
21	h	101	NS0	C18-C17-C19	-2.84	118.95	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	o	102	BCB	C4D-CHA-C1A	-2.84	117.80	121.25
21	q	102	NS0	C24-C23-C22	-2.84	118.95	122.92
13	O	102	BCB	C4-C3-C5	2.84	120.04	115.27
13	T	101	BCB	CHD-C1D-ND	-2.83	121.85	124.45
13	l	102	BCB	C1-C2-C3	-2.83	121.14	126.04
13	Z	101	BCB	CMB-C2B-C1B	-2.83	124.12	128.46
13	M	403	BCB	O2A-CGA-CBA	2.83	120.78	111.91
21	9	102	NS0	C18-C17-C19	-2.83	118.96	122.92
21	2	101	NS0	C18-C17-C19	-2.82	118.97	122.92
21	o	101	NS0	C13-C12-C14	-2.82	118.97	122.92
13	r	101	BCB	C1-C2-C3	-2.82	121.17	126.04
13	k	102	BCB	C4D-CHA-C1A	-2.82	117.82	121.25
11	C	406	UQ8	C7-C6-C1	-2.82	119.55	124.27
13	e	101	BCB	O2A-CGA-CBA	2.82	120.74	111.91
13	X	102	BCB	O2A-CGA-CBA	2.81	120.74	111.91
13	4	101	BCB	O2A-CGA-CBA	2.81	120.74	111.91
13	o	102	BCB	C1D-CHD-C4C	-2.81	119.99	126.06
13	B	202	BCB	C4-C3-C5	2.81	120.00	115.27
13	D	101	BCB	C2A-C1A-CHA	-2.81	118.95	123.86
13	M	403	BCB	O2D-CGD-O1D	-2.81	118.35	123.84
13	O	102	BCB	CMB-C2B-C1B	-2.81	124.15	128.46
13	W	302	BCB	CHB-C4A-NA	2.81	128.39	124.51
13	l	102	BCB	CHB-C4A-NA	2.81	128.39	124.51
14	M	404	BPB	CMC-C2C-C1C	-2.81	109.65	114.36
13	A	102	BCB	C4D-CHA-C1A	-2.81	117.83	121.25
13	e	101	BCB	CHD-C4C-C3C	-2.81	122.38	125.89
13	c	101	BCB	CMB-C2B-C1B	-2.80	124.17	128.46
13	q	101	BCB	C1-C2-C3	-2.79	121.21	126.04
13	7	102	BCB	C1B-CHB-C4A	-2.79	124.58	130.12
18	M	406	NS5	C23-C21-C20	2.79	123.23	118.94
13	4	101	BCB	C4-C3-C5	2.79	119.97	115.27
21	O	101	NS0	C24-C23-C22	-2.79	119.02	122.92
21	h	101	NS0	C13-C12-C14	-2.79	119.02	122.92
13	k	102	BCB	C4-C3-C5	2.78	119.95	115.27
13	M	403	BCB	C4B-CHC-C1C	-2.78	124.61	130.12
13	X	102	BCB	CHD-C4C-C3C	-2.78	122.41	125.89
13	i	101	BCB	O2A-CGA-CBA	2.78	120.63	111.91
21	X	101	NS0	C13-C12-C14	-2.78	119.03	122.92
13	M	403	BCB	C3D-C4D-ND	2.77	114.72	110.24
17	M	405	MQ7	C26-C27-C28	-2.76	121.01	127.66
17	M	405	MQ7	C29-C28-C30	2.76	119.92	115.27
13	M	402	BCB	C2A-C1A-CHA	-2.76	119.04	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	1	101	BCB	O2A-CGA-CBA	2.76	120.56	111.91
21	O	101	NS0	C18-C17-C19	-2.76	119.06	122.92
13	l	102	BCB	O2A-CGA-CBA	2.76	120.56	111.91
13	L	302	BCB	C1D-CHD-C4C	-2.76	120.11	126.06
13	7	102	BCB	CHB-C4A-NA	2.75	128.31	124.51
13	7	102	BCB	C1-C2-C3	-2.75	121.29	126.04
13	O	102	BCB	O2A-CGA-CBA	2.75	120.53	111.91
13	h	102	BCB	CHB-C4A-NA	2.75	128.31	124.51
18	M	406	NS5	C28-C26-C25	2.74	123.15	118.94
13	X	102	BCB	C1-C2-C3	-2.74	121.30	126.04
13	J	101	BCB	C4D-CHA-C1A	-2.74	117.91	121.25
20	W	301	PGV	O03-C19-C20	2.74	120.52	111.91
13	D	101	BCB	C3D-C4D-ND	2.74	114.67	110.24
13	L	303	BCB	C4-C3-C5	2.74	119.88	115.27
13	7	102	BCB	CHD-C1D-ND	-2.74	121.94	124.45
13	U	102	BCB	C4-C3-C5	2.74	119.88	115.27
13	E	101	BCB	CMB-C2B-C1B	-2.74	124.26	128.46
13	b	101	BCB	C4D-CHA-C1A	-2.73	117.92	121.25
13	r	101	BCB	CHD-C4C-C3C	-2.73	122.47	125.89
13	E	101	BCB	CHB-C4A-NA	2.73	128.29	124.51
13	D	101	BCB	O2A-CGA-CBA	2.73	120.47	111.91
13	i	101	BCB	C1D-CHD-C4C	-2.73	120.17	126.06
13	Q	402	BCB	CMB-C2B-C1B	-2.73	124.27	128.46
13	n	101	BCB	C4D-CHA-C1A	-2.73	117.93	121.25
21	o	101	NS0	C24-C23-C22	-2.73	119.10	122.92
21	7	101	NS0	C18-C17-C19	-2.72	119.11	122.92
13	o	102	BCB	CHB-C4A-NA	2.72	128.27	124.51
13	l	102	BCB	CHD-C4C-C3C	-2.72	122.49	125.89
13	0	102	BCB	C4-C3-C5	2.72	119.84	115.27
13	J	101	BCB	C4-C3-C5	2.72	119.84	115.27
13	Z	101	BCB	O2A-CGA-CBA	2.72	120.43	111.91
13	J	101	BCB	CMB-C2B-C1B	-2.72	124.29	128.46
13	U	102	BCB	C1D-CHD-C4C	-2.71	120.20	126.06
13	0	102	BCB	CHD-C4C-C3C	-2.71	122.50	125.89
13	q	101	BCB	C4-C3-C5	2.71	119.83	115.27
13	U	102	BCB	C2A-C1A-CHA	-2.71	119.12	123.86
13	R	102	BCB	C2A-C1A-CHA	-2.71	119.13	123.86
13	f	101	BCB	O2A-CGA-CBA	2.70	120.38	111.91
13	L	302	BCB	C3D-C4D-ND	2.70	114.60	110.24
11	L	305	UQ8	C1M-C1-C6	-2.70	120.00	124.40
13	f	101	BCB	C1B-CHB-C4A	-2.70	124.78	130.12
20	N	102	PGV	O01-C1-C2	2.70	117.31	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	7	102	BCB	O2A-CGA-CBA	2.69	120.36	111.91
13	3	101	BCB	CMB-C2B-C1B	-2.69	124.33	128.46
13	4	101	BCB	C1D-CHD-C4C	-2.69	120.26	126.06
21	D	103	NS0	C20-C21-C22	2.69	128.98	123.47
13	e	101	BCB	CHB-C4A-NA	2.69	128.22	124.51
13	M	403	BCB	CMB-C2B-C1B	-2.68	124.34	128.46
13	1	101	BCB	CHB-C4A-NA	2.68	128.22	124.51
13	n	101	BCB	C1B-CHB-C4A	-2.68	124.81	130.12
13	I	101	BCB	C1B-CHB-C4A	-2.68	124.82	130.12
13	M	402	BCB	CHD-C4C-C3C	-2.68	122.54	125.89
13	l	102	BCB	C4-C3-C5	2.68	119.77	115.27
13	n	101	BCB	CHD-C4C-C3C	-2.67	122.54	125.89
13	I	101	BCB	C6-C5-C3	-2.67	106.46	113.45
13	3	101	BCB	O2A-CGA-CBA	2.66	120.26	111.91
21	0	101	NS0	C24-C23-C22	-2.66	119.20	122.92
11	L	305	UQ8	C17-C18-C19	-2.66	121.25	127.66
13	n	101	BCB	CAA-CBA-CGA	-2.66	105.48	113.25
13	D	101	BCB	C1B-CHB-C4A	-2.66	124.85	130.12
11	L	305	UQ8	C10-C9-C11	2.66	119.74	115.27
13	q	101	BCB	C2A-C1A-CHA	-2.66	119.21	123.86
13	k	102	BCB	CHD-C4C-C3C	-2.65	122.57	125.89
20	N	102	PGV	O03-C19-C20	2.65	120.22	111.91
13	Z	101	BCB	CHD-C1D-ND	-2.65	122.02	124.45
13	h	102	BCB	C4D-CHA-C1A	-2.65	118.03	121.25
13	6	101	BCB	CMB-C2B-C1B	-2.64	124.40	128.46
13	b	101	BCB	O2A-CGA-CBA	2.64	120.20	111.91
13	3	101	BCB	C6-C5-C3	-2.64	106.53	113.45
13	Z	101	BCB	C1B-CHB-C4A	-2.64	124.88	130.12
13	E	101	BCB	C1-C2-C3	-2.64	121.47	126.04
17	M	405	MQ7	C36-C37-C38	-2.64	121.31	127.66
13	q	101	BCB	C4D-CHA-C1A	-2.64	118.04	121.25
13	U	102	BCB	CHB-C4A-NA	2.64	128.16	124.51
13	h	102	BCB	CAA-CBA-CGA	-2.63	105.56	113.25
13	6	101	BCB	CHB-C4A-NA	2.63	128.15	124.51
15	L	306	CDL	OB8-CB7-C71	2.63	120.16	111.91
15	L	306	CDL	CB4-OB6-CB5	-2.63	111.32	117.79
13	B	202	BCB	C2A-C1A-CHA	-2.63	119.27	123.86
15	M	409	CDL	OA8-CA7-C31	2.63	120.15	111.91
13	L	302	BCB	O2A-CGA-CBA	2.63	120.15	111.91
13	I	101	BCB	O2A-CGA-CBA	2.62	120.14	111.91
9	C	403	HEC	CBD-CAD-C3D	-2.62	108.15	112.62
13	7	102	BCB	C1D-CHD-C4C	-2.62	120.41	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	M	408	UQ8	C41-C42-C43	-2.62	103.28	111.88
13	R	102	BCB	CHD-C1D-ND	-2.62	122.05	124.45
13	i	101	BCB	C1B-CHB-C4A	-2.62	124.93	130.12
13	Z	101	BCB	CHB-C4A-NA	2.62	128.13	124.51
13	A	102	BCB	C2A-C1A-CHA	-2.61	119.29	123.86
13	q	101	BCB	CHB-C4A-NA	2.61	128.13	124.51
13	0	102	BCB	O2D-CGD-O1D	-2.61	118.73	123.84
13	R	102	BCB	C1D-CHD-C4C	-2.61	120.43	126.06
13	r	101	BCB	C4-C3-C5	2.61	119.66	115.27
13	A	102	BCB	C3D-C4D-ND	2.61	114.45	110.24
13	n	101	BCB	O2A-CGA-CBA	2.61	120.08	111.91
21	R	101	NS0	C16-C17-C19	2.60	122.94	118.94
13	M	402	BCB	CHB-C4A-NA	2.60	128.11	124.51
13	c	101	BCB	C4-C3-C5	2.60	119.65	115.27
13	I	101	BCB	CHB-C4A-NA	2.60	128.11	124.51
12	L	301	DGA	OG2-CB1-OB1	-2.60	117.42	123.70
11	A	101	UQ8	C37-C38-C39	-2.60	121.40	127.66
13	q	101	BCB	C3D-C4D-ND	2.59	114.43	110.24
21	A	103	NS0	C20-C21-C22	2.59	128.78	123.47
13	R	102	BCB	O2A-CGA-CBA	2.59	120.04	111.91
13	J	101	BCB	CHD-C4C-C3C	-2.59	122.65	125.89
13	f	101	BCB	C1D-CHD-C4C	-2.58	120.49	126.06
13	O	102	BCB	O2D-CGD-O1D	-2.58	118.79	123.84
13	1	101	BCB	C1B-CHB-C4A	-2.58	125.01	130.12
21	U	101	NS0	C20-C21-C22	2.58	128.75	123.47
13	N	101	BCB	C4D-CHA-C1A	-2.57	118.12	121.25
13	6	101	BCB	O2A-CGA-CBA	2.57	119.99	111.91
13	L	303	BCB	C2A-C1A-CHA	-2.57	119.36	123.86
13	Z	101	BCB	CAA-CBA-CGA	-2.57	105.73	113.25
13	6	101	BCB	CAA-CBA-CGA	-2.57	105.74	113.25
21	h	101	NS0	C20-C21-C22	2.57	128.74	123.47
13	Q	402	BCB	O2A-CGA-CBA	2.56	119.96	111.91
20	M	411	PGV	O03-C19-C20	2.56	119.96	111.91
13	n	101	BCB	CHB-C4A-NA	2.56	128.06	124.51
13	B	202	BCB	O2A-CGA-CBA	2.56	119.94	111.91
19	b	103	LMT	O1'-C1'-C2'	2.56	112.30	108.30
11	M	407	UQ8	C1M-C1-C6	-2.56	120.23	124.40
13	o	102	BCB	CHD-C1D-ND	-2.56	122.11	124.45
13	D	101	BCB	C1D-CHD-C4C	-2.55	120.55	126.06
19	T	102	LMT	O1'-C1'-C2'	2.55	112.29	108.30
13	A	102	BCB	CMB-C2B-C1B	-2.55	124.54	128.46
11	C	406	UQ8	C1M-C1-C6	-2.55	120.24	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	i	101	BCB	C2A-C1A-CHA	-2.55	119.40	123.86
13	I	101	BCB	C1D-CHD-C4C	-2.54	120.57	126.06
13	1	101	BCB	C1D-CHD-C4C	-2.54	120.57	126.06
15	H	301	CDL	OA8-CA7-C31	2.54	119.89	111.91
21	q	102	NS0	C16-C17-C19	2.54	122.84	118.94
13	o	102	BCB	C1-C2-C3	-2.54	121.66	126.04
13	L	302	BCB	CHD-C4C-C3C	-2.53	122.72	125.89
13	0	102	BCB	C1-C2-C3	-2.53	121.66	126.04
13	6	101	BCB	C1B-CHB-C4A	-2.53	125.10	130.12
13	O	102	BCB	CHD-C1D-ND	-2.53	122.13	124.45
13	D	101	BCB	C1-C2-C3	-2.53	121.67	126.04
20	Q	401	PGV	O03-C19-C20	2.53	119.85	111.91
13	q	101	BCB	O2A-CGA-CBA	2.53	119.84	111.91
13	X	102	BCB	C1B-CHB-C4A	-2.53	125.11	130.12
13	b	101	BCB	C1B-CHB-C4A	-2.53	125.11	130.12
13	N	101	BCB	CHC-C1C-NC	-2.52	121.02	124.51
13	q	101	BCB	CAA-CBA-CGA	-2.52	105.88	113.25
13	A	102	BCB	C1D-CHD-C4C	-2.52	120.61	126.06
13	f	101	BCB	C4-C3-C5	2.52	119.51	115.27
13	L	303	BCB	O2D-CGD-O1D	-2.52	118.92	123.84
13	D	101	BCB	C6-C5-C3	-2.52	106.86	113.45
15	M	409	CDL	OB8-CB7-C71	2.52	119.80	111.91
21	A	103	NS0	C13-C12-C14	-2.51	119.40	122.92
20	N	102	PGV	C03-C02-C01	-2.51	105.85	111.79
21	7	101	NS0	C20-C21-C22	2.51	128.62	123.47
13	1	101	BCB	CHD-C4C-C3C	-2.51	122.75	125.89
21	D	103	NS0	C13-C12-C14	-2.51	119.41	122.92
13	r	101	BCB	C1B-CHB-C4A	-2.51	125.15	130.12
13	W	302	BCB	C6-C5-C3	-2.51	106.89	113.45
21	k	101	NS0	C11-C12-C14	2.50	122.78	118.94
9	C	404	HEC	CAD-CBD-CGD	-2.50	106.75	113.76
11	A	101	UQ8	C15-C14-C16	2.50	119.47	115.27
13	n	101	BCB	CED-O2D-CGD	2.50	121.58	115.94
13	L	303	BCB	O1D-CGD-CBD	-2.49	119.39	124.48
13	B	202	BCB	O2D-CGD-O1D	-2.49	118.97	123.84
13	I	101	BCB	C4D-CHA-C1A	-2.49	118.22	121.25
21	k	101	NS0	C16-C17-C19	2.49	122.76	118.94
13	U	102	BCB	C1B-CHB-C4A	-2.49	125.19	130.12
13	b	101	BCB	CHB-C4A-NA	2.49	127.95	124.51
13	7	102	BCB	CHD-C4C-C3C	-2.48	122.79	125.89
13	L	303	BCB	C1B-CHB-C4A	-2.48	125.21	130.12
17	M	405	MQ7	C21-C22-C23	-2.47	121.70	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	W	302	BCB	C4D-CHA-C1A	-2.47	118.24	121.25
13	h	102	BCB	C3D-C4D-ND	2.46	114.22	110.24
13	1	101	BCB	C4-C3-C5	2.46	119.41	115.27
13	r	101	BCB	C1D-CHD-C4C	-2.46	120.75	126.06
21	k	101	NS0	C25-C23-C22	2.46	122.72	118.94
11	A	101	UQ8	C30-C29-C31	2.46	119.41	115.27
15	H	302	CDL	CB4-OB6-CB5	-2.46	111.74	117.79
13	N	101	BCB	CAA-CBA-CGA	-2.46	106.07	113.25
20	I	102	PGV	C02-O01-C1	-2.46	111.74	117.79
9	C	401	HEC	CBA-CAA-C2A	-2.46	108.47	112.60
13	i	101	BCB	CMB-C2B-C1B	-2.45	124.70	128.46
11	A	101	UQ8	C36-C37-C38	-2.45	103.83	111.88
13	3	101	BCB	C4D-CHA-C1A	-2.45	118.27	121.25
13	Q	402	BCB	CHB-C4A-NA	2.45	127.90	124.51
21	q	102	NS0	C20-C21-C22	2.45	128.49	123.47
13	4	101	BCB	CHD-C4C-C3C	-2.45	122.83	125.89
13	l	102	BCB	C1D-CHD-C4C	-2.45	120.78	126.06
13	1	101	BCB	CED-O2D-CGD	2.44	121.47	115.94
13	r	101	BCB	C4B-CHC-C1C	-2.44	125.28	130.12
13	B	202	BCB	C1-C2-C3	-2.44	121.82	126.04
13	l	102	BCB	CHC-C1C-NC	-2.44	121.13	124.51
13	b	101	BCB	C1D-CHD-C4C	-2.44	120.79	126.06
13	E	101	BCB	C4-C3-C5	2.44	119.37	115.27
11	M	407	UQ8	C15-C14-C16	2.44	119.37	115.27
11	L	305	UQ8	C12-C13-C14	-2.44	121.80	127.66
13	W	302	BCB	CAA-CBA-CGA	-2.43	106.14	113.25
21	l	101	NS0	C20-C21-C22	2.43	128.45	123.47
21	X	101	NS0	C16-C17-C19	2.43	122.67	118.94
17	M	405	MQ7	C45-C43-C44	2.43	119.97	114.60
21	D	103	NS0	C16-C17-C19	2.43	122.67	118.94
13	O	102	BCB	C4D-CHA-C1A	-2.42	118.30	121.25
11	M	407	UQ8	C8-C7-C6	-2.42	105.51	112.05
13	E	101	BCB	C1B-CHB-C4A	-2.42	125.32	130.12
13	T	101	BCB	C1D-CHD-C4C	-2.42	120.83	126.06
13	3	101	BCB	C1B-CHB-C4A	-2.42	125.32	130.12
13	k	102	BCB	O2A-CGA-CBA	2.42	119.50	111.91
13	q	101	BCB	CHC-C1C-NC	-2.42	121.17	124.51
14	L	304	BPB	CMA-C3A-C4A	-2.42	109.09	114.38
13	B	202	BCB	C1D-CHD-C4C	-2.41	120.85	126.06
13	U	102	BCB	CHD-C1D-ND	-2.41	122.24	124.45
13	o	102	BCB	C1B-CHB-C4A	-2.41	125.34	130.12
13	0	102	BCB	C1D-CHD-C4C	-2.41	120.86	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	e	101	BCB	C1B-CHB-C4A	-2.41	125.35	130.12
21	2	101	NS0	C25-C23-C22	2.41	122.63	118.94
13	r	101	BCB	O2D-CGD-O1D	-2.41	119.14	123.84
13	B	202	BCB	C4B-CHC-C1C	-2.40	125.36	130.12
13	4	101	BCB	C1B-CHB-C4A	-2.40	125.37	130.12
13	L	303	BCB	C1D-CHD-C4C	-2.39	120.89	126.06
13	h	102	BCB	O2A-CGA-CBA	2.39	119.42	111.91
13	E	101	BCB	CHD-C4C-C3C	-2.39	122.90	125.89
13	4	101	BCB	O2D-CGD-O1D	-2.39	119.16	123.84
13	A	102	BCB	O2A-CGA-CBA	2.39	119.39	111.91
13	3	101	BCB	CHC-C1C-NC	-2.38	121.22	124.51
13	h	102	BCB	C1B-CHB-C4A	-2.38	125.41	130.12
13	N	101	BCB	C1D-CHD-C4C	-2.38	120.93	126.06
13	i	101	BCB	CHD-C1D-ND	-2.38	122.27	124.45
14	M	404	BPB	CMA-C3A-C4A	-2.38	109.17	114.38
13	M	402	BCB	C1B-CHB-C4A	-2.37	125.42	130.12
13	M	403	BCB	C2A-C1A-CHA	-2.37	119.72	123.86
21	q	102	NS0	C11-C12-C14	2.37	122.58	118.94
13	X	102	BCB	C4B-CHC-C1C	-2.37	125.43	130.12
13	E	101	BCB	O2D-CGD-O1D	-2.37	119.21	123.84
13	L	303	BCB	O2A-CGA-CBA	2.37	119.33	111.91
13	Z	101	BCB	CHC-C1C-NC	-2.36	121.24	124.51
13	i	101	BCB	C1-O2A-CGA	2.36	122.64	116.44
13	3	101	BCB	C1D-CHD-C4C	-2.36	120.97	126.06
13	E	101	BCB	C4B-CHC-C1C	-2.36	125.44	130.12
13	9	101	BCB	O2A-CGA-CBA	2.36	119.31	111.91
13	4	101	BCB	CHD-C1D-ND	-2.36	122.29	124.45
13	W	302	BCB	C1B-CHB-C4A	-2.36	125.45	130.12
13	X	102	BCB	C2A-C1A-CHA	-2.35	119.74	123.86
17	M	405	MQ7	C19-C18-C20	2.35	119.23	115.27
13	D	101	BCB	C4D-CHA-C1A	-2.35	118.39	121.25
13	i	101	BCB	O2D-CGD-O1D	-2.35	119.24	123.84
13	R	102	BCB	C1-C2-C3	-2.35	121.98	126.04
13	R	102	BCB	O2D-CGD-O1D	-2.34	119.25	123.84
21	A	103	NS0	C16-C17-C19	2.34	122.54	118.94
13	r	101	BCB	C2A-C1A-CHA	-2.34	119.76	123.86
13	J	101	BCB	C1D-CHD-C4C	-2.34	121.00	126.06
13	c	101	BCB	CHD-C1D-ND	-2.34	122.31	124.45
21	l	101	NS0	C11-C12-C14	2.34	122.53	118.94
20	I	102	PGV	O03-C19-C20	2.34	119.24	111.91
21	U	101	NS0	C25-C23-C22	2.33	122.52	118.94
13	D	101	BCB	O2D-CGD-O1D	-2.33	119.27	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	O	101	NS0	C11-C12-C14	2.33	122.52	118.94
13	f	101	BCB	CHD-C4C-C3C	-2.33	122.97	125.89
13	X	102	BCB	C1D-CHD-C4C	-2.33	121.03	126.06
13	0	102	BCB	C4B-CHC-C1C	-2.33	125.50	130.12
13	q	101	BCB	C1D-CHD-C4C	-2.33	121.03	126.06
13	7	102	BCB	O2D-CGD-O1D	-2.33	119.29	123.84
18	M	406	NS5	C16-C15-C17	-2.33	119.67	122.92
17	M	405	MQ7	C2M-C2-C3	-2.33	120.61	124.40
13	3	101	BCB	CHB-C4A-NA	2.32	127.73	124.51
13	1	101	BCB	C2A-C1A-CHA	-2.32	119.80	123.86
13	3	101	BCB	C3D-C4D-ND	2.32	113.99	110.24
15	M	409	CDL	CA4-OA6-CA5	-2.32	112.08	117.79
13	L	303	BCB	CMD-C2D-C3D	-2.32	122.27	127.61
15	H	301	CDL	OB8-CB7-C71	2.32	119.19	111.91
13	Q	402	BCB	C1B-CHB-C4A	-2.32	125.53	130.12
13	W	302	BCB	C3D-C4D-ND	2.32	113.98	110.24
13	o	102	BCB	C2A-C1A-CHA	-2.32	119.81	123.86
21	U	101	NS0	C11-C12-C14	2.31	122.49	118.94
13	Q	402	BCB	CAA-CBA-CGA	-2.31	106.50	113.25
13	J	101	BCB	C1B-CHB-C4A	-2.31	125.54	130.12
13	f	101	BCB	C2A-C1A-CHA	-2.31	119.82	123.86
13	L	302	BCB	C4B-CHC-C1C	-2.31	125.55	130.12
13	B	202	BCB	C1B-CHB-C4A	-2.31	125.55	130.12
21	l	101	NS0	C16-C17-C19	2.31	122.48	118.94
13	M	403	BCB	C1B-CHB-C4A	-2.30	125.56	130.12
13	Z	101	BCB	C1D-CHD-C4C	-2.30	121.11	126.06
13	k	102	BCB	CED-O2D-CGD	2.30	121.13	115.94
13	R	102	BCB	C1B-CHB-C4A	-2.29	125.57	130.12
13	E	101	BCB	C1D-CHD-C4C	-2.29	121.11	126.06
13	M	403	BCB	CED-O2D-CGD	2.29	121.12	115.94
11	A	101	UQ8	C1M-C1-C6	-2.29	120.66	124.40
17	M	405	MQ7	C24-C23-C25	2.29	119.13	115.27
13	Q	402	BCB	CHC-C1C-NC	-2.29	121.35	124.51
13	n	101	BCB	C3D-C4D-ND	2.29	113.94	110.24
13	9	101	BCB	C1B-CHB-C4A	-2.28	125.59	130.12
13	6	101	BCB	C3D-C4D-ND	2.28	113.93	110.24
13	6	101	BCB	C1D-CHD-C4C	-2.28	121.14	126.06
13	X	102	BCB	C4-C3-C5	2.28	119.10	115.27
13	i	101	BCB	C1-C2-C3	-2.27	122.11	126.04
13	k	102	BCB	CAA-CBA-CGA	-2.27	106.61	113.25
9	C	403	HEC	O2D-CGD-CBD	2.27	121.33	114.03
11	M	408	UQ8	C46-C44-C45	2.27	119.61	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	3	101	BCB	C2A-C1A-CHA	-2.27	119.89	123.86
13	J	101	BCB	C2A-C1A-CHA	-2.27	119.89	123.86
13	U	102	BCB	CED-O2D-CGD	2.27	121.06	115.94
21	R	101	NS0	C11-C12-C14	2.27	122.42	118.94
21	l	101	NS0	C25-C23-C22	2.26	122.41	118.94
13	7	102	BCB	C2A-C1A-CHA	-2.26	119.91	123.86
13	7	102	BCB	C4B-CHC-C1C	-2.26	125.64	130.12
13	I	101	BCB	C3D-C4D-ND	2.26	113.89	110.24
13	0	102	BCB	C1B-CHB-C4A	-2.26	125.64	130.12
13	O	102	BCB	C1B-CHB-C4A	-2.26	125.65	130.12
13	Z	101	BCB	C4-C3-C5	2.25	119.06	115.27
13	n	101	BCB	C4-C3-C5	2.25	119.06	115.27
9	C	402	HEC	CMC-C2C-C1C	-2.25	125.00	128.46
9	C	403	HEC	CMC-C2C-C1C	-2.25	125.01	128.46
11	L	305	UQ8	C20-C19-C21	2.25	119.05	115.27
13	T	101	BCB	C4D-CHA-C1A	-2.25	118.52	121.25
21	A	103	NS0	C15-C14-C12	2.25	130.51	127.31
13	k	102	BCB	CHB-C4A-NA	2.25	127.62	124.51
13	M	402	BCB	O2D-CGD-O1D	-2.24	119.45	123.84
13	4	101	BCB	C4B-CHC-C1C	-2.24	125.67	130.12
13	h	102	BCB	C1D-CHD-C4C	-2.24	121.22	126.06
13	Q	402	BCB	C3D-C4D-ND	2.24	113.86	110.24
13	f	101	BCB	C4B-CHC-C1C	-2.24	125.68	130.12
13	T	101	BCB	CHB-C4A-NA	2.24	127.61	124.51
13	U	102	BCB	C1-C2-C3	-2.24	122.17	126.04
13	e	101	BCB	C3D-C4D-ND	2.24	113.86	110.24
13	b	101	BCB	C4A-NA-C1A	2.24	107.71	106.71
13	e	101	BCB	C4B-CHC-C1C	-2.24	125.69	130.12
17	M	405	MQ7	C31-C32-C33	-2.24	122.27	127.66
13	L	302	BCB	O2A-CGA-O1A	-2.24	117.95	123.59
13	e	101	BCB	CAA-CBA-CGA	-2.23	106.72	113.25
21	2	101	NS0	C11-C12-C14	2.23	122.37	118.94
13	o	102	BCB	O2D-CGD-O1D	-2.23	119.47	123.84
11	A	101	UQ8	C7-C6-C5	2.23	121.16	118.48
13	r	101	BCB	CHC-C1C-NC	-2.23	121.43	124.51
21	W	303	NS0	C16-C17-C19	2.23	122.36	118.94
13	M	403	BCB	C4-C3-C5	2.23	119.02	115.27
11	M	408	UQ8	C1M-C1-C6	-2.23	120.77	124.40
13	l	102	BCB	C2A-C1A-CHA	-2.23	119.97	123.86
13	M	402	BCB	O1D-CGD-CBD	-2.23	119.93	124.48
13	i	101	BCB	CHC-C1C-NC	-2.22	121.44	124.51
21	9	102	NS0	C16-C17-C19	2.22	122.35	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	M	409	CDL	OB6-CB5-OB7	-2.22	118.33	123.70
13	c	101	BCB	C4B-CHC-C1C	-2.22	125.72	130.12
13	c	101	BCB	C2A-C1A-CHA	-2.22	119.97	123.86
21	U	101	NS0	C16-C17-C19	2.22	122.35	118.94
13	M	402	BCB	C4B-CHC-C1C	-2.22	125.72	130.12
13	W	302	BCB	C1D-CHD-C4C	-2.22	121.27	126.06
9	C	401	HEC	O2D-CGD-CBD	2.22	121.15	114.03
17	M	405	MQ7	C14-C13-C15	2.21	119.00	115.27
13	e	101	BCB	CED-O2D-CGD	2.21	120.95	115.94
13	M	402	BCB	C4D-CHA-C1A	-2.21	118.55	121.25
13	b	101	BCB	CAA-CBA-CGA	-2.21	106.78	113.25
13	M	402	BCB	C1D-CHD-C4C	-2.21	121.29	126.06
13	Z	101	BCB	C3D-C4D-ND	2.21	113.81	110.24
11	M	407	UQ8	C7-C8-C9	-2.21	123.12	126.79
13	T	101	BCB	CAA-CBA-CGA	-2.20	106.82	113.25
13	M	403	BCB	C1-O2A-CGA	2.20	122.21	116.44
13	h	102	BCB	C2A-C1A-CHA	-2.20	120.02	123.86
13	E	101	BCB	O2A-CGA-O1A	-2.19	118.06	123.59
21	9	102	NS0	C20-C21-C22	2.19	127.97	123.47
13	k	102	BCB	C1D-CHD-C4C	-2.19	121.33	126.06
13	o	102	BCB	C4B-CHC-C1C	-2.19	125.77	130.12
13	T	101	BCB	C3D-C4D-ND	2.19	113.78	110.24
11	M	408	UQ8	C31-C32-C33	-2.19	104.68	111.88
13	b	101	BCB	C2A-C1A-CHA	-2.19	120.03	123.86
13	0	102	BCB	O2A-CGA-O1A	-2.19	118.07	123.59
13	b	101	BCB	C3D-C4D-ND	2.19	113.78	110.24
13	L	303	BCB	C4D-CHA-C1A	-2.19	118.59	121.25
12	L	301	DGA	OG1-CA1-OA1	-2.19	118.08	123.59
15	H	301	CDL	CB4-OB6-CB5	-2.19	112.41	117.79
13	7	102	BCB	C4-C3-C5	2.18	118.93	115.27
9	C	402	HEC	CAD-CBD-CGD	-2.17	107.66	113.76
13	A	102	BCB	O2D-CGD-O1D	-2.17	119.59	123.84
13	k	102	BCB	C3D-C4D-ND	2.17	113.75	110.24
11	M	408	UQ8	C32-C33-C34	-2.17	122.43	127.66
21	h	101	NS0	C16-C17-C19	2.17	122.28	118.94
13	b	101	BCB	C16-C15-C13	-2.17	108.90	115.92
13	L	302	BCB	C4D-CHA-C1A	-2.17	118.61	121.25
19	h	103	LMT	C1B-O1B-C4'	-2.17	112.60	117.96
13	M	403	BCB	CHB-C4A-NA	2.17	127.51	124.51
13	6	101	BCB	C2A-C1A-CHA	-2.16	120.08	123.86
21	X	101	NS0	C25-C23-C22	2.16	122.25	118.94
13	4	101	BCB	C1-C2-C3	-2.16	122.31	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	R	102	BCB	C4B-CHC-C1C	-2.16	125.84	130.12
13	n	101	BCB	C6-C5-C3	-2.16	107.80	113.45
11	A	101	UQ8	C12-C13-C14	-2.16	122.47	127.66
21	0	101	NS0	C20-C21-C22	2.16	127.89	123.47
13	c	101	BCB	C1B-CHB-C4A	-2.15	125.85	130.12
13	e	101	BCB	C4-C3-C5	2.15	118.89	115.27
21	9	102	NS0	C11-C12-C14	2.15	122.24	118.94
13	i	101	BCB	C4B-C3B-CAB	-2.15	122.98	127.13
13	U	102	BCB	O2D-CGD-O1D	-2.15	119.64	123.84
13	h	102	BCB	C4B-CHC-C1C	-2.15	125.87	130.12
15	H	302	CDL	OB8-CB7-C71	2.15	118.64	111.91
13	O	102	BCB	C2A-C1A-CHA	-2.15	120.11	123.86
13	f	101	BCB	O2D-CGD-O1D	-2.15	119.64	123.84
21	2	101	NS0	C16-C17-C19	2.14	122.23	118.94
13	1	101	BCB	C4B-CHC-C1C	-2.14	125.87	130.12
18	M	406	NS5	C18-C17-C15	2.14	130.37	127.31
13	I	101	BCB	CAA-CBA-CGA	-2.14	107.00	113.25
13	n	101	BCB	C4B-CHC-C1C	-2.14	125.88	130.12
13	X	102	BCB	O2D-CGD-O1D	-2.14	119.65	123.84
13	c	101	BCB	C1-C2-C3	-2.14	122.34	126.04
13	c	101	BCB	O2D-CGD-O1D	-2.14	119.66	123.84
21	W	303	NS0	C25-C23-C22	2.14	122.22	118.94
13	9	101	BCB	C11-C10-C8	-2.14	109.01	115.92
13	U	102	BCB	C4B-CHC-C1C	-2.14	125.88	130.12
21	0	101	NS0	C16-C17-C19	2.14	122.22	118.94
13	Q	402	BCB	C4B-CHC-C1C	-2.14	125.88	130.12
21	A	103	NS0	C25-C23-C22	2.14	122.22	118.94
13	B	202	BCB	CHC-C1C-NC	-2.13	121.56	124.51
13	W	302	BCB	CHC-C1C-NC	-2.13	121.56	124.51
13	D	101	BCB	C4B-C3B-CAB	-2.13	123.01	127.13
20	W	301	PGV	O01-C1-O02	-2.13	118.55	123.70
13	e	101	BCB	C6-C5-C3	-2.13	107.86	113.45
13	b	101	BCB	CHC-C1C-NC	-2.13	121.57	124.51
13	B	202	BCB	O2A-CGA-O1A	-2.13	118.22	123.59
13	N	101	BCB	CHB-C4A-NA	2.13	127.46	124.51
13	N	101	BCB	C6-C5-C3	-2.13	107.88	113.45
13	X	102	BCB	CED-O2D-CGD	2.12	120.73	115.94
11	A	101	UQ8	C46-C44-C45	2.12	119.28	114.60
13	J	101	BCB	C4B-CHC-C1C	-2.12	125.92	130.12
13	4	101	BCB	C2A-C1A-CHA	-2.12	120.16	123.86
13	A	102	BCB	CHC-C1C-NC	-2.11	121.59	124.51
13	1	101	BCB	CHC-C1C-NC	-2.11	121.59	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	R	102	BCB	CED-O2D-CGD	2.11	120.71	115.94
21	X	101	NS0	C20-C21-C22	2.11	127.80	123.47
13	f	101	BCB	C1-C2-C3	-2.10	122.41	126.04
15	L	306	CDL	OA8-CA7-OA9	-2.10	118.29	123.59
13	k	102	BCB	C4B-CHC-C1C	-2.10	125.96	130.12
21	O	101	NS0	C20-C21-C22	2.10	127.77	123.47
13	D	101	BCB	C4-C3-C5	2.09	118.79	115.27
13	T	101	BCB	CHC-C1C-NC	-2.09	121.62	124.51
21	9	102	NS0	C25-C23-C22	2.09	122.14	118.94
13	E	101	BCB	C2A-C1A-CHA	-2.09	120.21	123.86
13	9	101	BCB	CED-O2D-CGD	2.09	120.65	115.94
13	L	303	BCB	C1-O2A-CGA	2.08	121.91	116.44
13	3	101	BCB	C11-C10-C8	-2.08	109.19	115.92
13	A	102	BCB	C4-C3-C5	2.08	118.77	115.27
21	7	101	NS0	C25-C23-C22	2.08	122.14	118.94
13	l	102	BCB	O2D-CGD-O1D	-2.08	119.77	123.84
11	M	408	UQ8	C22-C23-C24	-2.08	122.65	127.66
11	A	101	UQ8	C26-C27-C28	-2.08	105.04	111.88
13	J	101	BCB	CED-O2D-CGD	2.08	120.64	115.94
13	h	102	BCB	CED-O2D-CGD	2.08	120.63	115.94
15	r	102	CDL	OB6-CB5-OB7	-2.08	118.69	123.70
13	L	302	BCB	C4B-C3B-CAB	-2.07	123.12	127.13
13	h	102	BCB	CHC-C1C-NC	-2.07	121.65	124.51
15	M	409	CDL	OA6-CA5-OA7	-2.07	118.70	123.70
13	7	102	BCB	O2A-CGA-O1A	-2.07	118.37	123.59
13	I	101	BCB	O2D-CGD-O1D	-2.07	119.80	123.84
13	9	101	BCB	C1D-CHD-C4C	-2.07	121.60	126.06
21	o	101	NS0	C15-C14-C12	2.07	130.26	127.31
13	6	101	BCB	CED-O2D-CGD	2.06	120.61	115.94
20	M	411	PGV	O03-C19-O04	-2.06	118.39	123.59
13	A	102	BCB	CBA-CAA-C2A	-2.06	107.78	113.86
21	o	101	NS0	C16-C17-C19	2.06	122.10	118.94
13	l	102	BCB	C4B-CHC-C1C	-2.06	126.04	130.12
17	M	405	MQ7	C16-C17-C18	-2.06	122.70	127.66
13	n	101	BCB	C1D-CHD-C4C	-2.06	121.62	126.06
13	3	101	BCB	C4B-C3B-CAB	-2.06	123.16	127.13
13	3	101	BCB	CED-O2D-CGD	2.06	120.59	115.94
11	M	408	UQ8	C37-C38-C39	-2.06	122.71	127.66
13	e	101	BCB	C1D-CHD-C4C	-2.06	121.62	126.06
13	6	101	BCB	C4A-NA-C1A	2.05	107.63	106.71
13	Q	402	BCB	C4B-C3B-CAB	-2.05	123.17	127.13
21	2	101	NS0	C20-C21-C22	2.05	127.67	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	O	102	BCB	C4B-CHC-C1C	-2.05	126.06	130.12
13	W	302	BCB	C2A-C1A-CHA	-2.04	120.28	123.86
13	1	101	BCB	C4B-C3B-CAB	-2.04	123.18	127.13
13	7	102	BCB	CED-O2D-CGD	2.04	120.56	115.94
13	D	101	BCB	CHC-C1C-NC	-2.04	121.69	124.51
21	W	303	NS0	C11-C12-C14	2.04	122.07	118.94
13	9	101	BCB	CMD-C2D-C3D	-2.04	122.92	127.61
13	i	101	BCB	C4B-CHC-C1C	-2.04	126.08	130.12
9	C	402	HEC	CMB-C2B-C1B	-2.04	125.33	128.46
13	f	101	BCB	CED-O2D-CGD	2.03	120.54	115.94
13	J	101	BCB	CHC-C1C-NC	-2.03	121.70	124.51
13	Z	101	BCB	CED-O2D-CGD	2.03	120.54	115.94
15	r	102	CDL	OB8-CB7-C71	2.03	118.28	111.91
21	o	101	NS0	C11-C12-C14	2.03	122.06	118.94
13	q	101	BCB	CED-O2D-CGD	2.03	120.53	115.94
13	3	101	BCB	C4-C3-C5	2.03	118.68	115.27
13	X	102	BCB	C6-C5-C3	-2.03	108.14	113.45
13	n	101	BCB	C2A-C1A-CHA	-2.02	120.32	123.86
21	h	101	NS0	C25-C23-C22	2.02	122.04	118.94
21	D	103	NS0	C25-C23-C22	2.02	122.04	118.94
13	U	102	BCB	CAA-CBA-CGA	-2.02	107.35	113.25
13	i	101	BCB	C16-C15-C13	-2.02	109.39	115.92
11	M	408	UQ8	C40-C39-C41	2.02	118.67	115.27
13	N	101	BCB	C3D-C4D-ND	2.02	113.50	110.24
13	J	101	BCB	O2D-CGD-O1D	-2.02	119.89	123.84
13	9	101	BCB	C4B-CHC-C1C	-2.01	126.13	130.12
15	M	409	CDL	CB6-CB4-CB3	-2.01	107.04	111.79
13	U	102	BCB	CHC-C1C-NC	-2.01	121.73	124.51
13	r	101	BCB	C4B-C3B-CAB	-2.01	123.25	127.13
15	L	306	CDL	OB6-CB5-OB7	-2.00	118.86	123.70
13	f	101	BCB	CHC-C1C-NC	-2.00	121.74	124.51
13	M	402	BCB	CMD-C2D-C3D	-2.00	123.01	127.61
13	L	303	BCB	CHC-C1C-NC	-2.00	121.75	124.51

All (76) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	L	302	BCB	NC
13	L	302	BCB	NA
13	L	303	BCB	NC
13	L	303	BCB	NA
13	M	402	BCB	NC

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Mol	Chain	Res	Type	Atom
13	M	402	BCB	NA
13	M	403	BCB	NC
13	M	403	BCB	NA
13	A	102	BCB	NC
13	A	102	BCB	NA
13	B	202	BCB	NC
13	B	202	BCB	NA
13	D	101	BCB	NC
13	D	101	BCB	NA
13	E	101	BCB	NC
13	E	101	BCB	NA
13	I	101	BCB	NC
13	I	101	BCB	NA
13	J	101	BCB	NC
13	J	101	BCB	NA
13	N	101	BCB	NC
13	N	101	BCB	NA
13	O	102	BCB	NC
13	O	102	BCB	NA
13	Q	402	BCB	NC
13	Q	402	BCB	NA
13	R	102	BCB	NC
13	R	102	BCB	NA
13	T	101	BCB	NC
13	T	101	BCB	NA
13	U	102	BCB	NC
13	U	102	BCB	NA
13	W	302	BCB	NC
13	W	302	BCB	NA
13	X	102	BCB	NC
13	X	102	BCB	NA
13	Z	101	BCB	NC
13	Z	101	BCB	NA
13	1	101	BCB	NC
13	1	101	BCB	NA
13	3	101	BCB	NC
13	3	101	BCB	NA
13	4	101	BCB	NC
13	4	101	BCB	NA
13	6	101	BCB	NC
13	6	101	BCB	NA
13	7	102	BCB	NC

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

All (884) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	402	HEC	C3D-CAD-CBD-CGD
11	M	408	UQ8	C29-C31-C32-C33
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

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Mol	Chain	Res	Type	Atoms
13	E	101	BCB	C14-C13-C15-C16
13	J	101	BCB	CHA-CBD-CGD-O1D
13	J	101	BCB	CHA-CBD-CGD-O2D
13	O	102	BCB	CHA-CBD-CGD-O1D
13	O	102	BCB	CHA-CBD-CGD-O2D
13	Q	402	BCB	CBD-CGD-O2D-CED
13	Q	402	BCB	C14-C13-C15-C16
13	R	102	BCB	CHA-CBD-CGD-O1D
13	R	102	BCB	CHA-CBD-CGD-O2D
13	W	302	BCB	CBD-CGD-O2D-CED
13	X	102	BCB	CHA-CBD-CGD-O1D
13	X	102	BCB	CHA-CBD-CGD-O2D
13	Z	101	BCB	CBD-CGD-O2D-CED
13	1	101	BCB	CHA-CBD-CGD-O1D
13	1	101	BCB	CHA-CBD-CGD-O2D
13	3	101	BCB	CBD-CGD-O2D-CED
13	4	101	BCB	CHA-CBD-CGD-O1D
13	4	101	BCB	CHA-CBD-CGD-O2D
13	7	102	BCB	C1A-C2A-CAA-CBA
13	7	102	BCB	CHA-CBD-CGD-O1D
13	7	102	BCB	CHA-CBD-CGD-O2D
13	b	101	BCB	CBD-CGD-O2D-CED
13	b	101	BCB	C2-C3-C5-C6
13	b	101	BCB	C4-C3-C5-C6
13	c	101	BCB	CHA-CBD-CGD-O1D
13	c	101	BCB	CHA-CBD-CGD-O2D
13	f	101	BCB	CHA-CBD-CGD-O1D
13	f	101	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	CHA-CBD-CGD-O1D
13	i	101	BCB	C11-C12-C13-C14
13	k	102	BCB	CBD-CGD-O2D-CED
13	o	102	BCB	CHA-CBD-CGD-O1D
13	o	102	BCB	CHA-CBD-CGD-O2D
13	q	101	BCB	C1A-C2A-CAA-CBA
13	q	101	BCB	C3A-C2A-CAA-CBA
13	r	101	BCB	C1A-C2A-CAA-CBA
13	r	101	BCB	CHA-CBD-CGD-O1D
13	r	101	BCB	CHA-CBD-CGD-O2D
14	L	304	BPB	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
15	L	306	CDL	O1-C1-CB2-OB2
15	H	301	CDL	CA2-OA2-PA1-OA3
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
15	H	302	CDL	CA2-OA2-PA1-OA4
15	H	302	CDL	CB2-OB2-PB2-OB3
15	H	302	CDL	CB2-OB2-PB2-OB4
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	CB3-OB5-PB2-OB2
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	b	102	LMT	C2-C1-O1'-C1'
19	k	103	LMT	O5'-C1'-O1'-C1
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	I	102	PGV	C04-O12-P-O11
20	I	102	PGV	C04-O12-P-O13
20	I	102	PGV	C04-O12-P-O14
20	Q	401	PGV	C04-O12-P-O13
20	W	301	PGV	C03-O11-P-O12
20	W	301	PGV	C04-O12-P-O14
21	R	101	NS0	C29-C28-C30-C31
21	R	101	NS0	C27-C28-C30-C31
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	n	101	BCB	CBD-CGD-O2D-CED
13	q	101	BCB	CBD-CGD-O2D-CED
13	Z	101	BCB	O1D-CGD-O2D-CED
13	Q	402	BCB	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	3	101	BCB	O1D-CGD-O2D-CED
13	h	102	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
13	W	302	BCB	O1D-CGD-O2D-CED
13	k	102	BCB	O1D-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
15	H	302	CDL	C11-CA5-OA6-CA4
13	b	101	BCB	O1D-CGD-O2D-CED
13	J	101	BCB	CBD-CGD-O2D-CED
13	o	102	BCB	CBD-CGD-O2D-CED
19	n	102	LMT	O5B-C5B-C6B-O6B
13	M	403	BCB	C2A-CAA-CBA-CGA
13	T	101	BCB	O1D-CGD-O2D-CED
13	6	101	BCB	O1D-CGD-O2D-CED
13	9	101	BCB	O1D-CGD-O2D-CED
12	L	301	DGA	OA1-CA1-OG1-CG1
19	b	103	LMT	O5'-C5'-C6'-O6'
13	e	101	BCB	O1D-CGD-O2D-CED
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	i	101	BCB	C3-C5-C6-C7
13	r	101	BCB	C3-C5-C6-C7
20	Q	401	PGV	C2-C1-O01-C02
13	X	102	BCB	CBD-CGD-O2D-CED
13	r	101	BCB	CBD-CGD-O2D-CED
19	M	410	LMT	O5'-C5'-C6'-O6'
13	q	101	BCB	O1D-CGD-O2D-CED
13	q	101	BCB	C8-C10-C11-C12
12	L	301	DGA	CA2-CA1-OG1-CG1
20	Q	401	PGV	O02-C1-O01-C02
13	L	303	BCB	C13-C15-C16-C17
13	L	302	BCB	C4-C3-C5-C6
18	M	406	NS5	C11-C10-C9-C8
21	q	102	NS0	C29-C28-C30-C31
13	L	302	BCB	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
18	M	406	NS5	C12-C10-C9-C8
21	q	102	NS0	C27-C28-C30-C31
19	n	102	LMT	C4B-C5B-C6B-O6B
11	L	305	UQ8	C14-C16-C17-C18
11	M	408	UQ8	C39-C41-C42-C43
11	A	101	UQ8	C19-C21-C22-C23
15	r	102	CDL	C31-CA7-OA8-CA6
13	A	102	BCB	O1D-CGD-O2D-CED
13	n	101	BCB	O1D-CGD-O2D-CED
15	r	102	CDL	OA9-CA7-OA8-CA6
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	6	101	BCB	C15-C16-C17-C18
13	I	101	BCB	O1D-CGD-O2D-CED
13	D	101	BCB	C15-C16-C17-C18
13	E	101	BCB	C10-C11-C12-C13
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	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
13	N	101	BCB	O1D-CGD-O2D-CED
13	X	102	BCB	C13-C15-C16-C17
13	n	101	BCB	C13-C15-C16-C17
21	O	101	NS0	C10-C11-C12-C13
15	M	409	CDL	C11-CA5-OA6-CA4
20	Q	401	PGV	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
13	J	101	BCB	C8-C10-C11-C12
19	b	103	LMT	C4'-C5'-C6'-O6'
13	A	102	BCB	C5-C6-C7-C8
13	D	101	BCB	C13-C15-C16-C17
13	I	101	BCB	C13-C15-C16-C17
13	Q	402	BCB	C13-C15-C16-C17
13	Q	402	BCB	C15-C16-C17-C18
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	r	101	BCB	C13-C15-C16-C17
19	b	102	LMT	O5B-C5B-C6B-O6B
15	L	306	CDL	CA5-C11-C12-C13
13	E	101	BCB	C8-C10-C11-C12
13	T	101	BCB	C10-C11-C12-C13
13	e	101	BCB	C5-C6-C7-C8
13	r	101	BCB	C8-C10-C11-C12
15	r	102	CDL	CA7-C31-C32-C33
13	A	102	BCB	C15-C16-C17-C18
21	0	101	NS0	C33-C35-C36-C37
15	r	102	CDL	C71-CB7-OB8-CB6
20	W	301	PGV	C27-C28-C29-C30
13	9	101	BCB	C2-C1-O2A-CGA
13	D	101	BCB	O1D-CGD-O2D-CED
15	r	102	CDL	C11-CA5-OA6-CA4
13	k	102	BCB	C13-C15-C16-C17
13	A	102	BCB	C12-C13-C15-C16
13	0	102	BCB	C11-C12-C13-C15
13	M	402	BCB	C15-C16-C17-C18
13	R	102	BCB	C10-C11-C12-C13
13	E	101	BCB	C13-C15-C16-C17
11	M	408	UQ8	C19-C21-C22-C23
11	A	101	UQ8	C14-C16-C17-C18
15	H	301	CDL	CB5-C51-C52-C53
15	H	301	CDL	O1-C1-CA2-OA2
15	H	302	CDL	O1-C1-CA2-OA2
13	W	302	BCB	C5-C6-C7-C8
13	1	101	BCB	C8-C10-C11-C12
13	r	101	BCB	C10-C11-C12-C13
19	B	201	LMT	O1'-C1-C2-C3
13	D	101	BCB	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
13	R	102	BCB	C8-C10-C11-C12
13	X	102	BCB	C15-C16-C17-C18
13	4	101	BCB	C10-C11-C12-C13
13	7	102	BCB	C5-C6-C7-C8
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	9	101	BCB	C10-C11-C12-C13
15	M	409	CDL	CA2-OA2-PA1-OA5
15	H	301	CDL	CA3-OA5-PA1-OA2
15	H	302	CDL	CA2-OA2-PA1-OA5
15	H	302	CDL	CA3-OA5-PA1-OA2
15	H	302	CDL	CB2-OB2-PB2-OB5
15	r	102	CDL	CB2-OB2-PB2-OB5
20	M	411	PGV	C03-O11-P-O12
20	D	102	PGV	C04-O12-P-O11
20	I	102	PGV	C03-O11-P-O12
20	N	102	PGV	C04-O12-P-O11
20	W	301	PGV	C04-O12-P-O11
20	M	411	PGV	C1-C2-C3-C4
13	J	101	BCB	O1D-CGD-O2D-CED
15	M	409	CDL	CB2-C1-CA2-OA2
15	H	301	CDL	CB2-C1-CA2-OA2
15	H	302	CDL	CB2-C1-CA2-OA2
15	M	409	CDL	OA7-CA5-OA6-CA4
15	r	102	CDL	OA7-CA5-OA6-CA4
19	M	410	LMT	C4'-C5'-C6'-O6'
13	A	102	BCB	CBA-CGA-O2A-C1
20	W	301	PGV	C2-C1-O01-C02
15	L	306	CDL	C79-C80-C81-C82
15	M	409	CDL	C13-C14-C15-C16
15	r	102	CDL	C53-C54-C55-C56
13	o	102	BCB	O1D-CGD-O2D-CED
13	M	402	BCB	C16-C17-C18-C20
13	c	101	BCB	C8-C10-C11-C12
15	H	301	CDL	C13-C14-C15-C16
15	H	301	CDL	C53-C54-C55-C56
15	r	102	CDL	O1-C1-CA2-OA2
15	H	301	CDL	C32-C33-C34-C35
13	N	101	BCB	C16-C17-C18-C19
13	7	102	BCB	C4-C3-C5-C6
21	O	101	NS0	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
13	7	102	BCB	C2-C3-C5-C6
13	L	303	BCB	C14-C13-C15-C16
13	M	402	BCB	C11-C10-C8-C9
13	M	402	BCB	C14-C13-C15-C16
15	H	302	CDL	CB5-C51-C52-C53
13	X	102	BCB	C10-C11-C12-C13
15	r	102	CDL	OB9-CB7-OB8-CB6
12	L	301	DGA	CB2-CB3-CB4-CB5
15	L	306	CDL	C11-C12-C13-C14
20	N	102	PGV	C04-C05-C06-O06
20	W	301	PGV	C04-C05-C06-O06
21	O	101	NS0	C10-C11-C12-C14
20	W	301	PGV	O02-C1-O01-C02
13	7	102	BCB	CBD-CGD-O2D-CED
15	H	301	CDL	C33-C34-C35-C36
19	M	410	LMT	C3-C4-C5-C6
19	b	102	LMT	C7-C8-C9-C10
20	M	411	PGV	C3-C4-C5-C6
20	M	411	PGV	C7-C8-C9-C10
13	N	101	BCB	C16-C17-C18-C20
13	O	102	BCB	C16-C17-C18-C19
13	O	102	BCB	C16-C17-C18-C20
13	9	101	BCB	C16-C17-C18-C20
13	f	101	BCB	C16-C17-C18-C20
12	L	301	DGA	CA2-CA3-CA4-CA5
20	N	102	PGV	C6-C7-C8-C9
20	Q	401	PGV	C6-C7-C8-C9
13	i	101	BCB	C13-C15-C16-C17
13	A	102	BCB	O1A-CGA-O2A-C1
20	Q	401	PGV	C5-C6-C7-C8
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	M	402	BCB	C16-C17-C18-C19
19	B	201	LMT	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
15	L	306	CDL	C51-CB5-OB6-CB4
15	H	301	CDL	C51-CB5-OB6-CB4
19	B	201	LMT	C1-C2-C3-C4
13	W	302	BCB	C13-C15-C16-C17
13	f	101	BCB	C16-C17-C18-C19
15	M	409	CDL	OB7-CB5-OB6-CB4
13	M	403	BCB	C2-C1-O2A-CGA
15	H	302	CDL	C59-C60-C61-C62
20	W	301	PGV	C26-C27-C28-C29
15	H	301	CDL	CA5-C11-C12-C13
13	9	101	BCB	CBA-CGA-O2A-C1
13	N	101	BCB	C13-C15-C16-C17
13	k	102	BCB	C10-C11-C12-C13
19	b	102	LMT	C1-C2-C3-C4
15	M	409	CDL	C51-CB5-OB6-CB4
15	M	409	CDL	C12-C13-C14-C15
19	M	410	LMT	C4-C5-C6-C7
13	o	102	BCB	C13-C15-C16-C17
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	J	101	BCB	C6-C7-C8-C10
13	N	101	BCB	C11-C12-C13-C15
13	X	102	BCB	C12-C13-C15-C16
13	4	101	BCB	C11-C10-C8-C7
13	7	102	BCB	C6-C7-C8-C10
13	c	101	BCB	C6-C7-C8-C10
13	i	101	BCB	C11-C12-C13-C15
13	T	101	BCB	C3-C5-C6-C7
13	1	101	BCB	C16-C17-C18-C19
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
20	D	102	PGV	C1-C2-C3-C4
20	D	102	PGV	C28-C29-C30-C31
13	X	102	BCB	O1D-CGD-O2D-CED
13	N	101	BCB	C5-C6-C7-C8
13	1	101	BCB	C13-C15-C16-C17
13	3	101	BCB	C15-C16-C17-C18
19	n	102	LMT	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
13	E	101	BCB	C5-C6-C7-C8
13	N	101	BCB	C3-C5-C6-C7
13	U	102	BCB	C10-C11-C12-C13
15	r	102	CDL	C33-C34-C35-C36
15	L	306	CDL	C11-CA5-OA6-CA4
15	H	301	CDL	C11-CA5-OA6-CA4
20	I	102	PGV	C2-C1-O01-C02
19	B	201	LMT	C2-C3-C4-C5
13	J	101	BCB	C15-C16-C17-C18
15	H	301	CDL	C51-C52-C53-C54
15	H	302	CDL	C51-C52-C53-C54
20	N	102	PGV	C5-C6-C7-C8
15	M	409	CDL	OB6-CB4-CB6-OB8
15	L	306	CDL	C32-C33-C34-C35
19	b	102	LMT	C11-C10-C9-C8
19	T	102	LMT	O5'-C5'-C6'-O6'
13	A	102	BCB	C14-C13-C15-C16
13	I	101	BCB	C14-C13-C15-C16
13	N	101	BCB	C11-C10-C8-C9
21	W	303	NS0	CA-CB-CG-CD1
15	H	302	CDL	C35-C36-C37-C38
13	9	101	BCB	O1A-CGA-O2A-C1
13	O	102	BCB	C1A-C2A-CAA-CBA
13	0	102	BCB	C1A-C2A-CAA-CBA
13	o	102	BCB	C1A-C2A-CAA-CBA
13	9	101	BCB	C16-C17-C18-C19
13	E	101	BCB	C15-C16-C17-C18
15	H	302	CDL	CB3-OB5-PB2-OB2
19	b	103	LMT	C1-C2-C3-C4
15	L	306	CDL	OA5-CA3-CA4-CA6
15	r	102	CDL	OB5-CB3-CB4-CB6
19	M	410	LMT	C2-C3-C4-C5
13	f	101	BCB	C15-C16-C17-C18
15	r	102	CDL	CA2-C1-CB2-OB2
20	W	301	PGV	C2-C3-C4-C5
20	D	102	PGV	C20-C21-C22-C23
15	M	409	CDL	CB3-CB4-CB6-OB8
15	H	302	CDL	CA3-CA4-CA6-OA8
15	H	302	CDL	CB3-CB4-CB6-OB8
15	H	302	CDL	C58-C59-C60-C61
15	r	102	CDL	C12-C13-C14-C15
13	l	102	BCB	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
15	H	301	CDL	C22-C23-C24-C25
15	H	302	CDL	C53-C54-C55-C56
13	c	101	BCB	C5-C6-C7-C8
15	L	306	CDL	C41-C42-C43-C44
12	L	301	DGA	CB3-CB4-CB5-CB6
20	W	301	PGV	O05-C05-C06-O06
20	W	301	PGV	C20-C21-C22-C23
19	k	103	LMT	C5-C6-C7-C8
15	H	301	CDL	C71-CB7-OB8-CB6
15	M	409	CDL	C40-C41-C42-C43
13	R	102	BCB	C13-C15-C16-C17
13	U	102	BCB	C13-C15-C16-C17
13	3	101	BCB	C13-C15-C16-C17
13	r	101	BCB	O1D-CGD-O2D-CED
12	L	301	DGA	CA5-CA6-CA7-CA8
20	M	411	PGV	C26-C27-C28-C29
13	7	102	BCB	CBA-CGA-O2A-C1
15	M	409	CDL	C31-CA7-OA8-CA6
21	q	102	NS0	C36-C37-C38-C39
13	e	101	BCB	C13-C15-C16-C17
13	f	101	BCB	C13-C15-C16-C17
13	l	102	BCB	C13-C15-C16-C17
20	Q	401	PGV	C15-C16-C17-C18
13	n	101	BCB	C15-C16-C17-C18
13	1	101	BCB	C16-C17-C18-C20
11	M	408	UQ8	C15-C14-C16-C17
21	U	101	NS0	C31-C32-C33-C34
11	M	408	UQ8	C13-C14-C16-C17
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	7	102	BCB	C11-C12-C13-C15
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

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Mol	Chain	Res	Type	Atoms
13	N	101	BCB	C14-C13-C15-C16
13	O	102	BCB	C14-C13-C15-C16
13	W	302	BCB	C14-C13-C15-C16
13	3	101	BCB	C11-C10-C8-C9
13	e	101	BCB	C11-C10-C8-C9
13	i	101	BCB	C14-C13-C15-C16
14	M	404	BPB	C11-C10-C8-C9
15	L	306	CDL	C53-C54-C55-C56
15	r	102	CDL	CB2-C1-CA2-OA2
15	M	409	CDL	C71-CB7-OB8-CB6
13	6	101	BCB	C8-C10-C11-C12
13	O	102	BCB	C13-C15-C16-C17
13	3	101	BCB	C4-C3-C5-C6
21	X	101	NS0	C34-C33-C35-C36
15	L	306	CDL	C72-C73-C74-C75
13	7	102	BCB	C8-C10-C11-C12
11	A	101	UQ8	C31-C32-C33-C34
19	h	103	LMT	O1'-C1-C2-C3
21	W	303	NS0	CA-CB-CG-CD2
15	L	306	CDL	C52-C53-C54-C55
13	O	102	BCB	C15-C16-C17-C18
13	N	101	BCB	C8-C10-C11-C12
20	I	102	PGV	O03-C01-C02-C03
15	r	102	CDL	C34-C35-C36-C37
15	H	301	CDL	C54-C55-C56-C57
15	M	409	CDL	OA9-CA7-OA8-CA6
21	U	101	NS0	CA-C-C7-C8
13	A	102	BCB	C10-C11-C12-C13
13	4	101	BCB	C15-C16-C17-C18
15	H	302	CDL	CA7-C31-C32-C33
20	N	102	PGV	O05-C05-C06-O06
15	L	306	CDL	OA5-CA3-CA4-OA6
13	c	101	BCB	CBA-CGA-O2A-C1
13	7	102	BCB	O1A-CGA-O2A-C1
15	M	409	CDL	C77-C78-C79-C80
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
13	b	101	BCB	C16-C17-C18-C20
20	D	102	PGV	O12-C04-C05-C06
19	B	201	LMT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
21	R	101	NS0	CA-C-C7-C8
21	R	101	NS0	CA-C-C7-C9
21	U	101	NS0	CA-C-C7-C9
21	X	101	NS0	C32-C33-C35-C36
13	M	403	BCB	C14-C13-C15-C16
13	7	102	BCB	C11-C10-C8-C9
13	k	102	BCB	C11-C10-C8-C9
15	L	306	CDL	C1-CB2-OB2-PB2
15	r	102	CDL	C1-CB2-OB2-PB2
19	k	103	LMT	C1-C2-C3-C4
15	H	302	CDL	C11-C12-C13-C14
15	r	102	CDL	C32-C33-C34-C35
20	M	411	PGV	C23-C24-C25-C26
20	Q	401	PGV	C27-C28-C29-C30
15	H	301	CDL	OB9-CB7-OB8-CB6
15	H	301	CDL	C40-C41-C42-C43
14	M	404	BPB	C13-C15-C16-C17
20	Q	401	PGV	C26-C27-C28-C29
20	N	102	PGV	C01-C02-C03-O11
15	H	301	CDL	C34-C35-C36-C37
13	L	302	BCB	C12-C13-C15-C16
13	M	403	BCB	C12-C13-C15-C16
13	B	202	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	o	102	BCB	C12-C13-C15-C16
13	q	101	BCB	C11-C10-C8-C7
13	Z	101	BCB	C10-C11-C12-C13
13	X	102	BCB	C16-C17-C18-C20
13	U	102	BCB	C15-C16-C17-C18
13	6	101	BCB	C16-C17-C18-C19
21	q	102	NS0	C36-C37-C38-C40
15	r	102	CDL	C36-C37-C38-C39
13	7	102	BCB	O1D-CGD-O2D-CED
13	T	101	BCB	C13-C15-C16-C17
15	H	302	CDL	CA6-CA4-OA6-CA5
15	r	102	CDL	CA6-CA4-OA6-CA5
21	A	103	NS0	C26-C27-C28-C29
21	U	101	NS0	C8-C7-C9-C10

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Mol	Chain	Res	Type	Atoms
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
21	o	101	NS0	C26-C27-C28-C29
13	J	101	BCB	C13-C15-C16-C17
11	M	408	UQ8	C30-C29-C31-C32
21	0	101	NS0	CA-C-C7-C8
21	9	102	NS0	CA-C-C7-C9
15	r	102	CDL	C1-CA2-OA2-PA1
15	H	302	CDL	OB5-CB3-CB4-OB6
20	N	102	PGV	O01-C02-C03-O11
13	6	101	BCB	C16-C17-C18-C20
13	U	102	BCB	CHA-CBD-CGD-O1D
13	i	101	BCB	CHA-CBD-CGD-O2D
13	l	102	BCB	CHA-CBD-CGD-O1D
15	M	409	CDL	OB9-CB7-OB8-CB6
15	M	409	CDL	C16-C17-C18-C19
15	H	302	CDL	OA6-CA4-CA6-OA8
21	R	101	NS0	C34-C33-C35-C36
21	9	102	NS0	CA-C-C7-C8
21	o	101	NS0	C34-C33-C35-C36
13	q	101	BCB	O1A-CGA-O2A-C1
21	0	101	NS0	CA-C-C7-C9
19	h	103	LMT	C7-C8-C9-C10
13	B	202	BCB	C14-C13-C15-C16
13	q	101	BCB	C11-C10-C8-C9
13	c	101	BCB	O1A-CGA-O2A-C1
15	M	409	CDL	C60-C61-C62-C63
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
13	e	101	BCB	C16-C17-C18-C20
15	L	306	CDL	CB3-OB5-PB2-OB2
15	H	301	CDL	CA2-OA2-PA1-OA5
15	r	102	CDL	CA3-OA5-PA1-OA2
20	Q	401	PGV	C04-O12-P-O11
15	M	409	CDL	C73-C74-C75-C76
15	H	302	CDL	C12-C13-C14-C15
11	M	408	UQ8	C40-C39-C41-C42

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Mol	Chain	Res	Type	Atoms
21	U	101	NS0	C34-C33-C35-C36
21	2	101	NS0	CA-C-C7-C8
21	7	101	NS0	C34-C33-C35-C36
19	b	103	LMT	O1'-C1-C2-C3
15	M	409	CDL	CA2-OA2-PA1-OA3
15	H	301	CDL	CA3-OA5-PA1-OA3
15	H	302	CDL	CA3-OA5-PA1-OA3
15	H	302	CDL	CB3-OB5-PB2-OB3
15	r	102	CDL	CB2-OB2-PB2-OB3
15	r	102	CDL	CB3-OB5-PB2-OB4
20	D	102	PGV	C04-O12-P-O13
20	I	102	PGV	C03-O11-P-O13
20	N	102	PGV	C04-O12-P-O14
20	Q	401	PGV	C04-O12-P-O14
20	W	301	PGV	C03-O11-P-O14
19	b	103	LMT	C2-C3-C4-C5
13	q	101	BCB	CBA-CGA-O2A-C1
15	r	102	CDL	C13-C14-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
19	n	102	LMT	C5-C6-C7-C8
20	N	102	PGV	C19-C20-C21-C22
15	r	102	CDL	C54-C55-C56-C57
15	H	301	CDL	C44-C45-C46-C47
13	o	102	BCB	CBA-CGA-O2A-C1
20	Q	401	PGV	C28-C29-C30-C31
9	C	404	HEC	C3D-CAD-CBD-CGD
11	M	408	UQ8	C38-C39-C41-C42
13	A	102	BCB	C11-C12-C13-C15
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	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
15	M	409	CDL	OA5-CA3-CA4-OA6
21	R	101	NS0	C32-C33-C35-C36
21	2	101	NS0	C26-C27-C28-C30
21	7	101	NS0	C26-C27-C28-C30
15	H	301	CDL	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
15	r	102	CDL	C11-C12-C13-C14
13	0	102	BCB	C10-C11-C12-C13
19	M	410	LMT	C9-C10-C11-C12
15	H	302	CDL	C57-C58-C59-C60
19	b	102	LMT	C4B-C5B-C6B-O6B
13	4	101	BCB	C13-C15-C16-C17
15	L	306	CDL	OB6-CB4-CB6-OB8
15	H	301	CDL	C21-C22-C23-C24
13	o	102	BCB	O1A-CGA-O2A-C1
21	X	101	NS0	CA-C-C7-C8
21	7	101	NS0	CA-C-C7-C8
21	l	101	NS0	C34-C33-C35-C36
13	L	302	BCB	C14-C13-C15-C16
13	T	101	BCB	C14-C13-C15-C16
13	f	101	BCB	C11-C10-C8-C9
13	f	101	BCB	C11-C12-C13-C14
13	b	101	BCB	C16-C17-C18-C19
13	N	101	BCB	C15-C16-C17-C18
13	I	101	BCB	C3-C5-C6-C7
11	L	305	UQ8	C5-C4-O4-C4M
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
20	I	102	PGV	C2-C3-C4-C5
21	7	101	NS0	C32-C33-C35-C36
21	o	101	NS0	C32-C33-C35-C36
15	L	306	CDL	C81-C82-C83-C84
20	D	102	PGV	C03-C02-O01-C1
15	M	409	CDL	OA5-CA3-CA4-CA6
20	W	301	PGV	O12-C04-C05-C06
13	D	101	BCB	C2-C1-O2A-CGA
13	N	101	BCB	C2-C1-O2A-CGA
13	7	102	BCB	C2-C1-O2A-CGA
13	e	101	BCB	C2-C1-O2A-CGA
13	O	102	BCB	C10-C11-C12-C13
21	O	101	NS0	CA-C-C7-C8
21	l	101	NS0	CA-C-C7-C8
11	M	408	UQ8	C28-C29-C31-C32
19	B	201	LMT	C3-C4-C5-C6
13	X	102	BCB	C8-C10-C11-C12
15	L	306	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
15	L	306	CDL	CA3-OA5-PA1-OA2
15	L	306	CDL	CB2-OB2-PB2-OB5
15	M	409	CDL	CB2-OB2-PB2-OB5
15	H	301	CDL	CB3-CB4-CB6-OB8
15	r	102	CDL	CB3-CB4-CB6-OB8
21	k	101	NS0	CA-C-C7-C8
13	f	101	BCB	C11-C10-C8-C7
21	2	101	NS0	CA-C-C7-C9
13	b	101	BCB	C11-C12-C13-C14
13	f	101	BCB	C14-C13-C15-C16
13	o	102	BCB	C14-C13-C15-C16
15	H	302	CDL	C32-C33-C34-C35
21	O	101	NS0	C31-C32-C33-C35
13	3	101	BCB	C2-C3-C5-C6
13	X	102	BCB	C16-C17-C18-C19
20	W	301	PGV	C11-C10-C9-C8
19	b	102	LMT	C6-C7-C8-C9
19	h	103	LMT	C9-C10-C11-C12
13	M	403	BCB	C15-C16-C17-C18
20	N	102	PGV	C1-C2-C3-C4
13	A	102	BCB	C4-C3-C5-C6
21	D	103	NS0	C34-C33-C35-C36
20	M	411	PGV	C25-C26-C27-C28
15	M	409	CDL	C62-C63-C64-C65
13	T	101	BCB	C2-C1-O2A-CGA
13	W	302	BCB	C2-C1-O2A-CGA
20	I	102	PGV	C1-C2-C3-C4
13	E	101	BCB	C3A-C2A-CAA-CBA
13	J	101	BCB	C3A-C2A-CAA-CBA
13	1	101	BCB	C3A-C2A-CAA-CBA
11	A	101	UQ8	C5-C4-O4-C4M
20	Q	401	PGV	C14-C15-C16-C17
13	X	102	BCB	CBA-CGA-O2A-C1
21	9	102	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
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
20	D	102	PGV	C29-C30-C31-C32
20	Q	401	PGV	C29-C30-C31-C32
20	W	301	PGV	C22-C23-C24-C25
12	L	301	DGA	OG1-CG1-CG2-CG3
15	H	301	CDL	C61-C62-C63-C64
13	f	101	BCB	CBA-CGA-O2A-C1
13	f	101	BCB	C8-C10-C11-C12
13	q	101	BCB	C5-C6-C7-C8
21	2	101	NS0	C34-C33-C35-C36
21	k	101	NS0	C34-C33-C35-C36
13	E	101	BCB	C1A-C2A-CAA-CBA
13	J	101	BCB	C1A-C2A-CAA-CBA
13	1	101	BCB	C1A-C2A-CAA-CBA
13	4	101	BCB	C1A-C2A-CAA-CBA
13	c	101	BCB	C1A-C2A-CAA-CBA
13	l	102	BCB	C1A-C2A-CAA-CBA
13	W	302	BCB	C12-C13-C15-C16
21	X	101	NS0	CA-C-C7-C9
21	h	101	NS0	C35-C36-C37-C38
9	C	401	HEC	CAA-CBA-CGA-O1A
9	C	402	HEC	CAA-CBA-CGA-O1A
11	L	305	UQ8	C3-C4-O4-C4M
15	M	409	CDL	C63-C64-C65-C66
20	D	102	PGV	C3-C4-C5-C6
13	B	202	BCB	C13-C15-C16-C17
13	O	102	BCB	C3-C5-C6-C7
13	0	102	BCB	C5-C6-C7-C8
20	M	411	PGV	C6-C7-C8-C9
15	H	302	CDL	OB5-CB3-CB4-CB6
20	I	102	PGV	C01-C02-C03-O11
20	I	102	PGV	C20-C21-C22-C23
13	J	101	BCB	C10-C11-C12-C13
9	C	401	HEC	CAA-CBA-CGA-O2A
11	L	305	UQ8	C20-C19-C21-C22
13	E	101	BCB	C4-C3-C5-C6
21	l	101	NS0	C32-C33-C35-C36
15	L	306	CDL	C80-C81-C82-C83
19	b	102	LMT	C5'-C4'-O1B-C1B
9	C	402	HEC	CAA-CBA-CGA-O2A
15	r	102	CDL	C14-C15-C16-C17
21	D	103	NS0	C-CA-CB-CG
19	b	103	LMT	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
11	A	101	UQ8	C39-C41-C42-C43
15	L	306	CDL	CB2-C1-CA2-OA2
11	L	305	UQ8	C12-C11-C9-C10
21	W	303	NS0	CA-C-C7-C8
13	3	101	BCB	C2-C1-O2A-CGA
13	q	101	BCB	C2-C1-O2A-CGA
21	D	103	NS0	C32-C33-C35-C36
21	O	101	NS0	CA-C-C7-C9
21	9	102	NS0	C32-C33-C35-C36
13	f	101	BCB	O1A-CGA-O2A-C1
13	D	101	BCB	C11-C10-C8-C9
13	0	102	BCB	CBA-CGA-O2A-C1
13	X	102	BCB	O1A-CGA-O2A-C1
13	0	102	BCB	O1A-CGA-O2A-C1
19	b	102	LMT	C3'-C4'-O1B-C1B
12	L	301	DGA	CA3-CA4-CA5-CA6
13	o	102	BCB	C5-C6-C7-C8
13	o	102	BCB	C10-C11-C12-C13
11	A	101	UQ8	C28-C29-C31-C32
21	O	101	NS0	C32-C33-C35-C36
21	2	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
20	M	411	PGV	C11-C12-C13-C14
11	A	101	UQ8	C2-C3-O3-C3M
13	c	101	BCB	C4-C3-C5-C6
21	0	101	NS0	C34-C33-C35-C36
13	D	101	BCB	C11-C10-C8-C7
13	O	102	BCB	C11-C10-C8-C7
13	X	102	BCB	C11-C10-C8-C7
13	D	101	BCB	C5-C6-C7-C8
20	Q	401	PGV	C13-C14-C15-C16
13	9	101	BCB	CAA-CBA-CGA-O2A
15	L	306	CDL	C32-C31-CA7-OA8
20	Q	401	PGV	O03-C19-C20-C21
13	A	102	BCB	C13-C15-C16-C17
13	O	102	BCB	CBA-CGA-O2A-C1
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	E	101	BCB	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
15	M	409	CDL	C39-C40-C41-C42
13	R	102	BCB	C11-C10-C8-C9
13	1	101	BCB	C14-C13-C15-C16
13	c	101	BCB	C6-C7-C8-C9
13	4	101	BCB	C3A-C2A-CAA-CBA
13	c	101	BCB	C3A-C2A-CAA-CBA
13	M	402	BCB	CAD-CBD-CGD-O2D
14	L	304	BPB	CAD-CBD-CGD-O2D
14	M	404	BPB	CAD-CBD-CGD-O2D
20	N	102	PGV	C03-C02-O01-C1
13	3	101	BCB	C16-C17-C18-C19
13	0	102	BCB	C8-C10-C11-C12
15	M	409	CDL	C80-C81-C82-C83
13	i	101	BCB	C4-C3-C5-C6
13	i	101	BCB	C2-C3-C5-C6
21	W	303	NS0	CA-C-C7-C9
21	k	101	NS0	C32-C33-C35-C36
11	A	101	UQ8	C24-C26-C27-C28
15	H	301	CDL	CA3-CA4-CA6-OA8
15	H	302	CDL	C31-C32-C33-C34
13	O	102	BCB	O1A-CGA-O2A-C1
12	L	301	DGA	OG2-CB1-CB2-CB3
15	M	409	CDL	C12-C11-CA5-OA6
15	M	409	CDL	C61-C62-C63-C64
15	H	301	CDL	C55-C56-C57-C58
20	D	102	PGV	O12-C04-C05-O05
13	M	403	BCB	CHA-CBD-CGD-O2D
13	E	101	BCB	CHA-CBD-CGD-O1D
13	E	101	BCB	CHA-CBD-CGD-O2D
13	U	102	BCB	CHA-CBD-CGD-O2D
13	0	102	BCB	CHA-CBD-CGD-O1D
13	0	102	BCB	CHA-CBD-CGD-O2D
13	l	102	BCB	CHA-CBD-CGD-O2D
9	C	404	HEC	CAD-CBD-CGD-O1D
13	B	202	BCB	C4-C3-C5-C6
13	1	101	BCB	CBA-CGA-O2A-C1
15	M	409	CDL	C59-C60-C61-C62
13	T	101	BCB	CAA-CBA-CGA-O2A
13	U	102	BCB	CAA-CBA-CGA-O2A
15	L	306	CDL	C40-C41-C42-C43
20	I	102	PGV	C31-C32-C33-C34
13	r	101	BCB	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
13	b	101	BCB	CAA-CBA-CGA-O2A
15	H	301	CDL	C20-C21-C22-C23
15	H	301	CDL	C71-C72-C73-C74
13	U	102	BCB	CBA-CGA-O2A-C1
13	4	101	BCB	C16-C17-C18-C20
13	I	101	BCB	C11-C10-C8-C9
13	7	102	BCB	C6-C7-C8-C9
13	7	102	BCB	C14-C13-C15-C16
13	k	102	BCB	C11-C12-C13-C14
20	Q	401	PGV	O04-C19-C20-C21
21	W	303	NS0	C11-C10-C9-C7
12	L	301	DGA	OB1-CB1-CB2-CB3
15	L	306	CDL	C82-C83-C84-C85
13	q	101	BCB	CAA-CBA-CGA-O2A
19	b	102	LMT	C9-C10-C11-C12
11	M	408	UQ8	C33-C34-C36-C37
13	c	101	BCB	C2-C3-C5-C6
15	M	409	CDL	C36-C37-C38-C39
13	R	102	BCB	CBA-CGA-O2A-C1
13	N	101	BCB	C1A-C2A-CAA-CBA
13	U	102	BCB	C1A-C2A-CAA-CBA
13	i	101	BCB	C1A-C2A-CAA-CBA
15	L	306	CDL	C12-C11-CA5-OA6
13	r	101	BCB	CBA-CGA-O2A-C1
9	C	404	HEC	CAD-CBD-CGD-O2D
13	9	101	BCB	CAA-CBA-CGA-O1A
15	L	306	CDL	C32-C31-CA7-OA9
15	r	102	CDL	C52-C51-CB5-OB6
15	H	302	CDL	OB7-CB5-OB6-CB4
15	M	409	CDL	CA3-OA5-PA1-OA3
15	r	102	CDL	CA3-OA5-PA1-OA3
13	1	101	BCB	O1A-CGA-O2A-C1
15	M	409	CDL	C52-C53-C54-C55
13	h	102	BCB	C13-C15-C16-C17
13	b	101	BCB	CAA-CBA-CGA-O1A
14	L	304	BPB	C8-C10-C11-C12
14	M	404	BPB	C15-C16-C17-C18
13	q	101	BCB	CAA-CBA-CGA-O1A
11	L	305	UQ8	C12-C11-C9-C8
11	A	101	UQ8	C38-C39-C41-C42
13	L	302	BCB	CAD-CBD-CGD-O1D
13	A	102	BCB	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
13	0	102	BCB	CAD-CBD-CGD-O1D
13	T	101	BCB	CAA-CBA-CGA-O1A
15	M	409	CDL	C12-C11-CA5-OA7
13	k	102	BCB	CAA-CBA-CGA-O2A
15	H	301	CDL	C16-C17-C18-C19
15	r	102	CDL	C12-C11-CA5-OA6
21	W	303	NS0	C35-C36-C37-C38
13	h	102	BCB	CAA-CBA-CGA-O2A
15	H	301	CDL	C12-C11-CA5-OA6
12	L	301	DGA	CA1-CA2-CA3-CA4
15	r	102	CDL	C52-C51-CB5-OB7
13	A	102	BCB	C2-C3-C5-C6
13	A	102	BCB	C11-C10-C8-C7
13	I	101	BCB	C11-C10-C8-C7
13	R	102	BCB	C11-C10-C8-C7
13	T	101	BCB	C12-C13-C15-C16
13	4	101	BCB	C6-C7-C8-C10
13	0	102	BCB	C12-C13-C15-C16
21	9	102	NS0	C26-C27-C28-C30
21	l	101	NS0	C26-C27-C28-C30
21	o	101	NS0	C26-C27-C28-C30
13	U	102	BCB	CAA-CBA-CGA-O1A
21	l	101	NS0	C10-C11-C12-C14
21	q	102	NS0	C10-C11-C12-C14
13	Z	101	BCB	CAA-CBA-CGA-O2A
13	k	102	BCB	C8-C10-C11-C12
21	A	103	NS0	C35-C36-C37-C38
13	W	302	BCB	CAA-CBA-CGA-O2A
15	r	102	CDL	C32-C31-CA7-OA8
13	f	101	BCB	C10-C11-C12-C13
13	o	102	BCB	C15-C16-C17-C18
15	r	102	CDL	C55-C56-C57-C58
20	D	102	PGV	C19-C20-C21-C22
13	k	102	BCB	CAA-CBA-CGA-O1A
13	i	101	BCB	CAA-CBA-CGA-O2A

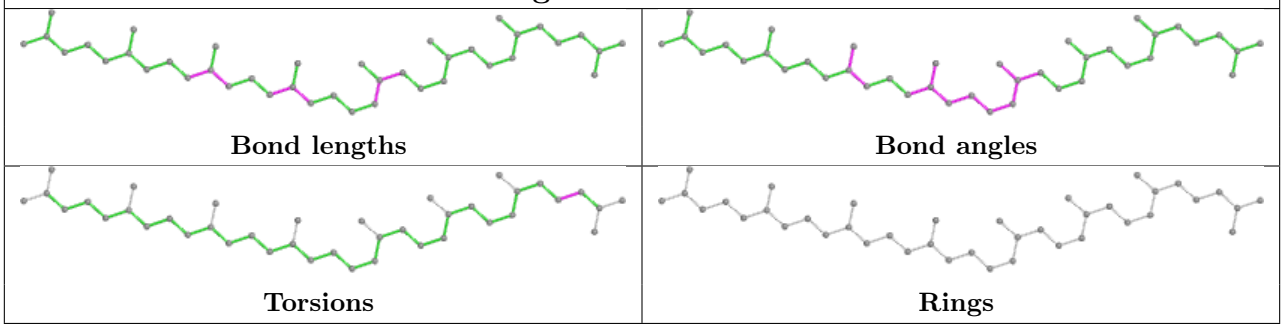
There are no ring outliers.

No monomer is involved in short contacts.

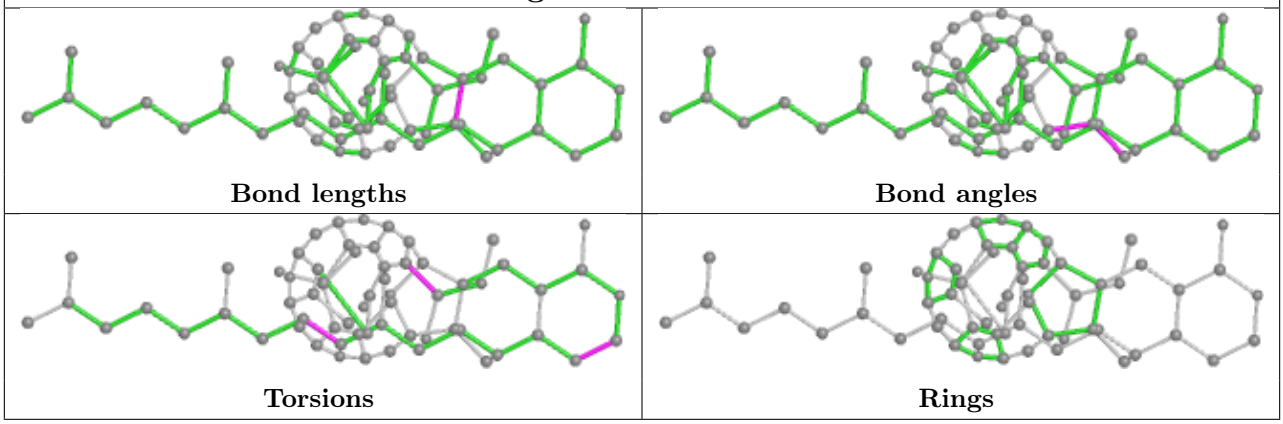
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

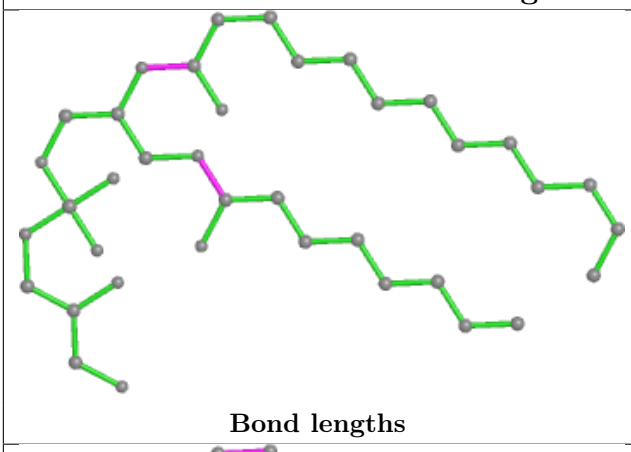
Ligand NS0 h 101



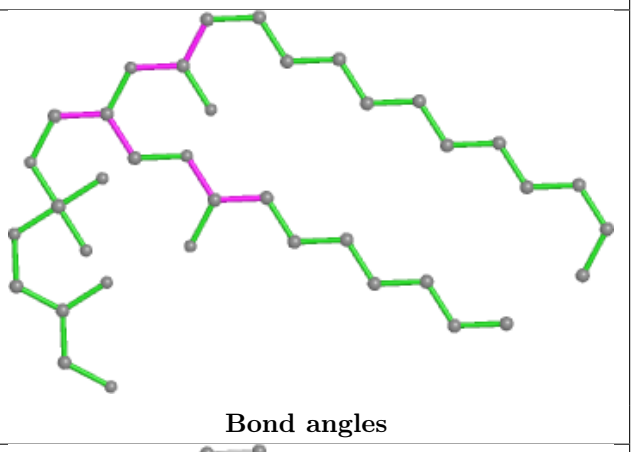
Ligand BPB L 304



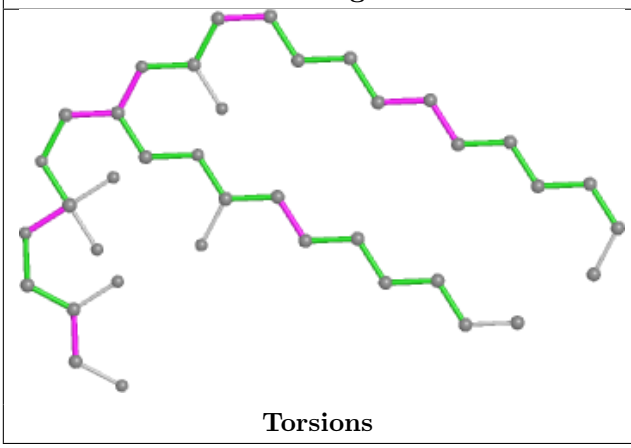
Ligand PGV N 102



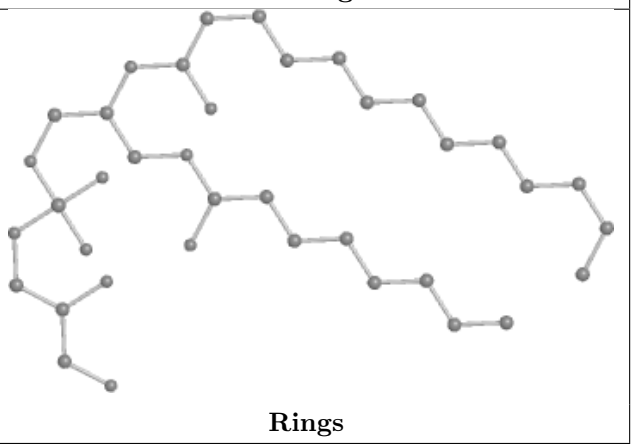
Bond lengths



Bond angles

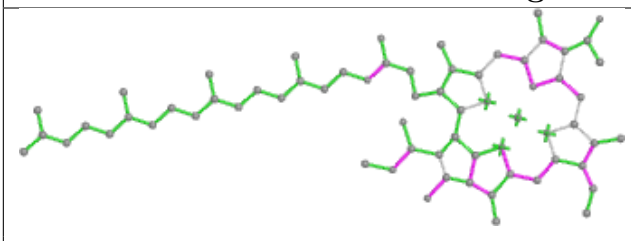


Torsions

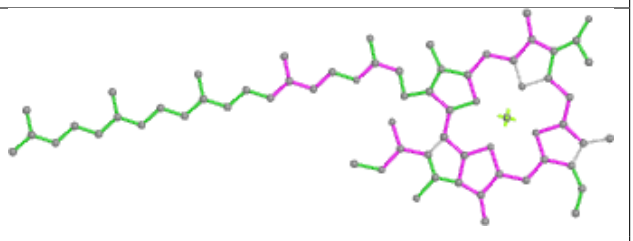


Rings

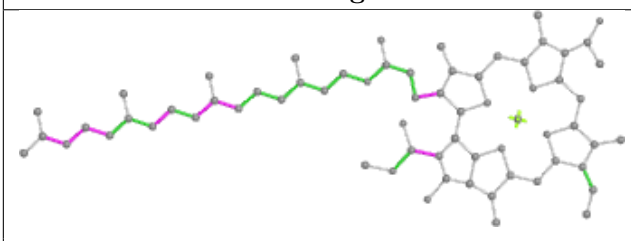
Ligand BCB 4 101



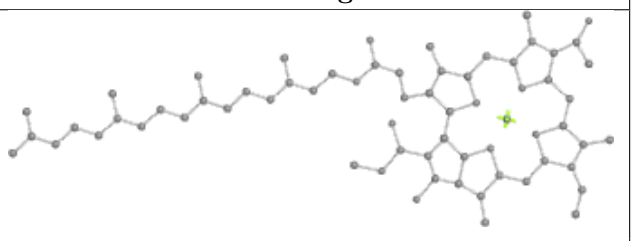
Bond lengths



Bond angles

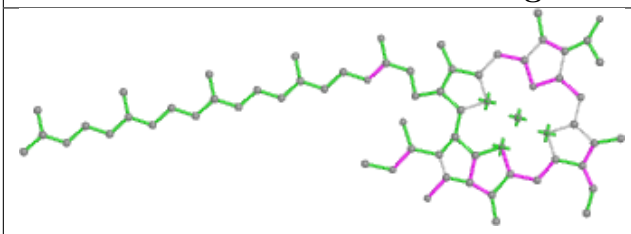


Torsions

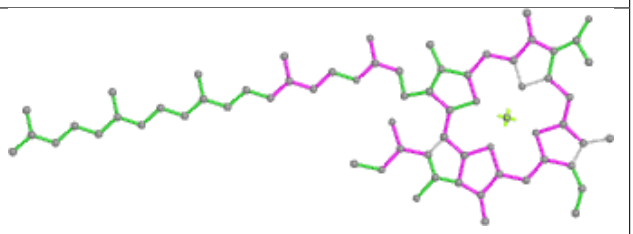


Rings

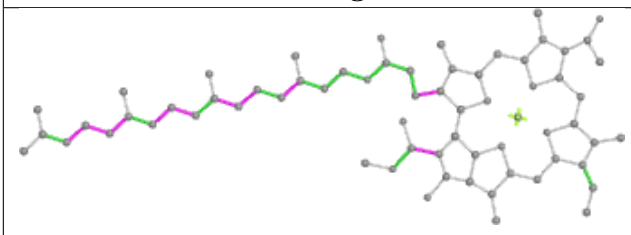
Ligand BCB E 101



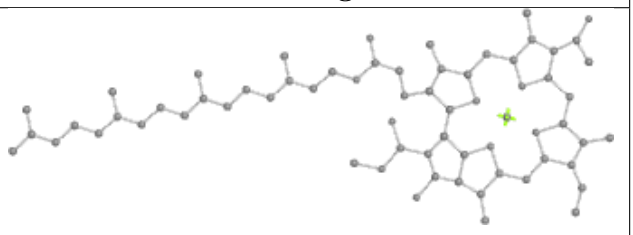
Bond lengths



Bond angles

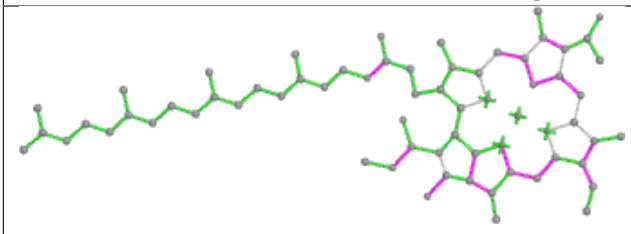


Torsions

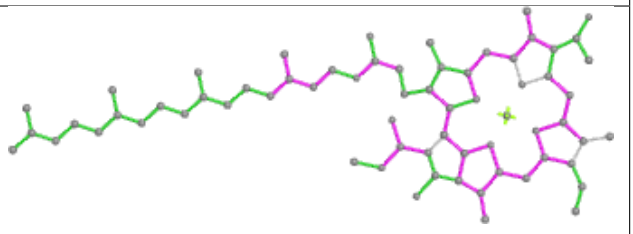


Rings

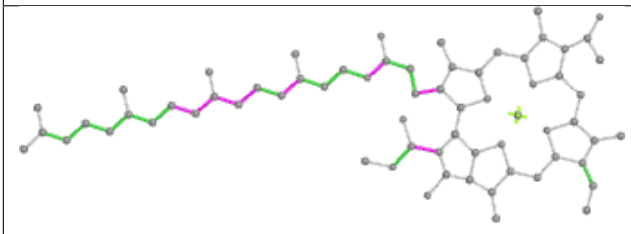
Ligand BCB c 101



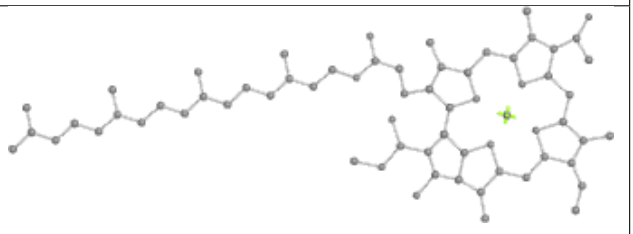
Bond lengths



Bond angles

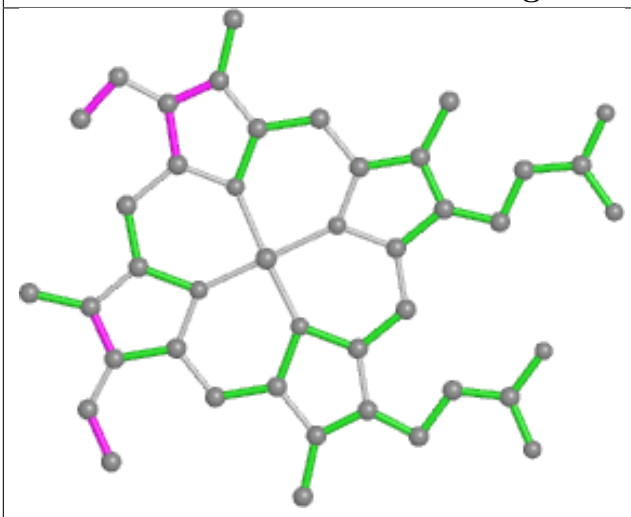


Torsions

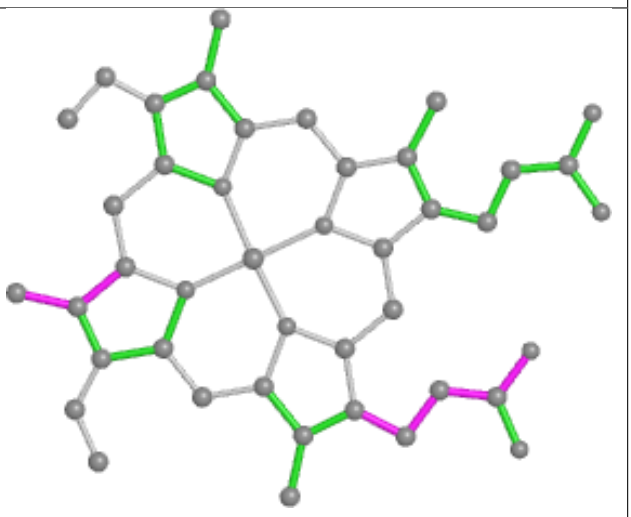


Rings

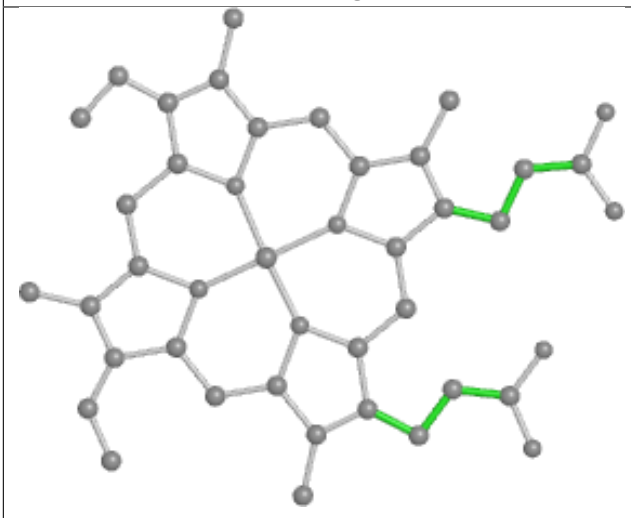
Ligand HEC C 403



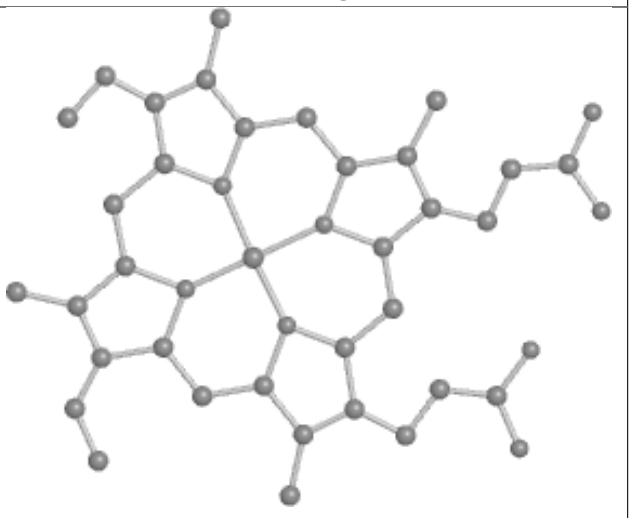
Bond lengths



Bond angles

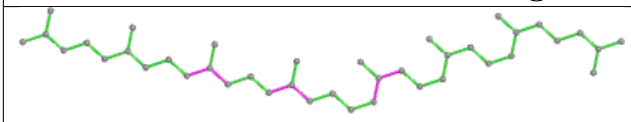


Torsions

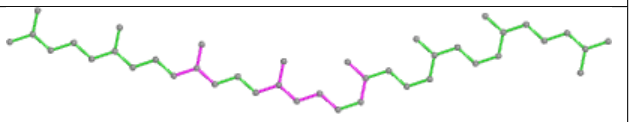


Rings

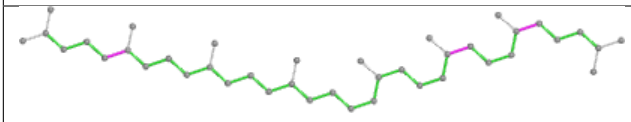
Ligand NS0 R 101



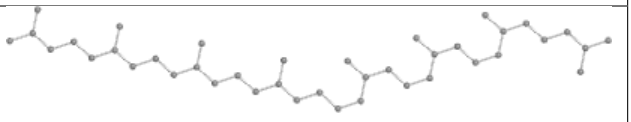
Bond lengths



Bond angles

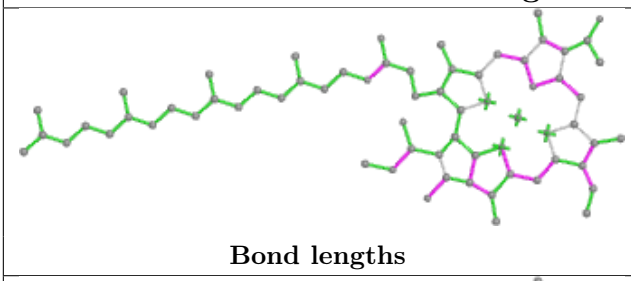


Torsions

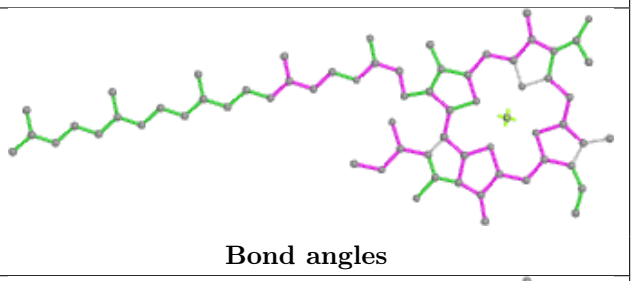


Rings

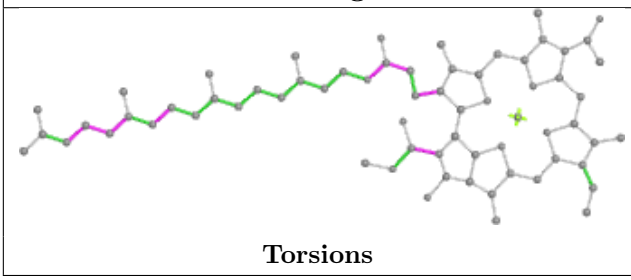
Ligand BCB U 102



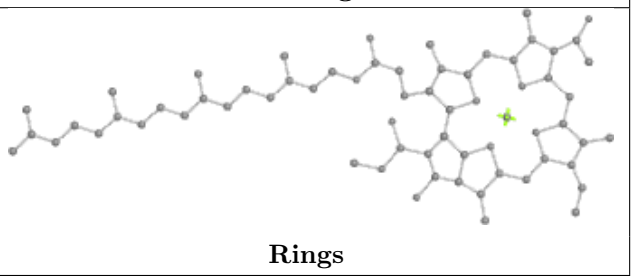
Bond lengths



Bond angles

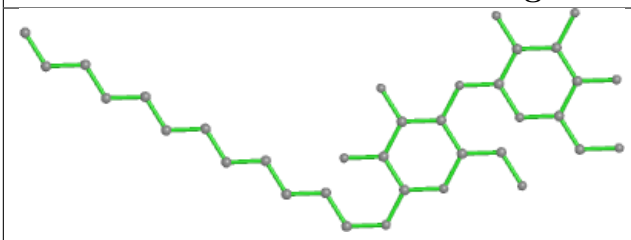


Torsions

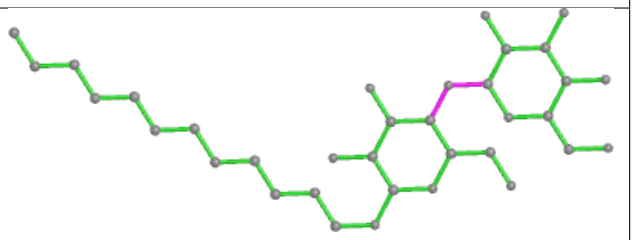


Rings

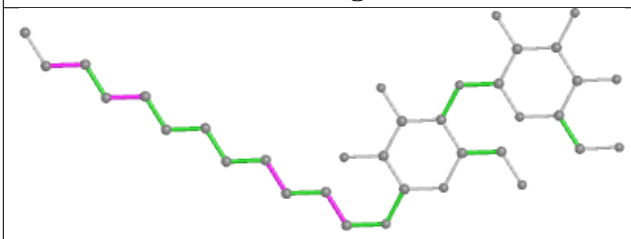
Ligand LMT h 103



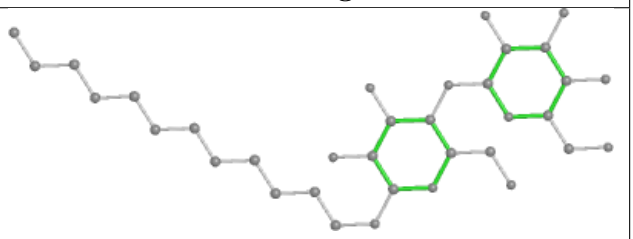
Bond lengths



Bond angles

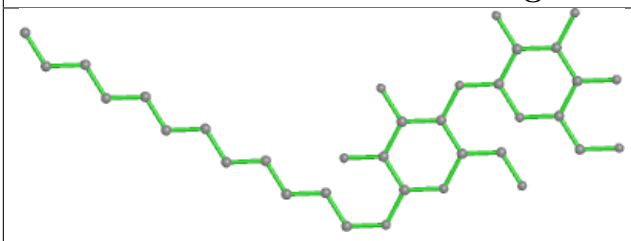


Torsions

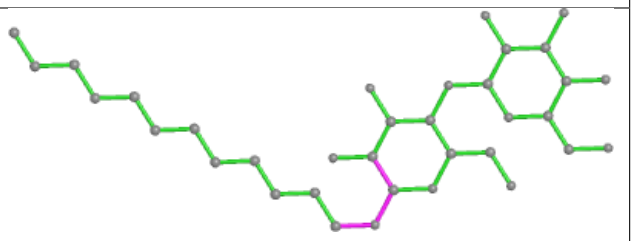


Rings

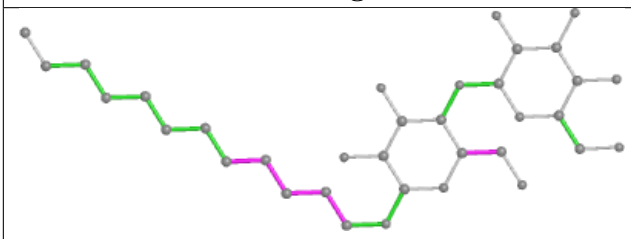
Ligand LMT b 103



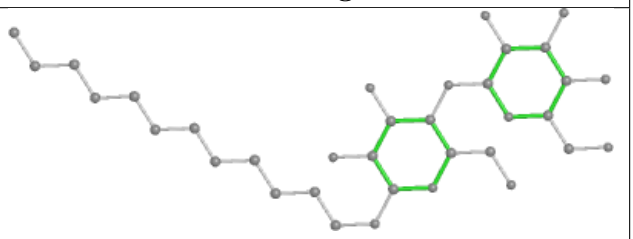
Bond lengths



Bond angles

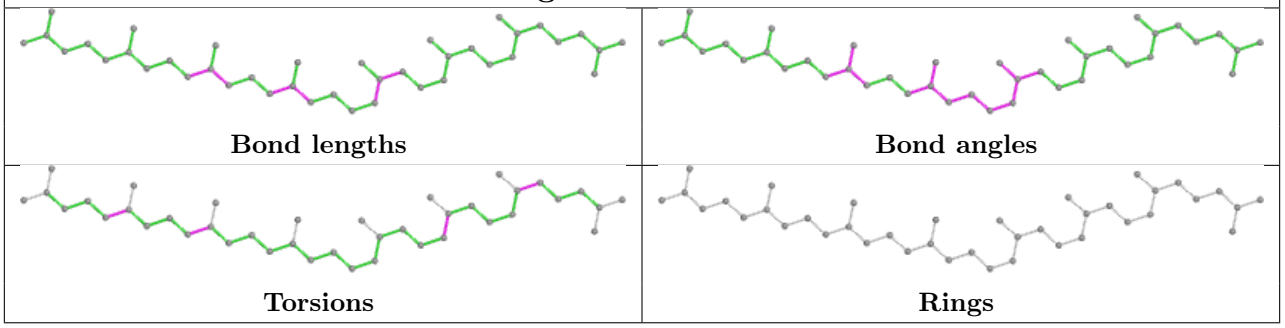


Torsions

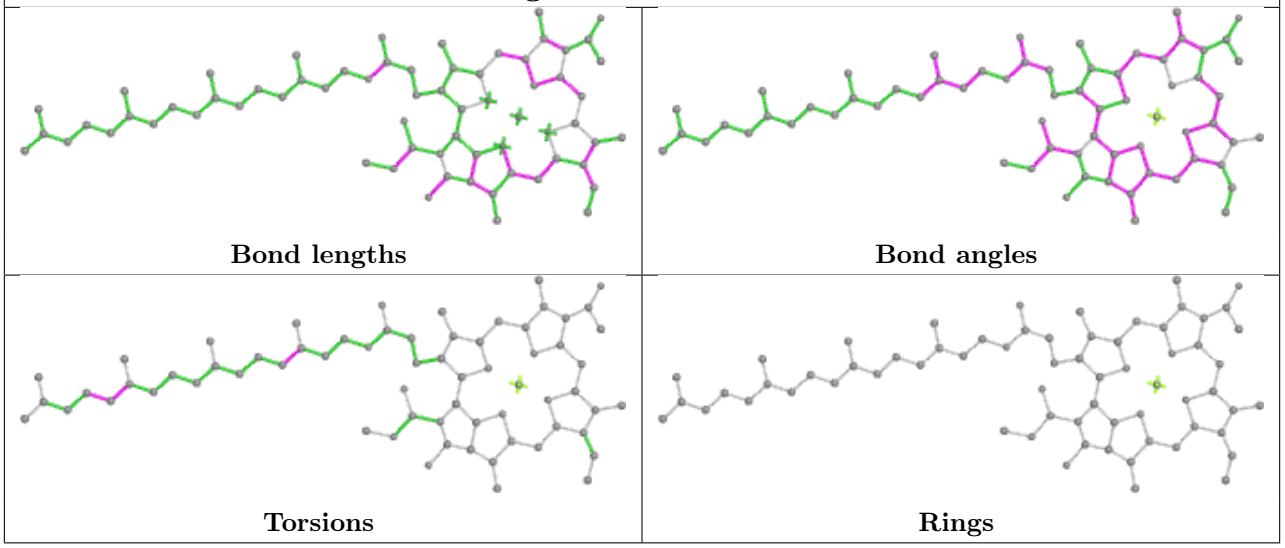


Rings

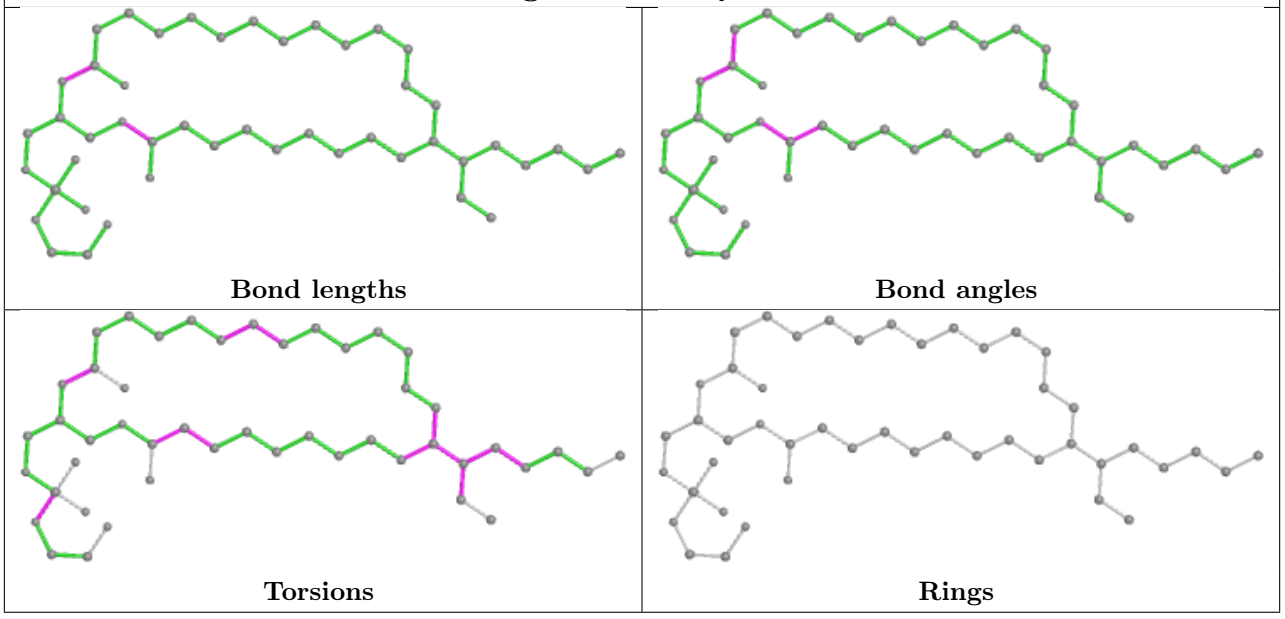
Ligand NS0 l 101



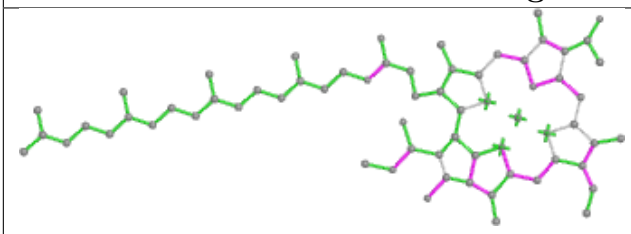
Ligand BCB B 202



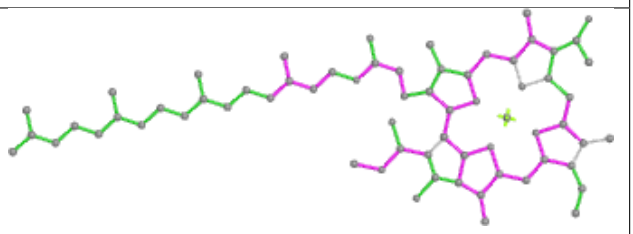
Ligand PGV Q 401



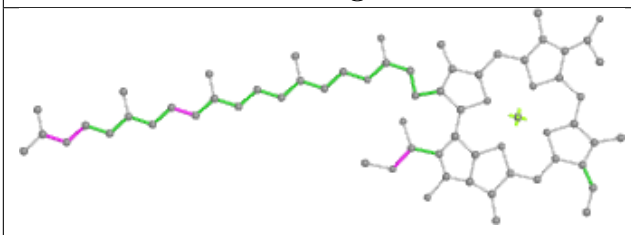
Ligand BCB 6 101



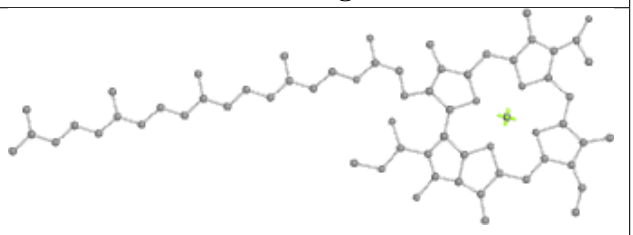
Bond lengths



Bond angles

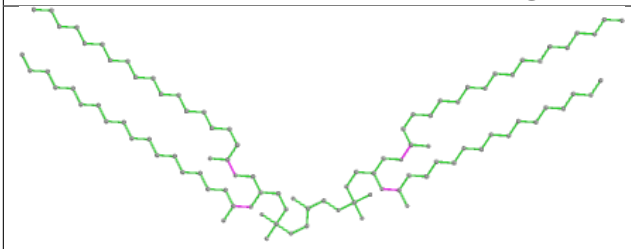


Torsions

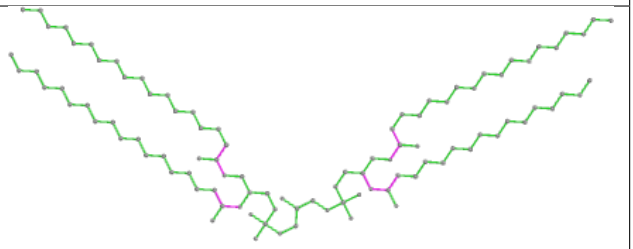


Rings

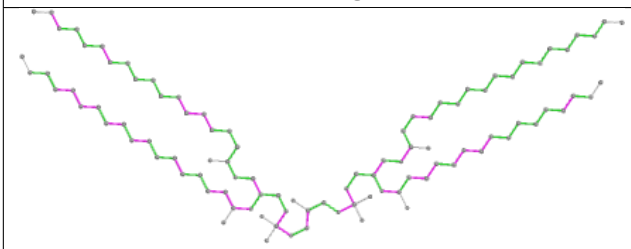
Ligand CDL H 301



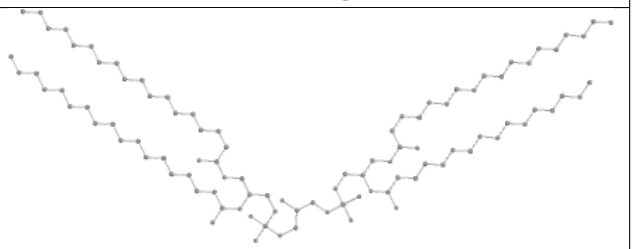
Bond lengths



Bond angles

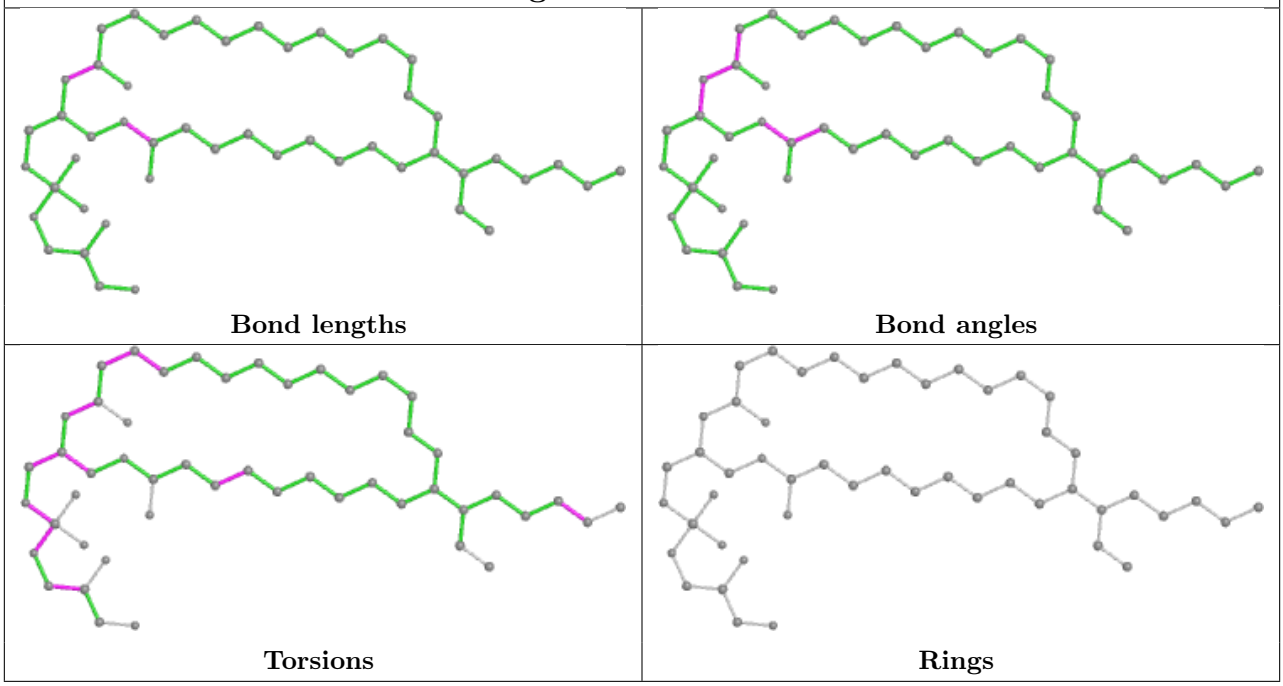


Torsions

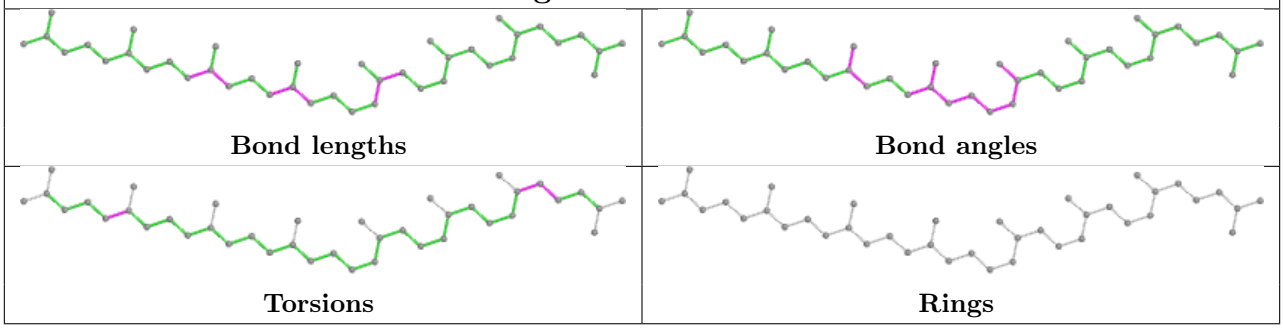


Rings

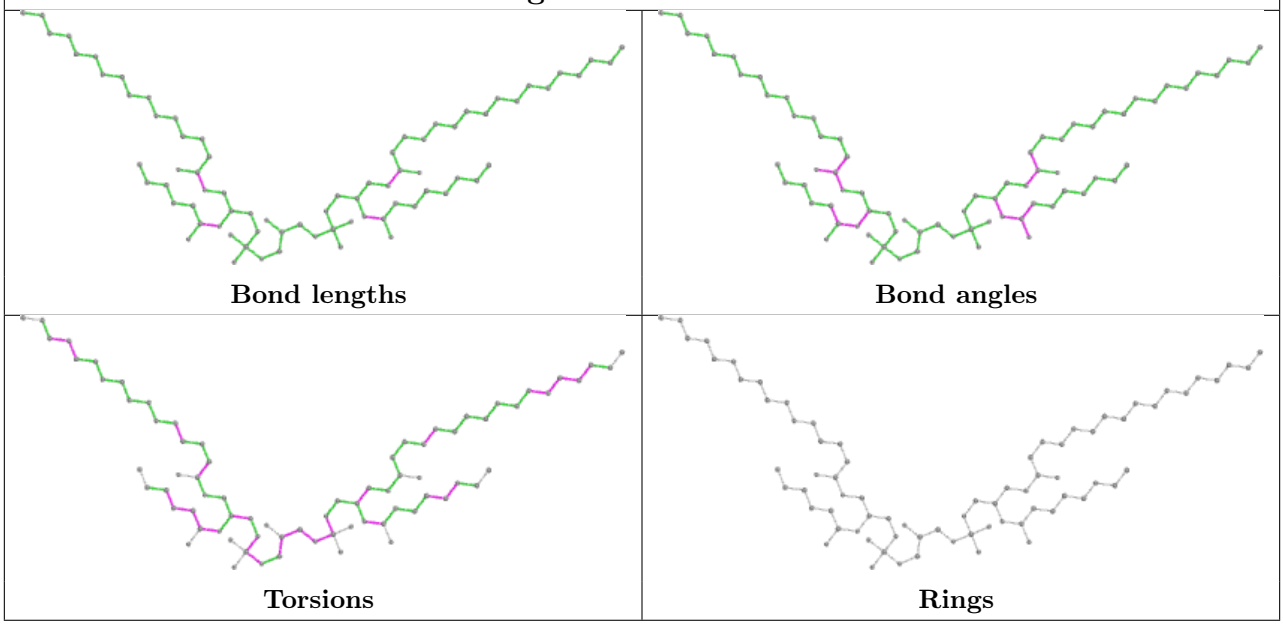
Ligand PGV I 102



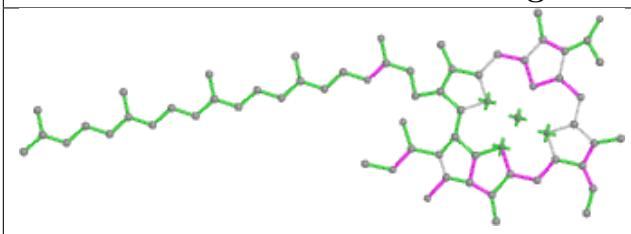
Ligand NS0 0 101



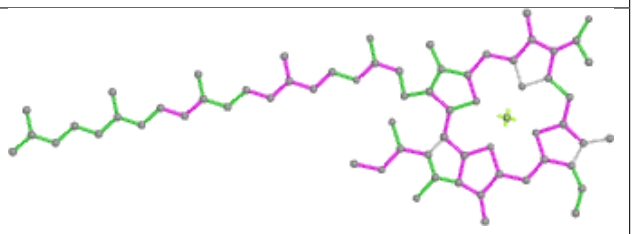
Ligand CDL L 306



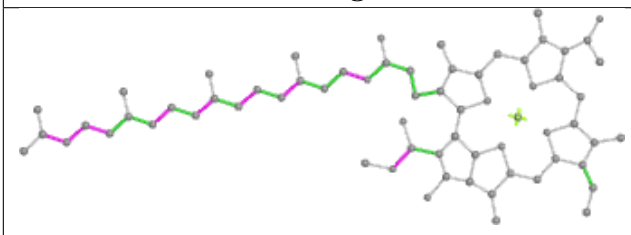
Ligand BCB 3 101



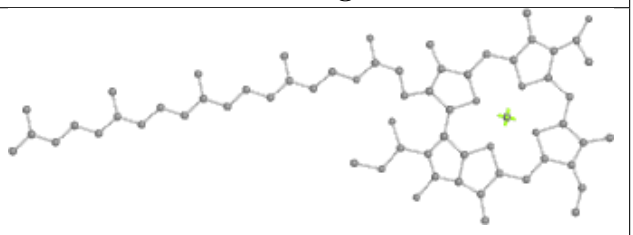
Bond lengths



Bond angles

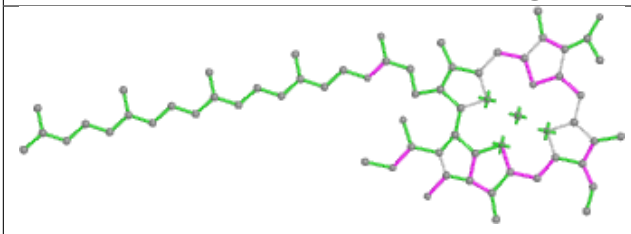


Torsions

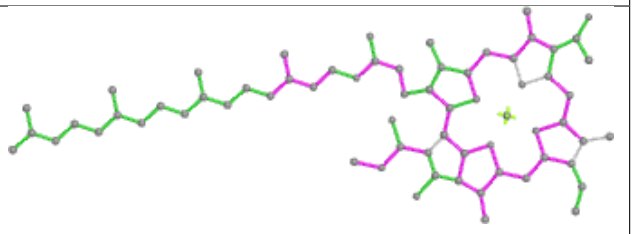


Rings

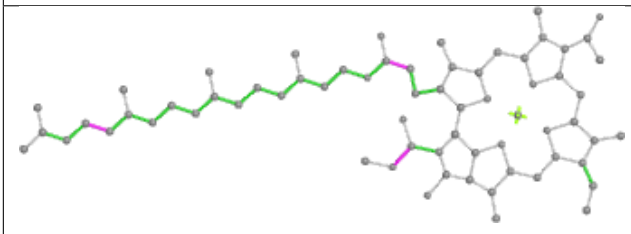
Ligand BCB h 102



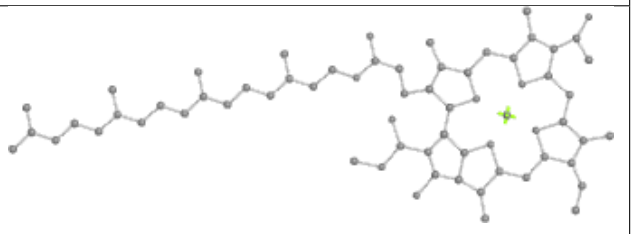
Bond lengths



Bond angles

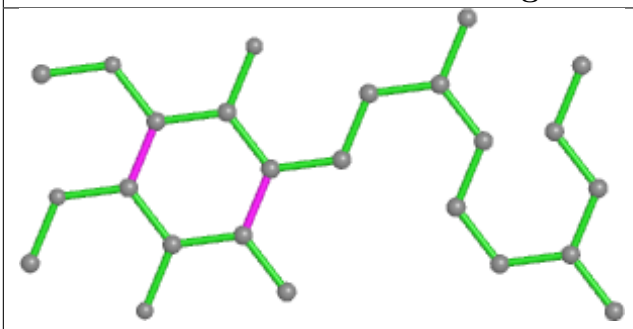


Torsions

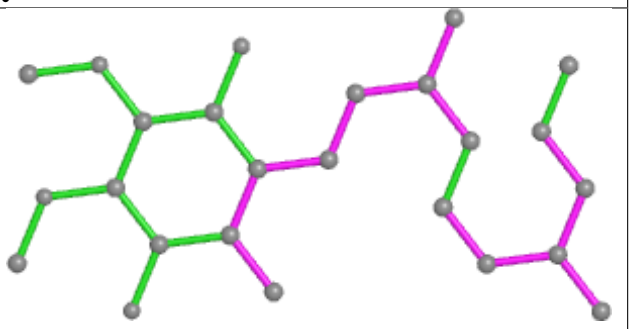


Rings

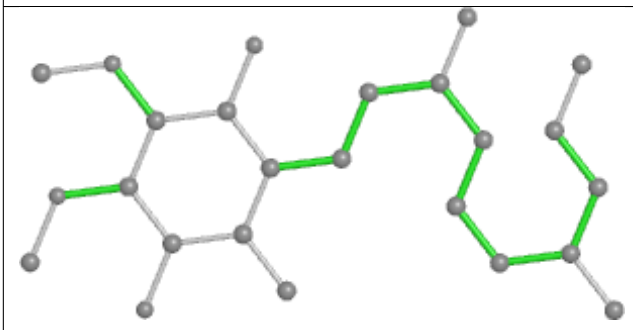
Ligand UQ8 M 407



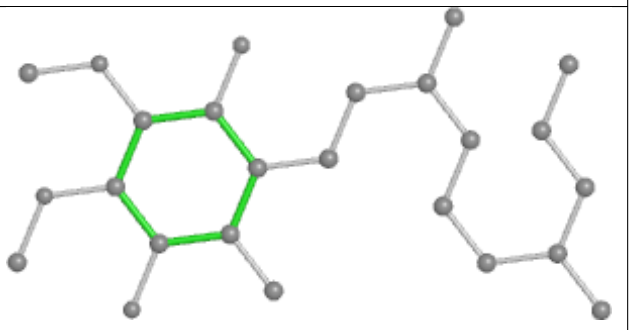
Bond lengths



Bond angles

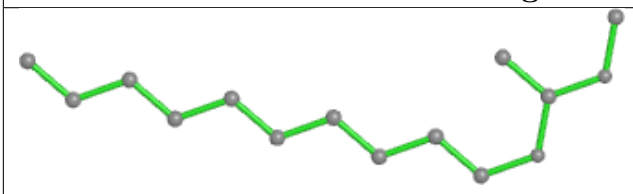


Torsions



Rings

Ligand LMT B 201



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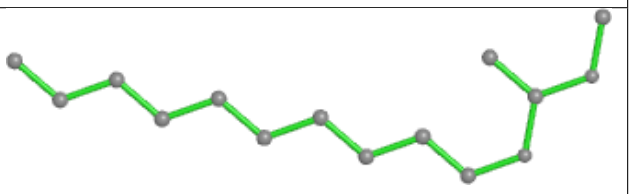
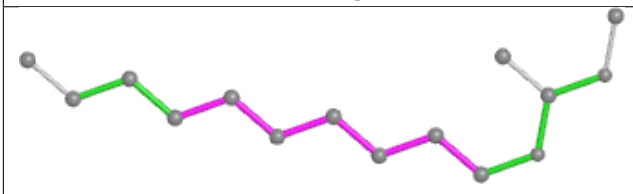
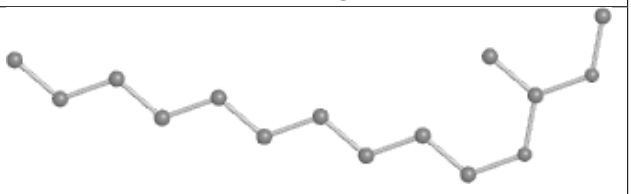


Bond angles

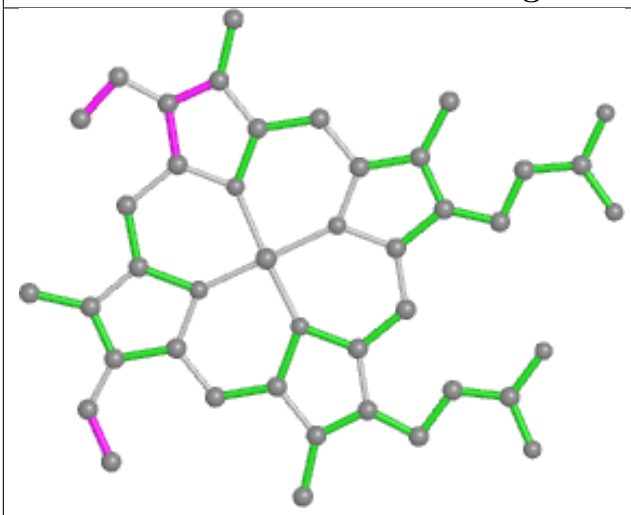


Torsions



Rings

Ligand HEC C 402



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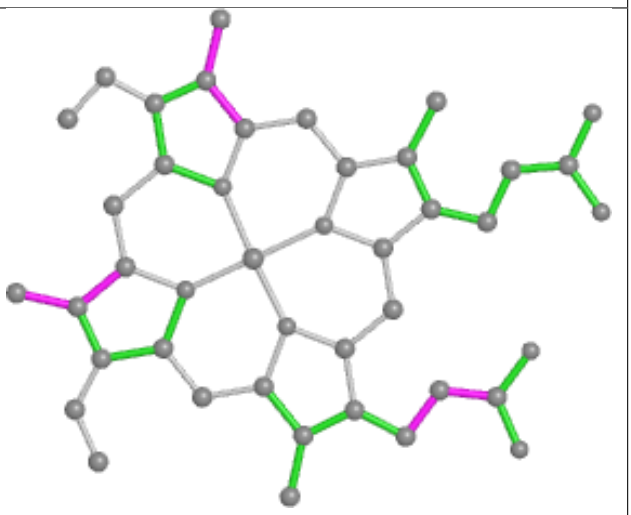
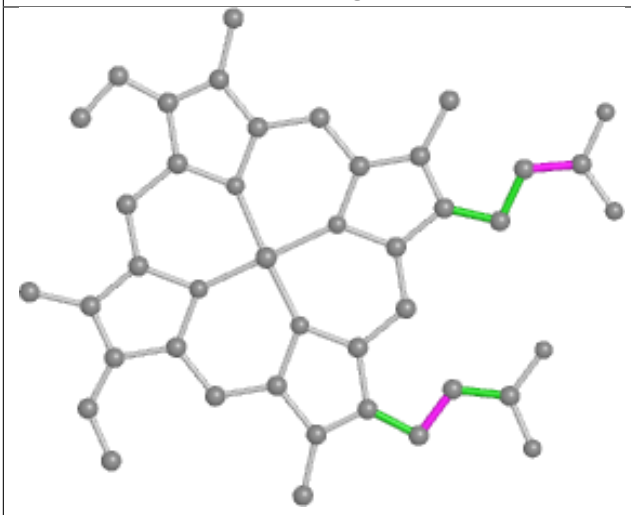
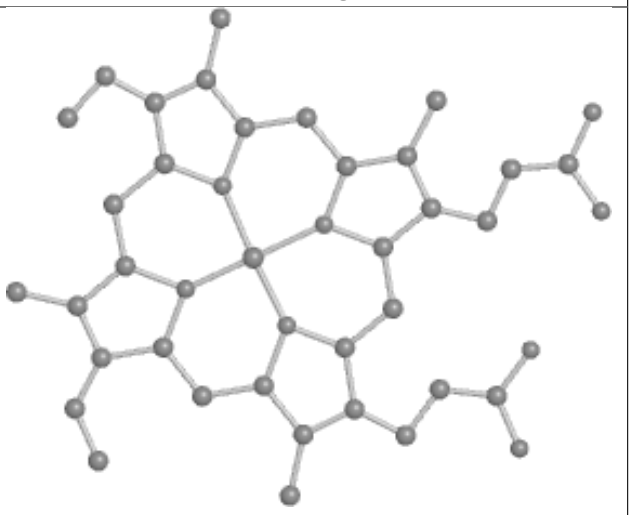


Bond angles

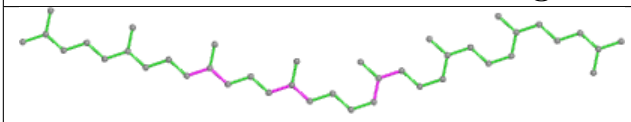


Torsions

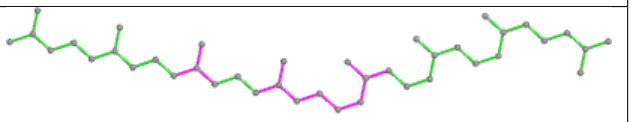


Rings

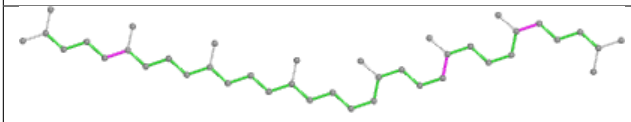
Ligand NS0 9 102



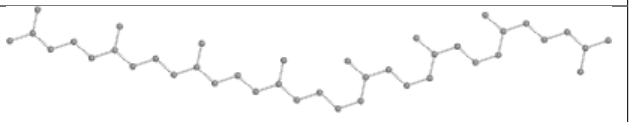
Bond lengths



Bond angles

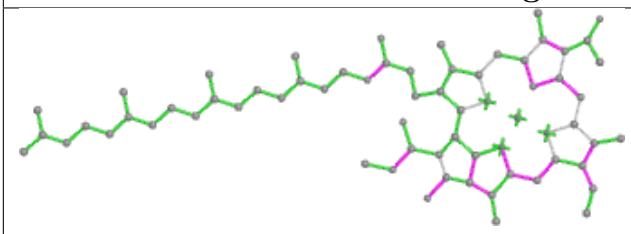


Torsions

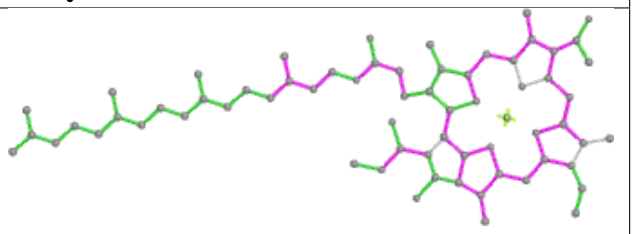


Rings

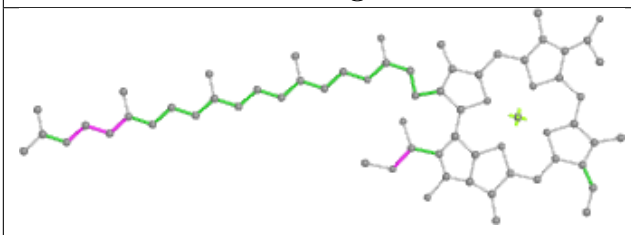
Ligand BCB Q 402



Bond lengths



Bond angles



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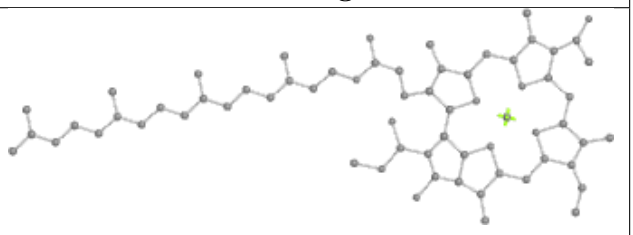
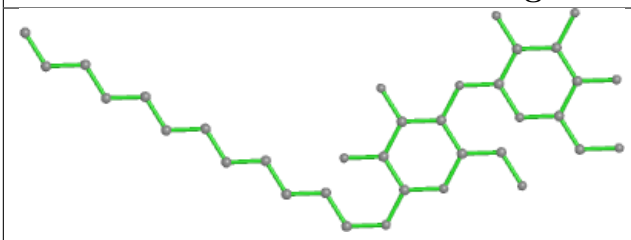
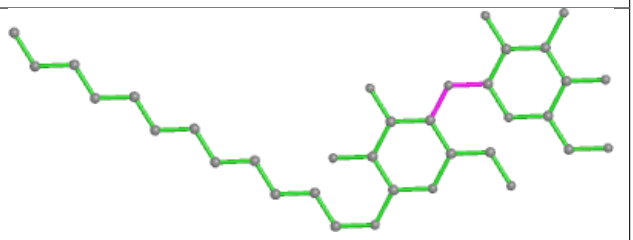


Rings

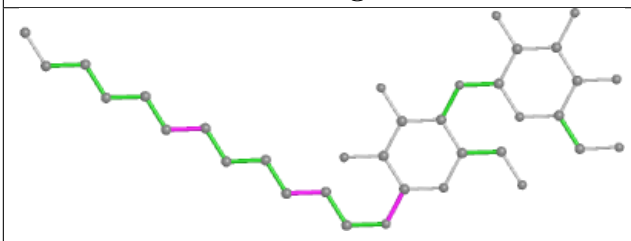
Ligand LMT k 103



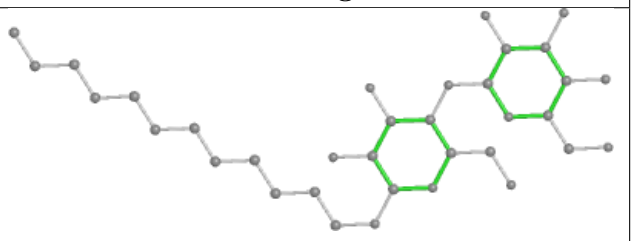
Bond lengths



Bond angles

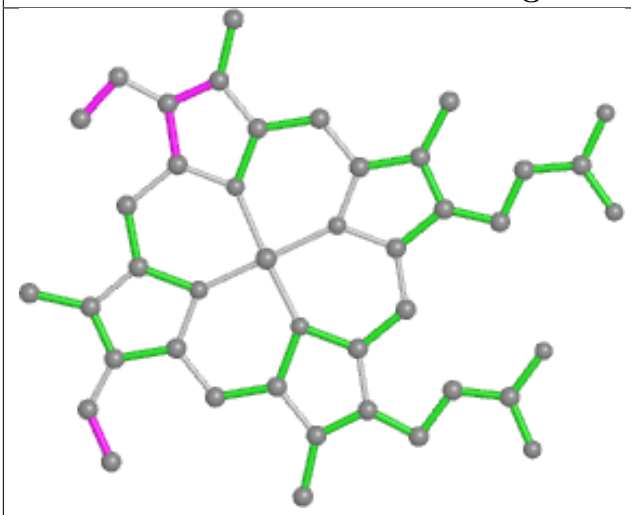


Torsions

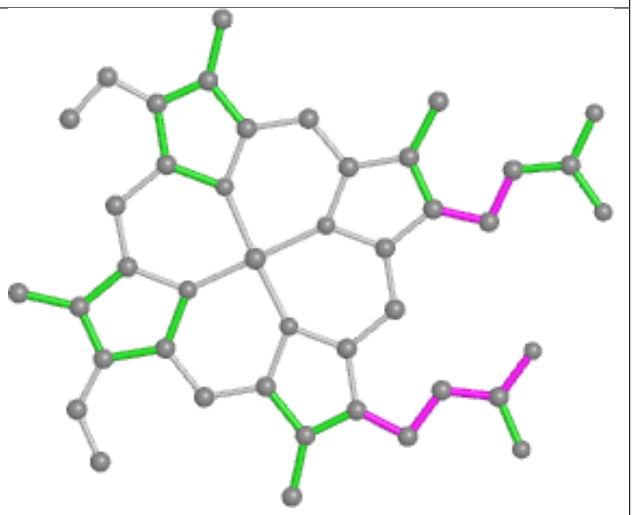


Rings

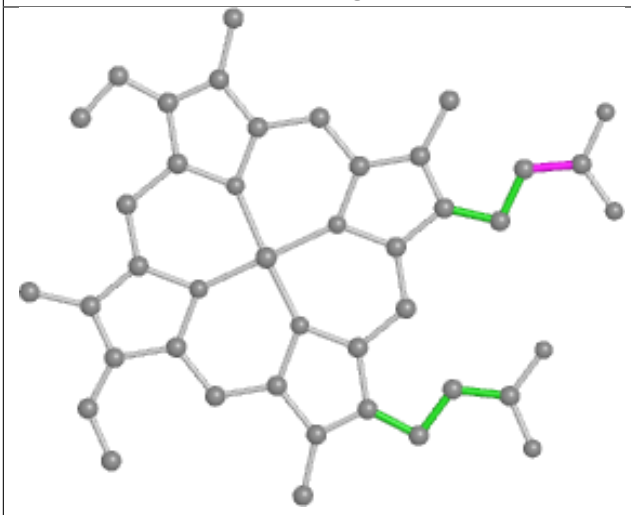
Ligand HEC C 401



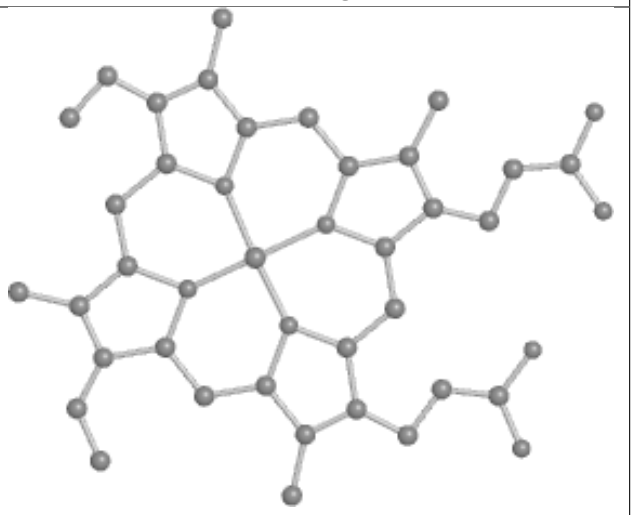
Bond lengths



Bond angles

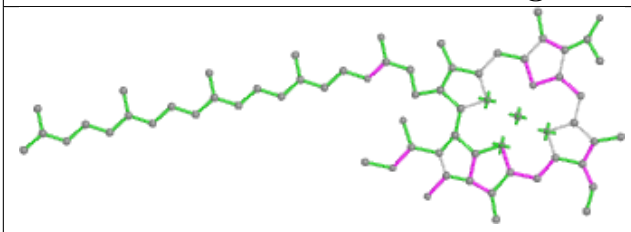


Torsions

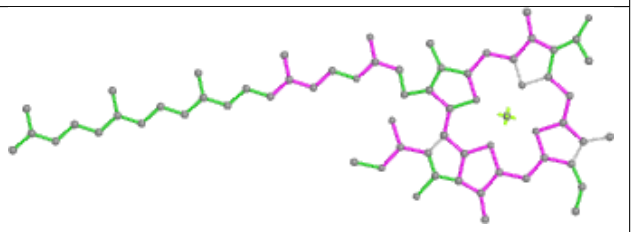


Rings

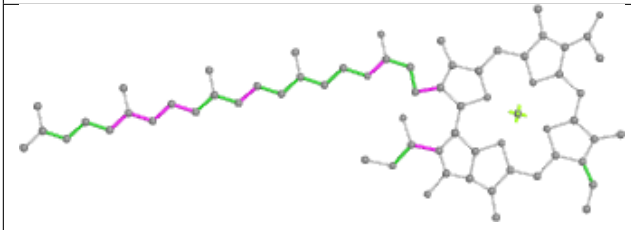
Ligand BCB 0 102



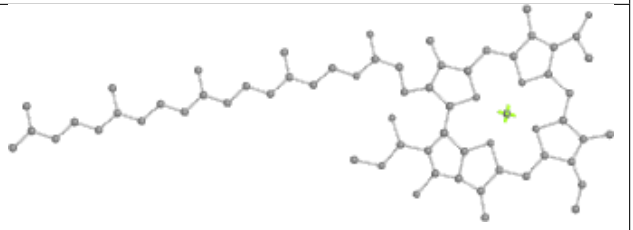
Bond lengths



Bond angles

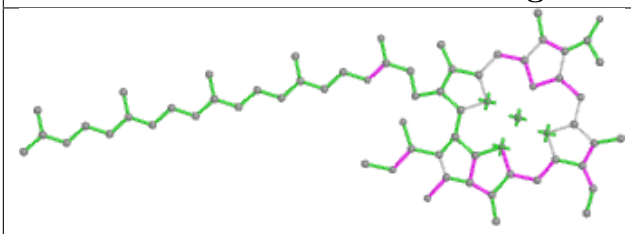


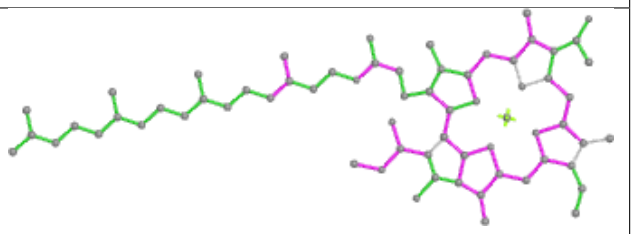
Torsions

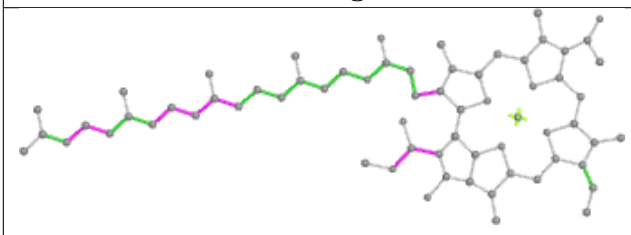


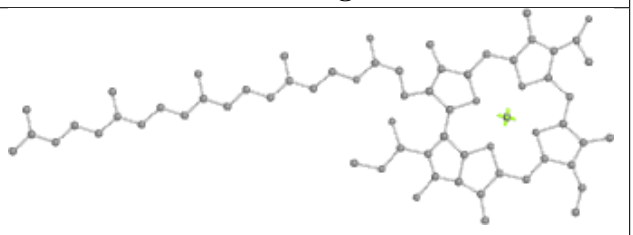
Rings

Ligand BCB J 101

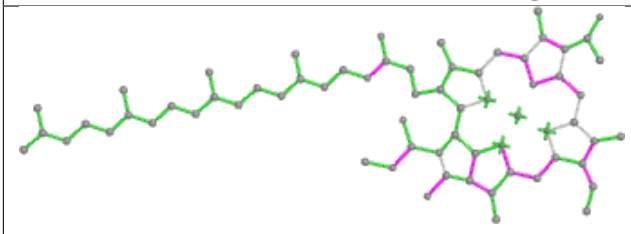

Bond lengths

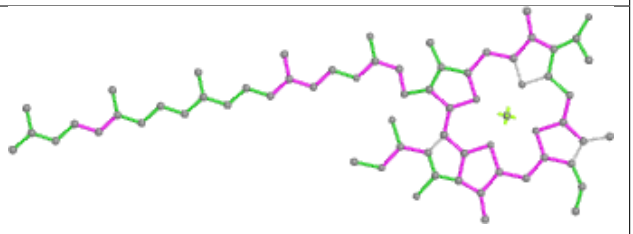

Bond angles

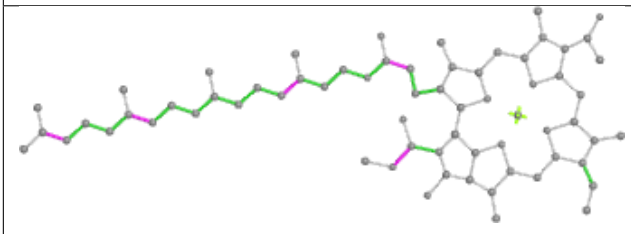

Torsions


Rings

Ligand BCB b 101


Bond lengths


Bond angles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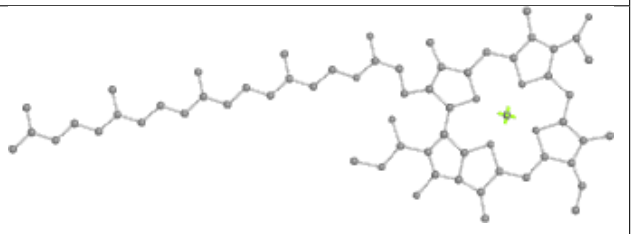
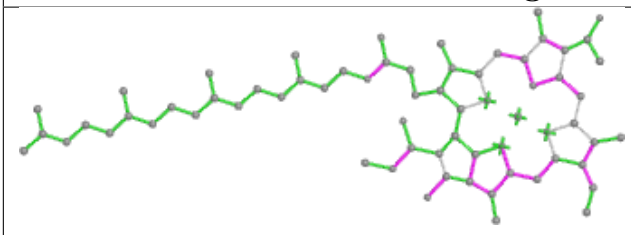
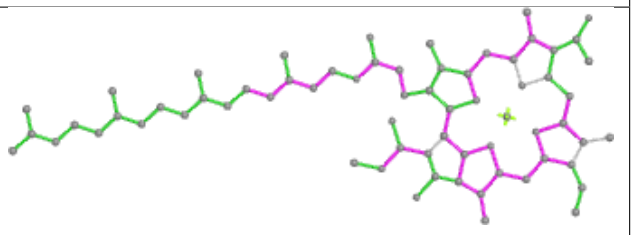
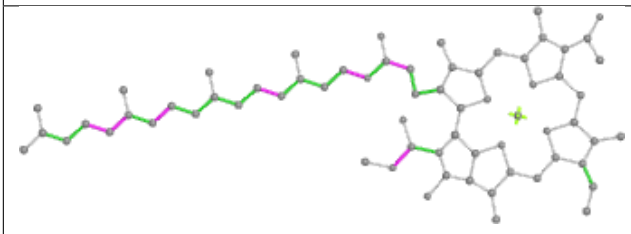

Rings

Ligand BCB T 101


Bond lengths


Bond angles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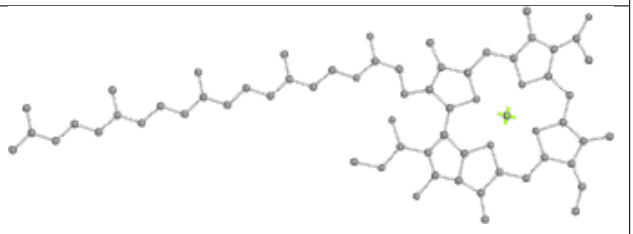
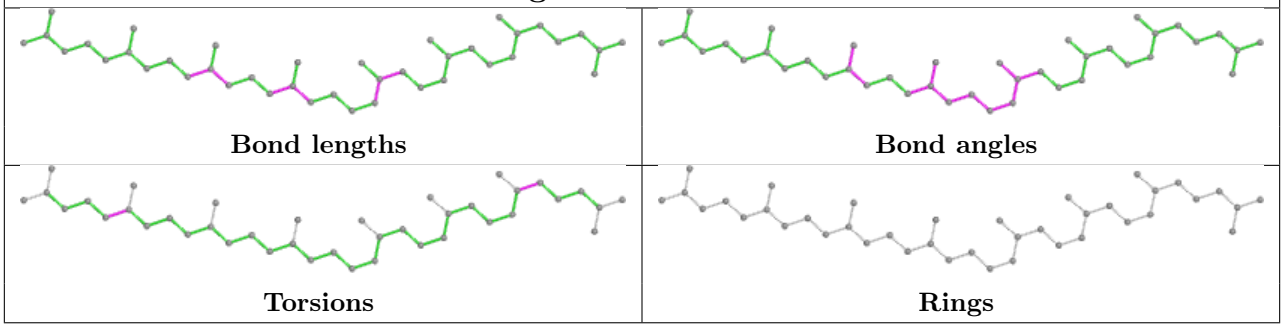
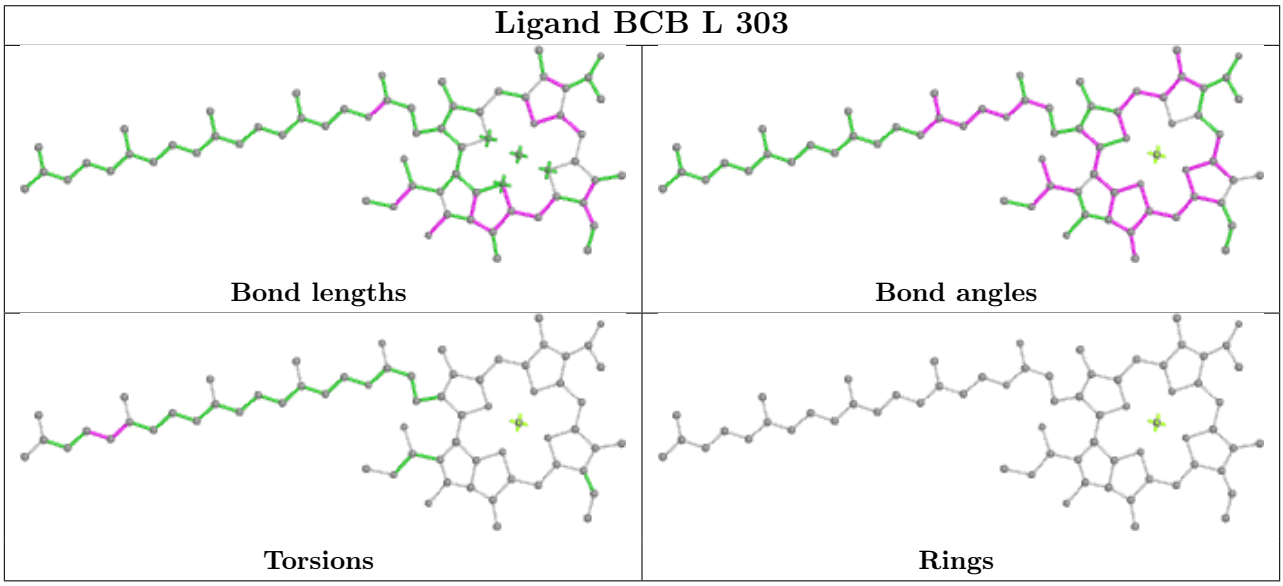

Rings

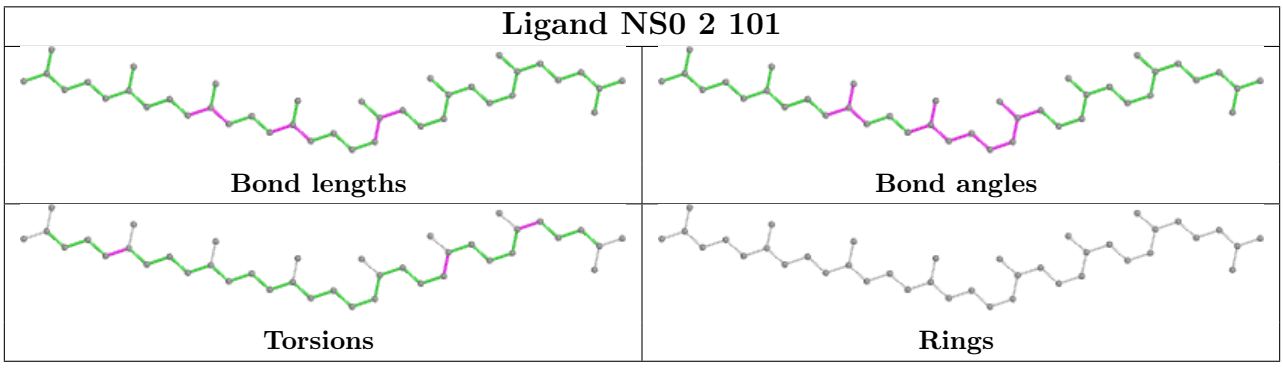
Ligand NS0 X 101



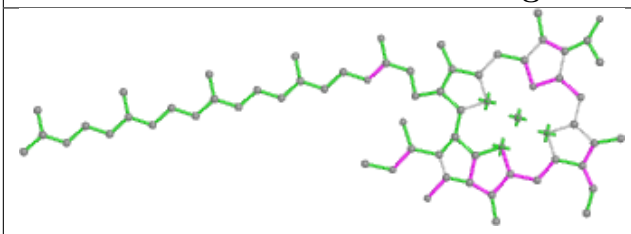
Ligand BCB L 303



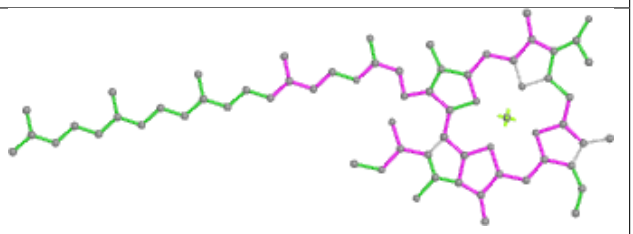
Ligand NS0 2 101



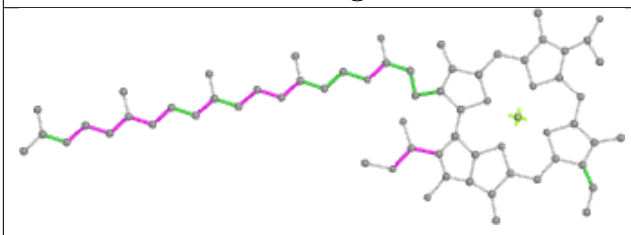
Ligand BCB A 102



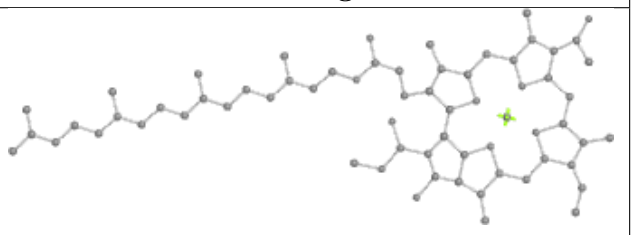
Bond lengths



Bond angles

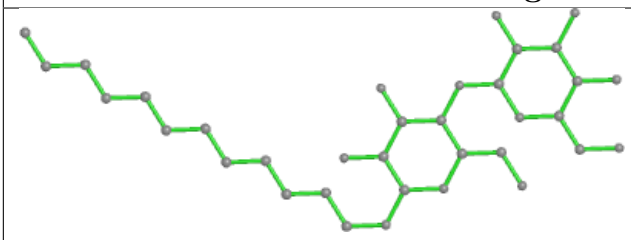


Torsions



Rings

Ligand LMT n 102



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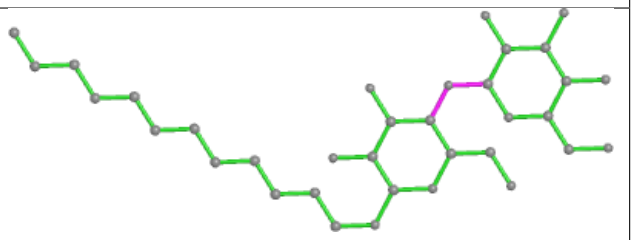
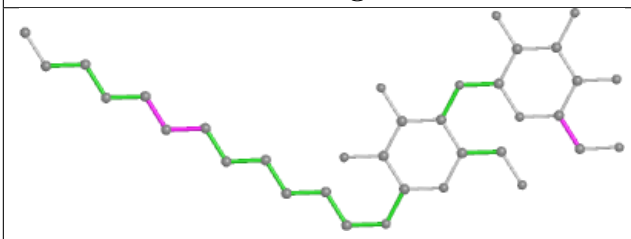
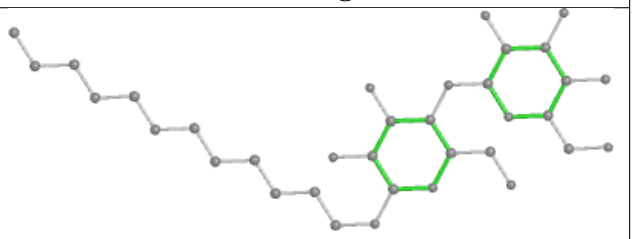


Bond angles

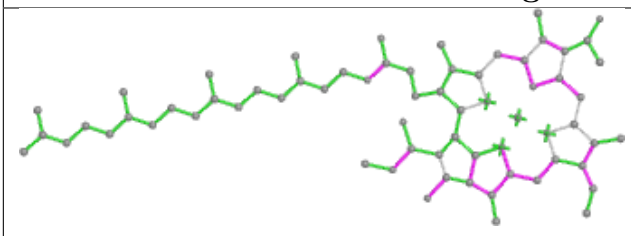


Torsions



Rings

Ligand BCB D 101



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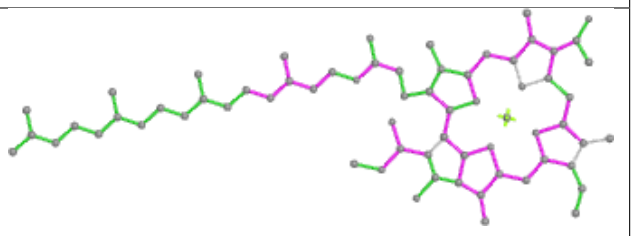
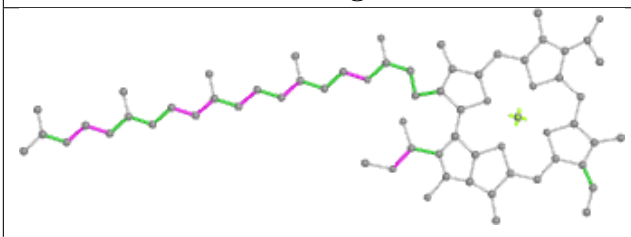
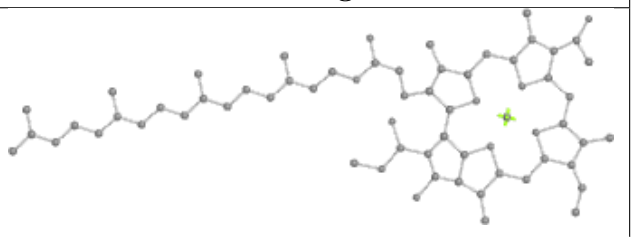


Bond angles

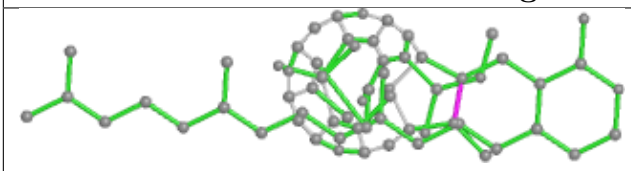


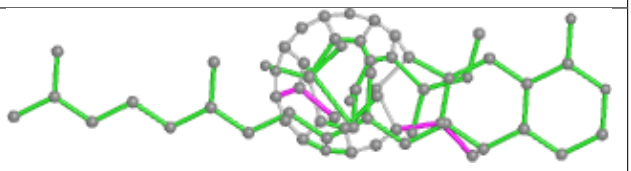
Torsions

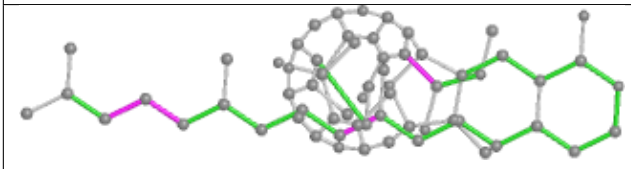


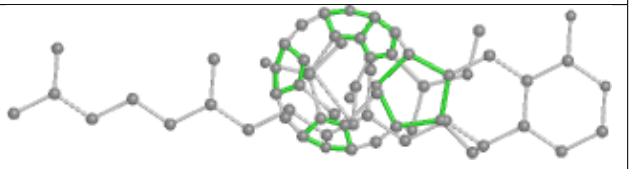
Rings

Ligand BPB M 404

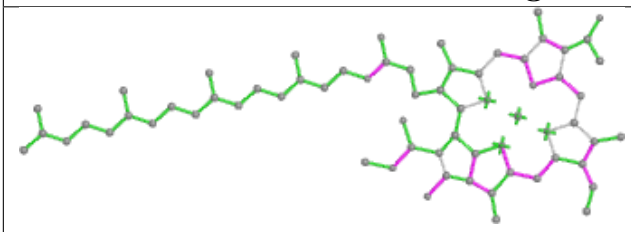

Bond lengths

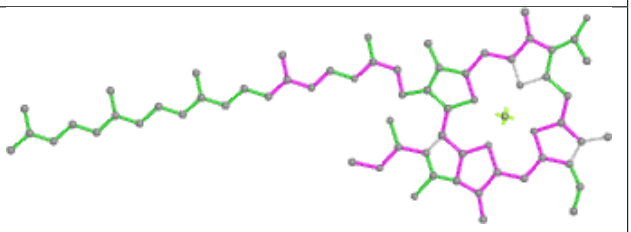

Bond angles

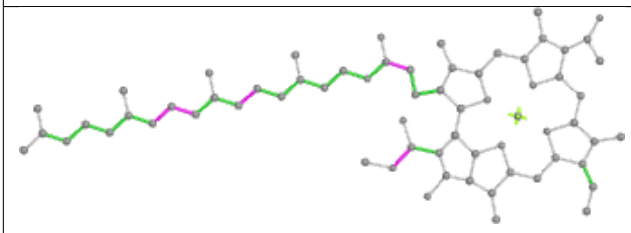

Torsions

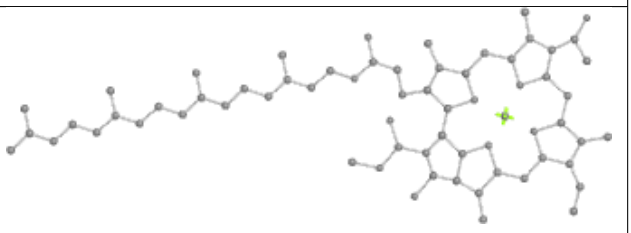

Rings

Ligand BCB Z 101

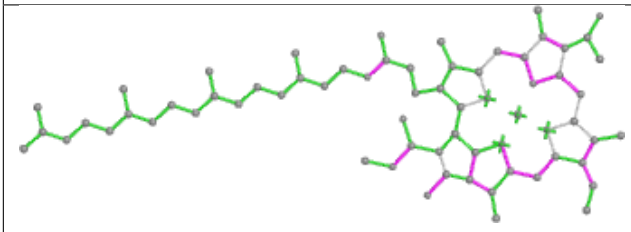

Bond lengths


Bond angles


Torsions


Rings

Ligand BCB N 101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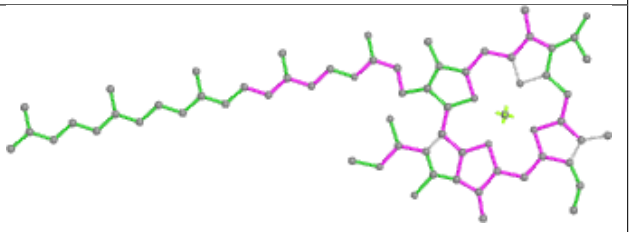
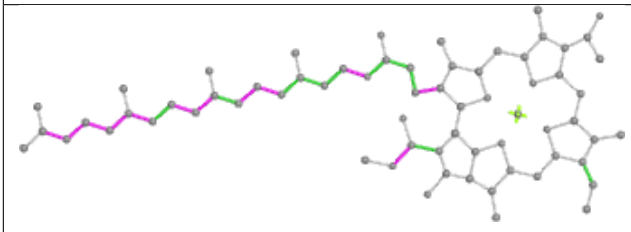
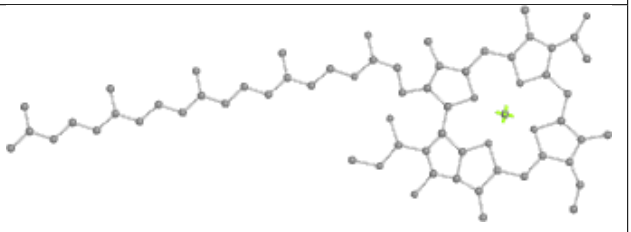
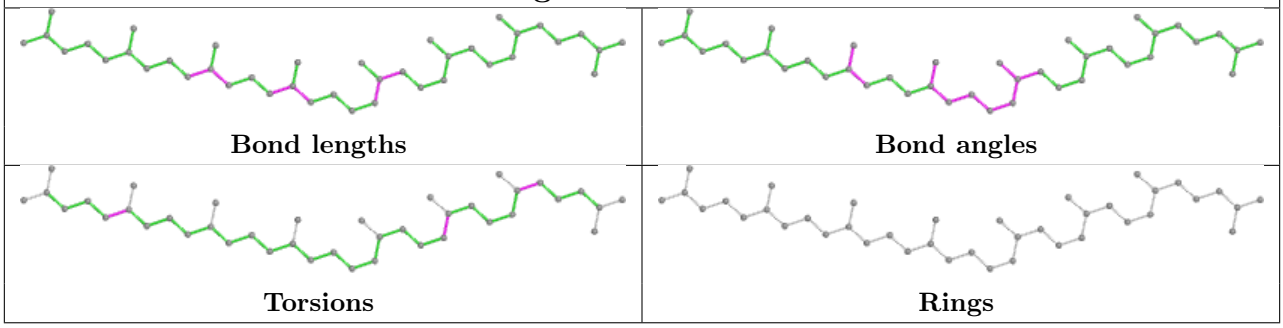

Bond angles

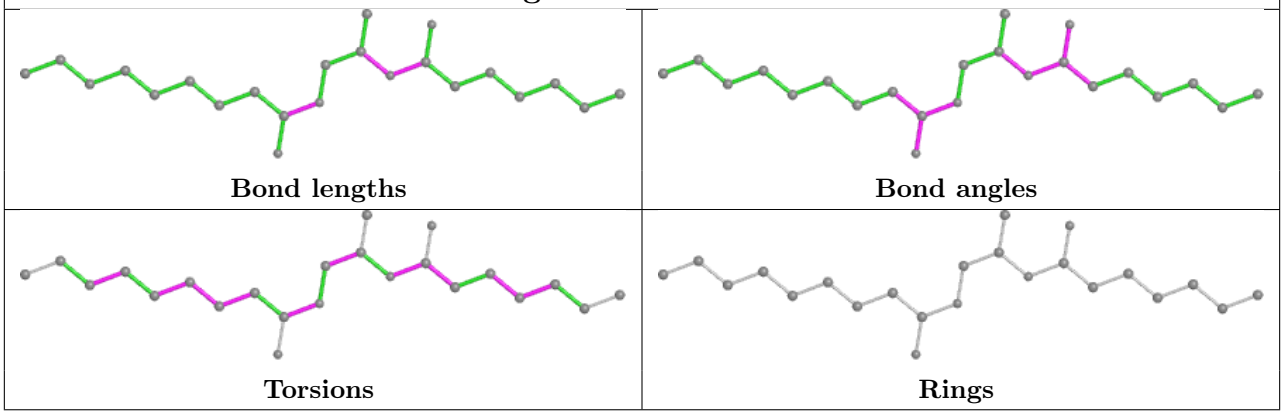

Torsions


Rings

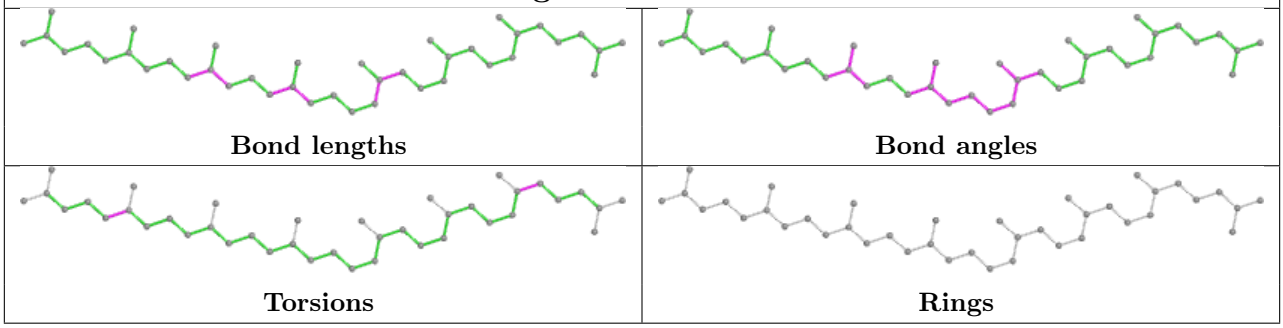
Ligand NS0 7 101



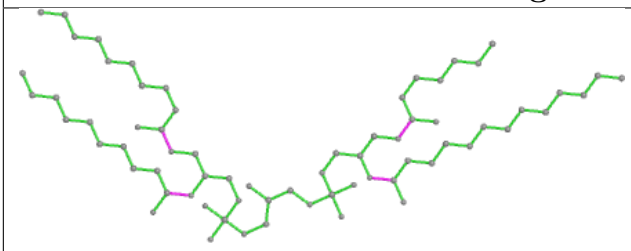
Ligand DGA L 301



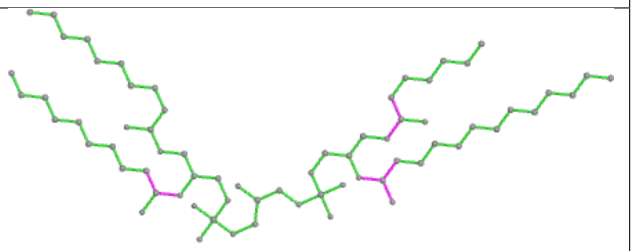
Ligand NS0 k 101



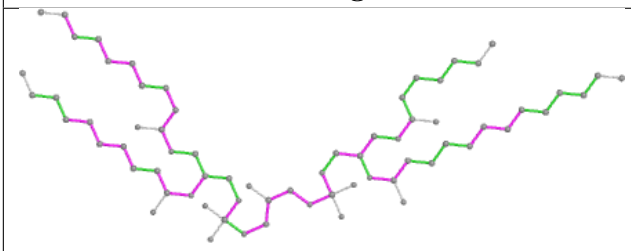
Ligand CDL r 102



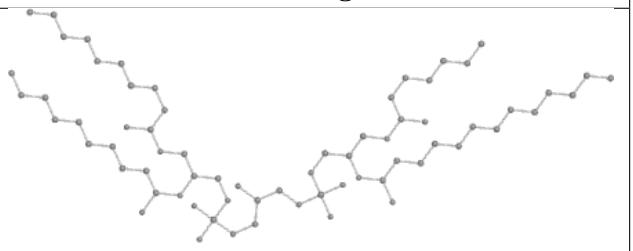
Bond lengths



Bond angles

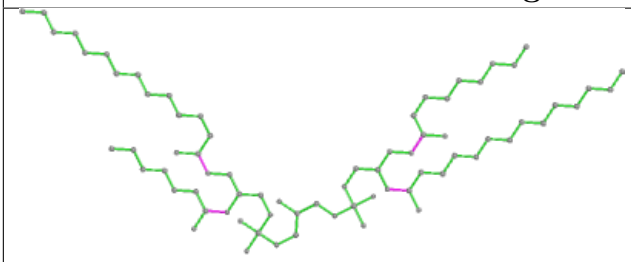


Torsions



Rings

Ligand CDL H 302



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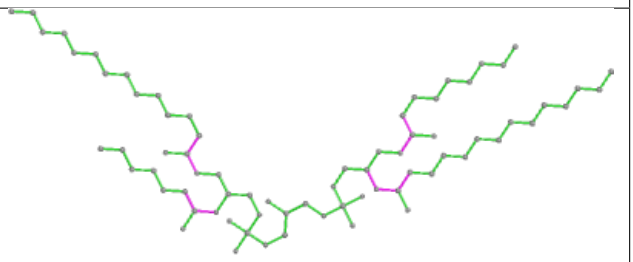
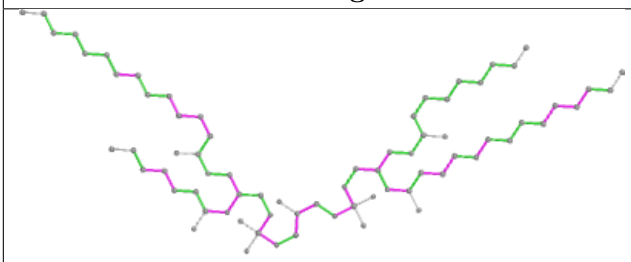


Bond angles



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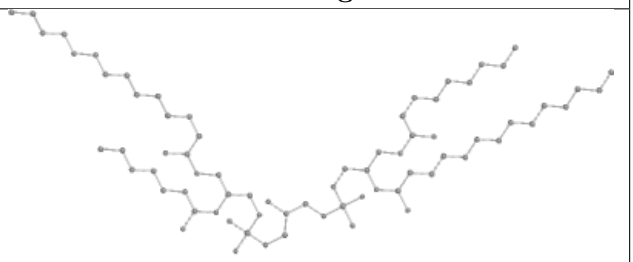
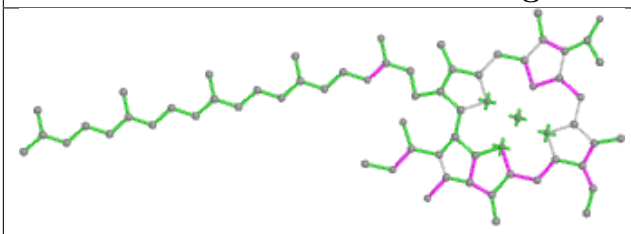
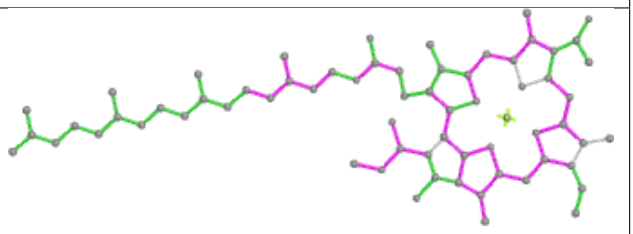


Rings

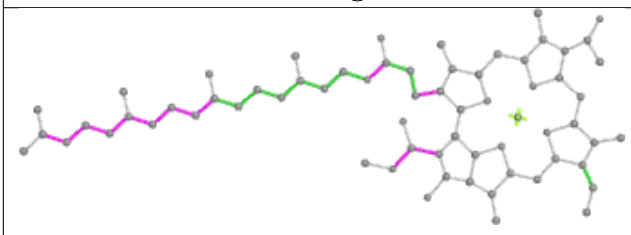
Ligand BCB X 102



Bond lengths



Bond angles



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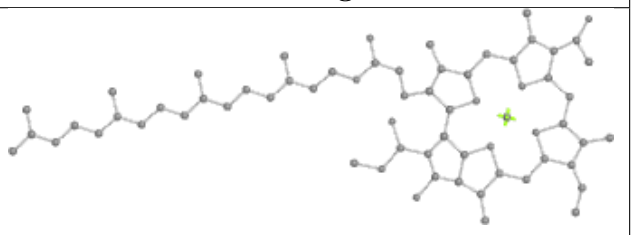
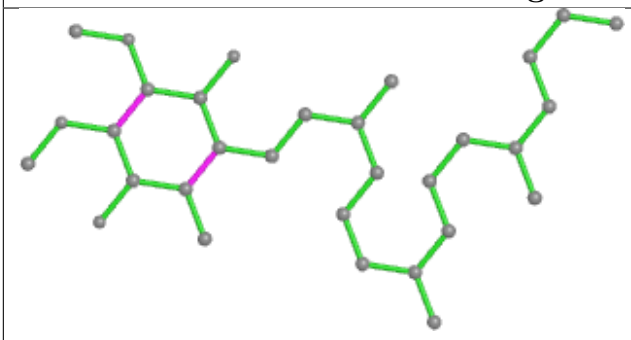
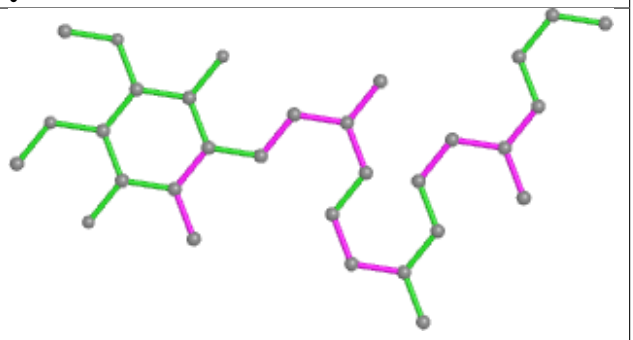


Rings

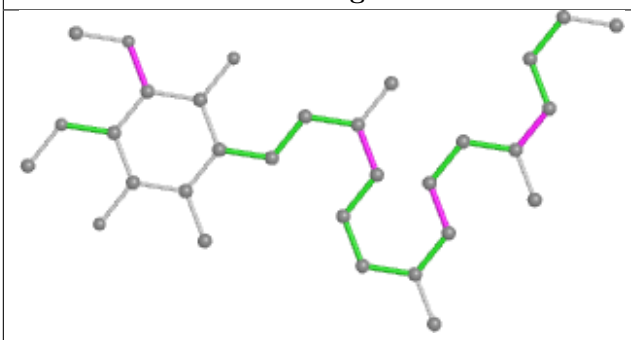
Ligand UQ8 L 305



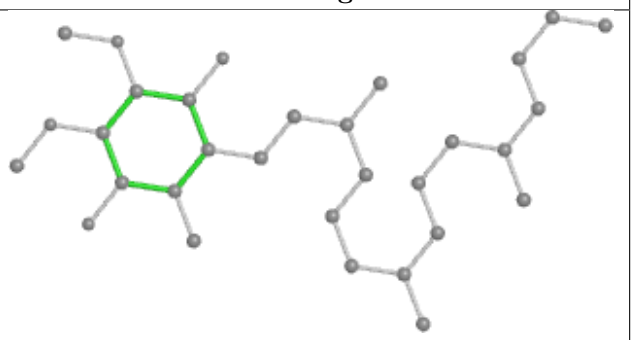
Bond lengths



Bond angles

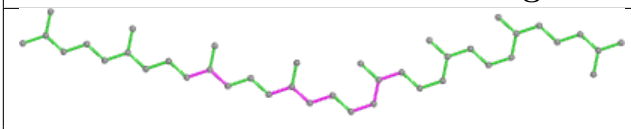


Torsions

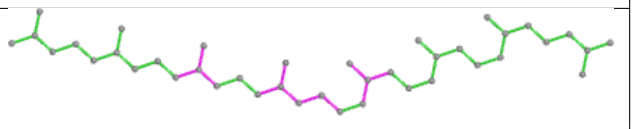


Rings

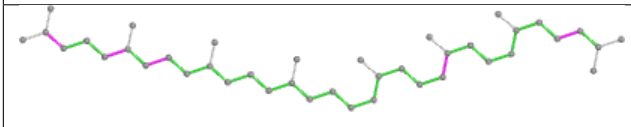
Ligand NS0 W 303



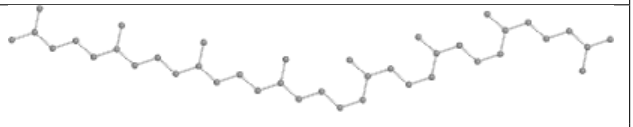
Bond lengths



Bond angles

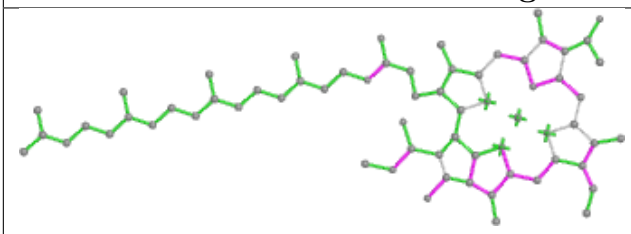


Torsions

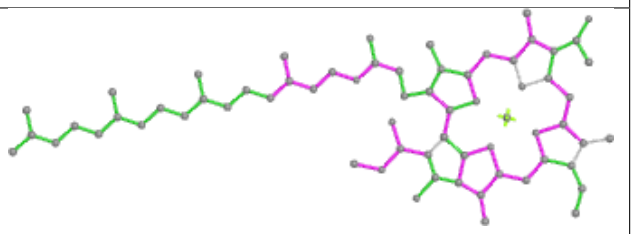


Rings

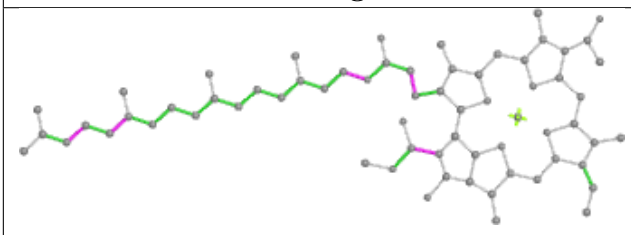
Ligand BCB M 403



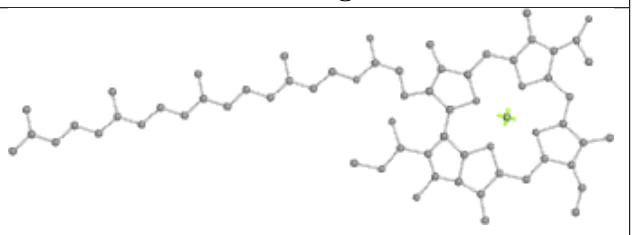
Bond lengths



Bond angles

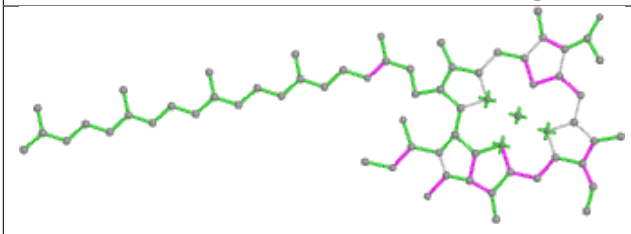


Torsions

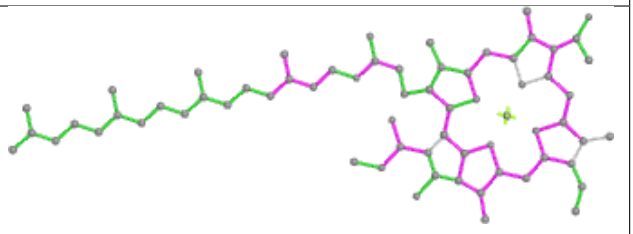


Rings

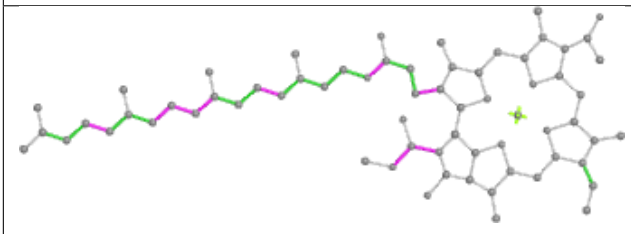
Ligand BCB r 101



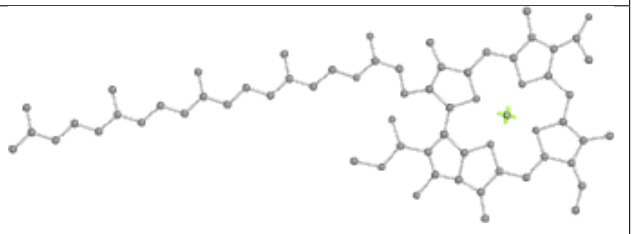
Bond lengths



Bond angles

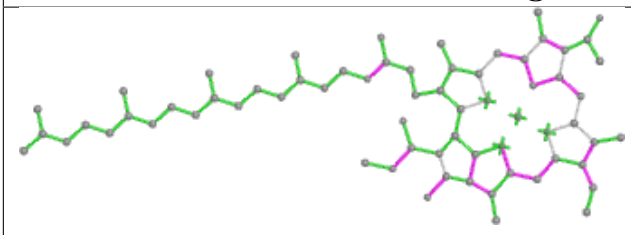


Torsions

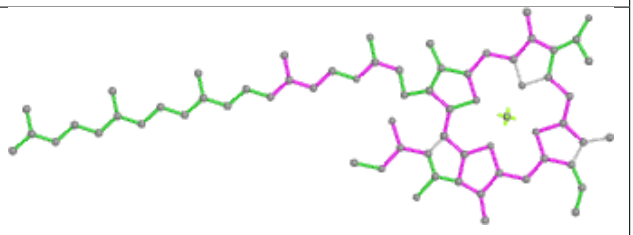


Rings

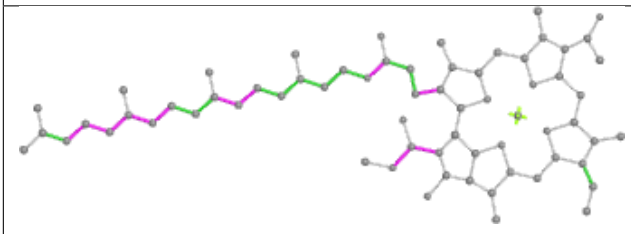
Ligand BCB o 102



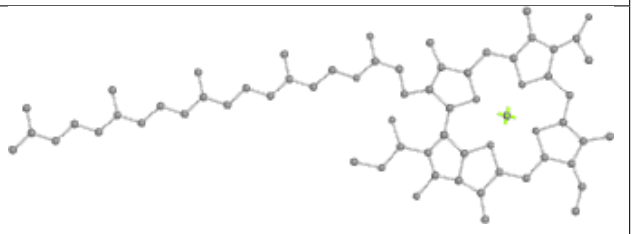
Bond lengths



Bond angles

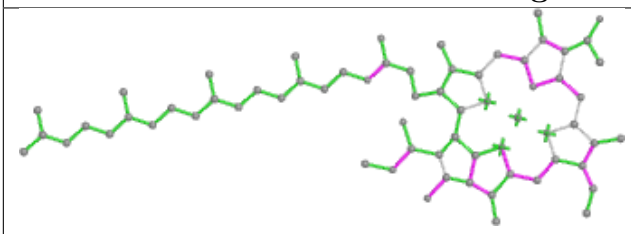


Torsions

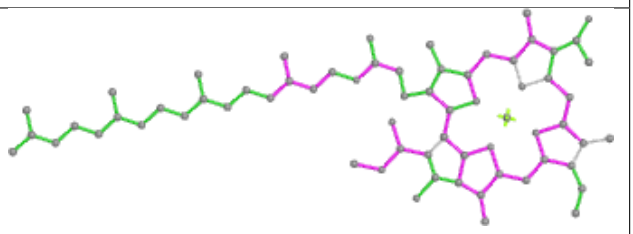


Rings

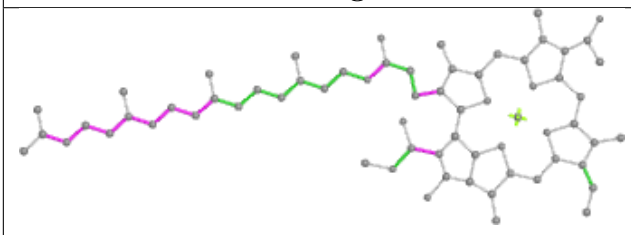
Ligand BCB f 101



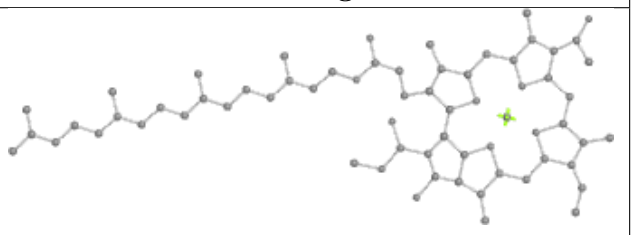
Bond lengths



Bond angles

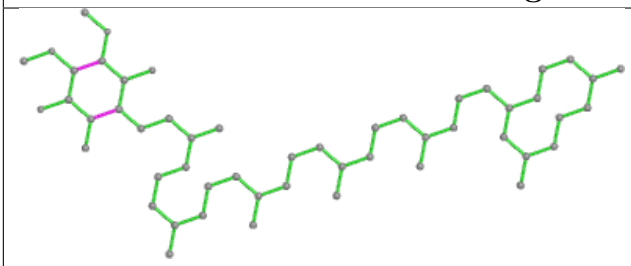


Torsions

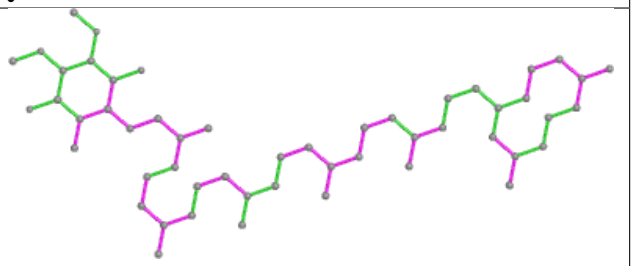


Rings

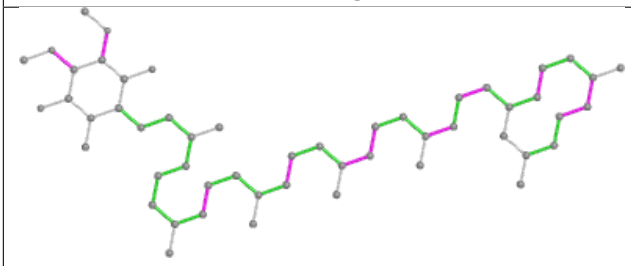
Ligand UQ8 A 101



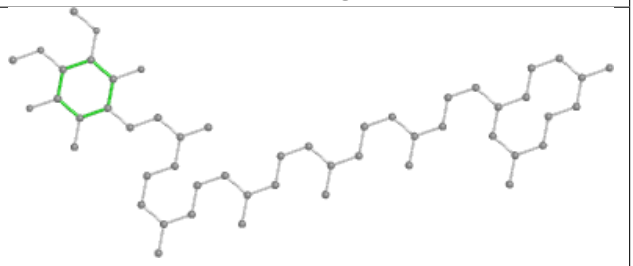
Bond lengths



Bond angles

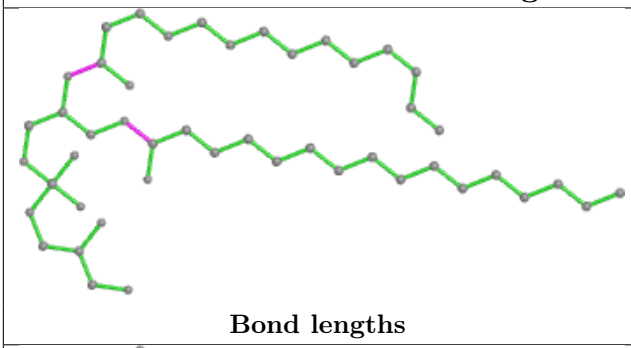


Torsions

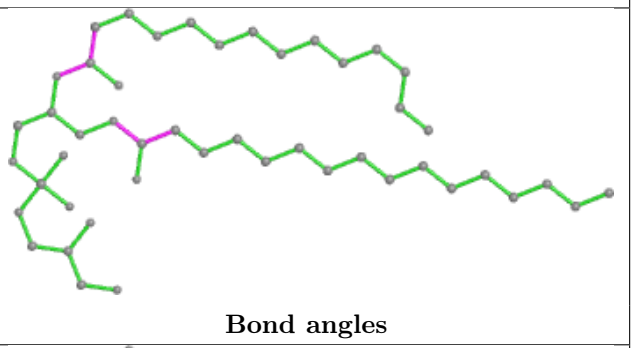


Rings

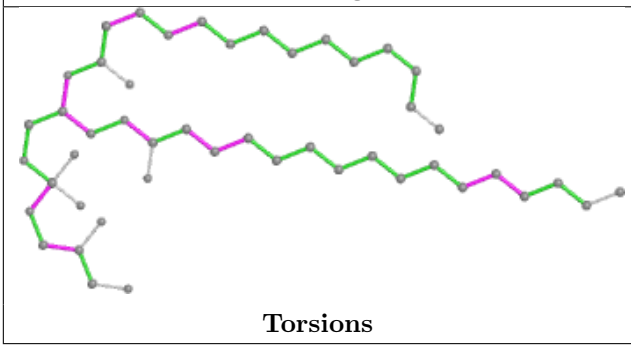
Ligand PGV D 102



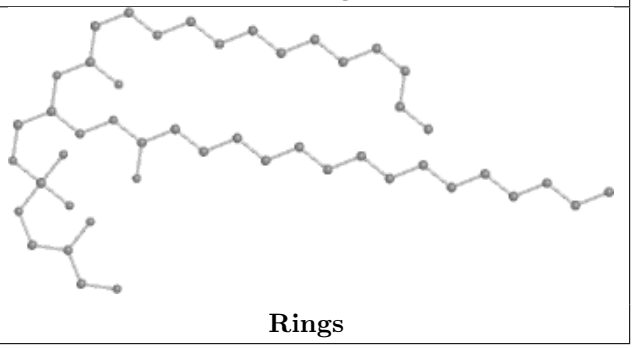
Bond lengths



Bond angles

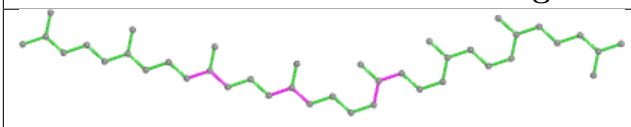


Torsions

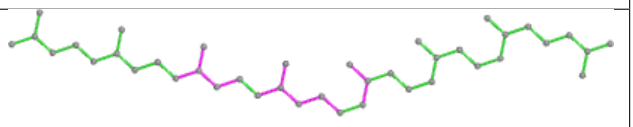


Rings

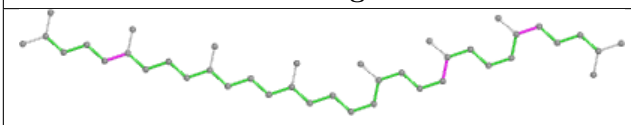
Ligand NS0 o 101



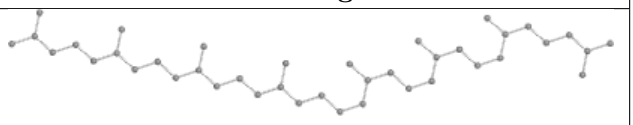
Bond lengths



Bond angles

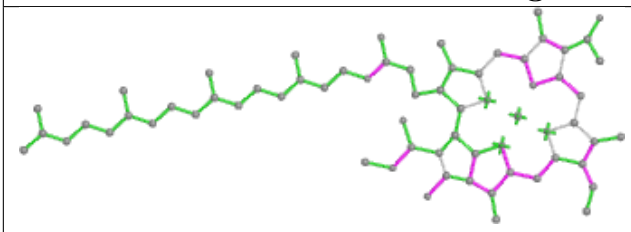


Torsions

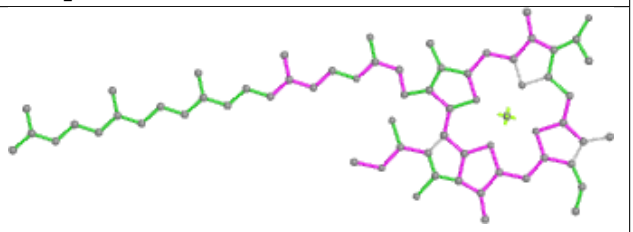


Rings

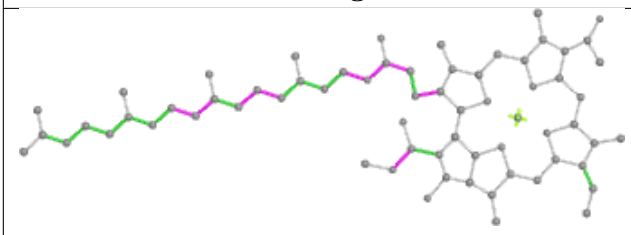
Ligand BCB q 101



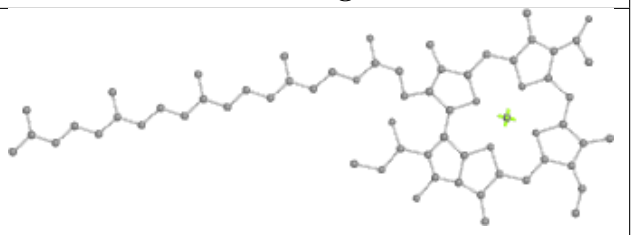
Bond lengths



Bond angles

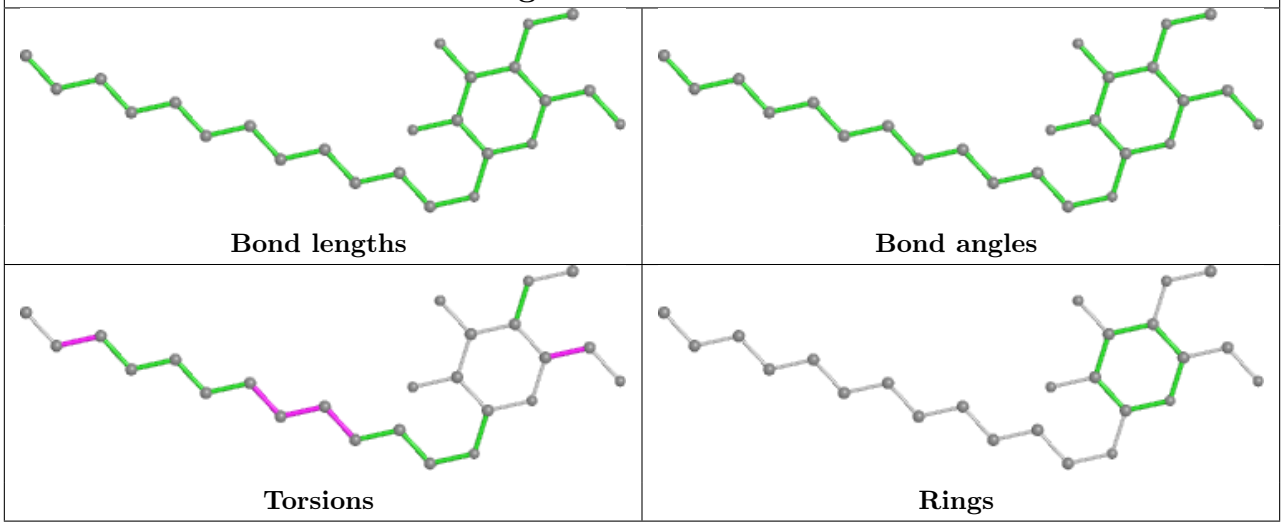


Torsions

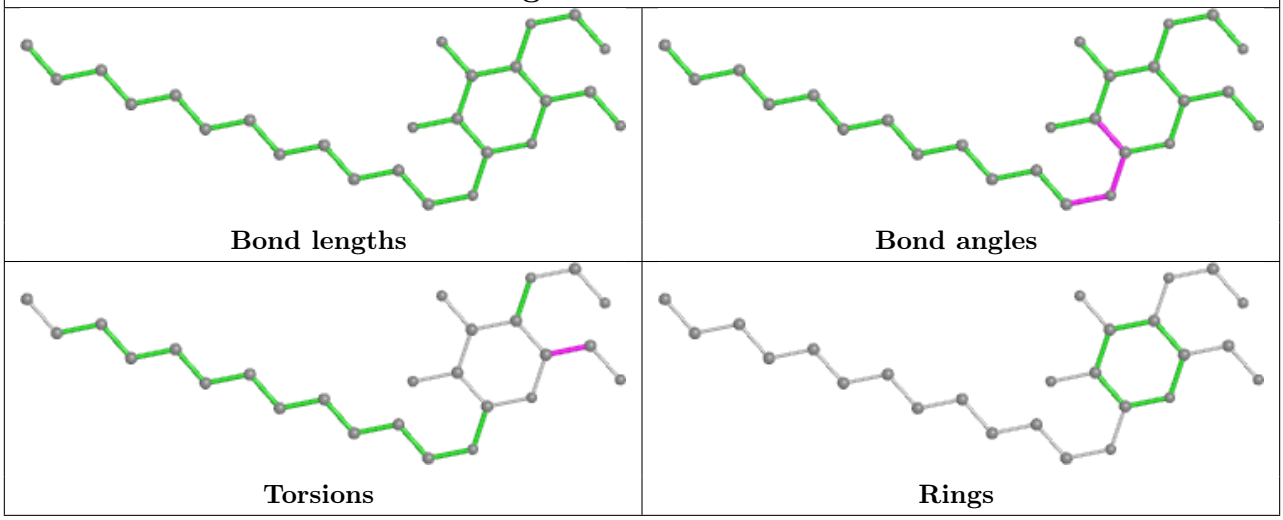


Rings

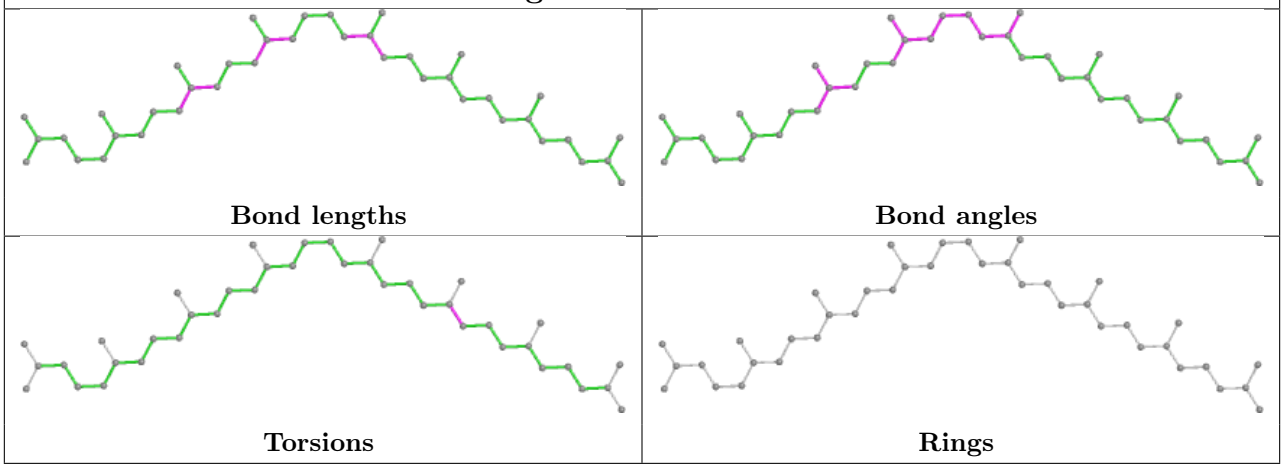
Ligand LMT M 410



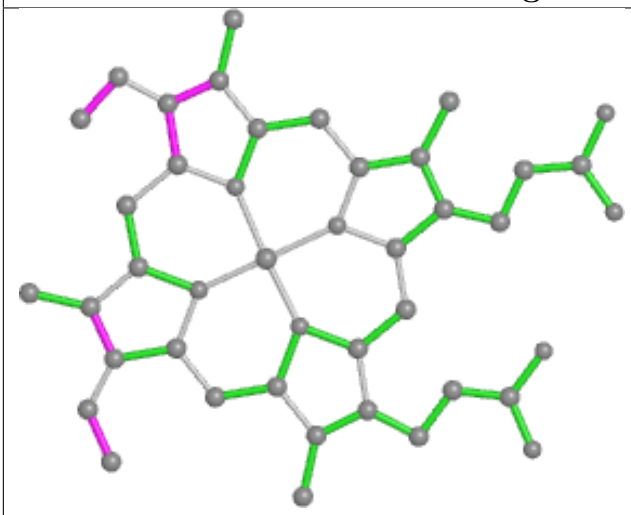
Ligand LMT T 102



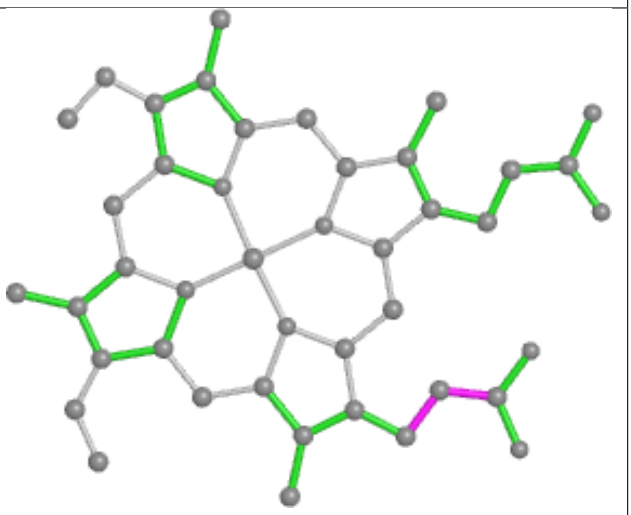
Ligand NS5 M 406



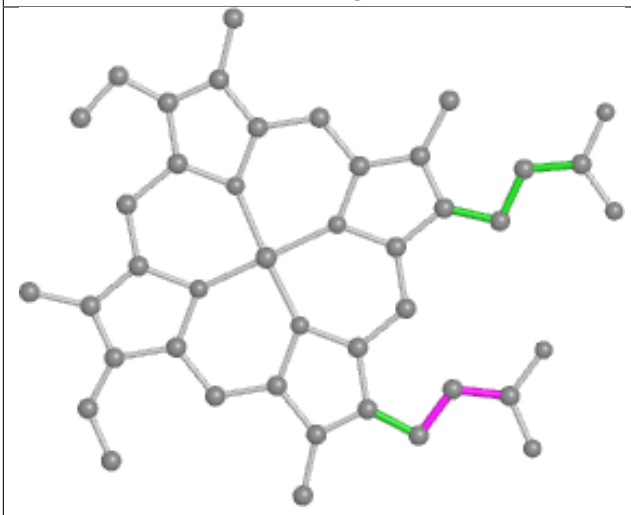
Ligand HEC C 404



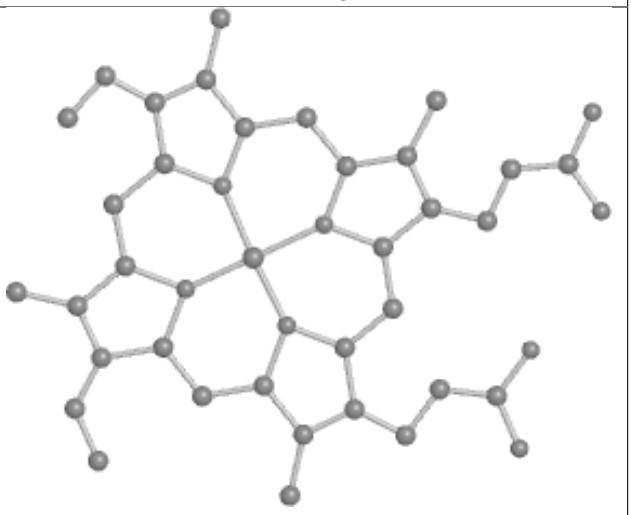
Bond lengths



Bond angles

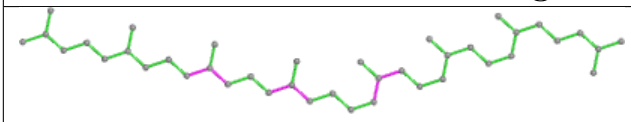


Torsions

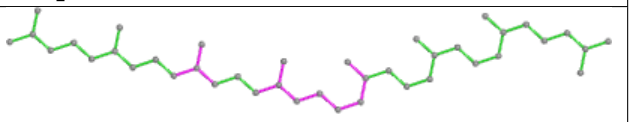


Rings

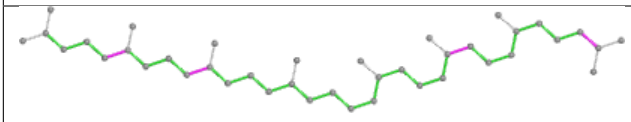
Ligand NS0 q 102



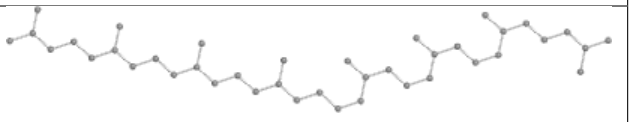
Bond lengths



Bond angles

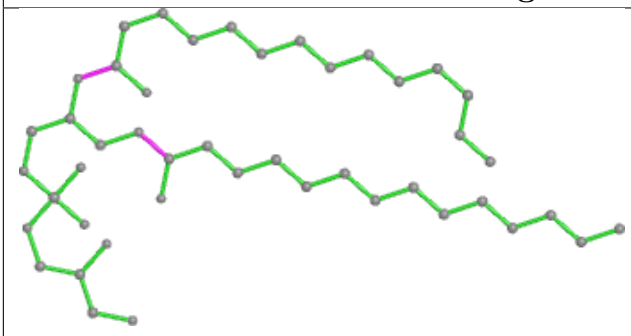


Torsions

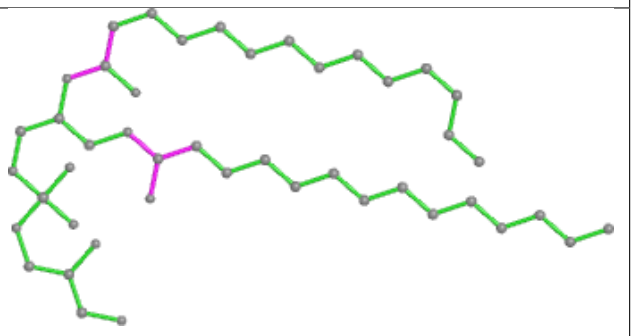


Rings

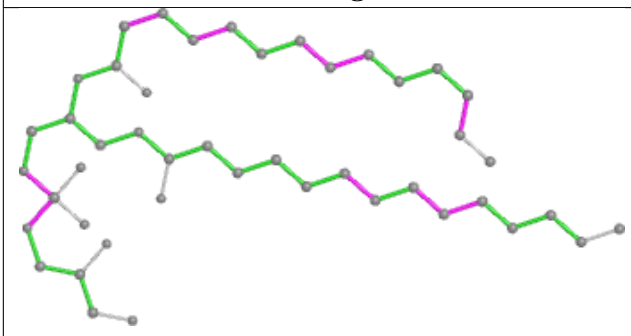
Ligand PGV M 411



Bond lengths



Bond angles



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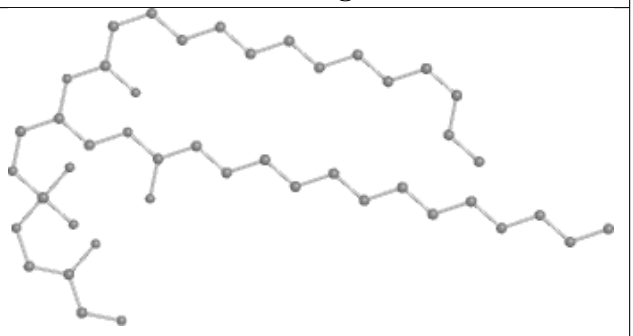
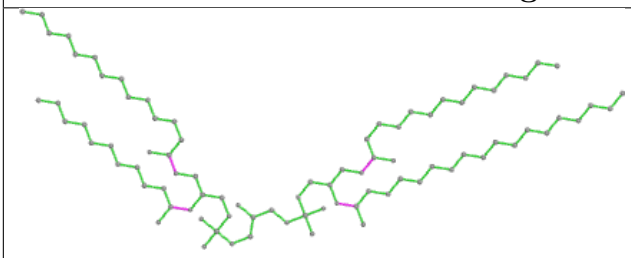
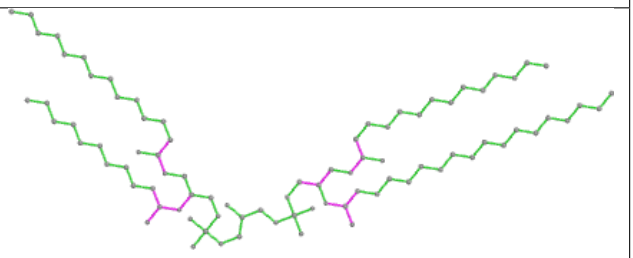


Rings

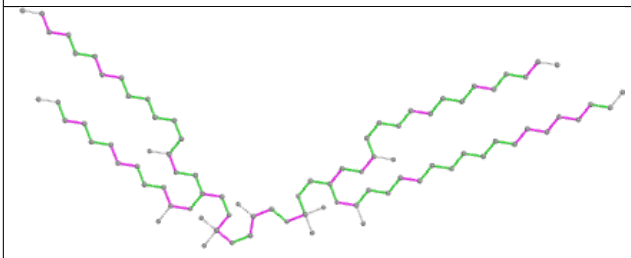
Ligand CDL M 409



Bond lengths



Bond angles



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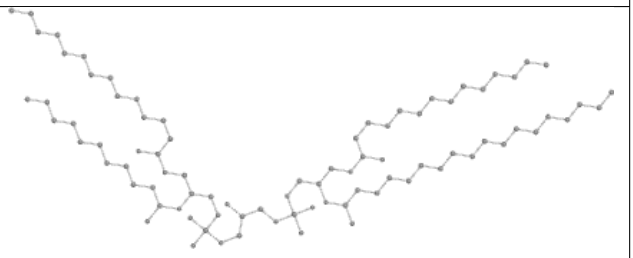
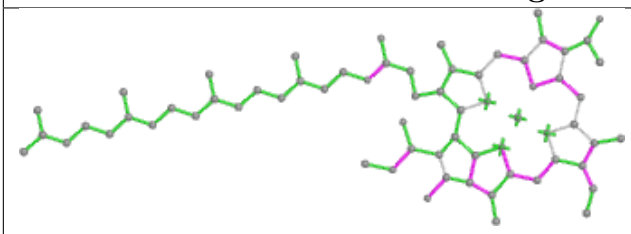


Rings

Ligand BCB e 101



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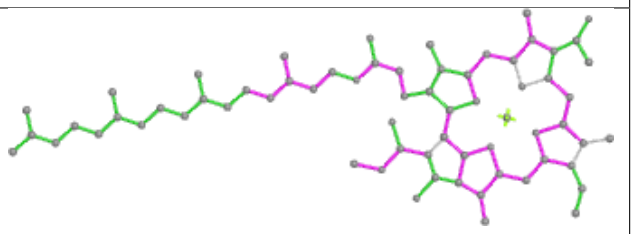
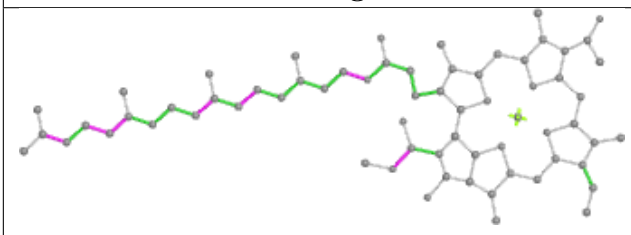
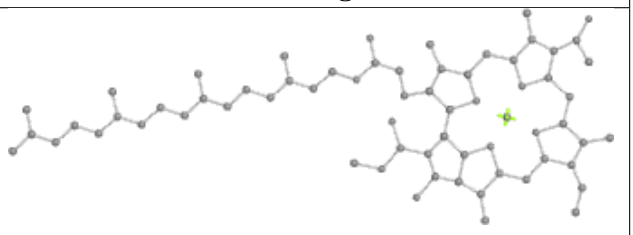


Bond angles

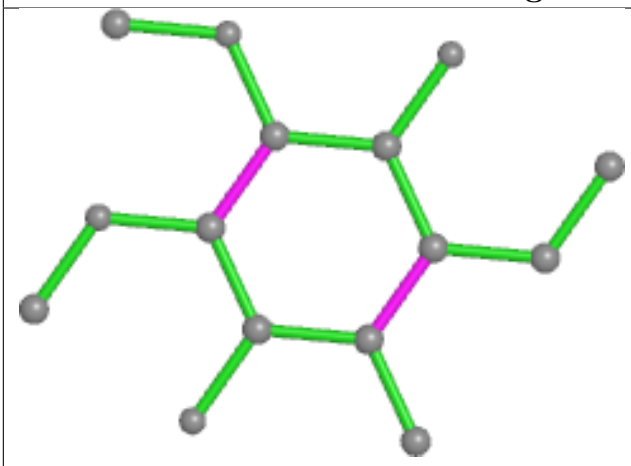


Torsions



Rings

Ligand UQ8 C 406



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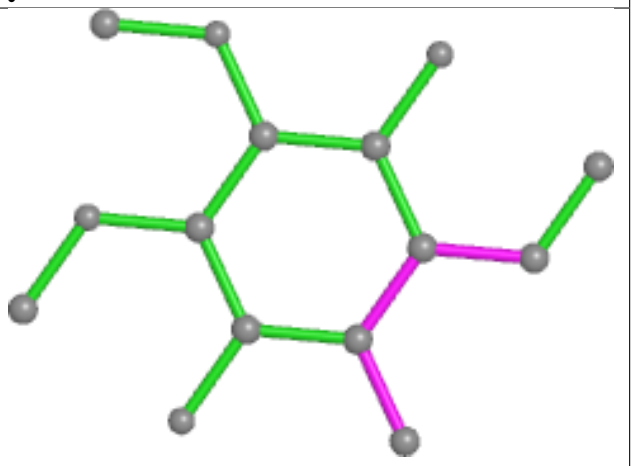
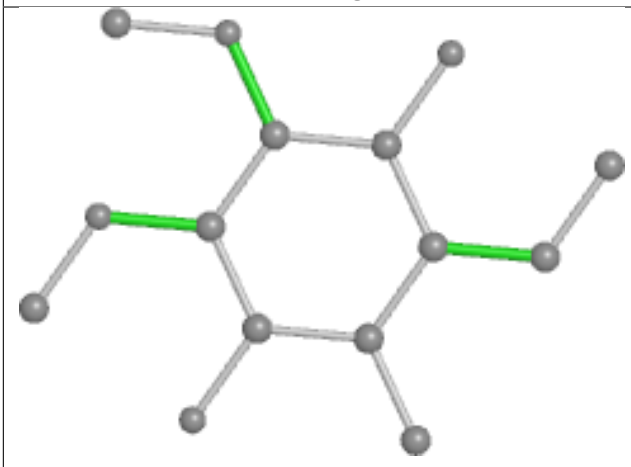


Bond angles



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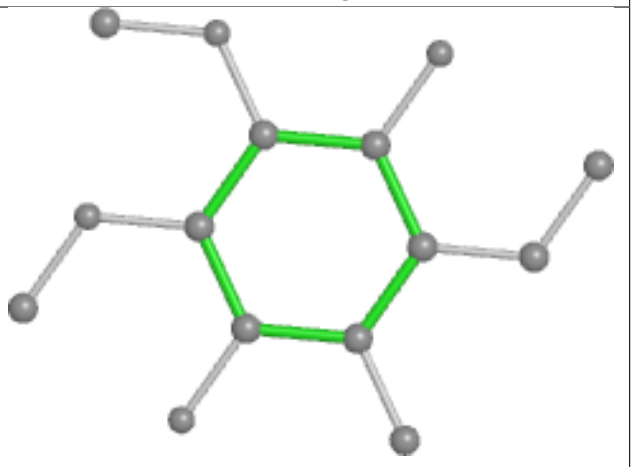
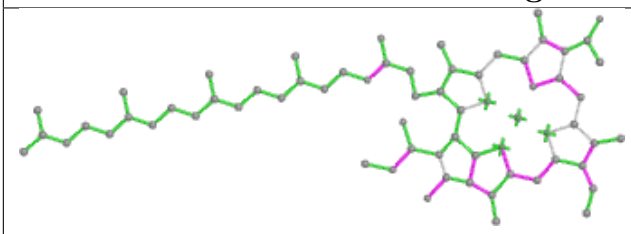
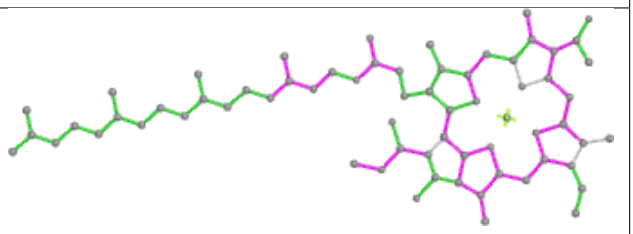


Rings

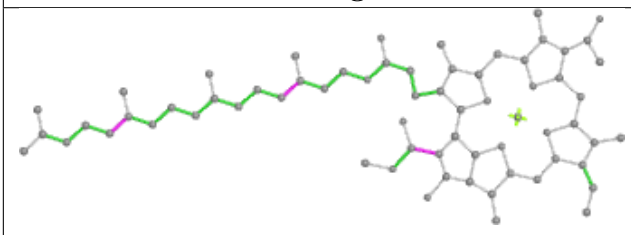
Ligand BCB L 302



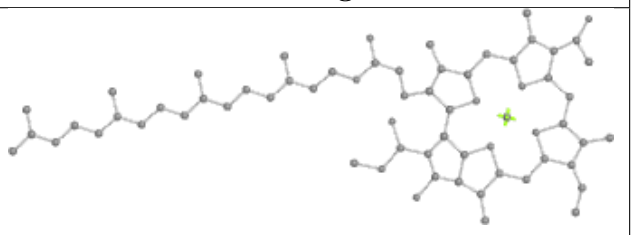
Bond lengths



Bond angles

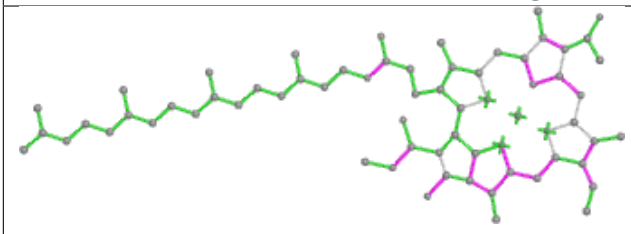


Torsions



Rings

Ligand BCB k 102



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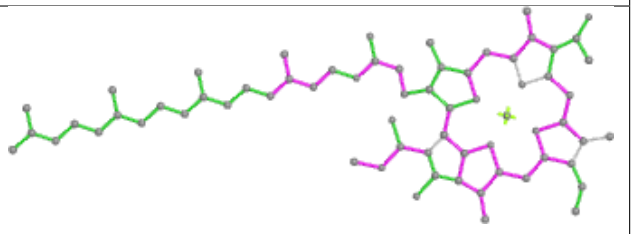
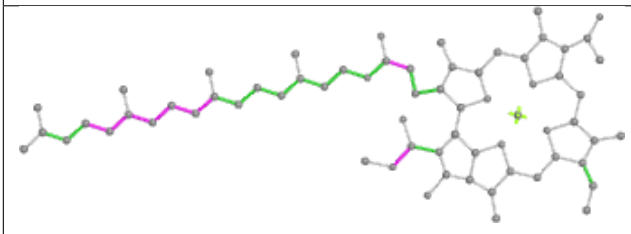
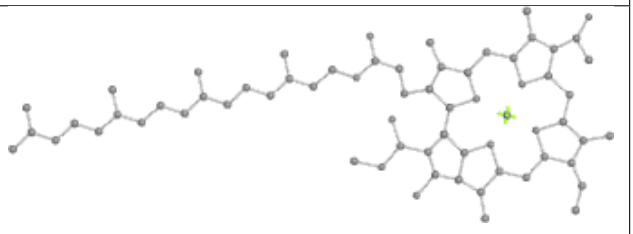


Bond angles

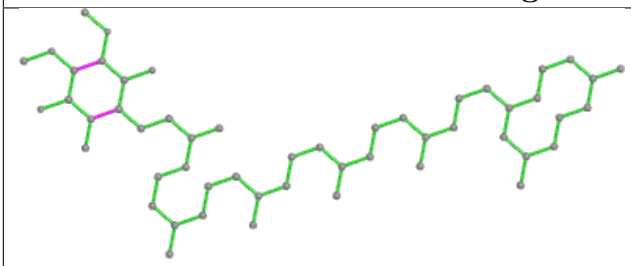


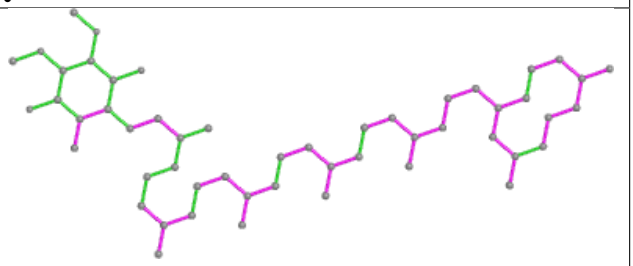
Torsions

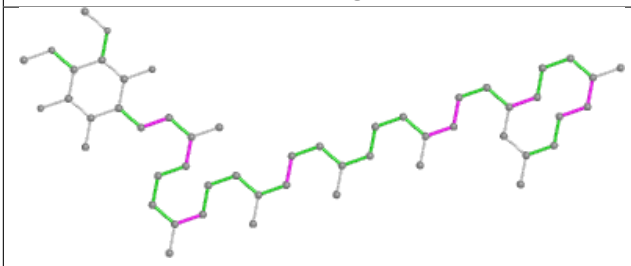


Rings

Ligand UQ8 M 408


Bond lengths


Bond angles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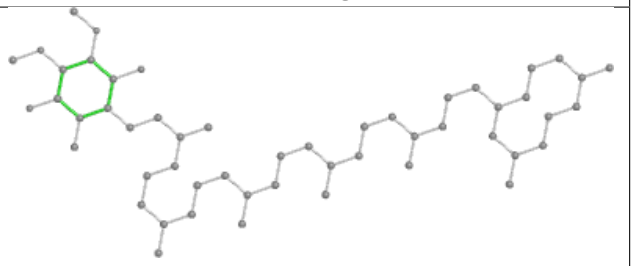
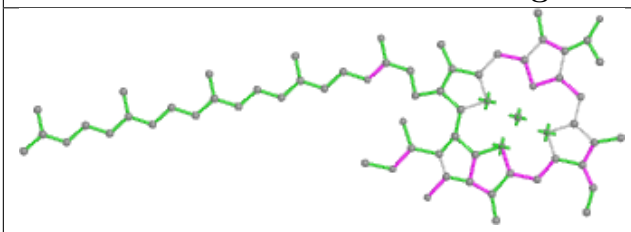

Rings

Ligand BCB l 102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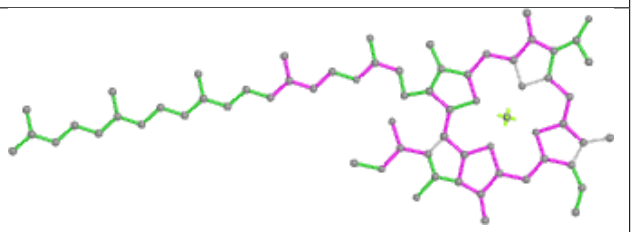
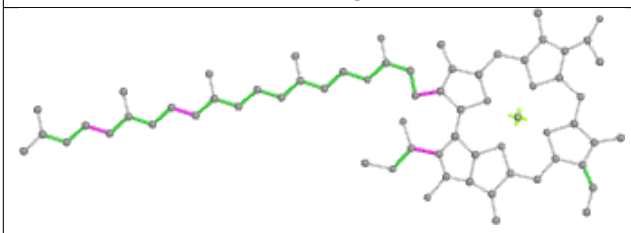
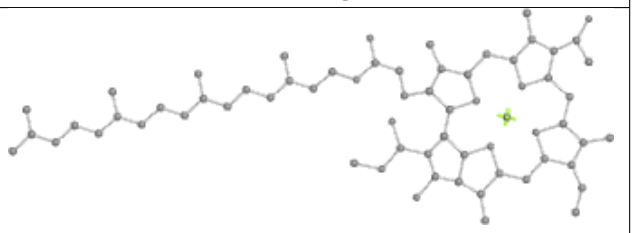
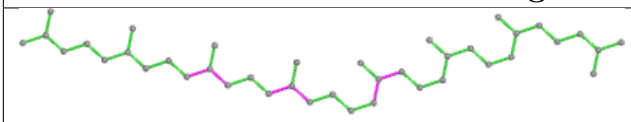

Bond angles


Torsions


Rings

Ligand NS0 O 101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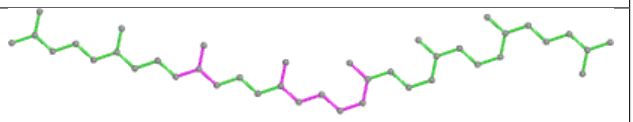
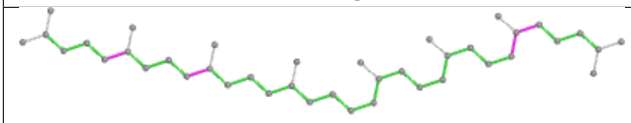
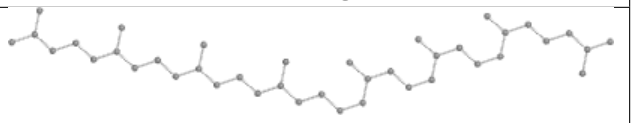
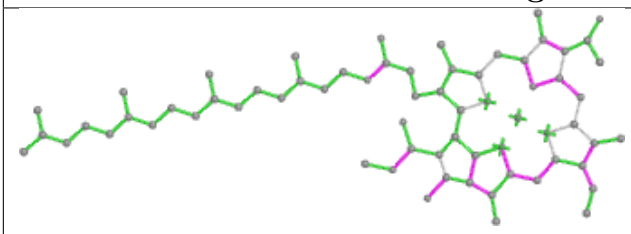

Bond angles

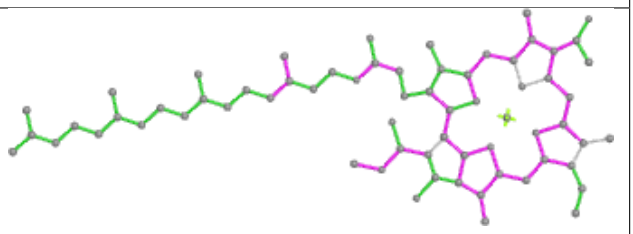

Torsions


Rings

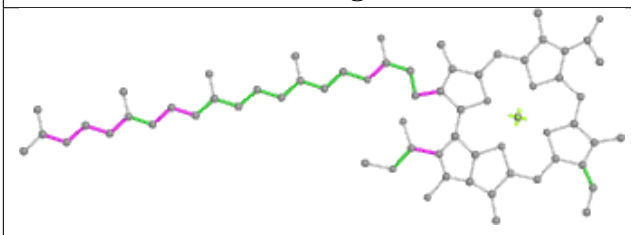
Ligand BCB 1 101



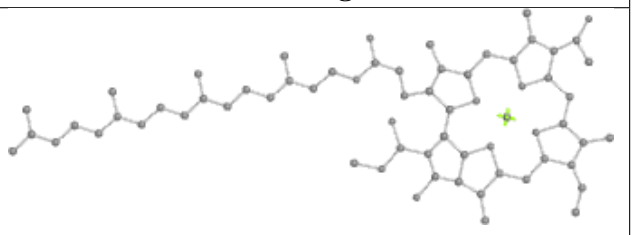
Bond lengths



Bond angles

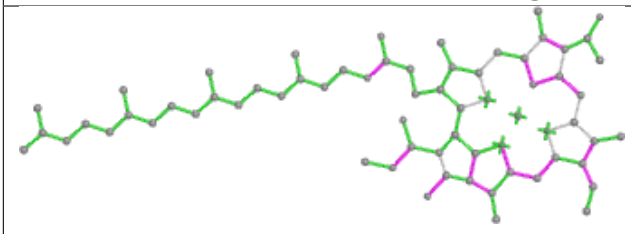


Torsions



Rings

Ligand BCB n 101



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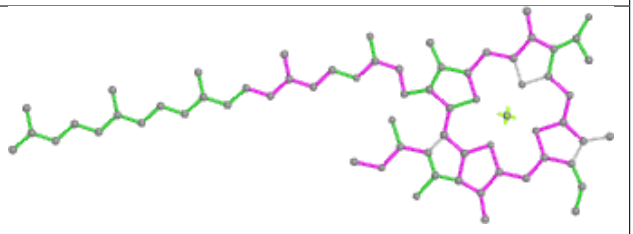
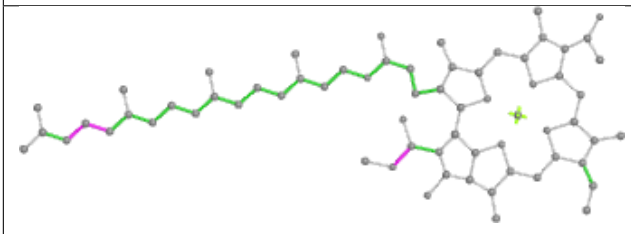
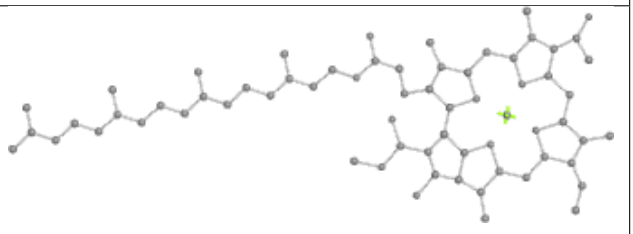


Bond angles

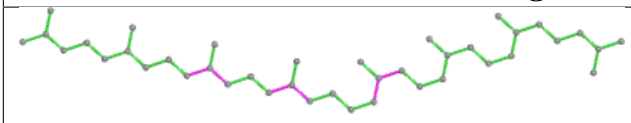


Torsions

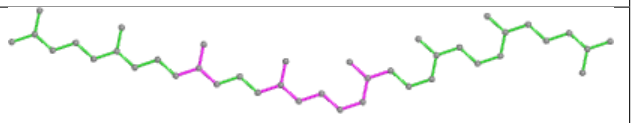


Rings

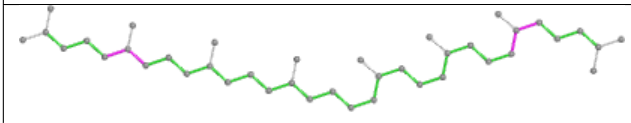
Ligand NS0 U 101



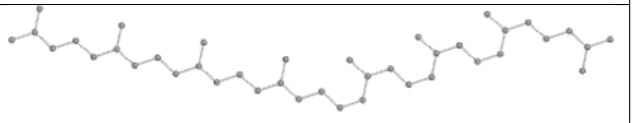
Bond lengths



Bond angles

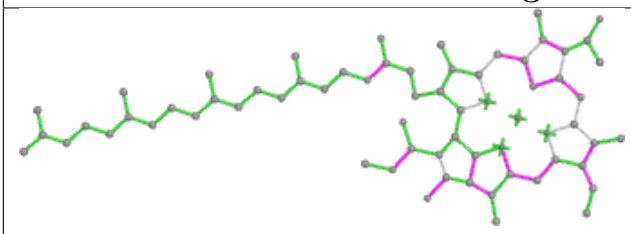


Torsions

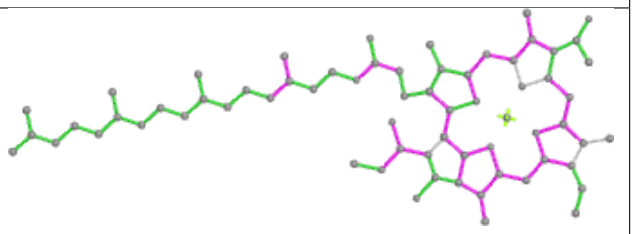


Rings

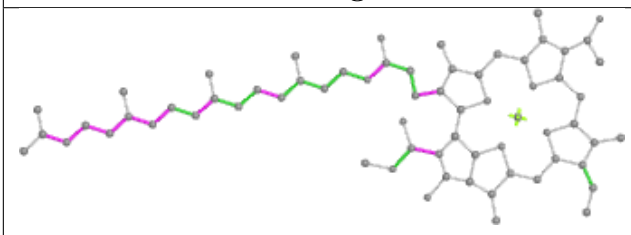
Ligand BCB O 102



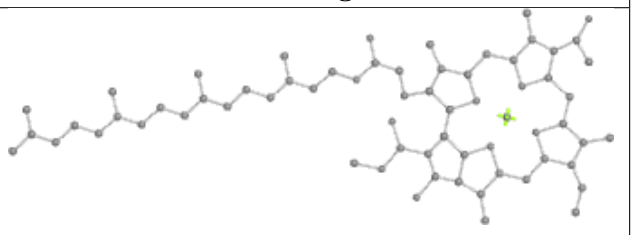
Bond lengths



Bond angles

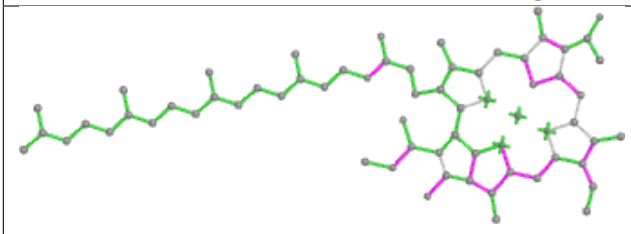


Torsions

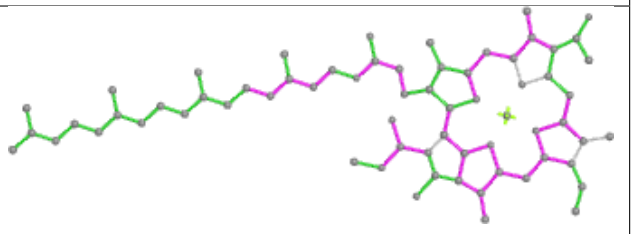


Rings

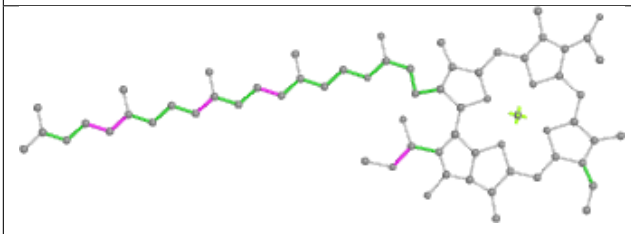
Ligand BCB I 101



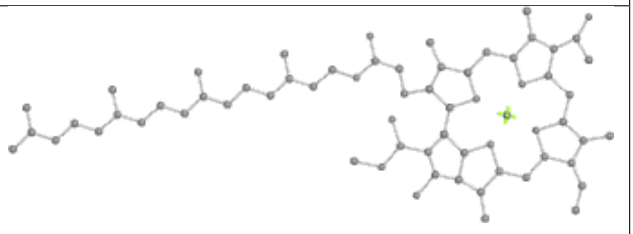
Bond lengths



Bond angles

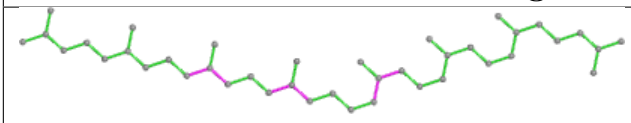


Torsions

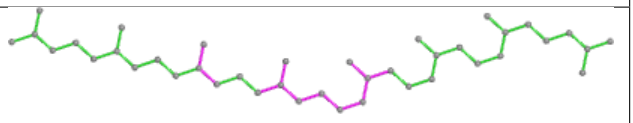


Rings

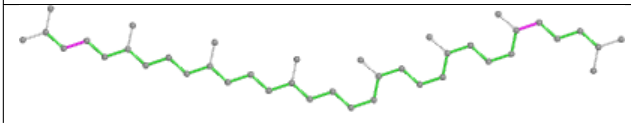
Ligand NS0 D 103



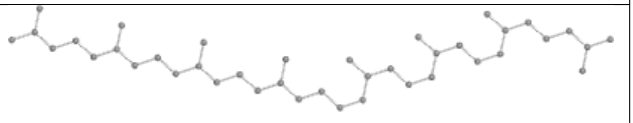
Bond lengths



Bond angles

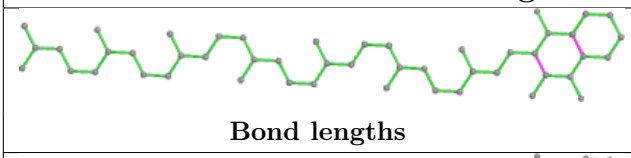


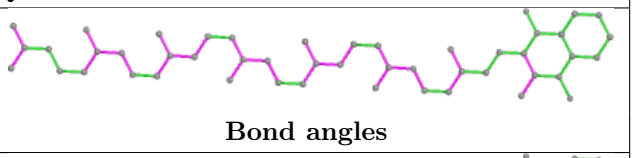
Torsions

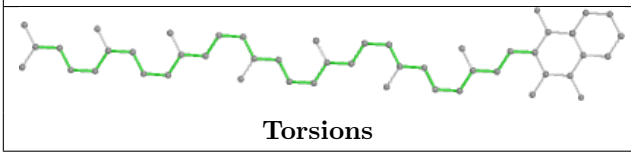


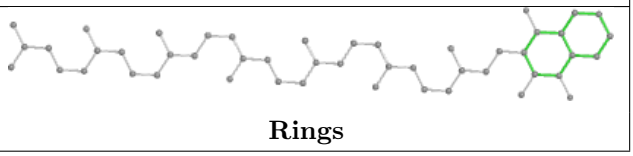
Rings

Ligand MQ7 M 405

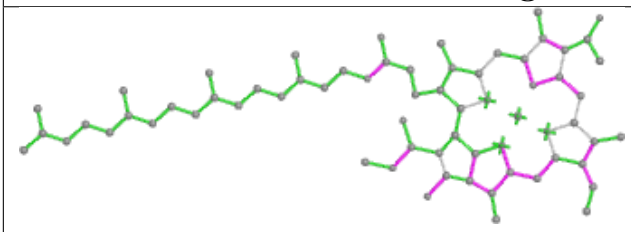

Bond lengths

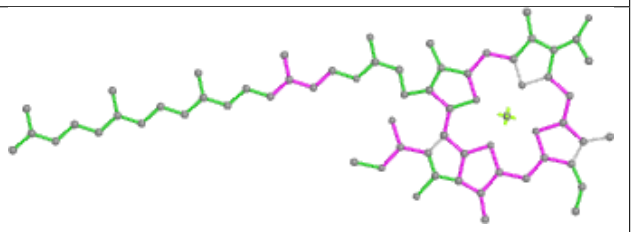

Bond angles

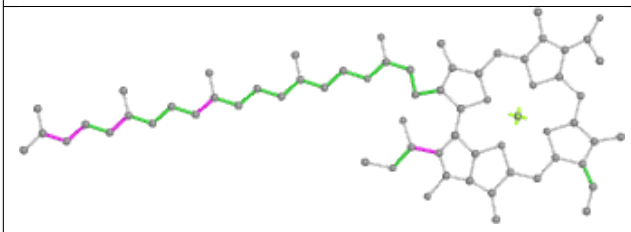

Torsions

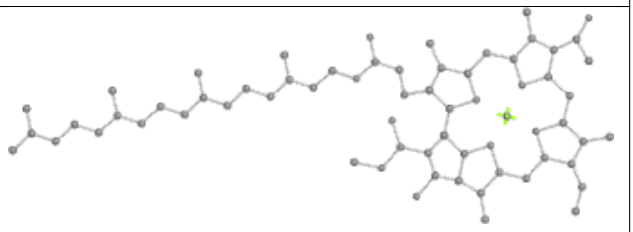

Rings

Ligand BCB M 402

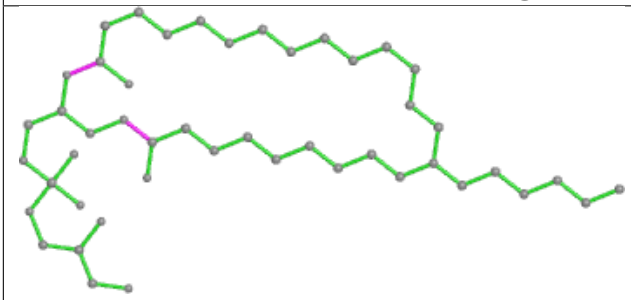

Bond lengths

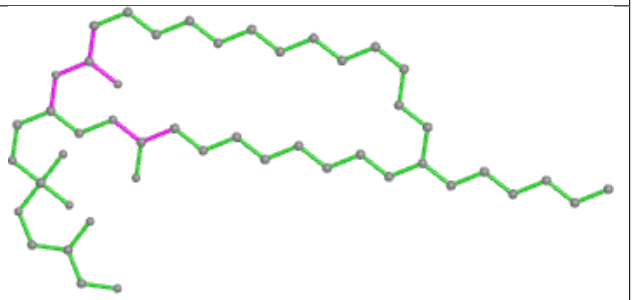

Bond angles

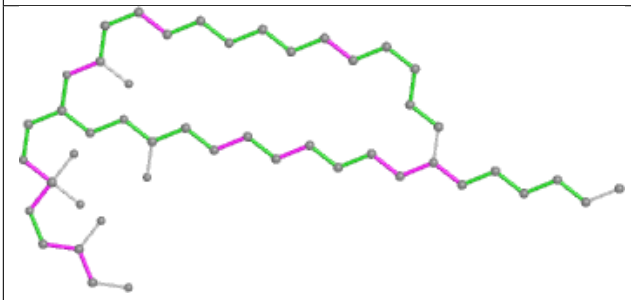

Torsions

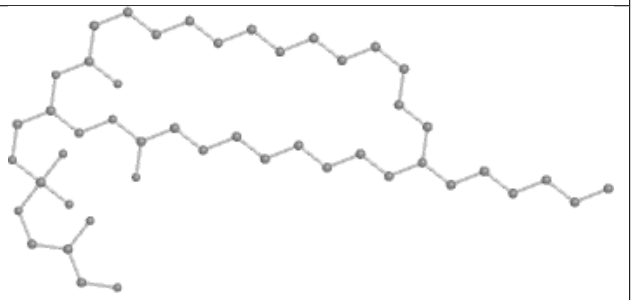

Rings

Ligand PGV W 301

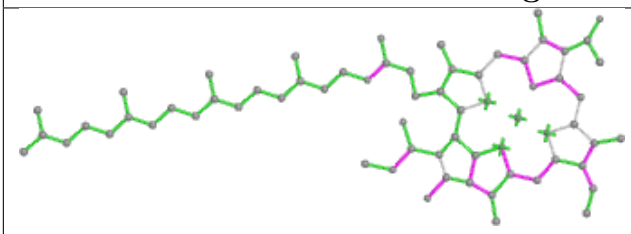

Bond lengths


Bond angles

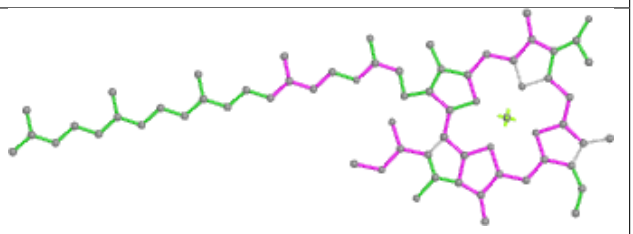

Torsions


Rings

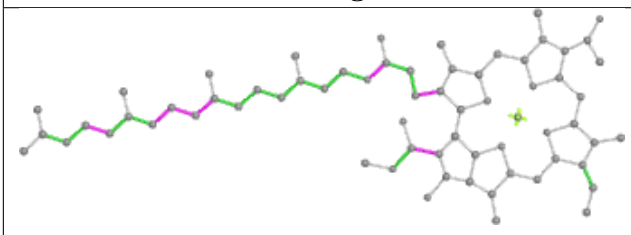
Ligand BCB R 102



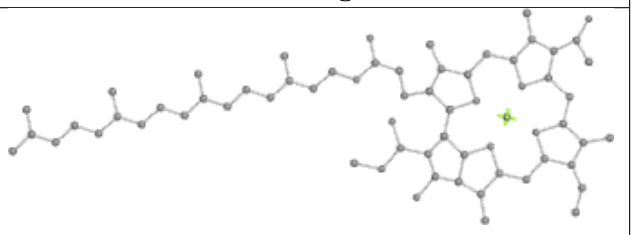
Bond lengths



Bond angles

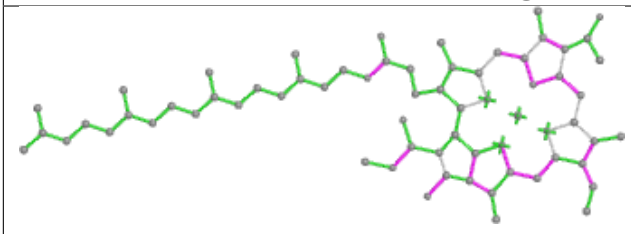


Torsions

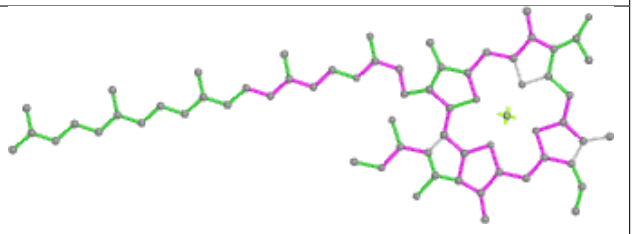


Rings

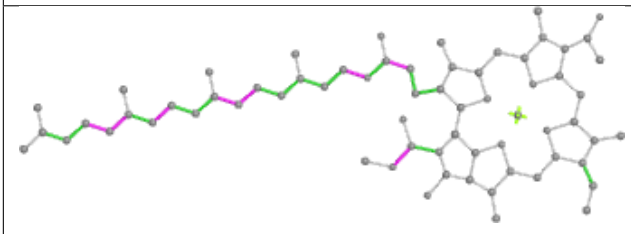
Ligand BCB W 302



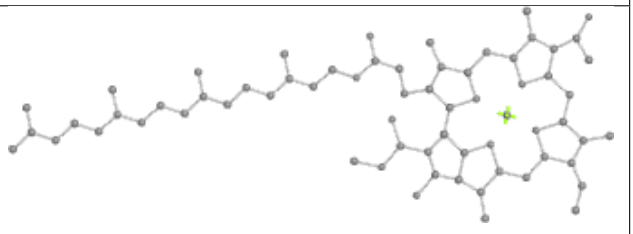
Bond lengths



Bond angles

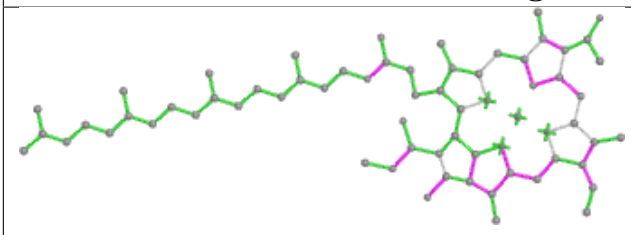


Torsions

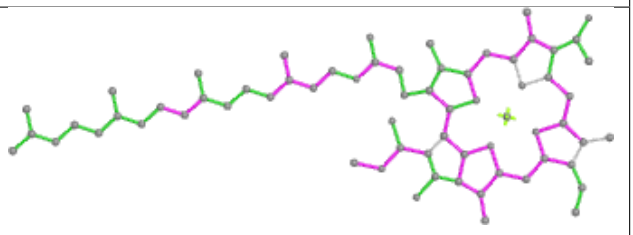


Rings

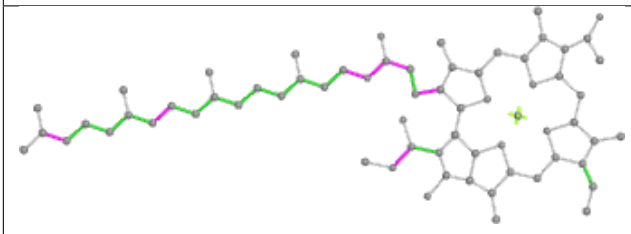
Ligand BCB 9 101



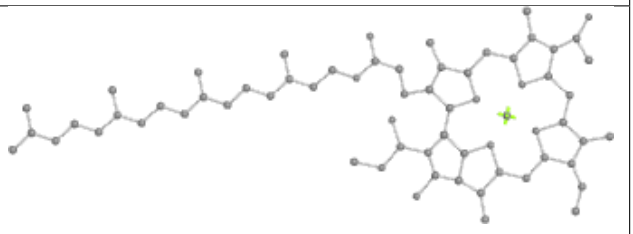
Bond lengths



Bond angles



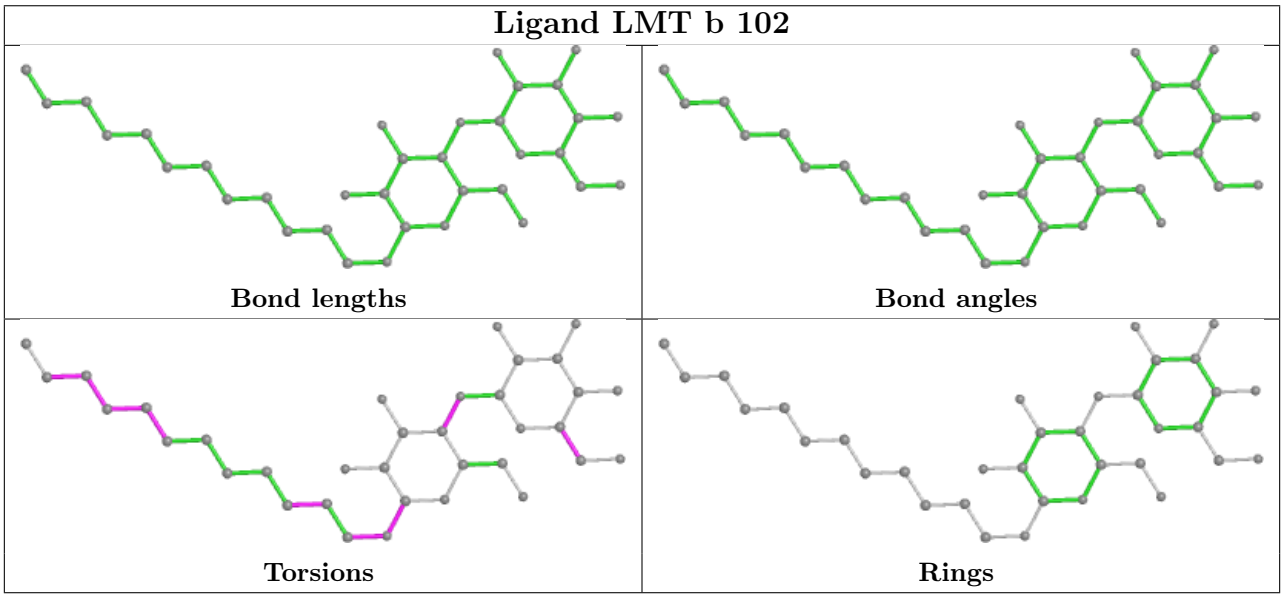
Torsions



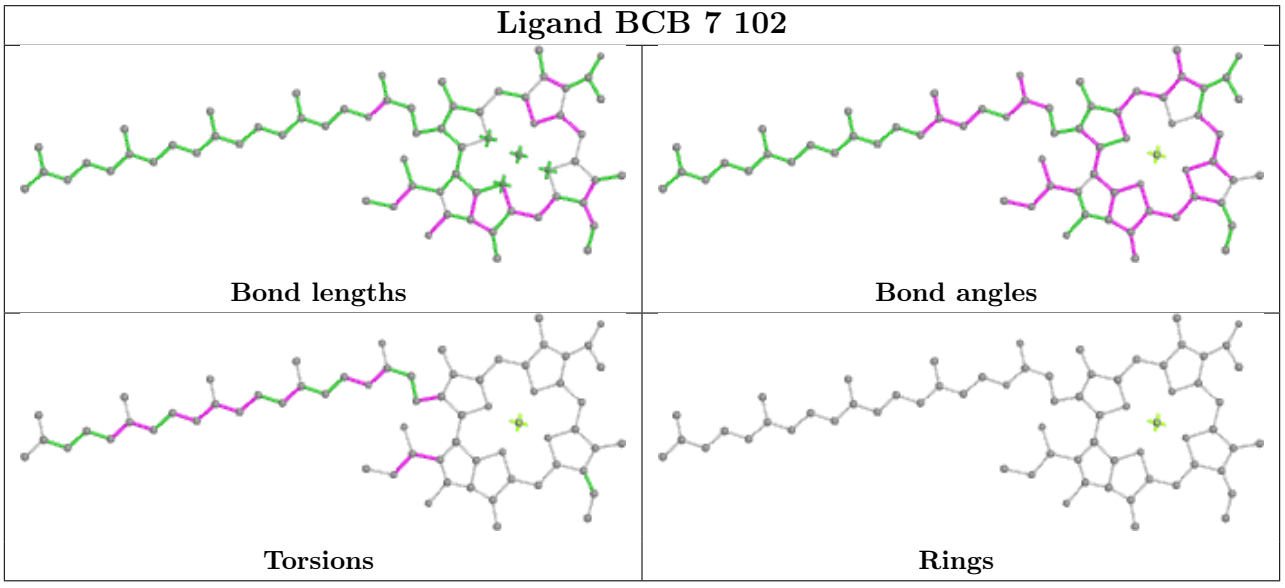
Rings

Ligand NS0 A 103

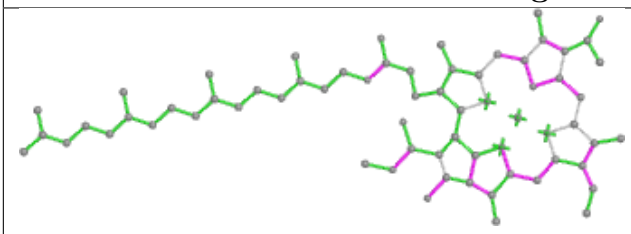
Ligand LMT b 102



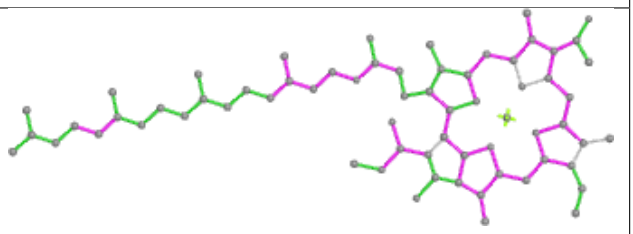
Ligand BCB 7 102



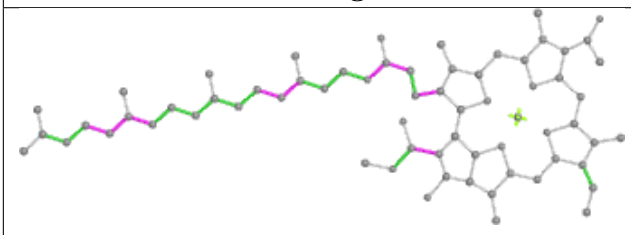
Ligand BCB i 101



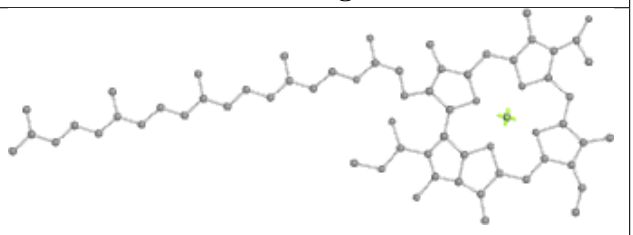
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

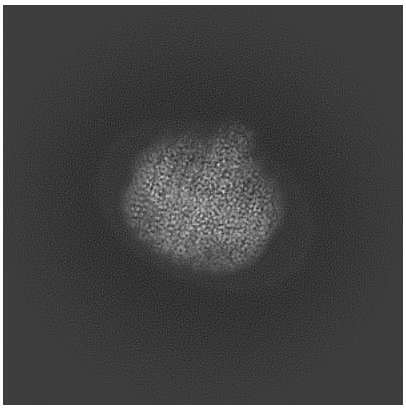
6 Map visualisation

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.

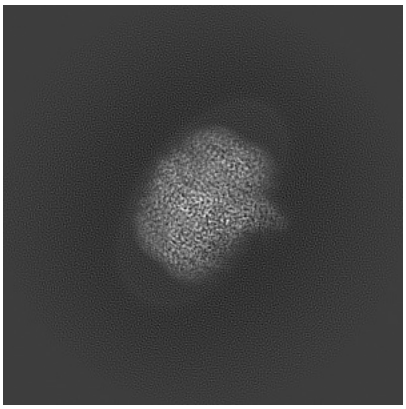
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

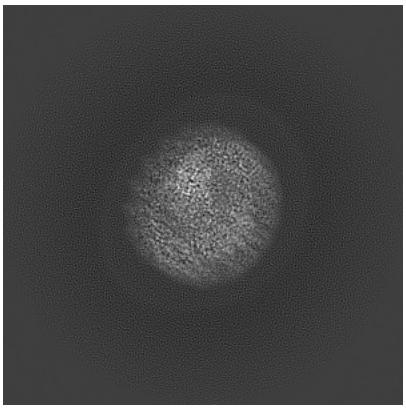
6.1.1 Primary map



X

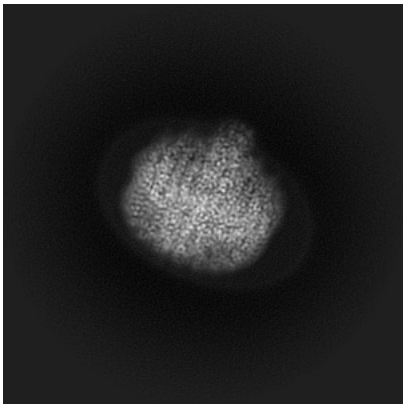


Y

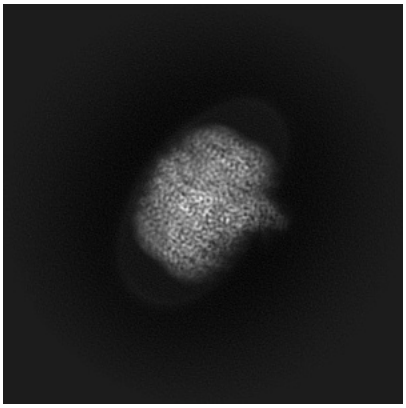


Z

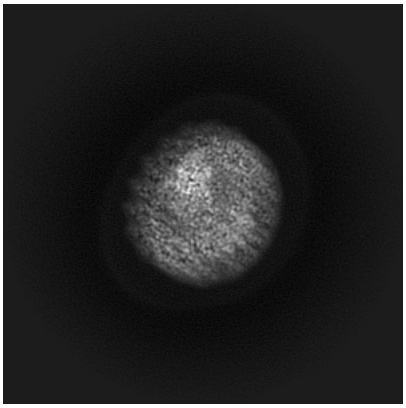
6.1.2 Raw map



X



Y

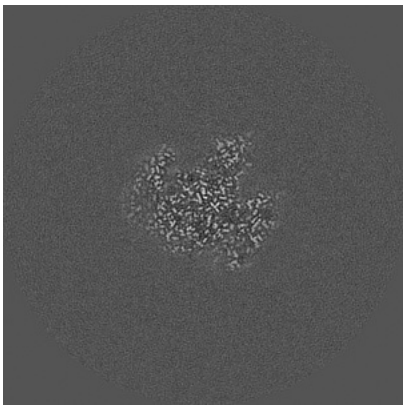


Z

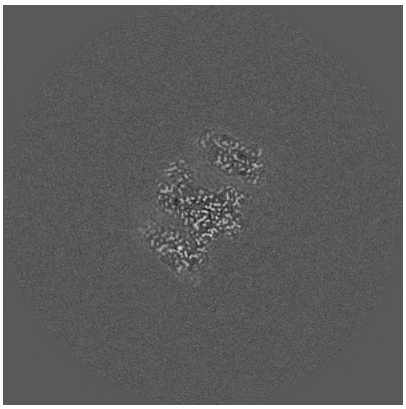
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

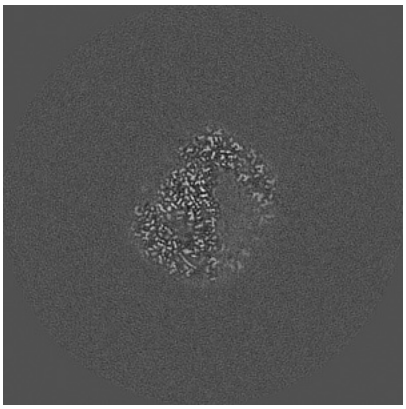
6.2.1 Primary map



X Index: 200

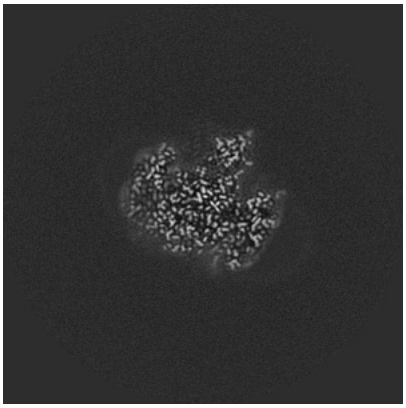


Y Index: 200

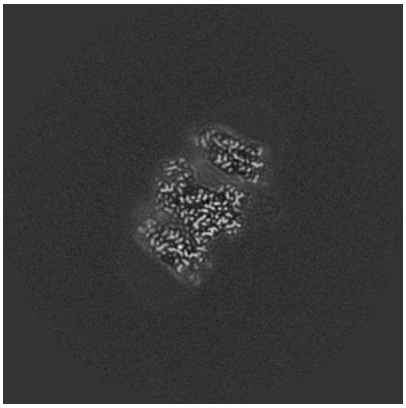


Z Index: 200

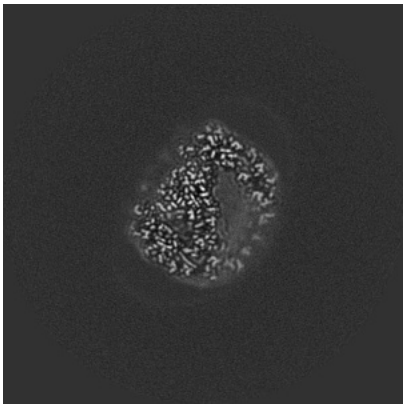
6.2.2 Raw map



X Index: 200



Y Index: 200

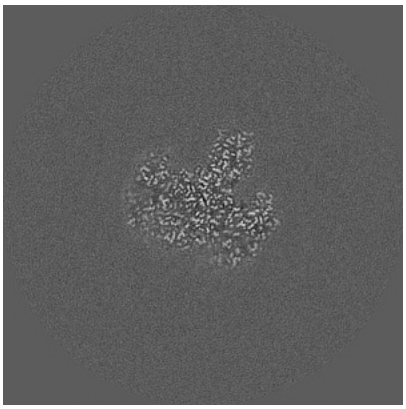


Z Index: 200

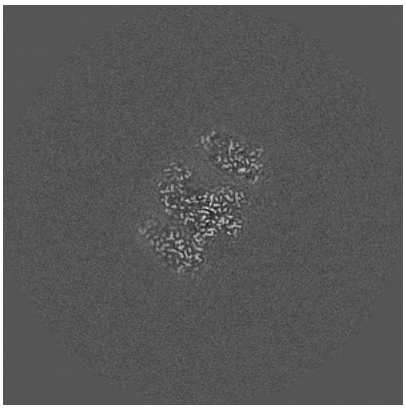
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

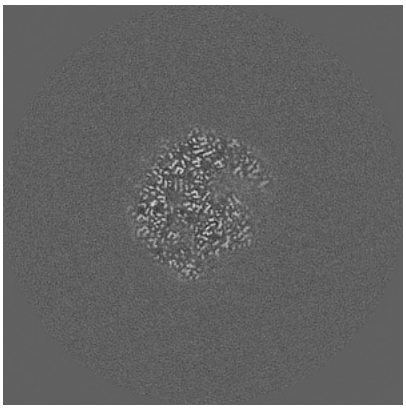
6.3.1 Primary map



X Index: 194

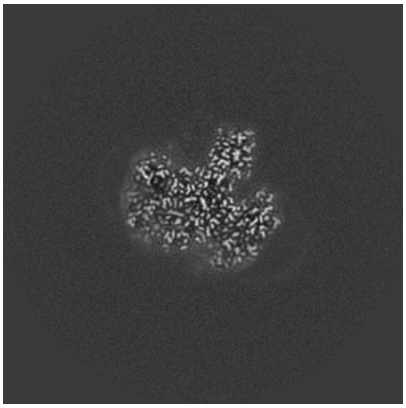


Y Index: 201

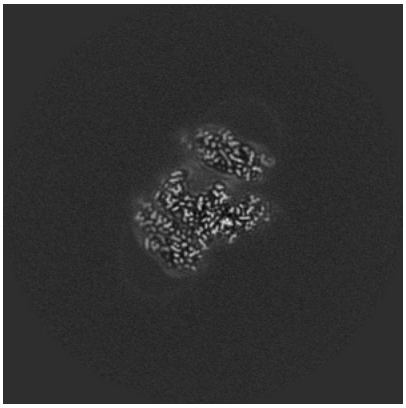


Z Index: 183

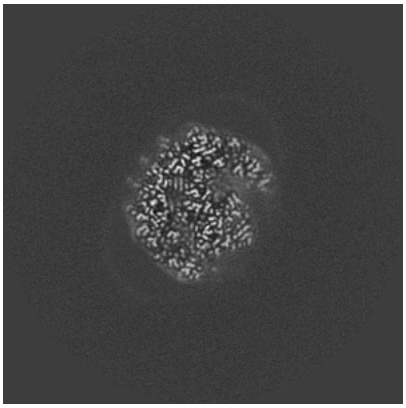
6.3.2 Raw map



X Index: 193



Y Index: 212

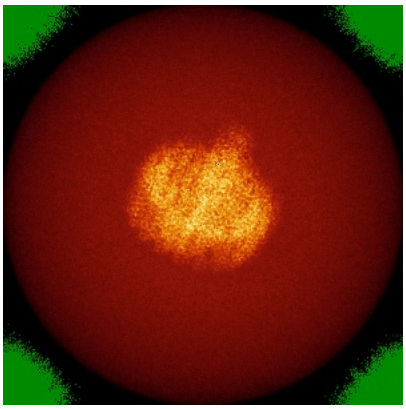


Z Index: 183

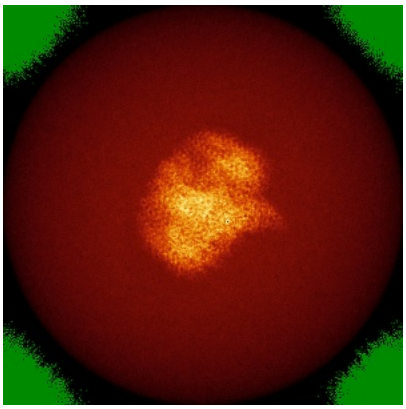
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

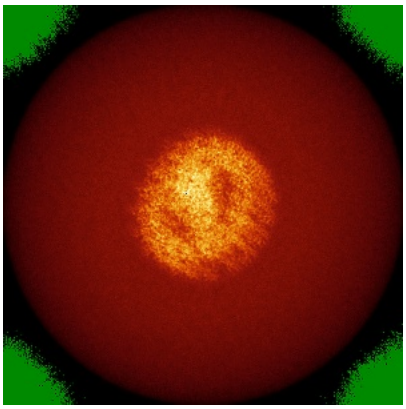
6.4.1 Primary map



X

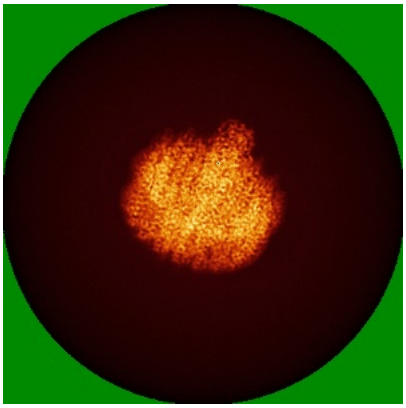


Y

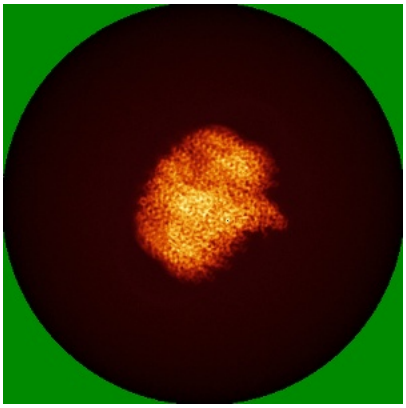


Z

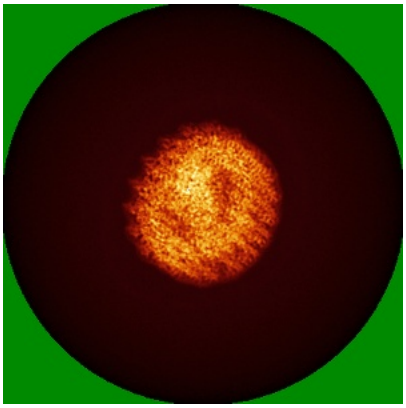
6.4.2 Raw map



X



Y

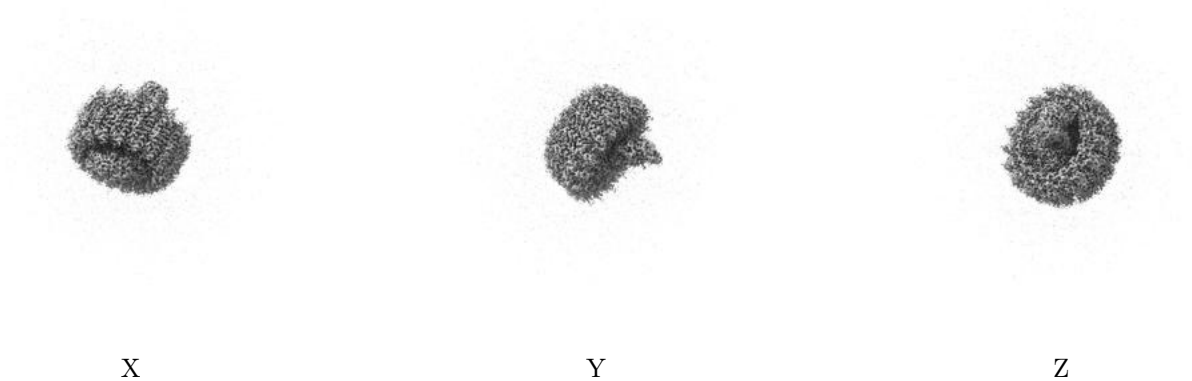


Z

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



X Y Z

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.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

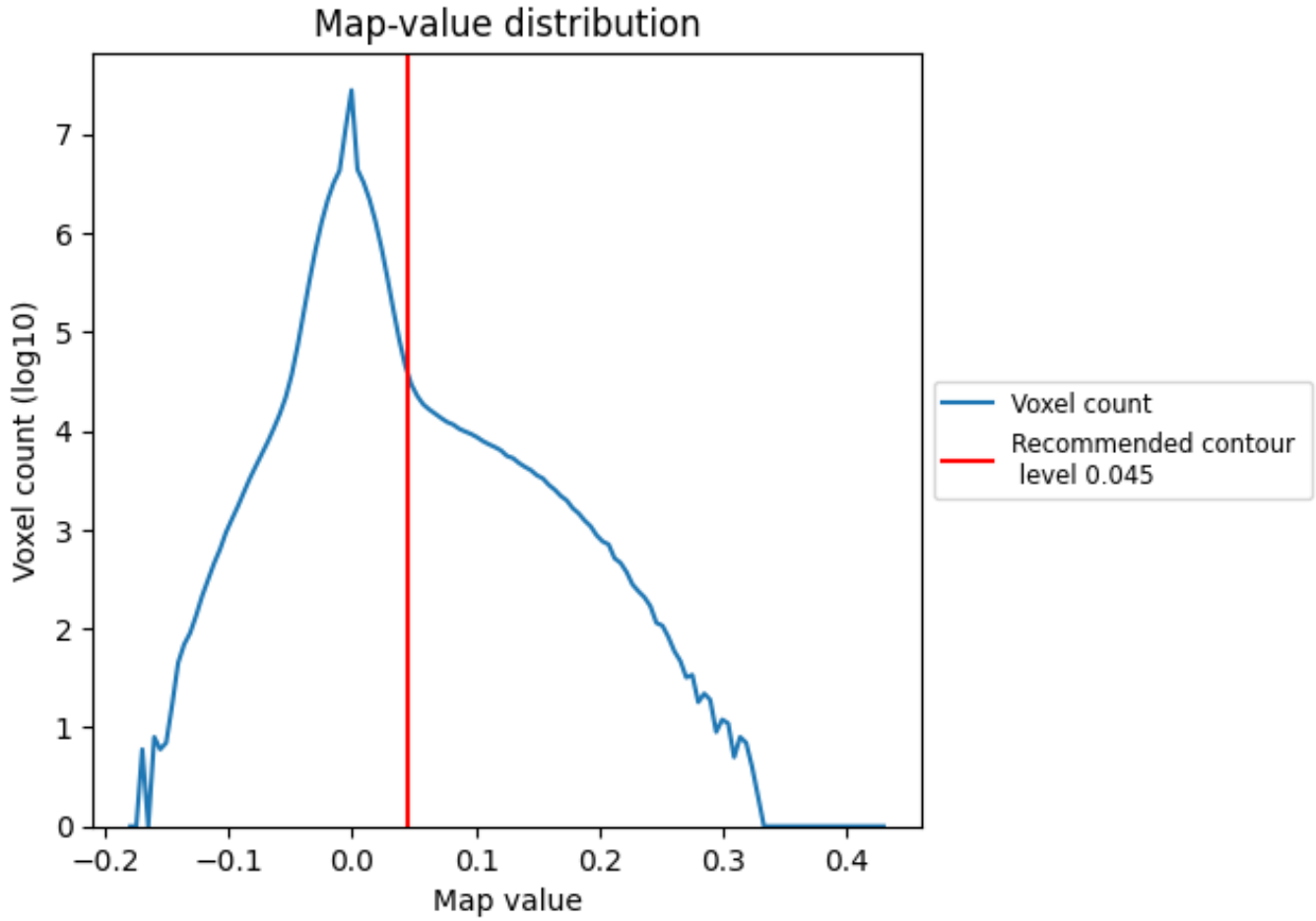
6.6 Mask visualisation (i)

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

7 Map analysis

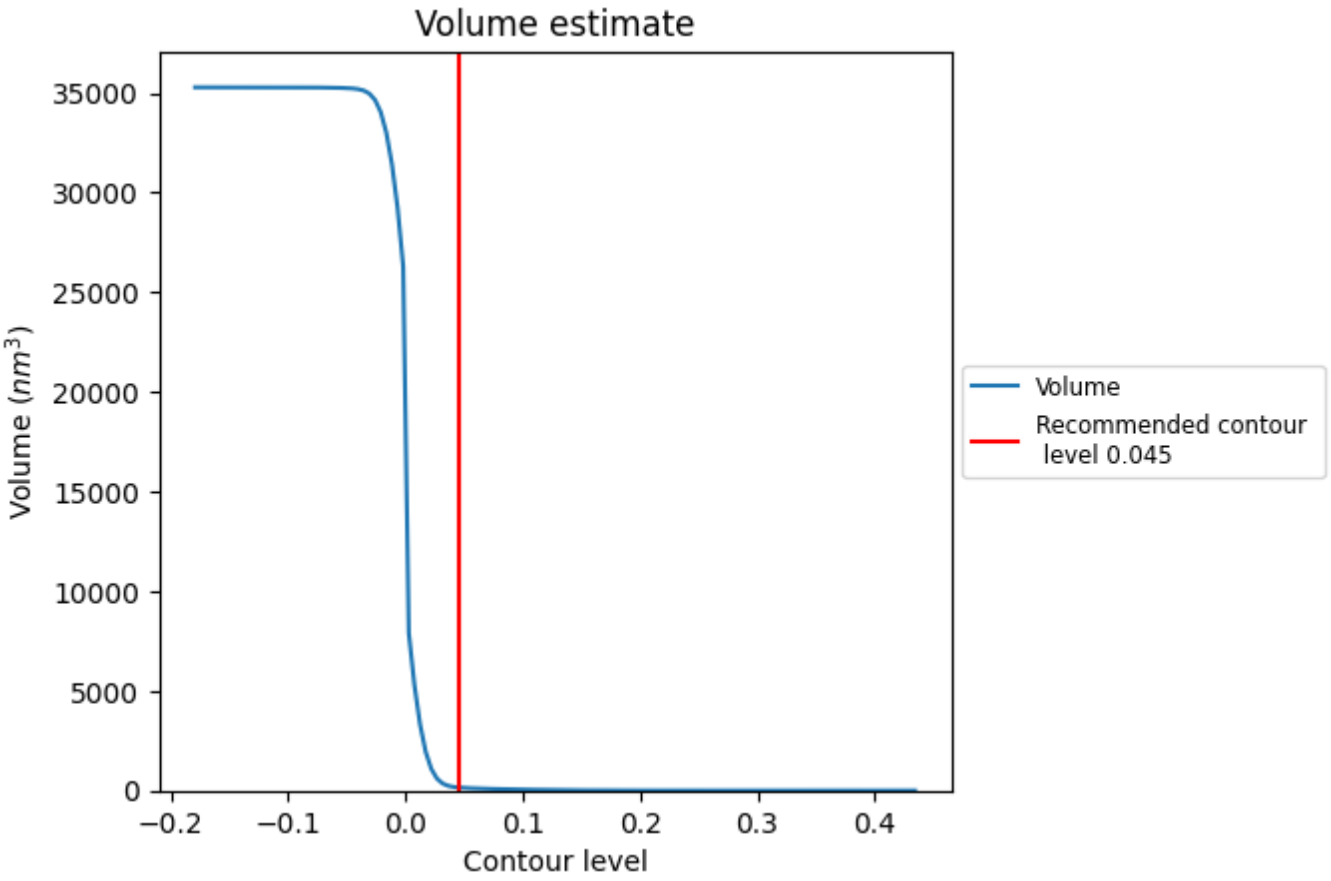
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

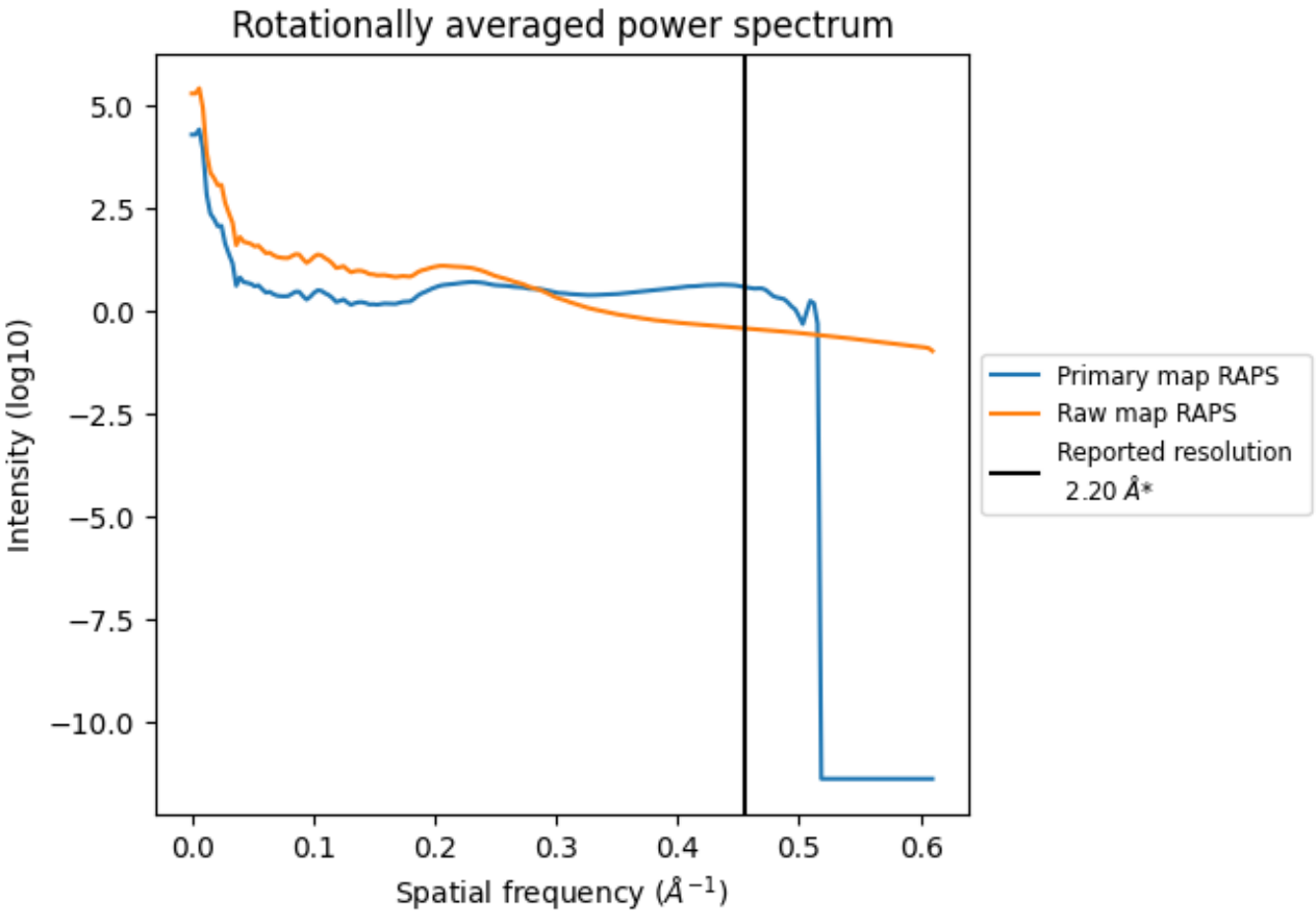
7.2 Volume estimate



The volume at the recommended contour level is 155 nm^3; 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 (i)

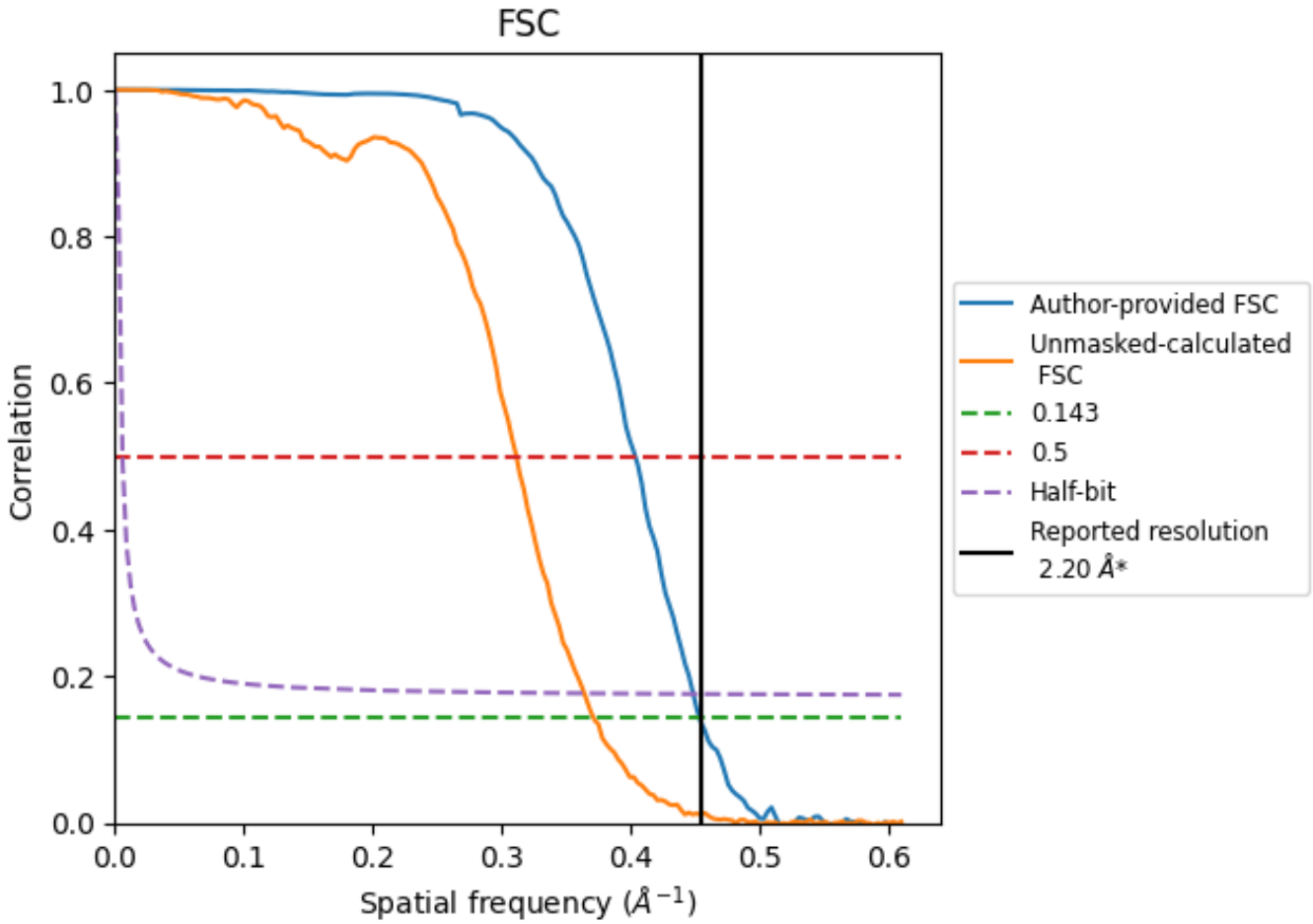


*Reported resolution corresponds to spatial frequency of 0.455 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.455 $Å^{-1}$

8.2 Resolution estimates (i)

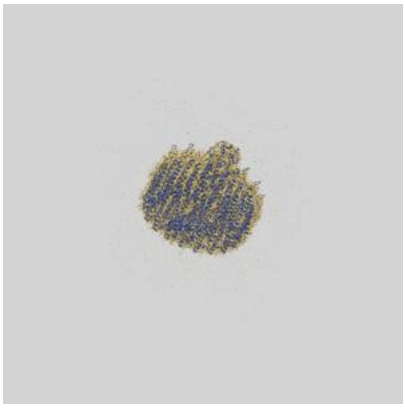
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.20	-	-
Author-provided FSC curve	2.21	2.48	2.23
Unmasked-calculated*	2.69	3.21	2.75

*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 %

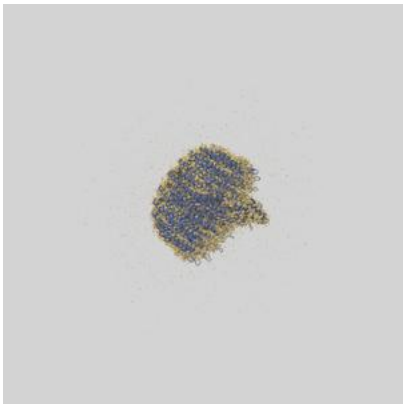
9 Map-model fit

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 22.

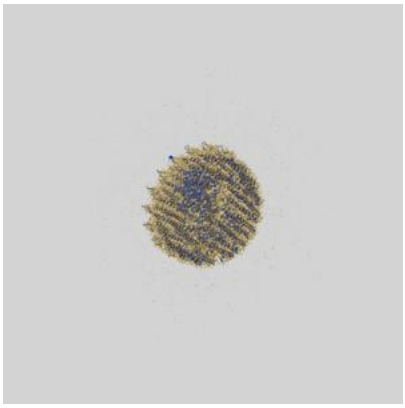
9.1 Map-model overlay



X



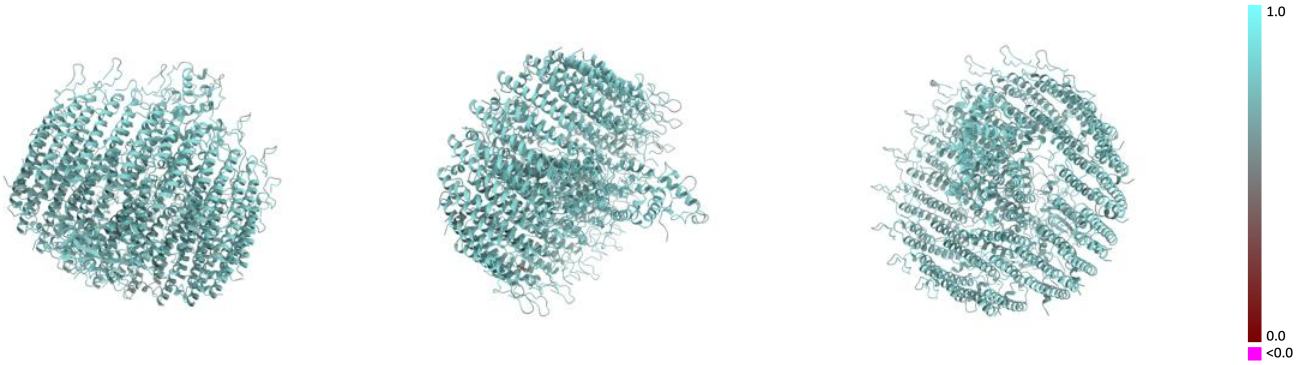
Y



Z

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.

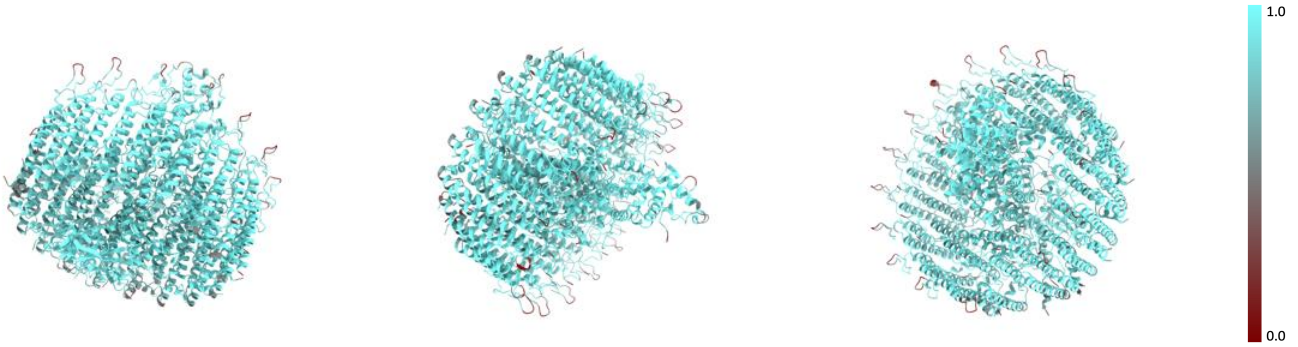
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

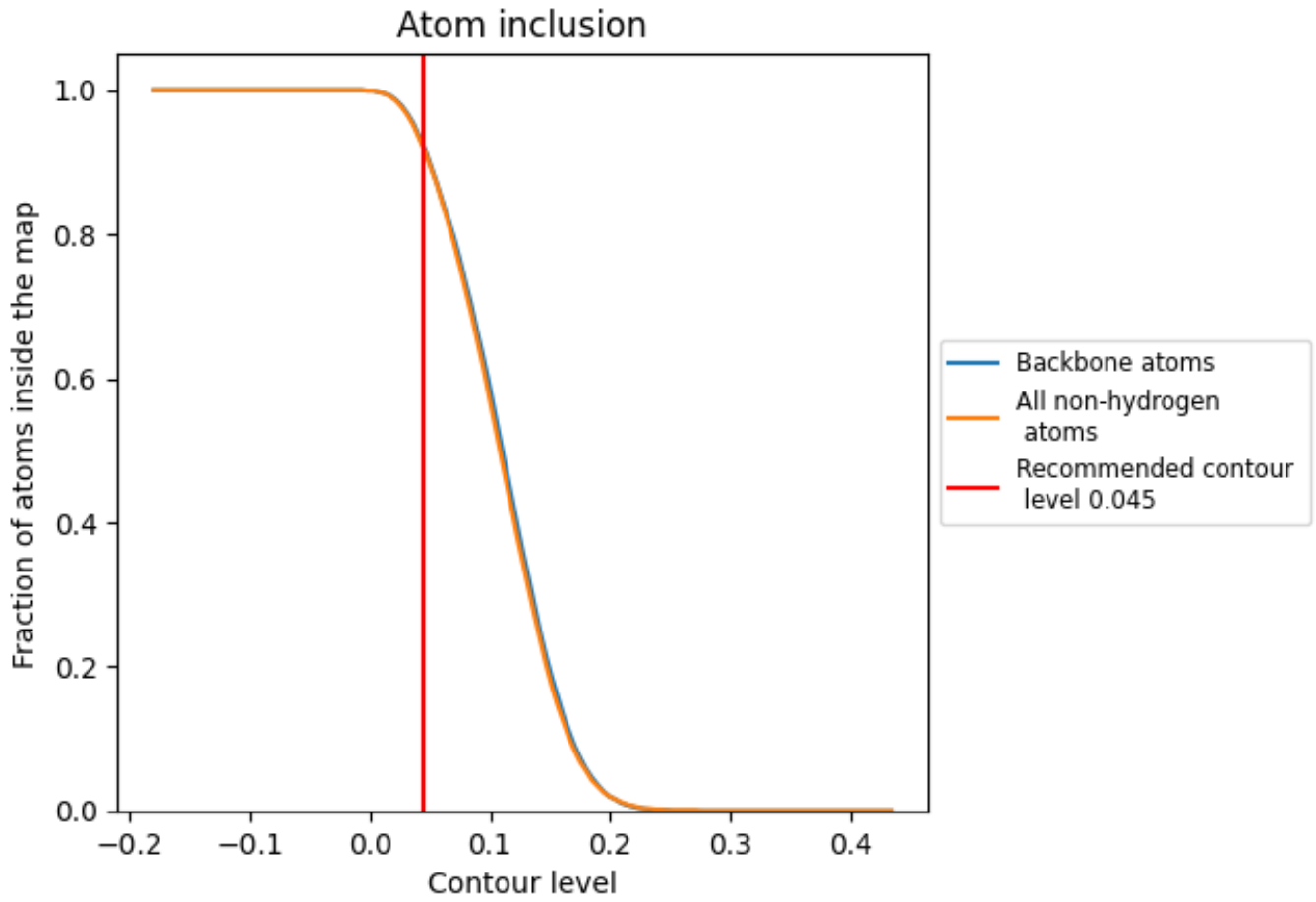
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (i)



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