Full wwPDB EM Validation Report ⓘ

Sep 8, 2026 – 03:21 am BST

PDB ID	:	6ET5 / pdb_00006et5
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	:	2.87 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

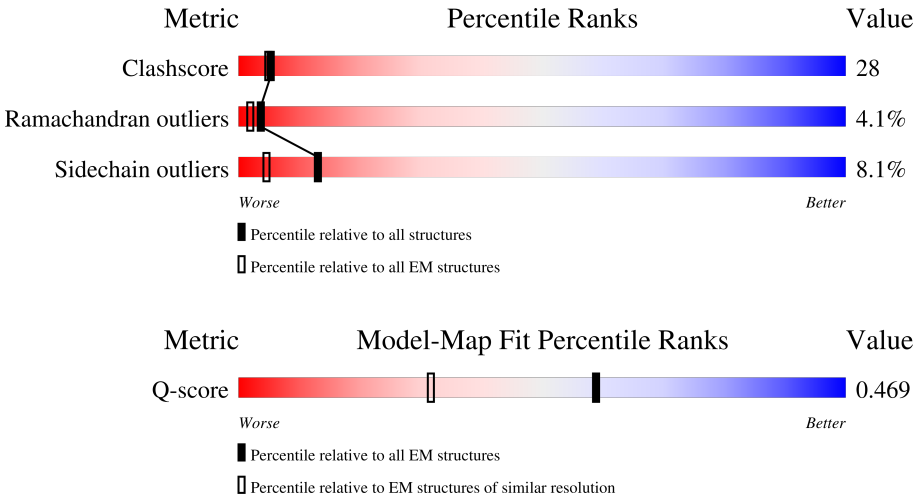
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance

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

The reported resolution of this entry is 2.87 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12062 (2.37 - 3.37)

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	77% 21%
2	L	274	67% 29%
3	M	323	80% 19%
4	H	258	9% 73% 22% 5%

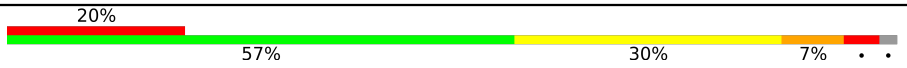
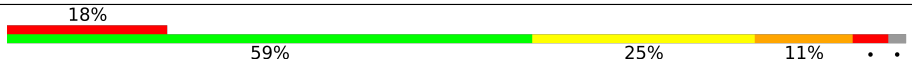
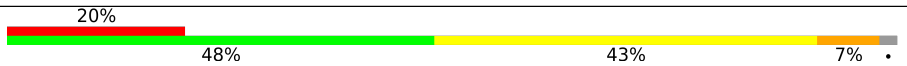
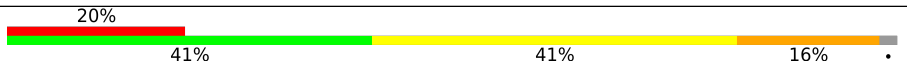
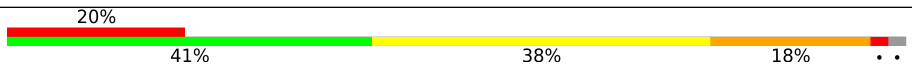
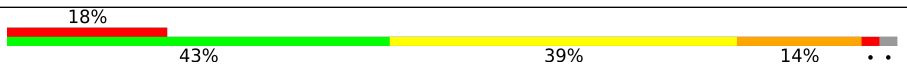
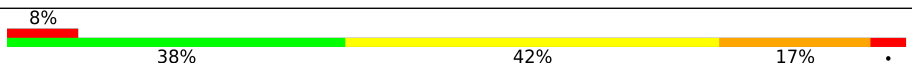
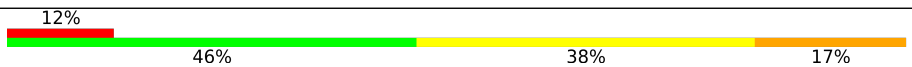
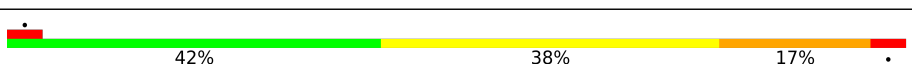
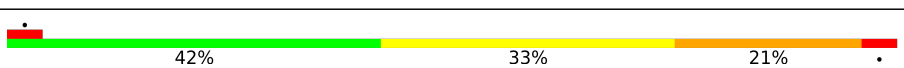
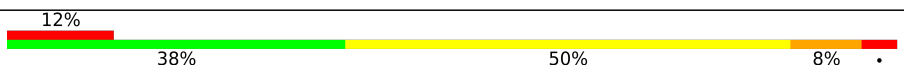
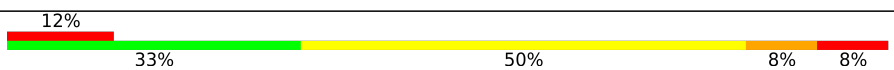
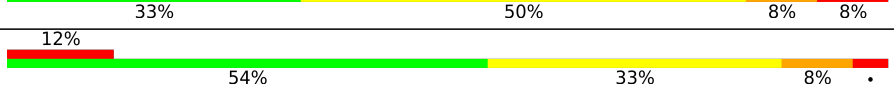
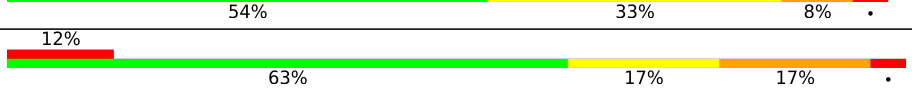
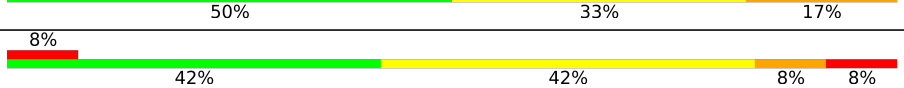
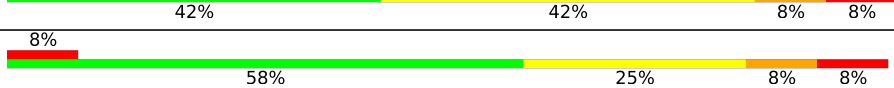
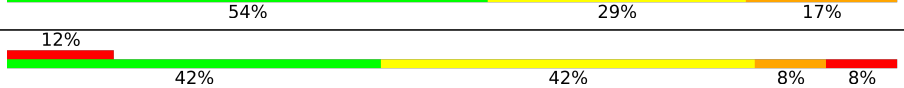
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Mol	Chain	Length	Quality of chain
5	3	59	7% 53% 32% 12%
5	6	59	10% 41% 44% 12%
5	F	59	12% 46% 42% 7%
5	K	59	10% 56% 31% 10%
5	P	59	8% 49% 32% 14%
5	S	59	8% 46% 41% 12%
5	V	59	8% 51% 37% 8%
5	Y	59	5% 44% 41% 12%
5	b	59	7% 53% 31% 12%
5	e	59	10% 53% 32% 12%
5	h	59	7% 53% 37% 7%
5	k	59	10% 46% 42% 8%
5	n	59	10% 49% 34% 14%
5	q	59	8% 42% 37% 14% 5%
5	t	59	10% 46% 39% 12%
5	w	59	7% 44% 37% 15%
5	z	59	7% 53% 34% 12%
6	1	56	20% 52% 38% 5%
6	4	56	20% 54% 34% 9%
6	7	56	20% 43% 46% 9%
6	G	56	20% 45% 38% 16%
6	N	56	18% 52% 32% 12%
6	Q	56	20% 48% 39% 9%
6	T	56	20% 39% 41% 11% 7%
6	W	56	20% 46% 46%

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Mol	Chain	Length	Quality of chain
6	Z	56	
6	c	56	
6	f	56	
6	i	56	
6	l	56	
6	o	56	
6	r	56	
6	u	56	
6	x	56	
7	2	24	
7	5	24	
7	I	24	
7	O	24	
7	R	24	
7	U	24	
7	X	24	
7	a	24	
7	d	24	
7	g	24	
7	j	24	
7	m	24	
7	p	24	
7	s	24	
7	v	24	
7	y	24	

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	408	X	-	-	-
11	UQ9	6	101	-	-	X	-
11	UQ9	L	304	-	-	X	-
17	NS0	1	102	-	X	-	-
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	-	-
8	HEC	C	401	X	-	-	-
8	HEC	C	402	X	-	-	-
8	HEC	C	403	X	-	-	-
8	HEC	C	404	X	-	-	-
9	BCB	1	101	X	-	-	-
9	BCB	3	101	X	-	-	-
9	BCB	4	101	X	-	-	-
9	BCB	6	102	X	-	-	-
9	BCB	7	101	X	-	-	-
9	BCB	F	101	X	-	-	-
9	BCB	G	101	X	-	-	-
9	BCB	K	101	X	-	-	-
9	BCB	L	301	X	-	-	-
9	BCB	L	302	X	-	-	-
9	BCB	M	406	X	-	-	-
9	BCB	M	407	X	-	-	-
9	BCB	N	101	X	-	-	-
9	BCB	P	101	X	-	-	-
9	BCB	Q	101	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	BCB	S	101	X	-	-	-
9	BCB	T	101	X	-	-	-
9	BCB	V	101	X	-	-	-
9	BCB	W	101	X	-	-	-
9	BCB	Y	101	X	-	-	-
9	BCB	Z	101	X	-	-	-
9	BCB	b	101	X	-	-	-
9	BCB	c	101	X	-	-	-
9	BCB	e	101	X	-	-	-
9	BCB	f	101	X	-	-	-
9	BCB	h	101	X	-	-	-
9	BCB	i	101	X	-	-	-
9	BCB	k	101	X	-	-	-
9	BCB	l	101	X	-	-	-
9	BCB	n	101	X	-	-	-
9	BCB	o	101	X	-	-	-
9	BCB	q	101	X	-	-	-
9	BCB	r	101	X	-	-	-
9	BCB	t	101	X	-	-	-
9	BCB	u	101	X	-	-	-
9	BCB	w	101	X	-	-	-
9	BCB	x	101	X	-	-	-
9	BCB	z	101	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.

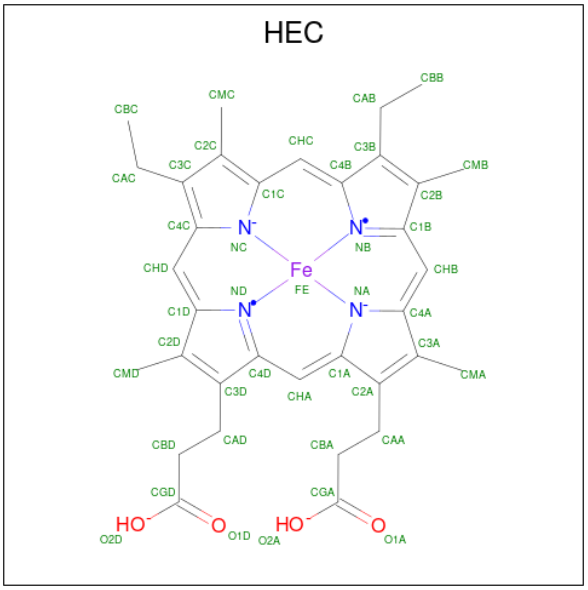
Mol	Chain	Residues	Atoms				AltConf	Trace
7	2	24	Total 199	C 137	N 31	O 31	0	0
7	I	24	Total 199	C 137	N 31	O 31	0	0
7	O	24	Total 199	C 137	N 31	O 31	0	0
7	R	24	Total 199	C 137	N 31	O 31	0	0
7	U	24	Total 199	C 137	N 31	O 31	0	0
7	X	24	Total 199	C 137	N 31	O 31	0	0
7	a	24	Total 199	C 137	N 31	O 31	0	0
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 HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



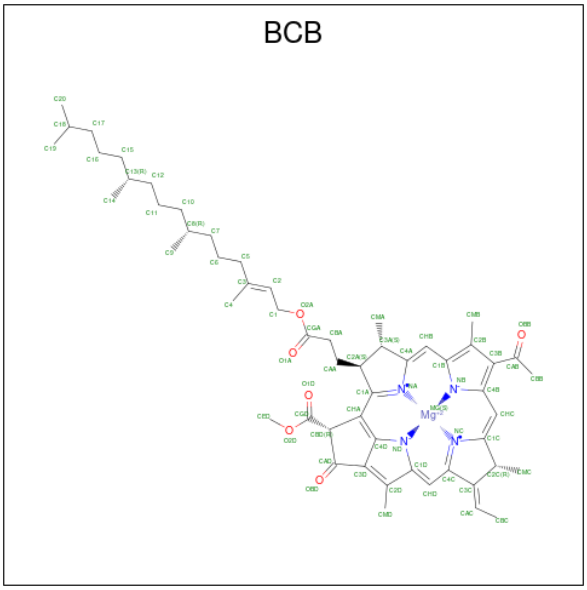
Mol	Chain	Residues	Atoms					AltConf
8	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
8	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
8	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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

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



Mol	Chain	Residues	Atoms					AltConf
9	L	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	L	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	M	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	M	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	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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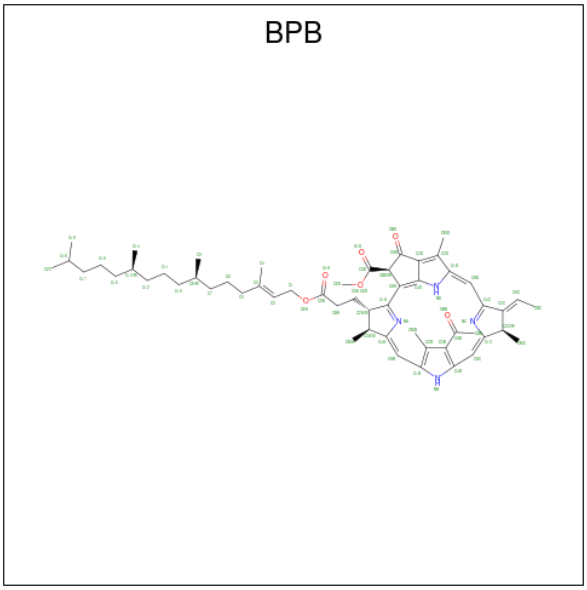
Mol	Chain	Residues	Atoms					AltConf
9	V	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	b	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	e	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	h	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	k	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	n	1	Total	C	Mg	N	O	0
			66	55	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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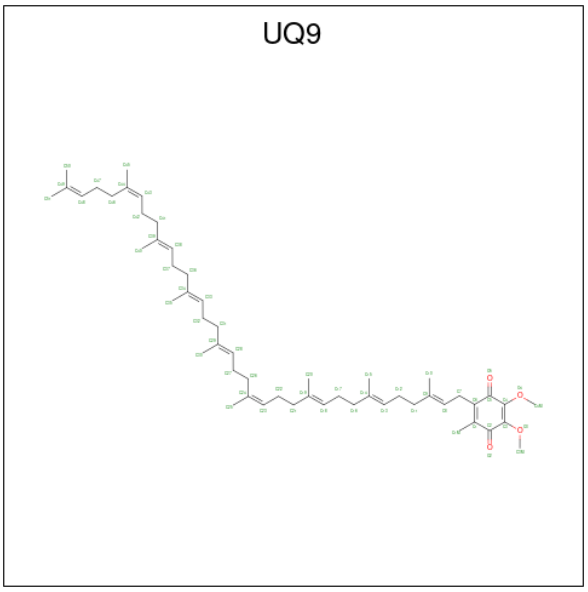
Mol	Chain	Residues	Atoms					AltConf
9	l	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	o	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	r	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	u	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	x	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	4	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 10 is BACTERIOPHEOPHYTIN B (CCD ID: 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 (CCD ID: UQ9) (formula: $C_{54}H_{82}O_4$).

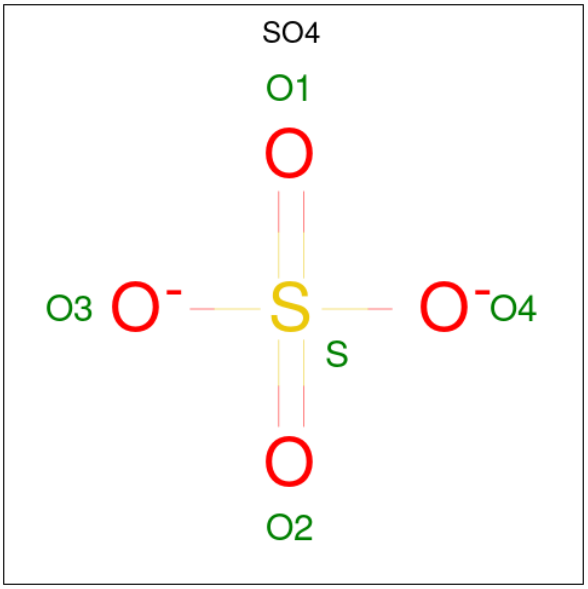


Mol	Chain	Residues	Atoms	AltConf
11	L	1	Total C O 58 54 4	0
11	6	1	Total C O 58 54 4	0

- Molecule 12 is FE (III) ION (CCD ID: FE) (formula: Fe).

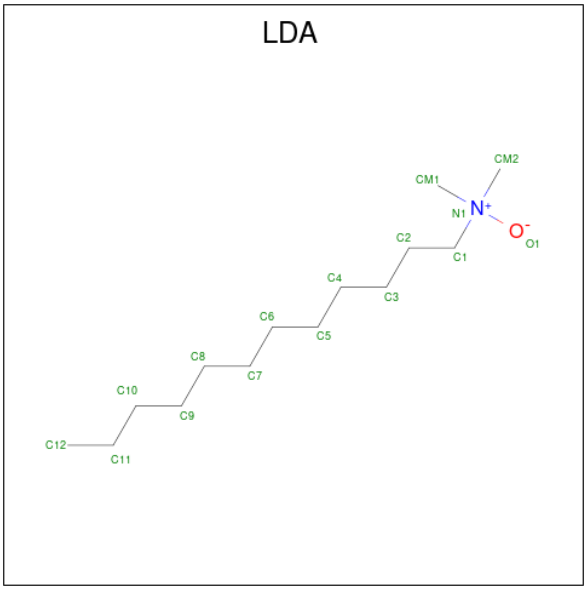
Mol	Chain	Residues	Atoms	AltConf
12	M	1	Total Fe 1 1	0

- Molecule 13 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



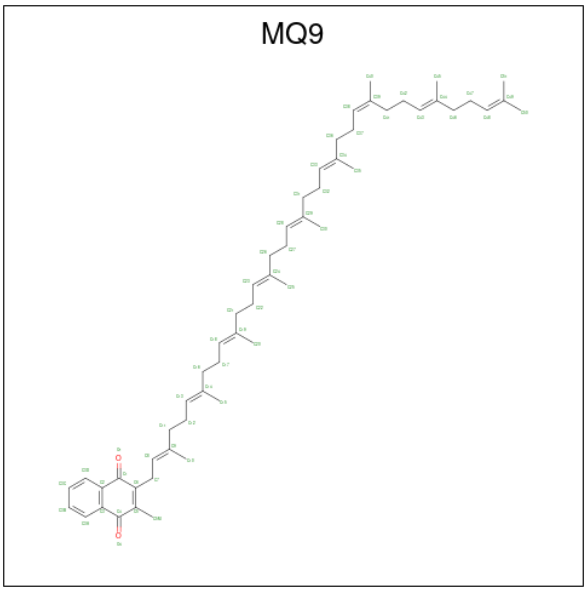
Mol	Chain	Residues	Atoms	AltConf
13	M	1	Total O S 5 4 1	0
13	M	1	Total O S 5 4 1	0
13	M	1	Total O S 5 4 1	0
13	M	1	Total O S 5 4 1	0
13	H	1	Total O S 5 4 1	0
13	H	1	Total O S 5 4 1	0
13	H	1	Total O S 5 4 1	0

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



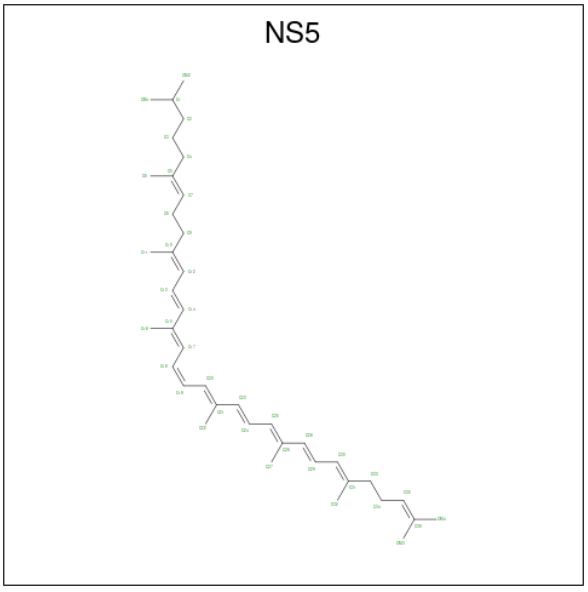
Mol	Chain	Residues	Atoms	AltConf
14	M	1	Total C N O 16 14 1 1	0
14	H	1	Total C N O 16 14 1 1	0

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



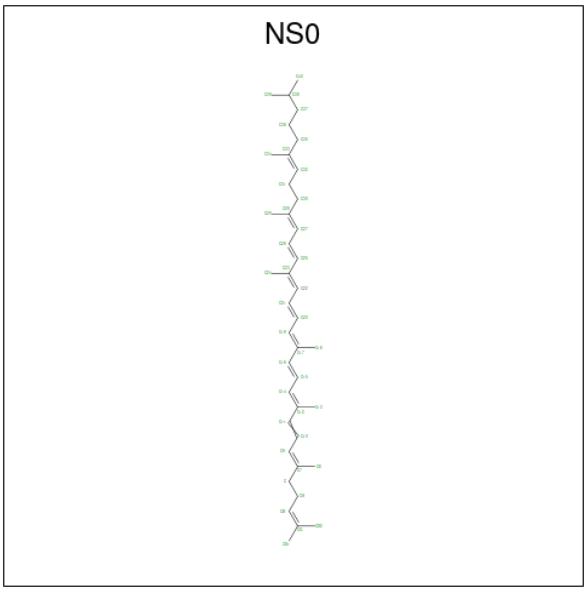
Mol	Chain	Residues	Atoms			AltConf
15	M	1	Total	C	O	0
			58	56	2	

- Molecule 16 is 15-cis-1,2-dihydroneurosporene (CCD ID: 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 (CCD ID: 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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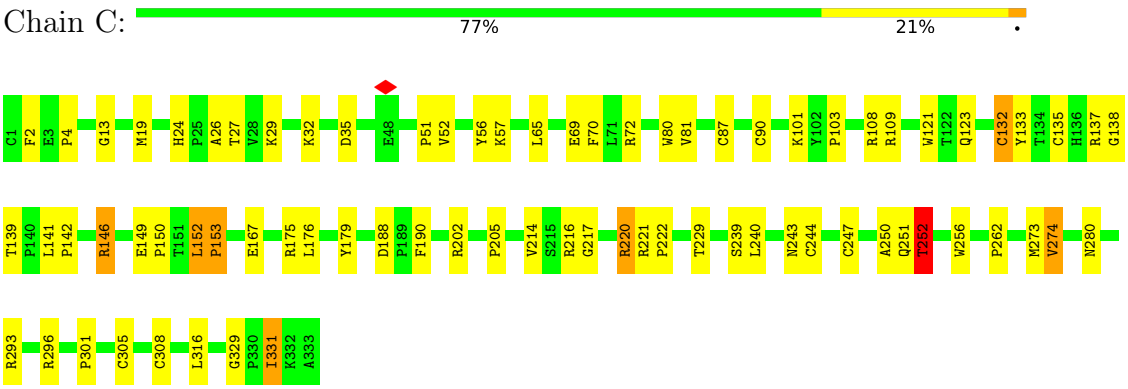
Mol	Chain	Residues	Atoms	AltConf
17	x	1	Total C 40 40	0
17	4	1	Total C 40 40	0
17	7	1	Total C 40 40	0

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.

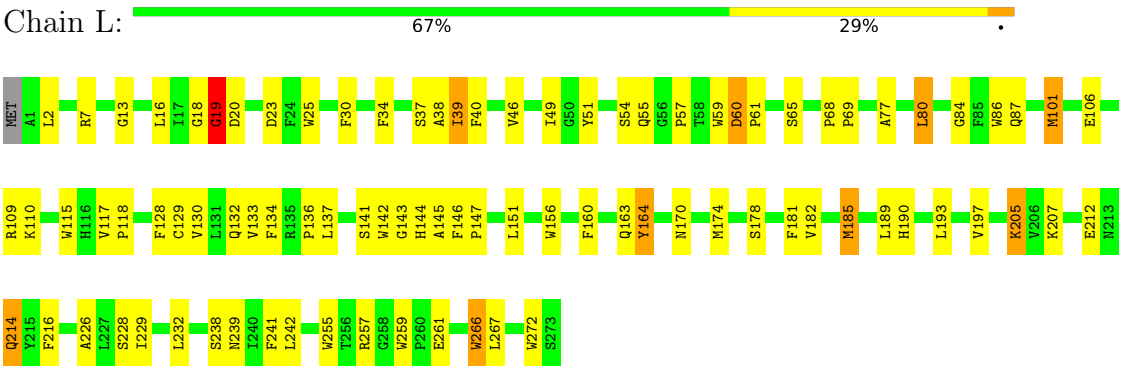
• Molecule 1: Photosynthetic reaction center cytochrome c subunit

Chain C:



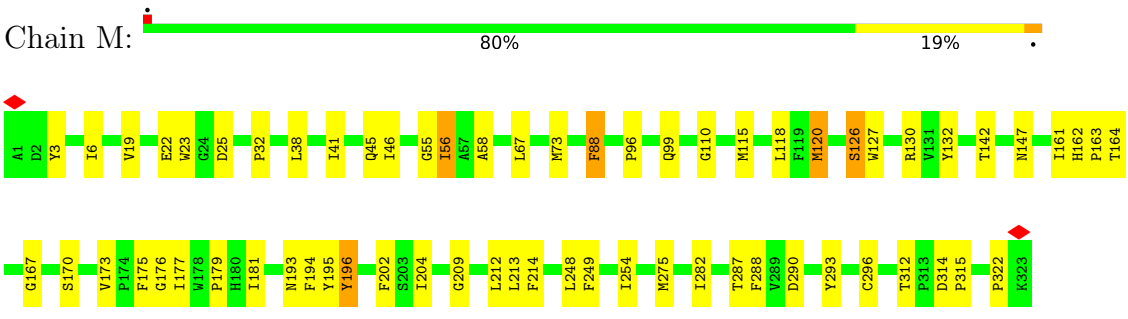
• Molecule 2: Reaction center protein L chain

Chain L:



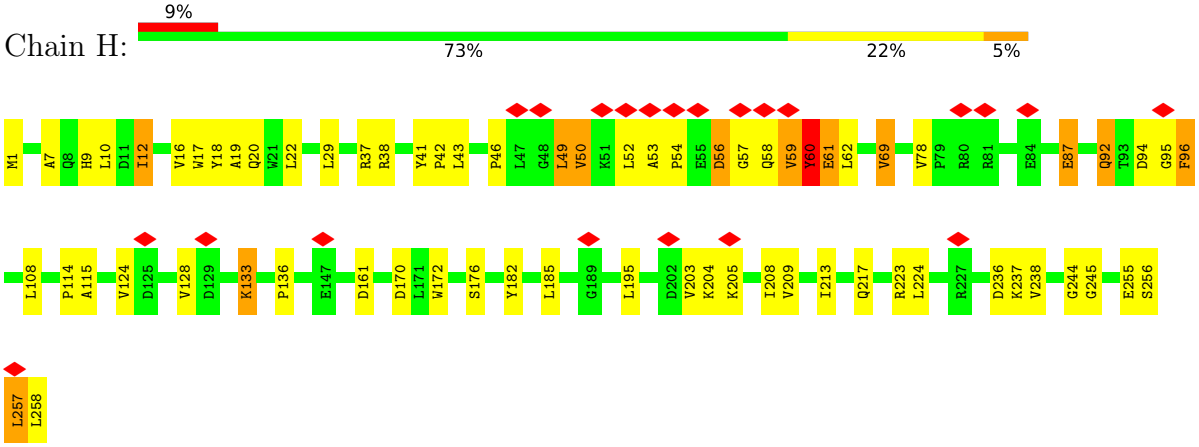
• Molecule 3: Reaction center protein M chain

Chain M:



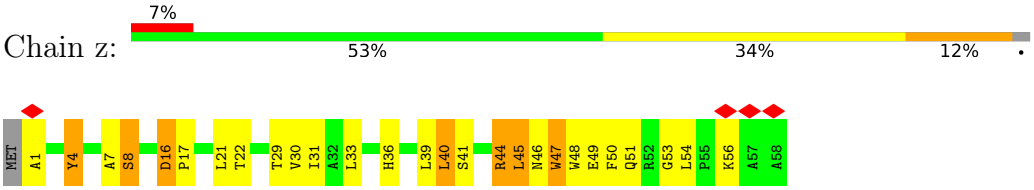
• Molecule 4: Reaction center protein H chain

Chain H:



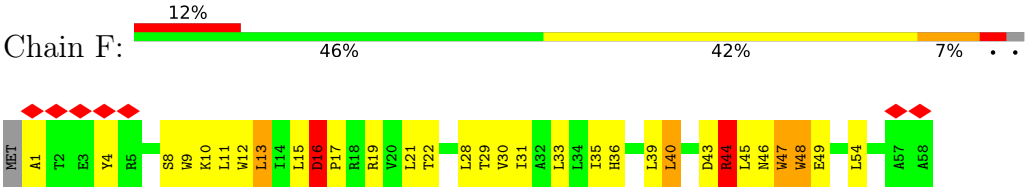
• Molecule 5: Light-harvesting protein B-1015 alpha chain

Chain z:



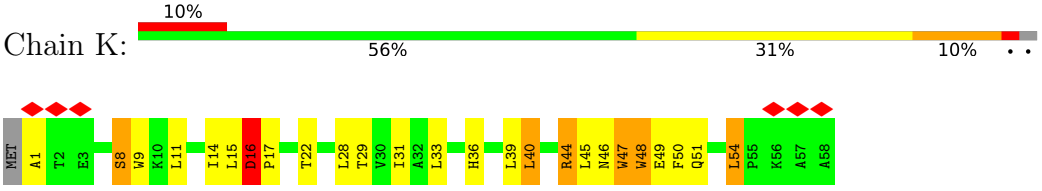
• Molecule 5: Light-harvesting protein B-1015 alpha chain

Chain F:



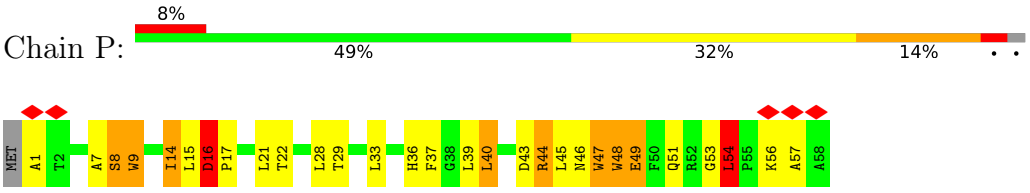
• Molecule 5: Light-harvesting protein B-1015 alpha chain

Chain K:



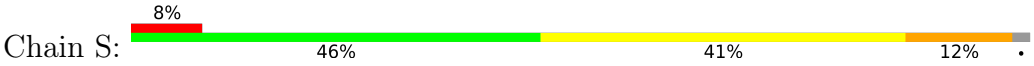
• Molecule 5: Light-harvesting protein B-1015 alpha chain

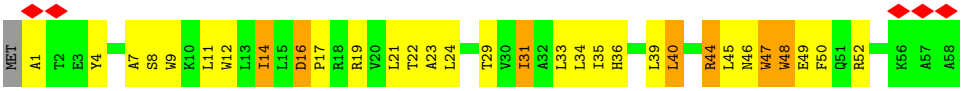
Chain P:



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

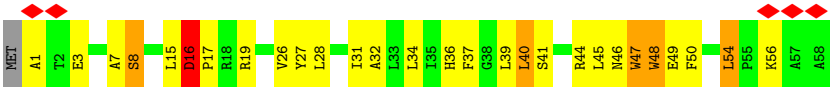
Chain S:





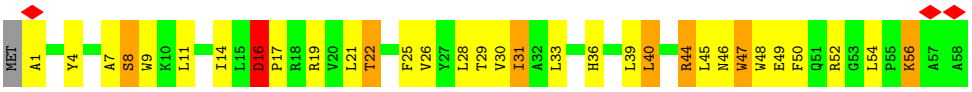
• Molecule 5: Light-harvesting protein B-1015 alpha chain





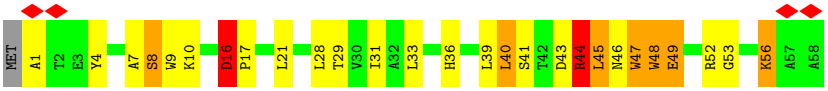
• Molecule 5: Light-harvesting protein B-1015 alpha chain





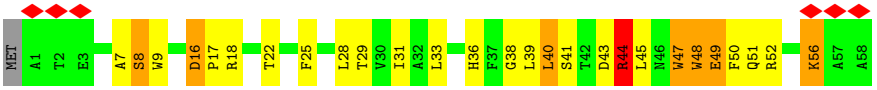
• Molecule 5: Light-harvesting protein B-1015 alpha chain





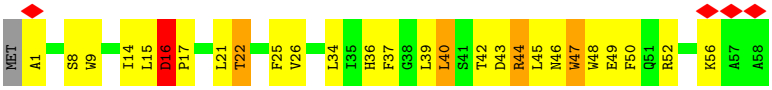
• Molecule 5: Light-harvesting protein B-1015 alpha chain





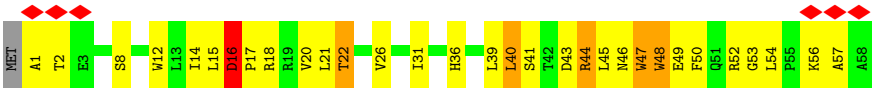
• Molecule 5: Light-harvesting protein B-1015 alpha chain





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





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

Chain n:

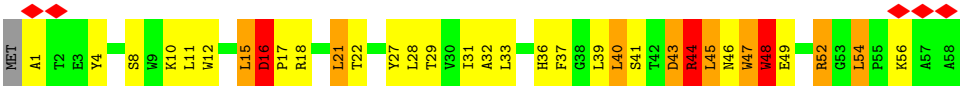




• Molecule 5: Light-harvesting protein B-1015 alpha chain

Chain q:

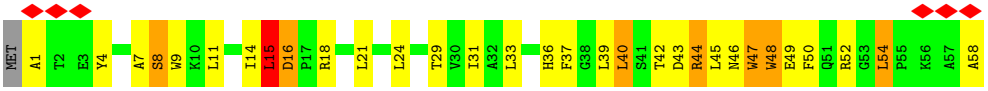




• Molecule 5: Light-harvesting protein B-1015 alpha chain

Chain t:

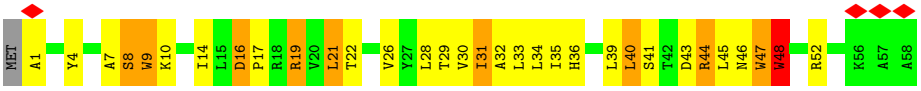




• Molecule 5: Light-harvesting protein B-1015 alpha chain

Chain w:

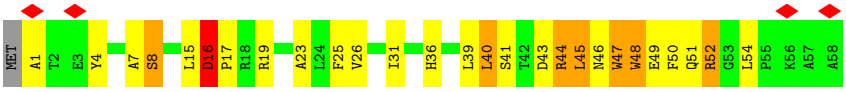




• Molecule 5: Light-harvesting protein B-1015 alpha chain

Chain 3:

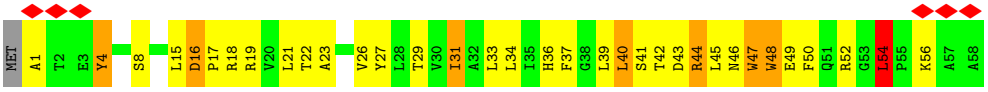




• Molecule 5: Light-harvesting protein B-1015 alpha chain

Chain 6:

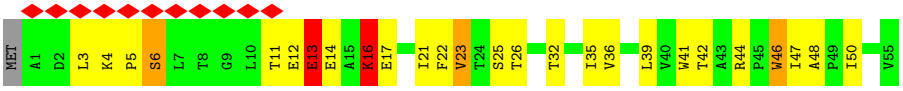




• Molecule 6: Light-harvesting protein B-1015 beta chain

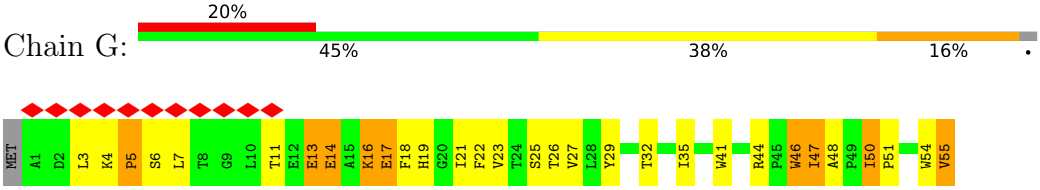
Chain 1:





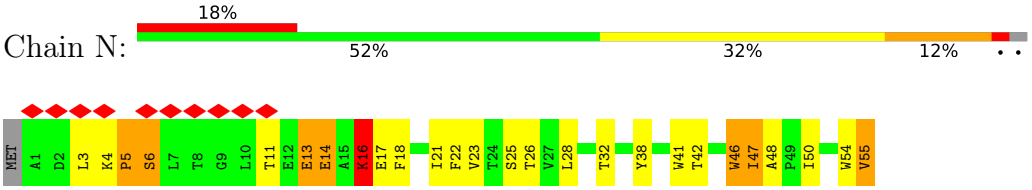
• Molecule 6: Light-harvesting protein B-1015 beta chain

Chain G:



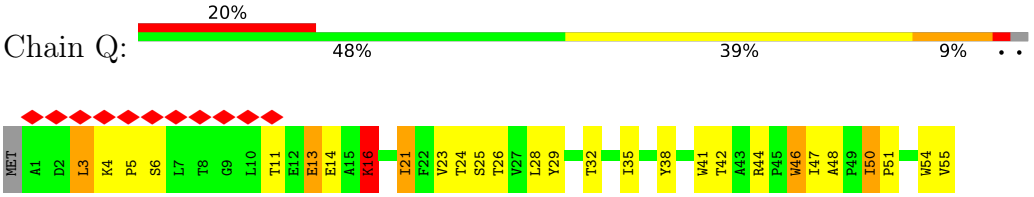
• Molecule 6: Light-harvesting protein B-1015 beta chain

Chain N:



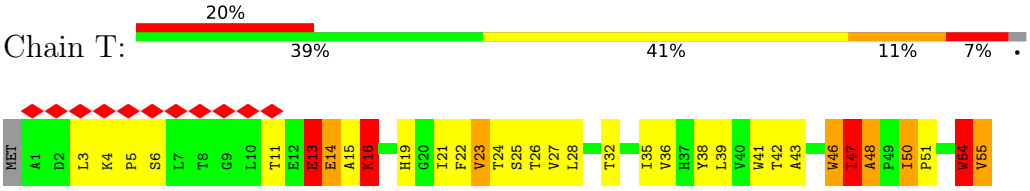
• Molecule 6: Light-harvesting protein B-1015 beta chain

Chain Q:



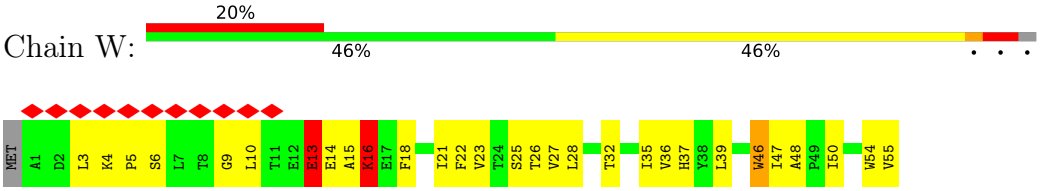
• Molecule 6: Light-harvesting protein B-1015 beta chain

Chain T:



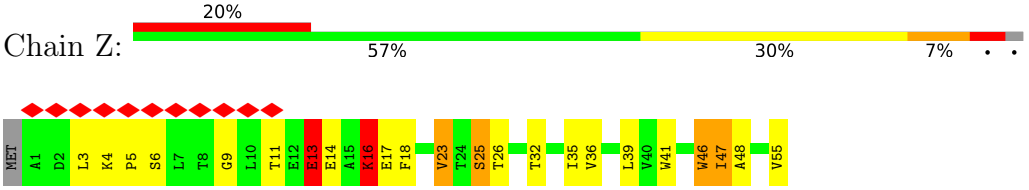
• Molecule 6: Light-harvesting protein B-1015 beta chain

Chain W:



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

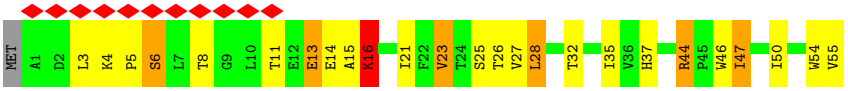
Chain Z:



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

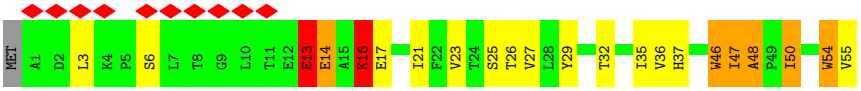
Chain c:





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





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





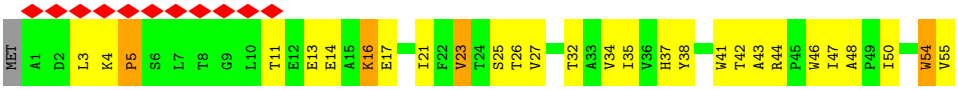
• Molecule 6: Light-harvesting protein B-1015 beta chain





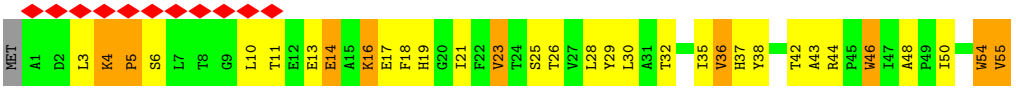
• Molecule 6: Light-harvesting protein B-1015 beta chain





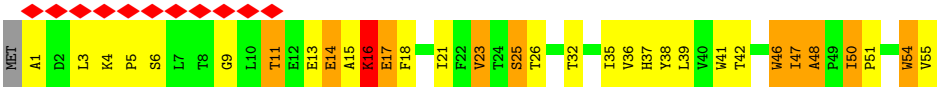
• Molecule 6: Light-harvesting protein B-1015 beta chain





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





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

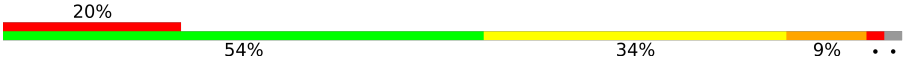
Chain x:

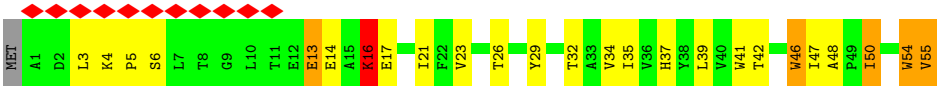




• Molecule 6: Light-harvesting protein B-1015 beta chain

Chain 4:

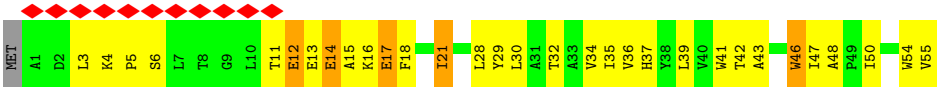




• Molecule 6: Light-harvesting protein B-1015 beta chain

Chain 7:

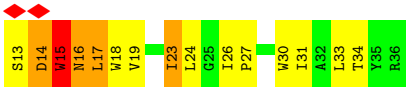




• Molecule 7: Light-harvesting protein B-1015 gamma chain

Chain 2:





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

Chain I:

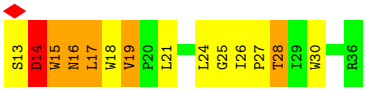




• Molecule 7: Light-harvesting protein B-1015 gamma chain

Chain O:

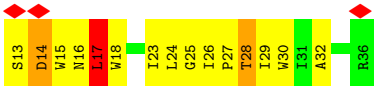




• Molecule 7: Light-harvesting protein B-1015 gamma chain

Chain R:

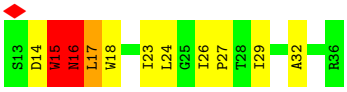




• Molecule 7: Light-harvesting protein B-1015 gamma chain

Chain U:

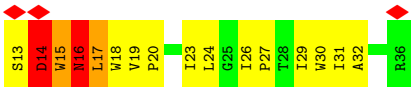




• Molecule 7: Light-harvesting protein B-1015 gamma chain

Chain X:

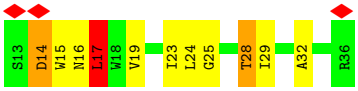




• Molecule 7: Light-harvesting protein B-1015 gamma chain

Chain a:

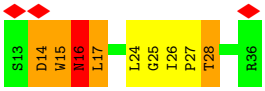




• Molecule 7: Light-harvesting protein B-1015 gamma chain

Chain d:

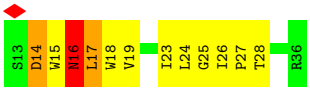




• Molecule 7: Light-harvesting protein B-1015 gamma chain

Chain g:

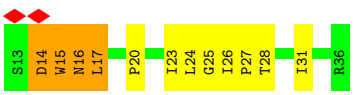




• Molecule 7: Light-harvesting protein B-1015 gamma chain

Chain j:

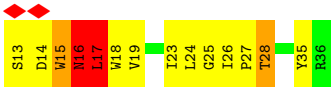




• Molecule 7: Light-harvesting protein B-1015 gamma chain

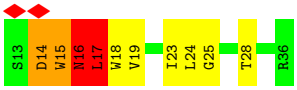
Chain m:





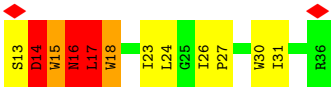
• Molecule 7: Light-harvesting protein B-1015 gamma chain





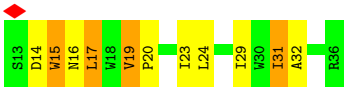
• Molecule 7: Light-harvesting protein B-1015 gamma chain





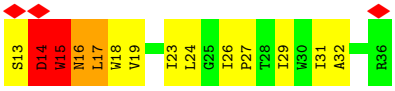
• Molecule 7: Light-harvesting protein B-1015 gamma chain



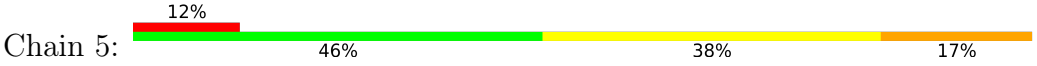


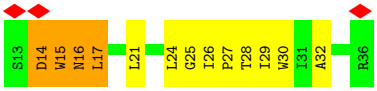
• Molecule 7: Light-harvesting protein B-1015 gamma chain





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





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	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: NS5, FME, UQ9, NS0, BPB, HEC, BCB, MQ9, LDA, FE, SO4

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	0.83	2/2670 (0.1%)	1.16	10/3639 (0.3%)
2	L	0.99	1/2259 (0.0%)	1.19	9/3084 (0.3%)
3	M	0.92	0/2659	1.14	7/3637 (0.2%)
4	H	0.72	0/2054	1.04	7/2803 (0.2%)
5	3	0.94	0/502	1.51	10/686 (1.5%)
5	6	0.92	0/502	1.39	9/686 (1.3%)
5	F	0.93	0/502	1.42	8/686 (1.2%)
5	K	0.91	0/502	1.47	9/686 (1.3%)
5	P	0.95	0/502	1.53	14/686 (2.0%)
5	S	0.92	0/502	1.41	5/686 (0.7%)
5	V	0.96	0/502	1.47	11/686 (1.6%)
5	Y	0.93	0/502	1.45	9/686 (1.3%)
5	b	0.95	0/502	1.52	9/686 (1.3%)
5	e	0.93	0/502	1.48	7/686 (1.0%)
5	h	0.86	0/502	1.35	5/686 (0.7%)
5	k	1.01	0/502	1.49	11/686 (1.6%)
5	n	0.90	0/502	1.42	10/686 (1.5%)
5	q	0.93	0/502	1.44	11/686 (1.6%)
5	t	0.93	0/502	1.44	9/686 (1.3%)
5	w	0.95	0/502	1.45	8/686 (1.2%)
5	z	0.97	0/502	1.46	7/686 (1.0%)
6	1	1.03	0/451	1.38	4/621 (0.6%)
6	4	1.02	0/451	1.42	7/621 (1.1%)
6	7	0.92	0/451	1.31	5/621 (0.8%)
6	G	0.91	0/451	1.35	7/621 (1.1%)
6	N	0.94	0/451	1.40	4/621 (0.6%)
6	Q	0.98	0/451	1.38	6/621 (1.0%)
6	T	0.98	0/451	1.42	6/621 (1.0%)
6	W	1.04	1/451 (0.2%)	1.40	7/621 (1.1%)
6	Z	1.01	0/451	1.36	7/621 (1.1%)
6	c	0.95	0/451	1.44	9/621 (1.4%)
6	f	0.93	0/451	1.38	6/621 (1.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
6	i	0.99	0/451	1.41	5/621 (0.8%)
6	l	0.94	0/451	1.32	4/621 (0.6%)
6	o	0.94	0/451	1.26	4/621 (0.6%)
6	r	0.92	0/451	1.34	5/621 (0.8%)
6	u	0.97	0/451	1.42	8/621 (1.3%)
6	x	1.04	0/451	1.47	9/621 (1.4%)
7	2	0.96	0/207	1.65	6/287 (2.1%)
7	5	0.73	0/207	1.39	4/287 (1.4%)
7	I	0.76	0/207	1.33	2/287 (0.7%)
7	O	0.86	0/207	1.54	5/287 (1.7%)
7	R	0.93	0/207	1.40	5/287 (1.7%)
7	U	0.85	0/207	1.47	5/287 (1.7%)
7	X	0.93	0/207	1.63	8/287 (2.8%)
7	a	0.77	0/207	1.40	3/287 (1.0%)
7	d	0.78	0/207	1.25	4/287 (1.4%)
7	g	0.73	0/207	1.34	4/287 (1.4%)
7	j	0.76	0/207	1.27	3/287 (1.0%)
7	m	0.83	0/207	1.58	6/287 (2.1%)
7	p	0.85	0/207	1.47	4/287 (1.4%)
7	s	0.84	0/207	1.46	7/287 (2.4%)
7	v	0.81	0/207	1.42	2/287 (0.7%)
7	y	0.90	0/207	1.52	6/287 (2.1%)
All	All	0.92	4/29155 (0.0%)	1.34	362/39974 (0.9%)

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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	152	LEU	N-CA	8.13	1.54	1.46
2	L	266	TRP	N-CA	-5.17	1.39	1.46
6	W	15	ALA	N-CA	5.05	1.52	1.46
1	C	153	PRO	CA-CB	5.01	1.62	1.53

All (362) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	P	48	TRP	CB-CA-C	-11.49	97.11	111.82
5	e	48	TRP	CB-CA-C	-11.29	97.36	111.82
5	b	48	TRP	CB-CA-C	-10.69	96.55	111.73
2	L	164	TYR	N-CA-C	-10.30	93.58	110.17
6	G	47	ILE	N-CA-C	9.80	119.83	110.42
5	e	56	LYS	N-CA-C	-9.76	103.49	114.62
5	Y	56	LYS	N-CA-C	-9.51	103.78	114.62
5	P	44	ARG	N-CA-C	-9.28	95.56	110.32
5	b	44	ARG	N-CA-C	-8.92	98.75	110.53
6	T	16	LYS	N-CA-C	-8.75	100.06	113.89
6	T	47	ILE	N-CA-CB	8.59	120.60	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	3	47	TRP	N-CA-C	-8.54	97.88	110.52
7	X	17	LEU	CB-CA-C	8.53	124.32	111.70
5	F	48	TRP	CB-CA-C	-8.49	97.08	111.26
5	n	56	LYS	N-CA-C	-8.39	105.06	114.62
6	x	47	ILE	N-CA-CB	8.20	121.07	110.57
7	m	17	LEU	CB-CA-C	8.20	124.44	111.73
5	K	48	TRP	CB-CA-C	-8.12	98.80	111.39
7	m	18	TRP	N-CA-C	-8.09	103.20	113.72
5	V	47	TRP	N-CA-C	-8.05	98.91	110.59
5	3	52	ARG	N-CA-C	-8.05	102.48	111.82
6	1	47	ILE	N-CA-CB	8.04	120.86	110.57
5	S	48	TRP	CB-CA-C	-8.03	101.88	109.83
5	e	47	TRP	N-CA-C	-8.00	99.00	110.59
6	c	50	ILE	CA-C-N	7.99	128.47	119.92
6	c	50	ILE	C-N-CA	7.99	128.47	119.92
7	p	17	LEU	CB-CA-C	7.98	123.51	111.70
5	w	52	ARG	N-CA-C	-7.98	103.44	113.02
5	t	48	TRP	CB-CA-C	-7.89	102.02	109.83
5	P	47	TRP	N-CA-C	-7.85	98.32	110.17
6	4	47	ILE	N-CA-CB	7.82	120.57	110.57
5	w	47	TRP	N-CA-C	-7.78	100.49	110.53
6	c	11	THR	N-CA-C	7.72	119.94	110.91
7	y	17	LEU	CB-CA-C	7.71	123.11	111.70
6	i	47	ILE	N-CA-CB	7.69	121.00	110.54
5	b	47	TRP	N-CA-C	-7.68	97.88	109.94
5	q	40	LEU	CA-CB-CG	7.59	142.87	116.30
6	1	16	LYS	N-CA-C	-7.53	101.80	113.02
5	k	48	TRP	CB-CA-C	-7.52	97.29	111.06
5	k	44	ARG	N-CA-C	-7.40	100.07	110.50
6	r	46	TRP	N-CA-C	7.40	120.79	111.69
5	S	47	TRP	N-CA-C	-7.39	99.87	110.59
6	Q	50	ILE	CA-C-N	7.38	129.06	119.84
6	Q	50	ILE	C-N-CA	7.38	129.06	119.84
5	V	44	ARG	N-CA-C	-7.34	100.84	110.53
5	S	44	ARG	N-CA-C	-7.34	98.65	110.32
5	6	44	ARG	N-CA-C	-7.29	100.72	110.55
7	2	18	TRP	N-CA-C	-7.28	104.26	113.72
7	2	17	LEU	CB-CA-C	7.25	122.41	111.76
5	V	16	ASP	CA-C-N	7.18	126.71	119.24
5	V	16	ASP	C-N-CA	7.18	126.71	119.24
7	v	15	TRP	N-CA-C	7.17	121.89	107.41
6	i	46	TRP	N-CA-C	7.09	120.41	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	r	17	GLU	N-CA-C	-7.06	103.58	111.28
5	h	16	ASP	CA-C-N	7.04	128.63	119.84
5	h	16	ASP	C-N-CA	7.04	128.63	119.84
5	z	44	ARG	N-CA-C	-7.03	100.79	110.35
6	7	46	TRP	N-CA-C	7.00	121.05	112.23
6	Z	11	THR	N-CA-C	6.97	119.06	110.91
6	W	47	ILE	N-CA-CB	6.94	119.46	110.57
5	K	47	TRP	N-CA-C	-6.93	100.55	110.59
6	l	16	LYS	N-CA-C	-6.91	103.97	112.88
6	x	17	GLU	N-CA-C	-6.90	103.84	111.36
6	x	50	ILE	CA-C-N	6.88	127.82	120.11
6	x	50	ILE	C-N-CA	6.88	127.82	120.11
6	f	46	TRP	N-CA-C	6.84	121.86	112.90
5	n	47	TRP	N-CA-C	-6.84	101.71	110.53
1	C	139	THR	CA-C-N	-6.82	113.17	120.47
1	C	139	THR	C-N-CA	-6.82	113.17	120.47
6	W	16	LYS	N-CA-C	-6.82	104.16	113.30
6	Z	9	GLY	N-CA-C	-6.80	101.52	111.03
5	b	45	LEU	N-CA-C	6.75	121.10	112.86
6	l	50	ILE	CA-C-N	6.75	127.67	120.11
6	l	50	ILE	C-N-CA	6.75	127.67	120.11
7	U	17	LEU	CB-CA-C	6.74	123.84	110.42
5	3	44	ARG	N-CA-C	-6.74	101.45	110.55
6	i	50	ILE	CA-C-N	6.73	127.65	120.11
6	i	50	ILE	C-N-CA	6.73	127.65	120.11
7	O	17	LEU	N-CA-C	6.70	117.98	108.54
5	F	47	TRP	N-CA-C	-6.67	100.02	110.36
5	k	16	ASP	CA-C-N	6.65	128.16	119.84
5	k	16	ASP	C-N-CA	6.65	128.16	119.84
6	T	50	ILE	CA-C-N	6.65	128.15	119.84
6	T	50	ILE	C-N-CA	6.65	128.15	119.84
5	e	44	ARG	N-CA-C	-6.63	101.60	110.55
6	i	16	LYS	N-CA-C	-6.58	104.82	112.92
5	k	40	LEU	CA-CB-CG	6.57	139.29	116.30
6	4	16	LYS	N-CA-C	-6.56	103.68	112.94
5	Y	52	ARG	N-CA-C	-6.56	105.02	113.16
6	c	47	ILE	N-CA-C	6.56	117.31	110.62
6	N	17	GLU	N-CA-C	-6.55	104.06	111.07
7	y	18	TRP	CB-CA-C	-6.54	98.27	109.65
3	M	196	TYR	N-CA-C	6.52	120.83	113.01
7	g	17	LEU	CA-C-N	6.52	130.22	120.31
7	g	17	LEU	C-N-CA	6.52	130.22	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	f	50	ILE	CA-C-N	6.51	126.46	120.21
6	f	50	ILE	C-N-CA	6.51	126.46	120.21
5	k	47	TRP	N-CA-C	-6.50	100.29	110.36
6	c	47	ILE	N-CA-CB	6.50	119.37	110.54
7	s	14	ASP	CA-C-N	-6.49	113.89	123.11
7	s	14	ASP	C-N-CA	-6.49	113.89	123.11
7	X	18	TRP	N-CA-C	-6.49	104.99	113.17
6	4	17	GLU	N-CA-C	-6.49	104.12	111.07
6	N	16	LYS	N-CA-C	-6.49	103.35	113.02
5	t	40	LEU	CA-CB-CG	6.48	138.97	116.30
6	Q	47	ILE	N-CA-CB	6.47	119.34	110.54
6	f	16	LYS	N-CA-C	-6.46	103.39	113.02
5	3	40	LEU	CA-CB-CG	6.46	138.91	116.30
5	P	16	ASP	CA-C-N	6.46	126.68	119.32
5	P	16	ASP	C-N-CA	6.46	126.68	119.32
6	G	46	TRP	N-CA-C	6.43	119.60	111.69
6	x	16	LYS	N-CA-C	-6.42	104.06	112.41
7	a	17	LEU	CA-C-N	6.42	132.37	121.14
7	a	17	LEU	C-N-CA	6.42	132.37	121.14
6	r	50	ILE	CA-C-N	6.41	126.36	120.21
6	r	50	ILE	C-N-CA	6.41	126.36	120.21
5	K	48	TRP	CA-CB-CG	6.40	125.77	113.60
5	6	48	TRP	CB-CA-C	-6.38	99.38	111.06
6	c	16	LYS	N-CA-C	-6.38	104.11	112.41
5	F	40	LEU	CA-CB-CG	6.38	138.63	116.30
5	3	16	ASP	CA-C-N	6.38	127.81	119.84
5	3	16	ASP	C-N-CA	6.38	127.81	119.84
7	R	17	LEU	N-CA-C	6.36	120.26	107.41
6	Z	17	GLU	N-CA-C	-6.36	104.43	111.36
6	1	46	TRP	N-CA-C	6.34	120.22	112.23
5	h	47	TRP	N-CA-C	-6.34	100.54	110.36
5	t	47	TRP	N-CA-C	-6.29	101.15	110.46
7	O	15	TRP	CB-CA-C	6.29	120.51	110.19
6	Z	47	ILE	N-CA-CB	6.26	119.97	110.58
6	W	50	ILE	CA-C-N	6.25	127.65	119.84
6	W	50	ILE	C-N-CA	6.25	127.65	119.84
6	7	17	GLU	N-CA-C	-6.24	104.39	111.07
2	L	60	ASP	CA-C-N	6.23	125.91	119.56
2	L	60	ASP	C-N-CA	6.23	125.91	119.56
7	v	17	LEU	CB-CA-C	6.23	122.81	110.42
6	u	47	ILE	N-CA-CB	6.22	119.91	110.58
7	s	15	TRP	N-CA-C	6.22	118.99	107.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	G	50	ILE	CA-C-N	6.20	127.59	119.84
6	G	50	ILE	C-N-CA	6.20	127.59	119.84
5	Y	44	ARG	N-CA-C	-6.19	101.32	110.48
7	p	17	LEU	CA-C-N	6.17	132.07	122.26
7	p	17	LEU	C-N-CA	6.17	132.07	122.26
3	M	25	ASP	N-CA-C	-6.16	105.60	113.23
5	z	47	TRP	N-CA-C	-6.16	100.82	110.36
5	6	16	ASP	CA-C-N	6.15	125.64	119.24
5	6	16	ASP	C-N-CA	6.15	125.64	119.24
7	R	18	TRP	CB-CA-C	-6.14	99.84	110.09
7	y	15	TRP	N-CA-C	6.13	118.40	108.41
5	q	44	ARG	N-CA-C	-6.13	102.88	110.41
6	x	47	ILE	N-CA-C	6.12	116.29	110.53
6	Z	16	LYS	N-CA-C	-6.12	103.29	112.54
6	7	50	ILE	CA-C-N	6.11	127.48	119.84
6	7	50	ILE	C-N-CA	6.11	127.48	119.84
5	V	54	LEU	CA-C-N	6.10	125.58	119.24
5	V	54	LEU	C-N-CA	6.10	125.58	119.24
5	q	47	TRP	N-CA-C	-6.09	101.95	110.35
5	n	40	LEU	CA-CB-CG	6.08	137.58	116.30
5	n	44	ARG	N-CA-C	-6.08	101.93	110.50
5	6	15	LEU	N-CA-C	6.07	121.56	114.04
6	o	50	ILE	CA-C-N	6.05	126.88	120.11
6	o	50	ILE	C-N-CA	6.05	126.88	120.11
6	G	17	GLU	N-CA-C	-6.04	104.62	111.14
7	s	17	LEU	CB-CA-C	6.04	122.43	110.42
5	t	44	ARG	N-CA-C	-6.03	102.00	110.50
5	n	52	ARG	N-CA-C	-6.01	105.94	113.28
7	X	15	TRP	CB-CA-C	6.00	120.04	110.19
5	Y	16	ASP	CA-C-N	6.00	126.16	119.32
5	Y	16	ASP	C-N-CA	6.00	126.16	119.32
7	O	17	LEU	CB-CA-C	6.00	120.58	111.70
5	b	44	ARG	N-CA-CB	-6.00	101.78	110.36
7	X	18	TRP	CB-CA-C	-6.00	100.08	110.09
5	b	40	LEU	CA-CB-CG	5.99	137.28	116.30
1	C	252	THR	CB-CA-C	-5.99	103.85	111.70
5	6	54	LEU	CA-C-N	5.99	125.47	119.24
5	6	54	LEU	C-N-CA	5.99	125.47	119.24
5	F	44	ARG	N-CA-C	-5.97	102.64	110.53
7	j	17	LEU	CB-CA-C	5.97	122.30	110.42
6	u	17	GLU	N-CA-C	-5.96	104.91	111.82
6	u	50	ILE	CA-C-N	5.95	127.28	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	u	50	ILE	C-N-CA	5.95	127.28	119.84
5	k	52	ARG	N-CA-C	-5.95	105.12	112.38
5	Y	40	LEU	CB-CA-C	5.94	121.23	110.72
1	C	152	LEU	N-CA-CB	-5.93	102.52	110.77
6	x	46	TRP	CA-C-N	-5.93	112.97	120.56
6	x	46	TRP	C-N-CA	-5.93	112.97	120.56
6	W	9	GLY	N-CA-C	-5.92	103.48	111.54
5	e	40	LEU	CA-CB-CG	5.92	137.03	116.30
5	Y	47	TRP	N-CA-C	-5.90	101.22	110.36
5	F	16	ASP	CA-C-N	5.87	127.18	119.84
5	F	16	ASP	C-N-CA	5.87	127.18	119.84
6	T	11	THR	N-CA-C	5.86	119.19	111.28
3	M	88	PHE	N-CA-C	5.84	118.11	111.11
5	P	40	LEU	CA-CB-CG	5.82	136.68	116.30
5	Y	40	LEU	CA-CB-CG	5.81	136.63	116.30
5	S	40	LEU	CA-CB-CG	5.79	136.56	116.30
6	G	11	THR	N-CA-C	5.78	119.22	111.24
6	Q	46	TRP	N-CA-C	5.78	118.79	111.69
1	C	146	ARG	N-CA-C	5.77	118.88	109.06
5	3	48	TRP	CB-CA-C	-5.77	101.33	110.04
6	f	47	ILE	N-CA-CB	5.77	119.23	110.58
7	2	17	LEU	CA-C-N	5.76	131.42	122.26
7	2	17	LEU	C-N-CA	5.76	131.42	122.26
5	q	54	LEU	CB-CA-C	5.75	115.28	111.20
2	L	7	ARG	N-CA-C	5.75	117.22	111.07
6	N	46	TRP	N-CA-C	5.75	119.47	112.23
5	q	54	LEU	CA-C-N	5.73	125.85	119.32
5	q	54	LEU	C-N-CA	5.73	125.85	119.32
7	j	17	LEU	CA-C-N	5.71	131.14	121.14
7	j	17	LEU	C-N-CA	5.71	131.14	121.14
5	P	56	LYS	N-CA-C	-5.71	105.59	113.18
6	4	50	ILE	CA-C-N	5.69	126.95	119.84
6	4	50	ILE	C-N-CA	5.69	126.95	119.84
5	n	15	LEU	N-CA-C	5.68	120.71	113.55
7	d	17	LEU	CB-CA-C	5.68	121.72	110.42
5	t	54	LEU	CA-C-N	5.67	125.78	119.32
5	t	54	LEU	C-N-CA	5.67	125.78	119.32
7	O	14	ASP	CA-C-N	-5.65	115.14	123.05
7	O	14	ASP	C-N-CA	-5.65	115.14	123.05
5	b	16	ASP	CA-C-N	5.64	126.89	119.84
5	b	16	ASP	C-N-CA	5.64	126.89	119.84
4	H	49	LEU	N-CA-C	5.63	117.59	108.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	t	15	LEU	N-CA-C	5.62	120.15	113.12
1	C	252	THR	N-CA-C	5.59	116.54	107.32
6	u	11	THR	N-CA-C	5.58	122.70	110.80
6	c	6	SER	N-CA-C	5.57	117.17	109.15
3	M	147	ASN	N-CA-C	-5.57	105.11	111.07
5	6	47	TRP	N-CA-C	-5.55	103.05	110.55
6	Q	16	LYS	N-CA-C	-5.55	105.72	112.88
7	d	17	LEU	CA-C-N	5.53	129.45	120.60
7	d	17	LEU	C-N-CA	5.53	129.45	120.60
7	5	17	LEU	CA-C-N	5.53	132.35	122.06
7	5	17	LEU	C-N-CA	5.53	132.35	122.06
5	t	44	ARG	N-CA-CB	-5.51	102.23	110.17
5	z	45	LEU	N-CA-C	5.51	119.59	112.86
7	I	17	LEU	CB-CA-C	5.51	121.38	110.42
7	p	18	TRP	N-CA-C	-5.51	106.56	113.72
5	q	15	LEU	N-CA-C	5.50	120.48	113.55
5	V	34	LEU	CB-CA-C	-5.50	102.25	110.88
7	g	17	LEU	CB-CA-C	5.47	121.30	110.42
5	z	56	LYS	N-CA-C	-5.46	106.54	113.43
6	W	46	TRP	CA-C-N	-5.46	113.58	120.56
6	W	46	TRP	C-N-CA	-5.46	113.58	120.56
5	K	44	ARG	N-CA-CB	-5.45	102.32	110.17
6	u	9	GLY	N-CA-C	-5.45	104.98	111.36
7	5	17	LEU	CB-CA-C	5.44	121.25	110.42
4	H	60	TYR	N-CA-C	-5.44	99.22	110.80
5	3	15	LEU	N-CA-C	5.44	120.57	113.88
5	z	40	LEU	CB-CA-C	5.43	120.33	110.72
7	R	18	TRP	N-CA-C	-5.43	106.33	113.17
1	C	274	VAL	N-CA-CB	5.42	117.92	110.54
5	n	44	ARG	N-CA-CB	-5.42	102.36	110.17
5	V	40	LEU	CA-CB-CG	5.42	135.27	116.30
5	w	40	LEU	CA-CB-CG	5.41	135.24	116.30
6	Q	11	THR	N-CA-C	5.41	122.32	110.80
3	M	254	ILE	N-CA-C	-5.40	107.54	113.43
5	3	44	ARG	N-CA-CB	-5.40	102.24	110.45
6	l	46	TRP	N-CA-C	5.40	119.97	112.90
7	a	15	TRP	N-CA-C	5.40	117.46	108.02
7	X	17	LEU	CA-C-N	5.38	131.42	122.54
7	X	17	LEU	C-N-CA	5.38	131.42	122.54
7	d	15	TRP	N-CA-C	5.38	117.17	108.34
5	z	44	ARG	N-CA-CB	-5.38	102.13	110.04
5	Y	44	ARG	N-CA-CB	-5.37	102.13	110.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	2	15	TRP	N-CA-C	5.37	117.16	108.41
3	M	173	VAL	CB-CA-C	-5.36	105.74	111.00
2	L	19	GLY	N-CA-C	5.36	125.89	113.18
5	K	40	LEU	CA-CB-CG	5.35	135.03	116.30
5	P	15	LEU	N-CA-C	5.35	120.29	113.55
5	b	52	ARG	N-CA-C	-5.35	106.76	113.28
7	s	17	LEU	CA-C-N	5.34	130.92	120.99
7	s	17	LEU	C-N-CA	5.34	130.92	120.99
7	U	18	TRP	CB-CA-C	-5.33	99.35	109.95
5	F	54	LEU	CA-C-N	5.32	125.38	119.32
5	F	54	LEU	C-N-CA	5.32	125.38	119.32
7	U	15	TRP	N-CA-C	5.30	118.07	107.62
5	k	48	TRP	CA-CB-CG	5.30	123.67	113.60
5	k	56	LYS	N-CA-C	-5.30	106.13	113.18
5	q	40	LEU	N-CA-CB	5.30	118.25	110.57
6	T	46	TRP	N-CA-C	5.29	118.89	112.23
6	u	16	LYS	N-CA-C	-5.29	106.06	112.88
5	P	48	TRP	CA-CB-CG	5.29	123.65	113.60
5	k	44	ARG	N-CA-CB	-5.27	102.58	110.17
6	Z	46	TRP	N-CA-C	5.27	119.80	112.90
5	n	54	LEU	CA-C-N	5.26	124.72	119.24
5	n	54	LEU	C-N-CA	5.26	124.72	119.24
7	y	17	LEU	CA-C-N	5.26	131.36	122.26
7	y	17	LEU	C-N-CA	5.26	131.36	122.26
5	z	30	VAL	N-CA-C	5.25	115.36	110.42
6	N	47	ILE	N-CA-CB	5.25	120.27	110.77
5	q	52	ARG	N-CA-C	-5.24	105.74	111.82
2	L	65	SER	N-CA-C	5.24	117.71	108.75
7	m	18	TRP	CB-CA-C	-5.24	100.76	109.55
7	R	17	LEU	CA-C-N	5.23	131.17	122.54
7	R	17	LEU	C-N-CA	5.23	131.17	122.54
3	M	195	TYR	N-CA-C	-5.23	105.66	111.36
6	o	17	GLU	N-CA-C	-5.23	105.66	111.36
5	6	40	LEU	CA-CB-CG	5.23	134.60	116.30
7	U	17	LEU	CA-C-N	5.22	131.76	121.58
7	U	17	LEU	C-N-CA	5.22	131.76	121.58
6	o	11	THR	N-CA-C	5.22	119.03	111.56
5	S	52	ARG	N-CA-C	-5.22	106.18	112.54
5	V	44	ARG	N-CA-CB	-5.21	102.91	110.36
5	P	44	ARG	N-CA-CB	-5.20	101.94	110.41
5	h	56	LYS	N-CA-C	-5.19	106.27	113.18
5	V	48	TRP	CB-CA-C	-5.19	100.44	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	G	47	ILE	N-CA-CB	5.18	116.61	110.55
5	w	48	TRP	N-CA-CB	5.17	119.24	110.49
4	H	170	ASP	N-CA-C	5.16	116.65	108.96
7	X	14	ASP	CA-C-N	-5.16	115.83	123.05
7	X	14	ASP	C-N-CA	-5.16	115.83	123.05
6	r	11	THR	N-CA-C	5.16	118.93	111.56
5	w	48	TRP	CA-C-N	-5.15	114.15	122.81
5	w	48	TRP	C-N-CA	-5.15	114.15	122.81
5	P	54	LEU	CA-C-N	5.15	125.19	119.32
5	P	54	LEU	C-N-CA	5.15	125.19	119.32
7	I	15	TRP	CB-CA-C	5.15	118.71	110.16
7	m	17	LEU	CA-C-N	5.15	130.45	122.26
7	m	17	LEU	C-N-CA	5.15	130.45	122.26
5	w	40	LEU	CB-CA-C	5.15	120.50	110.57
5	V	26	VAL	N-CA-C	5.14	115.36	110.42
5	t	40	LEU	CB-CA-C	5.14	120.48	110.57
5	P	40	LEU	N-CA-CB	5.13	118.37	110.46
6	x	9	GLY	N-CA-C	-5.13	101.01	113.18
5	w	9	TRP	N-CA-C	5.13	118.32	111.75
5	e	52	ARG	N-CA-C	-5.13	106.97	113.18
5	K	54	LEU	CA-C-N	5.13	126.25	119.84
5	K	54	LEU	C-N-CA	5.13	126.25	119.84
7	5	15	TRP	N-CA-C	5.12	117.71	107.62
1	C	81	VAL	CB-CA-C	-5.12	107.36	111.71
7	2	18	TRP	CB-CA-C	-5.12	100.95	109.55
1	C	146	ARG	CA-CB-CG	-5.11	103.88	114.10
6	u	46	TRP	N-CA-C	5.11	119.60	112.90
7	m	17	LEU	N-CA-C	5.11	116.93	107.73
2	L	38	ALA	N-CA-C	-5.10	105.41	110.97
5	q	16	ASP	CA-C-N	5.10	126.21	119.84
5	q	16	ASP	C-N-CA	5.10	126.21	119.84
6	Z	47	ILE	N-CA-C	5.09	115.87	110.72
5	3	40	LEU	CB-CA-C	5.09	120.14	110.27
5	k	15	LEU	N-CA-C	5.08	120.14	113.88
5	K	16	ASP	CA-C-N	5.08	126.19	119.84
5	K	16	ASP	C-N-CA	5.08	126.19	119.84
5	P	9	TRP	N-CA-C	5.08	118.26	111.75
4	H	50	VAL	N-CA-C	5.08	119.90	109.34
7	y	18	TRP	N-CA-C	-5.08	107.13	113.38
4	H	96	PHE	N-CA-C	5.08	117.40	110.24
7	g	18	TRP	CB-CA-C	-5.07	100.93	110.67
6	c	8	THR	CA-C-N	5.07	124.78	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	c	8	THR	C-N-CA	5.07	124.78	119.92
6	7	47	ILE	N-CA-CB	5.07	118.18	110.58
2	L	238	SER	N-CA-C	5.06	117.53	111.71
4	H	95	GLY	CA-C-N	5.06	128.03	120.90
4	H	95	GLY	C-N-CA	5.06	128.03	120.90
6	1	47	ILE	N-CA-C	5.04	115.27	110.53
5	e	48	TRP	CA-CB-CG	5.04	123.18	113.60
7	s	18	TRP	CB-CA-C	-5.04	99.17	110.21
1	C	149	GLU	N-CA-C	-5.03	103.20	110.40
2	L	20	ASP	N-CA-C	5.03	119.13	112.89
5	h	40	LEU	CA-CB-CG	5.03	133.90	116.30
6	f	17	GLU	N-CA-C	-5.01	105.70	111.07
5	n	9	TRP	N-CA-C	5.01	118.16	111.75
6	4	46	TRP	CA-C-N	-5.00	114.16	120.56
6	4	46	TRP	C-N-CA	-5.00	114.16	120.56

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

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Mol	Chain	Res	Type	Group
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
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)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2603	0	2587	86	0
2	L	2171	0	2098	85	0
3	M	2555	0	2452	55	0
4	H	2018	0	2020	56	0
5	3	487	0	506	43	0
5	6	487	0	506	72	0
5	F	487	0	506	50	0
5	K	487	0	506	36	0
5	P	487	0	506	37	0
5	S	487	0	506	40	0
5	V	487	0	506	27	0
5	Y	487	0	506	39	0
5	b	487	0	506	41	0
5	e	487	0	506	48	0
5	h	487	0	506	42	0
5	k	487	0	506	20	0
5	n	487	0	506	34	0
5	q	487	0	506	43	0
5	t	487	0	506	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	w	487	0	506	37	0
5	z	487	0	506	30	0
6	1	436	0	445	19	0
6	4	436	0	445	33	0
6	7	436	0	445	22	0
6	G	436	0	445	46	0
6	N	436	0	445	47	0
6	Q	436	0	445	39	0
6	T	436	0	445	52	0
6	W	436	0	445	29	0
6	Z	436	0	445	28	0
6	c	436	0	445	34	0
6	f	436	0	445	34	0
6	i	436	0	445	49	0
6	l	436	0	445	34	0
6	o	436	0	445	35	0
6	r	436	0	445	45	0
6	u	436	0	445	57	0
6	x	436	0	445	38	0
7	2	199	0	202	18	0
7	5	199	0	202	16	0
7	I	199	0	202	18	0
7	O	199	0	202	15	0
7	R	199	0	202	20	0
7	U	199	0	202	11	0
7	X	199	0	202	25	0
7	a	199	0	202	16	0
7	d	199	0	202	5	0
7	g	199	0	202	13	0
7	j	199	0	202	17	0
7	m	199	0	202	23	0
7	p	199	0	202	12	0
7	s	199	0	202	20	0
7	v	199	0	202	10	0
7	y	199	0	202	12	0
8	C	172	0	128	39	0
9	1	66	0	72	15	0
9	3	66	0	72	9	0
9	4	66	0	72	19	0
9	6	66	0	72	16	0
9	7	66	0	71	16	0
9	F	66	0	72	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	G	66	0	72	13	0
9	K	66	0	72	10	0
9	L	132	0	144	20	0
9	M	132	0	144	16	0
9	N	66	0	72	16	0
9	P	66	0	72	7	0
9	Q	66	0	72	16	0
9	S	66	0	72	8	0
9	T	66	0	72	17	0
9	V	66	0	72	8	0
9	W	66	0	72	11	0
9	Y	66	0	72	12	0
9	Z	66	0	72	15	0
9	b	66	0	72	8	0
9	c	66	0	72	14	0
9	e	66	0	72	18	0
9	f	66	0	72	11	0
9	h	66	0	72	10	0
9	i	66	0	72	12	0
9	k	66	0	72	7	0
9	l	66	0	72	17	0
9	n	66	0	72	8	0
9	o	66	0	72	16	0
9	q	66	0	69	6	0
9	r	66	0	72	11	0
9	t	66	0	72	10	0
9	u	66	0	72	8	0
9	w	66	0	72	3	0
9	x	66	0	72	9	0
9	z	66	0	72	10	0
10	L	65	0	74	11	0
10	M	65	0	74	6	0
11	6	58	0	82	39	0
11	L	58	0	82	21	0
12	M	1	0	0	0	0
13	H	15	0	0	0	0
13	M	20	0	0	0	0
14	H	16	0	31	0	0
14	M	16	0	31	3	0
15	M	58	0	80	4	0
16	M	40	0	60	4	0
17	1	40	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	4	40	0	0	6	0
17	7	40	0	0	7	0
17	G	40	0	0	20	0
17	N	40	0	0	13	0
17	Q	40	0	0	10	0
17	T	40	0	0	11	0
17	W	40	0	0	10	0
17	Z	40	0	0	4	0
17	c	40	0	0	6	0
17	f	40	0	0	11	0
17	i	40	0	0	14	0
17	l	40	0	0	14	0
17	o	40	0	0	7	0
17	r	40	0	0	10	0
17	u	40	0	0	12	0
17	x	40	0	0	8	0
All	All	31994	0	31930	1816	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 28.

All (1816) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:u:21:ILE:HG21	17:u:102:NS0:C8	1.22	1.63
6:o:47:ILE:CD1	7:m:17:LEU:HD22	1.30	1.57
6:u:47:ILE:CD1	7:s:17:LEU:HD22	1.30	1.57
6:r:21:ILE:CG2	17:r:102:NS0:C8	1.74	1.56
6:x:21:ILE:CG2	17:x:102:NS0:C8	1.77	1.56
5:F:44:ARG:HG2	6:N:54:TRP:CH2	1.07	1.55
5:F:44:ARG:CG	6:N:54:TRP:CH2	1.91	1.52
6:x:21:ILE:HG21	17:x:102:NS0:C8	1.07	1.52
9:6:102:BCB:HAA1	17:G:102:NS0:C34	1.42	1.48
6:Q:21:ILE:CG2	17:Q:102:NS0:C8	1.91	1.48
9:6:102:BCB:H3A	17:G:102:NS0:C34	1.44	1.47
6:u:21:ILE:CG2	17:u:102:NS0:C8	1.91	1.47
6:N:21:ILE:HG21	17:N:102:NS0:C8	1.45	1.45
5:b:44:ARG:HG2	6:f:54:TRP:CH2	1.51	1.44
1:C:132:CYS:SG	8:C:402:HEC:CAB	2.07	1.43
5:q:44:ARG:HG2	6:u:54:TRP:CH2	1.51	1.43
1:C:132:CYS:SG	8:C:402:HEC:HAB	1.58	1.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:CYS:SG	8:C:403:HEC:CAB	2.08	1.42
5:e:44:ARG:HG2	6:i:54:TRP:CH2	1.56	1.40
5:6:39:LEU:CD2	5:6:45:LEU:HD13	1.51	1.40
5:e:44:ARG:HG2	6:i:54:TRP:CZ3	1.58	1.39
6:T:21:ILE:CG2	17:T:102:NS0:C8	2.01	1.38
6:Q:21:ILE:CB	17:Q:102:NS0:C8	2.02	1.37
6:c:47:ILE:CD1	7:a:17:LEU:HD22	1.57	1.34
6:G:21:ILE:HB	17:G:102:NS0:C8	1.58	1.33
5:h:39:LEU:CD2	5:h:45:LEU:HD13	1.58	1.32
6:4:21:ILE:CG2	17:4:102:NS0:C8	2.08	1.32
6:o:47:ILE:HD11	7:m:17:LEU:CD2	1.61	1.31
6:r:21:ILE:CB	17:r:102:NS0:C8	2.08	1.31
6:u:47:ILE:HD11	7:s:17:LEU:CD2	1.59	1.30
6:o:54:TRP:CD1	6:o:55:VAL:H	1.47	1.30
6:Q:21:ILE:HG21	17:Q:102:NS0:C8	1.52	1.29
6:l:21:ILE:HG21	17:l:102:NS0:C8	1.61	1.29
5:6:18:ARG:HH12	5:6:19:ARG:CZ	1.45	1.29
6:T:21:ILE:CB	17:T:102:NS0:C8	2.11	1.29
1:C:247:CYS:SG	8:C:403:HEC:CAC	2.22	1.27
5:6:23:ALA:O	5:6:27:TYR:CD2	1.86	1.27
5:6:23:ALA:O	5:6:27:TYR:HD2	1.04	1.26
6:W:21:ILE:CG2	17:W:102:NS0:C8	2.13	1.26
5:b:44:ARG:HG2	6:f:54:TRP:CZ3	1.71	1.26
6:W:21:ILE:CB	17:W:102:NS0:C8	2.13	1.25
6:4:21:ILE:HG21	17:4:102:NS0:C8	1.62	1.25
6:T:21:ILE:HB	17:T:102:NS0:C8	1.65	1.25
1:C:135:CYS:SG	8:C:402:HEC:CAC	2.25	1.24
1:C:244:CYS:SG	8:C:403:HEC:HAB	1.74	1.23
6:N:21:ILE:CG2	17:N:102:NS0:C8	2.17	1.22
6:Z:47:ILE:CG2	7:X:17:LEU:HD13	1.70	1.21
6:W:21:ILE:HG21	17:W:102:NS0:C8	1.69	1.21
5:F:44:ARG:HG2	6:N:54:TRP:CZ3	1.76	1.20
9:6:102:BCB:C3A	17:G:102:NS0:C34	2.18	1.20
1:C:146:ARG:NH1	1:C:190:PHE:HB2	1.55	1.20
6:c:54:TRP:CD1	6:c:55:VAL:H	1.61	1.19
6:Q:21:ILE:HB	17:Q:102:NS0:C8	1.65	1.19
5:Y:4:TYR:CE2	6:Z:16:LYS:HD3	1.77	1.18
6:W:21:ILE:HB	17:W:102:NS0:C8	1.70	1.18
6:G:21:ILE:CB	17:G:102:NS0:C8	2.21	1.17
6:i:21:ILE:HB	17:i:102:NS0:C8	1.75	1.17
6:T:21:ILE:HG21	17:T:102:NS0:C8	1.64	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:4:TYR:HE2	6:G:16:LYS:HD3	1.01	1.15
6:T:54:TRP:CD1	6:T:55:VAL:H	1.64	1.15
2:L:25:TRP:O	5:3:19:ARG:NH1	1.79	1.15
5:K:39:LEU:HD22	5:K:45:LEU:HD23	1.15	1.15
6:4:54:TRP:CD1	6:4:55:VAL:H	1.65	1.15
6:o:21:ILE:CG2	17:o:102:NS0:C8	2.25	1.14
6:r:21:ILE:HB	17:r:102:NS0:C8	1.76	1.14
6:G:50:ILE:HD11	6:7:43:ALA:O	1.47	1.14
5:h:39:LEU:CD2	5:h:45:LEU:CD1	2.26	1.13
1:C:308:CYS:SG	8:C:404:HEC:CAC	2.36	1.13
3:M:209:GLY:O	3:M:213:LEU:HD13	1.48	1.13
5:h:39:LEU:HD22	5:h:45:LEU:CD1	1.77	1.13
6:c:47:ILE:HD11	7:a:17:LEU:HD22	1.26	1.13
5:6:39:LEU:HD22	5:6:45:LEU:HD13	1.20	1.13
6:o:54:TRP:CD1	6:o:55:VAL:N	2.17	1.13
4:H:57:GLY:H	5:w:19:ARG:HG3	1.14	1.12
5:6:39:LEU:CD2	5:6:45:LEU:CD1	2.27	1.12
6:i:21:ILE:CB	17:i:102:NS0:C8	2.27	1.12
5:6:39:LEU:HD23	5:6:45:LEU:CD1	1.78	1.12
5:b:44:ARG:CG	6:f:54:TRP:CH2	2.32	1.12
5:6:18:ARG:HH12	5:6:19:ARG:NE	1.48	1.12
6:l:54:TRP:CD1	6:l:55:VAL:H	1.67	1.11
5:3:45:LEU:CD2	9:4:101:BCB:HBC3	1.79	1.11
6:i:21:ILE:CG1	17:i:102:NS0:C8	2.27	1.11
6:o:47:ILE:HD11	7:m:17:LEU:CG	1.80	1.11
7:5:25:GLY:O	7:5:28:THR:HG22	1.49	1.11
5:b:44:ARG:HA	6:f:54:TRP:HZ3	1.01	1.10
6:x:21:ILE:CB	17:x:102:NS0:C8	2.29	1.10
6:c:47:ILE:HD13	7:a:17:LEU:HD22	1.33	1.10
6:o:47:ILE:CD1	7:m:17:LEU:CD2	2.20	1.10
5:e:44:ARG:CG	6:i:54:TRP:CH2	2.34	1.10
9:6:102:BCB:CAA	17:G:102:NS0:C34	2.30	1.09
6:G:54:TRP:CD1	6:G:55:VAL:H	1.72	1.08
6:4:21:ILE:CB	17:4:102:NS0:C8	2.30	1.08
5:q:44:ARG:CG	6:u:54:TRP:CH2	2.35	1.08
5:b:44:ARG:HA	6:f:54:TRP:CZ3	1.88	1.07
6:r:54:TRP:CD1	6:r:55:VAL:H	1.71	1.07
6:r:21:ILE:HG22	17:r:102:NS0:C8	1.73	1.07
6:c:47:ILE:HD11	7:a:17:LEU:CD2	1.84	1.07
6:o:47:ILE:HD13	7:m:17:LEU:HD22	1.11	1.07
5:3:45:LEU:HD21	9:4:101:BCB:HBC3	1.14	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:M:408:BPB:HHC	10:M:408:BPB:HBBB	1.35	1.06
6:G:21:ILE:CG2	17:G:102:NS0:C8	2.34	1.06
6:W:54:TRP:CD1	6:W:55:VAL:H	1.74	1.06
6:r:21:ILE:HG21	17:r:102:NS0:C8	1.52	1.06
5:F:4:TYR:CE2	6:G:16:LYS:HD3	1.90	1.05
9:7:101:BCB:C2	17:7:102:NS0:C29	2.33	1.05
5:h:39:LEU:HD22	5:h:45:LEU:HD13	1.08	1.05
6:u:47:ILE:CD1	7:s:17:LEU:CD2	2.25	1.05
5:q:47:TRP:O	5:q:48:TRP:HB2	1.55	1.05
6:u:47:ILE:HD13	7:s:17:LEU:HD22	1.27	1.05
6:Z:47:ILE:HG21	7:X:17:LEU:HD13	1.36	1.05
1:C:247:CYS:SG	8:C:403:HEC:HAC	1.95	1.04
6:o:47:ILE:HD11	7:m:17:LEU:HD22	1.06	1.04
6:4:54:TRP:CD1	6:4:55:VAL:N	2.26	1.04
5:q:44:ARG:HA	6:u:54:TRP:HZ3	1.21	1.04
6:i:54:TRP:CD1	6:i:55:VAL:H	1.76	1.04
5:6:37:PHE:HB3	11:6:101:UQ9:H35	1.35	1.04
6:l:21:ILE:CG2	17:l:102:NS0:C8	2.35	1.04
5:3:26:VAL:HG22	11:6:101:UQ9:H4M	1.38	1.03
6:l:54:TRP:CD1	6:l:55:VAL:N	2.26	1.03
5:Y:1:ALA:HB1	5:Y:4:TYR:HD2	1.21	1.03
6:T:54:TRP:CD1	6:T:55:VAL:N	2.26	1.03
6:o:21:ILE:HG21	17:o:102:NS0:C8	1.86	1.03
10:L:303:BPB:HHC	10:L:303:BPB:HBBB	1.34	1.03
5:t:39:LEU:HD22	5:t:45:LEU:HD22	1.38	1.03
6:4:21:ILE:HB	17:4:102:NS0:C8	1.88	1.03
6:x:54:TRP:CD1	6:x:55:VAL:H	1.75	1.03
5:e:44:ARG:CG	6:i:54:TRP:CZ3	2.42	1.02
1:C:146:ARG:HH12	1:C:190:PHE:HB2	0.90	1.02
7:2:16:ASN:O	7:2:17:LEU:HD23	1.59	1.02
2:L:18:GLY:HA2	5:6:19:ARG:HH21	1.23	1.02
5:K:45:LEU:HD21	9:N:101:BCB:HBC3	1.40	1.02
5:3:39:LEU:HD22	5:3:45:LEU:HD23	1.43	1.01
6:N:21:ILE:HD13	17:N:102:NS0:C8	1.90	1.01
5:Y:1:ALA:HB1	5:Y:4:TYR:CD2	1.95	1.01
9:F:101:BCB:HAA1	17:N:102:NS0:C34	1.91	1.01
5:Y:4:TYR:HE2	6:Z:16:LYS:HD3	0.86	1.01
6:Z:47:ILE:HG23	7:X:17:LEU:HD13	1.42	1.01
5:6:37:PHE:HB3	11:6:101:UQ9:C35	1.90	1.00
5:F:44:ARG:CG	6:N:54:TRP:CZ3	2.39	1.00
6:r:54:TRP:CD1	6:r:55:VAL:N	2.28	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:q:44:ARG:HA	6:u:54:TRP:CZ3	1.95	1.00
5:Y:45:LEU:HD22	9:Z:101:BCB:HBC1	1.44	0.99
6:i:21:ILE:HD13	17:i:102:NS0:C8	1.91	0.99
1:C:205:PRO:HG2	3:M:290:ASP:OD1	1.62	0.99
1:C:90:CYS:SG	8:C:401:HEC:CAC	2.50	0.99
7:j:24:LEU:O	7:j:28:THR:HG23	1.63	0.98
7:y:16:ASN:O	7:y:17:LEU:HD23	1.62	0.98
9:K:101:BCB:H93	17:N:102:NS0:C18	1.93	0.98
2:L:87:GLN:OE1	11:6:101:UQ9:H40A	1.62	0.98
5:K:39:LEU:CD2	5:K:45:LEU:HD23	1.93	0.98
6:c:54:TRP:CD1	6:c:55:VAL:N	2.31	0.97
5:S:45:LEU:HD22	9:T:101:BCB:HBC1	1.43	0.97
10:L:303:BPB:HHC	10:L:303:BPB:CBB	1.94	0.97
11:L:304:UQ9:H31A	11:L:304:UQ9:H35	1.46	0.97
6:f:54:TRP:CD1	6:f:55:VAL:H	1.83	0.96
6:G:54:TRP:CD1	6:G:55:VAL:N	2.32	0.96
6:i:21:ILE:HD13	17:i:102:NS0:C7	1.94	0.95
6:r:25:SER:OG	17:r:102:NS0:C14	2.14	0.95
7:O:16:ASN:O	7:O:17:LEU:HD23	1.67	0.95
5:K:39:LEU:HD22	5:K:45:LEU:CD2	1.95	0.95
5:6:18:ARG:NH1	5:6:19:ARG:CZ	2.29	0.95
5:t:39:LEU:CD2	5:t:45:LEU:HD13	1.95	0.95
6:i:54:TRP:CD1	6:i:55:VAL:N	2.35	0.94
5:t:42:THR:OG1	5:t:45:LEU:HD12	1.67	0.94
2:L:141:SER:OG	2:L:144:HIS:CD2	2.22	0.93
6:o:54:TRP:CG	6:o:55:VAL:H	1.85	0.93
5:3:26:VAL:HG22	11:6:101:UQ9:C4M	1.98	0.93
4:H:60:TYR:H	4:H:60:TYR:HD1	1.16	0.93
6:o:54:TRP:CG	6:o:55:VAL:N	2.35	0.93
5:t:39:LEU:HD22	5:t:45:LEU:HD13	1.48	0.92
6:u:21:ILE:CB	17:u:102:NS0:C8	2.48	0.92
5:S:45:LEU:CD2	9:T:101:BCB:HBC1	1.98	0.92
6:i:21:ILE:CD1	17:i:102:NS0:C8	2.47	0.92
9:N:101:BCB:CHB	7:I:24:LEU:HD21	2.00	0.92
5:P:45:LEU:HD22	9:Q:101:BCB:HBC1	1.50	0.91
5:t:39:LEU:HD22	5:t:45:LEU:CD2	1.99	0.91
6:u:47:ILE:HD11	7:s:17:LEU:CG	2.00	0.91
5:t:39:LEU:CD2	5:t:45:LEU:HD22	1.99	0.91
5:q:44:ARG:HG2	6:u:54:TRP:CZ3	2.05	0.91
6:Q:54:TRP:CD1	6:Q:55:VAL:H	1.88	0.91
6:N:21:ILE:CB	17:N:102:NS0:C8	2.49	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:45:LEU:CD2	9:Z:101:BCB:HBC1	2.00	0.90
6:W:54:TRP:CD1	6:W:55:VAL:N	2.39	0.90
6:f:54:TRP:CD1	6:f:55:VAL:N	2.39	0.90
5:h:39:LEU:HD23	5:h:45:LEU:CD1	1.98	0.90
5:F:29:THR:O	5:F:33:LEU:HD13	1.70	0.90
5:S:39:LEU:CD2	5:S:45:LEU:HD13	2.02	0.90
5:6:18:ARG:NH1	5:6:19:ARG:NE	2.20	0.90
6:u:54:TRP:CD1	6:u:55:VAL:H	1.90	0.89
6:u:47:ILE:HD11	7:s:17:LEU:HD22	0.90	0.89
5:6:23:ALA:C	5:6:27:TYR:HD2	1.80	0.89
6:N:54:TRP:CD1	6:N:55:VAL:N	2.40	0.89
7:U:16:ASN:O	7:U:17:LEU:HD23	1.72	0.89
6:u:54:TRP:CD1	6:u:55:VAL:N	2.40	0.89
6:r:44:ARG:NH1	6:u:50:ILE:HG13	1.87	0.89
5:6:23:ALA:HB1	5:6:27:TYR:HE2	1.37	0.89
5:P:48:TRP:O	5:P:49:GLU:HB2	1.71	0.88
7:g:16:ASN:O	7:g:17:LEU:HD23	1.73	0.88
5:P:44:ARG:HG3	6:T:54:TRP:CH2	2.07	0.88
1:C:214:VAL:O	1:C:214:VAL:HG12	1.71	0.88
5:e:44:ARG:HA	6:i:54:TRP:HZ3	1.39	0.88
6:x:54:TRP:CD1	6:x:55:VAL:N	2.41	0.88
7:v:16:ASN:O	7:v:17:LEU:HD23	1.73	0.88
5:t:42:THR:OG1	5:t:45:LEU:CD1	2.22	0.87
5:e:25:PHE:CD1	9:e:101:BCB:H92	2.08	0.87
4:H:52:LEU:HG	4:H:52:LEU:O	1.72	0.87
5:6:39:LEU:HD23	5:6:45:LEU:HD13	1.32	0.87
5:e:48:TRP:O	5:e:49:GLU:HB2	1.73	0.87
6:i:54:TRP:CG	6:i:55:VAL:N	2.36	0.87
6:c:47:ILE:CD1	7:a:17:LEU:CD2	2.45	0.86
6:c:47:ILE:HD11	7:a:17:LEU:CG	2.07	0.85
5:b:44:ARG:CG	6:f:54:TRP:CZ3	2.57	0.85
9:b:101:BCB:HAA1	17:f:102:NS0:C34	2.06	0.85
9:Y:101:BCB:H93	17:Z:102:NS0:C18	2.07	0.84
9:M:407:BCB:CBD	9:M:407:BCB:HAA2	2.07	0.84
5:h:42:THR:OG1	5:h:45:LEU:HD12	1.76	0.84
5:3:45:LEU:CD2	9:4:101:BCB:CBC	2.55	0.84
6:i:21:ILE:HG12	17:i:102:NS0:C8	2.07	0.84
9:L:301:BCB:H2C	9:M:407:BCB:H2C	1.60	0.84
5:6:39:LEU:HD23	5:6:45:LEU:HD11	1.59	0.84
9:7:101:BCB:CHB	7:5:24:LEU:HD21	2.06	0.84
6:N:54:TRP:CD1	6:N:55:VAL:H	1.96	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Z:47:ILE:HG23	7:X:17:LEU:CD1	2.07	0.83
6:l:23:VAL:HA	6:l:26:THR:HG22	1.60	0.83
5:t:39:LEU:CD2	5:t:45:LEU:CD2	2.57	0.83
5:t:39:LEU:HD22	5:t:45:LEU:CD1	2.08	0.83
5:6:37:PHE:CB	11:6:101:UQ9:H35	2.08	0.83
9:N:101:BCB:HHB	7:I:24:LEU:HD21	1.58	0.83
6:f:54:TRP:CG	6:f:55:VAL:N	2.42	0.83
5:F:4:TYR:HE2	6:G:16:LYS:CD	1.86	0.83
7:X:17:LEU:HD22	7:X:19:VAL:CG2	2.09	0.83
9:r:101:BCB:CHB	7:p:24:LEU:HD21	2.09	0.83
9:L:301:BCB:HMB1	9:L:301:BCB:HBB3	1.59	0.82
5:e:25:PHE:HD1	9:e:101:BCB:H92	1.43	0.82
7:g:24:LEU:O	7:g:28:THR:HG23	1.79	0.82
10:M:408:BPB:HHC	10:M:408:BPB:CBB	2.09	0.82
5:t:39:LEU:CD2	5:t:45:LEU:CD1	2.57	0.82
1:C:308:CYS:SG	8:C:404:HEC:HAC	2.17	0.82
7:p:24:LEU:O	7:p:28:THR:HG23	1.79	0.82
5:n:45:LEU:HD22	9:o:101:BCB:HBC1	1.60	0.82
6:l:54:TRP:CG	6:l:55:VAL:N	2.45	0.82
5:b:48:TRP:O	5:b:49:GLU:HB2	1.80	0.82
6:l:25:SER:OG	17:l:102:NS0:C14	2.28	0.82
6:c:54:TRP:CG	6:c:55:VAL:H	1.91	0.82
5:Y:28:LEU:HB3	9:Y:101:BCB:H12	1.61	0.81
2:L:226:ALA:HA	11:L:304:UQ9:C3M	2.11	0.81
1:C:135:CYS:SG	8:C:402:HEC:HAC	2.18	0.81
7:2:16:ASN:O	7:2:17:LEU:CD2	2.28	0.81
9:F:101:BCB:H93	17:G:102:NS0:C18	2.11	0.81
6:Z:47:ILE:CG2	7:X:17:LEU:CD1	2.54	0.81
7:5:25:GLY:O	7:5:28:THR:CG2	2.27	0.81
6:N:21:ILE:CD1	17:N:102:NS0:C8	2.58	0.81
6:x:54:TRP:CG	6:x:55:VAL:N	2.48	0.81
5:S:39:LEU:HD22	5:S:45:LEU:HD13	1.60	0.81
5:3:25:PHE:CE2	11:6:101:UQ9:H3M	2.16	0.81
7:5:25:GLY:C	7:5:28:THR:HG22	2.06	0.81
9:M:406:BCB:HBB2	9:M:406:BCB:HHC	1.60	0.81
9:1:101:BCB:CHB	7:y:24:LEU:HD21	2.10	0.81
1:C:146:ARG:HH12	1:C:190:PHE:CB	1.85	0.81
11:L:304:UQ9:H31A	11:L:304:UQ9:C35	2.11	0.80
4:H:57:GLY:N	5:w:19:ARG:HG3	1.95	0.80
4:H:58:GLN:HB3	4:H:61:GLU:HG3	1.62	0.80
6:u:54:TRP:CG	6:u:55:VAL:N	2.46	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:37:ARG:HD2	4:H:61:GLU:HG2	1.64	0.80
5:t:37:PHE:CZ	17:x:102:NS0:C40	2.64	0.80
5:6:21:LEU:HD11	6:7:18:PHE:HZ	1.46	0.80
5:6:23:ALA:HB1	5:6:27:TYR:CE2	2.16	0.80
6:N:54:TRP:CG	6:N:55:VAL:N	2.48	0.80
9:6:102:BCB:H71	17:7:102:NS0:C18	2.12	0.79
5:6:39:LEU:HD22	5:6:45:LEU:CD1	1.99	0.79
6:T:54:TRP:CG	6:T:55:VAL:N	2.47	0.79
7:d:16:ASN:O	7:d:17:LEU:HD23	1.83	0.79
1:C:135:CYS:SG	8:C:402:HEC:CBC	2.70	0.79
2:L:193:LEU:HD23	11:L:304:UQ9:C2	2.13	0.79
6:x:32:THR:HA	6:x:35:ILE:HD12	1.62	0.79
1:C:152:LEU:HD22	1:C:175:ARG:HA	1.65	0.79
9:M:407:BCB:HAA2	9:M:407:BCB:HBD	1.63	0.79
6:r:54:TRP:CG	6:r:55:VAL:N	2.49	0.79
7:X:16:ASN:O	7:X:17:LEU:HD23	1.83	0.79
5:F:44:ARG:HG3	6:N:54:TRP:CH2	2.15	0.79
9:V:101:BCB:H93	17:W:102:NS0:C18	2.13	0.78
7:2:24:LEU:HD21	9:4:101:BCB:CHB	2.13	0.78
9:P:101:BCB:H93	17:Q:102:NS0:C18	2.13	0.78
6:4:54:TRP:CG	6:4:55:VAL:N	2.48	0.78
1:C:205:PRO:CG	3:M:290:ASP:OD1	2.31	0.78
7:2:24:LEU:HD21	9:4:101:BCB:HHB	1.64	0.78
6:c:32:THR:HA	6:c:35:ILE:HD12	1.65	0.78
4:H:133:LYS:HD2	4:H:176:SER:HB2	1.66	0.78
7:I:16:ASN:O	7:I:17:LEU:HD23	1.84	0.78
5:h:39:LEU:HD22	5:h:45:LEU:CD2	2.13	0.78
5:e:45:LEU:CD2	9:f:101:BCB:HBC1	2.13	0.78
6:T:47:ILE:HD11	7:R:17:LEU:HD13	1.64	0.78
5:P:45:LEU:CD2	9:Q:101:BCB:HBC1	2.14	0.77
5:h:42:THR:OG1	5:h:45:LEU:CD1	2.32	0.77
6:Q:54:TRP:CD1	6:Q:55:VAL:N	2.51	0.77
9:1:101:BCB:HHB	7:y:24:LEU:HD21	1.66	0.77
6:G:21:ILE:HG21	17:G:102:NS0:C8	2.14	0.77
5:P:37:PHE:CE1	17:T:102:NS0:C40	2.68	0.77
5:h:39:LEU:HD22	5:h:45:LEU:HD22	1.66	0.77
9:e:101:BCB:H72	17:f:102:NS0:C18	2.15	0.77
9:Q:101:BCB:CHB	7:O:24:LEU:HD21	2.15	0.77
9:i:101:BCB:CHB	7:g:24:LEU:HD21	2.15	0.76
5:b:44:ARG:CA	6:f:54:TRP:HZ3	1.91	0.76
7:s:16:ASN:C	7:s:17:LEU:HG	2.10	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:CYS:SG	8:C:403:HEC:CBB	2.73	0.76
6:1:3:LEU:H	6:1:6:SER:HB3	1.50	0.76
5:V:36:HIS:CE1	9:W:101:BCB:HMD1	2.20	0.76
6:c:54:TRP:CG	6:c:55:VAL:N	2.45	0.76
9:S:101:BCB:HAA1	17:W:102:NS0:C34	2.16	0.75
6:c:47:ILE:HD11	7:a:17:LEU:CD1	2.16	0.75
4:H:258:LEU:HB3	5:F:19:ARG:HD2	1.69	0.75
5:3:39:LEU:CD2	5:3:45:LEU:HD23	2.16	0.75
5:P:36:HIS:CE1	9:Q:101:BCB:HMD1	2.22	0.75
5:P:44:ARG:CG	6:T:54:TRP:CH2	2.70	0.75
5:k:36:HIS:CE1	9:l:101:BCB:HMD1	2.22	0.75
1:C:132:CYS:SG	8:C:402:HEC:CBB	2.73	0.75
6:o:32:THR:HA	6:o:35:ILE:HD12	1.69	0.75
6:x:54:TRP:CG	6:x:55:VAL:H	2.02	0.75
7:m:16:ASN:C	7:m:17:LEU:HG	2.10	0.75
5:h:39:LEU:CD2	5:h:45:LEU:CD2	2.65	0.75
6:G:50:ILE:CD1	6:7:43:ALA:O	2.33	0.75
6:o:47:ILE:HD11	7:m:17:LEU:CD1	2.16	0.75
7:X:17:LEU:HD22	7:X:19:VAL:HG21	1.68	0.75
5:h:39:LEU:HD23	5:h:45:LEU:HD11	1.67	0.75
9:c:101:BCB:CHB	7:a:24:LEU:HD21	2.17	0.75
7:p:16:ASN:C	7:p:17:LEU:HG	2.12	0.74
4:H:37:ARG:CD	4:H:61:GLU:HG2	2.17	0.74
6:c:54:TRP:O	6:c:55:VAL:HG22	1.86	0.74
9:7:101:BCB:HHB	7:5:24:LEU:HD21	1.70	0.74
1:C:146:ARG:NH1	1:C:190:PHE:CB	2.46	0.74
6:u:21:ILE:HG22	17:u:102:NS0:C8	2.15	0.74
6:x:21:ILE:HB	17:x:102:NS0:C8	2.15	0.74
4:H:258:LEU:H	5:F:19:ARG:CD	2.00	0.74
9:f:101:BCB:CHB	7:d:24:LEU:HD21	2.16	0.74
5:Y:40:LEU:HD23	5:Y:47:TRP:CH2	2.22	0.74
6:Q:54:TRP:CG	6:Q:55:VAL:N	2.54	0.74
6:4:3:LEU:H	6:4:6:SER:HB3	1.52	0.74
7:p:16:ASN:O	7:p:17:LEU:HG	1.87	0.74
2:L:87:GLN:OE1	11:6:101:UQ9:C40	2.35	0.74
5:b:28:LEU:HB3	9:b:101:BCB:H12	1.68	0.74
5:P:37:PHE:CZ	17:T:102:NS0:C40	2.71	0.74
9:T:101:BCB:CHB	7:R:24:LEU:HD21	2.18	0.74
6:W:54:TRP:CG	6:W:55:VAL:H	2.02	0.74
6:l:54:TRP:HD1	6:l:55:VAL:H	1.32	0.74
5:S:44:ARG:HG2	6:W:54:TRP:CH2	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:b:101:BCB:H93	17:c:102:NS0:C18	2.18	0.73
6:4:54:TRP:HD1	6:4:55:VAL:H	1.29	0.73
5:q:44:ARG:CB	6:u:54:TRP:CH2	2.71	0.73
6:W:54:TRP:CG	6:W:55:VAL:N	2.48	0.73
5:b:36:HIS:CE1	9:c:101:BCB:HMD1	2.23	0.73
5:b:44:ARG:CA	6:f:54:TRP:CZ3	2.69	0.73
5:6:44:ARG:HG2	6:G:54:TRP:CH2	2.23	0.73
5:F:44:ARG:HA	6:N:54:TRP:HZ3	1.53	0.73
5:q:36:HIS:CE1	9:r:101:BCB:HMD1	2.24	0.73
2:L:18:GLY:CA	5:6:19:ARG:HH21	2.01	0.73
5:h:36:HIS:CE1	9:i:101:BCB:HMD1	2.24	0.73
2:L:51:TYR:HE1	5:z:40:LEU:HD11	1.54	0.73
2:L:190:HIS:ND1	11:L:304:UQ9:O2	2.22	0.73
5:q:44:ARG:HG2	6:u:54:TRP:CZ2	2.20	0.73
6:u:32:THR:HA	6:u:35:ILE:HD12	1.69	0.73
5:P:39:LEU:CD2	5:P:45:LEU:HD13	2.19	0.72
4:H:56:ASP:OD1	5:w:19:ARG:NH1	2.23	0.72
6:o:54:TRP:HD1	6:o:55:VAL:H	1.27	0.72
5:e:47:TRP:HE1	9:e:101:BCB:HBB3	1.54	0.72
5:w:36:HIS:CE1	9:x:101:BCB:HMD1	2.24	0.72
6:Q:25:SER:OG	17:Q:102:NS0:C14	2.36	0.72
5:Y:47:TRP:CE2	9:Y:101:BCB:H2C	2.24	0.72
5:h:39:LEU:HD22	5:h:45:LEU:CG	2.19	0.72
6:i:21:ILE:CD1	17:i:102:NS0:C7	2.66	0.72
5:F:44:ARG:CD	6:N:54:TRP:CH2	2.73	0.72
6:x:21:ILE:HG22	17:x:102:NS0:C8	2.13	0.72
5:e:44:ARG:CB	6:i:54:TRP:CH2	2.73	0.72
5:n:36:HIS:CE1	9:o:101:BCB:HMD1	2.25	0.72
5:Y:4:TYR:HE2	6:Z:16:LYS:CD	1.82	0.71
5:e:45:LEU:HD22	9:f:101:BCB:HBC1	1.70	0.71
6:l:18:PHE:HB2	17:l:102:NS0:CD1	2.20	0.71
5:h:39:LEU:CD2	5:h:45:LEU:HD22	2.19	0.71
5:6:23:ALA:C	5:6:27:TYR:CD2	2.62	0.71
5:z:45:LEU:HD22	9:1:101:BCB:HBC1	1.70	0.71
5:6:47:TRP:CE2	9:6:102:BCB:H2C	2.26	0.71
5:3:39:LEU:HD22	5:3:45:LEU:CD2	2.20	0.71
2:L:141:SER:OG	2:L:144:HIS:HD2	1.72	0.71
5:z:36:HIS:CE1	9:1:101:BCB:HMD1	2.26	0.71
6:T:47:ILE:HD12	6:T:48:ALA:N	2.05	0.71
6:Q:41:TRP:CG	7:O:14:ASP:OD1	2.43	0.71
2:L:226:ALA:HA	11:L:304:UQ9:H3MA	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1:25:SER:OG	17:1:102:NS0:C14	2.38	0.71
5:S:45:LEU:CD2	9:T:101:BCB:CBC	2.68	0.71
5:e:44:ARG:HA	6:i:54:TRP:CZ3	2.22	0.71
5:3:36:HIS:CE1	9:4:101:BCB:HMD1	2.26	0.71
5:Y:45:LEU:CD2	9:Z:101:BCB:CBC	2.69	0.70
6:W:23:VAL:HA	6:W:26:THR:HG22	1.74	0.70
6:N:3:LEU:H	6:N:6:SER:HB3	1.56	0.70
6:T:32:THR:HA	6:T:35:ILE:HD12	1.73	0.70
9:l:101:BCB:CBB	9:l:101:BCB:HMB1	2.21	0.70
5:q:10:LYS:HB2	17:o:102:NS0:CD1	2.22	0.70
2:L:241:PHE:HE2	10:L:303:BPB:H43	1.57	0.70
5:q:44:ARG:CG	6:u:54:TRP:CZ3	2.68	0.70
5:t:36:HIS:CE1	9:u:101:BCB:HMD1	2.27	0.70
5:3:45:LEU:HD21	9:4:101:BCB:CBC	2.06	0.70
6:c:47:ILE:HD11	7:a:17:LEU:HD13	1.74	0.70
6:r:3:LEU:H	6:r:6:SER:HB3	1.56	0.70
2:L:18:GLY:HA2	5:6:19:ARG:NH2	2.02	0.70
5:P:39:LEU:HD22	5:P:45:LEU:HD13	1.74	0.70
5:6:47:TRP:O	5:6:48:TRP:HB2	1.91	0.70
6:G:54:TRP:CG	6:G:55:VAL:N	2.50	0.70
9:Q:101:BCB:HHB	7:O:24:LEU:HD21	1.72	0.70
5:K:36:HIS:CE1	9:N:101:BCB:HMD1	2.27	0.69
6:r:54:TRP:HD1	6:r:55:VAL:H	1.32	0.69
3:M:209:GLY:O	3:M:213:LEU:CD1	2.33	0.69
3:M:213:LEU:N	3:M:213:LEU:HD12	2.06	0.69
6:T:54:TRP:HD1	6:T:55:VAL:H	1.30	0.69
6:G:26:THR:HB	17:G:102:NS0:C19	2.23	0.69
5:K:45:LEU:CD2	9:N:101:BCB:HBC3	2.21	0.69
6:f:13:GLU:HG2	6:f:14:GLU:N	2.07	0.69
7:O:16:ASN:O	7:O:17:LEU:CD2	2.41	0.69
6:N:21:ILE:HB	17:N:102:NS0:C8	2.23	0.69
6:7:30:LEU:HD21	9:7:101:BCB:H43	1.75	0.69
2:L:51:TYR:HE1	5:z:40:LEU:CD1	2.05	0.68
9:f:101:BCB:CBB	9:f:101:BCB:HMB1	2.24	0.68
5:n:45:LEU:CD2	9:o:101:BCB:HBC1	2.23	0.68
6:T:46:TRP:CE2	9:T:101:BCB:H2C	2.27	0.68
6:u:46:TRP:CE2	9:u:101:BCB:H2C	2.28	0.68
5:F:44:ARG:HG3	6:N:54:TRP:CZ3	2.27	0.68
6:r:44:ARG:HH11	6:u:50:ILE:HG13	1.57	0.68
5:F:40:LEU:HD23	5:F:47:TRP:CH2	2.28	0.68
9:K:101:BCB:HMB1	9:K:101:BCB:HBB3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:5:16:ASN:O	7:5:17:LEU:HD23	1.93	0.68
6:G:32:THR:HA	6:G:35:ILE:HD12	1.76	0.68
6:o:4:LYS:HB2	6:o:5:PRO:HD3	1.76	0.67
5:Y:36:HIS:CE1	9:Z:101:BCB:HMD1	2.28	0.67
6:Z:46:TRP:CE2	9:Z:101:BCB:H2C	2.29	0.67
5:n:39:LEU:CD2	5:n:45:LEU:HD13	2.24	0.67
6:u:21:ILE:HB	17:u:102:NS0:C8	2.24	0.67
5:k:44:ARG:HG2	6:o:54:TRP:CH2	2.30	0.67
6:l:21:ILE:CB	17:l:102:NS0:C8	2.71	0.67
1:C:90:CYS:SG	8:C:401:HEC:C3C	2.82	0.67
5:F:36:HIS:CE1	9:G:101:BCB:HMD1	2.30	0.67
6:r:23:VAL:HA	6:r:26:THR:HG22	1.77	0.67
1:C:214:VAL:O	1:C:214:VAL:CG1	2.43	0.67
5:K:45:LEU:HD21	9:N:101:BCB:CBC	2.23	0.67
9:h:101:BCB:HBB2	9:h:101:BCB:HMB1	1.75	0.67
6:Q:21:ILE:HG22	17:Q:102:NS0:C8	2.17	0.67
7:y:16:ASN:O	7:y:17:LEU:CD2	2.39	0.67
4:H:256:SER:C	4:H:258:LEU:OXT	2.38	0.66
5:V:47:TRP:O	5:V:48:TRP:HB2	1.94	0.66
5:V:49:GLU:HG3	5:V:50:PHE:N	2.11	0.66
5:e:9:TRP:HB2	6:f:16:LYS:HB3	1.76	0.66
5:6:37:PHE:HB3	11:6:101:UQ9:H35A	1.76	0.66
2:L:241:PHE:CE2	10:L:303:BPB:H43	2.31	0.66
5:K:39:LEU:CD2	5:K:45:LEU:CD2	2.66	0.66
5:e:36:HIS:CE1	9:f:101:BCB:HMD1	2.28	0.66
5:e:39:LEU:CD2	5:e:45:LEU:HD13	2.25	0.66
6:N:13:GLU:HG2	6:N:14:GLU:N	2.10	0.66
6:o:54:TRP:CD1	6:o:55:VAL:CA	2.78	0.66
1:C:262:PRO:HA	3:M:312:THR:HG21	1.78	0.66
9:S:101:BCB:H61	9:W:101:BCB:H102	1.77	0.66
5:3:47:TRP:CE2	9:3:101:BCB:H2C	2.31	0.66
5:z:47:TRP:HE3	5:z:47:TRP:H	1.42	0.66
6:1:32:THR:HA	6:1:35:ILE:HD12	1.77	0.66
9:Y:101:BCB:HBB2	17:c:102:NS0:C39	2.26	0.66
5:6:36:HIS:CE1	9:7:101:BCB:HMD1	2.31	0.66
6:W:46:TRP:CE2	9:W:101:BCB:H2C	2.30	0.66
9:f:101:BCB:HMB1	9:f:101:BCB:HBB2	1.77	0.66
4:H:56:ASP:HB2	5:w:22:THR:OG1	1.96	0.66
5:3:40:LEU:HB2	5:3:46:ASN:OD1	1.96	0.66
5:t:47:TRP:O	5:t:48:TRP:HB2	1.94	0.66
5:h:47:TRP:H	5:h:47:TRP:HE3	1.44	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:42:THR:OG1	5:6:45:LEU:HD12	1.95	0.66
6:T:21:ILE:HG22	17:T:102:NS0:C8	2.19	0.66
5:t:47:TRP:CE2	9:t:101:BCB:H2C	2.31	0.65
6:N:46:TRP:CE2	9:N:101:BCB:H2C	2.32	0.65
8:C:402:HEC:HMC1	8:C:402:HEC:HBC3	1.78	0.65
5:b:45:LEU:HD22	9:c:101:BCB:HBC1	1.78	0.65
5:t:39:LEU:HD23	5:t:45:LEU:CD1	2.26	0.65
6:G:54:TRP:HD1	6:G:55:VAL:H	1.36	0.65
5:e:44:ARG:CB	6:i:54:TRP:HH2	2.09	0.65
7:s:16:ASN:O	7:s:17:LEU:HG	1.95	0.65
5:e:44:ARG:HB3	6:i:54:TRP:HH2	1.60	0.65
5:n:45:LEU:HD22	9:o:101:BCB:CBC	2.27	0.65
6:Q:41:TRP:CD2	7:O:14:ASP:OD1	2.49	0.65
6:T:47:ILE:CD1	7:R:17:LEU:HD22	2.26	0.65
9:F:101:BCB:H142	9:N:101:BCB:H192	1.79	0.65
5:t:44:ARG:HG3	6:x:54:TRP:CH2	2.31	0.65
6:Q:32:THR:HA	6:Q:35:ILE:HD12	1.79	0.65
6:c:54:TRP:HD1	6:c:55:VAL:H	1.38	0.65
6:4:23:VAL:HA	6:4:26:THR:HG22	1.79	0.65
3:M:275:MET:HE2	3:M:275:MET:HA	1.79	0.65
9:W:101:BCB:CHB	7:U:24:LEU:HD21	2.26	0.65
9:o:101:BCB:HMB1	9:o:101:BCB:CBB	2.27	0.65
5:S:47:TRP:CE2	9:S:101:BCB:H2C	2.32	0.65
11:6:101:UQ9:H4MB	11:6:101:UQ9:C3M	2.26	0.65
6:o:47:ILE:HD13	7:m:17:LEU:CD2	2.05	0.65
7:j:16:ASN:C	7:j:17:LEU:HG	2.21	0.65
1:C:305:CYS:HB3	8:C:404:HEC:HAB	1.79	0.65
5:K:8:SER:HA	17:G:102:NS0:C	2.27	0.65
5:t:18:ARG:HD3	5:w:14:ILE:O	1.96	0.65
9:i:101:BCB:CBB	9:i:101:BCB:HMB1	2.26	0.65
1:C:247:CYS:SG	8:C:403:HEC:C3C	2.84	0.64
9:e:101:BCB:H102	17:f:102:NS0:C13	2.26	0.64
11:6:101:UQ9:C4M	11:6:101:UQ9:H3MB	2.27	0.64
6:T:41:TRP:NE1	7:R:14:ASP:HA	2.13	0.64
6:u:41:TRP:CG	7:s:14:ASP:OD1	2.50	0.64
9:L:301:BCB:H172	9:L:302:BCB:H111	1.78	0.64
5:V:47:TRP:CE2	9:V:101:BCB:H2C	2.32	0.64
11:L:304:UQ9:H35	11:L:304:UQ9:C31	2.18	0.64
5:6:27:TYR:HE1	11:6:101:UQ9:C5	2.11	0.64
6:u:46:TRP:CD2	9:u:101:BCB:H2C	2.33	0.64
5:6:19:ARG:HA	5:6:22:THR:HG22	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Z:41:TRP:HE1	7:X:13:SER:C	2.04	0.64
6:4:13:GLU:HG2	6:4:14:GLU:N	2.13	0.64
5:6:17:PRO:O	5:6:21:LEU:HD13	1.97	0.64
5:K:47:TRP:CE2	9:K:101:BCB:H2C	2.32	0.64
5:K:49:GLU:HG3	5:K:50:PHE:N	2.13	0.64
5:Y:45:LEU:HD22	9:Z:101:BCB:CBC	2.25	0.64
6:W:32:THR:HA	6:W:35:ILE:HD12	1.80	0.64
6:r:46:TRP:CD2	9:r:101:BCB:H2C	2.33	0.64
5:z:44:ARG:HA	6:4:54:TRP:CZ3	2.33	0.64
9:V:101:BCB:CBB	9:V:101:BCB:HMB1	2.28	0.64
5:h:47:TRP:CE2	9:h:101:BCB:H2C	2.32	0.64
5:q:44:ARG:CA	6:u:54:TRP:CZ3	2.79	0.64
8:C:403:HEC:HBB3	8:C:403:HEC:HMB3	1.78	0.64
9:6:102:BCB:C4A	17:G:102:NS0:C34	2.75	0.64
6:x:23:VAL:HA	6:x:26:THR:HG22	1.78	0.64
9:n:101:BCB:HMB1	9:n:101:BCB:HBB3	1.80	0.64
11:6:101:UQ9:H10A	11:6:101:UQ9:H13	1.80	0.64
9:T:101:BCB:HBB2	9:T:101:BCB:HMB1	1.80	0.64
2:L:266:TRP:CD1	2:L:266:TRP:C	2.76	0.63
5:S:45:LEU:HD21	9:T:101:BCB:CBC	2.26	0.63
6:G:13:GLU:HG2	6:G:14:GLU:N	2.12	0.63
9:W:101:BCB:HHB	7:U:24:LEU:HD21	1.80	0.63
6:i:23:VAL:HA	6:i:26:THR:HG22	1.80	0.63
9:o:101:BCB:HMB1	9:o:101:BCB:HBB2	1.78	0.63
11:6:101:UQ9:H35	11:6:101:UQ9:H30A	1.79	0.63
9:6:102:BCB:C2A	17:G:102:NS0:C34	2.76	0.63
1:C:202:ARG:HD3	8:C:403:HEC:O2A	1.99	0.63
3:M:32:PRO:HB3	3:M:45:GLN:HE21	1.63	0.63
5:P:40:LEU:HD23	5:P:47:TRP:CZ2	2.33	0.63
6:r:46:TRP:CE2	9:r:101:BCB:H2C	2.34	0.63
5:F:47:TRP:HE3	5:F:47:TRP:H	1.44	0.63
5:q:47:TRP:CD1	5:q:48:TRP:HD1	2.16	0.63
6:T:25:SER:OG	17:T:102:NS0:C14	2.46	0.63
5:q:44:ARG:CB	6:u:54:TRP:HH2	2.10	0.63
6:Q:46:TRP:CE2	9:Q:101:BCB:H2C	2.34	0.63
6:Q:46:TRP:CD2	9:Q:101:BCB:H2C	2.34	0.63
7:m:25:GLY:O	7:m:28:THR:HG22	1.99	0.63
5:K:40:LEU:HD23	5:K:47:TRP:CH2	2.34	0.63
9:i:101:BCB:H62	17:i:102:NS0:C24	2.29	0.63
6:o:54:TRP:CD1	6:o:55:VAL:HA	2.34	0.63
7:5:14:ASP:OD2	7:5:21:LEU:HD11	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:44:ARG:HA	6:T:54:TRP:HZ3	1.64	0.63
5:P:45:LEU:CD2	9:Q:101:BCB:CBC	2.76	0.63
5:S:36:HIS:CE1	9:T:101:BCB:HMD1	2.33	0.63
5:Y:39:LEU:CD2	5:Y:45:LEU:HD13	2.29	0.63
5:q:47:TRP:HE3	5:q:47:TRP:H	1.47	0.63
6:Z:32:THR:HA	6:Z:35:ILE:HD12	1.80	0.63
6:l:54:TRP:CD1	6:l:55:VAL:CA	2.82	0.63
5:Y:47:TRP:O	5:Y:48:TRP:HB2	1.98	0.62
5:q:37:PHE:CZ	17:u:102:NS0:C40	2.82	0.62
4:H:258:LEU:C	4:H:258:LEU:HD12	2.24	0.62
5:F:44:ARG:HA	6:N:54:TRP:CZ3	2.34	0.62
5:n:45:LEU:CD2	9:o:101:BCB:CBC	2.76	0.62
1:C:146:ARG:CZ	1:C:190:PHE:HB2	2.26	0.62
5:K:47:TRP:H	5:K:47:TRP:HE3	1.46	0.62
5:3:40:LEU:HD23	5:3:47:TRP:CH2	2.34	0.62
6:T:42:THR:HA	7:R:13:SER:OG	1.99	0.62
6:T:47:ILE:HD11	7:R:17:LEU:CD1	2.29	0.62
6:c:25:SER:OG	17:c:102:NS0:C14	2.46	0.62
5:F:29:THR:O	5:F:33:LEU:CD1	2.44	0.62
5:6:29:THR:O	5:6:33:LEU:HG	1.99	0.62
5:V:37:PHE:CE1	17:Z:102:NS0:C40	2.82	0.62
5:6:45:LEU:H	6:G:54:TRP:HH2	1.47	0.62
6:N:46:TRP:CD2	9:N:101:BCB:H2C	2.35	0.62
5:Y:45:LEU:HD21	9:Z:101:BCB:CBC	2.29	0.62
5:t:39:LEU:HD22	5:t:45:LEU:CG	2.30	0.62
6:N:41:TRP:HE1	7:I:13:SER:C	2.07	0.62
6:Q:21:ILE:CG1	17:Q:102:NS0:C8	2.77	0.62
4:H:56:ASP:OD2	5:w:22:THR:HG21	1.99	0.62
5:z:45:LEU:CD2	9:1:101:BCB:HBC1	2.30	0.62
5:k:47:TRP:CE2	9:k:101:BCB:H2C	2.35	0.62
6:W:46:TRP:CD2	9:W:101:BCB:H2C	2.34	0.62
1:C:90:CYS:HB3	1:C:103:PRO:HB2	1.81	0.61
3:M:41:ILE:HG22	3:M:41:ILE:O	1.98	0.61
9:z:101:BCB:HMB1	9:z:101:BCB:CBB	2.30	0.61
6:4:46:TRP:CD2	9:4:101:BCB:H2C	2.35	0.61
1:C:217:GLY:O	1:C:220:ARG:HG3	2.00	0.61
2:L:164:TYR:N	2:L:164:TYR:CD1	2.69	0.61
5:K:44:ARG:HG3	6:Q:54:TRP:CH2	2.35	0.61
5:P:40:LEU:HD23	5:P:47:TRP:CH2	2.35	0.61
5:S:47:TRP:H	5:S:47:TRP:HE3	1.44	0.61
5:q:11:LEU:HD11	5:q:15:LEU:HD22	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:u:18:PHE:HD1	17:u:102:NS0:CB	2.12	0.61
11:L:304:UQ9:H4MB	11:L:304:UQ9:O3	2.00	0.61
5:S:45:LEU:HD22	9:T:101:BCB:CBC	2.27	0.61
5:6:31:ILE:O	5:6:34:LEU:HB3	2.00	0.61
6:r:54:TRP:CD1	6:r:55:VAL:CA	2.83	0.61
9:T:101:BCB:HHB	7:R:24:LEU:HD21	1.82	0.61
2:L:272:TRP:CD1	2:L:272:TRP:C	2.78	0.61
5:n:47:TRP:O	5:n:48:TRP:HB2	2.01	0.61
5:n:44:ARG:CG	6:r:54:TRP:CH2	2.84	0.61
6:T:47:ILE:HD11	7:R:17:LEU:HD22	1.80	0.61
2:L:190:HIS:HA	11:L:304:UQ9:H1M	1.83	0.61
7:I:25:GLY:O	7:I:28:THR:HG22	2.01	0.61
6:N:25:SER:OG	17:N:102:NS0:C14	2.48	0.61
5:F:40:LEU:HD23	5:F:47:TRP:CZ2	2.36	0.61
5:F:44:ARG:HG2	6:N:54:TRP:HH2	0.80	0.61
6:i:21:ILE:HD13	17:i:102:NS0:C9	2.31	0.61
6:r:43:ALA:O	6:r:44:ARG:HG2	2.01	0.61
5:n:44:ARG:HA	6:r:54:TRP:CZ3	2.36	0.61
6:Z:46:TRP:CD2	9:Z:101:BCB:H2C	2.36	0.61
9:x:101:BCB:CHB	7:v:24:LEU:HD21	2.31	0.61
5:P:44:ARG:HA	6:T:54:TRP:CZ3	2.35	0.60
5:P:45:LEU:HD22	9:Q:101:BCB:CBC	2.27	0.60
5:q:1:ALA:HA	6:r:16:LYS:NZ	2.15	0.60
6:Q:13:GLU:HG2	6:Q:14:GLU:N	2.14	0.60
6:4:54:TRP:CD1	6:4:55:VAL:CA	2.83	0.60
9:L:301:BCB:HMB1	9:L:301:BCB:CBB	2.31	0.60
6:1:46:TRP:CD2	9:1:101:BCB:H2C	2.36	0.60
5:S:39:LEU:HD21	5:S:45:LEU:HD13	1.81	0.60
9:h:101:BCB:HAA1	17:l:102:NS0:C34	2.31	0.60
11:6:101:UQ9:H3MB	11:6:101:UQ9:O4	2.00	0.60
6:Q:38:TYR:O	6:Q:42:THR:HG23	2.00	0.60
5:F:45:LEU:HD22	9:G:101:BCB:HBC1	1.83	0.60
5:S:1:ALA:HB1	5:S:4:TYR:HB2	1.83	0.60
5:e:45:LEU:HD21	9:f:101:BCB:CBC	2.31	0.60
5:h:47:TRP:O	5:h:48:TRP:HB2	2.02	0.60
6:N:41:TRP:HH2	6:N:47:ILE:HG13	1.64	0.60
6:T:54:TRP:CD1	6:T:55:VAL:CA	2.84	0.60
9:o:101:BCB:HMB2	7:m:24:LEU:HD12	1.83	0.60
6:u:36:VAL:HA	6:u:39:LEU:HD12	1.82	0.60
1:C:108:ARG:NH1	8:C:401:HEC:O2D	2.35	0.60
2:L:115:TRP:O	2:L:118:PRO:HD2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:255:GLU:HA	4:H:255:GLU:OE2	2.00	0.60
6:W:54:TRP:O	6:W:55:VAL:HG22	2.01	0.60
5:K:28:LEU:HD21	17:N:102:NS0:C25	2.32	0.60
5:K:40:LEU:HD23	5:K:47:TRP:CZ2	2.36	0.60
5:Y:1:ALA:CB	5:Y:4:TYR:HD2	2.06	0.60
5:w:1:ALA:HA	6:x:16:LYS:NZ	2.17	0.60
6:i:46:TRP:CE2	9:i:101:BCB:H2C	2.36	0.60
6:x:46:TRP:CE2	9:x:101:BCB:H2C	2.36	0.60
5:z:45:LEU:CD2	9:1:101:BCB:CBC	2.79	0.60
5:F:1:ALA:HB1	5:F:4:TYR:HB2	1.83	0.60
5:n:44:ARG:HG2	6:r:54:TRP:CH2	2.37	0.60
6:c:13:GLU:HG2	6:c:14:GLU:N	2.16	0.60
5:q:47:TRP:CE2	9:q:101:BCB:H2C	2.36	0.60
6:c:46:TRP:CD2	9:c:101:BCB:H2C	2.36	0.60
9:l:101:BCB:HMB2	7:j:24:LEU:HD12	1.84	0.60
6:x:54:TRP:O	6:x:55:VAL:HG22	2.02	0.60
9:7:101:BCB:H2A	9:7:101:BCB:O1D	2.01	0.60
9:F:101:BCB:HBB2	9:F:101:BCB:HMB1	1.82	0.60
5:P:47:TRP:CE2	9:P:101:BCB:H2C	2.36	0.60
2:L:146:PHE:HZ	9:L:302:BCB:HBB2	1.67	0.60
9:L:302:BCB:HBB3	9:L:302:BCB:HHC	1.83	0.60
5:F:48:TRP:O	5:F:49:GLU:HB2	2.02	0.60
5:b:9:TRP:HB2	6:c:16:LYS:HB3	1.84	0.60
6:x:46:TRP:CD2	9:x:101:BCB:H2C	2.37	0.60
4:H:7:ALA:HA	5:q:52:ARG:HH12	1.66	0.60
5:q:28:LEU:HD21	17:r:102:NS0:C25	2.32	0.60
6:Q:23:VAL:HA	6:Q:26:THR:HG22	1.83	0.60
6:W:21:ILE:CG1	17:W:102:NS0:C8	2.79	0.60
6:f:46:TRP:CE2	9:f:101:BCB:H2C	2.37	0.60
6:u:23:VAL:HA	6:u:26:THR:HG22	1.84	0.60
1:C:239:SER:CB	1:C:305:CYS:SG	2.90	0.59
3:M:202:PHE:CE2	4:H:20:GLN:HG2	2.37	0.59
6:1:4:LYS:HB2	6:1:5:PRO:HD3	1.83	0.59
9:Y:101:BCB:CBB	9:Y:101:BCB:HMB1	2.32	0.59
6:o:21:ILE:HG23	17:o:102:NS0:C8	2.31	0.59
5:V:40:LEU:HB2	5:V:46:ASN:OD1	2.01	0.59
6:c:46:TRP:CE2	9:c:101:BCB:H2C	2.36	0.59
1:C:205:PRO:HG2	3:M:290:ASP:CG	2.28	0.59
5:z:45:LEU:HD22	9:1:101:BCB:CBC	2.32	0.59
5:3:45:LEU:HG	9:4:101:BCB:HBC1	1.84	0.59
11:L:304:UQ9:H3MB	11:L:304:UQ9:O4	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:47:TRP:O	5:F:48:TRP:HB2	2.02	0.59
9:k:101:BCB:HMB1	9:k:101:BCB:HBB3	1.83	0.59
5:t:44:ARG:CG	6:x:54:TRP:CH2	2.85	0.59
6:Q:29:TYR:O	6:Q:32:THR:HG22	2.03	0.59
9:1:101:BCB:HBB2	9:1:101:BCB:HMB1	1.83	0.59
9:Y:101:BCB:O2D	7:a:23:ILE:HG23	2.02	0.59
5:k:1:ALA:HA	6:l:16:LYS:HE3	1.83	0.59
11:6:101:UQ9:H4MB	11:6:101:UQ9:O3	2.00	0.59
6:f:46:TRP:CD2	9:f:101:BCB:H2C	2.38	0.59
7:v:17:LEU:HD22	7:v:19:VAL:CG2	2.33	0.59
5:3:1:ALA:HB1	5:3:4:TYR:HB2	1.83	0.59
5:6:18:ARG:NH1	5:6:19:ARG:CG	2.66	0.59
6:c:23:VAL:HA	6:c:26:THR:HG22	1.85	0.59
6:l:21:ILE:HG22	17:l:102:NS0:C10	2.32	0.59
5:b:47:TRP:CE2	9:b:101:BCB:H2C	2.37	0.59
6:7:11:THR:O	6:7:12:GLU:HB2	2.01	0.59
7:p:15:TRP:O	7:p:17:LEU:HD12	2.03	0.59
5:3:47:TRP:HE3	5:3:47:TRP:H	1.48	0.59
9:G:101:BCB:H122	17:G:102:NS0:C24	2.33	0.59
6:T:46:TRP:CD2	9:T:101:BCB:H2C	2.38	0.59
6:x:13:GLU:HG2	6:x:14:GLU:N	2.18	0.59
5:3:26:VAL:CG2	11:6:101:UQ9:H4M	2.25	0.58
5:6:27:TYR:HE1	11:6:101:UQ9:C4	2.16	0.58
6:r:54:TRP:CD1	6:r:55:VAL:HA	2.38	0.58
5:K:48:TRP:O	5:K:49:GLU:HB2	2.02	0.58
5:V:47:TRP:HE3	5:V:47:TRP:H	1.47	0.58
6:W:4:LYS:HB2	6:W:5:PRO:HD3	1.85	0.58
2:L:214:GLN:HG3	3:M:19:VAL:HB	1.85	0.58
9:6:102:BCB:H141	9:G:101:BCB:H193	1.86	0.58
9:G:101:BCB:H3A	9:G:101:BCB:H11	1.84	0.58
2:L:226:ALA:O	2:L:229:ILE:HG22	2.03	0.58
6:1:46:TRP:CE2	9:1:101:BCB:H2C	2.38	0.58
5:K:29:THR:O	5:K:33:LEU:HG	2.03	0.58
5:6:1:ALA:HB1	5:6:4:TYR:HB2	1.85	0.58
6:o:23:VAL:HA	6:o:26:THR:HG22	1.85	0.58
9:i:101:BCB:HMB1	9:i:101:BCB:HBB2	1.86	0.58
1:C:133:TYR:O	1:C:137:ARG:HD3	2.04	0.58
5:V:47:TRP:HB3	6:Z:47:ILE:CD1	2.34	0.58
5:k:40:LEU:HB2	5:k:46:ASN:OD1	2.02	0.58
5:n:39:LEU:HD22	5:n:45:LEU:HD13	1.85	0.58
5:6:40:LEU:HD23	5:6:47:TRP:CH2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Q:54:TRP:O	6:Q:55:VAL:HG22	2.03	0.58
5:3:25:PHE:CE2	11:6:101:UQ9:C3M	2.86	0.58
6:f:23:VAL:HA	6:f:26:THR:HG22	1.84	0.58
9:l:101:BCB:HMB1	9:l:101:BCB:HBB3	1.86	0.58
6:4:21:ILE:HG22	17:4:102:NS0:C8	2.25	0.58
6:4:54:TRP:CD1	6:4:55:VAL:HA	2.39	0.58
6:7:32:THR:O	6:7:36:VAL:HG23	2.04	0.58
7:R:16:ASN:C	7:R:17:LEU:HG	2.28	0.58
5:3:47:TRP:O	5:3:48:TRP:HB2	2.04	0.58
9:Z:101:BCB:HMB2	7:X:24:LEU:HD12	1.85	0.58
9:L:302:BCB:C1B	10:L:303:BPB:H20A	2.34	0.57
5:b:45:LEU:CD2	9:c:101:BCB:HBC1	2.34	0.57
6:c:4:LYS:HB2	6:c:5:PRO:HD3	1.85	0.57
2:L:146:PHE:CZ	9:L:302:BCB:HBB2	2.39	0.57
5:b:40:LEU:HB2	5:b:46:ASN:OD1	2.04	0.57
5:h:44:ARG:HA	6:l:54:TRP:CZ3	2.39	0.57
6:Q:4:LYS:HB2	6:Q:5:PRO:HD3	1.85	0.57
9:u:101:BCB:CHB	7:s:24:LEU:HD21	2.34	0.57
5:V:47:TRP:CB	6:Z:47:ILE:HD12	2.34	0.57
9:e:101:BCB:H121	17:f:102:NS0:C13	2.34	0.57
6:i:30:LEU:HB3	7:g:28:THR:HG22	1.85	0.57
9:l:101:BCB:H41	7:j:27:PRO:HB2	1.84	0.57
1:C:90:CYS:SG	8:C:401:HEC:HAC	2.41	0.57
6:T:4:LYS:HB2	6:T:5:PRO:HD3	1.86	0.57
6:l:46:TRP:CD2	9:l:101:BCB:H2C	2.39	0.57
6:o:47:ILE:HD11	7:m:17:LEU:HD13	1.86	0.57
6:4:46:TRP:CE2	9:4:101:BCB:H2C	2.39	0.57
5:K:14:ILE:HG13	17:G:102:NS0:CD2	2.34	0.57
6:T:54:TRP:O	6:T:55:VAL:HG22	2.04	0.57
6:4:54:TRP:O	6:4:55:VAL:HG22	2.04	0.57
5:P:29:THR:O	5:P:33:LEU:HG	2.05	0.57
5:n:47:TRP:CE2	9:n:101:BCB:H2C	2.39	0.57
6:N:26:THR:HB	17:N:102:NS0:C19	2.35	0.57
6:i:25:SER:OG	17:i:102:NS0:C14	2.53	0.57
7:g:14:ASP:OD1	7:g:17:LEU:O	2.23	0.57
4:H:257:LEU:C	4:H:258:LEU:OXT	2.47	0.57
5:S:49:GLU:HG3	5:S:50:PHE:N	2.19	0.57
5:6:21:LEU:HD11	6:7:18:PHE:CZ	2.35	0.57
5:6:47:TRP:HE3	5:6:47:TRP:H	1.51	0.57
1:C:52:VAL:HG13	1:C:56:TYR:CD2	2.40	0.57
5:z:29:THR:O	5:z:33:LEU:HG	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:n:40:LEU:HB2	5:n:46:ASN:OD1	2.05	0.57
9:l:101:BCB:C1B	7:j:24:LEU:HD11	2.35	0.57
6:o:46:TRP:CE2	9:o:101:BCB:H2C	2.39	0.57
5:e:47:TRP:O	5:e:48:TRP:HB2	2.05	0.57
6:r:32:THR:HA	6:r:35:ILE:HD12	1.85	0.57
6:u:41:TRP:HE1	7:s:13:SER:C	2.12	0.57
9:4:101:BCB:HBB2	9:4:101:BCB:HMB1	1.86	0.57
1:C:305:CYS:HB3	8:C:404:HEC:CAB	2.34	0.57
5:Y:47:TRP:HE3	5:Y:47:TRP:H	1.52	0.57
5:e:45:LEU:CD2	9:f:101:BCB:CBC	2.81	0.57
5:h:49:GLU:HG3	5:h:50:PHE:N	2.20	0.57
5:n:29:THR:O	5:n:33:LEU:HG	2.05	0.57
9:6:102:BCB:CBB	9:6:102:BCB:HMB1	2.35	0.57
9:x:101:BCB:HMB1	9:x:101:BCB:CBB	2.35	0.57
7:R:25:GLY:O	7:R:28:THR:HG22	2.05	0.57
2:L:133:VAL:C	2:L:136:PRO:HD2	2.30	0.56
3:M:3:TYR:HA	3:M:6:ILE:HD12	1.86	0.56
7:2:16:ASN:O	7:2:17:LEU:HG	2.04	0.56
5:b:44:ARG:CG	6:f:54:TRP:HH2	2.10	0.56
9:M:407:BCB:HMB3	9:M:407:BCB:CBB	2.35	0.56
6:1:44:ARG:HA	6:4:50:ILE:HD11	1.87	0.56
5:S:40:LEU:HD23	5:S:47:TRP:CZ2	2.40	0.56
5:e:47:TRP:CE2	9:e:101:BCB:H2C	2.40	0.56
2:L:170:ASN:HB2	2:L:259:TRP:CD1	2.40	0.56
3:M:38:LEU:HD22	3:M:46:ILE:HD11	1.87	0.56
4:H:258:LEU:H	5:F:19:ARG:HD3	1.70	0.56
5:P:44:ARG:HG3	6:T:54:TRP:CZ3	2.39	0.56
5:n:50:PHE:CE1	5:q:44:ARG:HG3	2.40	0.56
5:w:47:TRP:O	5:w:48:TRP:HB2	2.05	0.56
9:3:101:BCB:H71	17:4:102:NS0:C18	2.35	0.56
9:T:101:BCB:HMB1	9:T:101:BCB:CBB	2.34	0.56
7:j:14:ASP:OD1	7:j:17:LEU:O	2.23	0.56
1:C:146:ARG:NH2	1:C:188:ASP:OD1	2.38	0.56
9:M:406:BCB:HHC	9:M:406:BCB:CBB	2.32	0.56
5:w:47:TRP:CE2	9:w:101:BCB:H2C	2.40	0.56
1:C:132:CYS:CB	8:C:402:HEC:HAB	2.35	0.56
5:w:40:LEU:HB2	5:w:46:ASN:OD1	2.05	0.56
6:G:54:TRP:O	6:G:55:VAL:HG22	2.05	0.56
6:N:4:LYS:HB2	6:N:5:PRO:HD3	1.88	0.56
6:o:46:TRP:CD2	9:o:101:BCB:H2C	2.41	0.56
9:7:101:BCB:C1	17:7:102:NS0:C28	2.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L:301:BCB:H11	9:L:302:BCB:H2C	1.86	0.56
10:L:303:BPB:HBBB	10:L:303:BPB:CHC	2.23	0.56
3:M:213:LEU:CD1	3:M:213:LEU:N	2.69	0.56
6:1:23:VAL:HA	6:1:26:THR:HG22	1.87	0.56
5:V:47:TRP:HB3	6:Z:47:ILE:HD12	1.88	0.56
9:h:101:BCB:HMB1	9:h:101:BCB:CBB	2.36	0.56
7:X:16:ASN:O	7:X:17:LEU:CD2	2.52	0.56
5:z:47:TRP:CE2	9:z:101:BCB:H2C	2.40	0.56
5:3:49:GLU:HG3	5:3:50:PHE:N	2.20	0.56
5:n:45:LEU:H	6:r:54:TRP:HH2	1.54	0.56
5:z:49:GLU:HG3	5:z:50:PHE:N	2.21	0.56
5:t:40:LEU:HB2	5:t:46:ASN:OD1	2.06	0.56
5:6:27:TYR:CE1	11:6:101:UQ9:C4	2.89	0.56
2:L:109:ARG:HG2	2:L:109:ARG:HH11	1.70	0.56
9:L:301:BCB:H11	9:L:302:BCB:C2C	2.36	0.56
4:H:49:LEU:CD1	6:1:12:GLU:HB2	2.36	0.56
7:2:26:ILE:HB	7:2:27:PRO:HD3	1.88	0.56
5:b:44:ARG:CD	6:f:54:TRP:CH2	2.88	0.56
5:h:44:ARG:HG2	6:l:54:TRP:CH2	2.41	0.56
11:6:101:UQ9:H10A	11:6:101:UQ9:C13	2.36	0.56
2:L:51:TYR:CE1	5:z:40:LEU:HD11	2.39	0.55
5:z:44:ARG:HG3	6:4:54:TRP:CH2	2.41	0.55
9:1:101:BCB:HMB1	9:1:101:BCB:CBB	2.36	0.55
5:k:47:TRP:O	5:k:48:TRP:HB2	2.06	0.55
5:q:47:TRP:CD1	5:q:48:TRP:CD1	2.93	0.55
7:j:24:LEU:O	7:j:28:THR:CG2	2.45	0.55
7:v:17:LEU:HD22	7:v:19:VAL:HG21	1.88	0.55
7:5:25:GLY:CA	7:5:28:THR:HG22	2.36	0.55
5:K:11:LEU:HD11	5:K:15:LEU:HD22	1.88	0.55
11:6:101:UQ9:H8	11:6:101:UQ9:C1M	2.36	0.55
6:T:41:TRP:CD1	7:R:14:ASP:HA	2.42	0.55
1:C:256:TRP:CG	3:M:314:ASP:HB2	2.42	0.55
9:S:101:BCB:CBB	9:S:101:BCB:HMB1	2.36	0.55
5:6:44:ARG:CG	6:G:54:TRP:CH2	2.89	0.55
6:l:54:TRP:CD1	6:l:55:VAL:HA	2.40	0.55
1:C:252:THR:HG21	3:M:293:TYR:CD2	2.41	0.55
1:C:308:CYS:SG	8:C:404:HEC:CBC	2.94	0.55
2:L:205:LYS:HA	4:H:69:VAL:HG13	1.89	0.55
4:H:115:ALA:HB2	4:H:244:GLY:HA3	1.88	0.55
7:2:14:ASP:CG	7:2:17:LEU:O	2.49	0.55
5:e:44:ARG:CG	6:i:54:TRP:HH2	2.12	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:e:101:BCB:C12	17:f:102:NS0:C13	2.84	0.55
9:4:101:BCB:HMB1	9:4:101:BCB:CBB	2.36	0.55
1:C:205:PRO:CB	3:M:290:ASP:OD2	2.55	0.55
9:F:101:BCB:HMB1	9:F:101:BCB:CBB	2.35	0.55
9:S:101:BCB:HMB1	9:S:101:BCB:HBB2	1.89	0.55
5:w:40:LEU:HD23	5:w:47:TRP:CZ2	2.41	0.55
5:e:47:TRP:HE3	5:e:47:TRP:H	1.52	0.55
5:t:47:TRP:HE3	5:t:47:TRP:H	1.54	0.55
5:w:29:THR:O	5:w:33:LEU:HG	2.07	0.55
6:T:47:ILE:HD12	6:T:47:ILE:C	2.32	0.55
9:7:101:BCB:HMB1	9:7:101:BCB:CBB	2.36	0.55
5:F:28:LEU:HD21	17:G:102:NS0:C25	2.37	0.55
9:N:101:BCB:CBB	9:N:101:BCB:HMB1	2.37	0.55
9:K:101:BCB:HMB1	9:K:101:BCB:CBB	2.35	0.55
9:Y:101:BCB:HMB1	9:Y:101:BCB:HBB3	1.89	0.55
9:c:101:BCB:HBB2	9:c:101:BCB:HMB1	1.89	0.55
5:z:47:TRP:O	5:z:48:TRP:HB2	2.06	0.55
5:k:43:ASP:HB3	5:k:53:GLY:HA2	1.89	0.55
5:k:47:TRP:H	5:k:47:TRP:HE3	1.54	0.55
5:q:40:LEU:HB2	5:q:46:ASN:OD1	2.07	0.55
6:o:13:GLU:HG2	6:o:14:GLU:N	2.21	0.55
5:Y:9:TRP:HB2	6:Z:16:LYS:HB3	1.87	0.54
5:e:47:TRP:HE1	9:e:101:BCB:CBB	2.17	0.54
6:Z:23:VAL:HA	6:Z:26:THR:HG22	1.89	0.54
6:l:23:VAL:HA	6:l:26:THR:CG2	2.34	0.54
6:u:13:GLU:HG2	6:u:14:GLU:N	2.22	0.54
6:u:51:PRO:HG2	6:u:54:TRP:HB2	1.90	0.54
9:q:101:BCB:CBB	9:q:101:BCB:HMB1	2.37	0.54
6:Q:54:TRP:CG	6:Q:55:VAL:H	2.10	0.54
5:K:40:LEU:HB2	5:K:46:ASN:OD1	2.07	0.54
9:7:101:BCB:C3	17:7:102:NS0:C29	2.85	0.54
7:y:29:ILE:O	7:y:32:ALA:HB3	2.07	0.54
9:3:101:BCB:HED2	9:3:101:BCB:H2A	1.90	0.54
11:6:101:UQ9:C13	11:6:101:UQ9:C10	2.85	0.54
6:N:28:LEU:HD23	7:O:30:TRP:CE3	2.42	0.54
6:l:13:GLU:HG2	6:l:14:GLU:N	2.22	0.54
1:C:135:CYS:SG	8:C:402:HEC:C3C	2.92	0.54
9:K:101:BCB:H61	9:Q:101:BCB:H102	1.90	0.54
5:S:40:LEU:HD23	5:S:47:TRP:CH2	2.41	0.54
5:S:44:ARG:CG	6:W:54:TRP:CH2	2.90	0.54
6:W:28:LEU:O	6:W:32:THR:HG22	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:PRO:HB3	3:M:290:ASP:OD2	2.06	0.54
4:H:96:PHE:CZ	5:3:19:ARG:CZ	2.91	0.54
7:g:25:GLY:O	7:g:28:THR:OG1	2.25	0.54
7:m:15:TRP:C	7:m:17:LEU:H	2.15	0.54
5:z:44:ARG:CG	6:4:54:TRP:CH2	2.91	0.54
7:p:25:GLY:O	7:p:28:THR:OG1	2.25	0.54
7:y:26:ILE:HB	7:y:27:PRO:HD3	1.89	0.54
7:a:25:GLY:O	7:a:28:THR:HG22	2.08	0.54
5:h:40:LEU:HB2	5:h:46:ASN:OD1	2.07	0.54
6:l:18:PHE:CA	17:l:102:NS0:CD1	2.85	0.54
6:4:29:TYR:O	6:4:32:THR:HG22	2.08	0.54
10:M:408:BPB:H12	10:M:408:BPB:H19A	1.90	0.54
5:h:1:ALA:HA	6:i:16:LYS:NZ	2.23	0.54
5:t:44:ARG:HA	6:x:54:TRP:CZ3	2.43	0.54
5:6:39:LEU:HD22	5:6:45:LEU:HD22	1.90	0.54
5:h:49:GLU:HG2	5:h:52:ARG:NH1	2.23	0.53
9:N:101:BCB:HHB	7:I:24:LEU:CD2	2.33	0.53
7:g:16:ASN:O	7:g:17:LEU:CD2	2.51	0.53
5:P:47:TRP:O	5:P:48:TRP:HB2	2.08	0.53
5:h:44:ARG:HA	6:l:54:TRP:HZ3	1.73	0.53
6:Z:13:GLU:HG2	6:Z:14:GLU:N	2.23	0.53
7:5:25:GLY:HA2	7:5:28:THR:HG22	1.89	0.53
4:H:53:ALA:O	5:w:19:ARG:NH1	2.41	0.53
6:1:13:GLU:HG2	6:1:14:GLU:N	2.23	0.53
9:q:101:BCB:HAA1	17:u:102:NS0:C34	2.38	0.53
6:T:23:VAL:HA	6:T:26:THR:HG22	1.89	0.53
6:u:15:ALA:HA	6:u:17:GLU:OE1	2.09	0.53
5:P:17:PRO:O	5:P:21:LEU:HG	2.09	0.53
5:Y:39:LEU:HD22	5:Y:45:LEU:HD13	1.91	0.53
5:n:47:TRP:H	5:n:47:TRP:HE3	1.54	0.53
5:3:49:GLU:HG3	5:3:50:PHE:H	1.73	0.53
5:6:39:LEU:CD2	5:6:45:LEU:CD2	2.86	0.53
11:6:101:UQ9:C1M	11:6:101:UQ9:C8	2.85	0.53
6:G:46:TRP:CD2	9:G:101:BCB:H2C	2.44	0.53
6:i:46:TRP:CD2	9:i:101:BCB:H2C	2.43	0.53
2:L:25:TRP:NE1	2:L:30:PHE:HB2	2.24	0.53
3:M:290:ASP:OD1	3:M:290:ASP:O	2.27	0.53
6:1:39:LEU:O	6:1:42:THR:OG1	2.24	0.53
5:b:1:ALA:HA	6:c:16:LYS:NZ	2.24	0.53
6:i:21:ILE:HG12	17:i:102:NS0:CA	2.38	0.53
6:i:21:ILE:HD12	6:i:22:PHE:N	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:39:LEU:CD2	5:6:45:LEU:HD22	2.38	0.53
6:4:4:LYS:HB2	6:4:5:PRO:HD3	1.90	0.53
5:e:39:LEU:HD22	5:e:45:LEU:HD13	1.89	0.53
5:q:29:THR:O	5:q:33:LEU:HG	2.07	0.53
5:t:1:ALA:HA	6:u:16:LYS:HE3	1.91	0.53
1:C:252:THR:HG21	3:M:293:TYR:CE2	2.44	0.53
14:M:409:LDA:H61	4:H:17:TRP:CZ3	2.43	0.53
5:w:47:TRP:HE3	5:w:47:TRP:H	1.56	0.53
11:6:101:UQ9:C4M	11:6:101:UQ9:C3M	2.86	0.53
6:Q:41:TRP:CD1	7:O:14:ASP:OD1	2.61	0.53
9:L:301:BCB:HAA1	9:L:301:BCB:HBD	1.90	0.53
16:M:411:NS5:HM42	5:h:37:PHE:CE1	2.43	0.53
5:K:44:ARG:CG	6:Q:54:TRP:CH2	2.91	0.53
9:n:101:BCB:H102	17:o:102:NS0:C13	2.38	0.53
6:G:46:TRP:CE2	9:G:101:BCB:H2C	2.44	0.53
7:s:26:ILE:HB	7:s:27:PRO:HD3	1.91	0.53
7:5:25:GLY:HA2	7:5:28:THR:CG2	2.39	0.53
2:L:18:GLY:CA	5:6:19:ARG:NH2	2.66	0.53
2:L:130:VAL:HA	2:L:134:PHE:HD2	1.74	0.53
6:G:26:THR:CB	17:G:102:NS0:C19	2.85	0.53
6:T:54:TRP:CD1	6:T:55:VAL:HA	2.44	0.53
3:M:161:ILE:O	3:M:164:THR:HB	2.09	0.52
9:V:101:BCB:HMB1	9:V:101:BCB:HBB2	1.90	0.52
6:N:54:TRP:CD1	6:N:55:VAL:CA	2.91	0.52
9:N:101:BCB:H52	7:I:27:PRO:HB2	1.91	0.52
6:r:13:GLU:HG2	6:r:14:GLU:N	2.25	0.52
2:L:132:GLN:OE1	2:L:145:ALA:HB1	2.08	0.52
9:M:407:BCB:HMB3	9:M:407:BCB:HBB2	1.92	0.52
9:3:101:BCB:CBB	9:3:101:BCB:HMB1	2.38	0.52
6:u:47:ILE:HD11	7:s:17:LEU:CD1	2.39	0.52
6:u:47:ILE:HD13	7:s:17:LEU:CD2	2.16	0.52
6:x:21:ILE:CG1	17:x:102:NS0:C8	2.87	0.52
5:b:7:ALA:HB1	5:b:10:LYS:HD2	1.90	0.52
6:x:36:VAL:HA	6:x:39:LEU:HD12	1.91	0.52
5:F:39:LEU:CD2	5:F:45:LEU:HD13	2.39	0.52
6:r:30:LEU:HB3	7:p:28:THR:HG22	1.91	0.52
7:O:26:ILE:HB	7:O:27:PRO:HD3	1.91	0.52
2:L:129:CYS:O	2:L:133:VAL:HB	2.09	0.52
5:F:17:PRO:HB3	6:G:18:PHE:CZ	2.45	0.52
5:S:17:PRO:O	5:S:21:LEU:HG	2.10	0.52
5:Y:40:LEU:HB2	5:Y:46:ASN:OD1	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:k:49:GLU:HG3	5:k:50:PHE:N	2.24	0.52
6:G:23:VAL:O	6:G:27:VAL:HG23	2.10	0.52
6:l:18:PHE:HA	17:l:102:NS0:CD1	2.39	0.52
5:e:50:PHE:CZ	5:h:44:ARG:HG3	2.45	0.52
5:w:9:TRP:HB2	6:x:16:LYS:HB3	1.91	0.52
5:3:40:LEU:HD23	5:3:47:TRP:CZ2	2.44	0.52
6:u:25:SER:OG	17:u:102:NS0:C14	2.58	0.52
5:e:44:ARG:CA	6:i:54:TRP:HZ3	2.17	0.52
5:q:44:ARG:HB3	5:q:45:LEU:HD13	1.92	0.52
6:7:13:GLU:HG2	6:7:14:GLU:N	2.24	0.52
7:a:16:ASN:C	7:a:17:LEU:HG	2.31	0.52
5:K:47:TRP:O	5:K:48:TRP:HB2	2.09	0.52
6:r:18:PHE:HD1	17:r:102:NS0:CA	2.22	0.52
6:u:1:ALA:HB1	6:u:6:SER:OG	2.10	0.52
7:j:25:GLY:O	7:j:28:THR:OG1	2.19	0.52
1:C:52:VAL:HG21	1:C:70:PHE:HB2	1.91	0.52
5:z:44:ARG:HA	6:4:54:TRP:HZ3	1.73	0.52
5:F:44:ARG:CG	6:N:54:TRP:HH2	1.67	0.52
5:e:44:ARG:CA	6:i:54:TRP:CZ3	2.92	0.52
6:G:54:TRP:CD1	6:G:55:VAL:CA	2.92	0.52
6:c:28:LEU:O	6:c:32:THR:HG22	2.10	0.52
1:C:205:PRO:CG	3:M:290:ASP:CG	2.83	0.52
9:L:302:BCB:HHC	9:L:302:BCB:CBB	2.40	0.52
5:q:44:ARG:CA	6:u:54:TRP:CH2	2.93	0.52
6:G:29:TYR:O	6:G:32:THR:HG22	2.09	0.52
6:T:47:ILE:HD11	7:R:17:LEU:CD2	2.39	0.52
7:I:14:ASP:OD2	7:I:21:LEU:HD11	2.09	0.52
5:e:44:ARG:CB	6:i:54:TRP:CZ3	2.93	0.51
5:q:1:ALA:HB1	5:q:4:TYR:HB2	1.90	0.51
6:N:41:TRP:NE1	7:I:14:ASP:N	2.59	0.51
10:L:303:BPB:CBB	10:L:303:BPB:CHC	2.71	0.51
6:1:21:ILE:HD11	7:2:34:THR:HG22	1.91	0.51
6:l:3:LEU:H	6:l:6:SER:HB3	1.75	0.51
6:l:32:THR:HA	6:l:35:ILE:HD12	1.91	0.51
7:X:17:LEU:CD2	7:X:19:VAL:CG2	2.83	0.51
4:H:58:GLN:C	4:H:61:GLU:HB2	2.35	0.51
5:P:40:LEU:HB2	5:P:46:ASN:OD1	2.10	0.51
5:6:47:TRP:O	5:6:48:TRP:CB	2.59	0.51
6:Q:41:TRP:HE1	7:O:13:SER:C	2.19	0.51
6:r:43:ALA:C	6:r:44:ARG:HG2	2.35	0.51
9:Y:101:BCB:C2B	17:c:102:NS0:C39	2.88	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:27:TYR:CE1	11:6:101:UQ9:C5	2.93	0.51
9:c:101:BCB:HMB1	9:c:101:BCB:CBB	2.41	0.51
6:i:54:TRP:CD1	6:i:55:VAL:CA	2.92	0.51
6:l:18:PHE:CB	17:l:102:NS0:CD1	2.86	0.51
6:r:38:TYR:O	6:r:42:THR:HG23	2.11	0.51
17:7:102:NS0:CD1	17:7:102:NS0:C	2.86	0.51
7:g:24:LEU:O	7:g:28:THR:CG2	2.57	0.51
7:j:15:TRP:C	7:j:17:LEU:N	2.69	0.51
5:z:39:LEU:C	5:z:41:SER:H	2.17	0.51
5:V:49:GLU:HG3	5:V:50:PHE:H	1.74	0.51
9:3:101:BCB:HMD1	6:4:37:HIS:CE1	2.44	0.51
6:r:54:TRP:O	6:r:55:VAL:HG22	2.10	0.51
9:V:101:BCB:O2D	7:X:23:ILE:HG23	2.10	0.51
5:Y:47:TRP:CZ2	9:Y:101:BCB:H2C	2.45	0.51
5:6:40:LEU:HD23	5:6:47:TRP:CZ2	2.46	0.51
6:Z:41:TRP:NE1	7:X:14:ASP:N	2.59	0.51
9:r:101:BCB:HMB1	9:r:101:BCB:HBB2	1.92	0.51
7:U:16:ASN:O	7:U:17:LEU:CD2	2.52	0.51
9:F:101:BCB:HMA3	7:I:23:ILE:HG22	1.93	0.51
6:i:54:TRP:CD1	6:i:55:VAL:HA	2.46	0.51
17:l:102:NS0:C11	7:m:35:TYR:CE1	2.94	0.51
6:7:3:LEU:HB2	6:7:6:SER:HA	1.92	0.51
7:p:24:LEU:O	7:p:28:THR:CG2	2.54	0.51
5:F:47:TRP:CE2	9:F:101:BCB:H2C	2.46	0.51
5:K:47:TRP:CZ2	9:K:101:BCB:H2C	2.46	0.51
5:b:44:ARG:CB	6:f:54:TRP:CH2	2.94	0.51
9:t:101:BCB:HAA1	17:x:102:NS0:C34	2.41	0.51
9:t:101:BCB:C1B	9:x:101:BCB:HMB3	2.41	0.51
6:T:24:THR:O	6:T:28:LEU:HG	2.11	0.51
7:I:18:TRP:HA	7:I:21:LEU:HD12	1.93	0.51
1:C:150:PRO:HG3	1:C:176:LEU:HD13	1.93	0.51
8:C:402:HEC:HBC3	8:C:402:HEC:CMC	2.41	0.51
7:2:16:ASN:O	7:2:17:LEU:CG	2.59	0.51
5:6:18:ARG:HH22	5:6:19:ARG:HE	1.57	0.51
9:Q:101:BCB:H2A	9:Q:101:BCB:CGD	2.41	0.51
6:W:54:TRP:HD1	6:W:55:VAL:H	1.50	0.51
1:C:4:PRO:HD2	1:C:24:HIS:CE1	2.46	0.50
2:L:160:PHE:O	2:L:163:GLN:HB2	2.11	0.50
5:S:7:ALA:O	5:S:8:SER:C	2.54	0.50
9:6:102:BCB:C1B	9:G:101:BCB:HMB3	2.41	0.50
6:Q:3:LEU:H	6:Q:6:SER:HB3	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Q:44:ARG:NH1	6:T:50:ILE:HG13	2.25	0.50
9:Q:101:BCB:OBB	9:Q:101:BCB:HHC	2.11	0.50
9:Z:101:BCB:HMB1	9:Z:101:BCB:HBB2	1.93	0.50
6:l:4:LYS:HB2	6:l:5:PRO:HD3	1.93	0.50
1:C:308:CYS:SG	8:C:404:HEC:C3C	2.99	0.50
3:M:73:MET:HE1	3:M:88:PHE:CE1	2.46	0.50
3:M:120:MET:HG3	9:M:407:BCB:H202	1.93	0.50
5:S:35:ILE:HD12	9:T:101:BCB:O1D	2.11	0.50
5:V:7:ALA:O	5:V:8:SER:C	2.54	0.50
6:o:54:TRP:O	6:o:55:VAL:HG22	2.11	0.50
9:r:101:BCB:H2	17:r:102:NS0:C26	2.41	0.50
1:C:217:GLY:HA2	3:M:167:GLY:O	2.12	0.50
4:H:172:TRP:HB2	4:H:182:TYR:HB2	1.93	0.50
5:F:44:ARG:HG3	5:6:50:PHE:CE1	2.47	0.50
5:3:45:LEU:CG	9:4:101:BCB:CBC	2.89	0.50
9:T:101:BCB:H2	17:T:102:NS0:C26	2.42	0.50
6:W:13:GLU:HG2	6:W:14:GLU:N	2.27	0.50
2:L:51:TYR:CE1	5:z:40:LEU:CD1	2.92	0.50
3:M:176:GLY:C	3:M:179:PRO:HD2	2.37	0.50
5:F:35:ILE:HD12	9:G:101:BCB:O1D	2.12	0.50
9:N:101:BCB:HMB1	9:N:101:BCB:HBB2	1.94	0.50
9:W:101:BCB:HMB1	9:W:101:BCB:CBB	2.41	0.50
9:L:301:BCB:CBB	9:L:301:BCB:CMB	2.90	0.50
5:S:45:LEU:HD21	9:T:101:BCB:HBC1	1.83	0.50
6:f:36:VAL:HG22	7:g:23:ILE:HG12	1.93	0.50
6:i:54:TRP:CG	6:i:55:VAL:H	2.01	0.50
6:o:41:TRP:HH2	6:o:47:ILE:HG13	1.76	0.50
1:C:239:SER:OG	1:C:305:CYS:SG	2.65	0.50
2:L:130:VAL:HA	2:L:134:PHE:CD2	2.47	0.50
5:F:12:TRP:CD1	6:G:19:HIS:HB2	2.47	0.50
5:K:44:ARG:HA	6:Q:54:TRP:CZ3	2.47	0.50
5:K:45:LEU:CD2	9:N:101:BCB:CBC	2.85	0.50
9:e:101:BCB:CBB	9:i:101:BCB:HMC1	2.42	0.50
5:t:29:THR:O	5:t:33:LEU:HG	2.11	0.50
6:N:38:TYR:O	6:N:42:THR:HG23	2.12	0.50
9:W:101:BCB:HMB1	9:W:101:BCB:HBB2	1.93	0.50
6:l:46:TRP:CE2	9:l:101:BCB:H2C	2.47	0.50
5:w:28:LEU:HD22	9:x:101:BCB:HED1	1.94	0.50
5:3:39:LEU:CD2	5:3:45:LEU:CD2	2.87	0.50
6:N:21:ILE:CG1	17:N:102:NS0:C8	2.90	0.50
6:N:22:PHE:C	6:N:22:PHE:CD1	2.89	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:101:BCB:H2	17:W:102:NS0:C26	2.42	0.50
6:c:54:TRP:CD1	6:c:55:VAL:CA	2.93	0.50
1:C:247:CYS:SG	8:C:403:HEC:CBC	2.95	0.50
9:1:101:BCB:H2A	9:1:101:BCB:CGD	2.42	0.50
5:S:29:THR:O	5:S:33:LEU:HG	2.11	0.50
5:Y:25:PHE:HA	9:Y:101:BCB:H61	1.94	0.50
9:b:101:BCB:HMB1	9:b:101:BCB:HBB3	1.92	0.50
1:C:80:TRP:O	1:C:138:GLY:HA2	2.11	0.50
2:L:13:GLY:O	2:L:110:LYS:HE2	2.12	0.50
3:M:288:PHE:CD2	4:H:12:ILE:HD11	2.47	0.50
5:F:11:LEU:HD11	5:F:15:LEU:HD22	1.94	0.50
5:P:45:LEU:HD21	9:Q:101:BCB:CBC	2.41	0.50
5:n:45:LEU:HD21	9:o:101:BCB:CBC	2.42	0.50
11:6:101:UQ9:H8	11:6:101:UQ9:H1MA	1.93	0.50
6:Q:24:THR:O	6:Q:28:LEU:HG	2.12	0.50
6:T:3:LEU:HB2	6:T:6:SER:HA	1.93	0.50
6:i:32:THR:HA	6:i:35:ILE:HD12	1.94	0.50
7:X:29:ILE:O	7:X:32:ALA:HB3	2.12	0.50
2:L:34:PHE:HA	2:L:37:SER:OG	2.12	0.49
5:t:44:ARG:HA	6:x:54:TRP:HZ3	1.77	0.49
7:U:29:ILE:O	7:U:32:ALA:HB3	2.11	0.49
5:z:45:LEU:HD21	9:1:101:BCB:CBC	2.42	0.49
5:b:39:LEU:CD2	5:b:45:LEU:HD13	2.43	0.49
7:O:25:GLY:O	7:O:28:THR:HG22	2.12	0.49
1:C:121:TRP:CG	1:C:273:MET:HG3	2.47	0.49
5:S:47:TRP:CZ2	9:S:101:BCB:H2C	2.46	0.49
9:k:101:BCB:O2D	7:m:23:ILE:HG23	2.13	0.49
6:N:18:PHE:HB2	17:N:102:NS0:CG	2.43	0.49
9:l:101:BCB:H102	7:j:31:ILE:HD11	1.94	0.49
5:e:45:LEU:HD21	9:f:101:BCB:HBC1	1.86	0.49
9:e:101:BCB:HBB3	9:e:101:BCB:HHC	1.95	0.49
7:O:18:TRP:HA	7:O:21:LEU:HD12	1.95	0.49
7:d:26:ILE:HB	7:d:27:PRO:HD3	1.93	0.49
5:z:1:ALA:HB1	5:z:4:TYR:HB2	1.95	0.49
5:K:9:TRP:HB2	6:N:16:LYS:HB3	1.95	0.49
9:t:101:BCB:HBB2	9:t:101:BCB:HMB1	1.95	0.49
6:T:43:ALA:HB2	7:U:17:LEU:HD21	1.93	0.49
6:r:54:TRP:CG	6:r:55:VAL:H	2.07	0.49
6:7:41:TRP:CG	7:5:14:ASP:OD1	2.65	0.49
7:O:17:LEU:HD22	7:O:19:VAL:CG2	2.42	0.49
1:C:87:CYS:HB2	8:C:401:HEC:CAB	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:406:BCB:HBB2	9:M:406:BCB:CHC	2.39	0.49
6:G:3:LEU:HB2	6:G:6:SER:HA	1.95	0.49
7:p:14:ASP:OD1	7:p:17:LEU:O	2.31	0.49
4:H:43:LEU:HB2	4:H:54:PRO:HD3	1.95	0.49
5:K:45:LEU:H	6:Q:54:TRP:HH2	1.61	0.49
5:Y:7:ALA:O	5:Y:8:SER:C	2.56	0.49
9:w:101:BCB:H92	9:w:101:BCB:H51	1.93	0.49
6:N:41:TRP:HE1	7:I:14:ASP:N	2.11	0.49
7:a:19:VAL:O	7:a:23:ILE:HG13	2.12	0.49
5:Y:29:THR:O	5:Y:33:LEU:HG	2.13	0.49
2:L:170:ASN:OD1	2:L:170:ASN:C	2.56	0.49
4:H:258:LEU:C	4:H:258:LEU:CD1	2.85	0.49
5:F:47:TRP:CZ2	9:F:101:BCB:H2C	2.47	0.49
5:Y:40:LEU:HD23	5:Y:47:TRP:CZ2	2.47	0.49
9:Z:101:BCB:HHC	9:Z:101:BCB:OBB	2.13	0.49
9:M:406:BCB:CBB	9:M:406:BCB:CHC	2.91	0.48
16:M:411:NS5:HM42	5:h:37:PHE:HE1	1.77	0.48
5:q:1:ALA:HA	6:r:16:LYS:HZ1	1.76	0.48
9:Z:101:BCB:HMB1	9:Z:101:BCB:CBB	2.43	0.48
6:f:32:THR:HA	6:f:35:ILE:HD12	1.94	0.48
1:C:167:GLU:CD	1:C:167:GLU:H	2.21	0.48
6:f:54:TRP:CD1	6:f:55:VAL:CA	2.95	0.48
9:l:101:BCB:HMB1	9:l:101:BCB:HBB2	1.95	0.48
4:H:56:ASP:HA	5:w:19:ARG:CZ	2.43	0.48
5:P:1:ALA:HA	6:Q:16:LYS:NZ	2.29	0.48
5:q:47:TRP:NE1	5:q:48:TRP:CD1	2.81	0.48
5:S:47:TRP:O	5:S:48:TRP:HB2	2.13	0.48
5:k:12:TRP:HZ3	5:k:20:VAL:HG21	1.78	0.48
5:6:39:LEU:HD22	5:6:45:LEU:CG	2.43	0.48
6:G:54:TRP:CD1	6:G:55:VAL:HA	2.48	0.48
6:u:54:TRP:CG	6:u:55:VAL:H	2.15	0.48
9:7:101:BCB:HHB	7:5:24:LEU:CD2	2.41	0.48
2:L:193:LEU:HD22	2:L:216:PHE:CE2	2.48	0.48
4:H:136:PRO:HA	4:H:172:TRP:HA	1.94	0.48
5:F:10:LYS:O	5:F:13:LEU:HG	2.13	0.48
5:3:7:ALA:O	5:3:8:SER:C	2.56	0.48
6:T:21:ILE:CG1	17:T:102:NS0:C8	2.89	0.48
9:r:101:BCB:HMB1	9:r:101:BCB:CBB	2.44	0.48
6:u:41:TRP:CD2	7:s:14:ASP:OD1	2.66	0.48
9:V:101:BCB:HMD1	6:W:37:HIS:CE1	2.48	0.48
7:R:26:ILE:HB	7:R:27:PRO:HD3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:49:LEU:HG	6:1:12:GLU:HB2	1.95	0.48
5:S:16:ASP:HA	5:S:17:PRO:HD2	1.70	0.48
6:i:39:LEU:O	6:i:42:THR:OG1	2.31	0.48
9:o:101:BCB:C1B	7:m:24:LEU:HD11	2.44	0.48
6:7:46:TRP:CE2	9:7:101:BCB:H2C	2.49	0.48
5:Y:39:LEU:HD21	5:Y:45:LEU:HD13	1.94	0.48
9:Y:101:BCB:CMB	17:c:102:NS0:C39	2.91	0.48
5:6:39:LEU:HD22	5:6:45:LEU:CD2	2.44	0.48
6:f:36:VAL:CG2	7:g:23:ILE:HG12	2.44	0.48
6:4:39:LEU:O	6:4:42:THR:OG1	2.32	0.48
6:7:17:GLU:O	6:7:21:ILE:HD12	2.14	0.48
7:s:27:PRO:HA	7:s:30:TRP:NE1	2.29	0.48
2:L:77:ALA:HA	2:L:87:GLN:HE22	1.79	0.48
5:b:47:TRP:O	5:b:48:TRP:HB2	2.14	0.48
5:t:47:TRP:CZ2	9:t:101:BCB:H2C	2.49	0.48
9:w:101:BCB:CBB	9:w:101:BCB:HMB1	2.43	0.48
6:Z:4:LYS:HB2	6:Z:5:PRO:HD3	1.96	0.48
7:j:26:ILE:HB	7:j:27:PRO:HD3	1.95	0.48
2:L:80:LEU:HA	2:L:84:GLY:HA3	1.96	0.48
5:F:12:TRP:HD1	6:G:19:HIS:HB2	1.79	0.48
9:F:101:BCB:HMA3	7:I:23:ILE:CG2	2.44	0.48
5:b:29:THR:O	5:b:33:LEU:HG	2.13	0.48
9:e:101:BCB:CBB	9:e:101:BCB:HHC	2.44	0.48
5:n:25:PHE:HD1	9:n:101:BCB:H62	1.79	0.48
5:3:25:PHE:CD2	11:6:101:UQ9:H3M	2.48	0.48
6:l:54:TRP:O	6:l:55:VAL:HG22	2.13	0.48
2:L:193:LEU:HD23	11:L:304:UQ9:C3	2.44	0.47
4:H:60:TYR:CD1	4:H:60:TYR:N	2.70	0.47
5:V:1:ALA:HA	6:W:16:LYS:NZ	2.29	0.47
9:b:101:BCB:O1A	17:f:102:NS0:C34	2.62	0.47
6:4:54:TRP:CG	6:4:55:VAL:H	2.01	0.47
7:I:16:ASN:HA	7:I:18:TRP:HD1	1.79	0.47
7:X:19:VAL:HB	7:X:20:PRO:HD3	1.96	0.47
9:e:101:BCB:HBB1	9:i:101:BCB:HMC1	1.95	0.47
1:C:24:HIS:CD2	1:C:26:ALA:HB3	2.50	0.47
1:C:51:PRO:HA	1:C:65:LEU:O	2.15	0.47
7:2:16:ASN:C	7:2:17:LEU:HG	2.39	0.47
5:n:44:ARG:HG3	6:r:54:TRP:CH2	2.49	0.47
5:t:50:PHE:CE1	5:w:44:ARG:HG3	2.49	0.47
9:6:102:BCB:HMD1	6:7:37:HIS:CE1	2.49	0.47
6:u:38:TYR:O	6:u:42:THR:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:14:ASP:OD1	7:a:17:LEU:O	2.32	0.47
2:L:185:MET:HE3	2:L:189:LEU:HD11	1.96	0.47
9:L:301:BCB:HBD	9:L:301:BCB:O1A	2.14	0.47
5:z:40:LEU:HB2	5:z:46:ASN:OD1	2.13	0.47
5:P:16:ASP:HA	5:P:17:PRO:HD2	1.61	0.47
9:P:101:BCB:HBB3	9:P:101:BCB:HMB1	1.96	0.47
5:6:48:TRP:O	5:6:49:GLU:HB2	2.14	0.47
2:L:128:PHE:HD1	9:L:302:BCB:HBB1	1.79	0.47
3:M:115:MET:HB3	3:M:115:MET:HE2	1.67	0.47
3:M:127:TRP:O	3:M:130:ARG:HB3	2.14	0.47
9:M:407:BCB:CBB	9:M:407:BCB:CMB	2.92	0.47
5:e:16:ASP:HA	5:e:17:PRO:HD2	1.68	0.47
5:q:37:PHE:HZ	17:u:102:NS0:C40	2.26	0.47
9:q:101:BCB:H61	9:u:101:BCB:H91	1.96	0.47
5:t:39:LEU:HD21	5:t:45:LEU:HD22	1.93	0.47
9:r:101:BCB:HHB	7:p:24:LEU:HD21	1.94	0.47
7:R:15:TRP:C	7:R:17:LEU:H	2.22	0.47
5:k:18:ARG:HG2	5:n:14:ILE:HG23	1.97	0.47
7:R:27:PRO:HA	7:R:30:TRP:NE1	2.29	0.47
7:d:14:ASP:OD1	7:d:17:LEU:O	2.32	0.47
1:C:262:PRO:CA	3:M:312:THR:HG21	2.44	0.47
1:C:329:GLY:HA2	1:C:331:ILE:HD12	1.97	0.47
10:L:303:BPB:H2	10:L:303:BPB:H6A	1.64	0.47
4:H:96:PHE:HZ	5:3:19:ARG:CZ	2.28	0.47
6:1:21:ILE:HG21	17:1:102:NS0:CA	2.42	0.47
5:K:16:ASP:HA	5:K:17:PRO:HD2	1.65	0.47
9:K:101:BCB:HAA1	17:Q:102:NS0:C34	2.45	0.47
5:P:44:ARG:HG2	6:T:54:TRP:CH2	2.50	0.47
5:e:7:ALA:O	5:e:8:SER:C	2.57	0.47
5:e:39:LEU:HD21	5:e:45:LEU:HD13	1.97	0.47
5:t:49:GLU:HG3	5:t:50:PHE:N	2.30	0.47
5:6:23:ALA:CB	5:6:27:TYR:HE2	2.18	0.47
5:6:52:ARG:O	5:6:54:LEU:HD12	2.14	0.47
11:6:101:UQ9:H13	11:6:101:UQ9:C10	2.45	0.47
6:T:38:TYR:O	6:T:42:THR:HG23	2.15	0.47
6:r:30:LEU:HD13	7:p:28:THR:HG22	1.97	0.47
7:R:14:ASP:OD1	7:R:17:LEU:O	2.33	0.47
7:X:26:ILE:HB	7:X:27:PRO:HD3	1.97	0.47
7:m:15:TRP:O	7:m:17:LEU:HD12	2.15	0.47
5:K:1:ALA:HA	6:N:16:LYS:NZ	2.30	0.47
5:P:1:ALA:HA	6:Q:16:LYS:HZ2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:14:ILE:HD13	5:S:14:ILE:HA	1.76	0.47
5:Y:1:ALA:HA	6:Z:16:LYS:NZ	2.30	0.47
11:6:101:UQ9:H20	11:6:101:UQ9:H17	1.69	0.47
6:N:54:TRP:CD1	6:N:55:VAL:HA	2.49	0.47
6:x:50:ILE:HA	6:x:51:PRO:HD2	1.75	0.47
1:C:244:CYS:SG	8:C:403:HEC:C3B	2.95	0.47
5:b:44:ARG:NE	6:f:54:TRP:CZ2	2.83	0.47
9:Q:101:BCB:CBB	9:Q:101:BCB:HMB1	2.45	0.47
6:l:21:ILE:CG2	17:l:102:NS0:C10	2.93	0.47
7:I:14:ASP:OD1	7:I:17:LEU:O	2.33	0.47
5:k:2:THR:H	6:l:16:LYS:HE3	1.80	0.47
5:t:45:LEU:HD12	5:t:45:LEU:O	2.15	0.47
9:L:301:BCB:OBB	9:L:301:BCB:HHC	2.15	0.46
5:F:40:LEU:HB2	5:F:46:ASN:OD1	2.15	0.46
5:Y:45:LEU:HD21	9:Z:101:BCB:HBC1	1.87	0.46
5:t:39:LEU:CB	5:t:45:LEU:HD13	2.45	0.46
9:N:101:BCB:OBB	9:N:101:BCB:HHC	2.15	0.46
2:L:128:PHE:CD1	9:L:302:BCB:HBB1	2.51	0.46
4:H:29:LEU:HD23	4:H:29:LEU:HA	1.71	0.46
5:Y:17:PRO:O	5:Y:21:LEU:HG	2.16	0.46
5:t:7:ALA:O	5:t:8:SER:C	2.58	0.46
5:w:35:ILE:HD12	9:x:101:BCB:O1D	2.15	0.46
6:T:13:GLU:HG2	6:T:14:GLU:N	2.30	0.46
6:o:46:TRP:CZ2	9:o:101:BCB:HHC	2.49	0.46
7:m:15:TRP:C	7:m:17:LEU:N	2.73	0.46
5:F:45:LEU:CD1	5:6:48:TRP:HA	2.45	0.46
5:k:22:THR:O	5:k:26:VAL:HG23	2.15	0.46
5:6:26:VAL:O	5:6:29:THR:HB	2.15	0.46
9:6:102:BCB:HMB1	9:6:102:BCB:HBB3	1.97	0.46
6:T:41:TRP:CD1	7:R:14:ASP:CA	2.99	0.46
6:Z:47:ILE:HG21	7:X:17:LEU:CD1	2.26	0.46
7:j:15:TRP:C	7:j:17:LEU:H	2.23	0.46
15:M:410:MQ9:H422	5:3:23:ALA:HB2	1.98	0.46
5:F:45:LEU:HD12	5:6:48:TRP:HA	1.96	0.46
5:3:45:LEU:HG	9:4:101:BCB:CBC	2.45	0.46
9:z:101:BCB:HMB1	9:z:101:BCB:HBB3	1.97	0.46
5:b:43:ASP:HB3	5:b:53:GLY:HA2	1.97	0.46
5:b:49:GLU:C	5:e:44:ARG:HD2	2.41	0.46
6:i:13:GLU:HG2	6:i:14:GLU:N	2.31	0.46
6:o:43:ALA:C	6:o:44:ARG:HG2	2.40	0.46
9:L:301:BCB:H192	9:L:301:BCB:H162	1.82	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:54:LEU:HB3	5:P:57:ALA:O	2.16	0.46
5:S:40:LEU:HB2	5:S:46:ASN:OD1	2.16	0.46
5:t:39:LEU:HD23	5:t:45:LEU:HD11	1.94	0.46
6:Q:41:TRP:CE2	7:O:14:ASP:OD1	2.69	0.46
6:u:54:TRP:CD1	6:u:55:VAL:CA	2.98	0.46
7:m:19:VAL:O	7:m:23:ILE:HG13	2.15	0.46
1:C:135:CYS:SG	8:C:402:HEC:HBC3	2.53	0.46
2:L:40:PHE:CD1	2:L:40:PHE:C	2.94	0.46
3:M:67:LEU:HD12	3:M:67:LEU:HA	1.75	0.46
9:z:101:BCB:H93	17:1:102:NS0:C18	2.46	0.46
5:q:44:ARG:HB3	6:u:54:TRP:HH2	1.78	0.46
7:U:14:ASP:HB3	7:U:17:LEU:O	2.15	0.46
7:m:16:ASN:O	7:m:17:LEU:HG	2.15	0.46
2:L:151:LEU:HD13	3:M:196:TYR:HE1	1.81	0.46
3:M:314:ASP:HA	3:M:315:PRO:HD3	1.79	0.46
5:S:39:LEU:HA	5:S:39:LEU:HD23	1.83	0.46
5:V:17:PRO:HB3	6:W:18:PHE:CE2	2.50	0.46
5:Y:44:ARG:CG	6:c:54:TRP:CH2	2.99	0.46
5:e:48:TRP:HE1	9:e:101:BCB:HBB1	1.80	0.46
6:o:47:ILE:HD11	7:m:17:LEU:CB	2.45	0.46
6:x:4:LYS:HB2	6:x:5:PRO:HD3	1.96	0.46
7:g:26:ILE:HB	7:g:27:PRO:HD3	1.97	0.46
7:y:15:TRP:C	7:y:17:LEU:N	2.73	0.46
2:L:68:PRO:HB3	2:L:86:TRP:CD2	2.50	0.46
5:e:50:PHE:CE1	5:h:44:ARG:HG3	2.51	0.46
6:f:54:TRP:O	6:f:55:VAL:HG22	2.16	0.46
1:C:87:CYS:HB2	8:C:401:HEC:HAB	1.98	0.46
2:L:174:MET:HE3	9:M:406:BCB:HED2	1.97	0.46
9:M:407:BCB:OBB	9:M:407:BCB:HHC	2.16	0.46
4:H:52:LEU:O	4:H:52:LEU:CG	2.51	0.46
5:S:46:ASN:ND2	5:S:49:GLU:HB3	2.30	0.46
9:n:101:BCB:O2D	7:p:23:ILE:HG23	2.16	0.46
6:f:54:TRP:CD1	6:f:55:VAL:HA	2.51	0.46
6:o:44:ARG:NH2	6:r:48:ALA:O	2.40	0.46
6:7:46:TRP:CD2	9:7:101:BCB:H2C	2.51	0.46
1:C:146:ARG:NH1	1:C:179:TYR:CZ	2.84	0.45
1:C:244:CYS:CB	8:C:403:HEC:HAB	2.44	0.45
2:L:117:VAL:HB	2:L:118:PRO:HD3	1.98	0.45
9:S:101:BCB:O2D	7:U:23:ILE:HG23	2.16	0.45
5:Y:44:ARG:HG2	6:c:54:TRP:CH2	2.51	0.45
9:T:101:BCB:OBB	9:T:101:BCB:HHC	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:l:101:BCB:OBB	9:l:101:BCB:HHC	2.16	0.45
1:C:35:ASP:OD2	1:C:316:LEU:HA	2.16	0.45
3:M:212:LEU:HD23	3:M:212:LEU:C	2.41	0.45
4:H:58:GLN:HB3	4:H:61:GLU:CG	2.41	0.45
5:Y:21:LEU:HD11	6:Z:18:PHE:HE1	1.81	0.45
5:b:45:LEU:CD2	9:c:101:BCB:CBC	2.94	0.45
5:h:47:TRP:CZ2	9:h:101:BCB:H2C	2.51	0.45
5:w:16:ASP:HA	5:w:17:PRO:HD2	1.74	0.45
5:6:40:LEU:HB2	5:6:46:ASN:OD1	2.16	0.45
9:G:101:BCB:H2	9:G:101:BCB:H61	1.68	0.45
6:7:46:TRP:CZ2	9:7:101:BCB:HHC	2.51	0.45
4:H:258:LEU:CB	5:F:19:ARG:HD2	2.42	0.45
5:z:7:ALA:O	5:z:8:SER:C	2.59	0.45
5:P:7:ALA:O	5:P:8:SER:C	2.58	0.45
5:h:9:TRP:CD2	6:i:16:LYS:HG2	2.51	0.45
5:h:22:THR:O	5:h:26:VAL:HG23	2.17	0.45
5:6:39:LEU:C	5:6:41:SER:H	2.22	0.45
9:G:101:BCB:OBB	9:G:101:BCB:HHC	2.15	0.45
9:Z:101:BCB:H112	7:X:31:ILE:HD11	1.99	0.45
6:4:32:THR:HA	6:4:35:ILE:HD12	1.99	0.45
6:7:41:TRP:CD2	7:5:14:ASP:OD1	2.69	0.45
9:7:101:BCB:H112	7:5:30:TRP:CH2	2.51	0.45
5:b:7:ALA:O	5:b:8:SER:C	2.60	0.45
5:t:39:LEU:O	5:t:45:LEU:HD12	2.16	0.45
9:G:101:BCB:HMB1	9:G:101:BCB:CBB	2.46	0.45
9:7:101:BCB:H11	17:7:102:NS0:C28	2.31	0.45
6:W:54:TRP:CD1	6:W:55:VAL:CA	3.00	0.45
6:l:38:TYR:O	6:l:42:THR:HG23	2.16	0.45
1:C:52:VAL:HG13	1:C:56:TYR:HD2	1.81	0.45
15:M:410:MQ9:H421	15:M:410:MQ9:H403	1.75	0.45
5:k:16:ASP:HA	5:k:17:PRO:HD2	1.51	0.45
5:3:25:PHE:HD1	9:3:101:BCB:H8	1.82	0.45
6:f:21:ILE:HG22	17:f:102:NS0:C10	2.46	0.45
9:7:101:BCB:C5	17:7:102:NS0:C29	2.95	0.45
2:L:146:PHE:HB3	2:L:156:TRP:CD2	2.52	0.45
2:L:242:LEU:HD23	2:L:242:LEU:HA	1.69	0.45
9:L:301:BCB:HAA1	9:L:301:BCB:CBD	2.47	0.45
11:L:304:UQ9:H3MB	11:L:304:UQ9:C4M	2.47	0.45
3:M:248:LEU:HA	3:M:248:LEU:HD23	1.50	0.45
5:h:25:PHE:HD1	9:h:101:BCB:H8	1.80	0.45
9:t:101:BCB:H41	9:t:101:BCB:H61	1.71	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:47:ILE:HD12	6:G:48:ALA:N	2.32	0.45
6:c:44:ARG:HH12	6:f:50:ILE:HG13	1.82	0.45
6:7:39:LEU:O	6:7:42:THR:OG1	2.31	0.45
9:z:101:BCB:O2D	7:2:23:ILE:HG23	2.16	0.45
9:K:101:BCB:C1B	9:Q:101:BCB:HMB3	2.46	0.45
5:q:39:LEU:C	5:q:41:SER:H	2.24	0.45
5:6:44:ARG:HG2	6:G:54:TRP:CZ2	2.50	0.45
7:X:14:ASP:O	7:X:14:ASP:CG	2.60	0.45
1:C:13:GLY:HA3	1:C:19:MET:HE3	1.98	0.45
2:L:170:ASN:HB2	2:L:259:TRP:CG	2.52	0.45
5:P:53:GLY:O	5:P:54:LEU:C	2.60	0.45
9:h:101:BCB:O2D	7:j:23:ILE:HG23	2.17	0.45
5:q:18:ARG:HD3	5:t:14:ILE:O	2.17	0.45
9:W:101:BCB:HBA1	9:W:101:BCB:H3A	1.80	0.45
3:M:55:GLY:O	3:M:56:ILE:C	2.60	0.45
5:z:16:ASP:HA	5:z:17:PRO:HD2	1.70	0.45
5:q:12:TRP:CD1	6:r:19:HIS:HB2	2.52	0.45
5:q:47:TRP:CZ2	9:q:101:BCB:H2C	2.52	0.45
9:t:101:BCB:CED	7:v:23:ILE:HG23	2.47	0.45
5:3:43:ASP:OD1	5:3:52:ARG:HB3	2.17	0.45
6:l:30:LEU:HB3	7:j:28:THR:HG22	1.98	0.45
9:u:101:BCB:HMB1	9:u:101:BCB:CBB	2.48	0.45
9:z:101:BCB:HMB1	9:z:101:BCB:HBB2	1.99	0.44
5:P:14:ILE:HD13	5:P:14:ILE:HA	1.80	0.44
5:e:29:THR:O	5:e:33:LEU:HG	2.18	0.44
7:R:29:ILE:O	7:R:32:ALA:HB3	2.18	0.44
7:m:26:ILE:HB	7:m:27:PRO:HD3	1.99	0.44
6:1:13:GLU:OE1	6:1:14:GLU:O	2.35	0.44
5:K:17:PRO:HB3	6:N:18:PHE:CE2	2.52	0.44
5:w:1:ALA:HA	6:x:16:LYS:CE	2.48	0.44
11:6:101:UQ9:H50	11:6:101:UQ9:H47	1.74	0.44
6:c:21:ILE:HG22	17:c:102:NS0:C10	2.47	0.44
6:i:30:LEU:HB3	7:g:28:THR:CG2	2.47	0.44
6:r:44:ARG:NH2	6:u:48:ALA:O	2.44	0.44
7:v:14:ASP:OD1	7:v:17:LEU:O	2.36	0.44
11:L:304:UQ9:C3M	11:L:304:UQ9:H4MB	2.48	0.44
11:L:304:UQ9:H47A	11:L:304:UQ9:H50	1.69	0.44
3:M:162:HIS:O	3:M:163:PRO:C	2.60	0.44
7:2:15:TRP:C	7:2:17:LEU:N	2.75	0.44
5:V:40:LEU:HD23	5:V:47:TRP:CH2	2.52	0.44
5:Y:9:TRP:C	5:Y:11:LEU:H	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:b:47:TRP:H	5:b:47:TRP:HE3	1.60	0.44
5:b:48:TRP:O	5:b:49:GLU:CB	2.54	0.44
5:t:54:LEU:HD22	5:t:58:ALA:HB3	1.99	0.44
5:6:39:LEU:HD23	5:6:39:LEU:HA	1.87	0.44
6:G:35:ILE:H	6:G:35:ILE:HG13	1.53	0.44
6:T:28:LEU:O	6:T:32:THR:HG22	2.17	0.44
7:y:15:TRP:C	7:y:17:LEU:H	2.25	0.44
5:V:47:TRP:CZ2	9:V:101:BCB:H2C	2.52	0.44
5:e:38:GLY:O	5:e:41:SER:OG	2.32	0.44
5:n:15:LEU:O	5:n:16:ASP:HB3	2.18	0.44
9:n:101:BCB:HMD1	6:o:37:HIS:CE1	2.52	0.44
9:t:101:BCB:HMD1	6:u:37:HIS:CE1	2.53	0.44
6:7:29:TYR:O	6:7:32:THR:HG22	2.18	0.44
9:z:101:BCB:H61	9:4:101:BCB:H102	1.99	0.44
5:n:47:TRP:O	5:n:48:TRP:CB	2.66	0.44
6:W:3:LEU:HB2	6:W:6:SER:HA	1.99	0.44
6:i:3:LEU:H	6:i:6:SER:HB3	1.83	0.44
9:x:101:BCB:H112	7:v:31:ILE:HD11	1.98	0.44
1:C:132:CYS:CB	8:C:402:HEC:CAB	2.93	0.44
2:L:18:GLY:C	5:6:19:ARG:HD3	2.42	0.44
2:L:142:TRP:C	2:L:144:HIS:H	2.25	0.44
5:P:9:TRP:HB2	6:Q:16:LYS:HB3	1.99	0.44
5:n:7:ALA:O	5:n:8:SER:C	2.60	0.44
5:q:12:TRP:HA	5:q:12:TRP:CE3	2.53	0.44
5:t:39:LEU:HA	5:t:45:LEU:CD1	2.48	0.44
5:t:44:ARG:HG3	6:x:54:TRP:CZ3	2.53	0.44
5:w:7:ALA:O	5:w:8:SER:C	2.60	0.44
5:3:26:VAL:HG22	11:6:101:UQ9:H4MA	1.94	0.44
6:G:25:SER:OG	17:G:102:NS0:C14	2.66	0.44
6:Z:41:TRP:HE1	7:X:14:ASP:N	2.16	0.44
1:C:243:ASN:O	1:C:244:CYS:C	2.61	0.44
15:M:410:MQ9:H462	5:3:19:ARG:HB3	1.99	0.44
4:H:213:ILE:HG22	4:H:245:GLY:HA3	2.00	0.44
17:1:102:NS0:C34	5:w:32:ALA:HB1	2.48	0.44
5:K:45:LEU:HG	9:N:101:BCB:HBC1	1.99	0.44
5:w:1:ALA:HA	6:x:16:LYS:HZ2	1.83	0.44
9:6:102:BCB:OBB	9:6:102:BCB:HHC	2.17	0.44
9:Z:101:BCB:H2	9:Z:101:BCB:H62	1.83	0.44
1:C:152:LEU:HA	1:C:153:PRO:C	2.42	0.44
1:C:301:PRO:HG2	8:C:402:HEC:HBD1	1.98	0.44
9:z:101:BCB:H142	9:4:101:BCB:H172	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:47:TRP:H	5:P:47:TRP:HE3	1.61	0.44
9:h:101:BCB:H52	9:l:101:BCB:H91	2.00	0.44
5:3:39:LEU:HD23	5:3:39:LEU:HA	1.85	0.44
6:4:37:HIS:CE1	9:4:101:BCB:NA	2.85	0.44
2:L:39:ILE:HD11	15:M:410:MQ9:H321	2.00	0.44
5:Y:9:TRP:C	5:Y:11:LEU:N	2.74	0.44
9:e:101:BCB:HMD1	6:f:37:HIS:CE1	2.52	0.44
5:n:7:ALA:O	5:n:9:TRP:N	2.51	0.44
5:t:15:LEU:O	5:t:16:ASP:HB3	2.18	0.44
6:N:41:TRP:NE1	7:I:13:SER:HB2	2.33	0.44
2:L:25:TRP:CD1	2:L:30:PHE:HB2	2.53	0.43
2:L:272:TRP:C	2:L:272:TRP:HD1	2.22	0.43
3:M:22:GLU:HB3	3:M:23:TRP:CE3	2.53	0.43
3:M:202:PHE:CZ	4:H:20:GLN:HG2	2.52	0.43
4:H:19:ALA:O	4:H:22:LEU:HB3	2.18	0.43
6:1:21:ILE:HG23	6:1:22:PHE:N	2.32	0.43
7:2:27:PRO:HA	7:2:30:TRP:NE1	2.33	0.43
5:V:16:ASP:HA	5:V:17:PRO:HD2	1.69	0.43
5:t:42:THR:OG1	5:t:45:LEU:HD11	2.14	0.43
5:6:45:LEU:HD12	5:6:45:LEU:O	2.18	0.43
6:i:46:TRP:CZ2	9:i:101:BCB:HHC	2.53	0.43
6:r:4:LYS:HB2	6:r:5:PRO:HD3	1.99	0.43
7:R:13:SER:O	7:R:15:TRP:N	2.51	0.43
2:L:255:TRP:CZ2	2:L:257:ARG:HB2	2.53	0.43
3:M:132:TYR:CD1	3:M:132:TYR:C	2.95	0.43
5:S:31:ILE:O	5:S:34:LEU:HB2	2.18	0.43
9:t:101:BCB:HMB1	9:t:101:BCB:CBB	2.47	0.43
9:3:101:BCB:HMB1	9:3:101:BCB:HBB2	1.99	0.43
7:y:16:ASN:O	7:y:17:LEU:HG	2.18	0.43
4:H:12:ILE:O	4:H:16:VAL:HG23	2.18	0.43
5:F:16:ASP:HA	5:F:17:PRO:HD2	1.70	0.43
5:k:48:TRP:HA	5:n:45:LEU:HD12	2.01	0.43
5:k:49:GLU:HG3	5:k:50:PHE:H	1.83	0.43
5:6:44:ARG:HA	6:G:54:TRP:CZ3	2.52	0.43
6:W:25:SER:OG	17:W:102:NS0:C14	2.67	0.43
6:l:46:TRP:CZ2	9:l:101:BCB:HHC	2.54	0.43
9:o:101:BCB:H161	7:m:35:TYR:CE2	2.54	0.43
2:L:146:PHE:HZ	9:L:302:BCB:CBB	2.31	0.43
2:L:197:VAL:HG13	2:L:207:LYS:HB2	2.00	0.43
5:K:49:GLU:HG3	5:K:50:PHE:H	1.81	0.43
5:t:49:GLU:HG2	5:t:52:ARG:NH1	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:w:1:ALA:HB1	5:w:4:TYR:HB2	2.00	0.43
11:6:101:UQ9:H35	11:6:101:UQ9:H32A	1.65	0.43
11:6:101:UQ9:H18	11:6:101:UQ9:H22A	1.75	0.43
6:N:22:PHE:O	6:N:26:THR:HG22	2.18	0.43
9:c:101:BCB:O1A	9:c:101:BCB:H2A	2.18	0.43
7:U:26:ILE:HB	7:U:27:PRO:HD3	2.01	0.43
7:y:14:ASP:CG	7:y:17:LEU:O	2.61	0.43
10:M:408:BPB:ND	10:M:408:BPB:NC	2.67	0.43
5:S:12:TRP:CD1	6:T:19:HIS:HB2	2.54	0.43
5:b:39:LEU:C	5:b:41:SER:H	2.26	0.43
6:N:23:VAL:HA	6:N:26:THR:HG22	2.00	0.43
6:l:21:ILE:HB	17:l:102:NS0:C8	2.47	0.43
9:u:101:BCB:H142	9:u:101:BCB:H112	1.83	0.43
4:H:203:VAL:HG22	4:H:208:ILE:HD12	2.01	0.43
4:H:257:LEU:N	4:H:258:LEU:OXT	2.51	0.43
5:e:7:ALA:O	5:e:9:TRP:N	2.52	0.43
6:G:26:THR:OG1	17:G:102:NS0:C21	2.67	0.43
6:r:36:VAL:HG22	7:s:23:ILE:HG12	2.00	0.43
2:L:178:SER:O	2:L:182:VAL:HG23	2.18	0.43
11:L:304:UQ9:C35	11:L:304:UQ9:C31	2.86	0.43
7:2:33:LEU:HA	7:2:33:LEU:HD23	1.78	0.43
5:K:50:PHE:CZ	5:P:44:ARG:HB2	2.54	0.43
5:P:47:TRP:CZ2	9:P:101:BCB:H2C	2.52	0.43
5:Y:16:ASP:HA	5:Y:17:PRO:HD2	1.69	0.43
5:b:44:ARG:CB	6:f:54:TRP:CZ3	3.01	0.43
5:h:16:ASP:HA	5:h:17:PRO:HD2	1.56	0.43
5:h:39:LEU:HD23	5:h:39:LEU:HA	1.74	0.43
5:t:40:LEU:CB	5:t:46:ASN:OD1	2.67	0.43
5:3:16:ASP:HA	5:3:17:PRO:HD2	1.68	0.43
6:W:54:TRP:CD1	6:W:55:VAL:HA	2.54	0.43
6:Z:3:LEU:O	6:Z:6:SER:HB3	2.18	0.43
7:I:29:ILE:O	7:I:32:ALA:HB3	2.18	0.43
1:C:221:ARG:HA	1:C:222:PRO:HD3	1.88	0.43
2:L:229:ILE:HD12	2:L:232:LEU:HD23	2.00	0.43
7:2:13:SER:C	6:4:41:TRP:HE1	2.27	0.43
5:3:1:ALA:HA	6:4:16:LYS:NZ	2.33	0.43
9:r:101:BCB:OBB	9:r:101:BCB:HHC	2.19	0.43
6:x:24:THR:O	6:x:28:LEU:HG	2.19	0.43
3:M:58:ALA:HB2	3:M:126:SER:HB2	2.00	0.43
6:1:41:TRP:HE1	7:y:13:SER:C	2.26	0.43
5:P:39:LEU:HD23	5:P:39:LEU:HA	1.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:b:101:BCB:H3A	17:f:102:NS0:C34	2.49	0.43
5:k:39:LEU:HA	5:k:39:LEU:HD23	1.82	0.43
9:k:101:BCB:H41	9:k:101:BCB:H61	1.85	0.43
5:6:17:PRO:HB3	6:7:18:PHE:CE2	2.53	0.43
6:Z:36:VAL:HA	6:Z:39:LEU:HD12	2.00	0.43
6:f:47:ILE:HD12	6:f:48:ALA:O	2.19	0.43
9:l:101:BCB:HBA1	9:l:101:BCB:H3A	1.89	0.43
7:a:29:ILE:O	7:a:32:ALA:HB3	2.18	0.43
8:C:401:HEC:HMB1	8:C:401:HEC:HBB3	2.01	0.43
7:2:31:ILE:HD11	9:4:101:BCB:H112	2.00	0.43
5:t:9:TRP:C	5:t:11:LEU:H	2.27	0.43
6:c:54:TRP:CD1	6:c:55:VAL:HA	2.54	0.43
6:f:47:ILE:O	6:f:48:ALA:HB3	2.19	0.43
6:i:4:LYS:HB2	6:i:5:PRO:HD3	1.99	0.43
9:i:101:BCB:H61	9:i:101:BCB:H102	1.85	0.43
7:v:29:ILE:O	7:v:32:ALA:HB3	2.18	0.43
2:L:137:LEU:HD23	2:L:137:LEU:HA	1.82	0.42
2:L:239:ASN:HA	2:L:242:LEU:HB2	2.00	0.42
5:z:39:LEU:C	5:z:41:SER:N	2.77	0.42
9:k:101:BCB:HAA1	17:o:102:NS0:C34	2.48	0.42
5:w:22:THR:O	5:w:26:VAL:HG23	2.19	0.42
6:Q:50:ILE:HA	6:Q:51:PRO:HD2	1.78	0.42
6:i:3:LEU:HD12	6:i:6:SER:HA	2.00	0.42
3:M:249:PHE:CD1	3:M:249:PHE:C	2.97	0.42
5:S:1:ALA:HA	6:T:16:LYS:NZ	2.35	0.42
5:b:1:ALA:HB1	5:b:4:TYR:HB2	2.01	0.42
9:e:101:BCB:C10	17:f:102:NS0:C13	2.95	0.42
6:T:36:VAL:HA	6:T:39:LEU:HD12	2.01	0.42
9:i:101:BCB:HHB	7:g:24:LEU:HD21	1.99	0.42
1:C:250:ALA:O	1:C:251:GLN:C	2.62	0.42
4:H:18:TYR:O	4:H:19:ALA:C	2.61	0.42
5:V:40:LEU:HD23	5:V:47:TRP:CZ2	2.53	0.42
5:b:45:LEU:HD22	9:c:101:BCB:CBC	2.48	0.42
5:e:40:LEU:HD22	5:e:48:TRP:CD2	2.53	0.42
6:T:47:ILE:O	6:T:48:ALA:HB3	2.18	0.42
1:C:141:LEU:HA	1:C:142:PRO:HD3	1.72	0.42
8:C:403:HEC:HBC3	8:C:403:HEC:CMC	2.50	0.42
11:L:304:UQ9:H15A	11:L:304:UQ9:H17A	1.79	0.42
3:M:115:MET:HE1	5:h:34:LEU:HA	2.01	0.42
6:1:23:VAL:O	6:1:26:THR:HG22	2.19	0.42
5:K:44:ARG:HA	6:Q:54:TRP:HZ3	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:48:TRP:HA	5:V:45:LEU:HD22	2.01	0.42
5:V:47:TRP:HB2	6:Z:47:ILE:HD12	1.99	0.42
5:q:39:LEU:HD23	5:q:39:LEU:HA	1.87	0.42
6:c:3:LEU:HB2	6:c:6:SER:HA	2.00	0.42
9:l:101:BCB:CHB	7:j:24:LEU:HD11	2.49	0.42
1:C:256:TRP:CD1	3:M:314:ASP:HB2	2.54	0.42
3:M:118:LEU:HB2	16:M:411:NS5:H331	2.01	0.42
5:S:34:LEU:HD23	5:S:34:LEU:HA	1.75	0.42
5:V:28:LEU:HD21	17:W:102:NS0:C25	2.50	0.42
5:V:39:LEU:HD23	5:V:39:LEU:HA	1.73	0.42
5:b:16:ASP:HA	5:b:17:PRO:HD2	1.62	0.42
5:b:40:LEU:HD23	5:b:47:TRP:CZ2	2.54	0.42
5:h:15:LEU:O	5:h:16:ASP:HB3	2.20	0.42
5:k:21:LEU:HD12	5:k:21:LEU:HA	1.86	0.42
5:n:27:TYR:CZ	5:n:31:ILE:HD11	2.55	0.42
9:c:101:BCB:H2	9:c:101:BCB:H62	1.89	0.42
8:C:403:HEC:HBC3	8:C:403:HEC:HMC1	2.01	0.42
2:L:266:TRP:CD1	2:L:267:LEU:N	2.88	0.42
5:z:39:LEU:HD22	5:z:45:LEU:HD13	2.00	0.42
9:V:101:BCB:CED	7:X:23:ILE:HG23	2.49	0.42
9:h:101:BCB:C1B	9:l:101:BCB:HMB3	2.50	0.42
9:h:101:BCB:H111	9:h:101:BCB:H152	1.85	0.42
5:w:39:LEU:C	5:w:41:SER:H	2.26	0.42
5:3:25:PHE:CD1	9:3:101:BCB:H8	2.54	0.42
11:6:101:UQ9:C35	11:6:101:UQ9:H30A	2.49	0.42
6:u:21:ILE:HD13	17:u:102:NS0:C8	2.50	0.42
6:x:47:ILE:O	6:x:48:ALA:HB3	2.20	0.42
7:d:25:GLY:O	7:d:28:THR:HG22	2.20	0.42
10:L:303:BPB:H44	10:L:303:BPB:HBAA	1.94	0.42
11:L:304:UQ9:H1MB	11:L:304:UQ9:H7	1.72	0.42
5:F:45:LEU:CD2	9:G:101:BCB:HBC1	2.47	0.42
9:P:101:BCB:HED2	9:P:101:BCB:H2A	2.02	0.42
9:P:101:BCB:O2D	7:R:23:ILE:HG23	2.20	0.42
5:k:39:LEU:C	5:k:41:SER:H	2.27	0.42
9:o:101:BCB:H102	9:o:101:BCB:H61	1.70	0.42
6:x:39:LEU:O	6:x:42:THR:OG1	2.37	0.42
1:C:69:GLU:O	1:C:72:ARG:HB3	2.19	0.42
1:C:216:ARG:HH22	3:M:287:THR:HA	1.85	0.42
9:M:407:BCB:H91	9:M:407:BCB:H111	1.79	0.42
5:z:47:TRP:CZ2	9:z:101:BCB:H2C	2.55	0.42
5:t:24:LEU:HD23	5:t:24:LEU:HA	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:t:44:ARG:HG2	6:x:54:TRP:CH2	2.54	0.42
6:G:21:ILE:HG22	17:G:102:NS0:C8	2.37	0.42
7:X:16:ASN:O	7:X:17:LEU:HG	2.19	0.42
2:L:142:TRP:O	2:L:144:HIS:N	2.53	0.42
10:L:303:BPB:HHC	10:L:303:BPB:HBBA	1.95	0.42
3:M:193:ASN:C	3:M:193:ASN:OD1	2.62	0.42
14:M:409:LDA:O1	4:H:9:HIS:CE1	2.73	0.42
9:k:101:BCB:C1B	9:o:101:BCB:HMB3	2.50	0.42
5:n:39:LEU:HD21	5:n:45:LEU:HD13	2.00	0.42
5:q:49:GLU:HG2	5:q:52:ARG:NH1	2.34	0.42
5:t:40:LEU:HD21	5:t:48:TRP:CD2	2.55	0.42
6:W:22:PHE:CD1	6:W:22:PHE:C	2.98	0.42
3:M:204:ILE:HD11	9:M:407:BCB:C1B	2.50	0.42
4:H:38:ARG:HB3	4:H:78:VAL:HG12	2.01	0.42
5:F:44:ARG:CG	6:N:54:TRP:CZ2	2.82	0.42
5:F:44:ARG:NH1	6:G:46:TRP:O	2.34	0.42
9:P:101:BCB:HMB1	9:P:101:BCB:CBB	2.50	0.42
5:b:40:LEU:HD23	5:b:47:TRP:CH2	2.54	0.42
5:b:44:ARG:NH1	6:c:46:TRP:O	2.52	0.42
9:e:101:BCB:C11	17:f:102:NS0:C13	2.97	0.42
5:h:49:GLU:HG3	5:h:50:PHE:H	1.84	0.42
5:q:21:LEU:HD12	5:q:21:LEU:HA	1.81	0.42
6:u:4:LYS:HB2	6:u:5:PRO:HD3	2.01	0.42
7:5:29:ILE:O	7:5:32:ALA:HB3	2.20	0.42
1:C:222:PRO:HG3	3:M:99:GLN:HB2	2.02	0.41
2:L:226:ALA:HA	11:L:304:UQ9:H3MB	1.99	0.41
5:S:49:GLU:HG3	5:S:50:PHE:H	1.85	0.41
5:V:47:TRP:O	5:V:48:TRP:CB	2.64	0.41
5:b:7:ALA:O	5:b:9:TRP:N	2.53	0.41
5:w:28:LEU:HD23	5:w:28:LEU:HA	1.85	0.41
6:Q:3:LEU:HD12	6:Q:6:SER:HA	2.02	0.41
6:f:3:LEU:O	6:f:6:SER:HB3	2.20	0.41
6:x:1:ALA:HA	6:x:6:SER:HB2	2.00	0.41
6:x:54:TRP:CD1	6:x:55:VAL:CA	3.02	0.41
1:C:152:LEU:HB2	1:C:175:ARG:HG2	2.01	0.41
2:L:16:LEU:H	2:L:106:GLU:HG2	1.84	0.41
2:L:60:ASP:HA	2:L:61:PRO:HD3	1.82	0.41
3:M:120:MET:HE3	3:M:175:PHE:HE1	1.84	0.41
5:e:39:LEU:HD23	5:e:39:LEU:HA	1.70	0.41
5:t:44:ARG:O	5:t:45:LEU:HG	2.19	0.41
5:w:30:VAL:O	5:w:31:ILE:C	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:s:16:ASN:HA	7:s:18:TRP:HD1	1.85	0.41
2:L:146:PHE:HB2	2:L:147:PRO:HD2	2.02	0.41
11:L:304:UQ9:H25	11:L:304:UQ9:H22	1.79	0.41
4:H:41:TYR:HB3	4:H:42:PRO:HA	2.01	0.41
5:V:32:ALA:HB1	17:Z:102:NS0:C34	2.50	0.41
5:e:25:PHE:CD1	9:e:101:BCB:C9	2.94	0.41
5:n:9:TRP:CD2	6:o:16:LYS:HG2	2.55	0.41
5:w:16:ASP:HB3	5:w:19:ARG:HD2	2.02	0.41
6:G:3:LEU:H	6:G:6:SER:HB3	1.85	0.41
6:G:4:LYS:HB2	6:G:5:PRO:HD3	2.03	0.41
6:T:22:PHE:CD1	6:T:22:PHE:C	2.99	0.41
9:c:101:BCB:HBB2	7:a:23:ILE:HD12	2.02	0.41
2:L:68:PRO:HB2	2:L:69:PRO:HD2	2.03	0.41
5:K:39:LEU:HD23	5:K:39:LEU:HA	1.70	0.41
9:b:101:BCB:HMD1	6:c:37:HIS:CE1	2.56	0.41
5:e:28:LEU:HD21	17:f:102:NS0:C25	2.50	0.41
5:t:1:ALA:HB1	5:t:4:TYR:HB2	2.01	0.41
5:t:39:LEU:CA	5:t:45:LEU:HD13	2.50	0.41
5:t:47:TRP:O	5:t:48:TRP:CB	2.60	0.41
11:6:101:UQ9:H30A	11:6:101:UQ9:H32A	1.91	0.41
6:G:44:ARG:NH1	6:N:50:ILE:HG13	2.35	0.41
6:u:54:TRP:CD1	6:u:55:VAL:HA	2.55	0.41
1:C:80:TRP:CD1	1:C:133:TYR:HB2	2.56	0.41
2:L:101:MET:HB3	2:L:101:MET:HE2	1.75	0.41
4:H:92:GLN:HB2	4:H:94:ASP:O	2.21	0.41
4:H:114:PRO:HB2	4:H:244:GLY:HA2	2.01	0.41
9:S:101:BCB:H93	17:T:102:NS0:C18	2.50	0.41
5:V:39:LEU:C	5:V:41:SER:H	2.28	0.41
5:Y:49:GLU:HG3	5:Y:50:PHE:N	2.35	0.41
9:k:101:BCB:HBC3	9:k:101:BCB:CMC	2.50	0.41
5:n:37:PHE:CE1	17:r:102:NS0:C40	3.04	0.41
9:W:101:BCB:OBB	9:W:101:BCB:HHC	2.21	0.41
6:f:29:TYR:HA	6:f:32:THR:HG22	2.02	0.41
9:4:101:BCB:CGD	9:4:101:BCB:H2A	2.51	0.41
2:L:181:PHE:HB3	10:M:408:BPB:HBBA	2.03	0.41
5:z:44:ARG:HG2	6:4:54:TRP:CH2	2.56	0.41
5:b:40:LEU:HD22	5:b:48:TRP:CD2	2.56	0.41
5:e:48:TRP:O	5:e:49:GLU:CB	2.49	0.41
6:G:41:TRP:HH2	6:G:47:ILE:HG13	1.86	0.41
6:T:3:LEU:O	6:T:6:SER:HB3	2.20	0.41
6:u:3:LEU:HB2	6:u:6:SER:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:151:LEU:HD13	3:M:196:TYR:CE1	2.55	0.41
2:L:212:GLU:HB3	11:L:304:UQ9:H4MB	2.02	0.41
14:M:409:LDA:O1	4:H:9:HIS:HE1	2.03	0.41
5:h:39:LEU:HD21	5:h:45:LEU:HD22	1.99	0.41
5:n:40:LEU:HD23	5:n:47:TRP:CZ2	2.56	0.41
6:Z:25:SER:OG	17:Z:102:NS0:C14	2.69	0.41
6:r:29:TYR:O	6:r:32:THR:HG22	2.20	0.41
6:7:4:LYS:HB2	6:7:5:PRO:HD3	2.03	0.41
7:O:16:ASN:C	7:O:17:LEU:HG	2.44	0.41
1:C:109:ARG:NH2	1:C:280:ASN:O	2.53	0.41
4:H:60:TYR:OH	9:t:101:BCB:H192	2.21	0.41
5:F:9:TRP:CB	6:G:16:LYS:HB3	2.51	0.41
5:F:17:PRO:O	5:F:21:LEU:HG	2.21	0.41
5:e:39:LEU:HD22	5:e:45:LEU:HB3	2.02	0.41
9:q:101:BCB:HMD1	6:r:37:HIS:CE1	2.56	0.41
9:6:102:BCB:H143	9:6:102:BCB:H111	1.85	0.41
6:i:21:ILE:HD12	6:i:22:PHE:H	1.85	0.41
7:U:15:TRP:C	7:U:17:LEU:N	2.77	0.41
2:L:19:GLY:N	5:6:19:ARG:NH2	2.69	0.41
2:L:226:ALA:CA	11:L:304:UQ9:C3M	2.90	0.41
5:P:28:LEU:HD21	17:Q:102:NS0:C25	2.51	0.41
5:Y:22:THR:O	5:Y:26:VAL:HG23	2.21	0.41
9:Y:101:BCB:C1B	9:c:101:BCB:HMB3	2.51	0.41
5:e:36:HIS:CE1	17:i:102:NS0:C34	3.04	0.41
5:k:48:TRP:O	5:k:49:GLU:HB2	2.21	0.41
5:n:42:THR:OG1	5:n:44:ARG:O	2.33	0.41
5:q:16:ASP:HA	5:q:17:PRO:HD2	1.63	0.41
5:q:27:TYR:CZ	5:q:31:ILE:HD11	2.55	0.41
5:w:7:ALA:HB1	5:w:10:LYS:HD2	2.03	0.41
5:w:31:ILE:O	5:w:34:LEU:HB2	2.21	0.41
5:w:47:TRP:O	5:w:48:TRP:CB	2.69	0.41
5:3:47:TRP:O	5:3:48:TRP:CB	2.67	0.41
9:6:102:BCB:H141	9:6:102:BCB:H162	1.93	0.41
6:G:22:PHE:CD1	6:G:22:PHE:C	2.98	0.41
6:G:50:ILE:HA	6:G:51:PRO:HD2	1.84	0.41
6:N:28:LEU:O	6:N:32:THR:HG22	2.21	0.41
6:T:13:GLU:OE2	6:T:15:ALA:HB2	2.20	0.41
6:T:50:ILE:HA	6:T:51:PRO:HD2	1.83	0.41
9:l:101:BCB:HBB2	7:j:20:PRO:HA	2.03	0.41
6:r:4:LYS:H	6:r:4:LYS:HG3	1.74	0.41
6:r:28:LEU:HD23	7:s:30:TRP:CE3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:u:41:TRP:HH2	6:u:47:ILE:HG13	1.86	0.41
6:u:41:TRP:CD1	7:s:14:ASP:OD1	2.74	0.41
6:x:47:ILE:HG22	7:v:17:LEU:HD13	2.03	0.41
2:L:109:ARG:HG2	2:L:109:ARG:NH1	2.33	0.41
3:M:282:ILE:HA	3:M:282:ILE:HD13	1.78	0.41
5:z:49:GLU:OE2	5:3:43:ASP:HB2	2.21	0.41
5:Y:30:VAL:O	5:Y:31:ILE:C	2.64	0.41
5:n:24:LEU:HD21	17:o:102:NS0:C20	2.50	0.41
5:w:39:LEU:C	5:w:41:SER:N	2.79	0.41
5:3:49:GLU:OE2	5:6:43:ASP:HB2	2.21	0.41
6:Q:35:ILE:H	6:Q:35:ILE:HG13	1.70	0.41
6:c:13:GLU:OE2	6:c:15:ALA:HB2	2.21	0.41
6:i:50:ILE:HA	6:i:51:PRO:HD2	1.73	0.41
6:x:54:TRP:CD1	6:x:55:VAL:HA	2.56	0.41
7:j:20:PRO:O	7:j:24:LEU:HD13	2.21	0.41
3:M:96:PRO:HG3	3:M:110:GLY:HA3	2.01	0.40
16:M:411:NS5:H24	16:M:411:NS5:H221	1.94	0.40
4:H:60:TYR:O	4:H:62:LEU:N	2.54	0.40
9:1:101:BCB:H101	9:1:101:BCB:H61	1.79	0.40
5:F:19:ARG:HA	5:F:22:THR:HG22	2.03	0.40
5:S:39:LEU:HD22	5:S:45:LEU:CD1	2.43	0.40
5:h:1:ALA:HA	6:i:16:LYS:HZ1	1.85	0.40
5:w:21:LEU:HD12	5:w:21:LEU:HA	1.79	0.40
11:6:101:UQ9:H40	11:6:101:UQ9:H37	1.78	0.40
6:T:43:ALA:HB2	7:U:17:LEU:CD2	2.51	0.40
6:W:36:VAL:HA	6:W:39:LEU:HD12	2.03	0.40
9:u:101:BCB:H92	9:u:101:BCB:H61	1.94	0.40
4:H:108:LEU:HD21	4:H:244:GLY:C	2.47	0.40
5:z:39:LEU:HD23	5:z:39:LEU:HA	1.72	0.40
9:z:101:BCB:H162	9:z:101:BCB:H122	1.90	0.40
5:F:39:LEU:HD21	5:F:45:LEU:HD13	2.01	0.40
9:K:101:BCB:HMB3	9:Q:101:BCB:CHB	2.51	0.40
5:S:9:TRP:C	5:S:11:LEU:H	2.29	0.40
5:n:25:PHE:HD1	9:n:101:BCB:H8	1.86	0.40
6:o:38:TYR:O	6:o:42:THR:HG23	2.21	0.40
7:I:15:TRP:C	7:I:17:LEU:N	2.79	0.40
7:X:16:ASN:C	7:X:17:LEU:HG	2.46	0.40
1:C:216:ARG:NH2	3:M:287:THR:HA	2.37	0.40
2:L:77:ALA:HB2	11:6:101:UQ9:H36A	2.03	0.40
10:M:408:BPB:HBBB	10:M:408:BPB:CHC	2.24	0.40
9:1:101:BCB:HBA1	9:1:101:BCB:H3A	1.77	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:2:14:ASP:OD1	7:2:17:LEU:O	2.38	0.40
5:V:15:LEU:O	5:V:16:ASP:HB3	2.22	0.40
5:V:27:TYR:CE2	5:V:31:ILE:CD1	3.05	0.40
5:h:39:LEU:HA	5:h:45:LEU:CD1	2.52	0.40
9:3:101:BCB:OBB	9:3:101:BCB:HHC	2.21	0.40
9:T:101:BCB:H2A	9:T:101:BCB:CGD	2.52	0.40
6:r:46:TRP:CZ2	9:r:101:BCB:HHC	2.57	0.40
6:7:39:LEU:HD23	6:7:39:LEU:HA	1.75	0.40
2:L:54:SER:HA	2:L:59:TRP:CZ2	2.56	0.40
10:L:303:BPB:H7A	10:L:303:BPB:H11A	1.78	0.40
9:M:407:BCB:CMB	9:M:407:BCB:HBB3	2.51	0.40
6:1:44:ARG:HD3	6:4:50:ILE:HD11	2.04	0.40
9:K:101:BCB:CMC	9:K:101:BCB:HBC3	2.52	0.40
5:S:9:TRP:C	5:S:11:LEU:N	2.78	0.40
5:S:21:LEU:HA	5:S:21:LEU:HD23	1.86	0.40
5:S:23:ALA:O	5:S:24:LEU:C	2.65	0.40
5:h:37:PHE:CZ	17:l:102:NS0:C40	3.04	0.40
5:q:32:ALA:HB1	17:u:102:NS0:C34	2.52	0.40
5:w:39:LEU:HD23	5:w:39:LEU:HA	1.63	0.40
6:u:38:TYR:CD1	6:u:38:TYR:C	3.00	0.40
6:7:15:ALA:HA	6:7:17:GLU:OE1	2.21	0.40
7:X:27:PRO:HA	7:X:30:TRP:NE1	2.36	0.40
7:v:19:VAL:HB	7:v:20:PRO:HD3	2.03	0.40
7:5:26:ILE:HB	7:5:27:PRO:HD3	2.04	0.40
2:L:193:LEU:HD22	2:L:216:PHE:HE2	1.86	0.40
7:2:17:LEU:HD22	7:2:19:VAL:CG2	2.51	0.40
5:e:18:ARG:HD3	5:h:14:ILE:O	2.22	0.40
9:n:101:BCB:H52	9:r:101:BCB:H91	2.03	0.40
5:t:39:LEU:HA	5:t:45:LEU:HD13	2.04	0.40
5:t:49:GLU:HG2	5:t:52:ARG:HH12	1.86	0.40
5:6:40:LEU:HD22	5:6:48:TRP:CD2	2.57	0.40
11:6:101:UQ9:H25A	11:6:101:UQ9:H27	1.89	0.40
6:i:21:ILE:HD11	17:i:102:NS0:CA	2.51	0.40
6:x:3:LEU:HB2	6:x:6:SER:HA	2.02	0.40
6:x:22:PHE:CD1	6:x:22:PHE:C	2.99	0.40
7:y:19:VAL:O	7:y:23:ILE:HG13	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	331/333 (99%)	300 (91%)	31 (9%)	0	100 100
2	L	271/274 (99%)	251 (93%)	15 (6%)	5 (2%)	6 22
3	M	321/323 (99%)	301 (94%)	16 (5%)	4 (1%)	10 31
4	H	254/258 (98%)	231 (91%)	16 (6%)	7 (3%)	4 14
5	3	56/59 (95%)	45 (80%)	9 (16%)	2 (4%)	2 10
5	6	56/59 (95%)	43 (77%)	11 (20%)	2 (4%)	2 10
5	F	56/59 (95%)	46 (82%)	8 (14%)	2 (4%)	2 10
5	K	56/59 (95%)	47 (84%)	7 (12%)	2 (4%)	2 10
5	P	56/59 (95%)	46 (82%)	7 (12%)	3 (5%)	1 4
5	S	56/59 (95%)	43 (77%)	12 (21%)	1 (2%)	6 22
5	V	56/59 (95%)	48 (86%)	6 (11%)	2 (4%)	2 10
5	Y	56/59 (95%)	44 (79%)	10 (18%)	2 (4%)	2 10
5	b	56/59 (95%)	43 (77%)	9 (16%)	4 (7%)	1 2
5	e	56/59 (95%)	44 (79%)	9 (16%)	3 (5%)	1 4
5	h	56/59 (95%)	45 (80%)	9 (16%)	2 (4%)	2 10
5	k	56/59 (95%)	42 (75%)	11 (20%)	3 (5%)	1 4
5	n	56/59 (95%)	44 (79%)	9 (16%)	3 (5%)	1 4
5	q	56/59 (95%)	45 (80%)	7 (12%)	4 (7%)	1 2
5	t	56/59 (95%)	45 (80%)	9 (16%)	2 (4%)	2 10
5	w	56/59 (95%)	43 (77%)	10 (18%)	3 (5%)	1 4
5	z	56/59 (95%)	45 (80%)	7 (12%)	4 (7%)	1 2
6	1	53/56 (95%)	43 (81%)	7 (13%)	3 (6%)	1 4
6	4	53/56 (95%)	42 (79%)	8 (15%)	3 (6%)	1 4
6	7	53/56 (95%)	41 (77%)	8 (15%)	4 (8%)	1 2
6	G	53/56 (95%)	41 (77%)	9 (17%)	3 (6%)	1 4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	N	53/56 (95%)	40 (76%)	9 (17%)	4 (8%)	1	2
6	Q	53/56 (95%)	40 (76%)	11 (21%)	2 (4%)	2	9
6	T	53/56 (95%)	41 (77%)	9 (17%)	3 (6%)	1	4
6	W	53/56 (95%)	40 (76%)	10 (19%)	3 (6%)	1	4
6	Z	53/56 (95%)	42 (79%)	9 (17%)	2 (4%)	2	9
6	c	53/56 (95%)	43 (81%)	9 (17%)	1 (2%)	6	21
6	f	53/56 (95%)	43 (81%)	7 (13%)	3 (6%)	1	4
6	i	53/56 (95%)	39 (74%)	11 (21%)	3 (6%)	1	4
6	l	53/56 (95%)	42 (79%)	8 (15%)	3 (6%)	1	4
6	o	53/56 (95%)	43 (81%)	8 (15%)	2 (4%)	2	9
6	r	53/56 (95%)	40 (76%)	9 (17%)	4 (8%)	1	2
6	u	53/56 (95%)	43 (81%)	6 (11%)	4 (8%)	1	2
6	x	53/56 (95%)	42 (79%)	7 (13%)	4 (8%)	1	2
7	2	22/24 (92%)	19 (86%)	1 (4%)	2 (9%)	0	1
7	5	22/24 (92%)	18 (82%)	3 (14%)	1 (4%)	2	6
7	I	22/24 (92%)	19 (86%)	1 (4%)	2 (9%)	0	1
7	O	22/24 (92%)	18 (82%)	2 (9%)	2 (9%)	0	1
7	R	22/24 (92%)	18 (82%)	3 (14%)	1 (4%)	2	6
7	U	22/24 (92%)	18 (82%)	3 (14%)	1 (4%)	2	6
7	X	22/24 (92%)	18 (82%)	2 (9%)	2 (9%)	0	1
7	a	22/24 (92%)	17 (77%)	4 (18%)	1 (4%)	2	6
7	d	22/24 (92%)	17 (77%)	3 (14%)	2 (9%)	0	1
7	g	22/24 (92%)	17 (77%)	2 (9%)	3 (14%)	0	0
7	j	22/24 (92%)	17 (77%)	3 (14%)	2 (9%)	0	1
7	m	22/24 (92%)	18 (82%)	2 (9%)	2 (9%)	0	1
7	p	22/24 (92%)	18 (82%)	2 (9%)	2 (9%)	0	1
7	s	22/24 (92%)	19 (86%)	1 (4%)	2 (9%)	0	1
7	v	22/24 (92%)	17 (77%)	5 (23%)	0	100	100
7	y	22/24 (92%)	17 (77%)	3 (14%)	2 (9%)	0	1
All	All	3382/3527 (96%)	2831 (84%)	413 (12%)	138 (4%)	4	8

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	265 (94%)	16 (6%)	18 47
2	L	218/219 (100%)	207 (95%)	11 (5%)	22 51
3	M	249/249 (100%)	242 (97%)	7 (3%)	38 70
4	H	212/212 (100%)	191 (90%)	21 (10%)	7 22
5	3	50/51 (98%)	46 (92%)	4 (8%)	11 31
5	6	50/51 (98%)	46 (92%)	4 (8%)	11 31
5	F	50/51 (98%)	45 (90%)	5 (10%)	7 22
5	K	50/51 (98%)	46 (92%)	4 (8%)	11 31
5	P	50/51 (98%)	45 (90%)	5 (10%)	7 22
5	S	50/51 (98%)	46 (92%)	4 (8%)	11 31
5	V	50/51 (98%)	47 (94%)	3 (6%)	17 44
5	Y	50/51 (98%)	44 (88%)	6 (12%)	5 14
5	b	50/51 (98%)	46 (92%)	4 (8%)	11 31
5	e	50/51 (98%)	45 (90%)	5 (10%)	7 22
5	h	50/51 (98%)	47 (94%)	3 (6%)	17 44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	k	50/51 (98%)	46 (92%)	4 (8%)	11 31
5	n	50/51 (98%)	45 (90%)	5 (10%)	7 22
5	q	50/51 (98%)	44 (88%)	6 (12%)	5 14
5	t	50/51 (98%)	46 (92%)	4 (8%)	11 31
5	w	50/51 (98%)	45 (90%)	5 (10%)	7 22
5	z	50/51 (98%)	45 (90%)	5 (10%)	7 22
6	1	46/47 (98%)	40 (87%)	6 (13%)	4 11
6	4	46/47 (98%)	43 (94%)	3 (6%)	15 41
6	7	46/47 (98%)	40 (87%)	6 (13%)	4 11
6	G	46/47 (98%)	42 (91%)	4 (9%)	9 27
6	N	46/47 (98%)	42 (91%)	4 (9%)	9 27
6	Q	46/47 (98%)	43 (94%)	3 (6%)	15 41
6	T	46/47 (98%)	40 (87%)	6 (13%)	4 11
6	W	46/47 (98%)	44 (96%)	2 (4%)	26 57
6	Z	46/47 (98%)	42 (91%)	4 (9%)	9 27
6	c	46/47 (98%)	41 (89%)	5 (11%)	6 18
6	f	46/47 (98%)	41 (89%)	5 (11%)	6 18
6	i	46/47 (98%)	39 (85%)	7 (15%)	3 8
6	l	46/47 (98%)	40 (87%)	6 (13%)	4 11
6	o	46/47 (98%)	40 (87%)	6 (13%)	4 11
6	r	46/47 (98%)	41 (89%)	5 (11%)	6 18
6	u	46/47 (98%)	43 (94%)	3 (6%)	15 41
6	x	46/47 (98%)	42 (91%)	4 (9%)	9 27
7	2	21/21 (100%)	20 (95%)	1 (5%)	23 53
7	5	21/21 (100%)	20 (95%)	1 (5%)	23 53
7	I	21/21 (100%)	20 (95%)	1 (5%)	23 53
7	O	21/21 (100%)	19 (90%)	2 (10%)	8 24
7	R	21/21 (100%)	19 (90%)	2 (10%)	8 24
7	U	21/21 (100%)	20 (95%)	1 (5%)	23 53
7	X	21/21 (100%)	20 (95%)	1 (5%)	23 53
7	a	21/21 (100%)	19 (90%)	2 (10%)	8 24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	d	21/21 (100%)	19 (90%)	2 (10%)	8 24
7	g	21/21 (100%)	20 (95%)	1 (5%)	23 53
7	j	21/21 (100%)	21 (100%)	0	100 100
7	m	21/21 (100%)	17 (81%)	4 (19%)	1 4
7	p	21/21 (100%)	18 (86%)	3 (14%)	3 9
7	s	21/21 (100%)	18 (86%)	3 (14%)	3 9
7	v	21/21 (100%)	19 (90%)	2 (10%)	8 24
7	y	21/21 (100%)	19 (90%)	2 (10%)	8 24
All	All	2928/2963 (99%)	2690 (92%)	238 (8%)	13 30

All (238) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	2	PHE
1	C	27	THR
1	C	29	LYS
1	C	32	LYS
1	C	57	LYS
1	C	101	LYS
1	C	123	GLN
1	C	132	CYS
1	C	220	ARG
1	C	229	THR
1	C	240	LEU
1	C	252	THR
1	C	274	VAL
1	C	293	ARG
1	C	296	ARG
1	C	331	ILE
2	L	2	LEU
2	L	39	ILE
2	L	46	VAL
2	L	49	ILE
2	L	55	GLN
2	L	80	LEU
2	L	101	MET
2	L	185	MET
2	L	205	LYS
2	L	214	GLN

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Mol	Chain	Res	Type
2	L	228	SER
3	M	120	MET
3	M	126	SER
3	M	142	THR
3	M	181	ILE
3	M	194	PHE
3	M	214	PHE
3	M	296	CYS
4	H	12	ILE
4	H	56	ASP
4	H	60	TYR
4	H	69	VAL
4	H	87	GLU
4	H	92	GLN
4	H	124	VAL
4	H	128	VAL
4	H	133	LYS
4	H	161	ASP
4	H	185	LEU
4	H	195	LEU
4	H	204	LYS
4	H	205	LYS
4	H	209	VAL
4	H	217	GLN
4	H	223	ARG
4	H	224	LEU
4	H	236	ASP
4	H	237	LYS
4	H	238	VAL
5	z	4	TYR
5	z	21	LEU
5	z	22	THR
5	z	31	ILE
5	z	54	LEU
6	1	6	SER
6	1	16	LYS
6	1	17	GLU
6	1	23	VAL
6	1	36	VAL
6	1	50	ILE
7	2	23	ILE
5	F	13	LEU

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Mol	Chain	Res	Type
5	F	30	VAL
5	F	31	ILE
5	F	43	ASP
5	F	44	ARG
5	K	22	THR
5	K	31	ILE
5	K	51	GLN
5	K	54	LEU
5	P	14	ILE
5	P	22	THR
5	P	43	ASP
5	P	51	GLN
5	P	54	LEU
5	S	14	ILE
5	S	19	ARG
5	S	22	THR
5	S	31	ILE
5	V	3	GLU
5	V	19	ARG
5	V	56	LYS
5	Y	14	ILE
5	Y	19	ARG
5	Y	22	THR
5	Y	31	ILE
5	Y	54	LEU
5	Y	56	LYS
5	b	21	LEU
5	b	31	ILE
5	b	44	ARG
5	b	56	LYS
5	e	22	THR
5	e	31	ILE
5	e	44	ARG
5	e	51	GLN
5	e	56	LYS
5	h	21	LEU
5	h	22	THR
5	h	44	ARG
5	k	14	ILE
5	k	22	THR
5	k	31	ILE
5	k	45	LEU

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Mol	Chain	Res	Type
5	n	14	ILE
5	n	15	LEU
5	n	20	VAL
5	n	34	LEU
5	n	51	GLN
5	q	21	LEU
5	q	22	THR
5	q	44	ARG
5	q	45	LEU
5	q	54	LEU
5	q	56	LYS
5	t	15	LEU
5	t	21	LEU
5	t	31	ILE
5	t	43	ASP
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	3	51	GLN
5	6	4	TYR
5	6	31	ILE
5	6	54	LEU
5	6	56	LYS
6	G	13	GLU
6	G	16	LYS
6	G	17	GLU
6	G	55	VAL
6	N	6	SER
6	N	13	GLU
6	N	16	LYS
6	N	55	VAL
6	Q	3	LEU
6	Q	16	LYS
6	Q	21	ILE
6	T	14	GLU
6	T	16	LYS
6	T	23	VAL

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Mol	Chain	Res	Type
6	T	27	VAL
6	T	47	ILE
6	T	55	VAL
6	W	16	LYS
6	W	27	VAL
6	Z	16	LYS
6	Z	23	VAL
6	Z	25	SER
6	Z	55	VAL
6	c	16	LYS
6	c	23	VAL
6	c	27	VAL
6	c	28	LEU
6	c	44	ARG
6	f	13	GLU
6	f	14	GLU
6	f	16	LYS
6	f	25	SER
6	f	27	VAL
6	i	3	LEU
6	i	16	LYS
6	i	23	VAL
6	i	27	VAL
6	i	28	LEU
6	i	36	VAL
6	i	55	VAL
6	l	16	LYS
6	l	27	VAL
6	l	28	LEU
6	l	36	VAL
6	l	50	ILE
6	l	55	VAL
6	o	3	LEU
6	o	16	LYS
6	o	23	VAL
6	o	25	SER
6	o	27	VAL
6	o	34	VAL
6	r	4	LYS
6	r	16	LYS
6	r	23	VAL
6	r	36	VAL

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Mol	Chain	Res	Type
6	r	55	VAL
6	u	16	LYS
6	u	23	VAL
6	u	25	SER
6	x	16	LYS
6	x	21	ILE
6	x	25	SER
6	x	27	VAL
6	4	16	LYS
6	4	34	VAL
6	4	55	VAL
6	7	16	LYS
6	7	21	ILE
6	7	28	LEU
6	7	34	VAL
6	7	35	ILE
6	7	55	VAL
7	I	28	THR
7	O	19	VAL
7	O	28	THR
7	R	17	LEU
7	R	28	THR
7	U	16	ASN
7	X	16	ASN
7	a	17	LEU
7	a	28	THR
7	d	16	ASN
7	d	28	THR
7	g	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	s	31	ILE
7	v	19	VAL
7	v	31	ILE
7	y	14	ASP

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Mol	Chain	Res	Type
7	y	31	ILE
7	5	16	ASN

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

Mol	Chain	Res	Type
1	C	24	HIS
1	C	200	GLN
2	L	55	GLN
2	L	144	HIS
2	L	211	HIS
2	L	214	GLN
3	M	4	GLN
3	M	45	GLN
4	H	92	GLN
7	2	16	ASN
7	d	16	ASN
7	j	16	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	FME	H	1	4	8,9,10	0.58	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
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 oligosaccharides 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	$\#\|Z\|>2$
17	NS0	4	102	-	39,39,39	6.02	19 (48%)	44,46,46	3.61	21 (47%)
17	NS0	x	102	-	39,39,39	6.13	19 (48%)	44,46,46	3.59	20 (45%)
9	BCB	L	301	2	68,74,74	2.24	17 (25%)	79,115,115	2.64	30 (37%)
9	BCB	K	101	5	68,74,74	2.31	17 (25%)	79,115,115	2.97	28 (35%)
9	BCB	t	101	5	68,74,74	2.32	18 (26%)	79,115,115	2.68	25 (31%)
9	BCB	6	102	5	68,74,74	2.47	18 (26%)	79,115,115	2.80	24 (30%)
9	BCB	u	101	6	68,74,74	2.32	18 (26%)	79,115,115	2.68	20 (25%)
13	SO4	M	405	-	4,4,4	0.31	0	6,6,6	0.11	0
11	UQ9	6	101	-	58,58,58	3.85	16 (27%)	70,73,73	2.43	22 (31%)
13	SO4	H	302	-	4,4,4	0.38	0	6,6,6	0.25	0
17	NS0	c	102	6	39,39,39	6.09	19 (48%)	44,46,46	3.56	24 (54%)
17	NS0	i	102	-	39,39,39	6.04	19 (48%)	44,46,46	3.62	23 (52%)
9	BCB	Y	101	5	68,74,74	2.44	18 (26%)	79,115,115	2.71	26 (32%)
17	NS0	1	102	6	39,39,39	6.04	19 (48%)	44,46,46	3.64	24 (54%)
17	NS0	r	102	-	39,39,39	6.09	19 (48%)	44,46,46	3.59	23 (52%)
8	HEC	C	403	1	50,50,50	1.70	10 (20%)	68,82,82	1.97	16 (23%)
17	NS0	7	102	-	39,39,39	6.51	19 (48%)	44,46,46	3.56	26 (59%)
17	NS0	W	102	-	39,39,39	6.04	19 (48%)	44,46,46	3.68	23 (52%)
9	BCB	M	407	3	68,74,74	2.27	17 (25%)	79,115,115	2.55	27 (34%)
8	HEC	C	402	1	50,50,50	1.84	13 (26%)	68,82,82	1.96	20 (29%)
17	NS0	u	102	-	39,39,39	6.02	19 (48%)	44,46,46	3.60	21 (47%)
14	LDA	M	409	-	12,15,15	2.12	1 (8%)	14,17,17	0.88	0
9	BCB	W	101	6	68,74,74	2.33	18 (26%)	79,115,115	2.49	19 (24%)
8	HEC	C	401	1	50,50,50	1.85	12 (24%)	68,82,82	1.95	18 (26%)
10	BPB	L	303	-	57,70,70	2.68	15 (26%)	56,101,101	2.54	11 (19%)
9	BCB	V	101	5	68,74,74	2.34	18 (26%)	79,115,115	2.65	24 (30%)
15	MQ9	M	410	-	59,59,59	1.33	4 (6%)	72,75,75	2.22	25 (34%)
9	BCB	q	101	5	68,74,74	3.23	20 (29%)	79,115,115	2.78	24 (30%)
9	BCB	o	101	6	68,74,74	2.36	18 (26%)	79,115,115	2.94	24 (30%)
10	BPB	M	408	-	57,70,70	2.67	15 (26%)	56,101,101	2.57	19 (33%)
9	BCB	e	101	5	68,74,74	2.35	18 (26%)	79,115,115	2.82	22 (27%)
9	BCB	Q	101	6	68,74,74	2.33	16 (23%)	79,115,115	2.66	21 (26%)
11	UQ9	L	304	-	58,58,58	3.87	16 (27%)	70,73,73	2.62	23 (32%)
13	SO4	H	304	-	4,4,4	0.39	0	6,6,6	0.14	0
9	BCB	F	101	5	68,74,74	2.31	18 (26%)	79,115,115	2.96	23 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	BCB	i	101	6	68,74,74	2.35	18 (26%)	79,115,115	2.67	20 (25%)
17	NS0	T	102	-	39,39,39	6.15	19 (48%)	44,46,46	3.55	20 (45%)
9	BCB	L	302	2	68,74,74	2.31	20 (29%)	79,115,115	2.34	21 (26%)
17	NS0	o	102	6	39,39,39	6.06	19 (48%)	44,46,46	3.65	23 (52%)
13	SO4	H	303	-	4,4,4	0.36	0	6,6,6	0.10	0
17	NS0	N	102	-	39,39,39	5.94	19 (48%)	44,46,46	3.65	21 (47%)
9	BCB	h	101	5	68,74,74	2.36	17 (25%)	79,115,115	2.71	23 (29%)
14	LDA	H	301	-	12,15,15	2.16	1 (8%)	14,17,17	0.49	0
17	NS0	Z	102	-	39,39,39	6.07	19 (48%)	44,46,46	3.58	21 (47%)
9	BCB	T	101	6	68,74,74	2.39	17 (25%)	79,115,115	2.72	20 (25%)
9	BCB	l	101	6	68,74,74	2.31	18 (26%)	79,115,115	2.77	24 (30%)
9	BCB	S	101	5	68,74,74	2.34	17 (25%)	79,115,115	2.64	25 (31%)
9	BCB	k	101	5	68,74,74	2.24	17 (25%)	79,115,115	2.49	22 (27%)
13	SO4	M	402	-	4,4,4	0.39	0	6,6,6	0.48	0
13	SO4	M	403	-	4,4,4	0.32	0	6,6,6	0.09	0
9	BCB	N	101	6	68,74,74	2.39	20 (29%)	79,115,115	2.54	21 (26%)
17	NS0	Q	102	-	39,39,39	6.09	19 (48%)	44,46,46	3.54	23 (52%)
9	BCB	f	101	6	68,74,74	2.39	18 (26%)	79,115,115	2.64	21 (26%)
9	BCB	Z	101	6	68,74,74	2.33	18 (26%)	79,115,115	2.48	19 (24%)
9	BCB	z	101	5	68,74,74	2.32	17 (25%)	79,115,115	2.78	29 (36%)
9	BCB	4	101	6	68,74,74	2.35	17 (25%)	79,115,115	2.48	20 (25%)
9	BCB	M	406	3	68,74,74	2.53	19 (27%)	79,115,115	3.15	22 (27%)
16	NS5	M	411	-	39,39,39	0.78	0	44,46,46	1.99	10 (22%)
13	SO4	M	404	-	4,4,4	0.44	0	6,6,6	0.19	0
17	NS0	G	102	-	39,39,39	6.17	19 (48%)	44,46,46	3.58	23 (52%)
9	BCB	b	101	5	68,74,74	2.30	16 (23%)	79,115,115	2.68	26 (32%)
9	BCB	x	101	6	68,74,74	2.32	20 (29%)	79,115,115	2.64	17 (21%)
17	NS0	f	102	-	39,39,39	6.11	19 (48%)	44,46,46	3.62	23 (52%)
17	NS0	l	102	-	39,39,39	6.17	19 (48%)	44,46,46	3.55	22 (50%)
9	BCB	c	101	6	68,74,74	2.42	20 (29%)	79,115,115	2.49	18 (22%)
9	BCB	n	101	5	68,74,74	2.36	18 (26%)	79,115,115	2.68	23 (29%)
9	BCB	3	101	5	68,74,74	2.44	18 (26%)	79,115,115	2.70	22 (27%)
9	BCB	G	101	6	68,74,74	2.39	18 (26%)	79,115,115	2.81	19 (24%)
9	BCB	w	101	5	68,74,74	2.44	20 (29%)	79,115,115	2.85	22 (27%)
8	HEC	C	404	1	50,50,50	1.72	9 (18%)	68,82,82	1.88	16 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	BCB	1	101	6	68,74,74	2.41	19 (27%)	79,115,115	2.56	21 (26%)
9	BCB	7	101	6	68,74,74	2.41	16 (23%)	79,115,115	2.59	23 (29%)
9	BCB	P	101	5	68,74,74	2.44	17 (25%)	79,115,115	2.83	29 (36%)
9	BCB	r	101	6	68,74,74	2.32	19 (27%)	79,115,115	2.83	26 (32%)

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
17	NS0	4	102	-	-	14/43/43/43	-
17	NS0	x	102	-	-	14/43/43/43	-
9	BCB	L	301	2	3/3/21/26	10/41/137/137	-
9	BCB	K	101	5	2/2/21/26	20/41/137/137	-
9	BCB	t	101	5	2/2/21/26	21/41/137/137	-
9	BCB	6	102	5	2/2/21/26	19/41/137/137	-
9	BCB	u	101	6	2/2/21/26	17/41/137/137	-
17	NS0	c	102	6	-	13/43/43/43	-
11	UQ9	6	101	-	-	18/57/81/81	0/1/1/1
17	NS0	i	102	-	-	14/43/43/43	-
17	NS0	u	102	-	-	14/43/43/43	-
9	BCB	Y	101	5	2/2/21/26	19/41/137/137	-
17	NS0	1	102	6	-	16/43/43/43	-
17	NS0	r	102	-	-	14/43/43/43	-
8	HEC	C	403	1	1/1/3/7	8/14/54/54	-
17	NS0	7	102	-	-	17/43/43/43	-
17	NS0	W	102	-	-	13/43/43/43	-
9	BCB	M	407	3	2/2/21/26	16/41/137/137	-
8	HEC	C	402	1	1/1/3/7	7/14/54/54	-
14	LDA	M	409	-	-	9/13/13/13	-
9	BCB	W	101	6	2/2/21/26	18/41/137/137	-
8	HEC	C	401	1	1/1/3/7	7/14/54/54	-
10	BPB	L	303	-	1/1/18/23	16/37/105/105	0/5/6/6
9	BCB	V	101	5	2/2/21/26	24/41/137/137	-
15	MQ9	M	410	-	-	16/53/73/73	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BCB	q	101	5	2/2/21/26	21/41/137/137	-
9	BCB	o	101	6	2/2/21/26	23/41/137/137	-
10	BPB	M	408	-	1/1/18/23	15/37/105/105	0/5/6/6
9	BCB	e	101	5	2/2/21/26	21/41/137/137	-
9	BCB	Q	101	6	2/2/21/26	22/41/137/137	-
11	UQ9	L	304	-	-	16/57/81/81	0/1/1/1
17	NS0	T	102	-	-	15/43/43/43	-
9	BCB	F	101	5	2/2/21/26	18/41/137/137	-
9	BCB	i	101	6	2/2/21/26	21/41/137/137	-
17	NS0	o	102	6	-	14/43/43/43	-
9	BCB	L	302	2	2/2/21/26	10/41/137/137	-
17	NS0	N	102	-	-	15/43/43/43	-
17	NS0	Z	102	-	-	14/43/43/43	-
9	BCB	h	101	5	2/2/21/26	23/41/137/137	-
14	LDA	H	301	-	-	9/13/13/13	-
9	BCB	T	101	6	2/2/21/26	23/41/137/137	-
9	BCB	l	101	6	2/2/21/26	17/41/137/137	-
9	BCB	S	101	5	2/2/21/26	22/41/137/137	-
9	BCB	k	101	5	2/2/21/26	20/41/137/137	-
9	BCB	N	101	6	2/2/21/26	23/41/137/137	-
17	NS0	Q	102	-	-	14/43/43/43	-
9	BCB	f	101	6	2/2/21/26	17/41/137/137	-
9	BCB	Z	101	6	2/2/21/26	21/41/137/137	-
9	BCB	z	101	5	2/2/21/26	19/41/137/137	-
9	BCB	4	101	6	2/2/21/26	23/41/137/137	-
9	BCB	M	406	3	2/2/21/26	15/41/137/137	-
16	NS5	M	411	-	-	13/43/43/43	-
17	NS0	G	102	-	-	12/43/43/43	-
9	BCB	b	101	5	2/2/21/26	20/41/137/137	-
9	BCB	x	101	6	2/2/21/26	21/41/137/137	-
17	NS0	f	102	-	-	14/43/43/43	-
17	NS0	l	102	-	-	15/43/43/43	-
9	BCB	c	101	6	2/2/21/26	19/41/137/137	-
9	BCB	n	101	5	2/2/21/26	21/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BCB	3	101	5	2/2/21/26	16/41/137/137	-
9	BCB	G	101	6	2/2/21/26	20/41/137/137	-
9	BCB	w	101	5	2/2/21/26	17/41/137/137	-
8	HEC	C	404	1	1/1/3/7	7/14/54/54	-
9	BCB	1	101	6	2/2/21/26	23/41/137/137	-
9	BCB	7	101	6	2/2/21/26	14/41/137/137	-
9	BCB	P	101	5	2/2/21/26	21/41/137/137	-
9	BCB	r	101	6	2/2/21/26	20/41/137/137	-

All (1118) 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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
9	q	101	BCB	CBB-CAB	-14.60	1.21	1.50
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	OBB-CAB	10.77	1.47	1.23
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
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
9	P	101	BCB	C1D-ND	8.40	1.48	1.37
11	L	304	UQ9	C43-C44	8.36	1.53	1.33
11	6	101	UQ9	C33-C34	8.34	1.53	1.33
10	L	303	BPB	C1B-C2B	8.09	1.48	1.39
10	L	303	BPB	C1D-C2D	8.08	1.48	1.39
17	7	102	NS0	C32-C33	8.04	1.52	1.33
17	G	102	NS0	C32-C33	7.90	1.51	1.33
10	M	408	BPB	C1D-C2D	7.90	1.48	1.39
17	N	102	NS0	C32-C33	7.83	1.51	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	c	102	NS0	C32-C33	7.81	1.51	1.33
17	l	102	NS0	C32-C33	7.79	1.51	1.33
9	M	406	BCB	C4B-NB	7.76	1.47	1.37
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	408	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
9	K	101	BCB	C1D-ND	7.66	1.47	1.37
17	Z	102	NS0	C32-C33	7.64	1.51	1.33
9	6	102	BCB	C1D-ND	7.63	1.47	1.37
17	1	102	NS0	C32-C33	7.58	1.51	1.33
9	b	101	BCB	C1D-ND	7.56	1.47	1.37
9	L	302	BCB	C1D-ND	7.55	1.47	1.37
17	u	102	NS0	C32-C33	7.54	1.51	1.33
9	z	101	BCB	C1D-ND	7.53	1.47	1.37
9	h	101	BCB	C1D-ND	7.53	1.47	1.37
9	V	101	BCB	C1D-ND	7.51	1.47	1.37
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
9	t	101	BCB	C1D-ND	7.45	1.46	1.37
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
9	w	101	BCB	C1D-ND	7.37	1.46	1.37
17	7	102	NS0	CB-CG	7.37	1.53	1.32
9	M	406	BCB	C1D-ND	7.37	1.46	1.37
17	u	102	NS0	CB-CG	7.34	1.53	1.32
17	T	102	NS0	C10-C11	7.34	1.53	1.34
9	Y	101	BCB	C4B-NB	7.34	1.46	1.37
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
9	S	101	BCB	C1D-ND	7.24	1.46	1.37
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
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
9	Y	101	BCB	C1D-ND	7.14	1.46	1.37
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	409	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
9	7	101	BCB	C1D-ND	7.04	1.46	1.37
9	n	101	BCB	C1D-ND	7.04	1.46	1.37
17	G	102	NS0	C15-C16	7.01	1.52	1.34
11	6	101	UQ9	C7-C6	-7.00	1.40	1.51
9	w	101	BCB	C4B-NB	6.94	1.46	1.37
17	T	102	NS0	C26-C25	6.94	1.52	1.34
17	i	102	NS0	C15-C16	6.93	1.52	1.34
9	F	101	BCB	C1D-ND	6.92	1.46	1.37
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	3	101	BCB	C1D-ND	6.85	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	o	102	NS0	C15-C16	6.85	1.52	1.34
17	T	102	NS0	C15-C16	6.84	1.52	1.34
9	c	101	BCB	C4B-NB	6.84	1.46	1.37
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
10	M	408	BPB	C1B-C2B	6.80	1.47	1.39
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
9	q	101	BCB	C1D-ND	6.79	1.46	1.37
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	e	101	BCB	C1D-ND	6.71	1.46	1.37
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
9	c	101	BCB	C1D-ND	6.69	1.46	1.37
17	N	102	NS0	C15-C16	6.69	1.51	1.34
17	c	102	NS0	C15-C16	6.68	1.51	1.34
9	1	101	BCB	C4B-NB	6.66	1.46	1.37
9	k	101	BCB	C1D-ND	6.66	1.46	1.37
17	r	102	NS0	C26-C25	6.66	1.51	1.34
9	T	101	BCB	C1D-ND	6.62	1.45	1.37
17	7	102	NS0	C20-C21	6.59	1.53	1.36
17	W	102	NS0	C26-C25	6.58	1.51	1.34
9	i	101	BCB	C1D-ND	6.57	1.45	1.37
9	M	407	BCB	C1D-ND	6.55	1.45	1.37
9	3	101	BCB	C1B-NB	6.52	1.45	1.37
9	l	101	BCB	C1D-ND	6.51	1.45	1.37
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	1	101	BCB	C1D-ND	6.48	1.45	1.37
17	7	102	NS0	C16-C17	6.46	1.59	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	f	101	BCB	C1D-ND	6.46	1.45	1.37
17	G	102	NS0	C20-C21	6.43	1.52	1.36
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
9	T	101	BCB	C1B-NB	6.38	1.45	1.37
17	x	102	NS0	C20-C21	6.38	1.52	1.36
9	4	101	BCB	C4B-NB	6.38	1.45	1.37
17	l	102	NS0	C20-C21	6.38	1.52	1.36
9	F	101	BCB	C3D-C4D	-6.38	1.29	1.44
9	o	101	BCB	C1D-ND	6.37	1.45	1.37
17	Z	102	NS0	C20-C21	6.35	1.52	1.36
9	G	101	BCB	C1B-NB	6.34	1.45	1.37
9	f	101	BCB	C1B-NB	6.33	1.45	1.37
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
17	W	102	NS0	C20-C21	6.27	1.52	1.36
9	l	101	BCB	C3D-C4D	-6.27	1.30	1.44
15	M	410	MQ9	C6-C5	6.23	1.46	1.35
17	o	102	NS0	C20-C21	6.20	1.52	1.36
9	u	101	BCB	C1D-ND	6.20	1.45	1.37
9	N	101	BCB	C1D-ND	6.20	1.45	1.37
9	o	101	BCB	CAC-C3C	6.20	1.50	1.33
9	T	101	BCB	C3D-C4D	-6.19	1.30	1.44
17	N	102	NS0	C20-C21	6.19	1.52	1.36
9	f	101	BCB	C4B-NB	6.16	1.45	1.37
9	4	101	BCB	C1D-ND	6.14	1.45	1.37
9	W	101	BCB	C1D-ND	6.11	1.45	1.37
9	Q	101	BCB	C4B-NB	6.11	1.45	1.37
9	1	101	BCB	C3D-C4D	-6.06	1.30	1.44
9	l	101	BCB	CAC-C3C	6.04	1.50	1.33
9	6	102	BCB	O2D-CGD	6.04	1.47	1.33
9	Z	101	BCB	C1D-ND	6.03	1.45	1.37
9	r	101	BCB	C1D-ND	6.01	1.45	1.37
9	M	407	BCB	C3D-C4D	-6.00	1.30	1.44
9	x	101	BCB	C1D-ND	5.99	1.45	1.37
9	u	101	BCB	C4B-NB	5.99	1.45	1.37
9	L	301	BCB	C1D-ND	5.98	1.45	1.37
9	N	101	BCB	C4B-NB	5.98	1.45	1.37
9	i	101	BCB	C3D-C4D	-5.96	1.30	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	7	101	BCB	C4B-NB	5.96	1.45	1.37
9	n	101	BCB	C4B-NB	5.94	1.45	1.37
9	1	101	BCB	CAC-C3C	5.92	1.49	1.33
9	o	101	BCB	C3D-C4D	-5.92	1.30	1.44
9	L	301	BCB	O2D-CGD	5.90	1.47	1.33
9	M	406	BCB	C2C-C3C	-5.89	1.44	1.51
9	N	101	BCB	CAC-C3C	5.88	1.49	1.33
9	u	101	BCB	C3D-C4D	-5.88	1.30	1.44
9	K	101	BCB	C3D-C4D	-5.87	1.30	1.44
9	3	101	BCB	C4B-NB	5.86	1.45	1.37
9	S	101	BCB	C4B-NB	5.85	1.45	1.37
9	r	101	BCB	CAC-C3C	5.84	1.49	1.33
9	M	407	BCB	CAC-C3C	5.82	1.49	1.33
9	L	302	BCB	CAC-C3C	5.82	1.49	1.33
9	r	101	BCB	C3D-C4D	-5.79	1.31	1.44
9	k	101	BCB	C3D-C4D	-5.78	1.31	1.44
9	M	406	BCB	C3D-C4D	-5.78	1.31	1.44
9	q	101	BCB	C3D-C4D	-5.77	1.31	1.44
9	x	101	BCB	C3D-C4D	-5.77	1.31	1.44
9	F	101	BCB	CAC-C3C	5.76	1.49	1.33
9	i	101	BCB	C1B-NB	5.76	1.44	1.37
9	h	101	BCB	C3D-C4D	-5.76	1.31	1.44
9	W	101	BCB	C3D-C4D	-5.76	1.31	1.44
9	G	101	BCB	C4B-NB	5.75	1.44	1.37
9	Z	101	BCB	CAC-C3C	5.75	1.49	1.33
9	4	101	BCB	CAC-C3C	5.75	1.49	1.33
9	x	101	BCB	CAC-C3C	5.75	1.49	1.33
9	Z	101	BCB	C3D-C4D	-5.75	1.31	1.44
9	4	101	BCB	C3D-C4D	-5.74	1.31	1.44
9	L	301	BCB	CAC-C3C	5.72	1.49	1.33
9	L	301	BCB	C3D-C4D	-5.72	1.31	1.44
9	G	101	BCB	C3D-C4D	-5.71	1.31	1.44
9	3	101	BCB	C3D-C4D	-5.70	1.31	1.44
9	3	101	BCB	CAC-C3C	5.70	1.49	1.33
9	Q	101	BCB	C3D-C4D	-5.69	1.31	1.44
11	6	101	UQ9	C1M-C1	-5.67	1.38	1.50
9	P	101	BCB	C3D-C4D	-5.67	1.31	1.44
9	n	101	BCB	C3D-C4D	-5.66	1.31	1.44
9	Q	101	BCB	CAC-C3C	5.66	1.49	1.33
11	L	304	UQ9	C1M-C1	-5.65	1.38	1.50
9	u	101	BCB	CAC-C3C	5.64	1.48	1.33
9	e	101	BCB	C4B-NB	5.63	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	7	101	BCB	CAC-C3C	5.63	1.48	1.33
9	i	101	BCB	CAC-C3C	5.63	1.48	1.33
9	Y	101	BCB	CAC-C3C	5.60	1.48	1.33
9	f	101	BCB	C3D-C4D	-5.60	1.31	1.44
9	q	101	BCB	CAC-C3C	5.60	1.48	1.33
9	W	101	BCB	CAC-C3C	5.60	1.48	1.33
9	G	101	BCB	C1D-ND	5.59	1.44	1.37
9	Q	101	BCB	C2C-C3C	-5.59	1.44	1.51
9	T	101	BCB	C2C-C3C	-5.59	1.44	1.51
9	t	101	BCB	C3D-C4D	-5.58	1.31	1.44
10	M	408	BPB	CBD-CGD	-5.58	1.44	1.52
9	b	101	BCB	C3D-C4D	-5.58	1.31	1.44
9	V	101	BCB	C3D-C4D	-5.56	1.31	1.44
9	7	101	BCB	C1B-NB	5.56	1.44	1.37
9	Q	101	BCB	C1B-NB	5.56	1.44	1.37
9	Q	101	BCB	C1D-ND	5.54	1.44	1.37
9	e	101	BCB	O2A-CGA	5.54	1.49	1.33
9	S	101	BCB	C3D-C4D	-5.52	1.31	1.44
9	T	101	BCB	CAC-C3C	5.51	1.48	1.33
9	Y	101	BCB	C3D-C4D	-5.51	1.31	1.44
9	W	101	BCB	C4B-NB	5.48	1.44	1.37
9	u	101	BCB	C2C-C3C	-5.48	1.44	1.51
9	G	101	BCB	CAC-C3C	5.48	1.48	1.33
9	M	406	BCB	CAC-C3C	5.45	1.48	1.33
9	f	101	BCB	CAC-C3C	5.45	1.48	1.33
9	M	406	BCB	O2A-CGA	5.45	1.49	1.33
9	t	101	BCB	CAC-C3C	5.45	1.48	1.33
9	7	101	BCB	C3D-C4D	-5.44	1.31	1.44
9	M	407	BCB	O2D-CGD	5.42	1.46	1.33
9	Z	101	BCB	C1B-NB	5.42	1.44	1.37
9	o	101	BCB	C2C-C3C	-5.42	1.44	1.51
9	e	101	BCB	C3D-C4D	-5.41	1.32	1.44
9	4	101	BCB	C1B-NB	5.40	1.44	1.37
9	c	101	BCB	CAC-C3C	5.40	1.48	1.33
9	P	101	BCB	O2A-CGA	5.37	1.49	1.33
9	N	101	BCB	C1B-NB	5.37	1.44	1.37
9	K	101	BCB	C2C-C3C	-5.37	1.44	1.51
9	n	101	BCB	CAC-C3C	5.36	1.48	1.33
9	w	101	BCB	CAC-C3C	5.35	1.48	1.33
9	h	101	BCB	CAC-C3C	5.35	1.48	1.33
9	Z	101	BCB	C4B-NB	5.34	1.44	1.37
9	N	101	BCB	C3D-C4D	-5.34	1.32	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	f	101	BCB	C2C-C3C	-5.33	1.44	1.51
9	k	101	BCB	CAC-C3C	5.33	1.48	1.33
9	6	102	BCB	C4B-NB	5.32	1.44	1.37
9	L	301	BCB	C2C-C3C	-5.30	1.44	1.51
9	c	101	BCB	C1B-NB	5.28	1.44	1.37
9	w	101	BCB	C3D-C4D	-5.27	1.32	1.44
9	6	102	BCB	C3D-C4D	-5.27	1.32	1.44
9	x	101	BCB	C1B-NB	5.26	1.44	1.37
9	P	101	BCB	CAC-C3C	5.24	1.47	1.33
9	W	101	BCB	C2C-C3C	-5.22	1.44	1.51
9	6	102	BCB	CAC-C3C	5.22	1.47	1.33
9	l	101	BCB	C4B-NB	5.22	1.44	1.37
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	Z	101	BCB	C2C-C3C	-5.20	1.45	1.51
9	z	101	BCB	C4B-NB	5.19	1.44	1.37
10	L	303	BPB	C3B-C2B	5.19	1.48	1.39
9	W	101	BCB	C1B-NB	5.19	1.44	1.37
9	b	101	BCB	CAC-C3C	5.18	1.47	1.33
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	V	101	BCB	CAC-C3C	5.16	1.47	1.33
9	h	101	BCB	C1B-NB	5.16	1.44	1.37
9	M	406	BCB	C4D-ND	-5.16	1.30	1.37
9	S	101	BCB	C2C-C3C	-5.16	1.45	1.51
9	S	101	BCB	CAC-C3C	5.16	1.47	1.33
9	z	101	BCB	O2A-CGA	5.15	1.48	1.33
9	q	101	BCB	C2C-C3C	-5.15	1.45	1.51
10	M	408	BPB	C4D-CHA	5.14	1.47	1.39
9	L	302	BCB	C1B-NB	5.14	1.44	1.37
9	r	101	BCB	C4B-NB	5.13	1.44	1.37
9	n	101	BCB	C2C-C3C	-5.12	1.45	1.51
10	M	408	BPB	C3D-C4D	-5.12	1.33	1.41
9	G	101	BCB	C2C-C3C	-5.12	1.45	1.51
9	Y	101	BCB	O2A-CGA	5.11	1.48	1.33
9	6	102	BCB	C1B-NB	5.10	1.44	1.37
9	6	102	BCB	C2C-C3C	-5.10	1.45	1.51
9	P	101	BCB	C2C-C3C	-5.10	1.45	1.51
9	1	101	BCB	C1B-NB	5.09	1.44	1.37
9	q	101	BCB	C1B-NB	5.09	1.44	1.37
9	n	101	BCB	O2A-CGA	5.07	1.48	1.33
8	C	401	HEC	C4B-NB	-5.06	1.31	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	e	101	BCB	C2C-C3C	-5.05	1.45	1.51
9	e	101	BCB	CAC-C3C	5.05	1.47	1.33
9	x	101	BCB	O2A-CGA	5.03	1.48	1.33
9	i	101	BCB	C2C-C3C	-5.02	1.45	1.51
9	1	101	BCB	O2A-CGA	5.02	1.48	1.33
9	K	101	BCB	CAC-C3C	5.01	1.47	1.33
9	r	101	BCB	C2C-C3C	-5.01	1.45	1.51
9	L	302	BCB	C3D-C4D	-5.01	1.32	1.44
9	V	101	BCB	C2C-C3C	-5.01	1.45	1.51
9	z	101	BCB	CAC-C3C	5.00	1.47	1.33
9	P	101	BCB	C4B-NB	5.00	1.43	1.37
10	M	408	BPB	O2A-CGA	5.00	1.47	1.33
9	o	101	BCB	C4B-NB	4.99	1.43	1.37
9	c	101	BCB	CHC-C1C	4.97	1.48	1.37
9	7	101	BCB	C2C-C3C	-4.97	1.45	1.51
9	x	101	BCB	C4B-NB	4.96	1.43	1.37
10	L	303	BPB	CBD-CGD	-4.96	1.45	1.52
9	h	101	BCB	O2A-CGA	4.96	1.47	1.33
9	c	101	BCB	C2C-C3C	-4.95	1.45	1.51
9	z	101	BCB	C1B-NB	4.94	1.43	1.37
9	S	101	BCB	O2A-CGA	4.91	1.47	1.33
10	L	303	BPB	C3D-C4D	-4.91	1.34	1.41
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	Z	101	BCB	CHC-C1C	4.91	1.48	1.37
9	z	101	BCB	C3D-C4D	-4.91	1.33	1.44
9	N	101	BCB	C2C-C3C	-4.90	1.45	1.51
9	i	101	BCB	C4B-NB	4.88	1.43	1.37
9	i	101	BCB	O2A-CGA	4.87	1.47	1.33
9	K	101	BCB	C3B-C4B	4.87	1.50	1.41
9	T	101	BCB	C4B-NB	4.86	1.43	1.37
9	h	101	BCB	C2C-C3C	-4.86	1.45	1.51
9	b	101	BCB	C4B-NB	4.85	1.43	1.37
9	o	101	BCB	C1B-NB	4.84	1.43	1.37
9	k	101	BCB	C1B-NB	4.84	1.43	1.37
9	t	101	BCB	O2A-CGA	4.84	1.47	1.33
9	c	101	BCB	C3D-C4D	-4.83	1.33	1.44
9	P	101	BCB	C3B-C4B	4.83	1.50	1.41
9	l	101	BCB	C2C-C3C	-4.82	1.45	1.51
9	F	101	BCB	O2A-CGA	4.82	1.47	1.33
9	Y	101	BCB	C2C-C3C	-4.82	1.45	1.51
9	P	101	BCB	C1B-NB	4.80	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	V	101	BCB	C4B-NB	4.79	1.43	1.37
9	G	101	BCB	O2A-CGA	4.79	1.47	1.33
9	t	101	BCB	C2C-C3C	-4.79	1.45	1.51
9	F	101	BCB	C3B-C4B	4.78	1.50	1.41
9	M	407	BCB	O2A-CGA	4.77	1.47	1.33
9	l	101	BCB	O2A-CGA	4.77	1.47	1.33
9	V	101	BCB	O2A-CGA	4.76	1.47	1.33
9	x	101	BCB	C2C-C3C	-4.73	1.45	1.51
9	l	101	BCB	C1B-NB	4.72	1.43	1.37
8	C	403	HEC	C4B-NB	-4.72	1.32	1.40
9	7	101	BCB	O2A-CGA	4.70	1.47	1.33
9	Q	101	BCB	O2D-CGD	4.70	1.44	1.33
9	4	101	BCB	CHC-C1C	4.68	1.48	1.37
9	W	101	BCB	CHC-C1C	4.68	1.48	1.37
9	Y	101	BCB	C1B-NB	4.66	1.43	1.37
9	q	101	BCB	C4B-NB	4.66	1.43	1.37
9	w	101	BCB	CHC-C1C	4.66	1.48	1.37
9	4	101	BCB	C2C-C3C	-4.65	1.45	1.51
9	b	101	BCB	C1B-NB	4.64	1.43	1.37
9	Q	101	BCB	CHC-C1C	4.64	1.48	1.37
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	e	101	BCB	CHC-C1C	4.62	1.48	1.37
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	N	101	BCB	O2A-CGA	4.61	1.46	1.33
15	M	410	MQ9	C2-C3	4.57	1.48	1.40
9	z	101	BCB	CHC-C1C	4.54	1.47	1.37
9	N	101	BCB	O2D-CGD	4.54	1.44	1.33
9	Z	101	BCB	O2A-CGA	4.53	1.46	1.33
8	C	404	HEC	C4B-NB	-4.53	1.32	1.40
9	Y	101	BCB	CHC-C1C	4.53	1.47	1.37
9	q	101	BCB	C3B-C4B	4.53	1.49	1.41
9	N	101	BCB	CHC-C1C	4.52	1.47	1.37
9	h	101	BCB	C4B-NB	4.52	1.43	1.37
9	c	101	BCB	O2A-CGA	4.52	1.46	1.33
9	o	101	BCB	C3B-C4B	4.51	1.49	1.41
9	L	301	BCB	O2A-CGA	4.50	1.46	1.33
9	n	101	BCB	CHC-C1C	4.48	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	c	101	BCB	O2D-CGD	4.48	1.44	1.33
9	3	101	BCB	C2C-C3C	-4.48	1.45	1.51
9	M	406	BCB	CHD-C1D	4.47	1.47	1.38
9	7	101	BCB	CHC-C1C	4.47	1.47	1.37
9	6	102	BCB	CHD-C1D	4.46	1.47	1.38
9	V	101	BCB	C1B-NB	4.46	1.43	1.37
9	t	101	BCB	C4B-NB	4.44	1.43	1.37
9	q	101	BCB	CHC-C1C	4.44	1.47	1.37
9	1	101	BCB	CHC-C1C	4.43	1.47	1.37
9	S	101	BCB	C1B-NB	4.43	1.43	1.37
9	V	101	BCB	CHC-C1C	4.42	1.47	1.37
9	7	101	BCB	CHD-C1D	4.42	1.47	1.38
8	C	402	HEC	FE-NB	4.42	2.08	1.94
9	T	101	BCB	O2D-CGD	4.42	1.44	1.33
9	F	101	BCB	C4B-NB	4.42	1.43	1.37
9	u	101	BCB	O2A-CGA	4.40	1.46	1.33
9	M	407	BCB	C2C-C3C	-4.40	1.46	1.51
9	6	102	BCB	CHC-C1C	4.38	1.47	1.37
9	L	301	BCB	C4D-ND	-4.38	1.31	1.37
9	W	101	BCB	O2D-CGD	4.36	1.43	1.33
9	f	101	BCB	CHC-C1C	4.35	1.47	1.37
10	L	303	BPB	O2D-CGD	4.34	1.43	1.33
9	K	101	BCB	C1B-NB	4.34	1.43	1.37
9	1	101	BCB	C2C-C3C	-4.33	1.46	1.51
9	r	101	BCB	C3B-C4B	4.33	1.49	1.41
9	F	101	BCB	C2C-C3C	-4.33	1.46	1.51
9	x	101	BCB	O2D-CGD	4.32	1.43	1.33
9	o	101	BCB	CHC-C1C	4.31	1.47	1.37
9	r	101	BCB	C1B-NB	4.31	1.43	1.37
9	f	101	BCB	O2D-CGD	4.31	1.43	1.33
9	b	101	BCB	CHC-C1C	4.27	1.47	1.37
8	C	401	HEC	CBB-CAB	-4.27	1.32	1.51
9	L	302	BCB	CHC-C1C	4.27	1.47	1.37
9	t	101	BCB	C1B-NB	4.26	1.43	1.37
9	Z	101	BCB	O2D-CGD	4.26	1.43	1.33
9	t	101	BCB	C3B-C4B	4.26	1.49	1.41
9	G	101	BCB	CHD-C1D	4.25	1.46	1.38
9	3	101	BCB	CHC-C1C	4.25	1.47	1.37
9	T	101	BCB	O2A-CGA	4.25	1.45	1.33
9	n	101	BCB	C1B-NB	4.25	1.43	1.37
9	L	301	BCB	C1B-NB	4.25	1.43	1.37
9	b	101	BCB	C2C-C3C	-4.24	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	303	BPB	C4D-CHA	4.24	1.46	1.39
9	r	101	BCB	O2D-CGD	4.23	1.43	1.33
9	3	101	BCB	O2D-CGD	4.22	1.43	1.33
9	M	407	BCB	C4B-NB	4.21	1.43	1.37
8	C	403	HEC	FE-NB	4.21	2.07	1.94
10	L	303	BPB	O2A-CGA	4.21	1.45	1.33
9	V	101	BCB	C3D-C2D	4.20	1.50	1.39
9	L	302	BCB	CHD-C1D	4.19	1.46	1.38
9	w	101	BCB	C1B-NB	4.18	1.42	1.37
9	F	101	BCB	C1B-NB	4.18	1.42	1.37
9	T	101	BCB	CHD-C1D	4.18	1.46	1.38
9	n	101	BCB	C3B-C4B	4.18	1.48	1.41
9	7	101	BCB	O2D-CGD	4.18	1.43	1.33
9	z	101	BCB	C2C-C3C	-4.17	1.46	1.51
9	w	101	BCB	C2C-C3C	-4.17	1.46	1.51
9	P	101	BCB	CHD-C1D	4.17	1.46	1.38
9	L	301	BCB	C4B-NB	4.17	1.42	1.37
9	w	101	BCB	CHC-C4B	4.16	1.48	1.39
8	C	402	HEC	CBC-CAC	-4.16	1.32	1.51
9	L	302	BCB	O2D-CGD	4.13	1.43	1.33
9	h	101	BCB	C3D-C2D	4.12	1.50	1.39
9	4	101	BCB	O2A-CGA	4.12	1.45	1.33
9	z	101	BCB	C3D-C2D	4.11	1.50	1.39
9	6	102	BCB	C3B-C4B	4.11	1.48	1.41
9	h	101	BCB	CHD-C1D	4.11	1.46	1.38
9	r	101	BCB	CHC-C1C	4.11	1.46	1.37
9	1	101	BCB	O2D-CGD	4.11	1.43	1.33
9	N	101	BCB	CHD-C1D	4.10	1.46	1.38
9	h	101	BCB	CHD-C4C	4.10	1.48	1.39
9	4	101	BCB	C3B-C4B	4.10	1.48	1.41
9	M	406	BCB	OBD-CAD	4.09	1.29	1.22
9	F	101	BCB	O2D-CGD	4.08	1.43	1.33
9	u	101	BCB	C3B-C4B	4.08	1.48	1.41
9	Q	101	BCB	O2A-CGA	4.08	1.45	1.33
9	Y	101	BCB	O2D-CGD	4.07	1.43	1.33
8	C	401	HEC	FE-NB	4.07	2.07	1.94
10	L	303	BPB	C3D-C2D	4.07	1.46	1.39
9	3	101	BCB	C3B-C4B	4.07	1.48	1.41
9	h	101	BCB	CHC-C1C	4.06	1.46	1.37
9	w	101	BCB	CHD-C4C	4.06	1.48	1.39
9	w	101	BCB	C3B-C4B	4.05	1.48	1.41
9	c	101	BCB	CHD-C1D	4.04	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	e	101	BCB	C1B-NB	4.03	1.42	1.37
9	t	101	BCB	CHC-C1C	4.03	1.46	1.37
9	q	101	BCB	CHD-C1D	4.02	1.46	1.38
10	L	303	BPB	OBD-CAD	4.02	1.27	1.22
9	b	101	BCB	C3B-C4B	4.02	1.48	1.41
9	M	407	BCB	C4D-ND	-4.02	1.32	1.37
9	M	406	BCB	C3B-C4B	4.02	1.48	1.41
9	i	101	BCB	C3B-C4B	4.01	1.48	1.41
9	L	302	BCB	C2C-C3C	-4.00	1.46	1.51
9	V	101	BCB	O2D-CGD	3.99	1.42	1.33
9	k	101	BCB	CHD-C1D	3.99	1.46	1.38
9	x	101	BCB	CHB-C1B	3.98	1.48	1.39
9	k	101	BCB	C3B-C4B	3.98	1.48	1.41
9	K	101	BCB	C4B-NB	3.98	1.42	1.37
9	i	101	BCB	CHC-C1C	3.98	1.46	1.37
10	M	408	BPB	O2D-CGD	3.97	1.42	1.33
9	T	101	BCB	CHC-C1C	3.96	1.46	1.37
9	k	101	BCB	O2D-CGD	3.96	1.42	1.33
9	e	101	BCB	C3B-C4B	3.95	1.48	1.41
9	w	101	BCB	O2D-CGD	3.95	1.42	1.33
10	M	408	BPB	C3D-C2D	3.95	1.46	1.39
9	t	101	BCB	CHD-C1D	3.94	1.46	1.38
9	u	101	BCB	CHD-C1D	3.93	1.46	1.38
9	u	101	BCB	CHC-C1C	3.93	1.46	1.37
9	t	101	BCB	O2D-CGD	3.93	1.42	1.33
9	7	101	BCB	C3D-C2D	3.93	1.49	1.39
9	i	101	BCB	O2D-CGD	3.92	1.42	1.33
9	b	101	BCB	CHD-C1D	3.92	1.46	1.38
9	1	101	BCB	CHD-C1D	3.92	1.46	1.38
9	c	101	BCB	CHC-C4B	3.92	1.48	1.39
9	M	407	BCB	CHC-C1C	3.91	1.46	1.37
9	l	101	BCB	O2D-CGD	3.91	1.42	1.33
10	M	408	BPB	CHA-CBD	-3.91	1.46	1.51
9	V	101	BCB	CHD-C4C	3.91	1.48	1.39
9	S	101	BCB	C3D-C2D	3.90	1.49	1.39
9	P	101	BCB	O2D-CGD	3.90	1.42	1.33
9	4	101	BCB	O2D-CGD	3.90	1.42	1.33
9	n	101	BCB	O2D-CGD	3.89	1.42	1.33
9	i	101	BCB	CHD-C1D	3.88	1.45	1.38
8	C	401	HEC	CBC-CAC	-3.88	1.34	1.51
9	k	101	BCB	C4B-NB	3.88	1.42	1.37
9	S	101	BCB	CHD-C1D	3.88	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	z	101	BCB	CHD-C1D	3.88	1.45	1.38
9	f	101	BCB	CHB-C1B	3.87	1.48	1.39
9	3	101	BCB	CHB-C1B	3.87	1.48	1.39
9	n	101	BCB	CHD-C1D	3.87	1.45	1.38
9	k	101	BCB	CHC-C1C	3.87	1.46	1.37
8	C	404	HEC	FE-NB	3.86	2.06	1.94
9	z	101	BCB	C3B-C4B	3.86	1.48	1.41
9	S	101	BCB	C3B-C4B	3.86	1.48	1.41
9	x	101	BCB	CHC-C1C	3.86	1.46	1.37
9	7	101	BCB	C3B-C4B	3.86	1.48	1.41
9	i	101	BCB	CHB-C1B	3.86	1.48	1.39
9	S	101	BCB	CHC-C1C	3.85	1.46	1.37
9	z	101	BCB	CHD-C4C	3.85	1.48	1.39
9	L	301	BCB	CHC-C1C	3.84	1.46	1.37
9	u	101	BCB	C1B-NB	3.83	1.42	1.37
9	e	101	BCB	CHC-C4B	3.83	1.48	1.39
9	e	101	BCB	O2D-CGD	3.83	1.42	1.33
9	Z	101	BCB	CHD-C1D	3.82	1.45	1.38
9	V	101	BCB	CHD-C1D	3.82	1.45	1.38
9	l	101	BCB	CHC-C1C	3.82	1.46	1.37
9	k	101	BCB	C2C-C3C	-3.82	1.46	1.51
9	K	101	BCB	CHC-C1C	3.81	1.46	1.37
8	C	402	HEC	C1D-ND	-3.81	1.33	1.40
9	4	101	BCB	CHC-C4B	3.81	1.47	1.39
9	S	101	BCB	O2D-CGD	3.81	1.42	1.33
9	o	101	BCB	O2D-CGD	3.80	1.42	1.33
9	f	101	BCB	CHD-C1D	3.80	1.45	1.38
9	w	101	BCB	CHD-C1D	3.79	1.45	1.38
9	P	101	BCB	CHD-C4C	3.79	1.47	1.39
9	W	101	BCB	CHC-C4B	3.78	1.47	1.39
9	u	101	BCB	O2D-CGD	3.78	1.42	1.33
9	h	101	BCB	C3B-C4B	3.78	1.48	1.41
9	L	302	BCB	C3D-C2D	3.77	1.49	1.39
9	V	101	BCB	C3B-C4B	3.77	1.48	1.41
8	C	404	HEC	CBC-CAC	-3.77	1.34	1.51
9	q	101	BCB	O2D-CGD	3.76	1.42	1.33
9	6	102	BCB	CHD-C4C	3.74	1.47	1.39
9	q	101	BCB	CHB-C1B	3.74	1.47	1.39
9	k	101	BCB	C3D-C2D	3.74	1.49	1.39
9	n	101	BCB	C3D-C2D	3.74	1.49	1.39
9	b	101	BCB	O2D-CGD	3.73	1.42	1.33
9	t	101	BCB	C3D-C2D	3.73	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	Y	101	BCB	C3B-C4B	3.72	1.48	1.41
9	M	407	BCB	CHD-C1D	3.72	1.45	1.38
8	C	402	HEC	C4B-NB	-3.72	1.33	1.40
9	N	101	BCB	C3D-C2D	3.71	1.49	1.39
9	Y	101	BCB	CHC-C4B	3.71	1.47	1.39
8	C	403	HEC	CBC-CAC	-3.71	1.35	1.51
9	F	101	BCB	CHD-C1D	3.71	1.45	1.38
9	W	101	BCB	C3B-C4B	3.70	1.48	1.41
9	x	101	BCB	CHD-C1D	3.70	1.45	1.38
9	G	101	BCB	C3B-C4B	3.70	1.48	1.41
9	Q	101	BCB	C3D-C2D	3.70	1.49	1.39
9	3	101	BCB	CHD-C1D	3.70	1.45	1.38
9	T	101	BCB	C3B-C4B	3.69	1.48	1.41
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-C2D	3.68	1.49	1.39
9	z	101	BCB	O2D-CGD	3.68	1.42	1.33
9	F	101	BCB	CHB-C1B	3.66	1.47	1.39
9	G	101	BCB	CHC-C1C	3.65	1.45	1.37
9	z	101	BCB	CHC-C4B	3.65	1.47	1.39
9	l	101	BCB	C3B-C4B	3.65	1.47	1.41
9	h	101	BCB	O2D-CGD	3.64	1.42	1.33
9	G	101	BCB	CHC-C4B	3.64	1.47	1.39
9	W	101	BCB	C3D-C2D	3.63	1.49	1.39
9	S	101	BCB	CHB-C1B	3.62	1.47	1.39
9	r	101	BCB	CHD-C1D	3.62	1.45	1.38
8	C	402	HEC	CBB-CAB	-3.62	1.35	1.51
9	o	101	BCB	CHB-C1B	3.62	1.47	1.39
9	1	101	BCB	C3B-C4B	3.61	1.47	1.41
9	P	101	BCB	CHC-C1C	3.61	1.45	1.37
10	M	408	BPB	C4C-NC	-3.61	1.26	1.37
9	k	101	BCB	CHD-C4C	3.61	1.47	1.39
9	L	302	BCB	C4B-NB	3.60	1.42	1.37
9	c	101	BCB	CHB-C1B	3.60	1.47	1.39
9	o	101	BCB	CHD-C1D	3.59	1.45	1.38
9	1	101	BCB	CHC-C4B	3.58	1.47	1.39
8	C	403	HEC	CBB-CAB	-3.58	1.35	1.51
9	1	101	BCB	CHB-C1B	3.57	1.47	1.39
9	Z	101	BCB	C3D-C2D	3.56	1.48	1.39
9	G	101	BCB	CHB-C1B	3.55	1.47	1.39
9	c	101	BCB	C3D-C2D	3.55	1.48	1.39
9	6	102	BCB	CHB-C1B	3.55	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	l	101	BCB	CHB-C1B	3.55	1.47	1.39
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	b	101	BCB	CHC-C4B	3.54	1.47	1.39
9	e	101	BCB	C3D-C2D	3.54	1.48	1.39
9	q	101	BCB	CHD-C4C	3.53	1.47	1.39
9	Y	101	BCB	CHB-C1B	3.53	1.47	1.39
8	C	403	HEC	FE-NC	3.52	2.07	1.95
9	Q	101	BCB	CHC-C4B	3.52	1.47	1.39
9	f	101	BCB	C3B-C4B	3.52	1.47	1.41
17	7	102	NS0	C11-C12	3.51	1.53	1.45
9	b	101	BCB	CHD-C4C	3.51	1.47	1.39
9	P	101	BCB	CHB-C1B	3.51	1.47	1.39
8	C	402	HEC	FE-NC	3.51	2.07	1.95
9	L	302	BCB	OBD-CAD	3.50	1.28	1.22
9	Q	101	BCB	CHD-C1D	3.50	1.45	1.38
9	u	101	BCB	CHB-C1B	3.50	1.47	1.39
9	L	301	BCB	CHD-C1D	3.50	1.45	1.38
11	L	304	UQ9	C3-C2	-3.49	1.38	1.48
9	7	101	BCB	CHC-C4B	3.48	1.47	1.39
9	n	101	BCB	CHD-C4C	3.47	1.47	1.39
9	T	101	BCB	CHB-C1B	3.47	1.47	1.39
8	C	404	HEC	CBB-CAB	-3.46	1.36	1.51
9	e	101	BCB	CHB-C1B	3.46	1.47	1.39
9	4	101	BCB	C3D-C2D	3.45	1.48	1.39
9	L	302	BCB	C3B-C4B	3.45	1.47	1.41
9	4	101	BCB	CHD-C1D	3.44	1.45	1.38
9	N	101	BCB	C3B-C4B	3.43	1.47	1.41
9	7	101	BCB	CHD-C4C	3.43	1.47	1.39
9	3	101	BCB	C3D-C2D	3.43	1.48	1.39
9	F	101	BCB	CHC-C1C	3.42	1.45	1.37
9	N	101	BCB	CHC-C4B	3.41	1.47	1.39
9	M	407	BCB	C1B-NB	3.41	1.42	1.37
9	t	101	BCB	CHD-C4C	3.40	1.47	1.39
9	u	101	BCB	CHC-C4B	3.40	1.47	1.39
8	C	401	HEC	FE-NC	3.39	2.06	1.95
8	C	403	HEC	C1D-ND	-3.39	1.34	1.40
9	w	101	BCB	C3D-C2D	3.38	1.48	1.39
9	o	101	BCB	CHC-C4B	3.37	1.47	1.39
9	Y	101	BCB	CHD-C1D	3.37	1.44	1.38
9	G	101	BCB	C3D-C2D	3.37	1.48	1.39
9	6	102	BCB	C3D-C2D	3.36	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	b	101	BCB	CHB-C1B	3.36	1.46	1.39
9	h	101	BCB	CHB-C1B	3.35	1.46	1.39
9	Z	101	BCB	CHC-C4B	3.35	1.46	1.39
9	k	101	BCB	CHB-C1B	3.35	1.46	1.39
9	4	101	BCB	CHB-C1B	3.35	1.46	1.39
9	S	101	BCB	CHD-C4C	3.35	1.46	1.39
9	x	101	BCB	C3B-C4B	3.34	1.47	1.41
9	f	101	BCB	CHC-C4B	3.34	1.46	1.39
9	n	101	BCB	CHC-C4B	3.34	1.46	1.39
9	1	101	BCB	C3D-C2D	3.34	1.48	1.39
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	W	101	BCB	CHD-C1D	3.33	1.44	1.38
9	q	101	BCB	C3D-C2D	3.32	1.48	1.39
9	K	101	BCB	CHD-C4C	3.32	1.46	1.39
8	C	404	HEC	FE-NC	3.32	2.06	1.95
9	N	101	BCB	CHB-C1B	3.32	1.46	1.39
9	V	101	BCB	CHB-C1B	3.31	1.46	1.39
9	o	101	BCB	C3D-C2D	3.31	1.48	1.39
9	M	407	BCB	C3D-C2D	3.31	1.48	1.39
9	t	101	BCB	CHB-C1B	3.30	1.46	1.39
9	6	102	BCB	CHC-C4B	3.30	1.46	1.39
9	K	101	BCB	CHB-C1B	3.30	1.46	1.39
9	w	101	BCB	CHB-C1B	3.30	1.46	1.39
9	Q	101	BCB	C3B-C4B	3.30	1.47	1.41
9	K	101	BCB	CHD-C1D	3.29	1.44	1.38
9	i	101	BCB	CHC-C4B	3.29	1.46	1.39
9	L	302	BCB	CHD-C4C	3.29	1.46	1.39
9	e	101	BCB	CHD-C1D	3.29	1.44	1.38
9	Q	101	BCB	CHB-C1B	3.28	1.46	1.39
9	P	101	BCB	C3D-C2D	3.27	1.48	1.39
9	c	101	BCB	C3B-C4B	3.27	1.47	1.41
9	r	101	BCB	CHC-C4B	3.27	1.46	1.39
10	M	408	BPB	C3A-C2A	-3.27	1.51	1.54
9	T	101	BCB	C3D-C2D	3.27	1.48	1.39
9	Y	101	BCB	CHD-C4C	3.26	1.46	1.39
9	q	101	BCB	CHC-C4B	3.26	1.46	1.39
9	x	101	BCB	C3D-C2D	3.25	1.48	1.39
9	M	406	BCB	C1B-NB	3.24	1.41	1.37
9	3	101	BCB	CHD-C4C	3.24	1.46	1.39
9	t	101	BCB	CHC-C4B	3.24	1.46	1.39
9	W	101	BCB	OBD-CAD	3.24	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	G	101	BCB	OBD-CAD	3.22	1.28	1.22
9	M	406	BCB	CHC-C1C	3.22	1.44	1.37
9	u	101	BCB	CHD-C4C	3.22	1.46	1.39
9	S	101	BCB	CHC-C4B	3.21	1.46	1.39
9	r	101	BCB	CHB-C1B	3.20	1.46	1.39
9	T	101	BCB	OBD-CAD	3.19	1.28	1.22
17	7	102	NS0	C10-C9	3.19	1.53	1.43
8	C	404	HEC	C1D-ND	-3.18	1.34	1.40
8	C	401	HEC	C1D-ND	-3.18	1.34	1.40
9	F	101	BCB	C3D-C2D	3.17	1.47	1.39
9	K	101	BCB	C3D-C2D	3.17	1.47	1.39
9	3	101	BCB	CHC-C4B	3.17	1.46	1.39
9	u	101	BCB	C3D-C2D	3.16	1.47	1.39
10	L	303	BPB	CHA-CBD	-3.16	1.47	1.51
9	l	101	BCB	CHD-C4C	3.16	1.46	1.39
9	Q	101	BCB	OBD-CAD	3.16	1.27	1.22
8	C	402	HEC	C1B-NB	-3.15	1.32	1.38
9	c	101	BCB	CHD-C4C	3.15	1.46	1.39
9	W	101	BCB	CHB-C1B	3.15	1.46	1.39
9	N	101	BCB	OBD-CAD	3.14	1.27	1.22
9	f	101	BCB	CHD-C4C	3.14	1.46	1.39
9	Z	101	BCB	CHB-C1B	3.14	1.46	1.39
17	7	102	NS0	C26-C27	3.14	1.53	1.43
9	L	302	BCB	CHC-C4B	3.14	1.46	1.39
17	o	102	NS0	C10-C9	3.14	1.53	1.43
17	G	102	NS0	C16-C17	3.14	1.52	1.45
17	G	102	NS0	C11-C12	3.13	1.52	1.45
17	4	102	NS0	C10-C9	3.12	1.53	1.43
9	T	101	BCB	CHC-C4B	3.12	1.46	1.39
17	i	102	NS0	C10-C9	3.12	1.53	1.43
10	M	408	BPB	C3B-C2B	3.11	1.45	1.39
17	r	102	NS0	C10-C9	3.11	1.53	1.43
9	h	101	BCB	CHC-C4B	3.11	1.46	1.39
9	M	406	BCB	C3D-C2D	3.11	1.47	1.39
9	r	101	BCB	CHD-C4C	3.10	1.46	1.39
8	C	401	HEC	C1B-NB	-3.09	1.32	1.38
9	M	407	BCB	CHB-C1B	3.09	1.46	1.39
17	G	102	NS0	C10-C9	3.08	1.53	1.43
9	e	101	BCB	CHD-C4C	3.08	1.46	1.39
9	b	101	BCB	C3D-C2D	3.08	1.47	1.39
17	f	102	NS0	C11-C12	3.08	1.52	1.45
9	N	101	BCB	CHD-C4C	3.08	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	l	102	NS0	C11-C12	3.07	1.52	1.45
9	M	407	BCB	CHD-C4C	3.07	1.46	1.39
9	r	101	BCB	OBD-CAD	3.07	1.27	1.22
17	1	102	NS0	C10-C9	3.07	1.53	1.43
9	L	302	BCB	CHB-C1B	3.07	1.46	1.39
17	x	102	NS0	C10-C9	3.07	1.53	1.43
17	c	102	NS0	C10-C9	3.06	1.52	1.43
9	f	101	BCB	C3D-C2D	3.06	1.47	1.39
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	F	101	BCB	CHD-C4C	3.05	1.46	1.39
17	Q	102	NS0	C10-C9	3.05	1.52	1.43
17	T	102	NS0	C10-C9	3.04	1.52	1.43
9	l	101	BCB	CHC-C4B	3.04	1.46	1.39
9	x	101	BCB	CHC-C4B	3.04	1.46	1.39
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	l	101	BCB	C3D-C2D	3.02	1.47	1.39
9	7	101	BCB	OBD-CAD	3.02	1.27	1.22
9	7	101	BCB	CHB-C1B	3.02	1.46	1.39
17	Q	102	NS0	C11-C12	3.02	1.52	1.45
17	l	102	NS0	C16-C17	3.01	1.52	1.45
9	Z	101	BCB	C3B-C4B	3.01	1.46	1.41
9	M	407	BCB	CHC-C4B	3.01	1.46	1.39
9	z	101	BCB	CHB-C1B	3.01	1.46	1.39
9	i	101	BCB	CHD-C4C	3.00	1.46	1.39
9	1	101	BCB	CHD-C4C	3.00	1.46	1.39
9	x	101	BCB	OBD-CAD	3.00	1.27	1.22
17	f	102	NS0	C10-C9	3.00	1.52	1.43
10	M	408	BPB	OBD-CAD	3.00	1.26	1.22
17	W	102	NS0	C10-C9	3.00	1.52	1.43
17	c	102	NS0	C11-C12	3.00	1.52	1.45
17	l	102	NS0	C10-C9	3.00	1.52	1.43
17	r	102	NS0	C11-C12	2.99	1.52	1.45
9	n	101	BCB	CHB-C1B	2.99	1.46	1.39
17	1	102	NS0	C16-C17	2.99	1.52	1.45
9	l	101	BCB	OBD-CAD	2.99	1.27	1.22
10	M	408	BPB	C3B-C4B	2.99	1.46	1.41
17	o	102	NS0	C11-C12	2.98	1.52	1.45
9	K	101	BCB	CHC-C4B	2.98	1.46	1.39
9	G	101	BCB	MG-ND	-2.97	1.99	2.05
9	Z	101	BCB	OBD-CAD	2.97	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	i	101	BCB	OBD-CAD	2.97	1.27	1.22
9	r	101	BCB	C3D-C2D	2.96	1.47	1.39
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
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	6	102	BCB	OBD-CAD	2.93	1.27	1.22
9	M	406	BCB	CHB-C1B	2.93	1.46	1.39
17	Z	102	NS0	C16-C17	2.92	1.52	1.45
9	o	101	BCB	OBD-CAD	2.92	1.27	1.22
9	V	101	BCB	CHC-C4B	2.92	1.46	1.39
17	G	102	NS0	C20-C19	2.91	1.52	1.43
17	N	102	NS0	C10-C9	2.90	1.52	1.43
9	L	301	BCB	C3D-C2D	2.90	1.47	1.39
17	4	102	NS0	C26-C27	2.90	1.52	1.43
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	3	101	BCB	C4D-ND	-2.89	1.33	1.37
17	i	102	NS0	C16-C17	2.89	1.52	1.45
17	7	102	NS0	C20-C19	2.88	1.52	1.43
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
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	M	406	BCB	O2D-CGD	2.86	1.40	1.33
17	l	102	NS0	C21-C22	2.86	1.52	1.43
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
17	Q	102	NS0	C15-C14	2.86	1.52	1.43
9	k	101	BCB	CHC-C4B	2.85	1.45	1.39
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	F	101	BCB	CHC-C4B	2.85	1.45	1.39
9	4	101	BCB	OBD-CAD	2.85	1.27	1.22
17	i	102	NS0	C15-C14	2.84	1.52	1.43
17	1	102	NS0	C11-C12	2.84	1.52	1.45
17	f	102	NS0	C15-C14	2.84	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	4	102	NS0	C16-C17	2.83	1.52	1.45
9	u	101	BCB	OBD-CAD	2.83	1.27	1.22
10	L	303	BPB	C3B-C4B	2.83	1.46	1.41
17	Z	102	NS0	C11-C12	2.82	1.52	1.45
17	Z	102	NS0	C15-C14	2.82	1.52	1.43
8	C	401	HEC	C1C-NC	-2.81	1.34	1.39
17	x	102	NS0	C20-C19	2.81	1.52	1.43
17	T	102	NS0	C20-C19	2.81	1.52	1.43
17	Q	102	NS0	C20-C19	2.80	1.52	1.43
17	W	102	NS0	C16-C17	2.80	1.52	1.45
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
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
17	c	102	NS0	C16-C17	2.78	1.51	1.45
9	T	101	BCB	CHD-C4C	2.78	1.45	1.39
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
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
17	1	102	NS0	C15-C14	2.76	1.52	1.43
17	W	102	NS0	C20-C19	2.76	1.52	1.43
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	x	101	BCB	CHD-C4C	2.75	1.45	1.39
9	k	101	BCB	C4D-ND	-2.75	1.33	1.37
9	Y	101	BCB	C1B-C2B	2.74	1.49	1.43
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	M	410	MQ9	C38-C39	2.73	1.39	1.33
8	C	404	HEC	C1C-NC	-2.73	1.34	1.39
9	l	101	BCB	CHD-C1D	2.72	1.43	1.38
9	Z	101	BCB	CHD-C4C	2.72	1.45	1.39
17	r	102	NS0	C20-C19	2.72	1.51	1.43
17	u	102	NS0	C15-C14	2.72	1.51	1.43
17	u	102	NS0	C16-C17	2.72	1.51	1.45
9	Q	101	BCB	CHD-C4C	2.71	1.45	1.39
9	f	101	BCB	OBD-CAD	2.71	1.27	1.22
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	P	101	BCB	MG-ND	-2.71	2.00	2.05
17	c	102	NS0	C21-C22	2.71	1.51	1.43
9	F	101	BCB	OBD-CAD	2.70	1.27	1.22
9	1	101	BCB	C1B-C2B	2.70	1.49	1.43
9	P	101	BCB	CHC-C4B	2.70	1.45	1.39
17	4	102	NS0	C21-C22	2.69	1.51	1.43
17	c	102	NS0	C20-C19	2.69	1.51	1.43
17	4	102	NS0	C15-C14	2.69	1.51	1.43
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
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	r	101	BCB	CAA-C2A	-2.66	1.49	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
9	3	101	BCB	C1B-C2B	2.65	1.49	1.43
9	3	101	BCB	OBD-CAD	2.65	1.27	1.22
9	L	301	BCB	CHB-C1B	2.64	1.45	1.39
17	N	102	NS0	C25-C23	2.64	1.51	1.45
17	G	102	NS0	C25-C23	2.64	1.51	1.45
17	i	102	NS0	C25-C23	2.64	1.51	1.45
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	L	301	BCB	CHC-C4B	2.62	1.45	1.39
9	w	101	BCB	OBD-CAD	2.62	1.27	1.22
9	i	101	BCB	C3D-C2D	2.62	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	r	102	NS0	C25-C23	2.62	1.51	1.45
9	G	101	BCB	CHD-C4C	2.61	1.45	1.39
9	L	301	BCB	CHD-C4C	2.61	1.45	1.39
9	Y	101	BCB	OBD-CAD	2.61	1.27	1.22
17	u	102	NS0	C21-C22	2.61	1.51	1.43
17	N	102	NS0	C21-C22	2.61	1.51	1.43
9	Y	101	BCB	C4D-ND	-2.60	1.34	1.37
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	Z	101	BCB	CBD-CGD	-2.59	1.44	1.52
17	1	102	NS0	C21-C22	2.59	1.51	1.43
9	P	101	BCB	OBD-CAD	2.59	1.26	1.22
9	w	101	BCB	C4D-ND	-2.58	1.34	1.37
17	N	102	NS0	C20-C19	2.58	1.51	1.43
9	M	406	BCB	CHD-C4C	2.58	1.45	1.39
9	K	101	BCB	MG-ND	-2.58	2.00	2.05
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
17	4	102	NS0	C20-C19	2.56	1.51	1.43
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	V	101	BCB	OBD-CAD	2.54	1.26	1.22
9	4	101	BCB	CHD-C4C	2.53	1.45	1.39
8	C	404	HEC	C1B-NB	-2.53	1.33	1.38
9	L	301	BCB	MG-ND	-2.52	2.00	2.05
9	L	302	BCB	CBD-CGD	-2.51	1.44	1.52
9	e	101	BCB	C4D-ND	-2.50	1.34	1.37
9	z	101	BCB	OBD-CAD	2.49	1.26	1.22
11	L	304	UQ9	C6-C5	-2.48	1.39	1.46
9	k	101	BCB	OBD-CAD	2.48	1.26	1.22
9	1	101	BCB	OBD-CAD	2.47	1.26	1.22
17	W	102	NS0	C25-C23	2.47	1.51	1.45
9	o	101	BCB	CHD-C4C	2.47	1.44	1.39
9	1	101	BCB	CAA-C2A	-2.46	1.49	1.54
8	C	403	HEC	C1B-NB	-2.45	1.33	1.38
9	h	101	BCB	OBD-CAD	2.45	1.26	1.22
9	6	102	BCB	C1B-C2B	2.44	1.49	1.43
9	q	101	BCB	OBD-CAD	2.44	1.26	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	r	101	BCB	C2A-C1A	-2.44	1.46	1.52
9	W	101	BCB	CHD-C4C	2.42	1.44	1.39
9	c	101	BCB	C2A-C1A	-2.42	1.46	1.52
9	f	101	BCB	C1B-C2B	2.41	1.48	1.43
17	Q	102	NS0	C25-C23	2.40	1.51	1.45
9	F	101	BCB	MG-ND	-2.39	2.01	2.05
9	e	101	BCB	C2-C3	2.39	1.38	1.33
9	S	101	BCB	MG-ND	-2.39	2.01	2.05
9	z	101	BCB	C1B-C2B	2.37	1.48	1.43
9	c	101	BCB	CAA-C2A	-2.37	1.49	1.54
9	V	101	BCB	CAA-C2A	-2.35	1.49	1.54
9	M	406	BCB	CBD-CGD	-2.35	1.45	1.52
9	n	101	BCB	OBD-CAD	2.35	1.26	1.22
9	L	301	BCB	OBD-CAD	2.35	1.26	1.22
9	N	101	BCB	MG-ND	-2.34	2.01	2.05
9	x	101	BCB	C1B-C2B	2.34	1.48	1.43
8	C	402	HEC	C4C-NC	-2.34	1.35	1.39
9	o	101	BCB	MG-ND	-2.33	2.01	2.05
9	x	101	BCB	CAA-C2A	-2.33	1.49	1.54
9	l	101	BCB	MG-ND	-2.32	2.01	2.05
9	M	407	BCB	CAA-C2A	-2.32	1.49	1.54
9	e	101	BCB	OBD-CAD	2.31	1.26	1.22
9	r	101	BCB	CBD-CGD	-2.31	1.45	1.52
9	w	101	BCB	C3A-C2A	-2.31	1.48	1.54
9	i	101	BCB	CAA-C2A	-2.30	1.49	1.54
9	t	101	BCB	MG-ND	-2.29	2.01	2.05
9	F	101	BCB	C1B-C2B	2.29	1.48	1.43
9	l	101	BCB	C2A-C1A	-2.27	1.47	1.52
9	x	101	BCB	C2A-C1A	-2.26	1.47	1.52
9	c	101	BCB	OBD-CAD	2.25	1.26	1.22
8	C	402	HEC	CHD-C4C	-2.24	1.34	1.39
9	K	101	BCB	OBD-CAD	2.24	1.26	1.22
9	o	101	BCB	C2A-C1A	-2.23	1.47	1.52
9	t	101	BCB	C1B-C2B	2.23	1.48	1.43
9	1	101	BCB	CBD-CGD	-2.22	1.45	1.52
9	i	101	BCB	C1B-C2B	2.22	1.48	1.43
8	C	403	HEC	CAB-C3B	-2.21	1.45	1.51
9	L	302	BCB	C4D-ND	-2.21	1.34	1.37
8	C	401	HEC	C4C-NC	-2.20	1.35	1.39
8	C	402	HEC	C4C-C3C	-2.20	1.40	1.44
9	h	101	BCB	C4D-ND	-2.20	1.34	1.37
9	t	101	BCB	OBD-CAD	2.20	1.26	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	406	BCB	CHB-C4A	-2.20	1.32	1.37
8	C	403	HEC	C1C-NC	-2.18	1.35	1.39
9	b	101	BCB	OBD-CAD	2.18	1.26	1.22
9	W	101	BCB	MG-ND	-2.17	2.01	2.05
8	C	402	HEC	C4D-ND	-2.16	1.34	1.38
8	C	401	HEC	C4A-C3A	-2.16	1.41	1.45
9	u	101	BCB	C1B-C2B	2.16	1.48	1.43
9	x	101	BCB	MG-ND	-2.16	2.01	2.05
8	C	403	HEC	C4D-ND	-2.15	1.34	1.38
9	c	101	BCB	MG-ND	-2.14	2.01	2.05
9	w	101	BCB	C1B-C2B	2.13	1.48	1.43
9	W	101	BCB	C4D-ND	-2.13	1.34	1.37
9	N	101	BCB	C1B-C2B	2.13	1.48	1.43
8	C	402	HEC	C1C-NC	-2.12	1.35	1.39
8	C	404	HEC	C4D-C3D	2.12	1.48	1.45
9	M	406	BCB	CHC-C4B	2.12	1.44	1.39
9	N	101	BCB	C2A-C1A	-2.12	1.47	1.52
9	f	101	BCB	C2A-C1A	-2.12	1.47	1.52
9	S	101	BCB	C3B-C2B	2.11	1.49	1.42
9	c	101	BCB	C1B-C2B	2.11	1.48	1.43
8	C	401	HEC	C1A-C2A	-2.11	1.41	1.45
8	C	401	HEC	C4D-ND	-2.09	1.34	1.38
9	n	101	BCB	C1B-C2B	2.09	1.48	1.43
9	u	101	BCB	CBD-CGD	-2.09	1.45	1.52
9	T	101	BCB	C1B-C2B	2.08	1.48	1.43
9	L	302	BCB	CHB-C4A	-2.08	1.32	1.37
9	G	101	BCB	C1B-C2B	2.08	1.48	1.43
9	6	102	BCB	C1D-C2D	2.08	1.49	1.45
9	Z	101	BCB	CHB-C4A	-2.08	1.32	1.37
9	4	101	BCB	C2A-C1A	-2.07	1.47	1.52
15	M	410	MQ9	C43-C44	2.07	1.37	1.33
8	C	402	HEC	C1A-C2A	-2.05	1.41	1.45
9	w	101	BCB	CHB-C4A	-2.04	1.32	1.37
9	N	101	BCB	CHB-C4A	-2.04	1.32	1.37
9	L	302	BCB	C1B-C2B	2.03	1.48	1.43
9	V	101	BCB	CHB-C4A	-2.03	1.32	1.37
9	n	101	BCB	C3B-C2B	2.03	1.49	1.42
9	q	101	BCB	C4D-ND	-2.03	1.34	1.37
9	M	407	BCB	C3B-C4B	2.03	1.44	1.41
9	q	101	BCB	C3A-C2A	-2.02	1.48	1.54

All (1431) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	M	406	BCB	C1C-NC-C4C	-20.85	97.33	106.71
9	o	101	BCB	C1C-NC-C4C	-19.43	97.97	106.71
9	F	101	BCB	C1C-NC-C4C	-18.85	98.23	106.71
9	G	101	BCB	C1C-NC-C4C	-18.68	98.31	106.71
9	K	101	BCB	C1C-NC-C4C	-18.37	98.45	106.71
9	T	101	BCB	C1C-NC-C4C	-17.75	98.73	106.71
9	e	101	BCB	C1C-NC-C4C	-17.61	98.79	106.71
9	r	101	BCB	C1C-NC-C4C	-17.50	98.84	106.71
9	Q	101	BCB	C1C-NC-C4C	-17.47	98.85	106.71
9	x	101	BCB	C1C-NC-C4C	-17.31	98.92	106.71
9	q	101	BCB	C1C-NC-C4C	-16.91	99.10	106.71
9	P	101	BCB	C1C-NC-C4C	-16.75	99.18	106.71
9	i	101	BCB	C1C-NC-C4C	-16.70	99.20	106.71
9	t	101	BCB	C1C-NC-C4C	-16.69	99.20	106.71
9	l	101	BCB	C1C-NC-C4C	-16.66	99.22	106.71
9	h	101	BCB	C1C-NC-C4C	-16.61	99.24	106.71
9	6	102	BCB	C1C-NC-C4C	-16.55	99.27	106.71
9	n	101	BCB	C1C-NC-C4C	-16.50	99.29	106.71
9	u	101	BCB	C1C-NC-C4C	-16.40	99.33	106.71
9	N	101	BCB	C1C-NC-C4C	-16.20	99.42	106.71
9	f	101	BCB	C1C-NC-C4C	-16.07	99.48	106.71
9	S	101	BCB	C1C-NC-C4C	-15.90	99.56	106.71
9	Y	101	BCB	C1C-NC-C4C	-15.79	99.61	106.71
9	W	101	BCB	C1C-NC-C4C	-15.79	99.61	106.71
9	3	101	BCB	C1C-NC-C4C	-15.72	99.64	106.71
9	z	101	BCB	C1C-NC-C4C	-15.62	99.68	106.71
9	4	101	BCB	C1C-NC-C4C	-15.59	99.70	106.71
9	7	101	BCB	C1C-NC-C4C	-15.52	99.73	106.71
9	b	101	BCB	C1C-NC-C4C	-15.51	99.73	106.71
9	V	101	BCB	C1C-NC-C4C	-15.46	99.76	106.71
9	L	301	BCB	C1C-NC-C4C	-15.43	99.77	106.71
9	1	101	BCB	C1C-NC-C4C	-15.25	99.85	106.71
9	w	101	BCB	C1C-NC-C4C	-15.22	99.86	106.71
9	Z	101	BCB	C1C-NC-C4C	-15.22	99.86	106.71
9	k	101	BCB	C1C-NC-C4C	-14.86	100.03	106.71
9	c	101	BCB	C1C-NC-C4C	-14.55	100.16	106.71
9	M	407	BCB	C1C-NC-C4C	-13.32	100.72	106.71
9	L	302	BCB	C1C-NC-C4C	-11.97	101.33	106.71
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
17	Z	102	NS0	C20-C19-C17	-9.47	113.79	127.31
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
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	w	101	BCB	C4A-NA-C1A	-8.67	102.81	106.71
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
17	u	102	NS0	C15-C14-C12	-8.61	115.03	127.31
17	N	102	NS0	C15-C14-C12	-8.28	115.49	127.31
17	i	102	NS0	C15-C14-C12	-8.10	115.76	127.31
10	L	303	BPB	C2D-C1D-ND	8.05	115.08	109.53
10	L	303	BPB	O2D-CGD-CBD	7.79	120.87	111.00
10	M	408	BPB	O2D-CGD-CBD	7.73	120.80	111.00
11	L	304	UQ9	C7-C8-C9	-7.68	114.01	126.79
17	i	102	NS0	C10-C11-C12	-7.48	105.41	126.42
17	Z	102	NS0	C10-C11-C12	-7.33	105.84	126.42
17	u	102	NS0	C10-C11-C12	-7.32	105.86	126.42
17	4	102	NS0	C10-C11-C12	-7.27	105.98	126.42
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
10	L	303	BPB	C4D-ND-C1D	-7.17	101.54	108.83
17	N	102	NS0	C10-C11-C12	-7.15	106.34	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	x	102	NS0	C10-C11-C12	-7.05	106.62	126.42
17	r	102	NS0	C10-C11-C12	-7.01	106.72	126.42
17	u	102	NS0	C21-C22-C23	-7.00	117.32	127.31
17	c	102	NS0	C10-C11-C12	-6.98	106.82	126.42
17	o	102	NS0	C10-C11-C12	-6.92	106.97	126.42
17	W	102	NS0	C10-C11-C12	-6.86	107.15	126.42
17	N	102	NS0	C21-C22-C23	-6.82	117.57	127.31
17	G	102	NS0	C10-C11-C12	-6.72	107.55	126.42
11	6	101	UQ9	C7-C8-C9	-6.68	115.67	126.79
9	w	101	BCB	O2D-CGD-CBD	6.64	123.06	111.27
17	l	102	NS0	C10-C11-C12	-6.62	107.81	126.42
17	Q	102	NS0	C10-C11-C12	-6.57	107.97	126.42
17	Z	102	NS0	C21-C22-C23	-6.56	117.94	127.31
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	L	302	BCB	O2D-CGD-CBD	6.42	122.67	111.27
9	6	102	BCB	CED-O2D-CGD	6.38	130.38	115.94
9	6	102	BCB	CMD-C2D-C1D	6.31	135.83	124.71
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
17	W	102	NS0	C21-C22-C23	-6.27	118.36	127.31
17	W	102	NS0	C20-C21-C22	-6.27	110.63	123.47
17	r	102	NS0	C20-C21-C22	-6.25	110.66	123.47
17	o	102	NS0	C20-C21-C22	-6.24	110.69	123.47
9	P	101	BCB	CMD-C2D-C1D	6.22	135.68	124.71
17	f	102	NS0	C21-C22-C23	-6.22	118.44	127.31
9	i	101	BCB	CMD-C2D-C1D	6.21	135.67	124.71
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
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
17	G	102	NS0	C21-C22-C23	-6.14	118.54	127.31
10	M	408	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
10	M	408	BPB	C4D-ND-C1D	-6.10	102.63	108.83
17	o	102	NS0	C21-C22-C23	-6.07	118.64	127.31
9	b	101	BCB	CMD-C2D-C1D	6.07	135.42	124.71
9	V	101	BCB	C2D-C1D-ND	-6.07	105.63	110.10
8	C	403	HEC	C4B-NB-C1B	6.06	111.33	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	w	101	BCB	CMD-C2D-C1D	6.05	135.38	124.71
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
9	o	101	BCB	O2D-CGD-CBD	6.03	121.98	111.27
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
17	N	102	NS0	C20-C21-C22	-6.00	111.18	123.47
16	M	411	NS5	C19-C20-C21	-6.00	118.75	127.31
9	b	101	BCB	O2D-CGD-CBD	5.99	121.90	111.27
17	i	102	NS0	C21-C22-C23	-5.98	118.78	127.31
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	410	MQ9	C20-C19-C21	5.91	125.22	115.27
9	F	101	BCB	CMD-C2D-C1D	5.91	135.13	124.71
9	h	101	BCB	C4-C3-C5	5.90	125.20	115.27
9	l	101	BCB	CMD-C2D-C1D	5.87	135.06	124.71
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
9	G	101	BCB	O2D-CGD-CBD	5.83	121.63	111.27
9	1	101	BCB	O2D-CGD-CBD	5.82	121.60	111.27
9	K	101	BCB	CMD-C2D-C1D	5.81	134.94	124.71
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
9	N	101	BCB	O2D-CGD-CBD	5.78	121.54	111.27
11	6	101	UQ9	O2-C2-C3	-5.78	108.67	120.93
9	M	406	BCB	O2D-CGD-CBD	5.77	121.53	111.27
9	7	101	BCB	O2D-CGD-CBD	5.77	121.52	111.27
9	f	101	BCB	CMD-C2D-C1D	5.76	134.87	124.71
17	Q	102	NS0	C21-C22-C23	-5.74	119.12	127.31
9	Q	101	BCB	O2D-CGD-CBD	5.73	121.45	111.27
8	C	404	HEC	C4B-NB-C1B	5.71	110.97	105.07
17	4	102	NS0	C31-C32-C33	-5.70	113.93	127.66
9	Z	101	BCB	C2D-C1D-ND	-5.67	105.92	110.10
8	C	401	HEC	CBC-CAC-C3C	5.66	128.03	112.43
8	C	401	HEC	C4B-NB-C1B	5.63	110.89	105.07
17	x	102	NS0	C31-C32-C33	-5.62	114.12	127.66
9	r	101	BCB	CMD-C2D-C1D	5.61	134.60	124.71
9	q	101	BCB	CMD-C2D-C1D	5.61	134.60	124.71
17	u	102	NS0	C20-C21-C22	-5.58	112.04	123.47
10	L	303	BPB	C3D-C4D-ND	5.56	115.29	107.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	N	102	NS0	CA-CB-CG	-5.53	108.84	127.75
9	r	101	BCB	O2D-CGD-CBD	5.53	121.10	111.27
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	410	MQ9	C12-C13-C14	-5.51	114.39	127.66
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
9	i	101	BCB	O2D-CGD-CBD	5.48	121.00	111.27
9	t	101	BCB	C2D-C1D-ND	-5.47	106.07	110.10
11	6	101	UQ9	C6-C1-C2	5.47	123.51	119.18
10	M	408	BPB	C3D-C4D-ND	5.47	115.17	107.72
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
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
9	x	101	BCB	O2D-CGD-CBD	5.41	120.88	111.27
17	i	102	NS0	C31-C32-C33	-5.39	114.67	127.66
9	T	101	BCB	O2D-CGD-CBD	5.39	120.85	111.27
9	K	101	BCB	O2D-CGD-CBD	5.37	120.82	111.27
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
9	l	101	BCB	O2D-CGD-CBD	5.35	120.77	111.27
11	L	304	UQ9	C32-C33-C34	-5.34	114.81	127.66
8	C	403	HEC	CHC-C4B-NB	5.33	130.95	124.37
9	3	101	BCB	CMD-C2D-C1D	5.33	134.11	124.71
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
9	z	101	BCB	C2D-C1D-ND	-5.32	106.18	110.10
17	x	102	NS0	CA-CB-CG	-5.32	109.57	127.75
9	w	101	BCB	C2D-C1D-ND	-5.32	106.19	110.10
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
9	L	301	BCB	CMD-C2D-C1D	5.30	134.05	124.71
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
9	e	101	BCB	CMD-C2D-C1D	5.27	134.01	124.71
9	f	101	BCB	C2A-C1A-CHA	-5.27	114.64	123.86
9	G	101	BCB	C2D-C1D-ND	-5.27	106.22	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	3	101	BCB	O2D-CGD-CBD	5.26	120.62	111.27
8	C	402	HEC	C4B-NB-C1B	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
9	e	101	BCB	C4A-NA-C1A	-5.23	104.36	106.71
9	z	101	BCB	C4A-NA-C1A	-5.23	104.36	106.71
9	c	101	BCB	CMD-C2D-C1D	5.21	133.90	124.71
17	u	102	NS0	C27-C26-C25	-5.20	106.98	123.22
10	M	408	BPB	C2D-C1D-ND	5.20	113.11	109.53
9	M	407	BCB	CMD-C2D-C1D	5.20	133.87	124.71
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	b	101	BCB	C2D-C1D-ND	-5.18	106.29	110.10
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
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
9	q	101	BCB	O2D-CGD-CBD	5.13	120.39	111.27
11	6	101	UQ9	C17-C18-C19	-5.11	115.35	127.66
9	S	101	BCB	O2D-CGD-CBD	5.11	120.34	111.27
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
9	q	101	BCB	C4A-NA-C1A	-5.08	104.42	106.71
11	6	101	UQ9	C42-C43-C44	-5.07	115.44	127.66
9	K	101	BCB	C4-C3-C5	5.07	123.80	115.27
15	M	410	MQ9	C35-C34-C36	5.07	123.80	115.27
9	M	406	BCB	CMD-C2D-C1D	5.06	133.63	124.71
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
9	h	101	BCB	C2D-C1D-ND	-5.04	106.39	110.10
10	M	408	BPB	CBC-CAC-C3C	-5.03	113.34	126.70
9	Q	101	BCB	C2A-C1A-CHA	-5.02	115.07	123.86
9	u	101	BCB	C4-C3-C5	5.02	123.72	115.27
9	6	102	BCB	O2D-CGD-CBD	5.02	120.18	111.27
17	c	102	NS0	C27-C26-C25	-5.01	107.57	123.22
9	S	101	BCB	C4A-NA-C1A	-5.01	104.45	106.71
9	c	101	BCB	O2D-CGD-CBD	5.00	120.15	111.27
9	u	101	BCB	CMD-C2D-C1D	4.99	133.51	124.71
9	M	407	BCB	O2D-CGD-CBD	4.99	120.13	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	M	411	NS5	C18-C19-C20	4.98	133.68	123.47
9	3	101	BCB	C2A-C1A-CHA	-4.96	115.19	123.86
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	M	406	BCB	C2C-C1C-CHC	-4.94	112.01	123.64
17	Z	102	NS0	C31-C32-C33	-4.93	115.79	127.66
9	u	101	BCB	O2D-CGD-CBD	4.93	120.03	111.27
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
10	M	408	BPB	C2B-C1B-NB	4.89	112.91	109.53
9	F	101	BCB	CHC-C4B-NB	4.89	129.44	124.26
9	u	101	BCB	C2A-C1A-CHA	-4.88	115.32	123.86
11	L	304	UQ9	C27-C28-C29	-4.88	115.91	127.66
9	M	406	BCB	CHC-C4B-NB	4.87	129.41	124.26
17	u	102	NS0	CA-CB-CG	-4.87	111.11	127.75
9	Y	101	BCB	CMD-C2D-C1D	4.86	133.28	124.71
17	W	102	NS0	C31-C32-C33	-4.86	115.96	127.66
9	l	101	BCB	C2A-C1A-CHA	-4.86	115.36	123.86
9	1	101	BCB	C2A-C1A-CHA	-4.85	115.37	123.86
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	T	101	BCB	C2D-C1D-ND	-4.85	106.53	110.10
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
9	1	101	BCB	CMD-C2D-C1D	4.84	133.24	124.71
17	l	102	NS0	C27-C26-C25	-4.83	108.15	123.22
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
9	e	101	BCB	O2D-CGD-CBD	4.80	119.79	111.27
9	4	101	BCB	CMD-C2D-C1D	4.80	133.16	124.71
9	V	101	BCB	C4A-NA-C1A	-4.79	104.55	106.71
11	L	304	UQ9	C12-C13-C14	-4.78	116.15	127.66
15	M	410	MQ9	C31-C32-C33	-4.78	96.18	111.88
9	Y	101	BCB	C4D-CHA-C1A	-4.77	115.44	121.25
9	Z	101	BCB	C2A-C1A-CHA	-4.77	115.52	123.86
17	l	102	NS0	CD2-CG-CB	-4.76	108.88	122.65
9	M	407	BCB	CAA-C2A-C1A	-4.75	96.41	111.97
9	r	101	BCB	C2A-C1A-CHA	-4.74	115.56	123.86
17	G	102	NS0	CD1-CG-CB	-4.73	108.97	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	G	102	NS0	C27-C26-C25	-4.73	108.46	123.22
9	k	101	BCB	O2D-CGD-CBD	4.73	119.67	111.27
9	F	101	BCB	C2A-C1A-CHA	-4.72	115.60	123.86
17	N	102	NS0	CD1-CG-CB	-4.72	109.00	122.65
9	o	101	BCB	C2A-C1A-CHA	-4.72	115.61	123.86
9	K	101	BCB	CHC-C4B-NB	4.70	129.23	124.26
11	6	101	UQ9	C27-C28-C29	-4.70	116.34	127.66
9	L	301	BCB	C3D-C2D-C1D	-4.70	99.42	105.83
9	N	101	BCB	C2A-C1A-CHA	-4.70	115.65	123.86
9	z	101	BCB	O2D-CGD-CBD	4.69	119.61	111.27
9	3	101	BCB	C2D-C1D-ND	-4.69	106.65	110.10
17	r	102	NS0	C31-C32-C33	-4.69	116.37	127.66
9	G	101	BCB	CMD-C2D-C1D	4.69	132.97	124.71
9	i	101	BCB	C2A-C1A-CHA	-4.69	115.67	123.86
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
9	x	101	BCB	CMD-C2D-C1D	4.67	132.95	124.71
17	c	102	NS0	CD2-CG-CB	-4.67	109.15	122.65
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
9	T	101	BCB	CMD-C2D-C1D	4.66	132.93	124.71
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	L	301	BCB	C2C-C1C-CHC	-4.62	112.76	123.64
9	T	101	BCB	C2A-C1A-CHA	-4.61	115.80	123.86
8	C	403	HEC	C4C-NC-C1C	4.61	109.86	105.35
17	Z	102	NS0	CD2-CG-CB	-4.60	109.36	122.65
9	h	101	BCB	C2C-C1C-CHC	-4.60	112.81	123.64
9	t	101	BCB	O2D-CGD-CBD	4.60	119.44	111.27
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
8	C	402	HEC	CHD-C1D-ND	4.58	130.02	124.37
17	i	102	NS0	CD2-CG-CB	-4.58	109.42	122.65
17	o	102	NS0	CD1-CG-CB	-4.57	109.43	122.65
9	4	101	BCB	O2D-CGD-CBD	4.57	119.39	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	V	101	BCB	CMD-C2D-C1D	4.57	132.77	124.71
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
9	4	101	BCB	C2A-C1A-CHA	-4.57	115.88	123.86
17	i	102	NS0	CD1-CG-CB	-4.57	109.45	122.65
9	M	406	BCB	C4-C3-C5	4.56	122.95	115.27
9	i	101	BCB	C2D-C1D-ND	-4.56	106.75	110.10
17	r	102	NS0	CD2-CG-CB	-4.55	109.49	122.65
9	n	101	BCB	C2D-C1D-ND	-4.55	106.75	110.10
9	F	101	BCB	O2D-CGD-CBD	4.55	119.35	111.27
9	7	101	BCB	C2D-C1D-ND	-4.55	106.75	110.10
9	f	101	BCB	O2D-CGD-CBD	4.54	119.34	111.27
17	T	102	NS0	CD1-CG-CB	-4.54	109.53	122.65
8	C	404	HEC	CBC-CAC-C3C	4.53	124.92	112.43
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
9	n	101	BCB	O2D-CGD-CBD	4.53	119.31	111.27
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	HEC	CAD-C3D-C4D	4.51	132.54	124.66
17	f	102	NS0	C15-C16-C17	-4.51	113.76	126.42
9	Y	101	BCB	C2A-C1A-CHA	-4.50	115.98	123.86
9	Z	101	BCB	O2D-CGD-CBD	4.50	119.27	111.27
17	Z	102	NS0	CD1-CG-CB	-4.50	109.64	122.65
9	6	102	BCB	C2C-C1C-CHC	-4.49	113.06	123.64
17	l	102	NS0	C15-C16-C17	-4.49	113.80	126.42
9	o	101	BCB	CMD-C2D-C1D	4.49	132.63	124.71
9	F	101	BCB	C2D-C1D-ND	-4.49	106.80	110.10
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
9	h	101	BCB	CMD-C2D-C1D	4.44	132.54	124.71
9	Y	101	BCB	C4A-NA-C1A	-4.44	104.71	106.71
9	S	101	BCB	C2A-C1A-CHA	-4.43	116.11	123.86
17	N	102	NS0	C9-C10-C11	-4.43	109.39	123.22
9	V	101	BCB	C2C-C1C-CHC	-4.43	113.21	123.64
9	M	406	BCB	C1-O2A-CGA	4.43	128.06	116.44
9	x	101	BCB	C2A-C1A-CHA	-4.41	116.15	123.86
17	7	102	NS0	C27-C26-C25	-4.40	109.47	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	F	101	BCB	C4D-CHA-C1A	-4.40	115.89	121.25
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
9	t	101	BCB	C2C-C1C-CHC	-4.37	113.35	123.64
9	c	101	BCB	C2A-C1A-CHA	-4.36	116.23	123.86
9	7	101	BCB	C2A-C1A-CHA	-4.34	116.27	123.86
9	l	101	BCB	CHB-C1B-NB	-4.34	119.67	124.26
9	o	101	BCB	CHC-C1C-NC	-4.33	118.52	124.51
9	P	101	BCB	O2D-CGD-CBD	4.33	118.96	111.27
9	P	101	BCB	C2C-C1C-CHC	-4.33	113.44	123.64
10	L	303	BPB	C2B-C1B-NB	4.33	112.52	109.53
9	Y	101	BCB	O2D-CGD-CBD	4.33	118.96	111.27
9	k	101	BCB	C2D-C1D-ND	-4.33	106.92	110.10
9	3	101	BCB	C4D-CHA-C1A	-4.32	115.99	121.25
17	o	102	NS0	C9-C10-C11	-4.32	109.75	123.22
9	W	101	BCB	C2D-C1D-ND	-4.31	106.92	110.10
9	c	101	BCB	C4D-CHA-C1A	-4.30	116.01	121.25
17	W	102	NS0	C15-C16-C17	-4.30	114.33	126.42
9	S	101	BCB	CMD-C2D-C1D	4.29	132.28	124.71
9	n	101	BCB	C2C-C1C-CHC	-4.29	113.54	123.64
9	7	101	BCB	C4D-CHA-C1A	-4.28	116.04	121.25
9	P	101	BCB	C1-O2A-CGA	4.28	127.68	116.44
9	W	101	BCB	O2D-CGD-CBD	4.28	118.88	111.27
9	N	101	BCB	CMD-C2D-C1D	4.27	132.24	124.71
9	G	101	BCB	C2C-C1C-CHC	-4.27	113.59	123.64
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
9	w	101	BCB	C2C-C1C-CHC	-4.24	113.66	123.64
17	G	102	NS0	C9-C10-C11	-4.23	110.00	123.22
9	6	102	BCB	C2A-C1A-CHA	-4.23	116.46	123.86
9	F	101	BCB	C2C-C1C-CHC	-4.23	113.68	123.64
9	e	101	BCB	C2D-C1D-ND	-4.23	106.99	110.10
17	4	102	NS0	C15-C16-C17	-4.23	114.55	126.42
9	f	101	BCB	CHB-C1B-NB	-4.21	119.80	124.26
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	k	101	BCB	CMD-C2D-C1D	4.19	132.10	124.71
17	c	102	NS0	C29-C28-C30	4.19	122.31	115.27
8	C	402	HEC	CAD-CBD-CGD	-4.19	104.60	113.60
9	w	101	BCB	O2A-CGA-CBA	4.18	125.04	111.91
8	C	404	HEC	CHC-C4B-NB	4.17	129.52	124.37
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
9	G	101	BCB	C4D-CHA-C1A	-4.17	116.17	121.25
9	P	101	BCB	CHB-C4A-NA	4.17	130.28	124.51
9	V	101	BCB	O2D-CGD-CBD	4.17	118.67	111.27
17	Q	102	NS0	C29-C28-C30	4.16	122.28	115.27
9	1	101	BCB	C2D-C1D-ND	-4.16	107.04	110.10
15	M	410	MQ9	C30-C29-C31	4.15	122.25	115.27
9	c	101	BCB	C1-O2A-CGA	4.15	127.33	116.44
9	c	101	BCB	C2D-C1D-ND	-4.15	107.05	110.10
9	M	406	BCB	C2B-C1B-NB	-4.14	107.45	110.23
17	u	102	NS0	C15-C16-C17	-4.13	114.81	126.42
9	W	101	BCB	C4A-NA-C1A	-4.13	104.85	106.71
9	Q	101	BCB	CMD-C2D-C1D	4.13	131.99	124.71
9	t	101	BCB	CMD-C2D-C1D	4.12	131.97	124.71
17	f	102	NS0	C9-C10-C11	-4.12	110.37	123.22
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
9	Z	101	BCB	CMD-C2D-C1D	4.08	131.91	124.71
9	z	101	BCB	CMD-C2D-C1D	4.08	131.91	124.71
9	W	101	BCB	CMD-C2D-C1D	4.08	131.90	124.71
9	W	101	BCB	C2A-C1A-CHA	-4.07	116.74	123.86
17	u	102	NS0	C21-C20-C19	-4.07	115.14	123.47
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	408	BPB	O1D-CGD-CBD	-4.06	117.97	124.74
9	z	101	BCB	O2A-CGA-CBA	4.06	124.66	111.91
9	7	101	BCB	CHB-C4A-NA	4.06	130.13	124.51
8	C	404	HEC	CAD-C3D-C4D	4.06	131.75	124.66
9	L	302	BCB	CMD-C2D-C1D	4.05	131.86	124.71
17	7	102	NS0	C9-C10-C11	-4.05	110.57	123.22
9	M	407	BCB	C2D-C1D-ND	-4.05	107.12	110.10
17	T	102	NS0	C9-C10-C11	-4.04	110.62	123.22
9	K	101	BCB	C2A-C1A-CHA	-4.03	116.80	123.86
9	S	101	BCB	C2C-C1C-CHC	-4.03	114.14	123.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	r	102	NS0	C15-C16-C17	-4.03	115.10	126.42
9	b	101	BCB	C4A-NA-C1A	-4.03	104.90	106.71
9	Y	101	BCB	C3D-C2D-C1D	-4.03	100.34	105.83
9	Y	101	BCB	O2A-CGA-CBA	4.02	124.53	111.91
9	n	101	BCB	CMD-C2D-C1D	4.02	131.80	124.71
17	u	102	NS0	CD1-CG-CB	-4.02	111.03	122.65
9	3	101	BCB	C2C-C1C-CHC	-4.02	114.18	123.64
9	M	407	BCB	C2A-C1A-CHA	-4.02	116.84	123.86
9	4	101	BCB	CHD-C4C-C3C	-4.01	120.87	125.89
9	t	101	BCB	C4D-CHA-C1A	-4.01	116.37	121.25
8	C	401	HEC	CHC-C4B-NB	4.01	129.31	124.37
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
9	k	101	BCB	C2C-C1C-CHC	-4.00	114.23	123.64
17	x	102	NS0	C9-C10-C11	-4.00	110.75	123.22
9	c	101	BCB	CHB-C1B-NB	-3.99	120.03	124.26
15	M	410	MQ9	C45-C44-C46	3.98	121.96	115.27
9	k	101	BCB	C4A-NA-C1A	-3.97	104.92	106.71
9	G	101	BCB	C2A-C1A-CHA	-3.97	116.91	123.86
9	n	101	BCB	C4A-NA-C1A	-3.97	104.92	106.71
17	1	102	NS0	C15-C16-C17	-3.97	115.28	126.42
8	C	403	HEC	CHD-C1D-ND	3.97	129.26	124.37
17	i	102	NS0	C15-C16-C17	-3.96	115.28	126.42
9	z	101	BCB	C2C-C1C-CHC	-3.96	114.31	123.64
17	N	102	NS0	C15-C16-C17	-3.96	115.29	126.42
9	n	101	BCB	C4D-CHA-C1A	-3.96	116.43	121.25
9	3	101	BCB	C3D-C2D-C1D	-3.96	100.43	105.83
9	x	101	BCB	C2C-C1C-CHC	-3.96	114.33	123.64
17	i	102	NS0	C9-C10-C11	-3.95	110.88	123.22
9	M	406	BCB	C2D-C1D-ND	-3.95	107.19	110.10
9	N	101	BCB	C4D-CHA-C1A	-3.95	116.44	121.25
9	4	101	BCB	C2D-C1D-ND	-3.95	107.19	110.10
9	x	101	BCB	C4D-CHA-C1A	-3.95	116.44	121.25
9	M	407	BCB	C2C-C1C-CHC	-3.94	114.37	123.64
9	h	101	BCB	C2A-C1A-CHA	-3.93	116.99	123.86
9	x	101	BCB	C2D-C1D-ND	-3.93	107.21	110.10
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
9	b	101	BCB	CHD-C4C-C3C	-3.92	120.98	125.89
9	7	101	BCB	C2C-C1C-CHC	-3.92	114.42	123.64
17	Z	102	NS0	C29-C28-C30	3.91	121.86	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	o	101	BCB	CHB-C1B-NB	-3.91	120.12	124.26
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
9	e	101	BCB	C2C-C1C-CHC	-3.90	114.45	123.64
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
9	L	302	BCB	C2C-C1C-CHC	-3.90	114.47	123.64
9	Z	101	BCB	C2C-C1C-CHC	-3.90	114.47	123.64
9	1	101	BCB	C4A-NA-C1A	-3.89	104.96	106.71
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
9	L	302	BCB	C4A-NA-C1A	-3.87	104.97	106.71
17	c	102	NS0	C15-C16-C17	-3.87	115.56	126.42
8	C	403	HEC	CHA-C4D-ND	3.87	128.62	124.42
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
9	q	101	BCB	C2D-C1D-ND	-3.85	107.26	110.10
17	Z	102	NS0	C9-C10-C11	-3.84	111.22	123.22
9	k	101	BCB	CBC-CAC-C3C	-3.84	115.50	126.72
9	b	101	BCB	C2C-C1C-CHC	-3.83	114.62	123.64
15	M	410	MQ9	C21-C19-C18	-3.83	113.36	121.12
9	h	101	BCB	O2D-CGD-CBD	3.83	118.07	111.27
17	i	102	NS0	C29-C28-C30	3.83	121.71	115.27
9	K	101	BCB	C2C-C1C-CHC	-3.83	114.63	123.64
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	T	101	BCB	C2C-C1C-CHC	-3.81	114.66	123.64
9	k	101	BCB	O2A-CGA-CBA	3.81	123.87	111.91
8	C	402	HEC	CBB-CAB-C3B	3.81	122.93	112.43
9	z	101	BCB	C1D-ND-C4D	3.80	109.04	106.33
11	L	304	UQ9	C7-C6-C5	3.80	123.06	118.48
16	M	411	NS5	C4-C5-C7	-3.80	113.42	121.12
9	f	101	BCB	C4D-CHA-C1A	-3.80	116.62	121.25
9	M	406	BCB	CAB-C3B-C2B	-3.79	122.66	128.34
11	6	101	UQ9	C47-C48-C49	-3.79	114.80	127.75
9	P	101	BCB	C2A-C1A-CHA	-3.79	117.23	123.86
17	N	102	NS0	C29-C28-C30	3.78	121.63	115.27
9	i	101	BCB	CHC-C1C-NC	-3.78	119.29	124.51
17	c	102	NS0	C21-C20-C19	-3.78	115.73	123.47
9	G	101	BCB	CHB-C1B-NB	-3.77	120.26	124.26
15	M	410	MQ9	C46-C44-C43	-3.77	113.49	121.12
9	q	101	BCB	C3D-C2D-C1D	-3.77	100.69	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	N	102	NS0	C21-C20-C19	-3.77	115.76	123.47
9	o	101	BCB	CHC-C4B-NB	3.76	128.24	124.26
17	l	102	NS0	CD1-CG-CB	-3.76	111.78	122.65
9	L	302	BCB	C2D-C1D-ND	-3.75	107.34	110.10
9	K	101	BCB	CHC-C1C-NC	-3.75	119.33	124.51
8	C	402	HEC	CHC-C4B-NB	3.74	128.99	124.37
9	K	101	BCB	CHD-C4C-C3C	-3.74	121.21	125.89
16	M	411	NS5	C6-C5-C4	3.74	121.56	115.27
9	6	102	BCB	C2D-C1D-ND	-3.73	107.35	110.10
9	z	101	BCB	C1D-CHD-C4C	-3.73	118.01	126.06
9	Y	101	BCB	C2C-C1C-CHC	-3.73	114.86	123.64
9	L	302	BCB	O1D-CGD-CBD	-3.73	116.86	124.48
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
9	q	101	BCB	CAB-C3B-C2B	-3.72	122.77	128.34
17	l	102	NS0	C29-C28-C30	3.72	121.53	115.27
9	l	101	BCB	C2C-C1C-CHC	-3.72	114.89	123.64
9	e	101	BCB	CHD-C4C-C3C	-3.72	121.24	125.89
9	n	101	BCB	C2A-C1A-CHA	-3.72	117.36	123.86
9	7	101	BCB	CHB-C1B-NB	-3.71	120.33	124.26
17	7	102	NS0	C29-C28-C30	3.71	121.52	115.27
9	r	101	BCB	C2C-C1C-CHC	-3.71	114.90	123.64
9	P	101	BCB	C1D-CHD-C4C	-3.70	118.08	126.06
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	F	101	BCB	CHC-C1C-NC	-3.70	119.40	124.51
9	h	101	BCB	C1D-CHD-C4C	-3.69	118.10	126.06
8	C	401	HEC	CBB-CAB-C3B	3.67	122.56	112.43
9	L	301	BCB	OBD-CAD-C3D	-3.67	119.68	128.52
9	o	101	BCB	CHD-C4C-C3C	-3.66	121.31	125.89
16	M	411	NS5	C12-C13-C14	-3.66	111.79	123.22
17	G	102	NS0	C21-C20-C19	-3.66	115.97	123.47
17	T	102	NS0	C29-C28-C30	3.66	121.43	115.27
8	C	401	HEC	CHA-C4D-ND	3.66	128.39	124.42
8	C	403	HEC	CBC-CAC-C3C	3.66	122.51	112.43
9	f	101	BCB	C2D-C1D-ND	-3.65	107.41	110.10
9	z	101	BCB	CHD-C4C-C3C	-3.65	121.32	125.89
9	L	302	BCB	C1-O2A-CGA	3.65	126.02	116.44
9	Y	101	BCB	C2D-C1D-ND	-3.65	107.42	110.10
9	M	406	BCB	C3D-C4D-ND	3.65	116.14	110.24
9	L	302	BCB	CAB-C3B-C2B	-3.64	122.88	128.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	V	101	BCB	C2A-C1A-CHA	-3.63	117.51	123.86
9	q	101	BCB	C1-O2A-CGA	3.63	125.97	116.44
9	b	101	BCB	C2A-C1A-CHA	-3.63	117.51	123.86
9	N	101	BCB	C2C-C1C-CHC	-3.63	115.10	123.64
9	q	101	BCB	CHC-C1C-NC	-3.63	119.50	124.51
9	Y	101	BCB	CHD-C4C-C3C	-3.62	121.36	125.89
9	q	101	BCB	C2A-C1A-CHA	-3.61	117.54	123.86
9	c	101	BCB	C2C-C1C-CHC	-3.61	115.14	123.64
8	C	402	HEC	C4C-NC-C1C	3.61	108.88	105.35
9	r	101	BCB	O2A-C1-C2	3.60	118.11	108.64
9	3	101	BCB	CHB-C4A-NA	3.60	129.50	124.51
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	7	101	BCB	CMD-C2D-C1D	3.59	131.05	124.71
17	4	102	NS0	C21-C20-C19	-3.59	116.12	123.47
9	1	101	BCB	C4D-CHA-C1A	-3.59	116.88	121.25
9	t	101	BCB	C4A-NA-C1A	-3.59	105.09	106.71
9	V	101	BCB	C4D-CHA-C1A	-3.58	116.89	121.25
9	K	101	BCB	C3D-C2D-C1D	-3.58	100.94	105.83
9	w	101	BCB	O1D-CGD-CBD	-3.57	117.18	124.48
9	G	101	BCB	O2A-CGA-CBA	3.57	123.10	111.91
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	e	101	BCB	C2A-C1A-CHA	-3.55	117.65	123.86
9	4	101	BCB	C4A-NA-C1A	-3.55	105.11	106.71
9	Y	101	BCB	O2D-CGD-O1D	-3.55	116.89	123.84
9	P	101	BCB	C4D-CHA-C1A	-3.55	116.93	121.25
9	M	407	BCB	CAA-CBA-CGA	-3.54	102.90	113.25
8	C	401	HEC	CHA-C4D-C3D	-3.54	119.64	124.84
9	S	101	BCB	C2D-C1D-ND	-3.53	107.50	110.10
9	o	101	BCB	O2A-CGA-CBA	3.53	122.98	111.91
9	S	101	BCB	C1D-CHD-C4C	-3.53	118.45	126.06
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	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	L	301	BCB	CBB-CAB-C3B	-3.50	112.95	120.43
9	7	101	BCB	O2D-CGD-O1D	-3.50	116.99	123.84
9	1	101	BCB	CHB-C1B-NB	-3.50	120.56	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	6	101	UQ9	O2-C2-C1	-3.49	110.44	120.73
9	l	101	BCB	CHD-C4C-C3C	-3.49	121.52	125.89
9	1	101	BCB	C2C-C1C-CHC	-3.49	115.43	123.64
9	L	302	BCB	C3D-C2D-C1D	-3.49	101.07	105.83
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	L	302	BCB	C4D-C3D-CAD	-3.48	104.00	108.10
9	r	101	BCB	CHB-C4A-NA	3.48	129.32	124.51
9	F	101	BCB	O2D-CGD-O1D	-3.47	117.05	123.84
9	1	101	BCB	O2A-CGA-CBA	3.47	122.79	111.91
9	L	301	BCB	O2D-CGD-CBD	3.46	117.42	111.27
8	C	404	HEC	C4C-NC-C1C	3.46	108.74	105.35
8	C	404	HEC	CHD-C1D-ND	3.46	128.64	124.37
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	Q	101	BCB	CHC-C1C-NC	-3.45	119.74	124.51
9	k	101	BCB	C3D-C2D-C1D	-3.45	101.12	105.83
9	N	101	BCB	C4A-NA-C1A	-3.45	105.16	106.71
9	l	101	BCB	CHC-C1C-NC	-3.44	119.75	124.51
9	K	101	BCB	C1D-ND-C4D	-3.44	103.89	106.33
9	q	101	BCB	CHD-C4C-C3C	-3.44	121.59	125.89
9	M	407	BCB	O2A-CGA-CBA	3.44	122.69	111.91
9	Q	101	BCB	C2C-C1C-CHC	-3.43	115.56	123.64
9	w	101	BCB	C1D-CHD-C4C	-3.43	118.66	126.06
9	3	101	BCB	O2D-CGD-O1D	-3.43	117.13	123.84
9	e	101	BCB	C3D-C2D-C1D	-3.43	101.15	105.83
9	L	301	BCB	CHB-C4A-NA	3.42	129.25	124.51
9	q	101	BCB	C2C-C1C-CHC	-3.42	115.59	123.64
9	Y	101	BCB	OBD-CAD-C3D	-3.42	120.30	128.52
9	f	101	BCB	C1-O2A-CGA	3.42	125.40	116.44
9	k	101	BCB	C2A-C1A-CHA	-3.41	117.89	123.86
9	e	101	BCB	CAB-C3B-C2B	-3.41	123.23	128.34
16	M	411	NS5	C30-C29-C28	-3.41	112.58	123.22
9	z	101	BCB	C3D-C2D-C1D	-3.40	101.19	105.83
9	K	101	BCB	C1D-CHD-C4C	-3.40	118.72	126.06
9	w	101	BCB	CHD-C4C-C3C	-3.40	121.63	125.89
9	f	101	BCB	CHC-C1C-NC	-3.40	119.81	124.51
9	V	101	BCB	CAA-CBA-CGA	-3.39	103.34	113.25
9	F	101	BCB	C2B-C1B-NB	-3.39	107.96	110.23
9	P	101	BCB	C2D-C1D-ND	-3.39	107.61	110.10
9	3	101	BCB	C1-O2A-CGA	3.39	125.33	116.44
9	u	101	BCB	C2C-C1C-CHC	-3.38	115.68	123.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	w	101	BCB	C3D-C2D-C1D	-3.38	101.22	105.83
9	Q	101	BCB	C4D-CHA-C1A	-3.38	117.14	121.25
9	3	101	BCB	CHD-C4C-C3C	-3.38	121.67	125.89
8	C	403	HEC	CHA-C4D-C3D	-3.37	119.88	124.84
9	i	101	BCB	CHB-C1B-NB	-3.37	120.69	124.26
17	i	102	NS0	C14-C15-C16	-3.37	112.70	123.22
10	M	408	BPB	C1-O2A-CGA	3.37	125.28	116.44
9	M	407	BCB	C3D-C2D-C1D	-3.37	101.23	105.83
9	T	101	BCB	CHB-C4A-NA	3.37	129.17	124.51
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	r	101	BCB	C3D-C4D-ND	3.36	115.68	110.24
9	W	101	BCB	CHD-C4C-C3C	-3.36	121.68	125.89
9	h	101	BCB	C1-O2A-CGA	3.36	125.26	116.44
9	u	101	BCB	CHD-C4C-C3C	-3.36	121.69	125.89
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	k	101	BCB	C1D-CHD-C4C	-3.34	118.85	126.06
17	W	102	NS0	C21-C20-C19	-3.34	116.64	123.47
9	r	101	BCB	C1D-ND-C4D	-3.34	103.97	106.33
9	T	101	BCB	CHC-C1C-NC	-3.34	119.90	124.51
9	u	101	BCB	C2D-C1D-ND	-3.34	107.65	110.10
9	f	101	BCB	C2C-C1C-CHC	-3.33	115.79	123.64
9	Q	101	BCB	CHB-C1B-NB	-3.33	120.73	124.26
9	L	301	BCB	CHD-C4C-C3C	-3.33	121.72	125.89
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
8	C	403	HEC	CHB-C1B-NB	3.33	128.03	124.42
9	u	101	BCB	CHB-C1B-NB	-3.32	120.74	124.26
9	G	101	BCB	CHB-C4A-NA	3.32	129.11	124.51
9	t	101	BCB	C1D-CHD-C4C	-3.32	118.89	126.06
9	t	101	BCB	C2A-C1A-CHA	-3.32	118.05	123.86
9	i	101	BCB	C4D-CHA-C1A	-3.32	117.21	121.25
9	W	101	BCB	C4D-CHA-C1A	-3.31	117.22	121.25
15	M	410	MQ9	C5M-C5-C6	-3.31	119.00	124.40
9	P	101	BCB	C3D-C2D-C1D	-3.31	101.32	105.83
9	r	101	BCB	CHC-C1C-NC	-3.31	119.94	124.51
8	C	401	HEC	CHB-C1B-NB	3.30	128.00	124.42
9	o	101	BCB	C1-O2A-CGA	3.30	125.10	116.44
9	r	101	BCB	C4D-CHA-C1A	-3.29	117.24	121.25
9	x	101	BCB	O2A-CGA-CBA	3.29	122.24	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	o	102	NS0	C21-C20-C19	-3.29	116.73	123.47
17	Z	102	NS0	C14-C15-C16	-3.29	112.96	123.22
9	F	101	BCB	CHB-C1B-NB	-3.29	120.78	124.26
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	b	101	BCB	C3D-C2D-C1D	-3.28	101.36	105.83
9	4	101	BCB	C2C-C1C-CHC	-3.27	115.94	123.64
15	M	410	MQ9	C32-C31-C29	3.27	123.73	112.98
17	r	102	NS0	C14-C15-C16	-3.27	113.02	123.22
9	V	101	BCB	C1D-ND-C4D	3.27	108.66	106.33
9	M	406	BCB	CHC-C1C-NC	-3.27	120.00	124.51
9	S	101	BCB	CHD-C4C-C3C	-3.26	121.81	125.89
9	M	406	BCB	CHB-C4A-NA	3.26	129.02	124.51
17	i	102	NS0	C21-C20-C19	-3.26	116.80	123.47
9	6	102	BCB	C3D-C2D-C1D	-3.25	101.40	105.83
9	i	101	BCB	C2C-C1C-CHC	-3.24	116.00	123.64
9	Z	101	BCB	C4D-CHA-C1A	-3.24	117.30	121.25
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	G	101	BCB	CHC-C1C-NC	-3.24	120.04	124.51
17	r	102	NS0	C34-C33-C35	3.23	120.71	115.27
9	h	101	BCB	C3D-C2D-C1D	-3.23	101.42	105.83
9	S	101	BCB	C4D-CHA-C1A	-3.22	117.33	121.25
9	u	101	BCB	C4D-CHA-C1A	-3.22	117.33	121.25
9	6	102	BCB	C4D-CHA-C1A	-3.22	117.33	121.25
9	z	101	BCB	C1-O2A-CGA	3.22	124.89	116.44
15	M	410	MQ9	C12-C11-C9	-3.22	102.39	112.98
9	N	101	BCB	O2A-CGA-CBA	3.22	122.00	111.91
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
9	x	101	BCB	CHB-C1B-NB	-3.21	120.86	124.26
9	c	101	BCB	CHB-C4A-NA	3.21	128.95	124.51
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	4	101	BCB	C4D-CHA-C1A	-3.20	117.36	121.25
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	Q	101	BCB	C2D-C1D-ND	-3.20	107.75	110.10
9	Q	101	BCB	CHD-C4C-C3C	-3.19	121.89	125.89
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
8	C	401	HEC	CHD-C1D-ND	3.19	128.31	124.37
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
9	w	101	BCB	C2A-C1A-CHA	-3.19	118.29	123.86
9	Z	101	BCB	C4A-NA-C1A	-3.19	105.27	106.71
17	7	102	NS0	C21-C20-C19	-3.18	116.96	123.47
9	o	101	BCB	C3D-C4D-ND	3.18	115.38	110.24
9	S	101	BCB	C3D-C2D-C1D	-3.18	101.49	105.83
10	M	408	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	W	101	BCB	CHC-C1C-NC	-3.18	120.12	124.51
9	1	101	BCB	CHD-C4C-C3C	-3.17	121.92	125.89
9	o	101	BCB	C2C-C1C-CHC	-3.17	116.17	123.64
9	T	101	BCB	C1-O2A-CGA	3.17	124.75	116.44
9	M	407	BCB	O1D-CGD-CBD	-3.16	118.01	124.48
9	z	101	BCB	CBC-CAC-C3C	-3.15	117.50	126.72
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	z	101	BCB	CHD-C4C-NC	3.14	129.15	124.20
9	6	102	BCB	C1-C2-C3	3.14	131.47	126.04
9	l	101	BCB	C2D-C1D-ND	-3.13	107.79	110.10
9	M	407	BCB	C4D-C3D-CAD	-3.13	104.40	108.10
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	W	101	BCB	C2C-C1C-CHC	-3.12	116.29	123.64
9	k	101	BCB	CHD-C4C-C3C	-3.12	121.99	125.89
9	u	101	BCB	O2A-CGA-CBA	3.12	121.69	111.91
9	b	101	BCB	C1D-CHD-C4C	-3.12	119.34	126.06
17	c	102	NS0	C34-C33-C35	3.11	120.51	115.27
9	e	101	BCB	CHC-C1C-NC	-3.11	120.21	124.51
15	M	410	MQ9	C7-C6-C1	3.11	121.83	118.50
9	P	101	BCB	CHC-C4B-NB	3.11	127.55	124.26
9	Z	101	BCB	CHB-C1B-NB	-3.11	120.96	124.26
9	b	101	BCB	O2D-CGD-O1D	-3.11	117.76	123.84
8	C	404	HEC	CHB-C1B-NB	3.11	127.79	124.42
9	w	101	BCB	O2A-CGA-O1A	-3.11	115.75	123.59
9	n	101	BCB	C3D-C2D-C1D	-3.10	101.59	105.83
9	V	101	BCB	C1D-CHD-C4C	-3.10	119.38	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	M	407	BCB	OBB-CAB-CBB	3.09	126.59	119.73
9	L	301	BCB	C1D-CHD-C4C	-3.09	119.39	126.06
9	h	101	BCB	C4A-NA-C1A	-3.09	105.32	106.71
9	M	407	BCB	CBB-CAB-C3B	-3.09	113.83	120.43
9	z	101	BCB	C2A-C1A-CHA	-3.09	118.46	123.86
9	N	101	BCB	CHB-C4A-NA	3.09	128.78	124.51
15	M	410	MQ9	C16-C17-C18	-3.08	101.75	111.88
9	Y	101	BCB	C1D-CHD-C4C	-3.08	119.41	126.06
9	K	101	BCB	CHB-C4A-NA	3.08	128.77	124.51
8	C	404	HEC	C3B-C4B-NB	-3.08	106.74	110.17
8	C	402	HEC	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	h	101	BCB	CHB-C4A-NA	3.07	128.75	124.51
9	x	101	BCB	CHC-C1C-NC	-3.07	120.27	124.51
17	Q	102	NS0	C14-C15-C16	-3.06	113.66	123.22
9	c	101	BCB	C4A-NA-C1A	-3.06	105.33	106.71
17	u	102	NS0	C34-C33-C35	3.05	120.41	115.27
8	C	402	HEC	CHD-C1D-C2D	-3.05	118.25	126.73
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
9	T	101	BCB	C4D-CHA-C1A	-3.05	117.54	121.25
9	N	101	BCB	C2D-C1D-ND	-3.05	107.86	110.10
9	o	101	BCB	C1D-ND-C4D	-3.04	104.17	106.33
17	1	102	NS0	C34-C33-C35	3.04	120.39	115.27
9	w	101	BCB	CHD-C4C-NC	3.04	129.00	124.20
9	S	101	BCB	C1-O2A-CGA	3.04	124.42	116.44
15	M	410	MQ9	C25-C24-C23	-3.04	115.88	123.68
9	r	101	BCB	CHC-C4B-NB	3.04	127.47	124.26
9	o	101	BCB	C4D-CHA-C1A	-3.04	117.55	121.25
17	Z	102	NS0	C34-C33-C35	3.04	120.38	115.27
10	M	408	BPB	C4-C3-C5	3.03	120.37	115.27
9	l	101	BCB	C4D-CHA-C1A	-3.03	117.56	121.25
9	r	101	BCB	CHB-C1B-NB	-3.02	121.06	124.26
17	l	102	NS0	C34-C33-C35	3.02	120.35	115.27
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
9	L	302	BCB	CHB-C4A-NA	3.01	128.68	124.51
17	x	102	NS0	C34-C33-C35	3.01	120.33	115.27
9	T	101	BCB	C1D-CHD-C4C	-3.01	119.57	126.06
9	V	101	BCB	O2D-CGD-O1D	-3.01	117.96	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	M	407	BCB	CED-O2D-CGD	3.00	122.73	115.94
9	e	101	BCB	C1D-CHD-C4C	-3.00	119.58	126.06
15	M	410	MQ9	C31-C29-C28	-3.00	115.05	121.12
9	r	101	BCB	O1D-CGD-CBD	-2.99	118.36	124.48
9	3	101	BCB	CHB-C1B-NB	-2.98	121.10	124.26
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	6	102	BCB	CHB-C4A-NA	2.98	128.63	124.51
9	M	406	BCB	O2A-CGA-CBA	2.98	121.25	111.91
17	l	102	NS0	C21-C20-C19	-2.97	117.38	123.47
9	N	101	BCB	C3D-C2D-C1D	-2.97	101.78	105.83
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
17	T	102	NS0	C34-C33-C35	2.96	120.25	115.27
10	M	408	BPB	CMA-C3A-C4A	-2.95	107.91	114.38
9	F	101	BCB	OBD-CAD-C3D	-2.95	121.41	128.52
9	N	101	BCB	CHC-C1C-NC	-2.95	120.43	124.51
8	C	401	HEC	C4C-NC-C1C	2.95	108.24	105.35
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	408	BPB	CMC-C2C-C1C	-2.94	109.41	114.36
9	Z	101	BCB	O1D-CGD-CBD	-2.94	118.47	124.48
9	M	406	BCB	C3D-C2D-C1D	-2.94	101.82	105.83
17	G	102	NS0	C8-C7-C	2.94	120.21	115.27
17	f	102	NS0	C34-C33-C35	2.93	120.20	115.27
9	u	101	BCB	CHC-C1C-NC	-2.93	120.47	124.51
8	C	403	HEC	O2D-CGD-CBD	2.92	123.43	114.03
9	V	101	BCB	C3D-C2D-C1D	-2.92	101.84	105.83
9	K	101	BCB	C1-O2A-CGA	2.92	124.11	116.44
9	G	101	BCB	C4A-NA-C1A	-2.92	105.39	106.71
11	L	304	UQ9	C25-C24-C26	2.92	120.18	115.27
9	Y	101	BCB	CHB-C1B-NB	-2.92	121.17	124.26
9	b	101	BCB	CHD-C4C-NC	2.92	128.80	124.20
9	z	101	BCB	CHC-C1C-NC	-2.91	120.48	124.51
9	3	101	BCB	C1D-CHD-C4C	-2.91	119.78	126.06
9	6	102	BCB	C4A-NA-C1A	-2.91	105.40	106.71
9	L	301	BCB	C4D-C3D-CAD	-2.91	104.67	108.10
9	M	406	BCB	C4-C3-C2	-2.91	116.21	123.68
9	q	101	BCB	C4D-CHA-C1A	-2.91	117.71	121.25
9	L	302	BCB	CHD-C4C-C3C	-2.91	122.25	125.89
9	c	101	BCB	CHD-C1D-ND	-2.90	121.78	124.45
9	n	101	BCB	C5-C3-C2	-2.90	115.24	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	Z	102	NS0	C8-C7-C	2.90	120.15	115.27
8	C	402	HEC	CBC-CAC-C3C	2.90	120.42	112.43
17	Q	102	NS0	C8-C7-C	2.90	120.14	115.27
9	K	101	BCB	OBD-CAD-C3D	-2.89	121.56	128.52
9	e	101	BCB	O2A-CGA-O1A	-2.89	116.31	123.59
17	c	102	NS0	C8-C7-C	2.89	120.13	115.27
9	P	101	BCB	CHD-C4C-C3C	-2.88	122.28	125.89
17	7	102	NS0	C15-C16-C17	-2.88	118.32	126.42
9	h	101	BCB	CBC-CAC-C3C	-2.88	118.29	126.72
9	W	101	BCB	O2A-CGA-CBA	2.88	120.95	111.91
9	r	101	BCB	CBA-CAA-C2A	-2.88	105.36	113.86
9	7	101	BCB	CHC-C1C-NC	-2.88	120.53	124.51
9	f	101	BCB	C3D-C2D-C1D	-2.87	101.91	105.83
17	u	102	NS0	C8-C7-C	2.87	120.10	115.27
17	T	102	NS0	C8-C7-C	2.87	120.09	115.27
9	F	101	BCB	CHD-C4C-C3C	-2.86	122.31	125.89
9	L	301	BCB	C7-C6-C5	-2.86	105.58	113.36
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	N	101	BCB	O1D-CGD-CBD	-2.85	118.64	124.48
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	f	101	BCB	CHD-C4C-C3C	-2.84	122.33	125.89
9	V	101	BCB	C4-C3-C5	2.84	120.05	115.27
9	Y	101	BCB	CHC-C1C-NC	-2.84	120.59	124.51
9	P	101	BCB	CAA-C2A-C3A	-2.84	105.00	112.78
9	P	101	BCB	CHC-C1C-NC	-2.83	120.59	124.51
9	M	406	BCB	O2D-CGD-O1D	-2.83	118.30	123.84
17	4	102	NS0	C34-C33-C35	2.83	120.03	115.27
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	S	101	BCB	O2D-CGD-O1D	-2.82	118.33	123.84
9	S	101	BCB	O2A-CGA-CBA	2.82	120.74	111.91
9	r	101	BCB	C2D-C1D-ND	-2.81	108.03	110.10
9	M	406	BCB	CBB-CAB-C3B	-2.81	114.42	120.43
9	u	101	BCB	C1D-CHD-C4C	-2.81	119.99	126.06
9	P	101	BCB	O2A-C1-C2	2.81	116.02	108.64
9	z	101	BCB	CHB-C4A-NA	2.81	128.40	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	L	301	BCB	CHC-C4B-NB	2.81	127.23	124.26
8	C	402	HEC	CAB-C3B-C4B	2.81	128.45	124.81
9	t	101	BCB	C3D-C2D-C1D	-2.80	102.01	105.83
9	l	101	BCB	CHB-C4A-NA	2.80	128.38	124.51
9	l	101	BCB	CHC-C4B-NB	2.80	127.22	124.26
17	x	102	NS0	C8-C7-C	2.80	119.97	115.27
9	u	101	BCB	C3D-C4D-ND	2.79	114.75	110.24
9	Z	101	BCB	CHB-C4A-NA	2.79	128.37	124.51
9	e	101	BCB	O2D-CGD-O1D	-2.79	118.38	123.84
9	r	101	BCB	CHD-C1D-ND	-2.79	121.89	124.45
11	6	101	UQ9	C35-C34-C36	2.79	119.96	115.27
9	W	101	BCB	C3D-C2D-C1D	-2.79	102.03	105.83
17	G	102	NS0	C14-C15-C16	-2.78	114.53	123.22
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
9	l	101	BCB	C1D-CHD-C4C	-2.77	120.08	126.06
9	h	101	BCB	C4D-CHA-C1A	-2.77	117.88	121.25
9	n	101	BCB	O2D-CGD-O1D	-2.77	118.42	123.84
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
9	i	101	BCB	CHD-C4C-C3C	-2.76	122.44	125.89
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	4	101	BCB	CHC-C1C-NC	-2.76	120.70	124.51
9	l	101	BCB	C1D-ND-C4D	-2.76	104.38	106.33
9	n	101	BCB	O2A-CGA-CBA	2.76	120.56	111.91
9	o	101	BCB	C3D-C2D-C1D	-2.75	102.08	105.83
8	C	403	HEC	C3B-C4B-NB	-2.74	107.11	110.17
9	k	101	BCB	CHC-C1C-NC	-2.74	120.72	124.51
8	C	403	HEC	CAC-C3C-C4C	2.74	128.71	124.92
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
9	1	101	BCB	C3D-C2D-C1D	-2.73	102.11	105.83
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-NC	-2.72	120.75	124.51
9	o	101	BCB	CHB-C4A-NA	2.72	128.28	124.51
17	l	102	NS0	C14-C15-C16	-2.72	114.72	123.22
9	z	101	BCB	CHB-C1B-NB	-2.72	121.38	124.26
9	q	101	BCB	C1D-CHD-C4C	-2.72	120.19	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	f	102	NS0	C8-C7-C	2.72	119.85	115.27
9	1	101	BCB	O1D-CGD-CBD	-2.72	118.92	124.48
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	N	101	BCB	CHB-C1B-NB	-2.72	121.38	124.26
9	q	101	BCB	O2D-CGD-O1D	-2.72	118.53	123.84
9	6	102	BCB	C2B-C1B-NB	-2.71	108.41	110.23
16	M	411	NS5	C19-C18-C17	2.71	129.03	123.47
9	K	101	BCB	CBC-CAC-C3C	-2.71	118.79	126.72
9	n	101	BCB	C1D-CHD-C4C	-2.71	120.21	126.06
9	i	101	BCB	CHD-C1D-ND	-2.71	121.96	124.45
9	K	101	BCB	CHD-C4C-NC	2.71	128.47	124.20
9	L	301	BCB	C16-C15-C13	-2.70	107.18	115.92
15	M	410	MQ9	C15-C14-C16	2.70	119.82	115.27
8	C	401	HEC	CBD-CAD-C3D	-2.70	105.13	112.63
9	K	101	BCB	C3D-C4D-ND	2.69	114.60	110.24
9	Q	101	BCB	CHB-C4A-NA	2.69	128.24	124.51
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
17	f	102	NS0	C14-C15-C16	-2.69	114.83	123.22
8	C	402	HEC	CHA-C4D-ND	2.69	127.34	124.42
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	r	101	BCB	CHD-C4C-C3C	-2.69	122.53	125.89
9	P	101	BCB	OBD-CAD-C3D	-2.68	122.06	128.52
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
9	x	101	BCB	C3D-C2D-C1D	-2.68	102.17	105.83
9	4	101	BCB	OBB-CAB-C3B	-2.68	115.45	120.41
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	l	101	BCB	CAA-C2A-C1A	-2.67	103.22	111.97
9	L	301	BCB	CGD-CBD-CAD	-2.67	102.09	110.73
9	L	302	BCB	C1D-CHD-C4C	-2.67	120.31	126.06
17	Z	102	NS0	C24-C23-C25	2.66	122.28	118.08
8	C	402	HEC	O2A-CGA-CBA	2.66	122.57	114.03
9	L	301	BCB	OBB-CAB-CBB	2.66	125.62	119.73
9	x	101	BCB	CHB-C4A-NA	2.65	128.18	124.51
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	h	101	BCB	CHD-C4C-C3C	-2.65	122.58	125.89
9	b	101	BCB	CHC-C1C-NC	-2.65	120.85	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	w	101	BCB	CMA-C3A-C2A	-2.64	103.16	113.83
9	Q	101	BCB	CHD-C1D-ND	-2.64	122.03	124.45
9	x	101	BCB	C1D-CHD-C4C	-2.64	120.37	126.06
9	4	101	BCB	C3D-C2D-C1D	-2.63	102.24	105.83
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	n	101	BCB	CHD-C4C-C3C	-2.63	122.60	125.89
9	3	101	BCB	OBD-CAD-C3D	-2.63	122.20	128.52
9	M	406	BCB	C2A-C1A-CHA	-2.63	119.27	123.86
9	q	101	BCB	O2A-CGA-CBA	2.62	120.14	111.91
9	6	102	BCB	O2A-CGA-O1A	-2.62	116.99	123.59
9	n	101	BCB	C4D-C3D-CAD	-2.62	105.01	108.10
8	C	404	HEC	CHA-C4D-C3D	-2.61	121.00	124.84
8	C	403	HEC	O2D-CGD-O1D	-2.61	116.79	123.30
9	f	101	BCB	CHB-C4A-NA	2.61	128.12	124.51
9	h	101	BCB	C5-C3-C2	-2.61	115.84	121.12
9	7	101	BCB	C1D-CHD-C4C	-2.61	120.44	126.06
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	1	101	BCB	CHC-C1C-NC	-2.60	120.92	124.51
9	z	101	BCB	O2A-CGA-O1A	-2.59	117.05	123.59
9	t	101	BCB	OBD-CAD-C3D	-2.59	122.28	128.52
9	F	101	BCB	C3D-C2D-C1D	-2.59	102.30	105.83
9	S	101	BCB	CHD-C4C-NC	2.59	128.28	124.20
9	T	101	BCB	CHD-C4C-C3C	-2.59	122.66	125.89
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
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	M	407	BCB	CHC-C4B-NB	2.58	126.99	124.26
9	T	101	BCB	O1D-CGD-CBD	-2.58	119.20	124.48
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	w	101	BCB	C1D-ND-C4D	2.58	108.17	106.33
17	c	102	NS0	C24-C23-C25	2.58	122.14	118.08
8	C	401	HEC	CAA-CBA-CGA	-2.57	108.06	113.60
9	1	101	BCB	C1D-CHD-C4C	-2.57	120.52	126.06
9	k	101	BCB	CHD-C4C-NC	2.56	128.24	124.20
9	f	101	BCB	CHD-C1D-ND	-2.56	122.10	124.45
9	b	101	BCB	O2A-C1-C2	2.56	115.37	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	i	101	BCB	CMD-C2D-C3D	-2.56	121.73	127.61
9	P	101	BCB	CHD-C4C-NC	2.55	128.22	124.20
9	n	101	BCB	CHB-C1B-NB	-2.55	121.56	124.26
9	Q	101	BCB	O2A-CGA-CBA	2.55	119.91	111.91
9	i	101	BCB	O1D-CGD-CBD	-2.55	119.27	124.48
15	M	410	MQ9	C51-C49-C50	2.55	120.23	114.60
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
9	u	101	BCB	C3D-C2D-C1D	-2.54	102.37	105.83
9	M	406	BCB	CHD-C4C-C3C	-2.54	122.72	125.89
9	1	101	BCB	OBD-CAD-C3D	-2.54	122.42	128.52
17	x	102	NS0	CD1-CG-CD2	-2.54	109.00	114.60
9	M	407	BCB	C11-C12-C13	-2.53	107.73	115.92
9	n	101	BCB	CBC-CAC-C3C	-2.53	119.31	126.72
9	K	101	BCB	CHB-C1B-NB	-2.53	121.58	124.26
9	k	101	BCB	CHB-C4A-NA	2.53	128.00	124.51
17	l	102	NS0	C18-C17-C19	-2.53	119.39	122.92
9	l	101	BCB	OBD-CAD-C3D	-2.53	122.44	128.52
11	L	304	UQ9	C20-C19-C21	2.52	119.52	115.27
9	S	101	BCB	CHB-C4A-NA	2.52	128.00	124.51
8	C	401	HEC	CHA-C1A-NA	2.52	127.17	124.44
9	N	101	BCB	CHD-C1D-ND	-2.52	122.14	124.45
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
9	M	407	BCB	OBD-CAD-C3D	-2.52	122.47	128.52
8	C	401	HEC	C3B-C4B-NB	-2.52	107.37	110.17
17	u	102	NS0	CD1-CG-CD2	-2.51	109.06	114.60
9	b	101	BCB	OBD-CAD-C3D	-2.51	122.48	128.52
9	4	101	BCB	C1D-CHD-C4C	-2.51	120.65	126.06
9	e	101	BCB	CHD-C4C-NC	2.50	128.15	124.20
8	C	403	HEC	CHD-C1D-C2D	-2.50	119.78	126.73
9	Z	101	BCB	C1D-CHD-C4C	-2.50	120.67	126.06
17	o	102	NS0	C26-C25-C23	-2.50	119.40	126.42
9	r	101	BCB	C1D-CHD-C4C	-2.50	120.67	126.06
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
9	x	101	BCB	CHD-C4C-C3C	-2.49	122.77	125.89
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	L	302	BCB	CHD-C4C-NC	2.49	128.12	124.20
9	e	101	BCB	C4D-CHA-C1A	-2.49	118.22	121.25
9	q	101	BCB	CAA-C2A-C3A	-2.48	105.97	112.78
9	l	101	BCB	C3D-C4D-ND	2.48	114.25	110.24
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
9	L	301	BCB	C2D-C1D-ND	-2.48	108.28	110.10
11	L	304	UQ9	C30-C29-C31	2.48	119.44	115.27
9	t	101	BCB	CHD-C4C-C3C	-2.47	122.80	125.89
9	t	101	BCB	CHC-C1C-NC	-2.47	121.09	124.51
17	4	102	NS0	CD1-CG-CD2	-2.47	109.14	114.60
9	Z	101	BCB	CHD-C4C-C3C	-2.47	122.80	125.89
8	C	404	HEC	CMB-C2B-C1B	2.47	128.80	125.04
11	6	101	UQ9	C20-C19-C21	2.47	119.42	115.27
8	C	404	HEC	CHD-C1D-C2D	-2.47	119.88	126.73
9	Q	101	BCB	C3D-C2D-C1D	-2.46	102.47	105.83
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
9	P	101	BCB	C4A-NA-C1A	-2.46	105.60	106.71
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	L	301	BCB	O1D-CGD-CBD	-2.46	119.46	124.48
9	F	101	BCB	C1D-CHD-C4C	-2.45	120.76	126.06
9	Y	101	BCB	CHD-C4C-NC	2.45	128.07	124.20
10	M	408	BPB	C3B-C4B-NB	2.45	111.70	108.04
9	c	101	BCB	O2A-CGA-O1A	-2.45	117.42	123.59
9	i	101	BCB	CHB-C4A-NA	2.44	127.89	124.51
9	Q	101	BCB	C3D-C4D-ND	2.44	114.19	110.24
9	f	101	BCB	C4-C3-C5	2.44	119.38	115.27
9	l	101	BCB	C3D-C2D-C1D	-2.44	102.50	105.83
17	i	102	NS0	C37-C36-C35	-2.44	106.73	113.36
9	G	101	BCB	C1D-CHD-C4C	-2.44	120.80	126.06
9	z	101	BCB	C4D-C3D-CAD	-2.44	105.22	108.10
9	Z	101	BCB	CHD-C1D-ND	-2.43	122.22	124.45
17	f	102	NS0	C13-C12-C14	-2.43	119.51	122.92
9	W	101	BCB	CHB-C4A-NA	2.43	127.87	124.51
9	L	301	BCB	CHB-C1B-NB	-2.43	121.69	124.26
17	r	102	NS0	C24-C23-C25	2.43	121.90	118.08
17	Q	102	NS0	CD1-CG-CD2	-2.42	109.25	114.60
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	T	101	BCB	C4A-NA-C1A	-2.42	105.62	106.71
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	W	101	BCB	C1D-CHD-C4C	-2.41	120.85	126.06
9	z	101	BCB	C5-C3-C2	-2.41	116.24	121.12
9	c	101	BCB	C3D-C2D-C1D	-2.41	102.54	105.83
9	k	101	BCB	C4D-CHA-C1A	-2.41	118.32	121.25
9	L	301	BCB	CHD-C4C-NC	2.41	128.00	124.20
17	l	102	NS0	CD1-CG-CD2	-2.41	109.29	114.60
9	M	407	BCB	C1D-CHD-C4C	-2.41	120.87	126.06
9	Z	101	BCB	CHC-C1C-NC	-2.41	121.19	124.51
9	z	101	BCB	OBD-CAD-C3D	-2.40	122.74	128.52
9	3	101	BCB	CHC-C1C-NC	-2.40	121.19	124.51
9	q	101	BCB	C6-C5-C3	2.39	119.73	113.45
9	K	101	BCB	CBA-CAA-C2A	-2.39	106.80	113.86
9	n	101	BCB	CHC-C1C-NC	-2.39	121.20	124.51
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
9	u	101	BCB	OBB-CAB-C3B	-2.39	115.98	120.41
9	Q	101	BCB	OBB-CAB-C3B	-2.39	115.99	120.41
9	W	101	BCB	CHB-C1B-NB	-2.39	121.73	124.26
9	L	301	BCB	C4D-CHA-C1A	-2.39	118.34	121.25
16	M	411	NS5	C32-C31-C33	2.39	119.28	115.27
9	i	101	BCB	C3D-C2D-C1D	-2.39	102.58	105.83
9	e	101	BCB	O2A-C1-C2	2.38	114.89	108.64
9	t	101	BCB	CHB-C4A-NA	2.38	127.80	124.51
10	M	408	BPB	O2A-CGA-O1A	-2.38	117.59	123.59
9	4	101	BCB	CHD-C1D-ND	-2.38	122.27	124.45
9	S	101	BCB	CHC-C1C-NC	-2.38	121.23	124.51
8	C	403	HEC	CHA-C1A-NA	2.37	127.01	124.44
9	f	101	BCB	C4A-NA-C1A	-2.37	105.64	106.71
9	F	101	BCB	CHB-C4A-NA	2.37	127.79	124.51
11	6	101	UQ9	C45-C44-C46	2.37	119.26	115.27
9	4	101	BCB	CHB-C1B-NB	-2.37	121.75	124.26
10	M	408	BPB	CBB-CAB-C3B	-2.37	113.31	120.34
9	S	101	BCB	CHC-C4B-NB	2.37	126.76	124.26
17	7	102	NS0	C14-C15-C16	-2.37	115.83	123.22
9	z	101	BCB	CHC-C4B-NB	-2.37	121.75	124.26
17	1	102	NS0	CD1-CG-CD2	-2.37	109.38	114.60
9	V	101	BCB	CHC-C1C-NC	-2.36	121.25	124.51
9	Z	101	BCB	OBB-CAB-C3B	-2.36	116.04	120.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	F	101	BCB	CHC-C4B-C3B	-2.35	123.97	132.35
9	S	101	BCB	C4D-C3D-CAD	-2.35	105.32	108.10
8	C	402	HEC	CHB-C1B-NB	2.35	126.97	124.42
9	7	101	BCB	O2A-C1-C2	2.34	114.78	108.64
8	C	401	HEC	CHD-C1D-C2D	-2.34	120.23	126.73
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
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
8	C	402	HEC	C4A-NA-C1A	2.33	107.63	105.35
9	M	407	BCB	C4-C3-C5	2.33	119.19	115.27
10	M	408	BPB	OBD-CAD-CBD	-2.33	122.41	125.82
9	c	101	BCB	C1D-CHD-C4C	-2.33	121.03	126.06
8	C	404	HEC	CAB-C3B-C4B	2.32	127.83	124.81
9	7	101	BCB	O2A-CGA-CBA	2.32	119.19	111.91
17	l	102	NS0	C26-C25-C23	-2.32	119.89	126.42
9	o	101	BCB	C2D-C1D-ND	-2.32	108.39	110.10
8	C	403	HEC	C1A-CHA-C4D	-2.32	121.06	126.06
17	W	102	NS0	C18-C17-C19	-2.32	119.68	122.92
9	M	407	BCB	C6-C5-C3	-2.32	107.38	113.45
15	M	410	MQ9	C42-C43-C44	2.31	133.23	127.66
9	t	101	BCB	C1D-ND-C4D	2.31	107.97	106.33
9	i	101	BCB	OBD-CAD-C3D	-2.31	122.97	128.52
9	b	101	BCB	C1-O2A-CGA	2.31	122.50	116.44
9	M	407	BCB	CHD-C4C-C3C	-2.30	123.01	125.89
9	4	101	BCB	O2A-CGA-CBA	2.30	119.13	111.91
9	b	101	BCB	CAA-C2A-C1A	-2.30	104.44	111.97
9	M	407	BCB	C1-O2A-CGA	2.30	122.48	116.44
17	i	102	NS0	CD1-CG-CD2	-2.30	109.52	114.60
8	C	404	HEC	CHA-C4D-ND	2.30	126.92	124.42
8	C	402	HEC	C1A-CHA-C4D	-2.30	121.10	126.06
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
9	b	101	BCB	C4D-CHA-C1A	-2.30	118.46	121.25
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
9	Q	101	BCB	O1D-CGD-CBD	-2.29	119.80	124.48
17	Q	102	NS0	C24-C23-C25	2.29	121.69	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	o	102	NS0	C36-C35-C33	-2.29	107.46	113.45
9	L	302	BCB	C2A-C1A-CHA	-2.28	119.86	123.86
9	P	101	BCB	C5-C3-C2	-2.28	116.50	121.12
9	G	101	BCB	O1D-CGD-CBD	-2.28	119.81	124.48
9	L	301	BCB	C1-C2-C3	-2.28	122.10	126.04
9	K	101	BCB	C2B-C1B-NB	-2.28	108.70	110.23
17	W	102	NS0	C36-C35-C33	-2.28	107.49	113.45
9	k	101	BCB	C4D-C3D-CAD	-2.28	105.41	108.10
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
9	7	101	BCB	CAA-C2A-C3A	2.27	118.99	112.78
17	1	102	NS0	C37-C36-C35	-2.27	107.20	113.36
9	W	101	BCB	O1D-CGD-CBD	-2.27	119.84	124.48
9	T	101	BCB	C3D-C2D-C1D	-2.27	102.74	105.83
9	L	301	BCB	C2A-C1A-CHA	-2.27	119.90	123.86
9	K	101	BCB	C4D-CHA-C1A	-2.26	118.49	121.25
9	l	101	BCB	CMD-C2D-C3D	-2.26	122.41	127.61
8	C	402	HEC	O2A-CGA-O1A	-2.26	117.66	123.30
9	Y	101	BCB	CHB-C4A-NA	2.26	127.64	124.51
9	S	101	BCB	CHB-C1B-NB	-2.26	121.86	124.26
9	Q	101	BCB	O2A-CGA-O1A	-2.26	117.89	123.59
9	S	101	BCB	CMA-C3A-C2A	-2.26	104.72	113.83
9	V	101	BCB	C4D-C3D-CAD	-2.26	105.44	108.10
9	o	101	BCB	CHD-C1D-ND	-2.26	122.38	124.45
9	w	101	BCB	OBD-CAD-C3D	-2.25	123.10	128.52
9	6	102	BCB	CHC-C4B-C3B	-2.25	124.34	132.35
10	M	408	BPB	OBB-CAB-CBB	2.25	125.23	120.17
9	Q	101	BCB	C4A-NA-C1A	-2.25	105.69	106.71
15	M	410	MQ9	C47-C46-C44	2.25	120.37	112.98
9	N	101	BCB	O2A-CGA-O1A	-2.25	117.92	123.59
9	6	102	BCB	CHC-C4B-NB	2.25	126.64	124.26
9	h	101	BCB	CHD-C4C-NC	2.25	127.74	124.20
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	f	101	BCB	C1D-CHD-C4C	-2.24	121.22	126.06
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
8	C	401	HEC	C1A-CHA-C4D	-2.24	121.23	126.06
9	t	101	BCB	C4D-C3D-CAD	-2.24	105.46	108.10
17	r	102	NS0	CD1-CG-CD2	-2.24	109.67	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	V	101	BCB	OBD-CAD-C3D	-2.23	123.15	128.52
9	r	101	BCB	CMD-C2D-C3D	-2.23	122.48	127.61
9	r	101	BCB	C6-C5-C3	-2.23	107.61	113.45
10	M	408	BPB	CMA-C3A-C2A	-2.23	105.01	113.99
9	z	101	BCB	C4D-CHA-C1A	-2.23	118.54	121.25
8	C	402	HEC	C3B-C4B-NB	-2.22	107.69	110.17
9	F	101	BCB	CMD-C2D-C3D	-2.22	122.50	127.61
9	r	101	BCB	OBB-CAB-C3B	-2.22	116.29	120.41
9	6	102	BCB	CHB-C1B-NB	-2.22	121.91	124.26
9	3	101	BCB	CHD-C4C-NC	2.22	127.70	124.20
8	C	401	HEC	O2D-CGD-CBD	2.22	121.15	114.03
9	h	101	BCB	CHC-C1C-NC	-2.22	121.45	124.51
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
9	V	101	BCB	CHD-C4C-NC	2.21	127.69	124.20
9	r	101	BCB	C3D-C2D-C1D	-2.21	102.81	105.83
8	C	404	HEC	CAD-C3D-C2D	-2.21	123.76	127.88
9	S	101	BCB	CBC-CAC-C3C	-2.21	120.26	126.72
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
17	x	102	NS0	C26-C25-C23	-2.20	120.22	126.42
9	h	101	BCB	C4D-C3D-CAD	-2.20	105.50	108.10
9	N	101	BCB	CHD-C4C-C3C	-2.20	123.14	125.89
16	M	411	NS5	C14-C15-C17	-2.20	115.57	118.94
8	C	404	HEC	CHA-C1A-NA	2.20	126.81	124.44
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	q	101	BCB	CHD-C4C-NC	2.19	127.66	124.20
9	P	101	BCB	C3D-C4D-ND	2.19	113.78	110.24
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	e	101	BCB	C1-C2-C3	2.17	129.79	126.04
9	M	406	BCB	O1D-CGD-CBD	-2.17	120.05	124.48
9	o	101	BCB	CAB-C3B-C2B	-2.17	125.09	128.34
17	f	102	NS0	C37-C36-C35	-2.17	107.48	113.36
9	u	101	BCB	CHB-C4A-NA	2.17	127.51	124.51
9	K	101	BCB	CAA-C2A-C3A	-2.17	106.85	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	6	102	BCB	OBD-CAD-C3D	-2.16	123.32	128.52
9	4	101	BCB	O2A-CGA-O1A	-2.16	118.14	123.59
9	t	101	BCB	CBC-CAC-C3C	-2.16	120.41	126.72
17	G	102	NS0	C13-C12-C14	-2.16	119.90	122.92
9	G	101	BCB	CBA-CAA-C2A	-2.16	107.50	113.86
9	n	101	BCB	OBD-CAD-C3D	-2.15	123.33	128.52
9	o	101	BCB	O1D-CGD-CBD	-2.15	120.08	124.48
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	W	101	BCB	CMB-C2B-C3B	2.15	131.73	125.93
9	h	101	BCB	CAA-C2A-C3A	-2.15	106.90	112.78
8	C	402	HEC	CHA-C4D-C3D	-2.14	121.69	124.84
9	b	101	BCB	CAA-CBA-CGA	-2.14	107.00	113.25
9	q	101	BCB	OBD-CAD-C3D	-2.14	123.38	128.52
9	b	101	BCB	O1D-CGD-CBD	-2.14	120.11	124.48
9	M	407	BCB	C4D-CHA-C1A	-2.14	118.65	121.25
9	1	101	BCB	CHB-C4A-NA	2.14	127.47	124.51
9	6	102	BCB	CMD-C2D-C3D	-2.13	122.71	127.61
8	C	403	HEC	C4C-CHD-C1D	-2.13	121.28	126.34
9	N	101	BCB	C3D-C4D-ND	2.13	113.69	110.24
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	Y	101	BCB	CMA-C3A-C2A	-2.13	105.25	113.83
17	c	102	NS0	C26-C25-C23	-2.13	120.44	126.42
9	1	101	BCB	CMA-C3A-C2A	-2.13	105.25	113.83
9	P	101	BCB	CBC-CAC-C3C	-2.13	120.50	126.72
17	Z	102	NS0	C37-C36-C35	-2.13	107.58	113.36
9	Y	101	BCB	CAA-C2A-C1A	-2.13	105.01	111.97
17	Q	102	NS0	C25-C23-C22	-2.13	115.68	118.94
9	G	101	BCB	C3D-C2D-C1D	-2.12	102.93	105.83
9	L	301	BCB	C4A-NA-C1A	-2.12	105.75	106.71
8	C	401	HEC	C4A-NA-C1A	2.12	107.43	105.35
17	i	102	NS0	C40-C38-C39	2.12	120.30	110.51
9	i	101	BCB	C1D-CHD-C4C	-2.12	121.48	126.06
9	M	406	BCB	CMA-C3A-C4A	-2.12	106.08	111.77
9	T	101	BCB	CHB-C1B-NB	-2.12	122.01	124.26
9	x	101	BCB	O1D-CGD-CBD	-2.12	120.15	124.48
9	K	101	BCB	C4D-C3D-CAD	-2.12	105.60	108.10
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	M	410	MQ9	C25-C24-C26	2.12	118.83	115.27
9	t	101	BCB	C4-C3-C5	2.11	118.83	115.27
9	e	101	BCB	CBC-CAC-C3C	-2.11	120.54	126.72
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	w	101	BCB	CHC-C1C-NC	-2.11	121.60	124.51
17	T	102	NS0	C40-C38-C39	2.11	120.22	110.51
9	7	101	BCB	CHC-C4B-NB	-2.11	122.03	124.26
17	f	102	NS0	C18-C17-C19	-2.11	119.97	122.92
9	M	407	BCB	O2A-C1-C2	2.10	114.17	108.64
9	o	101	BCB	OBD-CAD-C3D	-2.10	123.45	128.52
9	G	101	BCB	O2A-CGA-O1A	-2.10	118.28	123.59
9	7	101	BCB	C3D-C4D-ND	2.10	113.64	110.24
9	r	101	BCB	CMB-C2B-C3B	2.10	131.61	125.93
17	Z	102	NS0	C40-C38-C39	2.10	120.20	110.51
9	n	101	BCB	CHB-C4A-NA	2.10	127.42	124.51
9	P	101	BCB	O2A-CGA-O1A	-2.10	118.29	123.59
9	V	101	BCB	CHB-C4A-NA	2.10	127.42	124.51
17	Q	102	NS0	C13-C12-C14	-2.10	119.98	122.92
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
9	6	102	BCB	C1D-CHD-C4C	-2.09	121.54	126.06
9	V	101	BCB	CHD-C4C-C3C	-2.09	123.27	125.89
17	1	102	NS0	C40-C38-C39	2.09	120.16	110.51
9	b	101	BCB	CBC-CAC-C3C	-2.09	120.60	126.72
9	L	302	BCB	CHC-C4B-NB	-2.09	122.04	124.26
9	N	101	BCB	O2D-CGD-O1D	-2.09	119.75	123.84
9	k	101	BCB	CHB-C1B-NB	-2.09	122.05	124.26
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	410	MQ9	C40-C39-C41	2.08	118.78	115.27
9	4	101	BCB	O2D-CGD-O1D	-2.08	119.77	123.84
9	7	101	BCB	C2B-C1B-NB	2.08	111.63	110.23
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	t	101	BCB	CHD-C4C-NC	2.06	127.45	124.20
9	K	101	BCB	O2A-CGA-CBA	2.06	118.38	111.91
16	M	411	NS5	C24-C25-C26	-2.06	124.37	127.31
15	M	410	MQ9	C26-C24-C23	2.06	125.28	121.12
9	N	101	BCB	C1D-CHD-C4C	-2.06	121.62	126.06
10	L	303	BPB	O2A-CGA-CBA	2.06	118.36	111.91
9	P	101	BCB	CMD-C2D-C3D	-2.05	122.89	127.61
9	M	407	BCB	CHD-C1D-ND	-2.05	122.57	124.45
17	Q	102	NS0	C40-C38-C39	2.05	119.95	110.51
9	7	101	BCB	C3D-C2D-C1D	-2.05	103.04	105.83
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
8	C	402	HEC	CHA-C1A-NA	2.04	126.64	124.44
9	f	101	BCB	O2A-CGA-O1A	-2.04	118.45	123.59
9	q	101	BCB	CHB-C4A-NA	2.04	127.33	124.51
17	i	102	NS0	C25-C23-C22	-2.04	115.82	118.94
9	S	101	BCB	CBA-CAA-C2A	-2.04	107.86	113.86
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
17	7	102	NS0	C37-C36-C35	-2.03	107.84	113.36
15	M	410	MQ9	O4-C4-C3	-2.03	118.28	121.56
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	M	407	BCB	CHC-C1C-NC	-2.03	121.71	124.51
9	o	101	BCB	C4B-C3B-C2B	2.02	111.62	108.36
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	410	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	HEC	CAD-CBD-CGD	-2.01	109.28	113.60
8	C	401	HEC	CMD-C2D-C1D	2.01	128.10	125.04
9	l	101	BCB	CHD-C4C-NC	2.01	127.37	124.20
9	S	101	BCB	C5-C3-C2	-2.01	117.06	121.12
9	4	101	BCB	CHB-C4A-NA	2.01	127.29	124.51
9	q	101	BCB	CMA-C3A-C2A	-2.01	105.74	113.83
15	M	410	MQ9	O1-C1-C2	-2.00	118.32	121.56
17	Q	102	NS0	C26-C25-C23	-2.00	120.79	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	N	101	BCB	C1-O2A-CGA	2.00	121.70	116.44
9	k	101	BCB	O1D-CGD-CBD	-2.00	120.39	124.48

All (83) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	C	401	HEC	NA
8	C	402	HEC	NA
8	C	403	HEC	NA
8	C	404	HEC	NA
9	L	301	BCB	NC
9	L	301	BCB	NA
9	L	301	BCB	ND
9	L	302	BCB	NC
9	L	302	BCB	NA
9	M	406	BCB	NC
9	M	406	BCB	NA
9	M	407	BCB	NC
9	M	407	BCB	NA
9	z	101	BCB	NC
9	z	101	BCB	NA
9	1	101	BCB	NC
9	1	101	BCB	NA
9	F	101	BCB	NC
9	F	101	BCB	NA
9	K	101	BCB	NC
9	K	101	BCB	NA
9	P	101	BCB	NC
9	P	101	BCB	NA
9	S	101	BCB	NC
9	S	101	BCB	NA
9	V	101	BCB	NC
9	V	101	BCB	NA
9	Y	101	BCB	NC
9	Y	101	BCB	NA
9	b	101	BCB	NC
9	b	101	BCB	NA
9	e	101	BCB	NC
9	e	101	BCB	NA
9	h	101	BCB	NC
9	h	101	BCB	NA
9	k	101	BCB	NC

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Mol	Chain	Res	Type	Atom
9	k	101	BCB	NA
9	n	101	BCB	NC
9	n	101	BCB	NA
9	q	101	BCB	NC
9	q	101	BCB	NA
9	t	101	BCB	NC
9	t	101	BCB	NA
9	w	101	BCB	NC
9	w	101	BCB	NA
9	3	101	BCB	NC
9	3	101	BCB	NA
9	6	102	BCB	NC
9	6	102	BCB	NA
9	G	101	BCB	NC
9	G	101	BCB	NA
9	N	101	BCB	NC
9	N	101	BCB	NA
9	Q	101	BCB	NC
9	Q	101	BCB	NA
9	T	101	BCB	NC
9	T	101	BCB	NA
9	W	101	BCB	NC
9	W	101	BCB	NA
9	Z	101	BCB	NC
9	Z	101	BCB	NA
9	c	101	BCB	NC
9	c	101	BCB	NA
9	f	101	BCB	NC
9	f	101	BCB	NA
9	i	101	BCB	NC
9	i	101	BCB	NA
9	l	101	BCB	NC
9	l	101	BCB	NA
9	o	101	BCB	NC
9	o	101	BCB	NA
9	r	101	BCB	NC
9	r	101	BCB	NA
9	u	101	BCB	NC
9	u	101	BCB	NA
9	x	101	BCB	NC
9	x	101	BCB	NA
9	4	101	BCB	NC

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Mol	Chain	Res	Type	Atom
9	4	101	BCB	NA
9	7	101	BCB	NC
9	7	101	BCB	NA
10	L	303	BPB	C13
10	M	408	BPB	C13

All (1118) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	401	HEC	C2C-C3C-CAC-CBC
8	C	402	HEC	C2C-C3C-CAC-CBC
9	M	407	BCB	CHA-CBD-CGD-O1D
9	M	407	BCB	CHA-CBD-CGD-O2D
9	M	407	BCB	CAD-CBD-CGD-O1D
9	M	407	BCB	CAD-CBD-CGD-O2D
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	C1A-C2A-CAA-CBA
9	F	101	BCB	C3A-C2A-CAA-CBA
9	F	101	BCB	O2A-C1-C2-C3
9	K	101	BCB	C1A-C2A-CAA-CBA
9	K	101	BCB	C3A-C2A-CAA-CBA
9	P	101	BCB	C1A-C2A-CAA-CBA
9	P	101	BCB	C3A-C2A-CAA-CBA
9	P	101	BCB	O1A-CGA-O2A-C1
9	P	101	BCB	CHA-CBD-CGD-O2D
9	P	101	BCB	CBD-CGD-O2D-CED
9	P	101	BCB	O2A-C1-C2-C3
9	S	101	BCB	C1A-C2A-CAA-CBA
9	S	101	BCB	C3A-C2A-CAA-CBA
9	V	101	BCB	O2A-C1-C2-C3
9	V	101	BCB	C2-C3-C5-C6
9	V	101	BCB	C4-C3-C5-C6
9	Y	101	BCB	C1A-C2A-CAA-CBA
9	Y	101	BCB	C3A-C2A-CAA-CBA
9	Y	101	BCB	O2A-C1-C2-C3
9	b	101	BCB	C1A-C2A-CAA-CBA
9	b	101	BCB	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
9	b	101	BCB	O2A-C1-C2-C3
9	e	101	BCB	C1A-C2A-CAA-CBA
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	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	q	101	BCB	C4-C3-C5-C6
9	t	101	BCB	O2A-C1-C2-C3
9	w	101	BCB	O2A-C1-C2-C3
9	3	101	BCB	C1A-C2A-CAA-CBA
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	CBD-CGD-O2D-CED
9	6	102	BCB	O2A-C1-C2-C3
9	G	101	BCB	CHA-CBD-CGD-O1D
9	G	101	BCB	CHA-CBD-CGD-O2D
9	N	101	BCB	CBA-CGA-O2A-C1
9	N	101	BCB	O1A-CGA-O2A-C1
9	N	101	BCB	CHA-CBD-CGD-O1D
9	N	101	BCB	CHA-CBD-CGD-O2D
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	T	101	BCB	CHA-CBD-CGD-O1D
9	T	101	BCB	CHA-CBD-CGD-O2D
9	W	101	BCB	CHA-CBD-CGD-O1D
9	f	101	BCB	CBA-CGA-O2A-C1
9	f	101	BCB	O1A-CGA-O2A-C1
9	f	101	BCB	CHA-CBD-CGD-O1D
9	i	101	BCB	CBA-CGA-O2A-C1
9	i	101	BCB	O1A-CGA-O2A-C1
9	i	101	BCB	CHA-CBD-CGD-O1D
9	l	101	BCB	C1A-C2A-CAA-CBA
9	l	101	BCB	CHA-CBD-CGD-O1D
9	l	101	BCB	CHA-CBD-CGD-O2D
9	o	101	BCB	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
9	o	101	BCB	CHA-CBD-CGD-O2D
9	r	101	BCB	CHA-CBD-CGD-O1D
9	r	101	BCB	CHA-CBD-CGD-O2D
9	u	101	BCB	CBA-CGA-O2A-C1
9	u	101	BCB	O1A-CGA-O2A-C1
9	u	101	BCB	CHA-CBD-CGD-O1D
9	x	101	BCB	CBA-CGA-O2A-C1
9	x	101	BCB	O1A-CGA-O2A-C1
9	x	101	BCB	CHA-CBD-CGD-O1D
9	x	101	BCB	CHA-CBD-CGD-O2D
9	4	101	BCB	C1A-C2A-CAA-CBA
9	4	101	BCB	C3A-C2A-CAA-CBA
9	4	101	BCB	CHA-CBD-CGD-O1D
9	4	101	BCB	CHA-CBD-CGD-O2D
9	4	101	BCB	C11-C10-C8-C9
10	L	303	BPB	O2A-C1-C2-C3
10	L	303	BPB	CBD-CGD-O2D-CED
10	L	303	BPB	C2C-C3C-CAC-CBC
10	M	408	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	409	LDA	N1-C1-C2-C3
14	H	301	LDA	C2-C1-N1-CM1
14	H	301	LDA	C2-C1-N1-CM2
15	M	410	MQ9	C9-C11-C12-C13
15	M	410	MQ9	C18-C19-C21-C22
15	M	410	MQ9	C20-C19-C21-C22
15	M	410	MQ9	C40-C39-C41-C42

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Mol	Chain	Res	Type	Atoms
15	M	410	MQ9	C43-C44-C46-C47
15	M	410	MQ9	C45-C44-C46-C47
15	M	410	MQ9	C44-C46-C47-C48
16	M	411	NS5	C7-C8-C9-C10
16	M	411	NS5	C13-C14-C15-C16
16	M	411	NS5	C13-C14-C15-C17
16	M	411	NS5	C25-C26-C28-C29
16	M	411	NS5	C27-C26-C28-C29
16	M	411	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
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

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Mol	Chain	Res	Type	Atoms
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
8	C	401	HEC	C4B-C3B-CAB-CBB
9	6	102	BCB	O1D-CGD-O2D-CED
8	C	401	HEC	C2B-C3B-CAB-CBB
9	7	101	BCB	O1D-CGD-O2D-CED
9	M	406	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
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	408	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
8	C	401	HEC	C4C-C3C-CAC-CBC
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

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Mol	Chain	Res	Type	Atoms
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
8	C	402	HEC	C4C-C3C-CAC-CBC
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
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	410	MQ9	C38-C39-C41-C42
9	M	407	BCB	C2A-CAA-CBA-CGA
9	c	101	BCB	C2A-CAA-CBA-CGA
8	C	403	HEC	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
8	C	404	HEC	C2C-C3C-CAC-CBC
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
8	C	402	HEC	C2B-C3B-CAB-CBB
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
9	M	406	BCB	C3-C5-C6-C7
9	P	101	BCB	C3-C5-C6-C7
9	o	101	BCB	C3-C5-C6-C7
16	M	411	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
8	C	404	HEC	C4C-C3C-CAC-CBC
17	1	102	NS0	CA-CB-CG-CD2
17	r	102	NS0	CA-CB-CG-CD1

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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	406	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	410	MQ9	C24-C26-C27-C28
15	M	410	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	408	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
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
8	C	403	HEC	C2B-C3B-CAB-CBB
9	M	407	BCB	C15-C16-C17-C18
9	K	101	BCB	C13-C15-C16-C17
9	M	407	BCB	C11-C10-C8-C9
9	M	407	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

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Mol	Chain	Res	Type	Atoms
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
8	C	403	HEC	C4C-C3C-CAC-CBC
17	f	102	NS0	C10-C11-C12-C14
9	M	406	BCB	C15-C16-C17-C18
9	z	101	BCB	C13-C15-C16-C17
9	Q	101	BCB	C5-C6-C7-C8
10	M	408	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
10	M	408	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

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Mol	Chain	Res	Type	Atoms
9	4	101	BCB	C5-C6-C7-C8
17	r	102	NS0	C35-C36-C37-C38
9	M	406	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	HEC	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
8	C	402	HEC	C4B-C3B-CAB-CBB
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
9	u	101	BCB	C10-C11-C12-C13
9	t	101	BCB	O1A-CGA-O2A-C1
9	M	407	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	408	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

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Mol	Chain	Res	Type	Atoms
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	411	NS5	C1-C2-C3-C4
9	f	101	BCB	O1D-CGD-O2D-CED
11	6	101	UQ9	C45-C44-C46-C47
16	M	411	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
9	k	101	BCB	C16-C17-C18-C19
9	M	406	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

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Mol	Chain	Res	Type	Atoms
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	409	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	408	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
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

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Mol	Chain	Res	Type	Atoms
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
9	M	406	BCB	O1A-CGA-O2A-C1
9	M	406	BCB	C16-C17-C18-C19
9	o	101	BCB	C16-C17-C18-C20
10	M	408	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	409	LDA	C3-C4-C5-C6
9	h	101	BCB	C15-C16-C17-C18
9	6	102	BCB	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
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	410	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
10	L	303	BPB	C11-C12-C13-C15
15	M	410	MQ9	C12-C11-C9-C8
14	M	409	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
8	C	404	HEC	C2B-C3B-CAB-CBB
9	7	101	BCB	C8-C10-C11-C12
9	L	302	BCB	CBD-CGD-O2D-CED
9	f	101	BCB	C16-C17-C18-C20
9	W	101	BCB	C15-C16-C17-C18
9	n	101	BCB	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
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	411	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
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	z	101	BCB	C1A-C2A-CAA-CBA
9	1	101	BCB	C1A-C2A-CAA-CBA
9	V	101	BCB	C1A-C2A-CAA-CBA
9	n	101	BCB	C1A-C2A-CAA-CBA
9	q	101	BCB	C1A-C2A-CAA-CBA
9	t	101	BCB	C1A-C2A-CAA-CBA
9	6	102	BCB	C1A-C2A-CAA-CBA
9	Z	101	BCB	C1A-C2A-CAA-CBA
9	f	101	BCB	C1A-C2A-CAA-CBA
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

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Mol	Chain	Res	Type	Atoms
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	409	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	406	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	408	BPB	C3-C5-C6-C7
9	T	101	BCB	C8-C10-C11-C12
9	4	101	BCB	C15-C16-C17-C18
9	h	101	BCB	C10-C11-C12-C13
8	C	403	HEC	C4B-C3B-CAB-CBB
9	N	101	BCB	C4-C3-C5-C6
17	i	102	NS0	C34-C33-C35-C36
9	L	302	BCB	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
9	M	407	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
9	l	101	BCB	C11-C12-C13-C14
10	M	408	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	406	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

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Mol	Chain	Res	Type	Atoms
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	407	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	HEC	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	407	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
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	M	407	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

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Mol	Chain	Res	Type	Atoms
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
9	7	101	BCB	C11-C12-C13-C15
10	L	303	BPB	C6-C7-C8-C10
10	M	408	BPB	C11-C12-C13-C15
17	T	102	NS0	C32-C33-C35-C36
9	M	406	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
9	M	406	BCB	CAD-CBD-CGD-O2D
9	6	102	BCB	CAD-CBD-CGD-O2D
10	M	408	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	409	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	L	302	BCB	CHA-CBD-CGD-O1D
9	P	101	BCB	CHA-CBD-CGD-O1D
9	V	101	BCB	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
9	V	101	BCB	CHA-CBD-CGD-O2D
9	Y	101	BCB	CHA-CBD-CGD-O1D
9	Y	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	3	101	BCB	CHA-CBD-CGD-O2D
9	W	101	BCB	CHA-CBD-CGD-O2D
9	f	101	BCB	CHA-CBD-CGD-O2D
9	M	407	BCB	O1A-CGA-O2A-C1
14	M	409	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
9	G	101	BCB	C1A-C2A-CAA-CBA
9	T	101	BCB	C1A-C2A-CAA-CBA
9	W	101	BCB	C1A-C2A-CAA-CBA
9	L	302	BCB	C2-C1-O2A-CGA
9	Q	101	BCB	C2-C3-C5-C6
10	M	408	BPB	O1A-CGA-O2A-C1
9	u	101	BCB	C16-C17-C18-C20
9	4	101	BCB	C16-C17-C18-C19
14	M	409	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

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Mol	Chain	Res	Type	Atoms
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	408	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
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

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Mol	Chain	Res	Type	Atoms
9	n	101	BCB	CBA-CGA-O2A-C1
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	407	BCB	C16-C17-C18-C20
9	b	101	BCB	C16-C17-C18-C19
9	b	101	BCB	C3-C5-C6-C7
9	N	101	BCB	C16-C17-C18-C19
8	C	401	HEC	C2A-CAA-CBA-CGA
9	6	102	BCB	CBA-CGA-O2A-C1
8	C	401	HEC	CAA-CBA-CGA-O2A
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	HEC	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	406	BCB	C3A-C2A-CAA-CBA
8	C	404	HEC	C4B-C3B-CAB-CBB
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	HEC	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
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	w	101	BCB	C1A-C2A-CAA-CBA
9	i	101	BCB	C1A-C2A-CAA-CBA
9	r	101	BCB	C1A-C2A-CAA-CBA
9	L	301	BCB	C6-C7-C8-C10
9	M	406	BCB	C12-C13-C15-C16
9	M	407	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	HEC	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
17	W	102	NS0	CA-CB-CG-CD2
16	M	411	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	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	409	LDA	C5-C6-C7-C8
9	l	101	BCB	C4-C3-C5-C6
11	6	101	UQ9	C40-C39-C41-C42

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Mol	Chain	Res	Type	Atoms
15	M	410	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	411	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	HEC	CAA-CBA-CGA-O2A
9	k	101	BCB	CAD-CBD-CGD-O2D
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	411	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
9	L	301	BCB	CHA-CBD-CGD-O1D
9	L	302	BCB	CHA-CBD-CGD-O2D
9	1	101	BCB	CHA-CBD-CGD-O1D
9	1	101	BCB	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
9	h	101	BCB	CHA-CBD-CGD-O1D
9	h	101	BCB	CHA-CBD-CGD-O2D
9	q	101	BCB	CHA-CBD-CGD-O1D
9	q	101	BCB	CHA-CBD-CGD-O2D
9	t	101	BCB	CHA-CBD-CGD-O1D
9	Q	101	BCB	CHA-CBD-CGD-O1D
9	Q	101	BCB	CHA-CBD-CGD-O2D
9	Z	101	BCB	CHA-CBD-CGD-O1D
9	Z	101	BCB	CHA-CBD-CGD-O2D
9	i	101	BCB	CHA-CBD-CGD-O2D
9	u	101	BCB	CHA-CBD-CGD-O2D
8	C	403	HEC	CAA-CBA-CGA-O1A
17	N	102	NS0	C32-C33-C35-C36
9	P	101	BCB	C2A-CAA-CBA-CGA
8	C	403	HEC	CAD-CBD-CGD-O1D
10	M	408	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	410	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
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

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Mol	Chain	Res	Type	Atoms
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
15	M	410	MQ9	C30-C29-C31-C32
9	M	406	BCB	C1A-C2A-CAA-CBA
9	N	101	BCB	C1A-C2A-CAA-CBA
9	o	101	BCB	C1A-C2A-CAA-CBA
9	u	101	BCB	C1A-C2A-CAA-CBA
9	x	101	BCB	C1A-C2A-CAA-CBA
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	HEC	CAA-CBA-CGA-O2A
9	q	101	BCB	CAA-CBA-CGA-O1A
9	G	101	BCB	C16-C17-C18-C19
15	M	410	MQ9	C11-C12-C13-C14
8	C	403	HEC	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	HEC	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.

66 monomers are involved in 659 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	4	102	NS0	6	0
17	x	102	NS0	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	L	301	BCB	12	0
9	K	101	BCB	10	0
9	t	101	BCB	10	0
9	6	102	BCB	16	0
9	u	101	BCB	8	0
11	6	101	UQ9	39	0
17	c	102	NS0	6	0
17	i	102	NS0	14	0
9	Y	101	BCB	12	0
17	1	102	NS0	4	0
17	r	102	NS0	10	0
8	C	403	HEC	13	0
17	7	102	NS0	7	0
17	W	102	NS0	10	0
9	M	407	BCB	11	0
8	C	402	HEC	13	0
17	u	102	NS0	12	0
14	M	409	LDA	3	0
9	W	101	BCB	11	0
8	C	401	HEC	7	0
10	L	303	BPB	11	0
9	V	101	BCB	8	0
15	M	410	MQ9	4	0
9	q	101	BCB	6	0
9	o	101	BCB	16	0
10	M	408	BPB	6	0
9	e	101	BCB	18	0
9	Q	101	BCB	16	0
11	L	304	UQ9	21	0
9	F	101	BCB	9	0
9	i	101	BCB	12	0
17	T	102	NS0	11	0
9	L	302	BCB	11	0
17	o	102	NS0	7	0
17	N	102	NS0	13	0
9	h	101	BCB	10	0
17	Z	102	NS0	4	0
9	T	101	BCB	17	0
9	l	101	BCB	17	0
9	S	101	BCB	8	0
9	k	101	BCB	7	0
9	N	101	BCB	16	0

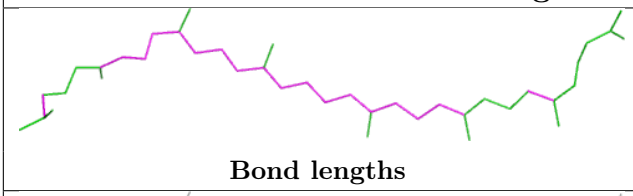
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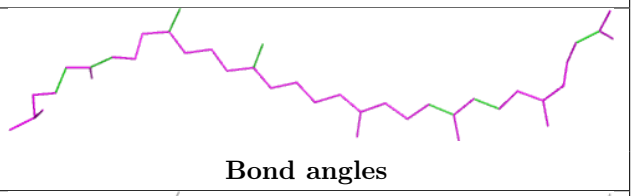
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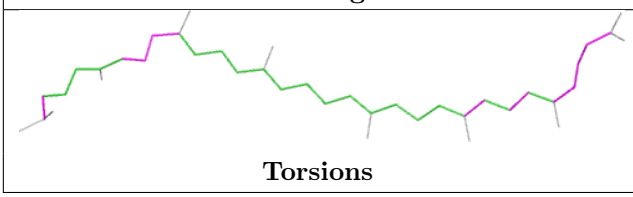
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	Q	102	NS0	10	0
9	f	101	BCB	11	0
9	Z	101	BCB	15	0
9	z	101	BCB	10	0
9	4	101	BCB	19	0
9	M	406	BCB	5	0
16	M	411	NS5	4	0
17	G	102	NS0	20	0
9	b	101	BCB	8	0
9	x	101	BCB	9	0
17	f	102	NS0	11	0
17	l	102	NS0	14	0
9	c	101	BCB	14	0
9	n	101	BCB	8	0
9	3	101	BCB	9	0
9	G	101	BCB	13	0
9	w	101	BCB	3	0
8	C	404	HEC	6	0
9	1	101	BCB	15	0
9	7	101	BCB	16	0
9	P	101	BCB	7	0
9	r	101	BCB	11	0

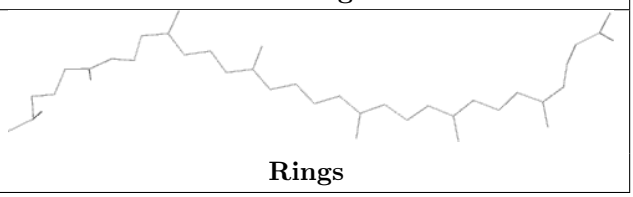
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand NS0 4 102

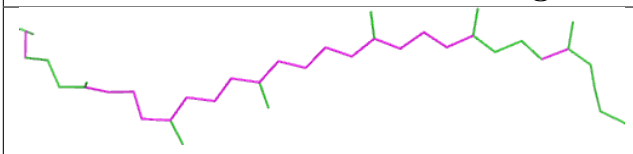

Bond lengths

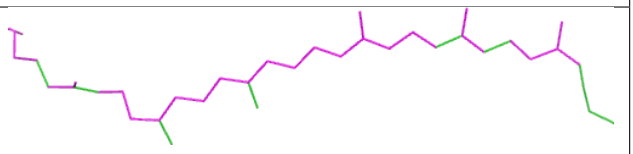

Bond angles

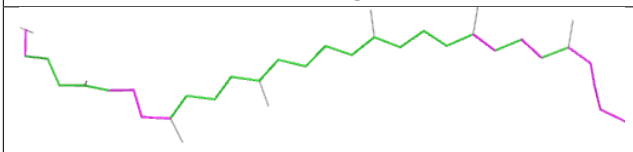

Torsions

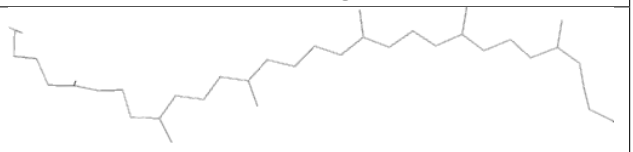

Rings

Ligand NS0 x 102

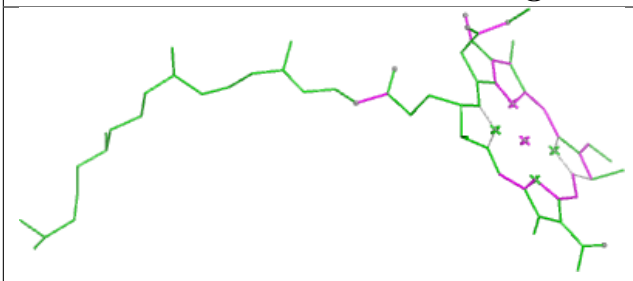

Bond lengths

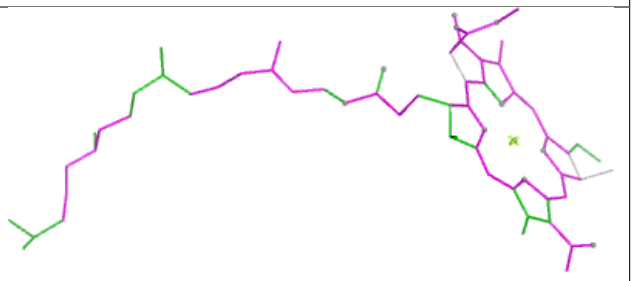

Bond angles

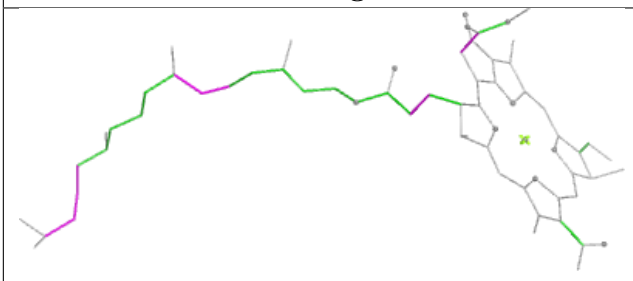

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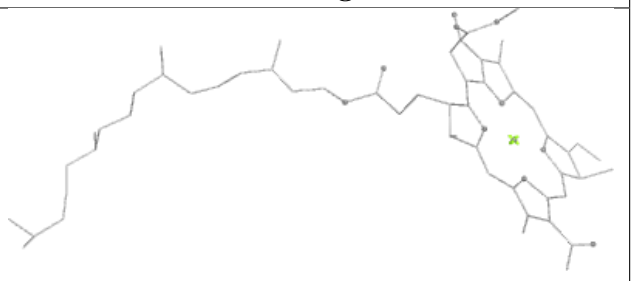

Rings

Ligand BCB L 301

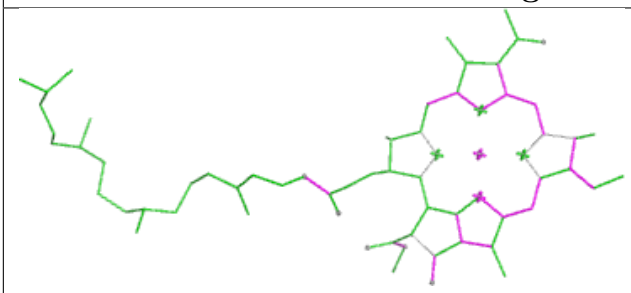

Bond lengths


Bond angles

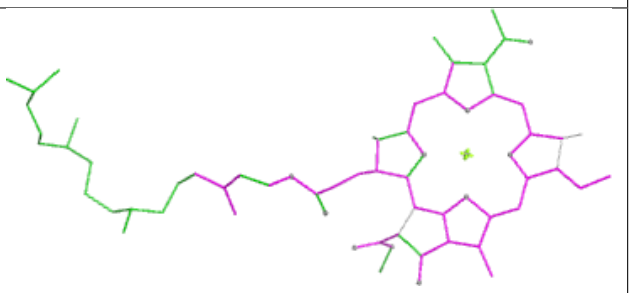

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Rings

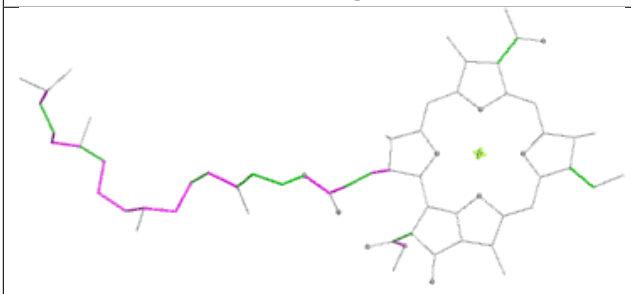
Ligand BCB K 101



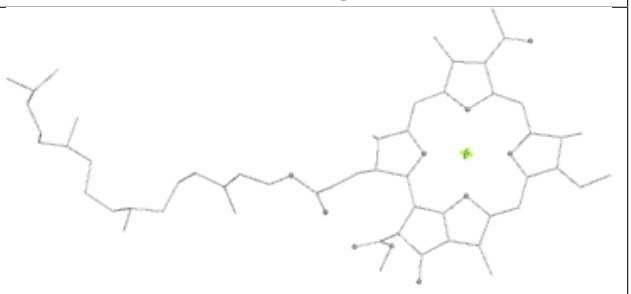
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Bond angles

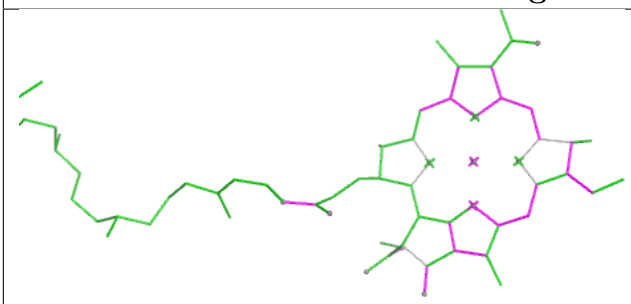


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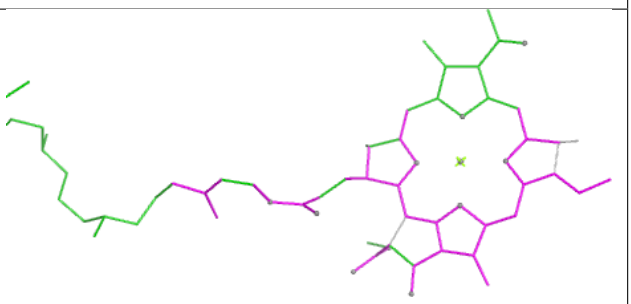


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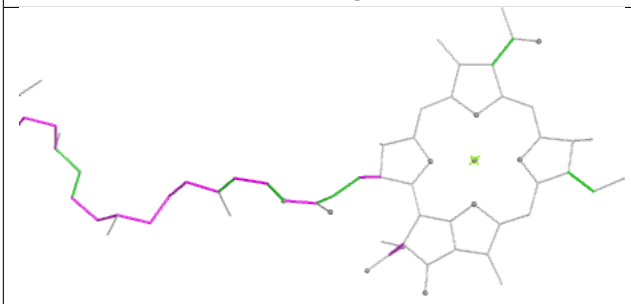
Ligand BCB t 101



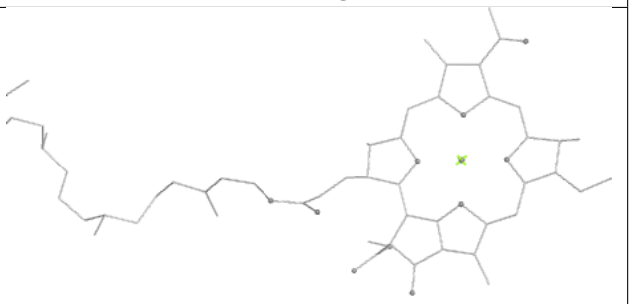
Bond lengths



Bond angles

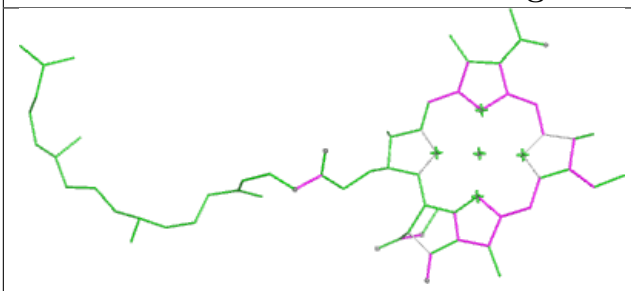


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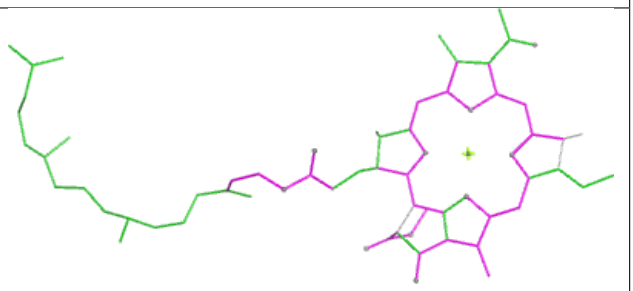


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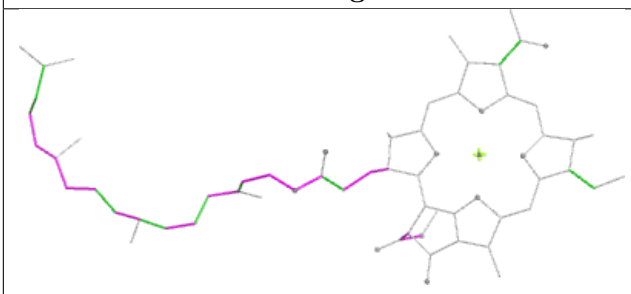
Ligand BCB 6 102



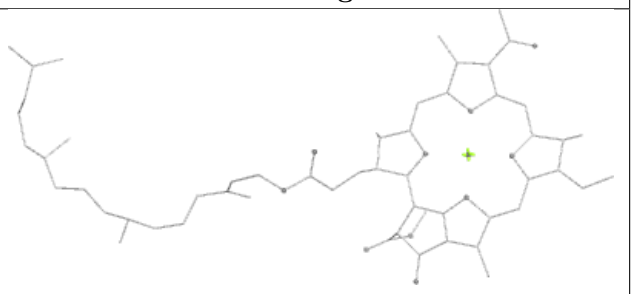
Bond lengths



Bond angles

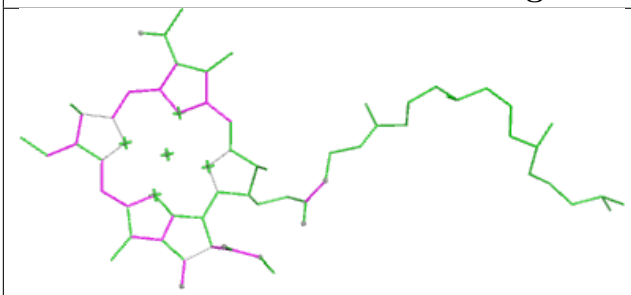


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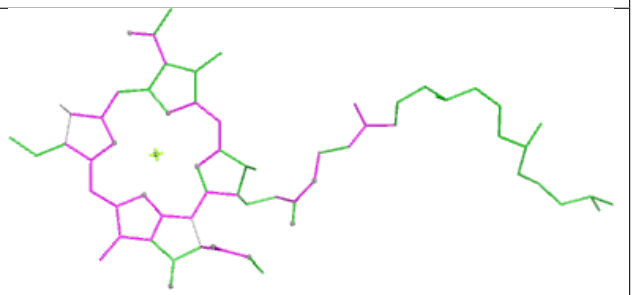


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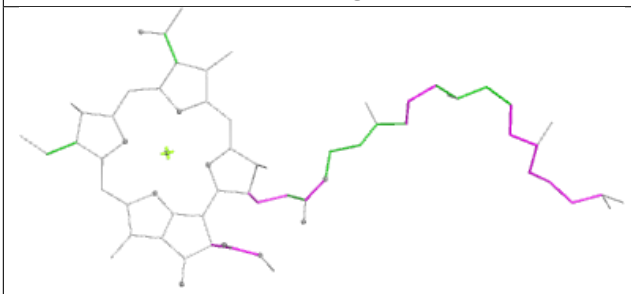
Ligand BCB u 101



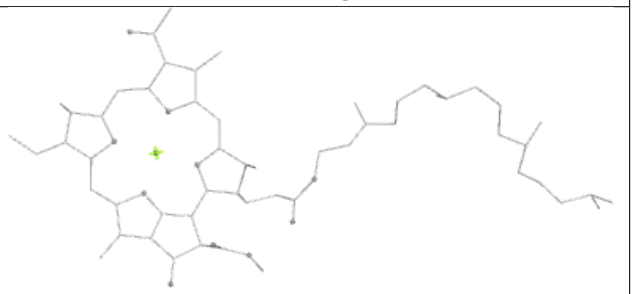
Bond lengths



Bond angles

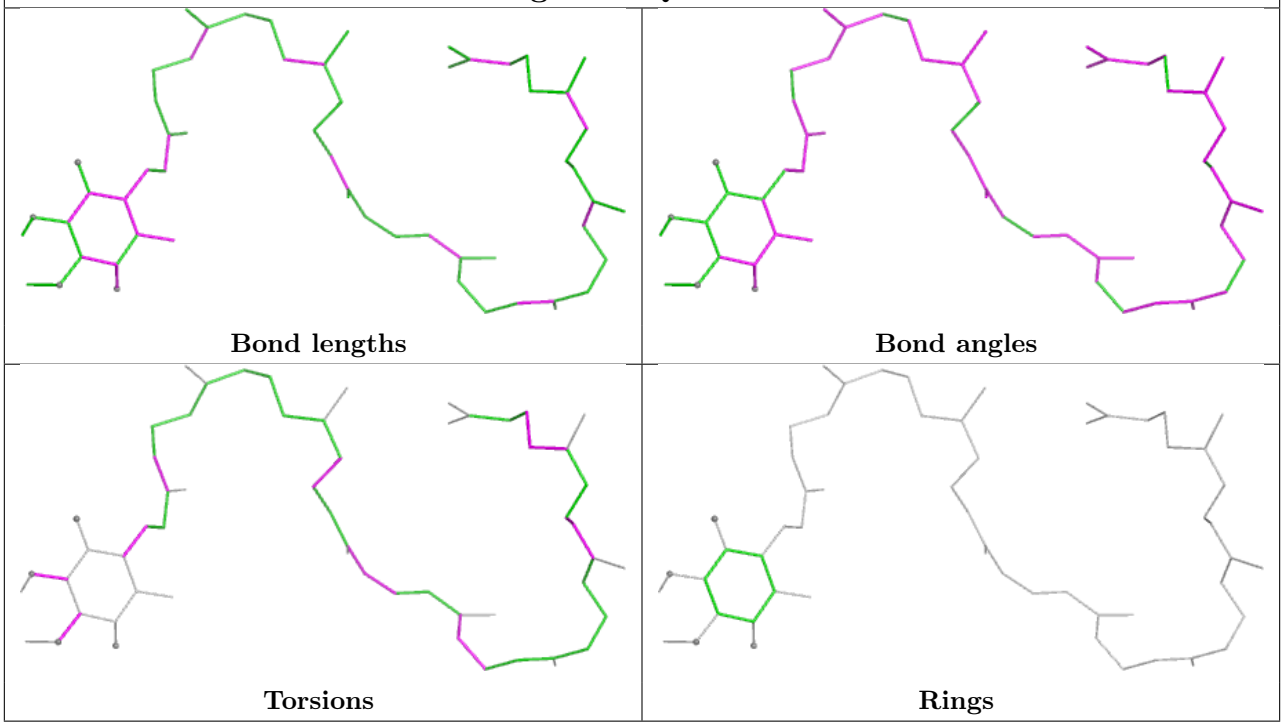


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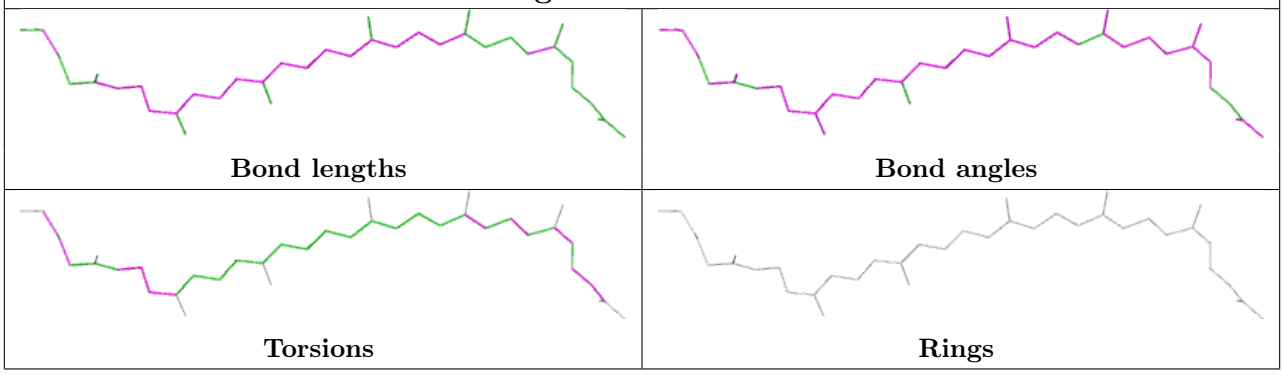


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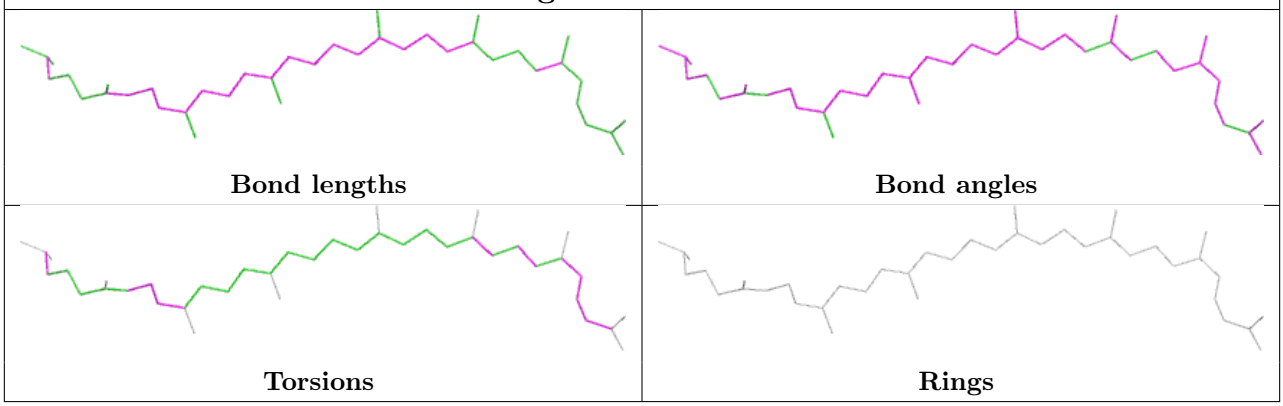
Ligand UQ9 6 101



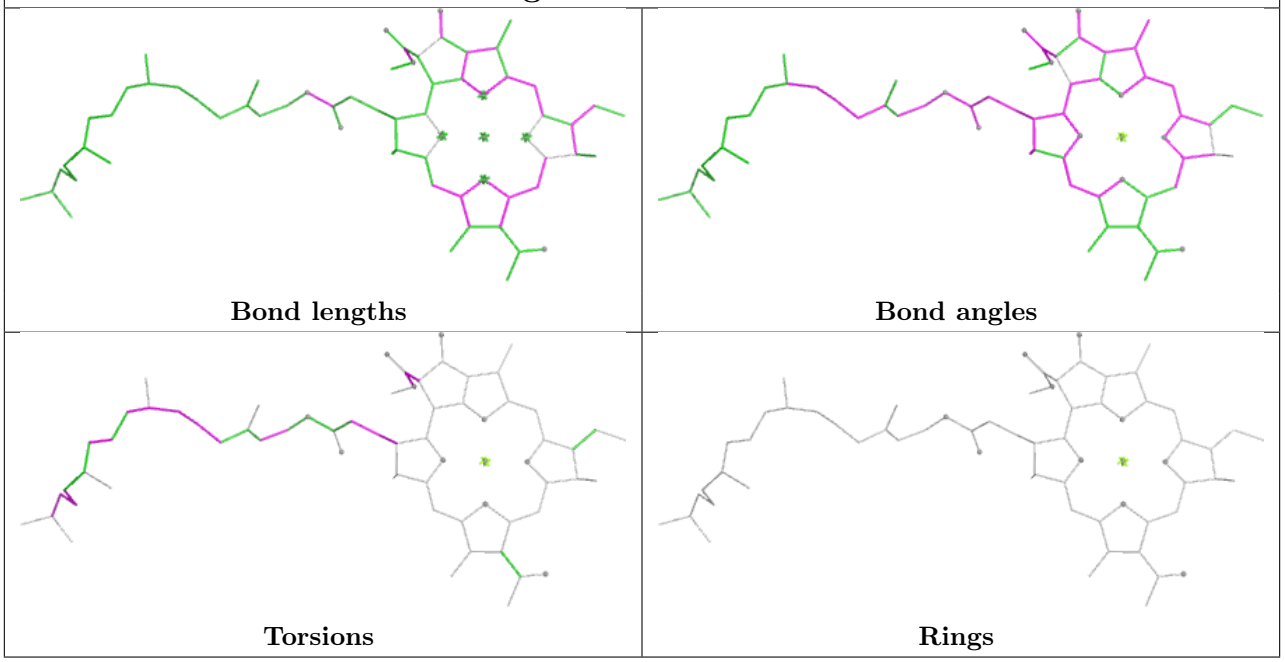
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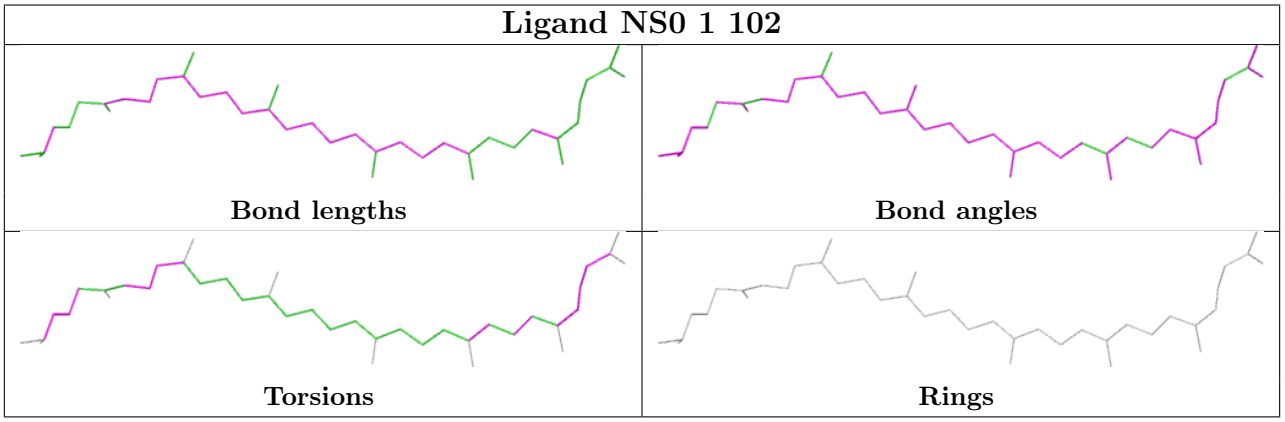
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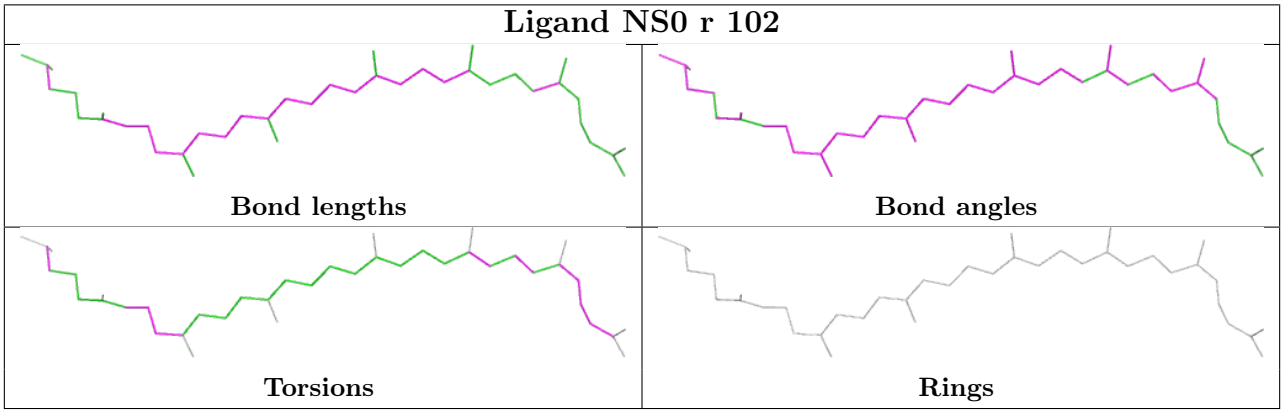
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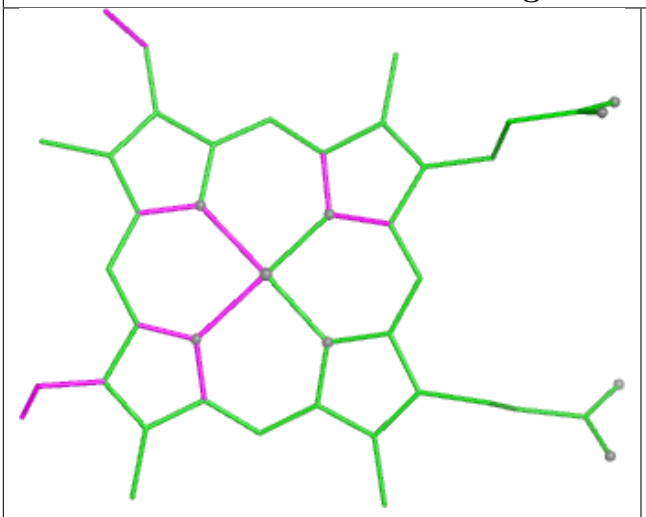
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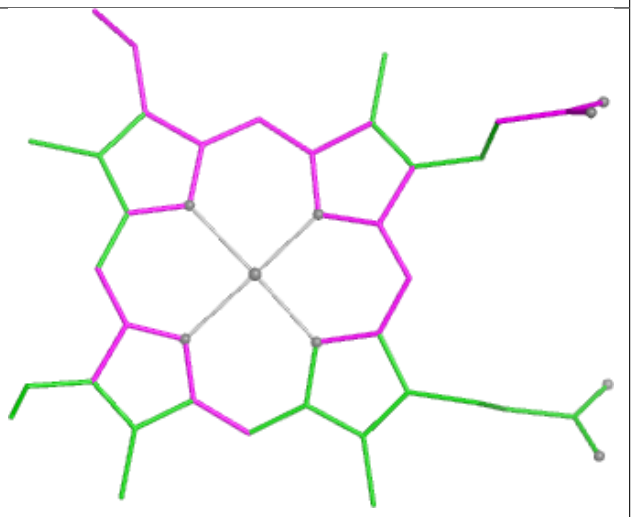
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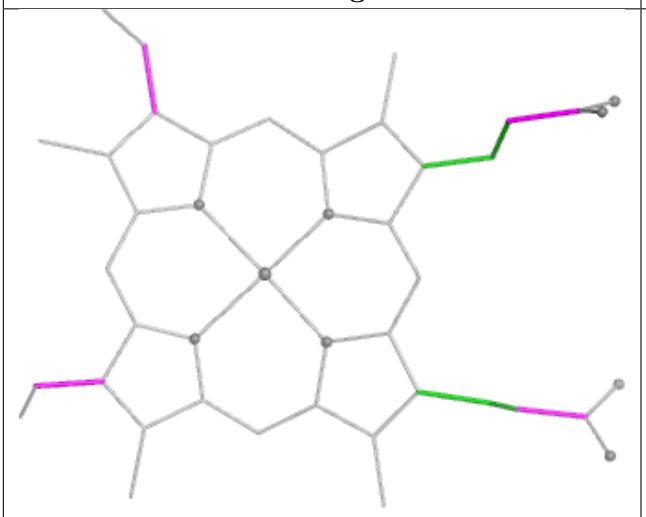
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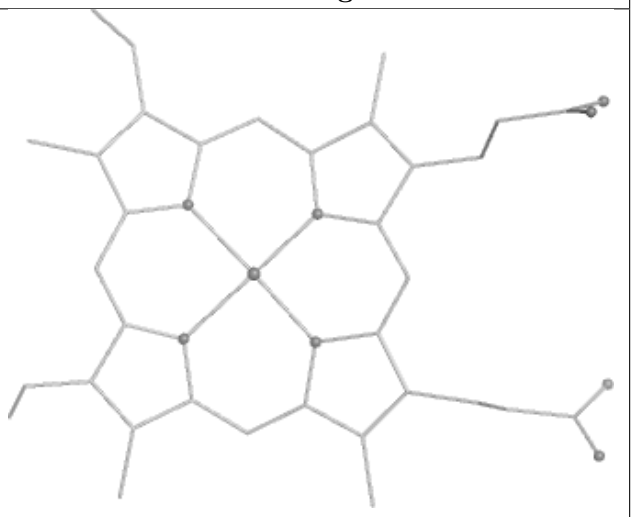
Bond lengths



Bond angles

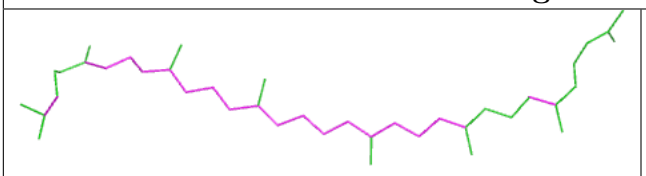


Torsions

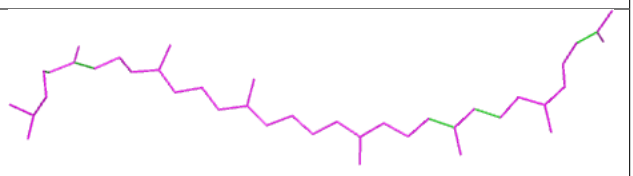


Rings

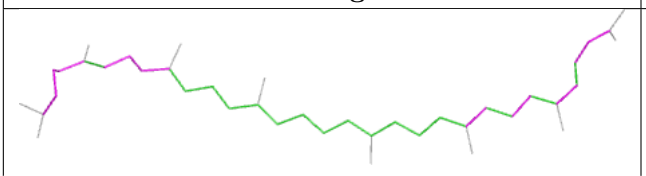
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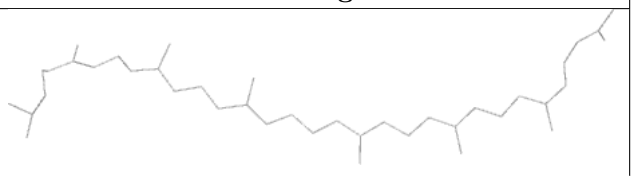
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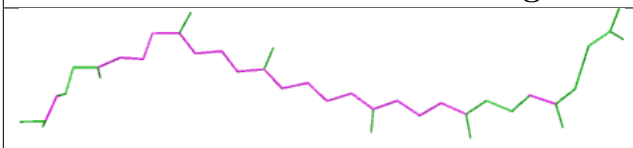


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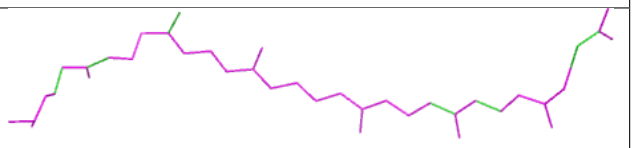


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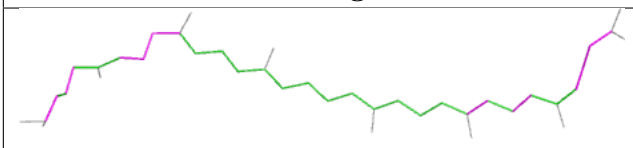
Ligand NS0 W 102



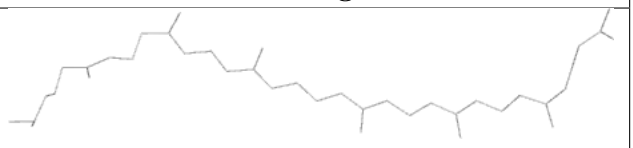
Bond lengths



Bond angles

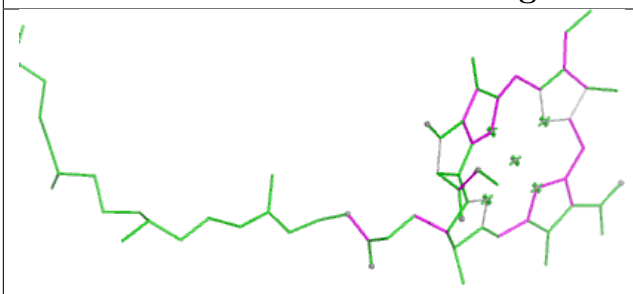


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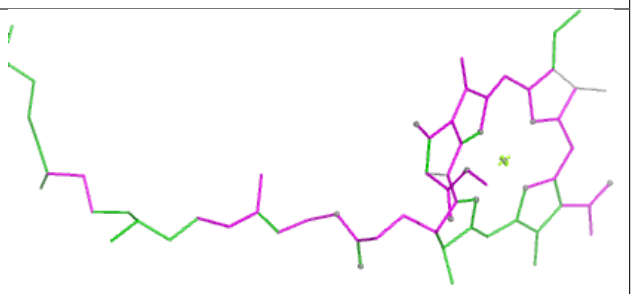


Rings

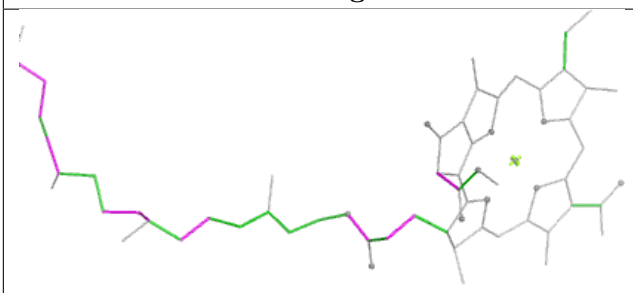
Ligand BCB M 407



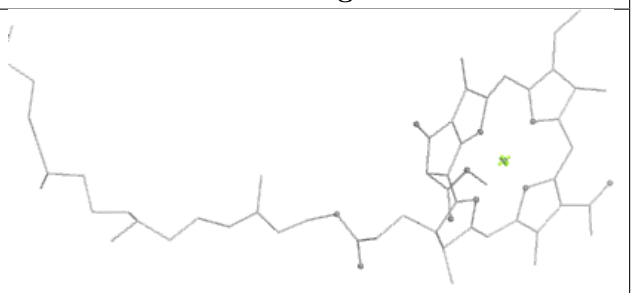
Bond lengths



Bond angles

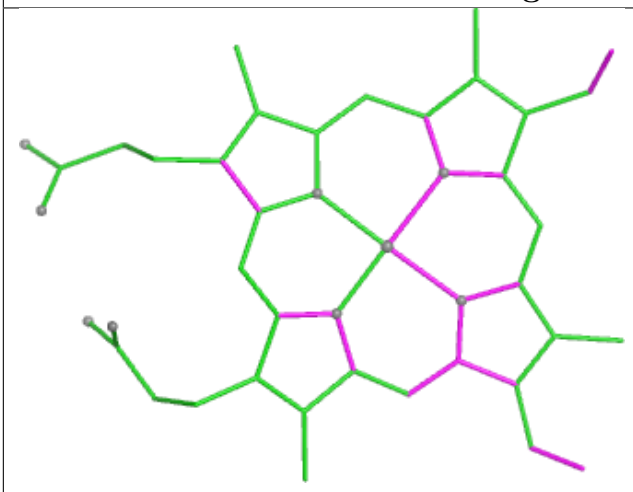


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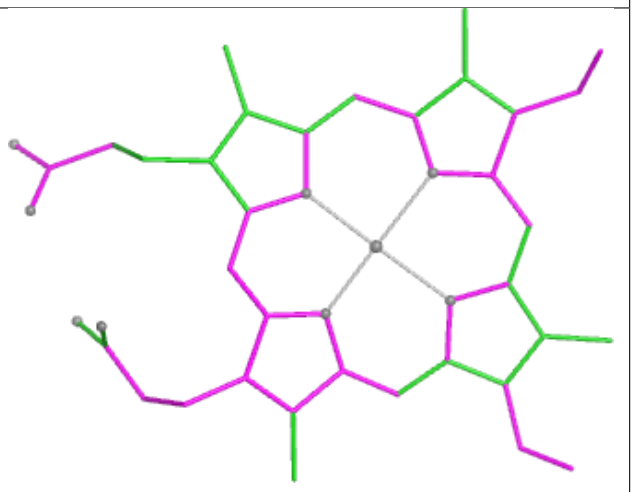


Rings

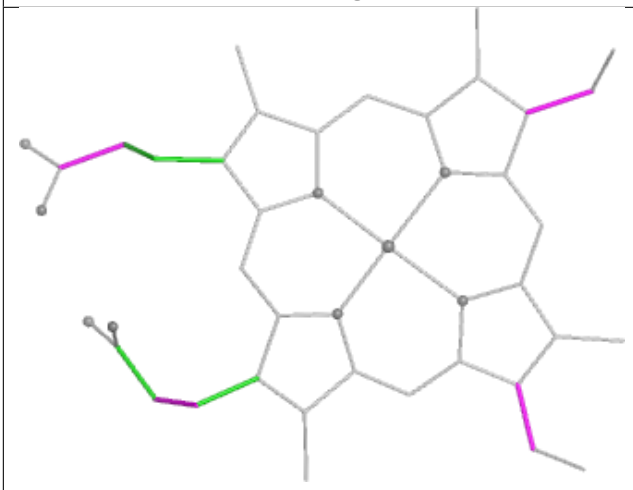
Ligand HEC C 402



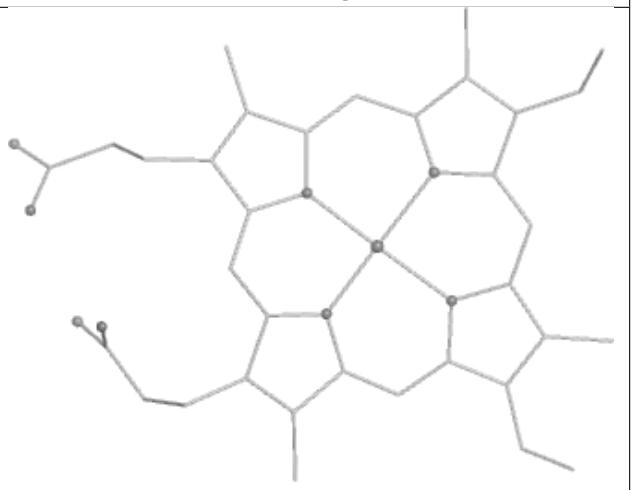
Bond lengths



Bond angles

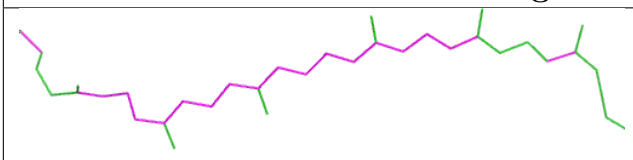


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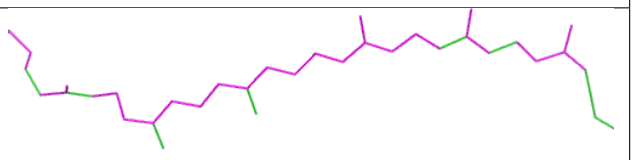


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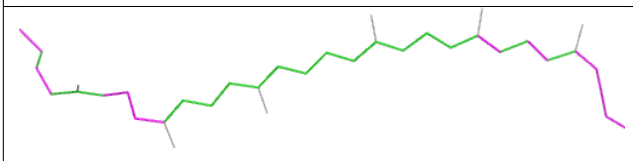
Ligand NS0 u 102



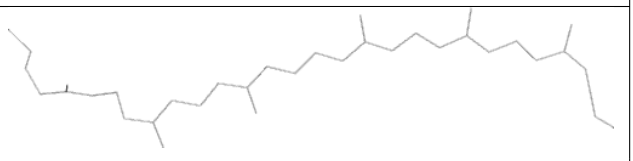
Bond lengths



Bond angles

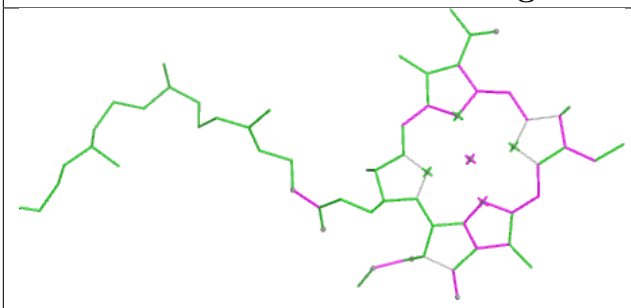


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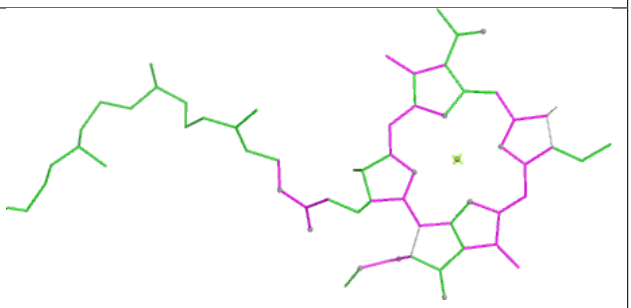


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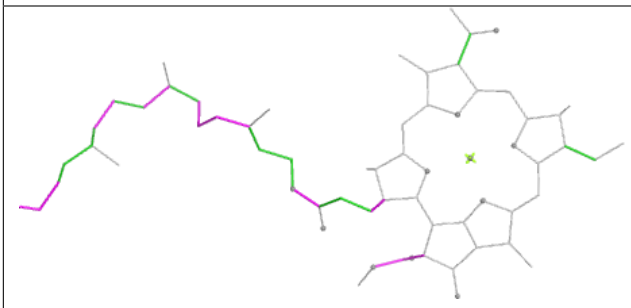
Ligand BCB W 101



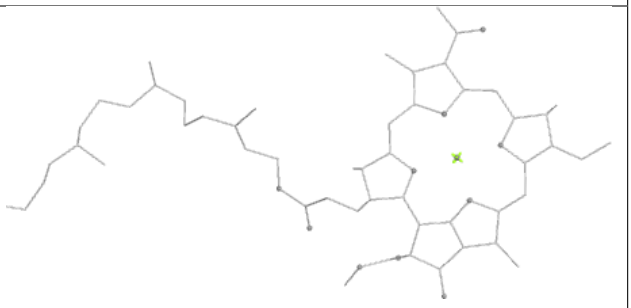
Bond lengths



Bond angles

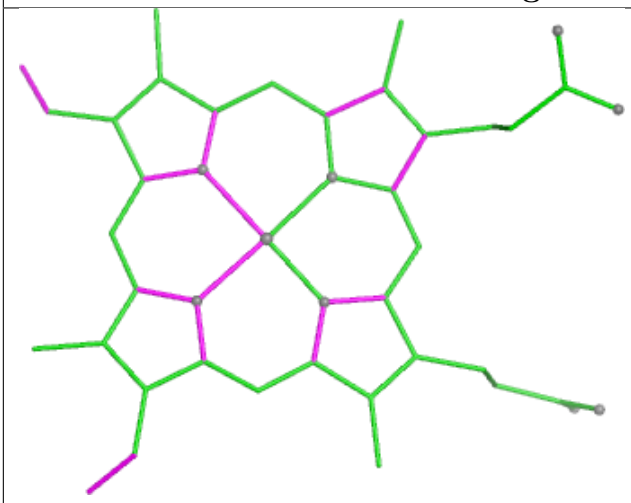


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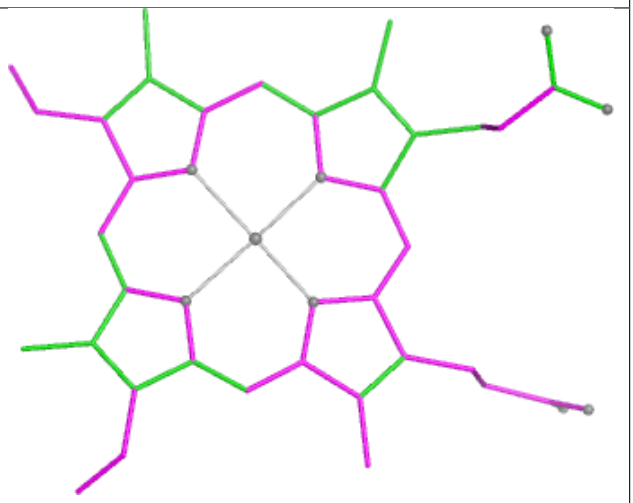


Rings

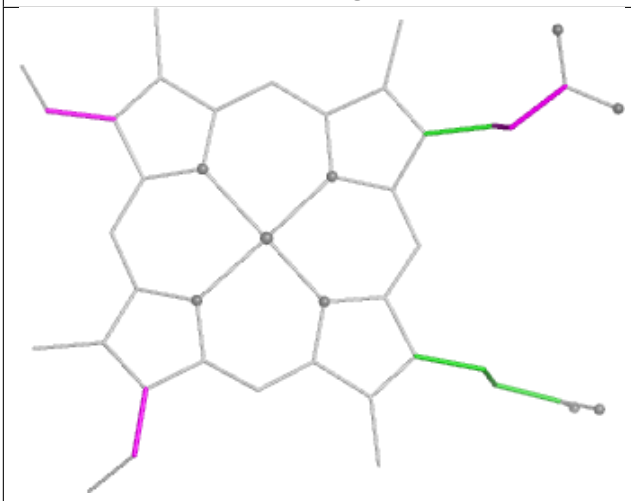
Ligand HEC C 401



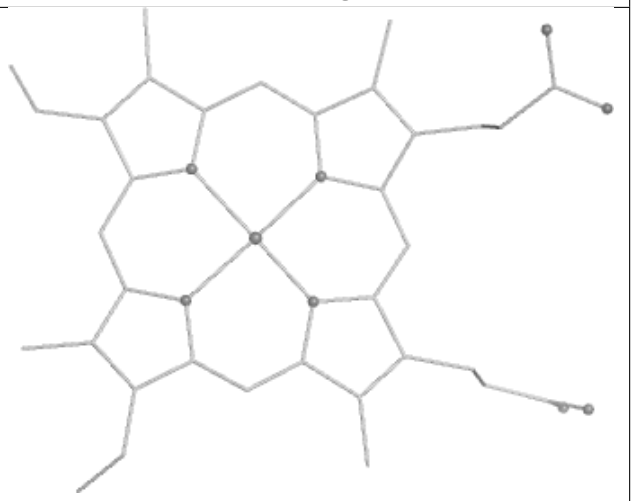
Bond lengths



Bond angles

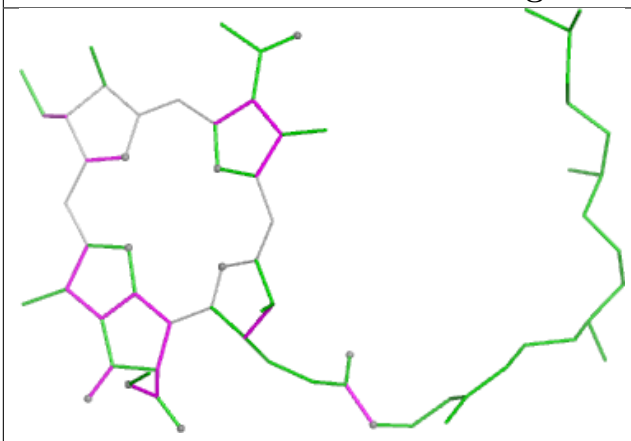


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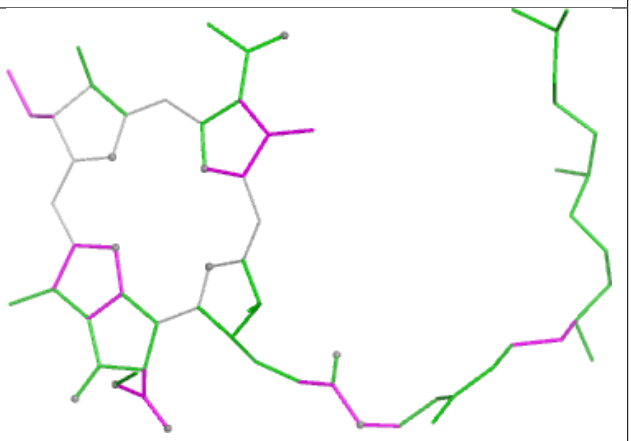


Rings

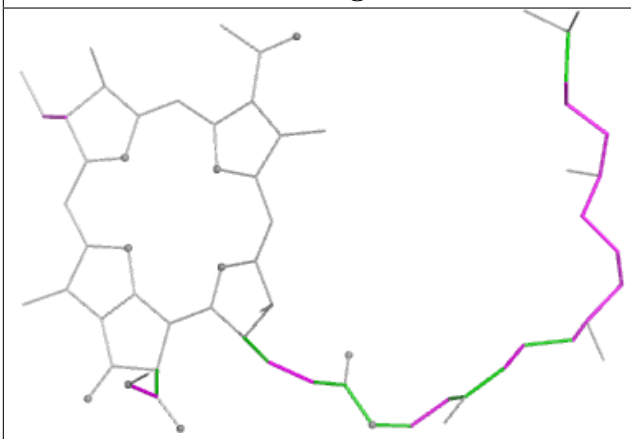
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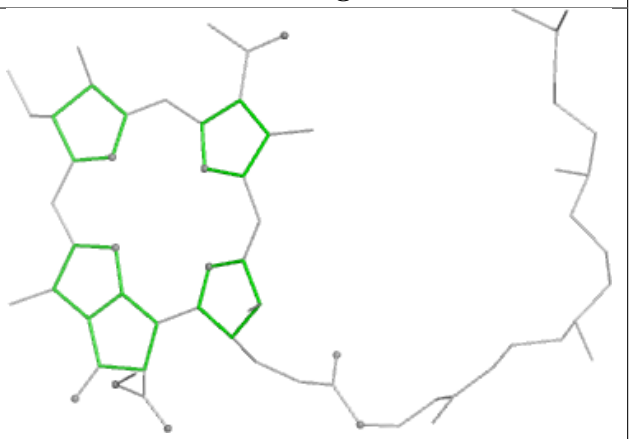
Bond lengths



Bond angles

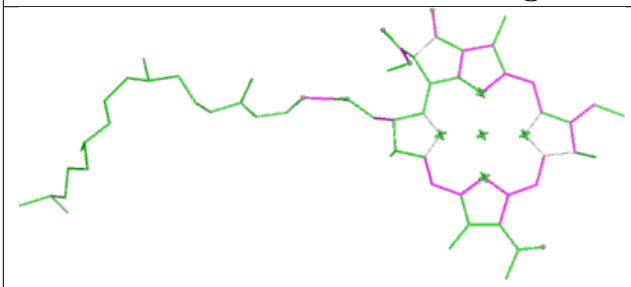


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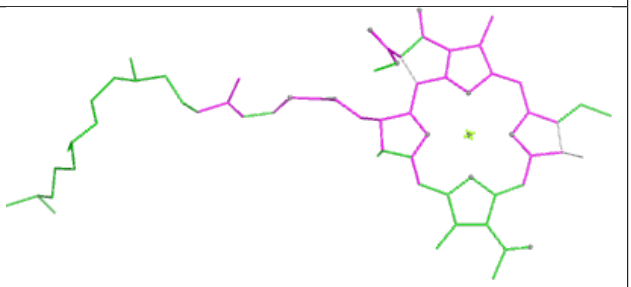


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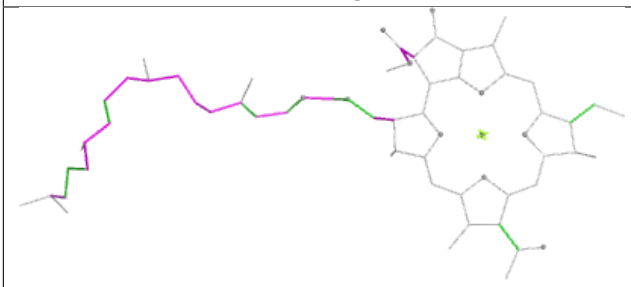
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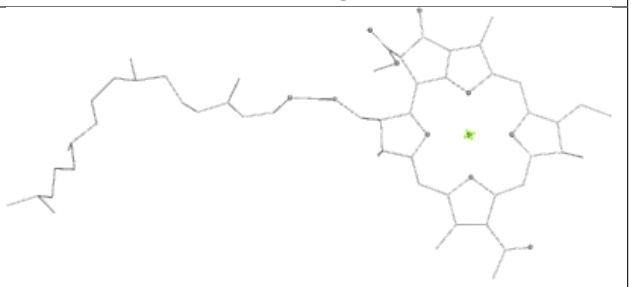
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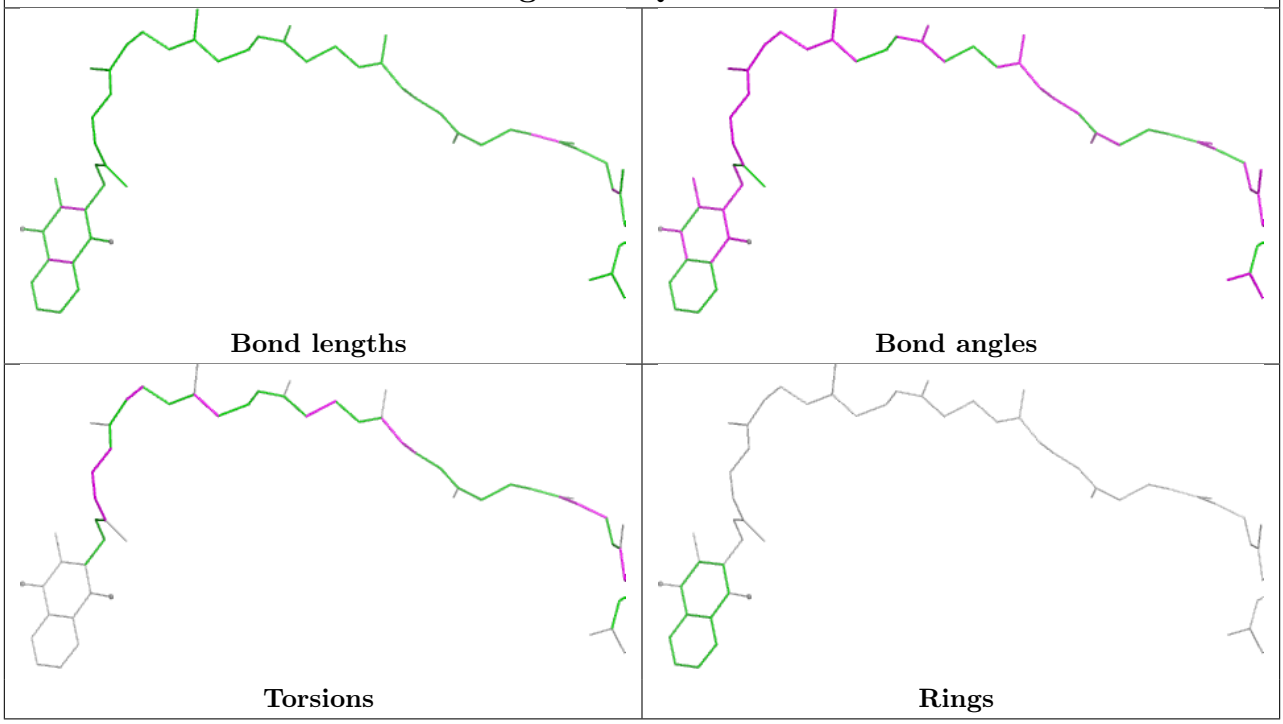


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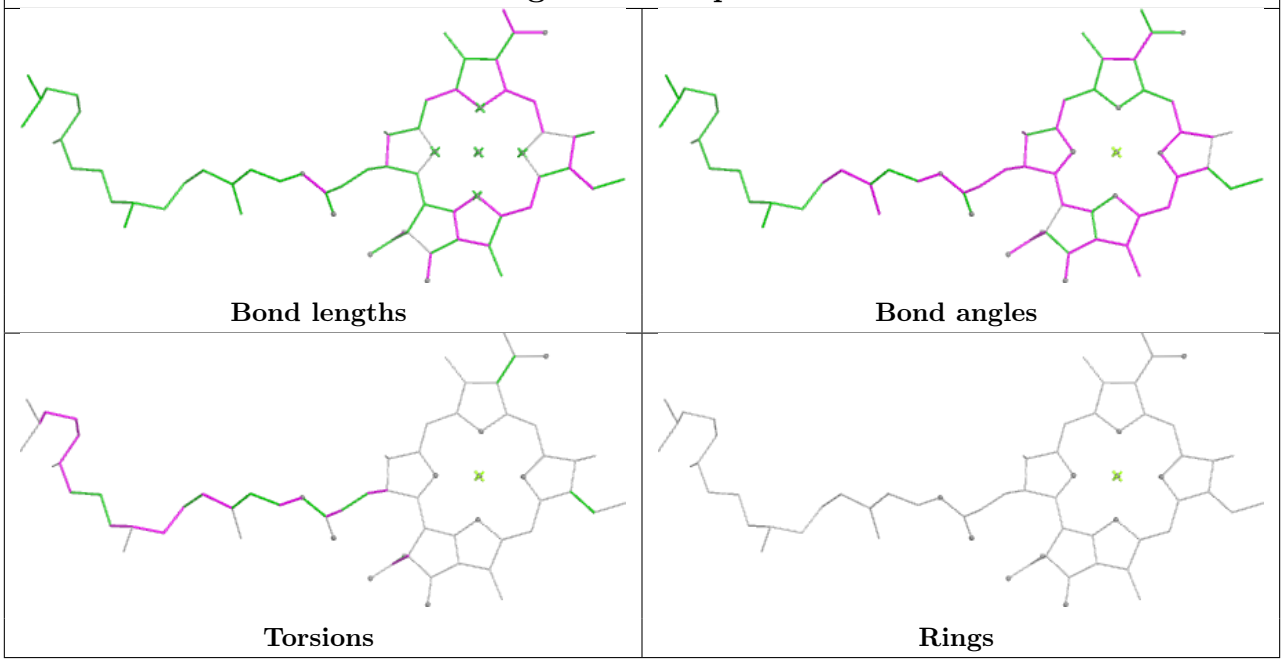


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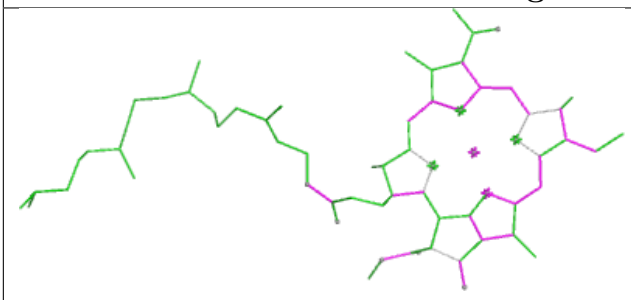
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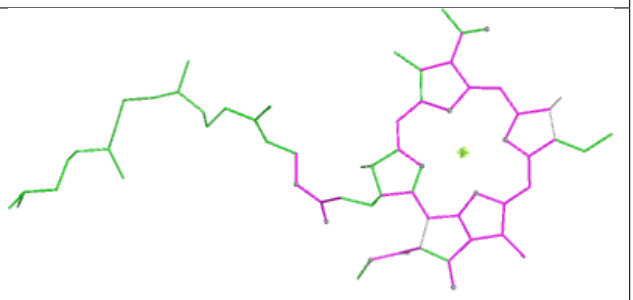
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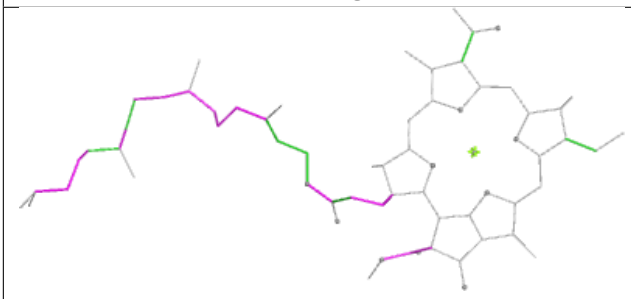
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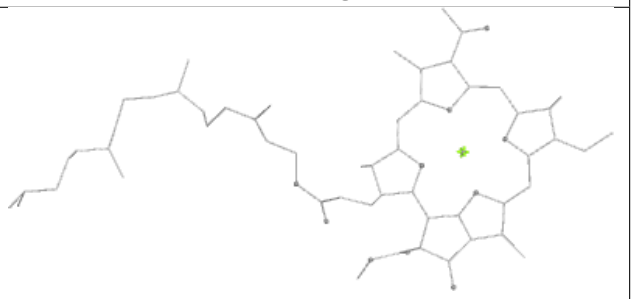
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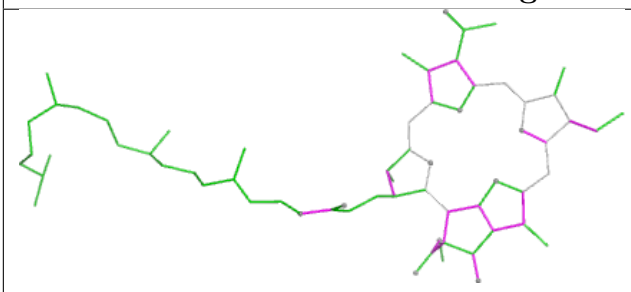


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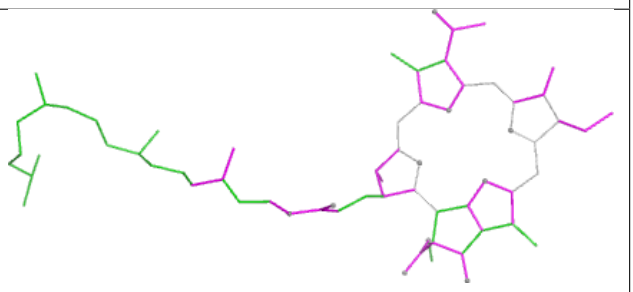


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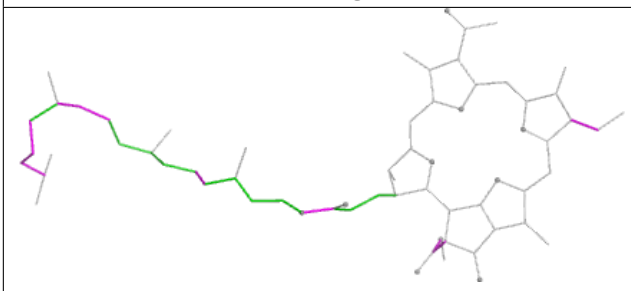
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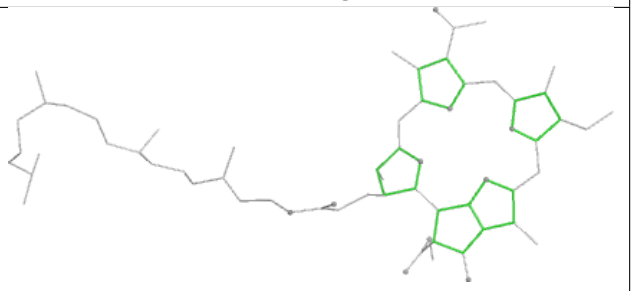
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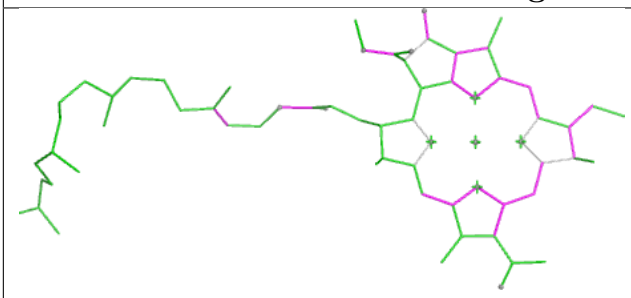


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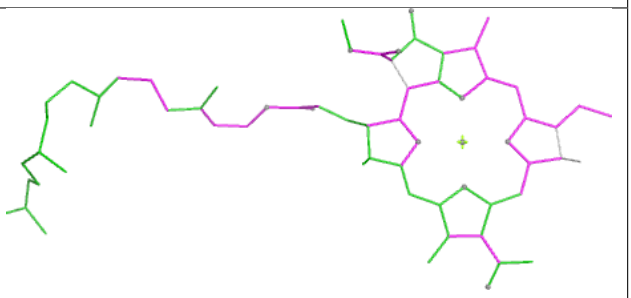


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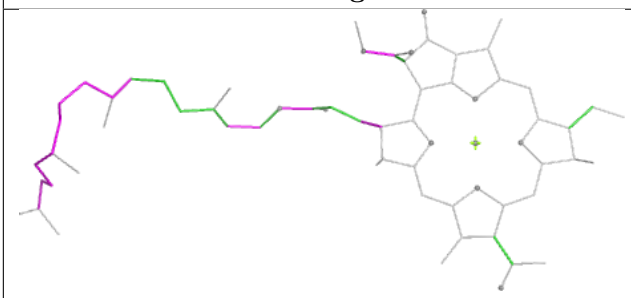
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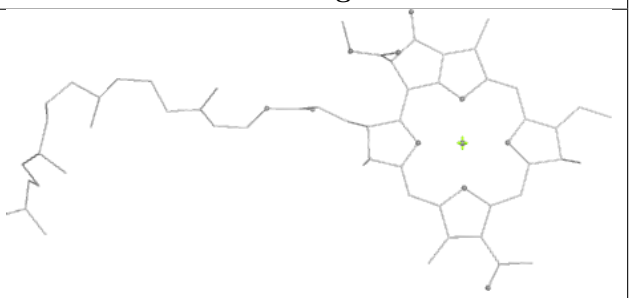
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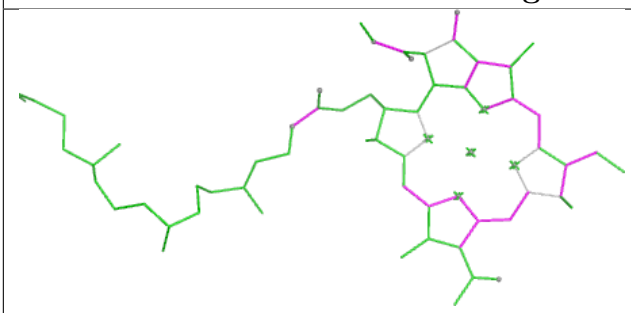


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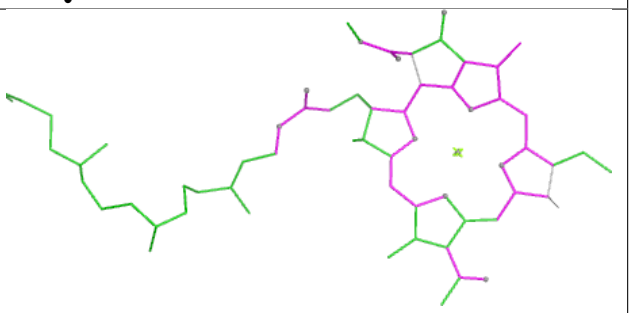


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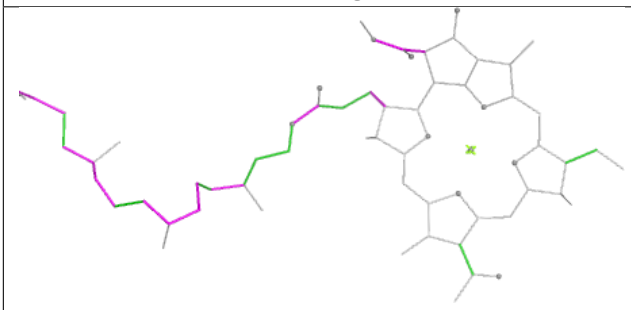
Ligand BCB Q 101



Bond lengths



Bond angles

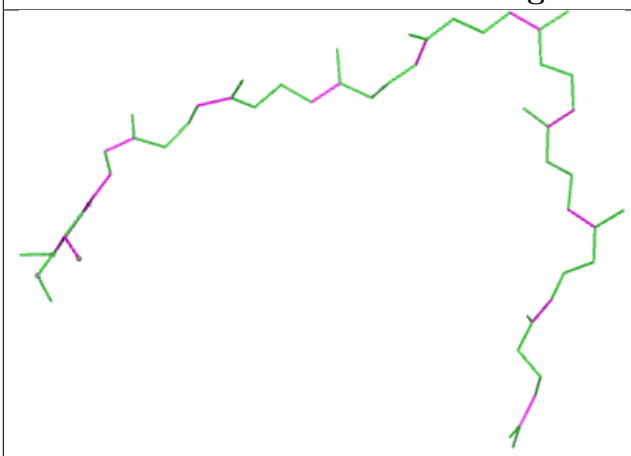


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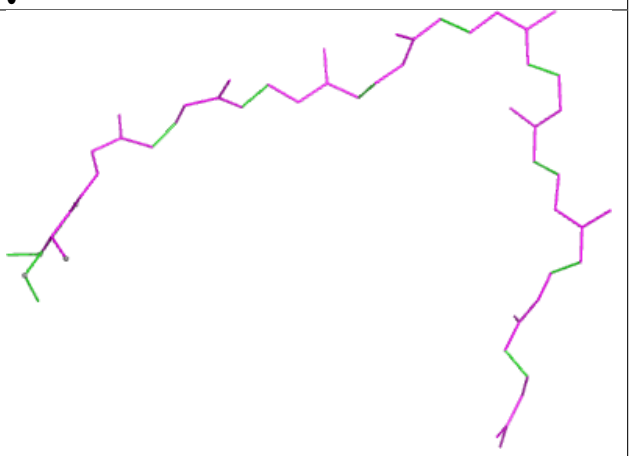


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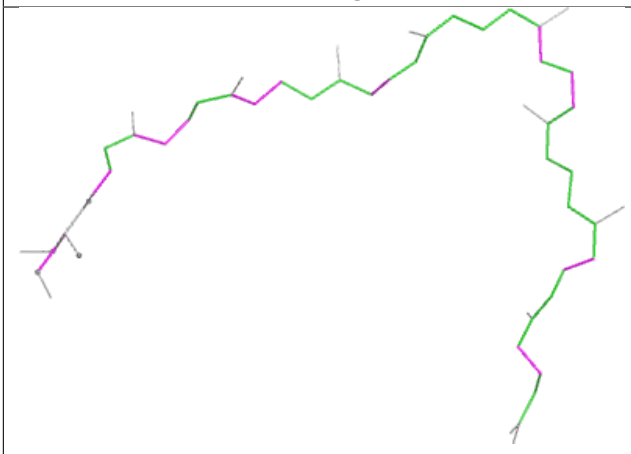
Ligand UQ9 L 304



Bond lengths



Bond angles

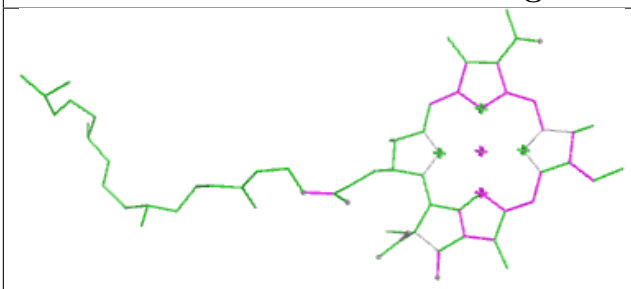


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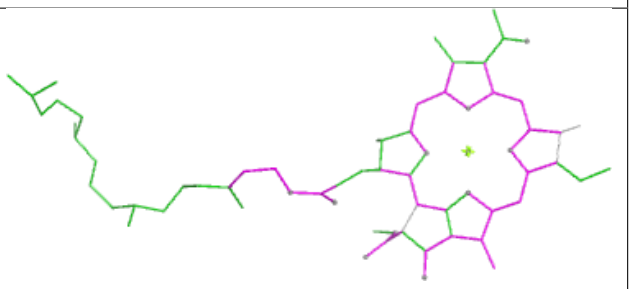


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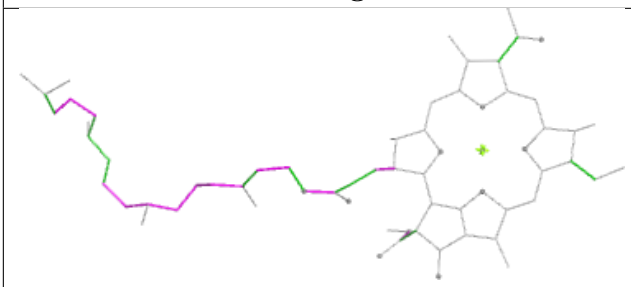
Ligand BCB F 101



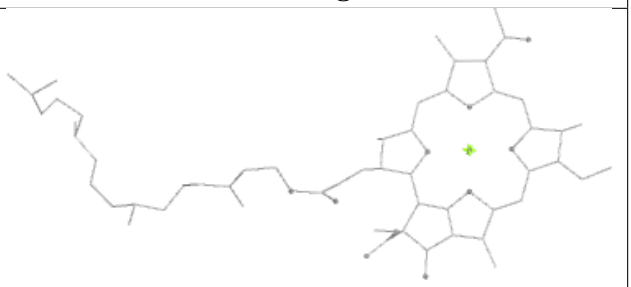
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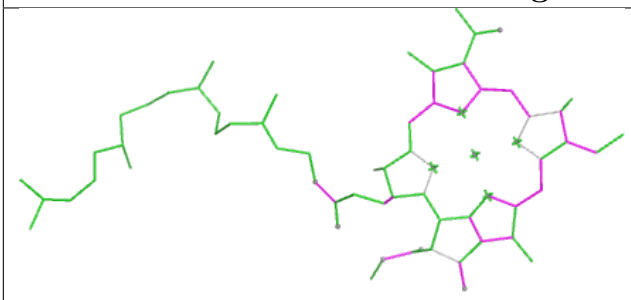


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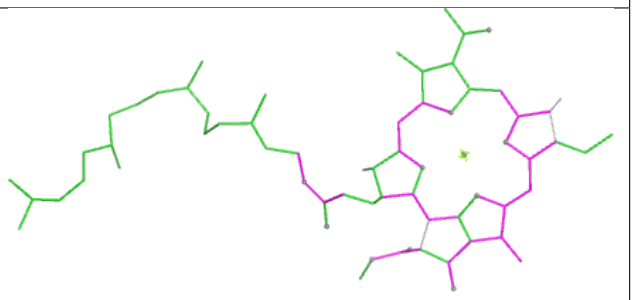


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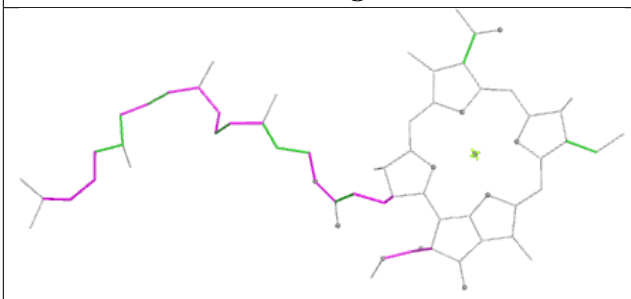
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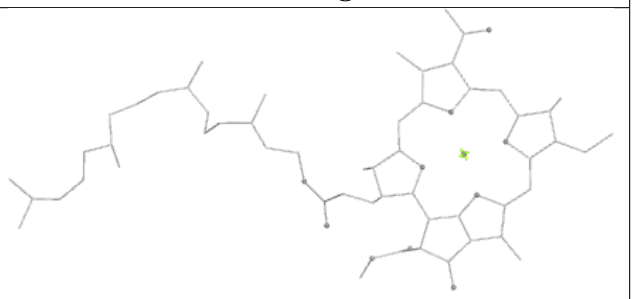
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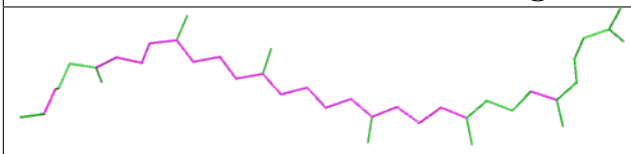


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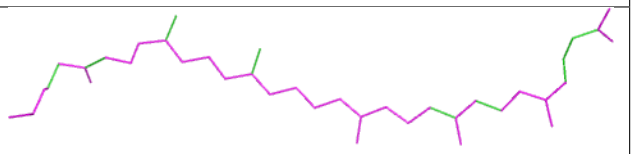


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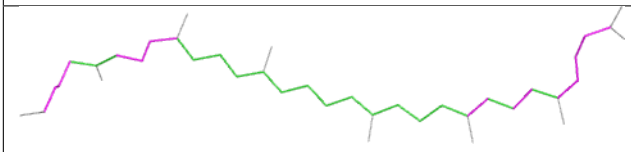
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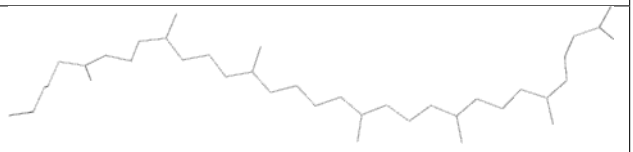
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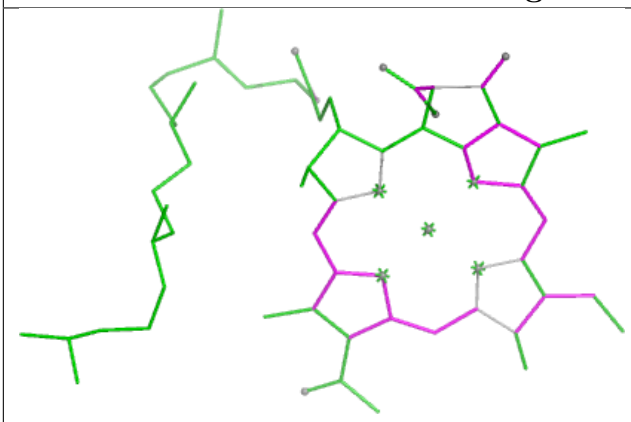


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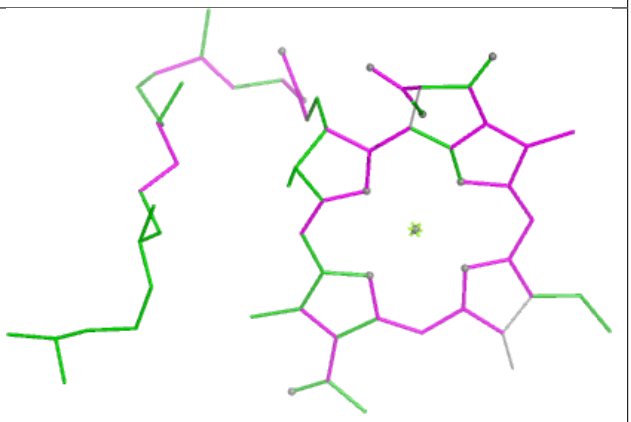


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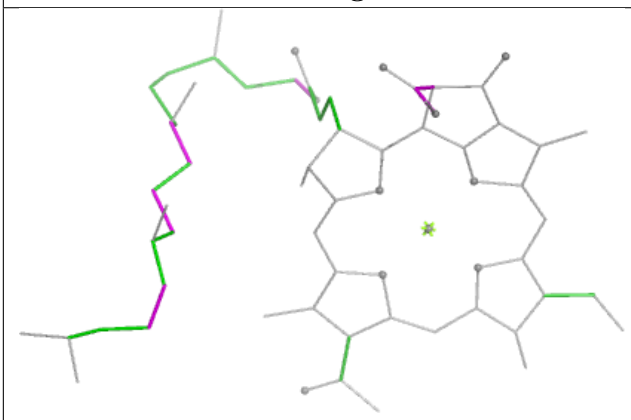
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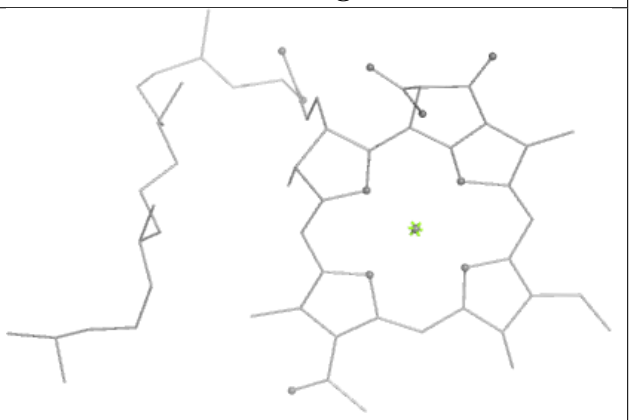
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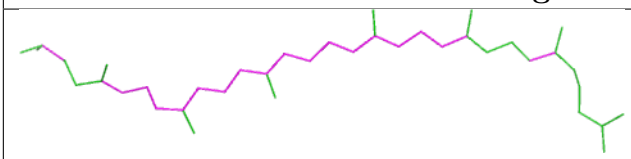


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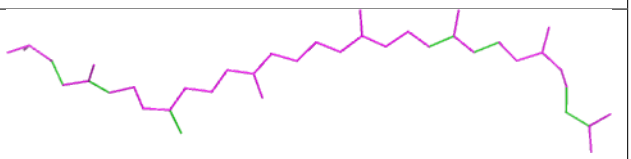


Rings

Ligand NS0 o 102



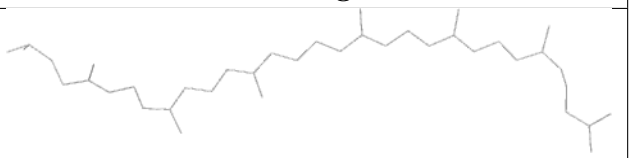
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Bond angles

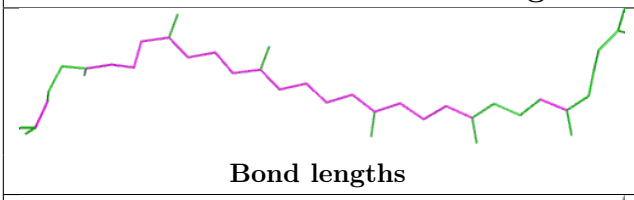


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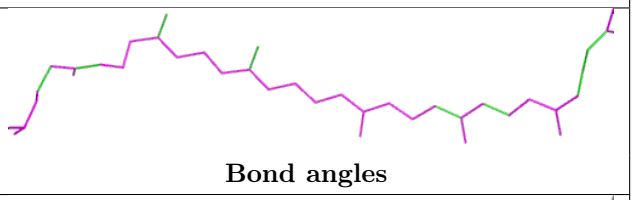


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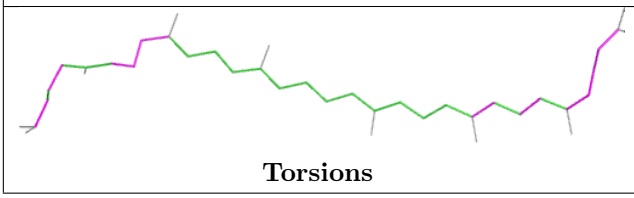
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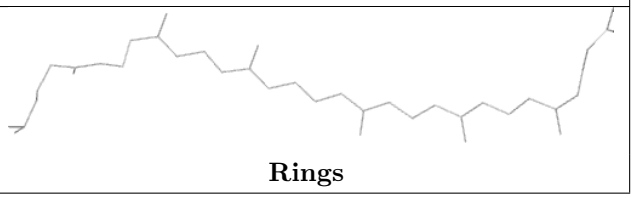
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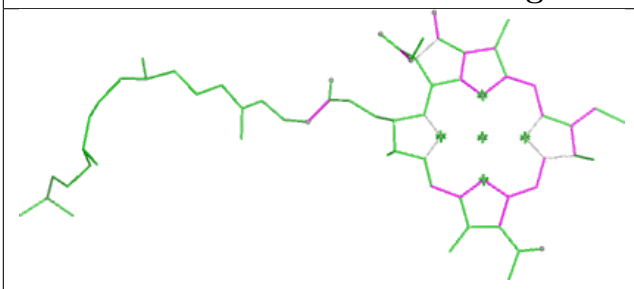


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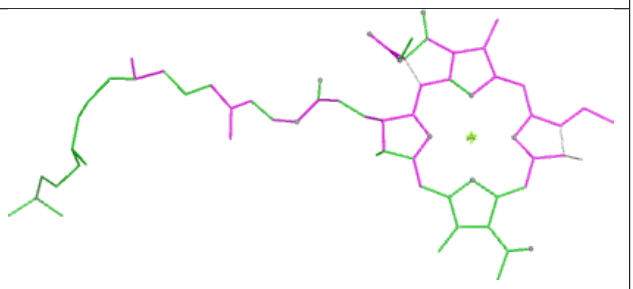


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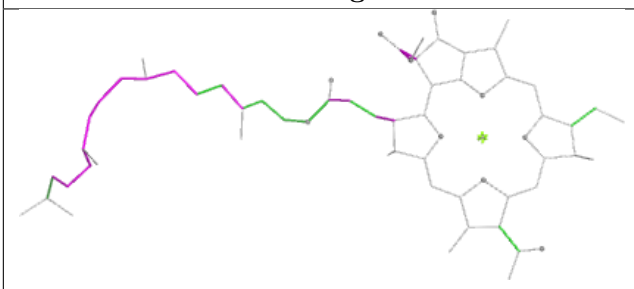
Ligand BCB h 101



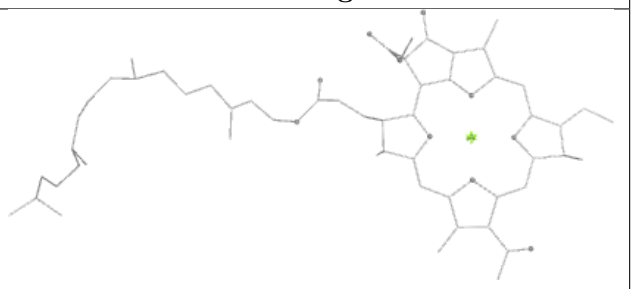
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Bond angles

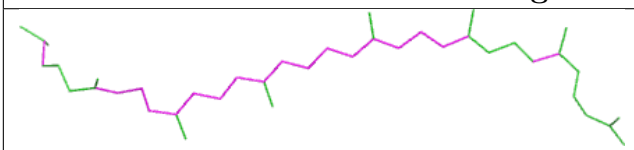


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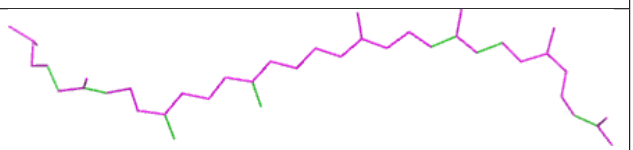


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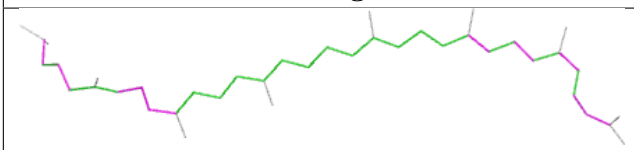
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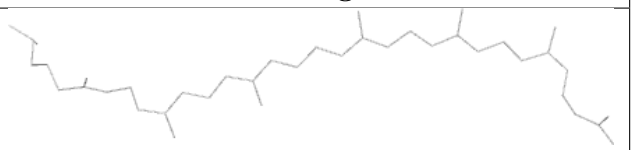
Bond lengths



Bond angles

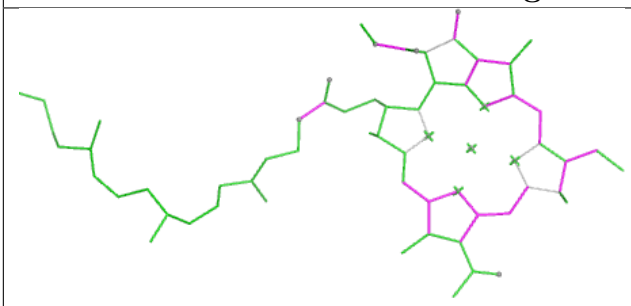


Torsions

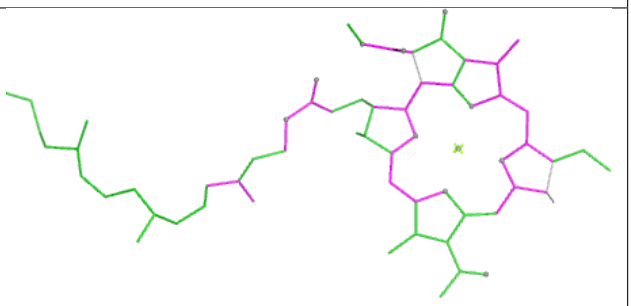


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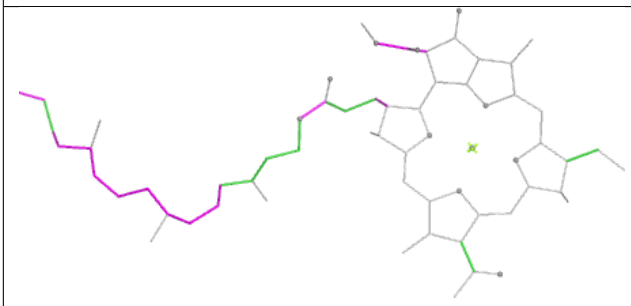
Ligand BCB T 101



Bond lengths



Bond angles

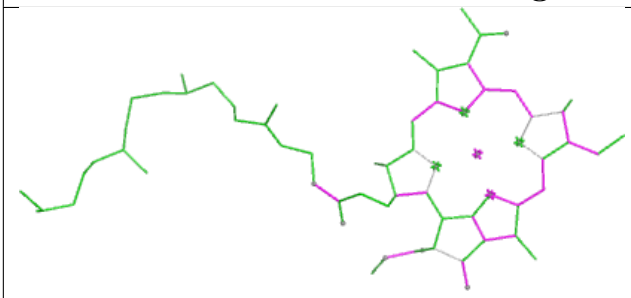


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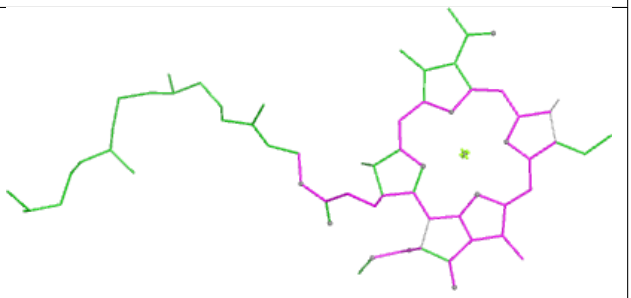


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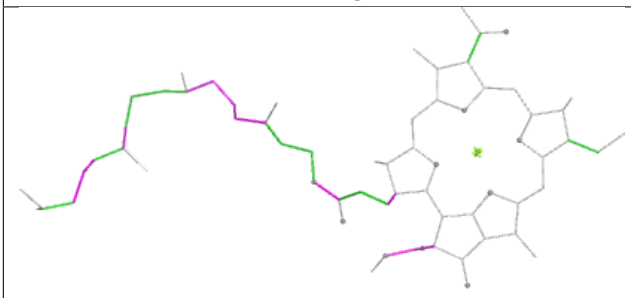
Ligand BCB l 101



Bond lengths



Bond angles

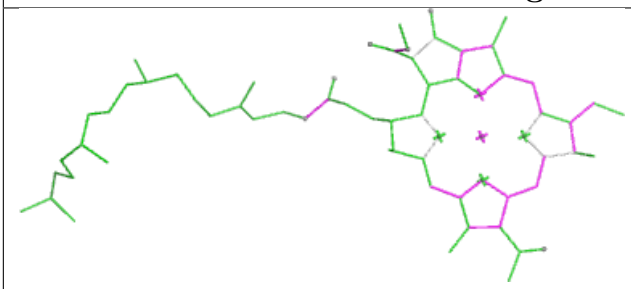


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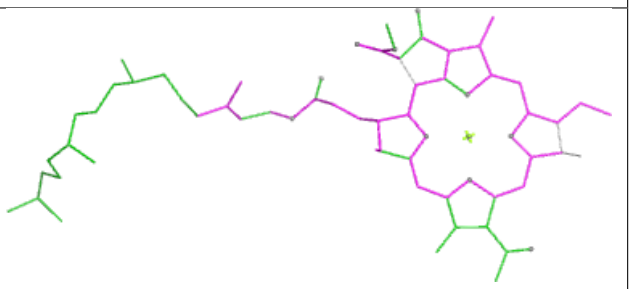


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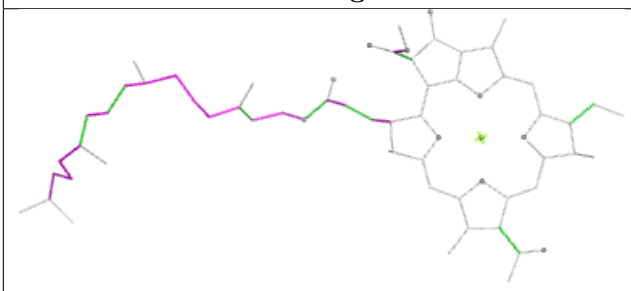
Ligand BCB S 101



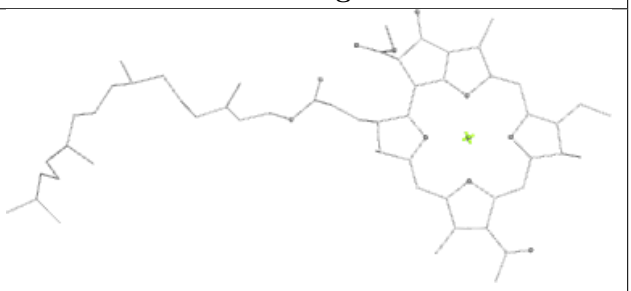
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Bond angles

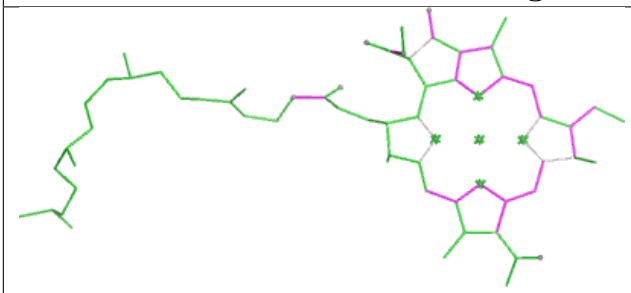


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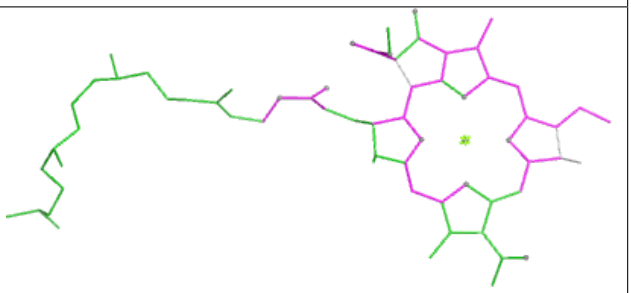


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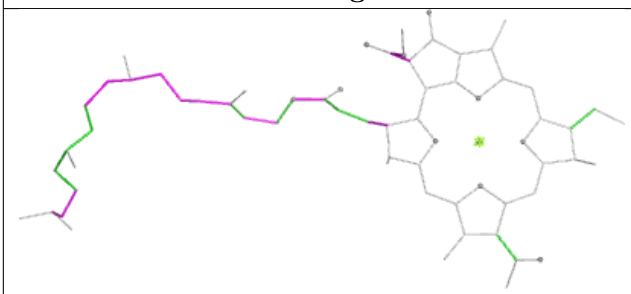
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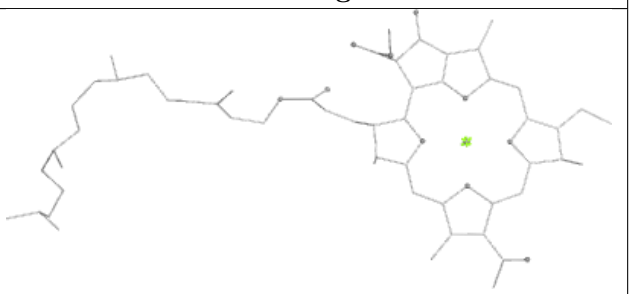
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Bond angles

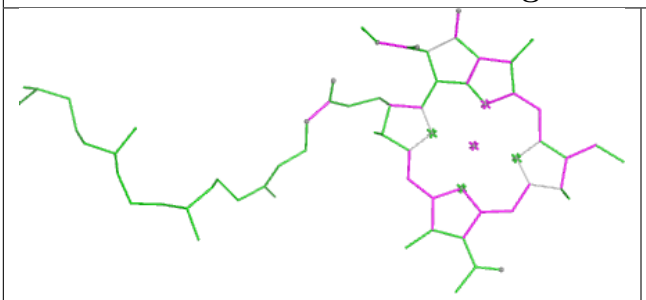


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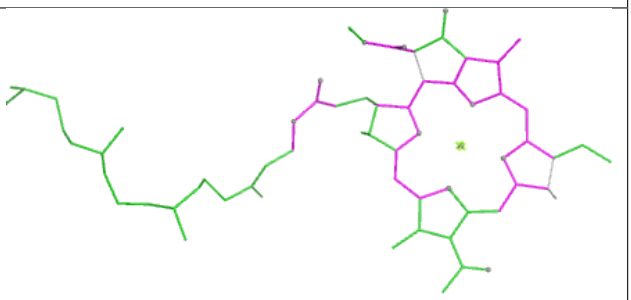


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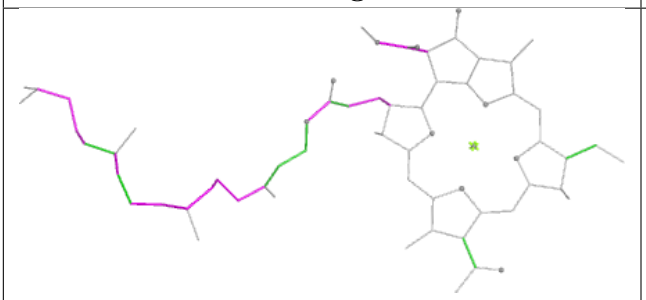
Ligand BCB N 101



Bond lengths



Bond angles

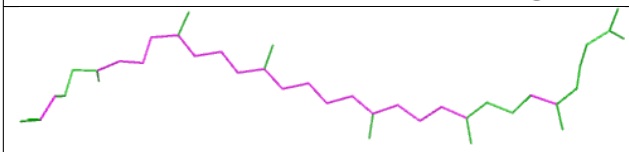


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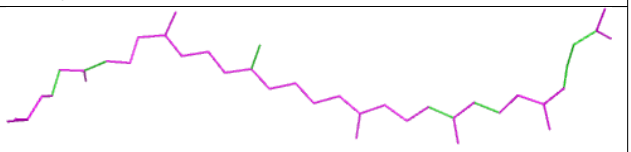


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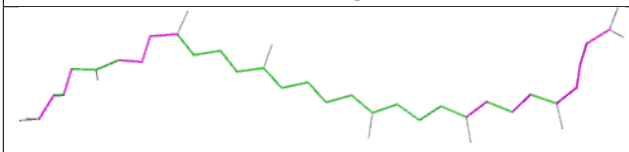
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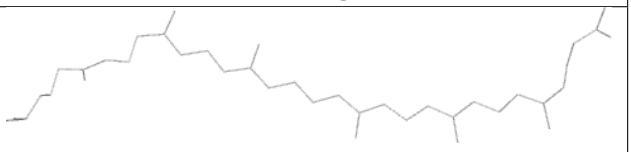
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Bond angles

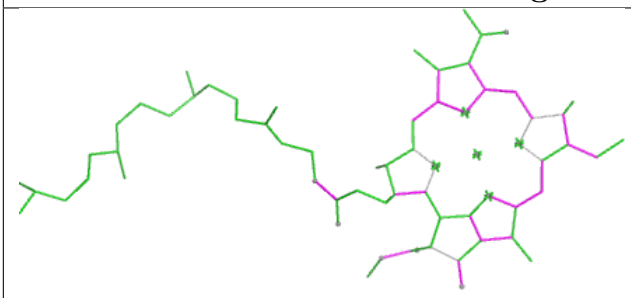


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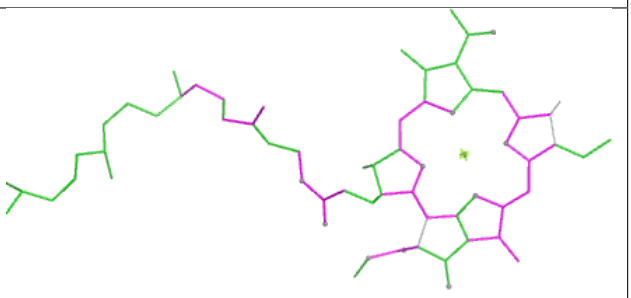


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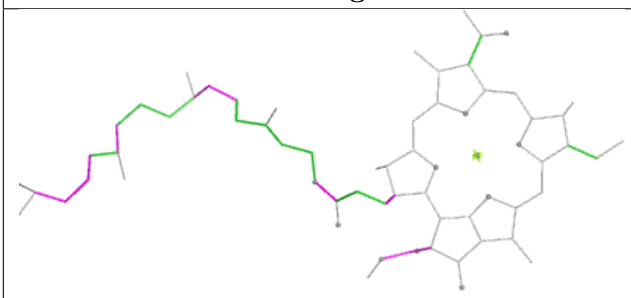
Ligand BCB f 101



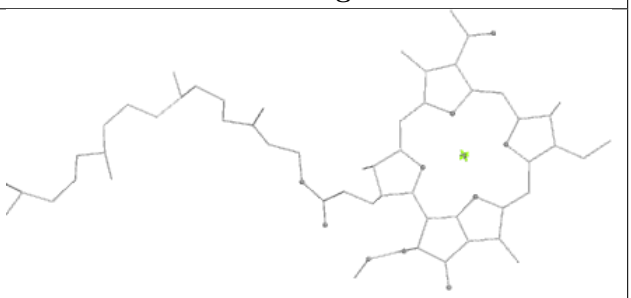
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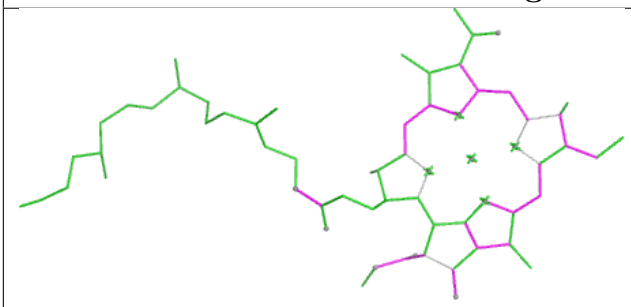


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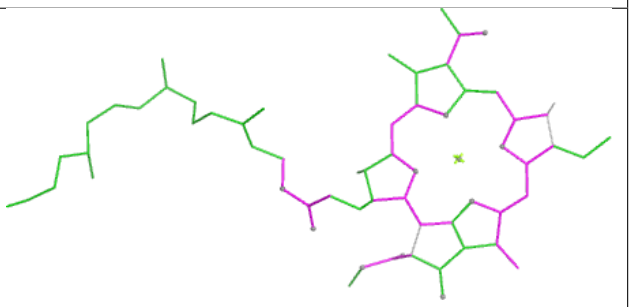


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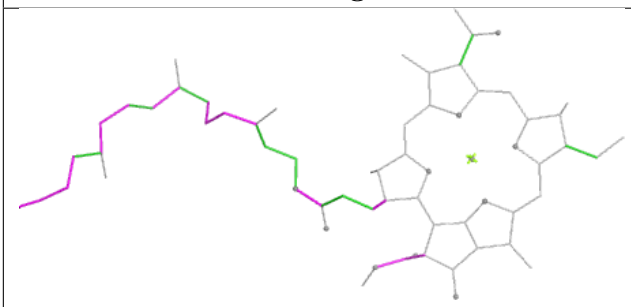
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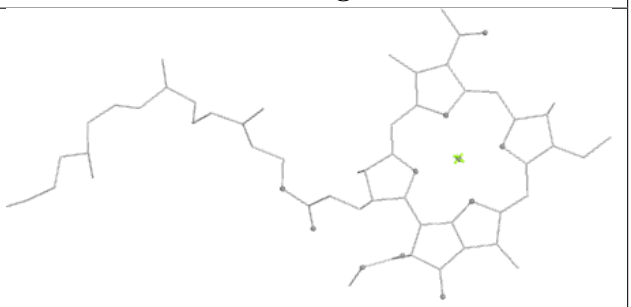
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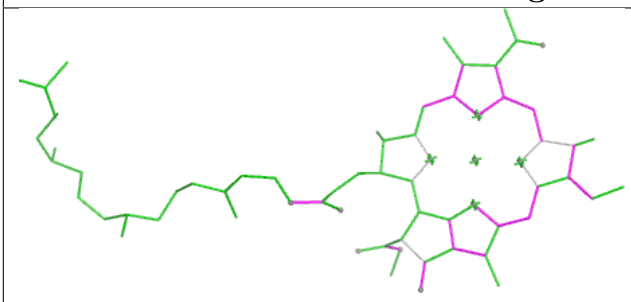


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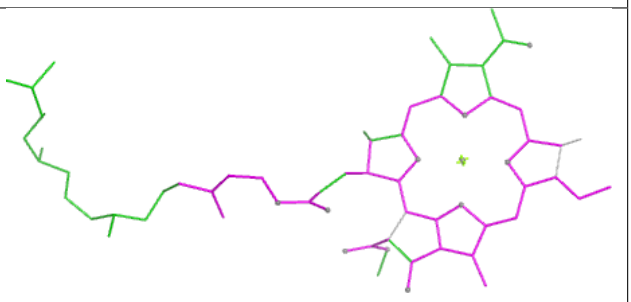


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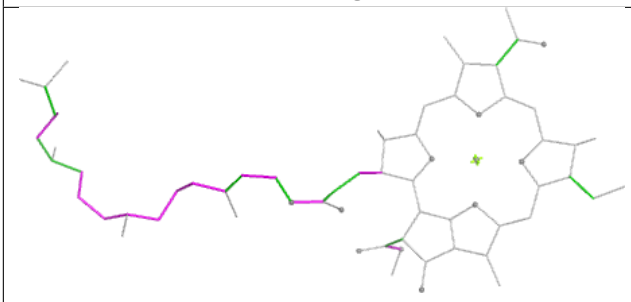
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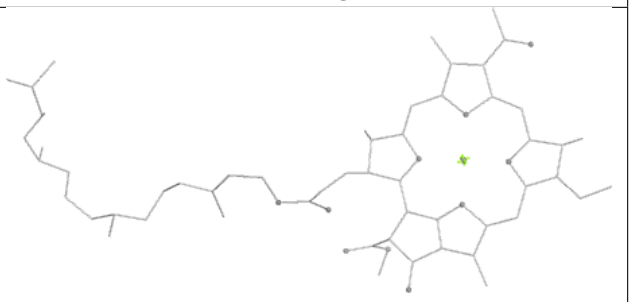
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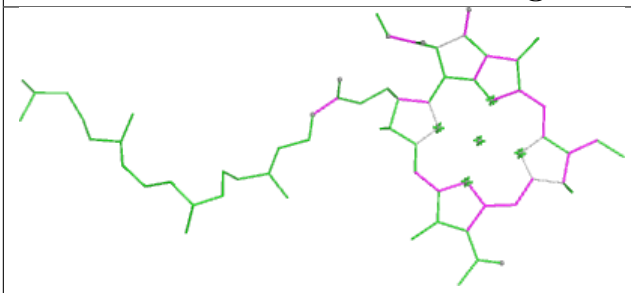


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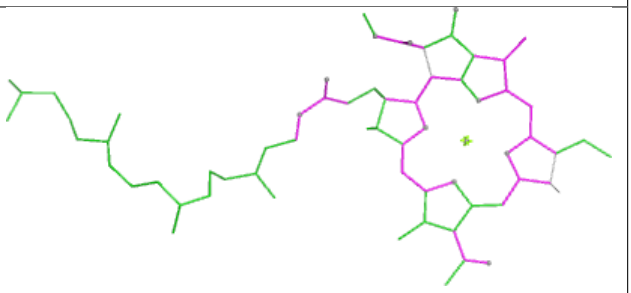


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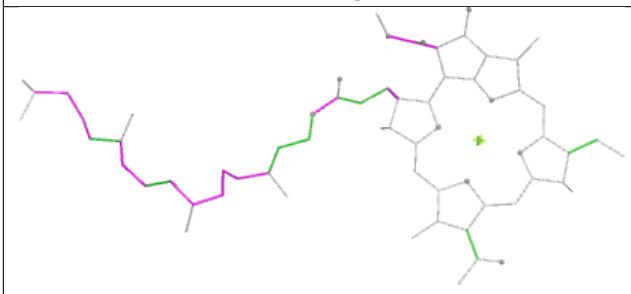
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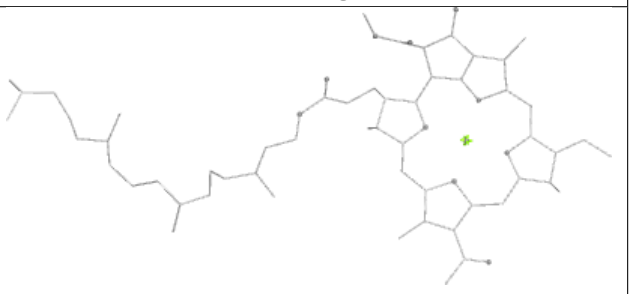
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Bond angles

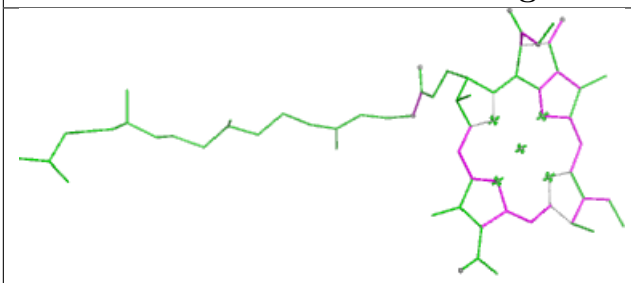


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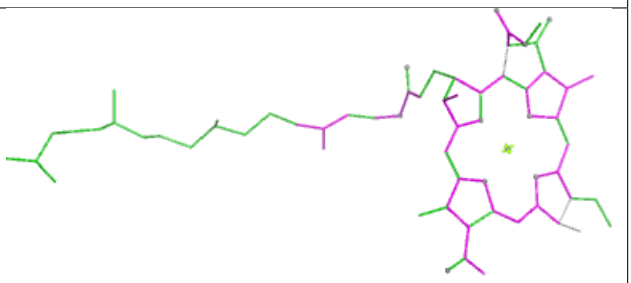


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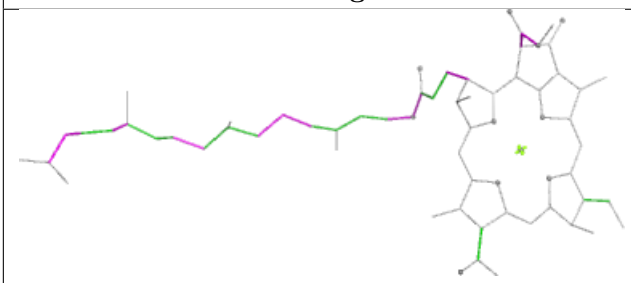
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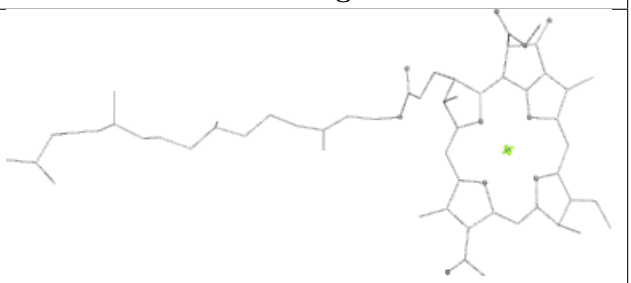
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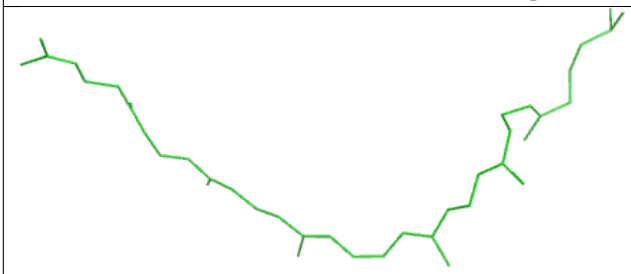


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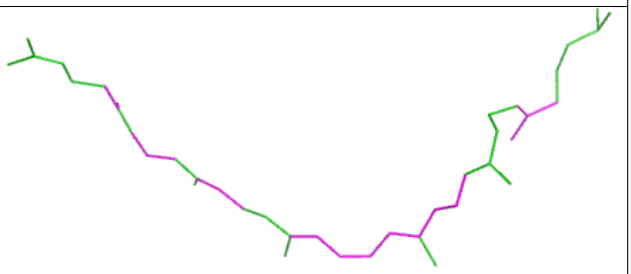


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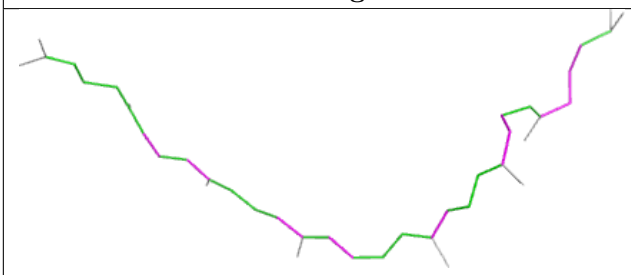
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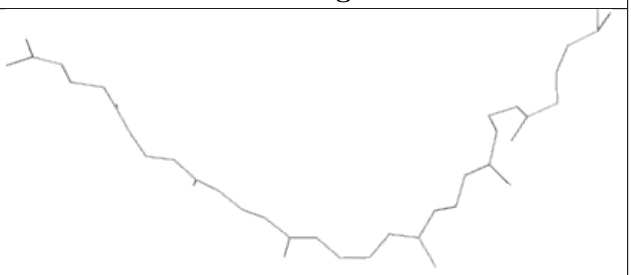
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Bond angles

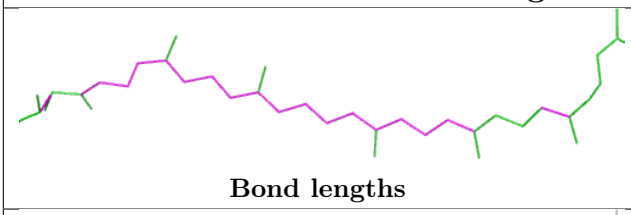


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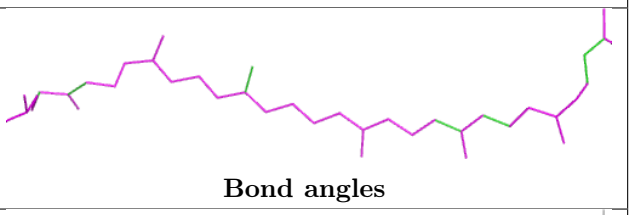


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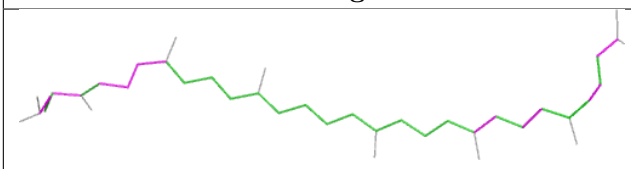
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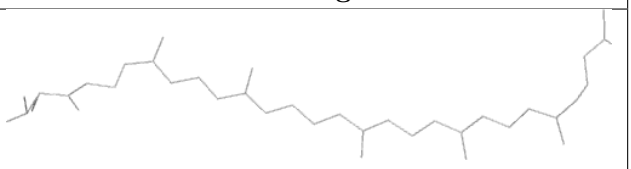
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Bond angles

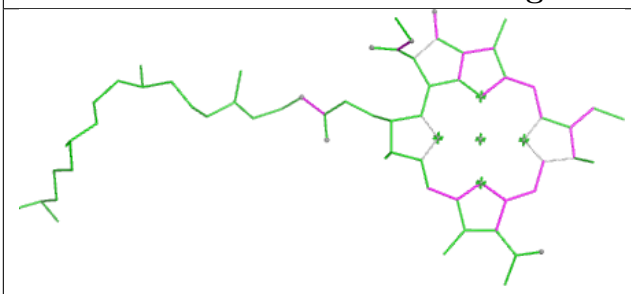


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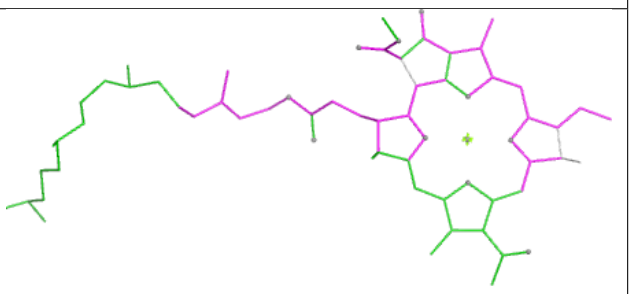


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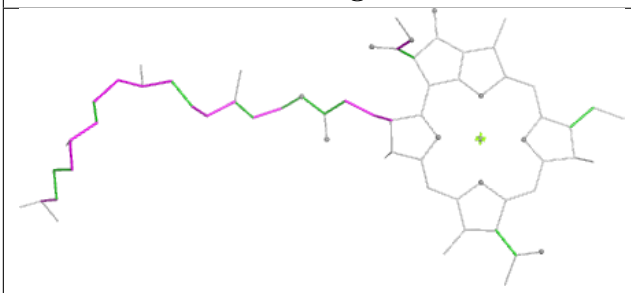
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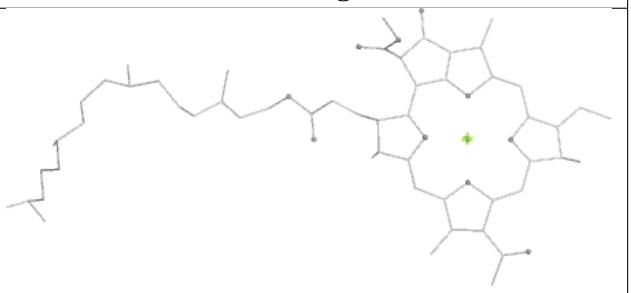
Bond lengths



Bond angles

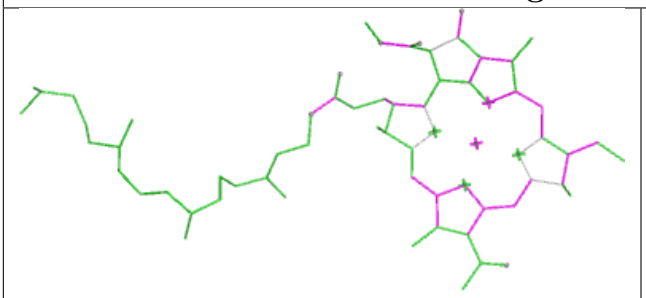


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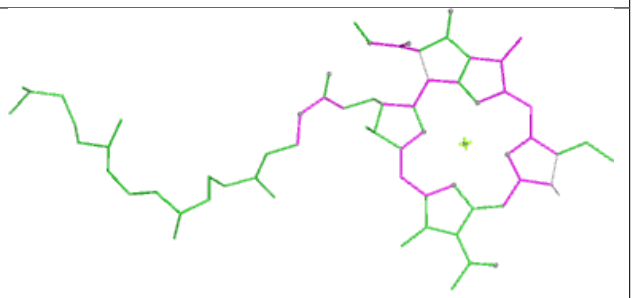


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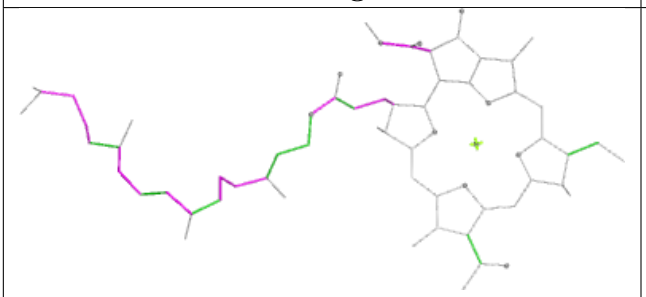
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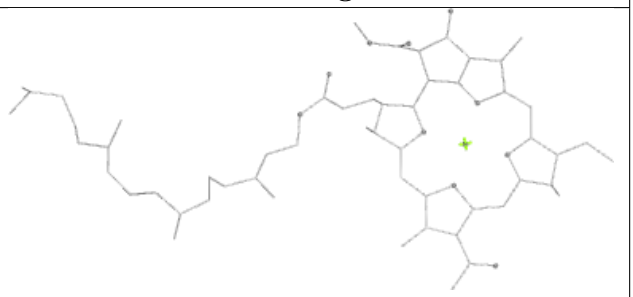
Bond lengths



Bond angles

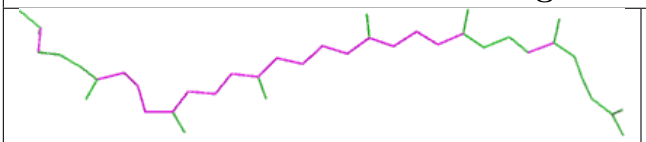


Torsions



Rings

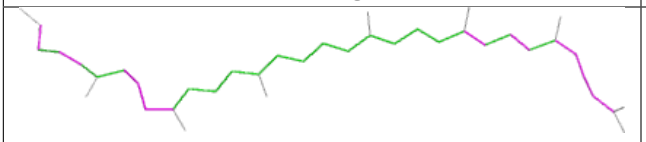
Ligand NS0 f 102



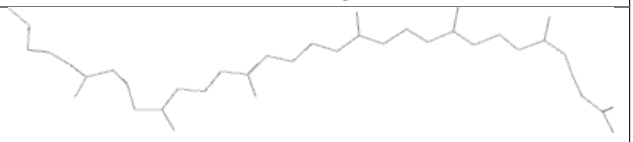
Bond lengths



Bond angles

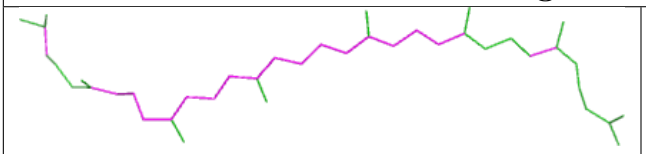


Torsions

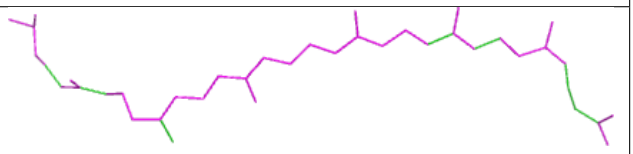


Rings

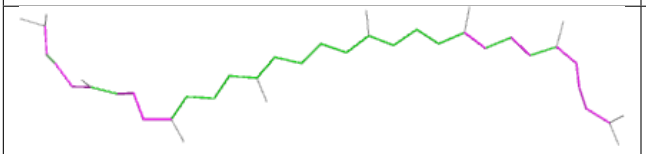
Ligand NS0 l 102



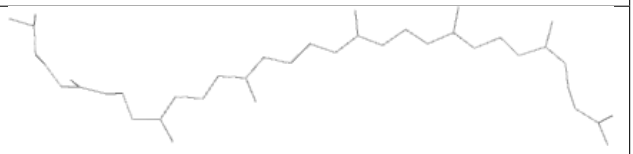
Bond lengths



Bond angles

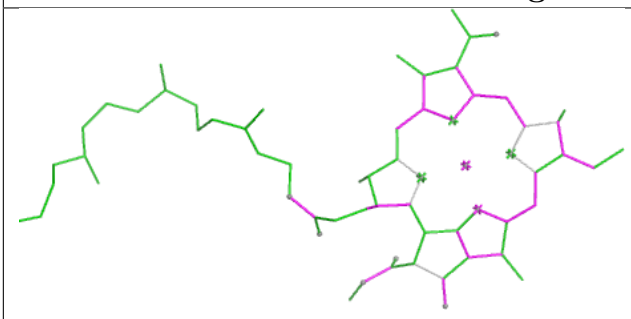


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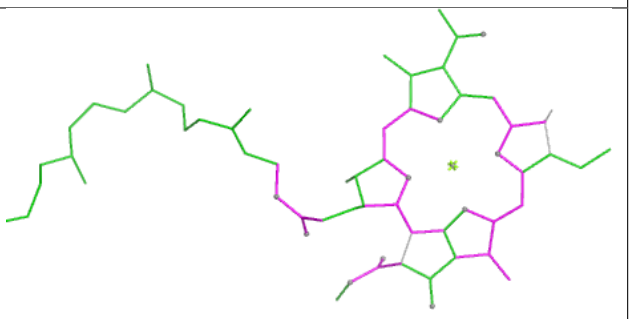


Rings

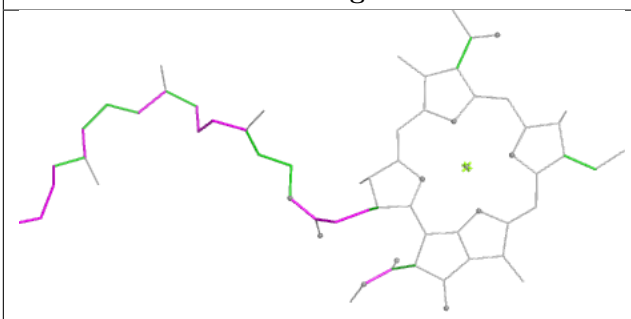
Ligand BCB c 101



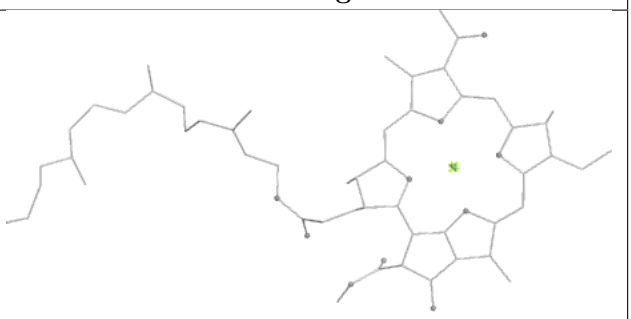
Bond lengths



Bond angles

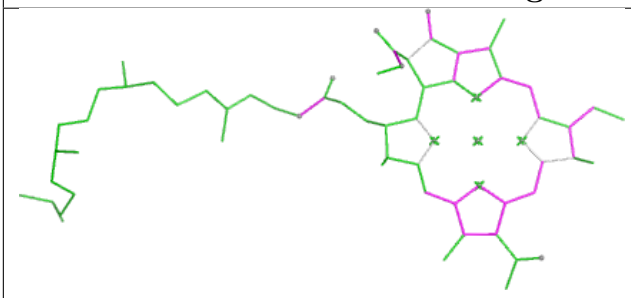


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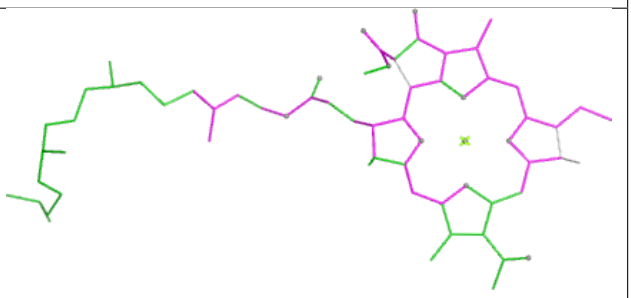


Rings

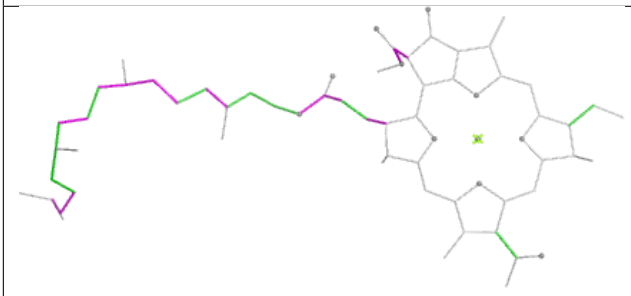
Ligand BCB n 101



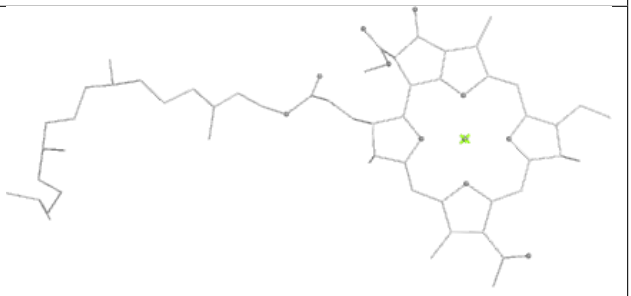
Bond lengths



Bond angles

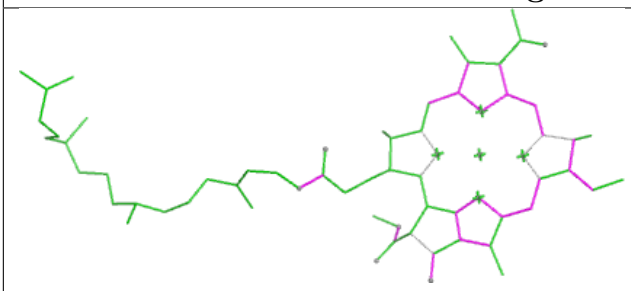


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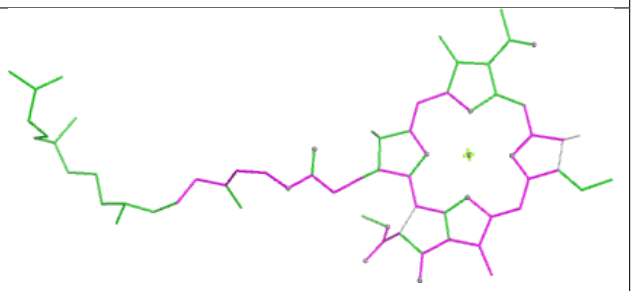


Rings

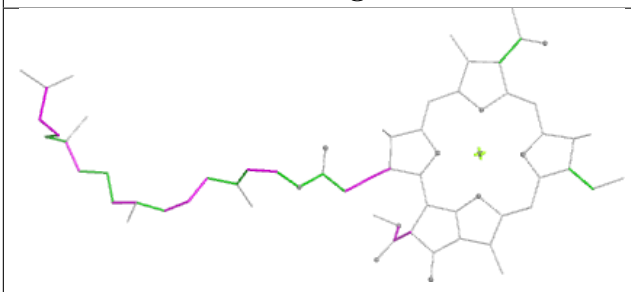
Ligand BCB 3 101



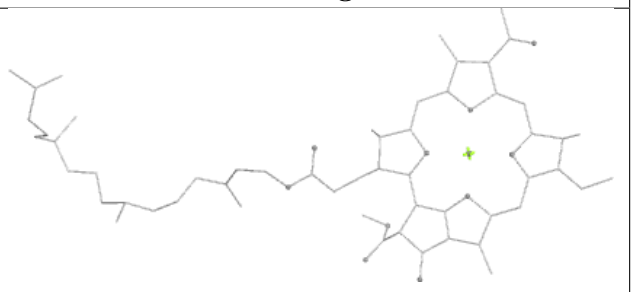
Bond lengths



Bond angles

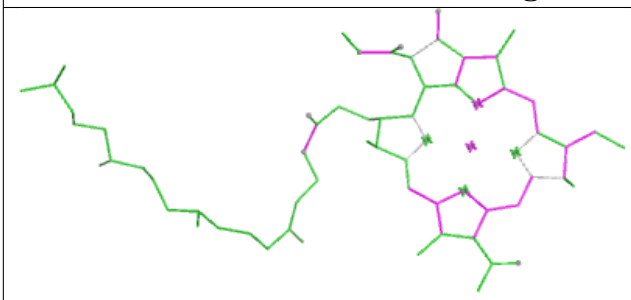


Torsions

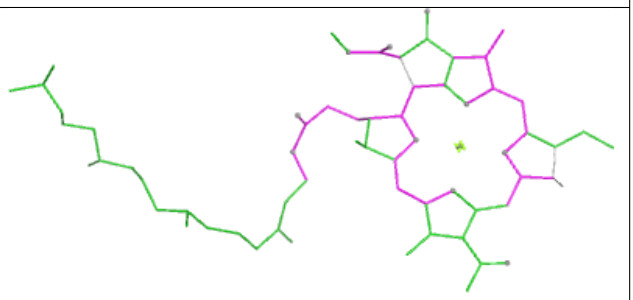


Rings

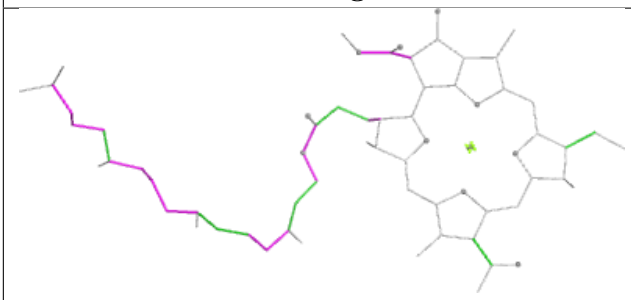
Ligand BCB G 101



Bond lengths



Bond angles

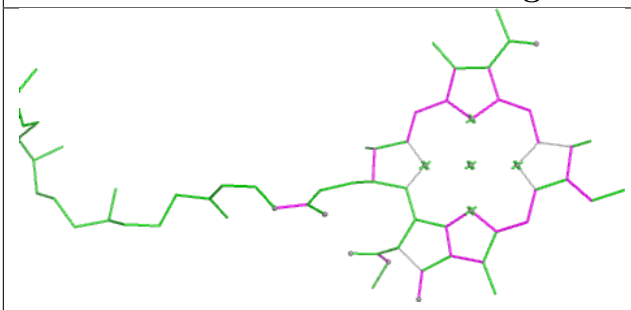


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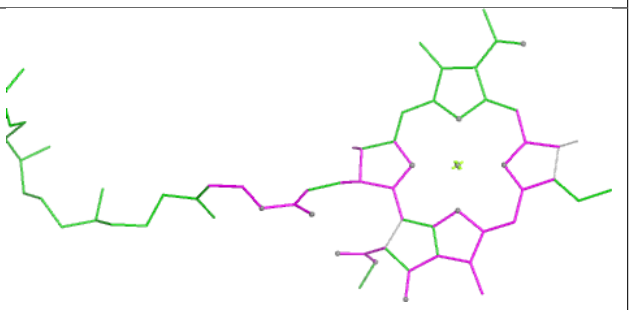


Rings

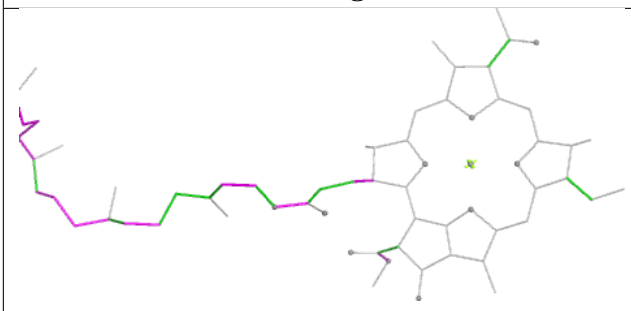
Ligand BCB w 101



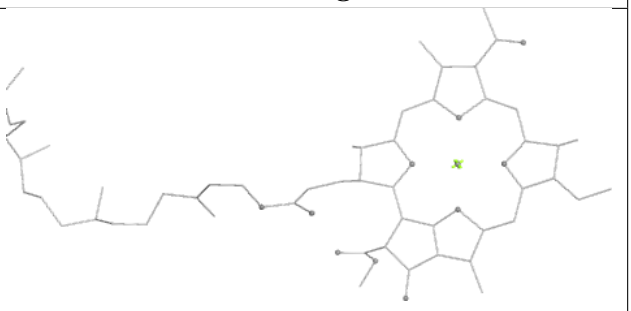
Bond lengths



Bond angles

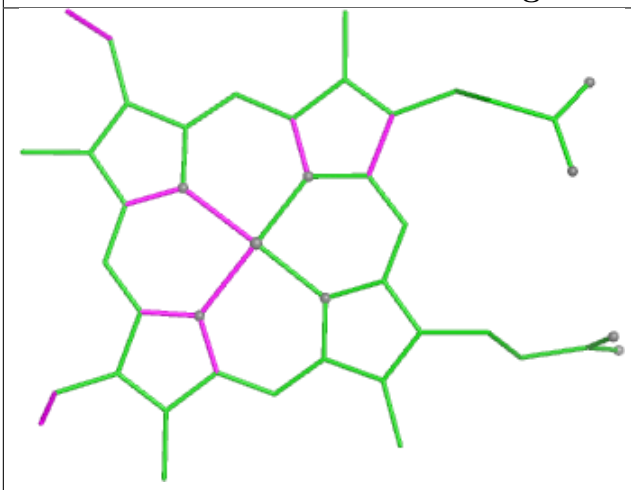


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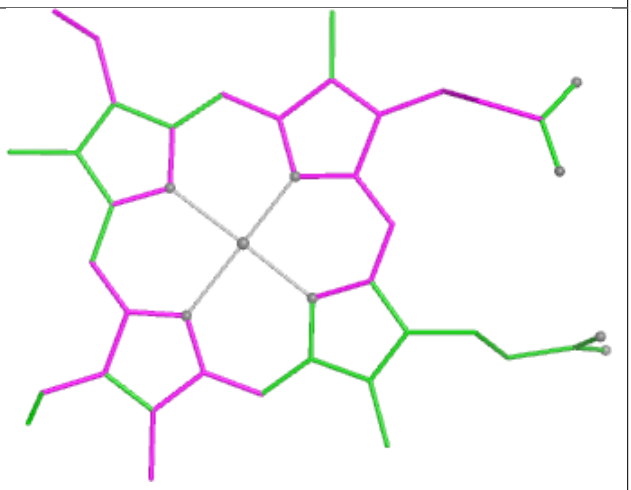


Rings

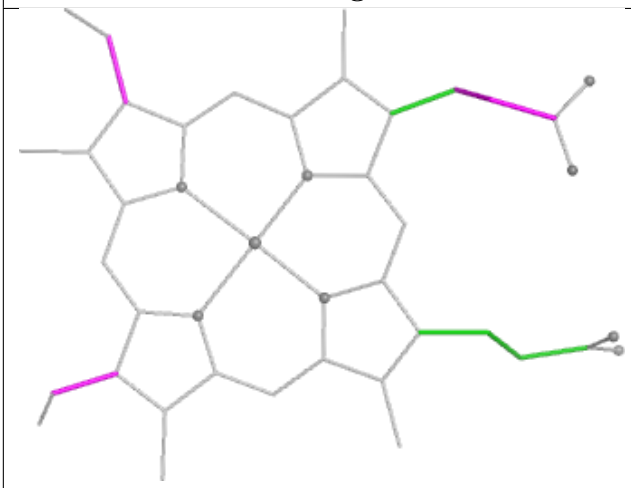
Ligand HEC C 404



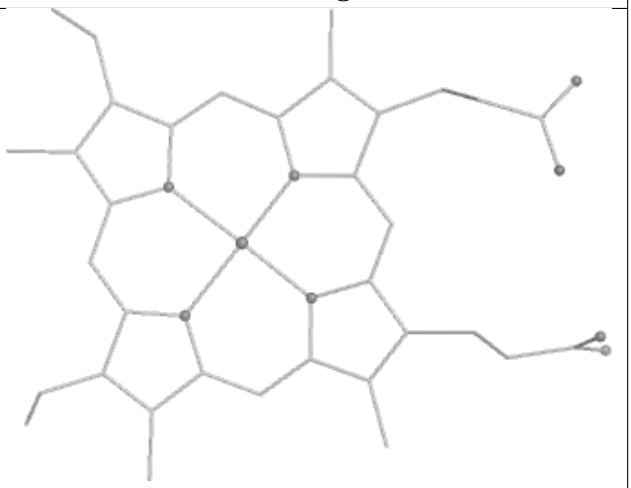
Bond lengths



Bond angles

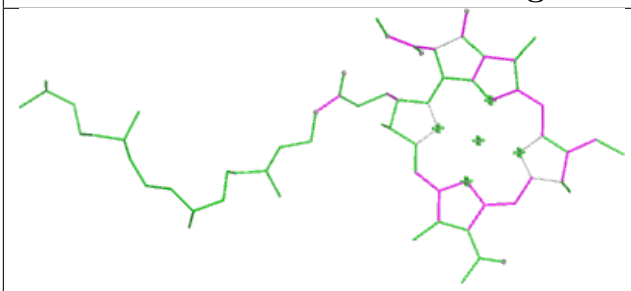


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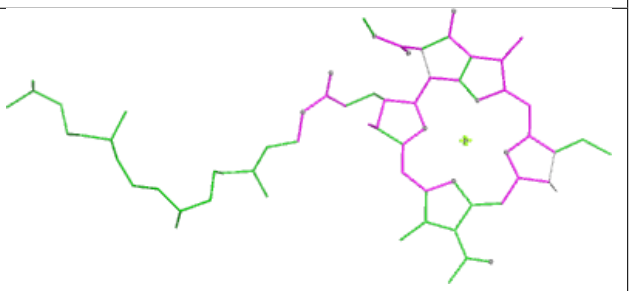


Rings

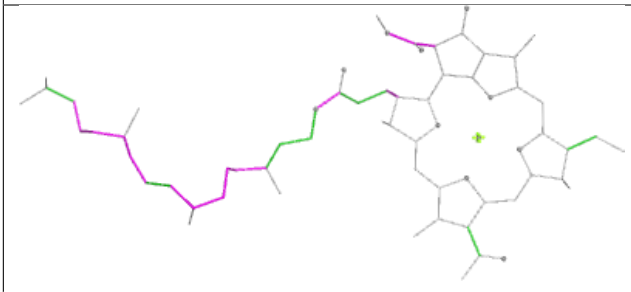
Ligand BCB 1 101



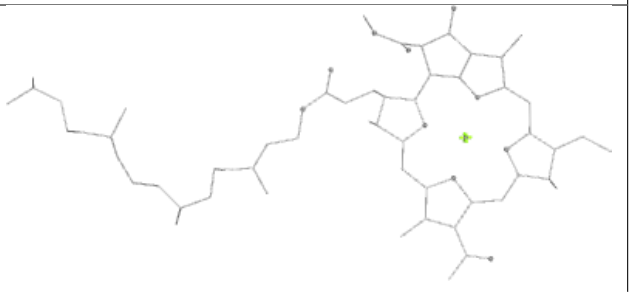
Bond lengths



Bond angles

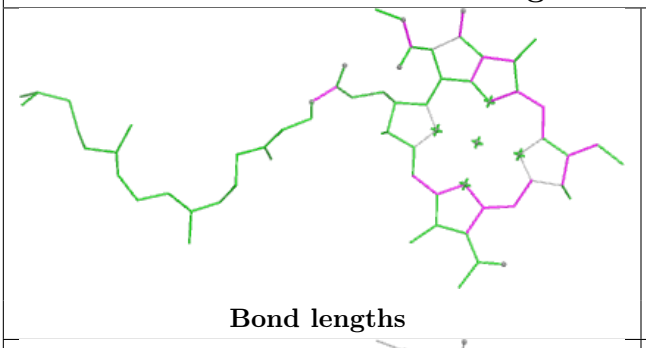


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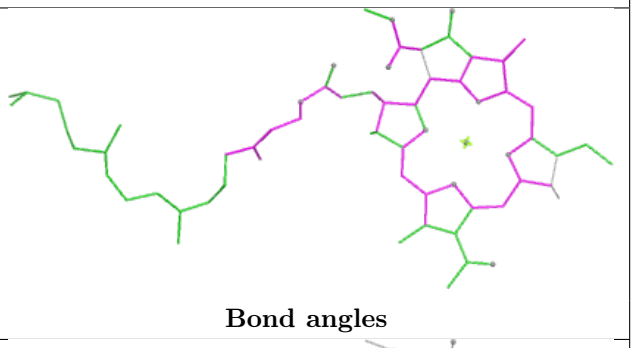


Rings

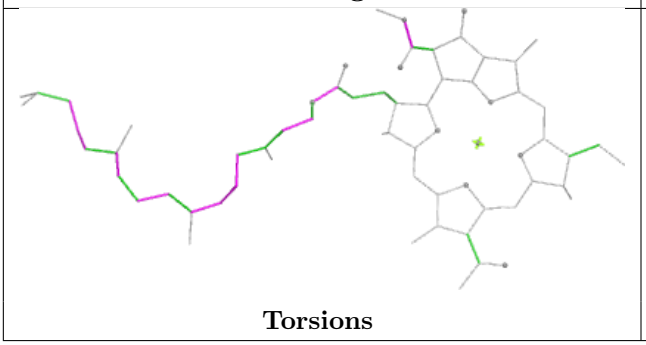
Ligand BCB 7 101



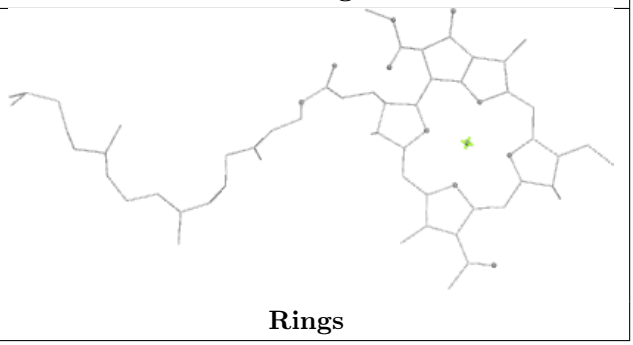
Bond lengths



Bond angles

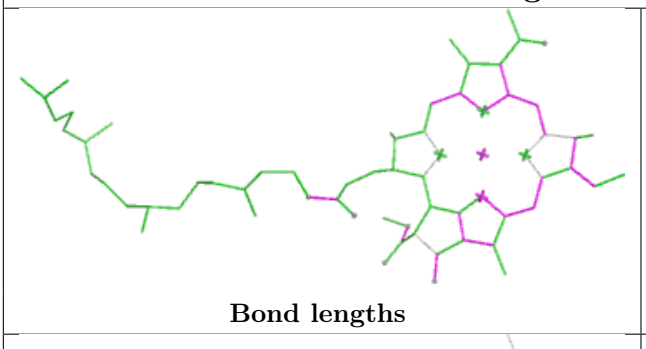


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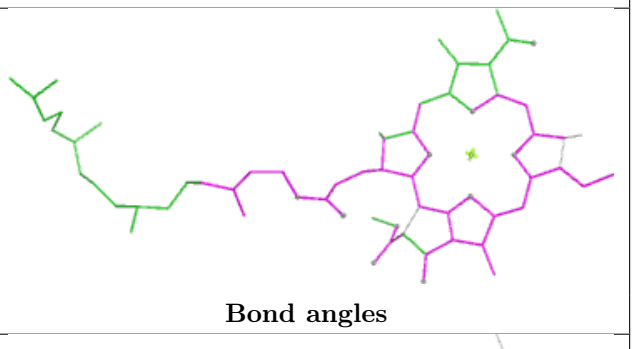


Rings

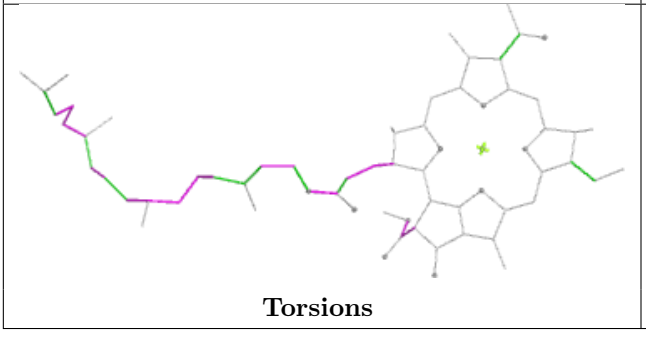
Ligand BCB P 101



Bond lengths



Bond angles

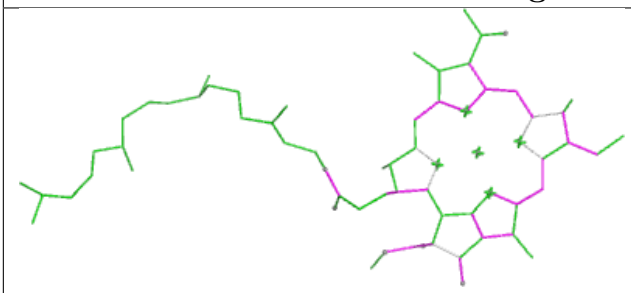


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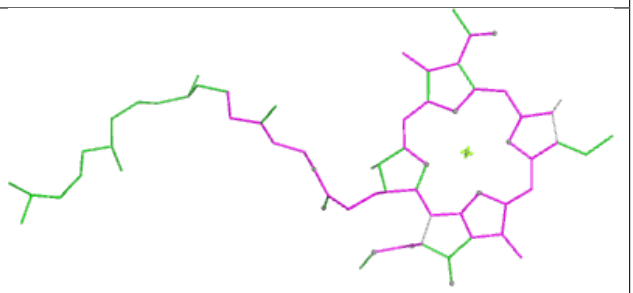


Rings

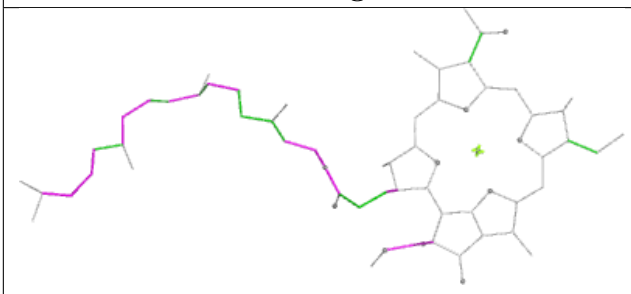
Ligand BCB r 101



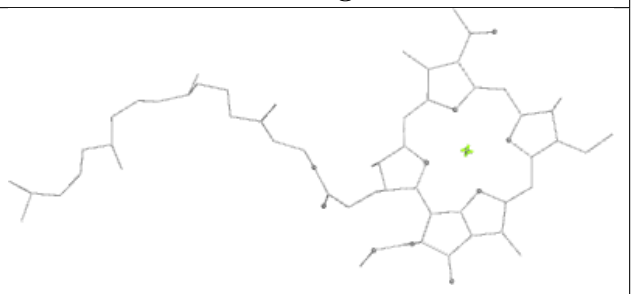
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage 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

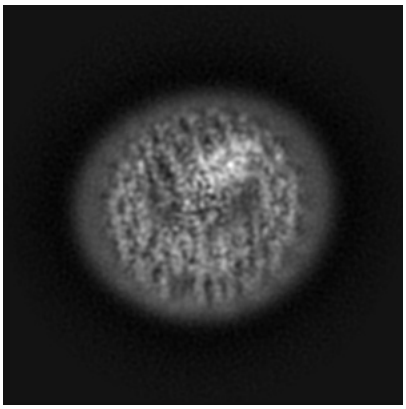
6 Map visualisation

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.

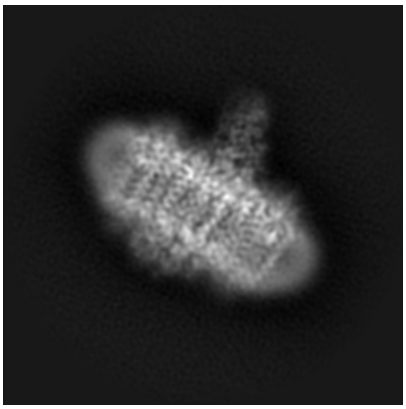
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

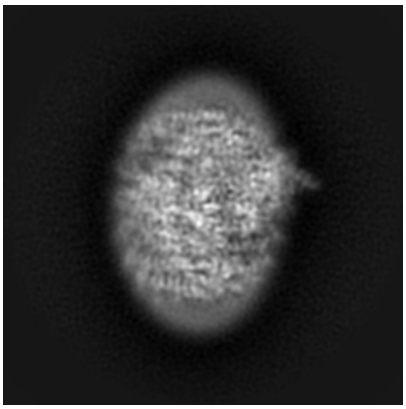
6.1.1 Primary map



X

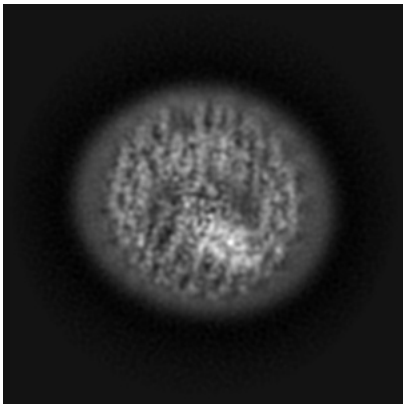


Y

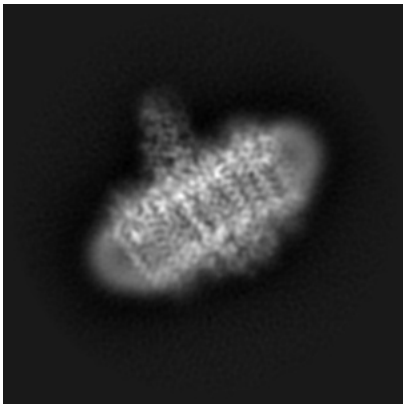


Z

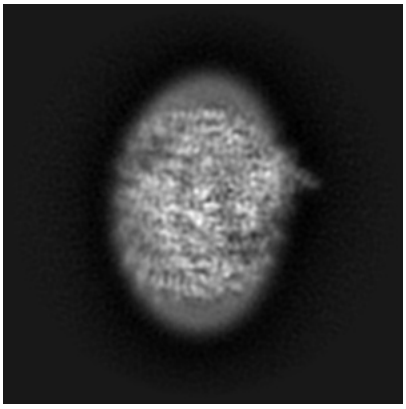
6.1.2 Raw map



X



Y

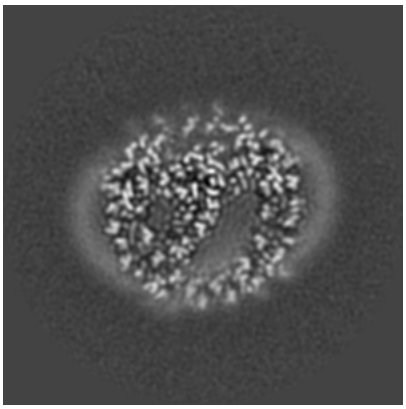


Z

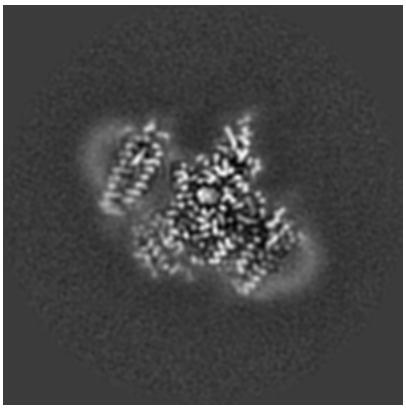
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

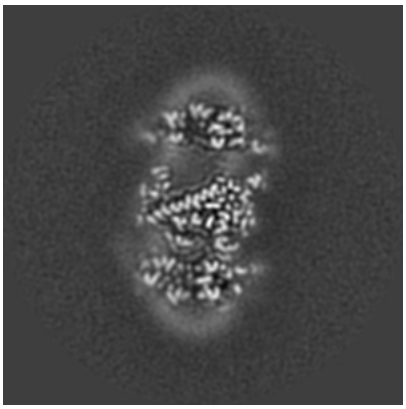
6.2.1 Primary map



X Index: 115

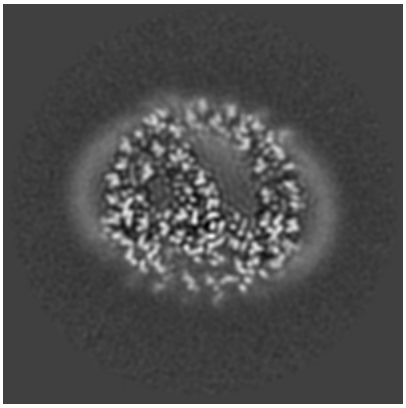


Y Index: 115

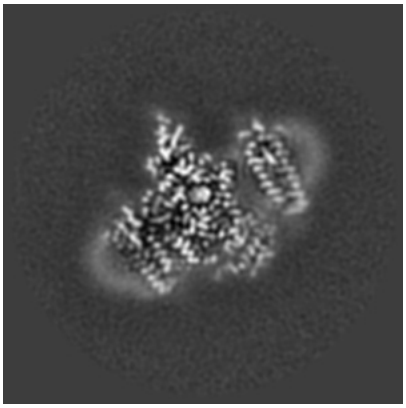


Z Index: 115

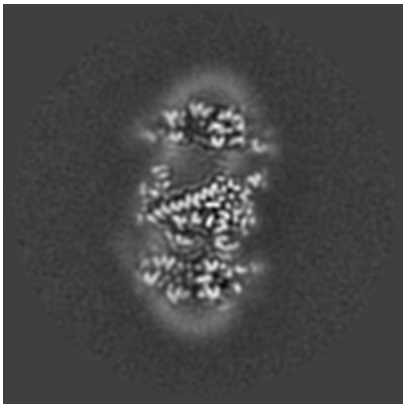
6.2.2 Raw map



X Index: 115



Y Index: 115

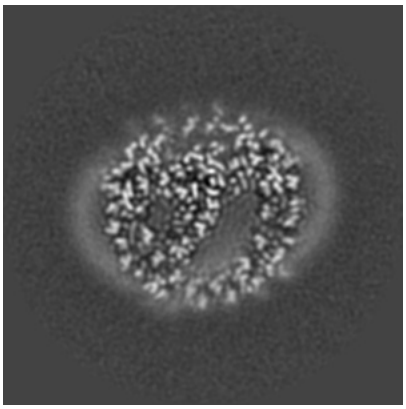


Z Index: 115

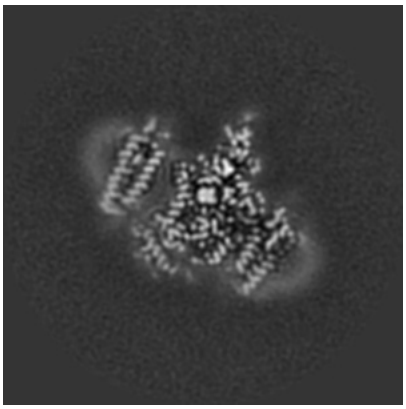
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

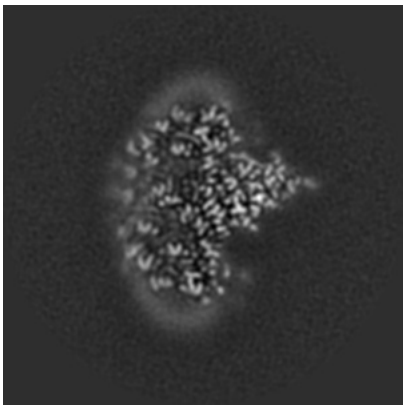
6.3.1 Primary map



X Index: 115

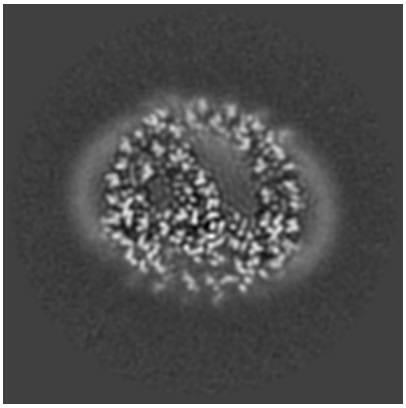


Y Index: 114

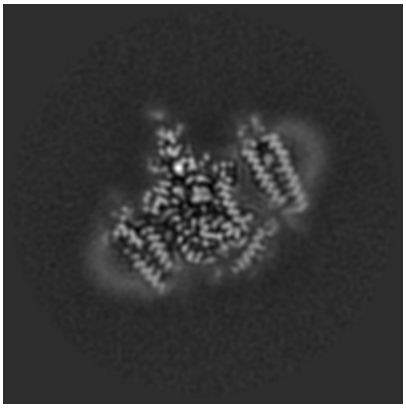


Z Index: 131

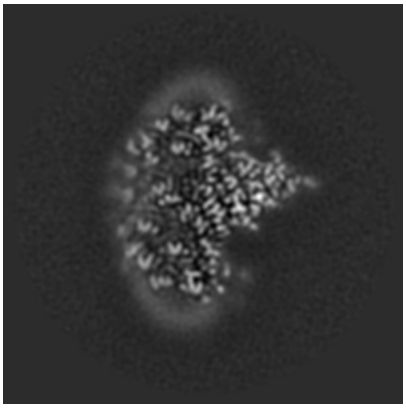
6.3.2 Raw map



X Index: 115



Y Index: 113

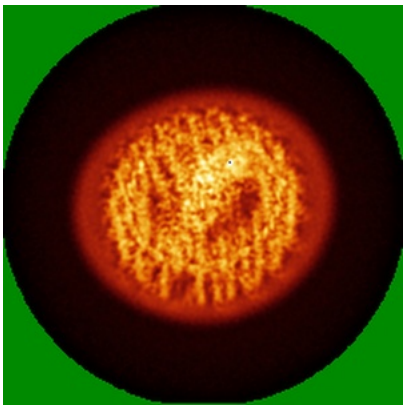


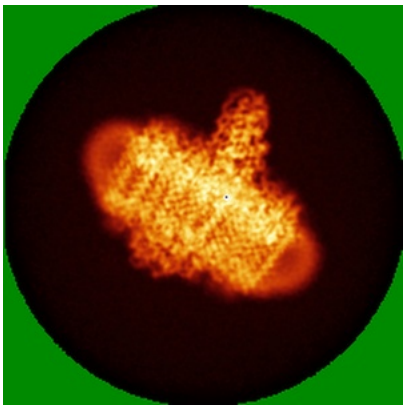
Z Index: 99

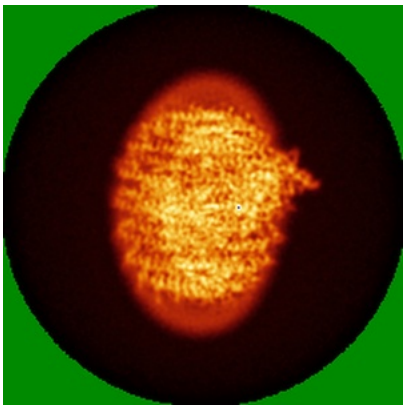
The images above show the largest variance slices of the map in three orthogonal directions.

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

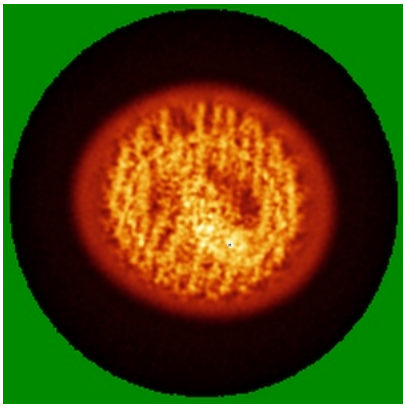
6.4.1 Primary map

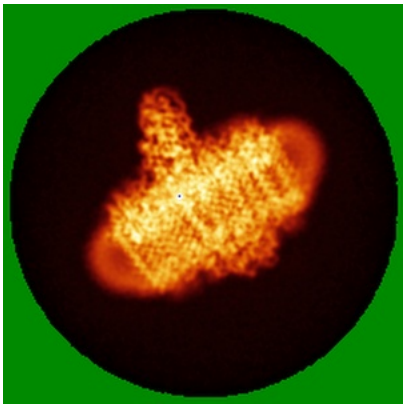

X

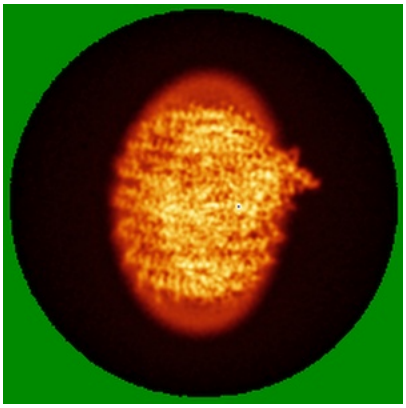

Y


Z

6.4.2 Raw map


X

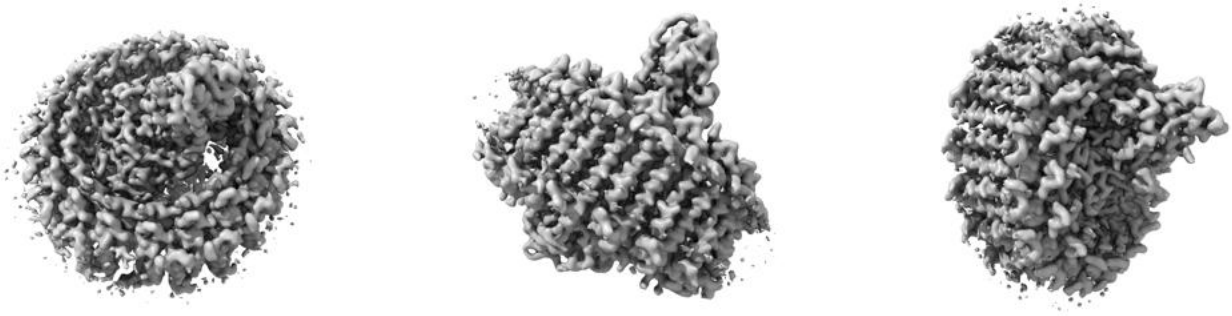

Y


Z

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

6.5 Orthogonal surface views (i)

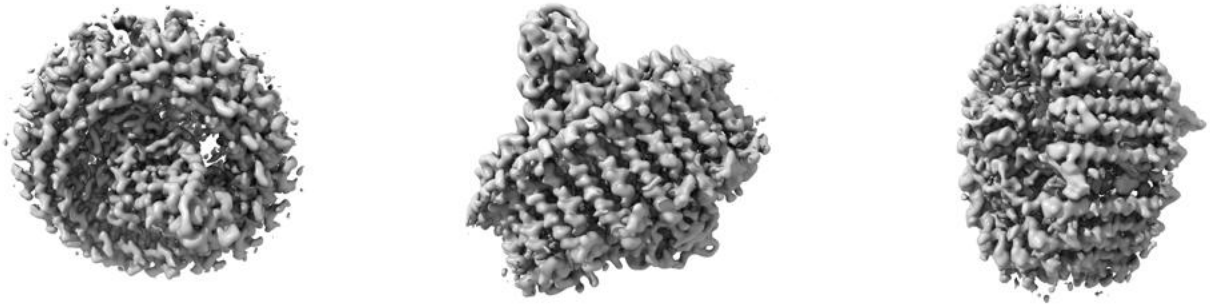
6.5.1 Primary map



X Y Z

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

6.5.2 Raw map



X Y Z

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

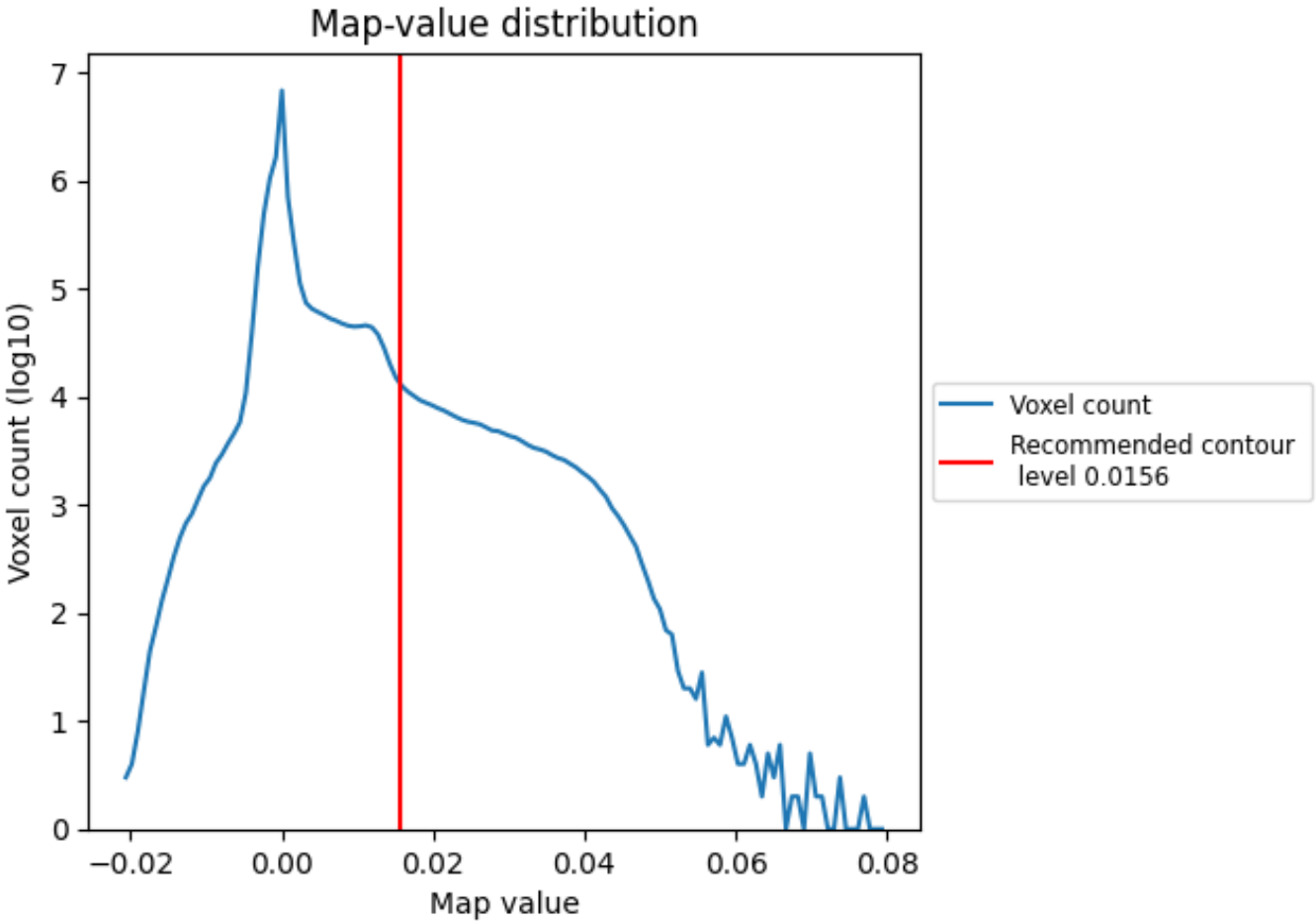
6.6 Mask visualisation (i)

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

7 Map analysis

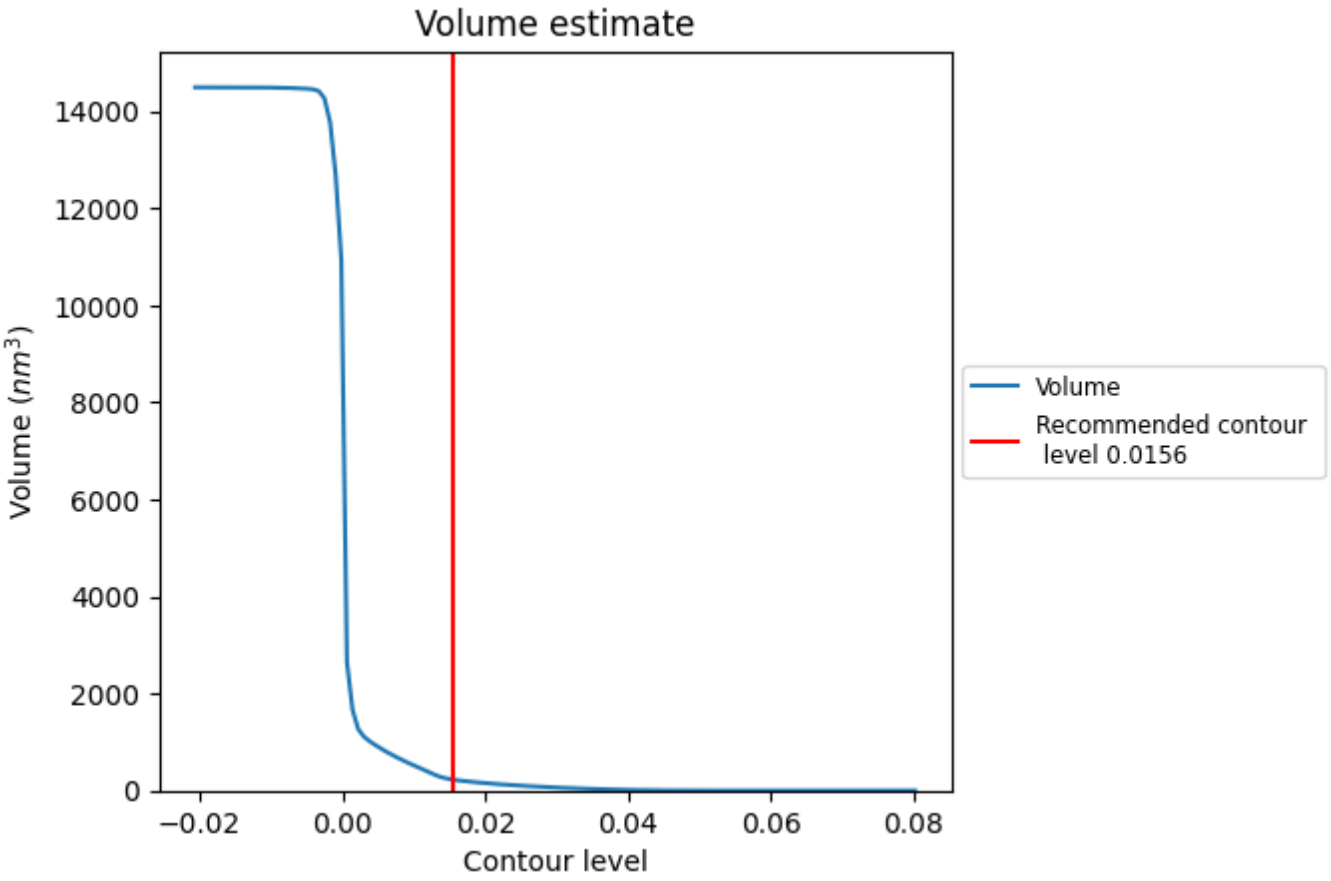
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

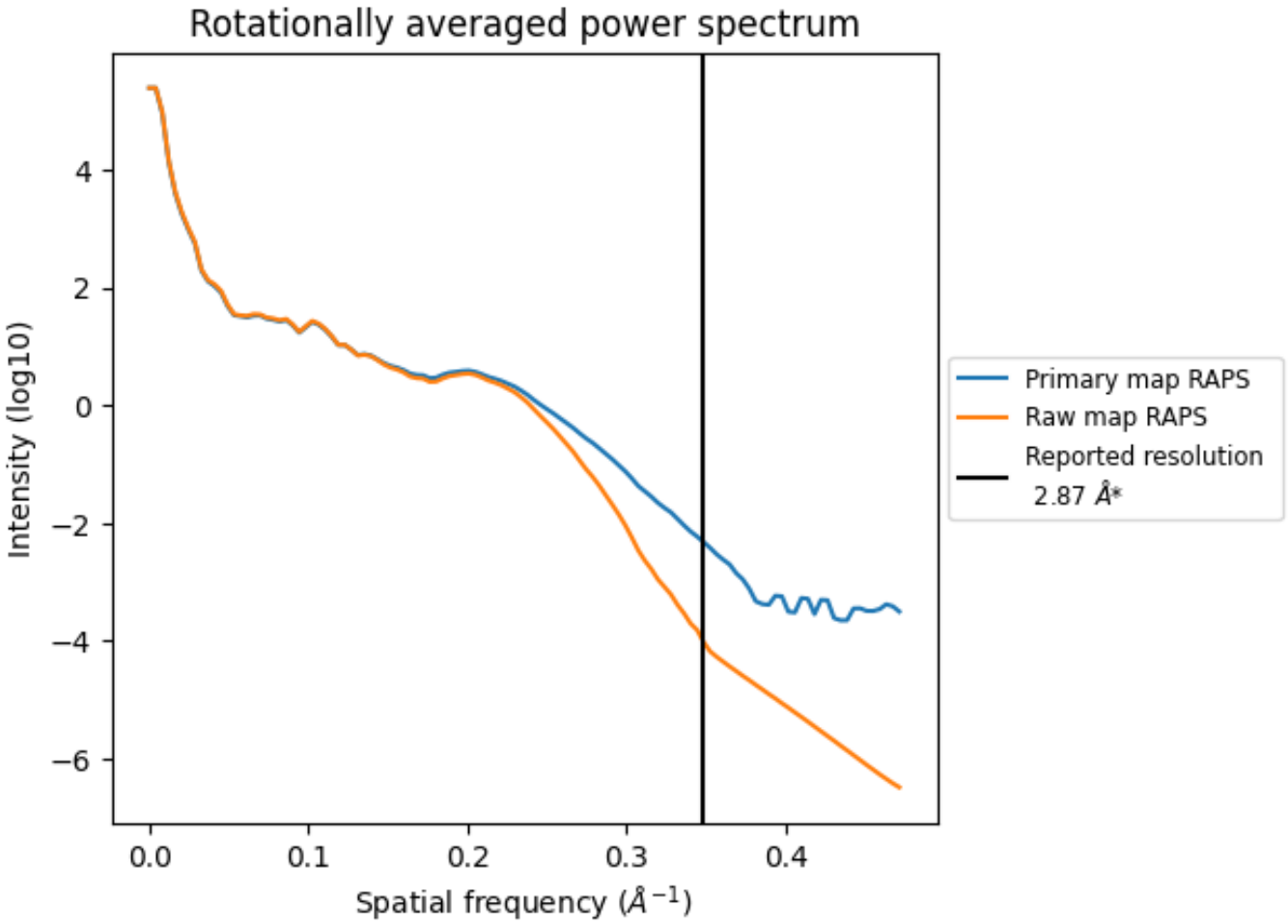
7.2 Volume estimate



The volume at the recommended contour level is 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)

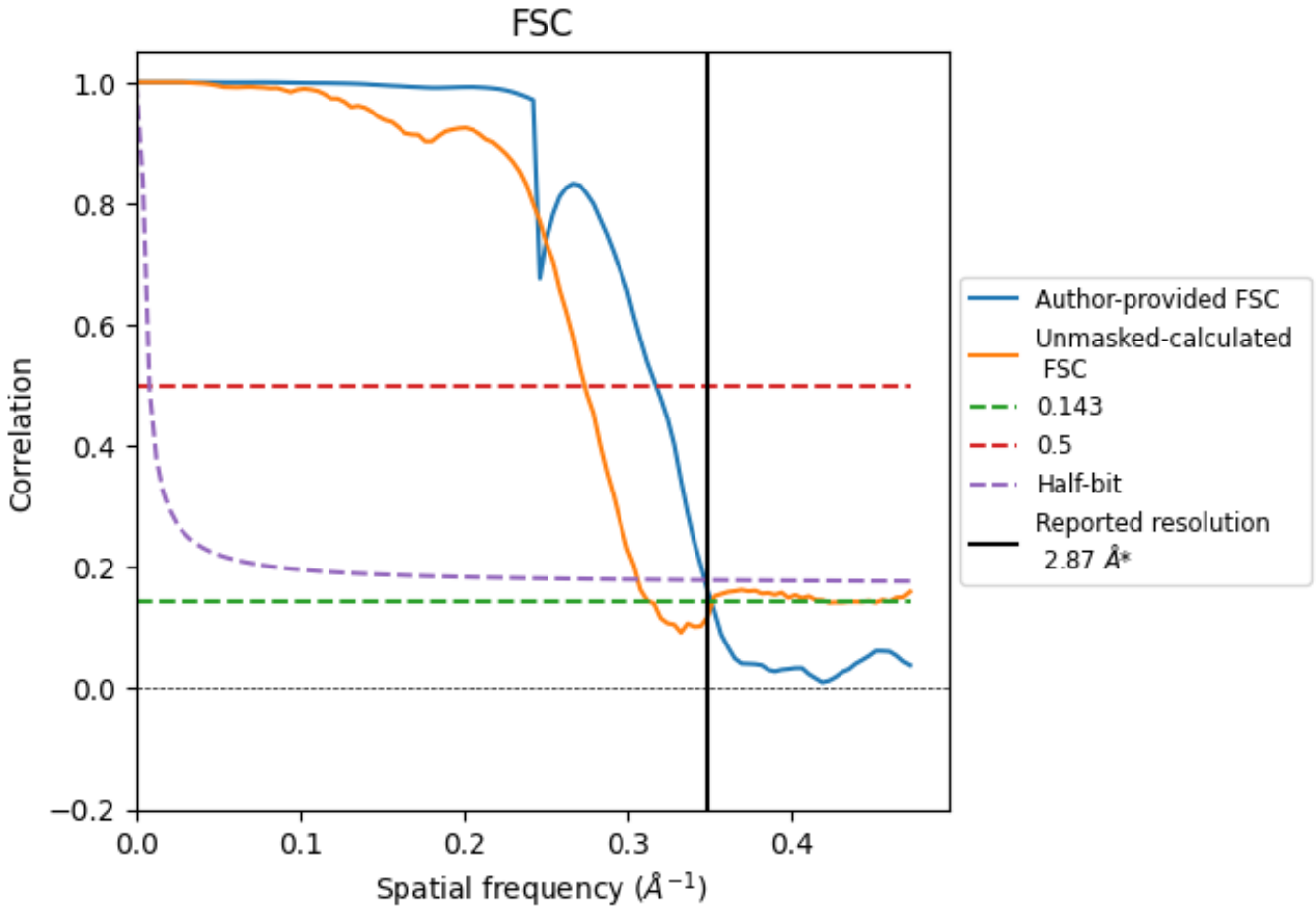


*Reported resolution corresponds to spatial frequency of 0.348 Å^{-1}

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)

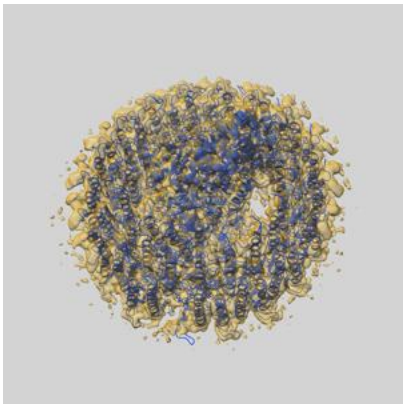
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.87	-	-
Author-provided FSC curve	2.85	3.16	2.88
Unmasked-calculated*	3.19	3.66	3.27

*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 %

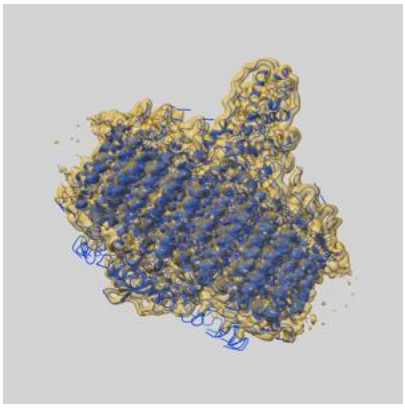
9 Map-model fit

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 19.

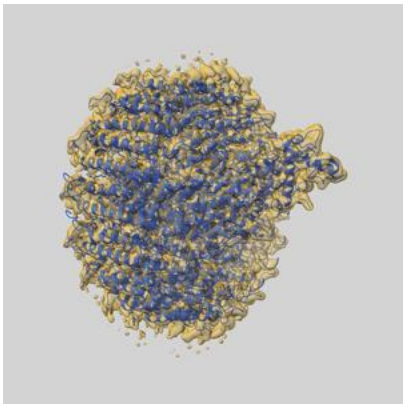
9.1 Map-model overlay



X



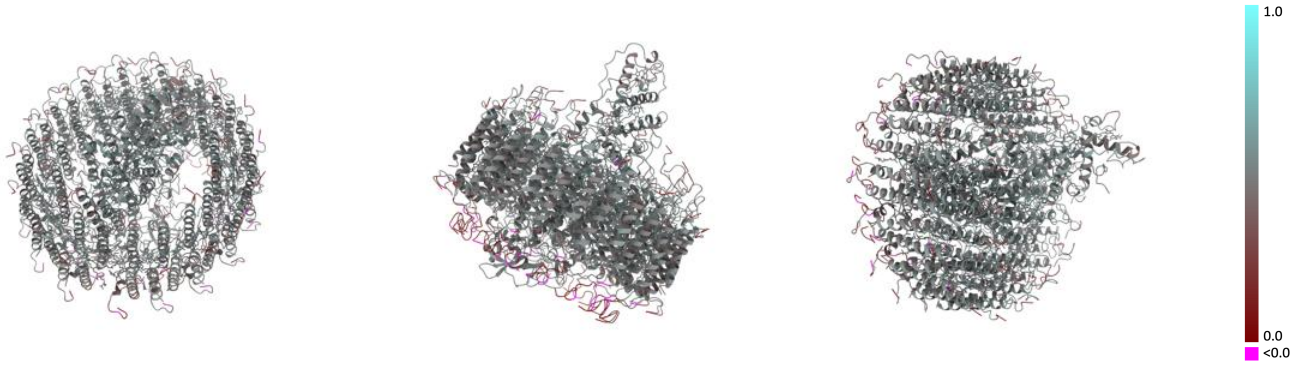
Y



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.

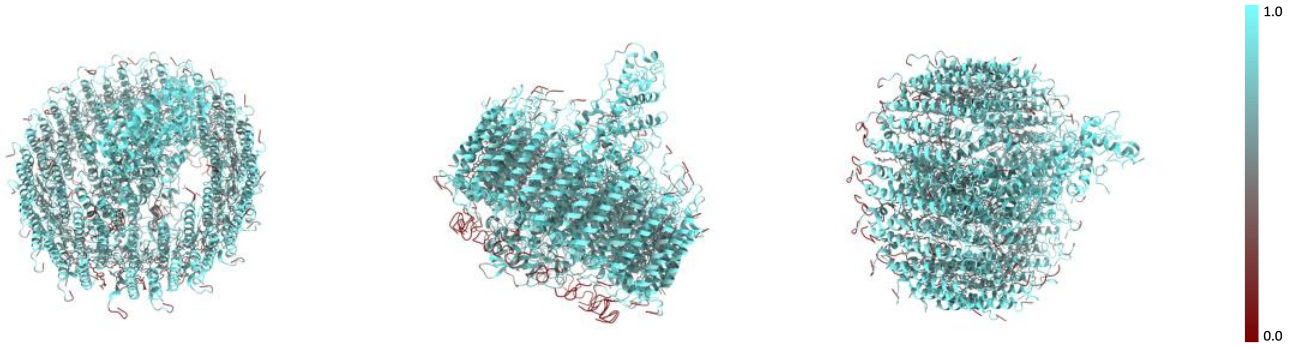
9.2 Q-score mapped to coordinate model (i)



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.

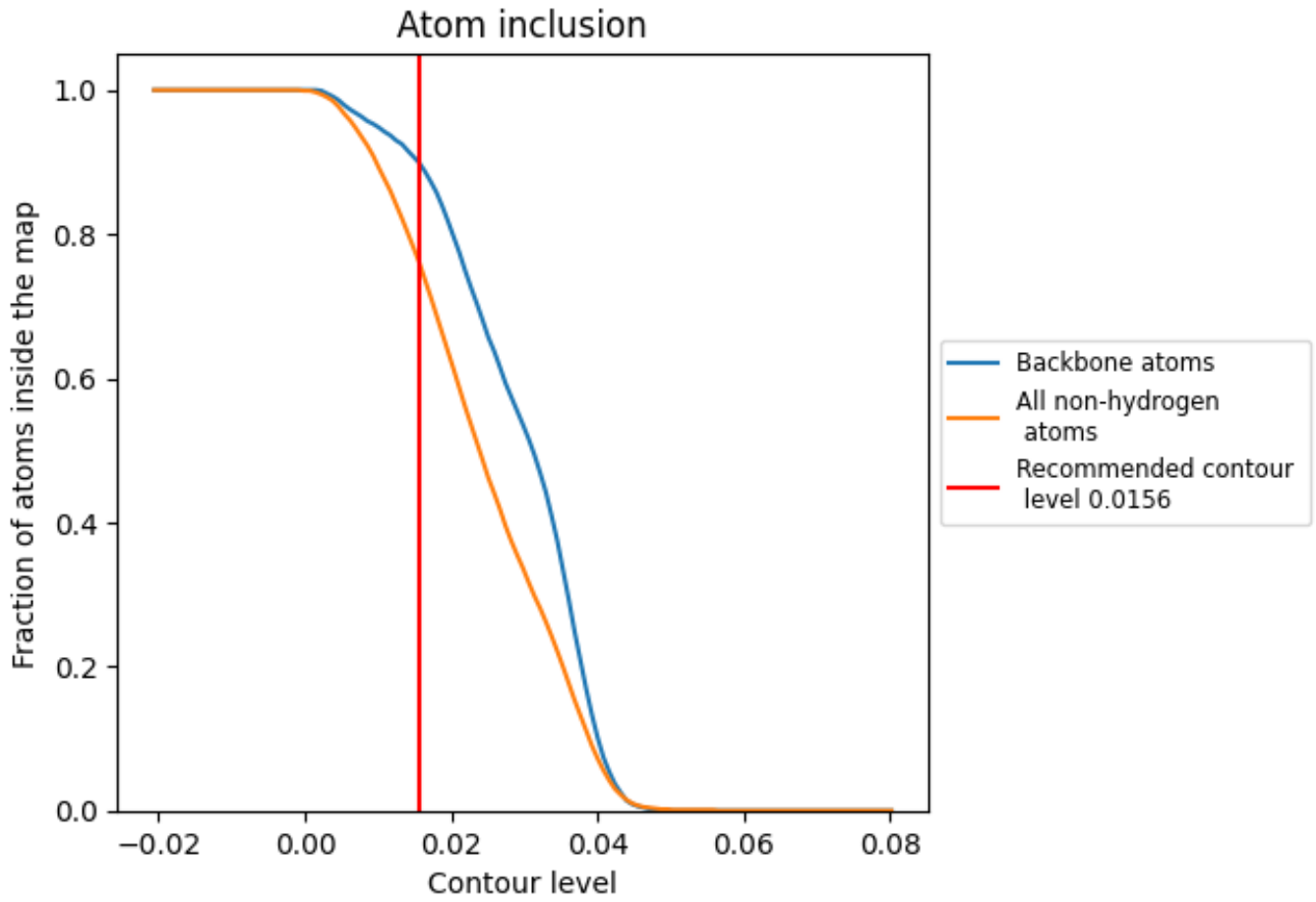
9.3 Atom inclusion mapped to coordinate model (i)



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	0.7610	0.4690
1	0.6930	0.4460
2	0.8080	0.4560
3	0.7880	0.4780
4	0.6890	0.4410
5	0.7310	0.4390
6	0.7020	0.4620
7	0.6530	0.4290
C	0.8860	0.5100
F	0.7130	0.4330
G	0.6440	0.4030
H	0.7060	0.4740
I	0.7930	0.4380
K	0.7640	0.4710
L	0.8380	0.5230
M	0.8380	0.5190
N	0.6910	0.4340
O	0.8190	0.4540
P	0.7770	0.4740
Q	0.6890	0.4420
R	0.7820	0.4430
S	0.7750	0.4760
T	0.7040	0.4310
U	0.8080	0.4460
V	0.7770	0.4840
W	0.6950	0.4290
X	0.7980	0.4380
Y	0.7840	0.4810
Z	0.6930	0.4240
a	0.6890	0.4280
b	0.7770	0.4800
c	0.6820	0.4320
d	0.7150	0.4370
e	0.7600	0.4720
f	0.7020	0.4280



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Chain	Atom inclusion	Q-score
g	0.7670	0.4430
h	0.7650	0.4820
i	0.6930	0.4330
j	0.6890	0.4310
k	0.7600	0.4730
l	0.6800	0.4370
m	0.7410	0.4320
n	0.7430	0.4710
o	0.6700	0.4190
p	0.7720	0.4490
q	0.7620	0.4670
r	0.6820	0.4260
s	0.8140	0.4490
t	0.7620	0.4760
u	0.6990	0.4280
v	0.7770	0.4320
w	0.7750	0.4780
x	0.7080	0.4330
y	0.8140	0.4540
z	0.7840	0.4870