Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 08:47 pm GMT

PDB ID	:	6ET5
EMDB ID	:	EMD-3951
Title	:	Reaction centre light harvesting complex 1 from Blc. virids
Authors	:	Qian, P.; Siebert, C.A.; Canniffe, D.P.; Wang, P.; Hunter, C.N.
Deposited on	:	2017-10-25
Resolution	:	3.00 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:

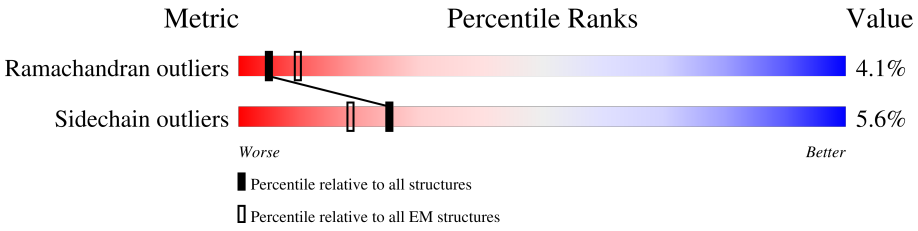
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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	154571	4023
Sidechain outliers	154315	3826

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	333	96%
2	L	274	93% 6%
3	M	323	96%
4	H	258	9% 91% 8%
5	3	59	7% 83% 14%
5	6	59	10% 80% 19%
5	F	59	12% 81% 17%
5	K	59	10% 85% 14%
5	P	59	8% 83% 15%

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Mol	Chain	Length	Quality of chain
5	S	59	8% 85% 14%
5	V	59	8% 86% 12%
5	Y	59	5% 85% 14%
5	b	59	7% 83% 14%
5	e	59	10% 81% 15%
5	h	59	7% 86% 10%
5	k	59	10% 83% 15%
5	n	59	10% 85% 14%
5	q	59	8% 78% 17%
5	t	59	10% 85% 14%
5	w	59	7% 80% 19%
5	z	59	7% 80% 19%
6	1	56	20% 86% 9%
6	4	56	20% 91% 7%
6	7	56	20% 88% 11%
6	G	56	20% 88% 11%
6	N	56	18% 82% 16%
6	Q	56	20% 89% 9%
6	T	56	20% 89% 5%
6	W	56	20% 91% 5%
6	Z	56	20% 91% 5%
6	c	56	20% 91% 7%
6	f	56	18% 91% 5%
6	i	56	20% 86% 11%
6	l	56	20% 86% 12%

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Mol	Chain	Length	Quality of chain
6	o	56	20% 86% 12%
6	r	56	20% 89% 9%
6	u	56	20% 88% 11%
6	x	56	18% 88% 11%
7	2	24	8% 83% 17%
7	5	24	12% 83% 17%
7	I	24	79% 21%
7	O	24	79% 17%
7	R	24	12% 83% 17%
7	U	24	83% 17%
7	X	24	12% 79% 21%
7	a	24	12% 83% 17%
7	d	24	12% 75% 21%
7	g	24	79% 17%
7	j	24	8% 83% 12%
7	m	24	8% 75% 17% 8%
7	p	24	8% 79% 12% 8%
7	s	24	8% 79% 12% 8%
7	v	24	92% 8%
7	y	24	12% 75% 21%

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
10	BPB	L	303	X	-	-	-
10	BPB	M	407	X	-	-	-
17	NS0	1	102	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	NS0	4	102	-	X	-	-
17	NS0	7	102	-	X	-	-
17	NS0	G	102	-	X	-	-
17	NS0	N	102	-	X	-	-
17	NS0	Q	102	-	X	-	-
17	NS0	T	102	-	X	-	-
17	NS0	W	102	-	X	-	-
17	NS0	Z	102	-	X	-	-
17	NS0	c	102	-	X	-	-
17	NS0	f	102	-	X	-	-
17	NS0	i	102	-	X	-	-
17	NS0	l	102	-	X	-	-
17	NS0	o	102	-	X	-	-
17	NS0	r	102	-	X	-	-
17	NS0	u	102	-	X	-	-
17	NS0	x	102	-	X	-	-

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 31994 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	333	Total	C	N	O	S	0	1
			2603	1640	467	478	18		

- 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
			2171	1459	350	355	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	323	Total	C	N	O	S	0	0
			2555	1702	419	423	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	258	Total	C	N	O	S	0	0
			2018	1292	344	380	2		

- Molecule 5 is a protein called Light-harvesting protein B-1015 alpha chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	z	58	Total	C	N	O	0	0
			487	327	83	77		
5	F	58	Total	C	N	O	0	0
			487	327	83	77		
5	K	58	Total	C	N	O	0	0
			487	327	83	77		
5	P	58	Total	C	N	O	0	0
			487	327	83	77		

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Mol	Chain	Residues	Atoms				AltConf	Trace
5	S	58	Total 487	C 327	N 83	O 77	0	0
5	V	58	Total 487	C 327	N 83	O 77	0	0
5	Y	58	Total 487	C 327	N 83	O 77	0	0
5	b	58	Total 487	C 327	N 83	O 77	0	0
5	e	58	Total 487	C 327	N 83	O 77	0	0
5	h	58	Total 487	C 327	N 83	O 77	0	0
5	k	58	Total 487	C 327	N 83	O 77	0	0
5	n	58	Total 487	C 327	N 83	O 77	0	0
5	q	58	Total 487	C 327	N 83	O 77	0	0
5	t	58	Total 487	C 327	N 83	O 77	0	0
5	w	58	Total 487	C 327	N 83	O 77	0	0
5	3	58	Total 487	C 327	N 83	O 77	0	0
5	6	58	Total 487	C 327	N 83	O 77	0	0

- Molecule 6 is a protein called Light-harvesting protein B-1015 beta chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	1	55	Total 436	C 293	N 68	O 75	0	0
6	G	55	Total 436	C 293	N 68	O 75	0	0
6	N	55	Total 436	C 293	N 68	O 75	0	0
6	Q	55	Total 436	C 293	N 68	O 75	0	0
6	T	55	Total 436	C 293	N 68	O 75	0	0
6	W	55	Total 436	C 293	N 68	O 75	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
6	Z	55	Total 436	C 293	N 68	O 75	0	0
6	c	55	Total 436	C 293	N 68	O 75	0	0
6	f	55	Total 436	C 293	N 68	O 75	0	0
6	i	55	Total 436	C 293	N 68	O 75	0	0
6	l	55	Total 436	C 293	N 68	O 75	0	0
6	o	55	Total 436	C 293	N 68	O 75	0	0
6	r	55	Total 436	C 293	N 68	O 75	0	0
6	u	55	Total 436	C 293	N 68	O 75	0	0
6	x	55	Total 436	C 293	N 68	O 75	0	0
6	4	55	Total 436	C 293	N 68	O 75	0	0
6	7	55	Total 436	C 293	N 68	O 75	0	0

- Molecule 7 is a protein called Light-harvesting protein B-1015 gamma chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	2	24	Total 199	C 137	N 31	O 31	0	0
7	I	24	Total 199	C 137	N 31	O 31	0	0
7	O	24	Total 199	C 137	N 31	O 31	0	0
7	R	24	Total 199	C 137	N 31	O 31	0	0
7	U	24	Total 199	C 137	N 31	O 31	0	0
7	X	24	Total 199	C 137	N 31	O 31	0	0
7	a	24	Total 199	C 137	N 31	O 31	0	0
7	d	24	Total 199	C 137	N 31	O 31	0	0

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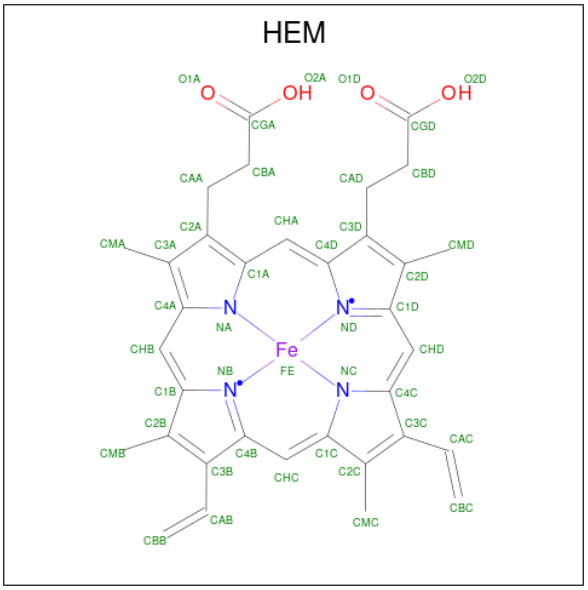
Mol	Chain	Residues	Atoms				AltConf	Trace
7	g	24	Total	C	N	O	0	0
			199	137	31	31		
7	j	24	Total	C	N	O	0	0
			199	137	31	31		
7	m	24	Total	C	N	O	0	0
			199	137	31	31		
7	p	24	Total	C	N	O	0	0
			199	137	31	31		
7	s	24	Total	C	N	O	0	0
			199	137	31	31		
7	v	24	Total	C	N	O	0	0
			199	137	31	31		
7	y	24	Total	C	N	O	0	0
			199	137	31	31		
7	5	24	Total	C	N	O	0	0
			199	137	31	31		

- Molecule 8 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
8	C	1	Total	C	Fe	N	O	0
			172	136	4	16	16	
8	C	1	Total	C	Fe	N	O	0
			172	136	4	16	16	
8	C	1	Total	C	Fe	N	O	0
			172	136	4	16	16	

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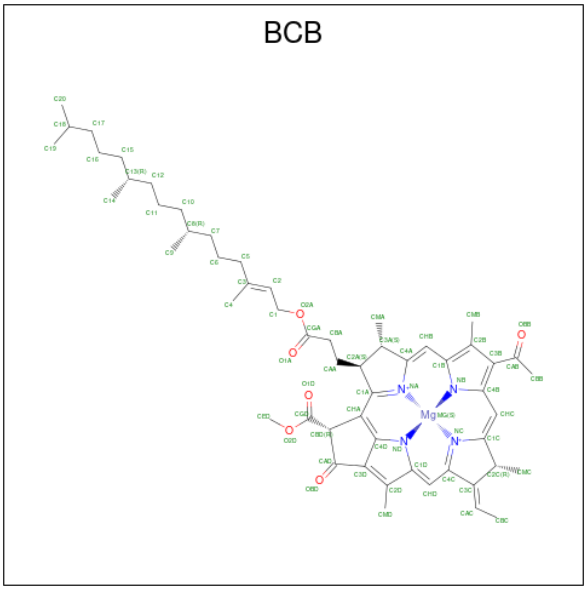
Mol	Chain	Residues	Atoms					AltConf
8	C	1	Total	C	Fe	N	O	0
			172	136	4	16	16	

- Molecule 9 is BACTERIOCHLOROPHYLL B (three-letter code: BCB) (formula: $C_{55}H_{72}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
9	L	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
9	L	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
9	M	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
9	M	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
9	z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	F	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	K	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	P	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	S	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
9	V	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	b	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	e	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	h	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	k	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	q	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	t	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	w	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	Q	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	T	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	Z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	c	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	f	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	i	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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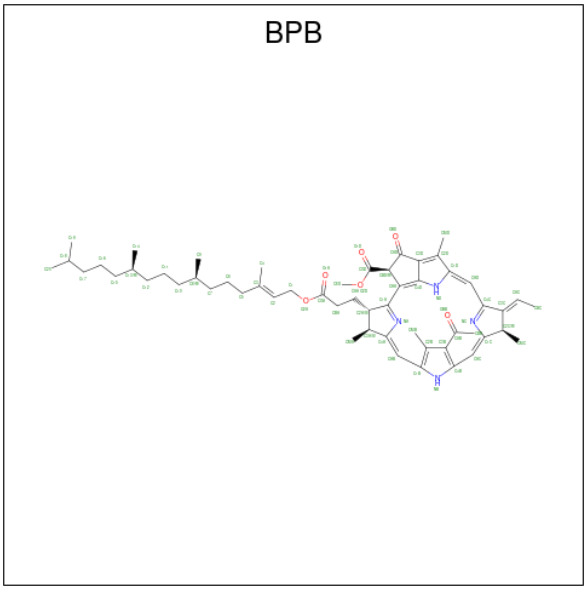
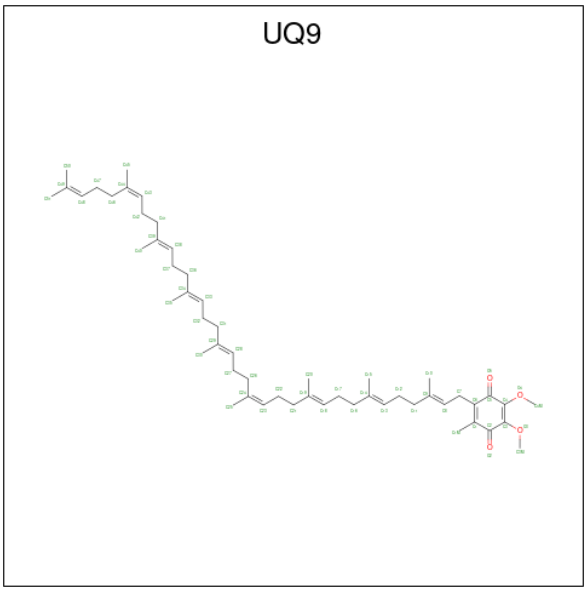
Mol	Chain	Residues	Atoms					AltConf
9	l	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	o	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	r	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	u	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	x	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	4	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 10 is BACTERIOPHEOPHYTIN B (three-letter code: BPB) (formula: $C_{55}H_{74}N_4O_6$).



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

- Molecule 11 is Ubiquinone-9 (three-letter code: UQ9) (formula: $C_{54}H_{82}O_4$).

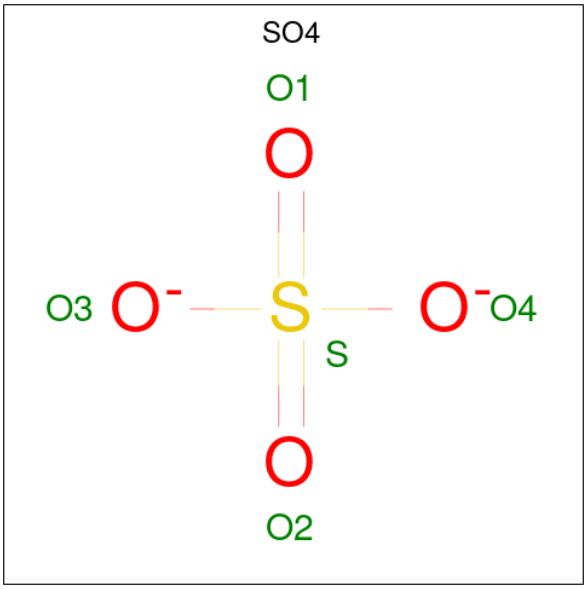


Mol	Chain	Residues	Atoms	AltConf
11	L	1	Total C O 58 54 4	0
11	6	1	Total C O 58 54 4	0

- Molecule 12 is FE (III) ION (three-letter code: FE) (formula: Fe).

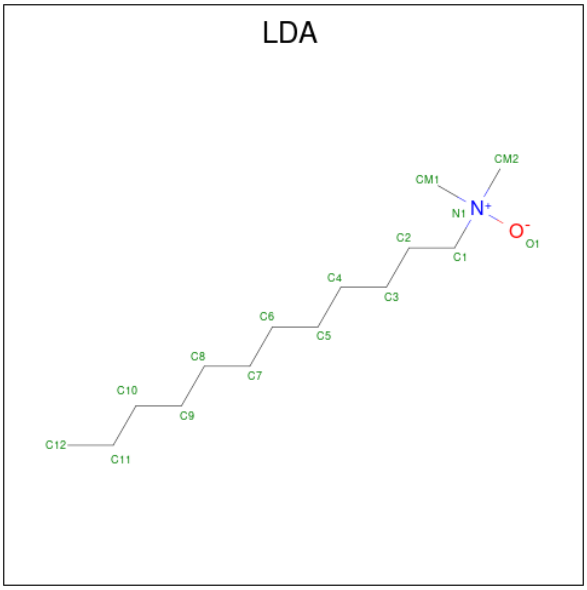
Mol	Chain	Residues	Atoms	AltConf
12	L	1	Total Fe 1 1	0

- Molecule 13 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



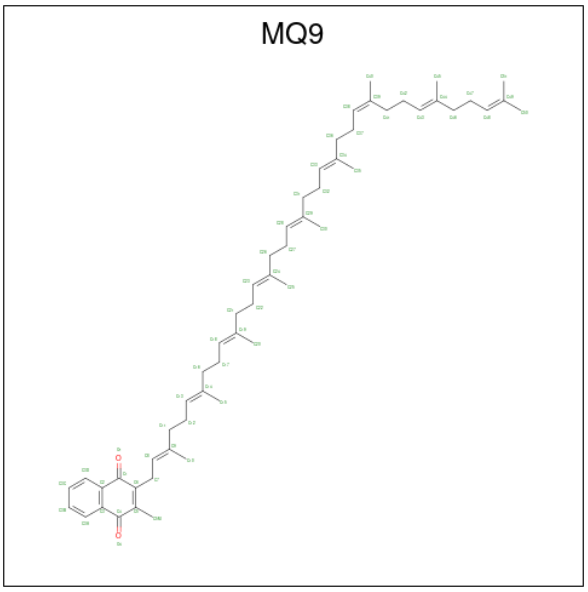
Mol	Chain	Residues	Atoms	AltConf
13	M	1	Total O S 20 16 4	0
13	M	1	Total O S 20 16 4	0
13	M	1	Total O S 20 16 4	0
13	M	1	Total O S 20 16 4	0
13	H	1	Total O S 15 12 3	0
13	H	1	Total O S 15 12 3	0
13	H	1	Total O S 15 12 3	0

- Molecule 14 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



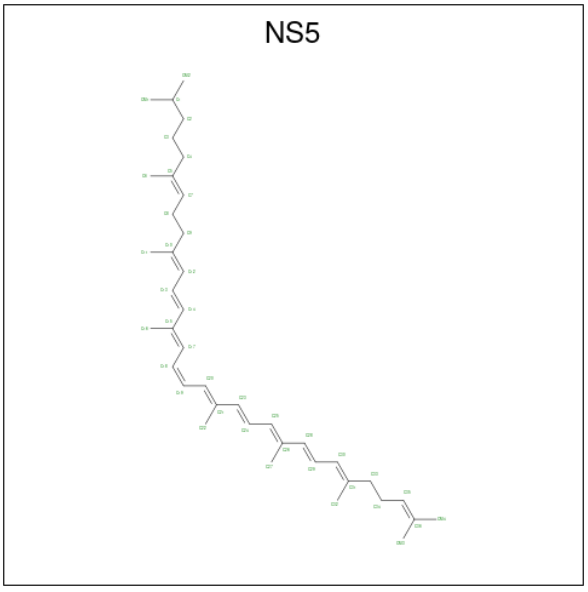
Mol	Chain	Residues	Atoms	AltConf
14	M	1	Total C N O 16 14 1 1	0
14	H	1	Total C N O 16 14 1 1	0

- Molecule 15 is MENAQUINONE-9 (three-letter code: MQ9) (formula: $C_{56}H_{80}O_2$).



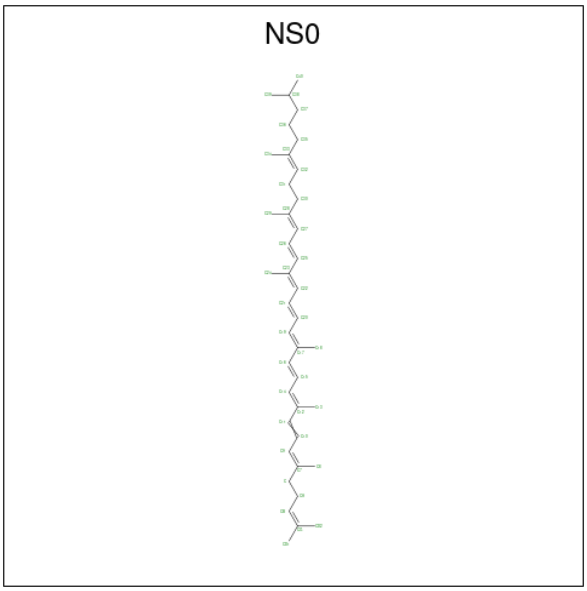
Mol	Chain	Residues	Atoms			AltConf
15	M	1	Total	C	O	0
			58	56	2	

- Molecule 16 is 15-cis-1,2-dihydroneurosporene (three-letter code: NS5) (formula: $C_{40}H_{60}$).



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

- Molecule 17 is all-trans-1,2-dihydroneurosporene (three-letter code: NS0) (formula: $C_{40}H_{60}$).



Mol	Chain	Residues	Atoms	AltConf
17	1	1	Total C 40 40	0
17	G	1	Total C 40 40	0
17	N	1	Total C 40 40	0
17	Q	1	Total C 40 40	0
17	T	1	Total C 40 40	0
17	W	1	Total C 40 40	0
17	Z	1	Total C 40 40	0
17	c	1	Total C 40 40	0
17	f	1	Total C 40 40	0
17	i	1	Total C 40 40	0
17	l	1	Total C 40 40	0
17	o	1	Total C 40 40	0
17	r	1	Total C 40 40	0
17	u	1	Total C 40 40	0

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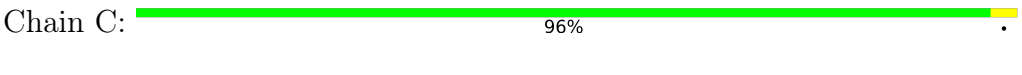
Mol	Chain	Residues	Atoms	AltConf
17	x	1	Total C 40 40	0
17	4	1	Total C 40 40	0
17	7	1	Total C 40 40	0

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.

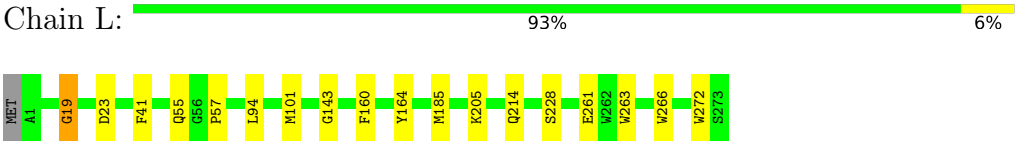
• Molecule 1: Photosynthetic reaction center cytochrome c subunit

Chain C:



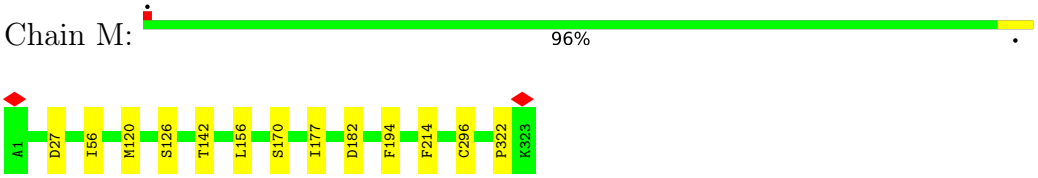
• Molecule 2: Reaction center protein L chain

Chain L:



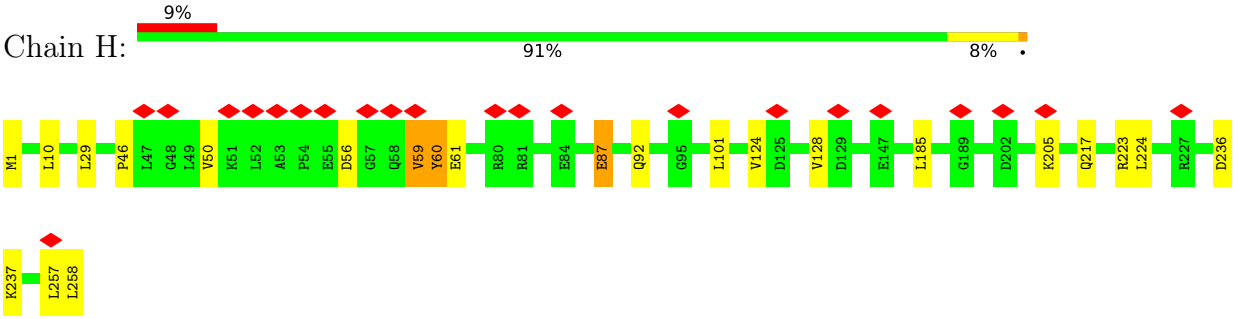
• Molecule 3: Reaction center protein M chain

Chain M:



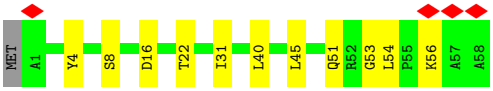
• Molecule 4: Reaction center protein H chain

Chain H:

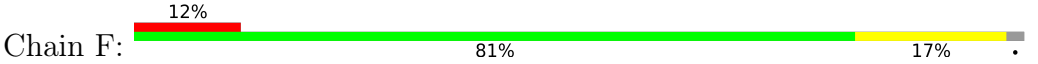


• Molecule 5: Light-harvesting protein B-1015 alpha chain

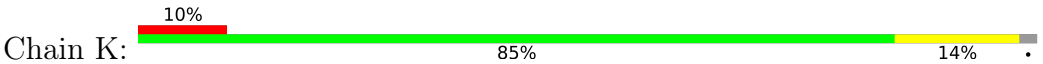
Chain z:

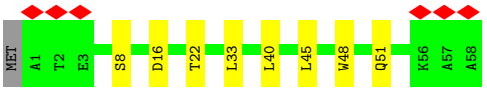


• Molecule 5: Light-harvesting protein B-1015 alpha chain

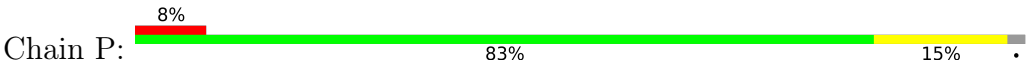


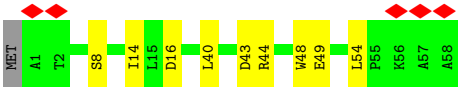
• Molecule 5: Light-harvesting protein B-1015 alpha chain



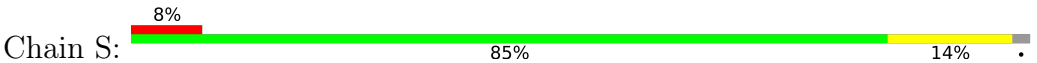


• Molecule 5: Light-harvesting protein B-1015 alpha chain

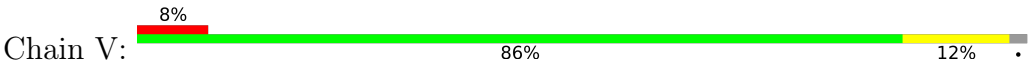


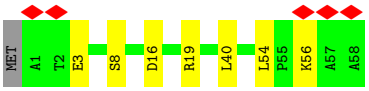


• Molecule 5: Light-harvesting protein B-1015 alpha chain

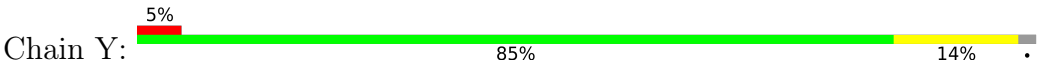


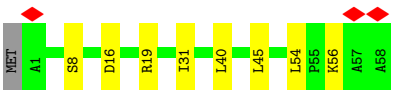
• Molecule 5: Light-harvesting protein B-1015 alpha chain





• Molecule 5: Light-harvesting protein B-1015 alpha chain



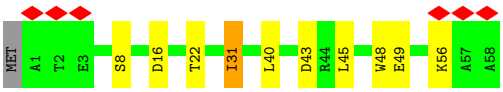


• Molecule 5: Light-harvesting protein B-1015 alpha chain

Chain b:

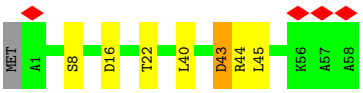
• Molecule 5: Light-harvesting protein B-1015 alpha chain

Chain e:



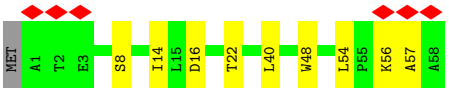
• Molecule 5: Light-harvesting protein B-1015 alpha chain

Chain h:



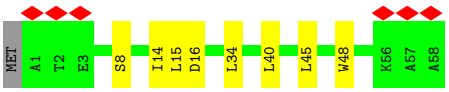
• Molecule 5: Light-harvesting protein B-1015 alpha chain

Chain k:



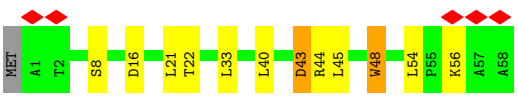
• Molecule 5: Light-harvesting protein B-1015 alpha chain

Chain n:



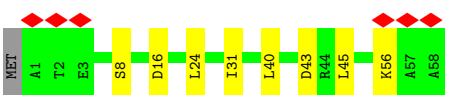
• Molecule 5: Light-harvesting protein B-1015 alpha chain

Chain q:



• Molecule 5: Light-harvesting protein B-1015 alpha chain

Chain t:

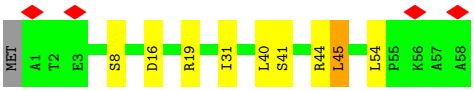


• Molecule 5: Light-harvesting protein B-1015 alpha chain

Chain w:

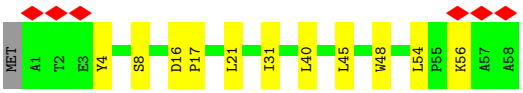
• Molecule 5: Light-harvesting protein B-1015 alpha chain

Chain 3:



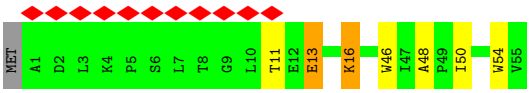
• Molecule 5: Light-harvesting protein B-1015 alpha chain

Chain 6:



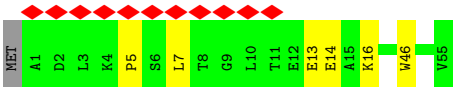
• Molecule 6: Light-harvesting protein B-1015 beta chain

Chain 1:



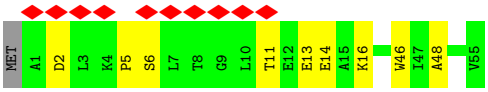
• Molecule 6: Light-harvesting protein B-1015 beta chain

Chain G:



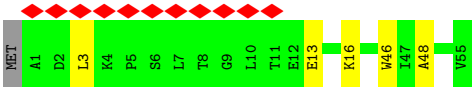
• Molecule 6: Light-harvesting protein B-1015 beta chain

Chain N:



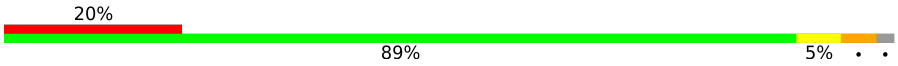
• Molecule 6: Light-harvesting protein B-1015 beta chain

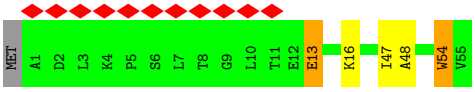
Chain Q:



• Molecule 6: Light-harvesting protein B-1015 beta chain

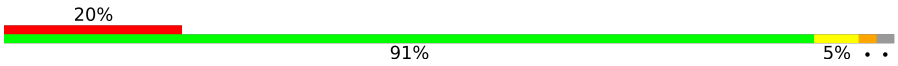
Chain T:

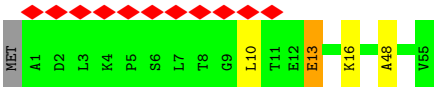




• Molecule 6: Light-harvesting protein B-1015 beta chain

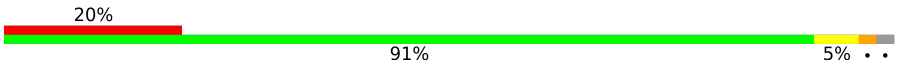
Chain W:

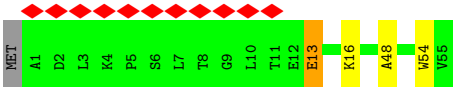




• Molecule 6: Light-harvesting protein B-1015 beta chain

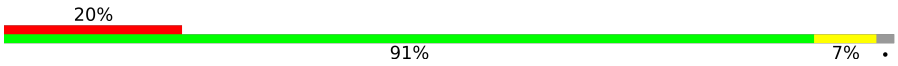
Chain Z:

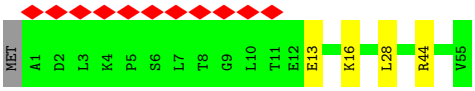




• Molecule 6: Light-harvesting protein B-1015 beta chain

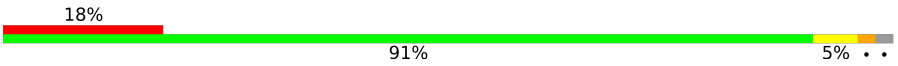
Chain c:

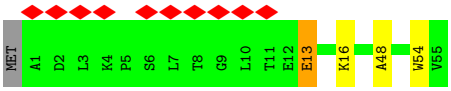




• Molecule 6: Light-harvesting protein B-1015 beta chain

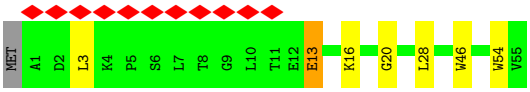
Chain f:





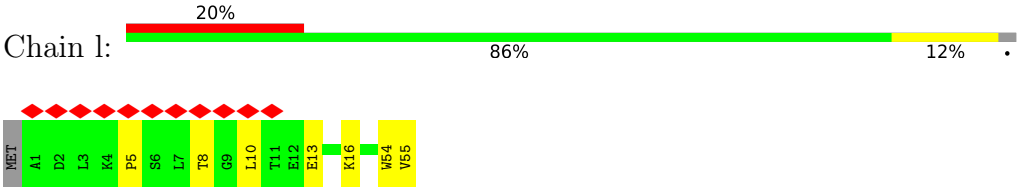
• Molecule 6: Light-harvesting protein B-1015 beta chain

Chain i:



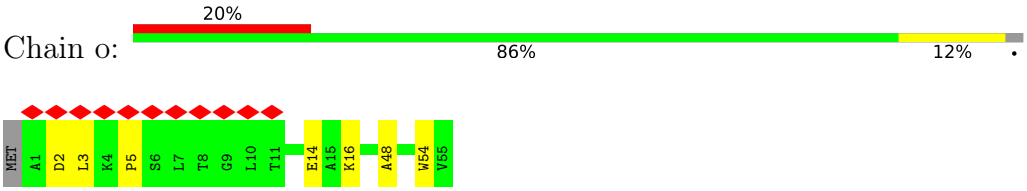
• Molecule 6: Light-harvesting protein B-1015 beta chain

Chain l:



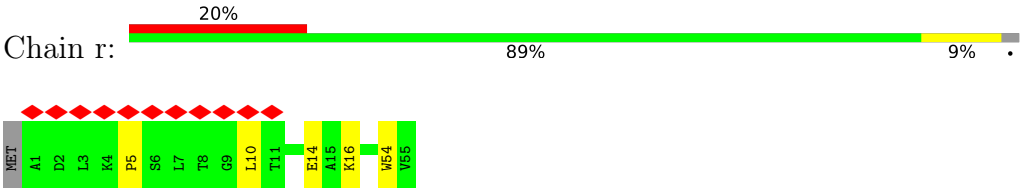
• Molecule 6: Light-harvesting protein B-1015 beta chain

Chain o:



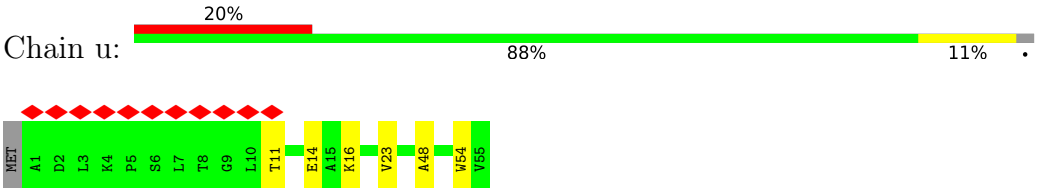
• Molecule 6: Light-harvesting protein B-1015 beta chain

Chain r:



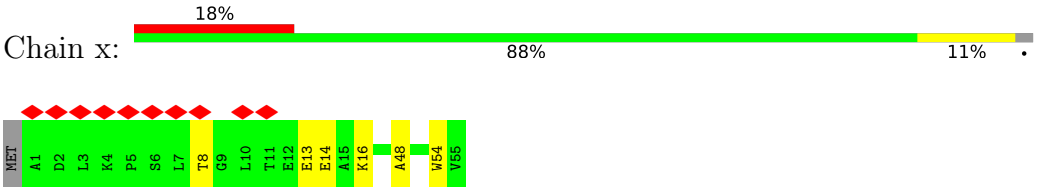
• Molecule 6: Light-harvesting protein B-1015 beta chain

Chain u:



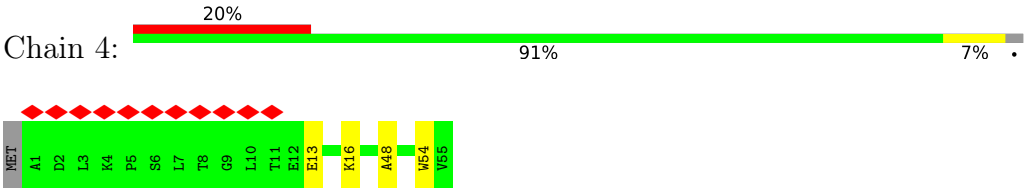
• Molecule 6: Light-harvesting protein B-1015 beta chain

Chain x:



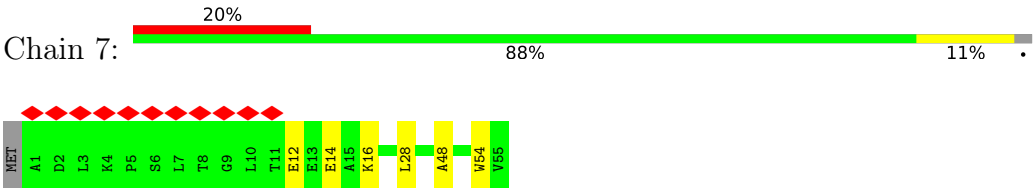
• Molecule 6: Light-harvesting protein B-1015 beta chain

Chain 4:



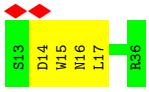
• Molecule 6: Light-harvesting protein B-1015 beta chain

Chain 7:



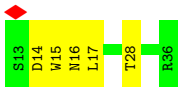
• Molecule 7: Light-harvesting protein B-1015 gamma chain

Chain 2:



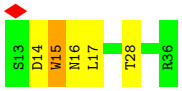
• Molecule 7: Light-harvesting protein B-1015 gamma chain

Chain I:



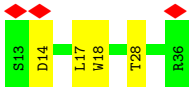
• Molecule 7: Light-harvesting protein B-1015 gamma chain

Chain O:



• Molecule 7: Light-harvesting protein B-1015 gamma chain

Chain R:

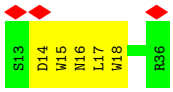


• Molecule 7: Light-harvesting protein B-1015 gamma chain

Chain U:

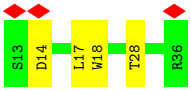
• Molecule 7: Light-harvesting protein B-1015 gamma chain

Chain X:



• Molecule 7: Light-harvesting protein B-1015 gamma chain

Chain a:



• Molecule 7: Light-harvesting protein B-1015 gamma chain

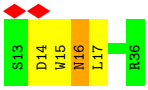
Chain d:

• Molecule 7: Light-harvesting protein B-1015 gamma chain

Chain g:

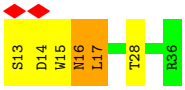
• Molecule 7: Light-harvesting protein B-1015 gamma chain

Chain j:



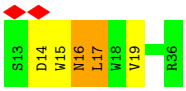
• Molecule 7: Light-harvesting protein B-1015 gamma chain

Chain m:



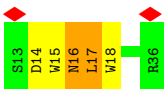
• Molecule 7: Light-harvesting protein B-1015 gamma chain

Chain p:



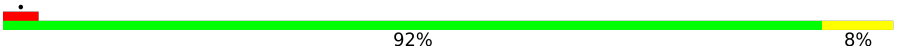
• Molecule 7: Light-harvesting protein B-1015 gamma chain

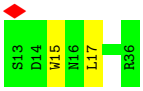
Chain s:



• Molecule 7: Light-harvesting protein B-1015 gamma chain

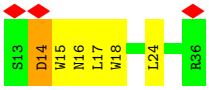
Chain v:





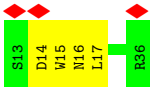
• Molecule 7: Light-harvesting protein B-1015 gamma chain

Chain y:



• Molecule 7: Light-harvesting protein B-1015 gamma chain

Chain 5:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	267726	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; gctf was used for CTF correction	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	2.25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.080	Depositor
Minimum map value	-0.021	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0156	Depositor
Map size (Å)	243.79999, 243.79999, 243.79999	wwPDB
Map dimensions	230, 230, 230	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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, BPB, SO4, FME, NS0, MQ9, LDA, NS5, HEM, BCB, UQ9

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	0.65	1/2670 (0.0%)	0.83	0/3639
2	L	0.82	3/2259 (0.1%)	0.91	3/3084 (0.1%)
3	M	0.77	0/2659	0.86	2/3637 (0.1%)
4	H	0.57	0/2054	0.81	1/2803 (0.0%)
5	3	0.73	0/502	1.24	4/686 (0.6%)
5	6	0.73	0/502	1.13	4/686 (0.6%)
5	F	0.76	1/502 (0.2%)	1.13	3/686 (0.4%)
5	K	0.70	0/502	1.17	5/686 (0.7%)
5	P	0.73	0/502	1.15	4/686 (0.6%)
5	S	0.69	0/502	1.11	2/686 (0.3%)
5	V	0.72	0/502	1.10	1/686 (0.1%)
5	Y	0.73	0/502	1.10	3/686 (0.4%)
5	b	0.77	1/502 (0.2%)	1.19	3/686 (0.4%)
5	e	0.76	1/502 (0.2%)	1.15	4/686 (0.6%)
5	h	0.65	0/502	1.05	2/686 (0.3%)
5	k	0.76	0/502	1.18	3/686 (0.4%)
5	n	0.70	0/502	1.11	2/686 (0.3%)
5	q	0.69	0/502	1.12	2/686 (0.3%)
5	t	0.72	0/502	1.15	5/686 (0.7%)
5	w	0.73	0/502	1.14	3/686 (0.4%)
5	z	0.73	0/502	1.11	3/686 (0.4%)
6	1	0.79	1/451 (0.2%)	0.98	0/621
6	4	0.77	0/451	0.96	0/621
6	7	0.71	0/451	0.88	0/621
6	G	0.67	1/451 (0.2%)	0.89	0/621
6	N	0.72	1/451 (0.2%)	0.96	0/621
6	Q	0.74	1/451 (0.2%)	0.94	1/621 (0.2%)
6	T	0.71	0/451	0.98	0/621
6	W	0.76	0/451	0.94	0/621
6	Z	0.76	0/451	0.96	0/621
6	c	0.68	0/451	0.94	0/621
6	f	0.72	0/451	0.94	0/621

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
6	i	0.77	1/451 (0.2%)	0.97	0/621
6	l	0.72	0/451	0.91	0/621
6	o	0.69	0/451	0.85	0/621
6	r	0.69	0/451	0.93	0/621
6	u	0.73	0/451	0.99	0/621
6	x	0.76	0/451	1.01	0/621
7	2	0.81	0/207	1.28	2/287 (0.7%)
7	5	0.63	0/207	1.12	2/287 (0.7%)
7	I	0.65	0/207	1.07	1/287 (0.3%)
7	O	0.78	0/207	1.16	3/287 (1.0%)
7	R	0.71	0/207	1.12	1/287 (0.3%)
7	U	0.67	0/207	1.21	3/287 (1.0%)
7	X	0.77	0/207	1.24	3/287 (1.0%)
7	a	0.61	0/207	1.05	1/287 (0.3%)
7	d	0.63	0/207	1.04	2/287 (0.7%)
7	g	0.60	0/207	1.11	1/287 (0.3%)
7	j	0.63	0/207	1.06	1/287 (0.3%)
7	m	0.66	0/207	1.20	2/287 (0.7%)
7	p	0.73	0/207	1.15	2/287 (0.7%)
7	s	0.75	0/207	1.20	3/287 (1.0%)
7	v	0.69	0/207	1.20	2/287 (0.7%)
7	y	0.77	0/207	1.26	4/287 (1.4%)
All	All	0.72	12/29155 (0.0%)	1.00	93/39974 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	H	0	2
5	3	0	2
5	V	0	1
5	e	0	1
5	h	0	1
5	k	0	1
5	q	0	2
5	w	0	1
6	1	0	2
6	T	0	2
6	W	0	1
6	Z	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
6	i	0	1
6	l	0	2
6	o	0	1
6	x	0	1
7	2	0	1
7	5	0	1
7	I	0	1
7	O	0	1
7	U	0	1
7	X	0	1
7	d	0	1
7	g	0	1
7	j	0	1
7	m	0	1
7	p	0	1
7	s	0	1
7	v	0	1
7	y	0	1
All	All	0	36

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	263	TRP	CB-CG	-7.30	1.37	1.50
5	b	48	TRP	CB-CG	-6.58	1.38	1.50
6	Q	46	TRP	CB-CG	-6.11	1.39	1.50
1	C	2	PHE	CB-CG	5.66	1.60	1.51
6	1	46	TRP	CB-CG	-5.54	1.40	1.50
5	F	48	TRP	CB-CG	-5.53	1.40	1.50
5	e	48	TRP	CB-CG	-5.38	1.40	1.50
6	i	46	TRP	CB-CG	-5.37	1.40	1.50
6	N	46	TRP	CB-CG	-5.35	1.40	1.50
2	L	266	TRP	CB-CG	-5.32	1.40	1.50
6	G	46	TRP	CB-CG	-5.20	1.40	1.50
2	L	41	PHE	CB-CG	-5.04	1.42	1.51

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	q	40	LEU	CA-CB-CG	11.99	142.87	115.30
5	k	40	LEU	CA-CB-CG	10.43	139.29	115.30
5	t	40	LEU	CA-CB-CG	10.29	138.97	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	3	40	LEU	CA-CB-CG	10.27	138.91	115.30
5	F	40	LEU	CA-CB-CG	10.14	138.63	115.30
5	n	40	LEU	CA-CB-CG	9.69	137.58	115.30
5	b	40	LEU	CA-CB-CG	9.55	137.28	115.30
5	e	40	LEU	CA-CB-CG	9.45	137.03	115.30
5	P	40	LEU	CA-CB-CG	9.29	136.68	115.30
5	Y	40	LEU	CA-CB-CG	9.27	136.63	115.30
5	S	40	LEU	CA-CB-CG	9.24	136.56	115.30
5	V	40	LEU	CA-CB-CG	8.68	135.27	115.30
5	w	40	LEU	CA-CB-CG	8.67	135.24	115.30
5	K	40	LEU	CA-CB-CG	8.58	135.03	115.30
5	6	40	LEU	CA-CB-CG	8.39	134.60	115.30
7	y	17	LEU	CB-CG-CD2	8.22	124.98	111.00
5	h	40	LEU	CA-CB-CG	8.09	133.90	115.30
5	z	40	LEU	CA-CB-CG	7.79	133.22	115.30
7	m	17	LEU	CB-CA-C	7.50	124.44	110.20
7	X	17	LEU	CB-CA-C	7.43	124.32	110.20
5	K	45	LEU	CA-CB-CG	7.42	132.38	115.30
5	3	45	LEU	CA-CB-CG	7.41	132.35	115.30
3	M	156	LEU	CB-CG-CD1	-7.36	98.48	111.00
7	U	17	LEU	CB-CA-C	7.18	123.84	110.20
7	p	17	LEU	CB-CA-C	7.01	123.51	110.20
7	2	17	LEU	CB-CG-CD2	6.99	122.89	111.00
5	b	48	TRP	CB-CA-C	-6.92	96.55	110.40
7	s	17	LEU	CB-CG-CD2	6.82	122.60	111.00
7	y	17	LEU	CB-CA-C	6.79	123.11	110.20
5	F	48	TRP	CB-CA-C	-6.66	97.08	110.40
5	P	48	TRP	CB-CA-C	-6.64	97.11	110.40
5	t	45	LEU	CA-CB-CG	6.64	130.57	115.30
7	v	17	LEU	CB-CA-C	6.64	122.81	110.20
5	k	48	TRP	CB-CA-C	-6.55	97.29	110.40
5	e	48	TRP	CB-CA-C	-6.52	97.36	110.40
2	L	164	TYR	N-CA-C	-6.45	93.58	111.00
7	s	17	LEU	CB-CA-C	6.44	122.43	110.20
7	2	17	LEU	CB-CA-C	6.43	122.41	110.20
5	h	45	LEU	CA-CB-CG	6.41	130.04	115.30
7	p	17	LEU	CB-CG-CD2	6.38	121.84	111.00
7	j	17	LEU	CB-CA-C	6.37	122.30	110.20
5	K	48	TRP	CA-CB-CG	6.35	125.77	113.70
5	6	45	LEU	CA-CB-CG	6.35	129.90	115.30
5	z	45	LEU	CB-CG-CD2	-6.26	100.36	111.00
5	e	45	LEU	CB-CG-CD2	-6.26	100.36	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	O	17	LEU	CB-CG-CD2	6.23	121.59	111.00
7	5	17	LEU	CB-CG-CD2	6.21	121.56	111.00
2	L	94	LEU	CA-CB-CG	-6.17	101.10	115.30
7	X	17	LEU	CB-CG-CD2	6.12	121.41	111.00
5	S	45	LEU	CA-CB-CG	6.10	129.34	115.30
4	H	29	LEU	CA-CB-CG	-6.10	101.27	115.30
7	d	17	LEU	CB-CA-C	6.07	121.72	110.20
7	y	18	TRP	CB-CA-C	-6.06	98.27	110.40
7	U	17	LEU	CB-CG-CD2	6.04	121.28	111.00
7	m	17	LEU	CB-CG-CD2	6.02	121.23	111.00
7	v	17	LEU	CB-CG-CD2	5.97	121.15	111.00
5	b	45	LEU	CB-CG-CD2	-5.91	100.95	111.00
7	I	17	LEU	CB-CA-C	5.88	121.38	110.20
7	g	17	LEU	CB-CA-C	5.84	121.30	110.20
7	5	17	LEU	CB-CA-C	5.82	121.25	110.20
5	Y	40	LEU	CB-CA-C	5.81	121.23	110.20
5	K	48	TRP	CB-CA-C	-5.80	98.80	110.40
5	6	21	LEU	CB-CG-CD2	-5.79	101.16	111.00
5	P	44	ARG	N-CA-C	-5.72	95.56	111.00
5	n	45	LEU	CB-CG-CD2	-5.66	101.38	111.00
7	s	18	TRP	CB-CA-C	-5.62	99.17	110.40
7	U	18	TRP	CB-CA-C	-5.52	99.35	110.40
5	6	48	TRP	CB-CA-C	-5.51	99.38	110.40
5	q	33	LEU	CB-CG-CD1	5.47	120.30	111.00
7	O	17	LEU	CB-CA-C	5.46	120.58	110.20
5	F	45	LEU	CB-CG-CD2	-5.46	101.72	111.00
5	e	31	ILE	CG1-CB-CG2	-5.46	99.39	111.40
5	w	40	LEU	CB-CA-C	5.42	120.50	110.20
5	t	40	LEU	CB-CA-C	5.41	120.48	110.20
5	w	39	LEU	CA-CB-CG	-5.39	102.89	115.30
5	K	33	LEU	CB-CG-CD2	-5.39	101.83	111.00
7	y	24	LEU	CB-CG-CD1	5.39	120.16	111.00
5	z	40	LEU	CB-CA-C	5.33	120.33	110.20
7	R	18	TRP	CB-CA-C	-5.28	99.84	110.40
5	3	19	ARG	NE-CZ-NH1	-5.27	117.67	120.30
5	k	48	TRP	CA-CB-CG	5.25	123.67	113.70
5	P	48	TRP	CA-CB-CG	5.24	123.65	113.70
5	3	40	LEU	CB-CA-C	5.23	120.14	110.20
5	t	40	LEU	CB-CG-CD2	-5.20	102.17	111.00
7	a	18	TRP	CB-CA-C	-5.18	100.05	110.40
7	d	18	TRP	CB-CA-C	-5.17	100.05	110.40
3	M	182	ASP	CB-CG-OD1	5.17	122.96	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	X	18	TRP	CB-CA-C	-5.16	100.08	110.40
2	L	19	GLY	N-CA-C	5.11	125.89	113.10
6	Q	3	LEU	CA-CB-CG	5.08	127.00	115.30
7	O	15	TRP	CB-CA-C	5.05	120.51	110.40
5	Y	45	LEU	CA-CB-CG	5.04	126.90	115.30
5	t	24	LEU	CB-CG-CD1	-5.01	102.49	111.00

There are no chirality outliers.

All (36) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	1	13	GLU	Peptide
6	1	16	LYS	Peptide
7	2	15	TRP	Peptide
5	3	45	LEU	Peptide
5	3	54	LEU	Peptide
7	5	15	TRP	Peptide
4	H	257	LEU	Peptide
4	H	59	VAL	Peptide
7	I	15	TRP	Peptide
7	O	15	TRP	Peptide
6	T	13	GLU	Peptide
6	T	54	TRP	Peptide
7	U	15	TRP	Peptide
5	V	54	LEU	Peptide
6	W	13	GLU	Peptide
7	X	15	TRP	Peptide
6	Z	13	GLU	Peptide
7	d	15	TRP	Peptide
5	e	43	ASP	Peptide
7	g	15	TRP	Peptide
5	h	43	ASP	Peptide
6	i	13	GLU	Peptide
7	j	15	TRP	Peptide
5	k	54	LEU	Peptide
6	l	13	GLU	Peptide
6	l	54	TRP	Peptide
7	m	15	TRP	Peptide
6	o	54	TRP	Peptide
7	p	15	TRP	Peptide
5	q	43	ASP	Peptide
5	q	48	TRP	Peptide

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Mol	Chain	Res	Type	Group
7	s	15	TRP	Peptide
7	v	15	TRP	Peptide
5	w	43	ASP	Peptide
6	x	54	TRP	Peptide
7	y	15	TRP	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	331/333 (99%)	300 (91%)	31 (9%)	0	100 100
2	L	271/274 (99%)	251 (93%)	15 (6%)	5 (2%)	8 37
3	M	321/323 (99%)	301 (94%)	16 (5%)	4 (1%)	13 48
4	H	254/258 (98%)	231 (91%)	16 (6%)	7 (3%)	5 25
5	3	56/59 (95%)	45 (80%)	9 (16%)	2 (4%)	3 19
5	6	56/59 (95%)	43 (77%)	11 (20%)	2 (4%)	3 19
5	F	56/59 (95%)	46 (82%)	8 (14%)	2 (4%)	3 19
5	K	56/59 (95%)	47 (84%)	7 (12%)	2 (4%)	3 19
5	P	56/59 (95%)	46 (82%)	7 (12%)	3 (5%)	2 11
5	S	56/59 (95%)	43 (77%)	12 (21%)	1 (2%)	8 37
5	V	56/59 (95%)	48 (86%)	6 (11%)	2 (4%)	3 19
5	Y	56/59 (95%)	44 (79%)	10 (18%)	2 (4%)	3 19
5	b	56/59 (95%)	43 (77%)	9 (16%)	4 (7%)	1 5
5	e	56/59 (95%)	44 (79%)	9 (16%)	3 (5%)	2 11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
5	h	56/59 (95%)	45 (80%)	9 (16%)	2 (4%)	3 19
5	k	56/59 (95%)	42 (75%)	11 (20%)	3 (5%)	2 11
5	n	56/59 (95%)	44 (79%)	9 (16%)	3 (5%)	2 11
5	q	56/59 (95%)	45 (80%)	7 (12%)	4 (7%)	1 5
5	t	56/59 (95%)	45 (80%)	9 (16%)	2 (4%)	3 19
5	w	56/59 (95%)	43 (77%)	10 (18%)	3 (5%)	2 11
5	z	56/59 (95%)	45 (80%)	7 (12%)	4 (7%)	1 5
6	1	53/56 (95%)	43 (81%)	7 (13%)	3 (6%)	1 10
6	4	53/56 (95%)	42 (79%)	8 (15%)	3 (6%)	1 10
6	7	53/56 (95%)	41 (77%)	8 (15%)	4 (8%)	1 5
6	G	53/56 (95%)	41 (77%)	9 (17%)	3 (6%)	1 10
6	N	53/56 (95%)	40 (76%)	9 (17%)	4 (8%)	1 5
6	Q	53/56 (95%)	40 (76%)	11 (21%)	2 (4%)	3 18
6	T	53/56 (95%)	41 (77%)	9 (17%)	3 (6%)	1 10
6	W	53/56 (95%)	40 (76%)	10 (19%)	3 (6%)	1 10
6	Z	53/56 (95%)	42 (79%)	9 (17%)	2 (4%)	3 18
6	c	53/56 (95%)	43 (81%)	9 (17%)	1 (2%)	8 36
6	f	53/56 (95%)	43 (81%)	7 (13%)	3 (6%)	1 10
6	i	53/56 (95%)	39 (74%)	11 (21%)	3 (6%)	1 10
6	l	53/56 (95%)	42 (79%)	8 (15%)	3 (6%)	1 10
6	o	53/56 (95%)	43 (81%)	8 (15%)	2 (4%)	3 18
6	r	53/56 (95%)	40 (76%)	9 (17%)	4 (8%)	1 5
6	u	53/56 (95%)	43 (81%)	6 (11%)	4 (8%)	1 5
6	x	53/56 (95%)	42 (79%)	7 (13%)	4 (8%)	1 5
7	2	22/24 (92%)	19 (86%)	1 (4%)	2 (9%)	1 3
7	5	22/24 (92%)	18 (82%)	3 (14%)	1 (4%)	2 14
7	I	22/24 (92%)	19 (86%)	1 (4%)	2 (9%)	1 3
7	O	22/24 (92%)	18 (82%)	2 (9%)	2 (9%)	1 3
7	R	22/24 (92%)	18 (82%)	3 (14%)	1 (4%)	2 14
7	U	22/24 (92%)	18 (82%)	3 (14%)	1 (4%)	2 14
7	X	22/24 (92%)	18 (82%)	2 (9%)	2 (9%)	1 3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
7	a	22/24 (92%)	17 (77%)	4 (18%)	1 (4%)	2 14
7	d	22/24 (92%)	17 (77%)	3 (14%)	2 (9%)	1 3
7	g	22/24 (92%)	17 (77%)	2 (9%)	3 (14%)	0 1
7	j	22/24 (92%)	17 (77%)	3 (14%)	2 (9%)	1 3
7	m	22/24 (92%)	18 (82%)	2 (9%)	2 (9%)	1 3
7	p	22/24 (92%)	18 (82%)	2 (9%)	2 (9%)	1 3
7	s	22/24 (92%)	19 (86%)	1 (4%)	2 (9%)	1 3
7	v	22/24 (92%)	17 (77%)	5 (23%)	0	100 100
7	y	22/24 (92%)	17 (77%)	3 (14%)	2 (9%)	1 3
All	All	3382/3527 (96%)	2831 (84%)	413 (12%)	138 (4%)	5 16

All (138) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	H	50	VAL
4	H	61	GLU
7	2	16	ASN
5	F	8	SER
5	K	8	SER
5	e	8	SER
5	n	8	SER
5	q	8	SER
5	t	8	SER
5	w	8	SER
5	3	8	SER
6	Q	13	GLU
6	T	13	GLU
6	T	54	TRP
6	4	13	GLU
7	I	14	ASP
7	I	16	ASN
7	O	14	ASP
7	O	16	ASN
7	X	14	ASP
7	X	16	ASN
7	d	16	ASN
7	g	16	ASN
7	j	16	ASN
7	m	16	ASN

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Mol	Chain	Res	Type
7	p	16	ASN
7	s	16	ASN
7	y	14	ASP
7	y	16	ASN
2	L	19	GLY
2	L	23	ASP
6	1	13	GLU
7	2	14	ASP
5	P	49	GLU
5	Y	8	SER
5	b	8	SER
5	k	8	SER
5	6	8	SER
6	G	14	GLU
6	N	11	THR
6	N	14	GLU
6	W	13	GLU
6	x	13	GLU
7	R	14	ASP
7	U	16	ASN
7	g	14	ASP
7	j	14	ASP
7	s	14	ASP
3	M	170	SER
4	H	60	TYR
4	H	87	GLU
5	z	8	SER
5	z	51	GLN
5	F	16	ASP
5	P	8	SER
5	e	16	ASP
5	e	49	GLU
5	h	8	SER
5	h	16	ASP
5	n	48	TRP
5	w	48	TRP
6	W	10	LEU
6	f	13	GLU
6	r	10	LEU
6	r	14	GLU
6	r	54	TRP
6	u	14	GLU

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Mol	Chain	Res	Type
6	u	54	TRP
6	x	8	THR
6	7	12	GLU
6	7	54	TRP
7	a	14	ASP
7	d	14	ASP
7	m	14	ASP
7	5	14	ASP
2	L	143	GLY
2	L	261	GLU
3	M	177	ILE
3	M	322	PRO
6	1	11	THR
5	P	16	ASP
5	S	16	ASP
5	V	16	ASP
5	Y	16	ASP
5	b	16	ASP
5	b	49	GLU
5	k	57	ALA
5	n	16	ASP
5	q	16	ASP
5	q	48	TRP
5	t	16	ASP
5	w	16	ASP
5	3	16	ASP
6	G	7	LEU
6	T	48	ALA
6	Z	13	GLU
6	c	13	GLU
6	i	13	GLU
6	i	20	GLY
6	l	8	THR
6	u	11	THR
6	x	14	GLU
6	7	14	GLU
2	L	57	PRO
4	H	10	LEU
4	H	46	PRO
5	z	16	ASP
5	K	16	ASP
5	V	8	SER

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Mol	Chain	Res	Type
5	k	16	ASP
5	q	43	ASP
5	6	16	ASP
6	Q	48	ALA
6	W	48	ALA
6	f	54	TRP
6	i	54	TRP
6	o	5	PRO
6	4	48	ALA
6	4	54	TRP
7	p	14	ASP
3	M	56	ILE
5	b	56	LYS
6	N	5	PRO
6	N	48	ALA
6	l	10	LEU
7	g	19	VAL
6	G	5	PRO
6	x	48	ALA
4	H	59	VAL
6	1	48	ALA
6	Z	48	ALA
6	l	5	PRO
6	o	48	ALA
6	r	5	PRO
5	z	53	GLY
6	f	48	ALA
6	u	48	ALA
6	7	48	ALA

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	281/281 (100%)	269 (96%)	12 (4%)	29	66
2	L	218/219 (100%)	210 (96%)	8 (4%)	34	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	M	249/249 (100%)	242 (97%)	7 (3%)	43 77
4	H	212/212 (100%)	197 (93%)	15 (7%)	14 46
5	3	50/51 (98%)	47 (94%)	3 (6%)	19 53
5	6	50/51 (98%)	45 (90%)	5 (10%)	7 29
5	F	50/51 (98%)	45 (90%)	5 (10%)	7 29
5	K	50/51 (98%)	48 (96%)	2 (4%)	31 68
5	P	50/51 (98%)	47 (94%)	3 (6%)	19 53
5	S	50/51 (98%)	45 (90%)	5 (10%)	7 29
5	V	50/51 (98%)	47 (94%)	3 (6%)	19 53
5	Y	50/51 (98%)	46 (92%)	4 (8%)	12 40
5	b	50/51 (98%)	47 (94%)	3 (6%)	19 53
5	e	50/51 (98%)	47 (94%)	3 (6%)	19 53
5	h	50/51 (98%)	47 (94%)	3 (6%)	19 53
5	k	50/51 (98%)	47 (94%)	3 (6%)	19 53
5	n	50/51 (98%)	47 (94%)	3 (6%)	19 53
5	q	50/51 (98%)	44 (88%)	6 (12%)	5 22
5	t	50/51 (98%)	47 (94%)	3 (6%)	19 53
5	w	50/51 (98%)	45 (90%)	5 (10%)	7 29
5	z	50/51 (98%)	45 (90%)	5 (10%)	7 29
6	1	46/47 (98%)	43 (94%)	3 (6%)	17 50
6	4	46/47 (98%)	45 (98%)	1 (2%)	52 81
6	7	46/47 (98%)	44 (96%)	2 (4%)	29 66
6	G	46/47 (98%)	44 (96%)	2 (4%)	29 66
6	N	46/47 (98%)	42 (91%)	4 (9%)	10 37
6	Q	46/47 (98%)	45 (98%)	1 (2%)	52 81
6	T	46/47 (98%)	44 (96%)	2 (4%)	29 66
6	W	46/47 (98%)	45 (98%)	1 (2%)	52 81
6	Z	46/47 (98%)	44 (96%)	2 (4%)	29 66
6	c	46/47 (98%)	43 (94%)	3 (6%)	17 50
6	f	46/47 (98%)	44 (96%)	2 (4%)	29 66
6	i	46/47 (98%)	43 (94%)	3 (6%)	17 50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	l	46/47 (98%)	44 (96%)	2 (4%)	29 66
6	o	46/47 (98%)	42 (91%)	4 (9%)	10 37
6	r	46/47 (98%)	45 (98%)	1 (2%)	52 81
6	u	46/47 (98%)	44 (96%)	2 (4%)	29 66
6	x	46/47 (98%)	45 (98%)	1 (2%)	52 81
7	2	21/21 (100%)	21 (100%)	0	100 100
7	5	21/21 (100%)	20 (95%)	1 (5%)	25 62
7	I	21/21 (100%)	20 (95%)	1 (5%)	25 62
7	O	21/21 (100%)	20 (95%)	1 (5%)	25 62
7	R	21/21 (100%)	19 (90%)	2 (10%)	8 32
7	U	21/21 (100%)	21 (100%)	0	100 100
7	X	21/21 (100%)	21 (100%)	0	100 100
7	a	21/21 (100%)	19 (90%)	2 (10%)	8 32
7	d	21/21 (100%)	19 (90%)	2 (10%)	8 32
7	g	21/21 (100%)	20 (95%)	1 (5%)	25 62
7	j	21/21 (100%)	20 (95%)	1 (5%)	25 62
7	m	21/21 (100%)	17 (81%)	4 (19%)	1 8
7	p	21/21 (100%)	18 (86%)	3 (14%)	3 15
7	s	21/21 (100%)	19 (90%)	2 (10%)	8 32
7	v	21/21 (100%)	21 (100%)	0	100 100
7	y	21/21 (100%)	20 (95%)	1 (5%)	25 62
All	All	2928/2963 (99%)	2765 (94%)	163 (6%)	25 56

All (163) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	2	PHE
1	C	29	LYS
1	C	32	LYS
1	C	38	TYR
1	C	57	LYS
1	C	132	CYS
1	C	220	ARG
1	C	252	THR
1	C	274	VAL

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Mol	Chain	Res	Type
1	C	293	ARG
1	C	296	ARG
1	C	331	ILE
2	L	55	GLN
2	L	101	MET
2	L	160	PHE
2	L	185	MET
2	L	205	LYS
2	L	214	GLN
2	L	228	SER
2	L	272	TRP
3	M	27	ASP
3	M	120	MET
3	M	126	SER
3	M	142	THR
3	M	194	PHE
3	M	214	PHE
3	M	296	CYS
4	H	56	ASP
4	H	60	TYR
4	H	87	GLU
4	H	92	GLN
4	H	101	LEU
4	H	124	VAL
4	H	128	VAL
4	H	185	LEU
4	H	205	LYS
4	H	217	GLN
4	H	223	ARG
4	H	224	LEU
4	H	236	ASP
4	H	237	LYS
4	H	258	LEU
5	z	4	TYR
5	z	22	THR
5	z	31	ILE
5	z	54	LEU
5	z	56	LYS
6	1	16	LYS
6	1	50	ILE
6	1	54	TRP
5	F	13	LEU

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Mol	Chain	Res	Type
5	F	31	ILE
5	F	43	ASP
5	F	44	ARG
5	F	56	LYS
5	K	22	THR
5	K	51	GLN
5	P	14	ILE
5	P	43	ASP
5	P	54	LEU
5	S	14	ILE
5	S	19	ARG
5	S	22	THR
5	S	31	ILE
5	S	56	LYS
5	V	3	GLU
5	V	19	ARG
5	V	56	LYS
5	Y	19	ARG
5	Y	31	ILE
5	Y	54	LEU
5	Y	56	LYS
5	b	31	ILE
5	b	44	ARG
5	b	56	LYS
5	e	22	THR
5	e	31	ILE
5	e	56	LYS
5	h	22	THR
5	h	43	ASP
5	h	44	ARG
5	k	14	ILE
5	k	22	THR
5	k	56	LYS
5	n	14	ILE
5	n	15	LEU
5	n	34	LEU
5	q	21	LEU
5	q	22	THR
5	q	44	ARG
5	q	45	LEU
5	q	54	LEU
5	q	56	LYS

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Mol	Chain	Res	Type
5	t	31	ILE
5	t	43	ASP
5	t	56	LYS
5	w	19	ARG
5	w	21	LEU
5	w	31	ILE
5	w	44	ARG
5	w	45	LEU
5	3	31	ILE
5	3	41	SER
5	3	44	ARG
5	6	4	TYR
5	6	17	PRO
5	6	31	ILE
5	6	54	LEU
5	6	56	LYS
6	G	13	GLU
6	G	16	LYS
6	N	2	ASP
6	N	6	SER
6	N	13	GLU
6	N	16	LYS
6	Q	16	LYS
6	T	16	LYS
6	T	47	ILE
6	W	16	LYS
6	Z	16	LYS
6	Z	54	TRP
6	c	16	LYS
6	c	28	LEU
6	c	44	ARG
6	f	13	GLU
6	f	16	LYS
6	i	3	LEU
6	i	16	LYS
6	i	28	LEU
6	l	16	LYS
6	l	55	VAL
6	o	2	ASP
6	o	3	LEU
6	o	14	GLU
6	o	16	LYS

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Mol	Chain	Res	Type
6	r	16	LYS
6	u	16	LYS
6	u	23	VAL
6	x	16	LYS
6	4	16	LYS
6	7	16	LYS
6	7	28	LEU
7	I	28	THR
7	O	28	THR
7	R	17	LEU
7	R	28	THR
7	a	17	LEU
7	a	28	THR
7	d	16	ASN
7	d	28	THR
7	g	16	ASN
7	j	16	ASN
7	m	13	SER
7	m	16	ASN
7	m	17	LEU
7	m	28	THR
7	p	16	ASN
7	p	17	LEU
7	p	19	VAL
7	s	16	ASN
7	s	17	LEU
7	y	14	ASP
7	5	16	ASN

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

Mol	Chain	Res	Type
1	C	24	HIS
1	C	54	GLN
2	L	55	GLN
2	L	144	HIS
2	L	211	HIS
3	M	45	GLN
4	H	92	GLN
5	Y	51	GLN

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	0.58	0	7,9,11	1.40	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FME	H	1	4	-	6/7/9/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	1	FME	CG-CB-CA	-2.16	106.94	112.95

There are no chirality outliers.

All (6) torsion outliers are listed below:

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

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 75 ligands modelled in this entry, 1 is monoatomic - leaving 74 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	$\#\|Z\| > 2$
9	BCB	l	101	-	54,74,74	2.43	17 (31%)	52,115,115	2.35	12 (23%)
9	BCB	e	101	-	54,74,74	2.50	18 (33%)	52,115,115	2.32	15 (28%)
13	SO4	M	402	-	4,4,4	0.32	0	6,6,6	0.09	0
13	SO4	M	403	-	4,4,4	0.44	0	6,6,6	0.19	0
13	SO4	H	303	-	4,4,4	0.36	0	6,6,6	0.10	0
15	MQ9	M	409	-	59,59,59	1.33	4 (6%)	72,75,75	2.22	25 (34%)
9	BCB	V	101	-	54,74,74	2.48	17 (31%)	52,115,115	2.29	14 (26%)
9	BCB	T	101	-	54,74,74	2.48	17 (31%)	52,115,115	2.40	14 (26%)
9	BCB	f	101	-	54,74,74	2.31	18 (33%)	52,115,115	2.18	13 (25%)
9	BCB	t	101	-	54,74,74	2.45	17 (31%)	52,115,115	2.30	15 (28%)
17	NS0	Z	102	-	39,39,39	6.07	19 (48%)	44,46,46	3.58	21 (47%)
17	NS0	G	102	-	39,39,39	6.17	19 (48%)	44,46,46	3.58	23 (52%)
8	HEM	C	401	1	41,50,50	1.46	4 (9%)	45,82,82	1.97	14 (31%)
9	BCB	i	101	-	54,74,74	2.35	17 (31%)	52,115,115	2.17	9 (17%)
13	SO4	M	404	-	4,4,4	0.31	0	6,6,6	0.11	0
9	BCB	z	101	-	54,74,74	2.45	17 (31%)	52,115,115	2.42	17 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	BCB	L	302	-	54,74,74	2.53	17 (31%)	52,115,115	2.48	13 (25%)
9	BCB	M	405	-	54,74,74	2.49	15 (27%)	52,115,115	2.47	13 (25%)
9	BCB	b	101	-	54,74,74	2.50	17 (31%)	52,115,115	2.41	18 (34%)
9	BCB	w	101	-	54,74,74	2.66	17 (31%)	52,115,115	2.53	15 (28%)
9	BCB	r	101	-	54,74,74	2.49	19 (35%)	52,115,115	2.43	14 (26%)
14	LDA	M	408	-	12,15,15	2.12	1 (8%)	14,17,17	0.88	0
9	BCB	Y	101	-	54,74,74	2.51	14 (25%)	52,115,115	2.33	15 (28%)
9	BCB	M	406	-	54,74,74	2.56	15 (27%)	52,115,115	2.68	18 (34%)
17	NS0	c	102	6	39,39,39	6.09	19 (48%)	44,46,46	3.56	24 (54%)
17	NS0	r	102	-	39,39,39	6.09	19 (48%)	44,46,46	3.59	23 (52%)
9	BCB	o	101	-	54,74,74	2.42	18 (33%)	52,115,115	2.34	13 (25%)
9	BCB	1	101	-	54,74,74	2.52	17 (31%)	52,115,115	2.38	13 (25%)
9	BCB	K	101	-	54,74,74	2.46	17 (31%)	52,115,115	2.45	17 (32%)
9	BCB	6	102	-	54,74,74	2.68	16 (29%)	52,115,115	2.46	15 (28%)
9	BCB	G	101	-	54,74,74	2.35	16 (29%)	52,115,115	2.31	14 (26%)
9	BCB	7	101	-	54,74,74	2.36	17 (31%)	52,115,115	2.45	17 (32%)
9	BCB	F	101	-	54,74,74	2.47	15 (27%)	52,115,115	2.24	12 (23%)
13	SO4	H	304	-	4,4,4	0.39	0	6,6,6	0.14	0
17	NS0	f	102	-	39,39,39	6.11	19 (48%)	44,46,46	3.62	23 (52%)
9	BCB	u	101	-	54,74,74	2.46	17 (31%)	52,115,115	2.35	13 (25%)
17	NS0	7	102	-	39,39,39	6.51	19 (48%)	44,46,46	3.56	26 (59%)
13	SO4	M	401	-	4,4,4	0.39	0	6,6,6	0.48	0
9	BCB	n	101	-	54,74,74	2.48	16 (29%)	52,115,115	2.40	14 (26%)
9	BCB	h	101	-	54,74,74	2.55	17 (31%)	52,115,115	2.37	15 (28%)
9	BCB	Q	101	-	54,74,74	2.35	16 (29%)	52,115,115	2.28	12 (23%)
8	HEM	C	403	1	41,50,50	1.39	6 (14%)	45,82,82	2.06	10 (22%)
9	BCB	q	101	-	54,74,74	3.04	20 (37%)	52,115,115	2.37	16 (30%)
17	NS0	l	102	-	39,39,39	6.17	19 (48%)	44,46,46	3.55	22 (50%)
11	UQ9	6	101	-	58,58,58	3.85	16 (27%)	70,73,73	2.43	22 (31%)
10	BPB	L	303	-	49,70,70	2.17	10 (20%)	47,101,101	1.99	7 (14%)
9	BCB	L	301	-	54,74,74	2.39	15 (27%)	52,115,115	2.36	20 (38%)
8	HEM	C	402	1	41,50,50	1.47	6 (14%)	45,82,82	2.13	12 (26%)
9	BCB	c	101	-	54,74,74	2.30	17 (31%)	52,115,115	2.31	13 (25%)
9	BCB	P	101	-	54,74,74	2.53	16 (29%)	52,115,115	2.43	19 (36%)
10	BPB	M	407	-	49,70,70	2.19	10 (20%)	47,101,101	2.24	13 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	NS0	4	102	-	39,39,39	6.02	19 (48%)	44,46,46	3.61	21 (47%)
9	BCB	S	101	-	54,74,74	2.51	17 (31%)	52,115,115	2.35	16 (30%)
9	BCB	Z	101	-	54,74,74	2.45	16 (29%)	52,115,115	2.30	12 (23%)
17	NS0	x	102	-	39,39,39	6.13	19 (48%)	44,46,46	3.59	20 (45%)
14	LDA	H	301	-	12,15,15	2.16	1 (8%)	14,17,17	0.49	0
17	NS0	W	102	-	39,39,39	6.04	19 (48%)	44,46,46	3.68	23 (52%)
17	NS0	Q	102	-	39,39,39	6.09	19 (48%)	44,46,46	3.54	23 (52%)
9	BCB	4	101	-	54,74,74	2.35	17 (31%)	52,115,115	2.18	13 (25%)
17	NS0	i	102	-	39,39,39	6.04	19 (48%)	44,46,46	3.62	23 (52%)
9	BCB	N	101	-	54,74,74	2.42	17 (31%)	52,115,115	2.35	13 (25%)
9	BCB	x	101	-	54,74,74	2.38	18 (33%)	52,115,115	2.27	12 (23%)
9	BCB	3	101	-	54,74,74	2.46	16 (29%)	52,115,115	2.39	15 (28%)
17	NS0	o	102	6	39,39,39	6.06	19 (48%)	44,46,46	3.65	23 (52%)
9	BCB	W	101	-	54,74,74	2.42	16 (29%)	52,115,115	2.20	12 (23%)
13	SO4	H	302	-	4,4,4	0.38	0	6,6,6	0.25	0
16	NS5	M	410	-	39,39,39	0.78	0	44,46,46	1.99	10 (22%)
17	NS0	1	102	6	39,39,39	6.04	19 (48%)	44,46,46	3.64	24 (54%)
8	HEM	C	404	1	41,50,50	1.38	5 (12%)	45,82,82	2.05	14 (31%)
11	UQ9	L	304	-	58,58,58	3.87	16 (27%)	70,73,73	2.62	23 (32%)
17	NS0	T	102	-	39,39,39	6.15	19 (48%)	44,46,46	3.55	20 (45%)
9	BCB	k	101	-	54,74,74	2.44	17 (31%)	52,115,115	2.28	14 (26%)
17	NS0	N	102	-	39,39,39	5.94	19 (48%)	44,46,46	3.65	21 (47%)
17	NS0	u	102	-	39,39,39	6.02	19 (48%)	44,46,46	3.60	21 (47%)

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
9	BCB	l	101	-	-	15/37/177/177	-
9	BCB	e	101	-	-	23/37/177/177	-
15	MQ9	M	409	-	-	16/53/73/73	0/2/2/2
9	BCB	V	101	-	-	24/37/177/177	-
9	BCB	T	101	-	-	21/37/177/177	-
9	BCB	f	101	-	-	15/37/177/177	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BCB	t	101	-	-	20/37/177/177	-
17	NS0	Z	102	-	-	14/43/43/43	-
17	NS0	G	102	-	-	12/43/43/43	-
8	HEM	C	401	1	-	3/12/54/54	-
9	BCB	i	101	-	-	18/37/177/177	-
9	BCB	z	101	-	-	19/37/177/177	-
9	BCB	L	302	-	-	8/37/177/177	-
9	BCB	M	405	-	-	14/37/177/177	-
9	BCB	b	101	-	-	20/37/177/177	-
9	BCB	w	101	-	-	16/37/177/177	-
9	BCB	r	101	-	-	17/37/177/177	-
14	LDA	M	408	-	-	9/13/13/13	-
9	BCB	Y	101	-	-	19/37/177/177	-
9	BCB	M	406	-	-	14/37/177/177	-
17	NS0	c	102	6	-	13/43/43/43	-
17	NS0	r	102	-	-	14/43/43/43	-
9	BCB	o	101	-	-	20/37/177/177	-
9	BCB	1	101	-	-	22/37/177/177	-
9	BCB	K	101	-	-	20/37/177/177	-
9	BCB	6	102	-	-	20/37/177/177	-
9	BCB	G	101	-	-	17/37/177/177	-
9	BCB	7	101	-	-	14/37/177/177	-
9	BCB	F	101	-	-	18/37/177/177	-
17	NS0	f	102	-	-	14/43/43/43	-
9	BCB	u	101	-	-	14/37/177/177	-
17	NS0	7	102	-	-	17/43/43/43	-
9	BCB	n	101	-	-	21/37/177/177	-
9	BCB	h	101	-	-	21/37/177/177	-
9	BCB	Q	101	-	-	21/37/177/177	-
8	HEM	C	403	1	-	6/12/54/54	-
9	BCB	q	101	-	-	20/37/177/177	-
17	NS0	l	102	-	-	15/43/43/43	-
11	UQ9	6	101	-	-	18/57/81/81	0/1/1/1
10	BPB	L	303	-	1/1/18/23	16/37/105/105	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BCB	L	301	-	-	9/37/177/177	-
8	HEM	C	402	1	-	6/12/54/54	-
9	BCB	c	101	-	-	21/37/177/177	-
10	BPB	M	407	-	1/1/18/23	15/37/105/105	0/5/6/6
9	BCB	P	101	-	-	21/37/177/177	-
17	NS0	4	102	-	-	14/43/43/43	-
9	BCB	S	101	-	-	22/37/177/177	-
9	BCB	Z	101	-	-	19/37/177/177	-
17	NS0	x	102	-	-	14/43/43/43	-
14	LDA	H	301	-	-	9/13/13/13	-
17	NS0	W	102	-	-	13/43/43/43	-
17	NS0	Q	102	-	-	14/43/43/43	-
9	BCB	4	101	-	-	21/37/177/177	-
17	NS0	i	102	-	-	14/43/43/43	-
9	BCB	N	101	-	-	20/37/177/177	-
9	BCB	x	101	-	-	18/37/177/177	-
9	BCB	3	101	-	-	16/37/177/177	-
17	NS0	o	102	6	-	14/43/43/43	-
9	BCB	W	101	-	-	16/37/177/177	-
16	NS5	M	410	-	-	13/43/43/43	-
17	NS0	1	102	6	-	16/43/43/43	-
8	HEM	C	404	1	-	5/12/54/54	-
11	UQ9	L	304	-	-	16/57/81/81	0/1/1/1
17	NS0	T	102	-	-	15/43/43/43	-
9	BCB	k	101	-	-	20/37/177/177	-
17	NS0	N	102	-	-	15/43/43/43	-
17	NS0	u	102	-	-	14/43/43/43	-

All (1038) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	7	102	NS0	C9-C7	19.00	1.53	1.34
17	i	102	NS0	C9-C7	18.33	1.53	1.34
17	c	102	NS0	C9-C7	18.32	1.53	1.34
17	r	102	NS0	C9-C7	18.22	1.53	1.34
17	1	102	NS0	C9-C7	18.18	1.53	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Q	102	NS0	C9-C7	18.15	1.52	1.34
17	G	102	NS0	C9-C7	18.14	1.52	1.34
17	x	102	NS0	C9-C7	18.08	1.52	1.34
17	o	102	NS0	C9-C7	18.05	1.52	1.34
17	7	102	NS0	C27-C28	18.03	1.52	1.34
17	f	102	NS0	C9-C7	17.96	1.52	1.34
17	4	102	NS0	C9-C7	17.94	1.52	1.34
17	Z	102	NS0	C9-C7	17.94	1.52	1.34
17	T	102	NS0	C27-C28	17.92	1.52	1.34
17	u	102	NS0	C9-C7	17.92	1.52	1.34
17	W	102	NS0	C9-C7	17.84	1.52	1.34
17	T	102	NS0	C9-C7	17.77	1.52	1.34
17	l	102	NS0	C9-C7	17.62	1.52	1.34
17	l	102	NS0	C27-C28	17.55	1.52	1.34
17	x	102	NS0	C27-C28	17.36	1.52	1.34
17	N	102	NS0	C9-C7	17.20	1.51	1.34
17	f	102	NS0	C27-C28	17.19	1.51	1.34
17	Z	102	NS0	C27-C28	17.17	1.51	1.34
17	G	102	NS0	C27-C28	17.03	1.51	1.34
17	W	102	NS0	C27-C28	16.99	1.51	1.34
17	r	102	NS0	C27-C28	16.93	1.51	1.34
17	Q	102	NS0	C27-C28	16.90	1.51	1.34
17	c	102	NS0	C27-C28	16.83	1.51	1.34
17	N	102	NS0	C27-C28	16.78	1.51	1.34
17	1	102	NS0	C27-C28	16.70	1.51	1.34
17	u	102	NS0	C27-C28	16.64	1.51	1.34
17	4	102	NS0	C27-C28	16.54	1.51	1.34
17	o	102	NS0	C27-C28	16.50	1.51	1.34
17	i	102	NS0	C27-C28	16.45	1.51	1.34
17	7	102	NS0	C14-C12	13.37	1.53	1.35
17	7	102	NS0	C19-C17	13.15	1.53	1.35
17	7	102	NS0	C22-C23	13.00	1.53	1.35
17	G	102	NS0	C19-C17	12.92	1.52	1.35
17	l	102	NS0	C14-C12	12.90	1.52	1.35
17	l	102	NS0	C19-C17	12.75	1.52	1.35
17	c	102	NS0	C19-C17	12.74	1.52	1.35
17	o	102	NS0	C14-C12	12.74	1.52	1.35
17	f	102	NS0	C19-C17	12.73	1.52	1.35
17	G	102	NS0	C22-C23	12.72	1.52	1.35
17	x	102	NS0	C19-C17	12.71	1.52	1.35
17	T	102	NS0	C19-C17	12.65	1.52	1.35
17	Q	102	NS0	C22-C23	12.64	1.52	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	o	102	NS0	C19-C17	12.60	1.52	1.35
17	r	102	NS0	C19-C17	12.55	1.52	1.35
17	Z	102	NS0	C19-C17	12.49	1.52	1.35
17	l	102	NS0	C22-C23	12.49	1.52	1.35
17	W	102	NS0	C19-C17	12.48	1.52	1.35
17	Q	102	NS0	C19-C17	12.48	1.52	1.35
17	u	102	NS0	C22-C23	12.47	1.52	1.35
17	W	102	NS0	C14-C12	12.42	1.52	1.35
17	i	102	NS0	C19-C17	12.42	1.52	1.35
17	x	102	NS0	C22-C23	12.40	1.52	1.35
17	G	102	NS0	C14-C12	12.39	1.52	1.35
17	1	102	NS0	C19-C17	12.38	1.52	1.35
17	N	102	NS0	C19-C17	12.37	1.52	1.35
17	f	102	NS0	C14-C12	12.36	1.52	1.35
17	T	102	NS0	C22-C23	12.33	1.52	1.35
17	i	102	NS0	C14-C12	12.33	1.52	1.35
17	c	102	NS0	C22-C23	12.33	1.52	1.35
17	4	102	NS0	C19-C17	12.31	1.52	1.35
17	f	102	NS0	C22-C23	12.31	1.52	1.35
17	r	102	NS0	C22-C23	12.29	1.52	1.35
17	1	102	NS0	C22-C23	12.26	1.52	1.35
17	r	102	NS0	C14-C12	12.25	1.52	1.35
17	o	102	NS0	C22-C23	12.24	1.52	1.35
17	Z	102	NS0	C22-C23	12.22	1.52	1.35
17	Z	102	NS0	C14-C12	12.21	1.52	1.35
17	T	102	NS0	C14-C12	12.21	1.52	1.35
17	x	102	NS0	C14-C12	12.20	1.52	1.35
17	u	102	NS0	C19-C17	12.20	1.52	1.35
17	4	102	NS0	C22-C23	12.20	1.52	1.35
17	1	102	NS0	C14-C12	12.17	1.51	1.35
17	4	102	NS0	C14-C12	12.17	1.51	1.35
17	W	102	NS0	C22-C23	12.12	1.51	1.35
17	N	102	NS0	C22-C23	12.11	1.51	1.35
17	i	102	NS0	C22-C23	12.09	1.51	1.35
17	Q	102	NS0	C14-C12	12.08	1.51	1.35
17	u	102	NS0	C14-C12	12.08	1.51	1.35
17	N	102	NS0	C14-C12	11.91	1.51	1.35
17	c	102	NS0	C14-C12	11.78	1.51	1.35
9	q	101	BCB	CBB-CAB	-9.54	1.21	1.49
11	L	304	UQ9	O2-C2	9.05	1.43	1.23
11	6	101	UQ9	O2-C2	8.89	1.42	1.23
11	L	304	UQ9	C28-C29	8.70	1.53	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	6	101	UQ9	C23-C24	8.66	1.53	1.33
11	6	101	UQ9	C18-C19	8.62	1.53	1.33
11	L	304	UQ9	C13-C14	8.61	1.53	1.33
11	L	304	UQ9	C8-C9	8.55	1.53	1.33
11	L	304	UQ9	C33-C34	8.52	1.53	1.33
11	L	304	UQ9	C38-C39	8.52	1.53	1.33
11	6	101	UQ9	C28-C29	8.50	1.53	1.33
11	6	101	UQ9	C8-C9	8.50	1.53	1.33
11	L	304	UQ9	C18-C19	8.50	1.53	1.33
11	L	304	UQ9	C23-C24	8.50	1.53	1.33
11	6	101	UQ9	C38-C39	8.50	1.53	1.33
11	6	101	UQ9	C43-C44	8.48	1.53	1.33
11	6	101	UQ9	C13-C14	8.44	1.53	1.33
11	L	304	UQ9	C43-C44	8.36	1.53	1.33
9	6	102	BCB	C1A-CHA	8.36	1.49	1.39
11	6	101	UQ9	C33-C34	8.34	1.53	1.33
17	7	102	NS0	C32-C33	8.04	1.52	1.33
9	M	406	BCB	C1A-CHA	8.01	1.48	1.39
17	G	102	NS0	C32-C33	7.90	1.51	1.33
17	N	102	NS0	C32-C33	7.83	1.51	1.33
9	q	101	BCB	OBB-CAB	7.82	1.47	1.22
17	c	102	NS0	C32-C33	7.81	1.51	1.33
17	l	102	NS0	C32-C33	7.79	1.51	1.33
17	r	102	NS0	C32-C33	7.74	1.51	1.33
17	4	102	NS0	C32-C33	7.73	1.51	1.33
17	f	102	NS0	C32-C33	7.72	1.51	1.33
10	M	407	BPB	CAC-C3C	7.71	1.53	1.33
17	W	102	NS0	C32-C33	7.70	1.51	1.33
17	Q	102	NS0	C32-C33	7.69	1.51	1.33
17	x	102	NS0	C32-C33	7.68	1.51	1.33
17	T	102	NS0	C32-C33	7.66	1.51	1.33
10	L	303	BPB	CAC-C3C	7.66	1.52	1.33
17	Z	102	NS0	C32-C33	7.64	1.51	1.33
17	1	102	NS0	C32-C33	7.58	1.51	1.33
17	u	102	NS0	C32-C33	7.54	1.51	1.33
17	i	102	NS0	C32-C33	7.47	1.50	1.33
11	L	304	UQ9	C48-C49	7.47	1.53	1.32
17	l	102	NS0	CB-CG	7.46	1.53	1.32
17	o	102	NS0	C32-C33	7.45	1.50	1.33
17	c	102	NS0	C10-C11	7.40	1.53	1.34
17	7	102	NS0	C10-C11	7.39	1.53	1.34
17	7	102	NS0	CB-CG	7.37	1.53	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	w	101	BCB	C3A-C2A	-7.35	1.48	1.54
17	u	102	NS0	CB-CG	7.34	1.53	1.32
17	T	102	NS0	C10-C11	7.34	1.53	1.34
17	r	102	NS0	C10-C11	7.33	1.53	1.34
17	c	102	NS0	CB-CG	7.33	1.53	1.32
11	6	101	UQ9	C48-C49	7.29	1.53	1.32
17	u	102	NS0	C10-C11	7.28	1.53	1.34
17	o	102	NS0	CB-CG	7.28	1.53	1.32
14	H	301	LDA	O1-N1	-7.28	1.25	1.42
17	G	102	NS0	C10-C11	7.27	1.53	1.34
17	Q	102	NS0	C10-C11	7.27	1.53	1.34
17	N	102	NS0	C10-C11	7.25	1.53	1.34
17	o	102	NS0	C10-C11	7.25	1.53	1.34
17	7	102	NS0	C15-C16	7.24	1.53	1.34
17	x	102	NS0	C10-C11	7.24	1.53	1.34
17	T	102	NS0	CB-CG	7.24	1.53	1.32
17	x	102	NS0	CB-CG	7.24	1.53	1.32
17	7	102	NS0	C26-C25	7.23	1.53	1.34
17	4	102	NS0	C10-C11	7.23	1.53	1.34
9	Y	101	BCB	C1A-CHA	7.23	1.47	1.39
17	r	102	NS0	CB-CG	7.22	1.53	1.32
17	W	102	NS0	C10-C11	7.21	1.53	1.34
17	4	102	NS0	CB-CG	7.19	1.53	1.32
17	i	102	NS0	CB-CG	7.19	1.53	1.32
17	i	102	NS0	C10-C11	7.19	1.53	1.34
17	Q	102	NS0	CB-CG	7.19	1.53	1.32
17	W	102	NS0	CB-CG	7.18	1.53	1.32
17	G	102	NS0	CB-CG	7.18	1.53	1.32
17	Z	102	NS0	CB-CG	7.17	1.53	1.32
17	Z	102	NS0	C10-C11	7.17	1.53	1.34
17	1	102	NS0	C10-C11	7.16	1.53	1.34
17	f	102	NS0	CB-CG	7.14	1.52	1.32
17	l	102	NS0	C10-C11	7.13	1.52	1.34
17	f	102	NS0	C10-C11	7.10	1.52	1.34
14	M	408	LDA	O1-N1	-7.09	1.25	1.42
17	N	102	NS0	CB-CG	7.08	1.52	1.32
17	l	102	NS0	C15-C16	7.07	1.52	1.34
17	1	102	NS0	CB-CG	7.06	1.52	1.32
17	G	102	NS0	C15-C16	7.01	1.52	1.34
11	6	101	UQ9	C7-C6	-7.00	1.40	1.51
17	T	102	NS0	C26-C25	6.94	1.52	1.34
17	i	102	NS0	C15-C16	6.93	1.52	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	e	101	BCB	C1A-CHA	6.92	1.47	1.39
17	f	102	NS0	C26-C25	6.90	1.52	1.34
17	f	102	NS0	C15-C16	6.89	1.52	1.34
17	x	102	NS0	C26-C25	6.87	1.52	1.34
17	l	102	NS0	C26-C25	6.87	1.52	1.34
9	P	101	BCB	C1A-CHA	6.87	1.47	1.39
17	o	102	NS0	C15-C16	6.85	1.52	1.34
17	T	102	NS0	C15-C16	6.84	1.52	1.34
17	4	102	NS0	C26-C25	6.84	1.52	1.34
17	u	102	NS0	C26-C25	6.83	1.52	1.34
17	Z	102	NS0	C26-C25	6.82	1.52	1.34
17	Z	102	NS0	C15-C16	6.81	1.52	1.34
17	x	102	NS0	C15-C16	6.80	1.52	1.34
17	r	102	NS0	C15-C16	6.80	1.52	1.34
17	Q	102	NS0	C15-C16	6.79	1.52	1.34
17	i	102	NS0	C26-C25	6.78	1.52	1.34
17	u	102	NS0	C15-C16	6.78	1.52	1.34
17	c	102	NS0	C26-C25	6.77	1.52	1.34
17	G	102	NS0	C26-C25	6.75	1.52	1.34
17	1	102	NS0	C15-C16	6.74	1.52	1.34
17	Q	102	NS0	C26-C25	6.74	1.51	1.34
11	L	304	UQ9	C7-C6	-6.73	1.40	1.51
9	o	101	BCB	CAC-C3C	6.71	1.50	1.33
17	W	102	NS0	C15-C16	6.71	1.51	1.34
17	N	102	NS0	C26-C25	6.70	1.51	1.34
17	o	102	NS0	C26-C25	6.69	1.51	1.34
17	4	102	NS0	C15-C16	6.69	1.51	1.34
17	1	102	NS0	C26-C25	6.69	1.51	1.34
17	N	102	NS0	C15-C16	6.69	1.51	1.34
17	c	102	NS0	C15-C16	6.68	1.51	1.34
17	r	102	NS0	C26-C25	6.66	1.51	1.34
17	7	102	NS0	C20-C21	6.59	1.53	1.36
9	n	101	BCB	C1A-CHA	6.59	1.47	1.39
9	F	101	BCB	C1A-CHA	6.58	1.47	1.39
17	W	102	NS0	C26-C25	6.58	1.51	1.34
9	l	101	BCB	CAC-C3C	6.55	1.50	1.33
17	Q	102	NS0	C20-C21	6.51	1.52	1.36
17	4	102	NS0	C20-C21	6.49	1.52	1.36
9	q	101	BCB	C3A-C2A	-6.46	1.48	1.54
17	7	102	NS0	C16-C17	6.46	1.59	1.45
9	h	101	BCB	CHD-C4C	6.44	1.48	1.37
17	G	102	NS0	C20-C21	6.43	1.52	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	1	101	BCB	CAC-C3C	6.42	1.49	1.33
17	c	102	NS0	C20-C21	6.40	1.52	1.36
17	f	102	NS0	C20-C21	6.40	1.52	1.36
17	T	102	NS0	C20-C21	6.39	1.52	1.36
17	r	102	NS0	C20-C21	6.39	1.52	1.36
17	x	102	NS0	C20-C21	6.38	1.52	1.36
9	w	101	BCB	CHD-C4C	6.38	1.48	1.37
17	l	102	NS0	C20-C21	6.38	1.52	1.36
9	N	101	BCB	CAC-C3C	6.37	1.49	1.33
17	Z	102	NS0	C20-C21	6.35	1.52	1.36
9	r	101	BCB	CAC-C3C	6.33	1.49	1.33
9	M	406	BCB	CAC-C3C	6.31	1.49	1.33
9	L	302	BCB	CAC-C3C	6.30	1.49	1.33
17	u	102	NS0	C20-C21	6.30	1.52	1.36
17	1	102	NS0	C20-C21	6.29	1.52	1.36
17	i	102	NS0	C20-C21	6.29	1.52	1.36
9	b	101	BCB	C1A-CHA	6.29	1.46	1.39
9	q	101	BCB	C1A-CHA	6.29	1.46	1.39
17	W	102	NS0	C20-C21	6.27	1.52	1.36
9	F	101	BCB	CAC-C3C	6.25	1.49	1.33
9	Z	101	BCB	CAC-C3C	6.23	1.49	1.33
9	4	101	BCB	CAC-C3C	6.23	1.49	1.33
9	x	101	BCB	CAC-C3C	6.23	1.49	1.33
15	M	409	MQ9	C6-C5	6.23	1.46	1.35
9	V	101	BCB	C3D-C2D	6.22	1.50	1.39
17	o	102	NS0	C20-C21	6.20	1.52	1.36
9	L	301	BCB	CAC-C3C	6.20	1.49	1.33
17	N	102	NS0	C20-C21	6.19	1.52	1.36
9	V	101	BCB	CHD-C4C	6.17	1.48	1.37
9	3	101	BCB	CAC-C3C	6.17	1.49	1.33
9	Q	101	BCB	CAC-C3C	6.13	1.49	1.33
9	u	101	BCB	CAC-C3C	6.11	1.48	1.33
9	h	101	BCB	C3D-C2D	6.11	1.50	1.39
9	7	101	BCB	CAC-C3C	6.10	1.48	1.33
9	3	101	BCB	C1A-CHA	6.10	1.46	1.39
9	i	101	BCB	CAC-C3C	6.10	1.48	1.33
9	z	101	BCB	CHD-C4C	6.10	1.48	1.37
9	z	101	BCB	C3D-C2D	6.09	1.50	1.39
9	V	101	BCB	C3A-C2A	-6.08	1.49	1.54
9	Y	101	BCB	CAC-C3C	6.07	1.48	1.33
9	q	101	BCB	CAC-C3C	6.06	1.48	1.33
9	V	101	BCB	C1A-CHA	6.06	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	W	101	BCB	CAC-C3C	6.06	1.48	1.33
9	k	101	BCB	C1A-CHA	6.04	1.46	1.39
9	6	102	BCB	O2D-CGD	6.04	1.47	1.33
9	P	101	BCB	CHD-C4C	6.02	1.47	1.37
9	z	101	BCB	C3A-C2A	-6.02	1.49	1.54
9	Z	101	BCB	CBD-CGD	-6.01	1.44	1.52
9	h	101	BCB	C3A-C2A	-6.01	1.49	1.54
9	T	101	BCB	CAC-C3C	5.97	1.48	1.33
9	Y	101	BCB	C3A-C2A	-5.97	1.49	1.54
9	6	102	BCB	CHD-C4C	5.96	1.47	1.37
9	G	101	BCB	CAC-C3C	5.93	1.48	1.33
9	M	405	BCB	CAC-C3C	5.91	1.48	1.33
9	f	101	BCB	CAC-C3C	5.91	1.48	1.33
9	L	301	BCB	O2D-CGD	5.90	1.47	1.33
9	t	101	BCB	CAC-C3C	5.90	1.48	1.33
9	M	405	BCB	CHA-CBD	-5.89	1.45	1.52
9	b	101	BCB	C3A-C2A	-5.86	1.49	1.54
9	c	101	BCB	CAC-C3C	5.85	1.48	1.33
9	S	101	BCB	C3A-C2A	-5.85	1.49	1.54
9	K	101	BCB	C1A-CHA	5.84	1.46	1.39
9	L	302	BCB	CBD-CGD	-5.83	1.44	1.52
9	L	301	BCB	C1A-CHA	5.82	1.46	1.39
9	7	101	BCB	C3D-C2D	5.81	1.49	1.39
9	n	101	BCB	CAC-C3C	5.80	1.48	1.33
9	L	301	BCB	C3A-C2A	-5.80	1.49	1.54
9	w	101	BCB	CAC-C3C	5.79	1.48	1.33
9	h	101	BCB	CAC-C3C	5.79	1.48	1.33
9	k	101	BCB	CHD-C4C	5.77	1.47	1.37
9	S	101	BCB	C3D-C2D	5.77	1.49	1.39
9	k	101	BCB	CAC-C3C	5.77	1.48	1.33
9	h	101	BCB	C1A-CHA	5.71	1.46	1.39
9	S	101	BCB	C3B-C2B	5.68	1.49	1.39
9	P	101	BCB	CAC-C3C	5.67	1.47	1.33
11	6	101	UQ9	C1M-C1	-5.67	1.38	1.50
9	q	101	BCB	CHD-C4C	5.67	1.47	1.37
9	l	101	BCB	C1A-CHA	5.66	1.46	1.39
9	6	102	BCB	CAC-C3C	5.66	1.47	1.33
11	L	304	UQ9	C1M-C1	-5.65	1.38	1.50
9	b	101	BCB	CHD-C4C	5.64	1.47	1.37
9	1	101	BCB	C3A-C2A	-5.64	1.49	1.54
9	T	101	BCB	C3A-C2A	-5.63	1.49	1.54
9	n	101	BCB	C3A-C2A	-5.63	1.49	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	b	101	BCB	CAC-C3C	5.61	1.47	1.33
9	V	101	BCB	CAC-C3C	5.59	1.47	1.33
9	n	101	BCB	CHD-C4C	5.59	1.47	1.37
9	S	101	BCB	CAC-C3C	5.59	1.47	1.33
10	M	407	BPB	CBD-CGD	-5.58	1.44	1.52
9	L	302	BCB	C3D-C2D	5.58	1.49	1.39
9	e	101	BCB	C3A-C2A	-5.56	1.49	1.54
9	6	102	BCB	C3A-C2A	-5.56	1.49	1.54
9	e	101	BCB	O2A-CGA	5.54	1.49	1.33
9	7	101	BCB	CHD-C4C	5.53	1.47	1.37
9	n	101	BCB	C3B-C2B	5.53	1.49	1.39
9	k	101	BCB	C3D-C2D	5.52	1.49	1.39
9	n	101	BCB	C3D-C2D	5.52	1.49	1.39
9	3	101	BCB	C3A-C2A	-5.50	1.49	1.54
9	t	101	BCB	C3D-C2D	5.50	1.49	1.39
9	t	101	BCB	CHD-C4C	5.50	1.47	1.37
9	N	101	BCB	C3D-C2D	5.48	1.49	1.39
9	u	101	BCB	C3A-C2A	-5.47	1.49	1.54
9	e	101	BCB	CAC-C3C	5.47	1.47	1.33
9	Q	101	BCB	C3D-C2D	5.47	1.49	1.39
9	M	405	BCB	CBD-CGD	-5.46	1.45	1.52
9	F	101	BCB	C3B-C2B	5.46	1.49	1.39
9	M	405	BCB	O2A-CGA	5.45	1.49	1.33
9	Y	101	BCB	C3D-C2D	5.43	1.49	1.39
9	K	101	BCB	CAC-C3C	5.43	1.47	1.33
9	M	406	BCB	O2D-CGD	5.42	1.46	1.33
9	S	101	BCB	CHD-C4C	5.42	1.46	1.37
9	z	101	BCB	CAC-C3C	5.42	1.47	1.33
9	t	101	BCB	C3B-C2B	5.39	1.49	1.39
9	K	101	BCB	CHD-C4C	5.38	1.46	1.37
9	P	101	BCB	O2A-CGA	5.37	1.49	1.33
9	t	101	BCB	C1A-CHA	5.37	1.45	1.39
9	r	101	BCB	CBD-CGD	-5.36	1.45	1.52
9	t	101	BCB	C3A-C2A	-5.36	1.49	1.54
9	P	101	BCB	C3B-C2B	5.36	1.49	1.39
9	W	101	BCB	C3D-C2D	5.35	1.49	1.39
9	L	302	BCB	CHD-C4C	5.35	1.46	1.37
9	W	101	BCB	C3A-C2A	-5.33	1.49	1.54
9	K	101	BCB	C3B-C2B	5.31	1.48	1.39
9	Y	101	BCB	CHD-C4C	5.31	1.46	1.37
9	6	102	BCB	C3B-C2B	5.29	1.48	1.39
9	K	101	BCB	C3A-C2A	-5.28	1.49	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	3	101	BCB	CHD-C4C	5.28	1.46	1.37
9	u	101	BCB	CHD-C4C	5.25	1.46	1.37
9	Z	101	BCB	C3D-C2D	5.25	1.48	1.39
9	c	101	BCB	C3D-C2D	5.23	1.48	1.39
9	N	101	BCB	C3A-C2A	-5.23	1.49	1.54
9	r	101	BCB	C3B-C2B	5.23	1.48	1.39
9	e	101	BCB	C3D-C2D	5.22	1.48	1.39
9	N	101	BCB	C3B-C2B	5.21	1.48	1.39
9	L	302	BCB	O2A-CGA	5.21	1.48	1.33
9	3	101	BCB	O2A-CGA	5.20	1.48	1.33
9	M	406	BCB	C3A-C2A	-5.19	1.50	1.54
9	3	101	BCB	C3B-C2B	5.19	1.48	1.39
10	L	303	BPB	C3B-C2B	5.19	1.48	1.39
9	Y	101	BCB	C3B-C2B	5.18	1.48	1.39
9	w	101	BCB	O2A-CGA	5.18	1.48	1.33
9	6	102	BCB	O2A-CGA	5.17	1.48	1.33
9	l	101	BCB	CHD-C4C	5.17	1.46	1.37
9	M	405	BCB	OBD-CAD	5.17	1.29	1.22
9	1	101	BCB	CBD-CGD	-5.16	1.45	1.52
9	c	101	BCB	CHD-C4C	5.15	1.46	1.37
9	z	101	BCB	O2A-CGA	5.15	1.48	1.33
9	o	101	BCB	C3B-C2B	5.15	1.48	1.39
9	f	101	BCB	CHD-C4C	5.15	1.46	1.37
9	w	101	BCB	C3B-C2B	5.15	1.48	1.39
9	T	101	BCB	C3B-C2B	5.14	1.48	1.39
9	F	101	BCB	C3A-C2A	-5.12	1.50	1.54
9	Y	101	BCB	O2A-CGA	5.11	1.48	1.33
9	M	405	BCB	C3B-C2B	5.10	1.48	1.39
9	L	302	BCB	CHA-CBD	-5.10	1.46	1.52
9	r	101	BCB	CHD-C4C	5.08	1.46	1.37
9	4	101	BCB	C3D-C2D	5.08	1.48	1.39
9	G	101	BCB	C3B-C2B	5.08	1.48	1.39
9	Q	101	BCB	C1A-CHA	5.07	1.45	1.39
9	n	101	BCB	O2A-CGA	5.07	1.48	1.33
9	e	101	BCB	CHD-C4C	5.06	1.46	1.37
9	N	101	BCB	CHD-C4C	5.06	1.46	1.37
9	P	101	BCB	C3A-C2A	-5.06	1.50	1.54
9	M	406	BCB	CHD-C4C	5.06	1.46	1.37
9	3	101	BCB	C3D-C2D	5.05	1.48	1.39
9	x	101	BCB	O2A-CGA	5.03	1.48	1.33
9	F	101	BCB	CHD-C4C	5.03	1.46	1.37
9	1	101	BCB	O2A-CGA	5.02	1.48	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	407	BPB	O2A-CGA	5.00	1.47	1.33
9	w	101	BCB	C3D-C2D	4.97	1.48	1.39
9	Z	101	BCB	C3A-C2A	-4.97	1.50	1.54
9	i	101	BCB	CHD-C4C	4.96	1.46	1.37
9	1	101	BCB	CHD-C4C	4.96	1.46	1.37
10	L	303	BPB	CBD-CGD	-4.96	1.45	1.52
9	G	101	BCB	C3D-C2D	4.96	1.48	1.39
9	h	101	BCB	O2A-CGA	4.96	1.47	1.33
9	6	102	BCB	C3D-C2D	4.95	1.48	1.39
9	r	101	BCB	C3A-C2A	-4.93	1.50	1.54
9	S	101	BCB	O2A-CGA	4.91	1.47	1.33
9	S	101	BCB	C1A-CHA	4.91	1.45	1.39
9	1	101	BCB	C3D-C2D	4.91	1.48	1.39
9	k	101	BCB	O2A-CGA	4.91	1.47	1.33
9	q	101	BCB	O2A-CGA	4.91	1.47	1.33
9	b	101	BCB	C3B-C2B	4.91	1.48	1.39
9	L	302	BCB	C3B-C2B	4.90	1.48	1.39
9	T	101	BCB	C1A-CHA	4.90	1.45	1.39
9	q	101	BCB	C3D-C2D	4.89	1.48	1.39
9	i	101	BCB	O2A-CGA	4.87	1.47	1.33
9	o	101	BCB	C3D-C2D	4.87	1.48	1.39
9	o	101	BCB	C3A-C2A	-4.87	1.50	1.54
9	h	101	BCB	C3B-C2B	4.86	1.48	1.39
9	k	101	BCB	C3B-C2B	4.86	1.48	1.39
9	M	406	BCB	C3D-C2D	4.86	1.48	1.39
9	u	101	BCB	CBD-CGD	-4.86	1.45	1.52
9	t	101	BCB	O2A-CGA	4.84	1.47	1.33
9	c	101	BCB	C3A-C2A	-4.82	1.50	1.54
9	w	101	BCB	C1A-CHA	4.82	1.45	1.39
9	W	101	BCB	C3B-C2B	4.82	1.48	1.39
9	F	101	BCB	O2A-CGA	4.82	1.47	1.33
9	Q	101	BCB	C3A-C2A	-4.81	1.50	1.54
9	P	101	BCB	C3D-C2D	4.81	1.48	1.39
9	T	101	BCB	C3D-C2D	4.80	1.48	1.39
9	b	101	BCB	O2A-CGA	4.80	1.47	1.33
9	o	101	BCB	O2A-CGA	4.80	1.47	1.33
9	K	101	BCB	O2A-CGA	4.80	1.47	1.33
9	7	101	BCB	C1A-CHA	4.80	1.45	1.39
9	G	101	BCB	O2A-CGA	4.79	1.47	1.33
9	z	101	BCB	C1A-CHA	4.78	1.45	1.39
9	x	101	BCB	C3D-C2D	4.78	1.48	1.39
9	M	406	BCB	O2A-CGA	4.77	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	l	101	BCB	O2A-CGA	4.77	1.47	1.33
9	l	101	BCB	C3A-C2A	-4.77	1.50	1.54
9	V	101	BCB	O2A-CGA	4.76	1.47	1.33
9	Q	101	BCB	C3B-C2B	4.73	1.47	1.39
9	7	101	BCB	O2A-CGA	4.70	1.47	1.33
9	u	101	BCB	C3B-C2B	4.70	1.47	1.39
9	Q	101	BCB	O2D-CGD	4.70	1.44	1.33
9	F	101	BCB	C3D-C2D	4.66	1.47	1.39
9	K	101	BCB	C3D-C2D	4.66	1.47	1.39
9	T	101	BCB	CHD-C4C	4.66	1.45	1.37
9	L	302	BCB	C1A-CHA	4.66	1.45	1.39
8	C	402	HEM	C1B-NB	-4.64	1.32	1.40
9	u	101	BCB	C3D-C2D	4.64	1.47	1.39
9	W	101	BCB	C1A-CHA	4.64	1.45	1.39
9	G	101	BCB	O2D-CGD	4.63	1.44	1.33
9	f	101	BCB	O2A-CGA	4.63	1.46	1.33
9	W	101	BCB	O2A-CGA	4.62	1.46	1.33
9	r	101	BCB	O2A-CGA	4.62	1.46	1.33
9	o	101	BCB	C1A-CHA	4.62	1.45	1.39
9	x	101	BCB	CHD-C4C	4.62	1.45	1.37
9	N	101	BCB	O2A-CGA	4.61	1.46	1.33
9	w	101	BCB	CHA-CBD	-4.61	1.46	1.52
10	M	407	BPB	CHA-CBD	-4.61	1.46	1.52
9	q	101	BCB	C3B-C2B	4.61	1.47	1.39
9	Z	101	BCB	CHD-C4C	4.58	1.45	1.37
9	Q	101	BCB	CHD-C4C	4.57	1.45	1.37
8	C	401	HEM	C1B-NB	-4.57	1.32	1.40
9	1	101	BCB	C3B-C2B	4.57	1.47	1.39
15	M	409	MQ9	C2-C3	4.57	1.48	1.40
9	M	405	BCB	C3D-C2D	4.56	1.47	1.39
9	e	101	BCB	C3B-C2B	4.55	1.47	1.39
9	4	101	BCB	C3B-C2B	4.54	1.47	1.39
9	1	101	BCB	C1A-CHA	4.54	1.44	1.39
9	N	101	BCB	O2D-CGD	4.54	1.44	1.33
9	Z	101	BCB	O2A-CGA	4.53	1.46	1.33
9	c	101	BCB	O2A-CGA	4.52	1.46	1.33
9	G	101	BCB	C3A-C2A	-4.51	1.50	1.54
9	b	101	BCB	C3D-C2D	4.51	1.47	1.39
9	i	101	BCB	CBD-CGD	-4.51	1.46	1.52
9	L	301	BCB	O2A-CGA	4.50	1.46	1.33
9	f	101	BCB	C3D-C2D	4.49	1.47	1.39
9	F	101	BCB	C3D-C4D	-4.49	1.29	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	W	101	BCB	CBD-CGD	-4.49	1.46	1.52
9	f	101	BCB	C3B-C2B	4.48	1.47	1.39
9	f	101	BCB	C3A-C2A	-4.48	1.50	1.54
9	c	101	BCB	O2D-CGD	4.48	1.44	1.33
9	4	101	BCB	CBD-CGD	-4.46	1.46	1.52
9	x	101	BCB	C3A-C2A	-4.45	1.50	1.54
9	L	302	BCB	OBD-CAD	4.45	1.28	1.22
9	7	101	BCB	C3B-C2B	4.44	1.47	1.39
9	G	101	BCB	CHD-C4C	4.44	1.45	1.37
9	M	406	BCB	CBD-CGD	-4.43	1.46	1.52
9	L	301	BCB	CHD-C4C	4.43	1.45	1.37
9	l	101	BCB	C3D-C2D	4.43	1.47	1.39
9	z	101	BCB	C3B-C2B	4.42	1.47	1.39
9	T	101	BCB	O2D-CGD	4.42	1.44	1.33
9	S	101	BCB	CHA-CBD	-4.41	1.47	1.52
9	u	101	BCB	O2A-CGA	4.40	1.46	1.33
9	M	405	BCB	CHD-C4C	4.40	1.45	1.37
9	l	101	BCB	C3D-C4D	-4.39	1.30	1.40
9	r	101	BCB	C1A-CHA	4.39	1.44	1.39
9	w	101	BCB	CBD-CGD	-4.38	1.46	1.52
9	W	101	BCB	O2D-CGD	4.36	1.43	1.33
9	M	406	BCB	C3B-C2B	4.36	1.47	1.39
10	L	303	BPB	O2D-CGD	4.34	1.43	1.33
9	l	101	BCB	C3B-C2B	4.34	1.47	1.39
9	r	101	BCB	C3D-C2D	4.33	1.47	1.39
9	4	101	BCB	CHD-C4C	4.33	1.45	1.37
9	L	301	BCB	CHA-CBD	-4.33	1.47	1.52
9	T	101	BCB	C3D-C4D	-4.32	1.30	1.40
9	x	101	BCB	O2D-CGD	4.32	1.43	1.33
9	k	101	BCB	C3A-C2A	-4.31	1.50	1.54
9	f	101	BCB	O2D-CGD	4.31	1.43	1.33
9	T	101	BCB	CBD-CGD	-4.29	1.46	1.52
9	4	101	BCB	C3A-C2A	-4.29	1.50	1.54
9	i	101	BCB	C3B-C2B	4.26	1.47	1.39
9	Z	101	BCB	O2D-CGD	4.26	1.43	1.33
9	T	101	BCB	O2A-CGA	4.25	1.45	1.33
9	o	101	BCB	CHD-C4C	4.25	1.44	1.37
9	L	301	BCB	C3D-C2D	4.25	1.47	1.39
9	Z	101	BCB	CHA-CBD	-4.24	1.47	1.52
9	x	101	BCB	C3B-C2B	4.23	1.47	1.39
9	r	101	BCB	O2D-CGD	4.23	1.43	1.33
9	u	101	BCB	C1A-CHA	4.23	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	3	101	BCB	O2D-CGD	4.22	1.43	1.33
9	G	101	BCB	C1A-CHA	4.22	1.44	1.39
10	L	303	BPB	O2A-CGA	4.21	1.45	1.33
9	N	101	BCB	CBD-CGD	-4.21	1.46	1.52
9	1	101	BCB	C3D-C4D	-4.20	1.30	1.40
9	7	101	BCB	O2D-CGD	4.18	1.43	1.33
9	W	101	BCB	CHD-C4C	4.18	1.44	1.37
9	x	101	BCB	C1A-CHA	4.16	1.44	1.39
9	Z	101	BCB	C3B-C2B	4.16	1.46	1.39
9	V	101	BCB	C3B-C2B	4.16	1.46	1.39
9	c	101	BCB	C3B-C2B	4.16	1.46	1.39
9	M	406	BCB	C3D-C4D	-4.14	1.30	1.40
9	L	302	BCB	O2D-CGD	4.13	1.43	1.33
9	Z	101	BCB	C1A-CHA	4.13	1.44	1.39
9	4	101	BCB	O2A-CGA	4.12	1.45	1.33
9	W	101	BCB	OBD-CAD	4.12	1.28	1.22
9	L	301	BCB	C3B-C2B	4.11	1.46	1.39
9	1	101	BCB	O2D-CGD	4.11	1.43	1.33
9	G	101	BCB	OBD-CAD	4.10	1.28	1.22
9	i	101	BCB	C3D-C4D	-4.10	1.30	1.40
9	F	101	BCB	O2D-CGD	4.08	1.43	1.33
9	Q	101	BCB	O2A-CGA	4.08	1.45	1.33
9	Y	101	BCB	O2D-CGD	4.07	1.43	1.33
10	L	303	BPB	C3D-C2D	4.07	1.46	1.39
9	o	101	BCB	C3D-C4D	-4.07	1.30	1.40
9	T	101	BCB	OBD-CAD	4.07	1.28	1.22
9	4	101	BCB	C1A-CHA	4.05	1.44	1.39
9	1	101	BCB	CHA-CBD	-4.04	1.47	1.52
9	u	101	BCB	C3D-C4D	-4.03	1.30	1.40
9	K	101	BCB	C3D-C4D	-4.02	1.30	1.40
10	L	303	BPB	OBD-CAD	4.02	1.27	1.22
9	Q	101	BCB	OBD-CAD	4.02	1.27	1.22
9	N	101	BCB	OBD-CAD	4.00	1.27	1.22
9	M	405	BCB	C1A-CHA	3.99	1.44	1.39
9	V	101	BCB	O2D-CGD	3.99	1.42	1.33
9	x	101	BCB	CBD-CGD	-3.98	1.47	1.52
9	M	405	BCB	C3A-C2A	-3.98	1.51	1.54
10	M	407	BPB	O2D-CGD	3.97	1.42	1.33
9	k	101	BCB	O2D-CGD	3.96	1.42	1.33
9	i	101	BCB	C1A-CHA	3.95	1.44	1.39
9	w	101	BCB	O2D-CGD	3.95	1.42	1.33
10	M	407	BPB	C3D-C2D	3.95	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	r	101	BCB	C3D-C4D	-3.95	1.31	1.40
9	k	101	BCB	C3D-C4D	-3.94	1.31	1.40
9	M	405	BCB	C3D-C4D	-3.94	1.31	1.40
9	o	101	BCB	CBD-CGD	-3.94	1.47	1.52
9	q	101	BCB	C3D-C4D	-3.93	1.31	1.40
9	b	101	BCB	CBD-CGD	-3.93	1.47	1.52
9	x	101	BCB	C3D-C4D	-3.93	1.31	1.40
9	t	101	BCB	O2D-CGD	3.93	1.42	1.33
9	i	101	BCB	O2D-CGD	3.92	1.42	1.33
9	h	101	BCB	C3D-C4D	-3.92	1.31	1.40
9	W	101	BCB	C3D-C4D	-3.92	1.31	1.40
9	r	101	BCB	OBD-CAD	3.91	1.27	1.22
9	K	101	BCB	CBD-CGD	-3.91	1.47	1.52
9	b	101	BCB	CHA-CBD	-3.91	1.47	1.52
9	l	101	BCB	O2D-CGD	3.91	1.42	1.33
9	Z	101	BCB	C3D-C4D	-3.91	1.31	1.40
9	4	101	BCB	CHA-CBD	-3.90	1.47	1.52
9	P	101	BCB	O2D-CGD	3.90	1.42	1.33
9	w	101	BCB	CHC-C4B	3.90	1.48	1.40
9	4	101	BCB	O2D-CGD	3.90	1.42	1.33
9	4	101	BCB	C3D-C4D	-3.90	1.31	1.40
8	C	404	HEM	C1B-NB	-3.90	1.33	1.40
9	n	101	BCB	O2D-CGD	3.89	1.42	1.33
9	L	301	BCB	C3D-C4D	-3.88	1.31	1.40
9	T	101	BCB	CHA-CBD	-3.88	1.47	1.52
9	G	101	BCB	C3D-C4D	-3.88	1.31	1.40
9	3	101	BCB	C3D-C4D	-3.87	1.31	1.40
9	Q	101	BCB	C3D-C4D	-3.86	1.31	1.40
9	K	101	BCB	CHA-CBD	-3.85	1.47	1.52
9	7	101	BCB	OBD-CAD	3.85	1.27	1.22
10	L	303	BPB	CHA-CBD	-3.85	1.47	1.52
9	l	101	BCB	CBD-CGD	-3.84	1.47	1.52
9	K	101	BCB	C3B-C4B	3.84	1.50	1.40
9	P	101	BCB	C3D-C4D	-3.84	1.31	1.40
9	n	101	BCB	C3D-C4D	-3.83	1.31	1.40
9	e	101	BCB	O2D-CGD	3.83	1.42	1.33
9	x	101	BCB	OBD-CAD	3.83	1.27	1.22
9	i	101	BCB	C3D-C2D	3.82	1.46	1.39
9	P	101	BCB	C3B-C4B	3.81	1.50	1.40
9	l	101	BCB	OBD-CAD	3.81	1.27	1.22
9	S	101	BCB	O2D-CGD	3.81	1.42	1.33
9	o	101	BCB	O2D-CGD	3.80	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	403	HEM	C1B-NB	-3.80	1.33	1.40
9	i	101	BCB	CHA-CBD	-3.79	1.47	1.52
9	Z	101	BCB	OBD-CAD	3.78	1.27	1.22
9	W	101	BCB	CHA-CBD	-3.78	1.47	1.52
9	i	101	BCB	OBD-CAD	3.78	1.27	1.22
9	S	101	BCB	CBD-CGD	-3.78	1.47	1.52
9	u	101	BCB	O2D-CGD	3.78	1.42	1.33
9	F	101	BCB	C3B-C4B	3.78	1.50	1.40
9	f	101	BCB	CBD-CGD	-3.78	1.47	1.52
9	f	101	BCB	C3D-C4D	-3.77	1.31	1.40
9	h	101	BCB	C4C-NC	3.77	1.38	1.35
9	q	101	BCB	O2D-CGD	3.76	1.42	1.33
9	t	101	BCB	C3D-C4D	-3.76	1.31	1.40
9	b	101	BCB	C3D-C4D	-3.76	1.31	1.40
9	V	101	BCB	C3D-C4D	-3.74	1.31	1.40
9	P	101	BCB	C4C-NC	3.74	1.38	1.35
9	6	102	BCB	OBD-CAD	3.73	1.27	1.22
9	L	302	BCB	C3A-C2A	-3.73	1.51	1.54
9	b	101	BCB	O2D-CGD	3.73	1.42	1.33
9	o	101	BCB	OBD-CAD	3.72	1.27	1.22
9	x	101	BCB	CHB-C1B	3.71	1.48	1.40
9	S	101	BCB	C3D-C4D	-3.70	1.31	1.40
10	L	303	BPB	C4C-NC	-3.69	1.26	1.37
9	K	101	BCB	O2D-CGD	3.69	1.42	1.33
9	Y	101	BCB	C3D-C4D	-3.69	1.31	1.40
9	z	101	BCB	O2D-CGD	3.68	1.42	1.33
9	f	101	BCB	C1A-CHA	3.66	1.43	1.39
9	c	101	BCB	CHC-C4B	3.65	1.48	1.40
9	N	101	BCB	CHA-CBD	-3.65	1.48	1.52
9	h	101	BCB	O2D-CGD	3.64	1.42	1.33
9	4	101	BCB	OBD-CAD	3.63	1.27	1.22
9	7	101	BCB	C3D-C4D	-3.63	1.31	1.40
9	7	101	BCB	CBD-CGD	-3.62	1.47	1.52
9	u	101	BCB	CHA-CBD	-3.62	1.48	1.52
9	u	101	BCB	OBD-CAD	3.61	1.27	1.22
9	L	301	BCB	CBD-CGD	-3.61	1.47	1.52
10	M	407	BPB	C4C-NC	-3.61	1.26	1.37
9	f	101	BCB	CHB-C1B	3.60	1.48	1.40
9	u	101	BCB	C4C-NC	3.60	1.38	1.35
9	e	101	BCB	C3D-C4D	-3.60	1.32	1.40
9	3	101	BCB	CHB-C1B	3.60	1.48	1.40
9	i	101	BCB	CHB-C1B	3.58	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	q	101	BCB	C3B-C4B	3.58	1.49	1.40
9	6	102	BCB	C4C-NC	3.57	1.38	1.35
9	o	101	BCB	C3B-C4B	3.57	1.49	1.40
9	w	101	BCB	C4C-NC	3.56	1.38	1.35
9	e	101	BCB	CHC-C4B	3.56	1.48	1.40
11	L	304	UQ9	C4-C5	-3.55	1.38	1.48
11	6	101	UQ9	C4-C5	-3.55	1.38	1.48
9	4	101	BCB	CHC-C4B	3.53	1.47	1.40
9	N	101	BCB	C3D-C4D	-3.53	1.32	1.40
9	z	101	BCB	C4C-NC	3.53	1.38	1.35
17	7	102	NS0	C11-C12	3.51	1.53	1.45
9	W	101	BCB	CHC-C4B	3.50	1.47	1.40
8	C	401	HEM	C4B-NB	-3.50	1.31	1.38
11	L	304	UQ9	C3-C2	-3.49	1.38	1.48
9	f	101	BCB	OBD-CAD	3.47	1.27	1.22
9	i	101	BCB	C4C-NC	3.47	1.38	1.35
9	w	101	BCB	C3D-C4D	-3.47	1.32	1.40
9	6	102	BCB	C3D-C4D	-3.46	1.32	1.40
9	q	101	BCB	CHB-C1B	3.46	1.47	1.40
9	F	101	BCB	OBD-CAD	3.46	1.27	1.22
8	C	402	HEM	C4D-ND	-3.46	1.34	1.40
9	Q	101	BCB	CBD-CGD	-3.45	1.47	1.52
9	e	101	BCB	CBD-CGD	-3.45	1.47	1.52
8	C	403	HEM	C4D-ND	-3.45	1.34	1.40
9	f	101	BCB	CHA-CBD	-3.44	1.48	1.52
9	t	101	BCB	C4C-NC	3.43	1.38	1.35
9	Y	101	BCB	CHC-C4B	3.43	1.47	1.40
9	r	101	BCB	C3B-C4B	3.43	1.49	1.40
9	x	101	BCB	CHA-CBD	-3.42	1.48	1.52
9	k	101	BCB	CHA-CBD	-3.42	1.48	1.52
9	i	101	BCB	C3A-C2A	-3.42	1.51	1.54
9	3	101	BCB	OBD-CAD	3.39	1.27	1.22
9	F	101	BCB	CHB-C1B	3.37	1.47	1.40
9	z	101	BCB	CHA-CBD	-3.37	1.48	1.52
9	t	101	BCB	C3B-C4B	3.37	1.49	1.40
9	r	101	BCB	CHA-CBD	-3.37	1.48	1.52
8	C	401	HEM	C4D-ND	-3.37	1.34	1.40
9	z	101	BCB	CHC-C4B	3.37	1.47	1.40
9	w	101	BCB	OBD-CAD	3.36	1.27	1.22
9	G	101	BCB	CHC-C4B	3.36	1.47	1.40
9	o	101	BCB	CHA-CBD	-3.35	1.48	1.52
9	Y	101	BCB	OBD-CAD	3.34	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	S	101	BCB	CHB-C1B	3.34	1.47	1.40
17	7	102	NS0	C25-C23	3.33	1.53	1.45
11	6	101	UQ9	C3-C2	-3.33	1.39	1.48
9	o	101	BCB	CHB-C1B	3.33	1.47	1.40
9	l	101	BCB	CHA-CBD	-3.33	1.48	1.52
9	P	101	BCB	OBD-CAD	3.31	1.26	1.22
9	c	101	BCB	CHB-C1B	3.31	1.47	1.40
9	n	101	BCB	C3B-C4B	3.31	1.48	1.40
9	1	101	BCB	CHC-C4B	3.30	1.47	1.40
9	k	101	BCB	CBD-CGD	-3.29	1.48	1.52
9	K	101	BCB	C4C-NC	3.28	1.38	1.35
9	c	101	BCB	C1A-CHA	3.28	1.43	1.39
9	1	101	BCB	CHB-C1B	3.28	1.47	1.40
10	M	407	BPB	C3A-C2A	-3.27	1.51	1.54
9	G	101	BCB	CHB-C1B	3.26	1.47	1.40
9	6	102	BCB	CHB-C1B	3.26	1.47	1.40
9	l	101	BCB	CHB-C1B	3.26	1.47	1.40
9	6	102	BCB	C3B-C4B	3.26	1.48	1.40
9	V	101	BCB	OBD-CAD	3.26	1.26	1.22
9	b	101	BCB	C4C-NC	3.26	1.38	1.35
9	b	101	BCB	CHC-C4B	3.25	1.47	1.40
9	k	101	BCB	C4C-NC	3.25	1.38	1.35
9	4	101	BCB	C3B-C4B	3.25	1.48	1.40
9	Y	101	BCB	CHB-C1B	3.24	1.47	1.40
9	u	101	BCB	C3B-C4B	3.23	1.48	1.40
9	Q	101	BCB	CHC-C4B	3.23	1.47	1.40
9	L	302	BCB	C3D-C4D	-3.23	1.32	1.40
9	3	101	BCB	C3B-C4B	3.22	1.48	1.40
9	P	101	BCB	CHB-C1B	3.22	1.47	1.40
8	C	403	HEM	C4B-NB	-3.21	1.32	1.38
9	w	101	BCB	C3B-C4B	3.21	1.48	1.40
9	u	101	BCB	CHB-C1B	3.21	1.47	1.40
9	z	101	BCB	OBD-CAD	3.19	1.26	1.22
9	7	101	BCB	CHC-C4B	3.19	1.47	1.40
17	7	102	NS0	C10-C9	3.19	1.53	1.43
9	b	101	BCB	C3B-C4B	3.19	1.48	1.40
9	M	406	BCB	CHA-CBD	-3.19	1.48	1.52
9	M	405	BCB	C3B-C4B	3.18	1.48	1.40
9	c	101	BCB	CBD-CGD	-3.18	1.48	1.52
9	k	101	BCB	OBD-CAD	3.18	1.26	1.22
9	T	101	BCB	CHB-C1B	3.18	1.47	1.40
9	i	101	BCB	C3B-C4B	3.18	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	1	101	BCB	OBD-CAD	3.18	1.26	1.22
9	1	101	BCB	C4C-NC	3.17	1.38	1.35
9	e	101	BCB	CHB-C1B	3.17	1.47	1.40
9	k	101	BCB	C3B-C4B	3.15	1.48	1.40
9	h	101	BCB	OBD-CAD	3.15	1.26	1.22
17	7	102	NS0	C26-C27	3.14	1.53	1.43
17	o	102	NS0	C10-C9	3.14	1.53	1.43
17	G	102	NS0	C16-C17	3.14	1.52	1.45
9	e	101	BCB	C3B-C4B	3.13	1.48	1.40
9	z	101	BCB	C3D-C4D	-3.13	1.33	1.40
9	N	101	BCB	C1A-CHA	3.13	1.43	1.39
17	G	102	NS0	C11-C12	3.13	1.52	1.45
9	q	101	BCB	OBD-CAD	3.13	1.26	1.22
9	M	405	BCB	CHD-C1D	3.13	1.47	1.40
9	q	101	BCB	CHA-CBD	-3.12	1.48	1.52
17	4	102	NS0	C10-C9	3.12	1.53	1.43
17	i	102	NS0	C10-C9	3.12	1.53	1.43
9	N	101	BCB	CHC-C4B	3.12	1.47	1.40
9	6	102	BCB	CHD-C1D	3.12	1.47	1.40
10	M	407	BPB	C3B-C2B	3.11	1.45	1.39
17	r	102	NS0	C10-C9	3.11	1.53	1.43
9	u	101	BCB	CHC-C4B	3.10	1.47	1.40
17	G	102	NS0	C10-C9	3.08	1.53	1.43
9	7	101	BCB	CHD-C1D	3.08	1.47	1.40
9	o	101	BCB	CHC-C4B	3.08	1.47	1.40
17	f	102	NS0	C11-C12	3.08	1.52	1.45
17	l	102	NS0	C11-C12	3.07	1.52	1.45
17	1	102	NS0	C10-C9	3.07	1.53	1.43
17	x	102	NS0	C10-C9	3.07	1.53	1.43
9	b	101	BCB	CHB-C1B	3.07	1.46	1.40
9	c	101	BCB	C3D-C4D	-3.07	1.33	1.40
9	z	101	BCB	C3B-C4B	3.06	1.48	1.40
8	C	404	HEM	C4B-NB	-3.06	1.32	1.38
17	c	102	NS0	C10-C9	3.06	1.52	1.43
9	S	101	BCB	C3B-C4B	3.06	1.48	1.40
9	7	101	BCB	C3B-C4B	3.06	1.48	1.40
17	7	102	NS0	C15-C14	3.06	1.52	1.43
17	Z	102	NS0	C10-C9	3.06	1.52	1.43
9	h	101	BCB	CHB-C1B	3.06	1.46	1.40
9	Z	101	BCB	CHC-C4B	3.05	1.46	1.40
9	k	101	BCB	CHB-C1B	3.05	1.46	1.40
9	4	101	BCB	CHB-C1B	3.05	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Q	102	NS0	C10-C9	3.05	1.52	1.43
9	f	101	BCB	CHC-C4B	3.05	1.46	1.40
17	T	102	NS0	C10-C9	3.04	1.52	1.43
9	n	101	BCB	CHC-C4B	3.04	1.46	1.40
17	T	102	NS0	C26-C27	3.03	1.52	1.43
17	u	102	NS0	C10-C9	3.02	1.52	1.43
9	n	101	BCB	OBD-CAD	3.02	1.26	1.22
9	q	101	BCB	CBD-CGD	-3.02	1.48	1.52
9	L	301	BCB	OBD-CAD	3.02	1.26	1.22
9	N	101	BCB	CHB-C1B	3.02	1.46	1.40
17	Q	102	NS0	C11-C12	3.02	1.52	1.45
9	V	101	BCB	CHB-C1B	3.02	1.46	1.40
17	l	102	NS0	C16-C17	3.01	1.52	1.45
9	t	101	BCB	CHB-C1B	3.01	1.46	1.40
9	6	102	BCB	CHC-C4B	3.00	1.46	1.40
9	S	101	BCB	C4C-NC	3.00	1.37	1.35
9	K	101	BCB	CHB-C1B	3.00	1.46	1.40
17	f	102	NS0	C10-C9	3.00	1.52	1.43
9	w	101	BCB	CHB-C1B	3.00	1.46	1.40
9	h	101	BCB	C3B-C4B	3.00	1.48	1.40
10	M	407	BPB	OBD-CAD	3.00	1.26	1.22
17	W	102	NS0	C10-C9	3.00	1.52	1.43
9	V	101	BCB	C3B-C4B	3.00	1.48	1.40
17	c	102	NS0	C11-C12	3.00	1.52	1.45
17	l	102	NS0	C10-C9	3.00	1.52	1.43
9	i	101	BCB	CHC-C4B	2.99	1.46	1.40
17	r	102	NS0	C11-C12	2.99	1.52	1.45
17	1	102	NS0	C16-C17	2.99	1.52	1.45
9	Q	101	BCB	CHB-C1B	2.98	1.46	1.40
17	o	102	NS0	C11-C12	2.98	1.52	1.45
9	q	101	BCB	C4C-NC	2.98	1.37	1.35
9	e	101	BCB	OBD-CAD	2.98	1.26	1.22
9	r	101	BCB	CHC-C4B	2.97	1.46	1.40
9	Y	101	BCB	C3B-C4B	2.96	1.48	1.40
9	q	101	BCB	CHC-C4B	2.96	1.46	1.40
9	Q	101	BCB	CHA-CBD	-2.96	1.48	1.52
17	7	102	NS0	C21-C22	2.95	1.52	1.43
17	x	102	NS0	C11-C12	2.95	1.52	1.45
17	f	102	NS0	C20-C19	2.95	1.52	1.43
9	W	101	BCB	C3B-C4B	2.94	1.48	1.40
9	G	101	BCB	C3B-C4B	2.94	1.48	1.40
9	t	101	BCB	CHC-C4B	2.94	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	T	101	BCB	C3B-C4B	2.94	1.48	1.40
17	W	102	NS0	C11-C12	2.93	1.52	1.45
17	G	102	NS0	C15-C14	2.93	1.52	1.43
17	l	102	NS0	C15-C14	2.93	1.52	1.43
9	G	101	BCB	CHD-C1D	2.93	1.46	1.40
9	F	101	BCB	C4C-NC	2.92	1.37	1.35
17	Z	102	NS0	C16-C17	2.92	1.52	1.45
9	S	101	BCB	CHC-C4B	2.91	1.46	1.40
17	G	102	NS0	C20-C19	2.91	1.52	1.43
17	N	102	NS0	C10-C9	2.90	1.52	1.43
17	4	102	NS0	C26-C27	2.90	1.52	1.43
9	e	101	BCB	CHA-CBD	-2.90	1.48	1.52
9	c	101	BCB	OBD-CAD	2.90	1.26	1.22
9	l	101	BCB	C3B-C4B	2.90	1.47	1.40
17	l	102	NS0	C26-C27	2.89	1.52	1.43
17	o	102	NS0	C16-C17	2.89	1.52	1.45
9	r	101	BCB	CHB-C1B	2.89	1.46	1.40
17	i	102	NS0	C16-C17	2.89	1.52	1.45
9	K	101	BCB	OBD-CAD	2.88	1.26	1.22
17	7	102	NS0	C20-C19	2.88	1.52	1.43
9	G	101	BCB	CBD-CGD	-2.88	1.48	1.52
17	r	102	NS0	C15-C14	2.88	1.52	1.43
17	T	102	NS0	C25-C23	2.88	1.52	1.45
17	x	102	NS0	C26-C27	2.88	1.52	1.43
9	1	101	BCB	C3B-C4B	2.87	1.47	1.40
17	x	102	NS0	C25-C23	2.87	1.52	1.45
17	u	102	NS0	C11-C12	2.87	1.52	1.45
17	Z	102	NS0	C26-C27	2.87	1.52	1.43
9	3	101	BCB	CHC-C4B	2.87	1.46	1.40
9	M	405	BCB	O2D-CGD	2.86	1.40	1.33
9	L	302	BCB	CHD-C1D	2.86	1.46	1.40
17	l	102	NS0	C21-C22	2.86	1.52	1.43
9	T	101	BCB	CHD-C1D	2.86	1.46	1.40
17	o	102	NS0	C15-C14	2.86	1.52	1.43
17	f	102	NS0	C16-C17	2.86	1.52	1.45
17	Q	102	NS0	C26-C27	2.86	1.52	1.43
9	c	101	BCB	CHA-CBD	-2.86	1.49	1.52
17	Q	102	NS0	C15-C14	2.86	1.52	1.43
17	f	102	NS0	C26-C27	2.85	1.52	1.43
17	r	102	NS0	C16-C17	2.85	1.52	1.45
9	h	101	BCB	CHA-CBD	-2.85	1.49	1.52
9	P	101	BCB	CHD-C1D	2.85	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	i	102	NS0	C15-C14	2.84	1.52	1.43
17	1	102	NS0	C11-C12	2.84	1.52	1.45
9	W	101	BCB	CHB-C1B	2.84	1.46	1.40
17	f	102	NS0	C15-C14	2.84	1.52	1.43
9	t	101	BCB	OBD-CAD	2.84	1.26	1.22
9	Z	101	BCB	CHB-C1B	2.83	1.46	1.40
9	L	302	BCB	CHC-C4B	2.83	1.46	1.40
17	4	102	NS0	C16-C17	2.83	1.52	1.45
17	Z	102	NS0	C11-C12	2.82	1.52	1.45
17	Z	102	NS0	C15-C14	2.82	1.52	1.43
9	b	101	BCB	OBD-CAD	2.81	1.26	1.22
9	T	101	BCB	CHC-C4B	2.81	1.46	1.40
17	x	102	NS0	C20-C19	2.81	1.52	1.43
17	T	102	NS0	C20-C19	2.81	1.52	1.43
9	z	101	BCB	CBD-CGD	-2.81	1.48	1.52
17	Q	102	NS0	C20-C19	2.80	1.52	1.43
9	f	101	BCB	C3B-C4B	2.80	1.47	1.40
9	h	101	BCB	CHC-C4B	2.80	1.46	1.40
17	W	102	NS0	C16-C17	2.80	1.52	1.45
9	h	101	BCB	CHD-C1D	2.79	1.46	1.40
17	i	102	NS0	C26-C27	2.79	1.52	1.43
17	W	102	NS0	C15-C14	2.79	1.52	1.43
17	N	102	NS0	C26-C27	2.79	1.52	1.43
9	N	101	BCB	CHD-C1D	2.79	1.46	1.40
17	Q	102	NS0	C16-C17	2.79	1.51	1.45
17	N	102	NS0	C11-C12	2.79	1.51	1.45
11	6	101	UQ9	C6-C1	2.78	1.40	1.35
9	M	406	BCB	CHB-C1B	2.78	1.46	1.40
17	c	102	NS0	C16-C17	2.78	1.51	1.45
9	n	101	BCB	CBD-CGD	-2.77	1.48	1.52
17	c	102	NS0	C26-C27	2.77	1.52	1.43
17	x	102	NS0	C15-C14	2.77	1.52	1.43
17	l	102	NS0	C25-C23	2.77	1.51	1.45
17	G	102	NS0	C21-C22	2.76	1.52	1.43
17	o	102	NS0	C20-C19	2.76	1.52	1.43
17	T	102	NS0	C11-C12	2.76	1.51	1.45
17	T	102	NS0	C16-C17	2.76	1.51	1.45
17	l	102	NS0	C20-C19	2.76	1.52	1.43
9	L	302	BCB	CHB-C1B	2.76	1.46	1.40
17	Z	102	NS0	C20-C19	2.76	1.52	1.43
17	f	102	NS0	C25-C23	2.76	1.51	1.45
17	r	102	NS0	C26-C27	2.76	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	T	101	BCB	C4C-NC	2.76	1.37	1.35
17	1	102	NS0	C15-C14	2.76	1.52	1.43
17	W	102	NS0	C20-C19	2.76	1.52	1.43
9	t	101	BCB	CHA-CBD	-2.76	1.49	1.52
17	u	102	NS0	C26-C27	2.75	1.52	1.43
17	f	102	NS0	C21-C22	2.75	1.52	1.43
17	T	102	NS0	C15-C14	2.75	1.52	1.43
17	4	102	NS0	C11-C12	2.75	1.51	1.45
17	u	102	NS0	C20-C19	2.75	1.52	1.43
9	L	302	BCB	C3B-C4B	2.75	1.47	1.40
17	1	102	NS0	C26-C27	2.74	1.51	1.43
17	G	102	NS0	C26-C27	2.73	1.51	1.43
17	c	102	NS0	C25-C23	2.73	1.51	1.45
9	l	101	BCB	CHC-C4B	2.73	1.46	1.40
8	C	404	HEM	C4D-ND	-2.73	1.35	1.40
15	M	409	MQ9	C38-C39	2.73	1.39	1.33
9	N	101	BCB	C3B-C4B	2.73	1.47	1.40
9	c	101	BCB	CHD-C1D	2.73	1.46	1.40
9	x	101	BCB	CHC-C4B	2.73	1.46	1.40
17	r	102	NS0	C20-C19	2.72	1.51	1.43
9	q	101	BCB	CHD-C1D	2.72	1.46	1.40
17	u	102	NS0	C15-C14	2.72	1.51	1.43
17	u	102	NS0	C16-C17	2.72	1.51	1.45
17	x	102	NS0	C16-C17	2.71	1.51	1.45
17	Z	102	NS0	C25-C23	2.71	1.51	1.45
17	i	102	NS0	C20-C19	2.71	1.51	1.43
9	7	101	BCB	CHB-C1B	2.71	1.46	1.40
17	c	102	NS0	C21-C22	2.71	1.51	1.43
9	M	406	BCB	CHC-C4B	2.70	1.46	1.40
17	4	102	NS0	C21-C22	2.69	1.51	1.43
9	z	101	BCB	CHB-C1B	2.69	1.46	1.40
17	c	102	NS0	C20-C19	2.69	1.51	1.43
17	4	102	NS0	C15-C14	2.69	1.51	1.43
9	k	101	BCB	CHD-C1D	2.68	1.46	1.40
9	r	101	BCB	C4C-NC	2.68	1.37	1.35
9	n	101	BCB	CHB-C1B	2.68	1.46	1.40
17	Q	102	NS0	C21-C22	2.68	1.51	1.43
17	1	102	NS0	C25-C23	2.67	1.51	1.45
17	u	102	NS0	C25-C23	2.67	1.51	1.45
17	N	102	NS0	C15-C14	2.67	1.51	1.43
9	K	101	BCB	CHC-C4B	2.67	1.46	1.40
9	x	101	BCB	C3B-C4B	2.67	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	V	101	BCB	C4C-NC	2.66	1.37	1.35
17	c	102	NS0	C15-C14	2.66	1.51	1.43
17	o	102	NS0	C26-C27	2.66	1.51	1.43
17	W	102	NS0	C26-C27	2.66	1.51	1.43
9	7	101	BCB	C3A-C2A	-2.66	1.52	1.54
17	T	102	NS0	C21-C22	2.66	1.51	1.43
17	x	102	NS0	C21-C22	2.66	1.51	1.43
17	i	102	NS0	C11-C12	2.65	1.51	1.45
17	N	102	NS0	C25-C23	2.64	1.51	1.45
9	t	101	BCB	CHD-C1D	2.64	1.46	1.40
17	G	102	NS0	C25-C23	2.64	1.51	1.45
17	i	102	NS0	C25-C23	2.64	1.51	1.45
9	u	101	BCB	CHD-C1D	2.64	1.46	1.40
11	L	304	UQ9	C6-C1	2.63	1.40	1.35
11	6	101	UQ9	C6-C5	-2.63	1.39	1.46
9	Q	101	BCB	C3B-C4B	2.63	1.47	1.40
9	b	101	BCB	CHD-C1D	2.62	1.46	1.40
9	1	101	BCB	CHD-C1D	2.62	1.46	1.40
17	r	102	NS0	C25-C23	2.62	1.51	1.45
9	M	405	BCB	CHB-C1B	2.61	1.46	1.40
17	u	102	NS0	C21-C22	2.61	1.51	1.43
9	c	101	BCB	C3B-C4B	2.61	1.47	1.40
17	N	102	NS0	C21-C22	2.61	1.51	1.43
9	V	101	BCB	CHC-C4B	2.60	1.46	1.40
17	Z	102	NS0	C21-C22	2.60	1.51	1.43
17	1	102	NS0	C20-C19	2.60	1.51	1.43
17	o	102	NS0	C21-C22	2.60	1.51	1.43
17	o	102	NS0	C25-C23	2.60	1.51	1.45
17	r	102	NS0	C21-C22	2.59	1.51	1.43
9	i	101	BCB	CHD-C1D	2.59	1.45	1.40
17	1	102	NS0	C21-C22	2.59	1.51	1.43
9	S	101	BCB	CHD-C1D	2.59	1.45	1.40
17	N	102	NS0	C20-C19	2.58	1.51	1.43
9	z	101	BCB	CHD-C1D	2.58	1.45	1.40
9	n	101	BCB	CHD-C1D	2.58	1.45	1.40
17	N	102	NS0	C16-C17	2.58	1.51	1.45
17	W	102	NS0	C21-C22	2.58	1.51	1.43
17	i	102	NS0	C21-C22	2.57	1.51	1.43
9	7	101	BCB	CHA-CBD	-2.56	1.49	1.52
9	V	101	BCB	CHA-CBD	-2.56	1.49	1.52
9	G	101	BCB	CHA-CBD	-2.56	1.49	1.52
17	4	102	NS0	C20-C19	2.56	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	4	102	NS0	C25-C23	2.56	1.51	1.45
10	L	303	BPB	C3A-C2A	-2.54	1.52	1.54
9	Z	101	BCB	CHD-C1D	2.54	1.45	1.40
9	S	101	BCB	OBD-CAD	2.54	1.25	1.22
9	k	101	BCB	CHC-C4B	2.53	1.45	1.40
9	V	101	BCB	CHD-C1D	2.53	1.45	1.40
9	V	101	BCB	CBD-CGD	-2.53	1.49	1.52
9	F	101	BCB	CHC-C4B	2.53	1.45	1.40
9	f	101	BCB	CHD-C1D	2.52	1.45	1.40
9	w	101	BCB	CHD-C1D	2.51	1.45	1.40
8	C	403	HEM	CHB-C1B	2.50	1.41	1.35
9	3	101	BCB	C4C-NC	2.48	1.37	1.35
11	L	304	UQ9	C6-C5	-2.48	1.39	1.46
9	t	101	BCB	CBD-CGD	-2.48	1.49	1.52
17	W	102	NS0	C25-C23	2.47	1.51	1.45
9	n	101	BCB	CHA-CBD	-2.46	1.49	1.52
8	C	402	HEM	C1D-ND	-2.46	1.33	1.38
9	M	406	BCB	CHD-C1D	2.44	1.45	1.40
9	F	101	BCB	CHD-C1D	2.43	1.45	1.40
9	x	101	BCB	CHD-C1D	2.43	1.45	1.40
9	3	101	BCB	CHD-C1D	2.42	1.45	1.40
9	Z	101	BCB	C3B-C4B	2.41	1.46	1.40
9	r	101	BCB	C1A-C2A	-2.40	1.46	1.51
17	Q	102	NS0	C25-C23	2.40	1.51	1.45
9	e	101	BCB	C2-C3	2.39	1.38	1.33
9	x	101	BCB	C4C-NC	2.39	1.37	1.35
8	C	402	HEM	C4B-NB	-2.38	1.33	1.38
9	c	101	BCB	C1A-C2A	-2.38	1.46	1.51
9	P	101	BCB	CHC-C4B	2.37	1.45	1.40
8	C	402	HEM	FE-NB	2.36	2.08	1.96
9	r	101	BCB	CHD-C1D	2.35	1.45	1.40
9	o	101	BCB	CHD-C1D	2.32	1.45	1.40
9	L	301	BCB	CHB-C1B	2.32	1.45	1.40
9	h	101	BCB	CBD-CGD	-2.31	1.49	1.52
9	L	301	BCB	CHC-C4B	2.29	1.45	1.40
9	l	101	BCB	C4C-NC	2.29	1.37	1.35
9	7	101	BCB	C4C-NC	2.29	1.37	1.35
9	4	101	BCB	C4C-NC	2.24	1.37	1.35
9	Q	101	BCB	CHD-C1D	2.24	1.45	1.40
9	L	301	BCB	CHD-C1D	2.24	1.45	1.40
9	L	302	BCB	C4C-NC	2.24	1.37	1.35
8	C	403	HEM	FE-NB	2.23	2.07	1.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	f	101	BCB	C4C-NC	2.20	1.37	1.35
9	3	101	BCB	CHA-CBD	-2.20	1.49	1.52
9	l	101	BCB	C1A-C2A	-2.20	1.47	1.51
9	x	101	BCB	C1A-C2A	-2.19	1.47	1.51
9	4	101	BCB	CHD-C1D	2.19	1.45	1.40
9	M	406	BCB	OBD-CAD	2.18	1.25	1.22
9	o	101	BCB	C1A-C2A	-2.16	1.47	1.51
8	C	401	HEM	FE-NB	2.14	2.07	1.96
9	Y	101	BCB	CHD-C1D	2.13	1.44	1.40
8	C	404	HEM	C4D-C3D	2.12	1.48	1.45
9	r	101	BCB	CAA-C2A	-2.11	1.49	1.54
8	C	403	HEM	C1D-ND	-2.11	1.34	1.38
9	W	101	BCB	CHD-C1D	2.09	1.44	1.40
9	P	101	BCB	CBD-CGD	-2.09	1.49	1.52
15	M	409	MQ9	C43-C44	2.07	1.37	1.33
9	K	101	BCB	CHD-C1D	2.06	1.44	1.40
9	e	101	BCB	CHD-C1D	2.05	1.44	1.40
9	q	101	BCB	CMA-C3A	-2.05	1.49	1.53
9	6	102	BCB	CHA-CBD	-2.04	1.49	1.52
9	o	101	BCB	C4C-NC	2.04	1.37	1.35
9	N	101	BCB	C1A-C2A	-2.03	1.47	1.51
9	f	101	BCB	C1A-C2A	-2.02	1.47	1.51
8	C	404	HEM	FE-NB	2.01	2.06	1.96
9	e	101	BCB	CMA-C3A	-2.00	1.49	1.53
8	C	402	HEM	CHB-C1B	2.00	1.40	1.35

All (1076) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	W	102	NS0	C20-C19-C17	-10.66	112.10	127.31
17	l	102	NS0	C20-C19-C17	-10.56	112.23	127.31
17	o	102	NS0	C20-C19-C17	-10.36	112.52	127.31
17	i	102	NS0	C20-C19-C17	-10.19	112.77	127.31
17	N	102	NS0	C20-C19-C17	-10.01	113.02	127.31
17	r	102	NS0	C20-C19-C17	-9.79	113.34	127.31
17	f	102	NS0	C15-C14-C12	-9.77	113.37	127.31
17	1	102	NS0	C20-C19-C17	-9.66	113.53	127.31
17	f	102	NS0	C20-C19-C17	-9.62	113.58	127.31
17	4	102	NS0	C20-C19-C17	-9.53	113.71	127.31
17	u	102	NS0	C20-C19-C17	-9.52	113.72	127.31
9	w	101	BCB	O2D-CGD-CBD	9.52	123.06	111.00
17	Z	102	NS0	C20-C19-C17	-9.47	113.79	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	7	102	NS0	C20-C19-C17	-9.44	113.84	127.31
17	G	102	NS0	C15-C14-C12	-9.40	113.89	127.31
17	G	102	NS0	C20-C19-C17	-9.36	113.95	127.31
17	x	102	NS0	C15-C14-C12	-9.34	113.98	127.31
17	x	102	NS0	C20-C19-C17	-9.22	114.16	127.31
9	L	302	BCB	O2D-CGD-CBD	9.21	122.67	111.00
17	W	102	NS0	C15-C14-C12	-9.19	114.19	127.31
17	Q	102	NS0	C15-C14-C12	-9.16	114.24	127.31
17	c	102	NS0	C20-C19-C17	-9.13	114.28	127.31
17	c	102	NS0	C15-C14-C12	-9.07	114.37	127.31
17	T	102	NS0	C15-C14-C12	-9.04	114.41	127.31
17	o	102	NS0	C15-C14-C12	-9.00	114.47	127.31
17	r	102	NS0	C15-C14-C12	-8.97	114.50	127.31
17	7	102	NS0	C15-C14-C12	-8.91	114.59	127.31
17	4	102	NS0	C15-C14-C12	-8.88	114.64	127.31
17	T	102	NS0	C20-C19-C17	-8.80	114.75	127.31
17	1	102	NS0	C15-C14-C12	-8.75	114.83	127.31
17	l	102	NS0	C15-C14-C12	-8.69	114.91	127.31
9	o	101	BCB	O2D-CGD-CBD	8.67	121.98	111.00
17	Z	102	NS0	C15-C14-C12	-8.64	114.98	127.31
17	Q	102	NS0	C20-C19-C17	-8.62	115.01	127.31
9	b	101	BCB	O2D-CGD-CBD	8.61	121.90	111.00
17	u	102	NS0	C15-C14-C12	-8.61	115.03	127.31
9	L	302	BCB	C4D-C3D-CAD	-8.39	104.00	116.53
9	G	101	BCB	O2D-CGD-CBD	8.39	121.63	111.00
9	1	101	BCB	O2D-CGD-CBD	8.37	121.60	111.00
9	N	101	BCB	O2D-CGD-CBD	8.32	121.54	111.00
9	M	405	BCB	O2D-CGD-CBD	8.31	121.53	111.00
9	7	101	BCB	O2D-CGD-CBD	8.31	121.52	111.00
17	N	102	NS0	C15-C14-C12	-8.28	115.49	127.31
9	Q	101	BCB	O2D-CGD-CBD	8.25	121.45	111.00
9	M	406	BCB	C4D-C3D-CAD	-8.12	104.40	116.53
17	i	102	NS0	C15-C14-C12	-8.10	115.76	127.31
9	r	101	BCB	O2D-CGD-CBD	7.97	121.10	111.00
9	f	101	BCB	CHA-C1A-C2A	-7.95	114.64	133.31
9	L	301	BCB	C4D-C3D-CAD	-7.95	104.67	116.53
9	i	101	BCB	O2D-CGD-CBD	7.90	121.00	111.00
9	x	101	BCB	O2D-CGD-CBD	7.80	120.88	111.00
10	L	303	BPB	O2D-CGD-CBD	7.79	120.87	111.00
9	T	101	BCB	O2D-CGD-CBD	7.78	120.85	111.00
9	Q	101	BCB	CHA-C1A-C2A	-7.77	115.07	133.31
9	K	101	BCB	O2D-CGD-CBD	7.75	120.82	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	M	407	BPB	O2D-CGD-CBD	7.73	120.80	111.00
9	3	101	BCB	CHA-C1A-C2A	-7.72	115.19	133.31
9	n	101	BCB	C4D-C3D-CAD	-7.71	105.01	116.53
9	l	101	BCB	O2D-CGD-CBD	7.71	120.77	111.00
11	L	304	UQ9	C7-C8-C9	-7.68	114.01	126.79
9	u	101	BCB	CHA-C1A-C2A	-7.66	115.32	133.31
9	l	101	BCB	CHA-C1A-C2A	-7.64	115.36	133.31
9	1	101	BCB	CHA-C1A-C2A	-7.64	115.37	133.31
9	3	101	BCB	O2D-CGD-CBD	7.60	120.62	111.00
9	Z	101	BCB	CHA-C1A-C2A	-7.57	115.52	133.31
9	z	101	BCB	C4D-C3D-CAD	-7.57	105.22	116.53
9	r	101	BCB	CHA-C1A-C2A	-7.56	115.56	133.31
9	F	101	BCB	CHA-C1A-C2A	-7.54	115.60	133.31
9	o	101	BCB	CHA-C1A-C2A	-7.54	115.61	133.31
9	N	101	BCB	CHA-C1A-C2A	-7.52	115.65	133.31
9	i	101	BCB	CHA-C1A-C2A	-7.51	115.67	133.31
9	S	101	BCB	C4D-C3D-CAD	-7.51	105.32	116.53
17	i	102	NS0	C10-C11-C12	-7.48	105.41	126.42
9	T	101	BCB	CHA-C1A-C2A	-7.46	115.80	133.31
9	k	101	BCB	C4D-C3D-CAD	-7.45	105.41	116.53
9	V	101	BCB	C4D-C3D-CAD	-7.43	105.44	116.53
9	4	101	BCB	CHA-C1A-C2A	-7.42	115.88	133.31
9	q	101	BCB	O2D-CGD-CBD	7.42	120.39	111.00
9	t	101	BCB	C4D-C3D-CAD	-7.41	105.46	116.53
9	h	101	BCB	C4D-C3D-CAD	-7.39	105.50	116.53
9	S	101	BCB	O2D-CGD-CBD	7.38	120.34	111.00
9	Y	101	BCB	CHA-C1A-C2A	-7.38	115.98	133.31
17	Z	102	NS0	C10-C11-C12	-7.33	105.84	126.42
9	S	101	BCB	CHA-C1A-C2A	-7.32	116.11	133.31
9	K	101	BCB	C4D-C3D-CAD	-7.32	105.60	116.53
17	u	102	NS0	C10-C11-C12	-7.32	105.86	126.42
9	x	101	BCB	CHA-C1A-C2A	-7.31	116.15	133.31
17	4	102	NS0	C10-C11-C12	-7.27	105.98	126.42
9	c	101	BCB	CHA-C1A-C2A	-7.27	116.23	133.31
9	7	101	BCB	CHA-C1A-C2A	-7.26	116.27	133.31
9	M	406	BCB	CMC-C2C-C1C	-7.25	102.17	114.36
9	6	102	BCB	O2D-CGD-CBD	7.25	120.18	111.00
17	1	102	NS0	C10-C11-C12	-7.24	106.08	126.42
17	T	102	NS0	C10-C11-C12	-7.24	106.09	126.42
9	c	101	BCB	O2D-CGD-CBD	7.23	120.15	111.00
9	N	101	BCB	C4D-C3D-CAD	-7.22	105.75	116.53
9	M	406	BCB	O2D-CGD-CBD	7.21	120.13	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	W	101	BCB	C4D-C3D-CAD	-7.21	105.77	116.53
9	6	102	BCB	CHA-C1A-C2A	-7.18	116.46	133.31
9	Z	101	BCB	C4D-C3D-CAD	-7.15	105.86	116.53
17	N	102	NS0	C10-C11-C12	-7.15	106.34	126.42
9	u	101	BCB	O2D-CGD-CBD	7.13	120.03	111.00
9	Y	101	BCB	C4D-C3D-CAD	-7.12	105.90	116.53
9	W	101	BCB	CHA-C1A-C2A	-7.06	116.74	133.31
17	x	102	NS0	C10-C11-C12	-7.05	106.62	126.42
9	K	101	BCB	CHA-C1A-C2A	-7.03	116.80	133.31
9	M	406	BCB	CHA-C1A-C2A	-7.01	116.84	133.31
17	r	102	NS0	C10-C11-C12	-7.01	106.72	126.42
9	q	101	BCB	C4D-C3D-CAD	-7.01	106.07	116.53
17	u	102	NS0	C21-C22-C23	-7.00	117.32	127.31
9	7	101	BCB	C4D-C3D-CAD	-6.99	106.09	116.53
9	G	101	BCB	CHA-C1A-C2A	-6.98	116.91	133.31
9	o	101	BCB	C4D-C3D-CAD	-6.98	106.11	116.53
17	c	102	NS0	C10-C11-C12	-6.98	106.82	126.42
9	h	101	BCB	CHA-C1A-C2A	-6.95	116.99	133.31
9	b	101	BCB	C4D-C3D-CAD	-6.94	106.16	116.53
9	e	101	BCB	O2D-CGD-CBD	6.94	119.79	111.00
9	4	101	BCB	C4D-C3D-CAD	-6.94	106.17	116.53
9	w	101	BCB	C4D-C3D-CAD	-6.93	106.19	116.53
17	o	102	NS0	C10-C11-C12	-6.92	106.97	126.42
9	e	101	BCB	C4D-C3D-CAD	-6.92	106.20	116.53
9	M	405	BCB	C4D-C3D-CAD	-6.91	106.21	116.53
9	1	101	BCB	C4D-C3D-CAD	-6.90	106.23	116.53
9	T	101	BCB	C4D-C3D-CAD	-6.89	106.24	116.53
17	W	102	NS0	C10-C11-C12	-6.86	107.15	126.42
9	P	101	BCB	CHA-C1A-C2A	-6.85	117.23	133.31
9	k	101	BCB	O2D-CGD-CBD	6.84	119.67	111.00
9	l	101	BCB	C4D-C3D-CAD	-6.83	106.34	116.53
17	N	102	NS0	C21-C22-C23	-6.82	117.57	127.31
9	z	101	BCB	O2D-CGD-CBD	6.80	119.61	111.00
9	n	101	BCB	CHA-C1A-C2A	-6.79	117.36	133.31
9	6	102	BCB	C4D-C3D-CAD	-6.75	106.45	116.53
9	F	101	BCB	C4D-C3D-CAD	-6.74	106.47	116.53
9	3	101	BCB	C4D-C3D-CAD	-6.73	106.48	116.53
9	V	101	BCB	CHA-C1A-C2A	-6.73	117.51	133.31
9	b	101	BCB	CHA-C1A-C2A	-6.73	117.51	133.31
17	G	102	NS0	C10-C11-C12	-6.72	107.55	126.42
9	q	101	BCB	CHA-C1A-C2A	-6.72	117.54	133.31
9	P	101	BCB	C4D-C3D-CAD	-6.71	106.51	116.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	Q	101	BCB	C4D-C3D-CAD	-6.69	106.55	116.53
11	6	101	UQ9	C7-C8-C9	-6.68	115.67	126.79
9	e	101	BCB	CHA-C1A-C2A	-6.67	117.65	133.31
9	t	101	BCB	O2D-CGD-CBD	6.66	119.44	111.00
9	4	101	BCB	O2D-CGD-CBD	6.62	119.39	111.00
17	l	102	NS0	C10-C11-C12	-6.62	107.81	126.42
9	F	101	BCB	O2D-CGD-CBD	6.59	119.35	111.00
9	f	101	BCB	O2D-CGD-CBD	6.59	119.34	111.00
9	c	101	BCB	C4D-C3D-CAD	-6.58	106.71	116.53
17	Q	102	NS0	C10-C11-C12	-6.57	107.97	126.42
9	k	101	BCB	CHA-C1A-C2A	-6.57	117.89	133.31
17	Z	102	NS0	C21-C22-C23	-6.56	117.94	127.31
9	n	101	BCB	O2D-CGD-CBD	6.56	119.31	111.00
9	Z	101	BCB	O2D-CGD-CBD	6.53	119.27	111.00
9	t	101	BCB	CHA-C1A-C2A	-6.50	118.05	133.31
17	f	102	NS0	C10-C11-C12	-6.49	108.17	126.42
11	L	304	UQ9	C6-C1-C2	6.47	124.29	119.18
17	i	102	NS0	C20-C21-C22	-6.44	110.29	123.47
9	w	101	BCB	CHA-C1A-C2A	-6.40	118.29	133.31
9	x	101	BCB	C4D-C3D-CAD	-6.39	106.98	116.53
9	6	102	BCB	CED-O2D-CGD	6.38	130.38	115.94
9	z	101	BCB	CHA-C1A-C2A	-6.32	118.46	133.31
17	7	102	NS0	C10-C11-C12	-6.30	108.72	126.42
17	1	102	NS0	C21-C22-C23	-6.29	118.34	127.31
9	P	101	BCB	O2D-CGD-CBD	6.29	118.96	111.00
9	Y	101	BCB	O2D-CGD-CBD	6.28	118.96	111.00
17	W	102	NS0	C21-C22-C23	-6.27	118.36	127.31
9	f	101	BCB	C4D-C3D-CAD	-6.27	107.17	116.53
17	W	102	NS0	C20-C21-C22	-6.27	110.63	123.47
9	i	101	BCB	C4D-C3D-CAD	-6.25	107.19	116.53
17	r	102	NS0	C20-C21-C22	-6.25	110.66	123.47
9	r	101	BCB	C4D-C3D-CAD	-6.25	107.20	116.53
17	o	102	NS0	C20-C21-C22	-6.24	110.69	123.47
9	W	101	BCB	O2D-CGD-CBD	6.22	118.88	111.00
17	f	102	NS0	C21-C22-C23	-6.22	118.44	127.31
9	u	101	BCB	C4D-C3D-CAD	-6.21	107.26	116.53
17	T	102	NS0	C21-C22-C23	-6.20	118.47	127.31
17	7	102	NS0	C20-C21-C22	-6.19	110.79	123.47
9	G	101	BCB	C4D-C3D-CAD	-6.19	107.29	116.53
17	4	102	NS0	C20-C21-C22	-6.18	110.81	123.47
17	c	102	NS0	C21-C22-C23	-6.18	118.48	127.31
17	x	102	NS0	C20-C21-C22	-6.15	110.87	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	G	102	NS0	C21-C22-C23	-6.14	118.54	127.31
10	M	407	BPB	C1A-C2A-C3A	-6.13	97.00	102.84
17	l	102	NS0	C20-C21-C22	-6.13	110.92	123.47
17	4	102	NS0	C21-C22-C23	-6.12	118.58	127.31
17	o	102	NS0	C21-C22-C23	-6.07	118.64	127.31
8	C	403	HEM	C1B-NB-C4B	6.06	111.33	105.07
9	V	101	BCB	O2D-CGD-CBD	6.06	118.67	111.00
17	x	102	NS0	C21-C22-C23	-6.04	118.69	127.31
17	1	102	NS0	C20-C21-C22	-6.04	111.11	123.47
17	Q	102	NS0	C20-C21-C22	-6.02	111.14	123.47
17	c	102	NS0	C20-C21-C22	-6.02	111.15	123.47
17	f	102	NS0	C20-C21-C22	-6.02	111.15	123.47
8	C	403	HEM	CHC-C4B-NB	6.00	130.95	124.43
17	N	102	NS0	C20-C21-C22	-6.00	111.18	123.47
16	M	410	NS5	C19-C20-C21	-6.00	118.75	127.31
17	i	102	NS0	C21-C22-C23	-5.98	118.78	127.31
9	M	405	BCB	CHA-C1A-C2A	-5.98	119.27	133.31
17	l	102	NS0	C21-C22-C23	-5.96	118.80	127.31
17	T	102	NS0	C20-C21-C22	-5.94	111.31	123.47
15	M	409	MQ9	C20-C19-C21	5.91	125.22	115.27
9	h	101	BCB	C4-C3-C5	5.90	125.20	115.27
10	L	303	BPB	CBC-CAC-C3C	-5.86	111.15	126.70
17	G	102	NS0	C20-C21-C22	-5.86	111.47	123.47
17	r	102	NS0	C21-C22-C23	-5.84	118.98	127.31
17	1	102	NS0	C31-C32-C33	-5.79	113.73	127.66
17	Z	102	NS0	C20-C21-C22	-5.78	111.63	123.47
11	6	101	UQ9	O2-C2-C3	-5.78	108.67	120.93
17	Q	102	NS0	C21-C22-C23	-5.74	119.12	127.31
9	L	302	BCB	CHA-C1A-C2A	-5.73	119.86	133.31
9	L	301	BCB	CHA-C1A-C2A	-5.71	119.90	133.31
8	C	404	HEM	C1B-NB-C4B	5.71	110.97	105.07
17	4	102	NS0	C31-C32-C33	-5.70	113.93	127.66
9	c	101	BCB	CMC-C2C-C1C	-5.66	104.84	114.36
8	C	401	HEM	C1B-NB-C4B	5.63	110.89	105.07
17	x	102	NS0	C31-C32-C33	-5.62	114.12	127.66
9	T	101	BCB	CMC-C2C-C1C	-5.59	104.97	114.36
9	h	101	BCB	O2D-CGD-CBD	5.59	118.07	111.00
17	u	102	NS0	C20-C21-C22	-5.58	112.04	123.47
17	N	102	NS0	CA-CB-CG	-5.53	108.84	127.75
11	L	304	UQ9	C42-C43-C44	-5.52	114.38	127.66
11	L	304	UQ9	C22-C23-C24	-5.52	114.38	127.66
15	M	409	MQ9	C12-C13-C14	-5.51	114.39	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	7	102	NS0	C21-C22-C23	-5.50	119.46	127.31
11	L	304	UQ9	O2-C2-C3	-5.48	109.30	120.93
11	6	101	UQ9	C6-C1-C2	5.47	123.51	119.18
9	M	405	BCB	CMC-C2C-C1C	-5.45	105.20	114.36
17	G	102	NS0	CA-CB-CG	-5.45	109.13	127.75
17	T	102	NS0	CA-CB-CG	-5.45	109.13	127.75
9	Z	101	BCB	CMC-C2C-C1C	-5.44	105.23	114.36
17	i	102	NS0	CA-CB-CG	-5.42	109.22	127.75
17	N	102	NS0	C31-C32-C33	-5.42	114.62	127.66
17	Q	102	NS0	CA-CB-CG	-5.42	109.24	127.75
17	i	102	NS0	C31-C32-C33	-5.39	114.67	127.66
17	o	102	NS0	CA-CB-CG	-5.37	109.39	127.75
17	f	102	NS0	CA-CB-CG	-5.37	109.40	127.75
17	f	102	NS0	C31-C32-C33	-5.35	114.79	127.66
11	L	304	UQ9	C32-C33-C34	-5.34	114.81	127.66
17	4	102	NS0	CA-CB-CG	-5.33	109.53	127.75
17	7	102	NS0	C16-C17-C19	5.33	127.11	118.94
17	Q	102	NS0	C31-C32-C33	-5.32	114.84	127.66
17	x	102	NS0	CA-CB-CG	-5.32	109.57	127.75
17	7	102	NS0	C31-C32-C33	-5.31	114.87	127.66
17	W	102	NS0	CA-CB-CG	-5.30	109.63	127.75
17	1	102	NS0	CA-CB-CG	-5.29	109.67	127.75
17	r	102	NS0	CA-CB-CG	-5.28	109.71	127.75
17	Z	102	NS0	CA-CB-CG	-5.28	109.72	127.75
8	C	402	HEM	C1B-NB-C4B	5.26	110.51	105.07
17	T	102	NS0	C31-C32-C33	-5.24	115.03	127.66
17	7	102	NS0	CA-CB-CG	-5.24	109.83	127.75
17	4	102	NS0	C27-C26-C25	-5.24	106.88	123.22
11	L	304	UQ9	C17-C18-C19	-5.23	115.06	127.66
17	u	102	NS0	C27-C26-C25	-5.20	106.98	123.22
17	i	102	NS0	C27-C26-C25	-5.19	107.03	123.22
17	Z	102	NS0	C27-C26-C25	-5.19	107.03	123.22
17	Q	102	NS0	C27-C26-C25	-5.18	107.04	123.22
9	n	101	BCB	C4-C3-C5	5.17	123.97	115.27
17	1	102	NS0	C27-C26-C25	-5.15	107.15	123.22
8	C	402	HEM	CHD-C1D-ND	5.15	130.02	124.43
11	6	101	UQ9	C32-C33-C34	-5.15	115.27	127.66
17	c	102	NS0	CA-CB-CG	-5.15	110.16	127.75
11	6	101	UQ9	C17-C18-C19	-5.11	115.35	127.66
17	u	102	NS0	C31-C32-C33	-5.10	115.37	127.66
17	T	102	NS0	C27-C26-C25	-5.09	107.34	123.22
11	6	101	UQ9	C42-C43-C44	-5.07	115.44	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	K	101	BCB	C4-C3-C5	5.07	123.80	115.27
9	L	301	BCB	O2D-CGD-CBD	5.07	117.42	111.00
15	M	409	MQ9	C35-C34-C36	5.07	123.80	115.27
9	z	101	BCB	CAA-C2A-C3A	-5.06	98.93	112.78
17	o	102	NS0	C31-C32-C33	-5.05	115.50	127.66
10	M	407	BPB	CBC-CAC-C3C	-5.03	113.34	126.70
9	u	101	BCB	C4-C3-C5	5.02	123.72	115.27
17	c	102	NS0	C27-C26-C25	-5.01	107.57	123.22
16	M	410	NS5	C18-C19-C20	4.98	133.68	123.47
17	N	102	NS0	C27-C26-C25	-4.95	107.75	123.22
11	6	101	UQ9	C22-C23-C24	-4.95	115.75	127.66
9	4	101	BCB	CMC-C2C-C1C	-4.94	106.05	114.36
17	Z	102	NS0	C31-C32-C33	-4.93	115.79	127.66
11	L	304	UQ9	C37-C38-C39	-4.92	115.81	127.66
11	6	101	UQ9	C37-C38-C39	-4.91	115.84	127.66
17	l	102	NS0	C31-C32-C33	-4.90	115.87	127.66
17	G	102	NS0	C31-C32-C33	-4.89	115.88	127.66
11	L	304	UQ9	C27-C28-C29	-4.88	115.91	127.66
17	u	102	NS0	CA-CB-CG	-4.87	111.11	127.75
17	W	102	NS0	C31-C32-C33	-4.86	115.96	127.66
17	o	102	NS0	C27-C26-C25	-4.85	108.08	123.22
17	r	102	NS0	C27-C26-C25	-4.85	108.09	123.22
9	e	101	BCB	C1-O2A-CGA	4.85	129.16	116.44
17	f	102	NS0	C27-C26-C25	-4.84	108.10	123.22
17	l	102	NS0	C27-C26-C25	-4.83	108.15	123.22
9	N	101	BCB	CMC-C2C-C1C	-4.81	106.27	114.36
17	u	102	NS0	CD2-CG-CB	-4.81	108.74	122.65
17	W	102	NS0	C27-C26-C25	-4.81	108.21	123.22
17	x	102	NS0	C27-C26-C25	-4.81	108.21	123.22
11	L	304	UQ9	C12-C13-C14	-4.78	116.15	127.66
15	M	409	MQ9	C31-C32-C33	-4.78	96.18	111.88
17	l	102	NS0	CD2-CG-CB	-4.76	108.88	122.65
9	L	302	BCB	O1D-CGD-CBD	-4.73	116.86	124.74
17	G	102	NS0	CD1-CG-CB	-4.73	108.97	122.65
17	G	102	NS0	C27-C26-C25	-4.73	108.46	123.22
17	N	102	NS0	CD1-CG-CB	-4.72	109.00	122.65
11	6	101	UQ9	C27-C28-C29	-4.70	116.34	127.66
17	r	102	NS0	C31-C32-C33	-4.69	116.37	127.66
8	C	404	HEM	CHC-C4B-NB	4.69	129.52	124.43
17	1	102	NS0	CD1-CG-CB	-4.68	109.13	122.65
9	l	101	BCB	C1-O2A-CGA	4.68	128.72	116.44
17	c	102	NS0	CD2-CG-CB	-4.67	109.15	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	l	102	NS0	CA-CB-CG	-4.67	111.80	127.75
17	f	102	NS0	CD1-CG-CB	-4.67	109.16	122.65
17	Q	102	NS0	CD1-CG-CB	-4.66	109.17	122.65
17	W	102	NS0	CD2-CG-CB	-4.64	109.23	122.65
17	x	102	NS0	CD1-CG-CB	-4.64	109.25	122.65
17	7	102	NS0	CD2-CG-CB	-4.62	109.29	122.65
9	q	101	BCB	C4-C3-C5	4.62	123.04	115.27
17	r	102	NS0	CD1-CG-CB	-4.62	109.29	122.65
9	G	101	BCB	CMC-C2C-C1C	-4.61	106.62	114.36
17	Z	102	NS0	CD2-CG-CB	-4.60	109.36	122.65
17	c	102	NS0	C31-C32-C33	-4.60	116.59	127.66
11	6	101	UQ9	C12-C13-C14	-4.59	116.61	127.66
17	N	102	NS0	CD2-CG-CB	-4.59	109.39	122.65
17	T	102	NS0	CD2-CG-CB	-4.58	109.40	122.65
17	4	102	NS0	CD1-CG-CB	-4.58	109.41	122.65
17	i	102	NS0	CD2-CG-CB	-4.58	109.42	122.65
9	x	101	BCB	CMC-C2C-C1C	-4.58	106.67	114.36
17	o	102	NS0	CD1-CG-CB	-4.57	109.43	122.65
17	W	102	NS0	CD1-CG-CB	-4.57	109.45	122.65
17	4	102	NS0	CD2-CG-CB	-4.57	109.45	122.65
17	i	102	NS0	CD1-CG-CB	-4.57	109.45	122.65
9	M	405	BCB	C4-C3-C5	4.56	122.95	115.27
17	r	102	NS0	CD2-CG-CB	-4.55	109.49	122.65
17	T	102	NS0	CD1-CG-CB	-4.54	109.53	122.65
9	w	101	BCB	O1D-CGD-CBD	-4.54	117.18	124.74
17	x	102	NS0	CD2-CG-CB	-4.53	109.56	122.65
17	o	102	NS0	CD2-CG-CB	-4.53	109.56	122.65
17	x	102	NS0	C15-C16-C17	-4.52	113.71	126.42
17	1	102	NS0	CD2-CG-CB	-4.52	109.58	122.65
8	C	402	HEM	CAD-C3D-C4D	4.51	132.54	124.66
9	1	101	BCB	CMC-C2C-C1C	-4.51	106.78	114.36
17	f	102	NS0	C15-C16-C17	-4.51	113.76	126.42
17	Z	102	NS0	CD1-CG-CB	-4.50	109.64	122.65
9	L	301	BCB	CMC-C2C-C1C	-4.50	106.80	114.36
8	C	401	HEM	CHC-C4B-NB	4.50	129.31	124.43
17	l	102	NS0	C15-C16-C17	-4.49	113.80	126.42
10	L	303	BPB	O1D-CGD-CBD	-4.48	117.27	124.74
17	G	102	NS0	CD2-CG-CB	-4.47	109.72	122.65
17	Q	102	NS0	CD2-CG-CB	-4.47	109.73	122.65
17	f	102	NS0	CD2-CG-CB	-4.46	109.75	122.65
9	u	101	BCB	C1-O2A-CGA	4.46	128.14	116.44
17	7	102	NS0	CD1-CG-CB	-4.45	109.77	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	403	HEM	CHD-C1D-ND	4.45	129.26	124.43
17	N	102	NS0	C9-C10-C11	-4.43	109.39	123.22
9	M	405	BCB	C1-O2A-CGA	4.43	128.06	116.44
17	7	102	NS0	C27-C26-C25	-4.40	109.47	123.22
17	Q	102	NS0	C9-C10-C11	-4.39	109.51	123.22
17	c	102	NS0	CD1-CG-CB	-4.39	109.95	122.65
17	o	102	NS0	C15-C16-C17	-4.38	114.11	126.42
9	P	101	BCB	O2A-CGA-CBA	4.38	125.65	111.91
9	e	101	BCB	O2A-CGA-CBA	4.38	125.64	111.91
17	o	102	NS0	C9-C10-C11	-4.32	109.75	123.22
8	C	402	HEM	CHD-C1D-C2D	-4.31	118.25	124.98
9	7	101	BCB	CMC-C2C-C1C	-4.31	107.13	114.36
17	W	102	NS0	C15-C16-C17	-4.30	114.33	126.42
9	P	101	BCB	C1-O2A-CGA	4.28	127.68	116.44
17	W	102	NS0	C9-C10-C11	-4.27	109.90	123.22
17	G	102	NS0	C15-C16-C17	-4.25	114.46	126.42
17	T	102	NS0	C15-C16-C17	-4.25	114.49	126.42
17	G	102	NS0	C9-C10-C11	-4.23	110.00	123.22
17	4	102	NS0	C15-C16-C17	-4.23	114.55	126.42
9	k	101	BCB	CBC-CAC-C3C	-4.22	115.50	126.70
17	l	102	NS0	C9-C10-C11	-4.21	110.08	123.22
9	1	101	BCB	C1-O2A-CGA	4.20	127.48	116.44
17	r	102	NS0	C29-C28-C30	4.20	122.33	115.27
17	u	102	NS0	C29-C28-C30	4.20	122.33	115.27
8	C	402	HEM	CHC-C4B-NB	4.20	128.99	124.43
17	c	102	NS0	C29-C28-C30	4.19	122.31	115.27
8	C	402	HEM	CAD-CBD-CGD	-4.19	104.60	113.60
9	w	101	BCB	O2A-CGA-CBA	4.18	125.04	111.91
9	i	101	BCB	C1-O2A-CGA	4.17	127.39	116.44
17	1	102	NS0	C29-C28-C30	4.17	122.29	115.27
17	Q	102	NS0	C29-C28-C30	4.16	122.28	115.27
15	M	409	MQ9	C30-C29-C31	4.15	122.25	115.27
9	c	101	BCB	C1-O2A-CGA	4.15	127.33	116.44
17	u	102	NS0	C15-C16-C17	-4.13	114.81	126.42
9	W	101	BCB	CMC-C2C-C1C	-4.12	107.44	114.36
17	f	102	NS0	C9-C10-C11	-4.12	110.37	123.22
9	r	101	BCB	CMC-C2C-C1C	-4.11	107.46	114.36
17	4	102	NS0	C29-C28-C30	4.10	122.17	115.27
9	G	101	BCB	C1-O2A-CGA	4.10	127.20	116.44
17	u	102	NS0	C9-C10-C11	-4.09	110.46	123.22
17	c	102	NS0	C9-C10-C11	-4.09	110.47	123.22
17	u	102	NS0	C21-C20-C19	-4.07	115.14	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	Q	102	NS0	C15-C16-C17	-4.07	114.99	126.42
17	Q	102	NS0	C21-C20-C19	-4.07	115.14	123.47
10	M	407	BPB	O1D-CGD-CBD	-4.06	117.97	124.74
9	z	101	BCB	O2A-CGA-CBA	4.06	124.66	111.91
8	C	404	HEM	CAD-C3D-C4D	4.06	131.75	124.66
17	7	102	NS0	C9-C10-C11	-4.05	110.57	123.22
9	M	406	BCB	O1D-CGD-CBD	-4.04	118.01	124.74
17	T	102	NS0	C9-C10-C11	-4.04	110.62	123.22
17	r	102	NS0	C15-C16-C17	-4.03	115.10	126.42
9	Y	101	BCB	O2A-CGA-CBA	4.02	124.53	111.91
17	u	102	NS0	CD1-CG-CB	-4.02	111.03	122.65
17	1	102	NS0	C9-C10-C11	-4.00	110.72	123.22
17	G	102	NS0	C29-C28-C30	4.00	122.00	115.27
17	x	102	NS0	C9-C10-C11	-4.00	110.75	123.22
15	M	409	MQ9	C45-C44-C46	3.98	121.96	115.27
17	1	102	NS0	C15-C16-C17	-3.97	115.28	126.42
17	i	102	NS0	C15-C16-C17	-3.96	115.28	126.42
17	N	102	NS0	C15-C16-C17	-3.96	115.29	126.42
17	i	102	NS0	C9-C10-C11	-3.95	110.88	123.22
17	4	102	NS0	C9-C10-C11	-3.93	110.96	123.22
17	W	102	NS0	C29-C28-C30	3.92	121.87	115.27
17	Z	102	NS0	C21-C20-C19	-3.92	115.44	123.47
17	Z	102	NS0	C29-C28-C30	3.91	121.86	115.27
17	Z	102	NS0	C15-C16-C17	-3.91	115.44	126.42
9	t	101	BCB	C1-O2A-CGA	3.91	126.70	116.44
17	r	102	NS0	C9-C10-C11	-3.90	111.04	123.22
9	n	101	BCB	C1-O2A-CGA	3.90	126.67	116.44
17	o	102	NS0	C29-C28-C30	3.89	121.82	115.27
9	6	102	BCB	O2A-CGA-CBA	3.87	124.06	111.91
8	C	404	HEM	CHD-C1D-ND	3.87	128.64	124.43
17	c	102	NS0	C15-C16-C17	-3.87	115.56	126.42
9	M	405	BCB	CHC-C1C-C2C	-3.86	112.01	122.60
9	W	101	BCB	C1-O2A-CGA	3.86	126.57	116.44
9	x	101	BCB	C1-O2A-CGA	3.86	126.56	116.44
17	Z	102	NS0	C9-C10-C11	-3.84	111.22	123.22
15	M	409	MQ9	C21-C19-C18	-3.83	113.36	121.12
9	L	302	BCB	CMC-C2C-C1C	-3.83	107.92	114.36
9	r	101	BCB	O1D-CGD-CBD	-3.83	118.36	124.74
17	i	102	NS0	C29-C28-C30	3.83	121.71	115.27
17	f	102	NS0	C29-C28-C30	3.83	121.71	115.27
17	1	102	NS0	C21-C20-C19	-3.82	115.65	123.47
9	k	101	BCB	O2A-CGA-CBA	3.81	123.87	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	L	304	UQ9	C7-C6-C5	3.80	123.06	118.48
16	M	410	NS5	C4-C5-C7	-3.80	113.42	121.12
9	M	405	BCB	CMA-C3A-C4A	-3.79	106.08	114.38
11	6	101	UQ9	C47-C48-C49	-3.79	114.80	127.75
17	N	102	NS0	C29-C28-C30	3.78	121.63	115.27
17	c	102	NS0	C21-C20-C19	-3.78	115.73	123.47
15	M	409	MQ9	C46-C44-C43	-3.77	113.49	121.12
9	W	101	BCB	CMB-C2B-C3B	3.77	131.73	124.68
17	N	102	NS0	C21-C20-C19	-3.77	115.76	123.47
9	Z	101	BCB	O1D-CGD-CBD	-3.77	118.47	124.74
17	l	102	NS0	CD1-CG-CB	-3.76	111.78	122.65
16	M	410	NS5	C6-C5-C4	3.74	121.56	115.27
17	T	102	NS0	C21-C20-C19	-3.72	115.85	123.47
9	F	101	BCB	O2A-CGA-CBA	3.72	123.59	111.91
10	L	303	BPB	C6-C7-C8	-3.72	103.89	115.92
17	l	102	NS0	C29-C28-C30	3.72	121.53	115.27
17	7	102	NS0	C29-C28-C30	3.71	121.52	115.27
9	r	101	BCB	CMB-C2B-C3B	3.70	131.61	124.68
8	C	404	HEM	C2C-C3C-C4C	-3.70	104.31	106.90
17	x	102	NS0	C29-C28-C30	3.70	121.49	115.27
17	N	102	NS0	C14-C15-C16	-3.70	111.68	123.22
9	l	101	BCB	CMC-C2C-C1C	-3.68	108.18	114.36
16	M	410	NS5	C12-C13-C14	-3.66	111.79	123.22
17	G	102	NS0	C21-C20-C19	-3.66	115.97	123.47
9	N	101	BCB	O1D-CGD-CBD	-3.66	118.64	124.74
17	T	102	NS0	C29-C28-C30	3.66	121.43	115.27
9	L	302	BCB	C1-O2A-CGA	3.65	126.02	116.44
9	V	101	BCB	C3D-CAD-CBD	3.65	112.41	107.61
11	L	304	UQ9	C47-C48-C49	-3.64	115.30	127.75
9	r	101	BCB	O2A-CGA-CBA	3.64	123.32	111.91
9	w	101	BCB	C1-O2A-CGA	3.63	125.98	116.44
9	q	101	BCB	C1-O2A-CGA	3.63	125.97	116.44
9	7	101	BCB	CMA-C3A-C4A	-3.62	106.44	114.38
9	n	101	BCB	C3D-CAD-CBD	3.62	112.37	107.61
9	r	101	BCB	O2A-C1-C2	3.60	118.11	108.64
9	V	101	BCB	O2A-CGA-CBA	3.60	123.20	111.91
11	L	304	UQ9	C1M-C1-C6	-3.60	118.53	124.40
9	L	301	BCB	CHC-C1C-C2C	-3.59	112.76	122.60
17	4	102	NS0	C21-C20-C19	-3.59	116.12	123.47
9	h	101	BCB	CHC-C1C-C2C	-3.57	112.81	122.60
9	G	101	BCB	O2A-CGA-CBA	3.57	123.10	111.91
8	C	401	HEM	CHD-C1D-ND	3.57	128.31	124.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	r	102	NS0	C21-C20-C19	-3.56	116.18	123.47
9	b	101	BCB	C4-C3-C5	3.56	121.26	115.27
9	Y	101	BCB	O2D-CGD-O1D	-3.55	116.89	123.84
9	M	406	BCB	CAA-CBA-CGA	-3.54	102.90	113.25
9	o	101	BCB	CMB-C2B-C3B	3.54	131.30	124.68
9	o	101	BCB	O2A-CGA-CBA	3.53	122.98	111.91
17	f	102	NS0	C21-C20-C19	-3.52	116.26	123.47
17	x	102	NS0	C21-C20-C19	-3.52	116.26	123.47
9	P	101	BCB	CMB-C2B-C3B	3.51	131.25	124.68
9	k	101	BCB	C1-O2A-CGA	3.51	125.65	116.44
9	c	101	BCB	O2A-CGA-CBA	3.51	122.91	111.91
9	t	101	BCB	C3D-CAD-CBD	3.50	112.22	107.61
9	7	101	BCB	O2D-CGD-O1D	-3.50	116.99	123.84
9	1	101	BCB	O1D-CGD-CBD	-3.50	118.92	124.74
11	6	101	UQ9	O2-C2-C1	-3.49	110.44	120.73
9	l	101	BCB	O2A-CGA-CBA	3.48	122.84	111.91
9	3	101	BCB	O2A-C1-C2	3.48	117.79	108.64
9	6	102	BCB	CHC-C1C-C2C	-3.48	113.06	122.60
9	Y	101	BCB	C3D-CAD-CBD	3.47	112.17	107.61
9	F	101	BCB	O2D-CGD-O1D	-3.47	117.05	123.84
9	z	101	BCB	CBC-CAC-C3C	-3.47	117.50	126.70
9	1	101	BCB	O2A-CGA-CBA	3.47	122.79	111.91
9	F	101	BCB	C1-O2A-CGA	3.45	125.51	116.44
11	L	304	UQ9	O2-C2-C1	-3.45	110.56	120.73
9	L	302	BCB	CMA-C3A-C4A	-3.45	106.83	114.38
9	M	406	BCB	C3D-CAD-CBD	3.45	112.14	107.61
9	M	406	BCB	O2A-CGA-CBA	3.44	122.69	111.91
9	3	101	BCB	O2D-CGD-O1D	-3.43	117.13	123.84
8	C	403	HEM	CHA-C4D-ND	3.43	128.62	124.38
9	V	101	BCB	CHC-C1C-C2C	-3.43	113.21	122.60
9	f	101	BCB	C1-O2A-CGA	3.42	125.40	116.44
16	M	410	NS5	C30-C29-C28	-3.41	112.58	123.22
9	V	101	BCB	CAA-CBA-CGA	-3.39	103.34	113.25
9	3	101	BCB	C1-O2A-CGA	3.39	125.33	116.44
9	t	101	BCB	CHC-C1C-C2C	-3.38	113.35	122.60
17	i	102	NS0	C14-C15-C16	-3.37	112.70	123.22
10	M	407	BPB	C1-O2A-CGA	3.37	125.28	116.44
17	u	102	NS0	C14-C15-C16	-3.37	112.71	123.22
9	w	101	BCB	CAA-C2A-C3A	-3.36	103.56	112.78
9	h	101	BCB	C1-O2A-CGA	3.36	125.26	116.44
9	b	101	BCB	CMB-C2B-C3B	3.36	130.96	124.68
9	L	301	BCB	C3D-CAD-CBD	3.35	112.02	107.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	K	101	BCB	C5-C3-C2	-3.34	114.35	121.12
17	c	102	NS0	C14-C15-C16	-3.34	112.79	123.22
9	P	101	BCB	CHC-C1C-C2C	-3.34	113.44	122.60
17	W	102	NS0	C21-C20-C19	-3.34	116.64	123.47
8	C	403	HEM	CHD-C1D-C2D	-3.33	119.78	124.98
9	i	101	BCB	O2A-CGA-CBA	3.33	122.36	111.91
9	t	101	BCB	O2A-CGA-CBA	3.33	122.35	111.91
9	3	101	BCB	CAA-CBA-CGA	-3.33	103.53	113.25
9	T	101	BCB	O1D-CGD-CBD	-3.32	119.20	124.74
15	M	409	MQ9	C5M-C5-C6	-3.31	119.00	124.40
9	n	101	BCB	CHC-C1C-C2C	-3.31	113.54	122.60
9	o	101	BCB	C1-O2A-CGA	3.30	125.10	116.44
9	P	101	BCB	CMC-C2C-C1C	-3.29	108.83	114.36
9	x	101	BCB	O2A-CGA-CBA	3.29	122.24	111.91
17	o	102	NS0	C21-C20-C19	-3.29	116.73	123.47
9	G	101	BCB	CHC-C1C-C2C	-3.29	113.59	122.60
17	Z	102	NS0	C14-C15-C16	-3.29	112.96	123.22
9	i	101	BCB	O1D-CGD-CBD	-3.29	119.27	124.74
9	3	101	BCB	O2A-CGA-CBA	3.29	122.22	111.91
9	S	101	BCB	C4-C3-C5	3.28	120.80	115.27
9	K	101	BCB	CMB-C2B-C3B	3.28	130.82	124.68
15	M	409	MQ9	C32-C31-C29	3.27	123.73	112.98
17	r	102	NS0	C14-C15-C16	-3.27	113.02	123.22
8	C	404	HEM	CHD-C1D-C2D	-3.26	119.88	124.98
9	w	101	BCB	CHC-C1C-C2C	-3.26	113.66	122.60
17	i	102	NS0	C21-C20-C19	-3.26	116.80	123.47
9	F	101	BCB	CHC-C1C-C2C	-3.26	113.68	122.60
9	4	101	BCB	CHD-C4C-C3C	-3.26	120.87	130.10
8	C	401	HEM	CBA-CAA-C2A	-3.25	107.07	112.62
8	C	401	HEM	CHA-C4D-ND	3.25	128.39	124.38
9	Y	101	BCB	O2A-C1-C2	3.24	117.15	108.64
17	W	102	NS0	C34-C33-C35	3.24	120.72	115.27
9	Z	101	BCB	CMB-C2B-C3B	3.24	130.73	124.68
17	r	102	NS0	C34-C33-C35	3.23	120.71	115.27
9	w	101	BCB	CMB-C2B-C3B	3.23	130.72	124.68
9	z	101	BCB	C1-O2A-CGA	3.22	124.89	116.44
15	M	409	MQ9	C12-C11-C9	-3.22	102.39	112.98
9	b	101	BCB	CHD-C4C-C3C	-3.22	120.98	130.10
9	N	101	BCB	O2A-CGA-CBA	3.22	122.00	111.91
9	t	101	BCB	CMB-C2B-C3B	3.21	130.69	124.68
9	f	101	BCB	O2A-CGA-CBA	3.21	121.98	111.91
9	P	101	BCB	O2D-CGD-O1D	-3.21	117.56	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	T	101	BCB	C4-C3-C5	3.20	120.66	115.27
17	7	102	NS0	C18-C17-C16	-3.20	113.03	118.08
17	Q	102	NS0	C34-C33-C35	3.20	120.65	115.27
9	z	101	BCB	O2D-CGD-O1D	-3.20	117.59	123.84
17	1	102	NS0	C14-C15-C16	-3.20	113.24	123.22
9	V	101	BCB	CAA-C2A-C3A	-3.19	104.03	112.78
9	z	101	BCB	O2A-C1-C2	3.19	117.02	108.64
10	L	303	BPB	CMB-C2B-C3B	3.19	130.65	124.68
11	6	101	UQ9	C1M-C1-C6	-3.19	119.19	124.40
17	N	102	NS0	C34-C33-C35	3.19	120.64	115.27
17	4	102	NS0	C14-C15-C16	-3.19	113.27	123.22
9	L	301	BCB	CED-O2D-CGD	3.19	123.14	115.94
17	7	102	NS0	C21-C20-C19	-3.18	116.96	123.47
10	M	407	BPB	O2A-CGA-CBA	3.18	121.89	111.91
9	K	101	BCB	O2D-CGD-O1D	-3.18	117.62	123.84
9	V	101	BCB	C1-O2A-CGA	3.18	124.78	116.44
9	S	101	BCB	C3D-CAD-CBD	3.18	111.79	107.61
9	L	301	BCB	O1D-CGD-CBD	-3.17	119.46	124.74
9	h	101	BCB	CBC-CAC-C3C	-3.17	118.29	126.70
9	T	101	BCB	C1-O2A-CGA	3.17	124.75	116.44
9	h	101	BCB	C3D-CAD-CBD	3.16	111.76	107.61
9	h	101	BCB	O2A-CGA-CBA	3.15	121.80	111.91
17	G	102	NS0	C34-C33-C35	3.14	120.56	115.27
9	6	102	BCB	C1-C2-C3	3.14	131.47	126.04
9	K	101	BCB	CHD-C4C-C3C	-3.14	121.21	130.10
9	N	101	BCB	CMB-C2B-C3B	3.13	130.54	124.68
9	Z	101	BCB	O2A-CGA-CBA	3.13	121.73	111.91
17	o	102	NS0	C34-C33-C35	3.13	120.54	115.27
9	e	101	BCB	CHD-C4C-C3C	-3.13	121.24	130.10
9	u	101	BCB	O2A-CGA-CBA	3.12	121.69	111.91
17	c	102	NS0	C34-C33-C35	3.11	120.51	115.27
15	M	409	MQ9	C7-C6-C1	3.11	121.83	118.50
9	b	101	BCB	O2D-CGD-O1D	-3.11	117.76	123.84
9	w	101	BCB	O2A-CGA-O1A	-3.11	115.75	123.59
9	o	101	BCB	CHD-C4C-C3C	-3.10	121.31	130.10
9	z	101	BCB	CHD-C4C-C3C	-3.10	121.32	130.10
9	6	102	BCB	CMA-C3A-C4A	-3.10	107.59	114.38
9	S	101	BCB	CHC-C1C-C2C	-3.09	114.14	122.60
9	Y	101	BCB	CHD-C4C-C3C	-3.08	121.36	130.10
15	M	409	MQ9	C16-C17-C18	-3.08	101.75	111.88
9	G	101	BCB	CMB-C2B-C3B	3.08	130.43	124.68
9	3	101	BCB	CHC-C1C-C2C	-3.07	114.18	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	402	HEM	CAD-C3D-C2D	-3.07	122.16	127.88
9	P	101	BCB	C1-C2-C3	3.07	131.35	126.04
17	T	102	NS0	C14-C15-C16	-3.07	113.65	123.22
9	Q	101	BCB	CMC-C2C-C1C	-3.06	109.21	114.36
17	Q	102	NS0	C14-C15-C16	-3.06	113.66	123.22
9	F	101	BCB	C3D-CAD-CBD	3.06	111.63	107.61
9	k	101	BCB	CHC-C1C-C2C	-3.06	114.23	122.60
17	u	102	NS0	C34-C33-C35	3.05	120.41	115.27
9	o	101	BCB	O2D-CGD-O1D	-3.05	117.88	123.84
17	i	102	NS0	C34-C33-C35	3.05	120.40	115.27
17	1	102	NS0	C34-C33-C35	3.04	120.39	115.27
9	S	101	BCB	C1-O2A-CGA	3.04	124.42	116.44
8	C	401	HEM	CHD-C1D-C2D	-3.04	120.23	124.98
15	M	409	MQ9	C25-C24-C23	-3.04	115.88	123.68
17	Z	102	NS0	C34-C33-C35	3.04	120.38	115.27
8	C	401	HEM	CHA-C4D-C3D	-3.03	119.64	125.33
10	M	407	BPB	C4-C3-C5	3.03	120.37	115.27
9	l	101	BCB	CHD-C4C-C3C	-3.03	121.52	130.10
9	z	101	BCB	CHC-C1C-C2C	-3.03	114.31	122.60
17	l	102	NS0	C34-C33-C35	3.02	120.35	115.27
9	x	101	BCB	CHC-C1C-C2C	-3.02	114.33	122.60
17	N	102	NS0	C8-C7-C	3.02	120.35	115.27
9	T	101	BCB	O2A-CGA-CBA	3.02	121.38	111.91
17	W	102	NS0	C14-C15-C16	-3.02	113.81	123.22
17	x	102	NS0	C34-C33-C35	3.01	120.33	115.27
9	V	101	BCB	O2D-CGD-O1D	-3.01	117.96	123.84
9	M	406	BCB	CHC-C1C-C2C	-3.00	114.37	122.60
9	q	101	BCB	CHD-C4C-C3C	-3.00	121.59	130.10
9	M	406	BCB	CED-O2D-CGD	3.00	122.73	115.94
15	M	409	MQ9	C31-C29-C28	-3.00	115.05	121.12
9	w	101	BCB	CHD-C4C-C3C	-2.99	121.63	130.10
9	7	101	BCB	CHC-C1C-C2C	-2.99	114.42	122.60
9	K	101	BCB	CBC-CAC-C3C	-2.98	118.79	126.70
9	b	101	BCB	O2A-CGA-CBA	2.98	121.26	111.91
9	t	101	BCB	O2D-CGD-O1D	-2.98	118.01	123.84
9	M	405	BCB	O2A-CGA-CBA	2.98	121.25	111.91
9	3	101	BCB	CHD-C4C-C3C	-2.98	121.67	130.10
9	e	101	BCB	CHC-C1C-C2C	-2.98	114.45	122.60
17	l	102	NS0	C21-C20-C19	-2.97	117.38	123.47
9	W	101	BCB	CHD-C4C-C3C	-2.97	121.68	130.10
9	L	302	BCB	CHC-C1C-C2C	-2.97	114.47	122.60
9	Z	101	BCB	CHC-C1C-C2C	-2.97	114.47	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	7	101	BCB	CMB-C2B-C3B	2.97	130.23	124.68
9	Q	101	BCB	O1D-CGD-CBD	-2.97	119.80	124.74
9	u	101	BCB	CHD-C4C-C3C	-2.97	121.69	130.10
17	o	102	NS0	C8-C7-C	2.96	120.25	115.27
17	i	102	NS0	C8-C7-C	2.96	120.25	115.27
9	P	101	BCB	C3D-CAD-CBD	2.96	111.50	107.61
9	z	101	BCB	C3D-CAD-CBD	2.96	111.50	107.61
17	T	102	NS0	C34-C33-C35	2.96	120.25	115.27
9	G	101	BCB	O1D-CGD-CBD	-2.96	119.81	124.74
9	L	301	BCB	CHD-C4C-C3C	-2.96	121.72	130.10
8	C	403	HEM	CHB-C1B-NB	2.95	128.03	124.38
10	M	407	BPB	CMA-C3A-C4A	-2.95	107.91	114.38
9	Y	101	BCB	CAA-CBA-CGA	-2.95	104.64	113.25
9	L	302	BCB	O2A-CGA-CBA	2.95	121.15	111.91
10	M	407	BPB	CMC-C2C-C1C	-2.94	109.41	114.36
9	W	101	BCB	O1D-CGD-CBD	-2.94	119.84	124.74
17	G	102	NS0	C8-C7-C	2.94	120.21	115.27
8	C	401	HEM	CHB-C1B-NB	2.93	128.00	124.38
17	f	102	NS0	C34-C33-C35	2.93	120.20	115.27
8	C	403	HEM	O2D-CGD-CBD	2.92	123.43	114.03
9	S	101	BCB	CHD-C4C-C3C	-2.92	121.81	130.10
9	K	101	BCB	C1-O2A-CGA	2.92	124.11	116.44
11	L	304	UQ9	C25-C24-C26	2.92	120.18	115.27
9	b	101	BCB	CHC-C1C-C2C	-2.91	114.62	122.60
9	M	405	BCB	C4-C3-C2	-2.91	116.21	123.68
9	K	101	BCB	CHC-C1C-C2C	-2.91	114.63	122.60
9	f	101	BCB	CMC-C2C-C1C	-2.91	109.48	114.36
9	n	101	BCB	C5-C3-C2	-2.90	115.24	121.12
9	3	101	BCB	C3D-CAD-CBD	2.90	111.43	107.61
17	Z	102	NS0	C8-C7-C	2.90	120.15	115.27
8	C	403	HEM	CHA-C4D-C3D	-2.90	119.88	125.33
9	T	101	BCB	CHC-C1C-C2C	-2.90	114.66	122.60
17	Q	102	NS0	C8-C7-C	2.90	120.14	115.27
9	Q	101	BCB	CHD-C4C-C3C	-2.90	121.89	130.10
9	r	101	BCB	CBA-CAA-C2A	-2.89	105.36	113.81
9	e	101	BCB	O2A-CGA-O1A	-2.89	116.31	123.59
9	1	101	BCB	CHD-C4C-C3C	-2.89	121.92	130.10
17	c	102	NS0	C8-C7-C	2.89	120.13	115.27
17	7	102	NS0	C15-C16-C17	-2.88	118.32	126.42
9	W	101	BCB	O2A-CGA-CBA	2.88	120.95	111.91
9	q	101	BCB	C3D-CAD-CBD	2.88	111.39	107.61
17	u	102	NS0	C8-C7-C	2.87	120.10	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	T	102	NS0	C8-C7-C	2.87	120.09	115.27
9	L	301	BCB	C7-C6-C5	-2.86	105.58	113.36
9	k	101	BCB	CHD-C4C-C3C	-2.86	121.99	130.10
17	7	102	NS0	C34-C33-C35	2.86	120.08	115.27
9	h	101	BCB	O2D-CGD-O1D	-2.86	118.25	123.84
9	4	101	BCB	C1-O2A-CGA	2.86	123.94	116.44
9	M	406	BCB	OBB-CAB-CBB	2.85	126.59	120.17
9	k	101	BCB	O2A-CGA-O1A	-2.85	116.39	123.59
11	L	304	UQ9	C45-C44-C46	2.85	120.06	115.27
17	o	102	NS0	C14-C15-C16	-2.85	114.33	123.22
11	6	101	UQ9	C30-C29-C31	2.85	120.06	115.27
9	M	406	BCB	CMB-C2B-C3B	2.84	130.00	124.68
9	V	101	BCB	C4-C3-C5	2.84	120.05	115.27
9	P	101	BCB	CAA-C2A-C3A	-2.84	105.00	112.78
9	M	405	BCB	O2D-CGD-O1D	-2.83	118.30	123.84
9	Q	101	BCB	CMB-C2B-C3B	2.83	129.98	124.68
17	4	102	NS0	C34-C33-C35	2.83	120.03	115.27
9	Y	101	BCB	CHC-C1C-C2C	-2.83	114.86	122.60
17	x	102	NS0	C14-C15-C16	-2.82	114.41	123.22
17	1	102	NS0	C8-C7-C	2.82	120.02	115.27
17	W	102	NS0	C8-C7-C	2.82	120.01	115.27
9	M	405	BCB	O1D-CGD-CBD	-2.82	120.05	124.74
9	S	101	BCB	O2D-CGD-O1D	-2.82	118.33	123.84
9	l	101	BCB	CHC-C1C-C2C	-2.82	114.89	122.60
9	S	101	BCB	O2A-CGA-CBA	2.82	120.74	111.91
9	r	101	BCB	CHC-C1C-C2C	-2.81	114.90	122.60
9	P	101	BCB	O2A-C1-C2	2.81	116.02	108.64
9	k	101	BCB	CMB-C2B-C3B	2.80	129.92	124.68
9	o	101	BCB	O1D-CGD-CBD	-2.80	120.08	124.74
9	T	101	BCB	CMB-C2B-C3B	2.80	129.91	124.68
17	x	102	NS0	C8-C7-C	2.80	119.97	115.27
9	e	101	BCB	O2D-CGD-O1D	-2.79	118.38	123.84
11	6	101	UQ9	C35-C34-C36	2.79	119.96	115.27
9	k	101	BCB	C3D-CAD-CBD	2.79	111.27	107.61
9	n	101	BCB	CBC-CAC-C3C	-2.78	119.31	126.70
17	G	102	NS0	C14-C15-C16	-2.78	114.53	123.22
9	b	101	BCB	O1D-CGD-CBD	-2.78	120.11	124.74
9	l	101	BCB	O2D-CGD-O1D	-2.78	118.41	123.84
17	4	102	NS0	C8-C7-C	2.78	119.94	115.27
9	Q	101	BCB	C1-O2A-CGA	2.78	123.73	116.44
17	l	102	NS0	C8-C7-C	2.77	119.94	115.27
8	C	403	HEM	CBB-CAB-C3B	-2.77	113.83	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	n	101	BCB	O2D-CGD-O1D	-2.77	118.42	123.84
9	L	302	BCB	CHD-C4C-C3C	-2.77	122.25	130.10
9	F	101	BCB	O2A-CGA-O1A	-2.76	116.62	123.59
17	7	102	NS0	C8-C7-C	2.76	119.92	115.27
8	C	404	HEM	CHB-C1B-NB	2.76	127.79	124.38
11	6	101	UQ9	C15-C14-C16	2.76	119.91	115.27
9	6	102	BCB	O2A-C1-C2	2.76	115.89	108.64
9	P	101	BCB	CHD-C4C-C3C	-2.76	122.28	130.10
9	x	101	BCB	O1D-CGD-CBD	-2.76	120.15	124.74
9	n	101	BCB	O2A-CGA-CBA	2.76	120.56	111.91
9	F	101	BCB	CHD-C4C-C3C	-2.75	122.31	130.10
9	f	101	BCB	CHD-C4C-C3C	-2.74	122.33	130.10
9	N	101	BCB	CHC-C1C-C2C	-2.74	115.10	122.60
9	S	101	BCB	CMB-C2B-C3B	2.73	129.79	124.68
9	G	101	BCB	O2D-CGD-O1D	-2.73	118.49	123.84
11	L	304	UQ9	C40-C39-C41	2.73	119.87	115.27
8	C	402	HEM	C4B-C3B-C2B	-2.73	104.95	107.11
9	L	301	BCB	CAA-CBA-CGA	-2.73	105.28	113.25
17	T	102	NS0	C24-C23-C25	2.72	122.37	118.08
9	c	101	BCB	CHC-C1C-C2C	-2.72	115.14	122.60
17	l	102	NS0	C14-C15-C16	-2.72	114.72	123.22
17	f	102	NS0	C8-C7-C	2.72	119.85	115.27
9	7	101	BCB	C1-O2A-CGA	2.72	123.58	116.44
9	n	101	BCB	CAA-C2A-C3A	-2.72	105.34	112.78
9	q	101	BCB	O2D-CGD-O1D	-2.72	118.53	123.84
16	M	410	NS5	C19-C18-C17	2.71	129.03	123.47
9	L	301	BCB	C16-C15-C13	-2.70	107.18	115.92
9	i	101	BCB	CHD-C4C-C3C	-2.70	122.44	130.10
15	M	409	MQ9	C15-C14-C16	2.70	119.82	115.27
8	C	401	HEM	CBD-CAD-C3D	-2.70	105.13	112.63
9	Z	101	BCB	C1-O2A-CGA	2.69	123.51	116.44
17	r	102	NS0	C8-C7-C	2.69	119.80	115.27
9	w	101	BCB	CMA-C3A-C2A	-2.69	103.16	113.99
17	f	102	NS0	C14-C15-C16	-2.69	114.83	123.22
9	P	101	BCB	CAA-CBA-CGA	-2.69	105.40	113.25
9	Y	101	BCB	C1-O2A-CGA	2.69	123.49	116.44
9	3	101	BCB	C6-C5-C3	-2.68	106.42	113.45
9	K	101	BCB	CAA-CBA-CGA	-2.68	105.41	113.25
11	6	101	UQ9	C40-C39-C41	2.68	119.77	115.27
9	V	101	BCB	C5-C3-C2	-2.67	115.71	121.12
9	r	101	BCB	CHD-C4C-C3C	-2.67	122.53	130.10
9	L	301	BCB	CGD-CBD-CAD	-2.67	102.09	110.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	Z	102	NS0	C24-C23-C25	2.66	122.28	118.08
8	C	402	HEM	O2A-CGA-CBA	2.66	122.57	114.03
9	h	101	BCB	CHD-C4C-C3C	-2.65	122.58	130.10
17	i	102	NS0	C24-C23-C25	2.65	122.25	118.08
17	G	102	NS0	C26-C25-C23	-2.65	118.97	126.42
9	n	101	BCB	CHD-C4C-C3C	-2.64	122.60	130.10
9	1	101	BCB	C3D-CAD-CBD	2.63	111.07	107.61
17	1	102	NS0	C24-C23-C25	2.63	122.22	118.08
17	N	102	NS0	C24-C23-C25	2.63	122.22	118.08
9	T	101	BCB	CHD-C4C-C3C	-2.63	122.66	130.10
9	q	101	BCB	O2A-CGA-CBA	2.62	120.14	111.91
9	1	101	BCB	CHC-C1C-C2C	-2.62	115.43	122.60
9	6	102	BCB	O2A-CGA-O1A	-2.62	116.99	123.59
8	C	403	HEM	O2D-CGD-O1D	-2.61	116.79	123.30
9	k	101	BCB	O1D-CGD-CBD	-2.61	120.39	124.74
9	h	101	BCB	C5-C3-C2	-2.61	115.84	121.12
9	M	405	BCB	CHD-C4C-C3C	-2.60	122.72	130.10
9	Q	101	BCB	O2D-CGD-O1D	-2.60	118.75	123.84
9	l	101	BCB	CAA-CBA-CGA	-2.60	105.65	113.25
9	V	101	BCB	CMB-C2B-C3B	2.60	129.54	124.68
9	z	101	BCB	O2A-CGA-O1A	-2.59	117.05	123.59
17	W	102	NS0	C26-C25-C23	-2.59	119.15	126.42
11	6	101	UQ9	C10-C9-C11	2.58	119.62	115.27
9	x	101	BCB	CHD-C4C-C3C	-2.58	122.77	130.10
11	L	304	UQ9	C35-C34-C36	2.58	119.62	115.27
11	6	101	UQ9	C25-C24-C26	2.58	119.62	115.27
9	6	102	BCB	O2D-CGD-O1D	-2.58	118.79	123.84
9	x	101	BCB	O2D-CGD-O1D	-2.58	118.79	123.84
9	u	101	BCB	C5-C3-C2	-2.58	115.90	121.12
9	Y	101	BCB	C6-C7-C8	-2.58	107.59	115.92
9	t	101	BCB	CHD-C4C-C3C	-2.58	122.80	130.10
9	q	101	BCB	CMB-C2B-C3B	2.58	129.50	124.68
17	c	102	NS0	C24-C23-C25	2.58	122.14	118.08
9	Z	101	BCB	CHD-C4C-C3C	-2.58	122.80	130.10
9	e	101	BCB	C3D-CAD-CBD	2.57	110.99	107.61
9	Z	101	BCB	C3D-CAD-CBD	2.57	110.99	107.61
9	Q	101	BCB	CHC-C1C-C2C	-2.57	115.56	122.60
9	b	101	BCB	O2A-C1-C2	2.56	115.37	108.64
9	u	101	BCB	O1D-CGD-CBD	-2.56	120.48	124.74
9	q	101	BCB	CHC-C1C-C2C	-2.56	115.59	122.60
9	Q	101	BCB	O2A-CGA-CBA	2.55	119.91	111.91
15	M	409	MQ9	C51-C49-C50	2.55	120.23	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	401	HEM	C2C-C3C-C4C	-2.55	105.12	106.90
9	K	101	BCB	C3D-CAD-CBD	2.54	110.95	107.61
17	7	102	NS0	C24-C23-C25	2.54	122.08	118.08
17	Z	102	NS0	CD1-CG-CD2	-2.54	109.00	114.60
17	x	102	NS0	CD1-CG-CD2	-2.54	109.00	114.60
9	M	406	BCB	C11-C12-C13	-2.53	107.73	115.92
9	u	101	BCB	CHC-C1C-C2C	-2.53	115.68	122.60
17	l	102	NS0	C18-C17-C19	-2.53	119.39	122.92
11	L	304	UQ9	C20-C19-C21	2.52	119.52	115.27
9	w	101	BCB	O2A-C1-C2	2.52	115.26	108.64
9	7	101	BCB	C4-C3-C5	2.52	119.51	115.27
9	c	101	BCB	O2D-CGD-O1D	-2.52	118.92	123.84
17	u	102	NS0	CD1-CG-CD2	-2.51	109.06	114.60
9	M	406	BCB	CHD-C4C-C3C	-2.50	123.01	130.10
9	6	102	BCB	C3D-CAD-CBD	2.50	110.89	107.61
17	o	102	NS0	C26-C25-C23	-2.50	119.40	126.42
9	Y	101	BCB	C6-C5-C3	-2.49	106.92	113.45
17	u	102	NS0	C24-C23-C25	2.49	122.00	118.08
9	3	101	BCB	C1-C2-C3	2.49	130.35	126.04
17	G	102	NS0	C36-C35-C33	-2.49	106.92	113.45
17	x	102	NS0	C24-C23-C25	2.49	122.00	118.08
9	t	101	BCB	CAA-C2A-C3A	-2.49	105.96	112.78
9	f	101	BCB	CHC-C1C-C2C	-2.49	115.79	122.60
9	q	101	BCB	CAA-C2A-C3A	-2.48	105.97	112.78
11	L	304	UQ9	C15-C14-C16	2.48	119.44	115.27
17	4	102	NS0	C24-C23-C25	2.48	121.98	118.08
11	L	304	UQ9	C30-C29-C31	2.48	119.44	115.27
17	4	102	NS0	CD1-CG-CD2	-2.47	109.14	114.60
8	C	404	HEM	CMB-C2B-C1B	2.47	128.80	125.04
11	6	101	UQ9	C20-C19-C21	2.47	119.42	115.27
11	6	101	UQ9	C50-C49-C51	2.46	120.04	114.60
9	6	102	BCB	C1-O2A-CGA	2.46	122.90	116.44
9	L	302	BCB	C5-C3-C2	-2.46	116.14	121.12
11	L	304	UQ9	C10-C9-C11	2.46	119.41	115.27
9	P	101	BCB	C4-C3-C5	2.46	119.40	115.27
9	N	101	BCB	CHD-C4C-C3C	-2.46	123.14	130.10
9	u	101	BCB	CMC-C2C-C1C	-2.46	110.24	114.36
9	u	101	BCB	CMB-C2B-C3B	2.45	129.26	124.68
9	F	101	BCB	CMB-C2B-C3B	2.45	129.26	124.68
9	N	101	BCB	C3D-CAD-CBD	2.45	110.83	107.61
9	c	101	BCB	O2A-CGA-O1A	-2.45	117.42	123.59
9	f	101	BCB	C4-C3-C5	2.44	119.38	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	i	102	NS0	C37-C36-C35	-2.44	106.73	113.36
17	f	102	NS0	C13-C12-C14	-2.43	119.51	122.92
9	4	101	BCB	CHC-C1C-C2C	-2.43	115.94	122.60
9	S	101	BCB	CBC-CAC-C3C	-2.43	120.26	126.70
9	W	101	BCB	C3D-CAD-CBD	2.43	110.80	107.61
9	L	301	BCB	CMB-C2B-C3B	2.43	129.22	124.68
17	r	102	NS0	C24-C23-C25	2.43	121.90	118.08
9	l	101	BCB	C3D-CAD-CBD	2.43	110.80	107.61
17	Q	102	NS0	CD1-CG-CD2	-2.42	109.25	114.60
9	L	301	BCB	OBB-CAB-CBB	2.42	125.62	120.17
9	Y	101	BCB	O2A-CGA-O1A	-2.42	117.48	123.59
9	z	101	BCB	C1-C2-C3	2.42	130.23	126.04
9	o	101	BCB	O2A-CGA-O1A	-2.42	117.50	123.59
17	r	102	NS0	C26-C25-C23	-2.41	119.63	126.42
9	b	101	BCB	C3D-CAD-CBD	2.41	110.78	107.61
9	z	101	BCB	C5-C3-C2	-2.41	116.24	121.12
9	V	101	BCB	CHD-C4C-C3C	-2.41	123.27	130.10
9	i	101	BCB	CHC-C1C-C2C	-2.41	116.00	122.60
17	l	102	NS0	CD1-CG-CD2	-2.41	109.29	114.60
9	K	101	BCB	CBA-CAA-C2A	-2.40	106.80	113.81
9	4	101	BCB	O1D-CGD-CBD	-2.40	120.74	124.74
9	q	101	BCB	C6-C5-C3	2.39	119.73	113.45
8	C	402	HEM	CHA-C4D-ND	2.39	127.34	124.38
9	c	101	BCB	CMB-C2B-C3B	2.39	129.16	124.68
9	F	101	BCB	C1-C2-C3	2.39	130.18	126.04
9	L	301	BCB	O2A-CGA-CBA	2.39	119.41	111.91
9	L	301	BCB	C4-C3-C5	2.39	119.29	115.27
16	M	410	NS5	C32-C31-C33	2.39	119.28	115.27
9	T	101	BCB	C3D-CAD-CBD	2.38	110.75	107.61
9	e	101	BCB	O2A-C1-C2	2.38	114.89	108.64
10	M	407	BPB	O2A-CGA-O1A	-2.38	117.59	123.59
9	7	101	BCB	C3D-CAD-CBD	2.38	110.73	107.61
9	l	101	BCB	O1D-CGD-CBD	-2.38	120.78	124.74
11	6	101	UQ9	C45-C44-C46	2.37	119.26	115.27
9	t	101	BCB	CBC-CAC-C3C	-2.37	120.41	126.70
17	7	102	NS0	C14-C15-C16	-2.37	115.83	123.22
17	1	102	NS0	CD1-CG-CD2	-2.37	109.38	114.60
9	6	102	BCB	O1D-CGD-CBD	-2.36	120.80	124.74
17	W	102	NS0	C24-C23-C25	2.36	121.79	118.08
17	o	102	NS0	C18-C17-C19	-2.36	119.62	122.92
9	o	101	BCB	CHC-C1C-C2C	-2.35	116.17	122.60
9	c	101	BCB	C3D-CAD-CBD	2.35	110.69	107.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	7	101	BCB	O2A-C1-C2	2.34	114.78	108.64
17	W	102	NS0	CD1-CG-CD2	-2.34	109.44	114.60
11	L	304	UQ9	C50-C49-C51	2.34	119.76	114.60
9	P	101	BCB	CBC-CAC-C3C	-2.34	120.50	126.70
9	n	101	BCB	CMB-C2B-C3B	2.34	129.05	124.68
17	N	102	NS0	C26-C25-C23	-2.33	119.86	126.42
17	f	102	NS0	C24-C23-C25	2.33	121.75	118.08
9	M	406	BCB	C4-C3-C5	2.33	119.19	115.27
9	6	102	BCB	CHD-C4C-C3C	-2.33	123.49	130.10
10	M	407	BPB	OBD-CAD-CBD	-2.33	122.41	125.82
9	7	101	BCB	O2A-CGA-CBA	2.32	119.19	111.91
9	e	101	BCB	CBC-CAC-C3C	-2.32	120.54	126.70
17	l	102	NS0	C26-C25-C23	-2.32	119.89	126.42
17	W	102	NS0	C18-C17-C19	-2.32	119.68	122.92
9	c	101	BCB	O1D-CGD-CBD	-2.32	120.88	124.74
9	M	406	BCB	C6-C5-C3	-2.32	107.38	113.45
15	M	409	MQ9	C42-C43-C44	2.31	133.23	127.66
8	C	404	HEM	CHA-C4D-C3D	-2.31	121.00	125.33
9	b	101	BCB	C1-O2A-CGA	2.31	122.50	116.44
9	W	101	BCB	CHC-C1C-C2C	-2.30	116.29	122.60
9	4	101	BCB	O2A-CGA-CBA	2.30	119.13	111.91
9	S	101	BCB	CMA-C3A-C2A	-2.30	104.72	113.99
9	M	406	BCB	C1-O2A-CGA	2.30	122.48	116.44
17	i	102	NS0	CD1-CG-CD2	-2.30	109.52	114.60
9	b	101	BCB	CBC-CAC-C3C	-2.30	120.60	126.70
17	o	102	NS0	CD1-CG-CD2	-2.30	109.53	114.60
17	f	102	NS0	CD1-CG-CD2	-2.30	109.53	114.60
17	o	102	NS0	C24-C23-C25	2.30	121.69	118.08
17	4	102	NS0	C37-C36-C35	-2.29	107.13	113.36
17	7	102	NS0	CD1-CG-CD2	-2.29	109.54	114.60
17	N	102	NS0	CD1-CG-CD2	-2.29	109.54	114.60
17	Q	102	NS0	C24-C23-C25	2.29	121.69	118.08
9	x	101	BCB	C3D-CAD-CBD	2.29	110.62	107.61
9	c	101	BCB	CHD-C4C-C3C	-2.29	123.61	130.10
8	C	404	HEM	CBB-CAB-C3B	-2.29	116.23	127.62
17	o	102	NS0	C36-C35-C33	-2.29	107.46	113.45
9	P	101	BCB	C5-C3-C2	-2.28	116.50	121.12
9	L	301	BCB	C1-C2-C3	-2.28	122.10	126.04
17	W	102	NS0	C36-C35-C33	-2.28	107.49	113.45
17	T	102	NS0	CD1-CG-CD2	-2.27	109.58	114.60
17	c	102	NS0	CD1-CG-CD2	-2.27	109.58	114.60
9	t	101	BCB	C5-C3-C2	-2.27	116.52	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	r	101	BCB	C3D-CAD-CBD	2.27	110.59	107.61
9	7	101	BCB	CAA-C2A-C3A	2.27	118.99	112.78
8	C	404	HEM	CMA-C3A-C4A	-2.27	124.98	128.46
17	1	102	NS0	C37-C36-C35	-2.27	107.20	113.36
9	o	101	BCB	C3D-CAD-CBD	2.27	110.59	107.61
8	C	402	HEM	O2A-CGA-O1A	-2.26	117.66	123.30
9	Q	101	BCB	O2A-CGA-O1A	-2.26	117.89	123.59
10	M	407	BPB	OBB-CAB-CBB	2.25	125.23	120.17
8	C	401	HEM	C4B-CHC-C1C	2.25	125.53	122.56
15	M	409	MQ9	C47-C46-C44	2.25	120.37	112.98
9	N	101	BCB	O2A-CGA-O1A	-2.25	117.92	123.59
9	f	101	BCB	O2D-CGD-O1D	-2.24	119.45	123.84
17	c	102	NS0	C13-C12-C14	-2.24	119.78	122.92
9	u	101	BCB	O2D-CGD-O1D	-2.24	119.46	123.84
9	1	101	BCB	O2D-CGD-O1D	-2.24	119.46	123.84
9	b	101	BCB	C5-C3-C2	-2.24	116.59	121.12
9	h	101	BCB	CMB-C2B-C3B	2.24	128.86	124.68
17	r	102	NS0	CD1-CG-CD2	-2.24	109.67	114.60
9	r	101	BCB	C6-C5-C3	-2.23	107.61	113.45
10	M	407	BPB	CMA-C3A-C2A	-2.23	105.01	113.99
9	z	101	BCB	CMB-C2B-C3B	2.23	128.84	124.68
9	q	101	BCB	O1D-CGD-CBD	-2.23	121.03	124.74
9	7	101	BCB	CHD-C4C-C3C	-2.23	123.79	130.10
8	C	401	HEM	O2D-CGD-CBD	2.22	121.15	114.03
9	L	302	BCB	O2A-CGA-O1A	-2.21	118.00	123.59
9	b	101	BCB	C6-C5-C3	2.21	119.26	113.45
8	C	404	HEM	CAD-C3D-C2D	-2.21	123.76	127.88
17	r	102	NS0	C13-C12-C14	-2.21	119.83	122.92
17	f	102	NS0	C26-C25-C23	-2.21	120.22	126.42
9	f	101	BCB	O1D-CGD-CBD	-2.21	121.07	124.74
17	x	102	NS0	C26-C25-C23	-2.20	120.22	126.42
16	M	410	NS5	C14-C15-C17	-2.20	115.57	118.94
9	T	101	BCB	O2A-CGA-O1A	-2.20	118.05	123.59
17	7	102	NS0	C18-C17-C19	-2.19	119.85	122.92
9	b	101	BCB	CAA-C2A-C3A	-2.19	106.79	112.78
9	7	101	BCB	C5-C3-C2	-2.18	116.70	121.12
17	o	102	NS0	C40-C38-C39	2.18	120.57	110.51
9	t	101	BCB	O2A-CGA-O1A	-2.18	118.09	123.59
9	Z	101	BCB	O2A-CGA-O1A	-2.18	118.09	123.59
17	G	102	NS0	CD1-CG-CD2	-2.18	109.79	114.60
17	l	102	NS0	C24-C23-C25	2.18	121.51	118.08
9	Y	101	BCB	CMA-C3A-C2A	-2.17	105.25	113.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	1	101	BCB	CMA-C3A-C2A	-2.17	105.25	113.99
9	4	101	BCB	CMB-C2B-C3B	2.17	128.74	124.68
9	e	101	BCB	C1-C2-C3	2.17	129.79	126.04
9	S	101	BCB	O1D-CGD-CBD	-2.17	121.13	124.74
17	f	102	NS0	C37-C36-C35	-2.17	107.48	113.36
9	K	101	BCB	CAA-C2A-C3A	-2.17	106.85	112.78
9	G	101	BCB	CBA-CAA-C2A	-2.16	107.50	113.81
9	4	101	BCB	O2A-CGA-O1A	-2.16	118.14	123.59
17	G	102	NS0	C13-C12-C14	-2.16	119.90	122.92
9	x	101	BCB	CMB-C2B-C3B	2.16	128.71	124.68
9	w	101	BCB	O2D-CGD-O1D	-2.15	119.63	123.84
9	e	101	BCB	C7-C6-C5	2.15	119.20	113.36
9	7	101	BCB	C1-C2-C3	2.15	129.76	126.04
9	h	101	BCB	CAA-C2A-C3A	-2.15	106.90	112.78
9	e	101	BCB	CMB-C2B-C3B	2.14	128.68	124.68
9	G	101	BCB	CHD-C4C-C3C	-2.14	124.03	130.10
9	b	101	BCB	CAA-CBA-CGA	-2.14	107.00	113.25
9	i	101	BCB	O2D-CGD-O1D	-2.13	119.67	123.84
9	r	101	BCB	C5-C3-C2	-2.13	116.81	121.12
9	k	101	BCB	CMA-C3A-C4A	-2.13	109.72	114.38
17	c	102	NS0	C26-C25-C23	-2.13	120.44	126.42
17	Z	102	NS0	C37-C36-C35	-2.13	107.58	113.36
17	Q	102	NS0	C25-C23-C22	-2.13	115.68	118.94
17	i	102	NS0	C40-C38-C39	2.12	120.30	110.51
17	4	102	NS0	C40-C38-C39	2.12	120.28	110.51
17	l	102	NS0	C40-C38-C39	2.12	120.28	110.51
9	q	101	BCB	CAA-CBA-CGA	-2.12	107.07	113.25
15	M	409	MQ9	C25-C24-C26	2.12	118.83	115.27
9	t	101	BCB	C4-C3-C5	2.11	118.83	115.27
10	L	303	BPB	C1-O2A-CGA	2.11	121.99	116.44
17	G	102	NS0	C40-C38-C39	2.11	120.25	110.51
17	N	102	NS0	C40-C38-C39	2.11	120.23	110.51
9	3	101	BCB	CMC-C2C-C1C	-2.11	110.82	114.36
9	o	101	BCB	CMA-C3A-C4A	-2.11	109.76	114.38
17	T	102	NS0	C40-C38-C39	2.11	120.22	110.51
17	f	102	NS0	C18-C17-C19	-2.11	119.97	122.92
9	M	406	BCB	O2A-C1-C2	2.10	114.17	108.64
9	G	101	BCB	O2A-CGA-O1A	-2.10	118.28	123.59
17	Z	102	NS0	C40-C38-C39	2.10	120.20	110.51
9	P	101	BCB	O2A-CGA-O1A	-2.10	118.29	123.59
8	C	402	HEM	CHB-C1B-NB	2.10	126.97	124.38
17	Q	102	NS0	C13-C12-C14	-2.10	119.98	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	7	102	NS0	C40-C38-C39	2.10	120.18	110.51
17	i	102	NS0	C18-C17-C19	-2.10	119.99	122.92
17	1	102	NS0	C40-C38-C39	2.09	120.16	110.51
9	3	101	BCB	CBC-CAC-C3C	-2.09	121.15	126.70
9	N	101	BCB	O2D-CGD-O1D	-2.09	119.75	123.84
9	4	101	BCB	C3D-CAD-CBD	2.09	110.35	107.61
17	u	102	NS0	C40-C38-C39	2.08	120.12	110.51
17	7	102	NS0	C26-C25-C23	-2.08	120.56	126.42
15	M	409	MQ9	C40-C39-C41	2.08	118.78	115.27
9	4	101	BCB	O2D-CGD-O1D	-2.08	119.77	123.84
17	c	102	NS0	C40-C38-C39	2.08	120.10	110.51
17	r	102	NS0	C25-C23-C22	-2.08	115.75	118.94
17	c	102	NS0	C36-C35-C33	-2.08	108.01	113.45
9	z	101	BCB	C4-C3-C5	2.08	118.77	115.27
9	W	101	BCB	O2A-CGA-O1A	-2.07	118.36	123.59
9	h	101	BCB	C9-C8-C7	-2.07	103.78	111.29
9	L	302	BCB	C11-C10-C8	-2.07	109.22	115.92
9	L	301	BCB	C11-C12-C13	-2.07	109.23	115.92
17	7	102	NS0	C13-C12-C14	-2.07	120.03	122.92
17	W	102	NS0	C40-C38-C39	2.06	120.03	110.51
9	K	101	BCB	O2A-CGA-CBA	2.06	118.38	111.91
16	M	410	NS5	C24-C25-C26	-2.06	124.37	127.31
15	M	409	MQ9	C26-C24-C23	2.06	125.28	121.12
9	G	101	BCB	C3D-CAD-CBD	2.06	110.31	107.61
10	L	303	BPB	O2A-CGA-CBA	2.06	118.36	111.91
8	C	404	HEM	CHA-C4D-ND	2.05	126.92	124.38
9	q	101	BCB	CMA-C3A-C2A	-2.05	105.74	113.99
17	Q	102	NS0	C40-C38-C39	2.05	119.95	110.51
9	K	101	BCB	O1D-CGD-CBD	-2.05	121.33	124.74
9	f	101	BCB	C6-C7-C8	-2.04	109.31	115.92
9	1	101	BCB	O2A-CGA-O1A	-2.04	118.44	123.59
17	1	102	NS0	C25-C23-C22	-2.04	115.81	118.94
9	S	101	BCB	CBA-CAA-C2A	-2.04	107.86	113.81
9	f	101	BCB	O2A-CGA-O1A	-2.04	118.45	123.59
17	i	102	NS0	C25-C23-C22	-2.04	115.82	118.94
9	L	301	BCB	C17-C16-C15	-2.03	103.89	113.24
17	1	102	NS0	C18-C17-C19	-2.03	120.08	122.92
9	k	101	BCB	O2D-CGD-O1D	-2.03	119.86	123.84
17	u	102	NS0	C26-C25-C23	-2.03	120.71	126.42
8	C	401	HEM	CAA-CBA-CGA	-2.03	108.06	113.76
17	7	102	NS0	C37-C36-C35	-2.03	107.84	113.36
15	M	409	MQ9	O4-C4-C3	-2.03	118.28	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	G	102	NS0	C24-C23-C25	2.03	121.27	118.08
17	c	102	NS0	C31-C30-C28	2.03	119.65	112.98
9	w	101	BCB	CBC-CAC-C3C	-2.02	121.33	126.70
9	T	101	BCB	O2D-CGD-O1D	-2.02	119.89	123.84
17	r	102	NS0	C18-C17-C19	-2.02	120.10	122.92
15	M	409	MQ9	C8-C7-C6	2.01	117.47	112.05
17	1	102	NS0	C26-C25-C23	-2.01	120.77	126.42
8	C	404	HEM	CAD-CBD-CGD	-2.01	109.28	113.60
8	C	401	HEM	CMD-C2D-C1D	2.01	128.10	125.04
9	S	101	BCB	C5-C3-C2	-2.01	117.06	121.12
15	M	409	MQ9	O1-C1-C2	-2.00	118.32	121.56
17	Q	102	NS0	C26-C25-C23	-2.00	120.79	126.42
9	N	101	BCB	C1-O2A-CGA	2.00	121.70	116.44

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	L	303	BPB	C13
10	M	407	BPB	C13

All (1068) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	M	406	BCB	CAD-CBD-CGD-O1D
9	M	406	BCB	CAD-CBD-CGD-O2D
9	z	101	BCB	C1A-C2A-CAA-CBA
9	z	101	BCB	O2A-C1-C2-C3
9	z	101	BCB	C2-C3-C5-C6
9	z	101	BCB	C4-C3-C5-C6
9	1	101	BCB	CBA-CGA-O2A-C1
9	1	101	BCB	O1A-CGA-O2A-C1
9	1	101	BCB	C11-C10-C8-C9
9	F	101	BCB	C3A-C2A-CAA-CBA
9	F	101	BCB	O2A-C1-C2-C3
9	K	101	BCB	C3A-C2A-CAA-CBA
9	P	101	BCB	C3A-C2A-CAA-CBA
9	P	101	BCB	O1A-CGA-O2A-C1
9	P	101	BCB	CBD-CGD-O2D-CED
9	P	101	BCB	O2A-C1-C2-C3
9	S	101	BCB	C3A-C2A-CAA-CBA
9	V	101	BCB	C1A-C2A-CAA-CBA
9	V	101	BCB	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
9	V	101	BCB	C2-C3-C5-C6
9	V	101	BCB	C4-C3-C5-C6
9	Y	101	BCB	C3A-C2A-CAA-CBA
9	Y	101	BCB	O2A-C1-C2-C3
9	b	101	BCB	C3A-C2A-CAA-CBA
9	b	101	BCB	O2A-C1-C2-C3
9	e	101	BCB	C3A-C2A-CAA-CBA
9	e	101	BCB	O2A-C1-C2-C3
9	e	101	BCB	C11-C12-C13-C15
9	h	101	BCB	C1A-C2A-CAA-CBA
9	k	101	BCB	C3A-C2A-CAA-CBA
9	k	101	BCB	CBD-CGD-O2D-CED
9	k	101	BCB	O2A-C1-C2-C3
9	n	101	BCB	C1A-C2A-CAA-CBA
9	q	101	BCB	C1A-C2A-CAA-CBA
9	q	101	BCB	C4-C3-C5-C6
9	t	101	BCB	C1A-C2A-CAA-CBA
9	t	101	BCB	O2A-C1-C2-C3
9	w	101	BCB	O2A-C1-C2-C3
9	3	101	BCB	C3A-C2A-CAA-CBA
9	3	101	BCB	C2A-CAA-CBA-CGA
9	3	101	BCB	CBD-CGD-O2D-CED
9	3	101	BCB	O2A-C1-C2-C3
9	6	102	BCB	C1A-C2A-CAA-CBA
9	6	102	BCB	CBD-CGD-O2D-CED
9	6	102	BCB	O2A-C1-C2-C3
9	N	101	BCB	CBA-CGA-O2A-C1
9	N	101	BCB	O1A-CGA-O2A-C1
9	Q	101	BCB	C1A-C2A-CAA-CBA
9	Q	101	BCB	C3A-C2A-CAA-CBA
9	Q	101	BCB	C14-C13-C15-C16
9	f	101	BCB	CBA-CGA-O2A-C1
9	f	101	BCB	O1A-CGA-O2A-C1
9	i	101	BCB	CBA-CGA-O2A-C1
9	i	101	BCB	O1A-CGA-O2A-C1
9	u	101	BCB	CBA-CGA-O2A-C1
9	u	101	BCB	O1A-CGA-O2A-C1
9	x	101	BCB	CBA-CGA-O2A-C1
9	x	101	BCB	O1A-CGA-O2A-C1
9	4	101	BCB	C3A-C2A-CAA-CBA
9	4	101	BCB	C11-C10-C8-C9
10	L	303	BPB	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
10	L	303	BPB	CBD-CGD-O2D-CED
10	L	303	BPB	C2C-C3C-CAC-CBC
10	M	407	BPB	C2C-C3C-CAC-CBC
11	L	304	UQ9	C19-C21-C22-C23
11	L	304	UQ9	C15-C14-C16-C17
11	L	304	UQ9	C13-C14-C16-C17
11	L	304	UQ9	C9-C11-C12-C13
11	L	304	UQ9	C12-C11-C9-C10
11	L	304	UQ9	C12-C11-C9-C8
11	L	304	UQ9	C1-C6-C7-C8
11	L	304	UQ9	C5-C6-C7-C8
11	6	101	UQ9	C39-C41-C42-C43
11	6	101	UQ9	C29-C31-C32-C33
11	6	101	UQ9	C30-C29-C31-C32
11	6	101	UQ9	C28-C29-C31-C32
11	6	101	UQ9	C25-C24-C26-C27
11	6	101	UQ9	C23-C24-C26-C27
11	6	101	UQ9	C12-C11-C9-C10
11	6	101	UQ9	C12-C11-C9-C8
14	M	408	LDA	N1-C1-C2-C3
14	H	301	LDA	C2-C1-N1-CM1
14	H	301	LDA	C2-C1-N1-CM2
15	M	409	MQ9	C9-C11-C12-C13
15	M	409	MQ9	C18-C19-C21-C22
15	M	409	MQ9	C20-C19-C21-C22
15	M	409	MQ9	C40-C39-C41-C42
15	M	409	MQ9	C43-C44-C46-C47
15	M	409	MQ9	C45-C44-C46-C47
15	M	409	MQ9	C44-C46-C47-C48
16	M	410	NS5	C7-C8-C9-C10
16	M	410	NS5	C13-C14-C15-C16
16	M	410	NS5	C13-C14-C15-C17
16	M	410	NS5	C25-C26-C28-C29
16	M	410	NS5	C27-C26-C28-C29
16	M	410	NS5	C28-C29-C30-C31
17	1	102	NS0	C9-C10-C11-C12
17	1	102	NS0	CA-CB-CG-CD1
17	G	102	NS0	C10-C11-C12-C14
17	G	102	NS0	C10-C11-C12-C13
17	G	102	NS0	C9-C10-C11-C12
17	N	102	NS0	C9-C10-C11-C12
17	N	102	NS0	C7-C-CA-CB

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Mol	Chain	Res	Type	Atoms
17	Q	102	NS0	C9-C10-C11-C12
17	T	102	NS0	C10-C11-C12-C13
17	T	102	NS0	C9-C10-C11-C12
17	T	102	NS0	C7-C-CA-CB
17	W	102	NS0	C9-C10-C11-C12
17	Z	102	NS0	C9-C10-C11-C12
17	Z	102	NS0	CA-CB-CG-CD2
17	Z	102	NS0	CA-CB-CG-CD1
17	c	102	NS0	C9-C10-C11-C12
17	c	102	NS0	C7-C-CA-CB
17	f	102	NS0	C9-C10-C11-C12
17	f	102	NS0	CA-CB-CG-CD2
17	i	102	NS0	C9-C10-C11-C12
17	i	102	NS0	C11-C10-C9-C7
17	l	102	NS0	C9-C10-C11-C12
17	l	102	NS0	CA-CB-CG-CD2
17	o	102	NS0	C9-C10-C11-C12
17	o	102	NS0	C7-C-CA-CB
17	r	102	NS0	C9-C10-C11-C12
17	r	102	NS0	CA-CB-CG-CD2
17	u	102	NS0	C9-C10-C11-C12
17	x	102	NS0	C9-C10-C11-C12
17	x	102	NS0	CA-CB-CG-CD1
17	4	102	NS0	C9-C10-C11-C12
17	4	102	NS0	CA-CB-CG-CD2
17	4	102	NS0	CA-CB-CG-CD1
17	7	102	NS0	C10-C11-C12-C14
17	7	102	NS0	C10-C11-C12-C13
17	7	102	NS0	C9-C10-C11-C12
17	7	102	NS0	C11-C10-C9-C7
17	7	102	NS0	C7-C-CA-CB
17	7	102	NS0	C-CA-CB-CG
9	6	102	BCB	O1D-CGD-O2D-CED
9	7	101	BCB	O1D-CGD-O2D-CED
9	M	405	BCB	CBD-CGD-O2D-CED
9	z	101	BCB	CBD-CGD-O2D-CED
9	K	101	BCB	CBD-CGD-O2D-CED
9	S	101	BCB	CBD-CGD-O2D-CED
9	V	101	BCB	CBD-CGD-O2D-CED
9	Y	101	BCB	CBD-CGD-O2D-CED
9	e	101	BCB	CBD-CGD-O2D-CED
9	h	101	BCB	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
9	n	101	BCB	CBD-CGD-O2D-CED
9	w	101	BCB	CBD-CGD-O2D-CED
9	4	101	BCB	CBD-CGD-O2D-CED
9	7	101	BCB	CBD-CGD-O2D-CED
10	M	407	BPB	CBD-CGD-O2D-CED
9	G	101	BCB	O1A-CGA-O2A-C1
9	T	101	BCB	O1A-CGA-O2A-C1
9	l	101	BCB	O1A-CGA-O2A-C1
9	o	101	BCB	O1A-CGA-O2A-C1
9	e	101	BCB	O1D-CGD-O2D-CED
9	h	101	BCB	O1D-CGD-O2D-CED
10	L	303	BPB	O1D-CGD-O2D-CED
9	T	101	BCB	CBA-CGA-O2A-C1
9	l	101	BCB	CBA-CGA-O2A-C1
17	W	102	NS0	CA-CB-CG-CD1
17	f	102	NS0	CA-CB-CG-CD1
17	i	102	NS0	CA-CB-CG-CD2
17	i	102	NS0	CA-CB-CG-CD1
17	x	102	NS0	CA-CB-CG-CD2
9	1	101	BCB	CBD-CGD-O2D-CED
9	b	101	BCB	CBD-CGD-O2D-CED
9	t	101	BCB	CBD-CGD-O2D-CED
9	Q	101	BCB	CBD-CGD-O2D-CED
9	T	101	BCB	CBD-CGD-O2D-CED
9	Z	101	BCB	CBD-CGD-O2D-CED
9	c	101	BCB	CBD-CGD-O2D-CED
9	f	101	BCB	CBD-CGD-O2D-CED
9	i	101	BCB	CBD-CGD-O2D-CED
9	o	101	BCB	CBD-CGD-O2D-CED
9	x	101	BCB	CBD-CGD-O2D-CED
9	z	101	BCB	O1A-CGA-O2A-C1
9	F	101	BCB	O1A-CGA-O2A-C1
9	k	101	BCB	O1A-CGA-O2A-C1
9	W	101	BCB	O1A-CGA-O2A-C1
9	Z	101	BCB	O1A-CGA-O2A-C1
9	c	101	BCB	O1A-CGA-O2A-C1
9	k	101	BCB	O1D-CGD-O2D-CED
9	3	101	BCB	O1D-CGD-O2D-CED
9	G	101	BCB	CBD-CGD-O2D-CED
9	W	101	BCB	CBD-CGD-O2D-CED
9	P	101	BCB	O1D-CGD-O2D-CED
9	F	101	BCB	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
9	Y	101	BCB	C3-C5-C6-C7
9	k	101	BCB	C3-C5-C6-C7
17	o	102	NS0	C33-C35-C36-C37
9	G	101	BCB	CBA-CGA-O2A-C1
9	W	101	BCB	CBA-CGA-O2A-C1
9	Z	101	BCB	CBA-CGA-O2A-C1
9	c	101	BCB	CBA-CGA-O2A-C1
9	o	101	BCB	CBA-CGA-O2A-C1
17	Q	102	NS0	CA-CB-CG-CD1
17	T	102	NS0	CA-CB-CG-CD1
17	u	102	NS0	CA-CB-CG-CD2
9	r	101	BCB	CBD-CGD-O2D-CED
9	u	101	BCB	CBD-CGD-O2D-CED
9	w	101	BCB	O1A-CGA-O2A-C1
9	b	101	BCB	C4-C3-C5-C6
9	k	101	BCB	C4-C3-C5-C6
9	b	101	BCB	C2-C3-C5-C6
9	k	101	BCB	C2-C3-C5-C6
15	M	409	MQ9	C38-C39-C41-C42
9	M	406	BCB	C2A-CAA-CBA-CGA
9	c	101	BCB	C2A-CAA-CBA-CGA
9	N	101	BCB	C3-C5-C6-C7
9	l	101	BCB	C3-C5-C6-C7
17	G	102	NS0	C33-C35-C36-C37
9	z	101	BCB	CBA-CGA-O2A-C1
9	P	101	BCB	CBA-CGA-O2A-C1
9	k	101	BCB	CBA-CGA-O2A-C1
9	Q	101	BCB	CBA-CGA-O2A-C1
17	N	102	NS0	CA-CB-CG-CD1
9	l	101	BCB	CBD-CGD-O2D-CED
9	V	101	BCB	O1D-CGD-O2D-CED
9	n	101	BCB	O1D-CGD-O2D-CED
9	w	101	BCB	O1D-CGD-O2D-CED
9	Q	101	BCB	O1A-CGA-O2A-C1
9	4	101	BCB	O1A-CGA-O2A-C1
17	1	102	NS0	C11-C10-C9-C7
17	W	102	NS0	C11-C10-C9-C7
17	Z	102	NS0	C11-C10-C9-C7
17	f	102	NS0	C11-C10-C9-C7
17	l	102	NS0	C11-C10-C9-C7
9	F	101	BCB	CBD-CGD-O2D-CED
9	z	101	BCB	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
9	M	405	BCB	C3-C5-C6-C7
9	P	101	BCB	C3-C5-C6-C7
9	o	101	BCB	C3-C5-C6-C7
16	M	410	NS5	C2-C3-C4-C5
17	N	102	NS0	C33-C35-C36-C37
17	x	102	NS0	C33-C35-C36-C37
9	F	101	BCB	CBA-CGA-O2A-C1
9	7	101	BCB	CBA-CGA-O2A-C1
17	G	102	NS0	CA-CB-CG-CD1
17	c	102	NS0	CA-CB-CG-CD1
17	o	102	NS0	CA-CB-CG-CD1
9	7	101	BCB	O1A-CGA-O2A-C1
9	S	101	BCB	O1D-CGD-O2D-CED
9	G	101	BCB	C3-C5-C6-C7
9	w	101	BCB	CBA-CGA-O2A-C1
9	4	101	BCB	CBA-CGA-O2A-C1
17	1	102	NS0	CA-CB-CG-CD2
17	r	102	NS0	CA-CB-CG-CD1
17	7	102	NS0	CA-CB-CG-CD1
9	K	101	BCB	C4-C3-C5-C6
9	S	101	BCB	C4-C3-C5-C6
9	h	101	BCB	C4-C3-C5-C6
9	n	101	BCB	C4-C3-C5-C6
9	t	101	BCB	C4-C3-C5-C6
11	L	304	UQ9	C30-C29-C31-C32
17	1	102	NS0	C29-C28-C30-C31
17	G	102	NS0	C29-C28-C30-C31
17	N	102	NS0	C29-C28-C30-C31
17	Q	102	NS0	C29-C28-C30-C31
17	T	102	NS0	C29-C28-C30-C31
17	W	102	NS0	C29-C28-C30-C31
17	Z	102	NS0	C29-C28-C30-C31
17	c	102	NS0	C29-C28-C30-C31
17	f	102	NS0	C29-C28-C30-C31
17	i	102	NS0	C29-C28-C30-C31
17	l	102	NS0	C29-C28-C30-C31
17	o	102	NS0	C29-C28-C30-C31
17	r	102	NS0	C29-C28-C30-C31
17	u	102	NS0	C29-C28-C30-C31
17	x	102	NS0	C29-C28-C30-C31
17	4	102	NS0	C29-C28-C30-C31
17	7	102	NS0	C29-C28-C30-C31

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Mol	Chain	Res	Type	Atoms
9	K	101	BCB	C2-C3-C5-C6
9	S	101	BCB	C2-C3-C5-C6
9	h	101	BCB	C2-C3-C5-C6
9	n	101	BCB	C2-C3-C5-C6
9	q	101	BCB	C2-C3-C5-C6
9	t	101	BCB	C2-C3-C5-C6
11	L	304	UQ9	C28-C29-C31-C32
17	1	102	NS0	C27-C28-C30-C31
17	G	102	NS0	C27-C28-C30-C31
17	N	102	NS0	C27-C28-C30-C31
17	Q	102	NS0	C27-C28-C30-C31
17	T	102	NS0	C27-C28-C30-C31
17	W	102	NS0	C27-C28-C30-C31
17	Z	102	NS0	C27-C28-C30-C31
17	c	102	NS0	C27-C28-C30-C31
17	f	102	NS0	C27-C28-C30-C31
17	i	102	NS0	C27-C28-C30-C31
17	l	102	NS0	C27-C28-C30-C31
17	o	102	NS0	C27-C28-C30-C31
17	r	102	NS0	C27-C28-C30-C31
17	u	102	NS0	C27-C28-C30-C31
17	x	102	NS0	C27-C28-C30-C31
17	4	102	NS0	C27-C28-C30-C31
17	7	102	NS0	C27-C28-C30-C31
9	N	101	BCB	C2A-CAA-CBA-CGA
9	M	405	BCB	O1D-CGD-O2D-CED
9	Y	101	BCB	O1D-CGD-O2D-CED
9	4	101	BCB	O1D-CGD-O2D-CED
11	L	304	UQ9	C14-C16-C17-C18
11	6	101	UQ9	C24-C26-C27-C28
11	6	101	UQ9	C19-C21-C22-C23
15	M	409	MQ9	C24-C26-C27-C28
15	M	409	MQ9	C39-C41-C42-C43
17	W	102	NS0	C7-C-CA-CB
17	Z	102	NS0	C7-C-CA-CB
17	l	102	NS0	C7-C-CA-CB
9	K	101	BCB	O1D-CGD-O2D-CED
9	Q	101	BCB	O1D-CGD-O2D-CED
10	M	407	BPB	O1D-CGD-O2D-CED
9	t	101	BCB	O1D-CGD-O2D-CED
9	u	101	BCB	C3-C5-C6-C7
9	1	101	BCB	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
9	i	101	BCB	O1D-CGD-O2D-CED
9	t	101	BCB	CBA-CGA-O2A-C1
9	N	101	BCB	CBD-CGD-O2D-CED
17	Q	102	NS0	C11-C10-C9-C7
17	4	102	NS0	C11-C10-C9-C7
9	Z	101	BCB	C5-C6-C7-C8
9	M	406	BCB	C15-C16-C17-C18
9	K	101	BCB	C13-C15-C16-C17
9	M	406	BCB	C11-C10-C8-C9
9	M	406	BCB	C14-C13-C15-C16
9	P	101	BCB	C14-C13-C15-C16
9	e	101	BCB	C11-C10-C8-C9
9	e	101	BCB	C14-C13-C15-C16
9	w	101	BCB	C11-C10-C8-C9
9	Q	101	BCB	C11-C10-C8-C9
9	W	101	BCB	C11-C10-C8-C9
9	Z	101	BCB	C11-C10-C8-C9
9	c	101	BCB	C11-C10-C8-C9
9	x	101	BCB	C11-C10-C8-C9
9	T	101	BCB	O1D-CGD-O2D-CED
9	Y	101	BCB	C13-C15-C16-C17
9	h	101	BCB	C5-C6-C7-C8
9	f	101	BCB	C13-C15-C16-C17
10	L	303	BPB	C15-C16-C17-C18
17	Z	102	NS0	C10-C11-C12-C13
17	c	102	NS0	C10-C11-C12-C13
17	f	102	NS0	C10-C11-C12-C13
17	i	102	NS0	C10-C11-C12-C13
17	o	102	NS0	C10-C11-C12-C13
17	f	102	NS0	C10-C11-C12-C14
9	M	405	BCB	C15-C16-C17-C18
9	z	101	BCB	C13-C15-C16-C17
9	Q	101	BCB	C5-C6-C7-C8
10	M	407	BPB	C13-C15-C16-C17
17	o	102	NS0	C35-C36-C37-C38
17	7	102	NS0	C35-C36-C37-C38
9	3	101	BCB	C5-C6-C7-C8
9	G	101	BCB	C10-C11-C12-C13
9	G	101	BCB	C13-C15-C16-C17
9	c	101	BCB	C13-C15-C16-C17
9	i	101	BCB	C13-C15-C16-C17
9	l	101	BCB	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
10	M	407	BPB	C15-C16-C17-C18
17	1	102	NS0	C35-C36-C37-C38
17	x	102	NS0	C35-C36-C37-C38
17	4	102	NS0	C35-C36-C37-C38
9	L	301	BCB	C5-C6-C7-C8
9	L	301	BCB	C13-C15-C16-C17
9	L	301	BCB	C15-C16-C17-C18
9	z	101	BCB	C15-C16-C17-C18
9	n	101	BCB	C5-C6-C7-C8
9	t	101	BCB	C13-C15-C16-C17
9	w	101	BCB	C15-C16-C17-C18
9	N	101	BCB	C13-C15-C16-C17
9	W	101	BCB	C5-C6-C7-C8
9	Z	101	BCB	C13-C15-C16-C17
9	Z	101	BCB	C15-C16-C17-C18
9	r	101	BCB	C13-C15-C16-C17
9	4	101	BCB	C5-C6-C7-C8
17	r	102	NS0	C35-C36-C37-C38
9	M	405	BCB	C5-C6-C7-C8
9	G	101	BCB	C8-C10-C11-C12
9	x	101	BCB	C5-C6-C7-C8
17	u	102	NS0	C35-C36-C37-C38
9	1	101	BCB	C10-C11-C12-C13
9	G	101	BCB	C15-C16-C17-C18
9	l	101	BCB	C13-C15-C16-C17
17	Q	102	NS0	C35-C36-C37-C38
17	l	102	NS0	C35-C36-C37-C38
8	C	404	HEM	C3D-CAD-CBD-CGD
9	q	101	BCB	C15-C16-C17-C18
9	t	101	BCB	C15-C16-C17-C18
9	T	101	BCB	C5-C6-C7-C8
9	h	101	BCB	C11-C12-C13-C15
9	q	101	BCB	C11-C12-C13-C15
9	3	101	BCB	C11-C10-C8-C7
9	o	101	BCB	C6-C7-C8-C10
9	r	101	BCB	C11-C10-C8-C7
9	c	101	BCB	C3-C5-C6-C7
17	G	102	NS0	C11-C10-C9-C7
17	T	102	NS0	C11-C10-C9-C7
17	u	102	NS0	C11-C10-C9-C7
9	x	101	BCB	O1D-CGD-O2D-CED
9	6	102	BCB	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
9	u	101	BCB	C10-C11-C12-C13
9	t	101	BCB	O1A-CGA-O2A-C1
9	M	406	BCB	C8-C10-C11-C12
11	L	304	UQ9	C39-C41-C42-C43
11	6	101	UQ9	C44-C46-C47-C48
17	1	102	NS0	C7-C-CA-CB
17	Q	102	NS0	C7-C-CA-CB
9	h	101	BCB	C13-C15-C16-C17
9	w	101	BCB	C13-C15-C16-C17
9	r	101	BCB	C10-C11-C12-C13
10	M	407	BPB	C10-C11-C12-C13
9	z	101	BCB	C8-C10-C11-C12
9	1	101	BCB	C13-C15-C16-C17
9	N	101	BCB	C15-C16-C17-C18
9	Q	101	BCB	C10-C11-C12-C13
9	c	101	BCB	C5-C6-C7-C8
9	f	101	BCB	C5-C6-C7-C8
9	o	101	BCB	C13-C15-C16-C17
9	x	101	BCB	C10-C11-C12-C13
9	x	101	BCB	C13-C15-C16-C17
9	4	101	BCB	C10-C11-C12-C13
17	T	102	NS0	C35-C36-C37-C38
9	c	101	BCB	O1D-CGD-O2D-CED
11	L	304	UQ9	C31-C32-C33-C34
9	V	101	BCB	C8-C10-C11-C12
9	w	101	BCB	C8-C10-C11-C12
9	u	101	BCB	C15-C16-C17-C18
9	4	101	BCB	C13-C15-C16-C17
17	Z	102	NS0	C35-C36-C37-C38
17	u	102	NS0	C33-C35-C36-C37
9	e	101	BCB	CBA-CGA-O2A-C1
9	Z	101	BCB	O1D-CGD-O2D-CED
9	k	101	BCB	C8-C10-C11-C12
9	7	101	BCB	C5-C6-C7-C8
16	M	410	NS5	C1-C2-C3-C4
9	f	101	BCB	O1D-CGD-O2D-CED
11	6	101	UQ9	C45-C44-C46-C47
16	M	410	NS5	C11-C10-C9-C8
9	W	101	BCB	C10-C11-C12-C13
9	l	101	BCB	C5-C6-C7-C8
9	b	101	BCB	O1D-CGD-O2D-CED
9	u	101	BCB	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
9	k	101	BCB	C16-C17-C18-C19
9	M	405	BCB	CBA-CGA-O2A-C1
17	N	102	NS0	C11-C10-C9-C7
17	c	102	NS0	C11-C10-C9-C7
17	o	102	NS0	C11-C10-C9-C7
17	r	102	NS0	C11-C10-C9-C7
17	x	102	NS0	C11-C10-C9-C7
14	H	301	LDA	C3-C4-C5-C6
9	z	101	BCB	C3-C5-C6-C7
9	3	101	BCB	C3-C5-C6-C7
17	1	102	NS0	C33-C35-C36-C37
9	F	101	BCB	O1D-CGD-O2D-CED
9	o	101	BCB	O1D-CGD-O2D-CED
9	K	101	BCB	C16-C17-C18-C19
9	n	101	BCB	C16-C17-C18-C20
9	f	101	BCB	C16-C17-C18-C19
9	G	101	BCB	O1D-CGD-O2D-CED
9	7	101	BCB	C13-C15-C16-C17
14	M	408	LDA	C2-C3-C4-C5
9	u	101	BCB	O1D-CGD-O2D-CED
9	F	101	BCB	C8-C10-C11-C12
9	V	101	BCB	C16-C17-C18-C20
9	q	101	BCB	C16-C17-C18-C20
9	Q	101	BCB	C16-C17-C18-C19
9	W	101	BCB	C16-C17-C18-C19
9	o	101	BCB	C16-C17-C18-C19
9	r	101	BCB	C16-C17-C18-C19
10	M	407	BPB	C16-C17-C18-C20
9	W	101	BCB	O1D-CGD-O2D-CED
9	K	101	BCB	C6-C7-C8-C9
9	V	101	BCB	C11-C12-C13-C14
9	b	101	BCB	C11-C12-C13-C14
9	t	101	BCB	C6-C7-C8-C9
9	T	101	BCB	C6-C7-C8-C9
14	H	301	LDA	C5-C6-C7-C8
9	Q	101	BCB	C15-C16-C17-C18
9	r	101	BCB	C15-C16-C17-C18
9	i	101	BCB	C2A-CAA-CBA-CGA
9	o	101	BCB	C2A-CAA-CBA-CGA
9	e	101	BCB	O1A-CGA-O2A-C1
17	T	102	NS0	C10-C11-C12-C14
9	b	101	BCB	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
9	h	101	BCB	C8-C10-C11-C12
9	T	101	BCB	C13-C15-C16-C17
9	L	302	BCB	C10-C11-C12-C13
9	N	101	BCB	C8-C10-C11-C12
9	l	101	BCB	O1D-CGD-O2D-CED
9	r	101	BCB	O1D-CGD-O2D-CED
9	z	101	BCB	C3A-C2A-CAA-CBA
9	V	101	BCB	C3A-C2A-CAA-CBA
9	h	101	BCB	C3A-C2A-CAA-CBA
9	n	101	BCB	C3A-C2A-CAA-CBA
9	q	101	BCB	C3A-C2A-CAA-CBA
9	t	101	BCB	C3A-C2A-CAA-CBA
9	w	101	BCB	C3A-C2A-CAA-CBA
9	6	102	BCB	C3A-C2A-CAA-CBA
9	G	101	BCB	C3A-C2A-CAA-CBA
9	W	101	BCB	C3A-C2A-CAA-CBA
9	Z	101	BCB	C3A-C2A-CAA-CBA
9	l	101	BCB	C3A-C2A-CAA-CBA
9	r	101	BCB	C3A-C2A-CAA-CBA
9	k	101	BCB	C16-C17-C18-C20
9	3	101	BCB	C16-C17-C18-C19
17	1	102	NS0	C36-C37-C38-C39
17	G	102	NS0	C36-C37-C38-C39
17	N	102	NS0	C36-C37-C38-C39
17	Q	102	NS0	C36-C37-C38-C39
17	T	102	NS0	C36-C37-C38-C39
17	W	102	NS0	C36-C37-C38-C39
17	c	102	NS0	C36-C37-C38-C39
17	r	102	NS0	C36-C37-C38-C39
17	u	102	NS0	C36-C37-C38-C39
17	x	102	NS0	C36-C37-C38-C39
9	7	101	BCB	O2A-C1-C2-C3
9	t	101	BCB	C3-C5-C6-C7
9	7	101	BCB	C3-C5-C6-C7
9	6	102	BCB	C5-C6-C7-C8
9	W	101	BCB	C4-C3-C5-C6
9	x	101	BCB	C4-C3-C5-C6
9	W	101	BCB	C2-C3-C5-C6
9	c	101	BCB	C2-C3-C5-C6
9	x	101	BCB	C2-C3-C5-C6
17	u	102	NS0	CA-CB-CG-CD1
9	i	101	BCB	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
9	M	405	BCB	O1A-CGA-O2A-C1
9	M	405	BCB	C16-C17-C18-C19
9	o	101	BCB	C16-C17-C18-C20
10	M	407	BPB	C16-C17-C18-C19
17	f	102	NS0	C36-C37-C38-C39
17	l	102	NS0	C36-C37-C38-C39
9	K	101	BCB	C5-C6-C7-C8
9	1	101	BCB	C3-C5-C6-C7
9	V	101	BCB	C3-C5-C6-C7
9	r	101	BCB	C5-C6-C7-C8
17	i	102	NS0	C35-C36-C37-C38
17	7	102	NS0	CA-CB-CG-CD2
14	M	408	LDA	C3-C4-C5-C6
9	h	101	BCB	C15-C16-C17-C18
9	6	102	BCB	C10-C11-C12-C13
17	Z	102	NS0	C36-C37-C38-C39
17	o	102	NS0	C36-C37-C38-C39
17	4	102	NS0	C36-C37-C38-C39
17	7	102	NS0	C36-C37-C38-C39
17	Q	102	NS0	C33-C35-C36-C37
9	e	101	BCB	C10-C11-C12-C13
9	n	101	BCB	C10-C11-C12-C13
17	N	102	NS0	CA-CB-CG-CD2
9	S	101	BCB	C13-C15-C16-C17
9	o	101	BCB	C8-C10-C11-C12
9	c	101	BCB	C4-C3-C5-C6
15	M	409	MQ9	C12-C11-C9-C10
9	z	101	BCB	C6-C7-C8-C10
9	K	101	BCB	C6-C7-C8-C10
9	P	101	BCB	C12-C13-C15-C16
9	V	101	BCB	C6-C7-C8-C10
9	V	101	BCB	C11-C12-C13-C15
9	V	101	BCB	C12-C13-C15-C16
9	b	101	BCB	C11-C12-C13-C15
9	b	101	BCB	C12-C13-C15-C16
9	e	101	BCB	C12-C13-C15-C16
9	t	101	BCB	C6-C7-C8-C10
9	w	101	BCB	C11-C10-C8-C7
9	i	101	BCB	C6-C7-C8-C10
9	o	101	BCB	C11-C12-C13-C15
9	4	101	BCB	C6-C7-C8-C10
9	7	101	BCB	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
10	L	303	BPB	C11-C12-C13-C15
15	M	409	MQ9	C12-C11-C9-C8
14	M	408	LDA	C1-C2-C3-C4
9	W	101	BCB	C16-C17-C18-C20
9	r	101	BCB	C16-C17-C18-C20
17	i	102	NS0	C36-C37-C38-C39
9	V	101	BCB	CBA-CGA-O2A-C1
9	F	101	BCB	C15-C16-C17-C18
9	Y	101	BCB	C15-C16-C17-C18
9	7	101	BCB	C8-C10-C11-C12
8	C	404	HEM	C2B-C3B-CAB-CBB
9	L	302	BCB	CBD-CGD-O2D-CED
9	f	101	BCB	C16-C17-C18-C20
9	W	101	BCB	C15-C16-C17-C18
8	C	404	HEM	C4B-C3B-CAB-CBB
9	n	101	BCB	C15-C16-C17-C18
9	S	101	BCB	C16-C17-C18-C19
9	V	101	BCB	C16-C17-C18-C19
9	Q	101	BCB	C16-C17-C18-C20
9	w	101	BCB	C10-C11-C12-C13
16	M	410	NS5	C12-C10-C9-C8
17	7	102	NS0	CA-C-C7-C9
9	L	302	BCB	C11-C10-C8-C9
9	z	101	BCB	C6-C7-C8-C9
9	V	101	BCB	C6-C7-C8-C9
9	V	101	BCB	C14-C13-C15-C16
9	b	101	BCB	C14-C13-C15-C16
9	h	101	BCB	C11-C12-C13-C14
9	k	101	BCB	C6-C7-C8-C9
9	q	101	BCB	C11-C10-C8-C9
9	3	101	BCB	C11-C10-C8-C9
9	o	101	BCB	C11-C12-C13-C14
9	r	101	BCB	C11-C10-C8-C9
9	7	101	BCB	C6-C7-C8-C9
10	L	303	BPB	C11-C12-C13-C14
14	H	301	LDA	C7-C8-C9-C10
17	1	102	NS0	C10-C11-C12-C13
17	N	102	NS0	C10-C11-C12-C13
17	u	102	NS0	C10-C11-C12-C13
17	N	102	NS0	C10-C11-C12-C14
17	Z	102	NS0	C10-C11-C12-C14
17	c	102	NS0	C10-C11-C12-C14

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Mol	Chain	Res	Type	Atoms
17	i	102	NS0	C10-C11-C12-C14
17	o	102	NS0	C10-C11-C12-C14
9	V	101	BCB	O1A-CGA-O2A-C1
9	Y	101	BCB	C16-C17-C18-C19
9	e	101	BCB	C16-C17-C18-C19
9	q	101	BCB	C16-C17-C18-C19
9	3	101	BCB	C16-C17-C18-C20
9	c	101	BCB	C16-C17-C18-C19
9	x	101	BCB	C16-C17-C18-C19
9	P	101	BCB	C10-C11-C12-C13
9	P	101	BCB	C13-C15-C16-C17
9	3	101	BCB	C15-C16-C17-C18
9	7	101	BCB	C15-C16-C17-C18
10	L	303	BPB	C3-C5-C6-C7
17	4	102	NS0	C33-C35-C36-C37
9	P	101	BCB	C15-C16-C17-C18
17	W	102	NS0	C35-C36-C37-C38
14	M	408	LDA	C6-C7-C8-C9
9	t	101	BCB	C8-C10-C11-C12
17	l	102	NS0	C33-C35-C36-C37
9	K	101	BCB	C16-C17-C18-C20
9	n	101	BCB	C16-C17-C18-C19
9	x	101	BCB	C3-C5-C6-C7
17	c	102	NS0	C35-C36-C37-C38
17	u	102	NS0	C7-C-CA-CB
9	t	101	BCB	C5-C6-C7-C8
9	Z	101	BCB	C10-C11-C12-C13
9	u	101	BCB	C5-C6-C7-C8
17	Z	102	NS0	C34-C33-C35-C36
17	7	102	NS0	CA-C-C7-C8
9	1	101	BCB	C5-C6-C7-C8
9	e	101	BCB	C15-C16-C17-C18
11	6	101	UQ9	C5-C6-C7-C8
9	M	405	BCB	C2-C1-O2A-CGA
17	i	102	NS0	C33-C35-C36-C37
9	k	101	BCB	C15-C16-C17-C18
14	H	301	LDA	C9-C10-C11-C12
9	w	101	BCB	C16-C17-C18-C19
9	i	101	BCB	C16-C17-C18-C19
9	q	101	BCB	C5-C6-C7-C8
9	T	101	BCB	C3-C5-C6-C7
10	M	407	BPB	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
9	T	101	BCB	C8-C10-C11-C12
9	4	101	BCB	C15-C16-C17-C18
9	h	101	BCB	C10-C11-C12-C13
9	P	101	BCB	CHA-CBD-CGD-O1D
9	P	101	BCB	CHA-CBD-CGD-O2D
9	V	101	BCB	CHA-CBD-CGD-O2D
9	3	101	BCB	CHA-CBD-CGD-O2D
9	N	101	BCB	C4-C3-C5-C6
17	i	102	NS0	C34-C33-C35-C36
9	L	302	BCB	C11-C10-C8-C7
9	M	406	BCB	C12-C13-C15-C16
9	F	101	BCB	C11-C10-C8-C7
9	P	101	BCB	C6-C7-C8-C10
9	V	101	BCB	C11-C10-C8-C7
9	Y	101	BCB	C11-C10-C8-C7
9	b	101	BCB	C11-C10-C8-C7
9	k	101	BCB	C6-C7-C8-C10
9	k	101	BCB	C11-C10-C8-C7
9	n	101	BCB	C11-C10-C8-C7
9	q	101	BCB	C11-C10-C8-C7
9	N	101	BCB	C6-C7-C8-C10
9	W	101	BCB	C11-C10-C8-C7
9	Z	101	BCB	C11-C10-C8-C7
9	c	101	BCB	C11-C12-C13-C15
9	f	101	BCB	C6-C7-C8-C10
9	l	101	BCB	C6-C7-C8-C10
9	4	101	BCB	C11-C10-C8-C7
17	Z	102	NS0	C32-C33-C35-C36
17	i	102	NS0	C32-C33-C35-C36
17	W	102	NS0	C33-C35-C36-C37
9	1	101	BCB	C11-C12-C13-C14
9	F	101	BCB	C6-C7-C8-C9
9	P	101	BCB	C6-C7-C8-C9
9	Y	101	BCB	C11-C10-C8-C9
9	b	101	BCB	C6-C7-C8-C9
9	e	101	BCB	C11-C12-C13-C14
9	n	101	BCB	C11-C10-C8-C9
9	q	101	BCB	C11-C12-C13-C14
9	N	101	BCB	C11-C12-C13-C14
9	T	101	BCB	C11-C12-C13-C14
9	f	101	BCB	C6-C7-C8-C9
9	l	101	BCB	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
9	l	101	BCB	C11-C12-C13-C14
10	M	407	BPB	C11-C12-C13-C14
9	Y	101	BCB	C10-C11-C12-C13
17	W	102	NS0	C10-C11-C12-C13
17	4	102	NS0	C10-C11-C12-C13
9	M	405	BCB	C16-C17-C18-C20
9	i	101	BCB	C16-C17-C18-C20
17	1	102	NS0	C10-C11-C12-C14
17	l	102	NS0	C10-C11-C12-C14
17	u	102	NS0	C10-C11-C12-C14
17	x	102	NS0	C10-C11-C12-C14
9	S	101	BCB	C3-C5-C6-C7
9	W	101	BCB	C3-C5-C6-C7
9	u	101	BCB	C13-C15-C16-C17
9	w	101	BCB	C5-C6-C7-C8
9	T	101	BCB	C10-C11-C12-C13
9	o	101	BCB	C5-C6-C7-C8
17	7	102	NS0	C34-C33-C35-C36
9	N	101	BCB	C2-C3-C5-C6
9	M	406	BCB	CBA-CGA-O2A-C1
9	1	101	BCB	C3A-C2A-CAA-CBA
9	T	101	BCB	C3A-C2A-CAA-CBA
9	f	101	BCB	C3A-C2A-CAA-CBA
17	G	102	NS0	CA-CB-CG-CD2
8	C	402	HEM	C3D-CAD-CBD-CGD
17	T	102	NS0	C33-C35-C36-C37
9	L	301	BCB	C16-C17-C18-C19
11	6	101	UQ9	C43-C44-C46-C47
9	M	406	BCB	C5-C6-C7-C8
9	e	101	BCB	C16-C17-C18-C20
9	N	101	BCB	C5-C6-C7-C8
11	L	304	UQ9	C5-C4-O4-C4M
9	F	101	BCB	C13-C15-C16-C17
9	S	101	BCB	C16-C17-C18-C20
9	k	101	BCB	C5-C6-C7-C8
17	f	102	NS0	C7-C-CA-CB
9	4	101	BCB	C4-C3-C5-C6
17	T	102	NS0	C34-C33-C35-C36
9	G	101	BCB	C2-C1-O2A-CGA
9	h	101	BCB	C6-C7-C8-C9
9	n	101	BCB	C6-C7-C8-C9
9	T	101	BCB	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
9	f	101	BCB	C11-C12-C13-C14
9	i	101	BCB	C11-C10-C8-C9
9	u	101	BCB	C14-C13-C15-C16
10	L	303	BPB	C14-C13-C15-C16
9	1	101	BCB	C1A-C2A-CAA-CBA
9	F	101	BCB	C1A-C2A-CAA-CBA
9	K	101	BCB	C1A-C2A-CAA-CBA
9	P	101	BCB	C1A-C2A-CAA-CBA
9	S	101	BCB	C1A-C2A-CAA-CBA
9	Y	101	BCB	C1A-C2A-CAA-CBA
9	b	101	BCB	C1A-C2A-CAA-CBA
9	e	101	BCB	C1A-C2A-CAA-CBA
9	k	101	BCB	C1A-C2A-CAA-CBA
9	3	101	BCB	C1A-C2A-CAA-CBA
9	Z	101	BCB	C1A-C2A-CAA-CBA
9	f	101	BCB	C1A-C2A-CAA-CBA
9	l	101	BCB	C1A-C2A-CAA-CBA
9	4	101	BCB	C1A-C2A-CAA-CBA
9	M	406	BCB	C16-C17-C18-C19
9	S	101	BCB	C15-C16-C17-C18
9	Y	101	BCB	C16-C17-C18-C20
9	x	101	BCB	C16-C17-C18-C20
9	F	101	BCB	C6-C7-C8-C10
9	P	101	BCB	C11-C10-C8-C7
9	S	101	BCB	C11-C10-C8-C7
9	b	101	BCB	C6-C7-C8-C10
9	e	101	BCB	C6-C7-C8-C10
9	h	101	BCB	C6-C7-C8-C10
9	h	101	BCB	C12-C13-C15-C16
9	G	101	BCB	C11-C10-C8-C7
9	N	101	BCB	C11-C10-C8-C7
9	N	101	BCB	C11-C12-C13-C15
9	Q	101	BCB	C11-C10-C8-C7
9	Q	101	BCB	C12-C13-C15-C16
9	T	101	BCB	C11-C12-C13-C15
9	Z	101	BCB	C11-C12-C13-C15
9	f	101	BCB	C11-C12-C13-C15
9	l	101	BCB	C11-C12-C13-C15
9	x	101	BCB	C11-C10-C8-C7
9	x	101	BCB	C11-C12-C13-C15
9	4	101	BCB	C2-C3-C5-C6
9	4	101	BCB	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
9	7	101	BCB	C11-C12-C13-C15
10	L	303	BPB	C6-C7-C8-C10
10	M	407	BPB	C11-C12-C13-C15
17	T	102	NS0	C32-C33-C35-C36
9	M	405	BCB	C8-C10-C11-C12
9	c	101	BCB	C16-C17-C18-C20
17	N	102	NS0	C35-C36-C37-C38
9	b	101	BCB	C2A-CAA-CBA-CGA
10	L	303	BPB	C13-C15-C16-C17
17	f	102	NS0	C33-C35-C36-C37
8	C	401	HEM	C2A-CAA-CBA-CGA
8	C	403	HEM	C2B-C3B-CAB-CBB
9	M	405	BCB	CAD-CBD-CGD-O2D
9	6	102	BCB	CAD-CBD-CGD-O2D
10	M	407	BPB	CAD-CBD-CGD-O2D
9	N	101	BCB	O1D-CGD-O2D-CED
9	Q	101	BCB	C4-C3-C5-C6
9	L	301	BCB	C16-C17-C18-C20
9	o	101	BCB	C15-C16-C17-C18
14	M	408	LDA	C11-C10-C9-C8
9	w	101	BCB	C16-C17-C18-C20
9	4	101	BCB	C16-C17-C18-C20
14	H	301	LDA	C6-C7-C8-C9
9	M	406	BCB	O1A-CGA-O2A-C1
14	M	408	LDA	C7-C8-C9-C10
9	b	101	BCB	C16-C17-C18-C20
17	7	102	NS0	C32-C33-C35-C36
9	z	101	BCB	C5-C6-C7-C8
9	b	101	BCB	C11-C10-C8-C9
9	Z	101	BCB	C11-C12-C13-C14
9	x	101	BCB	C11-C12-C13-C14
9	7	101	BCB	C11-C12-C13-C14
9	6	102	BCB	C2A-CAA-CBA-CGA
10	L	303	BPB	C10-C11-C12-C13
17	Q	102	NS0	C10-C11-C12-C13
17	l	102	NS0	C10-C11-C12-C13
17	r	102	NS0	C10-C11-C12-C13
17	x	102	NS0	C10-C11-C12-C13
17	Q	102	NS0	C10-C11-C12-C14
17	W	102	NS0	C10-C11-C12-C14
17	r	102	NS0	C10-C11-C12-C14
17	4	102	NS0	C10-C11-C12-C14

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Mol	Chain	Res	Type	Atoms
9	L	302	BCB	C2-C1-O2A-CGA
9	Q	101	BCB	C2-C3-C5-C6
10	M	407	BPB	O1A-CGA-O2A-C1
9	u	101	BCB	C16-C17-C18-C20
9	4	101	BCB	C16-C17-C18-C19
14	M	408	LDA	C9-C10-C11-C12
9	L	301	BCB	CAD-CBD-CGD-O1D
9	L	302	BCB	CAD-CBD-CGD-O1D
14	H	301	LDA	C2-C1-N1-O1
9	4	101	BCB	C3-C5-C6-C7
9	z	101	BCB	C11-C10-C8-C7
9	1	101	BCB	C11-C10-C8-C7
9	1	101	BCB	C11-C12-C13-C15
9	1	101	BCB	C12-C13-C15-C16
9	h	101	BCB	C11-C10-C8-C7
9	n	101	BCB	C6-C7-C8-C10
9	t	101	BCB	C12-C13-C15-C16
9	c	101	BCB	C11-C10-C8-C7
9	o	101	BCB	C11-C10-C8-C7
9	r	101	BCB	C11-C12-C13-C15
9	L	302	BCB	O1D-CGD-O2D-CED
9	Z	101	BCB	C3-C5-C6-C7
17	f	102	NS0	C35-C36-C37-C38
11	6	101	UQ9	C1-C6-C7-C8
9	K	101	BCB	C10-C11-C12-C13
9	e	101	BCB	C13-C15-C16-C17
9	P	101	BCB	C5-C6-C7-C8
10	M	407	BPB	CBA-CGA-O2A-C1
9	P	101	BCB	C11-C10-C8-C9
9	S	101	BCB	C11-C10-C8-C9
9	V	101	BCB	C11-C10-C8-C9
9	k	101	BCB	C11-C10-C8-C9
9	t	101	BCB	C14-C13-C15-C16
9	6	102	BCB	C14-C13-C15-C16
9	N	101	BCB	C11-C10-C8-C9
9	c	101	BCB	C11-C12-C13-C14
9	o	101	BCB	C6-C7-C8-C9
9	o	101	BCB	C11-C10-C8-C9
9	4	101	BCB	C6-C7-C8-C9
9	4	101	BCB	C11-C12-C13-C14
10	L	303	BPB	C6-C7-C8-C9
9	1	101	BCB	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
11	L	304	UQ9	C2-C3-O3-C3M
9	S	101	BCB	C5-C6-C7-C8
9	V	101	BCB	C5-C6-C7-C8
9	u	101	BCB	C16-C17-C18-C19
9	S	101	BCB	C2-C1-O2A-CGA
9	i	101	BCB	C2-C1-O2A-CGA
9	r	101	BCB	C2-C1-O2A-CGA
9	T	101	BCB	C16-C17-C18-C19
9	n	101	BCB	O1A-CGA-O2A-C1
9	i	101	BCB	C5-C6-C7-C8
11	L	304	UQ9	C44-C46-C47-C48
9	n	101	BCB	CBA-CGA-O2A-C1
9	1	101	BCB	CHA-CBD-CGD-O2D
9	V	101	BCB	CHA-CBD-CGD-O1D
9	Y	101	BCB	CHA-CBD-CGD-O2D
9	e	101	BCB	CHA-CBD-CGD-O1D
9	e	101	BCB	CHA-CBD-CGD-O2D
9	n	101	BCB	CHA-CBD-CGD-O1D
9	n	101	BCB	CHA-CBD-CGD-O2D
9	3	101	BCB	CHA-CBD-CGD-O1D
9	c	101	BCB	CHA-CBD-CGD-O1D
9	c	101	BCB	CHA-CBD-CGD-O2D
9	F	101	BCB	C5-C6-C7-C8
9	q	101	BCB	C6-C7-C8-C10
9	6	102	BCB	C11-C12-C13-C15
9	T	101	BCB	C11-C10-C8-C7
9	i	101	BCB	C11-C10-C8-C7
9	z	101	BCB	C11-C10-C8-C9
9	1	101	BCB	C14-C13-C15-C16
9	F	101	BCB	C11-C10-C8-C9
9	e	101	BCB	C6-C7-C8-C9
9	h	101	BCB	C11-C10-C8-C9
9	h	101	BCB	C14-C13-C15-C16
9	6	102	BCB	C11-C12-C13-C14
9	G	101	BCB	C11-C10-C8-C9
9	i	101	BCB	C6-C7-C8-C9
9	r	101	BCB	C11-C12-C13-C14
9	S	101	BCB	C10-C11-C12-C13
9	q	101	BCB	C13-C15-C16-C17
11	6	101	UQ9	C2-C3-O3-C3M
9	M	406	BCB	C16-C17-C18-C20
9	b	101	BCB	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
9	b	101	BCB	C3-C5-C6-C7
9	N	101	BCB	C16-C17-C18-C19
9	6	102	BCB	CBA-CGA-O2A-C1
8	C	401	HEM	CAA-CBA-CGA-O2A
8	C	402	HEM	C4B-C3B-CAB-CBB
8	C	403	HEM	C4B-C3B-CAB-CBB
9	F	101	BCB	C4-C3-C5-C6
17	c	102	NS0	C34-C33-C35-C36
17	l	102	NS0	CA-C-C7-C8
8	C	404	HEM	CAD-CBD-CGD-O2D
9	Z	101	BCB	C2-C3-C5-C6
9	o	101	BCB	C2-C3-C5-C6
9	L	302	BCB	C13-C15-C16-C17
9	x	101	BCB	C2A-CAA-CBA-CGA
9	M	405	BCB	C3A-C2A-CAA-CBA
11	6	101	UQ9	C5-C4-O4-C4M
9	Z	101	BCB	C4-C3-C5-C6
9	o	101	BCB	C4-C3-C5-C6
9	t	101	BCB	C11-C10-C8-C9
9	u	101	BCB	C11-C12-C13-C14
8	C	404	HEM	CAD-CBD-CGD-O1D
9	c	101	BCB	C15-C16-C17-C18
9	T	101	BCB	C16-C17-C18-C20
9	Z	101	BCB	C16-C17-C18-C20
9	S	101	BCB	O2A-C1-C2-C3
9	e	101	BCB	C8-C10-C11-C12
17	1	102	NS0	C34-C33-C35-C36
9	L	301	BCB	C6-C7-C8-C10
9	M	405	BCB	C12-C13-C15-C16
9	M	406	BCB	C11-C10-C8-C7
9	K	101	BCB	C11-C10-C8-C7
9	t	101	BCB	C11-C10-C8-C7
9	Q	101	BCB	C6-C7-C8-C10
10	L	303	BPB	C11-C10-C8-C7
9	N	101	BCB	C16-C17-C18-C20
9	z	101	BCB	C10-C11-C12-C13
9	i	101	BCB	C10-C11-C12-C13
8	C	401	HEM	CAA-CBA-CGA-O1A
9	1	101	BCB	C4-C3-C5-C6
9	i	101	BCB	C4-C3-C5-C6
17	l	102	NS0	C34-C33-C35-C36
17	4	102	NS0	C34-C33-C35-C36

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Mol	Chain	Res	Type	Atoms
17	W	102	NS0	CA-CB-CG-CD2
16	M	410	NS5	C18-C19-C20-C21
9	6	102	BCB	O1A-CGA-O2A-C1
17	G	102	NS0	CA-C-C7-C8
17	r	102	NS0	C34-C33-C35-C36
9	6	102	BCB	C2-C1-O2A-CGA
17	c	102	NS0	C32-C33-C35-C36
9	G	101	BCB	C11-C12-C13-C14
10	L	303	BPB	C8-C10-C11-C12
9	T	101	BCB	C1A-C2A-CAA-CBA
9	W	101	BCB	C1A-C2A-CAA-CBA
9	Y	101	BCB	C2A-CAA-CBA-CGA
9	r	101	BCB	O1A-CGA-O2A-C1
9	6	102	BCB	C4-C3-C5-C6
17	Q	102	NS0	C34-C33-C35-C36
17	x	102	NS0	C34-C33-C35-C36
9	Y	101	BCB	C5-C6-C7-C8
14	M	408	LDA	C5-C6-C7-C8
9	l	101	BCB	C4-C3-C5-C6
11	6	101	UQ9	C40-C39-C41-C42
15	M	409	MQ9	C14-C16-C17-C18
9	1	101	BCB	C2-C3-C5-C6
9	K	101	BCB	C12-C13-C15-C16
9	3	101	BCB	C11-C12-C13-C15
9	G	101	BCB	C2-C3-C5-C6
9	T	101	BCB	C6-C7-C8-C10
9	h	101	BCB	CAA-CBA-CGA-O2A
9	r	101	BCB	CBA-CGA-O2A-C1
16	M	410	NS5	C3-C4-C5-C6
17	N	102	NS0	C34-C33-C35-C36
9	K	101	BCB	C8-C10-C11-C12
9	x	101	BCB	C15-C16-C17-C18
9	F	101	BCB	C2-C3-C5-C6
9	i	101	BCB	C2-C3-C5-C6
17	l	102	NS0	C32-C33-C35-C36
9	L	301	BCB	C6-C7-C8-C9
9	K	101	BCB	C11-C10-C8-C9
9	Y	101	BCB	C6-C7-C8-C9
9	Q	101	BCB	C6-C7-C8-C9
8	C	403	HEM	CAA-CBA-CGA-O2A
8	C	402	HEM	C2B-C3B-CAB-CBB
9	k	101	BCB	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
9	q	101	BCB	C2-C1-O2A-CGA
9	S	101	BCB	CAA-CBA-CGA-O2A
9	n	101	BCB	CAA-CBA-CGA-O2A
17	u	102	NS0	C34-C33-C35-C36
17	1	102	NS0	C32-C33-C35-C36
17	Q	102	NS0	C32-C33-C35-C36
17	r	102	NS0	C32-C33-C35-C36
17	x	102	NS0	C32-C33-C35-C36
17	4	102	NS0	C32-C33-C35-C36
16	M	410	NS5	C20-C21-C23-C24
14	H	301	LDA	C4-C5-C6-C7
17	r	102	NS0	C33-C35-C36-C37
9	q	101	BCB	CAA-CBA-CGA-O2A
9	r	101	BCB	O2A-C1-C2-C3
9	L	301	BCB	C2A-CAA-CBA-CGA
17	o	102	NS0	CA-CB-CG-CD2
9	Z	101	BCB	C16-C17-C18-C19
8	C	403	HEM	CAA-CBA-CGA-O1A
17	N	102	NS0	C32-C33-C35-C36
9	P	101	BCB	C2A-CAA-CBA-CGA
8	C	403	HEM	CAD-CBD-CGD-O1D
9	Y	101	BCB	CHA-CBD-CGD-O1D
9	q	101	BCB	CHA-CBD-CGD-O2D
9	6	102	BCB	CHA-CBD-CGD-O2D
9	Q	101	BCB	CHA-CBD-CGD-O2D
10	M	407	BPB	CHA-CBD-CGD-O1D
9	Y	101	BCB	C6-C7-C8-C10
9	Q	101	BCB	C11-C12-C13-C15
9	T	101	BCB	C12-C13-C15-C16
9	1	101	BCB	C6-C7-C8-C9
9	S	101	BCB	C6-C7-C8-C9
9	q	101	BCB	C6-C7-C8-C9
9	q	101	BCB	C14-C13-C15-C16
9	N	101	BCB	C6-C7-C8-C9
9	T	101	BCB	C14-C13-C15-C16
15	M	409	MQ9	C29-C31-C32-C33
9	f	101	BCB	C15-C16-C17-C18
17	1	102	NS0	C30-C31-C32-C33
17	1	102	NS0	C-CA-CB-CG
17	G	102	NS0	C30-C31-C32-C33
17	N	102	NS0	C30-C31-C32-C33
17	Q	102	NS0	C30-C31-C32-C33

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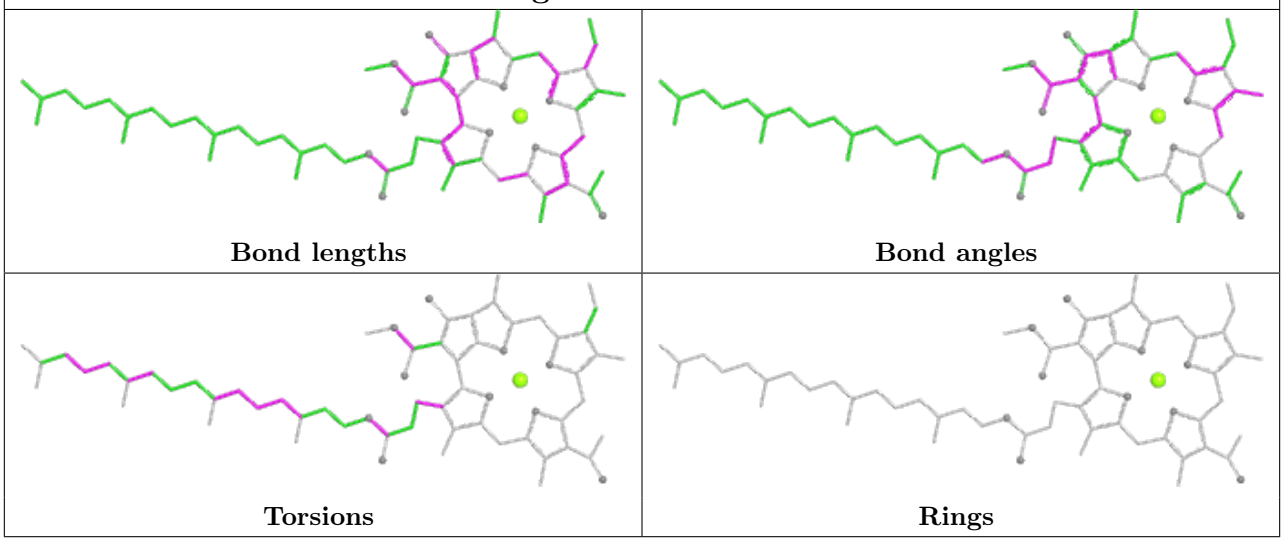
Mol	Chain	Res	Type	Atoms
17	T	102	NS0	C30-C31-C32-C33
17	T	102	NS0	C-CA-CB-CG
17	W	102	NS0	C30-C31-C32-C33
17	Z	102	NS0	C30-C31-C32-C33
17	c	102	NS0	C30-C31-C32-C33
17	f	102	NS0	C30-C31-C32-C33
17	i	102	NS0	C30-C31-C32-C33
17	l	102	NS0	C30-C31-C32-C33
17	o	102	NS0	C30-C31-C32-C33
17	r	102	NS0	C30-C31-C32-C33
17	u	102	NS0	C30-C31-C32-C33
17	x	102	NS0	C30-C31-C32-C33
17	4	102	NS0	C30-C31-C32-C33
17	7	102	NS0	C30-C31-C32-C33
8	C	402	HEM	C2A-CAA-CBA-CGA
15	M	409	MQ9	C30-C29-C31-C32
9	S	101	BCB	CAA-CBA-CGA-O1A
9	h	101	BCB	CAA-CBA-CGA-O1A
9	K	101	BCB	CAA-CBA-CGA-O2A
9	n	101	BCB	CAA-CBA-CGA-O1A
8	C	402	HEM	CAA-CBA-CGA-O2A
9	q	101	BCB	CAA-CBA-CGA-O1A
9	G	101	BCB	C16-C17-C18-C19
15	M	409	MQ9	C11-C12-C13-C14
8	C	403	HEM	CAD-CBD-CGD-O2D
9	K	101	BCB	O1A-CGA-O2A-C1
9	c	101	BCB	CAA-CBA-CGA-O2A
9	6	102	BCB	C11-C10-C8-C9
9	G	101	BCB	C4-C3-C5-C6
17	f	102	NS0	C34-C33-C35-C36
17	o	102	NS0	C34-C33-C35-C36
9	1	101	BCB	C6-C7-C8-C10
9	S	101	BCB	C6-C7-C8-C10
9	S	101	BCB	C12-C13-C15-C16
9	e	101	BCB	C11-C10-C8-C7
9	w	101	BCB	C12-C13-C15-C16
9	6	102	BCB	C11-C10-C8-C7
9	c	101	BCB	CAA-CBA-CGA-O1A
8	C	402	HEM	CAA-CBA-CGA-O1A
9	K	101	BCB	CAA-CBA-CGA-O1A
10	L	303	BPB	C2A-CAA-CBA-CGA

There are no ring outliers.

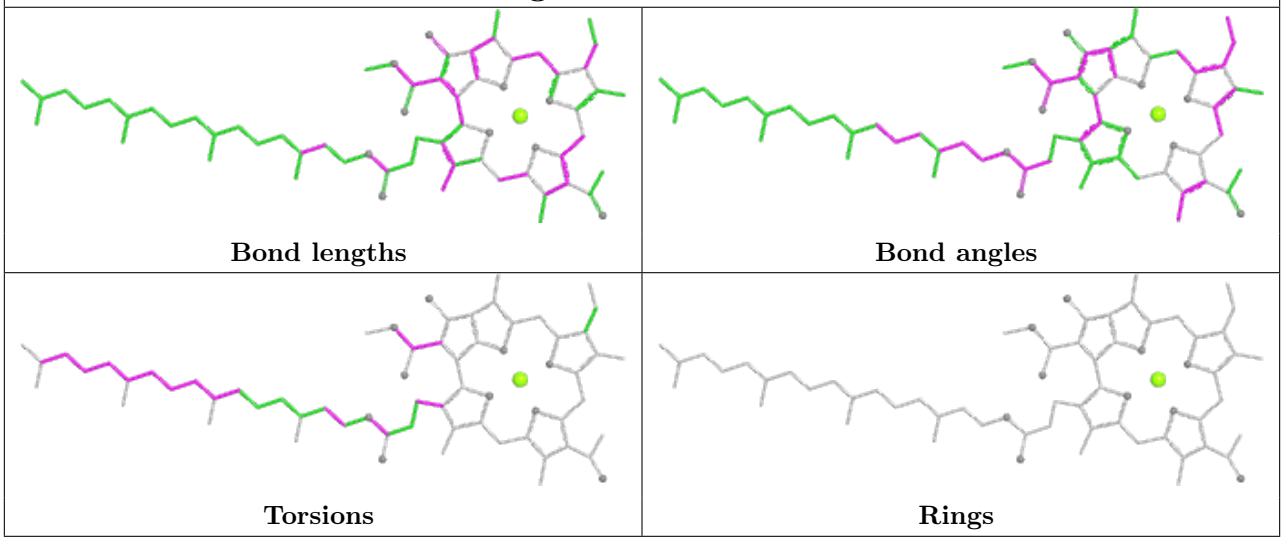
No monomer is involved in short contacts.

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.

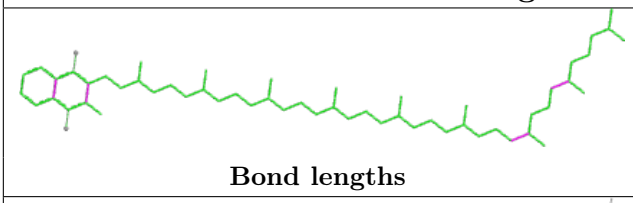
Ligand BCB l 101



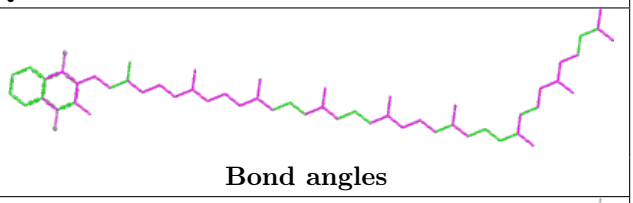
Ligand BCB e 101



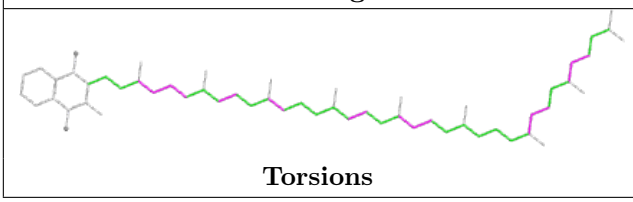
Ligand MQ9 M 409



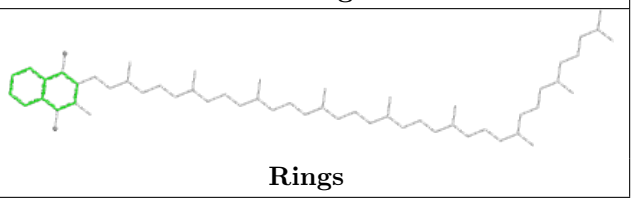
Bond lengths



Bond angles

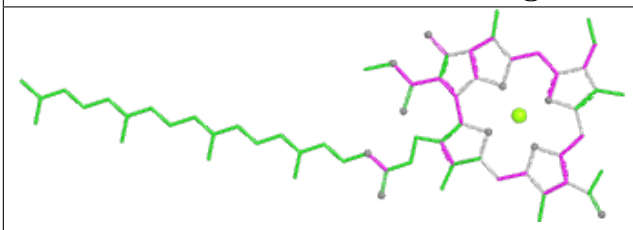


Torsions

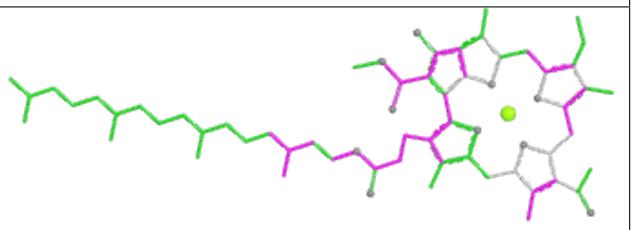


Rings

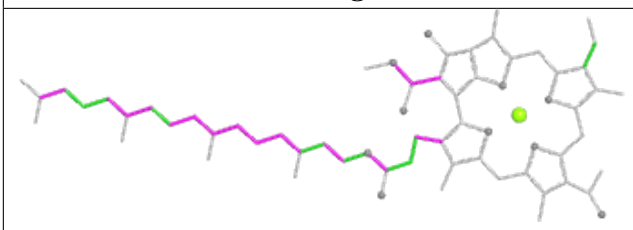
Ligand BCB V 101



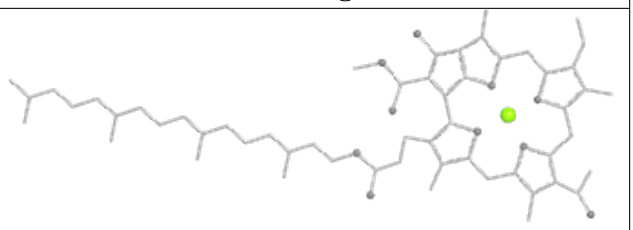
Bond lengths



Bond angles

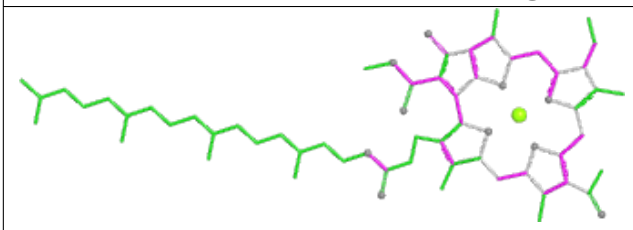


Torsions

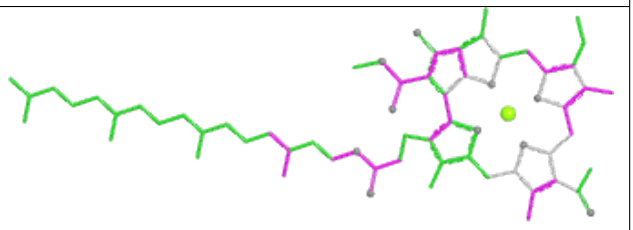


Rings

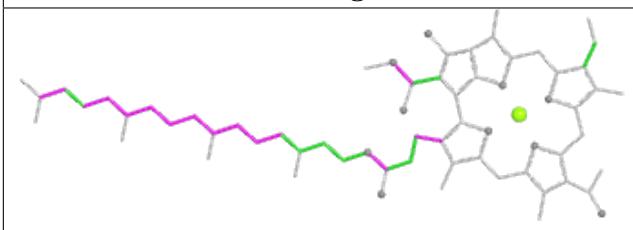
Ligand BCB T 101



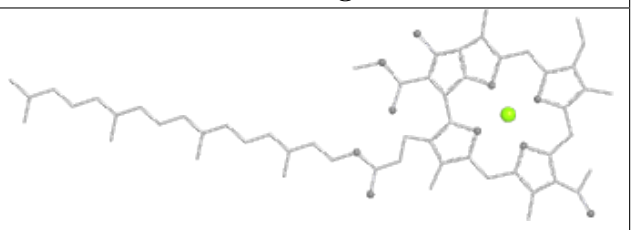
Bond lengths



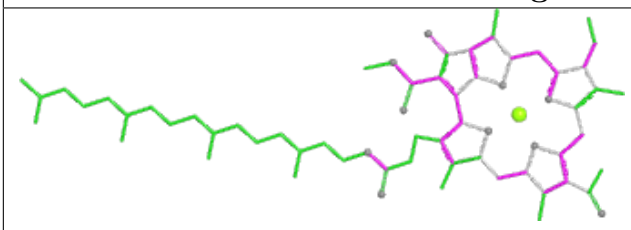
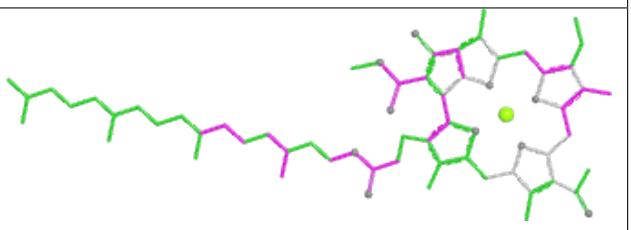
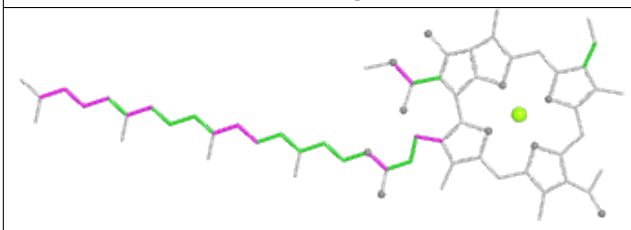
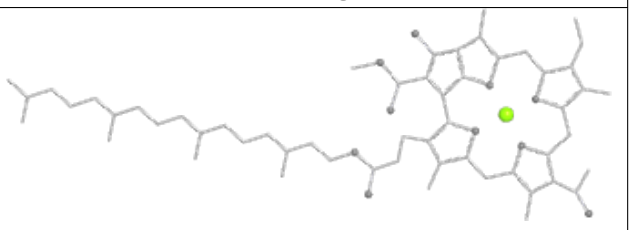
Bond angles

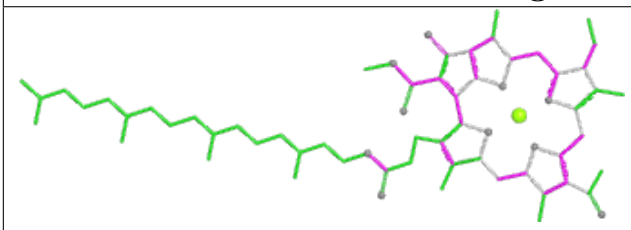
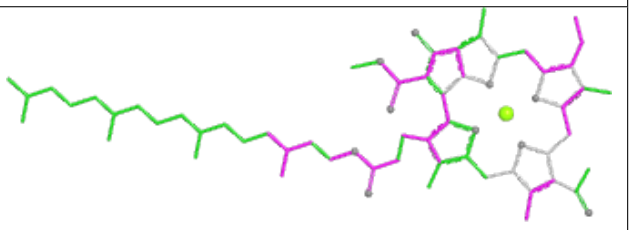
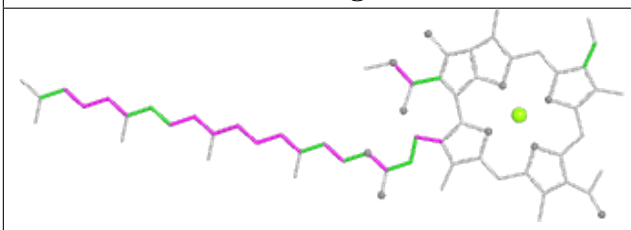
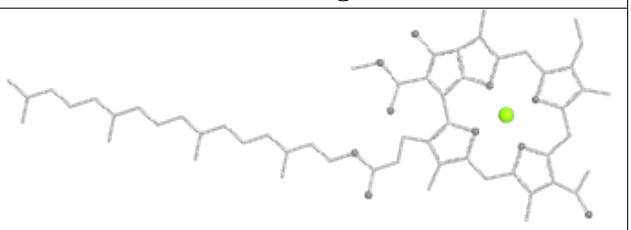


Torsions



Rings

Ligand BCB f 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCB t 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

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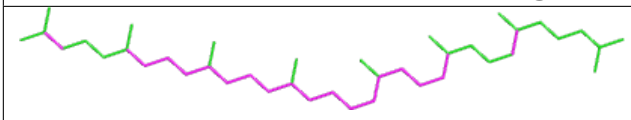
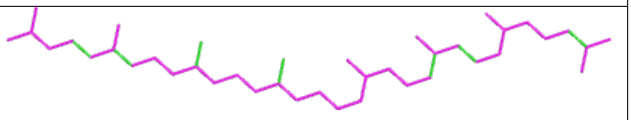
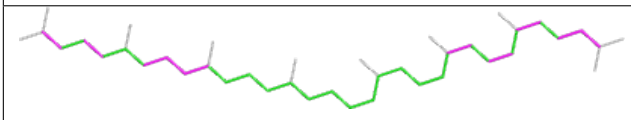
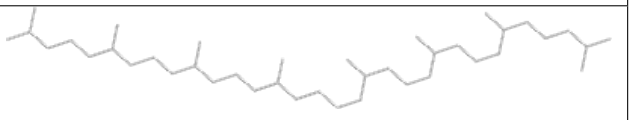
 Bond lengths	 Bond angles
 Torsions	 Rings

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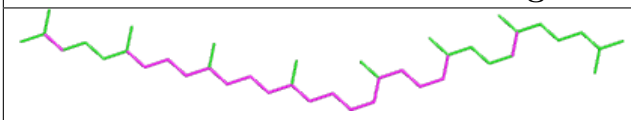
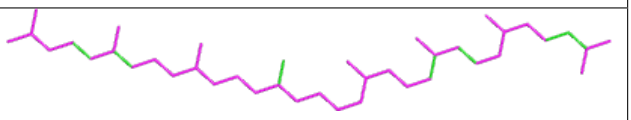
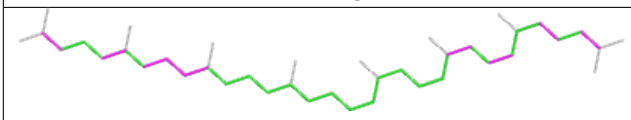
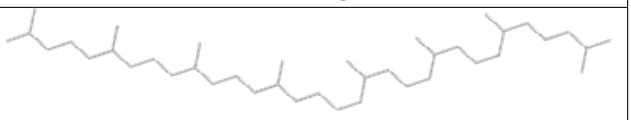
 Bond lengths	 Bond angles
 Torsions	 Rings

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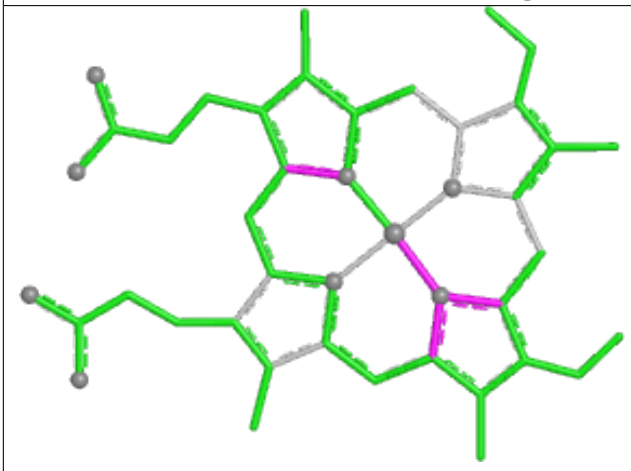
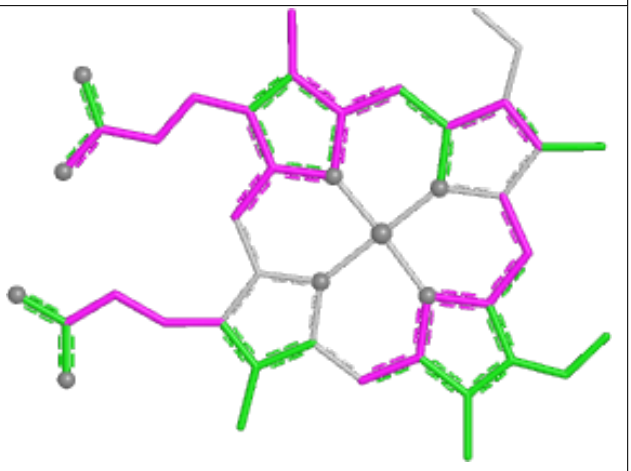
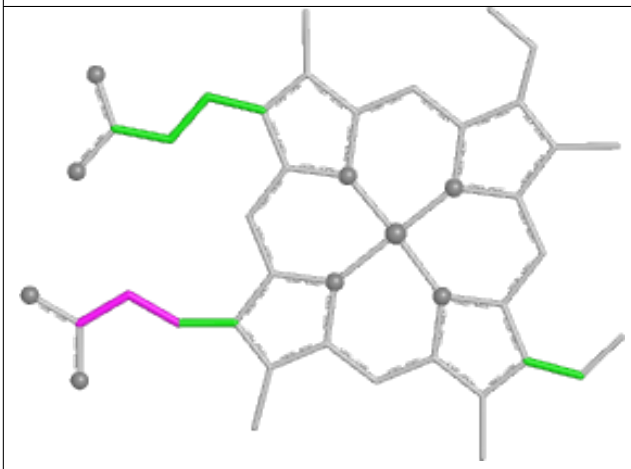
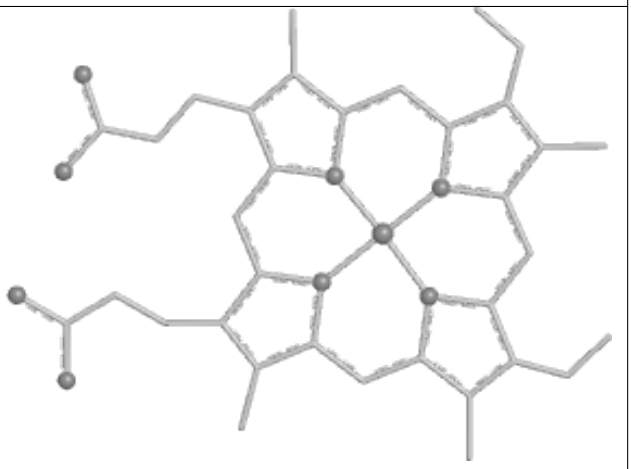
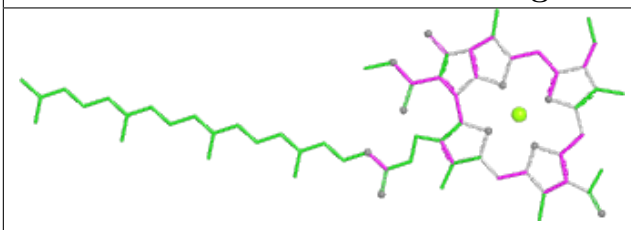
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCB i 101



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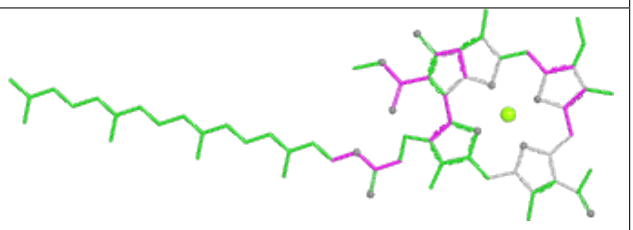

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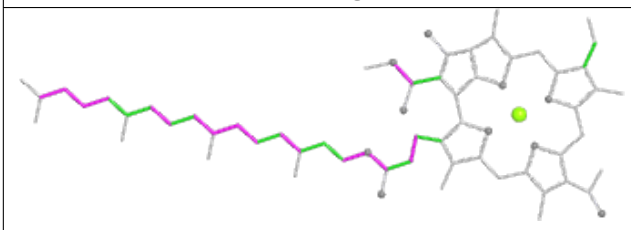

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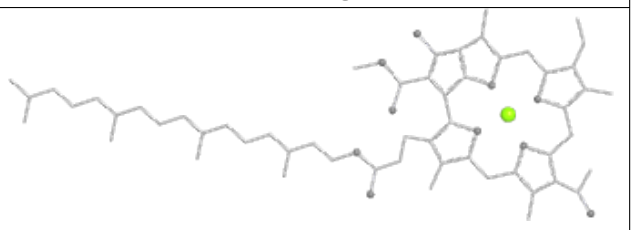
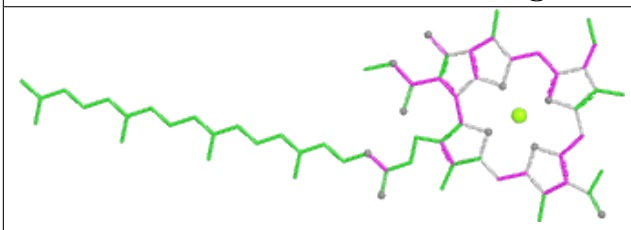


Rings

Ligand BCB z 101



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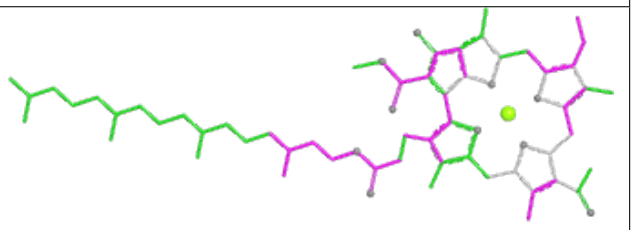

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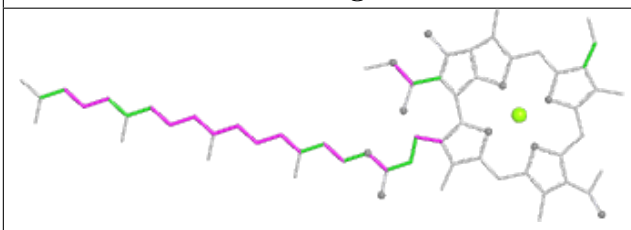

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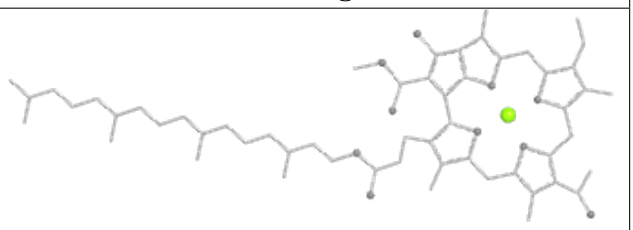
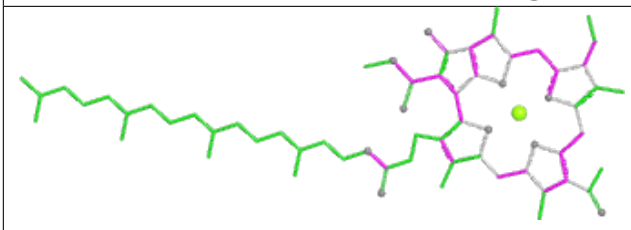


Rings

Ligand BCB L 302



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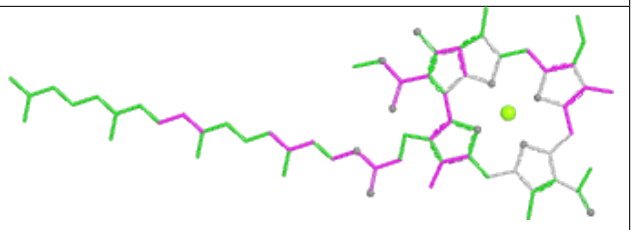
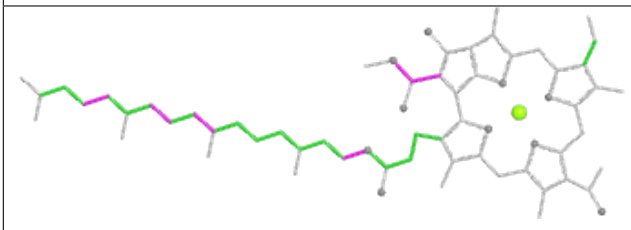


Bond angles



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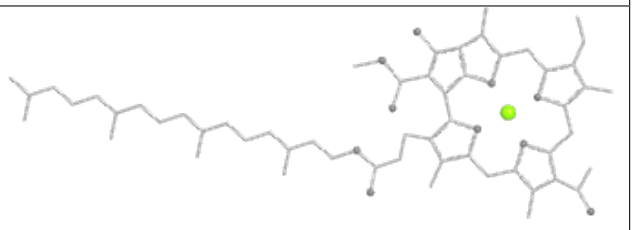
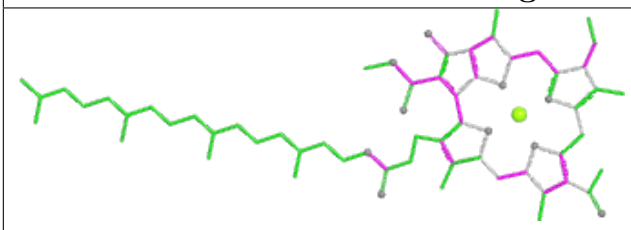
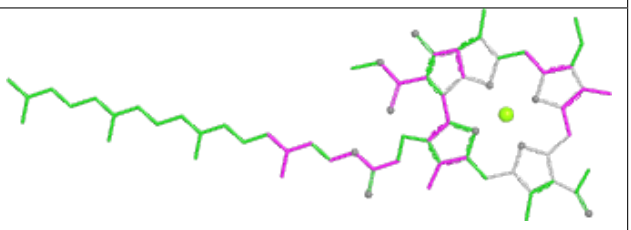
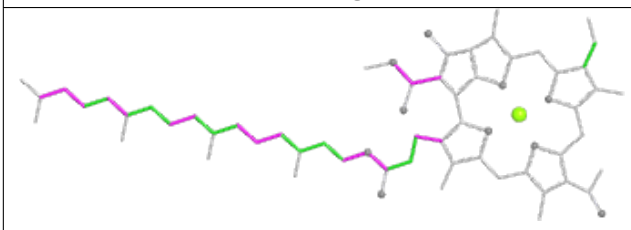
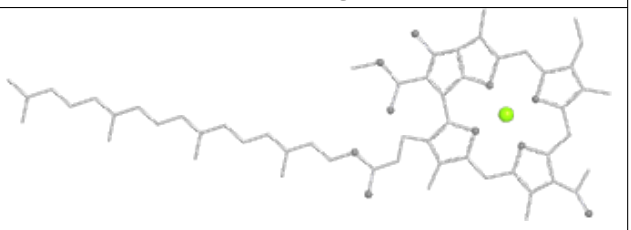


Rings

Ligand BCB M 405	
 Bond lengths	 Bond angles
 Torsions	 Rings

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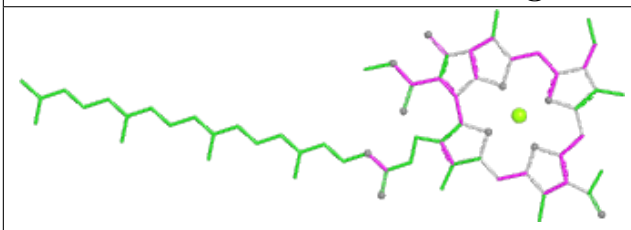
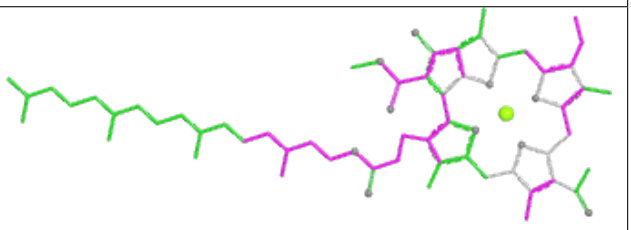
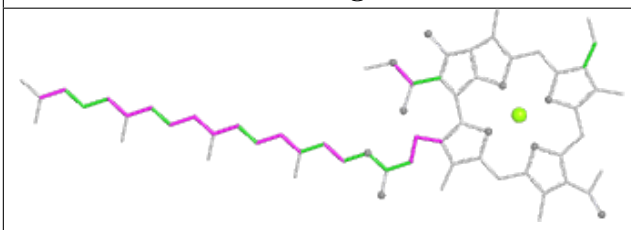
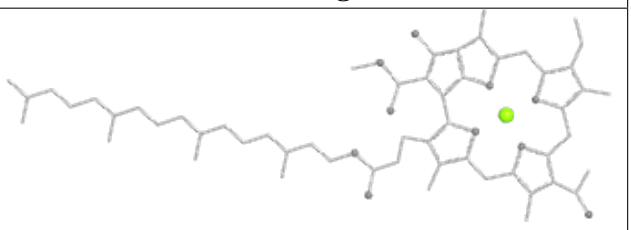
 Bond lengths	 Bond angles
 Torsions	 Rings

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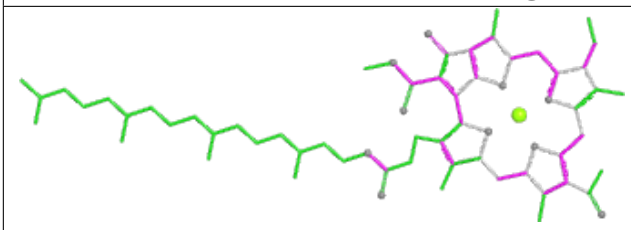
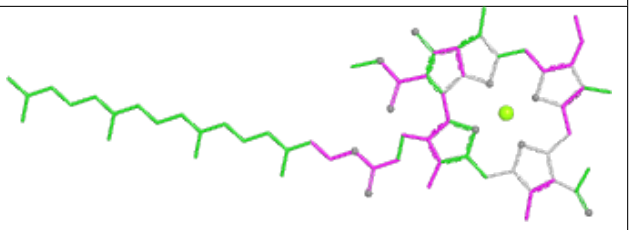
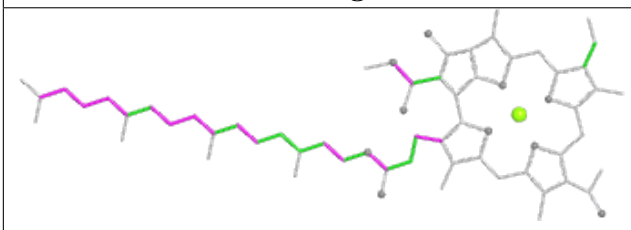
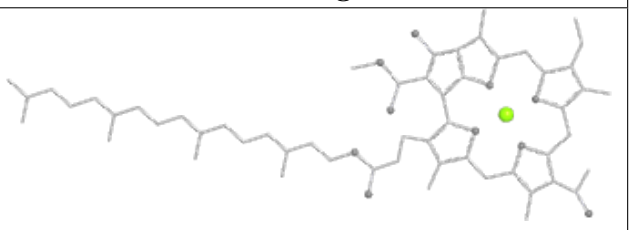
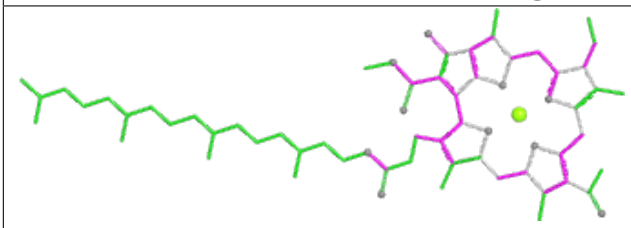
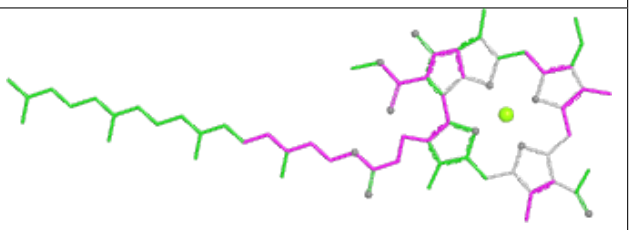
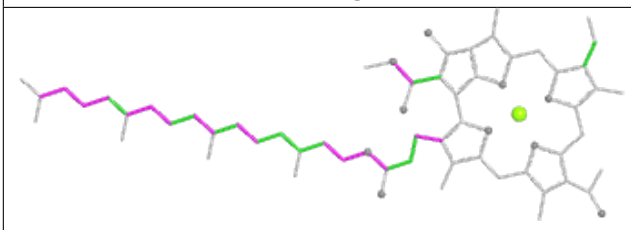
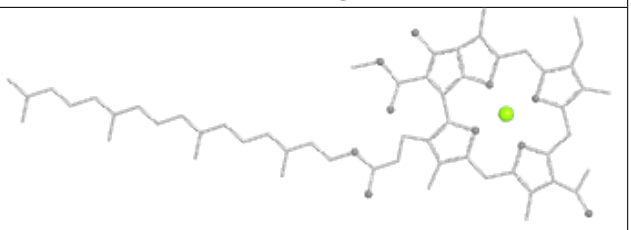
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCB r 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

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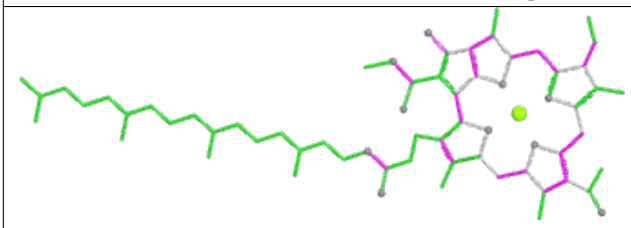
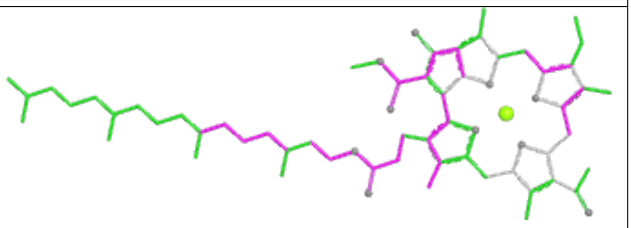
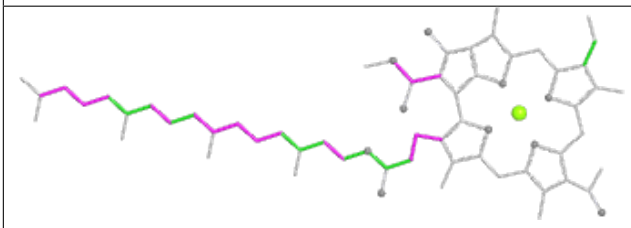
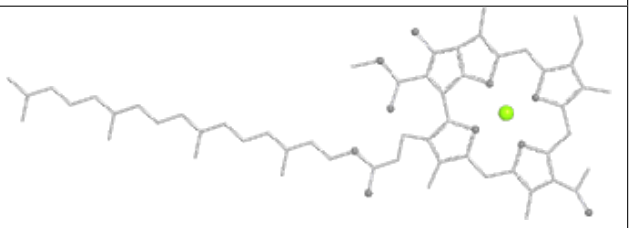
 Bond lengths	 Bond angles
 Torsions	 Rings

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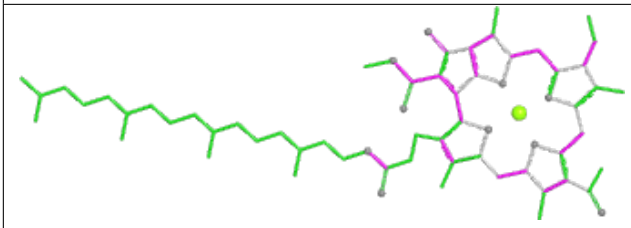
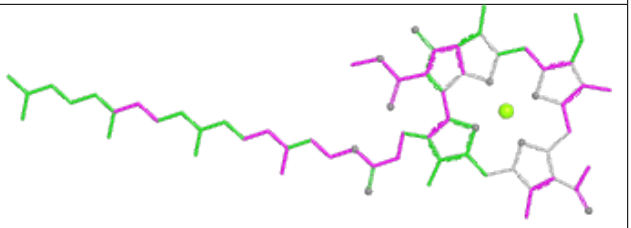
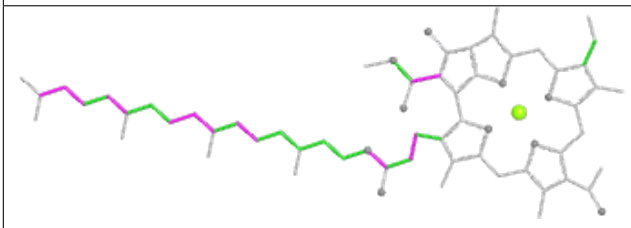
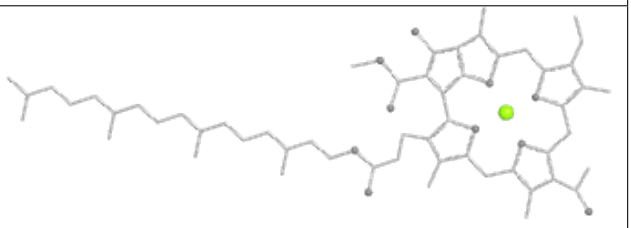
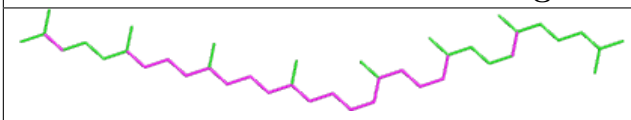
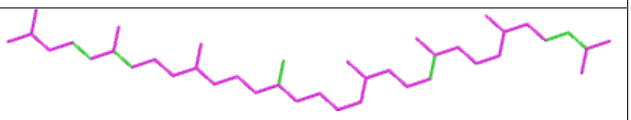
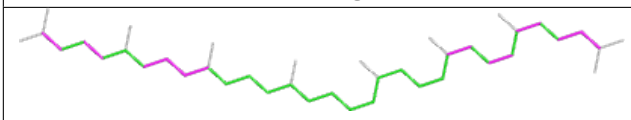
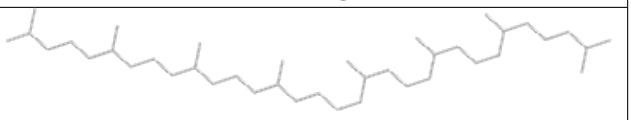
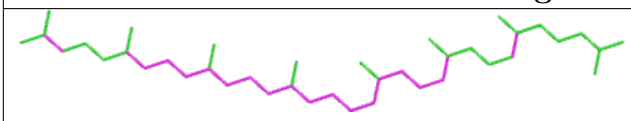
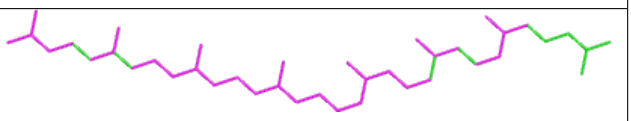
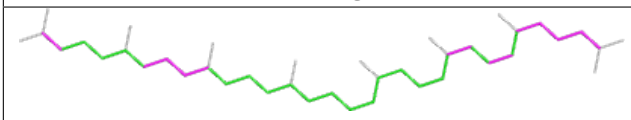
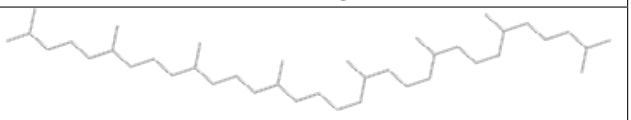
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NS0 c 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NS0 r 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

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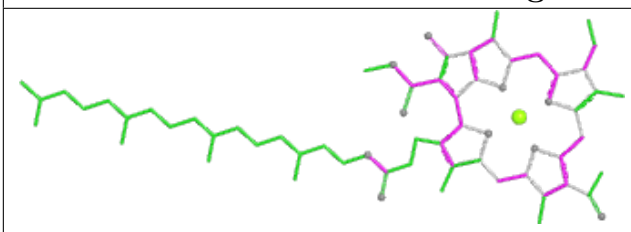
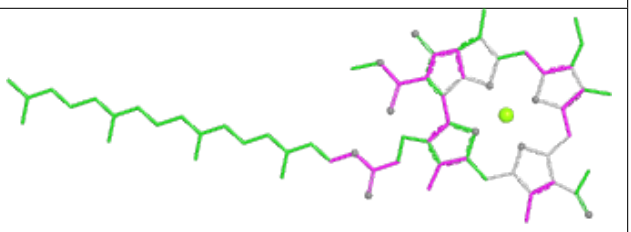
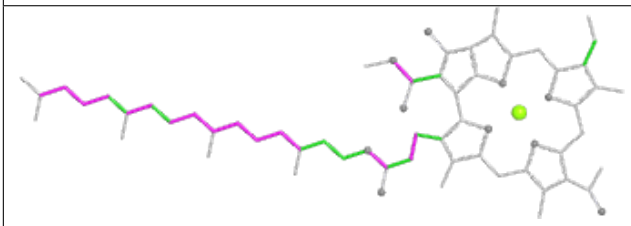
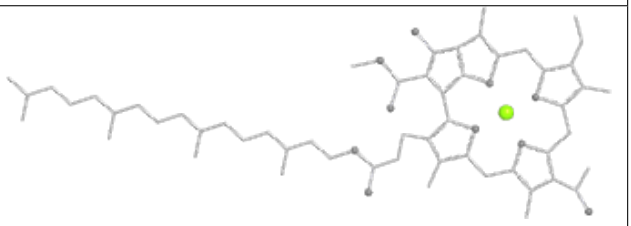
 Bond lengths	 Bond angles
 Torsions	 Rings

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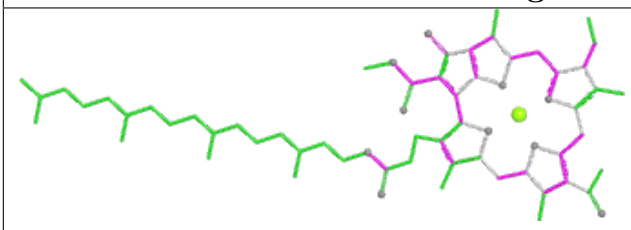

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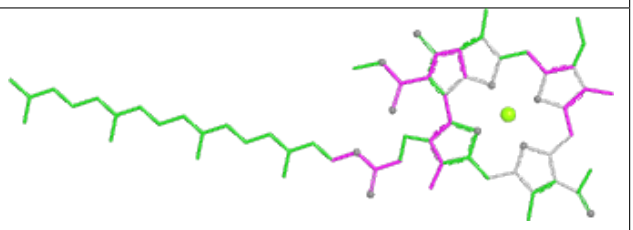

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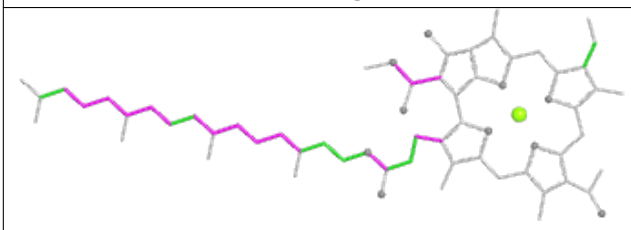

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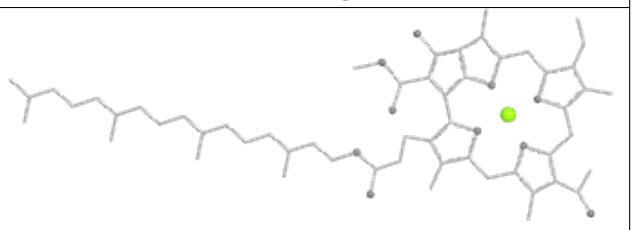

Rings

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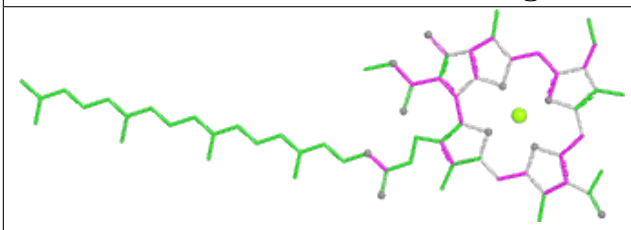

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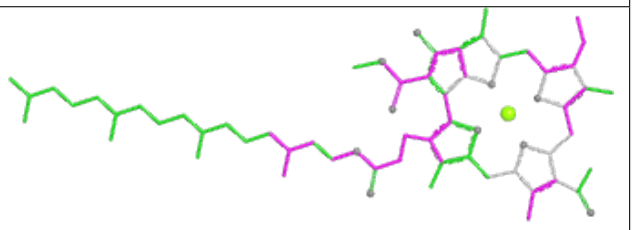

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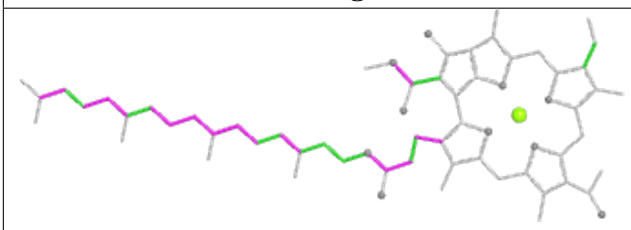

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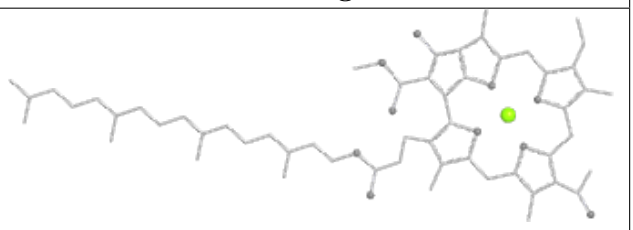

Rings

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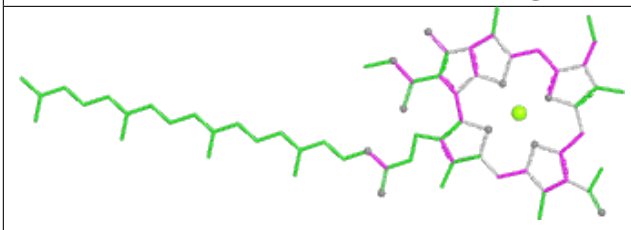

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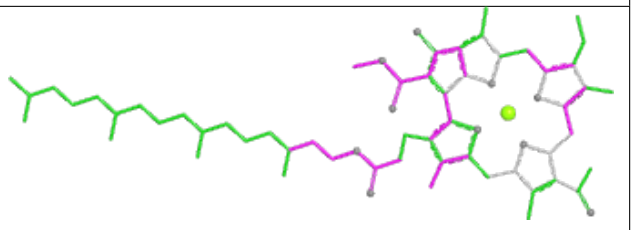

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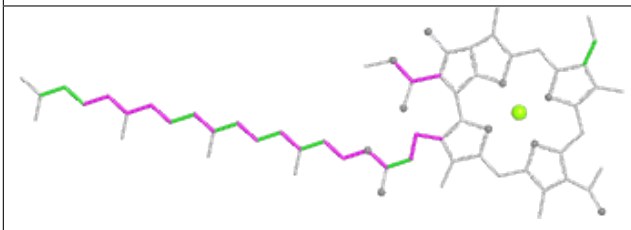

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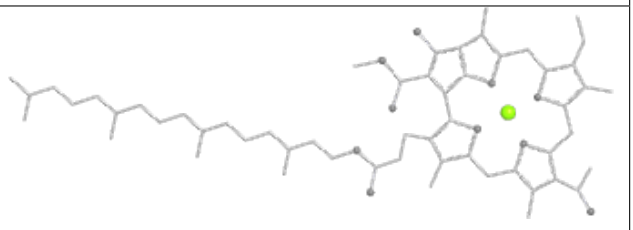

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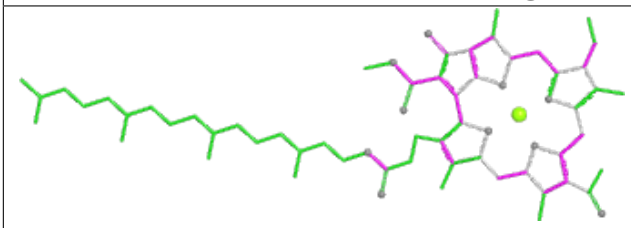
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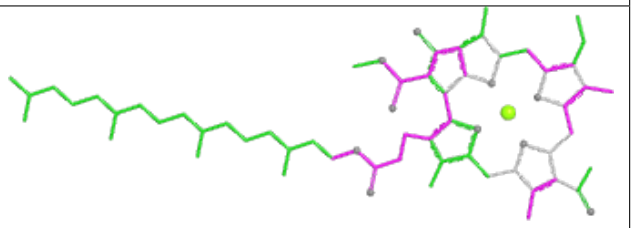
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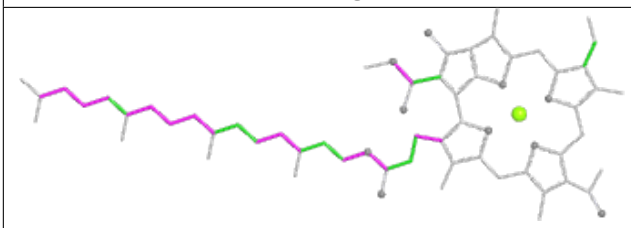
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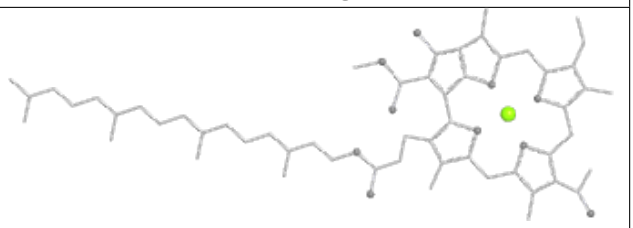
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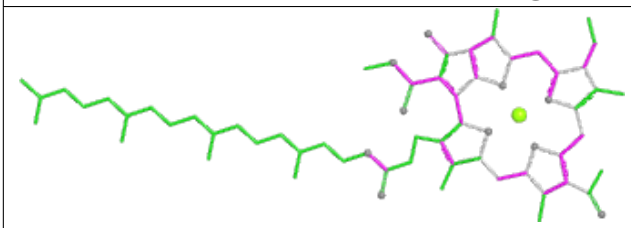
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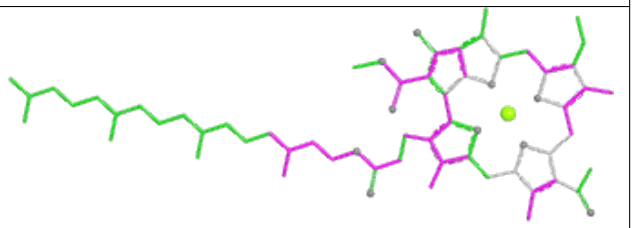
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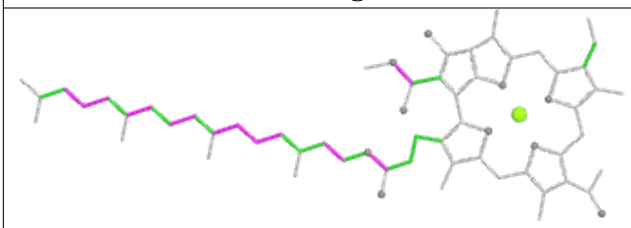
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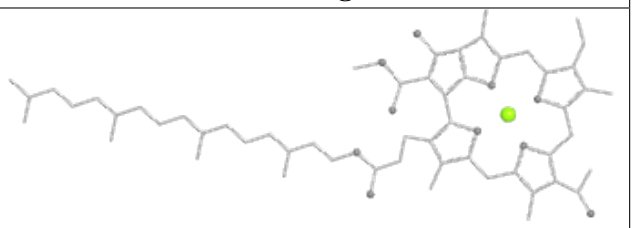
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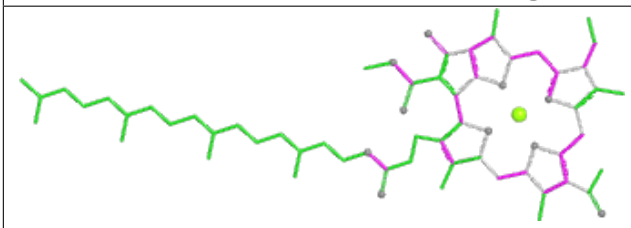
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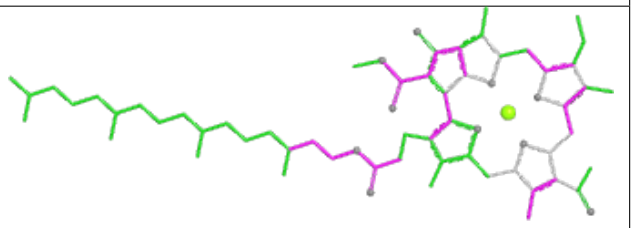
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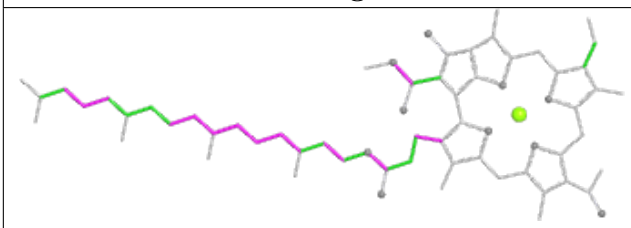
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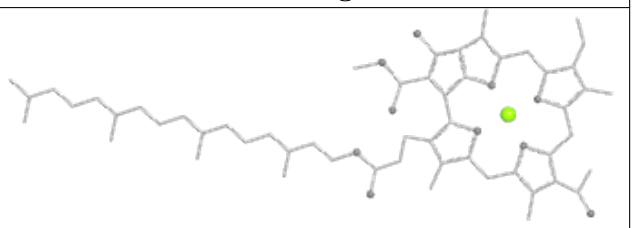
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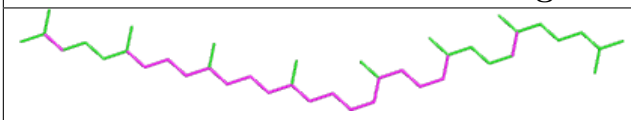
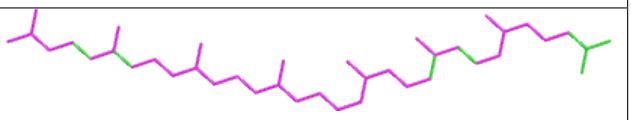
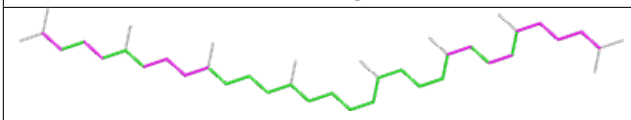
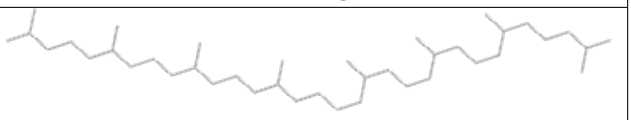
 Bond lengths	 Bond angles
 Torsions	 Rings

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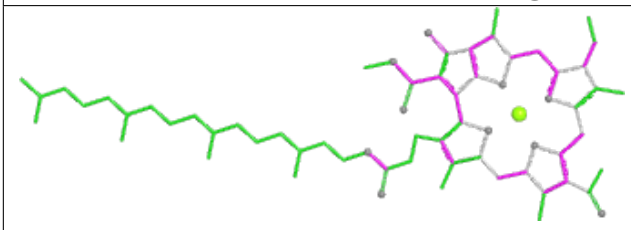
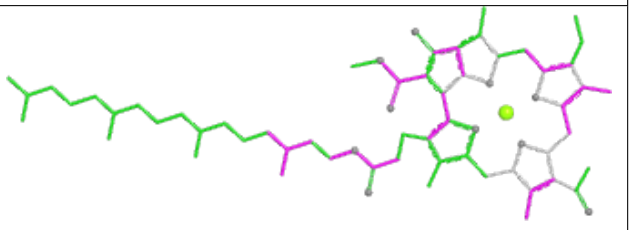
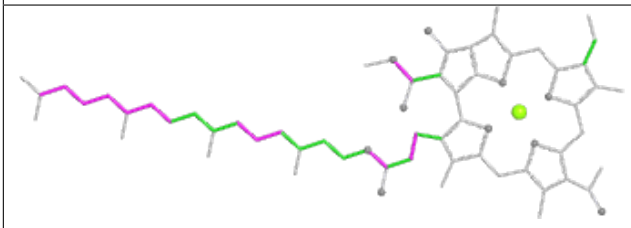
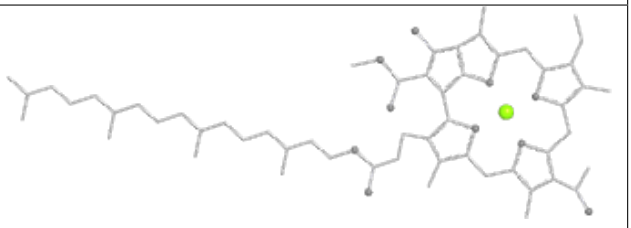
 Bond lengths	 Bond angles
 Torsions	 Rings

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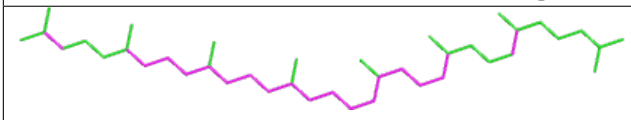
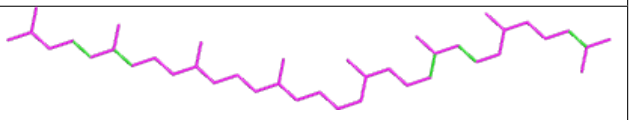
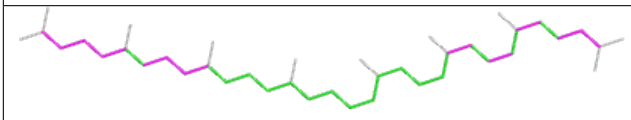
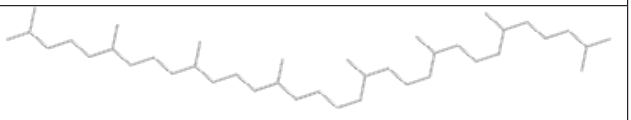
 Bond lengths	 Bond angles
 Torsions	 Rings

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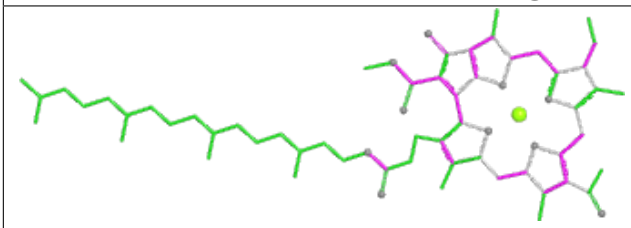
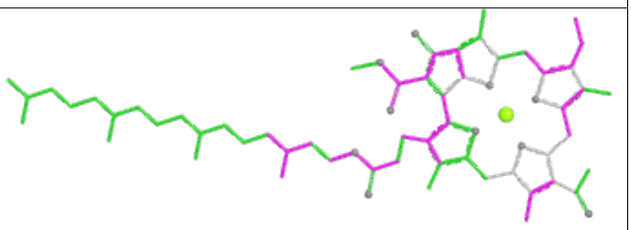
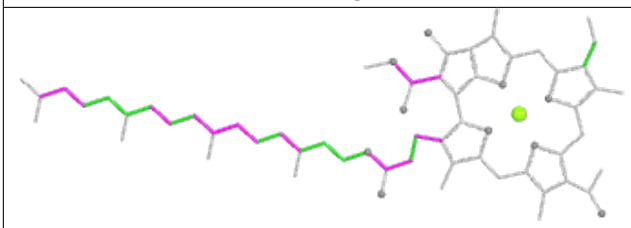
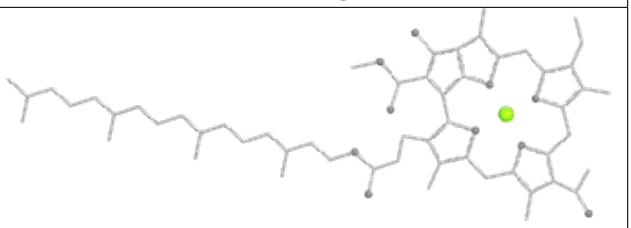
 Bond lengths	 Bond angles
 Torsions	 Rings

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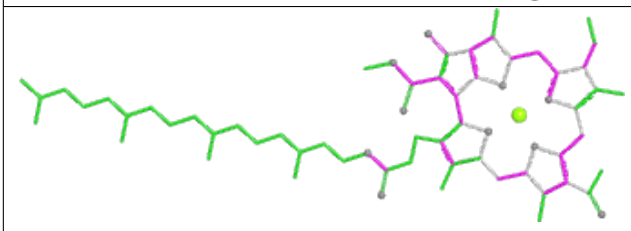
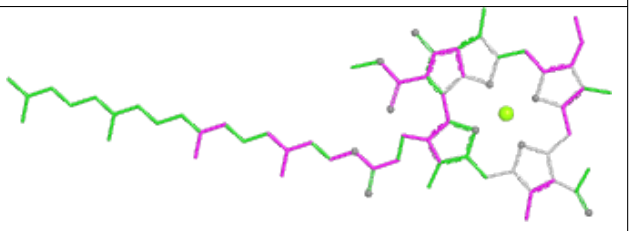
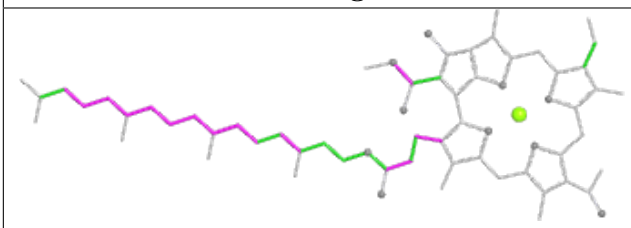
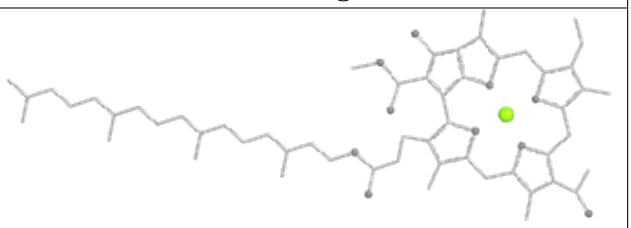
 Bond lengths	 Bond angles
 Torsions	 Rings

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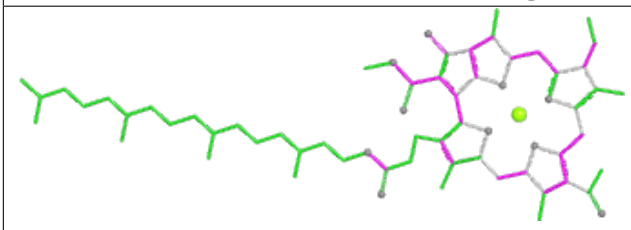
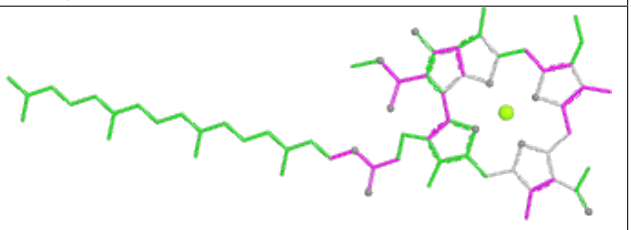
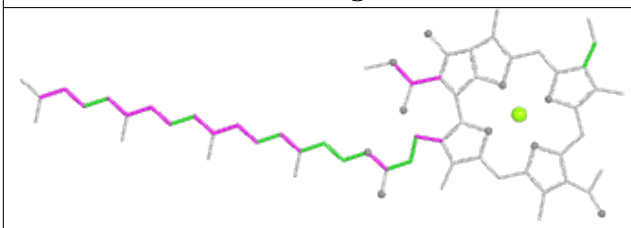
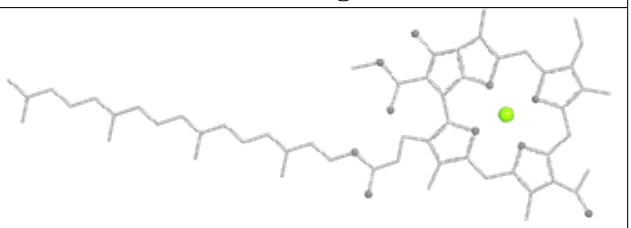
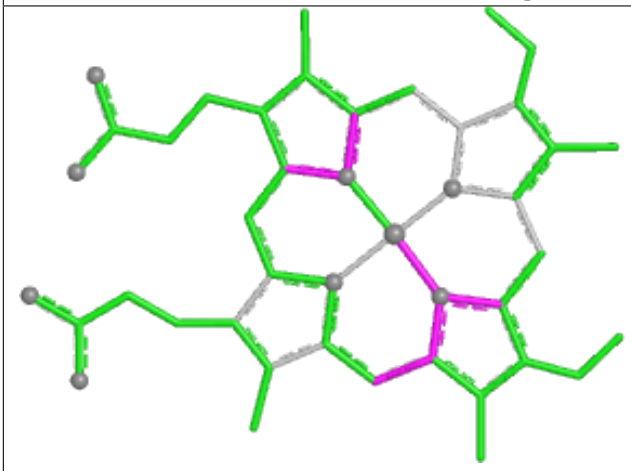
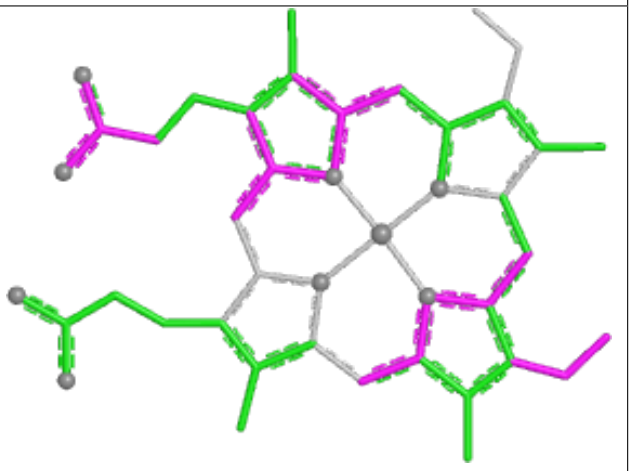
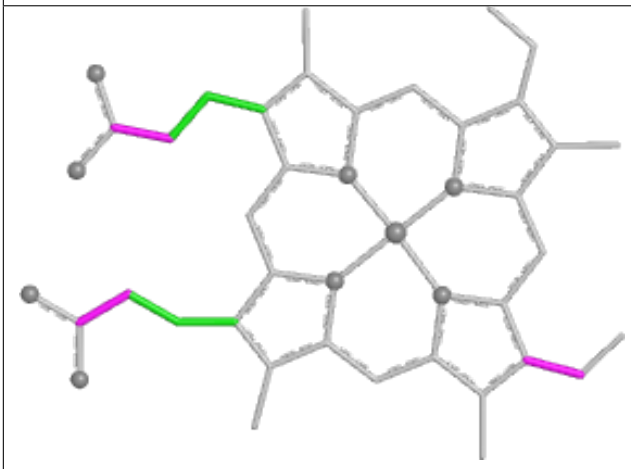
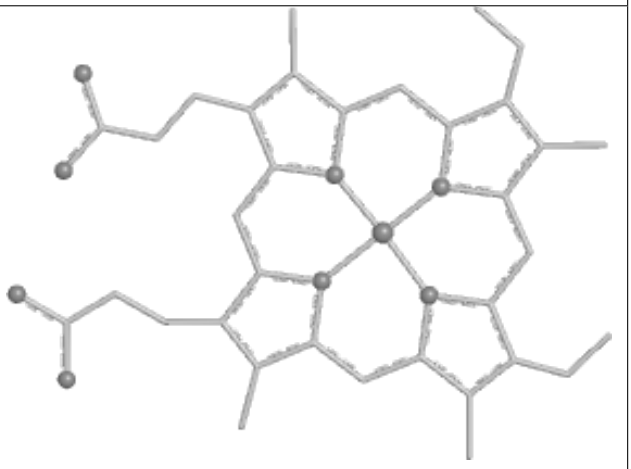
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HEM C 403	
	
Bond lengths	Bond angles
	
Torsions	Rings

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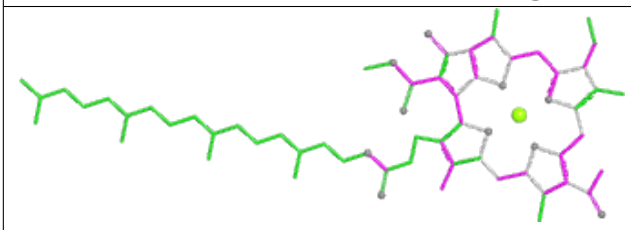	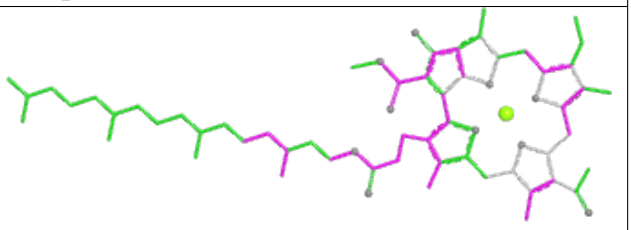
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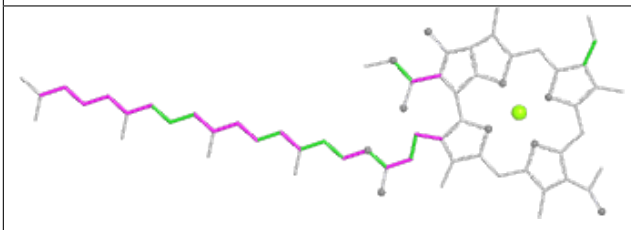	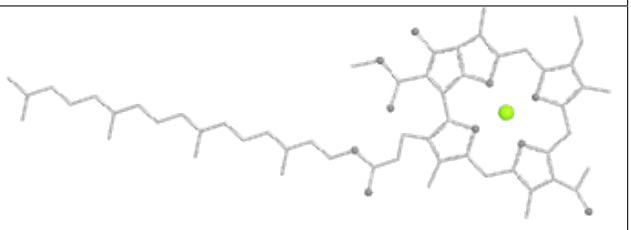
Torsions	Rings

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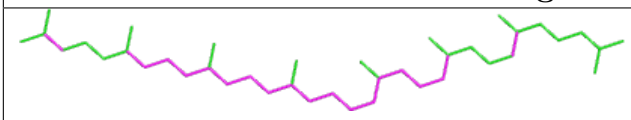
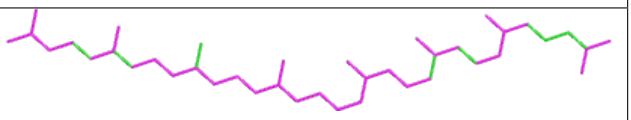
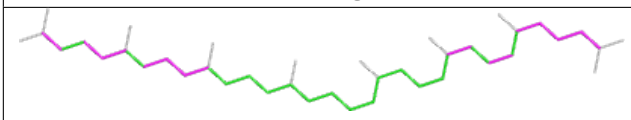
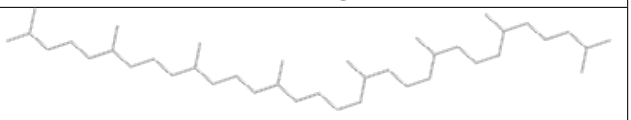
 Bond lengths	 Bond angles
 Torsions	 Rings

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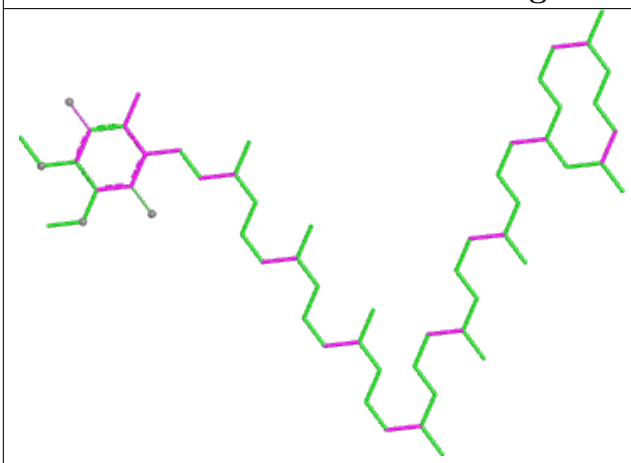
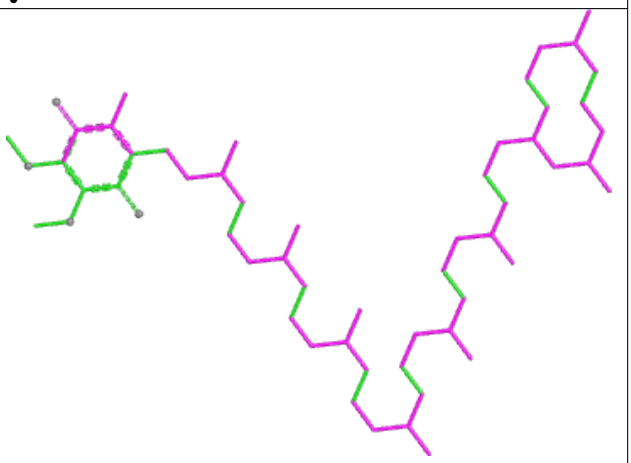
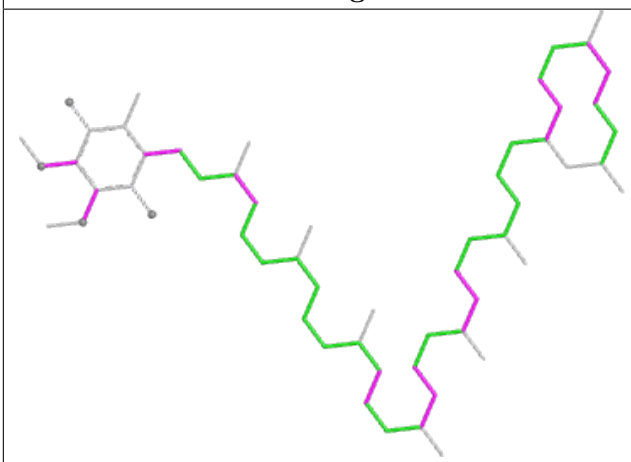
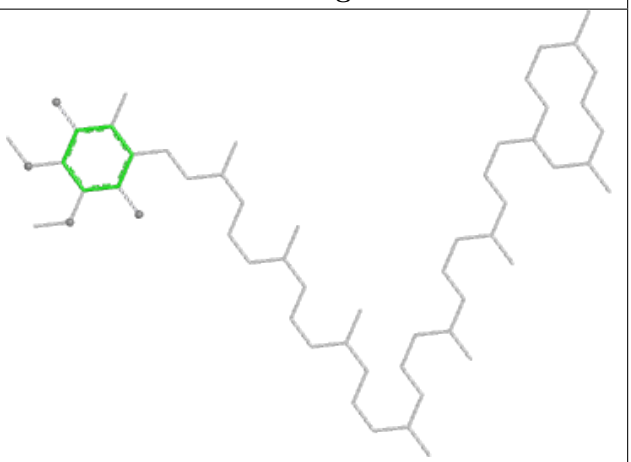
 Bond lengths	 Bond angles
 Torsions	 Rings

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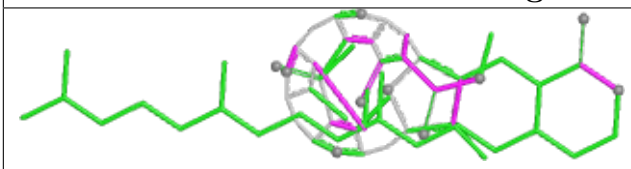
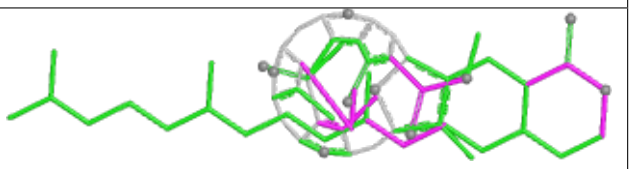
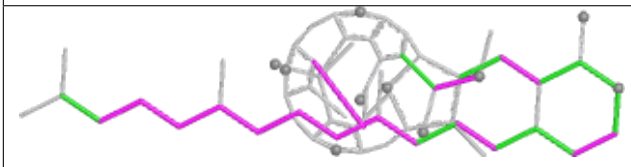
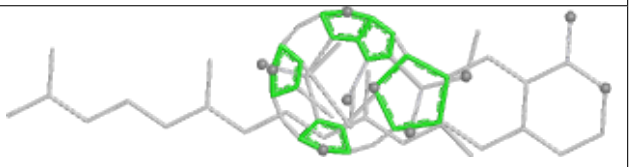
 Bond lengths	 Bond angles
 Torsions	 Rings

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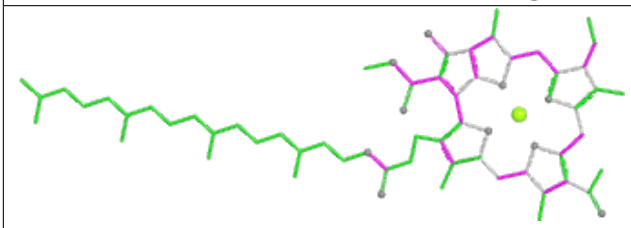
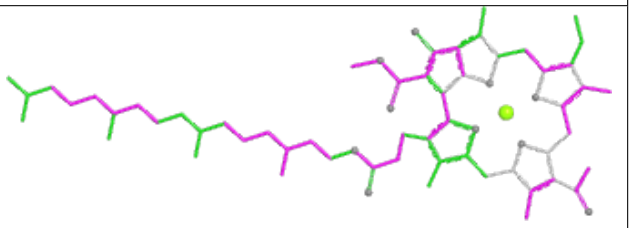
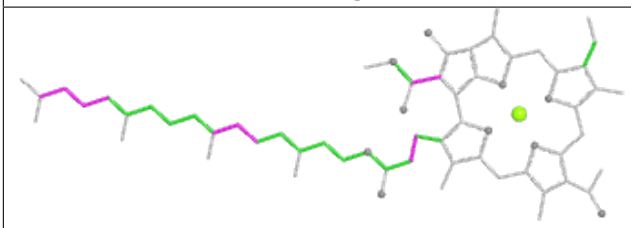
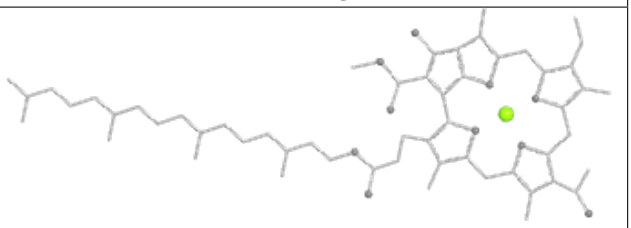
 Bond lengths	 Bond angles
 Torsions	 Rings

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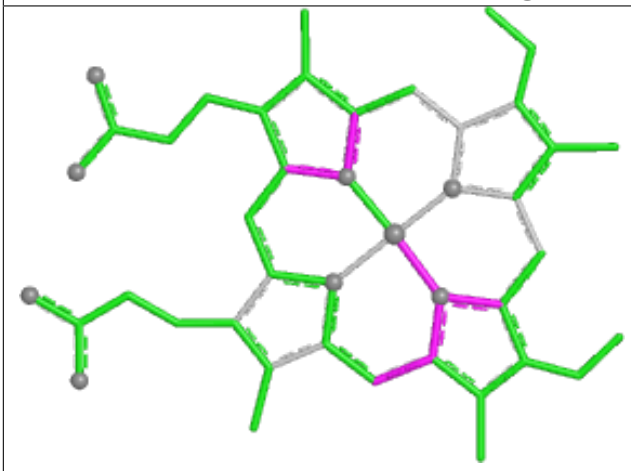
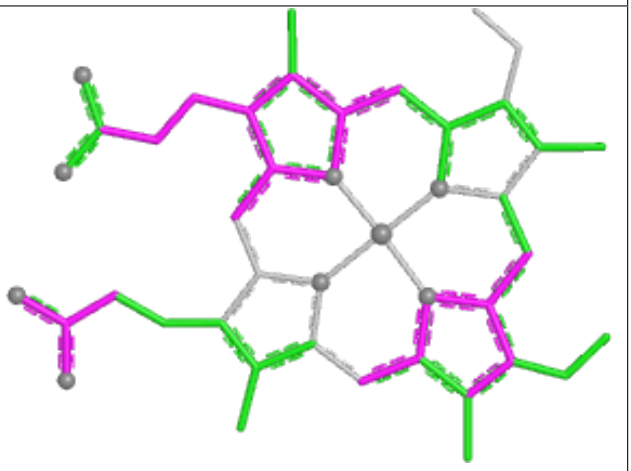
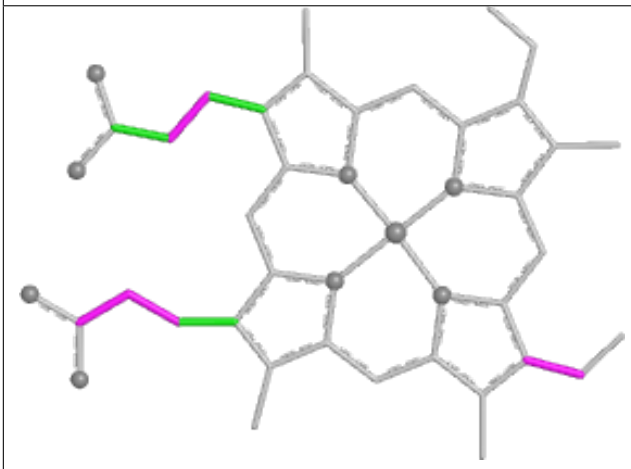
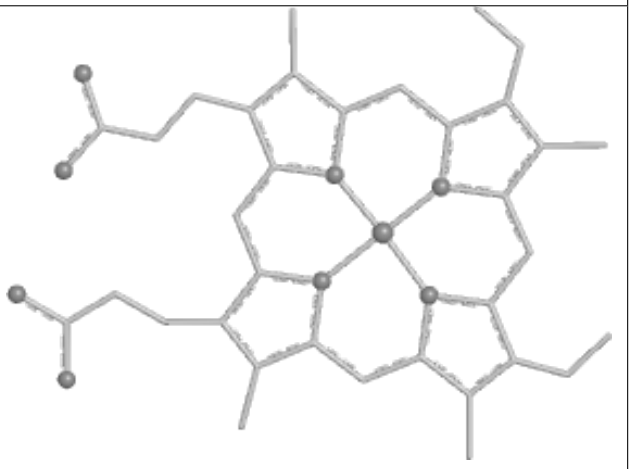
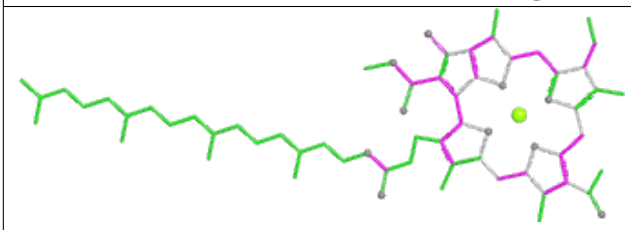
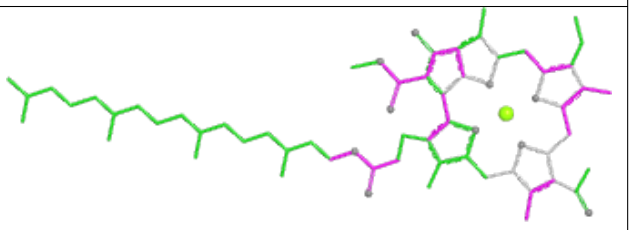
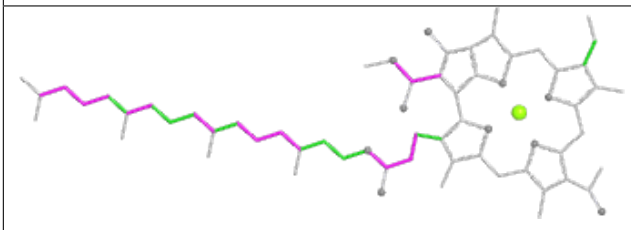
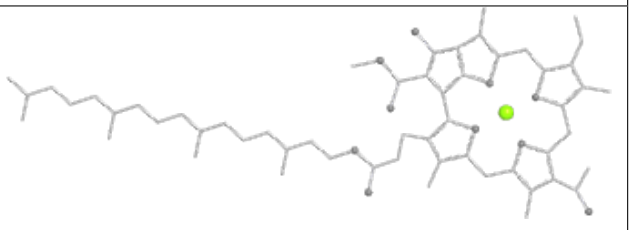
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCB c 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

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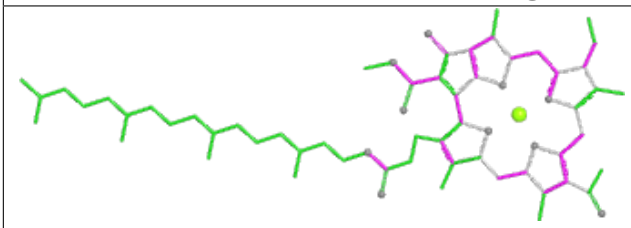
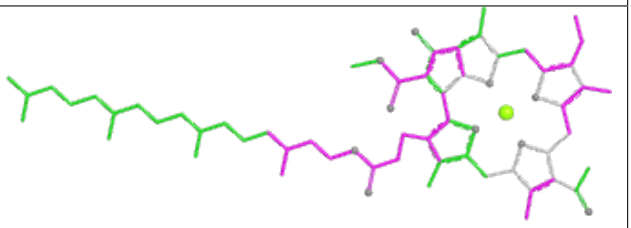
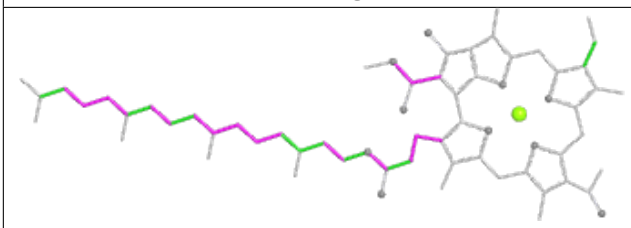
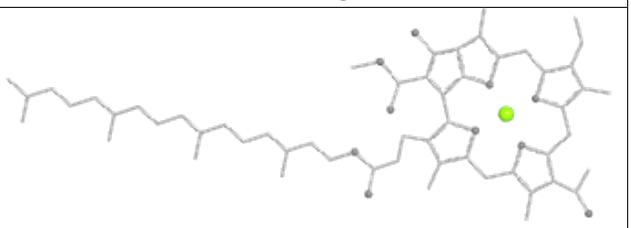
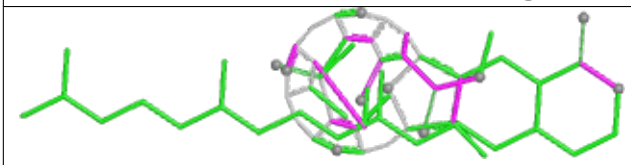
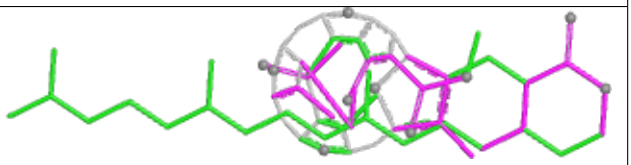
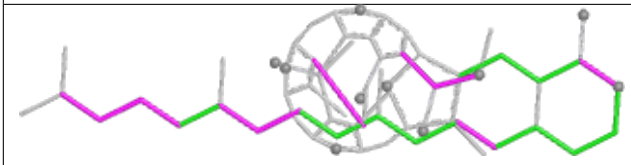
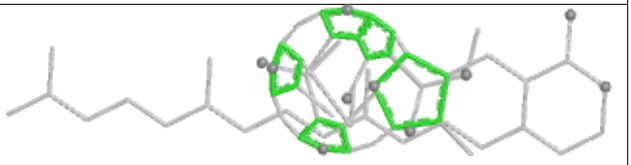
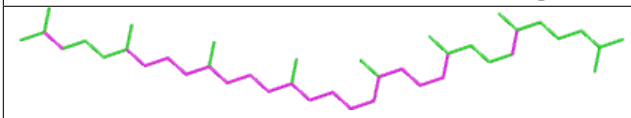
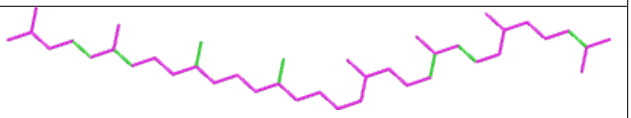
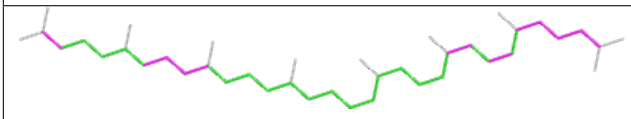
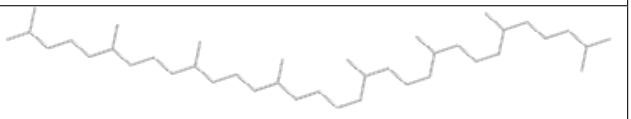
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BPB M 407	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NS0 4 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

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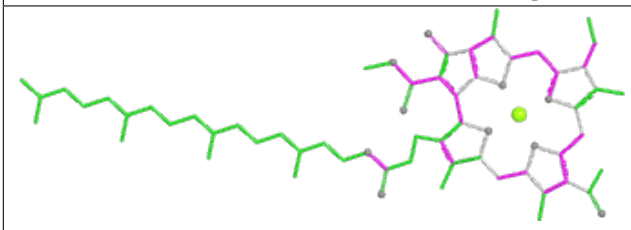
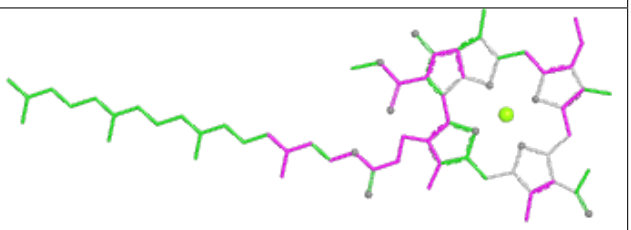
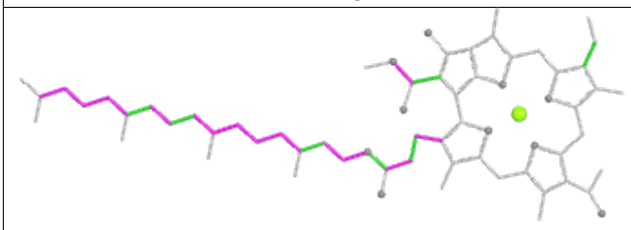
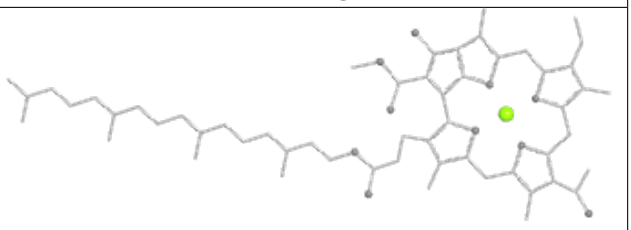
 Bond lengths	 Bond angles
 Torsions	 Rings

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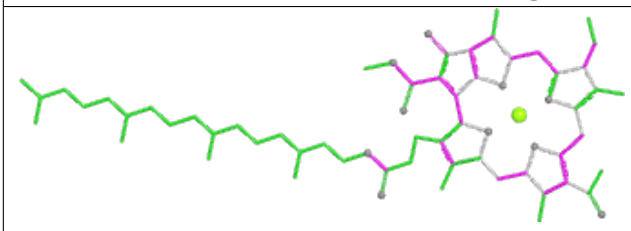
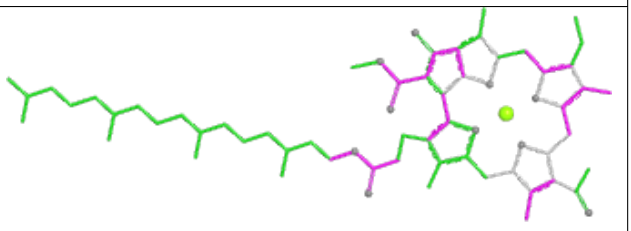
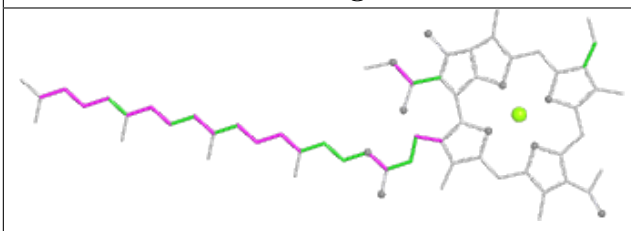
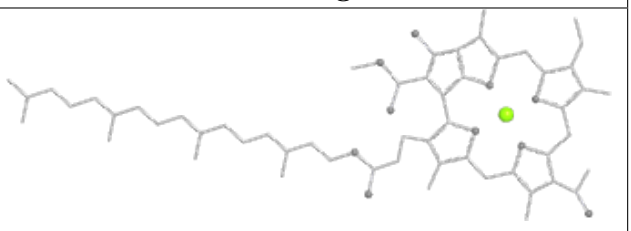
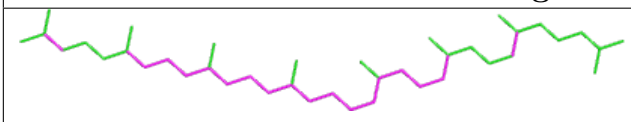
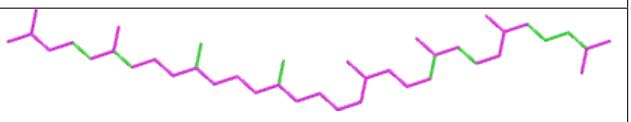
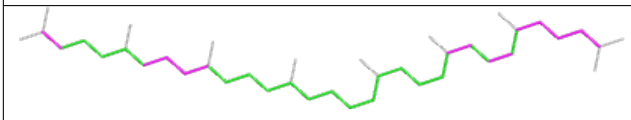
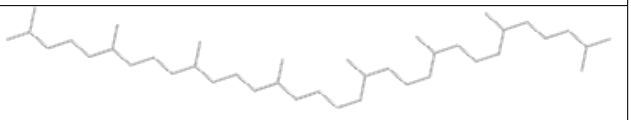
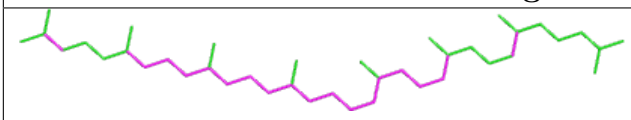
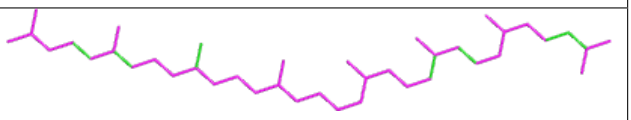
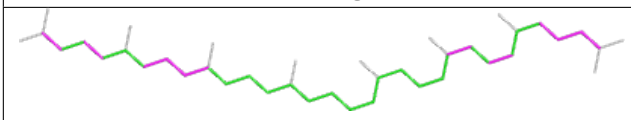
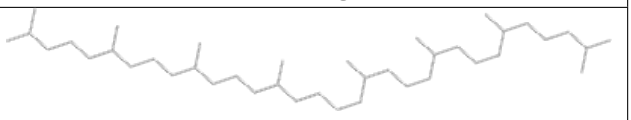
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NS0 x 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NS0 W 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

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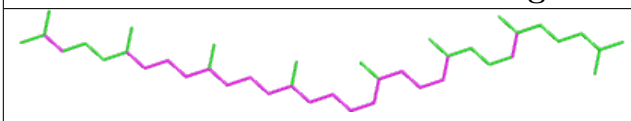
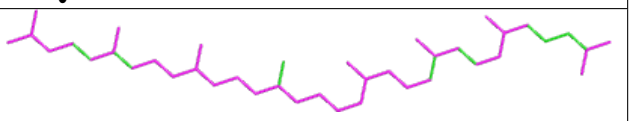
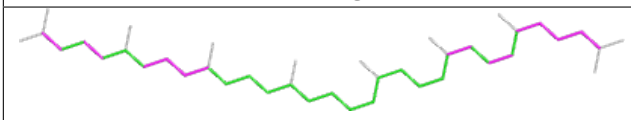
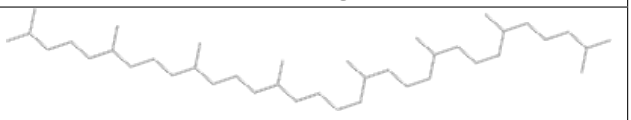
 Bond lengths	 Bond angles
 Torsions	 Rings

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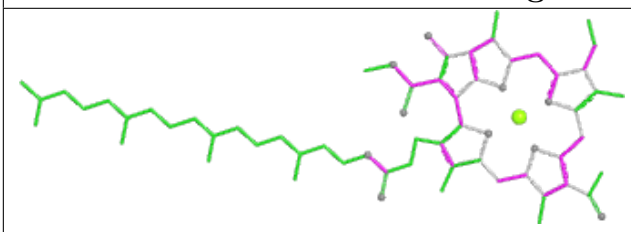
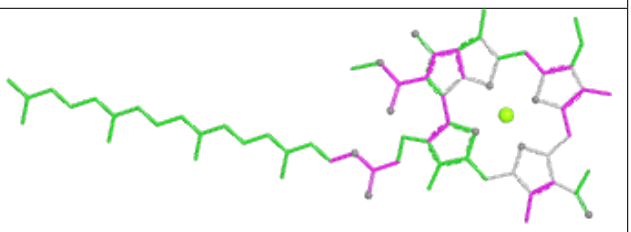
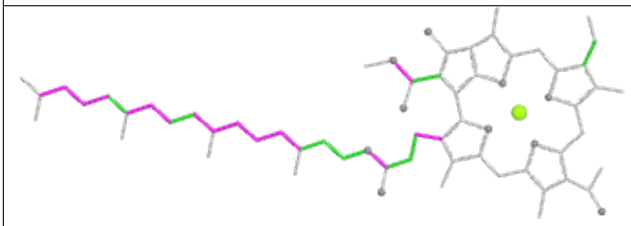
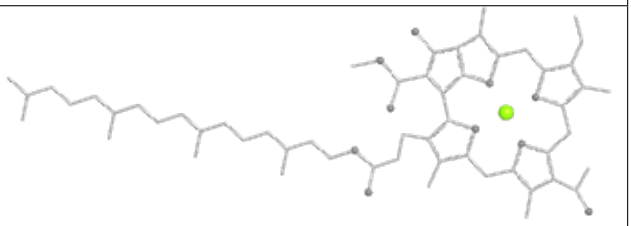
 Bond lengths	 Bond angles
 Torsions	 Rings

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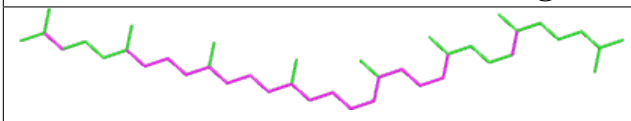
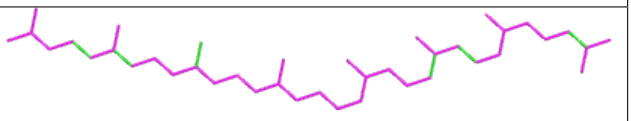
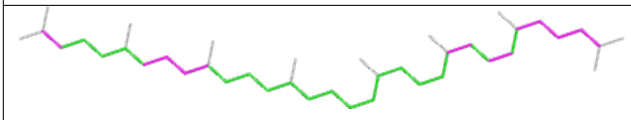
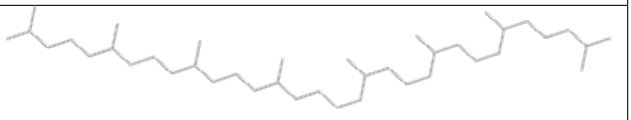
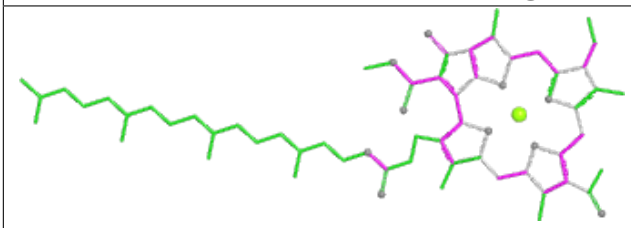
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCB N 101



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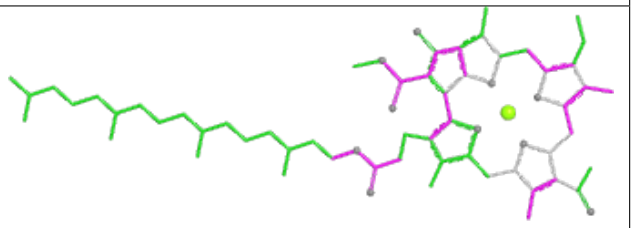

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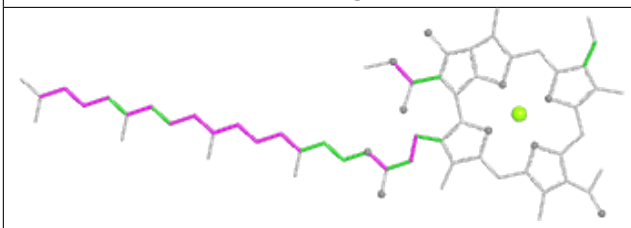

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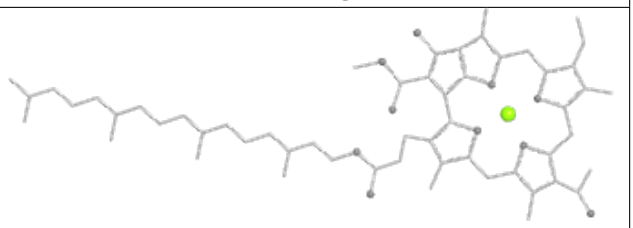
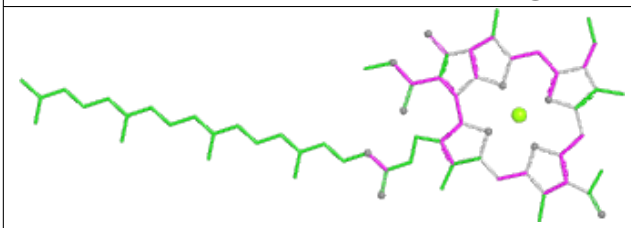


Rings

Ligand BCB x 101



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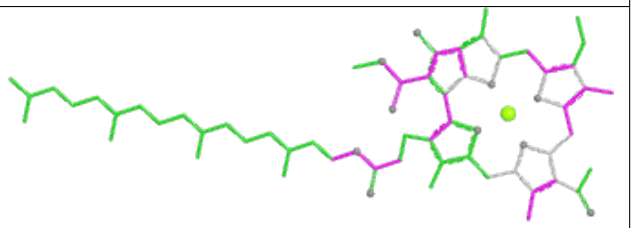

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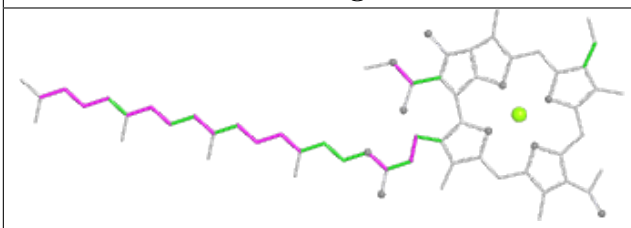

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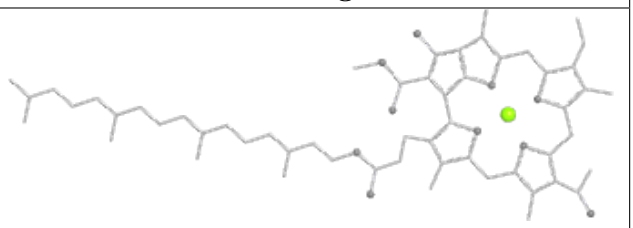
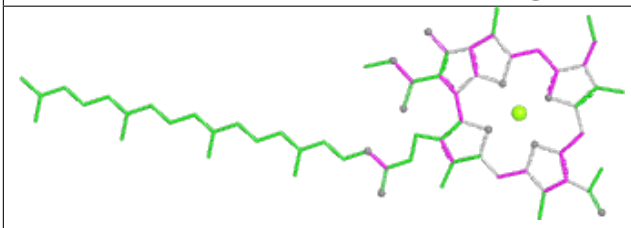


Rings

Ligand BCB 3 101



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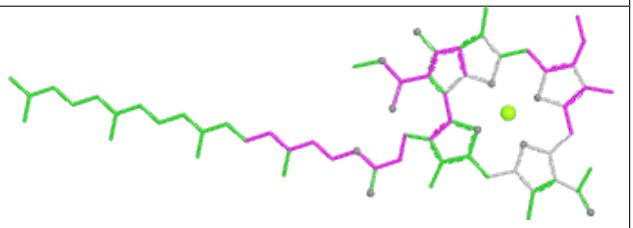

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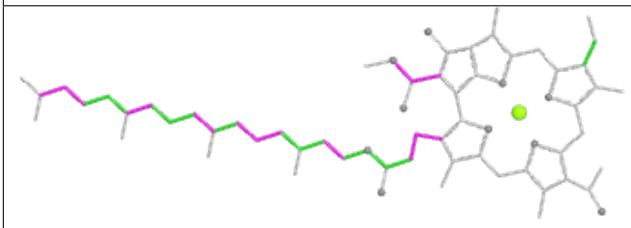

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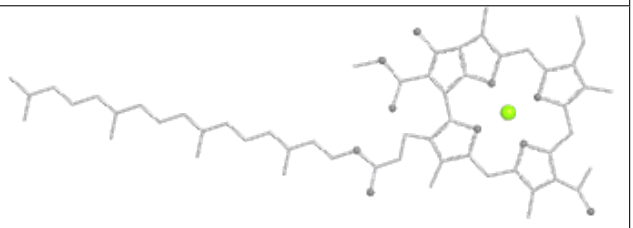

Rings

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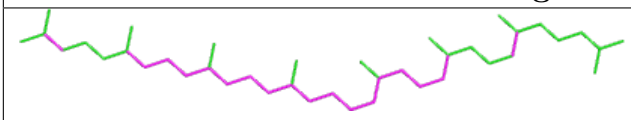
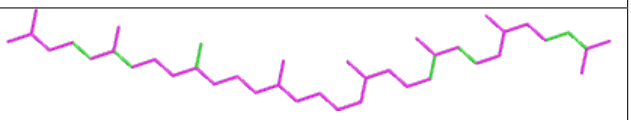
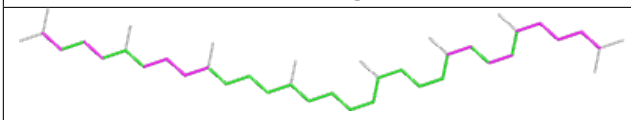
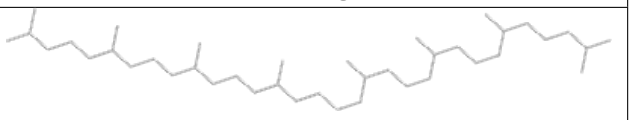
 Bond lengths	 Bond angles
 Torsions	 Rings

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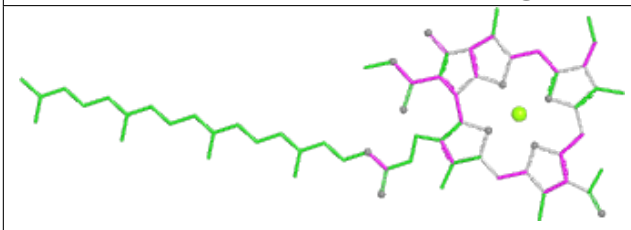
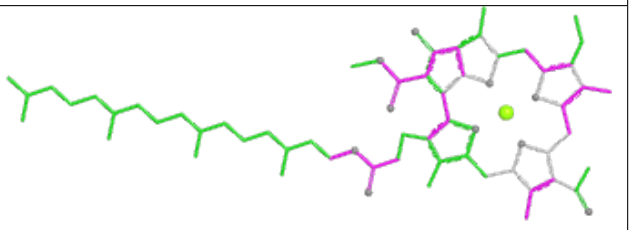
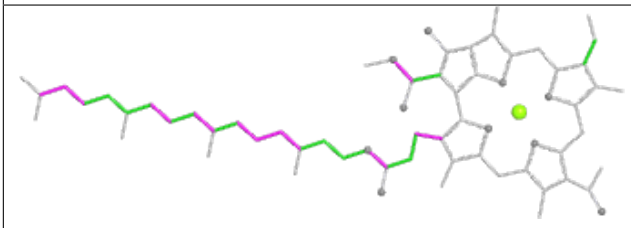
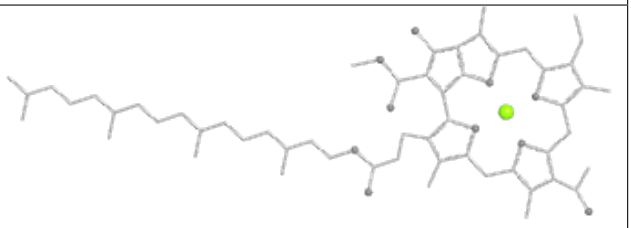
 Bond lengths	 Bond angles
 Torsions	 Rings

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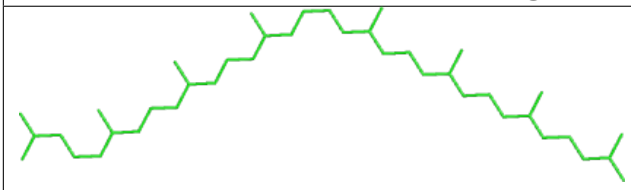
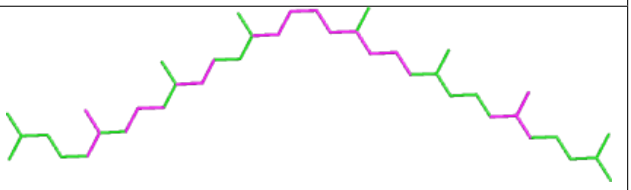
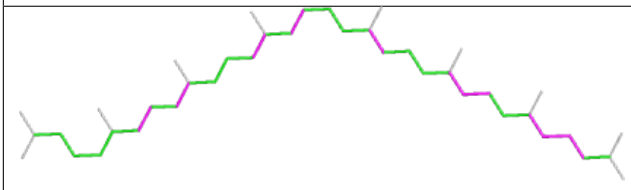
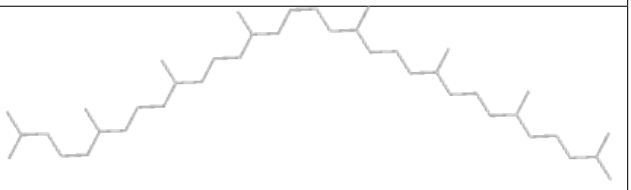
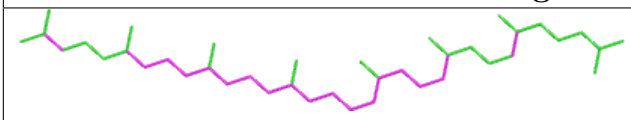
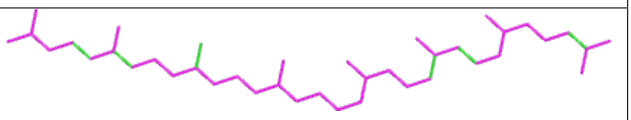
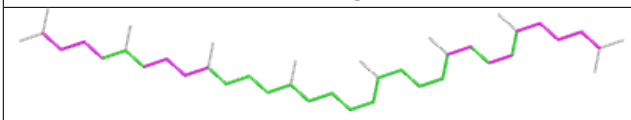
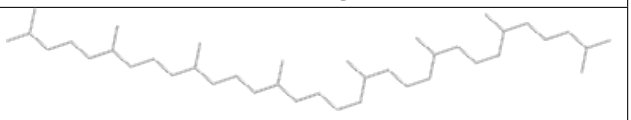
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NS0 1 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

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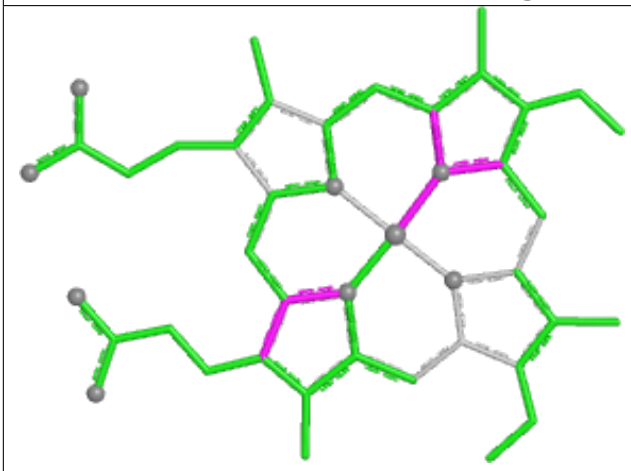
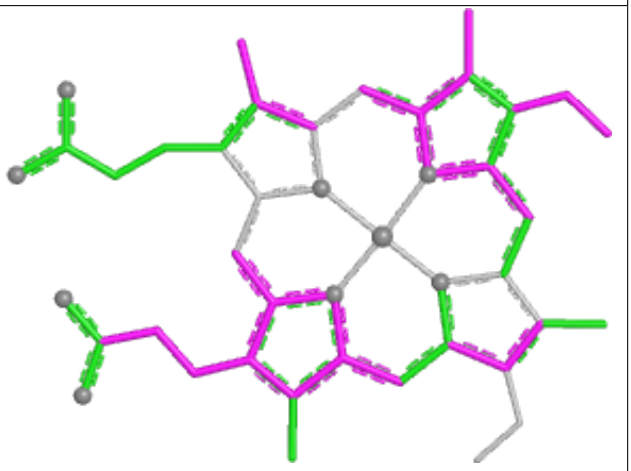
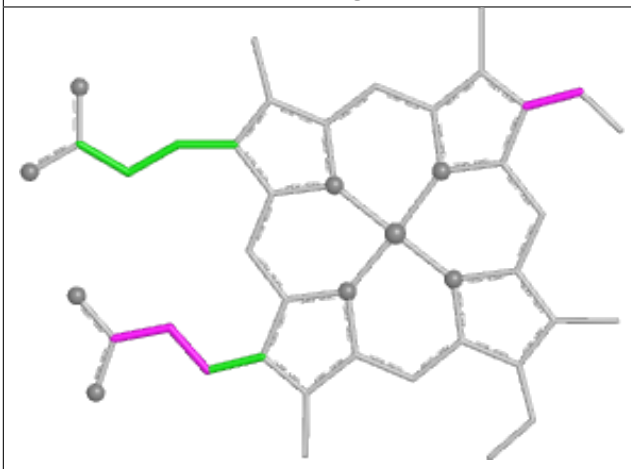
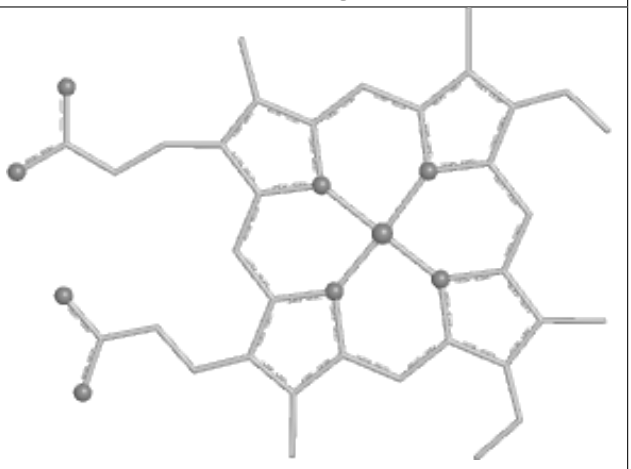
 Bond lengths	 Bond angles
 Torsions	 Rings

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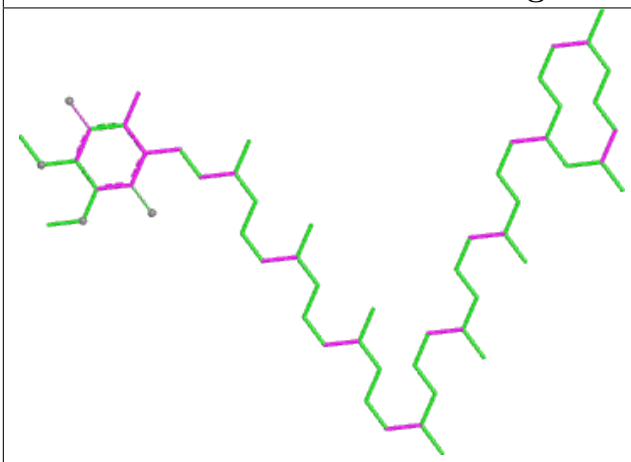
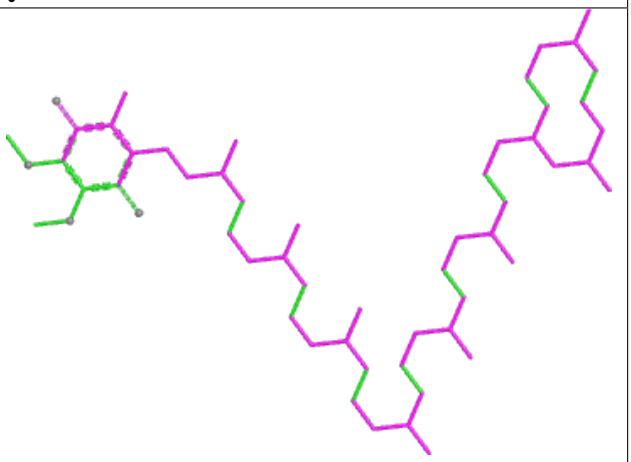
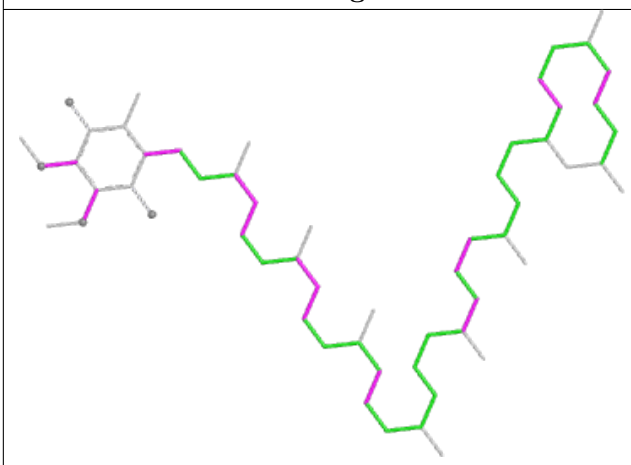
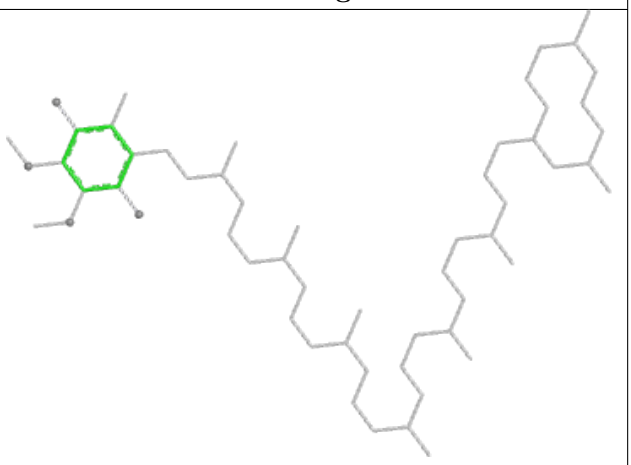
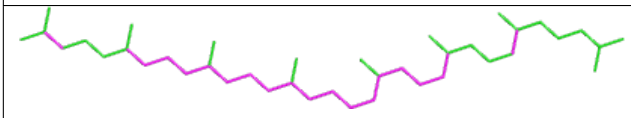
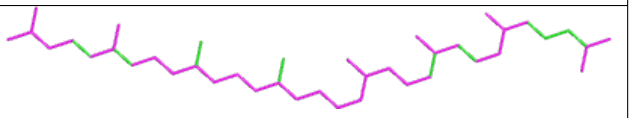
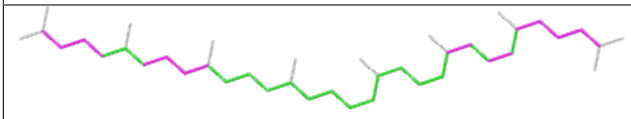
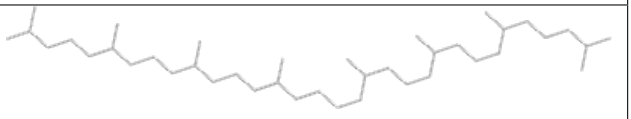
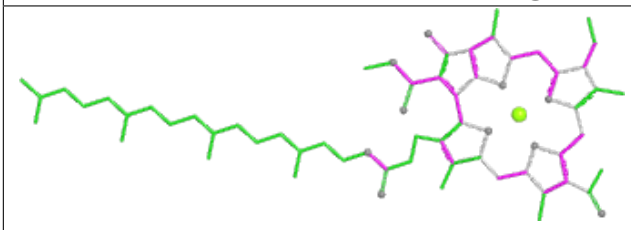
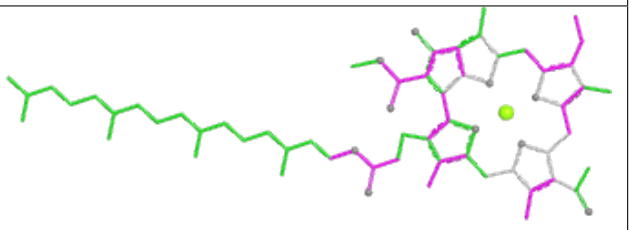
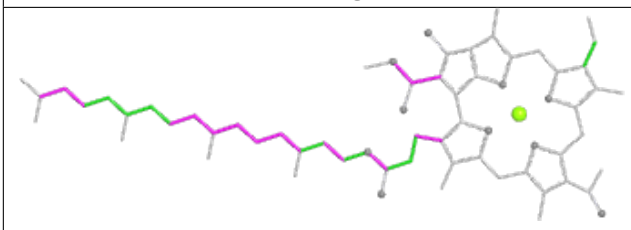
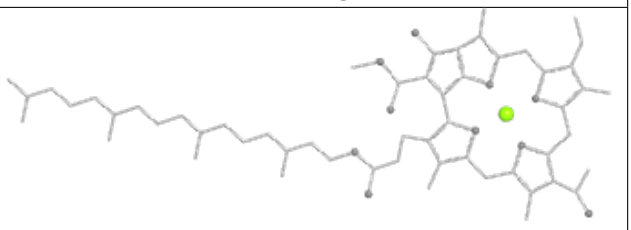
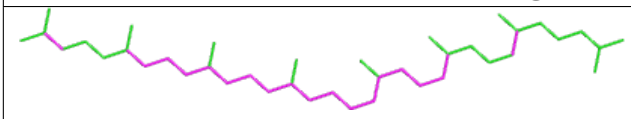
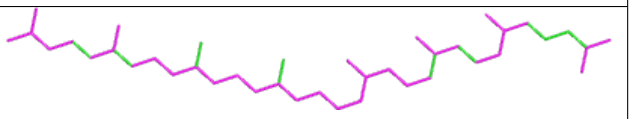
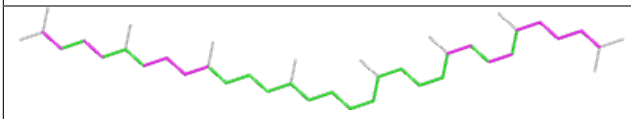
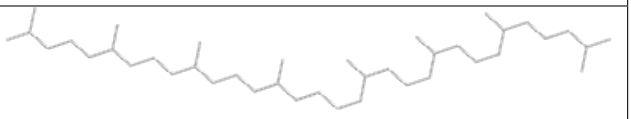
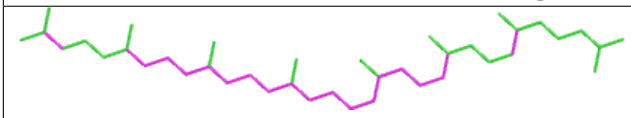
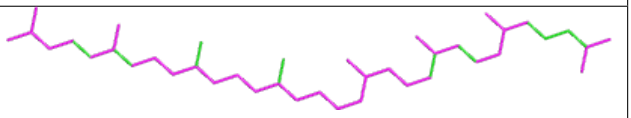
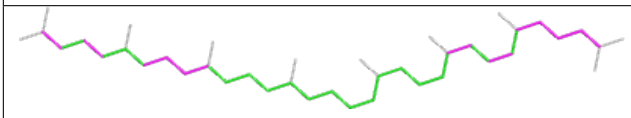
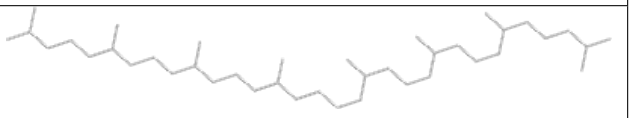
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NS0 T 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCB k 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NS0 N 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NS0 u 102	
 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)

The following chains have linkage breaks:

Continued on next page...

Continued from previous page...

Mol	Chain	Number of breaks

Mol	Chain	Number of breaks
4	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	53:ALA	C	54:PRO	N	3.10

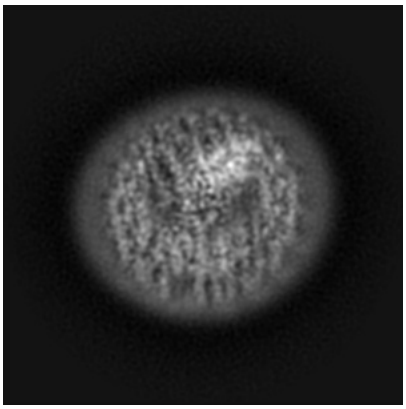
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-3951. These allow visual inspection of the internal detail of the map and identification of artifacts.

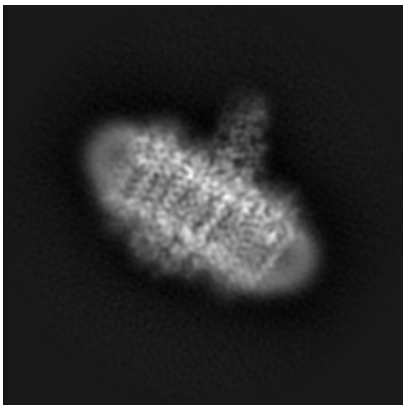
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

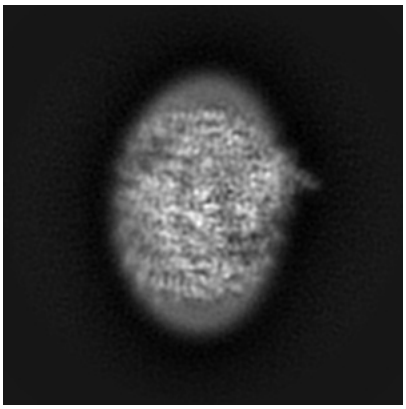
6.1.1 Primary map



X

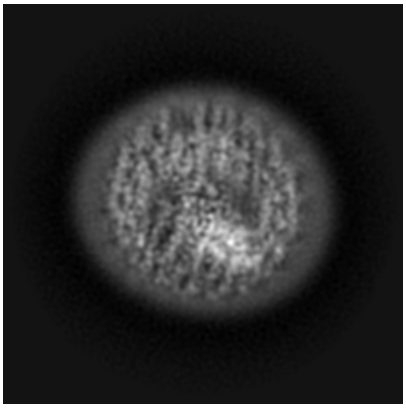


Y

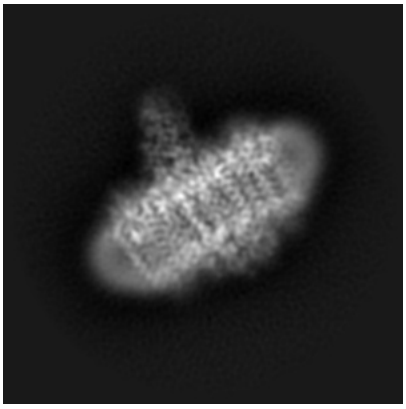


Z

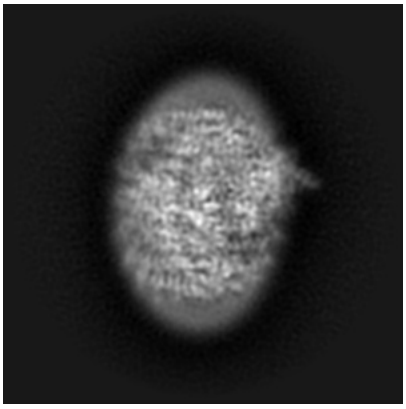
6.1.2 Raw map



X



Y

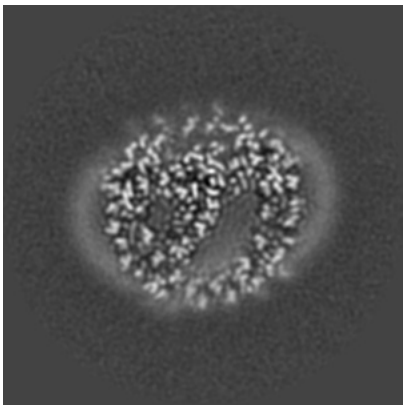


Z

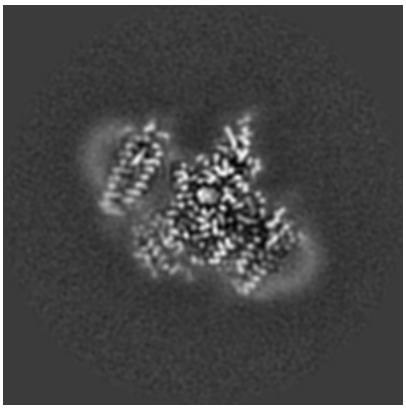
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

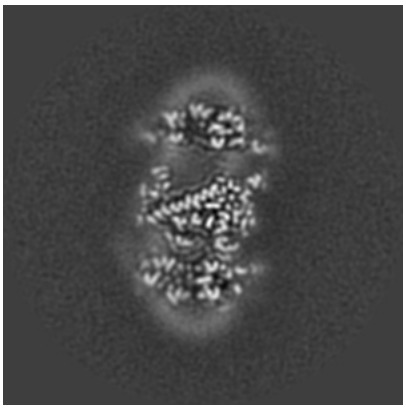
6.2.1 Primary map



X Index: 115

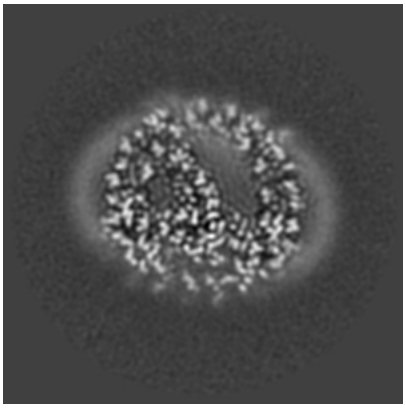


Y Index: 115

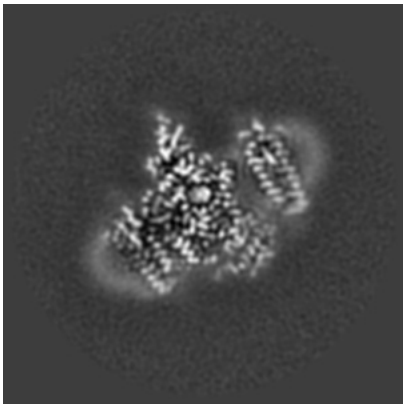


Z Index: 115

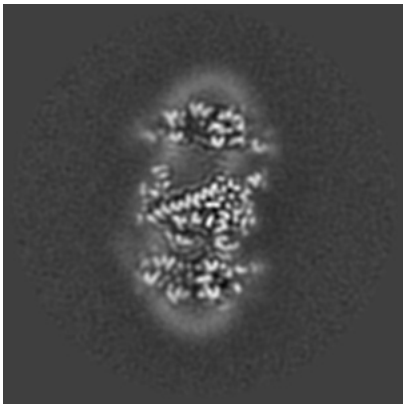
6.2.2 Raw map



X Index: 115



Y Index: 115

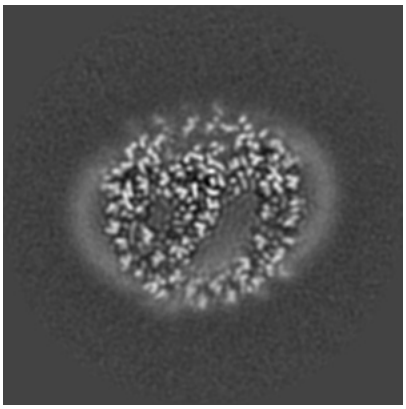


Z Index: 115

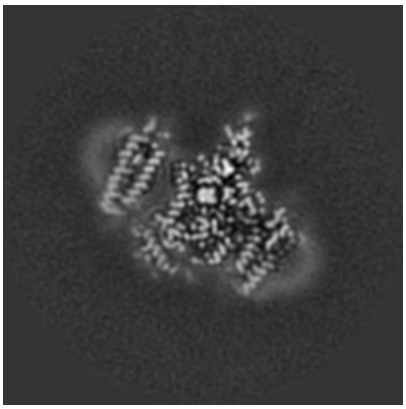
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

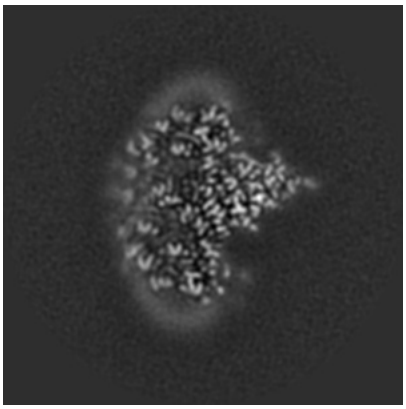
6.3.1 Primary map



X Index: 115

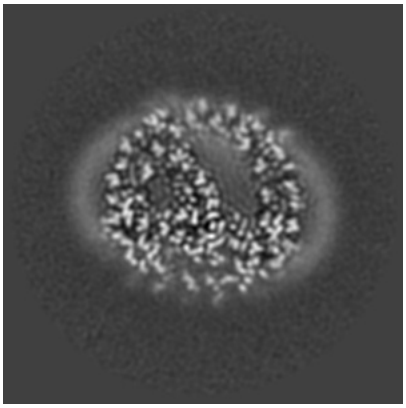


Y Index: 114

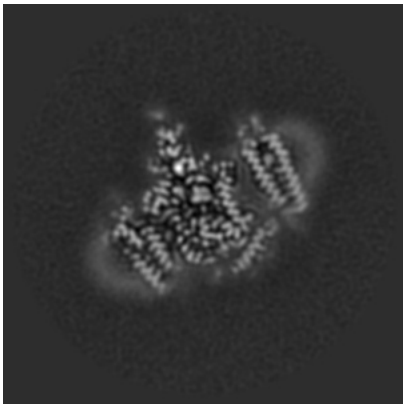


Z Index: 131

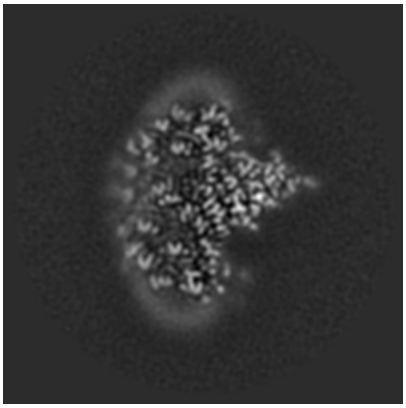
6.3.2 Raw map



X Index: 115



Y Index: 113

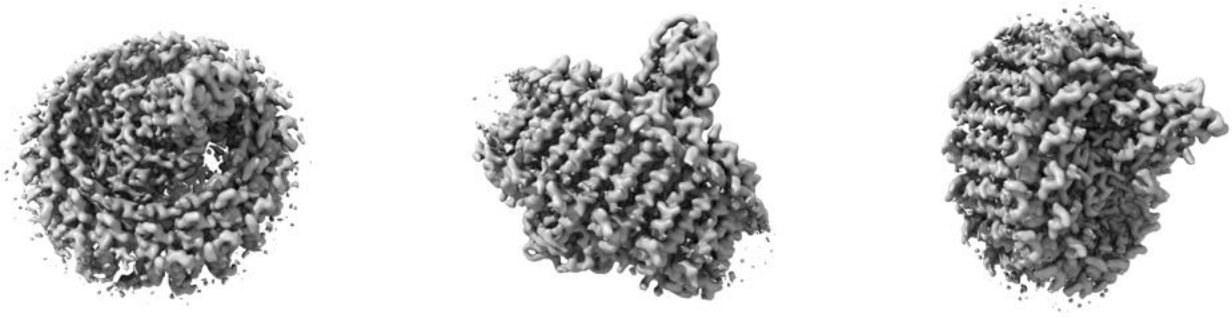


Z Index: 99

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

6.4 Orthogonal surface views (i)

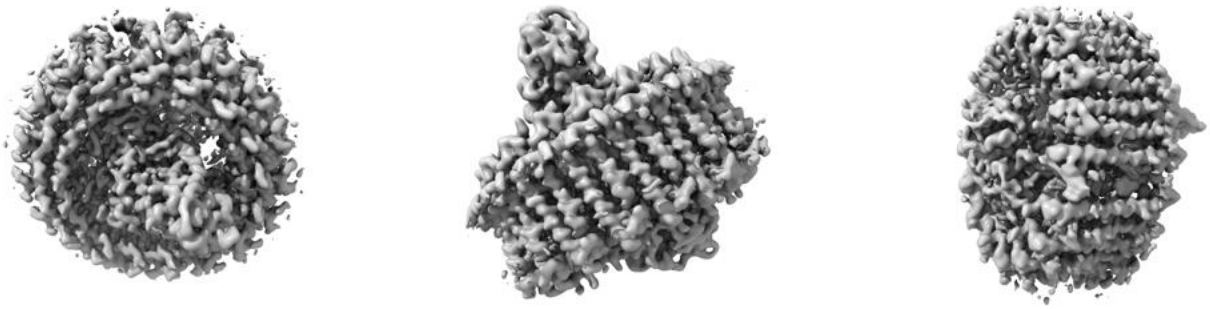
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0156. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

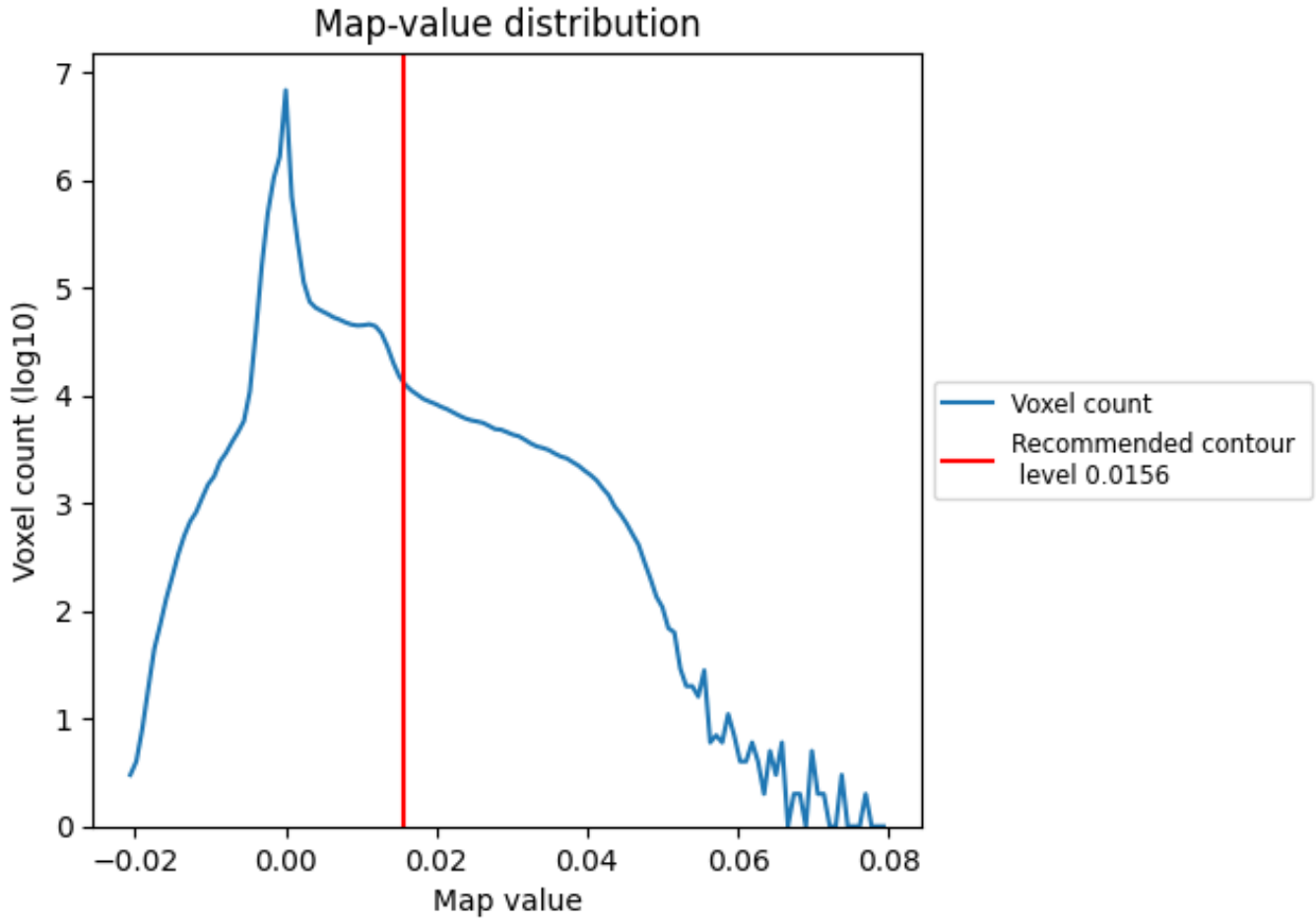
6.5 Mask visualisation (i)

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

7 Map analysis

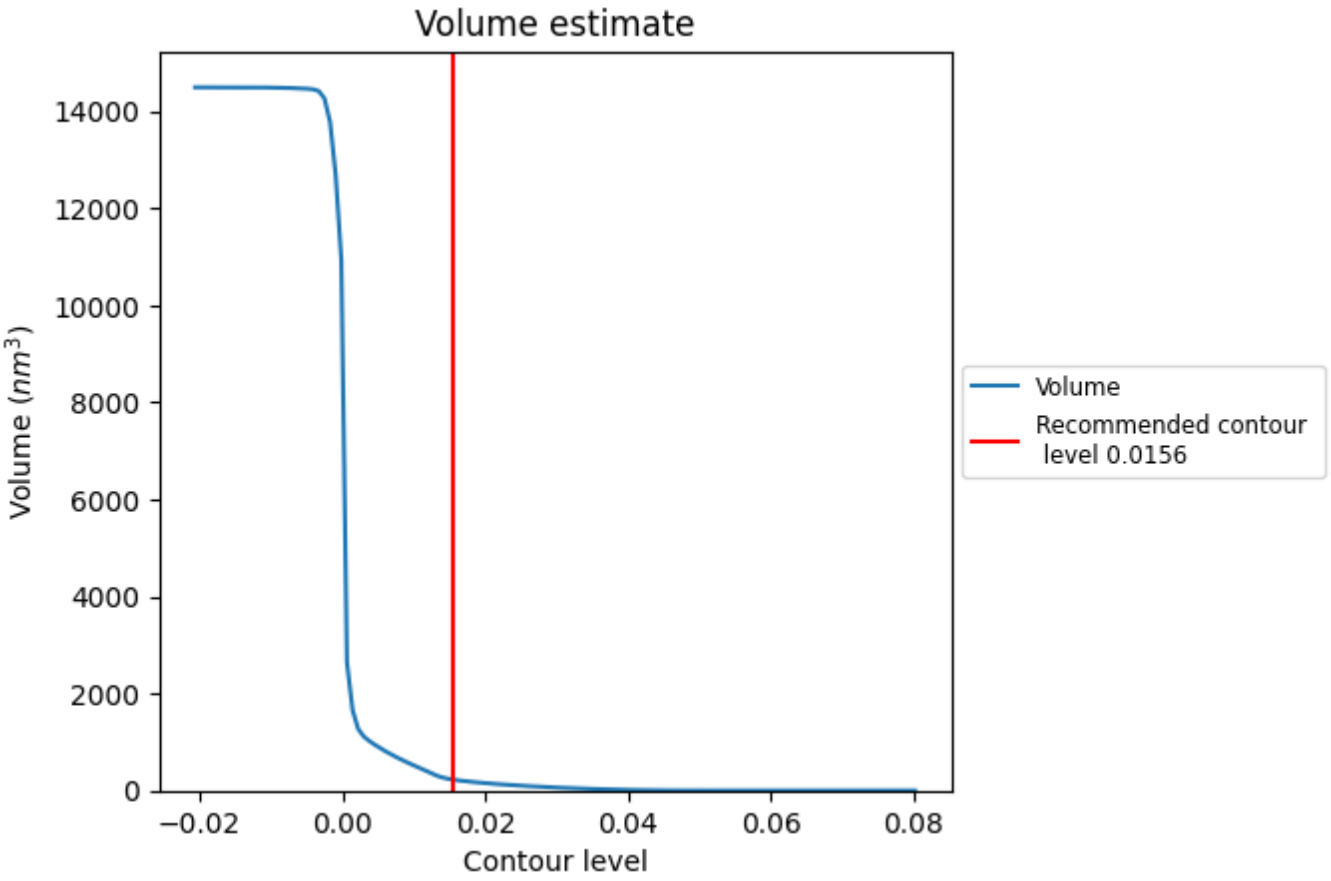
This section contains the results of statistical analysis of the map.

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.

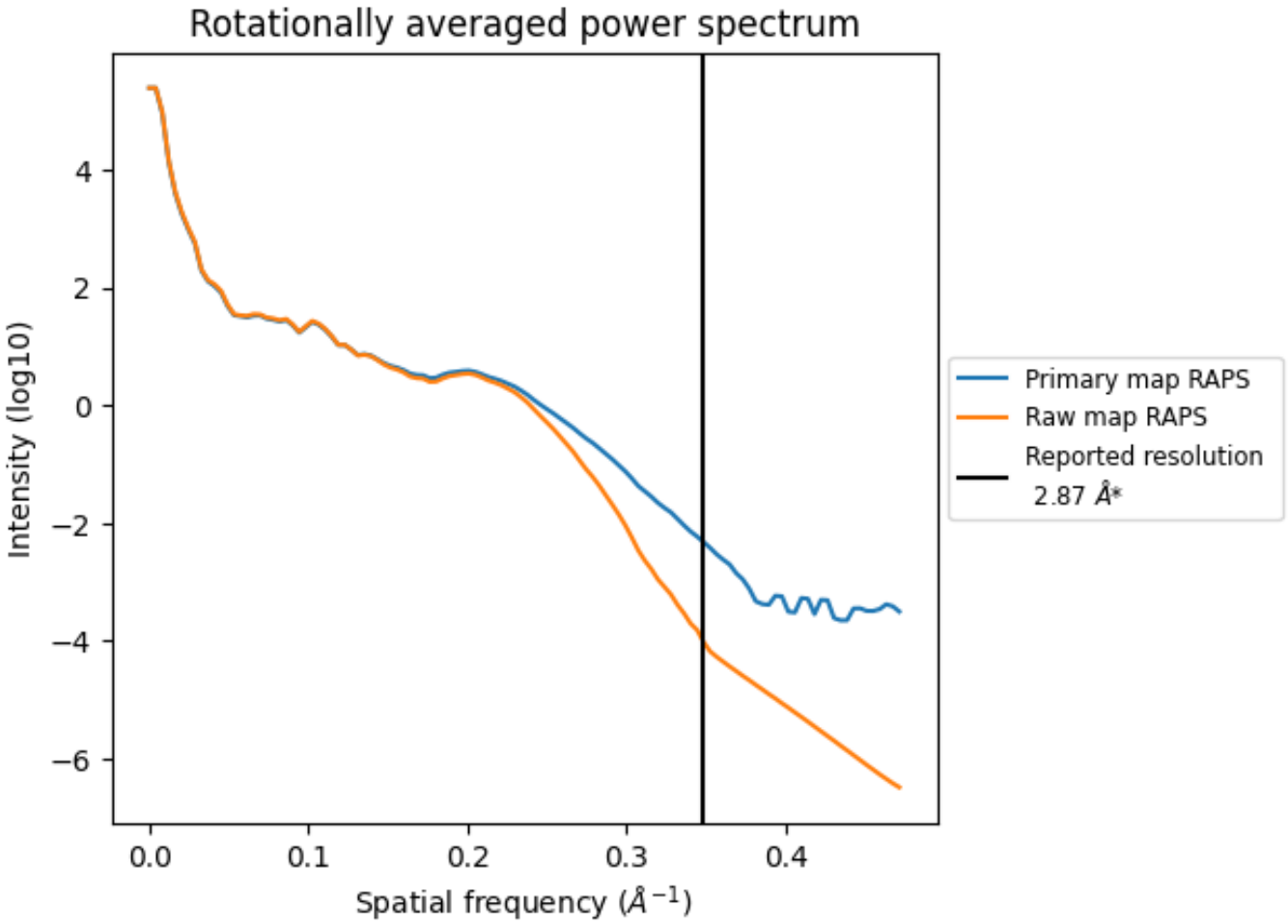
7.2 Volume estimate



The volume at the recommended contour level is 223 nm^3; this corresponds to an approximate mass of 202 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)

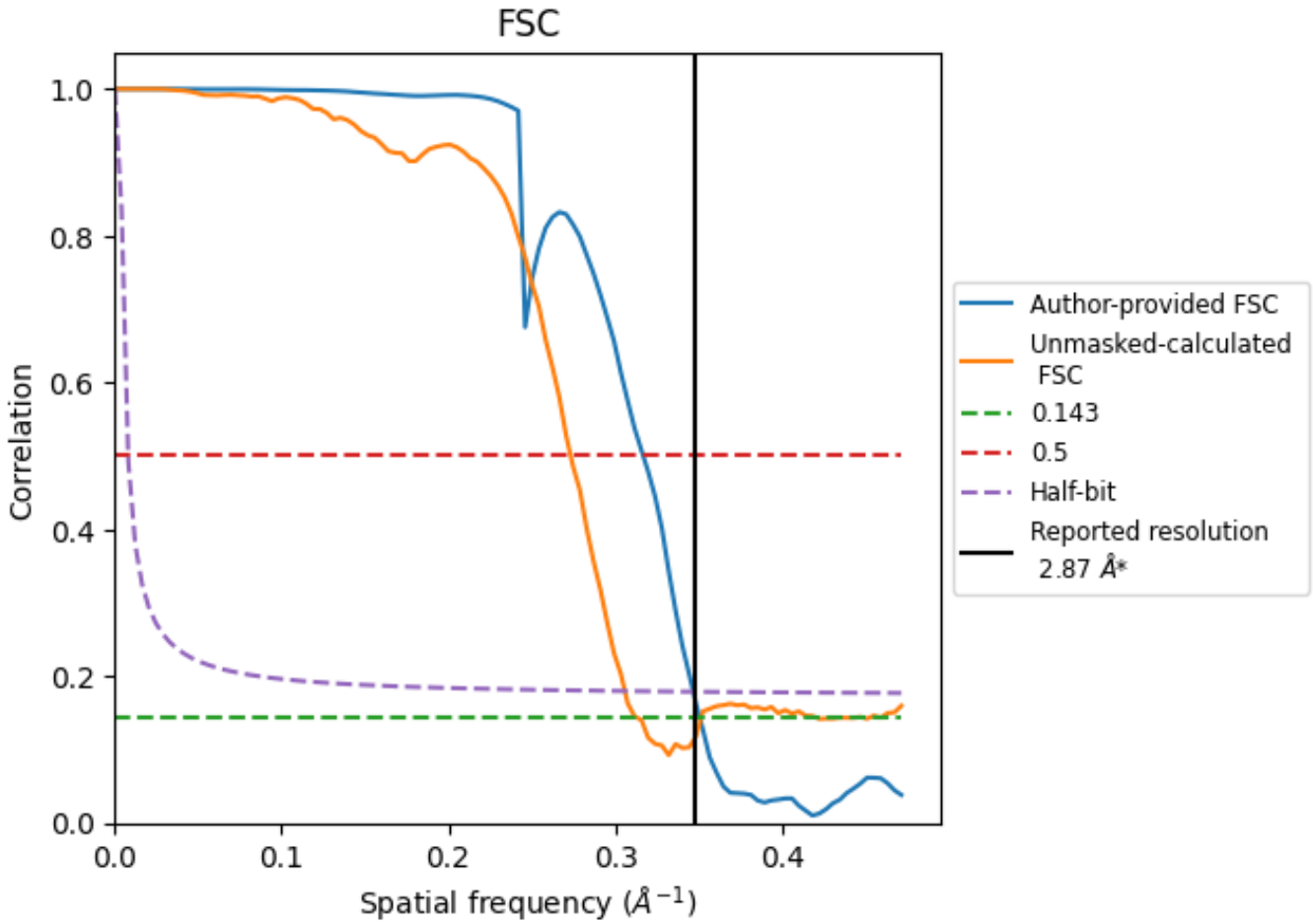


*Reported resolution corresponds to spatial frequency of 0.348 Å^{-1}

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 0.348 Å^{-1}

8.2 Resolution estimates (i)

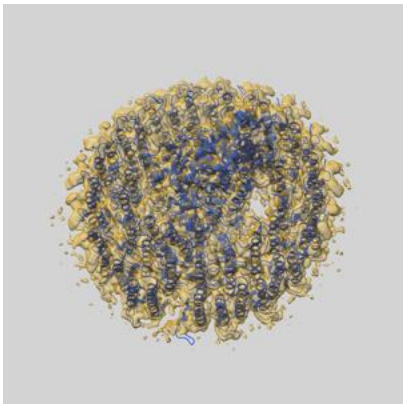
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.87	-	-
Author-provided FSC curve	2.85	3.16	2.88
Unmasked-calculated*	3.19	3.66	3.27

*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 3.19 differs from the reported value 2.87 by more than 10 %

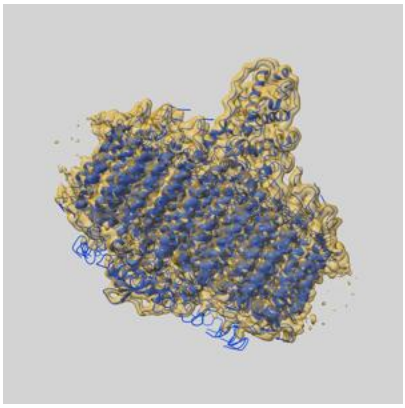
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-3951 and PDB model 6ET5. Per-residue inclusion information can be found in section 3 on page 18.

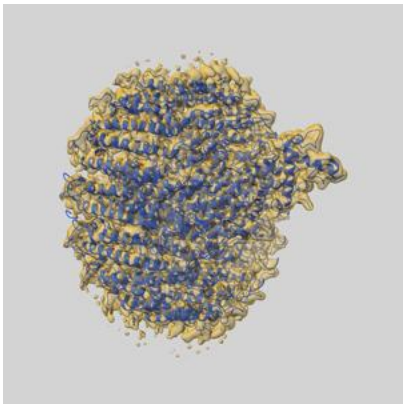
9.1 Map-model overlay



X



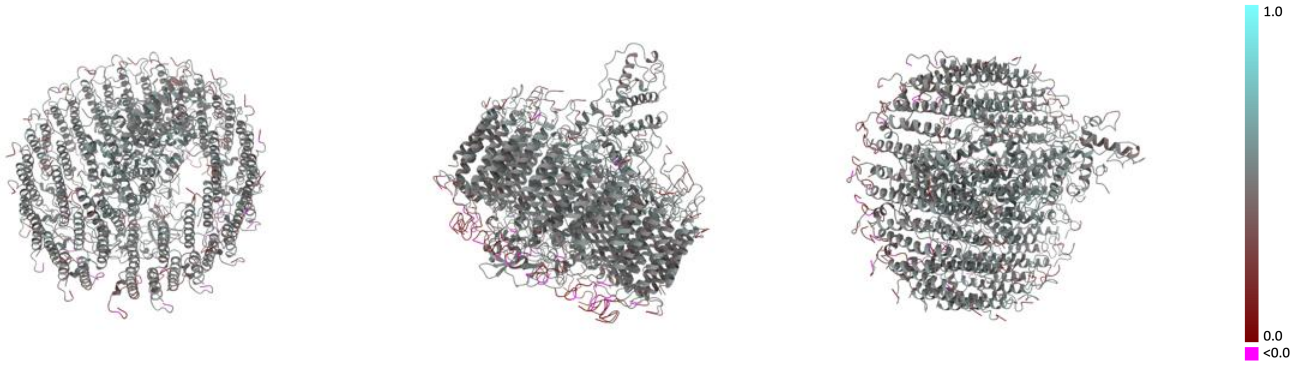
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0156 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.

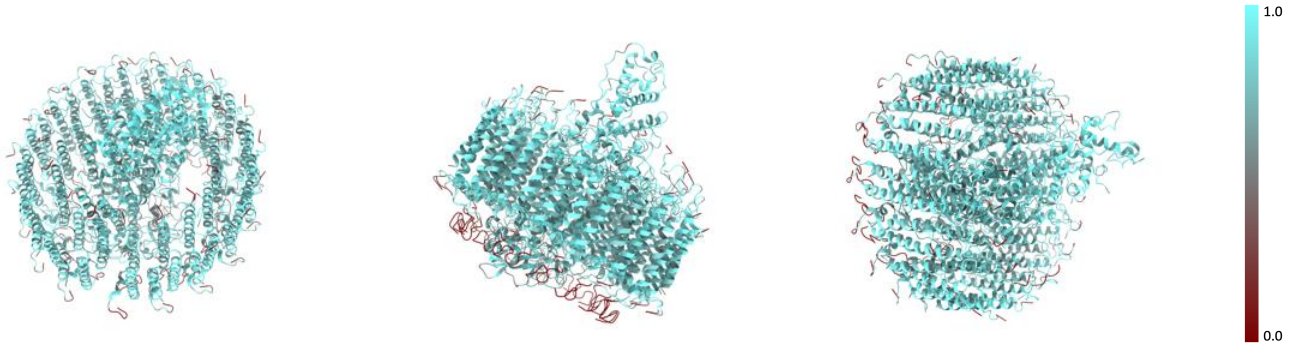
9.2 Q-score mapped to coordinate model (i)



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.

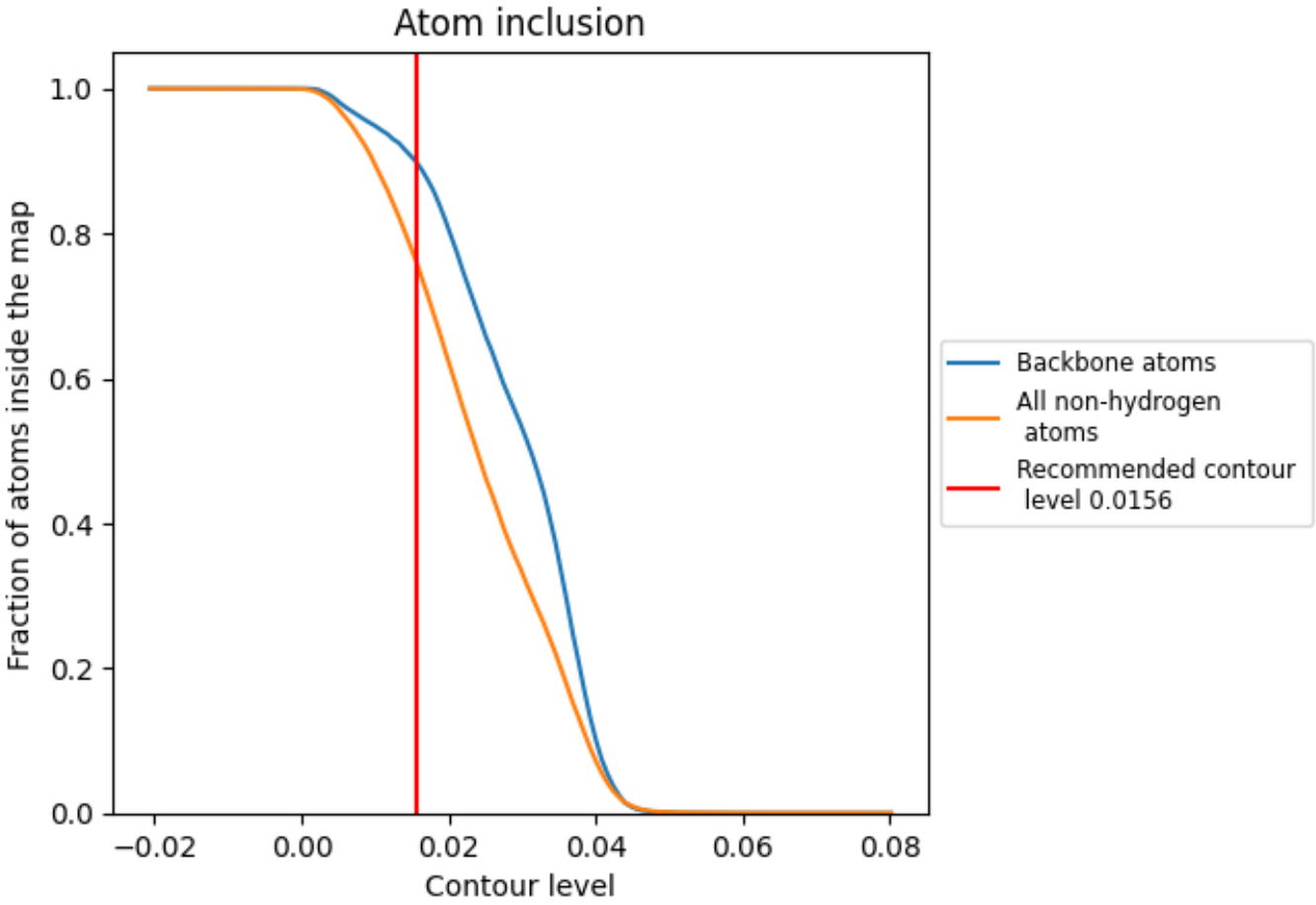
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0156).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 76% 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 (0.0156) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7607	0.4690
1	0.6930	0.4460
2	0.8083	0.4560
3	0.7880	0.4780
4	0.6893	0.4410
5	0.7306	0.4390
6	0.7022	0.4620
7	0.6535	0.4290
C	0.8859	0.5100
F	0.7129	0.4330
G	0.6441	0.4030
H	0.7061	0.4740
I	0.7927	0.4380
K	0.7636	0.4710
L	0.8381	0.5230
M	0.8377	0.5190
N	0.6911	0.4340
O	0.8187	0.4540
P	0.7767	0.4740
Q	0.6893	0.4420
R	0.7824	0.4430
S	0.7749	0.4760
T	0.7043	0.4310
U	0.8083	0.4460
V	0.7767	0.4840
W	0.6949	0.4290
X	0.7979	0.4380
Y	0.7842	0.4810
Z	0.6930	0.4240
a	0.6891	0.4280
b	0.7767	0.4800
c	0.6817	0.4320
d	0.7150	0.4370
e	0.7598	0.4720
f	0.7024	0.4280

Continued on next page...

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Chain	Atom inclusion	Q-score
g	0.7668	0.4430
h	0.7655	0.4820
i	0.6930	0.4330
j	0.6891	0.4310
k	0.7598	0.4730
l	0.6798	0.4370
m	0.7409	0.4320
n	0.7430	0.4710
o	0.6704	0.4190
p	0.7720	0.4490
q	0.7617	0.4670
r	0.6817	0.4260
s	0.8135	0.4490
t	0.7617	0.4760
u	0.6987	0.4280
v	0.7772	0.4320
w	0.7749	0.4780
x	0.7081	0.4330
y	0.8135	0.4540
z	0.7842	0.4870