Full wwPDB EM Validation Report ⓘ

Sep 15, 2026 – 04:28 pm BST

PDB ID	:	9H19 / pdb_00009h19
EMDB ID	:	EMD-51760
Title	:	Cryo-EM structure of RC-dLH complex model I from Gem. groenlandica strain TET16
Authors	:	Gardiner, A.; Qian, P.; Koblizek, M.; Jing, Y.; Joosten, M.; Jakobi, A.; Bina, D.; Mujakic, I.; Gardian, Z.; Kaftan, D.; Castro-Hartmann, P.
Deposited on	:	2024-10-09
Resolution	:	2.30 Å(reported)
Based on initial model	:	.

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:

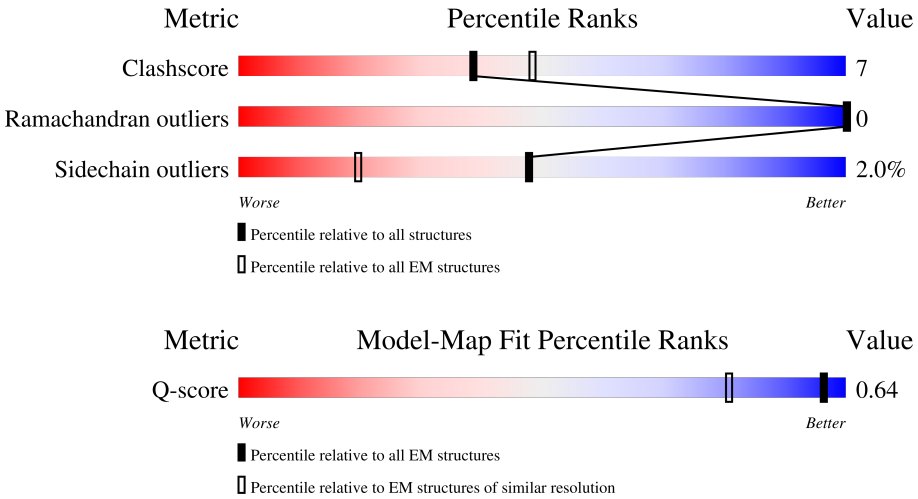
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 2.30 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	4254 (1.80 - 2.80)

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	Aa	71	11%, 92%, 6%
1	Ab	71	69%, 10%, 21%
1	Ac	71	65%, 14%, 21%

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Mol	Chain	Length	Quality of chain
1	Ad	71	69% 7% 24%
1	Ae	71	70% 13% 17%
1	Af	71	65% 14% 21%
1	Ag	71	6% 66% 14% 20%
1	Ah	71	70% 25%
1	Ai	71	68% 11% 20%
1	Aj	71	69% 10% 21%
1	Ak	71	73% 6% 21%
1	Al	71	87% 10%
1	Am	71	68% 6% 27%
1	An	71	76% 21%
1	Ao	71	69% 10% 21%
1	Ap	71	63% 14% 23%
2	BA	44	84% 7% 9%
2	BB	44	5% 59% 23% 7% 11%
2	BC	44	68% 23% 9%
2	BD	44	80% 11% 9%
2	BE	44	70% 16% 14%
2	BF	44	59% 30% 11%
2	BG	44	68% 20% 11%
2	BH	44	5% 77% 7% 5% 11%
2	BI	44	77% 9% 14%
2	BJ	44	84% 7% 9%
2	BK	44	7% 61% 27% 11%
2	BL	44	66% 23% 11%

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Mol	Chain	Length	Quality of chain
2	BM	44	77% 14% 9%
2	BN	44	66% 23% 11%
2	BO	44	70% 18% 11%
2	BP	44	66% 25% 9%
2	BQ	44	73% 16% 11%
2	BR	44	68% 20% 11%
2	BS	44	64% 25% 11%
2	BT	44	11% 70% 18% 11%
2	BU	44	5% 77% 11% 11%
2	BV	44	77% 16% 7%
2	BW	44	77% 14% 9%
2	BX	44	73% 18% 9%
2	Ba	44	11% 75% 7% 5% 14%
2	Bb	44	66% 20% 14%
2	Bc	44	66% 20% 14%
2	Bd	44	5% 73% 11% 16%
2	Be	44	5% 68% 18% 14%
2	Bf	44	68% 9% 23%
2	Bg	44	5% 70% 16% 14%
2	Bh	44	5% 66% 16% 18%
2	Bi	44	7% 68% 18% 14%
2	Bj	44	73% 14% 14%
2	Bk	44	75% 11% 14%
2	Bl	44	70% 14% 14%
2	Bm	44	70% 14% 14%

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Mol	Chain	Length	Quality of chain
2	Bn	44	75% 11% 14%
2	Bo	44	7% 66% 20% 14%
2	Bp	44	61% 18% 20%
3	S	204	45% 6% 50%
4	L	274	85% 14%
5	M	392	73% 12% 15%
6	H	60	12% 90% 10%
7	K	179	12% 88% 12%
8	C	373	70% 10% 20%
9	AA	56	79% 7% 14%
9	AB	56	68% 18% 14%
9	AC	56	71% 14% 14%
9	AD	56	66% 21% 12%
9	AE	56	73% 12% 12%
9	AF	56	71% 16% 12%
9	AG	56	5% 62% 25% 12%
9	AH	56	70% 16% 12%
9	AI	56	77% 11% 12%
9	AJ	56	77% 7% 14%
9	AK	56	5% 75% 11% 14%
9	AL	56	71% 14% 14%
9	AM	56	77% 11% 12%
9	AN	56	71% 14% 14%
9	AO	56	70% 16% 14%
9	AP	56	70% 14% 14%

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Mol	Chain	Length	Quality of chain
9	AQ	56	5% 71% 14% 12%
9	AR	56	80% 5% 14%
9	AS	56	68% 20% 12%
9	AT	56	5% 70% 14% 14%
9	AU	56	73% 12% 14%
9	AV	56	77% 9% 14%
9	AW	56	64% 23% 12%
9	AX	56	73% 12% 14%

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
11	BCL	Ao	101	-	-	X	-
19	HEC	C	402	X	-	-	-
19	HEC	C	403	X	-	-	-
19	HEC	C	404	X	-	-	-
19	HEC	C	405	X	-	-	-

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 49808 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 Light-harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Aa	69	Total	C	N	O	S	0	0
			520	340	90	86	4		
1	Ab	56	Total	C	N	O	S	0	0
			437	287	77	70	3		
1	Ac	56	Total	C	N	O	S	0	0
			440	289	77	70	4		
1	Ad	54	Total	C	N	O	S	0	0
			426	281	75	67	3		
1	Ae	59	Total	C	N	O	S	0	0
			454	298	80	73	3		
1	Af	56	Total	C	N	O	S	0	0
			440	289	77	70	4		
1	Ag	57	Total	C	N	O	S	0	0
			445	292	78	71	4		
1	Ah	53	Total	C	N	O	S	0	0
			411	272	69	67	3		
1	Ai	57	Total	C	N	O	S	0	0
			445	292	78	71	4		
1	Aj	56	Total	C	N	O	S	0	0
			437	287	77	70	3		
1	Ak	56	Total	C	N	O	S	0	0
			440	289	77	70	4		
1	Al	69	Total	C	N	O	S	0	0
			520	340	90	86	4		
1	Am	52	Total	C	N	O	S	0	0
			417	276	73	65	3		
1	An	56	Total	C	N	O	S	0	0
			440	289	77	70	4		
1	Ao	56	Total	C	N	O	S	0	0
			437	287	77	70	3		
1	Ap	55	Total	C	N	O	S	0	0
			432	284	76	69	3		

- Molecule 2 is a protein called Light-harvesting protein.

Mol	Chain	Residues	Atoms	AltConf	Trace
2	Ba	38	Total C N O S 324 218 55 50 1	0	0
2	Bb	38	Total C N O S 324 218 55 50 1	0	0
2	Bc	38	Total C N O S 324 218 55 50 1	0	0
2	Bd	37	Total C N O 316 213 54 49	0	0
2	Be	38	Total C N O S 324 218 55 50 1	0	0
2	Bf	34	Total C N O 292 200 51 41	0	0
2	Bg	38	Total C N O S 324 218 55 50 1	0	0
2	Bh	36	Total C N O 309 209 53 47	0	0
2	Bi	38	Total C N O S 324 218 55 50 1	0	0
2	Bj	38	Total C N O S 324 218 55 50 1	0	0
2	Bk	38	Total C N O S 324 218 55 50 1	0	0
2	Bl	38	Total C N O S 324 218 55 50 1	0	0
2	Bm	38	Total C N O S 324 218 55 50 1	0	0
2	Bn	38	Total C N O S 324 218 55 50 1	0	0
2	Bo	38	Total C N O S 324 218 55 50 1	0	0
2	Bp	35	Total C N O 300 204 52 44	0	0
2	BA	40	Total C N O S 332 222 57 52 1	0	0
2	BB	39	Total C N O S 328 220 56 51 1	0	0
2	BC	40	Total C N O S 332 222 57 52 1	0	0
2	BD	40	Total C N O S 332 222 57 52 1	0	0
2	BE	38	Total C N O S 324 218 55 50 1	0	0
2	BF	39	Total C N O S 328 220 56 51 1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	BG	39	Total	C	N	O	S	0	0
			328	220	56	51	1		
2	BH	39	Total	C	N	O	S	0	0
			328	220	56	51	1		
2	BI	38	Total	C	N	O	S	0	0
			324	218	55	50	1		
2	BJ	40	Total	C	N	O	S	0	0
			332	222	57	52	1		
2	BK	39	Total	C	N	O	S	0	0
			328	220	56	51	1		
2	BL	39	Total	C	N	O	S	0	0
			328	220	56	51	1		
2	BM	40	Total	C	N	O	S	0	0
			332	222	57	52	1		
2	BN	39	Total	C	N	O	S	0	0
			328	220	56	51	1		
2	BO	39	Total	C	N	O	S	0	0
			328	220	56	51	1		
2	BP	40	Total	C	N	O	S	0	0
			332	222	57	52	1		
2	BQ	39	Total	C	N	O	S	0	0
			328	220	56	51	1		
2	BR	39	Total	C	N	O	S	0	0
			328	220	56	51	1		
2	BS	39	Total	C	N	O	S	0	0
			328	220	56	51	1		
2	BT	39	Total	C	N	O	S	0	0
			328	220	56	51	1		
2	BU	39	Total	C	N	O	S	0	0
			328	220	56	51	1		
2	BV	41	Total	C	N	O	S	0	0
			341	228	59	53	1		
2	BW	40	Total	C	N	O	S	0	0
			332	222	57	52	1		
2	BX	40	Total	C	N	O	S	0	0
			332	222	57	52	1		

- Molecule 3 is a protein called reaction centre S sub unit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	S	103	Total	C	N	O	S	0	0
			800	498	150	148	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	271	Total	C	N	O	S	0	0
			2134	1435	346	342	11		

- Molecule 5 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	335	Total	C	N	O	S	0	0
			2697	1789	441	457	10		

- Molecule 6 is a protein called reaction centre Ht sub unit.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	60	Total	C	N	O	S	0	0
			510	338	85	85	2		

- Molecule 7 is a protein called reaction centre Hc sub unit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	179	Total	C	N	O	S	0	0
			1373	873	231	262	7		

- Molecule 8 is a protein called Photosynthetic reaction center cytochrome c subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	298	Total	C	N	O	S	0	0
			2330	1463	421	429	17		

- Molecule 9 is a protein called Light-harvesting protein.

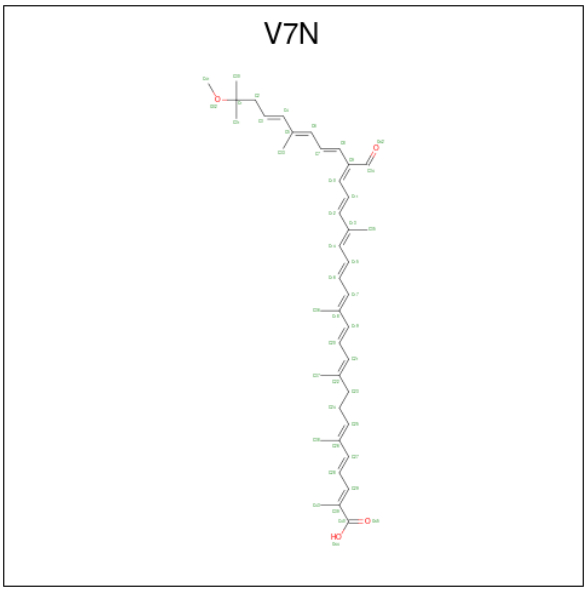
Mol	Chain	Residues	Atoms					AltConf	Trace
9	AA	48	Total	C	N	O	S	0	0
			391	262	65	60	4		
9	AB	48	Total	C	N	O	S	0	0
			391	262	65	60	4		
9	AC	48	Total	C	N	O	S	0	0
			391	262	65	60	4		
9	AD	49	Total	C	N	O	S	0	0
			400	267	67	62	4		
9	AE	49	Total	C	N	O	S	0	0
			400	267	67	62	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
9	AF	49	Total	C	N	O	S	0	0
			400	267	67	62	4		
9	AG	49	Total	C	N	O	S	0	0
			400	267	67	62	4		
9	AH	49	Total	C	N	O	S	0	0
			400	267	67	62	4		
9	AI	49	Total	C	N	O	S	0	0
			400	267	67	62	4		
9	AJ	48	Total	C	N	O	S	0	0
			391	262	65	60	4		
9	AK	48	Total	C	N	O	S	0	0
			392	262	66	61	3		
9	AL	48	Total	C	N	O	S	0	0
			391	262	65	60	4		
9	AM	49	Total	C	N	O	S	0	0
			400	267	67	62	4		
9	AN	48	Total	C	N	O	S	0	0
			392	262	66	61	3		
9	AO	48	Total	C	N	O	S	0	0
			391	262	65	60	4		
9	AP	48	Total	C	N	O	S	0	0
			391	262	65	60	4		
9	AQ	49	Total	C	N	O	S	0	0
			400	267	67	62	4		
9	AR	48	Total	C	N	O	S	0	0
			391	262	65	60	4		
9	AS	49	Total	C	N	O	S	0	0
			400	267	67	62	4		
9	AT	48	Total	C	N	O	S	0	0
			392	262	66	61	3		
9	AU	48	Total	C	N	O	S	0	0
			392	262	66	61	3		
9	AV	48	Total	C	N	O	S	0	0
			391	262	65	60	4		
9	AW	49	Total	C	N	O	S	0	0
			400	267	67	62	4		
9	AX	48	Total	C	N	O	S	0	0
			391	262	65	60	4		

- Molecule 10 is (2 {E},4 {E},6 {E},10 {E},12 {E},14 {E},16 {E},18 {E},20 {E},22 {Z},24 {E},26 {E},28 {E})-23-methanoyl-31-methoxy-2,6,10,14,19,27,31-heptamethyl-dotriaconta-2,4,6,10,12,14,16,18,20,22,24,26,28-tridecaenoic acid (CCD ID: V7N) (formula: $C_{41}H_{54}O_4$).



Mol	Chain	Residues	Atoms			AltConf
10	Aa	1	Total	C	O	0
			45	41	4	
10	Bb	1	Total	C	O	0
			45	41	4	
10	Bc	1	Total	C	O	0
			45	41	4	
10	Bd	1	Total	C	O	0
			45	41	4	
10	Be	1	Total	C	O	0
			45	41	4	
10	Bf	1	Total	C	O	0
			45	41	4	
10	Bg	1	Total	C	O	0
			45	41	4	
10	Bh	1	Total	C	O	0
			45	41	4	
10	Bi	1	Total	C	O	0
			45	41	4	
10	Bj	1	Total	C	O	0
			45	41	4	
10	Bk	1	Total	C	O	0
			45	41	4	
10	Bl	1	Total	C	O	0
			45	41	4	
10	Bm	1	Total	C	O	0
			45	41	4	
10	An	1	Total	C	O	0
			45	41	4	

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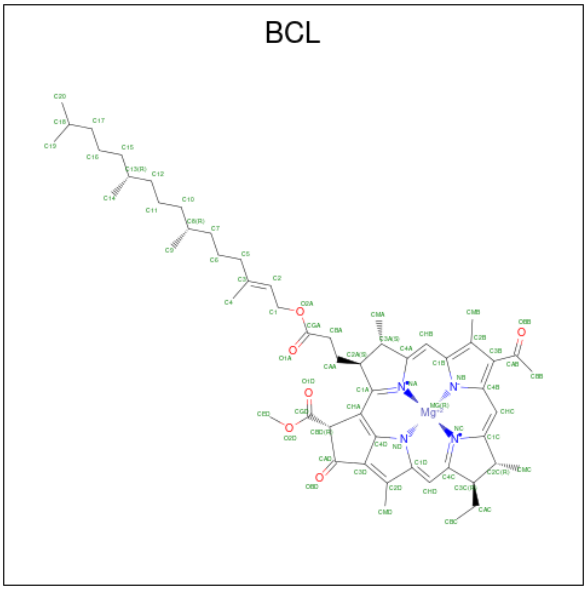
Mol	Chain	Residues	Atoms			AltConf
10	Bn	1	Total	C	O	0
			45	41	4	
10	Bp	1	Total	C	O	0
			45	41	4	
10	BA	1	Total	C	O	0
			45	41	4	
10	BB	1	Total	C	O	0
			45	41	4	
10	BC	1	Total	C	O	0
			45	41	4	
10	BD	1	Total	C	O	0
			45	41	4	
10	BF	1	Total	C	O	0
			45	41	4	
10	AF	1	Total	C	O	0
			45	41	4	
10	BG	1	Total	C	O	0
			45	41	4	
10	BH	1	Total	C	O	0
			45	41	4	
10	BI	1	Total	C	O	0
			45	41	4	
10	BJ	1	Total	C	O	0
			45	41	4	
10	BK	1	Total	C	O	0
			45	41	4	
10	AL	1	Total	C	O	0
			45	41	4	
10	BL	1	Total	C	O	0
			45	41	4	
10	BN	1	Total	C	O	0
			45	41	4	
10	BO	1	Total	C	O	0
			45	41	4	
10	BP	1	Total	C	O	0
			45	41	4	
10	BQ	1	Total	C	O	0
			45	41	4	
10	BR	1	Total	C	O	0
			45	41	4	
10	BS	1	Total	C	O	0
			45	41	4	

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Mol	Chain	Residues	Atoms	AltConf
10	BT	1	Total C O 45 41 4	0
10	BU	1	Total C O 45 41 4	0
10	BV	1	Total C O 45 41 4	0
10	BW	1	Total C O 45 41 4	0
10	BX	1	Total C O 45 41 4	0

- Molecule 11 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
11	Aa	1	Total C Mg N O 66 55 1 4 6	0
11	Ab	1	Total C Mg N O 66 55 1 4 6	0
11	Bb	1	Total C Mg N O 66 55 1 4 6	0
11	Ac	1	Total C Mg N O 66 55 1 4 6	0
11	Bc	1	Total C Mg N O 66 55 1 4 6	0
11	Ad	1	Total C Mg N O 66 55 1 4 6	0

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Mol	Chain	Residues	Atoms					AltConf
11	Bd	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	Ae	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	Be	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	Af	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	Bf	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	Bg	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	Ah	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	Bh	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	Ai	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	Bi	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	Aj	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	Bj	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	Ak	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	Bk	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	Al	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	Bl	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	Am	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	Bm	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	Bn	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	Ao	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	Bo	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
11	Bp	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	Bp	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	L	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	L	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	M	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	M	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	BA	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	BA	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	BB	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	AB	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	AC	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	BC	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	BD	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	AD	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	AE	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	BE	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	BF	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	AF	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	AG	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	BG	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	AH	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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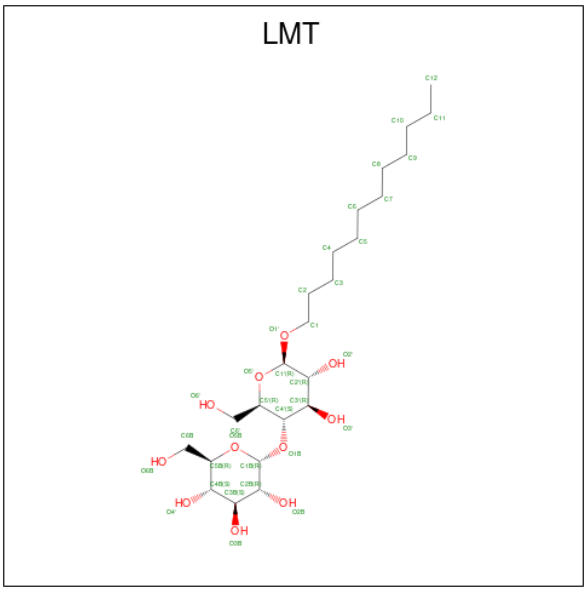
Mol	Chain	Residues	Atoms					AltConf
11	BH	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	AI	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	AI	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	BI	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	AJ	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	AJ	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	AK	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	BK	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	AL	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	BL	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	AM	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	AM	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	BN	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	AN	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	AO	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	BO	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	BP	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	AP	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	AQ	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	AQ	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	AQ	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
11	BR	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	AR	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	BS	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	AS	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	AT	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	AT	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	BU	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	AU	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	AV	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	BV	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	AW	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	AW	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	AW	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	AX	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	BX	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 12 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
12	Aa	1	Total	C	O	0
			35	24	11	
12	Ba	1	Total	C	O	0
			35	24	11	
12	Bb	1	Total	C	O	0
			35	24	11	
12	Bc	1	Total	C	O	0
			35	24	11	
12	Ad	1	Total	C	O	0
			35	24	11	
12	Bd	1	Total	C	O	0
			35	24	11	
12	Be	1	Total	C	O	0
			35	24	11	
12	Bf	1	Total	C	O	0
			35	24	11	
12	Bf	1	Total	C	O	0
			35	24	11	
12	Bh	1	Total	C	O	0
			35	24	11	
12	Bh	1	Total	C	O	0
			35	24	11	
12	Aj	1	Total	C	O	0
			35	24	11	
12	Bj	1	Total	C	O	0
			35	24	11	
12	Bj	1	Total	C	O	0
			35	24	11	

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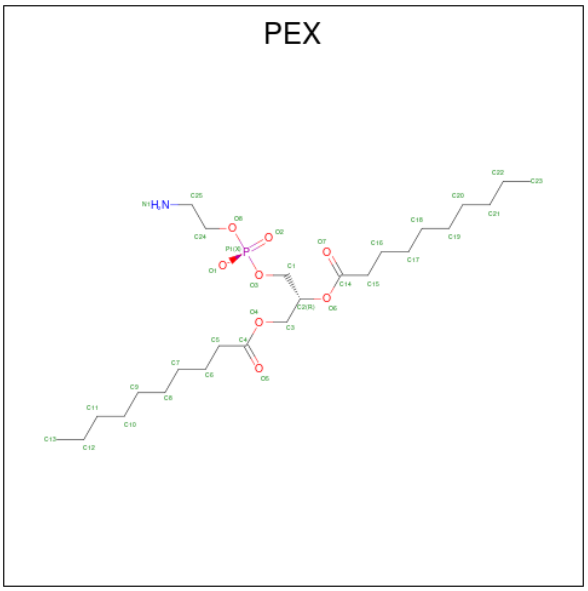
Mol	Chain	Residues	Atoms			AltConf
12	Bl	1	Total	C	O	0
			35	24	11	
12	Bo	1	Total	C	O	0
			35	24	11	
12	Bp	1	Total	C	O	0
			35	24	11	
12	L	1	Total	C	O	0
			35	24	11	
12	M	1	Total	C	O	0
			35	24	11	
12	K	1	Total	C	O	0
			35	24	11	
12	C	1	Total	C	O	0
			35	24	11	
12	BA	1	Total	C	O	0
			35	24	11	
12	BA	1	Total	C	O	0
			35	24	11	
12	BB	1	Total	C	O	0
			35	24	11	
12	BC	1	Total	C	O	0
			35	24	11	
12	BD	1	Total	C	O	0
			35	24	11	
12	BE	1	Total	C	O	0
			35	24	11	
12	BF	1	Total	C	O	0
			35	24	11	
12	BG	1	Total	C	O	0
			35	24	11	
12	BH	1	Total	C	O	0
			35	24	11	
12	BH	1	Total	C	O	0
			35	24	11	
12	BI	1	Total	C	O	0
			35	24	11	
12	BK	1	Total	C	O	0
			35	24	11	
12	BK	1	Total	C	O	0
			35	24	11	
12	BL	1	Total	C	O	0
			35	24	11	

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Mol	Chain	Residues	Atoms	AltConf
12	BM	1	Total C O 35 24 11	0
12	BO	1	Total C O 35 24 11	0
12	BO	1	Total C O 35 24 11	0
12	BQ	1	Total C O 35 24 11	0
12	BQ	1	Total C O 35 24 11	0
12	BR	1	Total C O 35 24 11	0
12	BS	1	Total C O 35 24 11	0
12	BU	1	Total C O 35 24 11	0
12	BU	1	Total C O 35 24 11	0
12	AW	1	Total C O 35 24 11	0
12	BW	1	Total C O 35 24 11	0
12	BW	1	Total C O 35 24 11	0
12	AX	1	Total C O 35 24 11	0

- Molecule 13 is 1,2-DIDECANOYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (CCD ID: PEX) (formula: $C_{25}H_{49}NO_8P$).



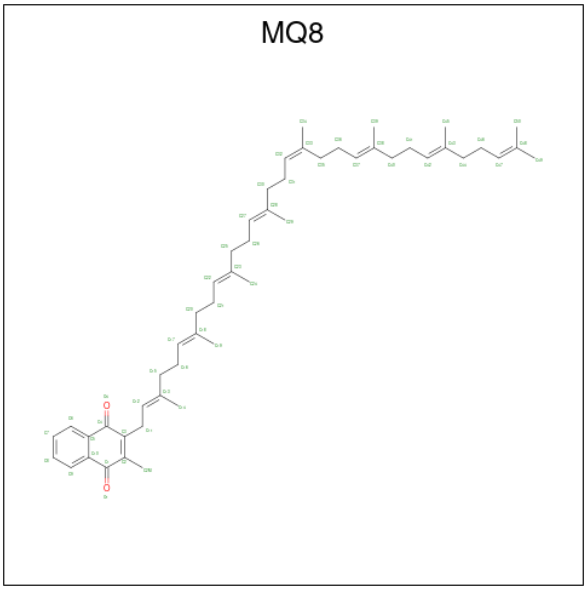
Mol	Chain	Residues	Atoms					AltConf
13	Ba	1	Total	C	N	O	P	0
			35	25	1	8	1	
13	Bc	1	Total	C	N	O	P	0
			35	25	1	8	1	
13	Be	1	Total	C	N	O	P	0
			35	25	1	8	1	
13	Be	1	Total	C	N	O	P	0
			35	25	1	8	1	
13	Bg	1	Total	C	N	O	P	0
			35	25	1	8	1	
13	Bh	1	Total	C	N	O	P	0
			35	25	1	8	1	
13	Aj	1	Total	C	N	O	P	0
			35	25	1	8	1	
13	Bk	1	Total	C	N	O	P	0
			35	25	1	8	1	
13	Bm	1	Total	C	N	O	P	0
			35	25	1	8	1	
13	Bn	1	Total	C	N	O	P	0
			35	25	1	8	1	
13	AA	1	Total	C	N	O	P	0
			35	25	1	8	1	
13	AD	1	Total	C	N	O	P	0
			35	25	1	8	1	
13	AE	1	Total	C	N	O	P	0
			35	25	1	8	1	
13	AJ	1	Total	C	N	O	P	0
			35	25	1	8	1	

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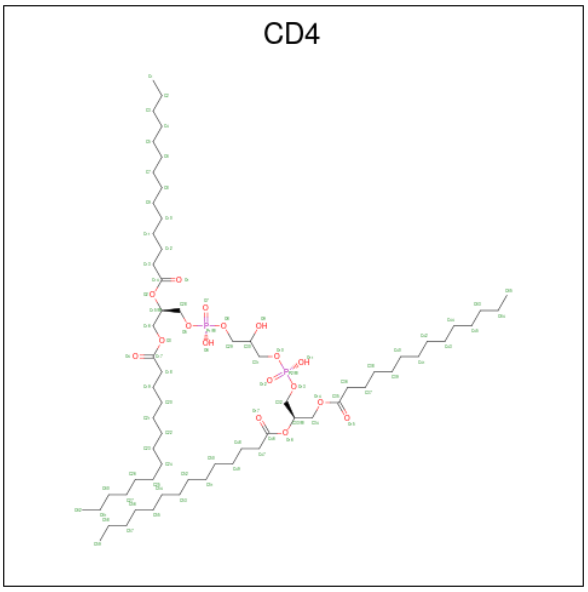
Mol	Chain	Residues	Atoms					AltConf
13	AP	1	Total	C	N	O	P	0
			35	25	1	8	1	
13	AS	1	Total	C	N	O	P	0
			35	25	1	8	1	
13	AT	1	Total	C	N	O	P	0
			35	25	1	8	1	

- Molecule 14 is MENAQUINONE 8 (CCD ID: MQ8) (formula: $C_{51}H_{72}O_2$).



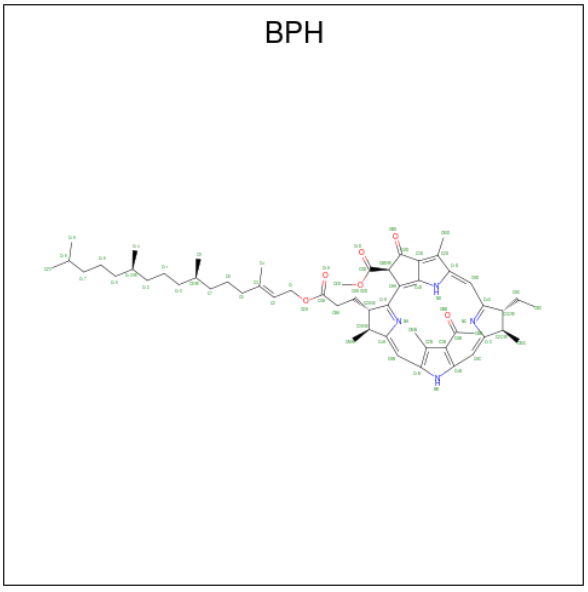
Mol	Chain	Residues	Atoms			AltConf
14	Ad	1	Total	C	O	0
			53	51	2	
14	L	1	Total	C	O	0
			53	51	2	
14	M	1	Total	C	O	0
			53	51	2	

- Molecule 15 is (2R,5R,11R,14R)-5,8,11-trihydroxy-5,11-dioxido-17-oxo-2,14-bis(tetradecanoyloxy)-4,6,10,12,16-pentaoxa-5,11-diphosphatriacont-1-yl tetradecanoate (CCD ID: CD4) (formula: $C_{65}H_{126}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
15	Af	1	Total	C	O	P	0
			84	65	17	2	
15	M	1	Total	C	O	P	0
			84	65	17	2	

- Molecule 16 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$).

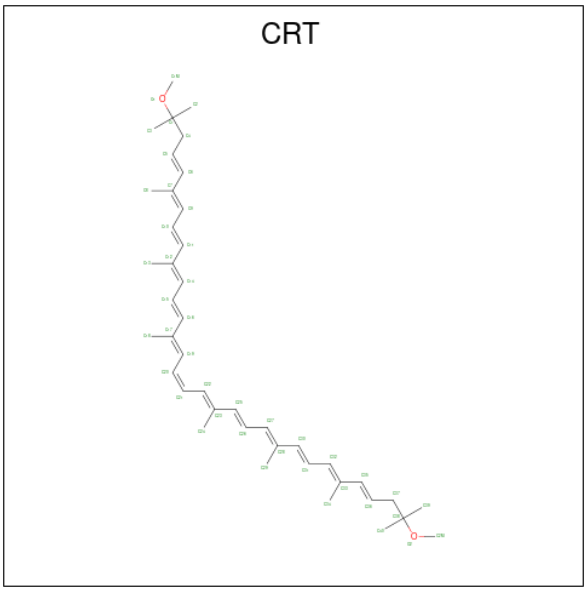


Mol	Chain	Residues	Atoms				AltConf
16	L	1	Total	C	N	O	0
			65	55	4	6	
16	M	1	Total	C	N	O	0
			65	55	4	6	

- Molecule 17 is FE (III) ION (CCD ID: FE) (formula: Fe).

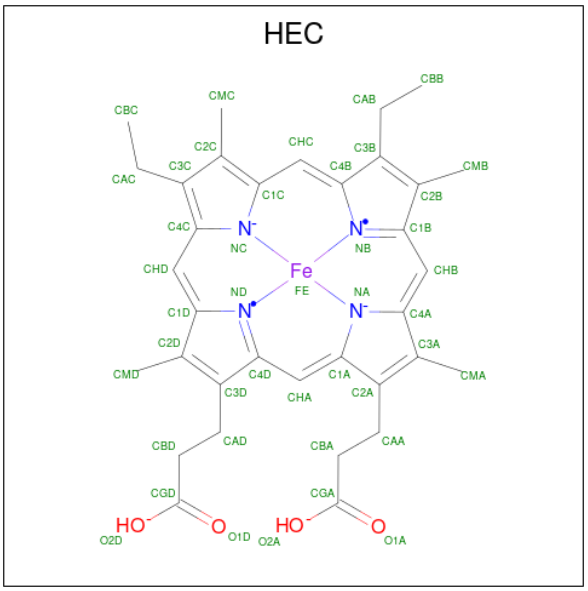
Mol	Chain	Residues	Atoms	AltConf
17	M	1	Total Fe 1 1	0

- Molecule 18 is SPIRILLOXANTHIN (CCD ID: CRT) (formula: $C_{42}H_{60}O_2$).



Mol	Chain	Residues	Atoms	AltConf
18	M	1	Total C O 44 42 2	0

- Molecule 19 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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

- Molecule 20 is water.

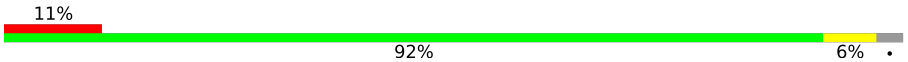
Mol	Chain	Residues	Atoms		AltConf
20	Aa	2	Total 2	O 2	0
20	Ac	1	Total 1	O 1	0
20	Ae	1	Total 1	O 1	0
20	Ag	1	Total 1	O 1	0
20	Bj	1	Total 1	O 1	0
20	Ak	1	Total 1	O 1	0
20	Al	2	Total 2	O 2	0
20	Am	3	Total 3	O 3	0
20	An	1	Total 1	O 1	0
20	S	2	Total 2	O 2	0
20	L	10	Total 10	O 10	0
20	M	8	Total 8	O 8	0
20	C	3	Total 3	O 3	0
20	AC	1	Total 1	O 1	0
20	BO	1	Total 1	O 1	0

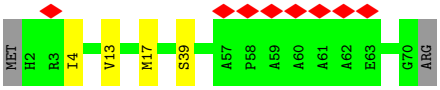
3 Residue-property plots (i)

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: Light-harvesting protein

Chain Aa:

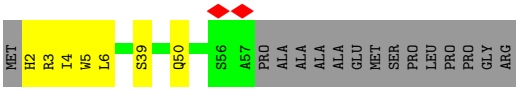




• Molecule 1: Light-harvesting protein

Chain Ab:

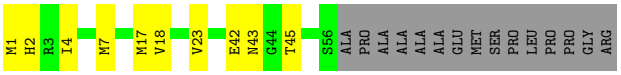




• Molecule 1: Light-harvesting protein

Chain Ac:

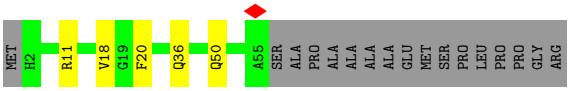




• Molecule 1: Light-harvesting protein

Chain Ad:

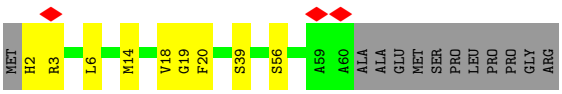




• Molecule 1: Light-harvesting protein

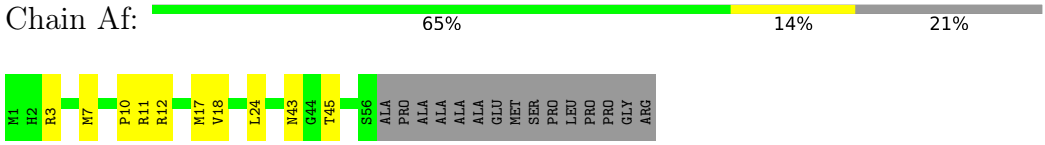
Chain Ae:





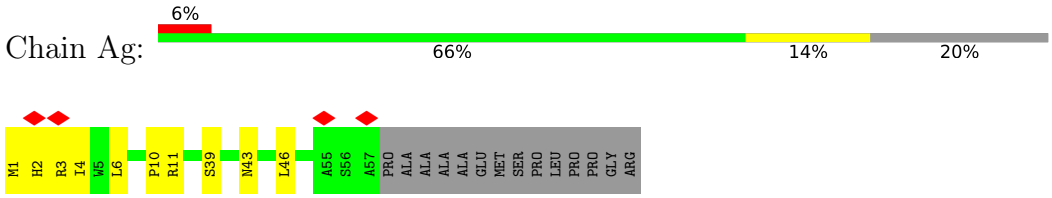
• Molecule 1: Light-harvesting protein

Chain Af:



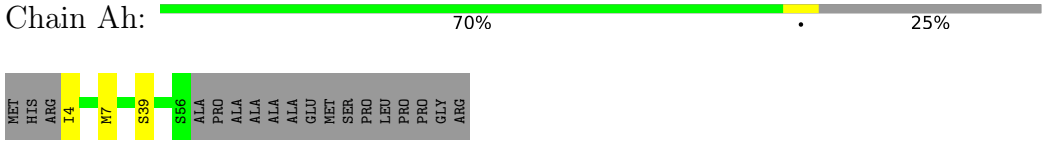
• Molecule 1: Light-harvesting protein

Chain Ag:



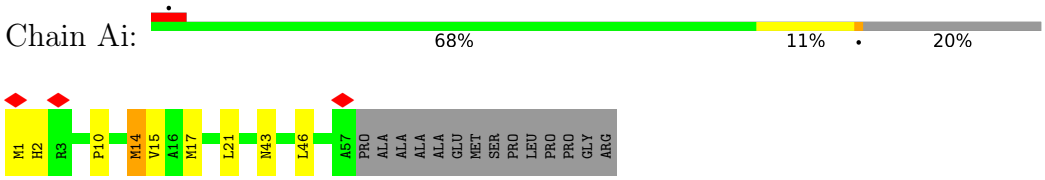
• Molecule 1: Light-harvesting protein

Chain Ah:



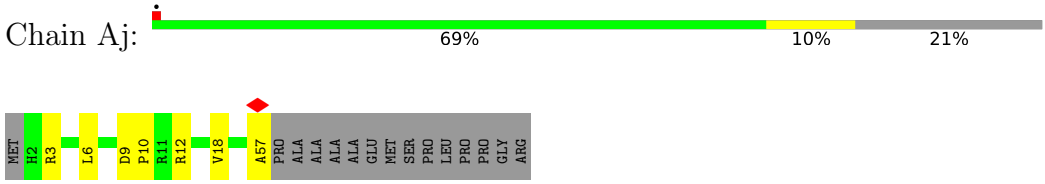
• Molecule 1: Light-harvesting protein

Chain Ai:



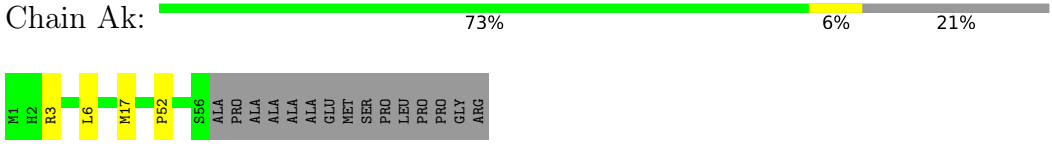
• Molecule 1: Light-harvesting protein

Chain Aj:



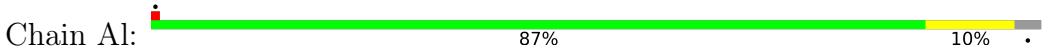
• Molecule 1: Light-harvesting protein

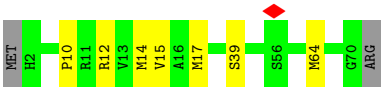
Chain Ak:



• Molecule 1: Light-harvesting protein

Chain Al:

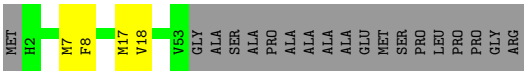




• Molecule 1: Light-harvesting protein

Chain Am:

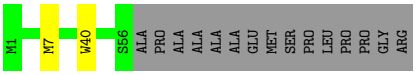




• Molecule 1: Light-harvesting protein

Chain An:

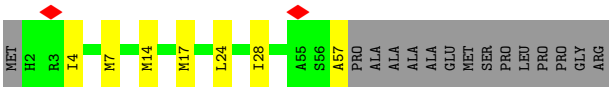




• Molecule 1: Light-harvesting protein

Chain Ao:

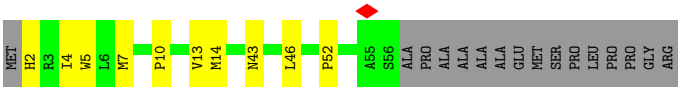




• Molecule 1: Light-harvesting protein

Chain Ap:

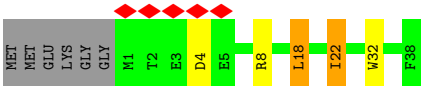




• Molecule 2: Light-harvesting protein

Chain Ba:





• Molecule 2: Light-harvesting protein

Chain Bb:

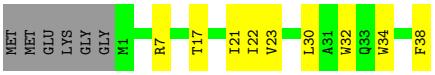




• Molecule 2: Light-harvesting protein

Chain Bc:

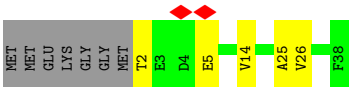




• Molecule 2: Light-harvesting protein

Chain Bd:

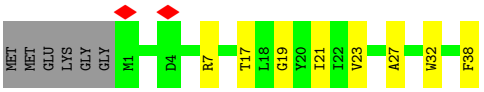




• Molecule 2: Light-harvesting protein

Chain Be:

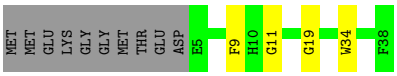




• Molecule 2: Light-harvesting protein

Chain Bf:





• Molecule 2: Light-harvesting protein

Chain Bg:





• Molecule 2: Light-harvesting protein

Chain Bh:





• Molecule 2: Light-harvesting protein

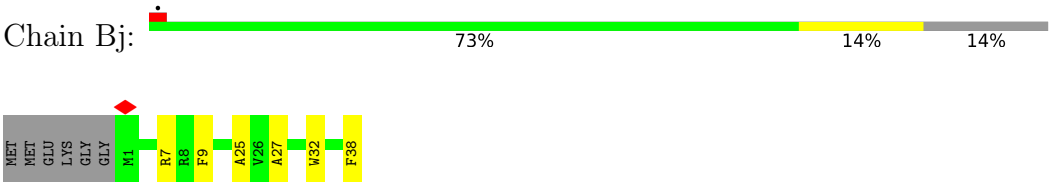
Chain Bi:





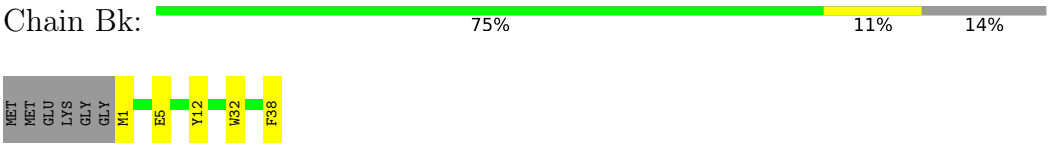
• Molecule 2: Light-harvesting protein

Chain Bj:



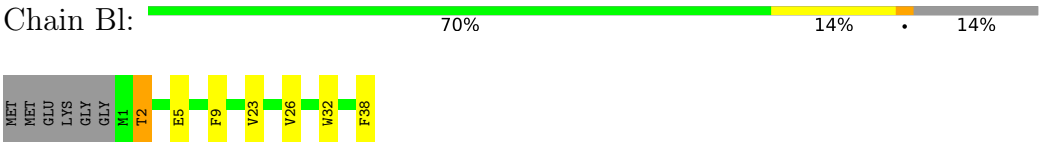
• Molecule 2: Light-harvesting protein

Chain Bk:



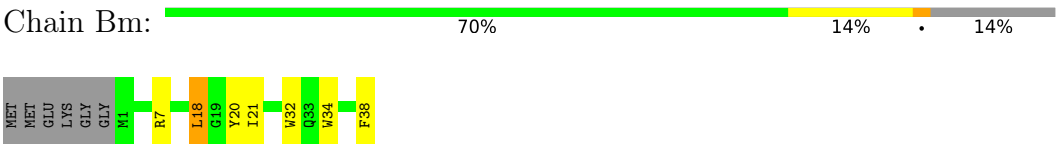
• Molecule 2: Light-harvesting protein

Chain Bl:



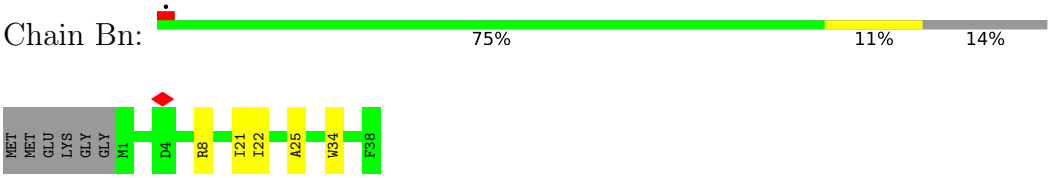
• Molecule 2: Light-harvesting protein

Chain Bm:



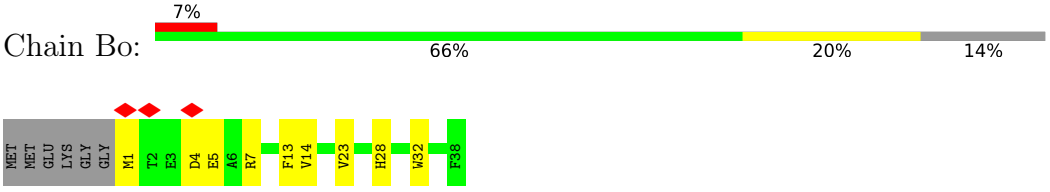
• Molecule 2: Light-harvesting protein

Chain Bn:



• Molecule 2: Light-harvesting protein

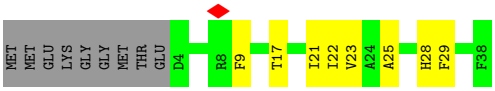
Chain Bo:



• Molecule 2: Light-harvesting protein

Chain Bp:

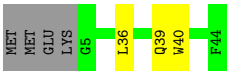




• Molecule 2: Light-harvesting protein

Chain BA:





• Molecule 2: Light-harvesting protein

Chain BB:





• Molecule 2: Light-harvesting protein

Chain BC:





• Molecule 2: Light-harvesting protein

Chain BD:

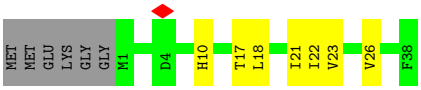




• Molecule 2: Light-harvesting protein

Chain BE:

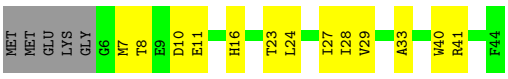




• Molecule 2: Light-harvesting protein

Chain BF:





• Molecule 2: Light-harvesting protein

Chain BG:

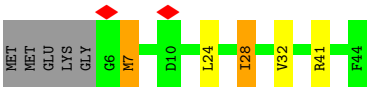




• Molecule 2: Light-harvesting protein

Chain BH:

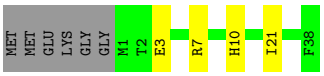




• Molecule 2: Light-harvesting protein

Chain BI:

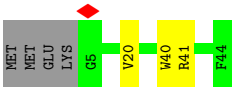




• Molecule 2: Light-harvesting protein

Chain BJ:

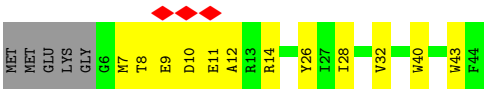




• Molecule 2: Light-harvesting protein

Chain BK:

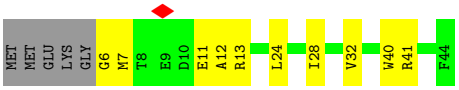




• Molecule 2: Light-harvesting protein

Chain BL:

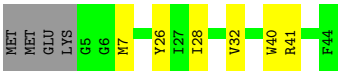




• Molecule 2: Light-harvesting protein

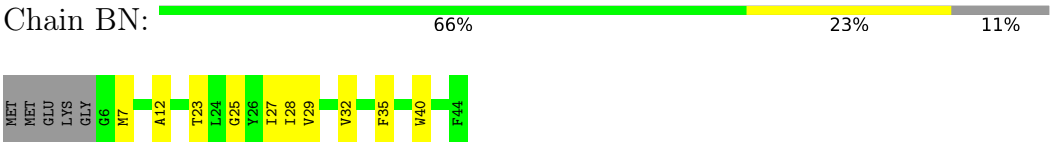
Chain BM:





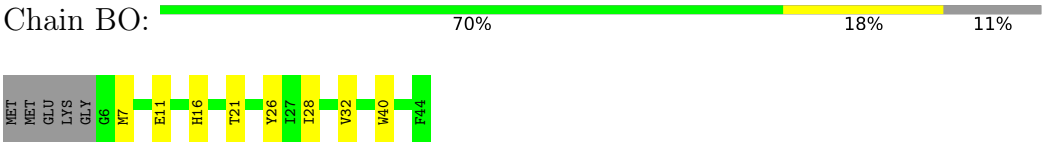
• Molecule 2: Light-harvesting protein

Chain BN:



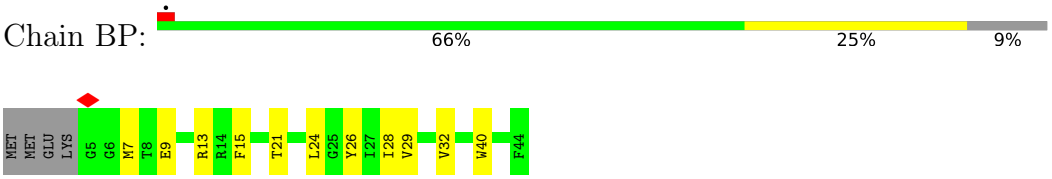
• Molecule 2: Light-harvesting protein

Chain BO:



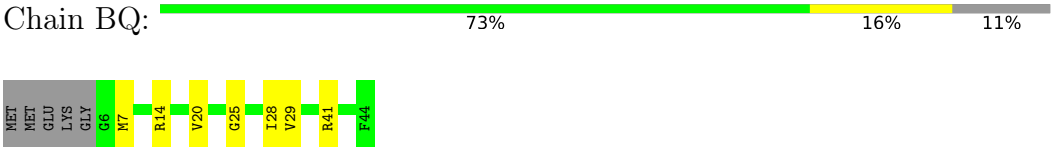
• Molecule 2: Light-harvesting protein

Chain BP:



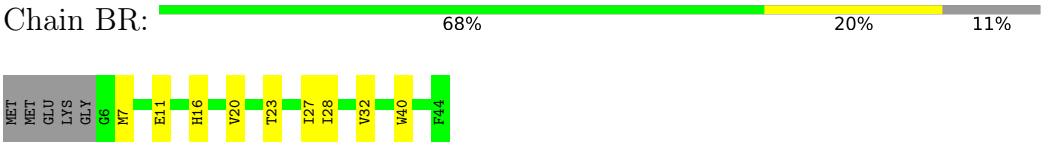
• Molecule 2: Light-harvesting protein

Chain BQ:



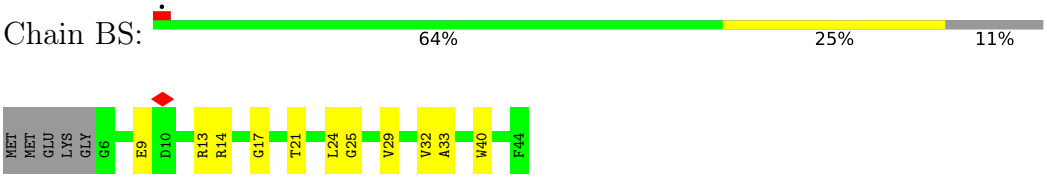
• Molecule 2: Light-harvesting protein

Chain BR:



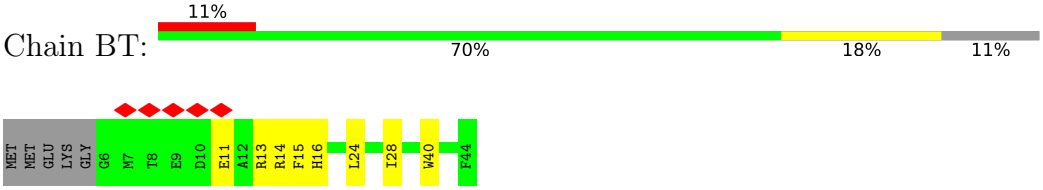
• Molecule 2: Light-harvesting protein

Chain BS:



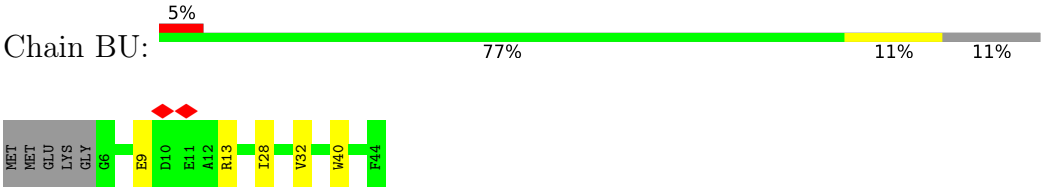
• Molecule 2: Light-harvesting protein

Chain BT:



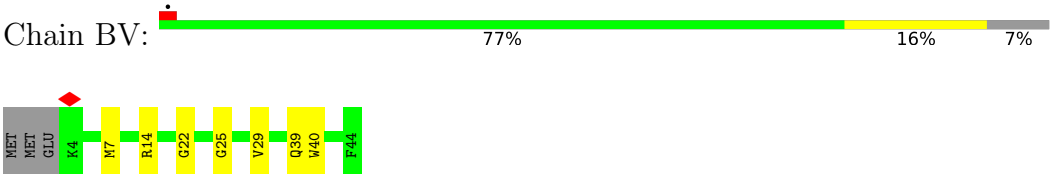
• Molecule 2: Light-harvesting protein

Chain BU:



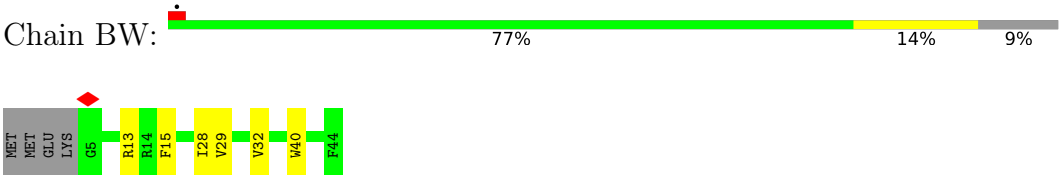
• Molecule 2: Light-harvesting protein

Chain BV:



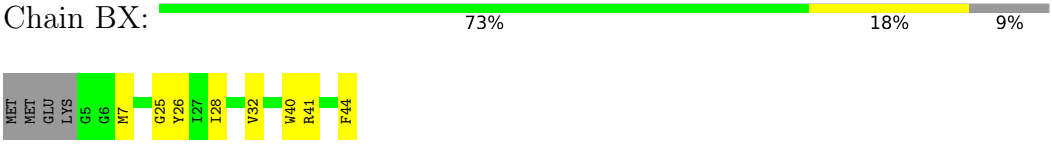
• Molecule 2: Light-harvesting protein

Chain BW:



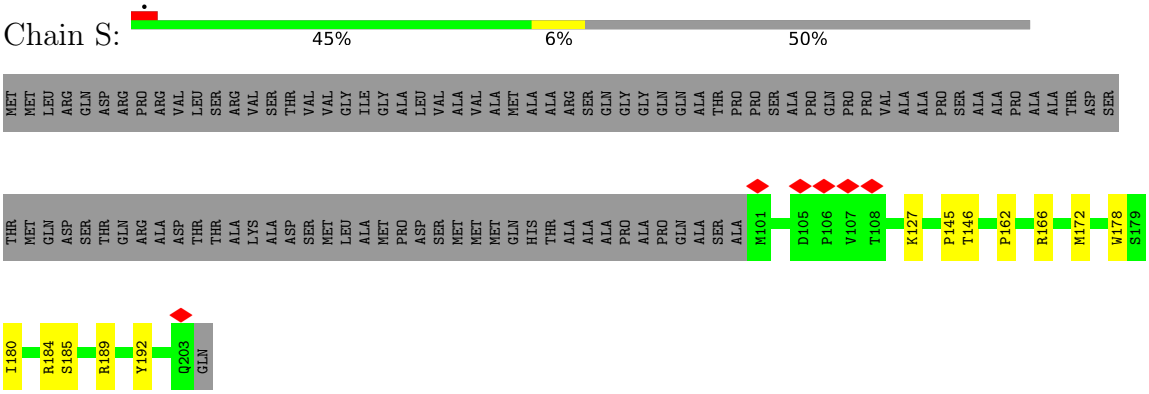
• Molecule 2: Light-harvesting protein

Chain BX:



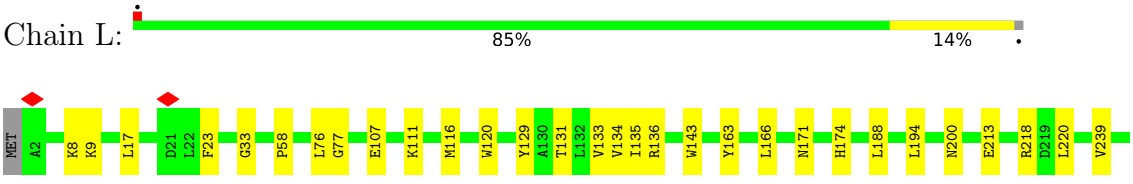
• Molecule 3: reaction centre S sub unit

Chain S:



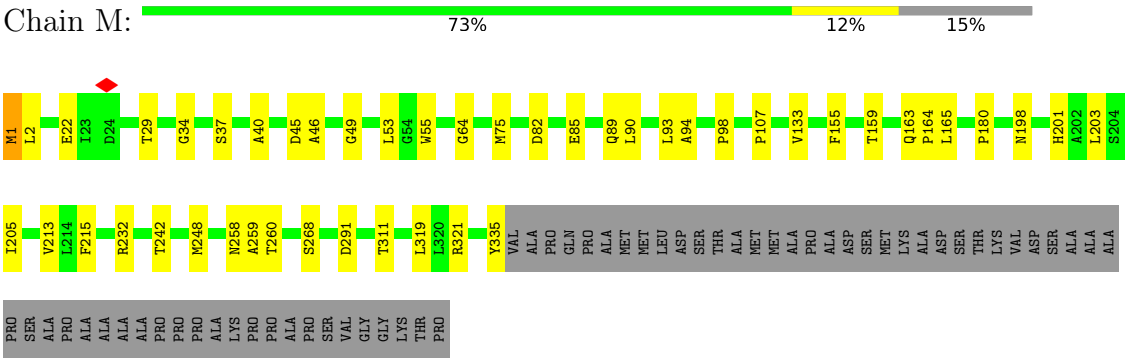
• Molecule 4: Reaction center protein L chain

Chain L:

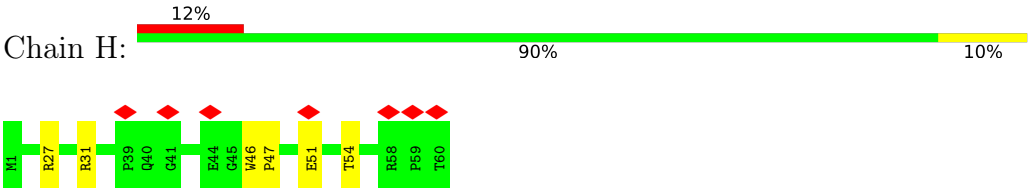




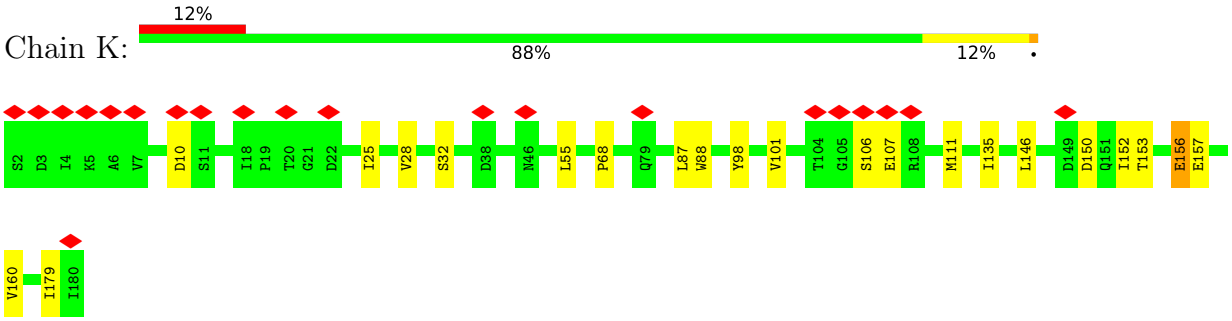
• Molecule 5: Reaction center protein M chain



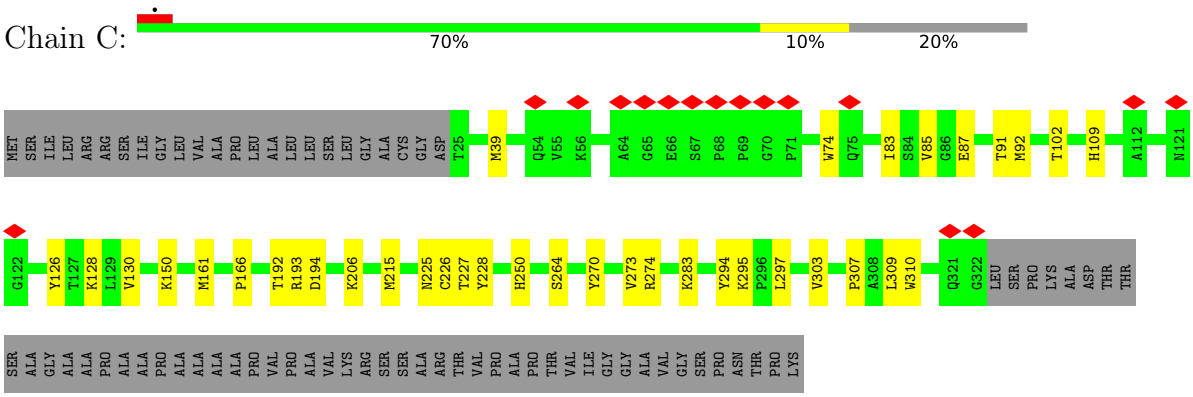
• Molecule 6: reaction centre Ht sub unit



• Molecule 7: reaction centre Hc sub unit



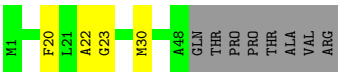
• Molecule 8: Photosynthetic reaction center cytochrome c subunit



• Molecule 9: Light-harvesting protein

Chain AA:

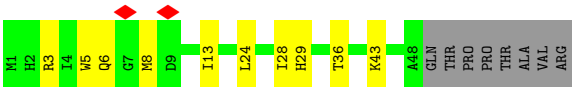




• Molecule 9: Light-harvesting protein

Chain AB:





• Molecule 9: Light-harvesting protein

Chain AC:

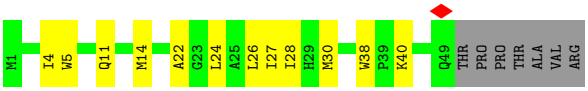




• Molecule 9: Light-harvesting protein

Chain AD:

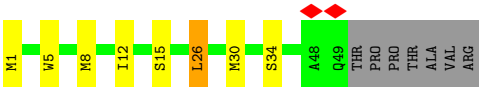




• Molecule 9: Light-harvesting protein

Chain AE:

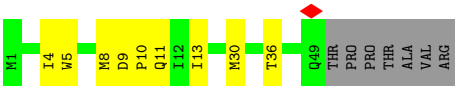




• Molecule 9: Light-harvesting protein

Chain AF:

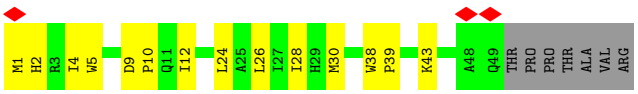




• Molecule 9: Light-harvesting protein

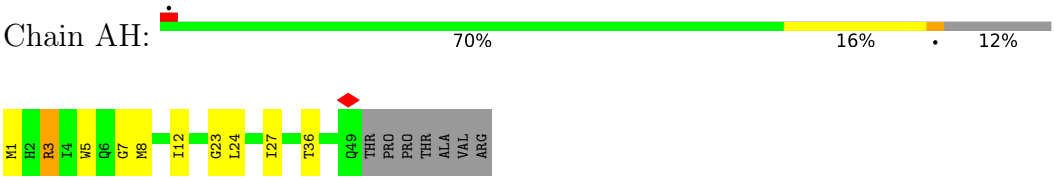
Chain AG:





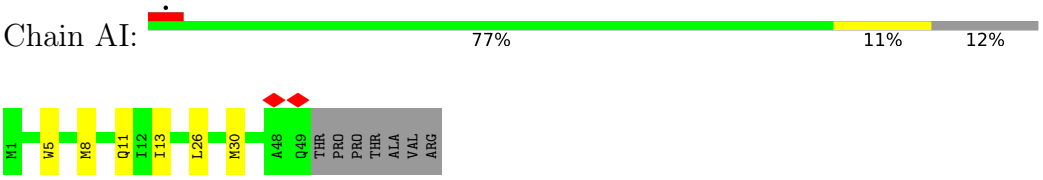
• Molecule 9: Light-harvesting protein

Chain AH:



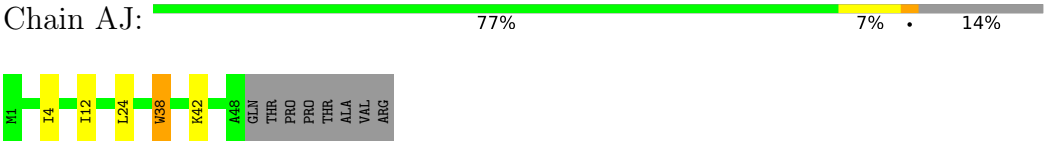
• Molecule 9: Light-harvesting protein

Chain AI:



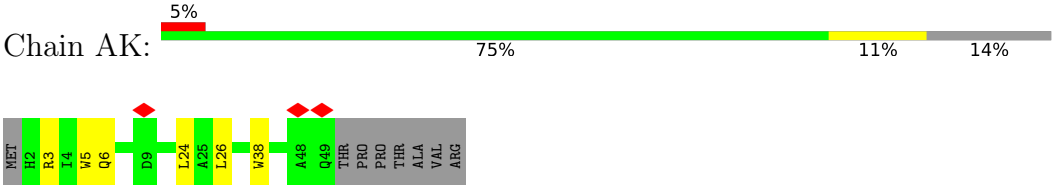
• Molecule 9: Light-harvesting protein

Chain AJ:



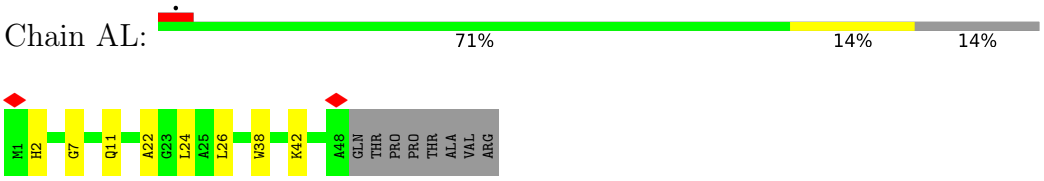
• Molecule 9: Light-harvesting protein

Chain AK:



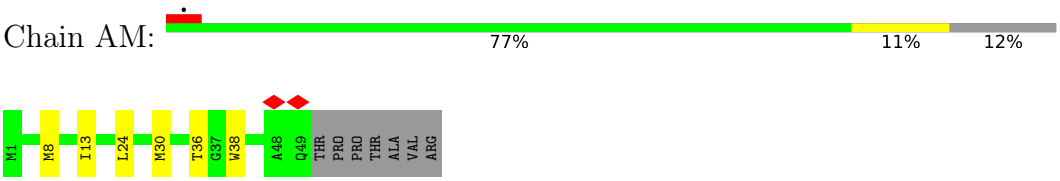
• Molecule 9: Light-harvesting protein

Chain AL:



• Molecule 9: Light-harvesting protein

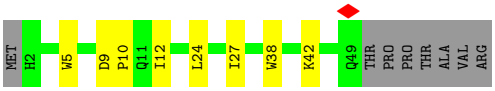
Chain AM:



• Molecule 9: Light-harvesting protein

Chain AN:

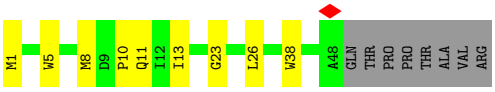




• Molecule 9: Light-harvesting protein

Chain AO:

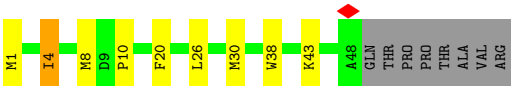




• Molecule 9: Light-harvesting protein

Chain AP:

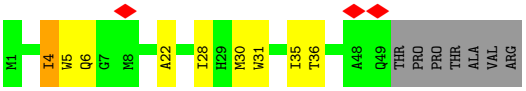




• Molecule 9: Light-harvesting protein

Chain AQ:

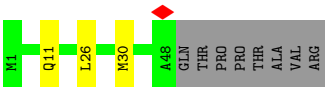




• Molecule 9: Light-harvesting protein

Chain AR:

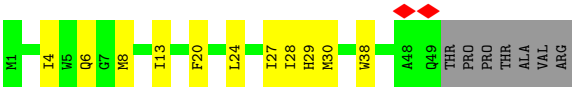




• Molecule 9: Light-harvesting protein

Chain AS:

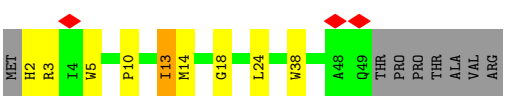




• Molecule 9: Light-harvesting protein

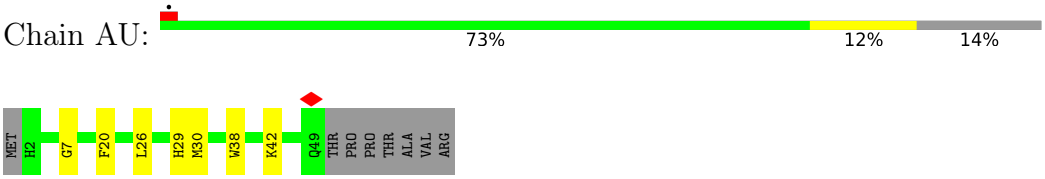
Chain AT:





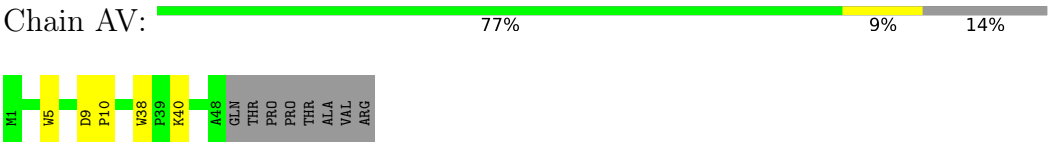
• Molecule 9: Light-harvesting protein

Chain AU:



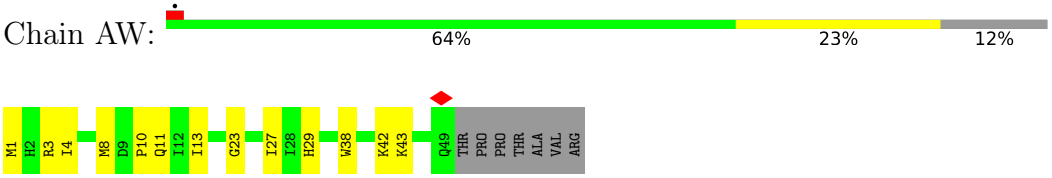
• Molecule 9: Light-harvesting protein

Chain AV:



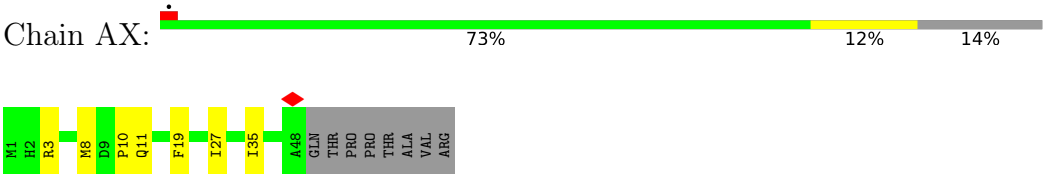
• Molecule 9: Light-harvesting protein

Chain AW:



• Molecule 9: Light-harvesting protein

Chain AX:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	129052	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF was performed within cryosparc	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.548	Depositor
Minimum map value	-0.226	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.0687	Depositor
Map size (Å)	439.19998, 439.19998, 439.19998	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.732, 0.732, 0.732	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: CD4, CRT, PEX, V7N, FE, BPH, BCL, HEC, LMT, MQ8

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	Aa	0.15	0/535	0.33	0/731
1	Ab	0.15	0/448	0.23	0/609
1	Ac	0.16	0/451	0.30	0/612
1	Ad	0.16	0/437	0.28	0/594
1	Ae	0.15	0/466	0.24	0/635
1	Af	0.16	0/451	0.28	0/612
1	Ag	0.16	0/456	0.26	0/619
1	Ah	0.16	0/421	0.27	0/573
1	Ai	0.15	0/456	0.27	0/619
1	Aj	0.15	0/448	0.24	0/609
1	Ak	0.15	0/451	0.22	0/612
1	Al	0.18	0/535	0.34	0/731
1	Am	0.17	0/428	0.24	0/582
1	An	0.17	0/451	0.27	0/612
1	Ao	0.15	0/448	0.27	0/609
1	Ap	0.14	0/443	0.26	0/602
2	BA	0.13	0/346	0.24	0/471
2	BB	0.14	0/342	0.28	0/466
2	BC	0.13	0/346	0.24	0/471
2	BD	0.14	0/346	0.24	0/471
2	BE	0.15	0/338	0.26	0/461
2	BF	0.13	0/342	0.23	0/466
2	BG	0.17	0/342	0.38	0/466
2	BH	0.13	0/342	0.25	0/466
2	BI	0.15	0/338	0.32	0/461
2	BJ	0.13	0/346	0.22	0/471
2	BK	0.14	0/342	0.27	0/466
2	BL	0.14	0/342	0.21	0/466
2	BM	0.13	0/346	0.22	0/471
2	BN	0.20	0/342	0.36	0/466
2	BO	0.14	0/342	0.29	0/466
2	BP	0.15	0/346	0.30	0/471

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
2	BQ	0.21	0/342	0.36	0/466
2	BR	0.14	0/342	0.24	0/466
2	BS	0.13	0/342	0.24	0/466
2	BT	0.16	0/342	0.30	0/466
2	BU	0.13	0/342	0.27	0/466
2	BV	0.15	0/355	0.34	0/482
2	BW	0.15	0/346	0.31	0/471
2	BX	0.14	0/346	0.30	0/471
2	Ba	0.15	0/338	0.23	0/461
2	Bb	0.20	0/338	0.35	0/461
2	Bc	0.18	0/338	0.29	0/461
2	Bd	0.16	0/330	0.22	0/451
2	Be	0.18	0/338	0.29	0/461
2	Bf	0.16	0/306	0.21	0/418
2	Bg	0.16	0/338	0.22	0/461
2	Bh	0.15	0/323	0.19	0/441
2	Bi	0.15	0/338	0.21	0/461
2	Bj	0.16	0/338	0.20	0/461
2	Bk	0.16	0/338	0.22	0/461
2	Bl	0.17	0/338	0.23	0/461
2	Bm	0.17	0/338	0.24	0/461
2	Bn	0.15	0/338	0.21	0/461
2	Bo	0.15	0/338	0.22	0/461
2	Bp	0.15	0/314	0.20	0/429
3	S	0.12	0/819	0.28	0/1112
4	L	0.15	0/2217	0.30	0/3031
5	M	0.18	0/2796	0.34	0/3821
6	H	0.14	0/529	0.27	0/716
7	K	0.14	0/1408	0.33	0/1925
8	C	0.18	0/2395	0.35	0/3268
9	AA	0.15	0/405	0.29	0/547
9	AB	0.17	0/405	0.36	0/547
9	AC	0.16	0/405	0.31	0/547
9	AD	0.16	0/414	0.33	0/559
9	AE	0.15	0/414	0.33	0/559
9	AF	0.16	0/414	0.30	0/559
9	AG	0.15	0/414	0.29	0/559
9	AH	0.16	0/414	0.36	0/559
9	AI	0.15	0/414	0.31	0/559
9	AJ	0.17	0/405	0.33	0/547
9	AK	0.16	0/406	0.32	0/549
9	AL	0.16	0/405	0.31	0/547
9	AM	0.15	0/414	0.29	0/559

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
9	AN	0.15	0/406	0.29	0/549
9	AO	0.14	0/405	0.30	0/547
9	AP	0.14	0/405	0.29	0/547
9	AQ	0.14	0/414	0.31	0/559
9	AR	0.14	0/405	0.28	0/547
9	AS	0.14	0/414	0.31	0/559
9	AT	0.14	0/406	0.31	0/549
9	AU	0.15	0/406	0.33	0/549
9	AV	0.15	0/405	0.30	0/547
9	AW	0.15	0/414	0.32	0/559
9	AX	0.17	0/405	0.38	0/547
All	All	0.16	0/40877	0.29	0/55591

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (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	Aa	520	0	532	3	0
1	Ab	437	0	450	5	0
1	Ac	440	0	457	7	0
1	Ad	426	0	440	2	0
1	Ae	454	0	467	5	0
1	Af	440	0	457	13	0
1	Ag	445	0	462	8	0
1	Ah	411	0	425	0	0
1	Ai	445	0	462	5	0
1	Aj	437	0	450	5	0
1	Ak	440	0	457	4	0
1	Al	520	0	532	6	0
1	Am	417	0	432	3	0
1	An	440	0	457	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Ao	437	0	450	8	0
1	Ap	432	0	445	9	0
2	BA	332	0	308	3	0
2	BB	328	0	305	12	0
2	BC	332	0	308	6	0
2	BD	332	0	308	7	0
2	BE	324	0	305	5	0
2	BF	328	0	305	12	0
2	BG	328	0	305	10	0
2	BH	328	0	305	4	0
2	BI	324	0	305	3	0
2	BJ	332	0	308	3	0
2	BK	328	0	305	10	0
2	BL	328	0	305	8	0
2	BM	332	0	308	6	0
2	BN	328	0	305	9	0
2	BO	328	0	305	6	0
2	BP	332	0	308	12	0
2	BQ	328	0	305	7	0
2	BR	328	0	305	5	0
2	BS	328	0	305	8	0
2	BT	328	0	305	10	0
2	BU	328	0	305	4	0
2	BV	341	0	321	8	0
2	BW	332	0	308	6	0
2	BX	332	0	308	7	0
2	Ba	324	0	305	3	0
2	Bb	324	0	305	9	0
2	Bc	324	0	305	7	0
2	Bd	316	0	293	3	0
2	Be	324	0	305	9	0
2	Bf	292	0	276	4	0
2	Bg	324	0	305	8	0
2	Bh	309	0	286	5	0
2	Bi	324	0	305	5	0
2	Bj	324	0	305	5	0
2	Bk	324	0	305	5	0
2	Bl	324	0	305	6	0
2	Bm	324	0	305	8	0
2	Bn	324	0	305	5	0
2	Bo	324	0	305	13	0
2	Bp	300	0	278	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	S	800	0	793	9	0
4	L	2134	0	2107	26	0
5	M	2697	0	2621	34	0
6	H	510	0	500	4	0
7	K	1373	0	1347	12	0
8	C	2330	0	2254	28	0
9	AA	391	0	394	5	0
9	AB	391	0	394	11	0
9	AC	391	0	394	9	0
9	AD	400	0	402	12	0
9	AE	400	0	402	6	0
9	AF	400	0	402	7	0
9	AG	400	0	402	11	0
9	AH	400	0	402	10	0
9	AI	400	0	402	7	0
9	AJ	391	0	394	5	0
9	AK	392	0	390	8	0
9	AL	391	0	394	7	0
9	AM	400	0	402	7	0
9	AN	392	0	390	8	0
9	AO	391	0	394	8	0
9	AP	391	0	394	10	0
9	AQ	400	0	402	7	0
9	AR	391	0	394	2	0
9	AS	400	0	402	10	0
9	AT	392	0	389	11	0
9	AU	392	0	390	7	0
9	AV	391	0	394	6	0
9	AW	400	0	402	14	0
9	AX	391	0	393	7	0
10	AF	45	0	0	0	0
10	AL	45	0	0	0	0
10	Aa	45	0	0	0	0
10	An	45	0	0	0	0
10	BA	45	0	0	0	0
10	BB	45	0	0	0	0
10	BC	45	0	0	0	0
10	BD	45	0	0	0	0
10	BF	45	0	0	0	0
10	BG	45	0	0	0	0
10	BH	45	0	0	0	0
10	BI	45	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	BJ	45	0	0	0	0
10	BK	45	0	0	0	0
10	BL	45	0	0	0	0
10	BN	45	0	0	0	0
10	BO	45	0	0	0	0
10	BP	45	0	0	0	0
10	BQ	45	0	0	0	0
10	BR	45	0	0	0	0
10	BS	45	0	0	1	0
10	BT	45	0	0	1	0
10	BU	45	0	0	0	0
10	BV	45	0	0	1	0
10	BW	45	0	0	0	0
10	BX	45	0	0	0	0
10	Bb	45	0	0	0	0
10	Bc	45	0	0	0	0
10	Bd	45	0	0	0	0
10	Be	45	0	0	0	0
10	Bf	45	0	0	0	0
10	Bg	45	0	0	0	0
10	Bh	45	0	0	0	0
10	Bi	45	0	0	0	0
10	Bj	45	0	0	0	0
10	Bk	45	0	0	0	0
10	Bl	45	0	0	0	0
10	Bm	45	0	0	0	0
10	Bn	45	0	0	0	0
10	Bp	45	0	0	0	0
11	AB	66	0	74	3	0
11	AC	66	0	74	2	0
11	AD	66	0	74	3	0
11	AE	66	0	74	4	0
11	AF	66	0	74	2	0
11	AG	66	0	74	1	0
11	AH	66	0	74	2	0
11	AI	132	0	142	5	0
11	AJ	132	0	146	3	0
11	AK	66	0	74	5	0
11	AL	66	0	74	3	0
11	AM	132	0	146	4	0
11	AN	66	0	74	3	0
11	AO	66	0	72	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	AP	66	0	74	2	0
11	AQ	198	0	217	5	0
11	AR	66	0	74	6	0
11	AS	66	0	74	3	0
11	AT	132	0	147	10	0
11	AU	66	0	73	2	0
11	AV	66	0	74	5	0
11	AW	198	0	216	7	0
11	AX	66	0	74	4	0
11	Aa	66	0	74	0	0
11	Ab	66	0	74	2	0
11	Ac	66	0	74	2	0
11	Ad	66	0	74	1	0
11	Ae	66	0	74	4	0
11	Af	66	0	74	2	0
11	Ah	66	0	74	1	0
11	Ai	66	0	72	0	0
11	Aj	66	0	74	2	0
11	Ak	66	0	74	2	0
11	Al	66	0	74	9	0
11	Am	66	0	74	9	0
11	Ao	66	0	74	26	0
11	BA	132	0	147	6	0
11	BB	66	0	74	3	0
11	BC	66	0	74	2	0
11	BD	66	0	74	4	0
11	BE	66	0	74	1	0
11	BF	66	0	74	3	0
11	BG	66	0	74	2	0
11	BH	66	0	71	1	0
11	BI	66	0	74	5	0
11	BK	66	0	74	1	0
11	BL	66	0	74	1	0
11	BN	66	0	74	3	0
11	BO	66	0	74	1	0
11	BP	66	0	74	2	0
11	BR	66	0	74	0	0
11	BS	66	0	74	1	0
11	BU	66	0	74	1	0
11	BV	66	0	74	0	0
11	BX	66	0	74	4	0
11	Bb	66	0	74	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	Bc	66	0	74	0	0
11	Bd	66	0	74	1	0
11	Be	66	0	74	3	0
11	Bf	66	0	74	1	0
11	Bg	66	0	74	1	0
11	Bh	66	0	74	1	0
11	Bi	66	0	74	1	0
11	Bj	66	0	74	3	0
11	Bk	66	0	74	1	0
11	Bl	66	0	74	4	0
11	Bm	66	0	74	3	0
11	Bn	66	0	74	2	0
11	Bo	66	0	74	3	0
11	Bp	132	0	148	12	0
11	L	132	0	148	3	0
11	M	132	0	147	3	0
12	AW	35	0	45	1	0
12	AX	35	0	42	2	0
12	Aa	35	0	46	0	0
12	Ad	35	0	45	2	0
12	Aj	35	0	46	0	0
12	BA	70	0	88	5	0
12	BB	35	0	45	2	0
12	BC	35	0	44	2	0
12	BD	35	0	45	1	0
12	BE	35	0	45	1	0
12	BF	35	0	45	2	0
12	BG	35	0	45	1	0
12	BH	70	0	87	3	0
12	BI	35	0	45	2	0
12	BK	70	0	90	1	0
12	BL	35	0	45	0	0
12	BM	35	0	45	2	0
12	BO	70	0	88	3	0
12	BQ	70	0	90	1	0
12	BR	35	0	45	1	0
12	BS	35	0	45	4	0
12	BU	70	0	90	0	0
12	BW	70	0	91	4	0
12	Ba	35	0	45	0	0
12	Bb	35	0	46	2	0
12	Bc	35	0	44	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	Bd	35	0	45	1	0
12	Be	35	0	45	1	0
12	Bf	70	0	86	3	0
12	Bh	70	0	89	2	0
12	Bj	70	0	88	2	0
12	Bl	35	0	44	0	0
12	Bo	35	0	44	3	0
12	Bp	35	0	44	1	0
12	C	35	0	45	0	0
12	K	35	0	46	1	0
12	L	35	0	46	0	0
12	M	35	0	46	2	0
13	AA	35	0	49	4	0
13	AD	35	0	49	3	0
13	AE	35	0	49	2	0
13	AJ	35	0	48	1	0
13	AP	35	0	49	2	0
13	AS	35	0	49	2	0
13	AT	35	0	45	2	0
13	Aj	35	0	49	2	0
13	Ba	35	0	49	1	0
13	Bc	35	0	49	4	0
13	Be	70	0	98	6	0
13	Bg	35	0	49	1	0
13	Bh	35	0	49	1	0
13	Bk	35	0	49	1	0
13	Bm	35	0	49	2	0
13	Bn	35	0	46	3	0
14	Ad	53	0	72	9	0
14	L	53	0	72	6	0
14	M	53	0	70	4	0
15	Af	84	0	124	9	0
15	M	84	0	124	1	0
16	L	65	0	76	6	0
16	M	65	0	76	4	0
17	M	1	0	0	0	0
18	M	44	0	60	0	0
19	C	172	0	122	6	0
20	AC	1	0	0	0	0
20	Aa	2	0	0	0	0
20	Ac	1	0	0	0	0
20	Ae	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	Ag	1	0	0	0	0
20	Ak	1	0	0	0	0
20	Al	2	0	0	0	0
20	Am	3	0	0	0	0
20	An	1	0	0	0	0
20	BO	1	0	0	0	0
20	Bj	1	0	0	0	0
20	C	3	0	0	0	0
20	L	10	0	0	0	0
20	M	8	0	0	0	0
20	S	2	0	0	0	0
All	All	49808	0	48618	719	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 7.

All (719) 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)
11:Ao:101:BCL:CED	2:Bo:23:VAL:HG12	1.84	1.08
11:Ao:101:BCL:HED3	2:Bo:23:VAL:HG12	1.46	0.97
11:Ao:101:BCL:H122	11:Ao:101:BCL:H91	1.56	0.86
11:Ao:101:BCL:HED1	2:Bo:23:VAL:HG12	1.56	0.86
11:Ao:101:BCL:H91	11:Ao:101:BCL:C14	2.09	0.83
11:Ao:101:BCL:H122	11:Ao:101:BCL:C9	2.07	0.82
11:AG:101:BCL:H102	9:AH:24:LEU:HD13	1.66	0.78
13:Be:1104:PEX:H37	11:AK:101:BCL:H91	1.66	0.77
11:Am:101:BCL:H43	2:Bm:20:TYR:CE1	2.23	0.74
2:BQ:28:ILE:HD12	2:BQ:28:ILE:H	1.52	0.73
2:BT:16:HIS:CE1	9:AT:2:HIS:HA	2.23	0.73
11:AE:1102:BCL:H172	9:AF:13:ILE:HG23	1.70	0.73
2:BN:28:ILE:HD12	2:BN:28:ILE:H	1.52	0.73
9:AH:7:GLY:H	2:BH:7:MET:HB3	1.53	0.72
13:Be:1104:PEX:H3	11:Be:1105:BCL:H193	1.70	0.71
9:AI:8:MET:HE2	9:AI:13:ILE:HD11	1.71	0.71
2:BB:29:VAL:HG12	11:AB:101:BCL:HED1	1.72	0.71
5:M:94:ALA:HB2	5:M:180:PRO:HG2	1.72	0.71
2:BL:7:MET:HG2	2:BL:11:GLU:HG3	1.74	0.70
11:Ao:101:BCL:CED	2:Bo:23:VAL:CG1	2.66	0.70
11:AK:101:BCL:O1A	2:BK:26:TYR:OH	2.10	0.70
9:AH:3:ARG:H	9:AH:3:ARG:HD2	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:152:ILE:HG13	7:K:156:GLU:HG3	1.73	0.69
7:K:111:MET:HE2	7:K:146:LEU:HD11	1.73	0.69
1:Ao:4:ILE:HD12	1:Ao:4:ILE:H	1.58	0.69
14:Ad:103:MQ8:H243	14:Ad:103:MQ8:H141	1.74	0.68
2:BU:9:GLU:OE2	2:BU:13:ARG:NH2	2.25	0.68
12:Bf:1203:LMT:H42	2:Bg:30:LEU:HG	1.75	0.68
11:Ao:101:BCL:HMB1	11:Ao:101:BCL:HBB3	1.76	0.68
2:BS:9:GLU:OE1	2:BS:13:ARG:NH2	2.27	0.68
2:Bk:1:MET:HG3	2:Bk:5:GLU:HB3	1.75	0.68
9:AX:10:PRO:HD3	2:BX:7:MET:HG3	1.75	0.68
11:Af:101:BCL:H172	2:Bf:19:GLY:HA3	1.77	0.67
2:Bm:21:ILE:HD13	11:Bm:103:BCL:H52	1.76	0.67
11:Ao:101:BCL:H91	11:Ao:101:BCL:C12	2.23	0.67
9:AQ:36:THR:O	2:BQ:41:ARG:NH1	2.27	0.67
9:AM:8:MET:HE3	9:AM:13:ILE:HD11	1.76	0.67
2:BI:3:GLU:OE1	2:BI:7:ARG:NH2	2.29	0.66
2:BP:29:VAL:HG22	11:AP:1102:BCL:HED1	1.78	0.66
2:Bn:21:ILE:HG22	11:AU:1001:BCL:H191	1.78	0.66
8:C:303:VAL:HG22	8:C:310:TRP:HD1	1.59	0.66
2:Bp:25:ALA:HB2	11:AR:101:BCL:H201	1.77	0.66
14:L:305:MQ8:H301	12:M:401:LMT:H81	1.78	0.66
1:Aj:3:ARG:HH12	2:Bj:7:ARG:HG3	1.61	0.65
1:Ak:17:MET:SD	11:Al:101:BCL:H143	2.37	0.65
9:AI:26:LEU:HD21	11:AI:102:BCL:H93	1.77	0.65
1:Al:64:MET:HE1	8:C:206:LYS:HB3	1.77	0.65
13:AA:1101:PEX:H44	13:AA:1101:PEX:H6	1.77	0.65
9:AO:26:LEU:HD21	11:AO:101:BCL:H93	1.78	0.65
2:BB:11:GLU:OE2	2:BB:14:ARG:NH2	2.29	0.64
9:AB:6:GLN:N	9:AB:6:GLN:OE1	2.31	0.64
2:Bp:23:VAL:HG12	11:Bp:1203:BCL:CED	2.28	0.64
11:AV:1001:BCL:H143	9:AW:23:GLY:HA3	1.78	0.64
8:C:87:GLU:O	8:C:91:THR:HG23	1.97	0.64
14:Ad:103:MQ8:H243	14:Ad:103:MQ8:H161	1.80	0.63
3:S:127:LYS:HG3	4:L:58:PRO:HA	1.81	0.63
11:AS:1102:BCL:H111	9:AT:24:LEU:HD13	1.81	0.63
2:BP:21:THR:HA	2:BP:24:LEU:HD12	1.81	0.63
9:AK:6:GLN:HA	2:BK:7:MET:HB3	1.80	0.62
1:Af:11:ARG:NH2	15:Af:102:CD4:O10	2.32	0.62
11:Al:101:BCL:CED	2:Bl:23:VAL:HG12	2.29	0.62
11:Ao:101:BCL:HED3	2:Bo:23:VAL:CG1	2.25	0.62
11:Bp:1203:BCL:HBB3	11:Bp:1203:BCL:HMB1	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:M:405:BCL:H141	16:M:406:BPH:H4C2	1.82	0.62
1:Af:7:MET:HE1	1:Ag:10:PRO:HB2	1.81	0.62
4:L:218:ARG:HD3	5:M:49:GLY:HA3	1.81	0.62
9:AT:18:GLY:HA3	11:AT:1103:BCL:H203	1.81	0.62
12:BC:102:LMT:H121	11:BD:101:BCL:H102	1.81	0.62
11:Be:1105:BCL:H13	9:AK:26:LEU:HD23	1.81	0.61
9:AB:3:ARG:HG2	9:AB:3:ARG:HH11	1.64	0.61
9:AL:26:LEU:HD11	11:AL:101:BCL:H71	1.82	0.61
9:AD:11:GLN:HG2	9:AE:8:MET:HE1	1.81	0.61
2:Bi:5:GLU:HG2	2:Bi:8:ARG:HH22	1.65	0.61
4:L:194:LEU:HD11	4:L:213:GLU:HB3	1.82	0.61
9:AH:1:MET:N	9:AH:1:MET:HE3	2.16	0.61
9:AO:8:MET:HB3	9:AO:13:ILE:HD11	1.83	0.61
1:Ac:43:ASN:O	1:Ac:45:THR:N	2.31	0.60
11:Am:101:BCL:HBB3	11:Am:101:BCL:HMB1	1.83	0.60
12:BF:102:LMT:H122	11:BG:102:BCL:H112	1.82	0.60
9:AE:5:TRP:CD1	2:BE:10:HIS:HB2	2.34	0.60
1:Af:11:ARG:HH21	15:Af:102:CD4:P2	2.24	0.60
11:Ao:101:BCL:H91	11:Ao:101:BCL:H143	1.83	0.60
2:BC:36:LEU:HD22	11:BD:101:BCL:H202	1.82	0.60
8:C:161:MET:HE1	8:C:297:LEU:HD21	1.83	0.60
14:L:305:MQ8:H192	11:M:404:BCL:H93	1.83	0.60
12:Ad:102:LMT:H92	12:Ad:102:LMT:H42	1.82	0.60
12:Bp:1201:LMT:H72	11:Bp:1203:BCL:CHD	2.32	0.60
8:C:192:THR:HG22	8:C:194:ASP:H	1.67	0.60
9:AH:1:MET:HE3	9:AH:1:MET:H1	1.66	0.59
1:Af:43:ASN:O	1:Af:45:THR:N	2.35	0.59
11:Am:101:BCL:C4	2:Bm:20:TYR:CE1	2.86	0.59
9:AL:24:LEU:HD23	11:BL:102:BCL:HED3	1.85	0.59
1:Ag:3:ARG:HG2	1:Ag:6:LEU:HB2	1.84	0.59
2:BG:40:TRP:HB2	12:BG:103:LMT:H21	1.85	0.58
2:BP:40:TRP:HB2	12:BQ:101:LMT:H22	1.85	0.58
1:Ap:4:ILE:HD12	1:Ap:4:ILE:H	1.67	0.58
11:AO:101:BCL:O1A	2:BO:26:TYR:OH	2.18	0.58
9:AA:30:MET:HE1	13:AA:1101:PEX:H14	1.84	0.58
11:Al:101:BCL:HMB3	11:Al:101:BCL:CBB	2.34	0.58
1:Ao:7:MET:HE1	1:Ap:10:PRO:HB2	1.85	0.58
2:BC:9:GLU:OE2	2:BC:13:ARG:NH2	2.32	0.58
1:Ag:2:HIS:HA	2:Bg:7:ARG:HH22	1.68	0.58
4:L:251:ILE:HA	4:L:255:PHE:HD2	1.69	0.58
9:AQ:22:ALA:HB1	11:AQ:102:BCL:H102	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:55:LEU:HD21	7:K:150:ASP:HB2	1.86	0.57
4:L:200:ASN:HB3	15:M:403:CD4:H54	1.85	0.57
12:BI:103:LMT:H5B	12:BI:103:LMT:H6D	1.85	0.57
2:Bn:34:TRP:HB2	12:AW:1201:LMT:H32	1.85	0.57
2:BS:33:ALA:HB2	12:BS:102:LMT:H122	1.86	0.57
13:Bc:1203:PEX:H6	13:Bc:1203:PEX:H35	1.87	0.57
9:AG:26:LEU:O	9:AG:30:MET:HG3	2.05	0.57
11:Ao:101:BCL:H91	11:Ao:101:BCL:H142	1.84	0.57
1:Ae:19:GLY:HA3	15:Af:102:CD4:H10	1.86	0.57
11:AJ:1103:BCL:H41	11:AJ:1103:BCL:H71	1.87	0.57
1:Ab:2:HIS:HB3	1:Ab:4:ILE:HG22	1.86	0.57
2:Be:7:ARG:NE	2:Be:7:ARG:HA	2.20	0.57
2:BS:14:ARG:NH1	10:BS:103:V7N:O45	2.35	0.56
13:Bn:102:PEX:O1	12:Bo:1201:LMT:O6'	2.21	0.56
7:K:68:PRO:HG2	7:K:87:LEU:HD11	1.87	0.56
9:AA:23:GLY:HA3	11:AX:1202:BCL:H162	1.86	0.56
11:Bh:1205:BCL:H72	11:Bh:1205:BCL:H41	1.87	0.56
8:C:92:MET:HE1	19:C:402:HEC:C4D	2.35	0.56
16:M:406:BPH:HBC3	16:M:406:BPH:HHD	1.88	0.56
11:AE:1102:BCL:HMA3	12:BE:102:LMT:H123	1.87	0.56
2:BL:24:LEU:O	2:BL:28:ILE:HG13	2.06	0.56
2:Bk:32:TRP:HH2	2:Bk:38:PHE:HB2	1.70	0.56
9:AL:2:HIS:CD2	2:BL:13:ARG:HE	2.24	0.56
2:Bh:27:ALA:HB1	12:Bh:1201:LMT:H91	1.88	0.56
1:Ao:14:MET:HA	1:Ao:14:MET:HE2	1.88	0.56
11:BN:101:BCL:HED1	9:AN:24:LEU:HG	1.88	0.56
2:BA:40:TRP:HB2	12:BA:104:LMT:H21	1.88	0.55
2:BK:11:GLU:OE2	2:BK:14:ARG:NH1	2.40	0.55
1:Ai:2:HIS:HB2	2:Bi:6:ALA:HB1	1.88	0.55
11:AQ:102:BCL:HED1	2:BQ:29:VAL:HG22	1.88	0.55
11:Ao:101:BCL:HMD3	2:Bo:28:HIS:CE1	2.40	0.55
9:AP:1:MET:SD	9:AP:1:MET:N	2.80	0.55
2:Bp:21:ILE:HG23	11:Bp:1204:BCL:H2	1.87	0.55
1:Ab:5:TRP:HE1	2:Bb:10:HIS:HD2	1.55	0.55
9:AC:24:LEU:HD23	11:BC:101:BCL:HED3	1.89	0.55
13:Bc:1203:PEX:H24	11:AN:101:BCL:H111	1.89	0.54
11:Ao:101:BCL:C17	11:Ao:101:BCL:C11	2.86	0.54
9:AA:20:PHE:HE1	11:AX:1202:BCL:H72	1.70	0.54
1:Ad:20:PHE:HD1	14:Ad:103:MQ8:H2M2	1.71	0.54
9:AF:11:GLN:NE2	9:AG:4:ILE:O	2.40	0.54
2:BF:10:ASP:OD2	2:BF:11:GLU:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:24:LEU:HD13	2:BB:28:ILE:HD11	1.88	0.54
2:Be:27:ALA:HB1	12:Be:1102:LMT:H91	1.88	0.54
11:Be:1105:BCL:H172	9:AK:26:LEU:HD23	1.89	0.54
1:Af:11:ARG:CZ	15:Af:102:CD4:H53	2.37	0.54
2:Bj:27:ALA:HB1	12:Bj:1201:LMT:H91	1.89	0.54
11:AV:1001:BCL:H18	9:AW:27:ILE:HD11	1.89	0.54
9:AE:5:TRP:HD1	2:BE:10:HIS:HB2	1.73	0.54
11:AQ:102:BCL:H2	11:AQ:102:BCL:H93	1.90	0.54
2:BX:28:ILE:O	2:BX:32:VAL:HG23	2.08	0.54
11:AM:101:BCL:H111	9:AN:24:LEU:HD13	1.90	0.54
3:S:185:SER:O	3:S:189:ARG:HG2	2.08	0.54
5:M:64:GLY:HA3	16:M:406:BPH:H5C1	1.89	0.54
2:Bd:25:ALA:HB1	13:Be:1101:PEX:H19	1.91	0.53
2:Bm:18:LEU:HD21	11:AW:1203:BCL:H152	1.89	0.53
2:Bm:34:TRP:HB2	12:AX:1201:LMT:H21	1.89	0.53
2:BP:24:LEU:O	2:BP:28:ILE:HG12	2.08	0.53
9:AK:3:ARG:NH1	2:BK:9:GLU:OE2	2.41	0.53
2:BR:7:MET:HB3	2:BR:11:GLU:HB2	1.90	0.53
1:Ab:3:ARG:HA	1:Ab:6:LEU:HD23	1.90	0.53
2:BF:16:HIS:HB2	9:AF:5:TRP:CD1	2.44	0.53
9:AM:36:THR:O	2:BM:41:ARG:NH1	2.41	0.53
2:BB:41:ARG:NH1	9:AB:36:THR:O	2.41	0.53
5:M:1:MET:HG2	5:M:2:LEU:H	1.73	0.53
2:BR:23:THR:O	2:BR:27:ILE:HG12	2.09	0.53
2:BB:9:GLU:HA	9:AB:6:GLN:HE21	1.73	0.53
2:BD:16:HIS:HB2	9:AD:5:TRP:CD1	2.44	0.53
2:BD:18:TYR:OH	9:AE:1:MET:SD	2.58	0.53
2:BX:25:GLY:HA2	2:BX:28:ILE:HD12	1.91	0.53
1:Ap:14:MET:HA	1:Ap:14:MET:HE2	1.90	0.53
5:M:82:ASP:HB3	5:M:85:GLU:HB2	1.91	0.53
11:Ac:101:BCL:HED1	2:Bc:23:VAL:HG12	1.91	0.52
9:AI:11:GLN:NE2	9:AJ:4:ILE:O	2.43	0.52
2:BN:28:ILE:O	2:BN:32:VAL:HG23	2.10	0.52
1:Ag:2:HIS:HA	2:Bg:7:ARG:HH12	1.74	0.52
11:Bb:1203:BCL:HAA1	13:AP:1101:PEX:H40	1.92	0.52
2:Be:32:TRP:HH2	2:Be:38:PHE:HB2	1.74	0.52
2:BB:40:TRP:HB2	12:BB:103:LMT:H21	1.90	0.52
1:Ai:14:MET:HA	1:Ai:17:MET:HG2	1.90	0.52
2:Bi:29:PHE:HD2	9:AF:30:MET:HE3	1.74	0.52
2:Bl:2:THR:HG23	2:Bl:5:GLU:H	1.74	0.52
7:K:98:TYR:OH	7:K:157:GLU:HG2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AD:26:LEU:O	9:AD:30:MET:HG3	2.10	0.52
11:BS:101:BCL:HMD3	9:AS:29:HIS:CE1	2.45	0.52
2:BP:40:TRP:HH2	9:AP:38:TRP:HB2	1.75	0.51
2:Bg:23:VAL:HG12	11:AI:101:BCL:HED1	1.91	0.51
2:BH:24:LEU:HD23	2:BH:28:ILE:HD11	1.92	0.51
9:AJ:38:TRP:HH2	2:BK:43:TRP:HB2	1.75	0.51
11:AW:1203:BCL:HED1	2:BW:29:VAL:HG12	1.90	0.51
14:Ad:103:MQ8:H161	14:Ad:103:MQ8:H212	1.92	0.51
9:AD:14:MET:HE2	9:AD:14:MET:HA	1.91	0.51
2:Bf:11:GLY:HA2	9:AJ:12:ILE:HD11	1.92	0.51
11:BD:101:BCL:H41	11:BD:101:BCL:H71	1.92	0.51
2:BH:28:ILE:O	2:BH:32:VAL:HG23	2.11	0.51
12:BO:104:LMT:H123	11:BP:101:BCL:H51	1.92	0.51
4:L:133:VAL:HG23	4:L:134:VAL:HG23	1.93	0.51
8:C:295:LYS:HG2	19:C:405:HEC:HAD2	1.91	0.51
9:AB:3:ARG:HG2	9:AB:3:ARG:NH1	2.25	0.51
9:AQ:30:MET:HB3	11:AQ:101:BCL:H191	1.93	0.51
1:Ai:1:MET:O	1:Ai:1:MET:HG3	2.11	0.51
9:AJ:24:LEU:HG	11:AJ:1103:BCL:CED	2.41	0.51
2:Bg:30:LEU:HD13	9:AI:30:MET:SD	2.51	0.51
11:Bn:103:BCL:HBB3	11:Ao:101:BCL:CHC	2.40	0.51
8:C:228:TYR:OH	19:C:405:HEC:O1A	2.29	0.51
2:BV:14:ARG:HH21	9:AW:3:ARG:HD3	1.76	0.51
11:Bo:1202:BCL:HBB3	11:Bp:1203:BCL:CHC	2.41	0.50
2:Bh:11:GLY:HA2	9:AG:12:ILE:HD11	1.92	0.50
2:Bi:32:TRP:HH2	2:Bi:38:PHE:HB2	1.75	0.50
3:S:145:PRO:O	8:C:193:ARG:NH1	2.31	0.50
7:K:88:TRP:HB2	7:K:98:TYR:HB2	1.94	0.50
9:AN:9:ASP:HB3	9:AN:12:ILE:HG13	1.93	0.50
9:AP:43:LYS:HG2	9:AQ:35:ILE:HA	1.92	0.50
13:Bm:102:PEX:H16	11:AW:1203:BCL:H91	1.93	0.50
2:BG:36:LEU:HD21	11:BH:104:BCL:H162	1.93	0.50
9:AL:7:GLY:HA2	2:BL:6:GLY:HA3	1.94	0.50
16:M:406:BPH:HHC	16:M:406:BPH:HBB3	1.94	0.50
1:Ac:1:MET:O	1:Ac:4:ILE:HG22	2.11	0.50
1:Af:11:ARG:NH2	15:Af:102:CD4:H53	2.27	0.50
11:Ao:101:BCL:CED	12:Bo:1201:LMT:H112	2.41	0.50
5:M:22:GLU:H	5:M:22:GLU:CD	2.20	0.50
9:AW:8:MET:HE3	9:AW:13:ILE:HD11	1.92	0.50
9:AW:29:HIS:CE1	11:AW:1204:BCL:HMD3	2.46	0.50
11:Ao:101:BCL:C11	11:Ao:101:BCL:C16	2.86	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Bp:1203:BCL:HMB1	11:Bp:1203:BCL:CBB	2.41	0.50
11:BA:101:BCL:H191	11:AB:101:BCL:H192	1.93	0.49
11:BA:101:BCL:C1A	12:BA:104:LMT:H111	2.41	0.49
2:BS:29:VAL:HG22	11:AS:1102:BCL:HED1	1.93	0.49
11:BI:102:BCL:H41	11:BI:102:BCL:H71	1.93	0.49
2:Ba:4:ASP:O	2:Ba:8:ARG:HD3	2.12	0.49
1:Af:18:VAL:HG13	11:Af:101:BCL:H43	1.94	0.49
11:Ao:101:BCL:HMB1	11:Ao:101:BCL:CBB	2.42	0.49
8:C:83:ILE:HG23	8:C:87:GLU:HB3	1.94	0.49
9:AS:8:MET:HE3	9:AS:13:ILE:HD11	1.94	0.49
11:AT:1102:BCL:H41	11:AT:1102:BCL:H8	1.95	0.49
11:Ak:101:BCL:H141	9:AC:19:PHE:CZ	2.47	0.49
11:Bl:1203:BCL:H43	11:Bl:1203:BCL:H3A	1.95	0.49
2:Ba:32:TRP:HE1	13:Ba:1101:PEX:H47	1.77	0.49
11:Bl:1203:BCL:HBB3	11:Am:101:BCL:CHC	2.42	0.49
9:AA:20:PHE:CE1	11:AX:1202:BCL:H72	2.47	0.49
9:AA:22:ALA:HB2	11:BA:101:BCL:H51	1.95	0.49
11:BB:101:BCL:HMD3	9:AB:29:HIS:CD2	2.48	0.49
2:BM:40:TRP:HB2	12:BM:1001:LMT:H11	1.94	0.49
2:BT:15:PHE:HE1	9:AT:10:PRO:HB3	1.78	0.49
2:Bc:30:LEU:HD21	13:AP:1101:PEX:H5	1.95	0.49
11:Am:101:BCL:H202	9:AX:19:PHE:CD1	2.48	0.49
5:M:34:GLY:HA2	5:M:49:GLY:HA2	1.94	0.49
2:BS:25:GLY:O	2:BS:29:VAL:HG12	2.13	0.49
2:Ba:18:LEU:O	2:Ba:22:ILE:HD12	2.13	0.49
14:L:305:MQ8:H341	14:L:305:MQ8:H361	1.46	0.49
8:C:307:PRO:HA	8:C:310:TRP:CE2	2.47	0.49
2:BF:24:LEU:O	2:BF:28:ILE:HG12	2.11	0.49
2:BK:8:THR:OG1	2:BK:10:ASP:OD1	2.27	0.49
9:AU:26:LEU:O	9:AU:30:MET:HG3	2.12	0.49
14:L:305:MQ8:H342	14:L:305:MQ8:H453	1.95	0.49
1:Ac:7:MET:HG2	1:Ad:11:ARG:HD2	1.95	0.48
2:Bc:34:TRP:HB2	12:Bc:1201:LMT:H22	1.95	0.48
9:AO:5:TRP:CD1	2:BO:16:HIS:HB2	2.48	0.48
2:BT:11:GLU:HB2	2:BT:14:ARG:HH12	1.77	0.48
8:C:74:TRP:HH2	8:C:85:VAL:HA	1.78	0.48
11:AH:101:BCL:H192	9:AI:8:MET:HE1	1.95	0.48
9:AX:3:ARG:HG3	9:AX:3:ARG:HH11	1.78	0.48
11:Am:101:BCL:H43	2:Bm:20:TYR:HE1	1.77	0.48
11:Ao:101:BCL:C17	11:Ao:101:BCL:H111	2.43	0.48
5:M:198:ASN:HB3	5:M:201:HIS:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BF:27:ILE:HD12	11:BF:101:BCL:H11	1.94	0.48
11:Ao:101:BCL:HED1	2:Bo:23:VAL:CG1	2.33	0.48
2:Bp:17:THR:O	2:Bp:21:ILE:HG12	2.14	0.48
4:L:17:LEU:HD13	4:L:107:GLU:HG2	1.93	0.48
2:BB:28:ILE:HD12	2:BB:28:ILE:H	1.78	0.48
11:BP:101:BCL:H102	11:BP:101:BCL:H142	1.94	0.48
9:AT:24:LEU:HG	11:AT:1102:BCL:CED	2.44	0.48
5:M:45:ASP:OD2	5:M:46:ALA:N	2.46	0.48
11:Bo:1202:BCL:HAA1	13:AT:1101:PEX:H42	1.95	0.48
16:L:303:BPH:HBC3	16:L:303:BPH:HHD	1.96	0.48
2:BB:33:ALA:HB1	12:BB:103:LMT:H92	1.95	0.48
9:AB:8:MET:HE2	9:AB:13:ILE:HD11	1.96	0.48
2:BE:17:THR:O	2:BE:21:ILE:HG12	2.14	0.48
1:Af:12:ARG:HG2	15:Af:102:CD4:H59	1.96	0.48
7:K:156:GLU:O	7:K:160:VAL:HG23	2.12	0.48
9:AG:38:TRP:HB2	2:BG:40:TRP:CH2	2.49	0.48
2:BP:40:TRP:CH2	9:AP:38:TRP:HB2	2.49	0.48
1:Aj:9:ASP:HB3	1:Aj:12:ARG:HD3	1.94	0.48
11:Am:101:BCL:H62	11:Am:101:BCL:H41	1.61	0.48
2:BC:40:TRP:HB2	12:BC:102:LMT:H22	1.96	0.48
9:AT:24:LEU:HG	11:AT:1102:BCL:HED2	1.95	0.48
1:Af:7:MET:HG2	1:Ag:11:ARG:HG3	1.96	0.48
3:S:180:ILE:HB	4:L:265:ASN:OD1	2.14	0.48
11:Al:101:BCL:HMB3	11:Al:101:BCL:HBB2	1.94	0.47
2:Bn:25:ALA:HB2	11:AU:1001:BCL:H193	1.95	0.47
9:AL:22:ALA:HB1	11:AL:101:BCL:H61	1.96	0.47
2:BN:25:GLY:O	2:BN:29:VAL:HG12	2.14	0.47
2:Bp:28:HIS:HB3	13:AS:1101:PEX:H11	1.96	0.47
2:BD:40:TRP:HB2	12:BD:102:LMT:H22	1.96	0.47
2:BU:28:ILE:O	2:BU:32:VAL:HG23	2.14	0.47
11:Bp:1203:BCL:H52	11:Bp:1203:BCL:H12	1.60	0.47
13:Aj:103:PEX:H1	5:M:165:LEU:HD21	1.95	0.47
13:Bm:102:PEX:H13	9:AX:27:ILE:HD13	1.94	0.47
11:Ao:101:BCL:H111	11:Ao:101:BCL:H171	1.95	0.47
5:M:98:PRO:HB3	5:M:107:PRO:HB3	1.95	0.47
2:BD:40:TRP:HH2	9:AD:38:TRP:HB2	1.78	0.47
11:AN:101:BCL:H101	11:AN:101:BCL:H62	1.54	0.47
1:Af:10:PRO:HB3	2:Bf:9:PHE:CE2	2.49	0.47
5:M:248:MET:HE3	5:M:260:THR:HG22	1.95	0.47
2:BP:7:MET:HE3	9:AP:10:PRO:HB3	1.95	0.47
11:Ao:101:BCL:O2D	12:Bo:1201:LMT:H112	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Am:101:BCL:CHD	12:AX:1201:LMT:H71	2.45	0.47
2:Bp:21:ILE:HG22	11:AR:101:BCL:H203	1.96	0.47
6:H:27:ARG:HG3	6:H:47:PRO:HB2	1.96	0.47
6:H:46:TRP:CE3	6:H:47:PRO:HA	2.50	0.47
9:AB:29:HIS:HE1	11:AB:101:BCL:C4B	2.21	0.47
2:BE:18:LEU:O	2:BE:22:ILE:HG13	2.14	0.47
2:BF:8:THR:OG1	2:BF:10:ASP:OD2	2.32	0.47
2:BF:23:THR:O	2:BF:27:ILE:HG12	2.15	0.47
11:AV:1001:BCL:HMA3	12:BW:101:LMT:H122	1.97	0.47
11:BI:102:BCL:HBA1	11:BI:102:BCL:H11	1.41	0.47
11:Al:101:BCL:HED3	2:Bl:23:VAL:HG12	1.96	0.47
8:C:126:TYR:O	8:C:130:VAL:HG23	2.15	0.47
8:C:270:TYR:HB3	8:C:274:ARG:HB2	1.96	0.47
9:AB:24:LEU:O	9:AB:28:ILE:HG12	2.15	0.47
2:BD:13:ARG:NH1	2:BD:13:ARG:HB2	2.29	0.47
11:AT:1103:BCL:H8	9:AU:20:PHE:HE1	1.80	0.47
2:BJ:40:TRP:CE2	2:BJ:41:ARG:HG3	2.50	0.47
2:Bb:34:TRP:HB2	12:Bb:1201:LMT:H31	1.97	0.46
12:Ad:102:LMT:H3'	4:L:77:GLY:HA2	1.96	0.46
2:Bo:7:ARG:NH1	9:AU:7:GLY:O	2.47	0.46
1:Ap:2:HIS:HB3	1:Ap:4:ILE:HD12	1.97	0.46
1:Ap:43:ASN:HB2	1:Ap:46:LEU:HD12	1.97	0.46
2:BB:8:THR:HG23	2:BB:11:GLU:HB2	1.97	0.46
12:BM:1001:LMT:H102	11:BN:101:BCL:HBB2	1.97	0.46
11:AS:1102:BCL:HAA1	11:AS:1102:BCL:CGD	2.44	0.46
2:BX:40:TRP:CE2	2:BX:41:ARG:HG3	2.50	0.46
11:Bg:103:BCL:H92	12:Bh:1201:LMT:H111	1.97	0.46
1:Ao:57:ALA:HB2	1:Ap:52:PRO:HA	1.96	0.46
2:BC:7:MET:HB3	2:BC:11:GLU:HG3	1.96	0.46
9:AE:26:LEU:HD21	13:AE:1101:PEX:H19	1.96	0.46
2:BW:13:ARG:HB2	2:BW:13:ARG:NH1	2.30	0.46
1:Aj:57:ALA:HB3	1:Ak:52:PRO:HA	1.97	0.46
11:Bj:1204:BCL:H72	13:AD:1101:PEX:H37	1.96	0.46
11:Ao:101:BCL:C17	11:Ao:101:BCL:H112	2.46	0.46
4:L:171:ASN:HB3	4:L:174:HIS:HB3	1.97	0.46
5:M:1:MET:HG2	5:M:2:LEU:N	2.30	0.46
14:Ad:103:MQ8:H241	14:Ad:103:MQ8:H261	1.60	0.46
2:Bm:32:TRP:HH2	2:Bm:38:PHE:HB2	1.79	0.46
13:Bn:102:PEX:H42	11:Bn:103:BCL:HAA1	1.98	0.46
11:AH:101:BCL:HED1	12:BH:103:LMT:H112	1.96	0.46
9:AP:26:LEU:O	9:AP:30:MET:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AV:9:ASP:N	9:AV:9:ASP:OD1	2.49	0.46
11:Ak:101:BCL:H112	11:Ak:101:BCL:H142	1.73	0.46
9:AC:1:MET:HE3	9:AC:1:MET:HA	1.96	0.46
2:BR:40:TRP:HB2	12:BR:102:LMT:H21	1.97	0.46
1:Ae:18:VAL:HG21	11:Ae:101:BCL:H122	1.97	0.46
11:Ae:101:BCL:HAA1	11:Ae:101:BCL:CGD	2.45	0.46
8:C:161:MET:HE2	8:C:161:MET:HA	1.97	0.46
2:BF:41:ARG:NH1	9:AF:36:THR:O	2.49	0.46
9:AO:10:PRO:HA	9:AO:13:ILE:HD12	1.98	0.46
9:AO:38:TRP:HB2	2:BO:40:TRP:CH2	2.51	0.46
11:Bk:103:BCL:HBB3	11:Al:101:BCL:CHC	2.45	0.46
4:L:166:LEU:HD21	8:C:225:ASN:HA	1.97	0.46
4:L:242:ALA:HB2	16:L:303:BPH:HAC2	1.98	0.46
2:BF:7:MET:SD	9:AF:10:PRO:HG3	2.56	0.46
9:AK:5:TRP:HB2	2:BK:12:ALA:HB1	1.98	0.46
2:BP:28:ILE:O	2:BP:32:VAL:HG23	2.16	0.46
9:AS:27:ILE:HD11	13:AS:1101:PEX:H21	1.97	0.46
11:BU:102:BCL:HMD3	9:AU:29:HIS:CE1	2.50	0.46
1:Af:24:LEU:HB3	11:Bf:1204:BCL:HED1	1.97	0.46
1:Al:14:MET:HE2	1:Al:14:MET:HA	1.97	0.46
1:Al:17:MET:HE2	1:Al:17:MET:HB3	1.87	0.46
2:Bo:4:ASP:OD1	2:Bo:5:GLU:N	2.49	0.46
4:L:239:VAL:HA	16:L:303:BPH:HBC1	1.98	0.46
2:BD:40:TRP:CH2	9:AD:38:TRP:HB2	2.51	0.46
3:S:172:MET:HE2	3:S:172:MET:HB3	1.82	0.46
16:L:303:BPH:HBB3	16:L:303:BPH:HHC	1.97	0.46
12:K:201:LMT:H1B	12:K:201:LMT:H3'	1.52	0.46
11:BF:101:BCL:H92	11:BF:101:BCL:H61	1.86	0.46
9:AG:1:MET:HB3	9:AG:2:HIS:H	1.50	0.46
11:Ad:101:BCL:H41	11:Ad:101:BCL:H62	1.66	0.45
2:Bf:34:TRP:HB2	12:Bf:1201:LMT:H21	1.98	0.45
1:Aj:3:ARG:HG3	1:Aj:6:LEU:HD12	1.97	0.45
11:Am:101:BCL:HMB1	11:Am:101:BCL:CBB	2.46	0.45
2:Bm:7:ARG:HD2	2:Bm:7:ARG:HA	1.67	0.45
2:Bp:29:PHE:HD1	9:AS:30:MET:HE2	1.81	0.45
5:M:259:ALA:N	14:M:408:MQ8:H2M3	2.31	0.45
2:BO:28:ILE:O	2:BO:32:VAL:HG23	2.15	0.45
11:AR:101:BCL:H61	11:AR:101:BCL:H41	1.68	0.45
11:Bl:1203:BCL:H18	13:AA:1101:PEX:H3	1.99	0.45
11:Ao:101:BCL:H112	11:Ao:101:BCL:H172	1.96	0.45
9:AR:11:GLN:NE2	9:AS:4:ILE:O	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:BS:102:LMT:O1B	12:BS:102:LMT:O6'	2.33	0.45
1:Ab:3:ARG:HH22	2:Bb:7:ARG:HG2	1.81	0.45
2:BL:40:TRP:CE2	2:BL:41:ARG:HG3	2.51	0.45
14:Ad:103:MQ8:H111	14:Ad:103:MQ8:H2M1	1.80	0.45
11:Ah:101:BCL:H12	11:Ah:101:BCL:H52	1.78	0.45
4:L:188:LEU:HD11	5:M:268:SER:HB3	1.98	0.45
9:AH:12:ILE:HD13	9:AH:12:ILE:HA	1.89	0.45
11:AM:101:BCL:O1A	2:BM:26:TYR:OH	2.34	0.45
2:BT:15:PHE:CE1	9:AT:10:PRO:HB3	2.51	0.45
9:AX:8:MET:O	2:BX:7:MET:HB2	2.17	0.45
11:AE:1102:BCL:HED3	2:BE:23:VAL:HG12	1.99	0.45
2:Bb:32:TRP:HH2	2:Bb:38:PHE:HB2	1.81	0.45
9:AC:11:GLN:NE2	9:AD:4:ILE:O	2.50	0.45
2:BS:17:GLY:O	2:BS:21:THR:HG22	2.16	0.45
4:L:23:PHE:O	4:L:33:GLY:HA2	2.17	0.45
8:C:215:MET:HB3	19:C:404:HEC:C4B	2.46	0.45
9:AI:26:LEU:HD11	11:AI:102:BCL:H101	1.99	0.45
2:BK:28:ILE:O	2:BK:32:VAL:HG23	2.17	0.45
1:Al:15:VAL:HG21	5:M:55:TRP:CD1	2.52	0.45
12:M:401:LMT:H3'	12:M:401:LMT:H1B	1.69	0.45
11:BA:101:BCL:CHC	11:BB:101:BCL:HBB3	2.47	0.45
9:AH:36:THR:O	2:BH:41:ARG:NH1	2.50	0.45
9:AV:5:TRP:HB3	2:BV:7:MET:HE1	1.98	0.45
12:Bd:1201:LMT:H5'	12:Bd:1201:LMT:H1B	1.85	0.45
11:Bi:102:BCL:H62	13:AE:1101:PEX:H42	1.99	0.45
2:Bo:32:TRP:CD1	13:AT:1101:PEX:H7	2.52	0.45
2:BP:7:MET:HE1	2:BP:15:PHE:CG	2.51	0.45
1:Ac:42:GLU:OE1	1:Ac:42:GLU:HA	2.17	0.44
1:Ao:17:MET:HE2	1:Ao:17:MET:HB3	1.84	0.44
9:AF:9:ASP:O	9:AF:13:ILE:HD12	2.17	0.44
9:AM:24:LEU:HG	11:AM:102:BCL:CED	2.48	0.44
9:AQ:6:GLN:HA	2:BQ:7:MET:HB2	1.98	0.44
9:AV:10:PRO:HG3	2:BV:7:MET:HG3	1.99	0.44
2:Bb:5:GLU:OE1	2:Bb:5:GLU:N	2.43	0.44
14:Ad:103:MQ8:H411	14:Ad:103:MQ8:H391	1.62	0.44
2:Bh:29:PHE:O	2:Bh:33:GLN:HG2	2.18	0.44
1:Ao:24:LEU:O	1:Ao:28:ILE:HG13	2.18	0.44
14:L:305:MQ8:H391	14:L:305:MQ8:H412	1.69	0.44
11:BE:101:BCL:H91	11:BE:101:BCL:H112	1.68	0.44
2:BF:29:VAL:HG23	11:AF:102:BCL:HED3	1.99	0.44
9:AN:42:LYS:HD2	9:AN:42:LYS:HA	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BQ:25:GLY:O	2:BQ:29:VAL:HG12	2.18	0.44
2:Bg:17:THR:O	2:Bg:21:ILE:HG12	2.18	0.44
2:Bh:32:TRP:HH2	2:Bh:38:PHE:HB2	1.81	0.44
1:Ak:3:ARG:HG3	1:Ak:6:LEU:HD12	1.98	0.44
9:AG:10:PRO:HG3	2:BG:7:MET:SD	2.57	0.44
2:BN:28:ILE:HD12	2:BN:28:ILE:N	2.28	0.44
11:AQ:102:BCL:CED	2:BQ:29:VAL:HG22	2.47	0.44
1:Aa:13:VAL:O	1:Aa:17:MET:HB2	2.17	0.44
2:Bp:28:HIS:CE1	11:Bp:1203:BCL:HMD3	2.53	0.44
11:M:404:BCL:H61	11:M:404:BCL:H41	1.64	0.44
6:H:31:ARG:NH1	6:H:51:GLU:O	2.49	0.44
8:C:109:HIS:CE1	8:C:128:LYS:HE3	2.52	0.44
9:AC:38:TRP:HB2	2:BC:40:TRP:CH2	2.52	0.44
9:AW:10:PRO:HB3	2:BW:15:PHE:CE1	2.53	0.44
14:Ad:103:MQ8:H141	14:Ad:103:MQ8:H161	1.57	0.44
2:Be:32:TRP:CD2	13:Be:1104:PEX:H5	2.52	0.44
3:S:166:ARG:HG2	3:S:178:TRP:HH2	1.83	0.44
9:AG:9:ASP:HB3	9:AG:12:ILE:HB	1.98	0.44
1:Ab:5:TRP:HE1	2:Bb:10:HIS:CD2	2.35	0.44
1:Ai:10:PRO:HB3	2:Bi:9:PHE:CE2	2.52	0.44
9:AP:4:ILE:H	9:AP:4:ILE:HG13	1.51	0.44
15:Af:102:CD4:H28	15:Af:102:CD4:H27	1.53	0.44
2:Bn:22:ILE:HD13	2:Bn:22:ILE:HA	1.88	0.44
9:AK:38:TRP:HB2	2:BK:40:TRP:CH2	2.53	0.44
2:BP:26:TYR:OH	11:AP:1102:BCL:O1A	2.33	0.44
11:BD:101:BCL:HED1	9:AD:24:LEU:HD23	2.00	0.44
2:BM:28:ILE:O	2:BM:32:VAL:HG23	2.18	0.44
9:AT:13:ILE:HG22	9:AT:14:MET:HE2	1.99	0.44
9:AV:38:TRP:HB2	2:BV:40:TRP:CH2	2.52	0.44
1:An:7:MET:HE2	1:An:7:MET:HB2	1.73	0.44
8:C:39:MET:HG2	8:C:227:THR:HB	1.99	0.44
8:C:283:LYS:HB2	8:C:283:LYS:HE2	1.77	0.44
2:BF:33:ALA:HB1	12:BF:102:LMT:H91	1.99	0.44
9:AM:30:MET:HE2	9:AM:30:MET:HB3	1.79	0.44
11:AM:102:BCL:H18	11:AM:102:BCL:H152	1.79	0.44
2:BO:7:MET:HG2	2:BO:11:GLU:HG3	1.98	0.44
8:C:294:TYR:CE2	8:C:295:LYS:HD2	2.53	0.43
11:AE:1102:BCL:H91	11:AE:1102:BCL:H112	1.82	0.43
11:AK:101:BCL:H192	11:AK:101:BCL:H161	1.86	0.43
11:BO:103:BCL:H142	11:BO:103:BCL:H112	1.80	0.43
2:BQ:14:ARG:HG2	2:BQ:14:ARG:HH11	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Bb:1203:BCL:H93	11:Bb:1203:BCL:H61	1.84	0.43
1:Aj:10:PRO:HB3	2:Bj:9:PHE:CZ	2.53	0.43
9:AO:38:TRP:HB2	2:BO:40:TRP:HH2	1.82	0.43
11:AR:101:BCL:H91	11:AR:101:BCL:H112	1.76	0.43
13:Bc:1203:PEX:H20	11:AN:101:BCL:H8	2.01	0.43
13:Bn:102:PEX:H35	13:Bn:102:PEX:H16	2.00	0.43
5:M:258:ASN:HA	14:M:408:MQ8:H2M2	2.00	0.43
11:BG:102:BCL:H202	11:BG:102:BCL:H162	1.77	0.43
12:BH:103:LMT:H122	12:BH:103:LMT:H92	1.79	0.43
2:BI:21:ILE:HG12	11:BI:102:BCL:H12	2.00	0.43
9:AJ:42:LYS:HG2	2:BK:43:TRP:O	2.19	0.43
11:AT:1102:BCL:H71	11:AT:1102:BCL:H112	1.55	0.43
2:Bc:32:TRP:HH2	2:Bc:38:PHE:HB2	1.82	0.43
1:Ag:1:MET:O	2:Bg:7:ARG:NH1	2.51	0.43
2:Bg:32:TRP:HH2	2:Bg:38:PHE:HB2	1.84	0.43
2:BB:8:THR:OG1	2:BB:9:GLU:N	2.50	0.43
11:AK:101:BCL:H61	11:AK:101:BCL:H112	2.01	0.43
9:AW:1:MET:O	9:AW:4:ILE:HG12	2.18	0.43
9:AW:42:LYS:HD2	9:AW:42:LYS:HA	1.74	0.43
2:BW:28:ILE:O	2:BW:32:VAL:HG23	2.18	0.43
13:Aj:103:PEX:H26	13:Aj:103:PEX:H3	1.82	0.43
11:Ao:101:BCL:H61	11:Ao:101:BCL:H92	1.63	0.43
1:Ap:5:TRP:HB3	1:Ap:10:PRO:HG3	2.00	0.43
9:AP:4:ILE:O	9:AP:8:MET:HE2	2.19	0.43
9:AV:38:TRP:HB2	2:BV:40:TRP:HH2	1.82	0.43
2:Be:32:TRP:CE2	13:Be:1104:PEX:H5	2.53	0.43
1:Ag:4:ILE:HD12	1:Ag:4:ILE:HA	1.87	0.43
2:Bp:23:VAL:HG12	11:Bp:1203:BCL:HED1	1.98	0.43
9:AQ:4:ILE:HD12	9:AQ:5:TRP:N	2.33	0.43
12:BW:103:LMT:O6B	12:BW:103:LMT:O4'	2.33	0.43
11:Aj:101:BCL:H52	11:Aj:101:BCL:H12	1.84	0.43
2:Bk:12:TYR:CE1	9:AC:12:ILE:HD11	2.53	0.43
3:S:146:THR:OG1	5:M:321:ARG:HD3	2.17	0.43
16:L:303:BPH:NC	5:M:213:VAL:HG22	2.34	0.43
2:BG:24:LEU:O	2:BG:28:ILE:HG13	2.18	0.43
2:BT:13:ARG:HE	2:BT:13:ARG:HB3	1.58	0.43
1:Af:17:MET:HE2	1:Af:17:MET:HB3	1.79	0.43
9:AD:40:LYS:HB3	9:AD:40:LYS:HE3	1.80	0.43
9:AM:38:TRP:HB2	2:BM:40:TRP:HH2	1.84	0.43
2:BS:40:TRP:CH2	9:AS:38:TRP:HB2	2.53	0.43
2:Bk:32:TRP:CE2	13:Bk:102:PEX:H5	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BP:7:MET:HE1	2:BP:15:PHE:CD1	2.54	0.43
2:Bc:22:ILE:CG2	9:AO:23:GLY:HA3	2.48	0.43
4:L:129:TYR:CD1	11:L:302:BCL:HBB1	2.54	0.43
5:M:75:MET:HG2	5:M:93:LEU:CB	2.49	0.43
5:M:203:LEU:HD23	5:M:203:LEU:HA	1.86	0.43
9:AH:3:ARG:H	9:AH:3:ARG:CD	2.28	0.43
2:BT:14:ARG:NH1	10:BT:101:V7N:O44	2.52	0.43
9:AW:38:TRP:HB2	2:BW:40:TRP:CH2	2.54	0.43
1:Af:3:ARG:HH11	1:Af:3:ARG:HB2	1.84	0.42
14:L:305:MQ8:H171	14:L:305:MQ8:H211	1.83	0.42
8:C:166:PRO:HG2	19:C:403:HEC:C1D	2.49	0.42
2:BG:28:ILE:O	2:BG:32:VAL:HG23	2.19	0.42
2:BV:25:GLY:O	2:BV:29:VAL:HG23	2.19	0.42
1:Aa:17:MET:HE2	1:Aa:17:MET:HB3	1.91	0.42
1:Al:12:ARG:NH2	5:M:29:THR:HB	2.34	0.42
4:L:131:THR:HA	4:L:135:ILE:HB	2.01	0.42
2:BG:39:GLN:H	2:BG:39:GLN:HG2	1.58	0.42
2:BJ:40:TRP:HB2	12:BK:101:LMT:H32	2.01	0.42
9:AK:24:LEU:HG	11:BK:102:BCL:HED1	2.01	0.42
9:AV:40:LYS:HE2	9:AV:40:LYS:HB3	1.70	0.42
11:Ab:101:BCL:HHC	11:Ab:101:BCL:OBB	2.19	0.42
13:Bg:102:PEX:H11	13:Bg:102:PEX:H16	1.86	0.42
2:Bl:32:TRP:HH2	2:Bl:38:PHE:HB2	1.84	0.42
11:AI:102:BCL:H62	11:AI:102:BCL:H41	1.90	0.42
11:BI:102:BCL:H11	11:BI:102:BCL:H51	1.76	0.42
2:BL:28:ILE:O	2:BL:32:VAL:HG23	2.19	0.42
11:AR:101:BCL:H142	9:AS:20:PHE:HD1	1.83	0.42
9:AW:38:TRP:CD1	2:BX:44:PHE:HB3	2.54	0.42
2:Bb:22:ILE:HD13	2:Bb:22:ILE:HA	1.86	0.42
2:Bk:12:TYR:CD1	9:AC:12:ILE:HD11	2.55	0.42
7:K:25:ILE:N	7:K:25:ILE:HD12	2.34	0.42
12:BA:104:LMT:H5B	12:BA:104:LMT:H6D	2.01	0.42
9:AD:24:LEU:O	9:AD:28:ILE:HG13	2.20	0.42
9:AM:38:TRP:HB2	2:BM:40:TRP:CH2	2.54	0.42
9:AS:24:LEU:O	9:AS:28:ILE:HG13	2.20	0.42
9:AU:42:LYS:HA	9:AU:42:LYS:HD3	1.68	0.42
4:L:8:LYS:HE2	4:L:8:LYS:HB3	1.64	0.42
9:AE:8:MET:HE2	9:AE:8:MET:HB3	1.79	0.42
9:AG:24:LEU:O	9:AG:28:ILE:HG13	2.20	0.42
2:Bb:31:ALA:HA	12:Bb:1201:LMT:H51	2.01	0.42
4:L:136:ARG:NH1	4:L:252:SER:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:335:TYR:HB2	8:C:264:SER:HB3	2.00	0.42
11:BA:101:BCL:CHA	12:BA:104:LMT:H111	2.50	0.42
12:BO:104:LMT:H121	12:BO:104:LMT:H92	1.87	0.42
2:BR:16:HIS:O	2:BR:20:VAL:HG22	2.19	0.42
2:BS:40:TRP:HH2	9:AS:38:TRP:HB2	1.84	0.42
11:Bd:1203:BCL:H52	11:Bd:1203:BCL:H8	1.80	0.42
2:Bh:22:ILE:HD13	2:Bh:22:ILE:HA	1.91	0.42
11:Bj:1204:BCL:C2B	13:AD:1101:PEX:H36	2.49	0.42
11:AC:101:BCL:H62	11:AC:101:BCL:H2	1.79	0.42
11:BC:101:BCL:H202	11:BC:101:BCL:H162	1.78	0.42
11:BF:101:BCL:H61	11:BF:101:BCL:H41	1.79	0.42
2:BN:35:PHE:HA	11:BN:101:BCL:H172	2.00	0.42
11:AO:101:BCL:H91	11:AO:101:BCL:H111	1.79	0.42
2:BR:28:ILE:O	2:BR:32:VAL:HG23	2.20	0.42
11:AT:1103:BCL:H62	11:AT:1103:BCL:H41	1.77	0.42
2:BU:40:TRP:CH2	9:AU:38:TRP:HB2	2.54	0.42
2:BX:26:TYR:HE2	11:BX:102:BCL:HBA1	1.84	0.42
11:BX:102:BCL:H142	11:BX:102:BCL:H111	1.80	0.42
11:Al:101:BCL:HBA1	11:Al:101:BCL:H3A	1.78	0.42
2:Bn:8:ARG:HE	2:Bn:8:ARG:HB3	1.66	0.42
1:Ap:7:MET:HE2	1:Ap:7:MET:HB2	1.97	0.42
1:Ap:10:PRO:HB3	2:Bp:9:PHE:CE2	2.55	0.42
4:L:163:TYR:HB3	8:C:226:CYS:SG	2.59	0.42
9:AO:1:MET:HE2	9:AO:1:MET:HA	2.01	0.42
12:BO:104:LMT:H5'	12:BO:104:LMT:H1B	1.73	0.42
11:AT:1103:BCL:H142	11:AT:1103:BCL:H112	1.84	0.42
11:Bp:1203:BCL:H61	11:Bp:1203:BCL:H101	1.41	0.42
4:L:116:MET:O	4:L:120:TRP:HD1	2.01	0.42
5:M:155:PHE:O	5:M:159:THR:HG23	2.20	0.42
5:M:319:LEU:HD21	8:C:250:HIS:NE2	2.35	0.42
2:BA:39:GLN:H	2:BA:39:GLN:HG2	1.62	0.42
9:AQ:28:ILE:HA	9:AQ:31:TRP:HB3	2.02	0.42
12:BW:103:LMT:H121	11:BX:102:BCL:H102	2.02	0.42
11:Ae:101:BCL:HED1	2:Be:23:VAL:HG12	2.01	0.42
13:Bh:1203:PEX:H16	13:Bh:1203:PEX:H33	2.01	0.42
9:AL:38:TRP:HB2	2:BL:40:TRP:CH2	2.54	0.42
2:BP:9:GLU:OE1	2:BP:13:ARG:NH2	2.53	0.42
3:S:184:ARG:NH1	3:S:184:ARG:HG3	2.35	0.41
11:L:302:BCL:HHC	11:L:302:BCL:HBB2	2.01	0.41
9:AH:5:TRP:HA	9:AH:8:MET:HE2	2.01	0.41
9:AI:5:TRP:CD1	2:BI:10:HIS:HB2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BT:40:TRP:CH2	9:AT:38:TRP:HB2	2.55	0.41
9:AT:3:ARG:HA	9:AT:3:ARG:HD3	1.79	0.41
9:AW:4:ILE:O	9:AW:8:MET:HE2	2.20	0.41
11:Ab:101:BCL:H12	2:Bb:20:TYR:HE1	1.85	0.41
2:Be:19:GLY:O	2:Be:23:VAL:HG23	2.20	0.41
1:Ao:14:MET:HE1	2:Bo:13:PHE:CE1	2.55	0.41
11:Bp:1203:BCL:H91	11:Bp:1203:BCL:H111	1.58	0.41
8:C:303:VAL:HG22	8:C:310:TRP:CD1	2.47	0.41
11:AI:102:BCL:HMA3	12:BI:103:LMT:H123	2.03	0.41
9:AL:42:LYS:HD2	9:AL:42:LYS:HA	1.77	0.41
11:AR:101:BCL:H142	9:AS:20:PHE:HA	2.02	0.41
2:BT:15:PHE:C	2:BT:15:PHE:CD2	2.98	0.41
12:Bj:1201:LMT:H5B	12:Bj:1201:LMT:H6D	2.01	0.41
2:BJ:40:TRP:CD2	2:BJ:41:ARG:HG3	2.55	0.41
2:BN:7:MET:SD	9:AN:10:PRO:HD3	2.61	0.41
9:AW:38:TRP:HB2	2:BW:40:TRP:HH2	1.85	0.41
13:Be:1104:PEX:H4	13:Be:1104:PEX:H6	1.82	0.41
2:BB:23:THR:O	2:BB:27:ILE:HG12	2.21	0.41
9:AG:38:TRP:HB2	2:BG:40:TRP:HH2	1.84	0.41
1:Ae:2:HIS:HB2	2:Be:7:ARG:NH2	2.36	0.41
1:Ai:43:ASN:HB2	1:Ai:46:LEU:HD12	2.02	0.41
11:Aj:101:BCL:HHC	11:Aj:101:BCL:OBB	2.21	0.41
2:Bj:25:ALA:HB1	13:AD:1101:PEX:H14	2.02	0.41
2:Bo:14:VAL:HG22	11:Bo:1202:BCL:H162	2.02	0.41
4:L:76:LEU:HA	4:L:143:TRP:CD1	2.56	0.41
5:M:201:HIS:O	5:M:205:ILE:HG12	2.19	0.41
11:AC:101:BCL:H143	9:AD:27:ILE:HD12	2.03	0.41
2:BC:28:ILE:O	2:BC:32:VAL:HG23	2.21	0.41
2:BN:12:ALA:HB1	9:AN:5:TRP:HB2	2.02	0.41
12:BS:102:LMT:H62	12:BS:102:LMT:H32	1.81	0.41
9:AW:11:GLN:HG2	9:AX:8:MET:HE3	2.03	0.41
1:Ac:17:MET:HE2	1:Ac:17:MET:HB3	1.89	0.41
2:Bc:17:THR:O	2:Bc:21:ILE:HG12	2.19	0.41
1:Ae:20:PHE:HA	15:Af:102:CD4:H3	2.03	0.41
12:Bf:1203:LMT:H12	13:AJ:1101:PEX:H3	2.02	0.41
2:Bo:1:MET:HE3	2:Bo:1:MET:HB3	1.92	0.41
11:AL:101:BCL:H102	9:AM:24:LEU:HD13	2.03	0.41
11:Ac:101:BCL:OBB	11:Ac:101:BCL:HHC	2.19	0.41
2:Bd:26:VAL:HG11	9:AN:27:ILE:HD13	2.03	0.41
11:Ae:101:BCL:H62	11:Ae:101:BCL:H41	1.83	0.41
11:Bj:1204:BCL:H141	9:AC:26:LEU:HD13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Al:10:PRO:HB3	2:Bl:9:PHE:CZ	2.56	0.41
11:Bl:1203:BCL:H72	11:AX:1202:BCL:H203	2.03	0.41
7:K:106:SER:OG	7:K:107:GLU:N	2.52	0.41
9:AB:43:LYS:HG2	9:AC:35:ILE:HA	2.01	0.41
2:BF:8:THR:H	2:BF:11:GLU:HB2	1.86	0.41
9:AR:26:LEU:O	9:AR:30:MET:HG3	2.21	0.41
12:BS:102:LMT:H82	11:AT:1102:BCL:HBB2	2.01	0.41
11:AV:1001:BCL:H62	11:AV:1001:BCL:H41	1.83	0.41
2:BV:39:GLN:H	2:BV:39:GLN:HG2	1.70	0.41
1:Ae:3:ARG:HG2	1:Ae:6:LEU:HD23	2.02	0.41
1:Ag:43:ASN:HB2	1:Ag:46:LEU:HD12	2.02	0.41
2:Bl:26:VAL:HG11	11:BA:101:BCL:H171	2.02	0.41
11:Bm:103:BCL:CGA	11:Bm:103:BCL:H3A	2.51	0.41
2:BD:29:VAL:HG12	11:AD:1102:BCL:CED	2.50	0.41
9:AP:43:LYS:HE2	9:AP:43:LYS:HB3	1.74	0.41
11:AT:1103:BCL:H102	11:AT:1103:BCL:H61	1.86	0.41
1:Ac:2:HIS:CD2	2:Bc:7:ARG:HB2	2.56	0.41
13:Bc:1203:PEX:H13	13:Bc:1203:PEX:H7	1.81	0.41
11:Al:101:BCL:CBB	11:Al:101:BCL:CMB	2.98	0.41
1:Am:7:MET:HE2	1:Am:7:MET:HB2	1.84	0.41
1:Am:17:MET:HE2	1:Am:17:MET:HB3	1.80	0.41
1:Ao:4:ILE:H	1:Ao:4:ILE:CD1	2.31	0.41
3:S:162:PRO:O	3:S:192:TYR:HB2	2.21	0.41
4:L:9:LYS:HD2	7:K:32:SER:HB3	2.02	0.41
5:M:232:ARG:NH2	7:K:157:GLU:OE1	2.53	0.41
5:M:321:ARG:HB3	5:M:321:ARG:CZ	2.50	0.41
14:M:408:MQ8:H291	14:M:408:MQ8:H312	1.69	0.41
2:BG:9:GLU:C	2:BG:9:GLU:OE1	2.64	0.41
11:AK:101:BCL:H143	11:AK:101:BCL:H111	1.88	0.41
9:AW:43:LYS:HG2	9:AX:35:ILE:HA	2.02	0.41
11:AW:1203:BCL:HMA3	12:BW:103:LMT:H123	2.02	0.41
2:Bd:2:THR:O	2:Bd:5:GLU:HG3	2.21	0.41
2:Bj:32:TRP:HH2	2:Bj:38:PHE:HB2	1.86	0.41
8:C:226:CYS:SG	19:C:404:HEC:CAB	3.09	0.41
2:BB:16:HIS:HB2	9:AB:5:TRP:HZ3	1.86	0.41
11:AD:1102:BCL:H161	11:AD:1102:BCL:H122	1.85	0.41
2:BL:7:MET:HE3	2:BL:12:ALA:HA	2.03	0.41
2:BN:23:THR:O	2:BN:27:ILE:HG12	2.21	0.41
2:BT:16:HIS:HD1	9:AT:5:TRP:CD1	2.37	0.41
11:BX:102:BCL:H61	11:BX:102:BCL:H41	1.80	0.41
2:Be:17:THR:O	2:Be:21:ILE:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:111:LYS:HB2	4:L:111:LYS:HE2	1.88	0.40
5:M:75:MET:HG2	5:M:93:LEU:HB3	2.02	0.40
8:C:87:GLU:HA	8:C:87:GLU:OE2	2.21	0.40
11:AJ:1102:BCL:H91	9:AK:24:LEU:HD13	2.03	0.40
1:Ak:17:MET:SD	11:Al:101:BCL:C14	3.06	0.40
1:Am:7:MET:HG2	1:Am:8:PHE:CE2	2.56	0.40
5:M:37:SER:HB3	5:M:40:ALA:HB3	2.02	0.40
5:M:163:GLN:HB3	5:M:164:PRO:HD3	2.02	0.40
7:K:55:LEU:CD2	7:K:150:ASP:HB2	2.50	0.40
11:AO:101:BCL:H62	9:AP:20:PHE:HZ	1.86	0.40
2:BT:24:LEU:O	2:BT:28:ILE:HG23	2.20	0.40
11:AW:1202:BCL:H52	11:AW:1202:BCL:H12	1.86	0.40
11:Bm:103:BCL:H93	11:AW:1202:BCL:H122	2.03	0.40
11:Ao:101:BCL:CBB	11:Ao:101:BCL:CMB	2.99	0.40
11:Bp:1203:BCL:CBB	11:Bp:1203:BCL:CMB	2.99	0.40
4:L:258:LYS:HE2	4:L:258:LYS:HB2	1.92	0.40
5:M:53:LEU:HD23	5:M:53:LEU:HA	1.86	0.40
5:M:89:GLN:O	5:M:93:LEU:HG	2.21	0.40
14:M:408:MQ8:H462	14:M:408:MQ8:H451	1.94	0.40
12:BA:104:LMT:H91	12:BA:104:LMT:H122	1.60	0.40
9:AD:22:ALA:HB1	11:AD:1102:BCL:H62	2.02	0.40
9:AG:5:TRP:CD1	2:BG:16:HIS:HB2	2.56	0.40
1:Ac:23:VAL:HG21	14:Ad:103:MQ8:H352	2.04	0.40
4:L:220:LEU:HD11	5:M:133:VAL:HG22	2.02	0.40
2:BA:36:LEU:HD13	11:BB:101:BCL:H171	2.04	0.40
11:AF:102:BCL:H61	11:AF:102:BCL:H41	1.85	0.40
9:AG:39:PRO:O	9:AG:43:LYS:HB2	2.21	0.40
11:AV:1001:BCL:H111	11:AV:1001:BCL:H72	1.76	0.40
2:BV:22:GLY:HA3	10:BV:101:V7N:C21	2.52	0.40
1:Aa:4:ILE:HD12	1:Aa:4:ILE:HA	1.86	0.40
15:Af:102:CD4:H30	15:Af:102:CD4:H31	1.25	0.40
2:Bp:22:ILE:HD13	2:Bp:22:ILE:HA	1.83	0.40
11:L:302:BCL:C1B	16:L:303:BPH:H202	2.52	0.40
6:H:46:TRP:CD2	6:H:47:PRO:HA	2.57	0.40
13:AA:1101:PEX:H33	13:AA:1101:PEX:H28	1.92	0.40
2:BF:40:TRP:CE2	2:BF:41:ARG:HG3	2.56	0.40
9:AH:23:GLY:O	9:AH:27:ILE:HG12	2.21	0.40
12:BH:103:LMT:H121	11:BI:102:BCL:H72	2.04	0.40
2:BN:40:TRP:CH2	9:AN:38:TRP:HB2	2.56	0.40
11:AO:101:BCL:H111	11:AO:101:BCL:H142	1.76	0.40
2:BU:40:TRP:HH2	9:AU:38:TRP:HB2	1.86	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	Aa	67/71 (94%)	64 (96%)	3 (4%)	0	100	100
1	Ab	54/71 (76%)	54 (100%)	0	0	100	100
1	Ac	54/71 (76%)	51 (94%)	3 (6%)	0	100	100
1	Ad	52/71 (73%)	52 (100%)	0	0	100	100
1	Ae	57/71 (80%)	57 (100%)	0	0	100	100
1	Af	54/71 (76%)	51 (94%)	3 (6%)	0	100	100
1	Ag	55/71 (78%)	55 (100%)	0	0	100	100
1	Ah	51/71 (72%)	49 (96%)	2 (4%)	0	100	100
1	Ai	55/71 (78%)	55 (100%)	0	0	100	100
1	Aj	54/71 (76%)	53 (98%)	1 (2%)	0	100	100
1	Ak	54/71 (76%)	54 (100%)	0	0	100	100
1	Al	67/71 (94%)	62 (92%)	5 (8%)	0	100	100
1	Am	50/71 (70%)	50 (100%)	0	0	100	100
1	An	54/71 (76%)	53 (98%)	1 (2%)	0	100	100
1	Ao	54/71 (76%)	54 (100%)	0	0	100	100
1	Ap	53/71 (75%)	53 (100%)	0	0	100	100
2	BA	38/44 (86%)	36 (95%)	2 (5%)	0	100	100
2	BB	37/44 (84%)	37 (100%)	0	0	100	100
2	BC	38/44 (86%)	38 (100%)	0	0	100	100
2	BD	38/44 (86%)	35 (92%)	3 (8%)	0	100	100
2	BE	36/44 (82%)	36 (100%)	0	0	100	100
2	BF	37/44 (84%)	37 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	BG	37/44 (84%)	37 (100%)	0	0	100	100
2	BH	37/44 (84%)	37 (100%)	0	0	100	100
2	BI	36/44 (82%)	36 (100%)	0	0	100	100
2	BJ	38/44 (86%)	35 (92%)	3 (8%)	0	100	100
2	BK	37/44 (84%)	37 (100%)	0	0	100	100
2	BL	37/44 (84%)	37 (100%)	0	0	100	100
2	BM	38/44 (86%)	36 (95%)	2 (5%)	0	100	100
2	BN	37/44 (84%)	36 (97%)	1 (3%)	0	100	100
2	BO	37/44 (84%)	37 (100%)	0	0	100	100
2	BP	38/44 (86%)	38 (100%)	0	0	100	100
2	BQ	37/44 (84%)	37 (100%)	0	0	100	100
2	BR	37/44 (84%)	37 (100%)	0	0	100	100
2	BS	37/44 (84%)	37 (100%)	0	0	100	100
2	BT	37/44 (84%)	35 (95%)	2 (5%)	0	100	100
2	BU	37/44 (84%)	37 (100%)	0	0	100	100
2	BV	39/44 (89%)	37 (95%)	2 (5%)	0	100	100
2	BW	38/44 (86%)	36 (95%)	2 (5%)	0	100	100
2	BX	38/44 (86%)	36 (95%)	2 (5%)	0	100	100
2	Ba	36/44 (82%)	36 (100%)	0	0	100	100
2	Bb	36/44 (82%)	35 (97%)	1 (3%)	0	100	100
2	Bc	36/44 (82%)	36 (100%)	0	0	100	100
2	Bd	35/44 (80%)	35 (100%)	0	0	100	100
2	Be	36/44 (82%)	36 (100%)	0	0	100	100
2	Bf	32/44 (73%)	32 (100%)	0	0	100	100
2	Bg	36/44 (82%)	36 (100%)	0	0	100	100
2	Bh	34/44 (77%)	34 (100%)	0	0	100	100
2	Bi	36/44 (82%)	36 (100%)	0	0	100	100
2	Bj	36/44 (82%)	36 (100%)	0	0	100	100
2	Bk	36/44 (82%)	36 (100%)	0	0	100	100
2	Bl	36/44 (82%)	36 (100%)	0	0	100	100
2	Bm	36/44 (82%)	36 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Bn	36/44 (82%)	36 (100%)	0	0	100	100
2	Bo	36/44 (82%)	36 (100%)	0	0	100	100
2	Bp	33/44 (75%)	33 (100%)	0	0	100	100
3	S	101/204 (50%)	99 (98%)	2 (2%)	0	100	100
4	L	269/274 (98%)	262 (97%)	7 (3%)	0	100	100
5	M	333/392 (85%)	327 (98%)	6 (2%)	0	100	100
6	H	58/60 (97%)	58 (100%)	0	0	100	100
7	K	177/179 (99%)	169 (96%)	8 (4%)	0	100	100
8	C	296/373 (79%)	287 (97%)	9 (3%)	0	100	100
9	AA	46/56 (82%)	46 (100%)	0	0	100	100
9	AB	46/56 (82%)	46 (100%)	0	0	100	100
9	AC	46/56 (82%)	46 (100%)	0	0	100	100
9	AD	47/56 (84%)	47 (100%)	0	0	100	100
9	AE	47/56 (84%)	47 (100%)	0	0	100	100
9	AF	47/56 (84%)	47 (100%)	0	0	100	100
9	AG	47/56 (84%)	47 (100%)	0	0	100	100
9	AH	47/56 (84%)	47 (100%)	0	0	100	100
9	AI	47/56 (84%)	47 (100%)	0	0	100	100
9	AJ	46/56 (82%)	45 (98%)	1 (2%)	0	100	100
9	AK	46/56 (82%)	46 (100%)	0	0	100	100
9	AL	46/56 (82%)	46 (100%)	0	0	100	100
9	AM	47/56 (84%)	47 (100%)	0	0	100	100
9	AN	46/56 (82%)	46 (100%)	0	0	100	100
9	AO	46/56 (82%)	46 (100%)	0	0	100	100
9	AP	46/56 (82%)	46 (100%)	0	0	100	100
9	AQ	47/56 (84%)	47 (100%)	0	0	100	100
9	AR	46/56 (82%)	46 (100%)	0	0	100	100
9	AS	47/56 (84%)	47 (100%)	0	0	100	100
9	AT	46/56 (82%)	46 (100%)	0	0	100	100
9	AU	46/56 (82%)	46 (100%)	0	0	100	100
9	AV	46/56 (82%)	46 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	AW	47/56 (84%)	47 (100%)	0	0	100	100
9	AX	46/56 (82%)	45 (98%)	1 (2%)	0	100	100
All	All	4695/5722 (82%)	4623 (98%)	72 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Aa	53/55 (96%)	52 (98%)	1 (2%)	50	69
1	Ab	45/55 (82%)	43 (96%)	2 (4%)	25	38
1	Ac	46/55 (84%)	45 (98%)	1 (2%)	45	65
1	Ad	44/55 (80%)	41 (93%)	3 (7%)	14	20
1	Ae	46/55 (84%)	43 (94%)	3 (6%)	15	22
1	Af	46/55 (84%)	46 (100%)	0	100	100
1	Ag	46/55 (84%)	45 (98%)	1 (2%)	45	65
1	Ah	43/55 (78%)	40 (93%)	3 (7%)	14	19
1	Ai	46/55 (84%)	43 (94%)	3 (6%)	15	22
1	Aj	45/55 (82%)	44 (98%)	1 (2%)	45	65
1	Ak	46/55 (84%)	46 (100%)	0	100	100
1	Al	53/55 (96%)	52 (98%)	1 (2%)	50	69
1	Am	44/55 (80%)	43 (98%)	1 (2%)	44	63
1	An	46/55 (84%)	45 (98%)	1 (2%)	45	65
1	Ao	45/55 (82%)	45 (100%)	0	100	100
1	Ap	45/55 (82%)	44 (98%)	1 (2%)	45	65
2	BA	30/34 (88%)	30 (100%)	0	100	100
2	BB	30/34 (88%)	27 (90%)	3 (10%)	7	9
2	BC	30/34 (88%)	28 (93%)	2 (7%)	15	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	BD	30/34 (88%)	30 (100%)	0	100 100
2	BE	30/34 (88%)	29 (97%)	1 (3%)	33 50
2	BF	30/34 (88%)	30 (100%)	0	100 100
2	BG	30/34 (88%)	30 (100%)	0	100 100
2	BH	30/34 (88%)	28 (93%)	2 (7%)	15 21
2	BI	30/34 (88%)	30 (100%)	0	100 100
2	BJ	30/34 (88%)	29 (97%)	1 (3%)	33 50
2	BK	30/34 (88%)	30 (100%)	0	100 100
2	BL	30/34 (88%)	30 (100%)	0	100 100
2	BM	30/34 (88%)	29 (97%)	1 (3%)	33 50
2	BN	30/34 (88%)	30 (100%)	0	100 100
2	BO	30/34 (88%)	29 (97%)	1 (3%)	33 50
2	BP	30/34 (88%)	30 (100%)	0	100 100
2	BQ	30/34 (88%)	29 (97%)	1 (3%)	33 50
2	BR	30/34 (88%)	30 (100%)	0	100 100
2	BS	30/34 (88%)	28 (93%)	2 (7%)	15 21
2	BT	30/34 (88%)	30 (100%)	0	100 100
2	BU	30/34 (88%)	30 (100%)	0	100 100
2	BV	31/34 (91%)	31 (100%)	0	100 100
2	BW	30/34 (88%)	30 (100%)	0	100 100
2	BX	30/34 (88%)	30 (100%)	0	100 100
2	Ba	30/34 (88%)	28 (93%)	2 (7%)	15 21
2	Bb	30/34 (88%)	30 (100%)	0	100 100
2	Bc	30/34 (88%)	30 (100%)	0	100 100
2	Bd	29/34 (85%)	28 (97%)	1 (3%)	32 49
2	Be	30/34 (88%)	30 (100%)	0	100 100
2	Bf	26/34 (76%)	26 (100%)	0	100 100
2	Bg	30/34 (88%)	30 (100%)	0	100 100
2	Bh	28/34 (82%)	28 (100%)	0	100 100
2	Bi	30/34 (88%)	29 (97%)	1 (3%)	33 50
2	Bj	30/34 (88%)	30 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	Bk	30/34 (88%)	30 (100%)	0	100 100
2	Bl	30/34 (88%)	29 (97%)	1 (3%)	33 50
2	Bm	30/34 (88%)	29 (97%)	1 (3%)	33 50
2	Bn	30/34 (88%)	30 (100%)	0	100 100
2	Bo	30/34 (88%)	30 (100%)	0	100 100
2	Bp	27/34 (79%)	27 (100%)	0	100 100
3	S	84/158 (53%)	84 (100%)	0	100 100
4	L	213/216 (99%)	210 (99%)	3 (1%)	59 76
5	M	272/311 (88%)	266 (98%)	6 (2%)	45 65
6	H	51/51 (100%)	50 (98%)	1 (2%)	48 67
7	K	146/146 (100%)	139 (95%)	7 (5%)	23 35
8	C	251/302 (83%)	247 (98%)	4 (2%)	55 73
9	AA	38/45 (84%)	38 (100%)	0	100 100
9	AB	38/45 (84%)	38 (100%)	0	100 100
9	AC	38/45 (84%)	38 (100%)	0	100 100
9	AD	39/45 (87%)	39 (100%)	0	100 100
9	AE	39/45 (87%)	34 (87%)	5 (13%)	4 4
9	AF	39/45 (87%)	37 (95%)	2 (5%)	21 32
9	AG	39/45 (87%)	39 (100%)	0	100 100
9	AH	39/45 (87%)	38 (97%)	1 (3%)	40 59
9	AI	39/45 (87%)	39 (100%)	0	100 100
9	AJ	38/45 (84%)	37 (97%)	1 (3%)	40 59
9	AK	38/45 (84%)	38 (100%)	0	100 100
9	AL	38/45 (84%)	37 (97%)	1 (3%)	40 59
9	AM	39/45 (87%)	39 (100%)	0	100 100
9	AN	38/45 (84%)	38 (100%)	0	100 100
9	AO	38/45 (84%)	37 (97%)	1 (3%)	40 59
9	AP	38/45 (84%)	37 (97%)	1 (3%)	40 59
9	AQ	39/45 (87%)	38 (97%)	1 (3%)	40 59
9	AR	38/45 (84%)	38 (100%)	0	100 100
9	AS	39/45 (87%)	38 (97%)	1 (3%)	40 59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
9	AT	38/45 (84%)	37 (97%)	1 (3%)	40 59
9	AU	38/45 (84%)	38 (100%)	0	100 100
9	AV	38/45 (84%)	38 (100%)	0	100 100
9	AW	39/45 (87%)	39 (100%)	0	100 100
9	AX	38/45 (84%)	37 (97%)	1 (3%)	40 59
All	All	3869/4504 (86%)	3790 (98%)	79 (2%)	48 67

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Aa	39	SER
2	Ba	18	LEU
2	Ba	22	ILE
1	Ab	39	SER
1	Ab	50	GLN
1	Ac	18	VAL
1	Ad	18	VAL
1	Ad	36	GLN
1	Ad	50	GLN
2	Bd	14	VAL
1	Ae	14	MET
1	Ae	39	SER
1	Ae	56	SER
1	Ag	39	SER
1	Ah	4	ILE
1	Ah	7	MET
1	Ah	39	SER
1	Ai	14	MET
1	Ai	15	VAL
1	Ai	21	LEU
2	Bi	15	THR
1	Aj	18	VAL
1	Al	39	SER
2	Bl	2	THR
1	Am	18	VAL
2	Bm	18	LEU
1	An	40	TRP
1	Ap	13	VAL
4	L	248	CYS
4	L	249	ILE

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Mol	Chain	Res	Type
4	L	250	VAL
5	M	1	MET
5	M	90	LEU
5	M	215	PHE
5	M	242	THR
5	M	291	ASP
5	M	311	THR
6	H	54	THR
7	K	10	ASP
7	K	28	VAL
7	K	101	VAL
7	K	135	ILE
7	K	153	THR
7	K	156	GLU
7	K	179	ILE
8	C	102	THR
8	C	150	LYS
8	C	273	VAL
8	C	309	LEU
2	BB	8	THR
2	BB	24	LEU
2	BB	28	ILE
2	BC	10	ASP
2	BC	24	LEU
9	AE	12	ILE
9	AE	15	SER
9	AE	26	LEU
9	AE	30	MET
9	AE	34	SER
2	BE	26	VAL
9	AF	4	ILE
9	AF	8	MET
9	AH	3	ARG
2	BH	7	MET
2	BH	28	ILE
9	AJ	38	TRP
2	BJ	20	VAL
9	AL	11	GLN
2	BM	7	MET
9	AO	11	GLN
2	BO	21	THR
9	AP	4	ILE

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Mol	Chain	Res	Type
9	AQ	4	ILE
2	BQ	20	VAL
2	BS	24	LEU
2	BS	32	VAL
9	AS	6	GLN
9	AT	13	ILE
9	AX	11	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
2	Ba	33	GLN
1	Ae	36	GLN
1	Ai	2	HIS
2	Bm	33	GLN
4	L	145	HIS
4	L	167	HIS
4	L	214	ASN
5	M	318	GLN
7	K	121	ASN
8	C	42	ASN
8	C	45	HIS
8	C	81	ASN
8	C	147	GLN
8	C	181	HIS
8	C	260	GLN
9	AB	29	HIS
9	AC	2	HIS
9	AD	49	GLN
9	AG	47	ASN
9	AK	47	ASN
9	AK	49	GLN
9	AL	2	HIS
9	AL	11	GLN
9	AO	6	GLN
9	AO	45	GLN
9	AS	11	GLN
9	AT	11	GLN
9	AU	49	GLN
9	AX	11	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 202 ligands modelled in this entry, 1 is monoatomic - leaving 201 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	$\#\|Z\| > 2$
11	BCL	AQ	101	2	69,74,74	1.14	5 (7%)	83,115,115	1.45	10 (12%)
12	LMT	BW	103	-	36,36,36	1.16	6 (16%)	47,47,47	1.03	3 (6%)
13	PEX	Be	1101	-	34,34,34	0.54	0	37,39,39	0.51	0
14	MQ8	M	408	-	54,54,54	0.46	1 (1%)	66,69,69	0.60	2 (3%)
12	LMT	Ba	1102	-	36,36,36	1.16	5 (13%)	47,47,47	0.98	2 (4%)
11	BCL	AJ	1103	2	69,74,74	1.15	5 (7%)	83,115,115	1.51	12 (14%)
11	BCL	BE	101	2	69,74,74	1.14	6 (8%)	83,115,115	1.43	12 (14%)
11	BCL	Bp	1203	1	69,74,74	1.76	16 (23%)	83,115,115	2.51	22 (26%)
11	BCL	Bm	103	2	69,74,74	1.15	5 (7%)	83,115,115	1.52	12 (14%)
12	LMT	BU	101	-	36,36,36	1.19	5 (13%)	47,47,47	1.04	1 (2%)
11	BCL	AK	101	9	69,74,74	1.16	5 (7%)	83,115,115	1.50	11 (13%)
10	V7N	Bc	1202	-	43,44,44	1.99	10 (23%)	44,54,54	1.67	10 (22%)
16	BPH	M	406	-	59,70,70	1.07	3 (5%)	61,101,101	1.91	6 (9%)
11	BCL	AT	1102	2	69,74,74	1.12	7 (10%)	83,115,115	1.46	12 (14%)
13	PEX	Bm	102	-	34,34,34	0.55	0	37,39,39	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	LMT	BE	102	-	36,36,36	1.17	5 (13%)	47,47,47	0.94	0
10	V7N	AL	102	-	43,44,44	1.96	9 (20%)	44,54,54	1.58	8 (18%)
10	V7N	Bb	1202	-	43,44,44	1.98	10 (23%)	44,54,54	1.59	9 (20%)
10	V7N	BD	103	-	43,44,44	1.98	9 (20%)	44,54,54	1.56	8 (18%)
12	LMT	BF	102	-	36,36,36	1.17	6 (16%)	47,47,47	0.98	2 (4%)
11	BCL	BK	102	2	69,74,74	1.12	4 (5%)	83,115,115	1.53	12 (14%)
11	BCL	Af	101	1	69,74,74	1.16	5 (7%)	83,115,115	1.45	12 (14%)
10	V7N	BA	102	-	43,44,44	1.98	10 (23%)	44,54,54	1.55	8 (18%)
10	V7N	BC	103	-	43,44,44	1.97	10 (23%)	44,54,54	1.61	10 (22%)
10	V7N	Bg	101	-	43,44,44	2.00	10 (23%)	44,54,54	1.65	9 (20%)
11	BCL	AR	101	9	69,74,74	1.13	5 (7%)	83,115,115	1.46	12 (14%)
13	PEX	AE	1101	-	34,34,34	0.54	0	37,39,39	0.57	0
10	V7N	BX	101	-	43,44,44	2.03	10 (23%)	44,54,54	1.55	9 (20%)
11	BCL	BS	101	2	69,74,74	1.13	5 (7%)	83,115,115	1.41	10 (12%)
11	BCL	AB	101	9	69,74,74	1.16	4 (5%)	83,115,115	1.43	11 (13%)
11	BCL	Ab	101	1	69,74,74	1.15	5 (7%)	83,115,115	1.45	12 (14%)
10	V7N	BQ	103	-	43,44,44	2.00	10 (23%)	44,54,54	1.59	8 (18%)
10	V7N	BO	102	-	43,44,44	2.00	10 (23%)	44,54,54	1.62	10 (22%)
11	BCL	Bj	1204	2	69,74,74	1.12	6 (8%)	83,115,115	1.51	10 (12%)
12	LMT	BU	103	-	36,36,36	1.16	5 (13%)	47,47,47	1.05	2 (4%)
13	PEX	Ba	1101	-	34,34,34	0.55	0	37,39,39	0.51	0
10	V7N	BG	101	-	43,44,44	1.99	10 (23%)	44,54,54	1.63	9 (20%)
19	HEC	C	402	8	50,50,50	1.87	5 (10%)	68,82,82	1.60	14 (20%)
11	BCL	BG	102	2	69,74,74	1.12	5 (7%)	83,115,115	1.45	12 (14%)
12	LMT	BH	101	11	36,36,36	1.17	5 (13%)	47,47,47	1.02	3 (6%)
12	LMT	M	401	-	36,36,36	1.17	5 (13%)	47,47,47	1.00	2 (4%)
11	BCL	Bh	1205	2	69,74,74	1.14	5 (7%)	83,115,115	1.50	12 (14%)
11	BCL	Al	101	1	69,74,74	1.75	18 (26%)	83,115,115	2.59	25 (30%)
10	V7N	Bf	1202	-	43,44,44	1.97	9 (20%)	44,54,54	1.69	10 (22%)
11	BCL	BR	101	2	69,74,74	1.11	4 (5%)	83,115,115	1.51	9 (10%)
11	BCL	Ak	101	1	69,74,74	1.17	5 (7%)	83,115,115	1.43	11 (13%)
10	V7N	BT	101	-	43,44,44	2.00	10 (23%)	44,54,54	1.54	8 (18%)
11	BCL	AQ	102	9	69,74,74	1.20	6 (8%)	83,115,115	1.47	9 (10%)
12	LMT	BG	103	-	36,36,36	1.18	6 (16%)	47,47,47	0.93	2 (4%)
11	BCL	Bp	1204	2	69,74,74	1.13	4 (5%)	83,115,115	1.45	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	LMT	BC	102	-	36,36,36	1.18	5 (13%)	47,47,47	0.98	1 (2%)
11	BCL	AW	1204	2	69,74,74	1.10	5 (7%)	83,115,115	1.37	9 (10%)
11	BCL	BN	101	2	69,74,74	1.13	4 (5%)	83,115,115	1.45	9 (10%)
12	LMT	Bf	1203	-	36,36,36	1.19	5 (13%)	47,47,47	1.00	3 (6%)
12	LMT	BQ	102	-	36,36,36	1.18	5 (13%)	47,47,47	0.98	2 (4%)
11	BCL	Bk	103	2	69,74,74	1.14	5 (7%)	83,115,115	3.62	12 (14%)
11	BCL	AQ	103	2	69,74,74	1.15	7 (10%)	83,115,115	1.41	11 (13%)
14	MQ8	L	305	-	54,54,54	0.38	1 (1%)	66,69,69	0.57	1 (1%)
11	BCL	AI	101	1	69,74,74	1.15	5 (7%)	83,115,115	1.46	12 (14%)
13	PEX	AA	1101	-	34,34,34	0.54	0	37,39,39	0.53	0
11	BCL	M	405	-	69,74,74	1.11	6 (8%)	83,115,115	1.47	8 (9%)
13	PEX	Bn	102	11	34,34,34	0.55	0	37,39,39	0.48	0
12	LMT	Ad	102	-	36,36,36	1.17	6 (16%)	47,47,47	1.03	2 (4%)
11	BCL	BA	101	-	69,74,74	1.17	6 (8%)	83,115,115	4.75	16 (19%)
12	LMT	AW	1201	-	36,36,36	1.15	6 (16%)	47,47,47	1.08	4 (8%)
10	V7N	Bn	101	-	43,44,44	1.97	10 (23%)	44,54,54	1.53	8 (18%)
11	BCL	Am	101	1	69,74,74	1.76	16 (23%)	83,115,115	2.57	24 (28%)
11	BCL	Ac	101	1	69,74,74	1.17	5 (7%)	83,115,115	1.50	12 (14%)
11	BCL	AC	101	9	69,74,74	1.13	6 (8%)	83,115,115	1.45	8 (9%)
11	BCL	AW	1202	1	69,74,74	1.17	6 (8%)	83,115,115	1.54	14 (16%)
10	V7N	BN	102	-	43,44,44	1.98	10 (23%)	44,54,54	1.58	9 (20%)
11	BCL	BA	103	2	69,74,74	1.12	6 (8%)	83,115,115	1.53	12 (14%)
12	LMT	C	401	-	36,36,36	1.16	5 (13%)	47,47,47	1.01	2 (4%)
12	LMT	Bh	1201	-	36,36,36	1.19	6 (16%)	47,47,47	1.01	2 (4%)
13	PEX	Be	1104	-	34,34,34	0.56	0	37,39,39	0.54	0
11	BCL	AD	1102	9	69,74,74	1.14	4 (5%)	83,115,115	1.40	10 (12%)
11	BCL	Bc	1204	2	69,74,74	1.15	5 (7%)	83,115,115	1.54	11 (13%)
11	BCL	AG	101	9	69,74,74	1.13	5 (7%)	83,115,115	1.37	8 (9%)
11	BCL	AP	1102	9	69,74,74	1.12	5 (7%)	83,115,115	1.44	9 (10%)
11	BCL	Bo	1202	2	69,74,74	1.13	5 (7%)	83,115,115	1.42	8 (9%)
11	BCL	Bl	1203	2	69,74,74	1.12	6 (8%)	83,115,115	1.48	11 (13%)
12	LMT	BK	101	-	36,36,36	1.16	5 (13%)	47,47,47	1.08	2 (4%)
11	BCL	Bn	103	2	69,74,74	1.16	4 (5%)	83,115,115	1.50	13 (15%)
12	LMT	AX	1201	-	36,36,36	1.14	6 (16%)	47,47,47	1.22	4 (8%)
10	V7N	Bm	101	-	43,44,44	2.01	9 (20%)	44,54,54	1.57	11 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	LMT	Aa	103	-	36,36,36	1.15	5 (13%)	47,47,47	0.91	1 (2%)
12	LMT	BQ	101	-	36,36,36	1.17	5 (13%)	47,47,47	1.01	2 (4%)
12	LMT	BS	102	-	36,36,36	1.17	6 (16%)	47,47,47	0.95	2 (4%)
12	LMT	BL	103	-	36,36,36	1.18	5 (13%)	47,47,47	1.01	1 (2%)
11	BCL	AH	101	9	69,74,74	1.17	5 (7%)	83,115,115	1.42	9 (10%)
11	BCL	AF	102	9	69,74,74	1.11	5 (7%)	83,115,115	1.45	9 (10%)
11	BCL	AM	102	2	69,74,74	1.13	6 (8%)	83,115,115	1.47	12 (14%)
19	HEC	C	404	8	50,50,50	1.75	5 (10%)	68,82,82	1.46	8 (11%)
11	BCL	Aj	101	1	69,74,74	1.17	6 (8%)	83,115,115	1.52	12 (14%)
11	BCL	AT	1103	9	69,74,74	1.14	5 (7%)	83,115,115	1.42	10 (12%)
12	LMT	L	304	-	36,36,36	1.13	5 (13%)	47,47,47	1.05	2 (4%)
13	PEX	Aj	103	-	34,34,34	0.55	0	37,39,39	0.54	0
13	PEX	Bh	1203	-	34,34,34	0.54	0	37,39,39	0.60	1 (2%)
10	V7N	Bh	1202	-	43,44,44	1.96	10 (23%)	44,54,54	1.61	8 (18%)
11	BCL	BX	102	2	69,74,74	1.12	4 (5%)	83,115,115	1.57	13 (15%)
11	BCL	BF	101	2	69,74,74	1.13	4 (5%)	83,115,115	1.49	12 (14%)
11	BCL	BI	102	2	69,74,74	1.12	5 (7%)	83,115,115	1.51	12 (14%)
12	LMT	Bj	1201	-	36,36,36	1.16	5 (13%)	47,47,47	0.96	2 (4%)
13	PEX	Bg	102	-	34,34,34	0.54	0	37,39,39	0.51	0
13	PEX	Bk	102	-	34,34,34	0.56	0	37,39,39	0.50	0
11	BCL	Ad	101	1	69,74,74	1.16	6 (8%)	83,115,115	1.43	10 (12%)
12	LMT	BB	103	-	36,36,36	1.17	6 (16%)	47,47,47	1.07	2 (4%)
11	BCL	Ah	101	1	69,74,74	1.16	6 (8%)	83,115,115	1.43	11 (13%)
13	PEX	Bc	1203	-	34,34,34	0.55	0	37,39,39	0.53	0
10	V7N	BV	101	-	43,44,44	1.97	10 (23%)	44,54,54	1.66	10 (22%)
10	V7N	Bp	1202	-	43,44,44	1.99	9 (20%)	44,54,54	1.59	8 (18%)
11	BCL	AV	1001	9	69,74,74	1.13	6 (8%)	83,115,115	1.46	11 (13%)
12	LMT	BO	101	-	36,36,36	1.19	6 (16%)	47,47,47	0.98	2 (4%)
11	BCL	AL	101	9	69,74,74	1.15	5 (7%)	83,115,115	1.47	12 (14%)
10	V7N	BB	102	-	43,44,44	2.00	10 (23%)	44,54,54	1.56	9 (20%)
13	PEX	AD	1101	-	34,34,34	0.55	0	37,39,39	0.54	0
10	V7N	An	101	-	43,44,44	2.02	9 (20%)	44,54,54	1.56	10 (22%)
11	BCL	Bf	1204	2	69,74,74	1.13	5 (7%)	83,115,115	1.40	9 (10%)
12	LMT	Bp	1201	-	36,36,36	1.19	6 (16%)	47,47,47	0.99	3 (6%)
11	BCL	AN	101	9	69,74,74	1.13	5 (7%)	83,115,115	1.43	11 (13%)
13	PEX	AP	1101	-	34,34,34	0.54	0	37,39,39	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	BCL	AE	1102	9	69,74,74	1.14	5 (7%)	83,115,115	1.45	12 (14%)
11	BCL	Bg	103	2	69,74,74	1.15	5 (7%)	83,115,115	1.47	10 (12%)
15	CD4	M	403	-	83,83,83	0.37	0	89,95,95	0.36	0
11	BCL	AU	1001	9,13	69,74,74	1.13	5 (7%)	83,115,115	1.47	10 (12%)
10	V7N	Bi	101	-	43,44,44	2.02	9 (20%)	44,54,54	1.61	9 (20%)
18	CRT	M	407	-	41,43,43	0.39	0	50,54,54	0.81	1 (2%)
12	LMT	Bo	1201	-	36,36,36	1.19	5 (13%)	47,47,47	0.94	2 (4%)
11	BCL	AJ	1102	9	69,74,74	1.13	4 (5%)	83,115,115	1.43	8 (9%)
10	V7N	BJ	101	-	43,44,44	1.95	9 (20%)	44,54,54	1.65	11 (25%)
11	BCL	L	302	4	69,74,74	1.12	6 (8%)	83,115,115	1.44	8 (9%)
12	LMT	BI	103	-	36,36,36	1.18	6 (16%)	47,47,47	0.98	2 (4%)
10	V7N	BS	103	-	43,44,44	2.04	9 (20%)	44,54,54	1.66	8 (18%)
13	PEX	AT	1101	-	34,34,34	0.55	0	37,39,39	0.51	0
11	BCL	Be	1105	2	69,74,74	1.13	4 (5%)	83,115,115	1.40	9 (10%)
14	MQ8	Ad	103	-	54,54,54	0.30	0	66,69,69	0.56	1 (1%)
11	BCL	Ai	101	1	69,74,74	1.16	5 (7%)	83,115,115	1.43	12 (14%)
11	BCL	AW	1203	9	69,74,74	1.15	5 (7%)	83,115,115	1.45	9 (10%)
12	LMT	Bj	1203	-	36,36,36	1.18	5 (13%)	47,47,47	0.98	2 (4%)
10	V7N	BF	103	-	43,44,44	2.00	10 (23%)	44,54,54	1.61	9 (20%)
10	V7N	BK	104	-	43,44,44	1.99	10 (23%)	44,54,54	1.60	8 (18%)
11	BCL	L	301	4	69,74,74	1.11	6 (8%)	83,115,115	1.45	12 (14%)
11	BCL	AM	101	9	69,74,74	1.16	5 (7%)	83,115,115	1.39	10 (12%)
12	LMT	BR	102	-	36,36,36	1.18	5 (13%)	47,47,47	0.96	2 (4%)
19	HEC	C	403	8	50,50,50	1.86	5 (10%)	68,82,82	1.40	7 (10%)
10	V7N	BP	102	-	43,44,44	1.97	10 (23%)	44,54,54	1.59	11 (25%)
12	LMT	BK	103	-	36,36,36	1.20	6 (16%)	47,47,47	1.13	3 (6%)
13	PEX	AS	1101	-	34,34,34	0.55	0	37,39,39	0.47	0
10	V7N	Bl	1202	-	43,44,44	2.02	10 (23%)	44,54,54	1.48	9 (20%)
10	V7N	Bk	101	-	43,44,44	1.97	10 (23%)	44,54,54	1.57	8 (18%)
11	BCL	Bd	1203	2	69,74,74	1.12	4 (5%)	83,115,115	1.53	14 (16%)
19	HEC	C	405	8	50,50,50	1.83	5 (10%)	68,82,82	1.38	6 (8%)
12	LMT	Bf	1201	-	36,36,36	1.21	6 (16%)	47,47,47	0.93	1 (2%)
11	BCL	Bb	1203	2	69,74,74	1.14	6 (8%)	83,115,115	1.37	9 (10%)
12	LMT	Aj	102	-	36,36,36	1.13	5 (13%)	47,47,47	1.09	2 (4%)
10	V7N	Bj	1202	-	43,44,44	2.00	10 (23%)	44,54,54	1.52	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	BCL	BO	103	2	69,74,74	1.12	5 (7%)	83,115,115	1.50	10 (12%)
11	BCL	AS	1102	-	69,74,74	1.14	6 (8%)	83,115,115	1.59	14 (16%)
11	BCL	BC	101	2	69,74,74	1.12	5 (7%)	83,115,115	1.55	11 (13%)
12	LMT	Bc	1201	-	36,36,36	1.19	6 (16%)	47,47,47	1.02	2 (4%)
10	V7N	Be	1103	-	43,44,44	2.02	9 (20%)	44,54,54	1.62	10 (22%)
11	BCL	BB	101	2	69,74,74	1.10	5 (7%)	83,115,115	1.59	13 (15%)
12	LMT	BO	104	11	36,36,36	1.14	6 (16%)	47,47,47	0.87	0
11	BCL	AO	101	12,9	69,74,74	1.14	5 (7%)	83,115,115	1.44	13 (15%)
12	LMT	Bd	1201	-	36,36,36	1.18	5 (13%)	47,47,47	0.88	0
12	LMT	Bb	1201	-	36,36,36	1.17	5 (13%)	47,47,47	1.01	1 (2%)
11	BCL	BU	102	2	69,74,74	1.12	4 (5%)	83,115,115	1.45	10 (12%)
12	LMT	K	201	-	36,36,36	1.15	5 (13%)	47,47,47	1.03	2 (4%)
12	LMT	BH	103	-	36,36,36	1.18	5 (13%)	47,47,47	0.94	1 (2%)
11	BCL	BH	104	12,2	69,74,74	1.11	4 (5%)	83,115,115	1.55	12 (14%)
11	BCL	AX	1202	-	69,74,74	1.13	5 (7%)	83,115,115	1.51	10 (12%)
13	PEX	AJ	1101	11	34,34,34	0.54	0	37,39,39	0.56	0
10	V7N	BR	103	-	43,44,44	2.00	10 (23%)	44,54,54	1.63	10 (22%)
12	LMT	BD	102	-	36,36,36	1.17	5 (13%)	47,47,47	1.07	2 (4%)
12	LMT	BW	101	-	36,36,36	1.21	6 (16%)	47,47,47	1.09	1 (2%)
12	LMT	BA	105	-	36,36,36	1.19	6 (16%)	47,47,47	1.08	2 (4%)
10	V7N	BI	101	-	43,44,44	1.98	10 (23%)	44,54,54	1.63	9 (20%)
11	BCL	Ao	101	1	69,74,74	1.76	17 (24%)	83,115,115	2.48	22 (26%)
10	V7N	BU	104	-	43,44,44	1.96	10 (23%)	44,54,54	1.56	8 (18%)
10	V7N	AF	101	-	43,44,44	1.97	10 (23%)	44,54,54	1.64	11 (25%)
12	LMT	Bl	1201	-	36,36,36	1.19	6 (16%)	47,47,47	0.97	1 (2%)
15	CD4	Af	102	-	83,83,83	0.41	1 (1%)	89,95,95	0.39	0
11	BCL	BD	101	2	69,74,74	1.14	4 (5%)	83,115,115	1.48	12 (14%)
11	BCL	Aa	102	1	69,74,74	1.18	6 (8%)	83,115,115	1.47	12 (14%)
10	V7N	BH	102	-	43,44,44	1.96	9 (20%)	44,54,54	1.59	8 (18%)
10	V7N	Bd	1202	-	43,44,44	1.97	9 (20%)	44,54,54	1.59	9 (20%)
10	V7N	BL	101	-	43,44,44	2.00	10 (23%)	44,54,54	1.58	9 (20%)
11	BCL	Bi	102	2	69,74,74	1.13	5 (7%)	83,115,115	1.39	10 (12%)
12	LMT	BA	104	-	36,36,36	1.18	5 (13%)	47,47,47	0.98	2 (4%)
11	BCL	BL	102	2	69,74,74	1.12	6 (8%)	83,115,115	1.41	10 (12%)
12	LMT	Bh	1204	-	36,36,36	1.16	5 (13%)	47,47,47	0.98	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	BCL	AI	102	9,13	69,74,74	1.14	5 (7%)	83,115,115	1.42	11 (13%)
12	LMT	Be	1102	-	36,36,36	1.17	5 (13%)	47,47,47	1.08	3 (6%)
10	V7N	BW	102	-	43,44,44	2.01	10 (23%)	44,54,54	1.58	9 (20%)
11	BCL	M	404	5	69,74,74	1.14	6 (8%)	83,115,115	1.46	9 (10%)
12	LMT	BM	1001	-	36,36,36	1.17	6 (16%)	47,47,47	1.00	1 (2%)
10	V7N	Aa	101	-	43,44,44	2.01	10 (23%)	44,54,54	1.60	11 (25%)
16	BPH	L	303	-	59,70,70	1.09	4 (6%)	61,101,101	1.86	8 (13%)
11	BCL	BP	101	2	69,74,74	1.12	4 (5%)	83,115,115	1.51	11 (13%)
11	BCL	Ae	101	1	69,74,74	1.17	7 (10%)	83,115,115	1.54	14 (16%)
11	BCL	BV	102	2	69,74,74	1.11	5 (7%)	83,115,115	1.42	10 (12%)

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
11	BCL	AQ	101	2	-	4/41/137/137	-
12	LMT	BW	103	-	-	6/21/61/61	0/2/2/2
13	PEX	Be	1101	-	-	12/38/38/38	-
14	MQ8	M	408	-	-	20/47/67/67	0/2/2/2
12	LMT	Ba	1102	-	-	5/21/61/61	0/2/2/2
11	BCL	AJ	1103	2	-	6/41/137/137	-
11	BCL	BE	101	2	-	8/41/137/137	-
11	BCL	Bp	1203	1	-	19/41/137/137	-
11	BCL	Bm	103	2	-	2/41/137/137	-
12	LMT	BU	101	-	-	9/21/61/61	0/2/2/2
11	BCL	AK	101	9	-	11/41/137/137	-
10	V7N	Bc	1202	-	-	14/53/53/53	-
16	BPH	M	406	-	-	6/37/105/105	0/5/6/6
11	BCL	AT	1102	2	-	10/41/137/137	-
13	PEX	Bm	102	-	-	9/38/38/38	-
12	LMT	BE	102	-	-	11/21/61/61	0/2/2/2
10	V7N	AL	102	-	-	6/53/53/53	-
10	V7N	Bb	1202	-	-	15/53/53/53	-
10	V7N	BD	103	-	-	5/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	LMT	BF	102	-	-	8/21/61/61	0/2/2/2
11	BCL	BK	102	2	-	15/41/137/137	-
11	BCL	Af	101	1	-	4/41/137/137	-
10	V7N	BA	102	-	-	6/53/53/53	-
10	V7N	BC	103	-	-	5/53/53/53	-
10	V7N	Bg	101	-	-	12/53/53/53	-
11	BCL	AR	101	9	-	8/41/137/137	-
13	PEX	AE	1101	-	-	18/38/38/38	-
10	V7N	BX	101	-	-	11/53/53/53	-
11	BCL	BS	101	2	-	9/41/137/137	-
11	BCL	AB	101	9	-	6/41/137/137	-
11	BCL	Ab	101	1	-	11/41/137/137	-
10	V7N	BQ	103	-	-	4/53/53/53	-
10	V7N	BO	102	-	-	11/53/53/53	-
11	BCL	Bj	1204	2	-	8/41/137/137	-
12	LMT	BU	103	-	-	5/21/61/61	0/2/2/2
13	PEX	Ba	1101	-	-	14/38/38/38	-
10	V7N	BG	101	-	-	5/53/53/53	-
19	HEC	C	402	8	1/1/3/7	6/14/54/54	-
11	BCL	BG	102	2	-	9/41/137/137	-
12	LMT	BH	101	11	-	6/21/61/61	0/2/2/2
12	LMT	M	401	-	-	10/21/61/61	0/2/2/2
11	BCL	Bh	1205	2	-	5/41/137/137	-
11	BCL	Al	101	1	-	22/41/137/137	-
10	V7N	Bf	1202	-	-	13/53/53/53	-
11	BCL	BR	101	2	-	9/41/137/137	-
11	BCL	Ak	101	1	-	8/41/137/137	-
10	V7N	BT	101	-	-	7/53/53/53	-
11	BCL	AQ	102	9	-	10/41/137/137	-
12	LMT	BG	103	-	-	6/21/61/61	0/2/2/2
11	BCL	Bp	1204	2	-	9/41/137/137	-
12	LMT	BC	102	-	-	10/21/61/61	0/2/2/2
11	BCL	AW	1204	2	-	6/41/137/137	-
11	BCL	BN	101	2	-	6/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	LMT	Bf	1203	-	-	8/21/61/61	0/2/2/2
12	LMT	BQ	102	-	-	6/21/61/61	0/2/2/2
11	BCL	Bk	103	2	-	2/41/137/137	-
11	BCL	AQ	103	2	-	9/41/137/137	-
14	MQ8	L	305	-	-	27/47/67/67	0/2/2/2
11	BCL	AI	101	1	-	5/41/137/137	-
13	PEX	AA	1101	-	-	15/38/38/38	-
11	BCL	M	405	-	-	5/41/137/137	-
13	PEX	Bn	102	11	-	15/38/38/38	-
12	LMT	Ad	102	-	-	13/21/61/61	0/2/2/2
11	BCL	BA	101	-	-	6/41/137/137	-
12	LMT	AW	1201	-	-	10/21/61/61	0/2/2/2
10	V7N	Bn	101	-	-	14/53/53/53	-
11	BCL	Am	101	1	-	11/41/137/137	-
11	BCL	Ac	101	1	-	7/41/137/137	-
11	BCL	AC	101	9	-	4/41/137/137	-
11	BCL	AW	1202	1	-	2/41/137/137	-
10	V7N	BN	102	-	-	5/53/53/53	-
11	BCL	BA	103	2	-	4/41/137/137	-
12	LMT	C	401	-	-	6/21/61/61	0/2/2/2
12	LMT	Bh	1201	-	-	6/21/61/61	0/2/2/2
13	PEX	Be	1104	-	-	19/38/38/38	-
11	BCL	AD	1102	9	-	4/41/137/137	-
11	BCL	Bc	1204	2	-	8/41/137/137	-
11	BCL	AG	101	9	-	7/41/137/137	-
11	BCL	AP	1102	9	-	5/41/137/137	-
11	BCL	Bo	1202	2	-	16/41/137/137	-
11	BCL	Bl	1203	2	-	8/41/137/137	-
12	LMT	BK	101	-	-	6/21/61/61	0/2/2/2
11	BCL	Bn	103	2	-	11/41/137/137	-
12	LMT	AX	1201	-	-	9/21/61/61	0/2/2/2
10	V7N	Bm	101	-	-	17/53/53/53	-
12	LMT	Aa	103	-	-	5/21/61/61	0/2/2/2
12	LMT	BQ	101	-	-	3/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	LMT	BS	102	-	-	13/21/61/61	0/2/2/2
12	LMT	BL	103	-	-	8/21/61/61	0/2/2/2
19	HEC	C	404	8	1/1/3/7	5/14/54/54	-
11	BCL	AF	102	9	-	10/41/137/137	-
11	BCL	AH	101	9	-	9/41/137/137	-
11	BCL	AM	102	2	-	11/41/137/137	-
11	BCL	Aj	101	1	-	4/41/137/137	-
11	BCL	AT	1103	9	-	9/41/137/137	-
12	LMT	L	304	-	-	10/21/61/61	0/2/2/2
13	PEX	Aj	103	-	-	10/38/38/38	-
13	PEX	Bh	1203	-	-	15/38/38/38	-
10	V7N	Bh	1202	-	-	9/53/53/53	-
11	BCL	BX	102	2	-	9/41/137/137	-
11	BCL	BF	101	2	-	12/41/137/137	-
11	BCL	BI	102	2	-	8/41/137/137	-
12	LMT	Bj	1201	-	-	5/21/61/61	0/2/2/2
13	PEX	Bg	102	-	-	21/38/38/38	-
13	PEX	Bk	102	-	-	19/38/38/38	-
11	BCL	Ad	101	1	-	5/41/137/137	-
12	LMT	BB	103	-	-	14/21/61/61	0/2/2/2
11	BCL	Ah	101	1	-	3/41/137/137	-
13	PEX	Bc	1203	-	-	21/38/38/38	-
10	V7N	BV	101	-	-	12/53/53/53	-
10	V7N	Bp	1202	-	-	10/53/53/53	-
11	BCL	AV	1001	9	-	6/41/137/137	-
12	LMT	BO	101	-	-	8/21/61/61	0/2/2/2
11	BCL	AL	101	9	-	4/41/137/137	-
10	V7N	BB	102	-	-	11/53/53/53	-
13	PEX	AD	1101	-	-	19/38/38/38	-
10	V7N	An	101	-	-	12/53/53/53	-
11	BCL	Bf	1204	2	-	13/41/137/137	-
12	LMT	Bp	1201	-	-	6/21/61/61	0/2/2/2
11	BCL	AN	101	9	-	6/41/137/137	-
13	PEX	AP	1101	-	-	18/38/38/38	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	BCL	AE	1102	9	-	10/41/137/137	-
11	BCL	Bg	103	2	-	11/41/137/137	-
15	CD4	M	403	-	-	18/94/94/94	-
11	BCL	AU	1001	9,13	-	4/41/137/137	-
10	V7N	Bi	101	-	-	9/53/53/53	-
18	CRT	M	407	-	-	3/51/51/51	-
12	LMT	Bo	1201	-	-	5/21/61/61	0/2/2/2
11	BCL	AJ	1102	9	-	7/41/137/137	-
10	V7N	BJ	101	-	-	15/53/53/53	-
11	BCL	L	302	4	-	6/41/137/137	-
12	LMT	BI	103	-	-	7/21/61/61	0/2/2/2
10	V7N	BS	103	-	-	14/53/53/53	-
13	PEX	AT	1101	-	-	13/38/38/38	-
11	BCL	Be	1105	2	-	4/41/137/137	-
14	MQ8	Ad	103	-	-	32/47/67/67	0/2/2/2
11	BCL	Ai	101	1	-	11/41/137/137	-
11	BCL	AW	1203	9	-	7/41/137/137	-
12	LMT	Bj	1203	-	-	6/21/61/61	0/2/2/2
10	V7N	BF	103	-	-	11/53/53/53	-
10	V7N	BK	104	-	-	7/53/53/53	-
11	BCL	L	301	4	-	2/41/137/137	-
11	BCL	AM	101	9	-	5/41/137/137	-
12	LMT	BR	102	-	-	7/21/61/61	0/2/2/2
19	HEC	C	403	8	1/1/3/7	2/14/54/54	-
10	V7N	BP	102	-	-	13/53/53/53	-
12	LMT	BK	103	-	-	7/21/61/61	0/2/2/2
13	PEX	AS	1101	-	-	16/38/38/38	-
10	V7N	Bl	1202	-	-	8/53/53/53	-
10	V7N	Bk	101	-	-	11/53/53/53	-
11	BCL	Bd	1203	2	-	7/41/137/137	-
19	HEC	C	405	8	1/1/3/7	4/14/54/54	-
12	LMT	Bf	1201	-	-	8/21/61/61	0/2/2/2
11	BCL	Bb	1203	2	-	7/41/137/137	-
12	LMT	Aj	102	-	-	10/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	V7N	Bj	1202	-	-	14/53/53/53	-
11	BCL	BO	103	2	-	8/41/137/137	-
11	BCL	AS	1102	-	-	7/41/137/137	-
11	BCL	BC	101	2	-	10/41/137/137	-
12	LMT	Bc	1201	-	-	7/21/61/61	0/2/2/2
10	V7N	Be	1103	-	-	12/53/53/53	-
11	BCL	BB	101	2	-	8/41/137/137	-
12	LMT	BO	104	11	-	8/21/61/61	0/2/2/2
11	BCL	AO	101	12,9	-	13/41/137/137	-
12	LMT	Bd	1201	-	-	9/21/61/61	0/2/2/2
12	LMT	Bb	1201	-	-	10/21/61/61	0/2/2/2
11	BCL	BU	102	2	-	9/41/137/137	-
12	LMT	K	201	-	-	9/21/61/61	0/2/2/2
12	LMT	BH	103	-	-	9/21/61/61	0/2/2/2
11	BCL	BH	104	12,2	-	6/41/137/137	-
11	BCL	AX	1202	-	-	5/41/137/137	-
13	PEX	AJ	1101	11	-	18/38/38/38	-
10	V7N	BR	103	-	-	10/53/53/53	-
12	LMT	BD	102	-	-	10/21/61/61	0/2/2/2
12	LMT	BW	101	-	-	6/21/61/61	0/2/2/2
12	LMT	BA	105	-	-	7/21/61/61	0/2/2/2
10	V7N	BI	101	-	-	6/53/53/53	-
11	BCL	Ao	101	1	-	21/41/137/137	-
10	V7N	BU	104	-	-	4/53/53/53	-
10	V7N	AF	101	-	-	17/53/53/53	-
12	LMT	Bl	1201	-	-	7/21/61/61	0/2/2/2
15	CD4	Af	102	-	-	22/94/94/94	-
11	BCL	BD	101	2	-	6/41/137/137	-
11	BCL	Aa	102	1	-	5/41/137/137	-
10	V7N	BH	102	-	-	2/53/53/53	-
10	V7N	Bd	1202	-	-	10/53/53/53	-
10	V7N	BL	101	-	-	6/53/53/53	-
11	BCL	Bi	102	2	-	4/41/137/137	-
12	LMT	BA	104	-	-	8/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	BCL	BL	102	2	-	3/41/137/137	-
12	LMT	Bh	1204	-	-	5/21/61/61	0/2/2/2
11	BCL	AI	102	9,13	-	7/41/137/137	-
12	LMT	Be	1102	-	-	9/21/61/61	0/2/2/2
10	V7N	BW	102	-	-	9/53/53/53	-
11	BCL	M	404	5	-	3/41/137/137	-
12	LMT	BM	1001	-	-	7/21/61/61	0/2/2/2
10	V7N	Aa	101	-	-	16/53/53/53	-
16	BPH	L	303	-	-	8/37/105/105	0/5/6/6
11	BCL	BP	101	2	-	8/41/137/137	-
11	BCL	Ae	101	1	-	7/41/137/137	-
11	BCL	BV	102	2	-	10/41/137/137	-

All (1156) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	C	403	HEC	C3D-C2D	8.01	1.53	1.36
19	C	405	HEC	C3D-C2D	7.89	1.53	1.36
19	C	404	HEC	C3D-C2D	7.88	1.53	1.36
19	C	402	HEC	C3D-C2D	7.74	1.53	1.36
10	BX	101	V7N	C28-C27	7.00	1.52	1.34
10	Be	1103	V7N	C28-C27	6.95	1.52	1.34
10	Bl	1202	V7N	C28-C27	6.94	1.52	1.34
10	Bj	1202	V7N	C28-C27	6.89	1.52	1.34
10	AF	101	V7N	C28-C27	6.88	1.52	1.34
10	Bc	1202	V7N	C28-C27	6.88	1.52	1.34
10	An	101	V7N	C28-C27	6.87	1.52	1.34
10	Bg	101	V7N	C28-C27	6.86	1.52	1.34
10	BA	102	V7N	C28-C27	6.86	1.52	1.34
10	BQ	103	V7N	C28-C27	6.86	1.52	1.34
10	BW	102	V7N	C28-C27	6.85	1.52	1.34
10	Bm	101	V7N	C28-C27	6.85	1.52	1.34
10	BC	103	V7N	C28-C27	6.85	1.52	1.34
10	BR	103	V7N	C28-C27	6.85	1.52	1.34
10	Aa	101	V7N	C28-C27	6.83	1.52	1.34
10	Bi	101	V7N	C28-C27	6.82	1.52	1.34
10	Bb	1202	V7N	C28-C27	6.82	1.52	1.34
10	BL	101	V7N	C28-C27	6.81	1.52	1.34
10	BO	102	V7N	C28-C27	6.81	1.52	1.34
10	BF	103	V7N	C28-C27	6.81	1.52	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	Bf	1202	V7N	C28-C27	6.81	1.52	1.34
10	Bp	1202	V7N	C28-C27	6.80	1.52	1.34
10	Bd	1202	V7N	C28-C27	6.80	1.52	1.34
10	Bn	101	V7N	C28-C27	6.79	1.52	1.34
10	BG	101	V7N	C28-C27	6.79	1.52	1.34
10	BN	102	V7N	C28-C27	6.79	1.52	1.34
10	BH	102	V7N	C28-C27	6.79	1.52	1.34
10	BU	104	V7N	C28-C27	6.77	1.52	1.34
10	BJ	101	V7N	C28-C27	6.77	1.52	1.34
10	BV	101	V7N	C28-C27	6.77	1.52	1.34
10	BB	102	V7N	C28-C27	6.76	1.52	1.34
10	BK	104	V7N	C28-C27	6.76	1.52	1.34
10	BS	103	V7N	C28-C27	6.76	1.52	1.34
10	BD	103	V7N	C28-C27	6.75	1.52	1.34
10	Bh	1202	V7N	C28-C27	6.74	1.52	1.34
10	BP	102	V7N	C28-C27	6.74	1.52	1.34
10	AL	102	V7N	C28-C27	6.74	1.51	1.34
10	Bk	101	V7N	C28-C27	6.74	1.51	1.34
10	BI	101	V7N	C28-C27	6.74	1.51	1.34
10	BT	101	V7N	C28-C27	6.71	1.51	1.34
19	C	402	HEC	FE-ND	5.41	2.11	1.94
11	Ae	101	BCL	MG-NA	5.15	2.18	2.06
11	Bp	1203	BCL	C3D-C4D	-5.15	1.32	1.44
11	Af	101	BCL	MG-NA	5.09	2.18	2.06
11	Aj	101	BCL	MG-NA	5.08	2.18	2.06
11	Ad	101	BCL	MG-NA	5.08	2.18	2.06
11	AM	101	BCL	MG-NA	5.08	2.18	2.06
11	Ah	101	BCL	MG-NA	5.07	2.18	2.06
19	C	403	HEC	FE-ND	5.06	2.10	1.94
11	BA	101	BCL	MG-NA	5.04	2.18	2.06
11	Ao	101	BCL	C3D-C4D	-5.04	1.32	1.44
11	AW	1202	BCL	MG-NA	5.03	2.18	2.06
11	Bm	103	BCL	MG-NA	5.00	2.18	2.06
11	Am	101	BCL	C3D-C4D	-4.99	1.32	1.44
11	AG	101	BCL	MG-NA	4.99	2.18	2.06
11	Al	101	BCL	C3D-C4D	-4.98	1.32	1.44
11	Ac	101	BCL	MG-NA	4.98	2.18	2.06
11	AD	1102	BCL	MG-NA	4.96	2.18	2.06
11	AH	101	BCL	MG-NA	4.96	2.18	2.06
11	Aa	102	BCL	MG-NA	4.94	2.18	2.06
11	Ai	101	BCL	MG-NA	4.94	2.18	2.06
11	AQ	102	BCL	MG-NA	4.94	2.18	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	BL	102	BCL	MG-NA	4.94	2.18	2.06
11	AV	1001	BCL	MG-NA	4.93	2.18	2.06
11	Bh	1205	BCL	MG-NA	4.91	2.17	2.06
11	AU	1001	BCL	MG-NA	4.90	2.17	2.06
11	AT	1103	BCL	MG-NA	4.90	2.17	2.06
11	AW	1203	BCL	MG-NA	4.90	2.17	2.06
11	Bp	1204	BCL	MG-NA	4.90	2.17	2.06
11	AI	102	BCL	MG-NA	4.89	2.17	2.06
11	BX	102	BCL	MG-NA	4.89	2.17	2.06
11	BD	101	BCL	MG-NA	4.88	2.17	2.06
11	AL	101	BCL	MG-NA	4.87	2.17	2.06
11	BO	103	BCL	MG-NA	4.87	2.17	2.06
11	BV	102	BCL	MG-NA	4.86	2.17	2.06
11	AB	101	BCL	MG-NA	4.86	2.17	2.06
11	Bd	1203	BCL	MG-NA	4.86	2.17	2.06
11	AN	101	BCL	MG-NA	4.86	2.17	2.06
11	L	302	BCL	MG-NA	4.85	2.17	2.06
11	AJ	1103	BCL	MG-NA	4.85	2.17	2.06
11	M	404	BCL	MG-NA	4.85	2.17	2.06
11	AC	101	BCL	MG-NA	4.84	2.17	2.06
11	Bf	1204	BCL	MG-NA	4.84	2.17	2.06
11	Bo	1202	BCL	MG-NA	4.83	2.17	2.06
11	AJ	1102	BCL	MG-NA	4.83	2.17	2.06
11	Ab	101	BCL	MG-NA	4.82	2.17	2.06
11	Bg	103	BCL	MG-NA	4.82	2.17	2.06
11	BK	102	BCL	MG-NA	4.82	2.17	2.06
11	BB	101	BCL	MG-NA	4.82	2.17	2.06
11	Ak	101	BCL	MG-NA	4.81	2.17	2.06
11	Bc	1204	BCL	MG-NA	4.80	2.17	2.06
11	Bb	1203	BCL	MG-NA	4.80	2.17	2.06
10	BS	103	V7N	C14-C13	4.79	1.42	1.35
11	Bi	102	BCL	MG-NA	4.79	2.17	2.06
11	BN	101	BCL	MG-NA	4.79	2.17	2.06
11	BP	101	BCL	MG-NA	4.79	2.17	2.06
11	Bn	103	BCL	MG-NA	4.78	2.17	2.06
11	M	405	BCL	MG-NA	4.78	2.17	2.06
11	AW	1204	BCL	MG-NA	4.77	2.17	2.06
11	AI	101	BCL	MG-NA	4.77	2.17	2.06
11	AP	1102	BCL	MG-NA	4.76	2.17	2.06
11	Bk	103	BCL	MG-NA	4.74	2.17	2.06
11	BE	101	BCL	MG-NA	4.73	2.17	2.06
11	BI	102	BCL	MG-NA	4.73	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	BG	102	BCL	MG-NA	4.73	2.17	2.06
11	AQ	101	BCL	MG-NA	4.72	2.17	2.06
11	BS	101	BCL	MG-NA	4.72	2.17	2.06
11	AM	102	BCL	MG-NA	4.72	2.17	2.06
11	Be	1105	BCL	MG-NA	4.70	2.17	2.06
19	C	405	HEC	FE-ND	4.69	2.09	1.94
11	BC	101	BCL	MG-NA	4.69	2.17	2.06
11	AQ	103	BCL	MG-NA	4.69	2.17	2.06
11	BF	101	BCL	MG-NA	4.68	2.17	2.06
11	AK	101	BCL	MG-NA	4.68	2.17	2.06
11	BH	104	BCL	MG-NA	4.68	2.17	2.06
11	BU	102	BCL	MG-NA	4.66	2.17	2.06
11	AO	101	BCL	MG-NA	4.66	2.17	2.06
10	BT	101	V7N	C14-C13	4.66	1.42	1.35
11	AX	1202	BCL	MG-NA	4.65	2.17	2.06
11	BR	101	BCL	MG-NA	4.65	2.17	2.06
10	BQ	103	V7N	C14-C13	4.64	1.41	1.35
10	Bi	101	V7N	C14-C13	4.64	1.41	1.35
11	AS	1102	BCL	MG-NA	4.63	2.17	2.06
11	AF	102	BCL	MG-NA	4.60	2.17	2.06
11	Bj	1204	BCL	MG-NA	4.59	2.17	2.06
10	BB	102	V7N	C14-C13	4.58	1.41	1.35
11	Bl	1203	BCL	MG-NA	4.57	2.17	2.06
11	BA	103	BCL	MG-NA	4.57	2.17	2.06
11	AR	101	BCL	MG-NA	4.57	2.17	2.06
10	Aa	101	V7N	C14-C13	4.57	1.41	1.35
10	BW	102	V7N	C14-C13	4.56	1.41	1.35
10	An	101	V7N	C14-C13	4.56	1.41	1.35
10	Bm	101	V7N	C14-C13	4.55	1.41	1.35
10	BX	101	V7N	C14-C13	4.53	1.41	1.35
11	Am	101	BCL	O2D-CGD	4.53	1.44	1.33
10	BF	103	V7N	C14-C13	4.53	1.41	1.35
11	AT	1102	BCL	MG-NA	4.53	2.17	2.06
10	Bi	101	V7N	C17-C18	4.53	1.41	1.35
10	BR	103	V7N	C14-C13	4.52	1.41	1.35
11	AE	1102	BCL	MG-NA	4.51	2.17	2.06
10	Be	1103	V7N	C14-C13	4.50	1.41	1.35
10	Bl	1202	V7N	C14-C13	4.49	1.41	1.35
10	BO	102	V7N	C14-C13	4.48	1.41	1.35
10	Bp	1202	V7N	C14-C13	4.47	1.41	1.35
10	Bg	101	V7N	C14-C13	4.46	1.41	1.35
10	Aa	101	V7N	C17-C18	4.44	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	BL	101	V7N	C14-C13	4.44	1.41	1.35
10	BG	101	V7N	C14-C13	4.44	1.41	1.35
10	BK	104	V7N	C14-C13	4.44	1.41	1.35
10	AL	102	V7N	C14-C13	4.43	1.41	1.35
10	BD	103	V7N	C14-C13	4.41	1.41	1.35
11	L	301	BCL	MG-NA	4.41	2.16	2.06
10	BS	103	V7N	C17-C18	4.41	1.41	1.35
10	Bf	1202	V7N	C14-C13	4.40	1.41	1.35
10	BX	101	V7N	C17-C18	4.38	1.41	1.35
10	BI	101	V7N	C14-C13	4.38	1.41	1.35
19	C	405	HEC	FE-NB	4.38	2.08	1.94
10	Bk	101	V7N	C14-C13	4.37	1.41	1.35
10	Bn	101	V7N	C14-C13	4.36	1.41	1.35
10	BL	101	V7N	C17-C18	4.36	1.41	1.35
10	Bj	1202	V7N	C14-C13	4.36	1.41	1.35
10	BV	101	V7N	C14-C13	4.36	1.41	1.35
11	Bp	1203	BCL	O2D-CGD	4.35	1.43	1.33
11	Ao	101	BCL	O2D-CGD	4.35	1.43	1.33
10	An	101	V7N	C17-C18	4.34	1.41	1.35
10	Bb	1202	V7N	C14-C13	4.34	1.41	1.35
10	Bm	101	V7N	C17-C18	4.34	1.41	1.35
10	BA	102	V7N	C14-C13	4.34	1.41	1.35
10	BU	104	V7N	C14-C13	4.33	1.41	1.35
10	BH	102	V7N	C14-C13	4.33	1.41	1.35
10	BW	102	V7N	C17-C18	4.33	1.41	1.35
10	BN	102	V7N	C14-C13	4.32	1.41	1.35
10	BR	103	V7N	C17-C18	4.31	1.41	1.35
10	BB	102	V7N	C17-C18	4.31	1.41	1.35
10	BP	102	V7N	C14-C13	4.31	1.41	1.35
10	Bc	1202	V7N	C14-C13	4.29	1.41	1.35
10	Bj	1202	V7N	C17-C18	4.28	1.41	1.35
10	Bl	1202	V7N	C17-C18	4.28	1.41	1.35
10	Bd	1202	V7N	C14-C13	4.28	1.41	1.35
10	BJ	101	V7N	C14-C13	4.28	1.41	1.35
10	Be	1103	V7N	C17-C18	4.25	1.41	1.35
10	BK	104	V7N	C17-C18	4.25	1.41	1.35
10	BO	102	V7N	C17-C18	4.22	1.41	1.35
10	BC	103	V7N	C14-C13	4.21	1.41	1.35
10	AF	101	V7N	C14-C13	4.21	1.41	1.35
11	Am	101	BCL	C4B-NB	-4.20	1.32	1.37
10	BF	103	V7N	C17-C18	4.19	1.41	1.35
10	Bp	1202	V7N	C17-C18	4.19	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	Bc	1202	V7N	C17-C18	4.18	1.41	1.35
10	Bh	1202	V7N	C14-C13	4.17	1.41	1.35
19	C	403	HEC	FE-NB	4.17	2.07	1.94
10	BI	101	V7N	C17-C18	4.17	1.41	1.35
10	BT	101	V7N	C17-C18	4.15	1.41	1.35
11	Al	101	BCL	O2D-CGD	4.15	1.43	1.33
10	BN	102	V7N	C17-C18	4.13	1.41	1.35
10	Bb	1202	V7N	C17-C18	4.13	1.41	1.35
10	BS	103	V7N	C21-C22	4.13	1.38	1.34
10	Bn	101	V7N	C17-C18	4.12	1.41	1.35
10	BP	102	V7N	C17-C18	4.12	1.41	1.35
10	BU	104	V7N	C17-C18	4.12	1.41	1.35
10	Bk	101	V7N	C17-C18	4.12	1.41	1.35
19	C	404	HEC	FE-ND	4.11	2.07	1.94
10	Bg	101	V7N	C17-C18	4.10	1.41	1.35
11	Ao	101	BCL	O2A-CGA	4.09	1.45	1.33
10	BD	103	V7N	C17-C18	4.08	1.41	1.35
10	AF	101	V7N	C17-C18	4.08	1.41	1.35
10	Bf	1202	V7N	C17-C18	4.07	1.41	1.35
10	BG	101	V7N	C17-C18	4.07	1.41	1.35
10	Be	1103	V7N	C21-C22	4.06	1.38	1.34
10	BA	102	V7N	C17-C18	4.05	1.41	1.35
10	BT	101	V7N	C21-C22	4.04	1.38	1.34
10	BV	101	V7N	C17-C18	4.03	1.41	1.35
11	Am	101	BCL	O2A-CGA	4.02	1.45	1.33
19	C	402	HEC	FE-NC	4.01	2.08	1.95
10	Bh	1202	V7N	C17-C18	4.01	1.41	1.35
10	An	101	V7N	C21-C22	3.99	1.38	1.34
10	BH	102	V7N	C17-C18	3.99	1.41	1.35
10	BC	103	V7N	C17-C18	3.99	1.41	1.35
11	Al	101	BCL	O2A-CGA	3.98	1.45	1.33
11	Bp	1203	BCL	O2A-CGA	3.96	1.44	1.33
10	BJ	101	V7N	C17-C18	3.93	1.41	1.35
16	M	406	BPH	CBD-CGD	-3.93	1.47	1.52
10	AL	102	V7N	C17-C18	3.92	1.41	1.35
19	C	402	HEC	FE-NB	3.92	2.07	1.94
10	Bd	1202	V7N	C17-C18	3.91	1.41	1.35
16	L	303	BPH	CBD-CGD	-3.90	1.47	1.52
10	BS	103	V7N	C6-C5	3.88	1.40	1.35
10	BQ	103	V7N	C17-C18	3.88	1.40	1.35
10	BG	101	V7N	C21-C22	3.87	1.38	1.34
10	Bg	101	V7N	C21-C22	3.86	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	Bd	1203	BCL	MG-NC	3.86	2.15	2.06
10	BR	103	V7N	C6-C5	3.85	1.40	1.35
10	Bi	101	V7N	C21-C22	3.85	1.38	1.34
10	Bm	101	V7N	C21-C22	3.85	1.38	1.34
10	BX	101	V7N	C21-C22	3.84	1.38	1.34
10	BI	101	V7N	C21-C22	3.83	1.38	1.34
10	BW	102	V7N	C21-C22	3.83	1.38	1.34
10	Bl	1202	V7N	C21-C22	3.82	1.38	1.34
10	Bp	1202	V7N	C21-C22	3.79	1.38	1.34
10	BL	101	V7N	C21-C22	3.79	1.38	1.34
10	BT	101	V7N	C6-C5	3.78	1.40	1.35
10	BF	103	V7N	C6-C5	3.77	1.40	1.35
10	Bi	101	V7N	C6-C5	3.77	1.40	1.35
10	BO	102	V7N	C6-C5	3.76	1.40	1.35
10	BN	102	V7N	C21-C22	3.75	1.38	1.34
10	BD	103	V7N	C21-C22	3.74	1.38	1.34
10	BK	104	V7N	C21-C22	3.74	1.38	1.34
10	Bd	1202	V7N	C21-C22	3.73	1.38	1.34
10	BB	102	V7N	C21-C22	3.73	1.38	1.34
10	Aa	101	V7N	C21-C22	3.72	1.38	1.34
10	BA	102	V7N	C21-C22	3.72	1.38	1.34
10	BO	102	V7N	C21-C22	3.72	1.38	1.34
10	Bc	1202	V7N	C21-C22	3.71	1.38	1.34
10	Bj	1202	V7N	C21-C22	3.70	1.38	1.34
10	Bj	1202	V7N	C6-C5	3.70	1.40	1.35
11	Ao	101	BCL	C4B-NB	-3.70	1.33	1.37
11	Al	101	BCL	C4B-NB	-3.70	1.33	1.37
11	AQ	103	BCL	MG-NC	3.70	2.15	2.06
10	BQ	103	V7N	C21-C22	3.68	1.38	1.34
10	BL	101	V7N	C6-C5	3.68	1.40	1.35
10	Bn	101	V7N	C21-C22	3.68	1.38	1.34
11	Bh	1205	BCL	MG-NC	3.67	2.15	2.06
11	AB	101	BCL	MG-NC	3.66	2.15	2.06
10	Aa	101	V7N	C6-C5	3.66	1.40	1.35
10	BB	102	V7N	C6-C5	3.65	1.40	1.35
10	BR	103	V7N	C21-C22	3.65	1.37	1.34
10	BP	102	V7N	C21-C22	3.65	1.37	1.34
10	BF	103	V7N	C21-C22	3.64	1.37	1.34
11	Bp	1203	BCL	C3B-C4B	3.63	1.47	1.41
11	BD	101	BCL	MG-NC	3.63	2.14	2.06
11	Bn	103	BCL	MG-NC	3.62	2.14	2.06
11	BO	103	BCL	MG-NC	3.62	2.14	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	BG	101	V7N	C6-C5	3.61	1.40	1.35
10	Bm	101	V7N	C6-C5	3.59	1.40	1.35
11	Bb	1203	BCL	MG-NC	3.59	2.14	2.06
10	Bf	1202	V7N	C21-C22	3.59	1.37	1.34
11	Bk	103	BCL	MG-NC	3.59	2.14	2.06
10	Bp	1202	V7N	C6-C5	3.58	1.40	1.35
11	Ae	101	BCL	MG-NC	3.58	2.14	2.06
11	Bo	1202	BCL	MG-NC	3.58	2.14	2.06
10	BW	102	V7N	C6-C5	3.57	1.40	1.35
11	BN	101	BCL	MG-NC	3.57	2.14	2.06
11	BK	102	BCL	MG-NC	3.57	2.14	2.06
10	Bh	1202	V7N	C21-C22	3.57	1.37	1.34
10	BQ	103	V7N	C6-C5	3.57	1.40	1.35
11	Bm	103	BCL	MG-NC	3.56	2.14	2.06
11	Bp	1203	BCL	CHD-C1D	3.56	1.45	1.38
10	BP	102	V7N	C6-C5	3.55	1.40	1.35
11	BA	101	BCL	MG-NC	3.55	2.14	2.06
10	Be	1103	V7N	C6-C5	3.54	1.40	1.35
11	Bp	1204	BCL	MG-NC	3.54	2.14	2.06
10	Bl	1202	V7N	C6-C5	3.54	1.40	1.35
10	AL	102	V7N	C21-C22	3.53	1.37	1.34
11	Be	1105	BCL	MG-NC	3.53	2.14	2.06
11	BS	101	BCL	MG-NC	3.53	2.14	2.06
10	BC	103	V7N	C21-C22	3.53	1.37	1.34
11	BP	101	BCL	MG-NC	3.53	2.14	2.06
10	BH	102	V7N	C21-C22	3.52	1.37	1.34
11	AW	1204	BCL	MG-NC	3.52	2.14	2.06
19	C	402	HEC	FE-NA	3.52	2.07	1.95
10	AF	101	V7N	C6-C5	3.51	1.40	1.35
11	Bc	1204	BCL	MG-NC	3.51	2.14	2.06
11	BC	101	BCL	MG-NC	3.51	2.14	2.06
10	Bk	101	V7N	C21-C22	3.51	1.37	1.34
10	BV	101	V7N	C6-C5	3.50	1.40	1.35
10	BC	103	V7N	C6-C5	3.50	1.40	1.35
11	Af	101	BCL	MG-NC	3.50	2.14	2.06
11	AJ	1103	BCL	MG-NC	3.50	2.14	2.06
11	Bf	1204	BCL	MG-NC	3.50	2.14	2.06
11	BE	101	BCL	MG-NC	3.49	2.14	2.06
11	BL	102	BCL	MG-NC	3.49	2.14	2.06
11	BV	102	BCL	MG-NC	3.48	2.14	2.06
11	AQ	101	BCL	MG-NC	3.48	2.14	2.06
10	Bb	1202	V7N	C6-C5	3.48	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	Bb	1202	V7N	C21-C22	3.48	1.37	1.34
11	Ad	101	BCL	MG-NC	3.48	2.14	2.06
10	BV	101	V7N	C21-C22	3.48	1.37	1.34
11	BG	102	BCL	MG-NC	3.47	2.14	2.06
11	Al	101	BCL	CHB-C1B	3.47	1.47	1.39
10	BJ	101	V7N	C6-C5	3.47	1.40	1.35
11	Ao	101	BCL	C3B-C4B	3.47	1.47	1.41
11	AU	1001	BCL	MG-NC	3.47	2.14	2.06
11	Ah	101	BCL	MG-NC	3.47	2.14	2.06
11	Ao	101	BCL	CHD-C1D	3.46	1.45	1.38
10	AF	101	V7N	C21-C22	3.46	1.37	1.34
11	AW	1202	BCL	MG-NC	3.46	2.14	2.06
11	Bg	103	BCL	MG-NC	3.46	2.14	2.06
11	Bp	1203	BCL	C4B-NB	-3.46	1.33	1.37
11	BX	102	BCL	MG-NC	3.45	2.14	2.06
10	BU	104	V7N	C6-C5	3.45	1.40	1.35
19	C	403	HEC	FE-NA	3.45	2.06	1.95
11	AM	102	BCL	MG-NC	3.45	2.14	2.06
11	Al	101	BCL	C3B-C4B	3.45	1.47	1.41
11	Am	101	BCL	C1D-ND	-3.45	1.33	1.37
19	C	403	HEC	FE-NC	3.44	2.06	1.95
11	Bi	102	BCL	MG-NC	3.44	2.14	2.06
10	BI	101	V7N	C6-C5	3.42	1.40	1.35
10	BN	102	V7N	C6-C5	3.42	1.40	1.35
11	Aj	101	BCL	MG-NC	3.42	2.14	2.06
11	AM	101	BCL	MG-NC	3.42	2.14	2.06
11	Al	101	BCL	C1D-ND	-3.42	1.33	1.37
10	BU	104	V7N	C21-C22	3.41	1.37	1.34
11	BF	101	BCL	MG-NC	3.41	2.14	2.06
11	Bp	1203	BCL	C1D-ND	-3.40	1.33	1.37
11	BR	101	BCL	MG-NC	3.40	2.14	2.06
10	An	101	V7N	C6-C5	3.40	1.40	1.35
11	Ab	101	BCL	MG-NC	3.39	2.14	2.06
10	BJ	101	V7N	C21-C22	3.39	1.37	1.34
11	AW	1203	BCL	MG-NC	3.39	2.14	2.06
11	BU	102	BCL	MG-NC	3.38	2.14	2.06
10	Bg	101	V7N	C6-C5	3.38	1.40	1.35
11	AD	1102	BCL	MG-NC	3.38	2.14	2.06
10	Bf	1202	V7N	C6-C5	3.37	1.40	1.35
11	AQ	102	BCL	C3B-C4B	3.36	1.47	1.41
11	Aa	102	BCL	MG-NC	3.36	2.14	2.06
11	Ac	101	BCL	MG-NC	3.36	2.14	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	AT	1102	BCL	MG-NC	3.36	2.14	2.06
11	L	302	BCL	MG-NC	3.36	2.14	2.06
11	Ai	101	BCL	MG-NC	3.35	2.14	2.06
11	Ak	101	BCL	MG-NC	3.35	2.14	2.06
10	BX	101	V7N	C6-C5	3.35	1.40	1.35
10	BK	104	V7N	C6-C5	3.35	1.40	1.35
19	C	405	HEC	FE-NC	3.35	2.06	1.95
11	BI	102	BCL	MG-NC	3.34	2.14	2.06
11	M	404	BCL	MG-NC	3.34	2.14	2.06
11	Am	101	BCL	CHB-C1B	3.32	1.46	1.39
11	Ao	101	BCL	C1D-ND	-3.32	1.33	1.37
11	AV	1001	BCL	MG-NC	3.31	2.14	2.06
19	C	404	HEC	FE-NB	3.31	2.05	1.94
11	Bp	1203	BCL	CHB-C1B	3.31	1.46	1.39
11	AH	101	BCL	MG-NC	3.30	2.14	2.06
10	Bh	1202	V7N	C6-C5	3.30	1.40	1.35
10	Bc	1202	V7N	C6-C5	3.30	1.40	1.35
10	BH	102	V7N	C6-C5	3.30	1.40	1.35
11	Ao	101	BCL	CHB-C1B	3.29	1.46	1.39
11	BB	101	BCL	MG-NC	3.29	2.14	2.06
10	BA	102	V7N	C6-C5	3.29	1.40	1.35
11	AJ	1102	BCL	MG-NC	3.28	2.14	2.06
11	AT	1103	BCL	MG-NC	3.27	2.14	2.06
11	Am	101	BCL	C3B-C4B	3.27	1.47	1.41
11	AC	101	BCL	MG-NC	3.26	2.14	2.06
11	AG	101	BCL	MG-NC	3.25	2.14	2.06
11	AK	101	BCL	MG-NC	3.25	2.14	2.06
11	AI	102	BCL	MG-NC	3.25	2.14	2.06
10	Bn	101	V7N	C6-C5	3.24	1.40	1.35
11	AN	101	BCL	MG-NC	3.24	2.14	2.06
11	L	301	BCL	MG-NC	3.23	2.14	2.06
19	C	405	HEC	FE-NA	3.23	2.06	1.95
11	AL	101	BCL	MG-NC	3.22	2.13	2.06
19	C	404	HEC	FE-NA	3.22	2.06	1.95
10	BD	103	V7N	C6-C5	3.21	1.40	1.35
11	Bj	1204	BCL	MG-NC	3.21	2.13	2.06
10	Bd	1202	V7N	C6-C5	3.20	1.40	1.35
11	AP	1102	BCL	MG-NC	3.19	2.13	2.06
16	L	303	BPH	C3B-C4B	3.19	1.47	1.41
11	BH	104	BCL	MG-NC	3.18	2.13	2.06
10	AL	102	V7N	C6-C5	3.18	1.40	1.35
10	Bk	101	V7N	C6-C5	3.17	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	AI	101	BCL	MG-NC	3.16	2.13	2.06
11	Bl	1203	BCL	MG-NC	3.15	2.13	2.06
11	Bp	1203	BCL	CHC-C4B	3.15	1.46	1.39
11	AX	1202	BCL	MG-NC	3.15	2.13	2.06
11	Ao	101	BCL	CHC-C4B	3.15	1.46	1.39
11	BA	103	BCL	MG-NC	3.14	2.13	2.06
11	Al	101	BCL	CHC-C4B	3.12	1.46	1.39
11	AF	102	BCL	MG-NC	3.11	2.13	2.06
11	AS	1102	BCL	MG-NC	3.09	2.13	2.06
11	AO	101	BCL	MG-NC	3.09	2.13	2.06
11	AR	101	BCL	MG-NC	3.05	2.13	2.06
11	Am	101	BCL	CHD-C1D	3.04	1.44	1.38
11	Aj	101	BCL	C3B-C4B	3.00	1.46	1.41
11	Ab	101	BCL	C3B-C4B	2.99	1.46	1.41
19	C	404	HEC	FE-NC	2.98	2.05	1.95
11	Al	101	BCL	CHD-C1D	2.98	1.44	1.38
11	Al	101	BCL	C3D-C2D	2.93	1.47	1.39
11	M	405	BCL	MG-NC	2.91	2.13	2.06
11	Ao	101	BCL	C3D-C2D	2.89	1.47	1.39
11	Am	101	BCL	C3D-C2D	2.88	1.47	1.39
11	Bp	1203	BCL	C3D-C2D	2.86	1.46	1.39
11	AE	1102	BCL	MG-NC	2.84	2.13	2.06
11	Bp	1203	BCL	OBD-CAD	2.83	1.27	1.22
11	AI	101	BCL	C3B-C4B	2.83	1.46	1.41
11	Ao	101	BCL	OBD-CAD	2.82	1.27	1.22
16	M	406	BPH	C3D-CAD	-2.82	1.41	1.47
12	Ad	102	LMT	O3'-C3'	-2.81	1.36	1.43
12	BD	102	LMT	O3'-C3'	-2.81	1.36	1.43
11	Am	101	BCL	CHC-C4B	2.81	1.45	1.39
12	Bc	1201	LMT	O3'-C3'	-2.80	1.36	1.43
12	BC	102	LMT	O3'-C3'	-2.80	1.36	1.43
12	BH	101	LMT	O3'-C3'	-2.80	1.36	1.43
11	Ac	101	BCL	C3B-C4B	2.79	1.46	1.41
11	Aa	102	BCL	C3B-C4B	2.77	1.46	1.41
11	BA	101	BCL	C3B-C4B	2.77	1.46	1.41
12	BG	103	LMT	O3'-C3'	-2.77	1.36	1.43
12	AX	1201	LMT	O2'-C2'	-2.76	1.36	1.43
11	AO	101	BCL	C3B-C4B	2.76	1.46	1.41
12	BI	103	LMT	O3'-C3'	-2.76	1.36	1.43
12	BE	102	LMT	O3'-C3'	-2.75	1.36	1.43
11	AR	101	BCL	C3B-C4B	2.75	1.46	1.41
12	AX	1201	LMT	O3'-C3'	-2.75	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	BA	104	LMT	O3'-C3'	-2.75	1.36	1.43
11	Ao	101	BCL	C1B-NB	-2.74	1.34	1.37
12	Bf	1201	LMT	O2'-C2'	-2.74	1.36	1.43
12	BB	103	LMT	O3'-C3'	-2.74	1.36	1.43
12	Bj	1203	LMT	O3'-C3'	-2.74	1.36	1.43
11	AQ	102	BCL	MG-NC	2.74	2.12	2.06
11	AW	1202	BCL	C3B-C4B	2.74	1.46	1.41
16	L	303	BPH	C3D-CAD	-2.73	1.41	1.47
12	Bp	1201	LMT	O3'-C3'	-2.73	1.36	1.43
12	BF	102	LMT	O3'-C3'	-2.73	1.36	1.43
11	Ae	101	BCL	C3B-C4B	2.72	1.46	1.41
12	Bd	1201	LMT	O3'-C3'	-2.72	1.36	1.43
11	L	301	BCL	C3B-C4B	2.72	1.46	1.41
12	BQ	102	LMT	O3'-C3'	-2.72	1.36	1.43
12	BQ	101	LMT	O3'-C3'	-2.72	1.36	1.43
12	BR	102	LMT	O3'-C3'	-2.71	1.36	1.43
12	BH	103	LMT	O3'-C3'	-2.71	1.36	1.43
12	Bo	1201	LMT	O3'-C3'	-2.71	1.36	1.43
11	AN	101	BCL	C3B-C4B	2.70	1.46	1.41
11	Ah	101	BCL	C3B-C4B	2.70	1.46	1.41
12	Bl	1201	LMT	O3'-C3'	-2.70	1.36	1.43
12	Bf	1203	LMT	O3'-C3'	-2.70	1.36	1.43
12	Ba	1102	LMT	O3'-C3'	-2.70	1.36	1.43
12	BL	103	LMT	O3'-C3'	-2.70	1.36	1.43
11	Ak	101	BCL	C3B-C4B	2.69	1.46	1.41
11	Al	101	BCL	OBD-CAD	2.69	1.27	1.22
12	Bj	1201	LMT	O2'-C2'	-2.68	1.36	1.43
12	BO	101	LMT	O3'-C3'	-2.68	1.36	1.43
12	BU	103	LMT	O3'-C3'	-2.68	1.36	1.43
12	AW	1201	LMT	O3'-C3'	-2.67	1.36	1.43
12	BC	102	LMT	O2'-C2'	-2.67	1.36	1.43
12	BA	105	LMT	O3'-C3'	-2.67	1.36	1.43
12	Bh	1204	LMT	O3'-C3'	-2.66	1.36	1.43
12	Bf	1201	LMT	O3'-C3'	-2.66	1.36	1.43
11	AI	102	BCL	C3B-C4B	2.66	1.46	1.41
12	Bc	1201	LMT	O2'-C2'	-2.66	1.36	1.43
12	Bh	1201	LMT	O3'-C3'	-2.66	1.36	1.43
12	BM	1001	LMT	O3'-C3'	-2.66	1.36	1.43
12	Be	1102	LMT	O3'-C3'	-2.65	1.36	1.43
12	Bj	1201	LMT	O3'-C3'	-2.65	1.36	1.43
12	BS	102	LMT	O3'-C3'	-2.65	1.36	1.43
12	BK	103	LMT	O3'-C3'	-2.65	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	Am	101	BCL	MG-NA	-2.65	2.00	2.06
12	Bp	1201	LMT	O2'-C2'	-2.65	1.36	1.43
12	BW	103	LMT	O3'-C3'	-2.64	1.36	1.43
11	L	302	BCL	C3B-C4B	2.64	1.46	1.41
11	AL	101	BCL	C3B-C4B	2.64	1.46	1.41
12	Bo	1201	LMT	O2'-C2'	-2.64	1.36	1.43
12	BK	101	LMT	O3'-C3'	-2.64	1.36	1.43
12	C	401	LMT	O3'-C3'	-2.64	1.36	1.43
12	BA	104	LMT	O2'-C2'	-2.63	1.36	1.43
12	BH	103	LMT	O2'-C2'	-2.63	1.36	1.43
11	Ai	101	BCL	C3B-C4B	2.63	1.45	1.41
11	AX	1202	BCL	C3B-C4B	2.63	1.45	1.41
12	Bl	1201	LMT	O2'-C2'	-2.63	1.36	1.43
12	K	201	LMT	O3'-C3'	-2.63	1.36	1.43
12	Bf	1203	LMT	O2'-C2'	-2.62	1.36	1.43
12	BO	104	LMT	O3'-C3'	-2.62	1.36	1.43
11	AC	101	BCL	C3B-C4B	2.62	1.45	1.41
11	M	404	BCL	C3B-C4B	2.61	1.45	1.41
11	Af	101	BCL	C3B-C4B	2.61	1.45	1.41
12	Aa	103	LMT	O3'-C3'	-2.61	1.36	1.43
11	AH	101	BCL	C3B-C4B	2.60	1.45	1.41
11	AS	1102	BCL	C3B-C4B	2.60	1.45	1.41
12	BW	101	LMT	O3'-C3'	-2.60	1.36	1.43
12	Bb	1201	LMT	O3'-C3'	-2.59	1.36	1.43
11	Bn	103	BCL	C3B-C4B	2.58	1.45	1.41
11	Al	101	BCL	C1B-NB	-2.58	1.34	1.37
11	AD	1102	BCL	C3B-C4B	2.57	1.45	1.41
12	Bj	1203	LMT	O2'-C2'	-2.57	1.36	1.43
11	Ao	101	BCL	CHD-C4C	2.57	1.46	1.39
11	BP	101	BCL	C3B-C4B	2.57	1.45	1.41
11	AW	1203	BCL	C3B-C4B	2.56	1.45	1.41
11	AE	1102	BCL	C3B-C4B	2.56	1.45	1.41
12	Ad	102	LMT	O2'-C2'	-2.56	1.36	1.43
11	BI	102	BCL	C3B-C4B	2.56	1.45	1.41
12	BR	102	LMT	O2'-C2'	-2.56	1.36	1.43
11	BE	101	BCL	C3B-C4B	2.56	1.45	1.41
11	AB	101	BCL	C3B-C4B	2.56	1.45	1.41
11	Bc	1204	BCL	C3B-C4B	2.55	1.45	1.41
11	Bp	1203	BCL	CHD-C4C	2.55	1.46	1.39
11	Am	101	BCL	OBD-CAD	2.55	1.26	1.22
12	BE	102	LMT	O2'-C2'	-2.55	1.37	1.43
12	Bb	1201	LMT	O2'-C2'	-2.54	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	BU	101	LMT	O3'-C3'	-2.54	1.37	1.43
12	BD	102	LMT	O2'-C2'	-2.54	1.37	1.43
12	Be	1102	LMT	O2'-C2'	-2.54	1.37	1.43
11	Al	101	BCL	MG-NA	-2.54	2.00	2.06
12	Bd	1201	LMT	O2'-C2'	-2.54	1.37	1.43
12	BQ	102	LMT	O2'-C2'	-2.54	1.37	1.43
12	L	304	LMT	O3'-C3'	-2.54	1.37	1.43
12	Bh	1201	LMT	O2'-C2'	-2.54	1.37	1.43
12	BB	103	LMT	O2'-C2'	-2.53	1.37	1.43
11	AQ	101	BCL	C3B-C4B	2.53	1.45	1.41
11	AT	1103	BCL	C3B-C4B	2.53	1.45	1.41
11	AJ	1102	BCL	C3B-C4B	2.52	1.45	1.41
12	BG	103	LMT	O2'-C2'	-2.52	1.37	1.43
11	AF	102	BCL	C3B-C4B	2.52	1.45	1.41
12	BE	102	LMT	O2B-C2B	-2.51	1.37	1.43
10	Bd	1202	V7N	C12-C13	-2.51	1.40	1.45
12	Bh	1204	LMT	O2'-C2'	-2.51	1.37	1.43
11	BG	102	BCL	C3B-C4B	2.49	1.45	1.41
12	BA	104	LMT	O2B-C2B	-2.49	1.37	1.43
12	Aj	102	LMT	O3'-C3'	-2.49	1.37	1.43
12	AW	1201	LMT	O2'-C2'	-2.49	1.37	1.43
12	BQ	101	LMT	O2'-C2'	-2.48	1.37	1.43
11	AV	1001	BCL	C3B-C4B	2.48	1.45	1.41
10	BD	103	V7N	C8-C9	-2.48	1.40	1.45
12	BL	103	LMT	O2'-C2'	-2.48	1.37	1.43
11	Be	1105	BCL	C3B-C4B	2.47	1.45	1.41
11	Bf	1204	BCL	C3B-C4B	2.47	1.45	1.41
11	AM	101	BCL	C3B-C4B	2.47	1.45	1.41
11	AM	102	BCL	C3B-C4B	2.47	1.45	1.41
11	Ad	101	BCL	C3B-C4B	2.46	1.45	1.41
11	BL	102	BCL	C3B-C4B	2.46	1.45	1.41
12	Bf	1201	LMT	O2B-C2B	-2.46	1.37	1.43
12	Ba	1102	LMT	O2'-C2'	-2.46	1.37	1.43
12	BH	103	LMT	O2B-C2B	-2.46	1.37	1.43
12	BO	101	LMT	O2'-C2'	-2.45	1.37	1.43
12	BF	102	LMT	O2'-C2'	-2.45	1.37	1.43
12	BU	101	LMT	O2B-C2B	-2.45	1.37	1.43
12	M	401	LMT	O3'-C3'	-2.45	1.37	1.43
12	Bo	1201	LMT	O2B-C2B	-2.45	1.37	1.43
11	Bj	1204	BCL	C3B-C4B	2.45	1.45	1.41
11	BH	104	BCL	C3B-C4B	2.45	1.45	1.41
11	BS	101	BCL	C3B-C4B	2.44	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	BW	101	LMT	O2'-C2'	-2.44	1.37	1.43
11	Am	101	BCL	C1B-NB	-2.44	1.34	1.37
12	Be	1102	LMT	O2B-C2B	-2.44	1.37	1.43
11	BU	102	BCL	C3B-C4B	2.43	1.45	1.41
12	BD	102	LMT	O2B-C2B	-2.43	1.37	1.43
12	BU	103	LMT	O2B-C2B	-2.43	1.37	1.43
12	BO	101	LMT	O2B-C2B	-2.43	1.37	1.43
11	AW	1204	BCL	C3B-C4B	2.42	1.45	1.41
10	Bk	101	V7N	C8-C9	-2.42	1.40	1.45
12	BW	103	LMT	O2'-C2'	-2.42	1.37	1.43
12	BL	103	LMT	O2B-C2B	-2.42	1.37	1.43
12	BI	103	LMT	O2'-C2'	-2.42	1.37	1.43
11	BA	103	BCL	C3B-C4B	2.42	1.45	1.41
11	AP	1102	BCL	C3B-C4B	2.41	1.45	1.41
11	BX	102	BCL	C3B-C4B	2.41	1.45	1.41
11	Bi	102	BCL	C3B-C4B	2.41	1.45	1.41
12	Bc	1201	LMT	O3B-C3B	-2.41	1.37	1.43
10	BC	103	V7N	C12-C13	-2.41	1.40	1.45
12	Bc	1201	LMT	O2B-C2B	-2.41	1.37	1.43
12	BQ	102	LMT	O3B-C3B	-2.41	1.37	1.43
10	BH	102	V7N	C12-C13	-2.41	1.40	1.45
10	AL	102	V7N	C8-C9	-2.40	1.40	1.45
10	BS	103	V7N	C8-C9	-2.40	1.40	1.45
12	Bh	1204	LMT	O2B-C2B	-2.40	1.37	1.43
10	Bf	1202	V7N	C12-C13	-2.40	1.40	1.45
11	Bp	1204	BCL	C3B-C4B	2.40	1.45	1.41
10	Bc	1202	V7N	C12-C13	-2.40	1.40	1.45
12	Bh	1201	LMT	O2B-C2B	-2.40	1.37	1.43
12	Bl	1201	LMT	O2B-C2B	-2.40	1.37	1.43
12	BW	101	LMT	O2B-C2B	-2.39	1.37	1.43
10	BK	104	V7N	C8-C9	-2.39	1.40	1.45
12	BA	104	LMT	O3B-C3B	-2.39	1.37	1.43
11	AG	101	BCL	C3B-C4B	2.39	1.45	1.41
12	BU	101	LMT	O3B-C3B	-2.39	1.37	1.43
12	Bf	1201	LMT	O3B-C3B	-2.39	1.37	1.43
12	BC	102	LMT	O3B-C3B	-2.39	1.37	1.43
12	BQ	102	LMT	O2B-C2B	-2.39	1.37	1.43
12	Bp	1201	LMT	O2B-C2B	-2.38	1.37	1.43
11	Am	101	BCL	CHD-C4C	2.38	1.45	1.39
10	Bn	101	V7N	C8-C9	-2.38	1.40	1.45
10	BN	102	V7N	C12-C13	-2.38	1.40	1.45
11	Bb	1203	BCL	C3B-C4B	2.38	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	BK	101	LMT	O3B-C3B	-2.38	1.37	1.43
12	BE	102	LMT	O3B-C3B	-2.38	1.37	1.43
12	Bf	1203	LMT	O2B-C2B	-2.38	1.37	1.43
12	Bd	1201	LMT	O2B-C2B	-2.38	1.37	1.43
12	BK	103	LMT	O3B-C3B	-2.37	1.37	1.43
12	BM	1001	LMT	O2B-C2B	-2.37	1.37	1.43
12	M	401	LMT	O3B-C3B	-2.37	1.37	1.43
11	Bo	1202	BCL	C3B-C4B	2.37	1.45	1.41
10	BA	102	V7N	C12-C13	-2.37	1.40	1.45
12	Be	1102	LMT	O3B-C3B	-2.37	1.37	1.43
12	L	304	LMT	O2B-C2B	-2.37	1.37	1.43
11	M	404	BCL	CHD-C1D	2.37	1.43	1.38
12	BQ	101	LMT	O3B-C3B	-2.37	1.37	1.43
12	K	201	LMT	O2B-C2B	-2.37	1.37	1.43
11	AU	1001	BCL	C3B-C4B	2.37	1.45	1.41
11	BF	101	BCL	C3B-C4B	2.36	1.45	1.41
12	Bj	1203	LMT	O2B-C2B	-2.36	1.37	1.43
12	Bo	1201	LMT	O3B-C3B	-2.36	1.37	1.43
12	BW	103	LMT	O3B-C3B	-2.36	1.37	1.43
10	Bb	1202	V7N	C12-C13	-2.36	1.40	1.45
12	Ad	102	LMT	O3B-C3B	-2.36	1.37	1.43
12	Bd	1201	LMT	O3B-C3B	-2.36	1.37	1.43
10	Bh	1202	V7N	C12-C13	-2.36	1.40	1.45
12	Bp	1201	LMT	O3B-C3B	-2.36	1.37	1.43
10	BG	101	V7N	C12-C13	-2.36	1.40	1.45
10	BJ	101	V7N	C12-C13	-2.36	1.40	1.45
11	BB	101	BCL	C1D-C2D	-2.36	1.40	1.45
12	BB	103	LMT	O2B-C2B	-2.36	1.37	1.43
12	Bf	1203	LMT	O3B-C3B	-2.36	1.37	1.43
12	M	401	LMT	O2B-C2B	-2.35	1.37	1.43
10	BX	101	V7N	C12-C13	-2.35	1.40	1.45
12	BB	103	LMT	O3B-C3B	-2.35	1.37	1.43
12	BI	103	LMT	O2B-C2B	-2.35	1.37	1.43
11	AJ	1103	BCL	C3B-C4B	2.35	1.45	1.41
10	Aa	101	V7N	C11-C12	2.35	1.40	1.34
12	BO	104	LMT	O3B-C3B	-2.35	1.37	1.43
12	Aj	102	LMT	O3B-C3B	-2.35	1.37	1.43
12	BI	103	LMT	O3B-C3B	-2.35	1.37	1.43
12	C	401	LMT	O2'-C2'	-2.35	1.37	1.43
10	BD	103	V7N	C12-C13	-2.34	1.40	1.45
10	BA	102	V7N	C8-C9	-2.34	1.40	1.45
12	BK	101	LMT	O2B-C2B	-2.34	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	BH	101	LMT	O3B-C3B	-2.34	1.37	1.43
11	BK	102	BCL	C3B-C4B	2.34	1.45	1.41
12	BM	1001	LMT	O2'-C2'	-2.34	1.37	1.43
12	BG	103	LMT	O3B-C3B	-2.34	1.37	1.43
11	BV	102	BCL	C3B-C4B	2.34	1.45	1.41
12	BW	101	LMT	O3B-C3B	-2.34	1.37	1.43
12	BG	103	LMT	O2B-C2B	-2.34	1.37	1.43
12	BM	1001	LMT	O3B-C3B	-2.34	1.37	1.43
10	AL	102	V7N	C12-C13	-2.34	1.40	1.45
10	BQ	103	V7N	C8-C9	-2.33	1.40	1.45
11	Al	101	BCL	C3C-C4C	-2.33	1.48	1.51
12	AW	1201	LMT	O2B-C2B	-2.33	1.37	1.43
10	Bi	101	V7N	C11-C12	2.33	1.40	1.34
12	BL	103	LMT	O3B-C3B	-2.33	1.37	1.43
12	L	304	LMT	O3B-C3B	-2.33	1.37	1.43
10	BH	102	V7N	C8-C9	-2.33	1.40	1.45
10	Bg	101	V7N	C8-C9	-2.33	1.40	1.45
10	Bh	1202	V7N	C8-C9	-2.33	1.40	1.45
12	BK	103	LMT	O2'-C2'	-2.33	1.37	1.43
11	AF	102	BCL	CHD-C1D	2.33	1.42	1.38
12	Ba	1102	LMT	O3B-C3B	-2.33	1.37	1.43
12	BQ	101	LMT	O2B-C2B	-2.33	1.37	1.43
11	BN	101	BCL	C3B-C4B	2.33	1.45	1.41
11	Bm	103	BCL	C3B-C4B	2.33	1.45	1.41
10	BI	101	V7N	C12-C13	-2.32	1.41	1.45
11	AQ	103	BCL	C3B-C4B	2.32	1.45	1.41
12	Bb	1201	LMT	O2B-C2B	-2.32	1.37	1.43
11	Bp	1203	BCL	C1B-NB	-2.32	1.34	1.37
10	BK	104	V7N	C12-C13	-2.32	1.41	1.45
12	K	201	LMT	O3B-C3B	-2.32	1.37	1.43
10	BC	103	V7N	C8-C9	-2.32	1.40	1.45
12	AW	1201	LMT	O3B-C3B	-2.32	1.37	1.43
12	BS	102	LMT	O2'-C2'	-2.32	1.37	1.43
10	BU	104	V7N	C12-C13	-2.32	1.41	1.45
10	Bd	1202	V7N	C8-C9	-2.32	1.40	1.45
10	BV	101	V7N	C12-C13	-2.31	1.41	1.45
10	BQ	103	V7N	C11-C12	2.31	1.40	1.34
11	AT	1102	BCL	C3B-C4B	2.31	1.45	1.41
12	Bl	1201	LMT	O3B-C3B	-2.31	1.37	1.43
12	BK	103	LMT	O2B-C2B	-2.31	1.37	1.43
11	Bk	103	BCL	C3B-C4B	2.31	1.45	1.41
10	Bg	101	V7N	C12-C13	-2.31	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	BO	104	LMT	O2'-C2'	-2.31	1.37	1.43
12	BF	102	LMT	O2B-C2B	-2.31	1.37	1.43
12	BH	103	LMT	O3B-C3B	-2.31	1.37	1.43
10	BP	102	V7N	C8-C9	-2.31	1.40	1.45
11	L	302	BCL	CHD-C1D	2.31	1.42	1.38
10	Bn	101	V7N	C12-C13	-2.31	1.41	1.45
12	BU	101	LMT	O2'-C2'	-2.31	1.37	1.43
10	BN	102	V7N	C8-C9	-2.31	1.40	1.45
12	Bb	1201	LMT	O3B-C3B	-2.31	1.37	1.43
10	AF	101	V7N	C12-C13	-2.31	1.41	1.45
12	AX	1201	LMT	O3B-C3B	-2.30	1.37	1.43
11	BD	101	BCL	C3B-C4B	2.30	1.45	1.41
11	BC	101	BCL	C3B-C4B	2.30	1.45	1.41
12	Aa	103	LMT	O3B-C3B	-2.30	1.37	1.43
12	Ba	1102	LMT	O2B-C2B	-2.30	1.37	1.43
10	Bc	1202	V7N	C8-C9	-2.30	1.40	1.45
12	BH	101	LMT	O2'-C2'	-2.30	1.37	1.43
10	BT	101	V7N	C11-C12	2.30	1.40	1.34
10	Bk	101	V7N	C12-C13	-2.30	1.41	1.45
12	BS	102	LMT	O3B-C3B	-2.30	1.37	1.43
10	Bf	1202	V7N	C8-C9	-2.30	1.40	1.45
11	Bh	1205	BCL	C3B-C4B	2.29	1.45	1.41
12	Bj	1203	LMT	O3B-C3B	-2.29	1.37	1.43
11	Bh	1205	BCL	C1D-C2D	-2.29	1.40	1.45
12	Bh	1204	LMT	O3B-C3B	-2.29	1.37	1.43
12	BS	102	LMT	O2B-C2B	-2.29	1.37	1.43
12	BW	103	LMT	O2B-C2B	-2.29	1.37	1.43
10	BW	102	V7N	C12-C13	-2.29	1.41	1.45
10	BJ	101	V7N	C19-C18	-2.29	1.41	1.45
10	BV	101	V7N	C19-C18	-2.29	1.41	1.45
10	Bp	1202	V7N	C12-C13	-2.29	1.41	1.45
10	Bj	1202	V7N	C11-C12	2.29	1.40	1.34
10	Bm	101	V7N	C11-C12	2.29	1.40	1.34
11	BR	101	BCL	C3B-C4B	2.29	1.45	1.41
12	Bj	1201	LMT	O3B-C3B	-2.29	1.37	1.43
10	BS	103	V7N	C12-C13	-2.29	1.41	1.45
12	BR	102	LMT	O2B-C2B	-2.28	1.37	1.43
12	BD	102	LMT	O3B-C3B	-2.28	1.37	1.43
12	BU	103	LMT	O3B-C3B	-2.28	1.37	1.43
12	K	201	LMT	O2'-C2'	-2.28	1.37	1.43
12	BA	105	LMT	O3B-C3B	-2.28	1.37	1.43
10	BO	102	V7N	C11-C12	2.28	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	BX	101	V7N	C8-C9	-2.28	1.40	1.45
11	AS	1102	BCL	CHD-C1D	2.28	1.42	1.38
11	Al	101	BCL	CHD-C4C	2.28	1.45	1.39
10	Bj	1202	V7N	C12-C13	-2.28	1.41	1.45
10	Be	1103	V7N	C12-C13	-2.28	1.41	1.45
10	BB	102	V7N	C11-C12	2.27	1.40	1.34
12	Be	1102	LMT	O4'-C4B	-2.27	1.37	1.43
10	BF	103	V7N	C11-C12	2.27	1.40	1.34
11	AL	101	BCL	CHD-C1D	2.27	1.42	1.38
12	Aj	102	LMT	O2B-C2B	-2.27	1.37	1.43
10	Bi	101	V7N	C7-C8	2.27	1.40	1.34
12	BR	102	LMT	O3B-C3B	-2.27	1.37	1.43
10	Bl	1202	V7N	C11-C12	2.27	1.40	1.34
10	An	101	V7N	C8-C9	-2.27	1.41	1.45
12	Aa	103	LMT	O2'-C2'	-2.27	1.37	1.43
12	Bj	1201	LMT	O2B-C2B	-2.27	1.37	1.43
11	AK	101	BCL	C3B-C4B	2.27	1.45	1.41
12	BO	104	LMT	O2B-C2B	-2.27	1.37	1.43
12	BH	101	LMT	O2B-C2B	-2.26	1.37	1.43
10	BI	101	V7N	C8-C9	-2.26	1.41	1.45
10	An	101	V7N	C12-C13	-2.26	1.41	1.45
12	BA	105	LMT	O2B-C2B	-2.26	1.37	1.43
10	Bg	101	V7N	C11-C12	2.26	1.40	1.34
10	BL	101	V7N	C12-C13	-2.26	1.41	1.45
10	BP	102	V7N	C12-C13	-2.26	1.41	1.45
10	BJ	101	V7N	C8-C9	-2.26	1.41	1.45
12	M	401	LMT	O2'-C2'	-2.26	1.37	1.43
12	Aa	103	LMT	O2B-C2B	-2.25	1.37	1.43
12	C	401	LMT	O3B-C3B	-2.25	1.37	1.43
10	Be	1103	V7N	C11-C12	2.25	1.40	1.34
12	Bh	1201	LMT	O3B-C3B	-2.25	1.37	1.43
12	Bf	1203	LMT	O4'-C4B	-2.25	1.37	1.43
11	BO	103	BCL	C3B-C4B	2.25	1.45	1.41
16	M	406	BPH	C3B-C4B	2.25	1.45	1.41
10	Bk	101	V7N	C11-C12	2.25	1.40	1.34
11	Am	101	BCL	CHC-C1C	-2.25	1.32	1.37
10	Bn	101	V7N	C11-C12	2.25	1.40	1.34
11	Bm	103	BCL	C1D-C2D	-2.25	1.40	1.45
11	BH	104	BCL	C3D-C4D	-2.24	1.39	1.44
10	Bp	1202	V7N	C11-C12	2.24	1.40	1.34
10	BH	102	V7N	C19-C18	-2.24	1.41	1.45
10	BU	104	V7N	C8-C9	-2.24	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	Bk	103	BCL	C3D-C4D	-2.24	1.39	1.44
10	Bp	1202	V7N	C8-C9	-2.24	1.41	1.45
11	Bl	1203	BCL	C3B-C4B	2.24	1.45	1.41
10	BT	101	V7N	C7-C8	2.24	1.40	1.34
10	BP	102	V7N	C11-C12	2.24	1.40	1.34
12	BB	103	LMT	O4'-C4B	-2.24	1.37	1.43
12	Ad	102	LMT	O2B-C2B	-2.24	1.37	1.43
10	BC	103	V7N	C19-C18	-2.23	1.41	1.45
11	Bm	103	BCL	C3D-C4D	-2.23	1.39	1.44
12	AX	1201	LMT	O2B-C2B	-2.23	1.37	1.43
10	An	101	V7N	C11-C12	2.23	1.40	1.34
11	AK	101	BCL	C3D-C4D	-2.23	1.39	1.44
11	AM	102	BCL	CBD-CGD	-2.23	1.45	1.52
11	Ao	101	BCL	MG-NA	-2.23	2.01	2.06
12	BA	105	LMT	O2'-C2'	-2.23	1.37	1.43
12	BF	102	LMT	O3B-C3B	-2.23	1.37	1.43
10	Be	1103	V7N	C8-C9	-2.22	1.41	1.45
15	Af	102	CD4	O10-C31	2.22	1.53	1.44
11	AR	101	BCL	CHD-C1D	2.22	1.42	1.38
11	L	301	BCL	O1A-CGA	-2.22	1.15	1.22
11	Bl	1203	BCL	CHD-C1D	2.22	1.42	1.38
10	BV	101	V7N	C8-C9	-2.22	1.41	1.45
11	AP	1102	BCL	CHD-C1D	2.22	1.42	1.38
12	BH	103	LMT	O4'-C4B	-2.22	1.37	1.43
10	BL	101	V7N	C11-C12	2.22	1.40	1.34
12	Bh	1204	LMT	O4'-C4B	-2.22	1.37	1.43
10	BT	101	V7N	C12-C13	-2.21	1.41	1.45
11	AE	1102	BCL	C3D-C4D	-2.21	1.39	1.44
10	Bc	1202	V7N	C11-C12	2.21	1.40	1.34
11	BA	103	BCL	C3D-C4D	-2.21	1.39	1.44
12	BF	102	LMT	O4'-C4B	-2.21	1.37	1.43
11	AO	101	BCL	CHD-C1D	2.21	1.42	1.38
11	Ad	101	BCL	C1D-C2D	-2.21	1.41	1.45
10	BG	101	V7N	C11-C12	2.21	1.40	1.34
12	C	401	LMT	O2B-C2B	-2.21	1.37	1.43
10	BR	103	V7N	C12-C13	-2.21	1.41	1.45
12	BQ	102	LMT	O4'-C4B	-2.21	1.37	1.43
10	AL	102	V7N	C11-C12	2.21	1.40	1.34
11	AM	102	BCL	C3D-C4D	-2.21	1.39	1.44
16	L	303	BPH	C1D-C2D	2.21	1.42	1.39
10	BB	102	V7N	C12-C13	-2.21	1.41	1.45
10	Bh	1202	V7N	C11-C12	2.21	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	BW	102	V7N	C11-C12	2.21	1.40	1.34
11	Bg	103	BCL	C3D-C4D	-2.21	1.39	1.44
11	AV	1001	BCL	CHD-C1D	2.21	1.42	1.38
11	AI	101	BCL	CHD-C1D	2.20	1.42	1.38
10	Bl	1202	V7N	C12-C13	-2.20	1.41	1.45
11	Bb	1203	BCL	C3D-C4D	-2.20	1.39	1.44
10	BU	104	V7N	C11-C12	2.20	1.40	1.34
10	BF	103	V7N	C12-C13	-2.20	1.41	1.45
11	Be	1105	BCL	C3D-C4D	-2.20	1.39	1.44
12	BL	103	LMT	O4'-C4B	-2.20	1.37	1.43
10	BP	102	V7N	C19-C18	-2.20	1.41	1.45
10	Bm	101	V7N	C7-C8	2.20	1.40	1.34
10	Bl	1202	V7N	C8-C9	-2.20	1.41	1.45
11	Ac	101	BCL	C3D-C4D	-2.20	1.39	1.44
11	L	301	BCL	CHD-C1D	2.20	1.42	1.38
10	BD	103	V7N	C11-C12	2.20	1.40	1.34
10	Bf	1202	V7N	C11-C12	2.20	1.40	1.34
10	Aa	101	V7N	C7-C8	2.19	1.40	1.34
10	AF	101	V7N	C19-C18	-2.19	1.41	1.45
10	Bp	1202	V7N	C7-C8	2.19	1.40	1.34
11	Bp	1203	BCL	C1D-C2D	2.19	1.49	1.45
11	Bp	1203	BCL	CHB-C4A	-2.19	1.32	1.37
11	M	405	BCL	CHD-C1D	2.19	1.42	1.38
11	BF	101	BCL	C3D-C4D	-2.19	1.39	1.44
11	AX	1202	BCL	CHD-C1D	2.19	1.42	1.38
12	BS	102	LMT	O1'-C1'	-2.19	1.36	1.40
10	BI	101	V7N	C11-C12	2.19	1.40	1.34
12	BW	103	LMT	O4'-C4B	-2.19	1.37	1.43
10	AL	102	V7N	C19-C18	-2.19	1.41	1.45
14	L	305	MQ8	C11-C12	-2.19	1.47	1.50
11	AH	101	BCL	CHD-C1D	2.19	1.42	1.38
12	L	304	LMT	O2'-C2'	-2.19	1.37	1.43
12	BO	101	LMT	O3B-C3B	-2.19	1.37	1.43
11	Bg	103	BCL	C3B-C4B	2.19	1.45	1.41
12	BG	103	LMT	O4'-C4B	-2.18	1.37	1.43
12	Bf	1201	LMT	O4'-C4B	-2.18	1.37	1.43
10	BR	103	V7N	C11-C12	2.18	1.40	1.34
11	AT	1102	BCL	CBD-CGD	-2.18	1.45	1.52
12	Aj	102	LMT	O2'-C2'	-2.18	1.37	1.43
10	BL	101	V7N	C8-C9	-2.18	1.41	1.45
12	C	401	LMT	O4'-C4B	-2.18	1.37	1.43
10	BO	102	V7N	C12-C13	-2.18	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	Aj	101	BCL	CHD-C1D	2.18	1.42	1.38
11	AT	1102	BCL	C3D-C4D	-2.18	1.39	1.44
11	BO	103	BCL	C3D-C4D	-2.18	1.39	1.44
11	M	405	BCL	C3D-C4D	-2.18	1.39	1.44
11	Ao	101	BCL	CHB-C4A	-2.18	1.32	1.37
10	Bl	1202	V7N	C7-C8	2.18	1.40	1.34
11	AI	101	BCL	C3D-C4D	-2.17	1.39	1.44
10	BA	102	V7N	C11-C12	2.17	1.40	1.34
11	AS	1102	BCL	C1D-C2D	-2.17	1.41	1.45
11	BI	102	BCL	C3D-C4D	-2.17	1.39	1.44
10	Bk	101	V7N	C19-C18	-2.17	1.41	1.45
12	Ba	1102	LMT	O4'-C4B	-2.17	1.37	1.43
11	AJ	1103	BCL	CBD-CGD	-2.17	1.45	1.52
10	BO	102	V7N	C19-C18	-2.17	1.41	1.45
12	BD	102	LMT	O4'-C4B	-2.17	1.37	1.43
11	AO	101	BCL	C3D-C4D	-2.17	1.39	1.44
11	Bc	1204	BCL	C3D-C4D	-2.17	1.39	1.44
12	BU	101	LMT	O4'-C4B	-2.17	1.37	1.43
10	AF	101	V7N	C8-C9	-2.17	1.41	1.45
10	AF	101	V7N	C11-C12	2.17	1.40	1.34
12	BK	103	LMT	O1'-C1'	-2.17	1.36	1.40
10	BG	101	V7N	C8-C9	-2.17	1.41	1.45
12	Bl	1201	LMT	O4'-C4B	-2.17	1.37	1.43
12	BR	102	LMT	O4'-C4B	-2.17	1.37	1.43
10	BN	102	V7N	C11-C12	2.17	1.40	1.34
11	BC	101	BCL	C1D-C2D	-2.17	1.41	1.45
11	Bh	1205	BCL	C3D-C4D	-2.17	1.39	1.44
10	BU	104	V7N	C19-C18	-2.17	1.41	1.45
11	Aj	101	BCL	C1D-C2D	-2.16	1.41	1.45
11	Ah	101	BCL	C1D-C2D	-2.16	1.41	1.45
12	BQ	101	LMT	O4'-C4B	-2.16	1.37	1.43
10	BL	101	V7N	C7-C8	2.16	1.40	1.34
10	BX	101	V7N	C11-C12	2.16	1.40	1.34
11	AK	101	BCL	CHD-C1D	2.16	1.42	1.38
10	BJ	101	V7N	C11-C12	2.16	1.40	1.34
12	Aj	102	LMT	O4'-C4B	-2.16	1.37	1.43
10	Bb	1202	V7N	C8-C9	-2.16	1.41	1.45
12	AX	1201	LMT	O4'-C4B	-2.16	1.37	1.43
10	BK	104	V7N	C11-C12	2.16	1.40	1.34
12	Bb	1201	LMT	O4'-C4B	-2.16	1.37	1.43
10	BK	104	V7N	C19-C18	-2.16	1.41	1.45
12	BK	103	LMT	O4'-C4B	-2.16	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	AE	1102	BCL	CHD-C1D	2.16	1.42	1.38
12	BA	104	LMT	O4'-C4B	-2.16	1.37	1.43
11	Ao	101	BCL	C1D-C2D	2.16	1.49	1.45
11	AW	1203	BCL	CHD-C1D	2.16	1.42	1.38
12	Bc	1201	LMT	O4'-C4B	-2.16	1.37	1.43
10	BF	103	V7N	C7-C8	2.16	1.40	1.34
10	Bj	1202	V7N	C8-C9	-2.16	1.41	1.45
10	BO	102	V7N	C7-C8	2.16	1.40	1.34
10	BQ	103	V7N	C7-C8	2.16	1.40	1.34
11	Bf	1204	BCL	C3D-C4D	-2.15	1.39	1.44
12	BE	102	LMT	O4'-C4B	-2.15	1.37	1.43
12	AW	1201	LMT	O4'-C4B	-2.15	1.37	1.43
11	L	302	BCL	C3D-C4D	-2.15	1.39	1.44
12	BK	101	LMT	O4'-C4B	-2.15	1.37	1.43
12	BW	101	LMT	O4'-C4B	-2.15	1.37	1.43
11	Bn	103	BCL	C3D-C4D	-2.15	1.39	1.44
10	Bj	1202	V7N	C7-C8	2.15	1.40	1.34
11	AM	101	BCL	C3D-C4D	-2.15	1.39	1.44
10	BF	103	V7N	C8-C9	-2.15	1.41	1.45
11	Bj	1204	BCL	C1D-C2D	-2.15	1.41	1.45
11	BB	101	BCL	C3D-C4D	-2.15	1.39	1.44
11	BP	101	BCL	C3D-C4D	-2.15	1.39	1.44
12	Ad	102	LMT	O4'-C4B	-2.15	1.37	1.43
10	BW	102	V7N	C8-C9	-2.15	1.41	1.45
11	Am	101	BCL	C1B-C2B	2.15	1.48	1.43
10	BG	101	V7N	C7-C8	2.14	1.40	1.34
10	Bm	101	V7N	C12-C13	-2.14	1.41	1.45
12	BK	101	LMT	O2'-C2'	-2.14	1.37	1.43
11	AD	1102	BCL	C3D-C4D	-2.14	1.39	1.44
10	BV	101	V7N	C11-C12	2.14	1.40	1.34
11	BL	102	BCL	C3D-C4D	-2.14	1.39	1.44
11	AQ	101	BCL	C3D-C4D	-2.14	1.39	1.44
11	BN	101	BCL	C3D-C4D	-2.14	1.39	1.44
12	BO	101	LMT	O1'-C1'	-2.14	1.36	1.40
10	Bh	1202	V7N	C19-C18	-2.14	1.41	1.45
11	Bo	1202	BCL	C3D-C4D	-2.14	1.39	1.44
11	Ai	101	BCL	C3D-C4D	-2.14	1.39	1.44
11	Bj	1204	BCL	CHD-C1D	2.14	1.42	1.38
10	BQ	103	V7N	C12-C13	-2.14	1.41	1.45
12	BI	103	LMT	O1'-C1'	-2.14	1.36	1.40
10	Bc	1202	V7N	C19-C18	-2.14	1.41	1.45
12	M	401	LMT	O4'-C4B	-2.14	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	AW	1202	BCL	CHD-C1D	2.14	1.42	1.38
10	Bb	1202	V7N	C11-C12	2.14	1.40	1.34
12	BU	103	LMT	O4'-C4B	-2.14	1.37	1.43
11	BA	103	BCL	CHD-C1D	2.14	1.42	1.38
10	Bb	1202	V7N	C19-C18	-2.14	1.41	1.45
10	Bi	101	V7N	C12-C13	-2.14	1.41	1.45
11	Bj	1204	BCL	C3D-C4D	-2.13	1.39	1.44
11	BE	101	BCL	C3D-C4D	-2.13	1.39	1.44
12	Bp	1201	LMT	O4'-C4B	-2.13	1.37	1.43
12	BI	103	LMT	O4'-C4B	-2.13	1.37	1.43
12	Aa	103	LMT	O4'-C4B	-2.13	1.38	1.43
10	BI	101	V7N	C19-C18	-2.13	1.41	1.45
10	BF	103	V7N	C19-C18	-2.13	1.41	1.45
12	BC	102	LMT	O4'-C4B	-2.13	1.38	1.43
10	Bg	101	V7N	C19-C18	-2.13	1.41	1.45
10	BS	103	V7N	C19-C18	-2.13	1.41	1.45
11	BX	102	BCL	C3D-C4D	-2.13	1.39	1.44
11	AQ	102	BCL	C1D-C2D	-2.13	1.41	1.45
10	Aa	101	V7N	C8-C9	-2.13	1.41	1.45
10	BX	101	V7N	C19-C18	-2.13	1.41	1.45
11	AT	1102	BCL	C1D-C2D	-2.13	1.41	1.45
10	BR	103	V7N	C8-C9	-2.13	1.41	1.45
10	BN	102	V7N	C19-C18	-2.13	1.41	1.45
11	Aa	102	BCL	CHD-C1D	2.13	1.42	1.38
11	AJ	1103	BCL	C3D-C4D	-2.13	1.39	1.44
11	Bl	1203	BCL	C3D-C4D	-2.13	1.39	1.44
12	Bf	1201	LMT	O1'-C1'	-2.12	1.36	1.40
11	AW	1202	BCL	C1D-C2D	-2.12	1.41	1.45
11	AP	1102	BCL	C3D-C4D	-2.12	1.39	1.44
11	BS	101	BCL	C3D-C4D	-2.12	1.39	1.44
11	AI	102	BCL	C3D-C4D	-2.12	1.39	1.44
10	Bb	1202	V7N	C7-C8	2.12	1.40	1.34
10	Bg	101	V7N	C7-C8	2.12	1.40	1.34
12	BH	101	LMT	O4'-C4B	-2.12	1.38	1.43
11	Ak	101	BCL	C3D-C4D	-2.12	1.39	1.44
11	AQ	103	BCL	C3D-C4D	-2.12	1.39	1.44
11	BC	101	BCL	C3D-C4D	-2.12	1.39	1.44
12	BB	103	LMT	O1'-C1'	-2.12	1.36	1.40
10	BC	103	V7N	C11-C12	2.12	1.40	1.34
12	BA	105	LMT	O1'-C1'	-2.12	1.36	1.40
10	BB	102	V7N	C8-C9	-2.12	1.41	1.45
11	BS	101	BCL	C1D-C2D	-2.12	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	AT	1103	BCL	C3D-C4D	-2.12	1.39	1.44
10	Bf	1202	V7N	C19-C18	-2.12	1.41	1.45
11	Bp	1204	BCL	C3D-C4D	-2.12	1.39	1.44
12	BM	1001	LMT	O4'-C4B	-2.11	1.38	1.43
11	AQ	103	BCL	C1D-C2D	-2.11	1.41	1.45
11	BR	101	BCL	C3D-C4D	-2.11	1.39	1.44
11	Ai	101	BCL	CHD-C1D	2.11	1.42	1.38
11	BV	102	BCL	C3D-C4D	-2.11	1.39	1.44
11	Ah	101	BCL	C3D-C4D	-2.11	1.39	1.44
12	Bh	1201	LMT	O4'-C4B	-2.11	1.38	1.43
11	AR	101	BCL	C3D-C4D	-2.11	1.39	1.44
11	BA	101	BCL	C1D-C2D	-2.11	1.41	1.45
11	BG	102	BCL	C3D-C4D	-2.11	1.39	1.44
11	AH	101	BCL	C3D-C4D	-2.11	1.39	1.44
11	Bi	102	BCL	C3D-C4D	-2.11	1.39	1.44
11	AM	101	BCL	CHD-C1D	2.11	1.42	1.38
10	BB	102	V7N	C7-C8	2.11	1.40	1.34
10	BN	102	V7N	C7-C8	2.11	1.40	1.34
11	BE	101	BCL	CHD-C1D	2.11	1.42	1.38
12	Bj	1201	LMT	O4'-C4B	-2.11	1.38	1.43
10	BX	101	V7N	C7-C8	2.11	1.40	1.34
11	Aj	101	BCL	C3D-C4D	-2.11	1.39	1.44
10	Aa	101	V7N	C12-C13	-2.11	1.41	1.45
11	BO	103	BCL	C1D-C2D	-2.11	1.41	1.45
12	Bj	1203	LMT	O4'-C4B	-2.11	1.38	1.43
11	L	302	BCL	O1A-CGA	-2.11	1.16	1.22
10	BO	102	V7N	C8-C9	-2.11	1.41	1.45
12	Bc	1201	LMT	O1'-C1'	-2.11	1.36	1.40
11	BU	102	BCL	C3D-C4D	-2.11	1.39	1.44
10	Be	1103	V7N	C7-C8	2.11	1.40	1.34
12	BO	101	LMT	O4'-C4B	-2.10	1.38	1.43
10	BD	103	V7N	C19-C18	-2.10	1.41	1.45
12	Bd	1201	LMT	O4'-C4B	-2.10	1.38	1.43
11	BK	102	BCL	C3D-C4D	-2.10	1.39	1.44
11	Ak	101	BCL	CHD-C1D	2.10	1.42	1.38
11	M	404	BCL	C3D-C4D	-2.10	1.39	1.44
11	Aa	102	BCL	C3D-C4D	-2.10	1.39	1.44
11	Ah	101	BCL	CHD-C1D	2.10	1.42	1.38
11	AQ	102	BCL	CBD-CGD	-2.10	1.45	1.52
12	Ad	102	LMT	O1'-C1'	-2.10	1.36	1.40
12	BS	102	LMT	O4'-C4B	-2.10	1.38	1.43
11	AI	102	BCL	CHD-C1D	2.10	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	Bm	101	V7N	C8-C9	-2.10	1.41	1.45
11	BA	101	BCL	CHD-C1D	2.10	1.42	1.38
10	BW	102	V7N	C7-C8	2.10	1.40	1.34
11	AU	1001	BCL	C3D-C4D	-2.10	1.39	1.44
10	BT	101	V7N	C8-C9	-2.10	1.41	1.45
11	M	404	BCL	O1A-CGA	-2.10	1.16	1.22
10	BW	102	V7N	C19-C18	-2.09	1.41	1.45
11	BL	102	BCL	C1D-C2D	-2.09	1.41	1.45
11	AG	101	BCL	C3D-C4D	-2.09	1.39	1.44
11	BD	101	BCL	C3D-C4D	-2.09	1.39	1.44
10	BA	102	V7N	C19-C18	-2.09	1.41	1.45
10	BL	101	V7N	C19-C18	-2.09	1.41	1.45
11	Ac	101	BCL	CHD-C1D	2.09	1.42	1.38
10	BB	102	V7N	C19-C18	-2.09	1.41	1.45
11	M	405	BCL	O1A-CGA	-2.09	1.16	1.22
11	Af	101	BCL	C3D-C4D	-2.08	1.39	1.44
11	AF	102	BCL	C3D-C4D	-2.08	1.39	1.44
12	AW	1201	LMT	O1'-C1'	-2.08	1.36	1.40
11	L	301	BCL	C3D-C4D	-2.08	1.39	1.44
11	Bp	1203	BCL	MG-NA	-2.08	2.01	2.06
11	BI	102	BCL	C1D-C2D	-2.08	1.41	1.45
11	Ae	101	BCL	C3D-C4D	-2.08	1.39	1.44
10	Bd	1202	V7N	C11-C12	2.08	1.39	1.34
11	AW	1204	BCL	C3D-C4D	-2.08	1.39	1.44
10	An	101	V7N	C7-C8	2.08	1.39	1.34
10	BS	103	V7N	C7-C8	2.08	1.39	1.34
11	AU	1001	BCL	CHD-C1D	2.08	1.42	1.38
11	AV	1001	BCL	C3D-C4D	-2.08	1.39	1.44
11	Ad	101	BCL	CHD-C1D	2.08	1.42	1.38
10	AF	101	V7N	C7-C8	2.08	1.39	1.34
10	Bh	1202	V7N	C7-C8	2.07	1.39	1.34
12	BM	1001	LMT	O1'-C1'	-2.07	1.36	1.40
11	M	405	BCL	C3B-C4B	2.07	1.44	1.41
12	K	201	LMT	O4'-C4B	-2.07	1.38	1.43
10	Bd	1202	V7N	C19-C18	-2.07	1.41	1.45
12	BU	103	LMT	O2'-C2'	-2.07	1.38	1.43
10	BR	103	V7N	C19-C18	-2.07	1.41	1.45
10	BH	102	V7N	C11-C12	2.07	1.39	1.34
11	Ae	101	BCL	CHD-C1D	2.07	1.42	1.38
11	AC	101	BCL	C3D-C4D	-2.07	1.39	1.44
10	Bc	1202	V7N	C7-C8	2.06	1.39	1.34
12	Bp	1201	LMT	O1'-C1'	-2.06	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	Ae	101	BCL	O1A-CGA	-2.06	1.16	1.22
11	AT	1103	BCL	CHD-C1D	2.06	1.42	1.38
12	BC	102	LMT	O2B-C2B	-2.06	1.38	1.43
12	Bo	1201	LMT	O4'-C4B	-2.06	1.38	1.43
11	Bd	1203	BCL	C3D-C4D	-2.06	1.39	1.44
11	AN	101	BCL	C3D-C4D	-2.06	1.39	1.44
10	Bn	101	V7N	C19-C18	-2.06	1.41	1.45
11	AJ	1102	BCL	C3D-C4D	-2.06	1.39	1.44
11	Al	101	BCL	C1D-C2D	2.05	1.49	1.45
10	BV	101	V7N	C7-C8	2.05	1.39	1.34
10	Bj	1202	V7N	C19-C18	-2.05	1.41	1.45
11	Bb	1203	BCL	CHD-C1D	2.05	1.42	1.38
11	AX	1202	BCL	C3D-C4D	-2.05	1.39	1.44
11	Al	101	BCL	C1B-C2B	2.05	1.48	1.43
12	BW	101	LMT	O1'-C1'	-2.05	1.36	1.40
11	AQ	102	BCL	O1A-CGA	-2.05	1.16	1.22
11	AL	101	BCL	C3D-C4D	-2.05	1.39	1.44
11	AC	101	BCL	C1D-C2D	-2.05	1.41	1.45
11	Bb	1203	BCL	C1D-C2D	-2.05	1.41	1.45
11	AS	1102	BCL	C3D-C4D	-2.05	1.39	1.44
10	BG	101	V7N	C19-C18	-2.05	1.41	1.45
11	AC	101	BCL	CHD-C1D	2.05	1.42	1.38
11	Bf	1204	BCL	C1D-C2D	-2.05	1.41	1.45
12	BF	102	LMT	O1'-C1'	-2.04	1.36	1.40
12	L	304	LMT	O4'-C4B	-2.04	1.38	1.43
11	AQ	103	BCL	CHD-C1D	2.04	1.42	1.38
12	BO	104	LMT	O4'-C4B	-2.04	1.38	1.43
11	Bo	1202	BCL	C1D-C2D	-2.04	1.41	1.45
11	Ab	101	BCL	CHD-C1D	2.04	1.42	1.38
11	AW	1203	BCL	C3D-C4D	-2.04	1.39	1.44
10	BU	104	V7N	C7-C8	2.04	1.39	1.34
11	Bi	102	BCL	C1D-C2D	-2.04	1.41	1.45
11	Ao	101	BCL	C1B-C2B	2.04	1.48	1.43
11	Bc	1204	BCL	C1D-C2D	-2.04	1.41	1.45
10	BA	102	V7N	C7-C8	2.04	1.39	1.34
12	BA	105	LMT	O4'-C4B	-2.04	1.38	1.43
11	Ab	101	BCL	C3D-C4D	-2.04	1.39	1.44
11	Ad	101	BCL	C3D-C4D	-2.04	1.39	1.44
11	BL	102	BCL	CHD-C1D	2.03	1.42	1.38
11	BB	101	BCL	C3B-C4B	2.03	1.44	1.41
10	BI	101	V7N	C7-C8	2.03	1.39	1.34
11	AV	1001	BCL	O1A-CGA	-2.03	1.16	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	Aa	101	V7N	C19-C18	-2.03	1.41	1.45
11	Af	101	BCL	C1D-C2D	-2.03	1.41	1.45
11	Aa	102	BCL	C5-C3	2.03	1.55	1.51
11	BA	103	BCL	C1D-C2D	-2.03	1.41	1.45
11	AB	101	BCL	C3D-C4D	-2.03	1.39	1.44
11	AM	102	BCL	CHD-C1D	2.03	1.42	1.38
11	Bk	103	BCL	C1D-C2D	-2.03	1.41	1.45
11	Ae	101	BCL	C1D-C2D	-2.03	1.41	1.45
11	BG	102	BCL	CHD-C1D	2.03	1.42	1.38
10	BR	103	V7N	C7-C8	2.03	1.39	1.34
11	Bl	1203	BCL	C1D-C2D	-2.02	1.41	1.45
11	AQ	101	BCL	CHD-C1D	2.02	1.42	1.38
11	AW	1204	BCL	C1D-C2D	-2.02	1.41	1.45
11	AT	1102	BCL	CHD-C1D	2.02	1.42	1.38
12	BG	103	LMT	O1'-C1'	-2.02	1.36	1.40
10	Bl	1202	V7N	C19-C18	-2.02	1.41	1.45
10	BQ	103	V7N	C19-C18	-2.02	1.41	1.45
11	AW	1202	BCL	C3D-C4D	-2.02	1.39	1.44
10	BP	102	V7N	C7-C8	2.02	1.39	1.34
11	BV	102	BCL	CHD-C1D	2.02	1.42	1.38
11	Bg	103	BCL	O1A-CGA	-2.02	1.16	1.22
11	BE	101	BCL	C1D-C2D	-2.02	1.41	1.45
11	BA	101	BCL	C3D-C4D	-2.01	1.39	1.44
14	M	408	MQ8	C11-C12	-2.01	1.47	1.50
12	BW	103	LMT	O1'-C1'	-2.01	1.36	1.40
10	BK	104	V7N	C7-C8	2.01	1.39	1.34
10	Bi	101	V7N	C19-C18	-2.01	1.41	1.45
11	Al	101	BCL	CHC-C1C	-2.01	1.32	1.37
10	Bn	101	V7N	C7-C8	2.01	1.39	1.34
12	Bh	1201	LMT	O1'-C1'	-2.01	1.36	1.40
11	Bd	1203	BCL	C3B-C4B	2.01	1.44	1.41
10	BT	101	V7N	C19-C18	-2.01	1.41	1.45
12	BO	104	LMT	O1'-C1'	-2.01	1.36	1.40
10	Bk	101	V7N	C7-C8	2.00	1.39	1.34
12	Bl	1201	LMT	O1'-C1'	-2.00	1.36	1.40
11	AN	101	BCL	CHD-C1D	2.00	1.42	1.38
12	AX	1201	LMT	O1'-C1'	-2.00	1.36	1.40
11	AG	101	BCL	CHD-C1D	2.00	1.42	1.38
11	AQ	103	BCL	O1A-CGA	-2.00	1.16	1.22
10	BC	103	V7N	C7-C8	2.00	1.39	1.34

All (1474) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	BA	101	BCL	O1D-CGD-CBD	-26.04	71.21	124.48
11	Bk	103	BCL	O2A-CGA-O1A	-25.35	59.61	123.59
11	BA	101	BCL	O2D-CGD-O1D	-24.00	76.91	123.84
11	BA	101	BCL	O2D-CGD-CBD	20.74	148.12	111.27
11	Bk	103	BCL	O2A-CGA-CBA	15.74	161.30	111.91
16	M	406	BPH	C4D-CHA-CBD	-10.98	103.55	108.52
16	L	303	BPH	C4D-CHA-CBD	-10.65	103.70	108.52
11	Bp	1203	BCL	C2B-C1B-NB	9.33	116.49	110.23
11	Ao	101	BCL	C2B-C1B-NB	9.24	116.43	110.23
11	Am	101	BCL	C2B-C1B-NB	9.14	116.36	110.23
11	Bp	1203	BCL	CHD-C1D-ND	-8.80	116.37	124.45
11	Al	101	BCL	CHD-C1D-ND	-8.69	116.47	124.45
11	Al	101	BCL	C2B-C1B-NB	8.51	115.94	110.23
11	Ao	101	BCL	CHD-C1D-ND	-8.46	116.67	124.45
11	Am	101	BCL	CHD-C1D-ND	-8.36	116.77	124.45
11	Ao	101	BCL	CMD-C2D-C1D	7.38	137.72	124.71
11	Bp	1203	BCL	CMD-C2D-C1D	7.35	137.66	124.71
11	Am	101	BCL	CMD-C2D-C1D	7.19	137.38	124.71
11	Al	101	BCL	CMD-C2D-C1D	7.12	137.27	124.71
19	C	404	HEC	C1D-ND-C4D	6.55	111.84	105.07
19	C	403	HEC	C1D-ND-C4D	6.49	111.78	105.07
19	C	405	HEC	C1D-ND-C4D	6.41	111.70	105.07
10	BS	103	V7N	C28-C27-C26	-6.37	108.52	126.42
11	Bp	1203	BCL	O2D-CGD-CBD	6.11	122.13	111.27
11	Al	101	BCL	C2D-C1D-ND	5.89	114.44	110.10
19	C	402	HEC	C1D-ND-C4D	5.83	111.10	105.07
11	Al	101	BCL	O2D-CGD-CBD	5.79	121.56	111.27
11	M	404	BCL	CHD-C1D-ND	-5.75	119.17	124.45
10	BN	102	V7N	C28-C27-C26	-5.70	110.40	126.42
11	Bk	103	BCL	O1A-CGA-CBA	-5.65	101.69	123.73
10	BK	104	V7N	C28-C27-C26	-5.65	110.55	126.42
10	BF	103	V7N	C28-C27-C26	-5.57	110.77	126.42
10	BJ	101	V7N	C28-C27-C26	-5.54	110.85	126.42
11	Bl	1203	BCL	CHD-C1D-ND	-5.53	119.37	124.45
10	Bi	101	V7N	C28-C27-C26	-5.52	110.92	126.42
10	BT	101	V7N	C28-C27-C26	-5.51	110.92	126.42
11	L	302	BCL	CHD-C1D-ND	-5.51	119.39	124.45
11	BP	101	BCL	CHD-C1D-ND	-5.51	119.39	124.45
11	Bj	1204	BCL	CHD-C1D-ND	-5.48	119.42	124.45
10	Bf	1202	V7N	C28-C27-C26	-5.48	111.03	126.42
11	BA	103	BCL	CHD-C1D-ND	-5.47	119.43	124.45
11	BH	104	BCL	CHD-C1D-ND	-5.45	119.44	124.45
11	AR	101	BCL	CHD-C1D-ND	-5.44	119.45	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	BQ	103	V7N	C28-C27-C26	-5.42	111.18	126.42
11	AS	1102	BCL	C4D-CHA-C1A	5.41	127.83	121.25
11	M	405	BCL	C4D-CHA-C1A	5.40	127.83	121.25
11	BK	102	BCL	CHD-C1D-ND	-5.40	119.49	124.45
11	BA	101	BCL	C4D-CHA-C1A	5.40	127.82	121.25
11	BU	102	BCL	CHD-C1D-ND	-5.39	119.50	124.45
10	BO	102	V7N	C28-C27-C26	-5.39	111.29	126.42
11	BN	101	BCL	CHD-C1D-ND	-5.36	119.52	124.45
11	AF	102	BCL	CHD-C1D-ND	-5.35	119.54	124.45
11	BG	102	BCL	CHD-C1D-ND	-5.34	119.55	124.45
11	AS	1102	BCL	CHD-C1D-ND	-5.34	119.55	124.45
10	BR	103	V7N	C28-C27-C26	-5.34	111.43	126.42
10	BU	104	V7N	C28-C27-C26	-5.32	111.46	126.42
11	AQ	103	BCL	CHD-C1D-ND	-5.32	119.56	124.45
10	AL	102	V7N	C28-C27-C26	-5.32	111.47	126.42
11	BD	101	BCL	CHD-C1D-ND	-5.32	119.57	124.45
11	Ao	101	BCL	O2D-CGD-CBD	5.32	120.71	111.27
11	AX	1202	BCL	CHD-C1D-ND	-5.30	119.58	124.45
11	AW	1204	BCL	CHD-C1D-ND	-5.30	119.59	124.45
11	BA	101	BCL	CHD-C1D-ND	-5.29	119.59	124.45
11	AP	1102	BCL	CHD-C1D-ND	-5.29	119.60	124.45
11	Bn	103	BCL	CHD-C1D-ND	-5.28	119.60	124.45
11	AR	101	BCL	C4D-CHA-C1A	5.27	127.66	121.25
11	BL	102	BCL	CHD-C1D-ND	-5.26	119.62	124.45
11	BR	101	BCL	CHD-C1D-ND	-5.26	119.62	124.45
11	AF	102	BCL	C4D-CHA-C1A	5.24	127.63	121.25
11	Bp	1204	BCL	CHD-C1D-ND	-5.24	119.64	124.45
11	BF	101	BCL	CHD-C1D-ND	-5.23	119.64	124.45
10	BV	101	V7N	C28-C27-C26	-5.21	111.78	126.42
11	Bg	103	BCL	CHD-C1D-ND	-5.21	119.67	124.45
11	AM	102	BCL	CHD-C1D-ND	-5.21	119.67	124.45
11	Bl	1203	BCL	C4D-CHA-C1A	5.20	127.58	121.25
10	Bb	1202	V7N	C28-C27-C26	-5.19	111.83	126.42
11	Bg	103	BCL	C4D-CHA-C1A	5.19	127.57	121.25
11	AX	1202	BCL	C4D-CHA-C1A	5.18	127.56	121.25
11	Ah	101	BCL	C4D-CHA-C1A	5.18	127.56	121.25
11	AW	1202	BCL	C4D-CHA-C1A	5.18	127.56	121.25
10	BB	102	V7N	C28-C27-C26	-5.18	111.86	126.42
10	BH	102	V7N	C28-C27-C26	-5.18	111.86	126.42
11	BC	101	BCL	CHD-C1D-ND	-5.18	119.69	124.45
11	Bo	1202	BCL	C4D-CHA-C1A	5.18	127.55	121.25
11	Bd	1203	BCL	CHD-C1D-ND	-5.18	119.70	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	Am	101	BCL	C2D-C1D-ND	5.16	113.91	110.10
11	Aa	102	BCL	C4D-CHA-C1A	5.16	127.53	121.25
11	Bj	1204	BCL	C4D-CHA-C1A	5.16	127.53	121.25
11	AJ	1102	BCL	C4D-CHA-C1A	5.16	127.53	121.25
11	Ae	101	BCL	C4D-CHA-C1A	5.16	127.53	121.25
11	BO	103	BCL	CHD-C1D-ND	-5.16	119.72	124.45
11	BI	102	BCL	C4D-CHA-C1A	5.15	127.52	121.25
11	Bn	103	BCL	C4D-CHA-C1A	5.15	127.52	121.25
11	Bp	1204	BCL	C4D-CHA-C1A	5.15	127.52	121.25
10	Bg	101	V7N	C28-C27-C26	-5.15	111.96	126.42
10	Bd	1202	V7N	C28-C27-C26	-5.15	111.96	126.42
10	Bh	1202	V7N	C28-C27-C26	-5.14	111.97	126.42
11	AE	1102	BCL	C4D-CHA-C1A	5.14	127.50	121.25
11	AQ	101	BCL	C4D-CHA-C1A	5.14	127.50	121.25
11	AQ	102	BCL	CHD-C1D-ND	-5.14	119.73	124.45
11	BA	103	BCL	C4D-CHA-C1A	5.13	127.50	121.25
11	Bf	1204	BCL	C4D-CHA-C1A	5.13	127.50	121.25
11	Al	101	BCL	C3D-C2D-C1D	-5.13	98.83	105.83
11	BV	102	BCL	CHD-C1D-ND	-5.13	119.74	124.45
11	Ad	101	BCL	C4D-CHA-C1A	5.12	127.48	121.25
10	BG	101	V7N	C28-C27-C26	-5.12	112.03	126.42
11	Bo	1202	BCL	CHD-C1D-ND	-5.12	119.75	124.45
11	BH	104	BCL	C4D-CHA-C1A	5.12	127.48	121.25
11	AN	101	BCL	C4D-CHA-C1A	5.12	127.47	121.25
11	BG	102	BCL	C4D-CHA-C1A	5.11	127.47	121.25
11	BN	101	BCL	C4D-CHA-C1A	5.11	127.47	121.25
10	BP	102	V7N	C28-C27-C26	-5.11	112.05	126.42
11	L	302	BCL	C4D-CHA-C1A	5.11	127.47	121.25
11	Be	1105	BCL	CHD-C1D-ND	-5.11	119.76	124.45
11	BK	102	BCL	C4D-CHA-C1A	5.10	127.46	121.25
11	Ab	101	BCL	C4D-CHA-C1A	5.09	127.45	121.25
11	Aa	102	BCL	CHD-C1D-ND	-5.09	119.78	124.45
11	AI	102	BCL	C4D-CHA-C1A	5.09	127.44	121.25
11	Ac	101	BCL	C4D-CHA-C1A	5.09	127.44	121.25
11	BS	101	BCL	CHD-C1D-ND	-5.08	119.78	124.45
11	AQ	101	BCL	CHD-C1D-ND	-5.08	119.78	124.45
11	BD	101	BCL	C4D-CHA-C1A	5.07	127.42	121.25
11	L	301	BCL	CHD-C1D-ND	-5.07	119.79	124.45
11	Bi	102	BCL	C4D-CHA-C1A	5.07	127.42	121.25
11	BO	103	BCL	C4D-CHA-C1A	5.06	127.41	121.25
11	Bd	1203	BCL	C4D-CHA-C1A	5.06	127.41	121.25
11	Be	1105	BCL	C4D-CHA-C1A	5.06	127.40	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	Af	101	BCL	C4D-CHA-C1A	5.06	127.40	121.25
11	BB	101	BCL	C4D-CHA-C1A	5.05	127.40	121.25
11	BF	101	BCL	C4D-CHA-C1A	5.05	127.40	121.25
11	Aj	101	BCL	C4D-CHA-C1A	5.05	127.39	121.25
10	BI	101	V7N	C28-C27-C26	-5.05	112.24	126.42
10	BD	103	V7N	C28-C27-C26	-5.04	112.24	126.42
11	Bc	1204	BCL	CHD-C1D-ND	-5.04	119.82	124.45
11	Bc	1204	BCL	C4D-CHA-C1A	5.04	127.39	121.25
11	BR	101	BCL	C4D-CHA-C1A	5.04	127.39	121.25
11	BX	102	BCL	CHD-C1D-ND	-5.03	119.83	124.45
10	BL	101	V7N	C28-C27-C26	-5.03	112.29	126.42
11	AW	1203	BCL	C4D-CHA-C1A	5.03	127.36	121.25
11	Ai	101	BCL	C4D-CHA-C1A	5.02	127.36	121.25
11	AQ	102	BCL	C4D-CHA-C1A	5.02	127.36	121.25
11	BU	102	BCL	C4D-CHA-C1A	5.02	127.36	121.25
11	AI	101	BCL	C4D-CHA-C1A	5.02	127.36	121.25
11	Ab	101	BCL	CHD-C1D-ND	-5.02	119.84	124.45
11	Al	101	BCL	C3C-C4C-CHD	-5.01	112.68	123.39
10	AF	101	V7N	C28-C27-C26	-5.01	112.33	126.42
11	AB	101	BCL	CHD-C1D-ND	-5.01	119.85	124.45
11	Am	101	BCL	O2D-CGD-CBD	5.01	120.17	111.27
11	BI	102	BCL	CHD-C1D-ND	-5.01	119.85	124.45
11	AC	101	BCL	C4D-CHA-C1A	5.00	127.34	121.25
11	Bk	103	BCL	CHD-C1D-ND	-5.00	119.86	124.45
11	AJ	1102	BCL	CHD-C1D-ND	-5.00	119.86	124.45
11	AV	1001	BCL	C4D-CHA-C1A	5.00	127.33	121.25
11	Bi	102	BCL	CHD-C1D-ND	-4.99	119.86	124.45
11	Bm	103	BCL	C4D-CHA-C1A	4.99	127.33	121.25
11	Al	101	BCL	CHD-C4C-NC	4.99	130.62	125.08
10	Aa	101	V7N	C28-C27-C26	-4.98	112.42	126.42
11	AJ	1103	BCL	CHD-C1D-ND	-4.98	119.88	124.45
11	Bf	1204	BCL	CHD-C1D-ND	-4.98	119.88	124.45
11	Ak	101	BCL	C4D-CHA-C1A	4.98	127.31	121.25
11	M	405	BCL	CHD-C1D-ND	-4.97	119.89	124.45
11	Bk	103	BCL	C4D-CHA-C1A	4.97	127.30	121.25
10	Bp	1202	V7N	C28-C27-C26	-4.96	112.47	126.42
11	M	404	BCL	C4D-CHA-C1A	4.96	127.29	121.25
11	BV	102	BCL	C4D-CHA-C1A	4.96	127.29	121.25
11	BX	102	BCL	C4D-CHA-C1A	4.96	127.29	121.25
11	AW	1203	BCL	CHD-C1D-ND	-4.96	119.90	124.45
11	Ai	101	BCL	CHD-C1D-ND	-4.95	119.90	124.45
11	BE	101	BCL	C4D-CHA-C1A	4.95	127.27	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	AP	1102	BCL	C4D-CHA-C1A	4.95	127.27	121.25
11	Bb	1203	BCL	CHD-C1D-ND	-4.94	119.91	124.45
11	AN	101	BCL	CHD-C1D-ND	-4.94	119.92	124.45
10	Bk	101	V7N	C28-C27-C26	-4.94	112.55	126.42
11	Am	101	BCL	C3D-C2D-C1D	-4.93	99.10	105.83
11	AI	102	BCL	CHD-C1D-ND	-4.93	119.93	124.45
11	AE	1102	BCL	CHD-C1D-ND	-4.92	119.93	124.45
11	BS	101	BCL	C4D-CHA-C1A	4.92	127.23	121.25
11	Bb	1203	BCL	C4D-CHA-C1A	4.91	127.23	121.25
11	AI	101	BCL	CHD-C1D-ND	-4.91	119.94	124.45
10	Bc	1202	V7N	C28-C27-C26	-4.91	112.63	126.42
11	AV	1001	BCL	CHD-C1D-ND	-4.91	119.94	124.45
11	BE	101	BCL	CHD-C1D-ND	-4.89	119.96	124.45
11	AB	101	BCL	C4D-CHA-C1A	4.89	127.20	121.25
11	Ac	101	BCL	CHD-C1D-ND	-4.89	119.96	124.45
11	AK	101	BCL	CHD-C1D-ND	-4.89	119.96	124.45
10	Bj	1202	V7N	C28-C27-C26	-4.88	112.70	126.42
11	AW	1202	BCL	CHD-C1D-ND	-4.88	119.97	124.45
11	BP	101	BCL	C4D-CHA-C1A	4.87	127.18	121.25
11	Af	101	BCL	CHD-C1D-ND	-4.87	119.97	124.45
11	AD	1102	BCL	CHD-C1D-ND	-4.87	119.97	124.45
11	Aj	101	BCL	CHD-C1D-ND	-4.86	119.99	124.45
11	AU	1001	BCL	CHD-C1D-ND	-4.86	119.99	124.45
11	Ad	101	BCL	CHD-C1D-ND	-4.86	119.99	124.45
11	AT	1103	BCL	CHD-C1D-ND	-4.85	119.99	124.45
11	AU	1001	BCL	C4D-CHA-C1A	4.85	127.15	121.25
11	AO	101	BCL	CHD-C1D-ND	-4.84	120.00	124.45
11	AG	101	BCL	CHD-C1D-ND	-4.84	120.00	124.45
11	Ao	101	BCL	C3D-C2D-C1D	-4.84	99.23	105.83
11	BC	101	BCL	C4D-CHA-C1A	4.83	127.13	121.25
11	AL	101	BCL	CHD-C1D-ND	-4.83	120.01	124.45
10	Bm	101	V7N	C28-C27-C26	-4.83	112.85	126.42
10	BA	102	V7N	C28-C27-C26	-4.83	112.86	126.42
11	Bc	1204	BCL	C1-C2-C3	-4.82	117.70	126.04
11	Bh	1205	BCL	CHD-C1D-ND	-4.82	120.02	124.45
11	AL	101	BCL	C4D-CHA-C1A	4.82	127.11	121.25
11	BL	102	BCL	C4D-CHA-C1A	4.81	127.11	121.25
11	AH	101	BCL	CHD-C1D-ND	-4.81	120.03	124.45
11	Ak	101	BCL	CHD-C1D-ND	-4.81	120.03	124.45
11	L	301	BCL	C4D-CHA-C1A	4.81	127.10	121.25
11	BB	101	BCL	CHD-C1D-ND	-4.81	120.04	124.45
11	Ae	101	BCL	CHD-C1D-ND	-4.81	120.04	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	Ao	101	BCL	C2D-C1D-ND	4.80	113.64	110.10
10	BW	102	V7N	C28-C27-C26	-4.80	112.93	126.42
11	Bm	103	BCL	CHD-C1D-ND	-4.79	120.05	124.45
11	Am	101	BCL	C4A-NA-C1A	4.78	108.85	106.71
16	L	303	BPH	C4D-ND-C1D	-4.77	103.98	108.83
16	M	406	BPH	C4D-ND-C1D	-4.76	103.98	108.83
10	An	101	V7N	C28-C27-C26	-4.76	113.04	126.42
11	Bp	1203	BCL	C3D-C2D-C1D	-4.76	99.34	105.83
11	Ah	101	BCL	CHD-C1D-ND	-4.75	120.09	124.45
11	AT	1102	BCL	CHD-C1D-ND	-4.74	120.09	124.45
11	AD	1102	BCL	C4D-CHA-C1A	4.73	127.00	121.25
11	AG	101	BCL	C4D-CHA-C1A	4.72	126.99	121.25
11	AW	1204	BCL	C4D-CHA-C1A	4.71	126.98	121.25
10	BC	103	V7N	C28-C27-C26	-4.71	113.19	126.42
11	Bh	1205	BCL	C4D-CHA-C1A	4.71	126.97	121.25
10	Be	1103	V7N	C28-C27-C26	-4.69	113.24	126.42
11	Bp	1203	BCL	C2D-C1D-ND	4.67	113.55	110.10
11	BR	101	BCL	C1-C2-C3	-4.66	117.98	126.04
11	AQ	103	BCL	C4D-CHA-C1A	4.64	126.90	121.25
11	AM	101	BCL	CHD-C1D-ND	-4.63	120.20	124.45
11	BH	104	BCL	C16-C15-C13	4.62	130.87	115.92
11	AC	101	BCL	CHD-C1D-ND	-4.62	120.20	124.45
11	AH	101	BCL	C4D-CHA-C1A	4.62	126.87	121.25
10	BX	101	V7N	C28-C27-C26	-4.62	113.44	126.42
11	AT	1103	BCL	C4D-CHA-C1A	4.58	126.83	121.25
10	Bn	101	V7N	C28-C27-C26	-4.57	113.57	126.42
11	Am	101	BCL	C3C-C4C-CHD	-4.56	113.65	123.39
11	AK	101	BCL	C4D-CHA-C1A	4.55	126.79	121.25
11	Al	101	BCL	C1D-ND-C4D	-4.55	103.10	106.33
11	AM	101	BCL	C4D-CHA-C1A	4.53	126.77	121.25
11	Am	101	BCL	CHD-C4C-NC	4.49	130.07	125.08
10	Bl	1202	V7N	C28-C27-C26	-4.42	114.00	126.42
11	M	405	BCL	C4A-NA-C1A	4.35	108.66	106.71
11	AJ	1103	BCL	C11-C10-C8	4.30	129.83	115.92
11	AO	101	BCL	C4D-CHA-C1A	4.26	126.44	121.25
11	AX	1202	BCL	C4A-NA-C1A	4.21	108.60	106.71
11	AM	102	BCL	C4D-CHA-C1A	4.20	126.37	121.25
11	BI	102	BCL	C1-C2-C3	-4.20	118.77	126.04
11	AK	101	BCL	C11-C10-C8	4.19	129.47	115.92
11	Bp	1203	BCL	CHD-C4C-NC	4.19	129.73	125.08
11	Ao	101	BCL	C3C-C4C-CHD	-4.17	114.49	123.39
11	AX	1202	BCL	C11-C10-C8	4.16	129.37	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	AJ	1103	BCL	C4D-CHA-C1A	4.15	126.30	121.25
11	Ao	101	BCL	CHD-C4C-NC	4.14	129.68	125.08
11	BA	103	BCL	C1D-ND-C4D	-4.13	103.40	106.33
11	Bj	1204	BCL	C1D-ND-C4D	-4.12	103.41	106.33
11	Bp	1203	BCL	C3C-C4C-CHD	-4.12	114.59	123.39
11	Bm	103	BCL	C1-C2-C3	-4.11	118.94	126.04
11	BB	101	BCL	C16-C15-C13	4.11	129.20	115.92
11	BP	101	BCL	C1-O2A-CGA	4.11	127.22	116.44
11	Bl	1203	BCL	C1D-ND-C4D	-4.08	103.43	106.33
11	L	302	BCL	C1D-ND-C4D	-4.01	103.48	106.33
10	Bn	101	V7N	C29-C28-C27	-4.00	110.72	123.22
11	Bj	1204	BCL	C4A-NA-C1A	3.97	108.49	106.71
11	AU	1001	BCL	C4A-NA-C1A	3.95	108.48	106.71
11	Bh	1205	BCL	C1-C2-C3	-3.95	119.21	126.04
11	AF	102	BCL	C4A-NA-C1A	3.94	108.48	106.71
11	AS	1102	BCL	C1D-ND-C4D	-3.94	103.54	106.33
11	AQ	102	BCL	C4A-NA-C1A	3.91	108.46	106.71
10	BB	102	V7N	C29-C28-C27	-3.89	111.09	123.22
10	BG	101	V7N	C29-C28-C27	-3.84	111.23	123.22
10	BC	103	V7N	C29-C28-C27	-3.83	111.28	123.22
11	BX	102	BCL	C11-C10-C8	3.81	128.22	115.92
11	AW	1202	BCL	C4A-NA-C1A	3.80	108.42	106.71
10	BW	102	V7N	C29-C28-C27	-3.79	111.39	123.22
11	AR	101	BCL	C1D-ND-C4D	-3.78	103.65	106.33
11	AR	101	BCL	C4A-NA-C1A	3.78	108.41	106.71
11	AL	101	BCL	C4A-NA-C1A	3.78	108.41	106.71
10	Bd	1202	V7N	C29-C28-C27	-3.77	111.46	123.22
11	Al	101	BCL	C4A-NA-C1A	3.75	108.39	106.71
10	BL	101	V7N	C29-C28-C27	-3.75	111.51	123.22
11	L	301	BCL	C1D-ND-C4D	-3.75	103.67	106.33
11	AT	1102	BCL	C4D-CHA-C1A	3.75	125.81	121.25
10	BA	102	V7N	C29-C28-C27	-3.74	111.54	123.22
11	Bp	1203	BCL	O2D-CGD-O1D	-3.74	116.53	123.84
10	BK	104	V7N	C29-C28-C27	-3.74	111.55	123.22
11	AO	101	BCL	C4A-NA-C1A	3.74	108.39	106.71
11	AX	1202	BCL	C1D-ND-C4D	-3.74	103.68	106.33
11	Bp	1203	BCL	C1D-ND-C4D	-3.73	103.68	106.33
11	BC	101	BCL	C1-C2-C3	-3.73	119.59	126.04
11	M	404	BCL	C1D-ND-C4D	-3.73	103.69	106.33
11	AM	102	BCL	C4A-NA-C1A	3.72	108.38	106.71
11	AP	1102	BCL	C1D-ND-C4D	-3.72	103.69	106.33
11	Al	101	BCL	O2D-CGD-O1D	-3.72	116.57	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	AT	1102	BCL	C11-C10-C8	-3.69	103.99	115.92
11	Ad	101	BCL	C4A-NA-C1A	3.68	108.36	106.71
11	AM	101	BCL	C4A-NA-C1A	3.68	108.36	106.71
10	Bj	1202	V7N	C29-C28-C27	-3.67	111.78	123.22
10	BI	101	V7N	C29-C28-C27	-3.67	111.78	123.22
11	Ai	101	BCL	C4A-NA-C1A	3.67	108.35	106.71
10	Aa	101	V7N	C29-C28-C27	-3.66	111.78	123.22
10	BJ	101	V7N	C29-C28-C27	-3.65	111.81	123.22
10	BU	104	V7N	C29-C28-C27	-3.65	111.82	123.22
10	Bb	1202	V7N	C29-C28-C27	-3.65	111.83	123.22
10	Bp	1202	V7N	C29-C28-C27	-3.65	111.84	123.22
11	AT	1103	BCL	C4A-NA-C1A	3.64	108.34	106.71
10	BP	102	V7N	C29-C28-C27	-3.64	111.85	123.22
11	AF	102	BCL	C1D-ND-C4D	-3.64	103.75	106.33
11	Ao	101	BCL	C1D-ND-C4D	-3.64	103.75	106.33
11	Am	101	BCL	C1-C2-C3	-3.63	119.76	126.04
10	Bk	101	V7N	C29-C28-C27	-3.63	111.90	123.22
11	AT	1102	BCL	CED-O2D-CGD	3.62	124.14	115.94
11	BA	101	BCL	C1D-ND-C4D	-3.61	103.77	106.33
11	Am	101	BCL	C1C-NC-C4C	-3.61	105.08	106.71
11	Bc	1204	BCL	C4A-NA-C1A	3.59	108.32	106.71
11	Aj	101	BCL	C4A-NA-C1A	3.59	108.32	106.71
11	Am	101	BCL	C1D-ND-C4D	-3.59	103.78	106.33
11	Am	101	BCL	CMB-C2B-C1B	3.59	130.83	125.37
11	BL	102	BCL	C4A-NA-C1A	3.58	108.32	106.71
11	BX	102	BCL	C4A-NA-C1A	3.58	108.32	106.71
11	AQ	102	BCL	C1D-ND-C4D	-3.58	103.79	106.33
10	Bc	1202	V7N	C29-C28-C27	-3.57	112.06	123.22
11	Bd	1203	BCL	C11-C10-C8	3.57	127.47	115.92
10	BH	102	V7N	C29-C28-C27	-3.57	112.09	123.22
11	BC	101	BCL	C11-C10-C8	3.56	127.44	115.92
10	BR	103	V7N	C29-C28-C27	-3.55	112.13	123.22
11	AB	101	BCL	C1D-ND-C4D	-3.55	103.81	106.33
11	AS	1102	BCL	C1-C2-C3	3.55	132.18	126.04
11	AW	1202	BCL	C1D-ND-C4D	-3.55	103.81	106.33
11	AI	102	BCL	C4A-NA-C1A	3.55	108.30	106.71
11	Af	101	BCL	C1D-ND-C4D	-3.55	103.81	106.33
11	AG	101	BCL	C4A-NA-C1A	3.54	108.30	106.71
11	AI	101	BCL	C4A-NA-C1A	3.54	108.30	106.71
11	Bp	1203	BCL	C1-C2-C3	-3.53	119.93	126.04
11	Ac	101	BCL	C4A-NA-C1A	3.53	108.30	106.71
11	Am	101	BCL	O2D-CGD-O1D	-3.53	116.93	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	Ae	101	BCL	C4A-NA-C1A	3.52	108.29	106.71
11	BA	101	BCL	CHA-C1A-NA	-3.52	118.35	126.40
11	BP	101	BCL	C1D-ND-C4D	-3.51	103.84	106.33
11	Bp	1203	BCL	CHC-C4B-NB	-3.50	120.55	124.26
11	AJ	1102	BCL	C4A-NA-C1A	3.50	108.28	106.71
10	Bi	101	V7N	C29-C28-C27	-3.49	112.33	123.22
10	BF	103	V7N	C29-C28-C27	-3.49	112.34	123.22
10	BV	101	V7N	C29-C28-C27	-3.48	112.36	123.22
11	Ao	101	BCL	O2D-CGD-O1D	-3.47	117.05	123.84
12	AX	1201	LMT	O5B-C5B-C4B	3.47	115.99	109.69
10	BI	101	V7N	C7-C6-C5	-3.47	122.36	127.31
11	Af	101	BCL	C4A-NA-C1A	3.47	108.27	106.71
11	AI	102	BCL	C1D-ND-C4D	-3.46	103.87	106.33
11	AM	102	BCL	C1D-ND-C4D	-3.46	103.87	106.33
11	Aj	101	BCL	C1D-ND-C4D	-3.46	103.88	106.33
10	An	101	V7N	C29-C28-C27	-3.46	112.41	123.22
10	Bg	101	V7N	C29-C28-C27	-3.46	112.42	123.22
11	Aa	102	BCL	C1D-ND-C4D	-3.46	103.88	106.33
11	BK	102	BCL	C1D-ND-C4D	-3.45	103.88	106.33
10	AL	102	V7N	C29-C28-C27	-3.45	112.44	123.22
11	AH	101	BCL	C4A-NA-C1A	3.45	108.26	106.71
10	Bf	1202	V7N	C29-C28-C27	-3.45	112.46	123.22
11	AW	1203	BCL	C4A-NA-C1A	3.44	108.25	106.71
11	Ac	101	BCL	C1D-ND-C4D	-3.44	103.89	106.33
11	AV	1001	BCL	C4A-NA-C1A	3.44	108.25	106.71
11	BN	101	BCL	C1D-ND-C4D	-3.43	103.90	106.33
11	BX	102	BCL	C1D-ND-C4D	-3.43	103.90	106.33
10	BX	101	V7N	C29-C28-C27	-3.42	112.53	123.22
11	AK	101	BCL	C1D-ND-C4D	-3.42	103.91	106.33
11	BD	101	BCL	C1D-ND-C4D	-3.42	103.91	106.33
11	Ad	101	BCL	C1D-ND-C4D	-3.41	103.91	106.33
11	Ai	101	BCL	C1D-ND-C4D	-3.41	103.91	106.33
10	Bc	1202	V7N	C35-C13-C14	-3.41	118.15	122.92
11	AC	101	BCL	CHA-C1A-NA	-3.40	118.60	126.40
11	BH	104	BCL	C1D-ND-C4D	-3.40	103.92	106.33
11	BU	102	BCL	C1D-ND-C4D	-3.40	103.92	106.33
11	AJ	1102	BCL	C1D-ND-C4D	-3.40	103.92	106.33
11	BO	103	BCL	C1D-ND-C4D	-3.40	103.92	106.33
11	AW	1203	BCL	C1D-ND-C4D	-3.40	103.92	106.33
11	Ac	101	BCL	C11-C10-C8	3.40	126.89	115.92
11	Al	101	BCL	C3D-C4D-ND	3.40	115.73	110.24
11	AV	1001	BCL	C1D-ND-C4D	-3.39	103.92	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	Ab	101	BCL	C1D-ND-C4D	-3.39	103.92	106.33
11	AE	1102	BCL	C4A-NA-C1A	3.39	108.23	106.71
11	AS	1102	BCL	CHA-C1A-NA	-3.39	118.64	126.40
11	AN	101	BCL	C4A-NA-C1A	3.39	108.23	106.71
12	AX	1201	LMT	C1B-O5B-C5B	3.38	120.33	113.69
11	AI	101	BCL	C1D-ND-C4D	-3.38	103.93	106.33
11	Ah	101	BCL	C1D-ND-C4D	-3.38	103.93	106.33
11	Ae	101	BCL	C1D-ND-C4D	-3.38	103.94	106.33
11	AQ	103	BCL	C1D-ND-C4D	-3.38	103.94	106.33
11	BO	103	BCL	C16-C15-C13	3.38	126.84	115.92
11	Ak	101	BCL	C1D-ND-C4D	-3.38	103.94	106.33
10	BS	103	V7N	C29-C28-C27	-3.37	112.69	123.22
10	BX	101	V7N	O44-C40-O45	-3.37	115.89	123.61
11	Bd	1203	BCL	C1D-ND-C4D	-3.37	103.94	106.33
11	AD	1102	BCL	C1D-ND-C4D	-3.37	103.94	106.33
10	Bc	1202	V7N	C15-C14-C13	-3.37	122.51	127.31
11	AC	101	BCL	C1D-ND-C4D	-3.36	103.94	106.33
11	BC	101	BCL	C1D-ND-C4D	-3.36	103.95	106.33
16	L	303	BPH	C3D-C4D-ND	3.36	112.30	107.72
11	BV	102	BCL	C4A-NA-C1A	3.36	108.22	106.71
11	Bc	1204	BCL	C1D-ND-C4D	-3.35	103.96	106.33
11	Bp	1203	BCL	C3D-C4D-ND	3.34	115.65	110.24
11	BV	102	BCL	C1D-ND-C4D	-3.34	103.96	106.33
11	Ao	101	BCL	CHC-C4B-NB	-3.34	120.72	124.26
11	AD	1102	BCL	C4A-NA-C1A	3.34	108.21	106.71
10	BT	101	V7N	C29-C28-C27	-3.34	112.80	123.22
11	BF	101	BCL	C1D-ND-C4D	-3.34	103.96	106.33
10	Bm	101	V7N	C29-C28-C27	-3.33	112.81	123.22
11	AN	101	BCL	C1D-ND-C4D	-3.33	103.97	106.33
11	Bf	1204	BCL	C1D-ND-C4D	-3.33	103.97	106.33
11	Bp	1204	BCL	C1D-ND-C4D	-3.33	103.97	106.33
10	BD	103	V7N	C29-C28-C27	-3.33	112.82	123.22
11	BP	101	BCL	C4A-NA-C1A	3.33	108.20	106.71
11	AG	101	BCL	C1D-ND-C4D	-3.33	103.97	106.33
11	BR	101	BCL	C1D-ND-C4D	-3.33	103.97	106.33
11	Bn	103	BCL	C1D-ND-C4D	-3.33	103.97	106.33
10	Bm	101	V7N	O44-C40-O45	-3.33	116.00	123.61
11	AM	101	BCL	C1D-ND-C4D	-3.32	103.97	106.33
11	AH	101	BCL	C1D-ND-C4D	-3.32	103.97	106.33
11	AT	1102	BCL	C1D-ND-C4D	-3.32	103.97	106.33
11	AU	1001	BCL	C1D-ND-C4D	-3.32	103.98	106.33
11	Ae	101	BCL	CHA-C1A-NA	-3.32	118.80	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	AK	101	BCL	C4A-NA-C1A	3.32	108.20	106.71
11	Bm	103	BCL	C1D-ND-C4D	-3.31	103.98	106.33
10	BN	102	V7N	C29-C28-C27	-3.31	112.88	123.22
11	AL	101	BCL	C1D-ND-C4D	-3.31	103.98	106.33
11	Bh	1205	BCL	C4A-NA-C1A	3.31	108.19	106.71
11	BG	102	BCL	C1D-ND-C4D	-3.31	103.98	106.33
11	Be	1105	BCL	C1D-ND-C4D	-3.31	103.98	106.33
11	Bi	102	BCL	C1D-ND-C4D	-3.30	103.99	106.33
11	AO	101	BCL	C1D-ND-C4D	-3.30	103.99	106.33
11	Bh	1205	BCL	C1D-ND-C4D	-3.30	103.99	106.33
11	Bo	1202	BCL	C1D-ND-C4D	-3.30	103.99	106.33
10	BW	102	V7N	C7-C6-C5	-3.30	122.60	127.31
11	Ah	101	BCL	C4A-NA-C1A	3.30	108.19	106.71
11	AC	101	BCL	C4A-NA-C1A	3.29	108.19	106.71
10	BO	102	V7N	C29-C28-C27	-3.29	112.95	123.22
11	AQ	101	BCL	C1D-ND-C4D	-3.29	104.00	106.33
10	Be	1103	V7N	C29-C28-C27	-3.29	112.96	123.22
11	Ah	101	BCL	CHA-C1A-NA	-3.29	118.87	126.40
11	AT	1103	BCL	C1D-ND-C4D	-3.29	104.00	106.33
11	Bg	103	BCL	C1D-ND-C4D	-3.28	104.00	106.33
11	Ak	101	BCL	CHA-C1A-NA	-3.28	118.88	126.40
11	Bb	1203	BCL	C1D-ND-C4D	-3.28	104.01	106.33
11	Aa	102	BCL	C4A-NA-C1A	3.27	108.18	106.71
11	M	405	BCL	CHA-C1A-NA	-3.27	118.90	126.40
12	BK	103	LMT	C1'-O5'-C5'	-3.27	107.27	113.69
11	BE	101	BCL	C1D-ND-C4D	-3.27	104.01	106.33
10	Be	1103	V7N	O44-C40-O45	-3.27	116.12	123.61
11	BX	102	BCL	C1-C2-C3	-3.27	120.39	126.04
10	Bh	1202	V7N	C29-C28-C27	-3.27	113.02	123.22
11	AS	1102	BCL	C4A-NA-C1A	3.27	108.17	106.71
16	M	406	BPH	C3D-C4D-ND	3.26	112.17	107.72
11	BL	102	BCL	C1D-ND-C4D	-3.26	104.02	106.33
10	BQ	103	V7N	C29-C28-C27	-3.26	113.05	123.22
11	BI	102	BCL	C1D-ND-C4D	-3.26	104.02	106.33
11	Bo	1202	BCL	CHA-C1A-NA	-3.25	118.95	126.40
11	AP	1102	BCL	C4A-NA-C1A	3.25	108.17	106.71
11	Aj	101	BCL	CHA-C1A-NA	-3.24	118.97	126.40
12	K	201	LMT	C1'-O5'-C5'	-3.24	107.32	113.69
19	C	402	HEC	C4C-NC-C1C	3.24	108.52	105.35
11	Ad	101	BCL	CHA-C1A-NA	-3.24	118.99	126.40
10	AF	101	V7N	O44-C40-O45	-3.23	116.21	123.61
11	Bk	103	BCL	C1D-ND-C4D	-3.23	104.04	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	BS	101	BCL	C1D-ND-C4D	-3.23	104.04	106.33
11	AU	1001	BCL	CHA-C1A-NA	-3.23	119.00	126.40
11	BB	101	BCL	C1D-ND-C4D	-3.23	104.04	106.33
10	Bg	101	V7N	C35-C13-C12	3.22	123.16	118.08
10	Bf	1202	V7N	C7-C6-C5	-3.22	122.71	127.31
11	AJ	1103	BCL	C1D-ND-C4D	-3.22	104.05	106.33
12	BU	101	LMT	C1'-O5'-C5'	-3.22	107.38	113.69
11	Ao	101	BCL	C3D-C4D-ND	3.21	115.44	110.24
10	Bk	101	V7N	C35-C13-C12	3.21	123.14	118.08
11	Aj	101	BCL	C11-C10-C8	3.21	126.29	115.92
11	Al	101	BCL	CMB-C2B-C1B	3.21	130.25	125.37
11	BD	101	BCL	CHA-C1A-NA	-3.20	119.07	126.40
11	Ak	101	BCL	C2A-C1A-CHA	3.20	129.45	123.86
11	Am	101	BCL	CHC-C4B-NB	-3.20	120.87	124.26
19	C	402	HEC	C4B-NB-C1B	3.20	108.38	105.07
11	AG	101	BCL	CHA-C1A-NA	-3.20	119.08	126.40
10	BW	102	V7N	O44-C40-O45	-3.20	116.29	123.61
11	Bm	103	BCL	CHA-C1A-NA	-3.20	119.08	126.40
16	M	406	BPH	OBD-CAD-CBD	-3.20	121.14	125.82
11	AW	1202	BCL	CHA-C1A-NA	-3.19	119.08	126.40
11	BI	102	BCL	CHA-C1A-NA	-3.19	119.09	126.40
10	BS	103	V7N	C35-C13-C14	-3.19	118.45	122.92
10	Aa	101	V7N	C35-C13-C14	-3.19	118.46	122.92
11	AI	102	BCL	CHA-C1A-NA	-3.19	119.10	126.40
12	BW	101	LMT	C1'-O5'-C5'	-3.19	107.44	113.69
11	Al	101	BCL	CHC-C4B-NB	-3.18	120.89	124.26
11	Bi	102	BCL	CHA-C1A-NA	-3.18	119.12	126.40
11	BC	101	BCL	C6-C7-C8	3.18	126.19	115.92
10	BQ	103	V7N	O44-C40-O45	-3.18	116.34	123.61
10	Be	1103	V7N	C7-C6-C5	-3.18	122.78	127.31
10	BH	102	V7N	C35-C13-C12	3.18	123.08	118.08
10	BJ	101	V7N	C35-C13-C12	3.17	123.08	118.08
10	Bg	101	V7N	O44-C40-O45	-3.17	116.35	123.61
11	Bm	103	BCL	C2A-C1A-CHA	3.17	129.40	123.86
10	BR	103	V7N	O44-C40-O45	-3.17	116.36	123.61
11	Bn	103	BCL	CHA-C1A-NA	-3.17	119.15	126.40
10	BJ	101	V7N	O44-C40-O45	-3.17	116.36	123.61
11	BK	102	BCL	CHA-C1A-NA	-3.16	119.15	126.40
11	Ao	101	BCL	C1-C2-C3	-3.16	120.57	126.04
10	An	101	V7N	O44-C40-O45	-3.16	116.37	123.61
10	AF	101	V7N	C35-C13-C12	3.16	123.06	118.08
11	Ac	101	BCL	CHA-C1A-NA	-3.16	119.16	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	Aa	101	V7N	O44-C40-O45	-3.16	116.38	123.61
10	Bj	1202	V7N	O44-C40-O45	-3.16	116.38	123.61
11	Bl	1203	BCL	C4A-NA-C1A	3.16	108.12	106.71
11	AE	1102	BCL	CHA-C1A-NA	-3.16	119.17	126.40
11	BN	101	BCL	CHA-C1A-NA	-3.15	119.17	126.40
11	Be	1105	BCL	C4A-NA-C1A	3.15	108.12	106.71
10	Bh	1202	V7N	O44-C40-O45	-3.15	116.40	123.61
11	BB	101	BCL	CHA-C1A-NA	-3.15	119.18	126.40
11	BS	101	BCL	CHA-C1A-NA	-3.15	119.18	126.40
12	Ad	102	LMT	C1'-O5'-C5'	-3.15	107.51	113.69
10	Bf	1202	V7N	O44-C40-O45	-3.15	116.41	123.61
11	Ae	101	BCL	C1-C2-C3	-3.15	120.60	126.04
11	M	405	BCL	C1D-ND-C4D	-3.14	104.10	106.33
10	BG	101	V7N	O44-C40-O45	-3.14	116.42	123.61
11	AQ	101	BCL	CHA-C1A-NA	-3.14	119.21	126.40
11	AM	101	BCL	CHA-C1A-NA	-3.14	119.21	126.40
11	Bg	103	BCL	CHA-C1A-NA	-3.14	119.22	126.40
11	Ao	101	BCL	CMB-C2B-C1B	3.14	130.14	125.37
11	BA	101	BCL	C17-C16-C15	3.13	127.64	113.24
11	Bd	1203	BCL	CHA-C1A-NA	-3.13	119.22	126.40
11	BA	103	BCL	CHA-C1A-NA	-3.13	119.22	126.40
11	BK	102	BCL	C1-C2-C3	-3.13	120.63	126.04
16	L	303	BPH	OBD-CAD-CBD	-3.13	121.23	125.82
10	BD	103	V7N	O44-C40-O45	-3.13	116.45	123.61
11	Af	101	BCL	CHA-C1A-NA	-3.13	119.23	126.40
10	BC	103	V7N	O44-C40-O45	-3.12	116.46	123.61
11	Bf	1204	BCL	CHA-C1A-NA	-3.12	119.25	126.40
10	Bi	101	V7N	O44-C40-O45	-3.12	116.47	123.61
12	L	304	LMT	C3'-C4'-C5'	-3.12	103.78	110.93
10	BB	102	V7N	O44-C40-O45	-3.12	116.47	123.61
11	Bp	1204	BCL	CHA-C1A-NA	-3.12	119.26	126.40
11	BA	103	BCL	C2A-C1A-CHA	3.12	129.31	123.86
10	BU	104	V7N	O44-C40-O45	-3.12	116.48	123.61
10	BO	102	V7N	O44-C40-O45	-3.11	116.48	123.61
10	Bh	1202	V7N	C35-C13-C12	3.11	122.98	118.08
10	BV	101	V7N	O44-C40-O45	-3.10	116.51	123.61
10	Bb	1202	V7N	O44-C40-O45	-3.10	116.51	123.61
11	L	302	BCL	C4A-NA-C1A	3.10	108.10	106.71
11	AV	1001	BCL	CHA-C1A-NA	-3.10	119.30	126.40
10	Bc	1202	V7N	O44-C40-O45	-3.10	116.52	123.61
10	BG	101	V7N	C36-C18-C19	3.10	122.96	118.08
11	AH	101	BCL	CHA-C1A-NA	-3.10	119.31	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	BH	104	BCL	C4A-NA-C1A	3.10	108.10	106.71
10	BK	104	V7N	C35-C13-C12	3.09	122.95	118.08
11	Ab	101	BCL	CHA-C1A-NA	-3.09	119.31	126.40
11	AT	1103	BCL	CHA-C1A-NA	-3.09	119.32	126.40
11	BX	102	BCL	CHA-C1A-NA	-3.09	119.33	126.40
10	AL	102	V7N	O44-C40-O45	-3.09	116.55	123.61
11	Bl	1203	BCL	CHA-C1A-NA	-3.08	119.34	126.40
11	AW	1203	BCL	CHA-C1A-NA	-3.08	119.34	126.40
10	Bl	1202	V7N	O44-C40-O45	-3.08	116.57	123.61
10	AF	101	V7N	C7-C6-C5	-3.08	122.92	127.31
10	Bp	1202	V7N	O44-C40-O45	-3.07	116.58	123.61
11	BO	103	BCL	CHA-C1A-NA	-3.07	119.36	126.40
11	BF	101	BCL	CHA-C1A-NA	-3.07	119.37	126.40
10	BF	103	V7N	C7-C6-C5	-3.07	122.93	127.31
10	BP	102	V7N	O44-C40-O45	-3.07	116.59	123.61
11	Bk	103	BCL	CHA-C1A-NA	-3.07	119.38	126.40
10	BQ	103	V7N	C36-C18-C19	3.07	122.91	118.08
10	BI	101	V7N	O44-C40-O45	-3.06	116.60	123.61
11	L	301	BCL	C2A-C1A-CHA	3.06	129.22	123.86
10	BV	101	V7N	C7-C6-C5	-3.06	122.94	127.31
11	AN	101	BCL	CHA-C1A-NA	-3.06	119.39	126.40
10	Bd	1202	V7N	O44-C40-O45	-3.06	116.61	123.61
11	AD	1102	BCL	CHA-C1A-NA	-3.06	119.39	126.40
11	AQ	102	BCL	CHA-C1A-NA	-3.06	119.40	126.40
10	BH	102	V7N	O44-C40-O45	-3.05	116.62	123.61
10	BA	102	V7N	C35-C13-C12	3.05	122.89	118.08
10	BC	103	V7N	C35-C13-C12	3.05	122.89	118.08
11	BF	101	BCL	C17-C16-C15	3.05	127.25	113.24
12	BU	103	LMT	C1'-O5'-C5'	-3.05	107.70	113.69
11	Bb	1203	BCL	CHA-C1A-NA	-3.05	119.42	126.40
11	BD	101	BCL	C2A-C1A-CHA	3.05	129.19	123.86
10	Be	1103	V7N	C36-C18-C17	-3.05	118.65	122.92
11	BU	102	BCL	CHA-C1A-NA	-3.05	119.42	126.40
12	BL	103	LMT	C1'-O5'-C5'	-3.05	107.71	113.69
12	BK	101	LMT	C3'-C4'-C5'	-3.05	103.94	110.93
11	BB	101	BCL	C1-C2-C3	3.04	131.31	126.04
11	AL	101	BCL	CHA-C1A-NA	-3.04	119.43	126.40
10	BF	103	V7N	O44-C40-O45	-3.04	116.65	123.61
11	AQ	102	BCL	CAB-C3B-C2B	3.04	132.89	128.34
10	Bd	1202	V7N	C36-C18-C19	3.04	122.86	118.08
10	BJ	101	V7N	C7-C6-C5	-3.04	122.98	127.31
11	Ai	101	BCL	CHA-C1A-NA	-3.03	119.45	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	BO	103	BCL	C4A-NA-C1A	3.03	108.07	106.71
10	BA	102	V7N	O44-C40-O45	-3.03	116.67	123.61
11	L	301	BCL	CHA-C1A-NA	-3.03	119.46	126.40
10	Bl	1202	V7N	C29-C28-C27	-3.03	113.76	123.22
11	AB	101	BCL	CHA-C1A-NA	-3.03	119.46	126.40
10	BO	102	V7N	C35-C13-C12	3.03	122.84	118.08
11	AP	1102	BCL	CHA-C1A-NA	-3.03	119.47	126.40
10	Bp	1202	V7N	C35-C13-C12	3.02	122.83	118.08
10	Bj	1202	V7N	C35-C13-C12	3.02	122.83	118.08
10	BL	101	V7N	O44-C40-O45	-3.02	116.70	123.61
10	Bf	1202	V7N	C35-C13-C12	3.02	122.83	118.08
11	BG	102	BCL	CHA-C1A-NA	-3.02	119.49	126.40
11	Am	101	BCL	C3D-C4D-ND	3.01	115.11	110.24
11	L	302	BCL	CHA-C1A-NA	-3.01	119.51	126.40
11	BB	101	BCL	C4A-NA-C1A	3.01	108.06	106.71
10	Bk	101	V7N	O44-C40-O45	-3.00	116.73	123.61
11	BB	101	BCL	C2A-C1A-CHA	3.00	129.11	123.86
11	AE	1102	BCL	C1D-ND-C4D	-3.00	104.20	106.33
11	AI	101	BCL	CHA-C1A-NA	-3.00	119.53	126.40
11	Am	101	BCL	O2A-CGA-CBA	3.00	121.31	111.91
10	Bd	1202	V7N	C35-C13-C12	2.99	122.79	118.08
10	BU	104	V7N	C35-C13-C12	2.99	122.79	118.08
10	BO	102	V7N	C35-C13-C14	-2.99	118.73	122.92
10	BS	103	V7N	O44-C40-O45	-2.99	116.77	123.61
11	Aa	102	BCL	CHA-C1A-NA	-2.99	119.56	126.40
10	BK	104	V7N	O44-C40-O45	-2.98	116.78	123.61
11	BR	101	BCL	CHA-C1A-NA	-2.98	119.58	126.40
11	Bh	1205	BCL	CHA-C1A-NA	-2.97	119.59	126.40
10	BT	101	V7N	O44-C40-O45	-2.97	116.81	123.61
10	Bf	1202	V7N	C36-C18-C19	2.97	122.75	118.08
11	AW	1204	BCL	C1D-ND-C4D	-2.97	104.23	106.33
10	BV	101	V7N	C35-C13-C12	2.97	122.75	118.08
10	BR	103	V7N	C35-C13-C14	-2.96	118.77	122.92
11	BE	101	BCL	CHA-C1A-NA	-2.96	119.62	126.40
11	BO	103	BCL	C2A-C1A-CHA	2.95	129.02	123.86
11	BH	104	BCL	CHA-C1A-NA	-2.95	119.64	126.40
11	BX	102	BCL	C2A-C1A-CHA	2.95	129.02	123.86
11	AJ	1102	BCL	CHA-C1A-NA	-2.95	119.64	126.40
11	AE	1102	BCL	C2A-C1A-CHA	2.95	129.02	123.86
10	BW	102	V7N	C35-C13-C12	2.95	122.72	118.08
11	AB	101	BCL	C2A-C1A-CHA	2.95	129.01	123.86
10	BI	101	V7N	C35-C13-C12	2.95	122.72	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	BD	103	V7N	C33-C5-C4	2.94	122.72	118.08
11	BV	102	BCL	CHA-C1A-NA	-2.94	119.67	126.40
11	AU	1001	BCL	C2A-C1A-CHA	2.94	129.00	123.86
11	L	302	BCL	C2A-C1A-CHA	2.93	128.99	123.86
11	BN	101	BCL	C2A-C1A-CHA	2.93	128.98	123.86
11	Al	101	BCL	C1C-NC-C4C	-2.93	105.39	106.71
10	Bn	101	V7N	C35-C13-C12	2.92	122.69	118.08
10	AL	102	V7N	C35-C13-C12	2.92	122.69	118.08
11	BC	101	BCL	CHA-C1A-NA	-2.92	119.70	126.40
11	AL	101	BCL	C11-C10-C8	2.92	125.36	115.92
11	M	405	BCL	C2A-C1A-CHA	2.92	128.97	123.86
12	Bb	1201	LMT	C1'-O5'-C5'	-2.91	107.97	113.69
11	AW	1202	BCL	C2A-C1A-CHA	2.91	128.96	123.86
11	AJ	1103	BCL	C4A-NA-C1A	2.91	108.02	106.71
11	AK	101	BCL	CHA-C1A-NA	-2.91	119.73	126.40
11	BA	103	BCL	C1-C2-C3	-2.91	121.01	126.04
11	AI	102	BCL	C2A-C1A-CHA	2.91	128.95	123.86
10	BQ	103	V7N	C35-C13-C12	2.91	122.66	118.08
11	AL	101	BCL	C17-C16-C15	2.90	126.58	113.24
10	BP	102	V7N	C35-C13-C12	2.90	122.65	118.08
11	M	404	BCL	CHA-C1A-NA	-2.90	119.75	126.40
10	BA	102	V7N	C36-C18-C19	2.90	122.64	118.08
11	AF	102	BCL	CHA-C1A-NA	-2.90	119.76	126.40
11	Bj	1204	BCL	CHA-C1A-NA	-2.90	119.76	126.40
10	Bm	101	V7N	C35-C13-C14	-2.90	118.87	122.92
11	AW	1204	BCL	CHA-C1A-NA	-2.90	119.77	126.40
11	M	404	BCL	C2A-C1A-CHA	2.90	128.92	123.86
11	Ad	101	BCL	C2A-C1A-CHA	2.89	128.92	123.86
10	Bl	1202	V7N	C35-C13-C12	2.89	122.63	118.08
11	Bl	1203	BCL	C2A-C1A-CHA	2.89	128.91	123.86
11	AM	102	BCL	CED-O2D-CGD	2.88	122.46	115.94
11	AQ	103	BCL	CHA-C1A-NA	-2.88	119.80	126.40
11	BP	101	BCL	CHA-C1A-NA	-2.88	119.80	126.40
11	Bm	103	BCL	C4A-NA-C1A	2.88	108.00	106.71
11	Bp	1204	BCL	C4A-NA-C1A	2.88	108.00	106.71
11	AQ	101	BCL	C1-C2-C3	-2.88	121.07	126.04
19	C	402	HEC	CAB-C3B-C4B	2.88	128.54	124.81
11	AB	101	BCL	C4A-NA-C1A	2.87	108.00	106.71
10	BB	102	V7N	C7-C6-C5	-2.87	123.21	127.31
11	Bc	1204	BCL	CHA-C1A-NA	-2.87	119.83	126.40
11	AR	101	BCL	CHA-C1A-NA	-2.87	119.83	126.40
11	BA	103	BCL	C4A-NA-C1A	2.86	107.99	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	BL	101	V7N	C35-C13-C14	-2.86	118.91	122.92
11	BL	102	BCL	CAB-C3B-C2B	2.86	132.63	128.34
11	AX	1202	BCL	CHA-C1A-NA	-2.86	119.84	126.40
11	Bp	1203	BCL	C4-C3-C5	2.86	120.08	115.27
10	BG	101	V7N	C35-C13-C14	-2.85	118.93	122.92
11	AJ	1103	BCL	CHA-C1A-NA	-2.85	119.86	126.40
10	An	101	V7N	C35-C13-C12	2.85	122.57	118.08
14	M	408	MQ8	C2M-C2-C3	-2.85	119.75	124.40
10	BR	103	V7N	C35-C13-C12	2.85	122.56	118.08
11	Bn	103	BCL	C16-C15-C13	2.84	125.11	115.92
11	AI	101	BCL	C2A-C1A-CHA	2.84	128.83	123.86
11	BC	101	BCL	C4A-NA-C1A	2.84	107.98	106.71
11	Bd	1203	BCL	C2A-C1A-CHA	2.84	128.82	123.86
10	Bl	1202	V7N	C35-C13-C14	-2.84	118.95	122.92
12	BA	105	LMT	C1'-O5'-C5'	-2.83	108.12	113.69
11	AV	1001	BCL	C2A-C1A-CHA	2.83	128.81	123.86
10	Bn	101	V7N	O44-C40-O45	-2.83	117.12	123.61
11	AW	1202	BCL	C11-C10-C8	2.83	125.07	115.92
11	Aj	101	BCL	C2A-C1A-CHA	2.83	128.81	123.86
10	BP	102	V7N	C7-C6-C5	-2.83	123.27	127.31
12	BD	102	LMT	C1'-O5'-C5'	-2.83	108.13	113.69
10	BN	102	V7N	C35-C13-C12	2.83	122.53	118.08
11	Bp	1203	BCL	C2A-C1A-CHA	-2.83	118.92	123.86
11	AO	101	BCL	CHA-C1A-NA	-2.83	119.93	126.40
11	BB	101	BCL	CAB-C3B-C2B	2.82	132.57	128.34
10	Be	1103	V7N	C35-C13-C14	-2.82	118.97	122.92
11	Be	1105	BCL	CHA-C1A-NA	-2.82	119.94	126.40
10	AF	101	V7N	C35-C13-C14	-2.82	118.97	122.92
11	BH	104	BCL	C11-C10-C8	2.82	125.03	115.92
10	Bi	101	V7N	C35-C13-C14	-2.82	118.97	122.92
10	BD	103	V7N	C35-C13-C12	2.82	122.52	118.08
10	BF	103	V7N	C35-C13-C12	2.82	122.52	118.08
11	AW	1203	BCL	C11-C10-C8	2.82	125.02	115.92
11	Bd	1203	BCL	CAB-C3B-C2B	2.81	132.55	128.34
11	BL	102	BCL	CHA-C1A-NA	-2.81	119.96	126.40
10	Bn	101	V7N	C36-C18-C19	2.81	122.51	118.08
10	Bh	1202	V7N	C36-C18-C19	2.81	122.50	118.08
11	Bf	1204	BCL	C4A-NA-C1A	2.80	107.97	106.71
10	Bi	101	V7N	C35-C13-C12	2.80	122.50	118.08
11	BK	102	BCL	C2A-C1A-CHA	2.80	128.76	123.86
11	Bf	1204	BCL	C2A-C1A-CHA	2.80	128.76	123.86
10	Bb	1202	V7N	C35-C13-C12	2.80	122.49	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	BL	101	V7N	C35-C13-C12	2.80	122.49	118.08
11	AC	101	BCL	C2A-C1A-CHA	2.80	128.75	123.86
12	BO	101	LMT	C1'-O5'-C5'	-2.80	108.20	113.69
11	Bp	1203	BCL	CMB-C2B-C1B	2.79	129.62	125.37
11	Bn	103	BCL	C1-C2-C3	-2.79	121.22	126.04
10	Bp	1202	V7N	C36-C18-C19	2.79	122.47	118.08
11	AN	101	BCL	C2A-C1A-CHA	2.79	128.74	123.86
11	Bh	1205	BCL	C2A-C1A-CHA	2.79	128.73	123.86
10	BF	103	V7N	C35-C13-C14	-2.78	119.02	122.92
11	Bb	1203	BCL	C4A-NA-C1A	2.78	107.96	106.71
11	Bd	1203	BCL	C6-C7-C8	-2.78	106.93	115.92
10	Bb	1202	V7N	C36-C18-C19	2.78	122.45	118.08
11	Bp	1204	BCL	C2A-C1A-CHA	2.77	128.71	123.86
10	Be	1103	V7N	C35-C13-C12	2.77	122.44	118.08
11	BR	101	BCL	C4A-NA-C1A	2.77	107.95	106.71
10	AF	101	V7N	C36-C18-C19	2.77	122.44	118.08
11	BA	101	BCL	C4A-NA-C1A	2.77	107.95	106.71
11	Al	101	BCL	O2A-CGA-CBA	2.77	120.59	111.91
10	Bm	101	V7N	C35-C13-C12	2.77	122.44	118.08
10	BB	102	V7N	C35-C13-C12	2.76	122.43	118.08
10	BX	101	V7N	C33-C5-C4	2.76	122.43	118.08
11	BD	101	BCL	C4A-NA-C1A	2.75	107.94	106.71
11	AW	1203	BCL	C2A-C1A-CHA	2.75	128.67	123.86
11	AP	1102	BCL	C2A-C1A-CHA	2.75	128.67	123.86
10	BJ	101	V7N	C35-C13-C14	-2.75	119.07	122.92
11	Ab	101	BCL	CAB-C3B-C2B	2.75	132.46	128.34
11	Al	101	BCL	CAA-CBA-CGA	-2.74	105.24	113.25
11	Bo	1202	BCL	C2A-C1A-CHA	2.74	128.65	123.86
11	AM	102	BCL	C1-C2-C3	-2.74	121.31	126.04
10	BS	103	V7N	C3-C4-C5	2.74	130.03	125.89
10	AL	102	V7N	C36-C18-C19	2.74	122.39	118.08
11	Ae	101	BCL	C2A-C1A-CHA	2.74	128.65	123.86
11	M	404	BCL	C4A-NA-C1A	2.73	107.94	106.71
11	BG	102	BCL	C4A-NA-C1A	2.73	107.94	106.71
11	AT	1102	BCL	C4A-NA-C1A	2.73	107.93	106.71
12	BQ	101	LMT	C1'-O5'-C5'	-2.73	108.33	113.69
10	BP	102	V7N	C35-C13-C14	-2.73	119.10	122.92
11	AL	101	BCL	C2A-C1A-CHA	2.73	128.63	123.86
11	BS	101	BCL	C2A-C1A-CHA	2.73	128.63	123.86
10	BI	101	V7N	C35-C13-C14	-2.72	119.11	122.92
10	BV	101	V7N	C16-C17-C18	-2.72	123.42	127.31
10	BC	103	V7N	C35-C13-C14	-2.72	119.11	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	Ao	101	BCL	O2A-CGA-CBA	2.72	120.45	111.91
11	Am	101	BCL	CHC-C1C-NC	2.72	128.27	124.51
12	M	401	LMT	C1'-O5'-C5'	-2.72	108.35	113.69
10	An	101	V7N	C7-C6-C5	-2.72	123.43	127.31
10	BN	102	V7N	C35-C13-C14	-2.72	119.12	122.92
11	AJ	1103	BCL	CED-O2D-CGD	2.72	122.08	115.94
11	BK	102	BCL	C4A-NA-C1A	2.71	107.93	106.71
11	BF	101	BCL	C1-C2-C3	-2.71	121.36	126.04
10	BB	102	V7N	C35-C13-C14	-2.71	119.13	122.92
10	BS	103	V7N	C35-C13-C12	2.71	122.34	118.08
11	AO	101	BCL	CED-O2D-CGD	2.71	122.06	115.94
10	Bf	1202	V7N	C35-C13-C14	-2.71	119.13	122.92
11	Ac	101	BCL	C2A-C1A-CHA	2.71	128.59	123.86
12	BI	103	LMT	C1'-O5'-C5'	-2.70	108.38	113.69
11	Bk	103	BCL	C2A-C1A-CHA	2.70	128.58	123.86
11	Al	101	BCL	C4-C3-C5	2.70	119.81	115.27
10	BG	101	V7N	C35-C13-C12	2.70	122.33	118.08
11	AG	101	BCL	C2A-C1A-CHA	2.70	128.58	123.86
11	L	301	BCL	CAB-C3B-C2B	2.70	132.38	128.34
10	Bg	101	V7N	C33-C5-C4	2.69	122.32	118.08
12	BF	102	LMT	C1'-O5'-C5'	-2.69	108.40	113.69
11	AT	1102	BCL	CHA-C1A-NA	-2.69	120.23	126.40
11	AO	101	BCL	CHC-C4B-NB	-2.69	121.41	124.26
11	BF	101	BCL	C2A-C1A-CHA	2.69	128.56	123.86
11	Am	101	BCL	C1D-CHD-C4C	-2.69	120.13	126.62
12	BW	103	LMT	C1'-O5'-C5'	-2.69	108.41	113.69
10	BO	102	V7N	C7-C6-C5	-2.69	123.47	127.31
11	Bg	103	BCL	C2A-C1A-CHA	2.69	128.56	123.86
12	Be	1102	LMT	C1'-O5'-C5'	-2.69	108.41	113.69
11	Al	101	BCL	C1-C2-C3	-2.68	121.40	126.04
10	Bj	1202	V7N	C35-C13-C14	-2.68	119.17	122.92
11	Ah	101	BCL	C2A-C1A-CHA	2.68	128.54	123.86
10	Bk	101	V7N	C35-C13-C14	-2.68	119.17	122.92
11	M	405	BCL	CAB-C3B-C2B	2.68	132.35	128.34
11	AU	1001	BCL	CHC-C4B-NB	-2.68	121.42	124.26
11	AM	102	BCL	CHA-C1A-NA	-2.67	120.27	126.40
10	Aa	101	V7N	C35-C13-C12	2.67	122.29	118.08
11	Bj	1204	BCL	C2A-C1A-CHA	2.67	128.53	123.86
11	BH	104	BCL	C2A-C1A-CHA	2.67	128.53	123.86
10	BT	101	V7N	C35-C13-C12	2.67	122.28	118.08
10	BQ	103	V7N	C36-C18-C17	-2.67	119.18	122.92
11	BP	101	BCL	C2A-C1A-CHA	2.67	128.52	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	Ao	101	BCL	C4-C3-C5	2.67	119.75	115.27
10	BC	103	V7N	C33-C5-C4	2.66	122.27	118.08
11	BE	101	BCL	C11-C10-C8	-2.66	107.31	115.92
11	AW	1202	BCL	C15-C13-C12	-2.66	98.14	112.13
11	AF	102	BCL	C2A-C1A-CHA	2.66	128.51	123.86
11	Ac	101	BCL	CAB-C3B-C2B	2.66	132.32	128.34
11	AQ	103	BCL	C4A-NA-C1A	2.65	107.90	106.71
11	BG	102	BCL	C2A-C1A-CHA	2.65	128.50	123.86
10	BN	102	V7N	C36-C18-C19	2.65	122.25	118.08
11	Bk	103	BCL	C4A-NA-C1A	2.65	107.90	106.71
11	AW	1204	BCL	CAB-C3B-C2B	2.65	132.31	128.34
10	BN	102	V7N	O44-C40-O45	-2.65	117.55	123.61
11	Al	101	BCL	C2A-C1A-CHA	-2.65	119.23	123.86
11	Bc	1204	BCL	C16-C15-C13	2.65	124.47	115.92
10	Bc	1202	V7N	C36-C18-C17	-2.65	119.22	122.92
11	Bd	1203	BCL	C4A-NA-C1A	2.64	107.89	106.71
11	AS	1102	BCL	C2A-C1A-CHA	2.64	128.48	123.86
12	BA	105	LMT	C3'-C4'-C5'	-2.64	104.87	110.93
10	Bh	1202	V7N	C33-C5-C4	2.64	122.24	118.08
11	BI	102	BCL	C2A-C1A-CHA	2.64	128.47	123.86
11	Ae	101	BCL	CAB-C3B-C2B	2.64	132.29	128.34
11	Ai	101	BCL	C2A-C1A-CHA	2.64	128.47	123.86
11	Al	101	BCL	CHC-C1C-NC	2.64	128.16	124.51
11	Bi	102	BCL	C2A-C1A-CHA	2.63	128.47	123.86
11	BI	102	BCL	CAB-C3B-C2B	2.63	132.28	128.34
11	BP	101	BCL	C11-C10-C8	2.63	124.43	115.92
10	BT	101	V7N	C35-C13-C14	-2.63	119.24	122.92
19	C	405	HEC	C4B-NB-C1B	2.63	107.79	105.07
10	BG	101	V7N	C36-C18-C17	-2.63	119.24	122.92
11	Bn	103	BCL	C2A-C1A-CHA	2.63	128.46	123.86
11	L	302	BCL	CHC-C4B-NB	-2.63	121.47	124.26
11	BE	101	BCL	C4A-NA-C1A	2.63	107.89	106.71
11	BK	102	BCL	C11-C10-C8	2.63	124.41	115.92
11	AE	1102	BCL	C6-C5-C3	2.62	120.34	113.45
10	Bc	1202	V7N	C33-C5-C4	2.62	122.21	118.08
11	Aa	102	BCL	C6-C5-C3	2.62	120.33	113.45
11	BU	102	BCL	C2A-C1A-CHA	2.62	128.44	123.86
11	BG	102	BCL	CAB-C3B-C2B	2.62	132.26	128.34
11	AH	101	BCL	C2A-C1A-CHA	2.62	128.44	123.86
11	AX	1202	BCL	C2A-C1A-CHA	2.62	128.43	123.86
19	C	402	HEC	C2A-C1A-NA	-2.61	107.78	110.32
10	BT	101	V7N	C36-C18-C19	2.61	122.20	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	Bk	103	BCL	C16-C15-C13	2.61	124.37	115.92
11	AI	101	BCL	CAB-C3B-C2B	2.61	132.25	128.34
16	M	406	BPH	C2D-C1D-ND	2.61	111.33	109.53
11	BV	102	BCL	C2A-C1A-CHA	2.61	128.42	123.86
11	AD	1102	BCL	C2A-C1A-CHA	2.61	128.42	123.86
11	Ad	101	BCL	CAB-C3B-C2B	2.61	132.25	128.34
11	Bj	1204	BCL	C1C-NC-C4C	2.61	107.88	106.71
10	Bp	1202	V7N	C33-C5-C4	2.61	122.18	118.08
10	Aa	101	V7N	C15-C14-C13	-2.61	123.59	127.31
12	BQ	102	LMT	C1'-O5'-C5'	-2.61	108.57	113.69
11	Am	101	BCL	CHB-C1B-NB	-2.60	121.50	124.26
19	C	403	HEC	C4B-NB-C1B	2.60	107.76	105.07
11	Bp	1203	BCL	CHB-C1B-NB	-2.60	121.50	124.26
11	AQ	101	BCL	C2A-C1A-CHA	2.60	128.41	123.86
11	BF	101	BCL	C4A-NA-C1A	2.60	107.88	106.71
10	BG	101	V7N	C15-C14-C13	-2.60	123.60	127.31
10	BL	101	V7N	C7-C6-C5	-2.60	123.60	127.31
11	AM	101	BCL	C2A-C1A-CHA	2.60	128.40	123.86
10	BH	102	V7N	C33-C5-C4	2.60	122.17	118.08
11	AR	101	BCL	C2A-C1A-CHA	2.60	128.40	123.86
10	An	101	V7N	C33-C5-C6	-2.59	119.29	122.92
10	Bj	1202	V7N	C36-C18-C19	2.59	122.16	118.08
10	Bm	101	V7N	C36-C18-C19	2.59	122.16	118.08
11	L	301	BCL	C4A-NA-C1A	2.59	107.87	106.71
10	Be	1103	V7N	C33-C5-C6	-2.59	119.29	122.92
11	BI	102	BCL	C4A-NA-C1A	2.59	107.87	106.71
10	Bk	101	V7N	C36-C18-C19	2.58	122.15	118.08
19	C	402	HEC	C3B-C4B-NB	-2.58	107.29	110.17
11	AQ	102	BCL	C2A-C1A-CHA	2.58	128.37	123.86
14	Ad	103	MQ8	C2M-C2-C3	-2.58	120.19	124.40
11	BO	103	BCL	CAB-C3B-C2B	2.58	132.20	128.34
10	Bn	101	V7N	C35-C13-C14	-2.58	119.31	122.92
10	An	101	V7N	C36-C18-C19	2.58	122.14	118.08
10	BK	104	V7N	C33-C5-C4	2.57	122.13	118.08
19	C	404	HEC	C2A-C1A-NA	-2.57	107.82	110.32
11	Ab	101	BCL	CHC-C4B-NB	-2.57	121.53	124.26
10	BC	103	V7N	C36-C18-C19	2.57	122.13	118.08
10	BX	101	V7N	C35-C13-C12	2.57	122.13	118.08
11	AT	1103	BCL	C2A-C1A-CHA	2.57	128.35	123.86
11	L	301	BCL	CHC-C4B-NB	-2.57	121.54	124.26
11	Aj	101	BCL	CHC-C4B-NB	-2.57	121.54	124.26
11	AE	1102	BCL	CHC-C4B-NB	-2.57	121.54	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	Ao	101	BCL	CHB-C1B-NB	-2.56	121.54	124.26
10	AF	101	V7N	C29-C28-C27	-2.56	115.22	123.22
11	Al	101	BCL	CHB-C1B-NB	-2.56	121.54	124.26
11	AQ	102	BCL	C4B-C3B-C2B	-2.56	104.25	108.36
11	Bn	103	BCL	CHC-C4B-NB	-2.55	121.55	124.26
11	AL	101	BCL	CHC-C4B-NB	-2.55	121.56	124.26
11	AW	1204	BCL	C4A-NA-C1A	2.55	107.85	106.71
12	Bl	1201	LMT	C1'-O5'-C5'	-2.55	108.68	113.69
10	BA	102	V7N	C33-C5-C4	2.55	122.10	118.08
11	AS	1102	BCL	O2A-C1-C2	-2.55	101.93	108.64
11	Ak	101	BCL	CHC-C4B-NB	-2.55	121.56	124.26
12	BB	103	LMT	C1'-O5'-C5'	-2.55	108.69	113.69
11	Bh	1205	BCL	C11-C10-C8	-2.55	107.68	115.92
19	C	402	HEC	C4A-NA-C1A	2.55	107.84	105.35
11	BC	101	BCL	C2A-C1A-CHA	2.55	128.31	123.86
11	BN	101	BCL	C4A-NA-C1A	2.54	107.85	106.71
11	Aj	101	BCL	CAB-C3B-C2B	2.54	132.15	128.34
11	AJ	1103	BCL	CAB-C3B-C2B	2.54	132.15	128.34
10	AL	102	V7N	C35-C13-C14	-2.54	119.37	122.92
12	C	401	LMT	C1'-O5'-C5'	-2.54	108.71	113.69
19	C	403	HEC	C4C-NC-C1C	2.54	107.83	105.35
11	Bn	103	BCL	C4A-NA-C1A	2.54	107.85	106.71
10	Bn	101	V7N	C33-C5-C4	2.53	122.07	118.08
11	M	404	BCL	C1-C2-C3	-2.53	121.66	126.04
12	BM	1001	LMT	C1'-O5'-C5'	-2.53	108.71	113.69
10	Bl	1202	V7N	C36-C18-C19	2.53	122.07	118.08
11	BU	102	BCL	C4A-NA-C1A	2.53	107.84	106.71
11	AB	101	BCL	CHC-C4B-NB	-2.53	121.58	124.26
11	AK	101	BCL	CHC-C4B-NB	-2.53	121.58	124.26
11	Aa	102	BCL	C2A-C1A-CHA	2.53	128.29	123.86
11	Ac	101	BCL	CHC-C4B-NB	-2.53	121.58	124.26
10	BD	103	V7N	C35-C13-C14	-2.53	119.38	122.92
19	C	402	HEC	CAB-C3B-C2B	-2.53	123.20	127.53
10	Bg	101	V7N	C36-C18-C17	-2.53	119.38	122.92
12	C	401	LMT	C3'-C4'-C5'	-2.53	105.13	110.93
10	BA	102	V7N	C35-C13-C14	-2.53	119.38	122.92
10	Bi	101	V7N	C36-C18-C19	2.53	122.06	118.08
19	C	404	HEC	C4A-NA-C1A	2.53	107.82	105.35
10	Bf	1202	V7N	C33-C5-C6	-2.53	119.39	122.92
10	Bg	101	V7N	C35-C13-C14	-2.53	119.39	122.92
10	BJ	101	V7N	C36-C18-C19	2.52	122.05	118.08
11	AC	101	BCL	CHC-C4B-NB	-2.52	121.58	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	AI	101	BCL	CHC-C4B-NB	-2.52	121.58	124.26
11	Bc	1204	BCL	C2A-C1A-CHA	2.52	128.27	123.86
12	Bh	1201	LMT	C1'-O5'-C5'	-2.52	108.74	113.69
11	BL	102	BCL	C2A-C1A-CHA	2.52	128.26	123.86
19	C	405	HEC	C4C-NC-C1C	2.52	107.81	105.35
11	AJ	1102	BCL	C2A-C1A-CHA	2.52	128.26	123.86
10	BX	101	V7N	C35-C13-C14	-2.52	119.40	122.92
10	BI	101	V7N	C33-C5-C6	-2.52	119.40	122.92
11	BH	104	BCL	CAB-C3B-C2B	2.51	132.11	128.34
11	BK	102	BCL	CAB-C3B-C2B	2.51	132.10	128.34
16	L	303	BPH	CMB-C2B-C3B	2.51	129.37	124.68
11	Bg	103	BCL	C4A-NA-C1A	2.51	107.83	106.71
11	Af	101	BCL	CAB-C3B-C2B	2.51	132.09	128.34
12	BU	103	LMT	C3'-C4'-C5'	-2.51	105.18	110.93
10	Bh	1202	V7N	C35-C13-C14	-2.50	119.42	122.92
10	An	101	V7N	C36-C18-C17	-2.50	119.42	122.92
10	BW	102	V7N	C35-C13-C14	-2.50	119.43	122.92
11	AO	101	BCL	CAB-C3B-C2B	2.50	132.08	128.34
11	Ao	101	BCL	CHC-C1C-NC	2.50	127.96	124.51
10	BU	104	V7N	C33-C5-C4	2.49	122.01	118.08
11	AM	101	BCL	CHC-C4B-NB	-2.49	121.62	124.26
12	Bj	1203	LMT	C3'-C4'-C5'	-2.49	105.21	110.93
11	AK	101	BCL	C2A-C1A-CHA	2.49	128.22	123.86
10	Bc	1202	V7N	C35-C13-C12	2.49	122.00	118.08
11	Bg	103	BCL	C6-C5-C3	2.49	119.98	113.45
11	AI	102	BCL	CHC-C4B-NB	-2.49	121.62	124.26
14	L	305	MQ8	C2M-C2-C3	-2.49	120.34	124.40
10	BV	101	V7N	C35-C13-C14	-2.49	119.44	122.92
11	Ab	101	BCL	C16-C15-C13	2.49	123.96	115.92
11	AT	1102	BCL	C2A-C1A-CHA	2.49	128.21	123.86
11	BK	102	BCL	C17-C16-C15	2.49	124.66	113.24
11	Al	101	BCL	C1D-CHD-C4C	-2.48	120.63	126.62
19	C	402	HEC	CHB-C1B-NB	2.48	127.12	124.42
10	AF	101	V7N	C33-C5-C6	-2.48	119.44	122.92
10	BW	102	V7N	C33-C5-C6	-2.48	119.44	122.92
19	C	403	HEC	C4A-NA-C1A	2.48	107.78	105.35
11	Af	101	BCL	C17-C16-C15	2.48	124.64	113.24
11	AM	102	BCL	C6-C5-C3	2.48	119.96	113.45
11	AD	1102	BCL	CHC-C4B-NB	-2.48	121.63	124.26
10	BV	101	V7N	C33-C5-C6	-2.47	119.46	122.92
10	BD	103	V7N	C36-C18-C19	2.47	121.97	118.08
11	Ae	101	BCL	CHC-C4B-NB	-2.47	121.64	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	Ab	101	BCL	C4A-NA-C1A	2.47	107.82	106.71
10	Bf	1202	V7N	C15-C14-C13	-2.47	123.78	127.31
11	Ak	101	BCL	C4A-NA-C1A	2.47	107.82	106.71
11	AN	101	BCL	CHC-C4B-NB	-2.47	121.64	124.26
11	AQ	101	BCL	CAB-C3B-C2B	2.47	132.04	128.34
11	Af	101	BCL	C2A-C1A-CHA	2.47	128.18	123.86
12	BQ	102	LMT	C3'-C4'-C5'	-2.47	105.27	110.93
10	Bd	1202	V7N	C33-C5-C4	2.47	121.96	118.08
11	AP	1102	BCL	CHC-C4B-NB	-2.47	121.65	124.26
16	L	303	BPH	C2D-C1D-ND	2.47	111.23	109.53
12	Bj	1203	LMT	C1'-O5'-C5'	-2.46	108.85	113.69
11	Ai	101	BCL	CAB-C3B-C2B	2.46	132.03	128.34
11	Bp	1203	BCL	O2A-CGA-CBA	2.46	119.63	111.91
11	BD	101	BCL	C6-C5-C3	2.46	119.91	113.45
10	BR	103	V7N	C36-C18-C19	2.46	121.95	118.08
11	Bp	1204	BCL	C16-C15-C13	2.46	123.87	115.92
11	Bh	1205	BCL	CAB-C3B-C2B	2.46	132.02	128.34
10	BW	102	V7N	C36-C18-C19	2.46	121.95	118.08
11	Af	101	BCL	CHC-C4B-NB	-2.46	121.66	124.26
11	Aa	102	BCL	CHC-C4B-NB	-2.46	121.66	124.26
11	BF	101	BCL	C16-C15-C13	2.46	123.86	115.92
10	BR	103	V7N	C7-C6-C5	-2.45	123.81	127.31
11	AW	1202	BCL	CHC-C4B-NB	-2.45	121.66	124.26
12	BA	104	LMT	C3'-C4'-C5'	-2.45	105.31	110.93
11	Ao	101	BCL	C2A-C1A-CHA	-2.45	119.58	123.86
11	Bk	103	BCL	CHC-C4B-NB	-2.44	121.67	124.26
12	BR	102	LMT	C1'-O5'-C5'	-2.44	108.89	113.69
11	Ai	101	BCL	CHC-C4B-NB	-2.44	121.67	124.26
11	AT	1103	BCL	CHC-C4B-NB	-2.44	121.67	124.26
11	BB	101	BCL	C6-C7-C8	-2.44	108.03	115.92
12	BH	101	LMT	C3'-C4'-C5'	-2.44	105.33	110.93
11	Ae	101	BCL	C17-C16-C15	2.44	124.44	113.24
11	AH	101	BCL	CHC-C4B-NB	-2.44	121.68	124.26
11	Ah	101	BCL	CAB-C3B-C2B	2.44	131.99	128.34
19	C	405	HEC	C4A-NA-C1A	2.44	107.73	105.35
10	Bi	101	V7N	C33-C5-C6	-2.44	119.51	122.92
10	BX	101	V7N	C36-C18-C19	2.43	121.91	118.08
11	AT	1102	BCL	CHC-C4B-NB	-2.43	121.68	124.26
11	AW	1202	BCL	CAB-C3B-C2B	2.43	131.98	128.34
10	BP	102	V7N	C36-C18-C17	-2.43	119.52	122.92
10	AL	102	V7N	C33-C5-C4	2.43	121.90	118.08
12	BH	101	LMT	C1'-O5'-C5'	-2.43	108.92	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	BN	101	BCL	CAB-C3B-C2B	2.43	131.97	128.34
11	AJ	1102	BCL	CHC-C4B-NB	-2.43	121.69	124.26
11	Ah	101	BCL	CHC-C4B-NB	-2.42	121.69	124.26
11	Am	101	BCL	CHB-C4A-NA	2.42	127.86	124.51
11	AO	101	BCL	C2A-C1A-CHA	2.42	128.09	123.86
11	AJ	1103	BCL	C6-C5-C3	2.42	119.81	113.45
11	AQ	101	BCL	C4A-NA-C1A	2.42	107.79	106.71
11	Bp	1203	BCL	CHC-C1C-NC	2.42	127.86	124.51
10	Bd	1202	V7N	C36-C18-C17	-2.42	119.53	122.92
10	BT	101	V7N	C36-C18-C17	-2.42	119.53	122.92
10	BX	101	V7N	O45-C40-C39	2.41	128.49	122.11
11	Ao	101	BCL	C1D-CHD-C4C	-2.41	120.80	126.62
10	BH	102	V7N	C35-C13-C14	-2.41	119.54	122.92
11	AN	101	BCL	CAB-C3B-C2B	2.41	131.96	128.34
11	AU	1001	BCL	CAB-C3B-C2B	2.41	131.95	128.34
10	Bh	1202	V7N	C36-C18-C17	-2.41	119.54	122.92
11	AJ	1103	BCL	C2A-C1A-CHA	2.41	128.08	123.86
11	AT	1102	BCL	CAB-C3B-C2B	2.41	131.95	128.34
10	BR	103	V7N	C36-C18-C17	-2.41	119.55	122.92
10	Bb	1202	V7N	C35-C13-C14	-2.41	119.55	122.92
11	AG	101	BCL	CHC-C4B-NB	-2.41	121.71	124.26
10	Bk	101	V7N	C33-C5-C4	2.40	121.86	118.08
11	BE	101	BCL	CAB-C3B-C2B	2.40	131.94	128.34
10	Bp	1202	V7N	C35-C13-C14	-2.40	119.56	122.92
12	BW	103	LMT	C3'-C4'-C5'	-2.40	105.42	110.93
11	BR	101	BCL	CAB-C3B-C2B	2.40	131.94	128.34
10	Bg	101	V7N	C36-C18-C19	2.40	121.86	118.08
11	Ab	101	BCL	OBB-CAB-CBB	-2.40	114.41	119.73
11	AQ	101	BCL	CHC-C4B-NB	-2.40	121.72	124.26
10	BO	102	V7N	C36-C18-C17	-2.40	119.56	122.92
11	Bn	103	BCL	CAB-C3B-C2B	2.40	131.93	128.34
10	An	101	V7N	C35-C13-C14	-2.40	119.56	122.92
12	BA	104	LMT	C1'-O5'-C5'	-2.40	108.98	113.69
10	Be	1103	V7N	C36-C18-C19	2.40	121.85	118.08
10	BV	101	V7N	C36-C18-C17	-2.40	119.57	122.92
10	Bm	101	V7N	C36-C18-C17	-2.40	119.57	122.92
11	AQ	103	BCL	O2D-CGD-CBD	2.40	115.52	111.27
10	BR	103	V7N	C33-C5-C6	-2.39	119.57	122.92
11	Bb	1203	BCL	CHC-C4B-NB	-2.39	121.72	124.26
11	L	301	BCL	C1C-NC-C4C	2.39	107.78	106.71
11	BA	101	BCL	C2A-C1A-CHA	2.39	128.03	123.86
10	BI	101	V7N	C36-C18-C17	-2.39	119.58	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	BQ	103	V7N	C35-C13-C14	-2.39	119.58	122.92
11	Aa	102	BCL	CAB-C3B-C2B	2.38	131.91	128.34
11	BE	101	BCL	CHC-C4B-NB	-2.38	121.73	124.26
11	Bj	1204	BCL	CHC-C4B-NB	-2.38	121.73	124.26
11	AV	1001	BCL	CHC-C4B-NB	-2.38	121.73	124.26
12	Bh	1204	LMT	C1'-O5'-C5'	-2.38	109.01	113.69
10	BK	104	V7N	C36-C18-C17	-2.38	119.59	122.92
10	BQ	103	V7N	C33-C5-C4	2.38	121.82	118.08
11	BA	101	BCL	CHC-C4B-NB	-2.38	121.74	124.26
11	BS	101	BCL	CAB-C3B-C2B	2.38	131.90	128.34
19	C	404	HEC	CAB-C3B-C4B	-2.37	121.73	124.81
11	Ab	101	BCL	CMB-C2B-C1B	-2.37	121.75	125.37
11	Ab	101	BCL	C2A-C1A-CHA	2.37	128.01	123.86
11	BR	101	BCL	C2A-C1A-CHA	2.37	128.01	123.86
10	BS	103	V7N	C36-C18-C19	2.37	121.82	118.08
11	BU	102	BCL	CAB-C3B-C2B	2.37	131.90	128.34
10	Bc	1202	V7N	C16-C17-C18	-2.37	123.93	127.31
12	BG	103	LMT	C3'-C4'-C5'	-2.37	105.49	110.93
10	Aa	101	V7N	C36-C18-C17	-2.37	119.61	122.92
12	Bj	1201	LMT	C3'-C4'-C5'	-2.37	105.50	110.93
10	BU	104	V7N	C36-C18-C19	2.37	121.80	118.08
11	BD	101	BCL	CAB-C3B-C2B	2.36	131.88	128.34
16	L	303	BPH	OBB-CAB-CBB	-2.36	114.85	120.17
11	BK	102	BCL	CHC-C4B-NB	-2.36	121.76	124.26
11	Bf	1204	BCL	CHC-C4B-NB	-2.36	121.76	124.26
11	BI	102	BCL	CHC-C4B-NB	-2.36	121.76	124.26
16	M	406	BPH	CMD-C2D-C3D	2.36	129.09	124.68
11	Bo	1202	BCL	CHC-C4B-NB	-2.36	121.76	124.26
12	Bc	1201	LMT	C1'-O5'-C5'	-2.36	109.06	113.69
11	BX	102	BCL	CAB-C3B-C2B	2.36	131.87	128.34
19	C	403	HEC	C2A-C1A-NA	-2.36	108.03	110.32
10	BU	104	V7N	C35-C13-C14	-2.35	119.62	122.92
10	Bj	1202	V7N	C36-C18-C17	-2.35	119.63	122.92
11	AW	1203	BCL	CHC-C4B-NB	-2.35	121.77	124.26
11	AI	102	BCL	CAB-C3B-C2B	2.35	131.86	128.34
11	Be	1105	BCL	CAB-C3B-C2B	2.35	131.86	128.34
11	BX	102	BCL	CHC-C4B-NB	-2.35	121.77	124.26
11	AM	102	BCL	CHC-C4B-NB	-2.35	121.77	124.26
12	Ad	102	LMT	C3'-C4'-C5'	-2.35	105.55	110.93
12	Bo	1201	LMT	C3'-C4'-C5'	-2.35	105.55	110.93
19	C	404	HEC	C4C-NC-C1C	2.35	107.64	105.35
10	BO	102	V7N	C33-C5-C6	-2.35	119.64	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	Bj	1204	BCL	CAB-C3B-C2B	2.34	131.85	128.34
11	Ab	101	BCL	C4B-C3B-C2B	-2.34	104.59	108.36
11	Bo	1202	BCL	C4A-NA-C1A	2.34	107.76	106.71
11	Bi	102	BCL	CHC-C4B-NB	-2.34	121.78	124.26
11	BE	101	BCL	C2A-C1A-CHA	2.34	127.96	123.86
11	AH	101	BCL	C6-C5-C3	2.34	119.59	113.45
10	Aa	101	V7N	C36-C18-C19	2.34	121.76	118.08
10	BL	101	V7N	C36-C18-C19	2.34	121.76	118.08
10	Bp	1202	V7N	C36-C18-C17	-2.34	119.65	122.92
10	BH	102	V7N	C36-C18-C19	2.34	121.76	118.08
12	AW	1201	LMT	C3'-C4'-C5'	-2.34	105.57	110.93
12	BK	101	LMT	C1'-O5'-C5'	-2.34	109.10	113.69
10	BL	101	V7N	C36-C18-C17	-2.33	119.65	122.92
10	BN	102	V7N	C33-C5-C4	2.33	121.75	118.08
11	Bj	1204	BCL	C2D-C1D-ND	2.33	111.82	110.10
11	BG	102	BCL	CHC-C4B-NB	-2.33	121.79	124.26
11	AJ	1103	BCL	CHC-C4B-NB	-2.33	121.79	124.26
11	Am	101	BCL	C4-C3-C5	2.32	119.18	115.27
11	Aj	101	BCL	OBB-CAB-CBB	-2.32	114.58	119.73
11	Bd	1203	BCL	C17-C16-C15	2.32	123.92	113.24
12	Bh	1201	LMT	C3B-C4B-C5B	-2.32	106.09	110.24
10	Be	1103	V7N	C16-C17-C18	-2.32	123.99	127.31
11	L	301	BCL	C4B-C3B-C2B	-2.32	104.62	108.36
11	BP	101	BCL	CHC-C4B-NB	-2.32	121.80	124.26
11	BC	101	BCL	CHC-C4B-NB	-2.32	121.80	124.26
11	L	301	BCL	OBB-CAB-CBB	-2.32	114.59	119.73
11	BB	101	BCL	C1-O2A-CGA	2.32	122.53	116.44
11	Be	1105	BCL	CHC-C4B-NB	-2.32	121.80	124.26
11	BC	101	BCL	CAB-C3B-C2B	2.32	131.81	128.34
10	Bn	101	V7N	C36-C18-C17	-2.32	119.68	122.92
11	AS	1102	BCL	CHC-C4B-NB	-2.32	121.81	124.26
10	BC	103	V7N	C15-C14-C13	-2.32	124.01	127.31
11	BI	102	BCL	C1C-NC-C4C	2.31	107.75	106.71
11	Ad	101	BCL	CHC-C4B-NB	-2.31	121.81	124.26
11	Aj	101	BCL	C4B-C3B-C2B	-2.31	104.64	108.36
11	BA	103	BCL	CAB-C3B-C2B	2.31	131.80	128.34
11	BO	103	BCL	CHC-C4B-NB	-2.31	121.81	124.26
12	Ba	1102	LMT	C1'-O5'-C5'	-2.31	109.16	113.69
11	Bb	1203	BCL	C2A-C1A-CHA	2.30	127.89	123.86
11	Bp	1203	BCL	C1D-CHD-C4C	-2.30	121.06	126.62
11	AX	1202	BCL	CHC-C4B-NB	-2.30	121.82	124.26
11	AR	101	BCL	CHC-C4B-NB	-2.30	121.82	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	Aj	101	BCL	CMB-C2B-C1B	-2.30	121.87	125.37
11	AW	1204	BCL	O2D-CGD-CBD	2.30	115.36	111.27
11	Bi	102	BCL	C4A-NA-C1A	2.30	107.74	106.71
11	AO	101	BCL	CMB-C2B-C1B	-2.30	121.87	125.37
11	BU	102	BCL	CHC-C4B-NB	-2.30	121.83	124.26
11	Ae	101	BCL	OBB-CAB-CBB	-2.30	114.64	119.73
12	BD	102	LMT	C3'-C4'-C5'	-2.29	105.67	110.93
11	AT	1103	BCL	O2A-C1-C2	-2.29	102.61	108.64
10	Bl	1202	V7N	C7-C6-C5	-2.29	124.04	127.31
11	Bh	1205	BCL	CHC-C4B-NB	-2.29	121.83	124.26
12	AW	1201	LMT	C1'-O5'-C5'	-2.29	109.19	113.69
11	BD	101	BCL	CHC-C4B-NB	-2.29	121.83	124.26
11	BN	101	BCL	CHC-C4B-NB	-2.29	121.83	124.26
12	BC	102	LMT	C1'-O5'-C5'	-2.29	109.19	113.69
11	L	301	BCL	CMB-C2B-C1B	-2.29	121.88	125.37
13	Bh	1203	PEX	C3-C2-C1	2.29	117.20	111.79
10	BL	101	V7N	C33-C5-C6	-2.29	119.72	122.92
11	BF	101	BCL	CHC-C4B-NB	-2.28	121.84	124.26
12	Bp	1201	LMT	C3B-C4B-C5B	-2.28	106.17	110.24
11	Bc	1204	BCL	CHC-C4B-NB	-2.28	121.84	124.26
11	Ak	101	BCL	CAB-C3B-C2B	2.28	131.75	128.34
11	Bp	1204	BCL	CHC-C4B-NB	-2.28	121.84	124.26
12	BG	103	LMT	C1'-O5'-C5'	-2.28	109.22	113.69
11	BL	102	BCL	CHC-C4B-NB	-2.28	121.85	124.26
11	AS	1102	BCL	CAB-C3B-C2B	2.28	131.75	128.34
10	BF	103	V7N	C36-C18-C17	-2.27	119.74	122.92
12	Bf	1203	LMT	C3'-C4'-C5'	-2.27	105.72	110.93
11	BE	101	BCL	C1C-NC-C4C	2.27	107.73	106.71
11	Be	1105	BCL	C2A-C1A-CHA	2.27	127.83	123.86
11	Ac	101	BCL	OBB-CAB-CBB	-2.27	114.70	119.73
11	Bm	103	BCL	CHC-C4B-NB	-2.27	121.86	124.26
11	BD	101	BCL	O2D-CGD-CBD	2.27	115.30	111.27
11	AI	101	BCL	C4B-C3B-C2B	-2.27	104.71	108.36
11	Bl	1203	BCL	CHC-C4B-NB	-2.27	121.86	124.26
11	AT	1102	BCL	C6-C5-C3	2.26	119.39	113.45
12	BB	103	LMT	C3B-C4B-C5B	-2.26	106.20	110.24
11	BV	102	BCL	CHC-C4B-NB	-2.26	121.86	124.26
19	C	405	HEC	C2A-C1A-NA	-2.26	108.12	110.32
11	Bf	1204	BCL	CAB-C3B-C2B	2.26	131.72	128.34
11	AI	101	BCL	CMB-C2B-C1B	-2.26	121.93	125.37
11	AW	1202	BCL	OBB-CAB-CBB	-2.26	114.73	119.73
12	Bo	1201	LMT	C1'-O5'-C5'	-2.25	109.26	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	BH	102	V7N	C36-C18-C17	-2.25	119.77	122.92
19	C	405	HEC	CAA-CBA-CGA	-2.25	108.75	113.60
11	BR	101	BCL	CHC-C4B-NB	-2.25	121.87	124.26
12	BR	102	LMT	C3'-C4'-C5'	-2.25	105.77	110.93
12	Bf	1203	LMT	C1'-O5'-C5'	-2.25	109.27	113.69
11	AQ	103	BCL	CAB-C3B-C2B	2.25	131.71	128.34
11	Ac	101	BCL	C4B-C3B-C2B	-2.25	104.74	108.36
19	C	403	HEC	CAA-CBA-CGA	-2.25	108.77	113.60
16	L	303	BPH	CMD-C2D-C3D	2.25	128.88	124.68
11	BS	101	BCL	CHC-C4B-NB	-2.25	121.88	124.26
12	Aa	103	LMT	C1'-O5'-C5'	-2.24	109.28	113.69
11	Ac	101	BCL	CMB-C2B-C1B	-2.24	121.95	125.37
11	AR	101	BCL	CAB-C3B-C2B	2.24	131.70	128.34
12	Be	1102	LMT	C3'-C4'-C5'	-2.24	105.79	110.93
10	Bm	101	V7N	C33-C5-C4	2.24	121.61	118.08
12	Aj	102	LMT	C2'-C3'-C4'	2.24	114.80	109.68
11	AS	1102	BCL	C11-C10-C8	-2.24	108.68	115.92
10	BK	104	V7N	C35-C13-C14	-2.24	119.78	122.92
11	AW	1204	BCL	CHC-C4B-NB	-2.24	121.89	124.26
19	C	404	HEC	CHA-C4D-ND	2.24	126.85	124.42
11	BG	102	BCL	C1-C2-C3	-2.24	122.17	126.04
11	Bk	103	BCL	CAB-C3B-C2B	2.24	131.69	128.34
11	M	405	BCL	CHC-C4B-NB	-2.24	121.89	124.26
12	Bp	1201	LMT	C1'-O5'-C5'	-2.24	109.30	113.69
11	AQ	103	BCL	CHC-C4B-NB	-2.24	121.89	124.26
11	BX	102	BCL	C1C-NC-C4C	2.24	107.71	106.71
11	BX	102	BCL	C16-C15-C13	2.23	123.14	115.92
11	Aa	102	BCL	C4B-C3B-C2B	-2.23	104.77	108.36
11	BA	101	BCL	O2A-C1-C2	-2.23	102.77	108.64
10	BF	103	V7N	C36-C18-C19	2.23	121.59	118.08
11	BA	103	BCL	C1C-NC-C4C	2.23	107.71	106.71
11	AO	101	BCL	C4B-C3B-C2B	-2.23	104.77	108.36
11	AW	1202	BCL	C4B-C3B-C2B	-2.23	104.77	108.36
11	BO	103	BCL	C11-C10-C8	-2.23	108.72	115.92
10	BC	103	V7N	C36-C18-C17	-2.23	119.80	122.92
11	AF	102	BCL	CHC-C4B-NB	-2.23	121.90	124.26
11	BA	103	BCL	CHC-C4B-NB	-2.22	121.90	124.26
11	AM	101	BCL	O2A-C1-C2	-2.22	102.79	108.64
14	M	408	MQ8	C11-C3-C4	2.22	120.88	118.50
11	BS	101	BCL	O2D-CGD-CBD	2.22	115.21	111.27
11	Am	101	BCL	CED-O2D-CGD	2.22	120.95	115.94
11	BA	103	BCL	C2D-C1D-ND	2.21	111.74	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	AI	101	BCL	OBB-CAB-CBB	-2.21	114.83	119.73
11	Aa	102	BCL	CMB-C2B-C1B	-2.21	122.00	125.37
11	AT	1103	BCL	CAB-C3B-C2B	2.21	131.65	128.34
11	Bl	1203	BCL	C2D-C1D-ND	2.21	111.73	110.10
11	AK	101	BCL	CMB-C2B-C1B	-2.21	122.00	125.37
11	AQ	103	BCL	C2A-C1A-CHA	2.21	127.72	123.86
11	Ai	101	BCL	C16-C15-C13	2.21	123.06	115.92
11	M	404	BCL	CHC-C4B-NB	-2.21	121.92	124.26
11	Bm	103	BCL	CAB-C3B-C2B	2.21	131.65	128.34
11	BH	104	BCL	CHC-C4B-NB	-2.20	121.92	124.26
12	Be	1102	LMT	O5B-C5B-C4B	2.20	113.69	109.69
11	AL	101	BCL	OBB-CAB-CBB	-2.20	114.86	119.73
10	Bm	101	V7N	C33-C5-C6	-2.20	119.84	122.92
12	AX	1201	LMT	C3'-C4'-C5'	-2.20	105.89	110.93
11	AL	101	BCL	C4B-C3B-C2B	-2.20	104.83	108.36
10	BU	104	V7N	C36-C18-C17	-2.20	119.85	122.92
11	Bp	1203	BCL	CHD-C1D-C2D	2.20	130.08	125.48
10	Bc	1202	V7N	C36-C18-C19	2.19	121.53	118.08
11	BB	101	BCL	O2D-CGD-CBD	2.19	115.17	111.27
19	C	403	HEC	C3C-C4C-NC	-2.19	107.70	110.15
11	AW	1204	BCL	C2A-C1A-CHA	2.19	127.69	123.86
11	Ae	101	BCL	C4B-C3B-C2B	-2.19	104.84	108.36
12	K	201	LMT	O1'-C1'-C2'	2.19	111.72	108.30
12	Aj	102	LMT	C3B-C4B-C5B	-2.19	106.33	110.24
11	AE	1102	BCL	C11-C10-C8	-2.19	108.84	115.92
12	BS	102	LMT	C1'-O5'-C5'	-2.19	109.39	113.69
10	BO	102	V7N	C36-C18-C19	2.19	121.52	118.08
10	Aa	101	V7N	C7-C6-C5	-2.18	124.19	127.31
11	AU	1001	BCL	O2A-C1-C2	-2.18	102.90	108.64
11	Ae	101	BCL	C16-C15-C13	2.18	122.98	115.92
11	BV	102	BCL	CAB-C3B-C2B	2.18	131.61	128.34
11	AI	102	BCL	CMB-C2B-C1B	-2.18	122.05	125.37
11	Ah	101	BCL	C4B-C3B-C2B	-2.18	104.85	108.36
11	AW	1202	BCL	C16-C15-C13	2.18	122.97	115.92
10	BG	101	V7N	C33-C5-C4	2.18	121.51	118.08
11	AI	102	BCL	C4B-C3B-C2B	-2.18	104.86	108.36
10	Bi	101	V7N	C36-C18-C17	-2.18	119.87	122.92
11	AB	101	BCL	O2D-CGD-CBD	2.18	115.14	111.27
11	AM	102	BCL	C2A-C1A-CHA	2.18	127.66	123.86
12	Bc	1201	LMT	C3'-C4'-C5'	-2.18	105.94	110.93
12	BH	101	LMT	C3B-C4B-C5B	-2.18	106.36	110.24
11	Aa	102	BCL	OBB-CAB-CBB	-2.17	114.91	119.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	BT	101	V7N	O45-C40-C39	2.17	127.85	122.11
11	Ak	101	BCL	C4B-C3B-C2B	-2.17	104.86	108.36
11	Al	101	BCL	CHB-C4A-NA	2.17	127.52	124.51
11	Bg	103	BCL	CHC-C4B-NB	-2.17	121.96	124.26
11	AK	101	BCL	C1C-NC-C4C	2.17	107.68	106.71
10	BV	101	V7N	O45-C40-C39	2.17	127.84	122.11
10	Bd	1202	V7N	C35-C13-C14	-2.17	119.88	122.92
10	BB	102	V7N	C36-C18-C19	2.17	121.50	118.08
10	BB	102	V7N	C33-C5-C6	-2.17	119.89	122.92
10	BR	103	V7N	C3-C4-C5	2.16	129.16	125.89
11	Bb	1203	BCL	CAB-C3B-C2B	2.16	131.58	128.34
11	AL	101	BCL	CAB-C3B-C2B	2.16	131.58	128.34
19	C	404	HEC	C3C-C4C-NC	-2.16	107.73	110.15
10	BP	102	V7N	C33-C5-C6	-2.16	119.89	122.92
11	AS	1102	BCL	CAA-C2A-C1A	2.16	119.06	111.97
11	Af	101	BCL	OBB-CAB-CBB	-2.16	114.94	119.73
10	Bi	101	V7N	C7-C6-C5	-2.16	124.23	127.31
11	AK	101	BCL	CAB-C3B-C2B	2.16	131.57	128.34
11	Bi	102	BCL	O2D-CGD-CBD	2.15	115.10	111.27
11	Bl	1203	BCL	CAB-C3B-C2B	2.15	131.57	128.34
11	Af	101	BCL	C4B-C3B-C2B	-2.15	104.89	108.36
10	BK	104	V7N	C36-C18-C19	2.15	121.47	118.08
11	Ak	101	BCL	CMB-C2B-C1B	-2.15	122.09	125.37
11	Bd	1203	BCL	CHC-C4B-NB	-2.15	121.98	124.26
11	Ai	101	BCL	C4B-C3B-C2B	-2.15	104.90	108.36
11	Bo	1202	BCL	CAB-C3B-C2B	2.15	131.56	128.34
11	AS	1102	BCL	C2D-C1D-ND	2.15	111.69	110.10
12	Bf	1201	LMT	C1'-O5'-C5'	-2.15	109.47	113.69
10	AF	101	V7N	O45-C40-C39	2.15	127.78	122.11
19	C	402	HEC	CAD-CBD-CGD	-2.15	108.98	113.60
12	Bj	1201	LMT	C1'-O5'-C5'	-2.15	109.48	113.69
11	AB	101	BCL	CAB-C3B-C2B	2.14	131.55	128.34
11	Ak	101	BCL	OBB-CAB-CBB	-2.14	114.98	119.73
11	Ad	101	BCL	C4B-C3B-C2B	-2.14	104.91	108.36
11	BF	101	BCL	CAB-C3B-C2B	2.14	131.55	128.34
19	C	404	HEC	C4B-NB-C1B	2.14	107.28	105.07
11	AV	1001	BCL	C16-C15-C13	2.14	122.84	115.92
11	AN	101	BCL	C4B-C3B-C2B	-2.14	104.92	108.36
10	BB	102	V7N	C36-C18-C17	-2.14	119.93	122.92
10	Bl	1202	V7N	C36-C18-C17	-2.14	119.93	122.92
11	AO	101	BCL	C1-C2-C3	-2.14	122.35	126.04
11	AG	101	BCL	CAB-C3B-C2B	2.13	131.53	128.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	AD	1102	BCL	CAB-C3B-C2B	2.13	131.53	128.34
11	Bm	103	BCL	O2D-CGD-CBD	2.13	115.06	111.27
12	BS	102	LMT	C3B-C4B-C5B	-2.13	106.44	110.24
11	BU	102	BCL	C17-C16-C15	2.13	123.03	113.24
11	Ao	101	BCL	CHB-C4A-NA	2.13	127.46	124.51
10	An	101	V7N	O45-C40-C39	2.13	127.73	122.11
12	BK	103	LMT	O1B-C4'-C3'	2.13	112.94	107.28
11	BF	101	BCL	C6-C5-C3	2.13	119.04	113.45
11	AO	101	BCL	OBB-CAB-CBB	-2.13	115.02	119.73
12	AX	1201	LMT	C1'-O5'-C5'	-2.13	109.51	113.69
11	AR	101	BCL	C4B-C3B-C2B	-2.13	104.94	108.36
11	Ah	101	BCL	CMB-C2B-C1B	-2.12	122.13	125.37
11	AQ	103	BCL	C6-C5-C3	2.12	119.03	113.45
11	Bl	1203	BCL	O2D-CGD-CBD	2.12	115.04	111.27
11	Bd	1203	BCL	O2D-CGD-O1D	-2.12	119.69	123.84
11	BA	101	BCL	C4B-C3B-C2B	-2.12	104.94	108.36
11	BP	101	BCL	CAB-C3B-C2B	2.12	131.52	128.34
10	BD	103	V7N	C36-C18-C17	-2.12	119.95	122.92
11	AT	1102	BCL	C1-C2-C3	-2.12	122.38	126.04
10	AF	101	V7N	C37-C22-C23	2.12	118.83	115.27
11	AU	1001	BCL	C4B-C3B-C2B	-2.12	104.95	108.36
11	AQ	103	BCL	O2D-CGD-O1D	-2.11	119.71	123.84
10	Bf	1202	V7N	C33-C5-C4	2.11	121.41	118.08
11	AI	101	BCL	O2D-CGD-CBD	2.11	115.02	111.27
11	AD	1102	BCL	C4B-C3B-C2B	-2.11	104.96	108.36
12	BH	103	LMT	C1'-O5'-C5'	-2.11	109.54	113.69
11	AX	1202	BCL	C1C-NC-C4C	2.11	107.65	106.71
11	AF	102	BCL	C1C-NC-C4C	2.11	107.65	106.71
11	BH	104	BCL	C4B-C3B-C2B	-2.11	104.97	108.36
11	BG	102	BCL	O2D-CGD-CBD	2.11	115.01	111.27
11	Bn	103	BCL	C4B-C3B-C2B	-2.11	104.97	108.36
11	AH	101	BCL	C4B-C3B-C2B	-2.10	104.97	108.36
11	Bl	1203	BCL	C1C-NC-C4C	2.10	107.65	106.71
11	AV	1001	BCL	CAB-C3B-C2B	2.10	131.49	128.34
10	Bg	101	V7N	C16-C17-C18	-2.10	124.31	127.31
11	Ai	101	BCL	OBB-CAB-CBB	-2.10	115.07	119.73
11	AM	102	BCL	CAB-C3B-C2B	2.10	131.49	128.34
11	BE	101	BCL	C4B-C3B-C2B	-2.10	104.98	108.36
11	Bh	1205	BCL	C6-C5-C3	2.10	118.96	113.45
10	BI	101	V7N	C36-C18-C19	2.10	121.38	118.08
11	Bd	1203	BCL	O2D-CGD-CBD	2.10	114.99	111.27
11	Af	101	BCL	CMB-C2B-C1B	-2.10	122.18	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	Bj	1202	V7N	C33-C5-C4	2.10	121.38	118.08
12	BQ	101	LMT	C3B-C4B-C5B	-2.10	106.50	110.24
10	BA	102	V7N	C36-C18-C17	-2.10	119.99	122.92
19	C	402	HEC	C3C-C4C-NC	-2.09	107.81	110.15
12	Bh	1204	LMT	C3'-C4'-C5'	-2.09	106.13	110.93
12	Bp	1201	LMT	C3'-C4'-C5'	-2.09	106.13	110.93
11	AW	1202	BCL	CMB-C2B-C1B	-2.09	122.18	125.37
10	Bb	1202	V7N	C7-C6-C5	-2.09	124.33	127.31
12	Ba	1102	LMT	C3'-C4'-C5'	-2.09	106.14	110.93
11	BD	101	BCL	C11-C10-C8	2.09	122.67	115.92
10	AL	102	V7N	C15-C14-C13	-2.09	124.33	127.31
11	AN	101	BCL	CMB-C2B-C1B	-2.09	122.19	125.37
11	AE	1102	BCL	C4B-C3B-C2B	-2.09	105.00	108.36
11	AI	102	BCL	OBB-CAB-CBB	-2.08	115.11	119.73
11	BH	104	BCL	O2D-CGD-CBD	2.08	114.97	111.27
11	BN	101	BCL	O2D-CGD-CBD	2.08	114.97	111.27
10	BX	101	V7N	C15-C14-C13	-2.08	124.34	127.31
11	AP	1102	BCL	CAB-C3B-C2B	2.08	131.46	128.34
11	BL	102	BCL	OBB-CAB-CBB	-2.08	115.12	119.73
11	AB	101	BCL	C4B-C3B-C2B	-2.08	105.02	108.36
10	Bl	1202	V7N	C33-C5-C6	-2.08	120.01	122.92
10	Bj	1202	V7N	O45-C40-C39	2.08	127.59	122.11
12	BI	103	LMT	C3'-C4'-C5'	-2.08	106.17	110.93
10	BC	103	V7N	C16-C17-C18	-2.08	124.35	127.31
10	BP	102	V7N	C16-C17-C18	-2.08	124.35	127.31
11	AQ	101	BCL	C4B-C3B-C2B	-2.07	105.02	108.36
10	AF	101	V7N	C36-C18-C17	-2.07	120.02	122.92
12	BK	103	LMT	O5B-C5B-C4B	2.07	113.46	109.69
11	Ae	101	BCL	CMB-C2B-C1B	-2.07	122.21	125.37
11	BI	102	BCL	C4B-C3B-C2B	-2.07	105.03	108.36
11	BD	101	BCL	O2D-CGD-O1D	-2.07	119.79	123.84
11	BG	102	BCL	C4B-C3B-C2B	-2.07	105.03	108.36
10	BP	102	V7N	C36-C18-C19	2.07	121.34	118.08
11	AR	101	BCL	CMB-C2B-C1B	-2.07	122.22	125.37
11	Bg	103	BCL	O2D-CGD-CBD	2.07	114.94	111.27
10	BS	103	V7N	C36-C18-C17	-2.07	120.03	122.92
11	AB	101	BCL	C17-C16-C15	2.07	122.74	113.24
10	BJ	101	V7N	C15-C14-C13	-2.07	124.36	127.31
12	BO	101	LMT	C3'-C4'-C5'	-2.07	106.19	110.93
11	AF	102	BCL	CAB-C3B-C2B	2.07	131.44	128.34
11	Al	101	BCL	C6-C5-C3	-2.07	108.04	113.45
11	BK	102	BCL	C4B-C3B-C2B	-2.06	105.04	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	AM	102	BCL	C1C-NC-C4C	2.06	107.63	106.71
11	BX	102	BCL	C4B-C3B-C2B	-2.06	105.04	108.36
11	AX	1202	BCL	C4B-C3B-C2B	-2.06	105.05	108.36
11	AN	101	BCL	OBB-CAB-CBB	-2.06	115.17	119.73
11	AJ	1103	BCL	C4B-C3B-C2B	-2.06	105.05	108.36
11	AT	1103	BCL	C4B-C3B-C2B	-2.06	105.05	108.36
10	Bm	101	V7N	C3-C4-C5	2.06	129.00	125.89
10	Aa	101	V7N	C33-C5-C6	-2.06	120.04	122.92
10	BF	103	V7N	C33-C5-C6	-2.06	120.04	122.92
10	BN	102	V7N	C36-C18-C17	-2.06	120.04	122.92
11	AJ	1102	BCL	C4B-C3B-C2B	-2.06	105.05	108.36
11	BA	101	BCL	CMB-C2B-C1B	-2.06	122.24	125.37
11	Bp	1204	BCL	O2D-CGD-CBD	2.06	114.92	111.27
19	C	402	HEC	C2B-C1B-NB	-2.06	107.42	109.88
11	AC	101	BCL	C4B-C3B-C2B	-2.06	105.05	108.36
11	AM	101	BCL	C4B-C3B-C2B	-2.06	105.05	108.36
11	BA	101	BCL	C2D-C1D-ND	2.05	111.62	110.10
11	AP	1102	BCL	OBB-CAB-CBB	-2.05	115.18	119.73
10	BO	102	V7N	O45-C40-C39	2.05	127.53	122.11
11	AR	101	BCL	C1C-NC-C4C	2.05	107.63	106.71
11	BB	101	BCL	CHC-C4B-NB	-2.05	122.08	124.26
11	Ad	101	BCL	CMB-C2B-C1B	-2.05	122.24	125.37
11	AR	101	BCL	OBB-CAB-CBB	-2.05	115.18	119.73
11	BG	102	BCL	O2D-CGD-O1D	-2.05	119.83	123.84
11	Ah	101	BCL	OBB-CAB-CBB	-2.05	115.19	119.73
11	Ai	101	BCL	CMB-C2B-C1B	-2.05	122.25	125.37
11	BP	101	BCL	C4B-C3B-C2B	-2.05	105.06	108.36
11	BA	103	BCL	CAA-CBA-CGA	2.05	119.24	113.25
12	AW	1201	LMT	C3B-C4B-C5B	-2.05	106.59	110.24
11	Am	101	BCL	CAA-CBA-CGA	-2.05	107.28	113.25
10	BW	102	V7N	O45-C40-C39	2.04	127.51	122.11
11	AD	1102	BCL	OBB-CAB-CBB	-2.04	115.20	119.73
11	BU	102	BCL	C4B-C3B-C2B	-2.04	105.07	108.36
11	Bi	102	BCL	CAB-C3B-C2B	2.04	131.40	128.34
11	BS	101	BCL	C6-C5-C3	2.04	118.81	113.45
11	AV	1001	BCL	C4B-C3B-C2B	-2.04	105.08	108.36
11	Bd	1203	BCL	CHC-C1C-NC	-2.04	121.69	124.51
11	BA	101	BCL	OBB-CAB-CBB	-2.04	115.22	119.73
11	AQ	102	BCL	CHC-C4B-NB	-2.04	122.10	124.26
12	M	401	LMT	C3'-C4'-C5'	-2.04	106.25	110.93
11	Be	1105	BCL	C4B-C3B-C2B	-2.03	105.09	108.36
11	Bg	103	BCL	CAB-C3B-C2B	2.03	131.39	128.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	BN	102	V7N	C15-C14-C13	-2.03	124.41	127.31
19	C	402	HEC	CAA-C2A-C3A	-2.03	124.09	127.88
12	L	304	LMT	C1'-O5'-C5'	-2.03	109.70	113.69
10	BJ	101	V7N	C36-C18-C17	-2.03	120.08	122.92
11	BE	101	BCL	C6-C5-C3	2.03	118.78	113.45
11	Bf	1204	BCL	C4B-C3B-C2B	-2.03	105.09	108.36
12	BF	102	LMT	C3'-C4'-C5'	-2.03	106.27	110.93
11	BS	101	BCL	C4A-NA-C1A	2.03	107.62	106.71
11	Bc	1204	BCL	C17-C16-C15	2.03	122.56	113.24
11	Bn	103	BCL	OBB-CAB-CBB	-2.03	115.24	119.73
11	AV	1001	BCL	C17-C16-C15	-2.03	103.92	113.24
18	M	407	CRT	C20-C21-C22	2.03	127.63	123.47
10	Bd	1202	V7N	O45-C40-C39	2.03	127.46	122.11
10	Bm	101	V7N	C15-C14-C13	-2.03	124.42	127.31
11	AE	1102	BCL	C1C-NC-C4C	2.03	107.62	106.71
10	Aa	101	V7N	O45-C40-C39	2.02	127.45	122.11
11	Bm	103	BCL	C4B-C3B-C2B	-2.02	105.11	108.36
11	AS	1102	BCL	C4B-C3B-C2B	-2.02	105.11	108.36
11	Bh	1205	BCL	C4B-C3B-C2B	-2.02	105.11	108.36
11	AE	1102	BCL	CAB-C3B-C2B	2.02	131.37	128.34
10	BJ	101	V7N	C33-C5-C6	-2.02	120.10	122.92
10	Bb	1202	V7N	C36-C18-C17	-2.02	120.10	122.92
11	Bi	102	BCL	C4B-C3B-C2B	-2.02	105.12	108.36
11	Bn	103	BCL	O2D-CGD-CBD	2.02	114.85	111.27
11	M	404	BCL	C4B-C3B-C2B	-2.02	105.12	108.36
11	Bm	103	BCL	O2D-CGD-O1D	-2.02	119.90	123.84
11	Bb	1203	BCL	C4B-C3B-C2B	-2.01	105.12	108.36
11	BL	102	BCL	C4B-C3B-C2B	-2.01	105.12	108.36
12	AW	1201	LMT	O5B-C5B-C4B	2.01	113.35	109.69
11	BI	102	BCL	O2D-CGD-CBD	2.01	114.85	111.27
11	AW	1203	BCL	C4B-C3B-C2B	-2.01	105.12	108.36
19	C	402	HEC	C2C-C1C-NC	-2.01	107.02	110.08
12	Bf	1203	LMT	O1'-C1'-C2'	2.01	111.44	108.30
11	Bp	1203	BCL	CMD-C2D-C3D	-2.01	122.99	127.61
11	BV	102	BCL	C1-O2A-CGA	2.01	121.71	116.44
11	Bc	1204	BCL	CAB-C3B-C2B	2.01	131.35	128.34
11	AM	101	BCL	CAB-C3B-C2B	2.01	131.35	128.34
10	Bk	101	V7N	C36-C18-C17	-2.01	120.11	122.92
12	BW	103	LMT	C3B-C4B-C5B	-2.00	106.66	110.24
10	BP	102	V7N	O45-C40-C39	2.00	127.40	122.11
10	Bb	1202	V7N	C33-C5-C6	-2.00	120.12	122.92
11	Ao	101	BCL	CHD-C1D-C2D	2.00	129.68	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	BV	102	BCL	C1C-NC-C4C	2.00	107.61	106.71
10	BJ	101	V7N	O45-C40-C39	2.00	127.39	122.11
11	L	302	BCL	C1-C2-C3	2.00	129.50	126.04

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	C	402	HEC	NA
19	C	403	HEC	NA
19	C	404	HEC	NA
19	C	405	HEC	NA

All (1845) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	Aa	101	V7N	C30-C1-C2-C3
10	Aa	101	V7N	C31-C1-C2-C3
10	Aa	101	V7N	O42-C34-C9-C10
10	Aa	101	V7N	O42-C34-C9-C8
10	Bb	1202	V7N	C31-C1-C2-C3
10	Bb	1202	V7N	O42-C34-C9-C10
10	Bb	1202	V7N	O42-C34-C9-C8
10	Bc	1202	V7N	C26-C27-C28-C29
10	Bc	1202	V7N	O42-C34-C9-C10
10	Bc	1202	V7N	O42-C34-C9-C8
10	Bd	1202	V7N	O32-C1-C2-C3
10	Bd	1202	V7N	C25-C26-C27-C28
10	Bd	1202	V7N	C38-C26-C27-C28
10	Bd	1202	V7N	O42-C34-C9-C8
10	Be	1103	V7N	C30-C1-C2-C3
10	Be	1103	V7N	C31-C1-C2-C3
10	Be	1103	V7N	C26-C27-C28-C29
10	Be	1103	V7N	O42-C34-C9-C10
10	Be	1103	V7N	O42-C34-C9-C8
10	Bf	1202	V7N	C30-C1-C2-C3
10	Bf	1202	V7N	C31-C1-C2-C3
10	Bf	1202	V7N	O32-C1-C2-C3
10	Bf	1202	V7N	O42-C34-C9-C10
10	Bf	1202	V7N	O42-C34-C9-C8
10	Bg	101	V7N	C11-C12-C13-C14
10	Bg	101	V7N	C11-C12-C13-C35
10	Bg	101	V7N	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
10	Bg	101	V7N	C38-C26-C27-C28
10	Bg	101	V7N	C26-C27-C28-C29
10	Bg	101	V7N	O42-C34-C9-C10
10	Bg	101	V7N	O42-C34-C9-C8
10	Bh	1202	V7N	C11-C12-C13-C14
10	Bh	1202	V7N	C11-C12-C13-C35
10	Bh	1202	V7N	C25-C26-C27-C28
10	Bh	1202	V7N	C38-C26-C27-C28
10	Bh	1202	V7N	C26-C27-C28-C29
10	Bh	1202	V7N	O42-C34-C9-C10
10	Bh	1202	V7N	O42-C34-C9-C8
10	Bi	101	V7N	C30-C1-C2-C3
10	Bi	101	V7N	C31-C1-C2-C3
10	Bi	101	V7N	O32-C1-C2-C3
10	Bi	101	V7N	O42-C34-C9-C10
10	Bi	101	V7N	O42-C34-C9-C8
10	Bj	1202	V7N	O32-C1-C2-C3
10	Bj	1202	V7N	C25-C26-C27-C28
10	Bj	1202	V7N	C38-C26-C27-C28
10	Bj	1202	V7N	C26-C27-C28-C29
10	Bj	1202	V7N	O42-C34-C9-C10
10	Bj	1202	V7N	O42-C34-C9-C8
10	Bk	101	V7N	C2-C1-O32-C41
10	Bk	101	V7N	C30-C1-O32-C41
10	Bk	101	V7N	C31-C1-O32-C41
10	Bk	101	V7N	C26-C27-C28-C29
10	Bk	101	V7N	O42-C34-C9-C10
10	Bk	101	V7N	O42-C34-C9-C8
10	Bl	1202	V7N	C26-C27-C28-C29
10	Bl	1202	V7N	O42-C34-C9-C10
10	Bl	1202	V7N	O42-C34-C9-C8
10	Bm	101	V7N	C30-C1-C2-C3
10	Bm	101	V7N	C31-C1-C2-C3
10	Bm	101	V7N	O32-C1-C2-C3
10	Bm	101	V7N	C2-C1-O32-C41
10	Bm	101	V7N	C31-C1-O32-C41
10	Bm	101	V7N	C25-C26-C27-C28
10	Bm	101	V7N	C38-C26-C27-C28
10	Bm	101	V7N	C26-C27-C28-C29
10	Bm	101	V7N	O42-C34-C9-C10
10	Bm	101	V7N	C3-C4-C5-C33
10	Bm	101	V7N	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
10	Bm	101	V7N	C7-C8-C9-C10
10	An	101	V7N	O32-C1-C2-C3
10	An	101	V7N	C26-C27-C28-C29
10	An	101	V7N	O42-C34-C9-C10
10	An	101	V7N	O42-C34-C9-C8
10	An	101	V7N	C3-C4-C5-C33
10	Bn	101	V7N	C2-C1-O32-C41
10	Bn	101	V7N	O42-C34-C9-C10
10	Bn	101	V7N	O42-C34-C9-C8
10	Bp	1202	V7N	C2-C1-O32-C41
10	Bp	1202	V7N	O42-C34-C9-C10
10	Bp	1202	V7N	O42-C34-C9-C8
10	BA	102	V7N	O42-C34-C9-C10
10	BA	102	V7N	O42-C34-C9-C8
10	BB	102	V7N	O32-C1-C2-C3
10	BB	102	V7N	C25-C26-C27-C28
10	BB	102	V7N	C38-C26-C27-C28
10	BB	102	V7N	C26-C27-C28-C29
10	BB	102	V7N	O42-C34-C9-C10
10	BB	102	V7N	O42-C34-C9-C8
10	BC	103	V7N	O42-C34-C9-C10
10	BC	103	V7N	O42-C34-C9-C8
10	BD	103	V7N	C26-C27-C28-C29
10	BD	103	V7N	O42-C34-C9-C10
10	BD	103	V7N	O42-C34-C9-C8
10	BF	103	V7N	C30-C1-C2-C3
10	BF	103	V7N	C31-C1-C2-C3
10	BF	103	V7N	C26-C27-C28-C29
10	BF	103	V7N	O42-C34-C9-C10
10	BF	103	V7N	O42-C34-C9-C8
10	AF	101	V7N	O32-C1-C2-C3
10	AF	101	V7N	C17-C18-C19-C20
10	AF	101	V7N	C36-C18-C19-C20
10	AF	101	V7N	C25-C26-C27-C28
10	AF	101	V7N	C38-C26-C27-C28
10	AF	101	V7N	O42-C34-C9-C10
10	AF	101	V7N	O42-C34-C9-C8
10	AF	101	V7N	C7-C8-C9-C10
10	BG	101	V7N	O42-C34-C9-C10
10	BG	101	V7N	O42-C34-C9-C8
10	BH	102	V7N	O42-C34-C9-C10
10	BH	102	V7N	O42-C34-C9-C8

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Mol	Chain	Res	Type	Atoms
10	BI	101	V7N	O42-C34-C9-C10
10	BI	101	V7N	O42-C34-C9-C8
10	BJ	101	V7N	C30-C1-C2-C3
10	BJ	101	V7N	O42-C34-C9-C10
10	BJ	101	V7N	O42-C34-C9-C8
10	BK	104	V7N	C26-C27-C28-C29
10	BK	104	V7N	O42-C34-C9-C10
10	BK	104	V7N	O42-C34-C9-C8
10	AL	102	V7N	C26-C27-C28-C29
10	AL	102	V7N	O42-C34-C9-C8
10	BL	101	V7N	C25-C26-C27-C28
10	BL	101	V7N	O42-C34-C9-C10
10	BL	101	V7N	O42-C34-C9-C8
10	BN	102	V7N	O42-C34-C9-C8
10	BO	102	V7N	C26-C27-C28-C29
10	BO	102	V7N	O42-C34-C9-C10
10	BO	102	V7N	O42-C34-C9-C8
10	BP	102	V7N	C30-C1-C2-C3
10	BP	102	V7N	C31-C1-C2-C3
10	BP	102	V7N	C11-C12-C13-C14
10	BP	102	V7N	C11-C12-C13-C35
10	BP	102	V7N	C25-C26-C27-C28
10	BP	102	V7N	C38-C26-C27-C28
10	BP	102	V7N	O42-C34-C9-C10
10	BP	102	V7N	O42-C34-C9-C8
10	BQ	103	V7N	C25-C26-C27-C28
10	BQ	103	V7N	C38-C26-C27-C28
10	BQ	103	V7N	O42-C34-C9-C10
10	BQ	103	V7N	O42-C34-C9-C8
10	BR	103	V7N	O32-C1-C2-C3
10	BR	103	V7N	O42-C34-C9-C8
10	BS	103	V7N	C30-C1-C2-C3
10	BS	103	V7N	C31-C1-C2-C3
10	BS	103	V7N	C21-C22-C23-C24
10	BS	103	V7N	C37-C22-C23-C24
10	BS	103	V7N	O42-C34-C9-C10
10	BS	103	V7N	O42-C34-C9-C8
10	BS	103	V7N	C3-C4-C5-C33
10	BS	103	V7N	C3-C4-C5-C6
10	BT	101	V7N	C22-C23-C24-C25
10	BT	101	V7N	C25-C26-C27-C28
10	BT	101	V7N	C38-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
10	BT	101	V7N	C26-C27-C28-C29
10	BT	101	V7N	O42-C34-C9-C8
10	BU	104	V7N	O42-C34-C9-C10
10	BU	104	V7N	O42-C34-C9-C8
10	BV	101	V7N	O32-C1-C2-C3
10	BV	101	V7N	O42-C34-C9-C10
10	BV	101	V7N	O42-C34-C9-C8
10	BW	102	V7N	O32-C1-C2-C3
10	BW	102	V7N	O42-C34-C9-C10
10	BW	102	V7N	O42-C34-C9-C8
10	BX	101	V7N	C22-C23-C24-C25
10	BX	101	V7N	C26-C27-C28-C29
10	BX	101	V7N	O42-C34-C9-C10
10	BX	101	V7N	O42-C34-C9-C8
10	BX	101	V7N	C29-C39-C40-O44
10	BX	101	V7N	C29-C39-C40-O45
10	BX	101	V7N	C43-C39-C40-O44
10	BX	101	V7N	C43-C39-C40-O45
11	Ab	101	BCL	C2-C3-C5-C6
11	Ab	101	BCL	C4-C3-C5-C6
11	Bc	1204	BCL	C4C-C3C-CAC-CBC
11	Ad	101	BCL	C2-C3-C5-C6
11	Ad	101	BCL	C4-C3-C5-C6
11	Ak	101	BCL	C1A-C2A-CAA-CBA
11	Bk	103	BCL	O1A-CGA-O2A-C1
11	Al	101	BCL	C2A-CAA-CBA-CGA
11	Al	101	BCL	C2C-C3C-CAC-CBC
11	Al	101	BCL	C4C-C3C-CAC-CBC
11	Al	101	BCL	C6-C7-C8-C9
11	Am	101	BCL	C2-C3-C5-C6
11	Am	101	BCL	C4-C3-C5-C6
11	Bn	103	BCL	C1A-C2A-CAA-CBA
11	Bp	1203	BCL	C2C-C3C-CAC-CBC
11	Bp	1203	BCL	C4C-C3C-CAC-CBC
11	M	404	BCL	C2-C3-C5-C6
11	M	404	BCL	C4-C3-C5-C6
11	BA	101	BCL	O1D-CGD-O2D-CED
11	BB	101	BCL	C4C-C3C-CAC-CBC
11	BC	101	BCL	C1A-C2A-CAA-CBA
11	AE	1102	BCL	C4-C3-C5-C6
11	BE	101	BCL	C4-C3-C5-C6
11	BF	101	BCL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
11	BF	101	BCL	C3A-C2A-CAA-CBA
11	BF	101	BCL	C2-C3-C5-C6
11	BF	101	BCL	C4-C3-C5-C6
11	BF	101	BCL	C14-C13-C15-C16
11	AH	101	BCL	C2-C3-C5-C6
11	AH	101	BCL	C4-C3-C5-C6
11	AI	102	BCL	C4-C3-C5-C6
11	BI	102	BCL	CBA-CGA-O2A-C1
11	BI	102	BCL	O1A-CGA-O2A-C1
11	BI	102	BCL	C4C-C3C-CAC-CBC
11	BK	102	BCL	C4C-C3C-CAC-CBC
11	AO	101	BCL	C2-C3-C5-C6
11	AO	101	BCL	C4-C3-C5-C6
11	AP	1102	BCL	C2-C3-C5-C6
11	AP	1102	BCL	C4-C3-C5-C6
11	AQ	101	BCL	C1A-C2A-CAA-CBA
11	AQ	103	BCL	C2-C3-C5-C6
11	AQ	103	BCL	C4-C3-C5-C6
11	AR	101	BCL	C2-C3-C5-C6
11	AR	101	BCL	C4-C3-C5-C6
11	AT	1102	BCL	C2-C3-C5-C6
11	AT	1102	BCL	C4-C3-C5-C6
11	AT	1103	BCL	C2-C3-C5-C6
11	AT	1103	BCL	C4-C3-C5-C6
11	BU	102	BCL	C1A-C2A-CAA-CBA
11	AV	1001	BCL	C2-C3-C5-C6
11	AV	1001	BCL	C4-C3-C5-C6
11	BX	102	BCL	C2-C3-C5-C6
11	BX	102	BCL	C4-C3-C5-C6
12	Bb	1201	LMT	O5'-C1'-O1'-C1
12	Bd	1201	LMT	O5'-C1'-O1'-C1
12	Bf	1201	LMT	C2-C1-O1'-C1'
12	Aj	102	LMT	C2'-C1'-O1'-C1
12	Aj	102	LMT	O5'-C1'-O1'-C1
12	L	304	LMT	C2'-C1'-O1'-C1
12	L	304	LMT	O5'-C1'-O1'-C1
12	K	201	LMT	C2'-C1'-O1'-C1
12	K	201	LMT	O5'-C1'-O1'-C1
12	C	401	LMT	C2'-C1'-O1'-C1
12	C	401	LMT	O5'-C1'-O1'-C1
12	BA	104	LMT	C2-C1-O1'-C1'
12	BF	102	LMT	C2-C1-O1'-C1'

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Mol	Chain	Res	Type	Atoms
12	BG	103	LMT	C2-C1-O1'-C1'
12	BH	101	LMT	C2'-C1'-O1'-C1
12	BH	101	LMT	O5'-C1'-O1'-C1
12	BH	101	LMT	C2-C1-O1'-C1'
12	BK	101	LMT	C2'-C1'-O1'-C1
12	BK	101	LMT	O5'-C1'-O1'-C1
12	BL	103	LMT	C2'-C1'-O1'-C1
12	BL	103	LMT	O5'-C1'-O1'-C1
12	BL	103	LMT	C2-C1-O1'-C1'
12	BR	102	LMT	C2-C1-O1'-C1'
12	BS	102	LMT	C2-C1-O1'-C1'
12	BU	101	LMT	C2'-C1'-O1'-C1
12	BU	101	LMT	O5'-C1'-O1'-C1
12	BU	101	LMT	C2-C1-O1'-C1'
12	AX	1201	LMT	C2-C1-O1'-C1'
13	Ba	1101	PEX	C24-O8-P1-O1
13	Ba	1101	PEX	C24-O8-P1-O2
13	Bc	1203	PEX	C1-O3-P1-O2
13	Bc	1203	PEX	C24-O8-P1-O1
13	Bc	1203	PEX	C24-O8-P1-O2
13	Bc	1203	PEX	C24-O8-P1-O3
13	Be	1101	PEX	C1-O3-P1-O1
13	Be	1101	PEX	O6-C2-C3-O4
13	Be	1104	PEX	C1-O3-P1-O1
13	Be	1104	PEX	C1-O3-P1-O2
13	Be	1104	PEX	C15-C14-O6-C2
13	Bg	102	PEX	C15-C14-O6-C2
13	Bh	1203	PEX	C24-O8-P1-O2
13	Bh	1203	PEX	O5-C4-O4-C3
13	Aj	103	PEX	C1-O3-P1-O2
13	Aj	103	PEX	C24-O8-P1-O3
13	Aj	103	PEX	O7-C14-O6-C2
13	Bk	102	PEX	C1-O3-P1-O2
13	Bk	102	PEX	C24-O8-P1-O2
13	Bk	102	PEX	O6-C2-C3-O4
13	Bm	102	PEX	C1-O3-P1-O1
13	Bm	102	PEX	C15-C14-O6-C2
13	Bn	102	PEX	C1-O3-P1-O1
13	Bn	102	PEX	C24-O8-P1-O1
13	Bn	102	PEX	C24-O8-P1-O3
13	AE	1101	PEX	C1-O3-P1-O1
13	AE	1101	PEX	O8-C24-C25-N1

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Mol	Chain	Res	Type	Atoms
13	AJ	1101	PEX	C1-O3-P1-O2
13	AP	1101	PEX	C15-C14-O6-C2
13	AS	1101	PEX	C15-C14-O6-C2
13	AT	1101	PEX	C1-O3-P1-O2
14	Ad	103	MQ8	C12-C13-C15-C16
14	Ad	103	MQ8	C14-C13-C15-C16
14	Ad	103	MQ8	C16-C17-C18-C19
14	Ad	103	MQ8	C16-C17-C18-C20
14	Ad	103	MQ8	C21-C22-C23-C25
14	Ad	103	MQ8	C24-C23-C25-C26
14	Ad	103	MQ8	C27-C28-C30-C31
14	Ad	103	MQ8	C29-C28-C30-C31
14	Ad	103	MQ8	C33-C35-C36-C37
14	Ad	103	MQ8	C39-C38-C40-C41
14	Ad	103	MQ8	C41-C42-C43-C44
14	Ad	103	MQ8	C41-C42-C43-C45
14	L	305	MQ8	C20-C21-C22-C23
14	L	305	MQ8	C21-C22-C23-C24
14	L	305	MQ8	C21-C22-C23-C25
14	L	305	MQ8	C39-C38-C40-C41
14	L	305	MQ8	C40-C41-C42-C43
14	L	305	MQ8	C41-C42-C43-C44
14	L	305	MQ8	C41-C42-C43-C45
14	M	408	MQ8	C3-C11-C12-C13
14	M	408	MQ8	C11-C12-C13-C14
14	M	408	MQ8	C11-C12-C13-C15
14	M	408	MQ8	C16-C17-C18-C19
14	M	408	MQ8	C16-C17-C18-C20
14	M	408	MQ8	C38-C40-C41-C42
14	M	408	MQ8	C42-C43-C44-C46
14	M	408	MQ8	C45-C43-C44-C46
14	M	408	MQ8	C46-C47-C48-C50
15	Af	102	CD4	C13-C14-O2-C15
15	Af	102	CD4	O1-C14-O2-C15
15	Af	102	CD4	O4-C17-O3-C16
15	Af	102	CD4	C18-C17-O3-C16
15	Af	102	CD4	C28-O5-P1-O7
15	Af	102	CD4	C29-O8-P1-O6
15	Af	102	CD4	C29-O8-P1-O7
15	Af	102	CD4	O8-C29-C30-O9
15	M	403	CD4	C32-O13-P2-O10
15	M	403	CD4	C32-O13-P2-O11

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Mol	Chain	Res	Type	Atoms
15	M	403	CD4	C32-O13-P2-O12
15	M	403	CD4	O17-C46-O16-C33
15	M	403	CD4	C47-C46-O16-C33
12	Aj	102	LMT	C5'-C4'-O1B-C1B
12	K	201	LMT	C3'-C4'-O1B-C1B
12	BK	101	LMT	C3'-C4'-O1B-C1B
12	BW	101	LMT	C3'-C4'-O1B-C1B
11	Ao	101	BCL	C8-C10-C11-C12
12	M	401	LMT	C3'-C4'-O1B-C1B
12	BK	103	LMT	C3'-C4'-O1B-C1B
12	BU	101	LMT	C3'-C4'-O1B-C1B
12	BS	102	LMT	C3'-C4'-O1B-C1B
12	AX	1201	LMT	O5B-C1B-O1B-C4'
13	Be	1104	PEX	O5-C4-O4-C3
13	Bg	102	PEX	O5-C4-O4-C3
13	Bn	102	PEX	O5-C4-O4-C3
13	AD	1101	PEX	O5-C4-O4-C3
13	AJ	1101	PEX	O5-C4-O4-C3
13	AS	1101	PEX	O5-C4-O4-C3
12	BI	103	LMT	O5B-C5B-C6B-O6B
12	AW	1201	LMT	O5B-C1B-O1B-C4'
13	Be	1104	PEX	O7-C14-O6-C2
13	Bg	102	PEX	O7-C14-O6-C2
13	Bm	102	PEX	O7-C14-O6-C2
13	AJ	1101	PEX	O7-C14-O6-C2
13	AP	1101	PEX	O7-C14-O6-C2
13	AS	1101	PEX	O7-C14-O6-C2
11	Bn	103	BCL	C3-C5-C6-C7
13	Be	1104	PEX	C5-C4-O4-C3
13	Bh	1203	PEX	C5-C4-O4-C3
13	Bn	102	PEX	C5-C4-O4-C3
13	AD	1101	PEX	C5-C4-O4-C3
13	Aj	103	PEX	C15-C14-O6-C2
13	AJ	1101	PEX	C15-C14-O6-C2
12	BB	103	LMT	O5B-C1B-O1B-C4'
19	C	404	HEC	C2B-C3B-CAB-CBB
10	Bf	1202	V7N	C37-C22-C23-C24
11	Ac	101	BCL	C4-C3-C5-C6
11	Ae	101	BCL	C4-C3-C5-C6
11	BD	101	BCL	C4-C3-C5-C6
11	Ac	101	BCL	C2-C3-C5-C6
11	AE	1102	BCL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
11	BE	101	BCL	C2-C3-C5-C6
11	AI	102	BCL	C2-C3-C5-C6
14	Ad	103	MQ8	C22-C23-C25-C26
14	Ad	103	MQ8	C37-C38-C40-C41
14	L	305	MQ8	C37-C38-C40-C41
11	Bo	1202	BCL	C2A-CAA-CBA-CGA
11	BD	101	BCL	C2A-CAA-CBA-CGA
11	BS	101	BCL	C2A-CAA-CBA-CGA
11	Al	101	BCL	C3-C5-C6-C7
13	Bg	102	PEX	C5-C4-O4-C3
13	AJ	1101	PEX	C5-C4-O4-C3
13	AS	1101	PEX	C5-C4-O4-C3
12	BO	104	LMT	C5'-C4'-O1B-C1B
14	Ad	103	MQ8	C21-C22-C23-C24
14	Ad	103	MQ8	C31-C32-C33-C34
14	Ad	103	MQ8	C36-C37-C38-C39
14	L	305	MQ8	C31-C32-C33-C34
14	M	408	MQ8	C41-C42-C43-C45
14	Ad	103	MQ8	C31-C32-C33-C35
14	Ad	103	MQ8	C36-C37-C38-C40
14	L	305	MQ8	C31-C32-C33-C35
14	M	408	MQ8	C41-C42-C43-C44
10	Bh	1202	V7N	C27-C28-C29-C39
10	AF	101	V7N	C27-C28-C29-C39
10	AL	102	V7N	C27-C28-C29-C39
10	BW	102	V7N	C27-C28-C29-C39
12	Bc	1201	LMT	O5B-C5B-C6B-O6B
12	AX	1201	LMT	O5'-C5'-C6'-O6'
12	BC	102	LMT	O5B-C1B-O1B-C4'
11	Al	101	BCL	CBA-CGA-O2A-C1
12	Bd	1201	LMT	O5B-C5B-C6B-O6B
12	K	201	LMT	O5'-C5'-C6'-O6'
12	C	401	LMT	O5B-C5B-C6B-O6B
12	BG	103	LMT	O5'-C5'-C6'-O6'
13	AE	1101	PEX	C15-C14-O6-C2
12	Aa	103	LMT	O5'-C5'-C6'-O6'
12	Ad	102	LMT	O5B-C5B-C6B-O6B
12	Bp	1201	LMT	O5'-C5'-C6'-O6'
12	BQ	102	LMT	O5B-C5B-C6B-O6B
12	BS	102	LMT	O5'-C5'-C6'-O6'
12	BI	103	LMT	C4B-C5B-C6B-O6B
12	Bf	1203	LMT	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
12	AX	1201	LMT	C4'-C5'-C6'-O6'
16	L	303	BPH	C8-C10-C11-C12
12	Aj	102	LMT	O5B-C5B-C6B-O6B
12	M	401	LMT	O5B-C5B-C6B-O6B
12	C	401	LMT	C4'-C5'-C6'-O6'
19	C	404	HEC	C4B-C3B-CAB-CBB
14	M	408	MQ8	C46-C47-C48-C49
10	Bb	1202	V7N	C37-C22-C23-C24
10	Bk	101	V7N	C37-C22-C23-C24
10	AF	101	V7N	C37-C22-C23-C24
11	Aa	102	BCL	C4-C3-C5-C6
11	Bg	103	BCL	C4-C3-C5-C6
11	Al	101	BCL	C4-C3-C5-C6
11	AF	102	BCL	C4-C3-C5-C6
11	AM	102	BCL	C4-C3-C5-C6
14	L	305	MQ8	C34-C33-C35-C36
14	M	408	MQ8	C29-C28-C30-C31
10	Bk	101	V7N	C21-C22-C23-C24
10	AF	101	V7N	C21-C22-C23-C24
11	Aa	102	BCL	C2-C3-C5-C6
11	Ae	101	BCL	C2-C3-C5-C6
11	Bg	103	BCL	C2-C3-C5-C6
11	Al	101	BCL	C2-C3-C5-C6
11	BD	101	BCL	C2-C3-C5-C6
11	AF	102	BCL	C2-C3-C5-C6
11	AM	102	BCL	C2-C3-C5-C6
14	L	305	MQ8	C32-C33-C35-C36
12	BD	102	LMT	O5B-C5B-C6B-O6B
12	BH	103	LMT	O5B-C5B-C6B-O6B
12	AW	1201	LMT	O5B-C5B-C6B-O6B
11	Al	101	BCL	O1A-CGA-O2A-C1
12	M	401	LMT	O5'-C1'-O1'-C1
12	BO	101	LMT	O5'-C1'-O1'-C1
10	Be	1103	V7N	C22-C23-C24-C25
10	Bf	1202	V7N	C22-C23-C24-C25
10	Bh	1202	V7N	C22-C23-C24-C25
10	Bl	1202	V7N	C22-C23-C24-C25
10	Bn	101	V7N	C22-C23-C24-C25
14	Ad	103	MQ8	C13-C15-C16-C17
14	L	305	MQ8	C23-C25-C26-C27
14	L	305	MQ8	C28-C30-C31-C32
13	AA	1101	PEX	C5-C4-O4-C3

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Mol	Chain	Res	Type	Atoms
12	L	304	LMT	O5'-C5'-C6'-O6'
12	K	201	LMT	C4'-C5'-C6'-O6'
12	Be	1102	LMT	O5B-C1B-O1B-C4'
12	Bd	1201	LMT	C4B-C5B-C6B-O6B
14	L	305	MQ8	C36-C37-C38-C39
13	AE	1101	PEX	O7-C14-O6-C2
14	Ad	103	MQ8	C11-C12-C13-C15
14	L	305	MQ8	C36-C37-C38-C40
12	AW	1201	LMT	C4B-C5B-C6B-O6B
13	AA	1101	PEX	O5-C4-O4-C3
13	Bk	102	PEX	C5-C4-O4-C3
13	AE	1101	PEX	C5-C4-O4-C3
12	BH	103	LMT	C4B-C5B-C6B-O6B
12	BK	103	LMT	C4B-C5B-C6B-O6B
10	Bk	101	V7N	C27-C28-C29-C39
10	Bm	101	V7N	C27-C28-C29-C39
10	BT	101	V7N	C27-C28-C29-C39
11	BV	102	BCL	C8-C10-C11-C12
12	BQ	102	LMT	C4B-C5B-C6B-O6B
11	Bp	1203	BCL	C5-C6-C7-C8
11	AO	101	BCL	C8-C10-C11-C12
11	AR	101	BCL	C5-C6-C7-C8
12	C	401	LMT	O5'-C5'-C6'-O6'
12	BK	103	LMT	O5B-C5B-C6B-O6B
10	Aa	101	V7N	C37-C22-C23-C24
12	BD	102	LMT	C4B-C5B-C6B-O6B
10	Bf	1202	V7N	C21-C22-C23-C24
11	Ab	101	BCL	C11-C12-C13-C14
11	Bd	1203	BCL	C11-C12-C13-C14
11	Ai	101	BCL	C14-C13-C15-C16
11	Bj	1204	BCL	C11-C10-C8-C9
11	Ak	101	BCL	C11-C10-C8-C9
11	Am	101	BCL	C14-C13-C15-C16
11	Bn	103	BCL	C11-C12-C13-C14
11	Bp	1203	BCL	C11-C10-C8-C9
11	AC	101	BCL	C6-C7-C8-C9
11	AK	101	BCL	C14-C13-C15-C16
11	AN	101	BCL	C11-C10-C8-C9
11	AO	101	BCL	C11-C12-C13-C14
11	BU	102	BCL	C11-C12-C13-C14
11	AW	1203	BCL	C14-C13-C15-C16
11	AM	102	BCL	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
10	Aa	101	V7N	C38-C26-C27-C28
10	Bb	1202	V7N	C38-C26-C27-C28
10	Bf	1202	V7N	C38-C26-C27-C28
10	Bk	101	V7N	C38-C26-C27-C28
10	Bn	101	V7N	C11-C12-C13-C35
10	BD	103	V7N	C38-C26-C27-C28
10	BF	103	V7N	C38-C26-C27-C28
10	BI	101	V7N	C3-C4-C5-C33
10	BJ	101	V7N	C3-C4-C5-C33
10	BK	104	V7N	C38-C26-C27-C28
10	AL	102	V7N	C38-C26-C27-C28
10	BL	101	V7N	C38-C26-C27-C28
10	BL	101	V7N	C3-C4-C5-C33
10	BO	102	V7N	C38-C26-C27-C28
10	BO	102	V7N	C3-C4-C5-C33
10	BR	103	V7N	C38-C26-C27-C28
10	BU	104	V7N	C38-C26-C27-C28
10	BV	101	V7N	C38-C26-C27-C28
10	BV	101	V7N	C3-C4-C5-C33
10	BX	101	V7N	C36-C18-C19-C20
12	BC	102	LMT	C2B-C1B-O1B-C4'
10	Aa	101	V7N	C25-C26-C27-C28
10	Bb	1202	V7N	C25-C26-C27-C28
10	Bf	1202	V7N	C25-C26-C27-C28
10	Bk	101	V7N	C25-C26-C27-C28
10	Bp	1202	V7N	C25-C26-C27-C28
10	BD	103	V7N	C25-C26-C27-C28
10	BF	103	V7N	C25-C26-C27-C28
10	BI	101	V7N	C3-C4-C5-C6
10	BJ	101	V7N	C3-C4-C5-C6
10	BK	104	V7N	C25-C26-C27-C28
10	AL	102	V7N	C25-C26-C27-C28
10	BL	101	V7N	C3-C4-C5-C6
10	BO	102	V7N	C3-C4-C5-C6
10	BR	103	V7N	C25-C26-C27-C28
10	BU	104	V7N	C25-C26-C27-C28
10	BV	101	V7N	C3-C4-C5-C6
12	Be	1102	LMT	O5B-C5B-C6B-O6B
12	Bh	1201	LMT	O5B-C5B-C6B-O6B
12	BR	102	LMT	O5B-C5B-C6B-O6B
12	BR	102	LMT	O5'-C5'-C6'-O6'
12	Aj	102	LMT	C4B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
12	BR	102	LMT	C4B-C5B-C6B-O6B
12	BR	102	LMT	C4'-C5'-C6'-O6'
13	Bn	102	PEX	C4-C5-C6-C7
11	Ao	101	BCL	C15-C16-C17-C18
12	BB	103	LMT	O5'-C5'-C6'-O6'
12	Bp	1201	LMT	C4'-C5'-C6'-O6'
11	Al	101	BCL	C13-C15-C16-C17
11	AO	101	BCL	C10-C11-C12-C13
11	BS	101	BCL	C10-C11-C12-C13
11	AT	1102	BCL	C5-C6-C7-C8
13	Bm	102	PEX	C14-C15-C16-C17
11	Bf	1204	BCL	C8-C10-C11-C12
11	Ao	101	BCL	C5-C6-C7-C8
11	Ao	101	BCL	C13-C15-C16-C17
11	Bp	1203	BCL	C8-C10-C11-C12
11	BF	101	BCL	C5-C6-C7-C8
11	BF	101	BCL	C15-C16-C17-C18
12	BB	103	LMT	C4'-C5'-C6'-O6'
14	Ad	103	MQ8	C46-C47-C48-C50
14	L	305	MQ8	C46-C47-C48-C50
14	Ad	103	MQ8	C11-C12-C13-C14
13	Ba	1101	PEX	C14-C15-C16-C17
13	AS	1101	PEX	C4-C5-C6-C7
12	Bh	1201	LMT	C4B-C5B-C6B-O6B
11	Ao	101	BCL	C10-C11-C12-C13
13	Be	1104	PEX	C5-C6-C7-C8
12	Bb	1201	LMT	O5B-C5B-C6B-O6B
11	Ao	101	BCL	C2-C1-O2A-CGA
11	BP	101	BCL	C2-C1-O2A-CGA
12	BE	102	LMT	C3'-C4'-O1B-C1B
11	Am	101	BCL	C5-C6-C7-C8
13	Bc	1203	PEX	C4-C5-C6-C7
12	Bd	1201	LMT	C5'-C4'-O1B-C1B
13	Bc	1203	PEX	C17-C18-C19-C20
19	C	403	HEC	C3D-CAD-CBD-CGD
11	AJ	1102	BCL	C8-C10-C11-C12
11	Bp	1203	BCL	C6-C7-C8-C10
13	Bk	102	PEX	O5-C4-O4-C3
13	AE	1101	PEX	O5-C4-O4-C3
10	Bb	1202	V7N	C27-C28-C29-C39
10	Bn	101	V7N	C27-C28-C29-C39
10	Bp	1202	V7N	C27-C28-C29-C39

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Mol	Chain	Res	Type	Atoms
10	BA	102	V7N	C27-C28-C29-C39
10	BC	103	V7N	C27-C28-C29-C39
10	BJ	101	V7N	C27-C28-C29-C39
10	BJ	101	V7N	C5-C6-C7-C8
10	BN	102	V7N	C27-C28-C29-C39
11	Ai	101	BCL	C10-C11-C12-C13
11	Bp	1203	BCL	C13-C15-C16-C17
12	Bj	1201	LMT	O1'-C1-C2-C3
12	Bo	1201	LMT	O1'-C1-C2-C3
12	BQ	102	LMT	O1'-C1-C2-C3
12	BS	102	LMT	O1'-C1-C2-C3
12	Aa	103	LMT	C4'-C5'-C6'-O6'
12	Ad	102	LMT	C4B-C5B-C6B-O6B
12	BI	103	LMT	C4'-C5'-C6'-O6'
12	BM	1001	LMT	O5'-C1'-O1'-C1
10	Bc	1202	V7N	C22-C23-C24-C25
10	Bg	101	V7N	C22-C23-C24-C25
10	Bj	1202	V7N	C22-C23-C24-C25
10	An	101	V7N	C22-C23-C24-C25
10	AF	101	V7N	C22-C23-C24-C25
14	Ad	103	MQ8	C38-C40-C41-C42
14	M	408	MQ8	C13-C15-C16-C17
12	AX	1201	LMT	O1'-C1-C2-C3
10	Bb	1202	V7N	C26-C27-C28-C29
10	Bn	101	V7N	C26-C27-C28-C29
10	Bp	1202	V7N	C26-C27-C28-C29
10	BJ	101	V7N	C26-C27-C28-C29
10	BV	101	V7N	C26-C27-C28-C29
12	Bj	1203	LMT	O5B-C5B-C6B-O6B
12	BI	103	LMT	O5'-C5'-C6'-O6'
12	BU	101	LMT	O5B-C5B-C6B-O6B
12	BU	103	LMT	O5B-C5B-C6B-O6B
11	BO	103	BCL	C15-C16-C17-C18
11	AQ	102	BCL	C8-C10-C11-C12
12	BU	101	LMT	O1'-C1-C2-C3
12	BA	104	LMT	O1'-C1-C2-C3
12	BK	101	LMT	O1'-C1-C2-C3
12	BW	101	LMT	O1'-C1-C2-C3
11	Ai	101	BCL	C13-C15-C16-C17
11	AL	101	BCL	C13-C15-C16-C17
11	BP	101	BCL	C8-C10-C11-C12
12	BU	103	LMT	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
12	AW	1201	LMT	O5'-C5'-C6'-O6'
12	BU	101	LMT	C4B-C5B-C6B-O6B
12	AW	1201	LMT	C4'-C5'-C6'-O6'
11	Ac	101	BCL	C15-C16-C17-C18
13	Ba	1101	PEX	C24-O8-P1-O3
13	Be	1101	PEX	C1-O3-P1-O8
13	Be	1104	PEX	C1-O3-P1-O8
13	Bg	102	PEX	C1-O3-P1-O8
13	Bh	1203	PEX	C1-O3-P1-O8
13	Aj	103	PEX	C1-O3-P1-O8
13	Bk	102	PEX	C24-O8-P1-O3
13	Bm	102	PEX	C1-O3-P1-O8
13	Bn	102	PEX	C1-O3-P1-O8
13	AD	1101	PEX	C24-O8-P1-O3
13	AE	1101	PEX	C1-O3-P1-O8
13	AE	1101	PEX	C24-O8-P1-O3
13	AJ	1101	PEX	C1-O3-P1-O8
13	AP	1101	PEX	C24-O8-P1-O3
13	AT	1101	PEX	C1-O3-P1-O8
13	AT	1101	PEX	C24-O8-P1-O3
15	Af	102	CD4	C29-O8-P1-O5
15	Af	102	CD4	C31-O10-P2-O13
15	M	403	CD4	C28-O5-P1-O8
15	M	403	CD4	C29-O8-P1-O5
13	Bh	1203	PEX	C4-C5-C6-C7
12	Bc	1201	LMT	C4B-C5B-C6B-O6B
12	Ad	102	LMT	O5B-C1B-O1B-C4'
11	Bo	1202	BCL	C13-C15-C16-C17
12	C	401	LMT	C4B-C5B-C6B-O6B
11	Bj	1204	BCL	C4-C3-C5-C6
11	BK	102	BCL	C4-C3-C5-C6
12	BE	102	LMT	O1'-C1-C2-C3
11	Bc	1204	BCL	C2A-CAA-CBA-CGA
12	Bf	1201	LMT	O1'-C1-C2-C3
10	BI	101	V7N	C27-C28-C29-C39
10	BS	103	V7N	C27-C28-C29-C39
12	BS	102	LMT	C4'-C5'-C6'-O6'
13	AP	1101	PEX	C4-C5-C6-C7
12	BE	102	LMT	C5'-C4'-O1B-C1B
13	AA	1101	PEX	C15-C14-O6-C2
11	AI	101	BCL	C15-C16-C17-C18
12	Be	1102	LMT	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
12	AW	1201	LMT	C2-C3-C4-C5
13	Bg	102	PEX	C18-C19-C20-C21
13	Bh	1203	PEX	C7-C8-C9-C10
13	AT	1101	PEX	C7-C8-C9-C10
11	AO	101	BCL	C16-C17-C18-C19
11	BV	102	BCL	C16-C17-C18-C19
12	Aa	103	LMT	C4-C5-C6-C7
12	Ba	1102	LMT	C11-C10-C9-C8
12	Ad	102	LMT	C7-C8-C9-C10
12	Bd	1201	LMT	C3'-C4'-O1B-C1B
12	Bj	1201	LMT	C5-C6-C7-C8
12	Bj	1203	LMT	C7-C8-C9-C10
12	L	304	LMT	C2-C3-C4-C5
12	K	201	LMT	C4-C5-C6-C7
12	BK	103	LMT	C7-C8-C9-C10
13	AS	1101	PEX	C9-C10-C11-C12
13	AA	1101	PEX	O7-C14-O6-C2
12	Aa	103	LMT	C3-C4-C5-C6
12	BD	102	LMT	O1'-C1-C2-C3
12	Bp	1201	LMT	O1'-C1-C2-C3
12	BM	1001	LMT	C3-C4-C5-C6
12	BG	103	LMT	C4'-C5'-C6'-O6'
12	BB	103	LMT	O1'-C1-C2-C3
12	BH	103	LMT	O1'-C1-C2-C3
12	BM	1001	LMT	O1'-C1-C2-C3
12	BO	104	LMT	C3-C4-C5-C6
11	Bd	1203	BCL	C3-C5-C6-C7
12	Bb	1201	LMT	C2'-C1'-O1'-C1
12	Bd	1201	LMT	C2'-C1'-O1'-C1
12	M	401	LMT	C2'-C1'-O1'-C1
12	BA	105	LMT	C2'-C1'-O1'-C1
12	BM	1001	LMT	C2'-C1'-O1'-C1
12	BS	102	LMT	C2'-C1'-O1'-C1
13	Be	1104	PEX	C17-C18-C19-C20
11	Bp	1203	BCL	C16-C17-C18-C20
11	Bb	1203	BCL	C4-C3-C5-C6
11	L	302	BCL	C4-C3-C5-C6
12	BF	102	LMT	C6-C7-C8-C9
12	BG	103	LMT	O1'-C1-C2-C3
13	Be	1101	PEX	C15-C16-C17-C18
11	AH	101	BCL	C11-C10-C8-C9
11	AQ	102	BCL	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
11	BS	101	BCL	C6-C7-C8-C9
13	Bg	102	PEX	C4-C5-C6-C7
12	BE	102	LMT	C7-C8-C9-C10
12	BW	103	LMT	C5-C6-C7-C8
12	AX	1201	LMT	C3-C4-C5-C6
13	Bk	102	PEX	C15-C16-C17-C18
11	BK	102	BCL	C2A-CAA-CBA-CGA
10	Bi	101	V7N	C38-C26-C27-C28
10	Bp	1202	V7N	C38-C26-C27-C28
10	AF	101	V7N	C3-C4-C5-C33
10	BG	101	V7N	C38-C26-C27-C28
10	BJ	101	V7N	C38-C26-C27-C28
10	BP	102	V7N	C3-C4-C5-C33
10	BS	103	V7N	C38-C26-C27-C28
10	BW	102	V7N	C3-C4-C5-C33
13	Bn	102	PEX	C5-C6-C7-C8
13	AJ	1101	PEX	C5-C6-C7-C8
13	AJ	1101	PEX	C7-C8-C9-C10
10	Bi	101	V7N	C25-C26-C27-C28
10	An	101	V7N	C3-C4-C5-C6
10	AF	101	V7N	C3-C4-C5-C6
10	BG	101	V7N	C25-C26-C27-C28
10	BJ	101	V7N	C25-C26-C27-C28
10	BO	102	V7N	C25-C26-C27-C28
10	BP	102	V7N	C3-C4-C5-C6
10	BS	103	V7N	C25-C26-C27-C28
10	BW	102	V7N	C3-C4-C5-C6
12	Be	1102	LMT	C6-C7-C8-C9
12	Bh	1201	LMT	C5-C6-C7-C8
12	BI	103	LMT	C6-C7-C8-C9
12	BM	1001	LMT	C4-C5-C6-C7
13	AE	1101	PEX	C4-C5-C6-C7
12	Aa	103	LMT	C2-C3-C4-C5
12	BS	102	LMT	C3-C4-C5-C6
13	Bm	102	PEX	C18-C19-C20-C21
13	AJ	1101	PEX	C16-C17-C18-C19
13	AS	1101	PEX	C18-C19-C20-C21
11	Al	101	BCL	C16-C17-C18-C19
11	AM	102	BCL	C16-C17-C18-C19
11	AM	102	BCL	C16-C17-C18-C20
12	BA	105	LMT	O5'-C1'-O1'-C1
12	BS	102	LMT	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
11	Ak	101	BCL	C8-C10-C11-C12
11	BU	102	BCL	C10-C11-C12-C13
10	BS	103	V7N	C22-C23-C24-C25
12	Bf	1203	LMT	C6-C7-C8-C9
13	Be	1101	PEX	C7-C8-C9-C10
15	M	403	CD4	C20-C21-C22-C23
12	BW	103	LMT	O1'-C1-C2-C3
13	AT	1101	PEX	C17-C18-C19-C20
13	AA	1101	PEX	C4-C5-C6-C7
11	Bp	1204	BCL	C5-C6-C7-C8
12	Bl	1201	LMT	C4'-C5'-C6'-O6'
12	BD	102	LMT	O5B-C1B-O1B-C4'
11	Bf	1204	BCL	C3A-C2A-CAA-CBA
11	Bg	103	BCL	C3A-C2A-CAA-CBA
11	Bn	103	BCL	C3A-C2A-CAA-CBA
11	Bp	1204	BCL	C3A-C2A-CAA-CBA
11	BC	101	BCL	C3A-C2A-CAA-CBA
11	AQ	101	BCL	C3A-C2A-CAA-CBA
11	AT	1102	BCL	C3A-C2A-CAA-CBA
11	BU	102	BCL	C3A-C2A-CAA-CBA
12	Ba	1102	LMT	C2-C1-O1'-C1'
12	Ad	102	LMT	C2-C1-O1'-C1'
12	Bp	1201	LMT	C2-C1-O1'-C1'
12	BB	103	LMT	C2-C1-O1'-C1'
12	BQ	101	LMT	C2-C1-O1'-C1'
11	Bp	1203	BCL	C16-C17-C18-C19
11	AO	101	BCL	C16-C17-C18-C20
12	BW	103	LMT	O5B-C5B-C6B-O6B
12	BC	102	LMT	C1-C2-C3-C4
13	AD	1101	PEX	C15-C16-C17-C18
10	Bn	101	V7N	C29-C39-C40-O44
10	Bn	101	V7N	C29-C39-C40-O45
10	Bn	101	V7N	C43-C39-C40-O44
10	Bn	101	V7N	C43-C39-C40-O45
11	Ac	101	BCL	O2A-C1-C2-C3
12	Bh	1204	LMT	O1'-C1-C2-C3
12	BB	103	LMT	C5-C6-C7-C8
11	Bf	1204	BCL	C10-C11-C12-C13
11	Ai	101	BCL	C4-C3-C5-C6
11	Bo	1202	BCL	C4-C3-C5-C6
11	BC	101	BCL	C4-C3-C5-C6
11	AX	1202	BCL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
14	Ad	103	MQ8	C34-C33-C35-C36
16	L	303	BPH	C4-C3-C5-C6
11	Bb	1203	BCL	C2-C3-C5-C6
11	Bo	1202	BCL	C2-C3-C5-C6
11	AX	1202	BCL	C2-C3-C5-C6
14	Ad	103	MQ8	C32-C33-C35-C36
16	L	303	BPH	C2-C3-C5-C6
12	Bf	1203	LMT	O1'-C1-C2-C3
12	BA	105	LMT	C5-C6-C7-C8
12	BK	103	LMT	C11-C10-C9-C8
12	BS	102	LMT	C7-C8-C9-C10
12	BS	102	LMT	C6-C7-C8-C9
12	Ad	102	LMT	C5-C6-C7-C8
13	Bn	102	PEX	C17-C18-C19-C20
13	AS	1101	PEX	C5-C6-C7-C8
12	Bc	1201	LMT	C1-C2-C3-C4
11	BB	101	BCL	C2-C1-O2A-CGA
13	Be	1101	PEX	C6-C7-C8-C9
13	Bk	102	PEX	C9-C10-C11-C12
11	AM	102	BCL	C10-C11-C12-C13
12	K	201	LMT	C1-C2-C3-C4
12	BO	101	LMT	C4'-C5'-C6'-O6'
12	BH	101	LMT	C3-C4-C5-C6
13	Bg	102	PEX	C6-C7-C8-C9
11	BE	101	BCL	C15-C16-C17-C18
11	BX	102	BCL	C10-C11-C12-C13
13	AE	1101	PEX	C18-C19-C20-C21
13	Bh	1203	PEX	C14-C15-C16-C17
12	BA	104	LMT	C11-C10-C9-C8
14	Ad	103	MQ8	C46-C47-C48-C49
14	L	305	MQ8	C46-C47-C48-C49
13	AP	1101	PEX	C7-C8-C9-C10
11	BB	101	BCL	C4-C3-C5-C6
14	L	305	MQ8	C19-C18-C20-C21
10	Aa	101	V7N	C21-C22-C23-C24
10	Bb	1202	V7N	C21-C22-C23-C24
11	Bg	103	BCL	C12-C13-C15-C16
11	Ai	101	BCL	C2-C3-C5-C6
11	Ao	101	BCL	C11-C12-C13-C15
11	L	302	BCL	C2-C3-C5-C6
11	M	405	BCL	C12-C13-C15-C16
11	BB	101	BCL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
11	BC	101	BCL	C2-C3-C5-C6
11	BF	101	BCL	C12-C13-C15-C16
11	BI	102	BCL	C11-C12-C13-C15
11	BR	101	BCL	C12-C13-C15-C16
11	BS	101	BCL	C6-C7-C8-C10
11	AW	1203	BCL	C12-C13-C15-C16
14	L	305	MQ8	C17-C18-C20-C21
14	M	408	MQ8	C27-C28-C30-C31
12	BA	104	LMT	C9-C10-C11-C12
10	BF	103	V7N	C5-C6-C7-C8
11	AW	1204	BCL	C16-C17-C18-C20
13	Bc	1203	PEX	O7-C14-O6-C2
11	BX	102	BCL	C2A-CAA-CBA-CGA
11	BF	101	BCL	C8-C10-C11-C12
11	Bf	1204	BCL	C15-C16-C17-C18
11	BU	102	BCL	C15-C16-C17-C18
12	Ad	102	LMT	C4-C5-C6-C7
12	L	304	LMT	C5-C6-C7-C8
12	BL	103	LMT	C1-C2-C3-C4
12	BI	103	LMT	O5'-C1'-O1'-C1
11	Bc	1204	BCL	C5-C6-C7-C8
11	Al	101	BCL	C10-C11-C12-C13
12	BK	101	LMT	C1-C2-C3-C4
14	Ad	103	MQ8	C43-C44-C46-C47
14	L	305	MQ8	C38-C40-C41-C42
12	L	304	LMT	C3-C4-C5-C6
12	BA	104	LMT	C5-C6-C7-C8
13	Ba	1101	PEX	C15-C14-O6-C2
13	Bc	1203	PEX	C15-C14-O6-C2
13	Be	1101	PEX	C15-C14-O6-C2
13	AD	1101	PEX	C15-C14-O6-C2
12	Bf	1201	LMT	C6-C7-C8-C9
12	BF	102	LMT	C7-C8-C9-C10
13	Be	1101	PEX	O7-C14-O6-C2
13	AD	1101	PEX	O7-C14-O6-C2
12	Bc	1201	LMT	O5B-C1B-O1B-C4'
13	AP	1101	PEX	O6-C2-C3-O4
15	Af	102	CD4	O16-C33-C34-O14
12	Bl	1201	LMT	O5B-C5B-C6B-O6B
12	BE	102	LMT	O5B-C5B-C6B-O6B
11	Bj	1204	BCL	C2-C3-C5-C6
11	Bg	103	BCL	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
11	BI	102	BCL	C11-C12-C13-C14
11	BR	101	BCL	C14-C13-C15-C16
12	Ad	102	LMT	O5'-C5'-C6'-O6'
11	BB	101	BCL	C2A-CAA-CBA-CGA
11	AS	1102	BCL	C2A-CAA-CBA-CGA
12	BK	101	LMT	C4-C5-C6-C7
10	Be	1103	V7N	C3-C4-C5-C33
10	Bl	1202	V7N	C3-C4-C5-C33
10	BN	102	V7N	C38-C26-C27-C28
16	L	303	BPH	C2C-C3C-CAC-CBC
12	BS	102	LMT	C2-C3-C4-C5
10	Be	1103	V7N	C3-C4-C5-C6
10	BN	102	V7N	C25-C26-C27-C28
12	M	401	LMT	C1-C2-C3-C4
11	Bf	1204	BCL	C1A-C2A-CAA-CBA
11	Bg	103	BCL	C1A-C2A-CAA-CBA
11	Bp	1204	BCL	C1A-C2A-CAA-CBA
11	AT	1102	BCL	C1A-C2A-CAA-CBA
11	BV	102	BCL	C16-C17-C18-C20
13	Ba	1101	PEX	O7-C14-O6-C2
10	AF	101	V7N	C5-C6-C7-C8
12	BD	102	LMT	C1-C2-C3-C4
11	BC	101	BCL	C15-C16-C17-C18
11	Ao	101	BCL	CBA-CGA-O2A-C1
13	AD	1101	PEX	C11-C10-C9-C8
13	AP	1101	PEX	C15-C16-C17-C18
13	AT	1101	PEX	C4-C5-C6-C7
12	BG	103	LMT	O5B-C5B-C6B-O6B
11	AT	1103	BCL	C8-C10-C11-C12
12	M	401	LMT	C2-C3-C4-C5
12	BS	102	LMT	C5-C6-C7-C8
12	BW	101	LMT	C5-C6-C7-C8
12	AX	1201	LMT	C5-C6-C7-C8
13	Be	1104	PEX	C15-C16-C17-C18
11	BO	103	BCL	C10-C11-C12-C13
10	Bm	101	V7N	C1-C2-C3-C4
12	Bj	1203	LMT	O1'-C1-C2-C3
12	AW	1201	LMT	C3-C4-C5-C6
12	BF	102	LMT	O5B-C5B-C6B-O6B
11	M	405	BCL	C4-C3-C5-C6
11	AQ	101	BCL	C4-C3-C5-C6
14	M	408	MQ8	C36-C37-C38-C40

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Mol	Chain	Res	Type	Atoms
11	BB	101	BCL	C2C-C3C-CAC-CBC
11	BK	102	BCL	C2C-C3C-CAC-CBC
11	AQ	102	BCL	C2-C3-C5-C6
11	BR	101	BCL	C2-C3-C5-C6
12	Ad	102	LMT	C5'-C4'-O1B-C1B
12	Bf	1201	LMT	C5-C6-C7-C8
12	Bj	1203	LMT	C6-C7-C8-C9
12	BE	102	LMT	C5-C6-C7-C8
12	BC	102	LMT	C7-C8-C9-C10
11	AW	1204	BCL	C16-C17-C18-C19
13	Be	1101	PEX	C1-C2-C3-O4
13	Bg	102	PEX	C1-C2-C3-O4
12	BB	103	LMT	C9-C10-C11-C12
12	Aj	102	LMT	O5B-C1B-O1B-C4'
13	AS	1101	PEX	C15-C16-C17-C18
12	BO	104	LMT	C3'-C4'-O1B-C1B
10	Aa	101	V7N	C2-C1-O32-C41
10	Bc	1202	V7N	C2-C1-O32-C41
10	Be	1103	V7N	C2-C1-O32-C41
10	Bg	101	V7N	C2-C1-O32-C41
10	An	101	V7N	C2-C1-O32-C41
12	Bf	1203	LMT	C5-C6-C7-C8
12	BW	101	LMT	C4'-C5'-C6'-O6'
12	M	401	LMT	C4B-C5B-C6B-O6B
11	AB	101	BCL	C10-C11-C12-C13
11	BK	102	BCL	C8-C10-C11-C12
12	Bf	1201	LMT	O5'-C5'-C6'-O6'
12	Bp	1201	LMT	O5B-C5B-C6B-O6B
12	BA	104	LMT	O5B-C5B-C6B-O6B
11	AQ	102	BCL	C4-C3-C5-C6
11	BR	101	BCL	C4-C3-C5-C6
15	Af	102	CD4	C49-C50-C51-C52
11	BK	102	BCL	C2-C3-C5-C6
11	Al	101	BCL	C16-C17-C18-C20
12	BH	103	LMT	O5'-C5'-C6'-O6'
11	BN	101	BCL	C15-C16-C17-C18
13	AJ	1101	PEX	C3-C2-O6-C14
12	M	401	LMT	O5'-C5'-C6'-O6'
11	AJ	1103	BCL	C2A-CAA-CBA-CGA
11	BV	102	BCL	C2-C1-O2A-CGA
12	Bh	1201	LMT	O1'-C1-C2-C3
12	Bp	1201	LMT	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
12	BH	101	LMT	C6-C7-C8-C9
12	BO	101	LMT	C5-C6-C7-C8
12	Aj	102	LMT	O5'-C5'-C6'-O6'
12	AX	1201	LMT	O5B-C5B-C6B-O6B
12	BC	102	LMT	C6-C7-C8-C9
12	BC	102	LMT	C9-C10-C11-C12
11	AR	101	BCL	C10-C11-C12-C13
12	BK	103	LMT	C9-C10-C11-C12
11	Am	101	BCL	C16-C17-C18-C19
12	BO	101	LMT	C11-C10-C9-C8
10	Aa	101	V7N	C30-C1-O32-C41
10	Bc	1202	V7N	C30-C1-O32-C41
10	Bd	1202	V7N	C31-C1-O32-C41
10	Be	1103	V7N	C31-C1-O32-C41
10	Bg	101	V7N	C31-C1-O32-C41
10	Bl	1202	V7N	C30-C1-O32-C41
10	Bl	1202	V7N	C31-C1-O32-C41
10	An	101	V7N	C30-C1-O32-C41
10	An	101	V7N	C31-C1-O32-C41
10	Bn	101	V7N	C30-C1-O32-C41
10	Bp	1202	V7N	C31-C1-O32-C41
18	M	407	CRT	C2-C1-O1-C1M
18	M	407	CRT	C3-C1-O1-C1M
15	M	403	CD4	O14-C35-C36-C37
12	BC	102	LMT	C4'-C5'-C6'-O6'
11	Be	1105	BCL	C5-C6-C7-C8
11	BA	101	BCL	C10-C11-C12-C13
11	Ao	101	BCL	O1A-CGA-O2A-C1
10	Bb	1202	V7N	C30-C1-C2-C3
10	Bd	1202	V7N	C30-C1-C2-C3
10	Bj	1202	V7N	C30-C1-C2-C3
10	An	101	V7N	C30-C1-C2-C3
10	BB	102	V7N	C30-C1-C2-C3
10	AF	101	V7N	C30-C1-C2-C3
10	BJ	101	V7N	C31-C1-C2-C3
10	BR	103	V7N	C30-C1-C2-C3
10	BV	101	V7N	C30-C1-C2-C3
10	BW	102	V7N	C30-C1-C2-C3
11	L	302	BCL	C4B-C3B-CAB-OBB
11	L	302	BCL	C4B-C3B-CAB-CBB
12	L	304	LMT	C11-C10-C9-C8
11	AD	1102	BCL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
14	Ad	103	MQ8	C19-C18-C20-C21
11	Ab	101	BCL	C11-C12-C13-C15
11	Ai	101	BCL	C12-C13-C15-C16
11	Al	101	BCL	C6-C7-C8-C10
11	Bn	103	BCL	C11-C12-C13-C15
11	Bo	1202	BCL	C6-C7-C8-C10
11	AF	102	BCL	C11-C12-C13-C15
11	AM	102	BCL	C11-C12-C13-C15
11	AO	101	BCL	C11-C12-C13-C15
11	AQ	101	BCL	C2-C3-C5-C6
16	L	303	BPH	C11-C12-C13-C15
16	M	406	BPH	C11-C10-C8-C7
11	Bo	1202	BCL	C6-C7-C8-C9
11	Bo	1202	BCL	C14-C13-C15-C16
11	Bp	1203	BCL	C6-C7-C8-C9
11	Bp	1203	BCL	C11-C12-C13-C14
11	M	405	BCL	C14-C13-C15-C16
11	AM	102	BCL	C11-C12-C13-C14
11	BX	102	BCL	C11-C12-C13-C14
16	M	406	BPH	C11-C10-C8-C9
13	Be	1104	PEX	C11-C10-C9-C8
10	Aa	101	V7N	O32-C1-C2-C3
10	Be	1103	V7N	O32-C1-C2-C3
10	BF	103	V7N	O32-C1-C2-C3
10	BJ	101	V7N	O32-C1-C2-C3
10	BP	102	V7N	O32-C1-C2-C3
10	BS	103	V7N	O32-C1-C2-C3
12	BU	103	LMT	O5B-C1B-O1B-C4'
10	Aa	101	V7N	C3-C4-C5-C33
10	Bf	1202	V7N	C3-C4-C5-C33
10	BR	103	V7N	C3-C4-C5-C33
11	Aa	102	BCL	C16-C17-C18-C20
11	AI	101	BCL	C16-C17-C18-C20
10	Bl	1202	V7N	C3-C4-C5-C6
10	Bn	101	V7N	C11-C12-C13-C14
10	BB	102	V7N	C3-C4-C5-C6
10	BF	103	V7N	C3-C4-C5-C6
10	BR	103	V7N	C3-C4-C5-C6
13	Bn	102	PEX	C18-C19-C20-C21
13	Ba	1101	PEX	C10-C11-C12-C13
13	Bc	1203	PEX	C14-C15-C16-C17
15	M	403	CD4	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
13	Aj	103	PEX	C11-C10-C9-C8
11	Ao	101	BCL	C16-C17-C18-C20
11	AW	1203	BCL	C5-C6-C7-C8
11	AS	1102	BCL	C3-C5-C6-C7
14	M	408	MQ8	C33-C35-C36-C37
13	Ba	1101	PEX	C9-C10-C11-C12
13	Aj	103	PEX	C17-C18-C19-C20
13	Be	1104	PEX	O8-C24-C25-N1
13	AS	1101	PEX	O8-C24-C25-N1
13	AP	1101	PEX	C5-C4-O4-C3
13	Bm	102	PEX	C7-C8-C9-C10
11	AD	1102	BCL	C2-C3-C5-C6
14	Ad	103	MQ8	C17-C18-C20-C21
11	AE	1102	BCL	C10-C11-C12-C13
13	Be	1104	PEX	C19-C20-C21-C22
12	BM	1001	LMT	C6-C7-C8-C9
11	Ae	101	BCL	C2A-CAA-CBA-CGA
11	AW	1204	BCL	C2A-CAA-CBA-CGA
11	Al	101	BCL	C3A-C2A-CAA-CBA
11	BG	102	BCL	C3A-C2A-CAA-CBA
12	Bl	1201	LMT	C2-C1-O1'-C1'
12	M	401	LMT	C2-C1-O1'-C1'
12	K	201	LMT	C2-C1-O1'-C1'
12	BD	102	LMT	C2-C1-O1'-C1'
12	BW	103	LMT	C2-C1-O1'-C1'
12	Bo	1201	LMT	C9-C10-C11-C12
13	AP	1101	PEX	C1-C2-C3-O4
15	Af	102	CD4	C32-C33-C34-O14
13	AJ	1101	PEX	C19-C20-C21-C22
12	Bh	1201	LMT	C6-C7-C8-C9
12	BQ	102	LMT	C4-C5-C6-C7
11	AK	101	BCL	O2A-C1-C2-C3
14	L	305	MQ8	C29-C28-C30-C31
12	Bl	1201	LMT	C2-C3-C4-C5
15	Af	102	CD4	C28-O5-P1-O8
15	M	403	CD4	C31-O10-P2-O13
12	BB	103	LMT	O5B-C5B-C6B-O6B
12	BC	102	LMT	C3-C4-C5-C6
13	Be	1104	PEX	O3-C1-C2-O6
13	Bn	102	PEX	O3-C1-C2-O6
13	AS	1101	PEX	O3-C1-C2-O6
12	Ba	1102	LMT	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
12	BA	105	LMT	C6-C7-C8-C9
11	AI	101	BCL	C16-C17-C18-C19
13	Bg	102	PEX	C15-C16-C17-C18
12	Bf	1203	LMT	C4'-C5'-C6'-O6'
12	Ad	102	LMT	C3-C4-C5-C6
13	AA	1101	PEX	O6-C2-C3-O4
11	Bh	1205	BCL	C5-C6-C7-C8
12	L	304	LMT	C4'-C5'-C6'-O6'
12	BW	103	LMT	C5'-C4'-O1B-C1B
11	Bo	1202	BCL	C10-C11-C12-C13
10	Aa	101	V7N	C22-C23-C24-C25
10	BA	102	V7N	C22-C23-C24-C25
15	Af	102	CD4	O8-C29-C30-C31
12	Bj	1201	LMT	C6-C7-C8-C9
12	BH	101	LMT	C7-C8-C9-C10
11	Am	101	BCL	C2-C1-O2A-CGA
11	Bo	1202	BCL	C2-C1-O2A-CGA
11	BG	102	BCL	C2-C1-O2A-CGA
11	AO	101	BCL	C2-C1-O2A-CGA
11	AW	1203	BCL	C2-C1-O2A-CGA
12	BR	102	LMT	O1'-C1-C2-C3
11	Bf	1204	BCL	C14-C13-C15-C16
11	Bg	103	BCL	C11-C12-C13-C14
11	AQ	103	BCL	C6-C7-C8-C9
13	AD	1101	PEX	C17-C18-C19-C20
12	BH	103	LMT	C4-C5-C6-C7
11	Am	101	BCL	C8-C10-C11-C12
12	Bh	1204	LMT	C3-C4-C5-C6
13	AT	1101	PEX	C9-C10-C11-C12
11	Bd	1203	BCL	C2A-CAA-CBA-CGA
11	Be	1105	BCL	C2A-CAA-CBA-CGA
11	Aa	102	BCL	C16-C17-C18-C19
11	Aa	102	BCL	C8-C10-C11-C12
13	AP	1101	PEX	C11-C10-C9-C8
10	Bc	1202	V7N	C38-C26-C27-C28
10	BB	102	V7N	C3-C4-C5-C33
10	BF	103	V7N	C3-C4-C5-C33
10	BX	101	V7N	C17-C18-C19-C20
11	Bg	103	BCL	C4C-C3C-CAC-CBC
11	Bh	1205	BCL	C4C-C3C-CAC-CBC
11	BE	101	BCL	C4C-C3C-CAC-CBC
11	BX	102	BCL	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
14	M	408	MQ8	C36-C37-C38-C39
12	BF	102	LMT	C3-C4-C5-C6
13	Bk	102	PEX	C11-C10-C9-C8
11	BK	102	BCL	C10-C11-C12-C13
13	Bn	102	PEX	O3-C1-C2-C3
13	AA	1101	PEX	O3-C1-C2-C3
13	AP	1101	PEX	O3-C1-C2-C3
13	AS	1101	PEX	O3-C1-C2-C3
12	Bb	1201	LMT	C3-C4-C5-C6
13	AD	1101	PEX	C6-C7-C8-C9
11	Al	101	BCL	C11-C10-C8-C7
11	Bo	1202	BCL	C12-C13-C15-C16
11	Bp	1203	BCL	C11-C12-C13-C15
11	AQ	103	BCL	C6-C7-C8-C10
12	BO	101	LMT	O5'-C5'-C6'-O6'
12	BQ	102	LMT	C5-C6-C7-C8
13	AP	1101	PEX	C17-C18-C19-C20
13	AT	1101	PEX	C6-C7-C8-C9
10	Bc	1202	V7N	C13-C14-C15-C16
10	BB	102	V7N	C5-C6-C7-C8
11	Am	101	BCL	C16-C17-C18-C20
12	BU	103	LMT	C1-C2-C3-C4
13	Ba	1101	PEX	C4-C5-C6-C7
12	BO	101	LMT	O5B-C5B-C6B-O6B
13	AJ	1101	PEX	C6-C7-C8-C9
11	Ao	101	BCL	C16-C17-C18-C19
12	BA	104	LMT	C7-C8-C9-C10
13	Bk	102	PEX	C5-C6-C7-C8
12	Bf	1203	LMT	C3-C4-C5-C6
13	Bm	102	PEX	C19-C20-C21-C22
11	Ab	101	BCL	CAD-CBD-CGD-O2D
11	Bd	1203	BCL	CAD-CBD-CGD-O2D
11	Ae	101	BCL	CAD-CBD-CGD-O2D
11	Af	101	BCL	CAD-CBD-CGD-O2D
11	Bf	1204	BCL	CAD-CBD-CGD-O2D
11	Bg	103	BCL	CAD-CBD-CGD-O2D
11	Ai	101	BCL	CAD-CBD-CGD-O2D
11	Bi	102	BCL	CAD-CBD-CGD-O2D
11	Ak	101	BCL	CAD-CBD-CGD-O2D
11	Bm	103	BCL	CAD-CBD-CGD-O2D
11	Bn	103	BCL	CAD-CBD-CGD-O2D
11	Bo	1202	BCL	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
11	Bp	1204	BCL	CAD-CBD-CGD-O2D
11	L	301	BCL	CAD-CBD-CGD-O2D
11	BB	101	BCL	CAD-CBD-CGD-O2D
11	AC	101	BCL	CAD-CBD-CGD-O2D
11	AE	1102	BCL	CAD-CBD-CGD-O2D
11	AG	101	BCL	CAD-CBD-CGD-O2D
11	AI	102	BCL	CAD-CBD-CGD-O2D
11	AJ	1103	BCL	CAD-CBD-CGD-O2D
11	BK	102	BCL	CAD-CBD-CGD-O2D
11	AM	101	BCL	CAD-CBD-CGD-O2D
11	AM	102	BCL	CAD-CBD-CGD-O2D
11	AO	101	BCL	CAD-CBD-CGD-O2D
11	AR	101	BCL	CAD-CBD-CGD-O2D
11	AS	1102	BCL	CAD-CBD-CGD-O2D
11	AT	1103	BCL	CAD-CBD-CGD-O2D
11	AU	1001	BCL	CAD-CBD-CGD-O2D
11	AV	1001	BCL	CAD-CBD-CGD-O2D
11	AW	1202	BCL	CAD-CBD-CGD-O2D
13	AE	1101	PEX	C3-C2-O6-C14
16	M	406	BPH	CAD-CBD-CGD-O2D
13	AP	1101	PEX	C9-C10-C11-C12
11	Am	101	BCL	C15-C16-C17-C18
11	Bl	1203	BCL	C4-C3-C5-C6
12	BO	104	LMT	O5'-C1'-O1'-C1
11	BN	101	BCL	C8-C10-C11-C12
12	Bl	1201	LMT	O5'-C5'-C6'-O6'
13	Bk	102	PEX	C1-C2-C3-O4
13	Ba	1101	PEX	O3-C1-C2-O6
11	AF	102	BCL	C15-C16-C17-C18
12	AW	1201	LMT	C6-C7-C8-C9
11	Ao	101	BCL	CBD-CGD-O2D-CED
12	BA	105	LMT	C4B-C5B-C6B-O6B
13	AP	1101	PEX	O5-C4-O4-C3
12	Be	1102	LMT	C4-C5-C6-C7
12	BI	103	LMT	C2'-C1'-O1'-C1
12	BE	102	LMT	C11-C10-C9-C8
13	Be	1104	PEX	O6-C2-C3-O4
13	AJ	1101	PEX	O6-C2-C3-O4
15	Af	102	CD4	O2-C15-C16-O3
12	BD	102	LMT	C4'-C5'-C6'-O6'
11	Bb	1203	BCL	C5-C6-C7-C8
12	BB	103	LMT	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
12	BQ	101	LMT	C1-C2-C3-C4
11	Bp	1204	BCL	C4-C3-C5-C6
13	Bg	102	PEX	C19-C20-C21-C22
13	AE	1101	PEX	C16-C17-C18-C19
11	Bf	1204	BCL	C11-C10-C8-C9
11	AG	101	BCL	C14-C13-C15-C16
11	BO	103	BCL	C11-C12-C13-C14
12	Bd	1201	LMT	C3-C4-C5-C6
12	BW	101	LMT	O5'-C5'-C6'-O6'
12	Bh	1204	LMT	C2-C3-C4-C5
11	Bj	1204	BCL	C2A-CAA-CBA-CGA
12	Bf	1203	LMT	C7-C8-C9-C10
10	Bb	1202	V7N	C3-C4-C5-C33
10	Bc	1202	V7N	C3-C4-C5-C33
10	Bi	101	V7N	C3-C4-C5-C33
11	AS	1102	BCL	C5-C6-C7-C8
16	M	406	BPH	C15-C16-C17-C18
10	Aa	101	V7N	C3-C4-C5-C6
10	Bb	1202	V7N	C3-C4-C5-C6
10	Bf	1202	V7N	C3-C4-C5-C6
10	Bi	101	V7N	C3-C4-C5-C6
10	BV	101	V7N	C25-C26-C27-C28
11	Al	101	BCL	C1A-C2A-CAA-CBA
11	BG	102	BCL	C1A-C2A-CAA-CBA
11	BB	101	BCL	C13-C15-C16-C17
11	AK	101	BCL	C8-C10-C11-C12
13	Bn	102	PEX	C7-C8-C9-C10
12	Be	1102	LMT	C4B-C5B-C6B-O6B
13	Bh	1203	PEX	C9-C10-C11-C12
12	BE	102	LMT	C1-C2-C3-C4
13	Ba	1101	PEX	C1-O3-P1-O8
13	Bc	1203	PEX	C1-O3-P1-O8
13	Bh	1203	PEX	C24-O8-P1-O3
13	AA	1101	PEX	C1-O3-P1-O8
13	AJ	1101	PEX	C24-O8-P1-O3
15	Af	102	CD4	C32-O13-P2-O10
12	L	304	LMT	C5'-C4'-O1B-C1B
12	M	401	LMT	C6-C7-C8-C9
12	BO	101	LMT	C4B-C5B-C6B-O6B
19	C	404	HEC	C2C-C3C-CAC-CBC
10	BK	104	V7N	C37-C22-C23-C24
13	Bh	1203	PEX	C2-C1-O3-P1

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Mol	Chain	Res	Type	Atoms
11	M	405	BCL	C2-C3-C5-C6
12	Ad	102	LMT	C3'-C4'-O1B-C1B
13	Bc	1203	PEX	C15-C16-C17-C18
13	Bg	102	PEX	C1-O3-P1-O2
13	Bh	1203	PEX	C1-O3-P1-O2
13	Aj	103	PEX	C1-O3-P1-O1
13	Aj	103	PEX	C24-O8-P1-O1
13	Bk	102	PEX	C24-O8-P1-O1
13	AD	1101	PEX	C24-O8-P1-O1
13	AD	1101	PEX	C24-O8-P1-O2
13	AE	1101	PEX	C24-O8-P1-O2
13	AJ	1101	PEX	C1-O3-P1-O1
13	AP	1101	PEX	C24-O8-P1-O2
13	AT	1101	PEX	C1-O3-P1-O1
13	AT	1101	PEX	C24-O8-P1-O2
15	Af	102	CD4	C28-O5-P1-O6
15	Af	102	CD4	C31-O10-P2-O12
15	M	403	CD4	C28-O5-P1-O6
15	M	403	CD4	C28-O5-P1-O7
15	M	403	CD4	C29-O8-P1-O7
13	AE	1101	PEX	C20-C21-C22-C23
13	Ba	1101	PEX	O3-C1-C2-C3
13	Bk	102	PEX	O3-C1-C2-C3
13	AD	1101	PEX	O3-C1-C2-C3
12	Ba	1102	LMT	C7-C8-C9-C10
13	Bm	102	PEX	O8-C24-C25-N1
11	BL	102	BCL	C2A-CAA-CBA-CGA
12	AW	1201	LMT	C1-C2-C3-C4
12	BE	102	LMT	C3-C4-C5-C6
13	Bg	102	PEX	C25-C24-O8-P1
11	Am	101	BCL	C10-C11-C12-C13
11	BA	103	BCL	C15-C16-C17-C18
10	BS	103	V7N	C1-C2-C3-C4
12	Bl	1201	LMT	C5-C6-C7-C8
11	BO	103	BCL	C4-C3-C5-C6
11	Bd	1203	BCL	C11-C12-C13-C15
11	Ak	101	BCL	C3A-C2A-CAA-CBA
11	Am	101	BCL	C12-C13-C15-C16
11	Ao	101	BCL	C2C-C3C-CAC-CBC
11	AK	101	BCL	C12-C13-C15-C16
11	BK	102	BCL	C6-C7-C8-C10
11	BR	101	BCL	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
11	AT	1103	BCL	C11-C10-C8-C7
11	AV	1001	BCL	C6-C7-C8-C10
13	Bg	102	PEX	O3-C1-C2-O6
13	AA	1101	PEX	O3-C1-C2-O6
13	AD	1101	PEX	O3-C1-C2-O6
13	AP	1101	PEX	O3-C1-C2-O6
10	Bf	1202	V7N	C27-C28-C29-C39
11	L	302	BCL	C2B-C3B-CAB-OBB
11	L	302	BCL	C2B-C3B-CAB-CBB
12	Bb	1201	LMT	C5'-C4'-O1B-C1B
12	BG	103	LMT	C6-C7-C8-C9
13	Bk	102	PEX	C18-C19-C20-C21
11	AH	101	BCL	C3-C5-C6-C7
12	Bd	1201	LMT	C4'-C5'-C6'-O6'
10	Bd	1202	V7N	O42-C34-C9-C10
10	BJ	101	V7N	C7-C8-C9-C10
10	AL	102	V7N	O42-C34-C9-C10
10	BN	102	V7N	O42-C34-C9-C10
10	BO	102	V7N	C7-C8-C9-C10
10	BR	103	V7N	O42-C34-C9-C10
10	BT	101	V7N	O42-C34-C9-C10
12	Ba	1102	LMT	O1'-C1-C2-C3
16	L	303	BPH	C4C-C3C-CAC-CBC
13	Ba	1101	PEX	O6-C2-C3-O4
13	AS	1101	PEX	O6-C2-C3-O4
13	AE	1101	PEX	C19-C20-C21-C22
11	Ao	101	BCL	O1D-CGD-O2D-CED
13	AE	1101	PEX	C11-C10-C9-C8
11	Aj	101	BCL	C15-C16-C17-C18
11	Bp	1204	BCL	C2-C3-C5-C6
11	Aj	101	BCL	C6-C7-C8-C9
11	Al	101	BCL	C11-C10-C8-C9
11	AF	102	BCL	C11-C12-C13-C14
11	AT	1103	BCL	C11-C10-C8-C9
11	AX	1202	BCL	C6-C7-C8-C9
11	Ao	101	BCL	C3-C5-C6-C7
10	BW	102	V7N	C22-C23-C24-C25
14	L	305	MQ8	C33-C35-C36-C37
11	AC	101	BCL	C2A-CAA-CBA-CGA
12	BB	103	LMT	C6-C7-C8-C9
13	Be	1104	PEX	C9-C10-C11-C12
12	BO	104	LMT	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
12	BU	103	LMT	C2B-C1B-O1B-C4'
15	Af	102	CD4	C38-C39-C40-C41
12	BD	102	LMT	C5'-C4'-O1B-C1B
12	BH	103	LMT	C9-C10-C11-C12
12	Bc	1201	LMT	C2B-C1B-O1B-C4'
11	AJ	1102	BCL	C4-C3-C5-C6
12	BE	102	LMT	C6-C7-C8-C9
10	BK	104	V7N	C21-C22-C23-C24
11	Bl	1203	BCL	C2-C3-C5-C6
12	BC	102	LMT	O5'-C5'-C6'-O6'
12	BB	103	LMT	C5'-C4'-O1B-C1B
12	K	201	LMT	C3-C4-C5-C6
13	Be	1104	PEX	O3-C1-C2-C3
13	Bg	102	PEX	O3-C1-C2-C3
11	BH	104	BCL	C2A-CAA-CBA-CGA
11	BI	102	BCL	C2A-CAA-CBA-CGA
11	BO	103	BCL	C2A-CAA-CBA-CGA
12	Bb	1201	LMT	C2-C3-C4-C5
11	Bc	1204	BCL	C2-C1-O2A-CGA
11	BA	101	BCL	C2-C1-O2A-CGA
11	AI	102	BCL	C2-C1-O2A-CGA
11	AM	101	BCL	C2-C1-O2A-CGA
11	AU	1001	BCL	C2-C1-O2A-CGA
11	AX	1202	BCL	C2-C1-O2A-CGA
12	Aj	102	LMT	C11-C10-C9-C8
12	AX	1201	LMT	C2-C3-C4-C5
15	Af	102	CD4	C35-C36-C37-C38
11	BI	102	BCL	C3-C5-C6-C7
12	Bh	1204	LMT	C9-C10-C11-C12
13	AT	1101	PEX	C15-C16-C17-C18
12	BF	102	LMT	O1'-C1-C2-C3
11	BA	101	BCL	C13-C15-C16-C17
11	AW	1204	BCL	C4-C3-C5-C6
12	Bb	1201	LMT	C7-C8-C9-C10
12	BA	105	LMT	C5'-C4'-O1B-C1B
11	BX	102	BCL	C8-C10-C11-C12
12	Bo	1201	LMT	C3-C4-C5-C6
13	AS	1101	PEX	C6-C7-C8-C9
10	Aa	101	V7N	C31-C1-O32-C41
10	Bc	1202	V7N	C31-C1-O32-C41
10	Bd	1202	V7N	C30-C1-O32-C41
10	Be	1103	V7N	C30-C1-O32-C41

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Mol	Chain	Res	Type	Atoms
10	Bg	101	V7N	C30-C1-O32-C41
10	Bm	101	V7N	C30-C1-O32-C41
10	Bn	101	V7N	C31-C1-O32-C41
10	Bp	1202	V7N	C30-C1-O32-C41
10	BC	103	V7N	C22-C23-C24-C25
10	BJ	101	V7N	C22-C23-C24-C25
13	Bg	102	PEX	O6-C2-C3-O4
13	Bg	102	PEX	C24-O8-P1-O3
13	Bk	102	PEX	C1-O3-P1-O8
13	AD	1101	PEX	C1-O3-P1-O8
13	AP	1101	PEX	C1-O3-P1-O8
13	AS	1101	PEX	C1-O3-P1-O8
11	AK	101	BCL	C15-C16-C17-C18
10	BV	101	V7N	C31-C1-C2-C3
10	BW	102	V7N	C31-C1-C2-C3
11	AM	102	BCL	C15-C16-C17-C18
13	AA	1101	PEX	C1-C2-C3-O4
11	Bf	1204	BCL	C11-C10-C8-C7
11	BC	101	BCL	C11-C12-C13-C15
11	AQ	102	BCL	C6-C7-C8-C10
13	Aj	103	PEX	C9-C10-C11-C12
11	BC	101	BCL	CAA-CBA-CGA-O2A
11	BR	101	BCL	C11-C10-C8-C9
11	AV	1001	BCL	C6-C7-C8-C9
10	BO	102	V7N	C9-C10-C11-C12
12	BS	102	LMT	C5'-C4'-O1B-C1B
11	Bi	102	BCL	C2A-CAA-CBA-CGA
10	Bc	1202	V7N	O32-C1-C2-C3
11	AU	1001	BCL	C16-C17-C18-C19
13	Bg	102	PEX	C2-C1-O3-P1
13	Bk	102	PEX	C2-C1-O3-P1
12	Bj	1201	LMT	C7-C8-C9-C10
12	Bd	1201	LMT	C6-C7-C8-C9
10	Aa	101	V7N	C19-C20-C21-C22
10	BO	102	V7N	C5-C6-C7-C8
10	BX	101	V7N	C27-C28-C29-C39
12	BQ	102	LMT	C1-C2-C3-C4
13	Bg	102	PEX	C7-C8-C9-C10
12	BD	102	LMT	C2B-C1B-O1B-C4'
13	Be	1101	PEX	O8-C24-C25-N1
13	Bc	1203	PEX	O3-C1-C2-O6
10	Bg	101	V7N	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
19	C	402	HEC	C2B-C3B-CAB-CBB
10	BG	101	V7N	C26-C27-C28-C29
11	Bf	1204	BCL	C4-C3-C5-C6
11	BA	101	BCL	C4-C3-C5-C6
11	BA	103	BCL	C4-C3-C5-C6
11	AG	101	BCL	C4-C3-C5-C6
11	AK	101	BCL	C4-C3-C5-C6
11	BS	101	BCL	C4-C3-C5-C6
11	BA	101	BCL	C2-C3-C5-C6
11	AJ	1102	BCL	C2-C3-C5-C6
11	AK	101	BCL	C13-C15-C16-C17
11	Ab	101	BCL	C2-C1-O2A-CGA
11	L	301	BCL	C2-C1-O2A-CGA
11	AR	101	BCL	C2-C1-O2A-CGA
11	AT	1102	BCL	C2-C1-O2A-CGA
11	Bn	103	BCL	C13-C15-C16-C17
12	Bf	1201	LMT	C4-C5-C6-C7
11	Bf	1204	BCL	C2A-CAA-CBA-CGA
11	BC	101	BCL	C2A-CAA-CBA-CGA
11	BP	101	BCL	C2A-CAA-CBA-CGA
12	Bo	1201	LMT	C2-C3-C4-C5
10	Bj	1202	V7N	C19-C20-C21-C22
12	BO	104	LMT	O1'-C1-C2-C3
13	Be	1101	PEX	C5-C6-C7-C8
10	BP	102	V7N	C37-C22-C23-C24
12	BF	102	LMT	C4'-C5'-C6'-O6'
11	Bd	1203	BCL	C11-C10-C8-C9
11	Ao	101	BCL	C6-C7-C8-C9
11	BF	101	BCL	C6-C7-C8-C9
11	BG	102	BCL	C6-C7-C8-C9
11	BN	101	BCL	C11-C12-C13-C14
11	BP	101	BCL	C6-C7-C8-C9
11	BU	102	BCL	C14-C13-C15-C16
11	AJ	1103	BCL	C16-C17-C18-C19
11	AU	1001	BCL	C16-C17-C18-C20
11	Ac	101	BCL	C8-C10-C11-C12
11	BO	103	BCL	C13-C15-C16-C17
12	BM	1001	LMT	C11-C10-C9-C8
13	Be	1101	PEX	C11-C10-C9-C8
13	Bh	1203	PEX	C19-C20-C21-C22
13	AE	1101	PEX	C7-C8-C9-C10
11	Bb	1203	BCL	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
12	Be	1102	LMT	C5-C6-C7-C8
11	Aj	101	BCL	C16-C17-C18-C19
16	L	303	BPH	O2A-C1-C2-C3
19	C	402	HEC	C1A-C2A-CAA-CBA
12	Ad	102	LMT	O5'-C1'-O1'-C1
12	BC	102	LMT	O5'-C1'-O1'-C1
19	C	405	HEC	C2C-C3C-CAC-CBC
10	Bj	1202	V7N	C11-C12-C13-C35
12	Bo	1201	LMT	C1-C2-C3-C4
12	BD	102	LMT	C5-C6-C7-C8
11	Bb	1203	BCL	C1A-C2A-CAA-CBA
11	Bi	102	BCL	C1A-C2A-CAA-CBA
11	Bl	1203	BCL	C1A-C2A-CAA-CBA
11	Bo	1202	BCL	C1A-C2A-CAA-CBA
11	BE	101	BCL	C1A-C2A-CAA-CBA
11	BK	102	BCL	C1A-C2A-CAA-CBA
11	BN	101	BCL	C1A-C2A-CAA-CBA
11	AQ	103	BCL	C1A-C2A-CAA-CBA
11	BR	101	BCL	C1A-C2A-CAA-CBA
11	BC	101	BCL	C11-C10-C8-C7
11	AE	1102	BCL	C6-C7-C8-C10
11	AH	101	BCL	C11-C10-C8-C7
11	BP	101	BCL	C11-C12-C13-C15
11	BX	102	BCL	C5-C6-C7-C8
10	BI	101	V7N	C5-C6-C7-C8
12	Bj	1201	LMT	C3-C4-C5-C6
11	BH	104	BCL	C13-C15-C16-C17
15	M	403	CD4	C9-C10-C11-C12
11	Ak	101	BCL	C2A-CAA-CBA-CGA
11	AI	101	BCL	C2A-CAA-CBA-CGA
11	AS	1102	BCL	C4-C3-C5-C6
12	BW	103	LMT	C3'-C4'-O1B-C1B
11	Ac	101	BCL	C5-C6-C7-C8
12	Bf	1201	LMT	C2-C3-C4-C5
11	AS	1102	BCL	C10-C11-C12-C13
11	AT	1102	BCL	C3-C5-C6-C7
10	Bm	101	V7N	O42-C34-C9-C8
12	Be	1102	LMT	O1'-C1-C2-C3
11	AQ	102	BCL	C5-C6-C7-C8
11	BG	102	BCL	C15-C16-C17-C18
13	Bc	1203	PEX	C5-C6-C7-C8
14	Ad	103	MQ8	C18-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
14	L	305	MQ8	C18-C20-C21-C22
19	C	405	HEC	CAA-CBA-CGA-O2A
13	Bc	1203	PEX	C19-C20-C21-C22
11	BD	101	BCL	C3-C5-C6-C7
11	AJ	1103	BCL	C3-C5-C6-C7
11	Bn	103	BCL	C4-C3-C5-C6
11	Bk	103	BCL	C2-C1-O2A-CGA
11	BF	101	BCL	C2-C1-O2A-CGA
11	AF	102	BCL	C2-C1-O2A-CGA
11	BK	102	BCL	C2-C1-O2A-CGA
10	BP	102	V7N	C21-C22-C23-C24
11	Bc	1204	BCL	C2C-C3C-CAC-CBC
11	BA	103	BCL	C2-C3-C5-C6
11	BS	101	BCL	C2-C3-C5-C6
11	AQ	103	BCL	C8-C10-C11-C12
11	Ab	101	BCL	C6-C7-C8-C9
11	Bj	1204	BCL	C14-C13-C15-C16
11	Bp	1203	BCL	C14-C13-C15-C16
15	M	403	CD4	O15-C35-C36-C37
12	Bh	1204	LMT	C1-C2-C3-C4
12	Bj	1203	LMT	C11-C10-C9-C8
11	BV	102	BCL	C15-C16-C17-C18
11	Bg	103	BCL	C8-C10-C11-C12
12	BO	101	LMT	C3-C4-C5-C6
13	Ba	1101	PEX	C5-C6-C7-C8
10	Bc	1202	V7N	C37-C22-C23-C24
11	BV	102	BCL	C4-C3-C5-C6
14	M	408	MQ8	C34-C33-C35-C36
10	Bc	1202	V7N	C25-C26-C27-C28
11	Bp	1204	BCL	C4C-C3C-CAC-CBC
11	AT	1102	BCL	C4C-C3C-CAC-CBC
11	AW	1204	BCL	C2-C3-C5-C6
14	L	305	MQ8	C27-C28-C30-C31
19	C	402	HEC	C2A-CAA-CBA-CGA
12	BL	103	LMT	C7-C8-C9-C10
13	AT	1101	PEX	C5-C6-C7-C8
11	M	405	BCL	CAA-CBA-CGA-O2A
11	AL	101	BCL	C15-C16-C17-C18
13	Bk	102	PEX	O3-C1-C2-O6
12	Aj	102	LMT	C4-C5-C6-C7
11	M	404	BCL	C8-C10-C11-C12
13	AA	1101	PEX	O4-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
12	BA	105	LMT	O5B-C5B-C6B-O6B
10	Bd	1202	V7N	C2-C1-O32-C41
12	Aj	102	LMT	C2B-C1B-O1B-C4'
11	Bf	1204	BCL	C12-C13-C15-C16
11	Bj	1204	BCL	C12-C13-C15-C16
11	Bp	1203	BCL	C12-C13-C15-C16
11	BO	103	BCL	C2-C3-C5-C6
11	BV	102	BCL	C2-C3-C5-C6
12	BO	104	LMT	C2'-C1'-O1'-C1
11	AB	101	BCL	C16-C17-C18-C19
12	BH	103	LMT	C11-C10-C9-C8
13	Bc	1203	PEX	O6-C2-C3-O4
13	AJ	1101	PEX	C15-C16-C17-C18
13	Bc	1203	PEX	O6-C14-C15-C16
12	BU	101	LMT	C5-C6-C7-C8
11	Bb	1203	BCL	C2A-CAA-CBA-CGA
12	Bb	1201	LMT	C4B-C5B-C6B-O6B
13	Bn	102	PEX	C15-C16-C17-C18
11	BH	104	BCL	CAA-CBA-CGA-O2A
13	AD	1101	PEX	O6-C14-C15-C16
10	BV	101	V7N	C37-C22-C23-C24
11	Ak	101	BCL	C4-C3-C5-C6
11	Ao	101	BCL	C4-C3-C5-C6
11	AB	101	BCL	C4-C3-C5-C6
11	BG	102	BCL	C4-C3-C5-C6
11	AW	1203	BCL	C4-C3-C5-C6
14	L	305	MQ8	C14-C13-C15-C16
13	Be	1104	PEX	C16-C17-C18-C19
19	C	405	HEC	CAA-CBA-CGA-O1A
11	Bn	103	BCL	C2-C3-C5-C6
11	AS	1102	BCL	C2-C3-C5-C6
12	BO	104	LMT	C11-C10-C9-C8
11	AJ	1103	BCL	C16-C17-C18-C20
11	Ao	101	BCL	C11-C12-C13-C14
11	AJ	1102	BCL	C6-C7-C8-C9
11	BK	102	BCL	C6-C7-C8-C9
11	AM	101	BCL	C11-C10-C8-C9
11	AM	102	BCL	C11-C10-C8-C9
11	BP	101	BCL	C11-C12-C13-C14
12	BB	103	LMT	C3-C4-C5-C6
13	AP	1101	PEX	C10-C11-C12-C13
11	Bb	1203	BCL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
11	Bi	102	BCL	C3A-C2A-CAA-CBA
11	Bl	1203	BCL	C3A-C2A-CAA-CBA
11	BE	101	BCL	C3A-C2A-CAA-CBA
11	BK	102	BCL	C3A-C2A-CAA-CBA
11	BN	101	BCL	C3A-C2A-CAA-CBA
11	AQ	103	BCL	C3A-C2A-CAA-CBA
11	BR	101	BCL	C3A-C2A-CAA-CBA
11	Bp	1203	BCL	CAA-CBA-CGA-O2A
11	AF	102	BCL	CAA-CBA-CGA-O2A
11	BK	102	BCL	CAA-CBA-CGA-O2A
11	BS	101	BCL	CAA-CBA-CGA-O2A
11	BV	102	BCL	CAA-CBA-CGA-O2A
12	AW	1201	LMT	C5'-C4'-O1B-C1B
11	Ac	101	BCL	CAD-CBD-CGD-O2D
11	Ad	101	BCL	CAD-CBD-CGD-O2D
11	Ah	101	BCL	CAD-CBD-CGD-O2D
11	Aj	101	BCL	CAD-CBD-CGD-O2D
11	Al	101	BCL	CAD-CBD-CGD-O2D
11	Bl	1203	BCL	CAD-CBD-CGD-O2D
11	Ao	101	BCL	CAD-CBD-CGD-O2D
11	Bp	1203	BCL	CAD-CBD-CGD-O2D
11	BA	103	BCL	CAD-CBD-CGD-O2D
11	AB	101	BCL	CAD-CBD-CGD-O2D
11	BD	101	BCL	CAD-CBD-CGD-O2D
11	BF	101	BCL	CAD-CBD-CGD-O2D
11	AF	102	BCL	CAD-CBD-CGD-O2D
11	BG	102	BCL	CAD-CBD-CGD-O2D
11	AH	101	BCL	CAD-CBD-CGD-O2D
11	BH	104	BCL	CAD-CBD-CGD-O2D
11	AI	101	BCL	CAD-CBD-CGD-O2D
11	BI	102	BCL	CAD-CBD-CGD-O2D
11	AK	101	BCL	CAD-CBD-CGD-O2D
11	BN	101	BCL	CAD-CBD-CGD-O2D
11	AN	101	BCL	CAD-CBD-CGD-O2D
11	BO	103	BCL	CAD-CBD-CGD-O2D
11	BS	101	BCL	CAD-CBD-CGD-O2D
11	AT	1102	BCL	CAD-CBD-CGD-O2D
11	BU	102	BCL	CAD-CBD-CGD-O2D
11	AW	1203	BCL	CAD-CBD-CGD-O2D
11	BX	102	BCL	CAD-CBD-CGD-O2D
13	AD	1101	PEX	C5-C6-C7-C8
11	Bo	1202	BCL	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
13	AJ	1101	PEX	C18-C19-C20-C21
11	Bc	1204	BCL	CAA-CBA-CGA-O2A
11	Ai	101	BCL	CAA-CBA-CGA-O2A
11	AP	1102	BCL	CAA-CBA-CGA-O2A
11	AR	101	BCL	CAA-CBA-CGA-O2A
11	AT	1103	BCL	CAA-CBA-CGA-O2A
13	Bc	1203	PEX	O4-C4-C5-C6
13	Bn	102	PEX	C16-C17-C18-C19
14	L	305	MQ8	C12-C13-C15-C16
11	Bh	1205	BCL	CAA-CBA-CGA-O2A
10	Bc	1202	V7N	C3-C4-C5-C6
10	Bj	1202	V7N	C11-C12-C13-C14
10	BA	102	V7N	C17-C18-C19-C20
10	BC	103	V7N	C17-C18-C19-C20
10	BO	102	V7N	C11-C12-C13-C14
12	BW	101	LMT	C1-C2-C3-C4
10	Bb	1202	V7N	C22-C23-C24-C25
13	Bc	1203	PEX	C1-C2-C3-O4
13	AS	1101	PEX	C1-C2-C3-O4
12	BE	102	LMT	C9-C10-C11-C12
10	AF	101	V7N	C26-C27-C28-C29
12	BQ	101	LMT	C5'-C4'-O1B-C1B
11	Af	101	BCL	O2A-C1-C2-C3
11	Bo	1202	BCL	O2A-C1-C2-C3
11	BD	101	BCL	O2A-C1-C2-C3
11	AE	1102	BCL	O2A-C1-C2-C3
11	AN	101	BCL	O2A-C1-C2-C3
11	AO	101	BCL	O2A-C1-C2-C3
11	AT	1102	BCL	O2A-C1-C2-C3
12	Bf	1201	LMT	C7-C8-C9-C10
13	AA	1101	PEX	C19-C20-C21-C22
11	Af	101	BCL	C2A-CAA-CBA-CGA
11	AL	101	BCL	CAA-CBA-CGA-O2A
11	AN	101	BCL	CAA-CBA-CGA-O2A
11	Bo	1202	BCL	CHA-CBD-CGD-O2D
11	Bp	1204	BCL	CHA-CBD-CGD-O2D
11	BR	101	BCL	CHA-CBD-CGD-O2D
11	AG	101	BCL	CAA-CBA-CGA-O2A
11	AJ	1102	BCL	CAA-CBA-CGA-O2A
11	AW	1203	BCL	C2-C3-C5-C6
14	M	408	MQ8	C32-C33-C35-C36
11	AE	1102	BCL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
13	Bc	1203	PEX	O3-C1-C2-C3
10	Bj	1202	V7N	C30-C1-O32-C41
10	Bj	1202	V7N	C31-C1-O32-C41
12	BF	102	LMT	C4-C5-C6-C7
11	AQ	102	BCL	C15-C16-C17-C18
11	Bj	1204	BCL	CAA-CBA-CGA-O2A
11	Ao	101	BCL	CAA-CBA-CGA-O2A
11	AH	101	BCL	CAA-CBA-CGA-O2A
11	AI	102	BCL	CAA-CBA-CGA-O2A
11	AM	101	BCL	CAA-CBA-CGA-O2A
12	BL	103	LMT	C2-C3-C4-C5
12	BR	102	LMT	C6-C7-C8-C9
19	C	402	HEC	CAA-CBA-CGA-O2A
11	Bl	1203	BCL	CAA-CBA-CGA-O2A
11	AD	1102	BCL	CAA-CBA-CGA-O2A
10	Bd	1202	V7N	C31-C1-C2-C3
10	Bj	1202	V7N	C31-C1-C2-C3
10	An	101	V7N	C31-C1-C2-C3
10	BB	102	V7N	C31-C1-C2-C3
10	BR	103	V7N	C31-C1-C2-C3
16	M	406	BPH	CHA-CBD-CGD-O2D
11	Ae	101	BCL	C13-C15-C16-C17
11	Bp	1203	BCL	C15-C16-C17-C18
12	Bf	1203	LMT	C4-C5-C6-C7
11	Al	101	BCL	CAA-CBA-CGA-O2A
11	Al	101	BCL	C12-C13-C15-C16
11	AC	101	BCL	C6-C7-C8-C10
11	BG	102	BCL	C2-C3-C5-C6
11	AJ	1102	BCL	C6-C7-C8-C10
11	AQ	103	BCL	C11-C10-C8-C7
11	BU	102	BCL	C11-C12-C13-C15
12	Bh	1201	LMT	C7-C8-C9-C10
11	BC	101	BCL	C8-C10-C11-C12
11	AW	1202	BCL	C15-C16-C17-C18
11	Ab	101	BCL	CAA-CBA-CGA-O2A
11	Ai	101	BCL	C6-C7-C8-C9
11	Bn	103	BCL	C6-C7-C8-C9
16	L	303	BPH	C11-C12-C13-C14
10	Bb	1202	V7N	C5-C6-C7-C8
18	M	407	CRT	C20-C21-C22-C23
19	C	404	HEC	CAD-CBD-CGD-O2D
11	Bl	1203	BCL	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
11	AE	1102	BCL	C5-C6-C7-C8
11	AB	101	BCL	C16-C17-C18-C20
12	Bl	1201	LMT	C5'-C4'-O1B-C1B
11	BV	102	BCL	C2A-CAA-CBA-CGA
10	Bb	1202	V7N	O32-C1-C2-C3
13	Bg	102	PEX	C9-C10-C11-C12
12	BA	104	LMT	O5B-C1B-O1B-C4'
10	BA	102	V7N	C36-C18-C19-C20
16	M	406	BPH	C2C-C3C-CAC-CBC
11	Bh	1205	BCL	CAA-CBA-CGA-O1A
11	Bd	1203	BCL	C1A-C2A-CAA-CBA
11	Be	1105	BCL	C1A-C2A-CAA-CBA
11	Bp	1203	BCL	C1A-C2A-CAA-CBA
11	BH	104	BCL	C1A-C2A-CAA-CBA
11	AW	1204	BCL	C1A-C2A-CAA-CBA
19	C	402	HEC	CAA-CBA-CGA-O1A
10	Bp	1202	V7N	C23-C24-C25-C26
11	AT	1103	BCL	C2-C1-O2A-CGA
11	Bc	1204	BCL	CAA-CBA-CGA-O1A
11	BH	104	BCL	CAA-CBA-CGA-O1A
11	AR	101	BCL	CAA-CBA-CGA-O1A
11	BS	101	BCL	CAA-CBA-CGA-O1A
13	Bc	1203	PEX	O5-C4-C5-C6
13	AD	1101	PEX	O7-C14-C15-C16
13	Be	1104	PEX	C1-C2-C3-O4
15	Af	102	CD4	C28-C15-C16-O3
12	BH	103	LMT	C5-C6-C7-C8
12	Ad	102	LMT	C2B-C1B-O1B-C4'
11	Bj	1204	BCL	CAA-CBA-CGA-O1A
11	AP	1102	BCL	CAA-CBA-CGA-O1A
11	AT	1103	BCL	CAA-CBA-CGA-O1A
11	Bc	1204	BCL	C13-C15-C16-C17
11	AJ	1103	BCL	C8-C10-C11-C12
19	C	402	HEC	C3A-C2A-CAA-CBA
11	AK	101	BCL	CAA-CBA-CGA-O2A
11	Ai	101	BCL	CAA-CBA-CGA-O1A
11	AH	101	BCL	CAA-CBA-CGA-O1A
11	BK	102	BCL	CAA-CBA-CGA-O1A
13	Bc	1203	PEX	O7-C14-C15-C16
13	AA	1101	PEX	C1-O3-P1-O1
13	AD	1101	PEX	C1-O3-P1-O2
15	M	403	CD4	C31-O10-P2-O12

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Mol	Chain	Res	Type	Atoms
19	C	405	HEC	C2B-C3B-CAB-CBB
11	Ao	101	BCL	CAA-CBA-CGA-O1A
11	AF	102	BCL	CAA-CBA-CGA-O1A
11	AQ	102	BCL	C3-C5-C6-C7
12	Bb	1201	LMT	C3'-C4'-O1B-C1B
12	BB	103	LMT	C2-C3-C4-C5
13	Bh	1203	PEX	C15-C16-C17-C18
11	Af	101	BCL	C10-C11-C12-C13
13	Bh	1203	PEX	O8-C24-C25-N1
13	Bk	102	PEX	O8-C24-C25-N1
13	AA	1101	PEX	O8-C24-C25-N1
11	Ab	101	BCL	CAA-CBA-CGA-O1A
11	AJ	1102	BCL	CAA-CBA-CGA-O1A
11	AL	101	BCL	CAA-CBA-CGA-O1A
11	AM	101	BCL	CAA-CBA-CGA-O1A
11	AN	101	BCL	CAA-CBA-CGA-O1A
12	BL	103	LMT	C5'-C4'-O1B-C1B
12	Bj	1203	LMT	C4B-C5B-C6B-O6B
11	Bg	103	BCL	C16-C17-C18-C19
10	BR	103	V7N	C26-C27-C28-C29
11	Bp	1203	BCL	CAA-CBA-CGA-O1A
11	AD	1102	BCL	CAA-CBA-CGA-O1A
11	AG	101	BCL	CAA-CBA-CGA-O1A
11	AI	102	BCL	CAA-CBA-CGA-O1A
11	BV	102	BCL	CAA-CBA-CGA-O1A
19	C	403	HEC	CAD-CBD-CGD-O2D
13	AJ	1101	PEX	O4-C4-C5-C6
11	Bf	1204	BCL	C2-C3-C5-C6
11	AK	101	BCL	C2-C3-C5-C6
13	AE	1101	PEX	C25-C24-O8-P1
13	AT	1101	PEX	C25-C24-O8-P1
12	Bc	1201	LMT	C5-C6-C7-C8
13	Bh	1203	PEX	C6-C7-C8-C9
13	Bk	102	PEX	C16-C17-C18-C19
11	Ad	101	BCL	CAA-CBA-CGA-O2A
11	Be	1105	BCL	CAA-CBA-CGA-O2A
11	BG	102	BCL	CAA-CBA-CGA-O2A
11	BE	101	BCL	C10-C11-C12-C13
11	AI	102	BCL	C15-C16-C17-C18
11	Ab	101	BCL	C14-C13-C15-C16
11	Ae	101	BCL	C11-C12-C13-C14
11	Ae	101	BCL	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
11	Bp	1204	BCL	C11-C12-C13-C14
11	AQ	103	BCL	C11-C10-C8-C9
12	BB	103	LMT	C3'-C4'-O1B-C1B
11	AF	102	BCL	C16-C17-C18-C20
11	Bm	103	BCL	CAA-CBA-CGA-O2A
11	AO	101	BCL	CAA-CBA-CGA-O2A
11	AQ	102	BCL	CAA-CBA-CGA-O2A
11	BU	102	BCL	CAA-CBA-CGA-O2A
13	AA	1101	PEX	O6-C14-C15-C16
19	C	404	HEC	CAD-CBD-CGD-O1D
11	Al	101	BCL	CAA-CBA-CGA-O1A
12	BU	101	LMT	C2-C3-C4-C5
11	Ah	101	BCL	CAA-CBA-CGA-O2A
11	AE	1102	BCL	CAA-CBA-CGA-O2A
11	Ab	101	BCL	C6-C7-C8-C10
11	Ai	101	BCL	C6-C7-C8-C10
11	Ak	101	BCL	C11-C10-C8-C7
11	Bn	103	BCL	C6-C7-C8-C10
11	Bo	1202	BCL	C3A-C2A-CAA-CBA
11	AG	101	BCL	C2-C3-C5-C6
11	AG	101	BCL	C12-C13-C15-C16
11	AN	101	BCL	C11-C10-C8-C7
11	AV	1001	BCL	C12-C13-C15-C16
11	Ad	101	BCL	CAA-CBA-CGA-O1A
11	AQ	102	BCL	CAA-CBA-CGA-O1A
15	M	403	CD4	C19-C20-C21-C22
11	AB	101	BCL	CAA-CBA-CGA-O2A
11	BL	102	BCL	CAA-CBA-CGA-O2A
12	BH	103	LMT	C6-C7-C8-C9
12	L	304	LMT	C3'-C4'-O1B-C1B
10	BJ	101	V7N	C11-C12-C13-C14
10	BV	101	V7N	C11-C12-C13-C14
10	Bm	101	V7N	C5-C6-C7-C8
12	BL	103	LMT	C9-C10-C11-C12
12	Bc	1201	LMT	C2-C1-O1'-C1'
13	AD	1101	PEX	C9-C10-C11-C12
12	BK	103	LMT	O5'-C1'-O1'-C1
11	Bl	1203	BCL	CAA-CBA-CGA-O1A
11	BL	102	BCL	CAA-CBA-CGA-O1A
11	AO	101	BCL	CAA-CBA-CGA-O1A
14	Ad	103	MQ8	C28-C30-C31-C32
11	Bh	1205	BCL	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
11	AH	101	BCL	C8-C10-C11-C12
11	AX	1202	BCL	C8-C10-C11-C12
11	BP	101	BCL	CAA-CBA-CGA-O2A
11	AP	1102	BCL	C5-C6-C7-C8
11	Ah	101	BCL	CAA-CBA-CGA-O1A
11	AE	1102	BCL	CAA-CBA-CGA-O1A
11	AK	101	BCL	CAA-CBA-CGA-O1A
11	BE	101	BCL	C5-C6-C7-C8
11	BP	101	BCL	C5-C6-C7-C8
12	Bb	1201	LMT	C4-C5-C6-C7
13	Bg	102	PEX	O6-C14-C15-C16
12	Be	1102	LMT	C4'-C5'-C6'-O6'

There are no ring outliers.

139 monomers are involved in 333 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	AQ	101	BCL	1	0
12	BW	103	LMT	3	0
13	Be	1101	PEX	1	0
14	M	408	MQ8	4	0
11	AJ	1103	BCL	2	0
11	BE	101	BCL	1	0
11	Bp	1203	BCL	11	0
11	Bm	103	BCL	3	0
11	AK	101	BCL	5	0
16	M	406	BPH	4	0
11	AT	1102	BCL	5	0
13	Bm	102	PEX	2	0
12	BE	102	LMT	1	0
12	BF	102	LMT	2	0
11	BK	102	BCL	1	0
11	Af	101	BCL	2	0
11	AR	101	BCL	6	0
13	AE	1101	PEX	2	0
11	BS	101	BCL	1	0
11	AB	101	BCL	3	0
11	Ab	101	BCL	2	0
11	Bj	1204	BCL	3	0
13	Ba	1101	PEX	1	0
19	C	402	HEC	1	0
11	BG	102	BCL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	M	401	LMT	2	0
11	Bh	1205	BCL	1	0
11	Al	101	BCL	9	0
11	Ak	101	BCL	2	0
10	BT	101	V7N	1	0
11	AQ	102	BCL	4	0
12	BG	103	LMT	1	0
11	Bp	1204	BCL	1	0
12	BC	102	LMT	2	0
11	AW	1204	BCL	1	0
11	BN	101	BCL	3	0
12	Bf	1203	LMT	2	0
11	Bk	103	BCL	1	0
14	L	305	MQ8	6	0
11	AI	101	BCL	1	0
13	AA	1101	PEX	4	0
11	M	405	BCL	1	0
13	Bn	102	PEX	3	0
12	Ad	102	LMT	2	0
11	BA	101	BCL	6	0
12	AW	1201	LMT	1	0
11	Am	101	BCL	9	0
11	Ac	101	BCL	2	0
11	AC	101	BCL	2	0
11	AW	1202	BCL	2	0
12	Bh	1201	LMT	2	0
13	Be	1104	PEX	5	0
11	AD	1102	BCL	3	0
11	AG	101	BCL	1	0
11	AP	1102	BCL	2	0
11	Bo	1202	BCL	3	0
11	Bl	1203	BCL	4	0
12	BK	101	LMT	1	0
11	Bn	103	BCL	2	0
12	AX	1201	LMT	2	0
12	BQ	101	LMT	1	0
12	BS	102	LMT	4	0
11	AH	101	BCL	2	0
11	AF	102	BCL	2	0
11	AM	102	BCL	2	0
19	C	404	HEC	2	0
11	Aj	101	BCL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	AT	1103	BCL	5	0
13	Aj	103	PEX	2	0
13	Bh	1203	PEX	1	0
11	BX	102	BCL	4	0
11	BF	101	BCL	3	0
11	BI	102	BCL	5	0
12	Bj	1201	LMT	2	0
13	Bg	102	PEX	1	0
13	Bk	102	PEX	1	0
11	Ad	101	BCL	1	0
12	BB	103	LMT	2	0
11	Ah	101	BCL	1	0
13	Bc	1203	PEX	4	0
10	BV	101	V7N	1	0
11	AV	1001	BCL	5	0
11	AL	101	BCL	3	0
13	AD	1101	PEX	3	0
11	Bf	1204	BCL	1	0
12	Bp	1201	LMT	1	0
11	AN	101	BCL	3	0
13	AP	1101	PEX	2	0
11	AE	1102	BCL	4	0
11	Bg	103	BCL	1	0
15	M	403	CD4	1	0
11	AU	1001	BCL	2	0
12	Bo	1201	LMT	3	0
11	AJ	1102	BCL	1	0
11	L	302	BCL	3	0
12	BI	103	LMT	2	0
10	BS	103	V7N	1	0
13	AT	1101	PEX	2	0
11	Be	1105	BCL	3	0
14	Ad	103	MQ8	9	0
11	AW	1203	BCL	4	0
11	AM	101	BCL	2	0
12	BR	102	LMT	1	0
19	C	403	HEC	1	0
13	AS	1101	PEX	2	0
11	Bd	1203	BCL	1	0
19	C	405	HEC	2	0
12	Bf	1201	LMT	1	0
11	Bb	1203	BCL	2	0

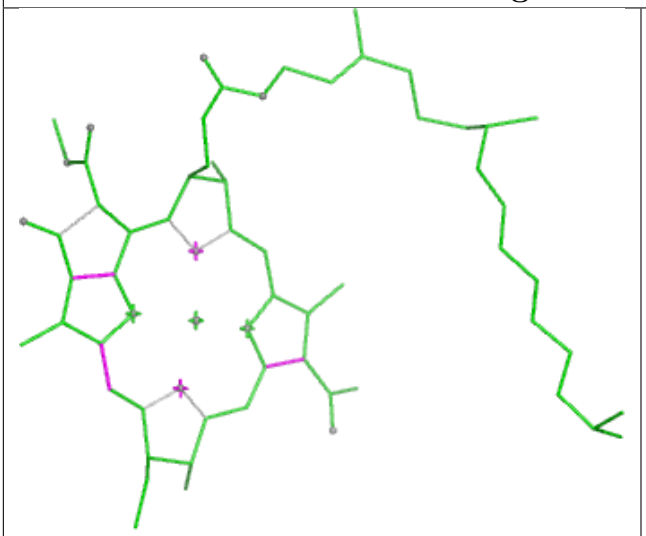
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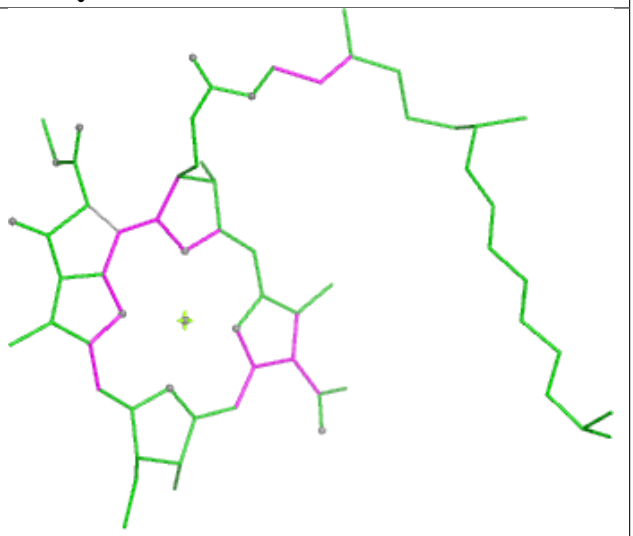
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	BO	103	BCL	1	0
11	AS	1102	BCL	3	0
11	BC	101	BCL	2	0
12	Bc	1201	LMT	1	0
11	BB	101	BCL	3	0
12	BO	104	LMT	3	0
11	AO	101	BCL	5	0
12	Bd	1201	LMT	1	0
12	Bb	1201	LMT	2	0
11	BU	102	BCL	1	0
12	K	201	LMT	1	0
12	BH	103	LMT	3	0
11	BH	104	BCL	1	0
11	AX	1202	BCL	4	0
13	AJ	1101	PEX	1	0
12	BD	102	LMT	1	0
12	BW	101	LMT	1	0
11	Ao	101	BCL	26	0
15	Af	102	CD4	9	0
11	BD	101	BCL	4	0
11	Bi	102	BCL	1	0
12	BA	104	LMT	5	0
11	BL	102	BCL	1	0
11	AI	102	BCL	4	0
12	Be	1102	LMT	1	0
11	M	404	BCL	2	0
12	BM	1001	LMT	2	0
16	L	303	BPH	6	0
11	BP	101	BCL	2	0
11	Ae	101	BCL	4	0

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

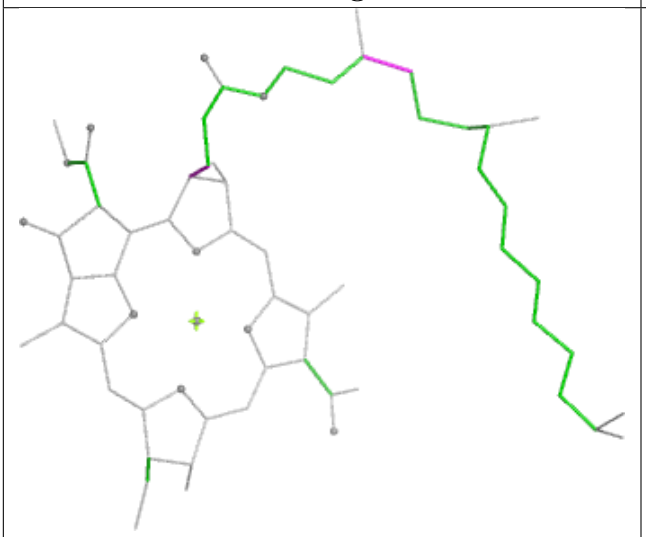
Ligand BCL AQ 101



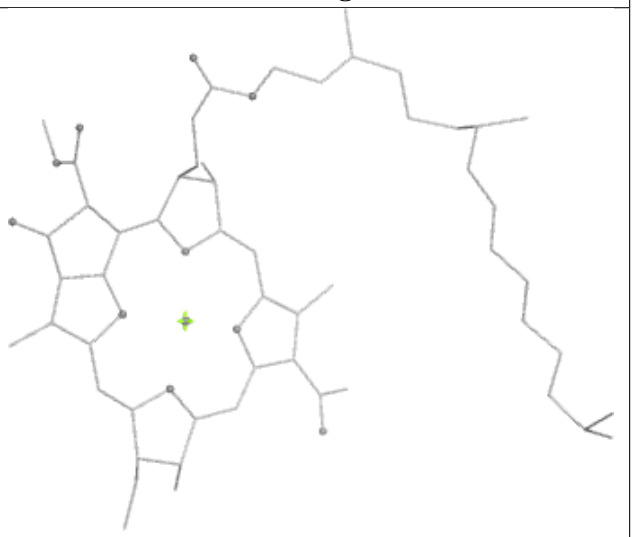
Bond lengths



Bond angles

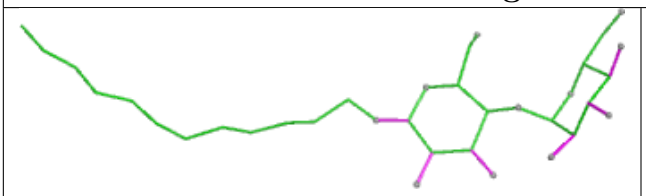


Torsions

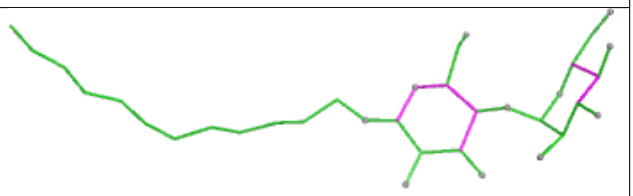


Rings

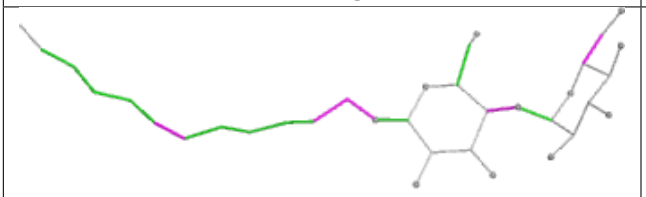
Ligand LMT BW 103



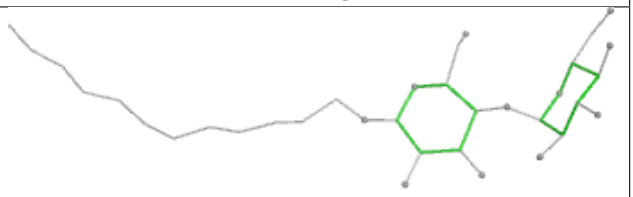
Bond lengths



Bond angles

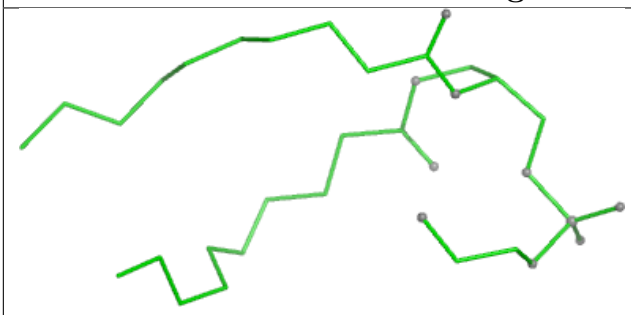


Torsions

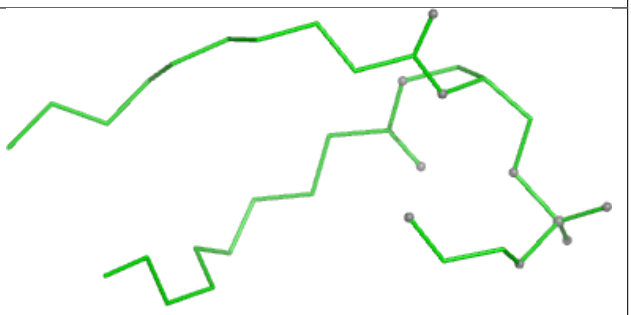


Rings

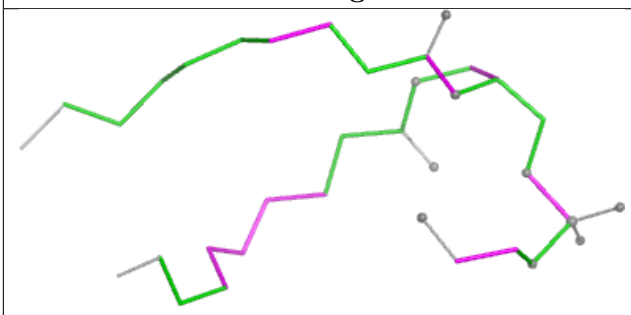
Ligand PEX Be 1101



Bond lengths



Bond angles

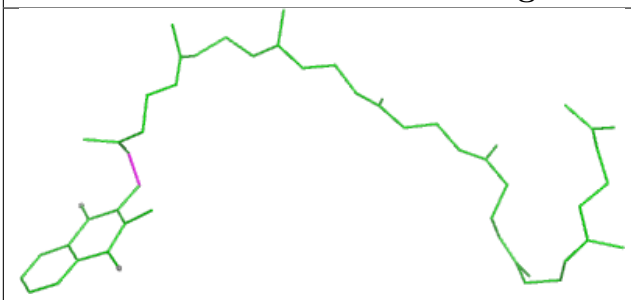


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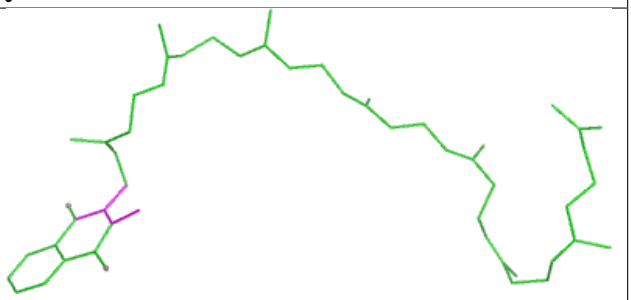


Rings

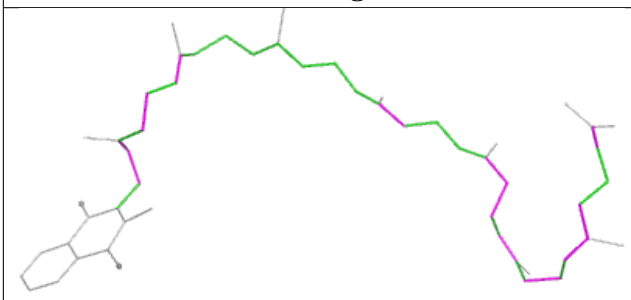
Ligand MQ8 M 408



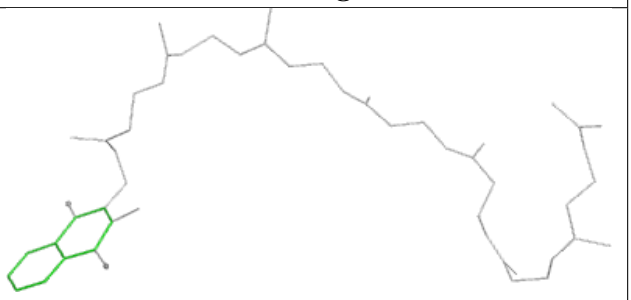
Bond lengths



Bond angles

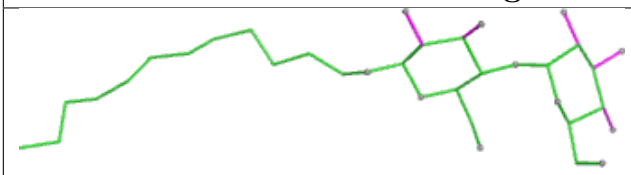


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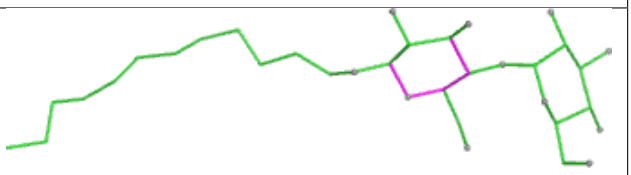


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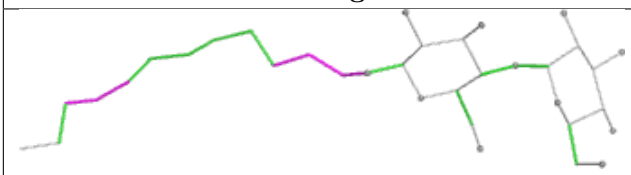
Ligand LMT Ba 1102



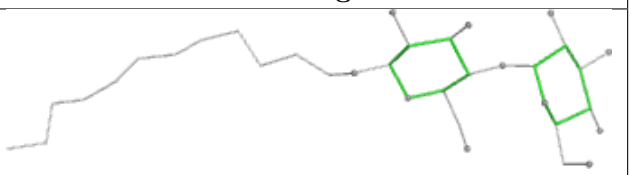
Bond lengths



Bond angles

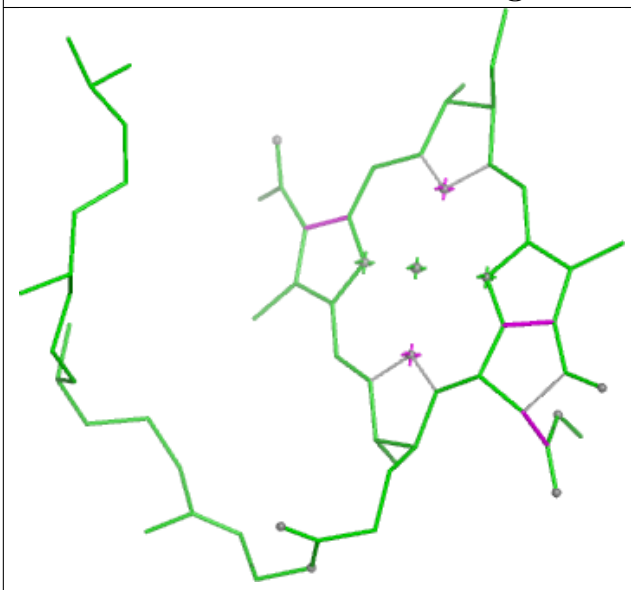


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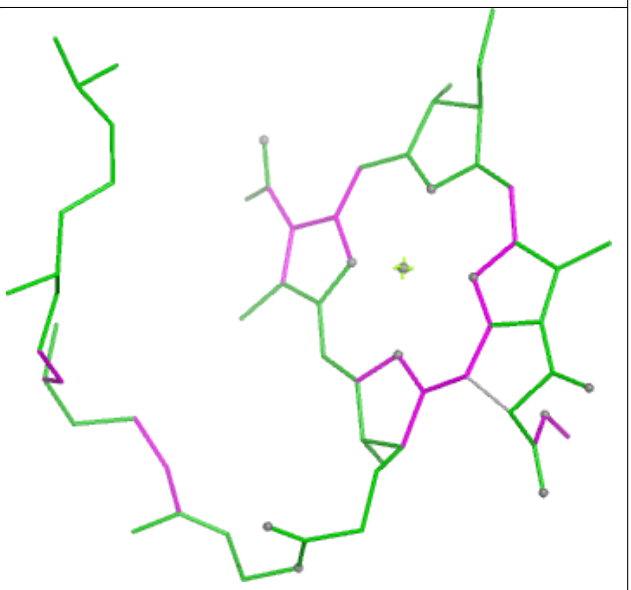


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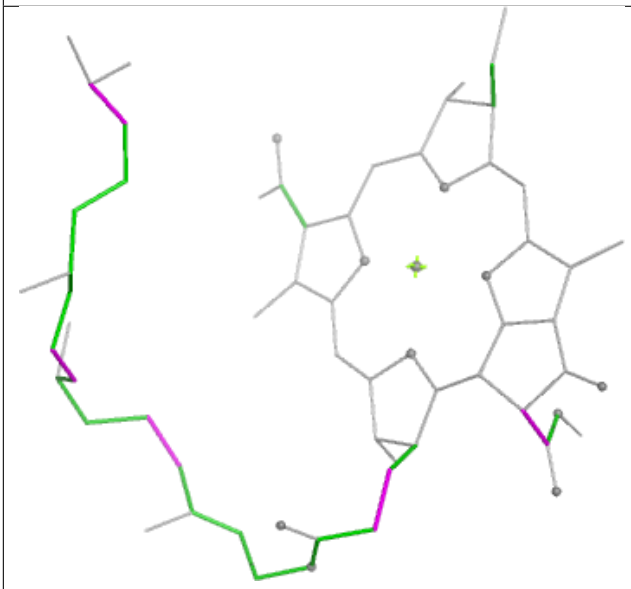
Ligand BCL AJ 1103



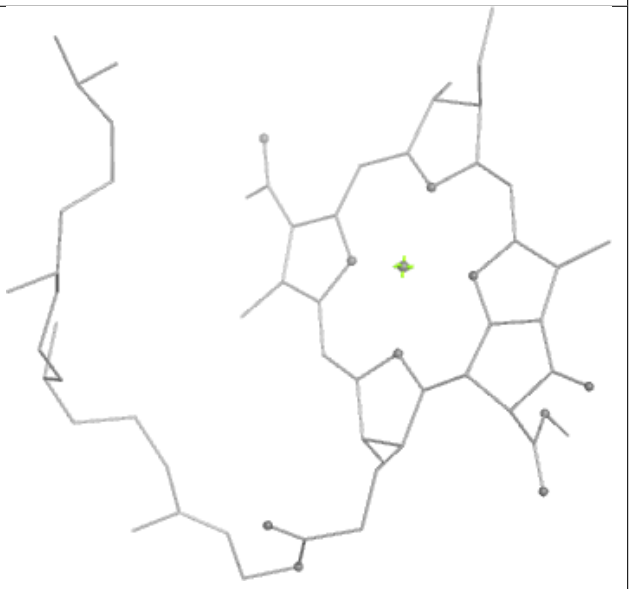
Bond lengths



Bond angles

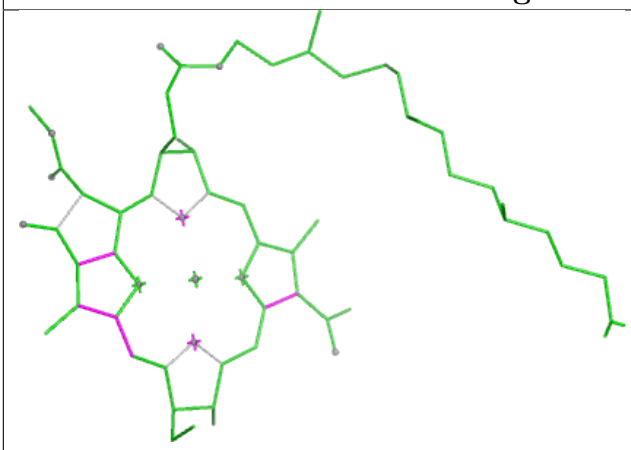


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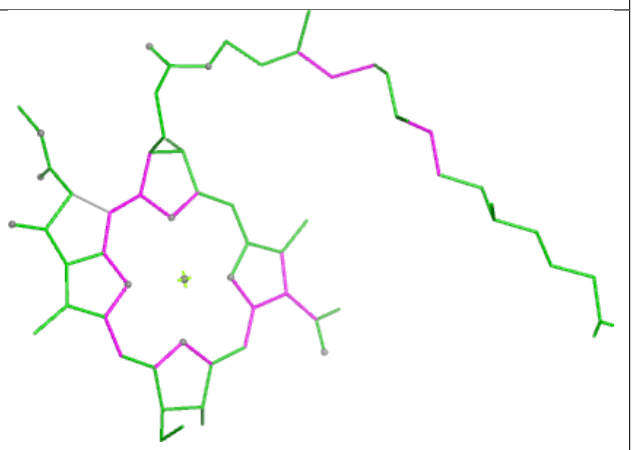


Rings

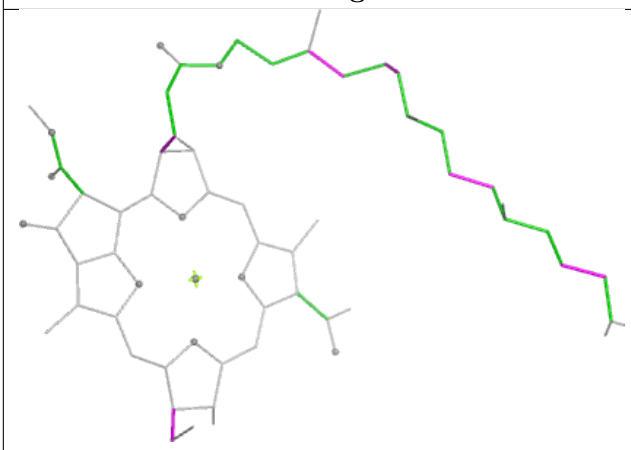
Ligand BCL BE 101



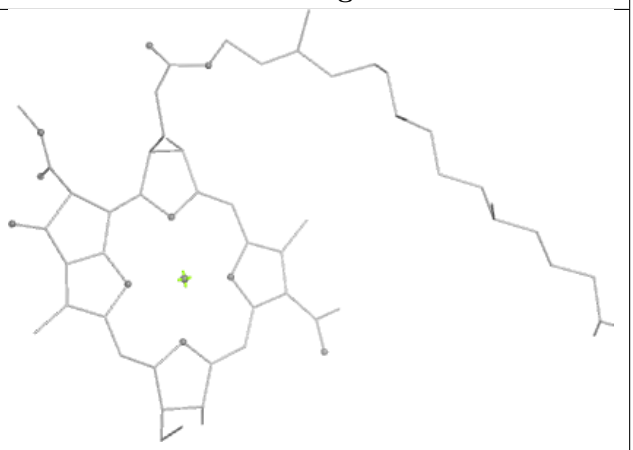
Bond lengths



Bond angles

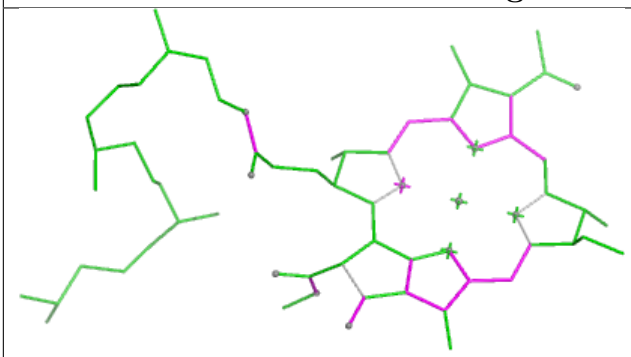


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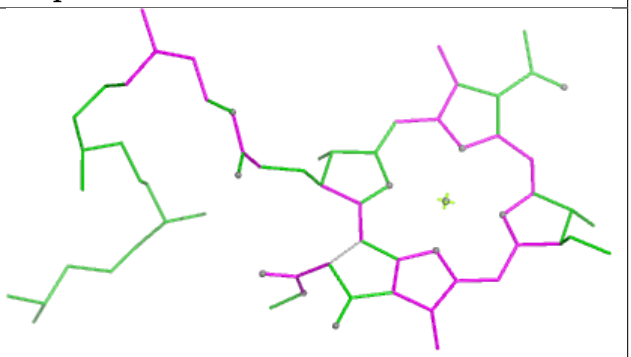


Rings

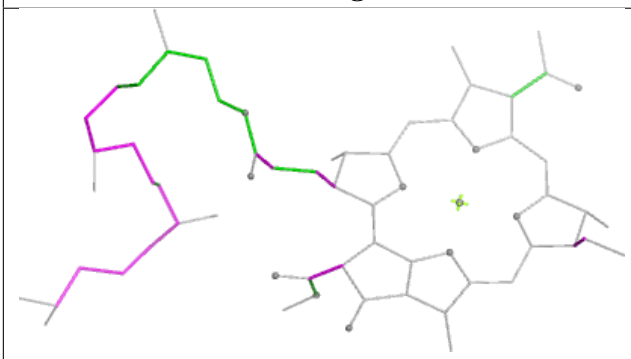
Ligand BCL Bp 1203



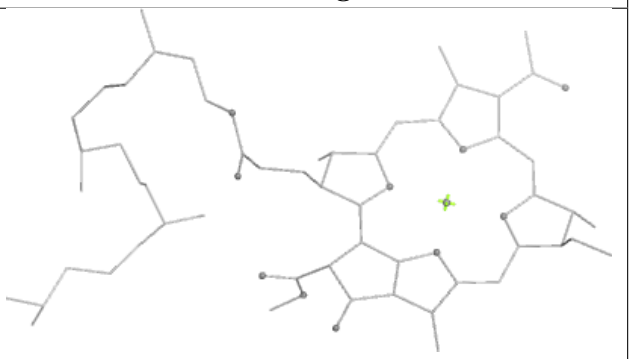
Bond lengths



Bond angles

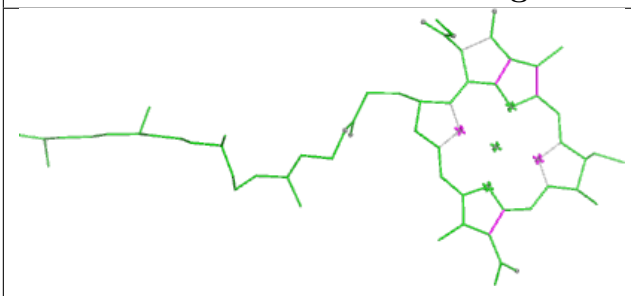


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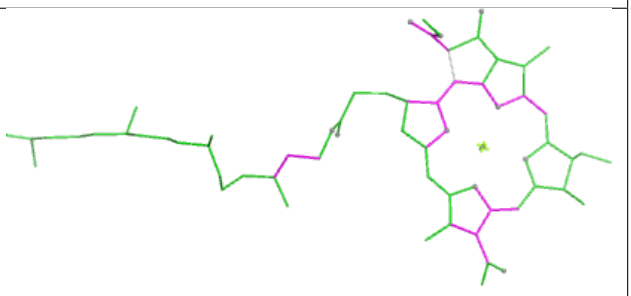


Rings

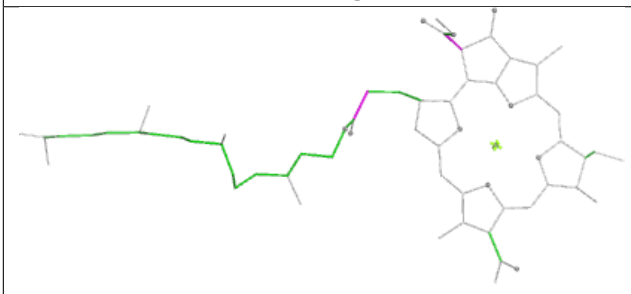
Ligand BCL Bm 103



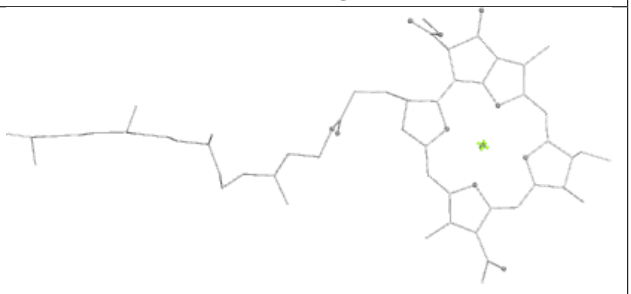
Bond lengths



Bond angles

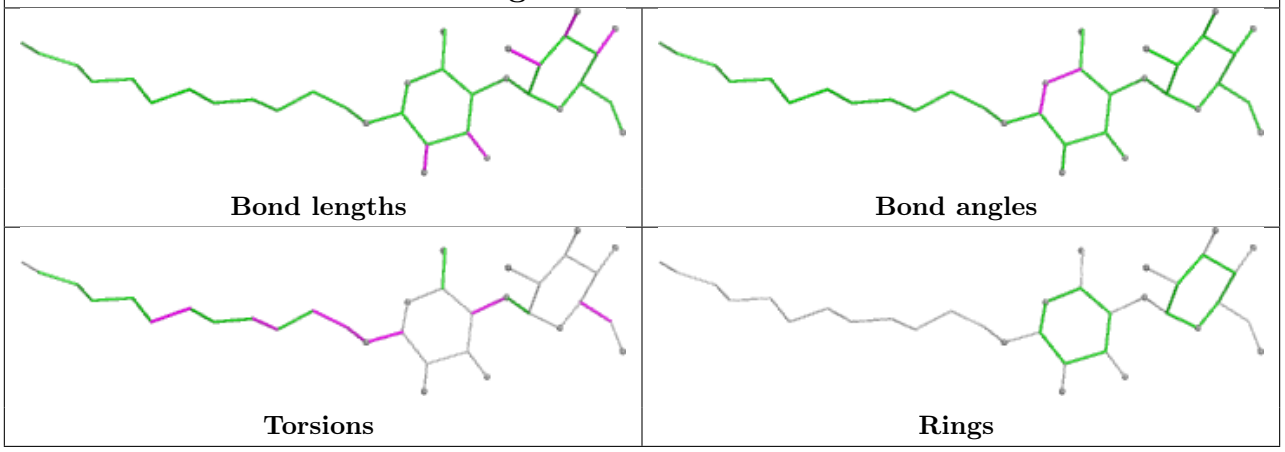


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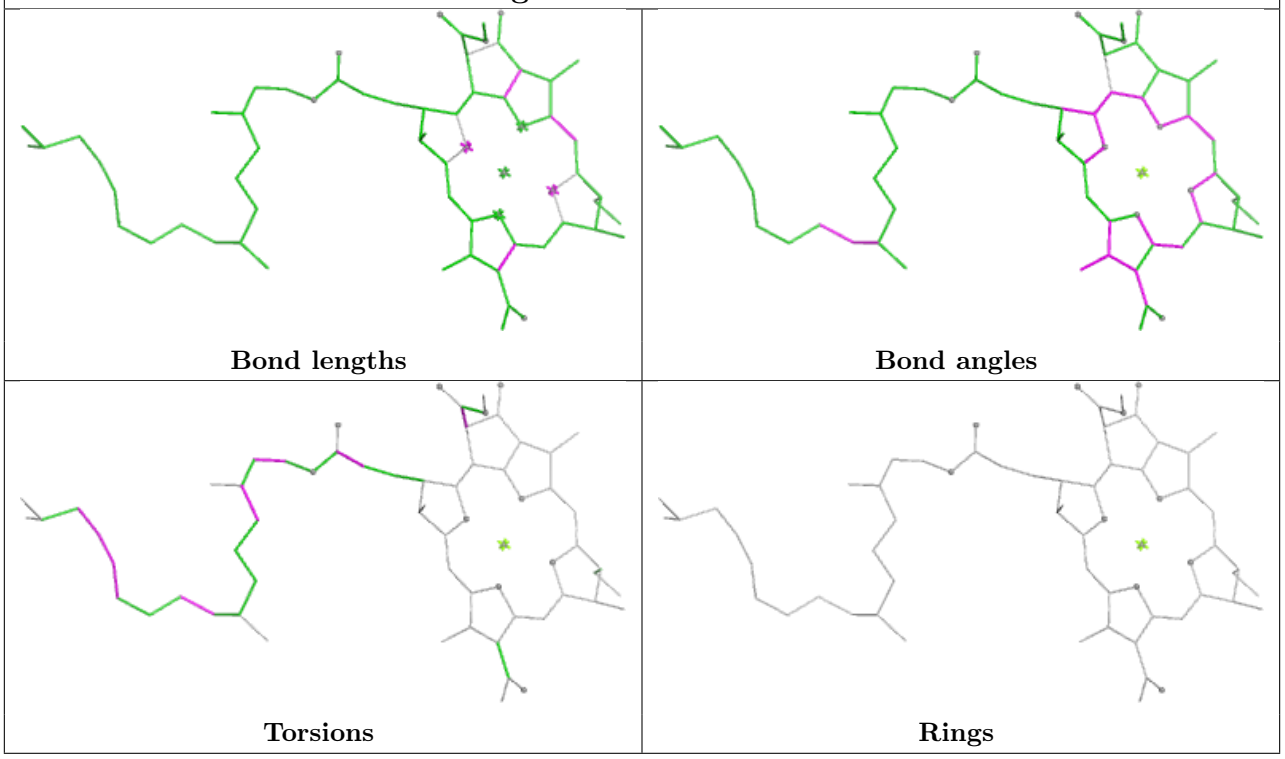


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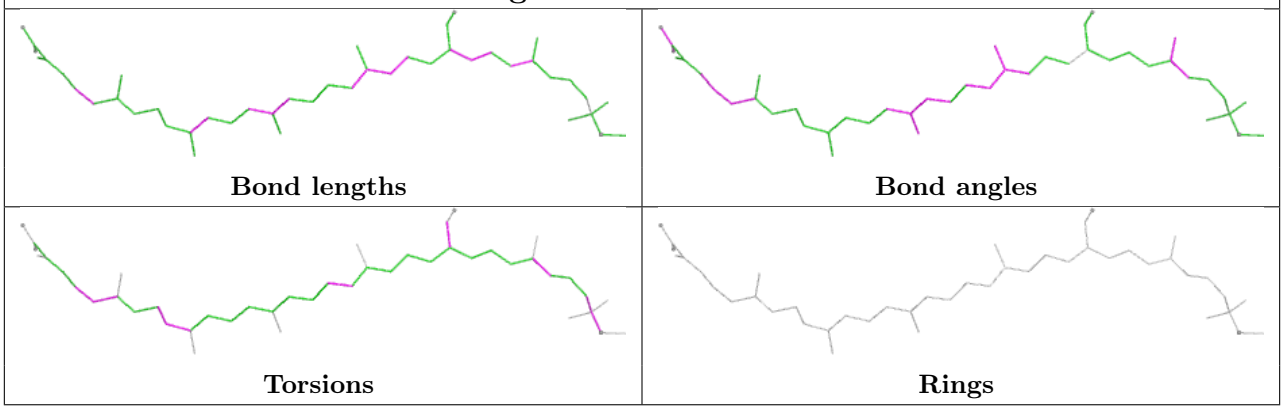
Ligand LMT BU 101



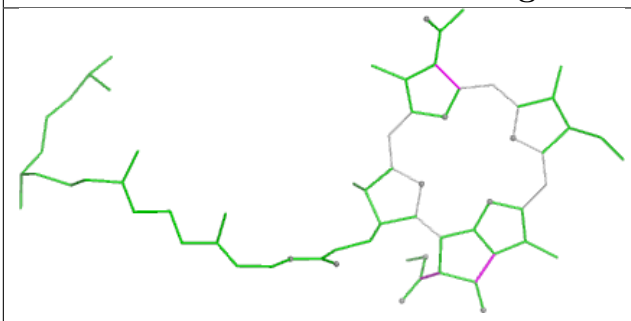
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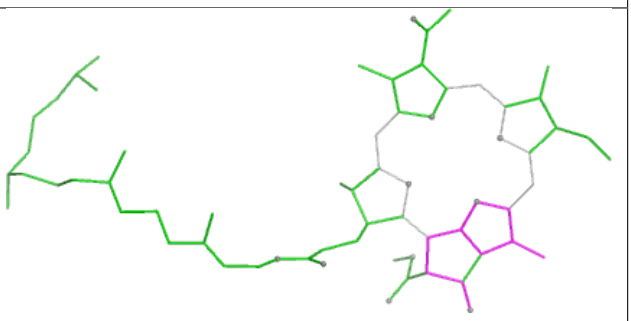
Ligand V7N Bc 1202



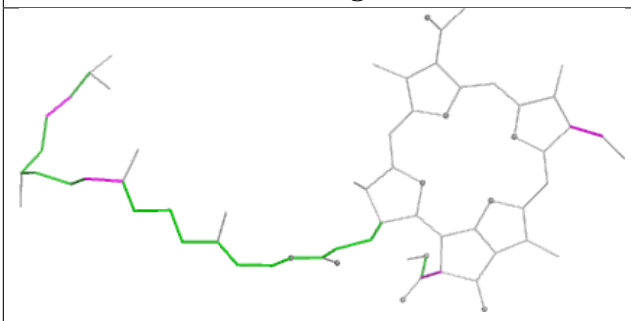
Ligand BPH M 406



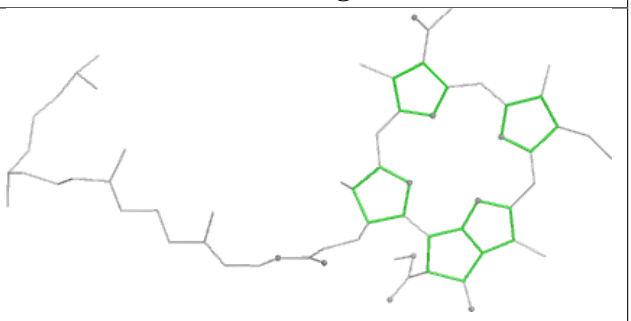
Bond lengths



Bond angles

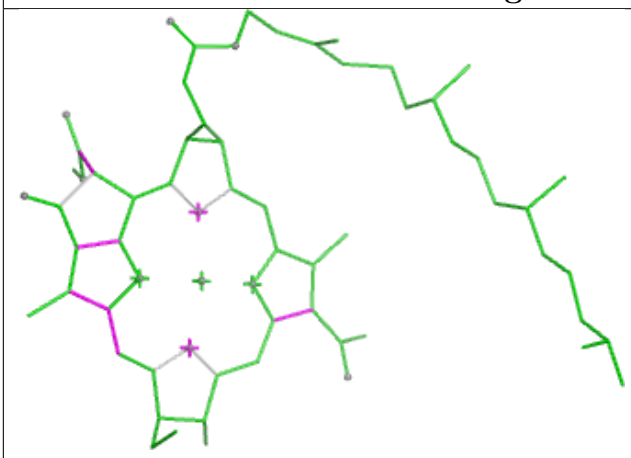


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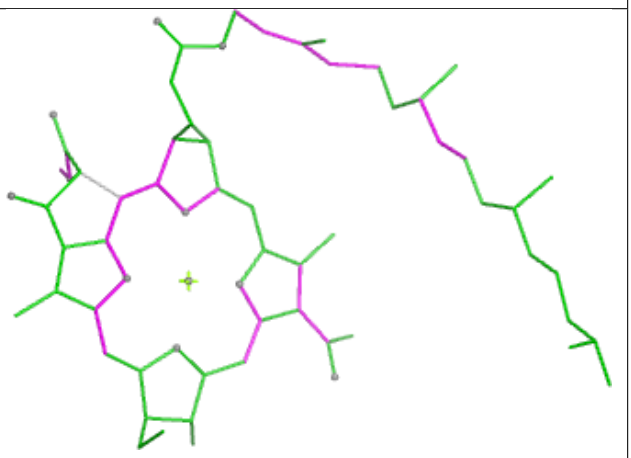


Rings

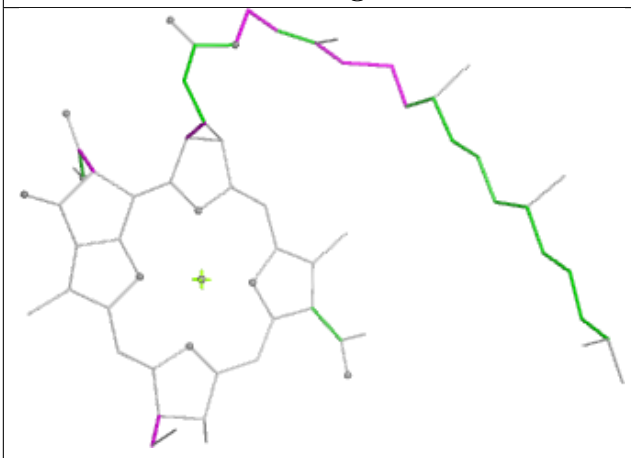
Ligand BCL AT 1102



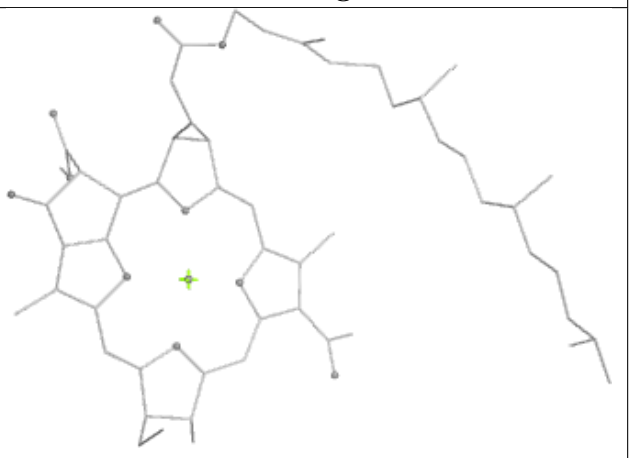
Bond lengths



Bond angles

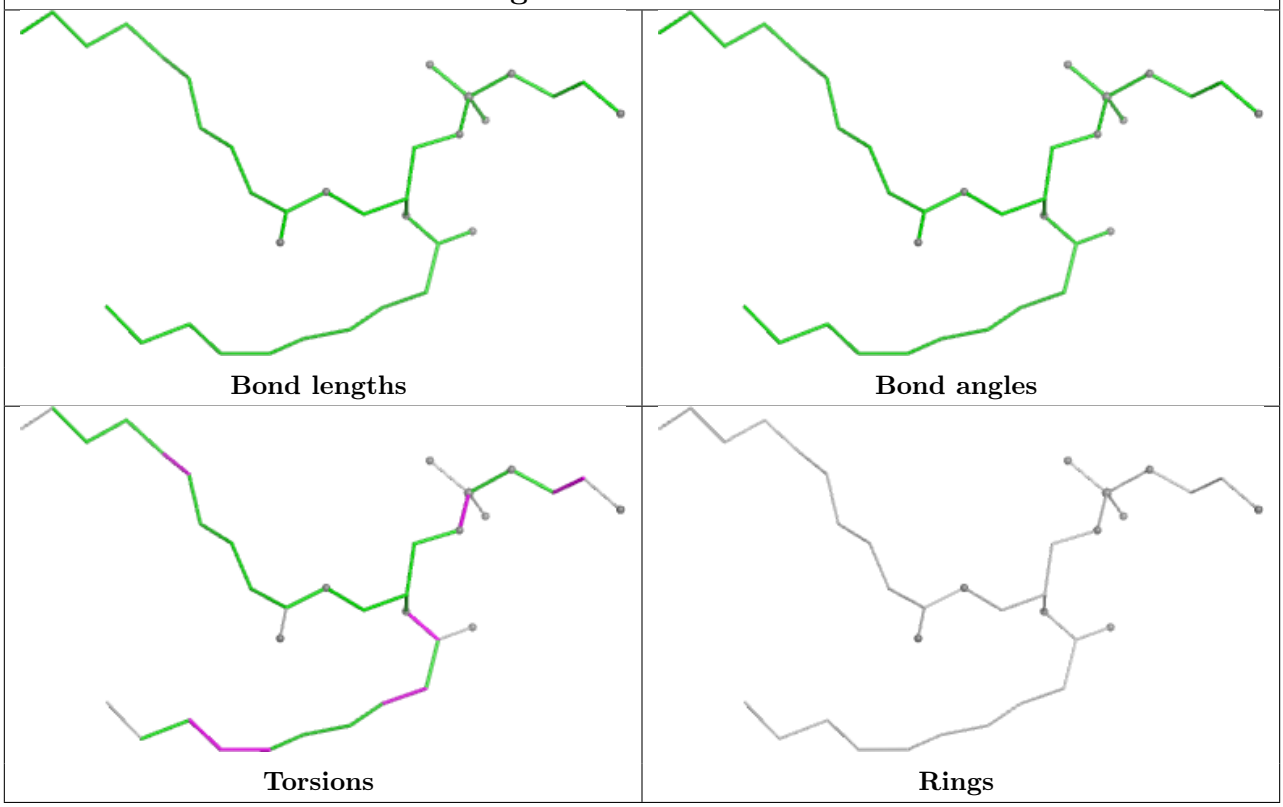


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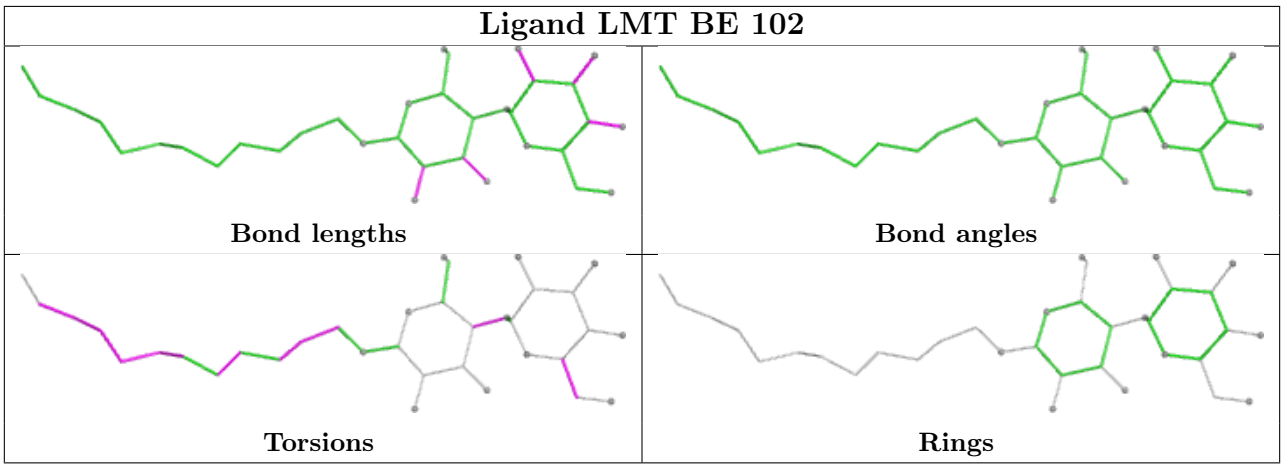


Rings

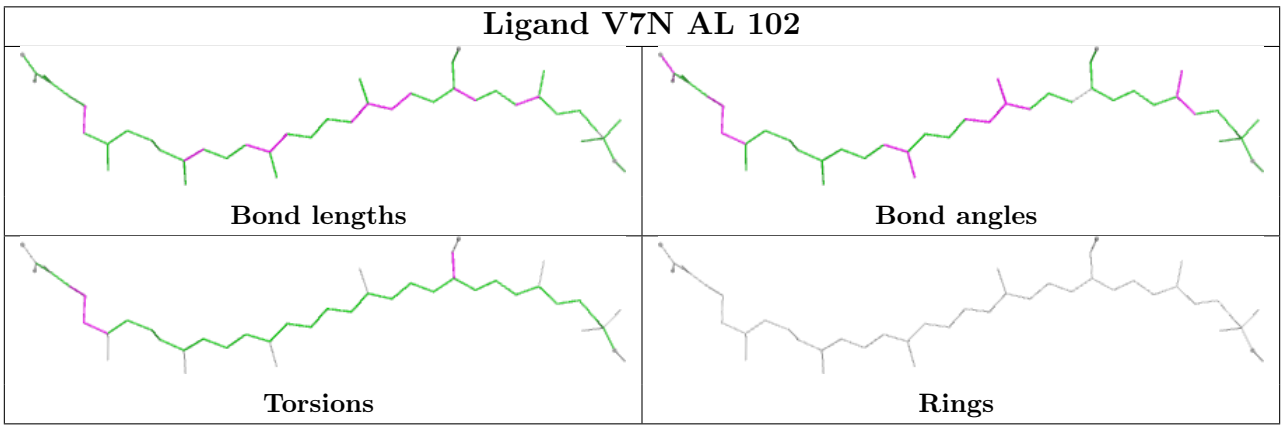
Ligand PEX Bm 102



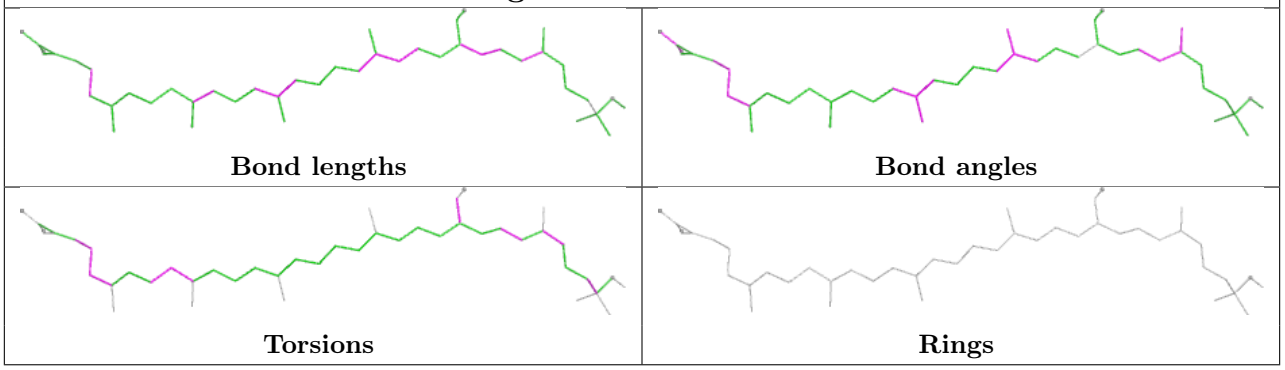
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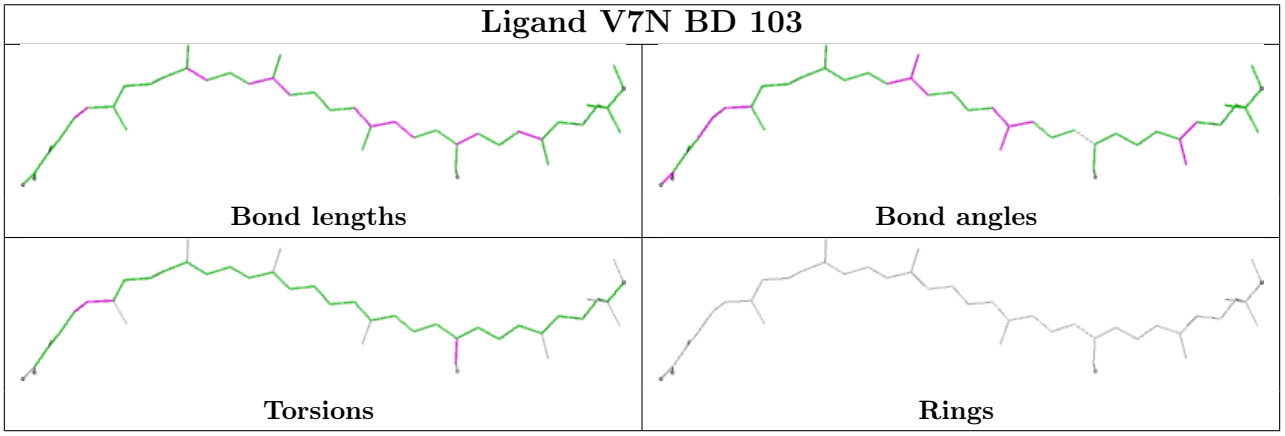
Ligand V7N AL 102



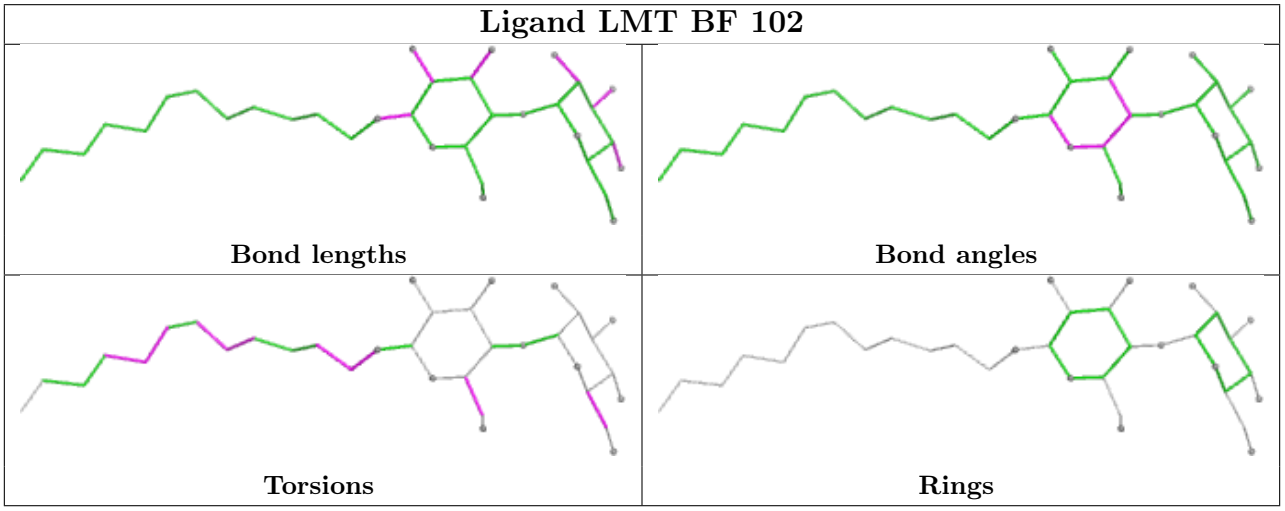
Ligand V7N Bb 1202



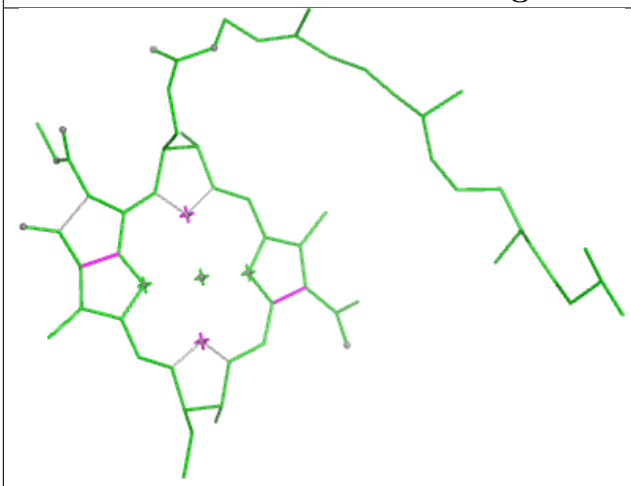
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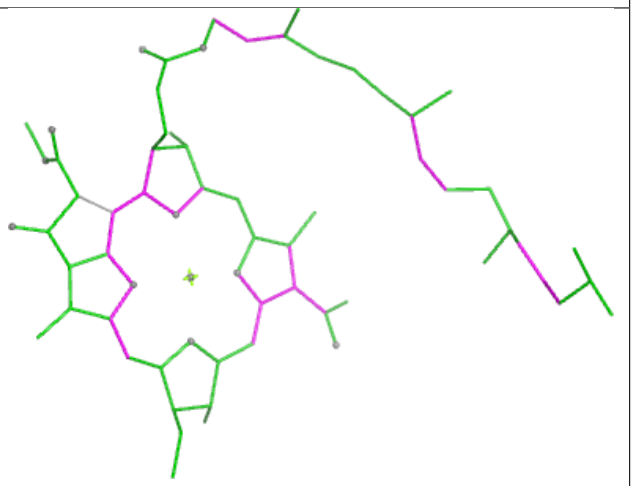
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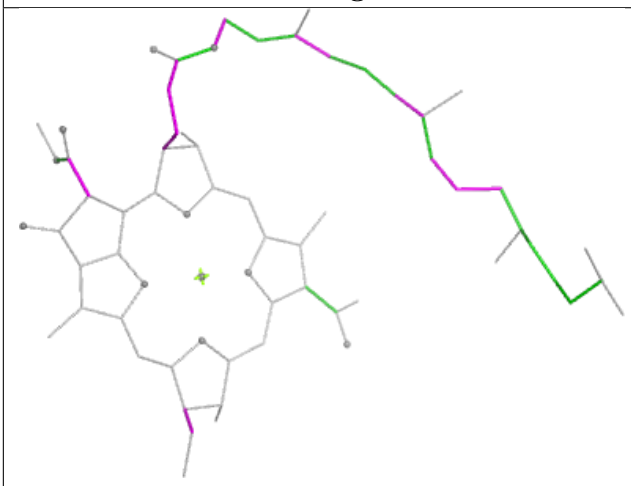
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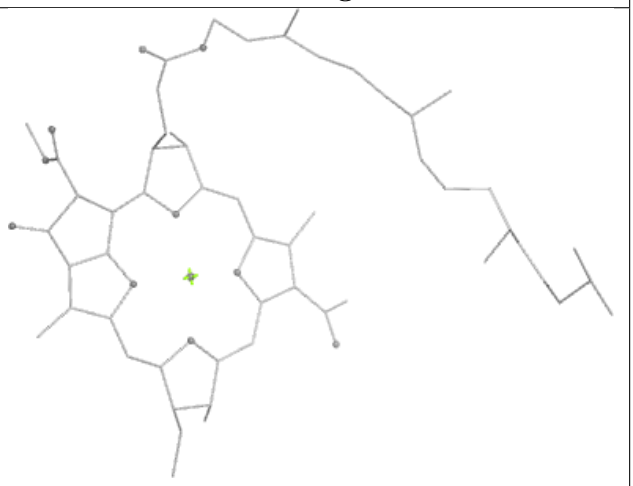
Bond lengths



Bond angles

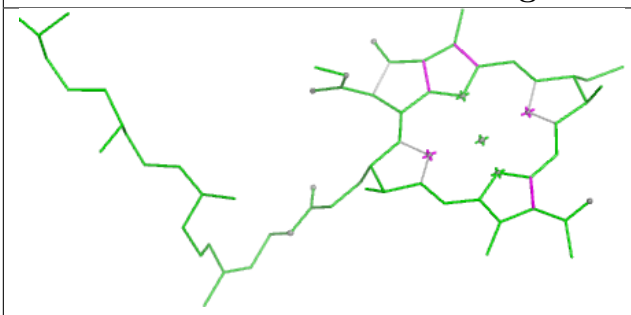


Torsions

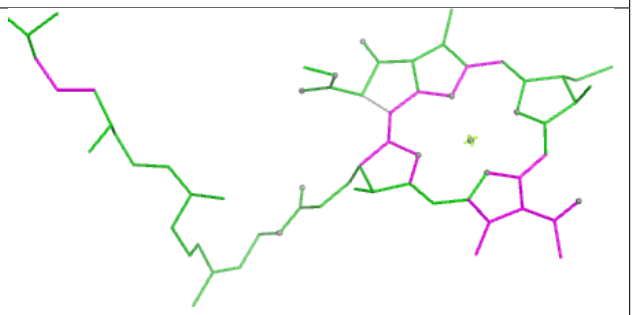


Rings

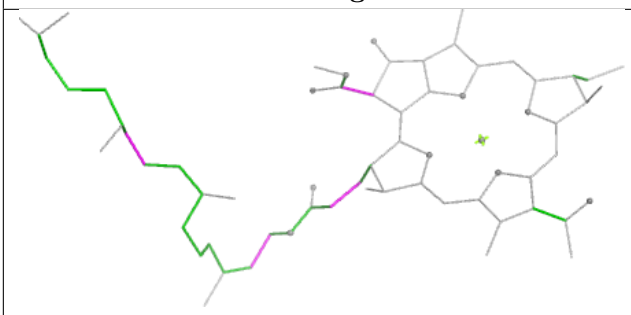
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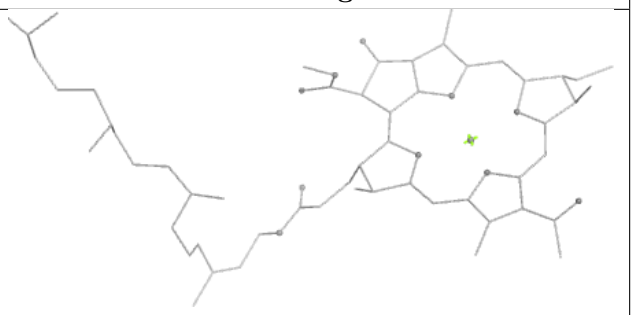
Bond lengths



Bond angles

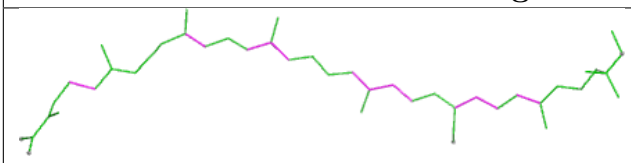


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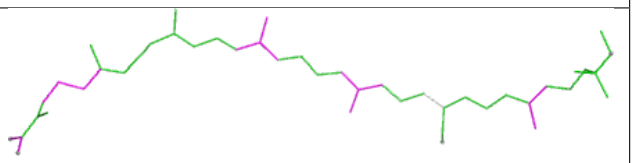


Rings

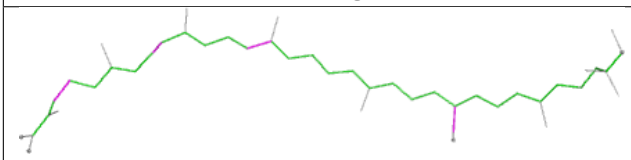
Ligand V7N BA 102



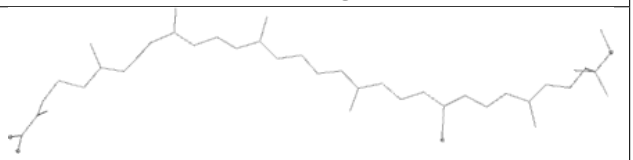
Bond lengths



Bond angles

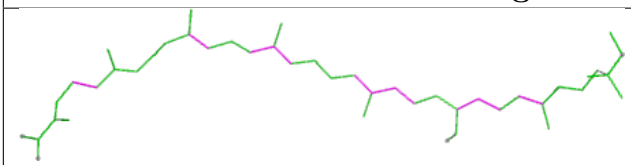


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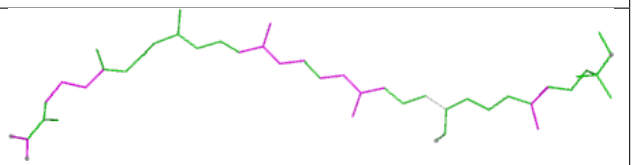


Rings

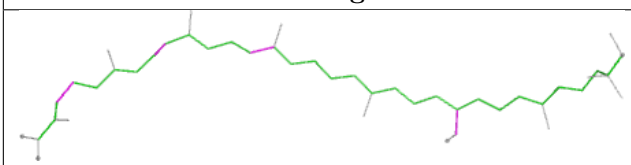
Ligand V7N BC 103



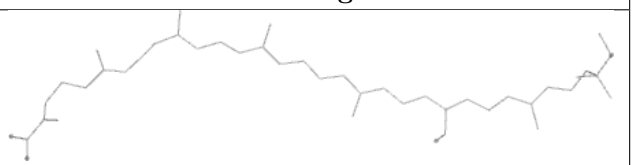
Bond lengths



Bond angles

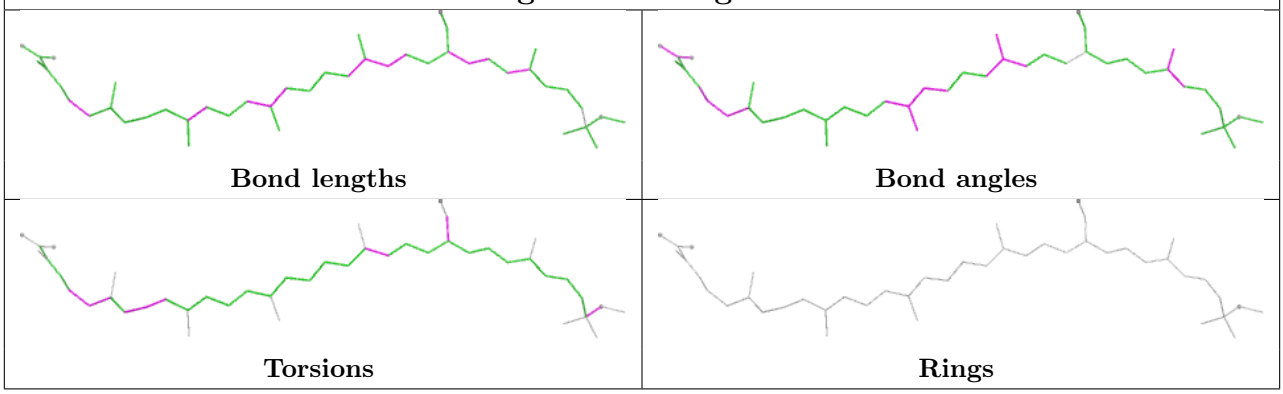


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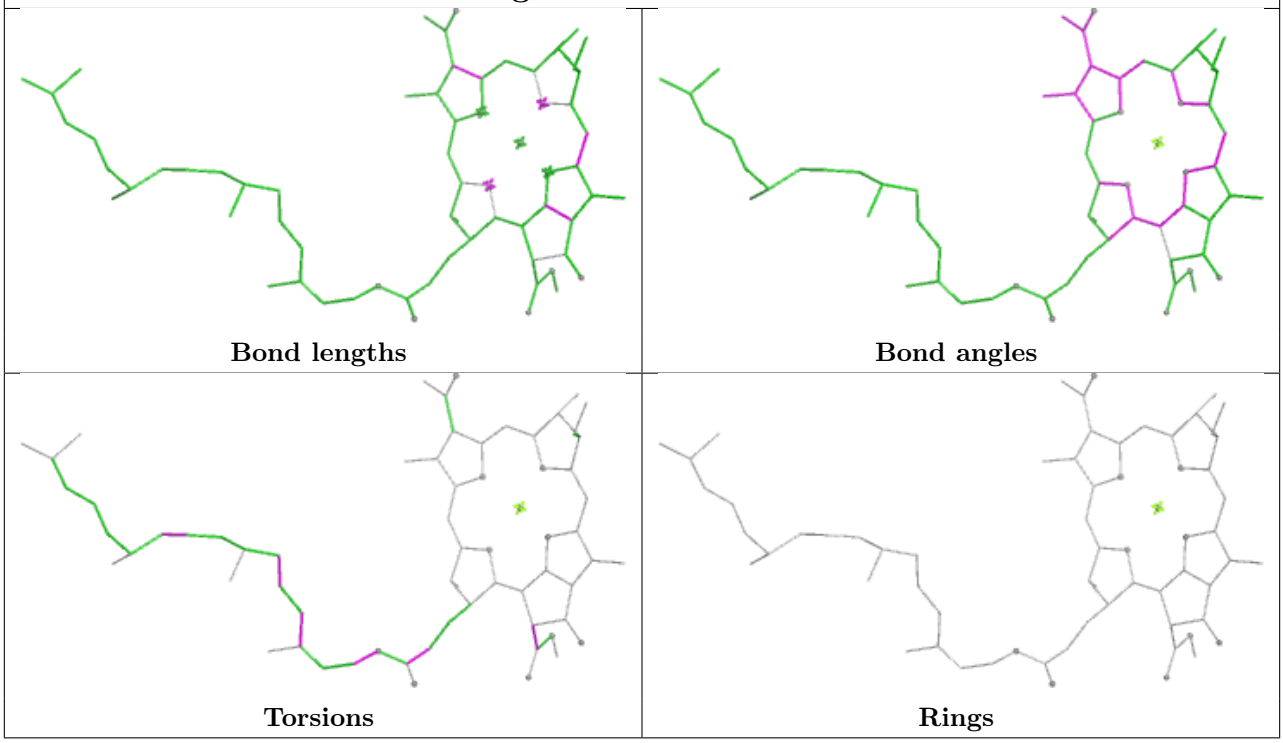


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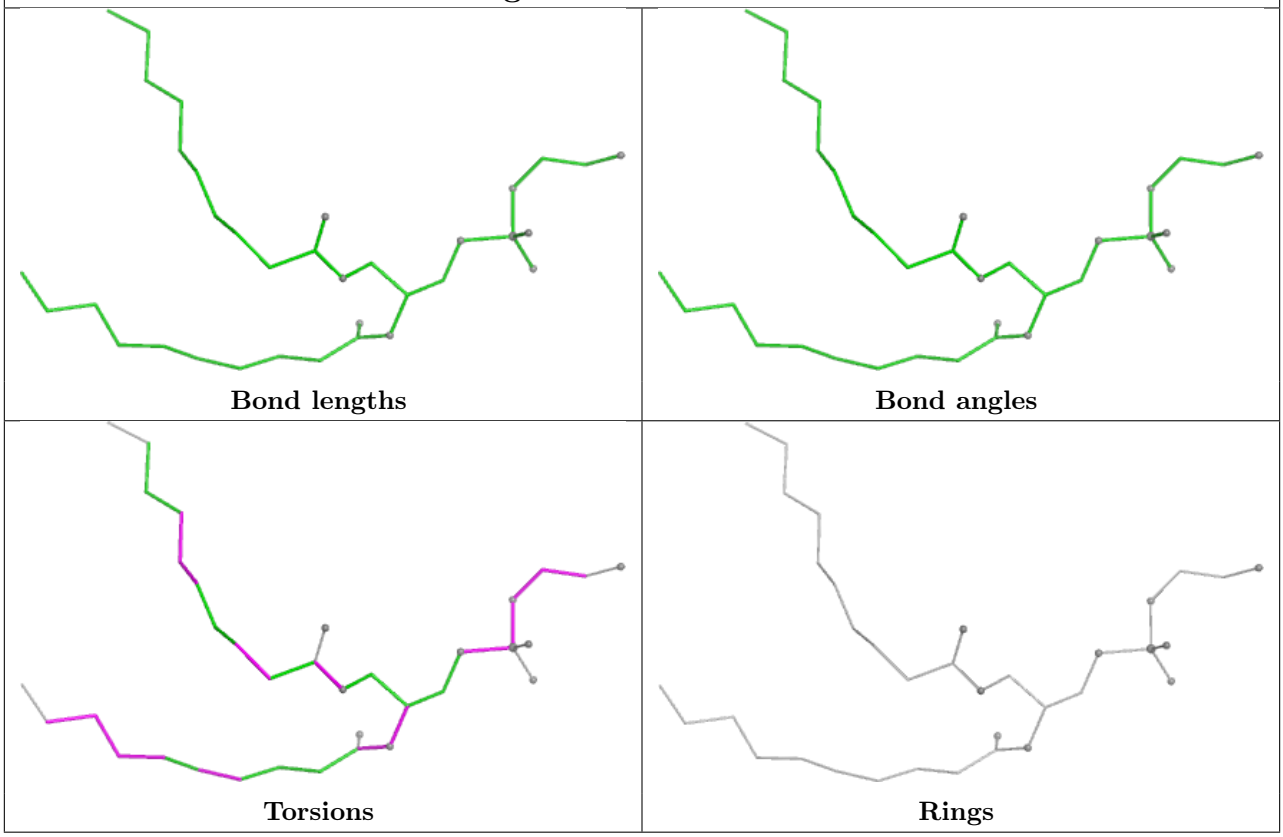
Ligand V7N Bg 101



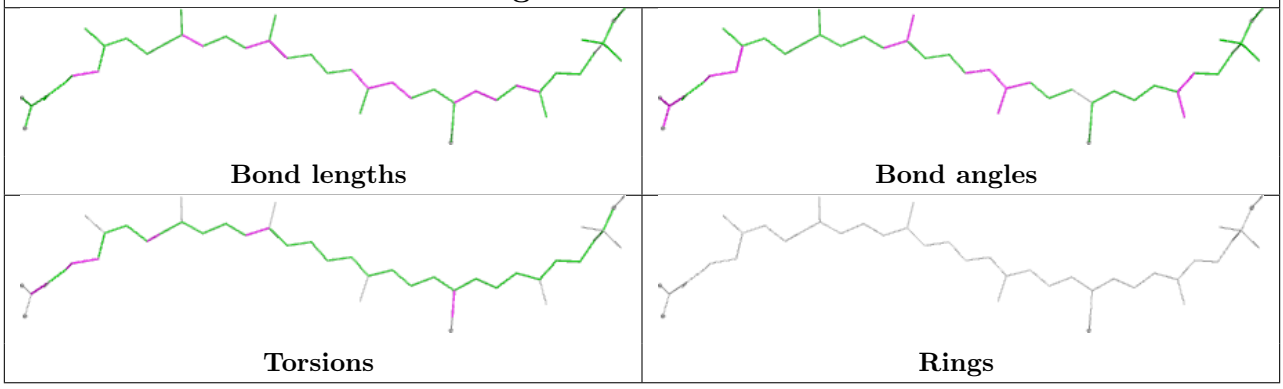
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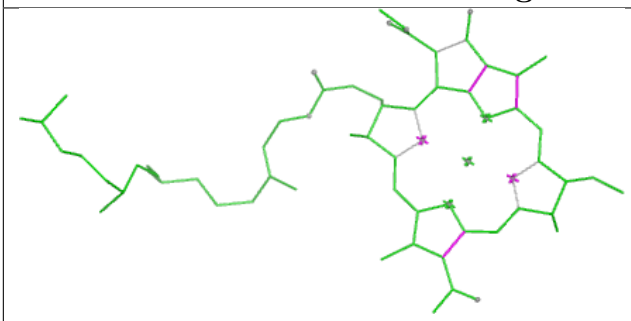
Ligand PEX AE 1101



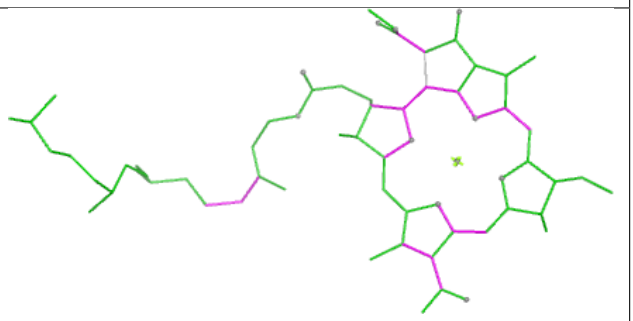
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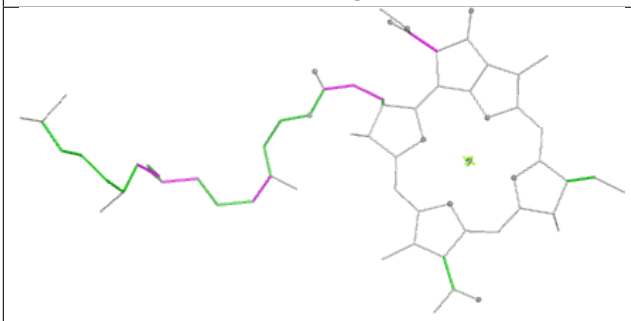
Ligand BCL BS 101



Bond lengths



Bond angles



Torsions

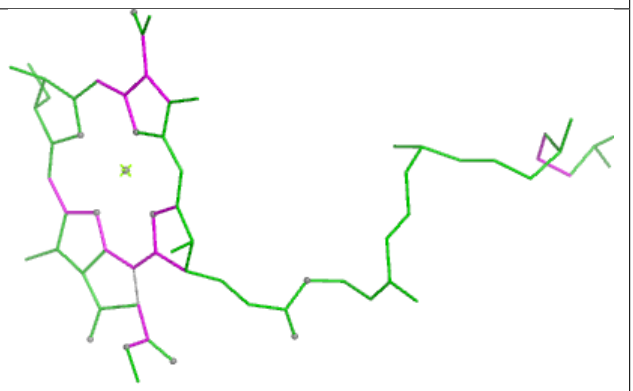


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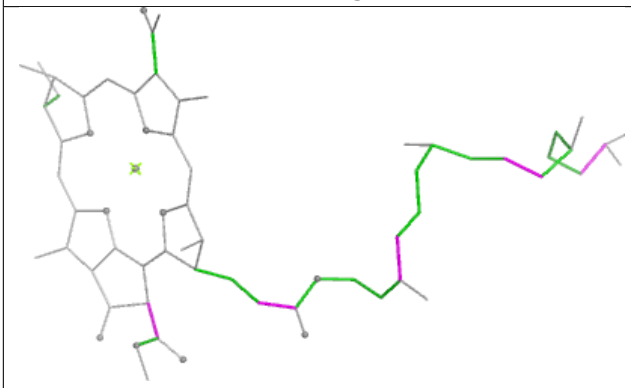
Ligand BCL AB 101



Bond lengths



Bond angles

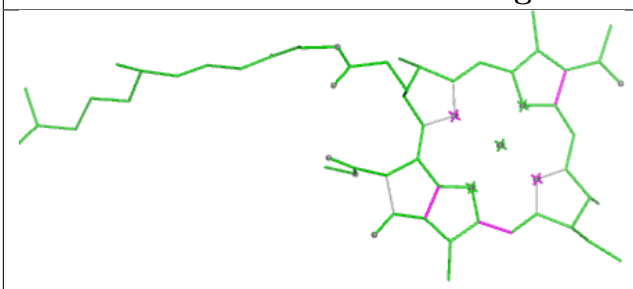


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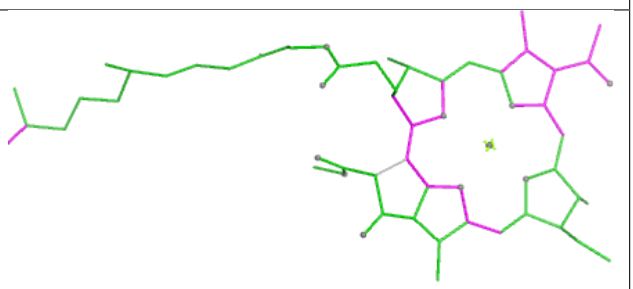


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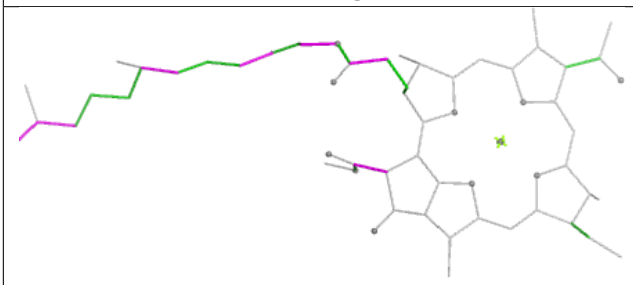
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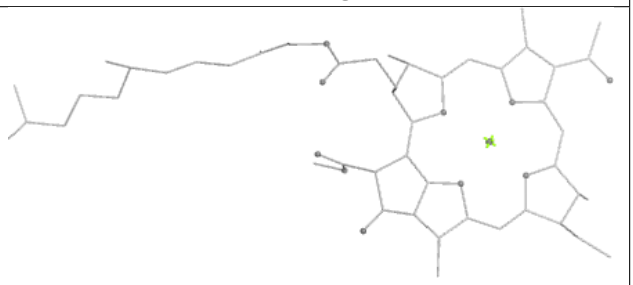
Bond lengths



Bond angles

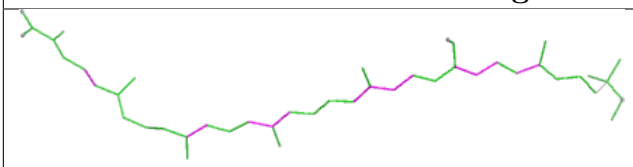


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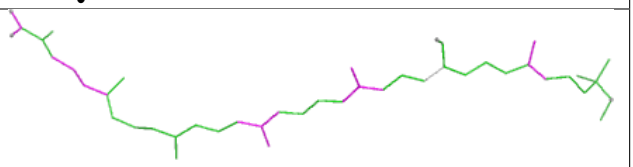


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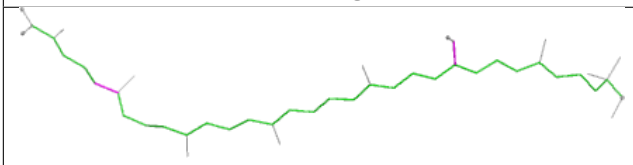
Ligand V7N BQ 103



Bond lengths



Bond angles

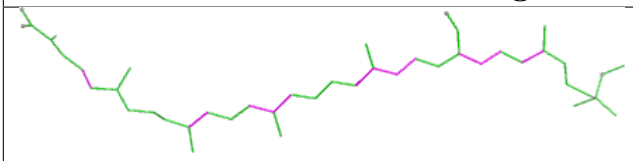


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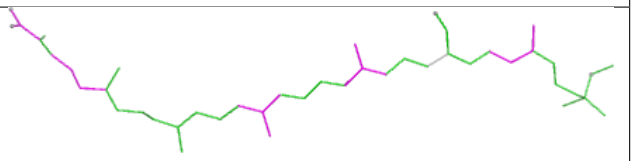


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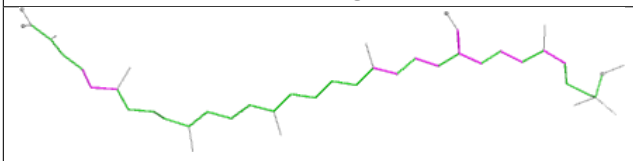
Ligand V7N BO 102



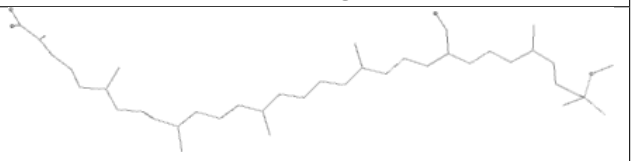
Bond lengths



Bond angles

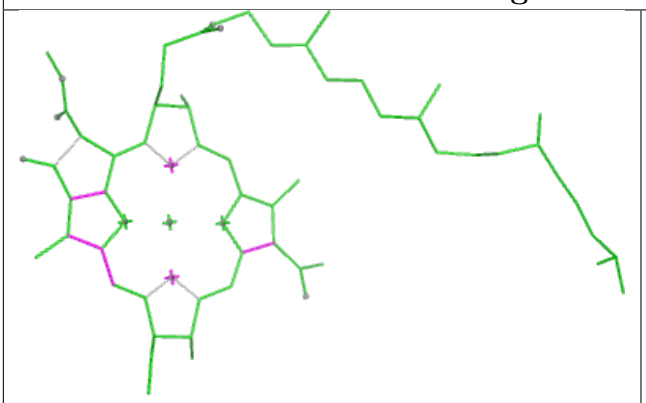


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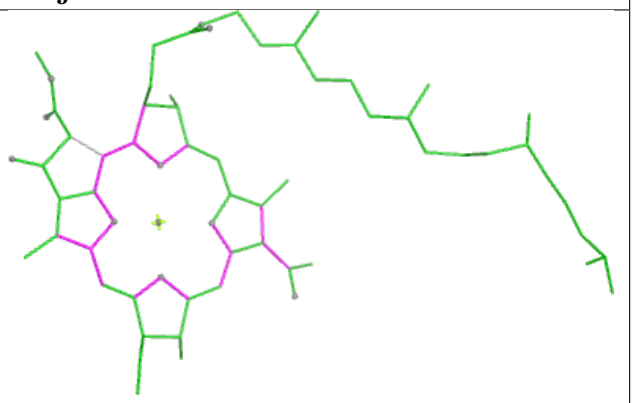


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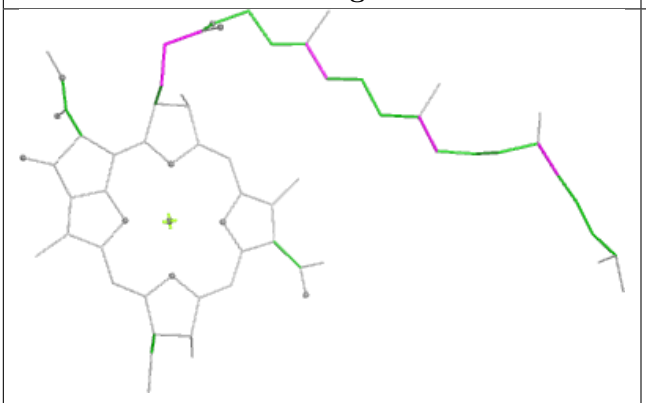
Ligand BCL Bj 1204



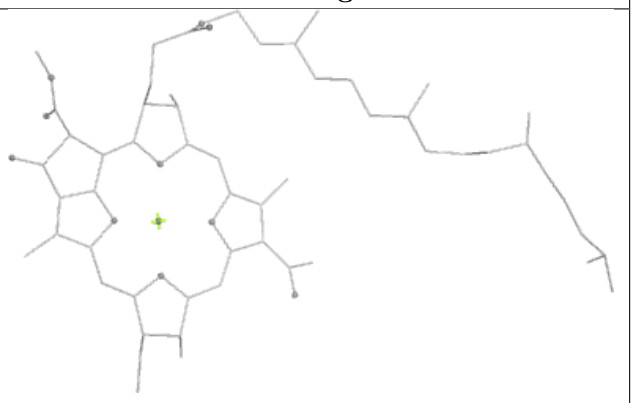
Bond lengths



Bond angles

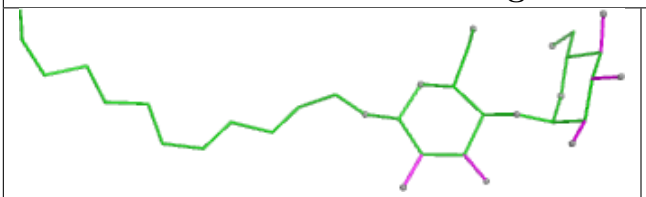


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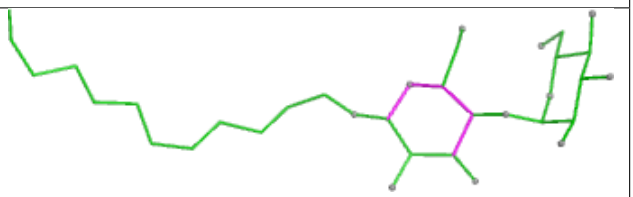


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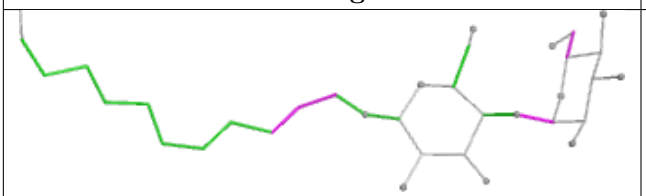
Ligand LMT BU 103



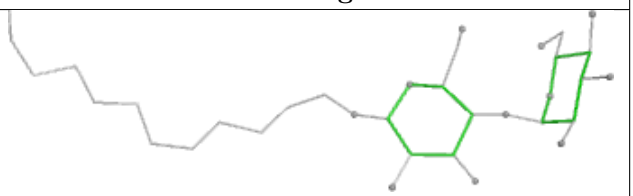
Bond lengths



Bond angles

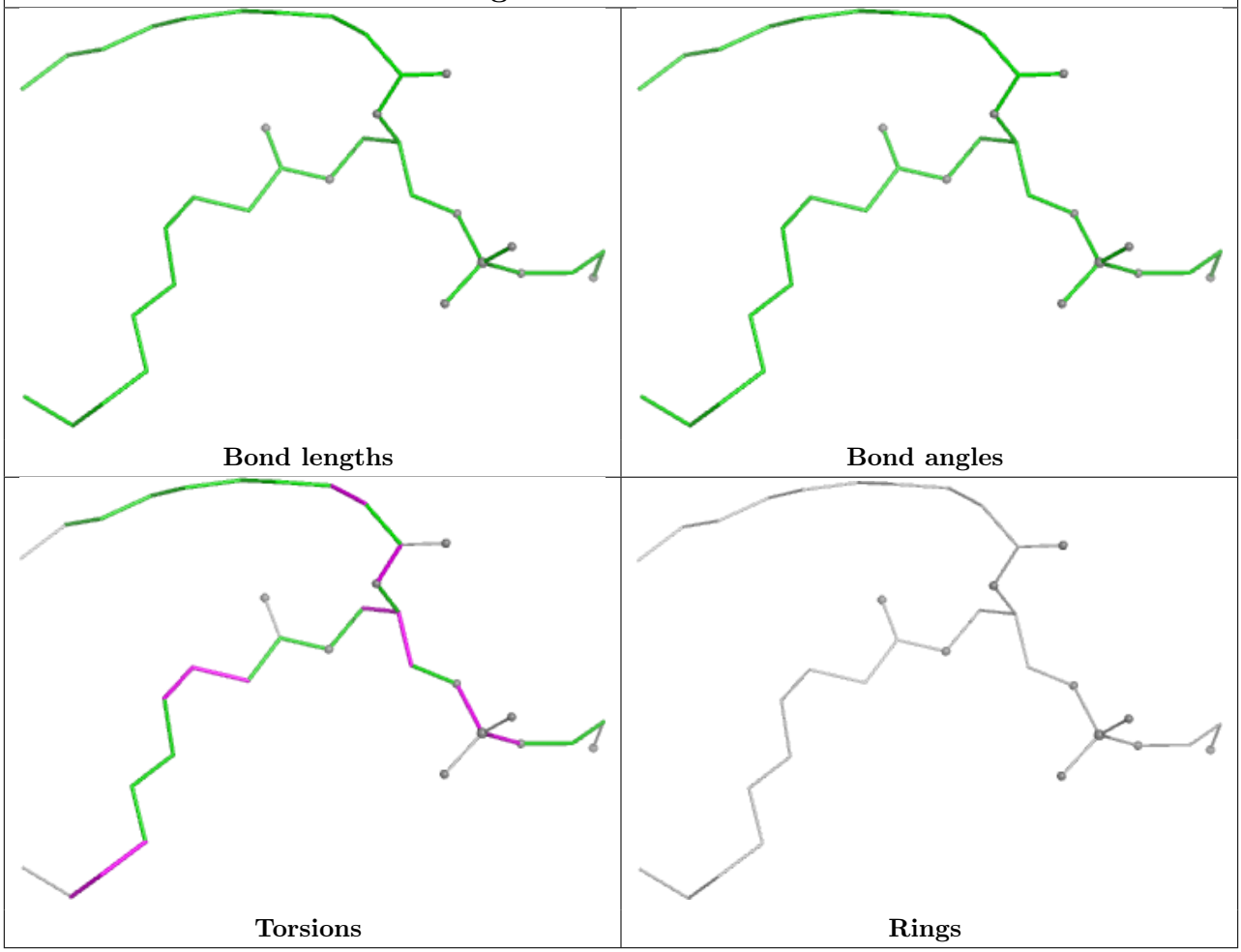


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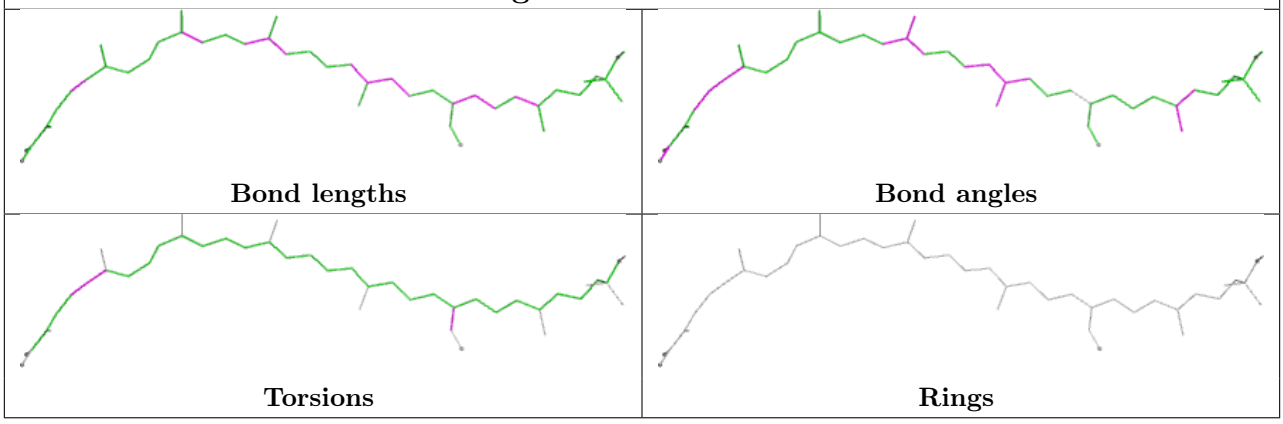


Rings

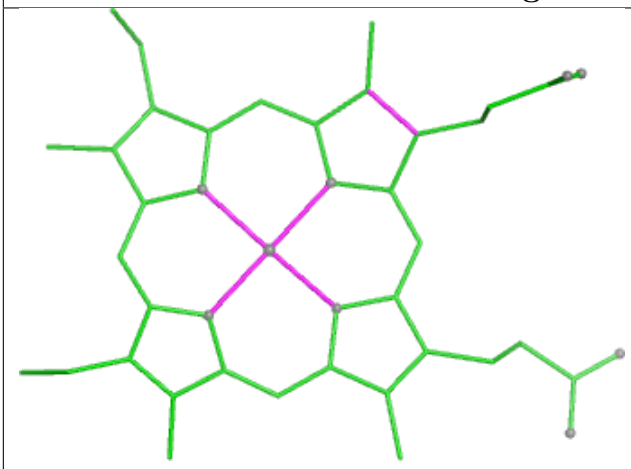
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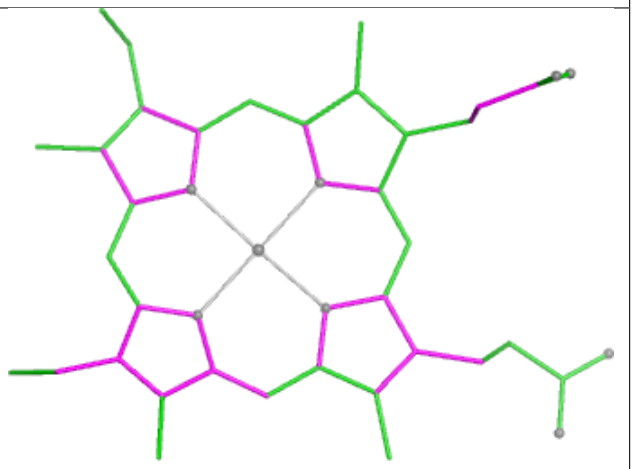
Ligand V7N BG 101



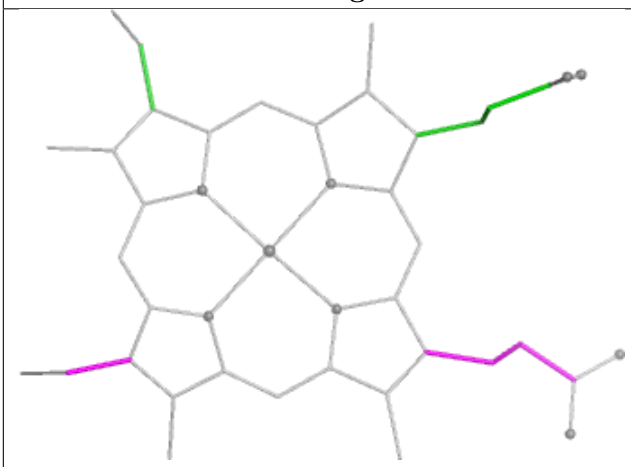
Ligand HEC C 402



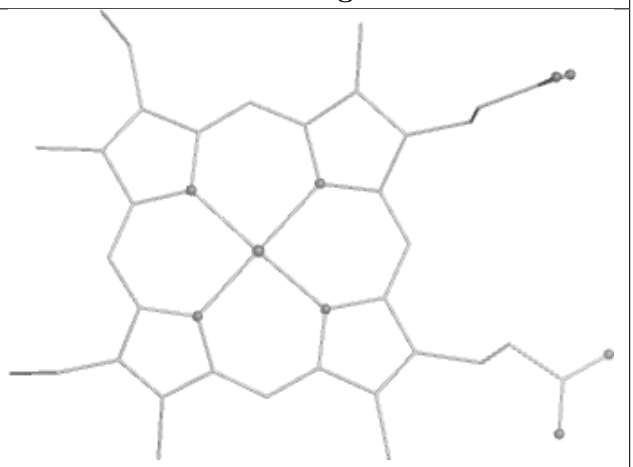
Bond lengths



Bond angles

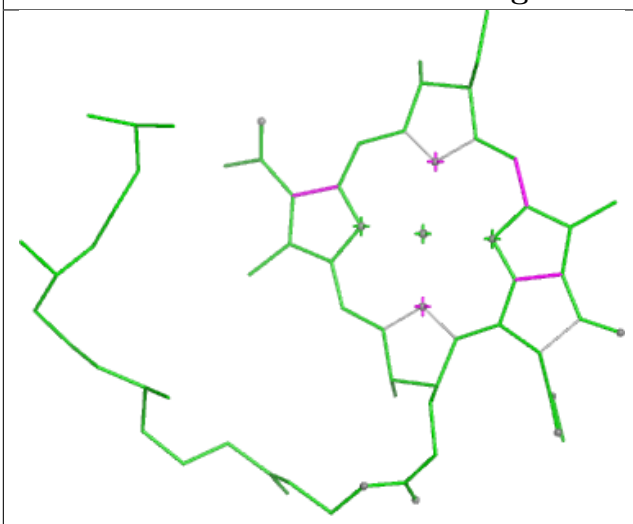


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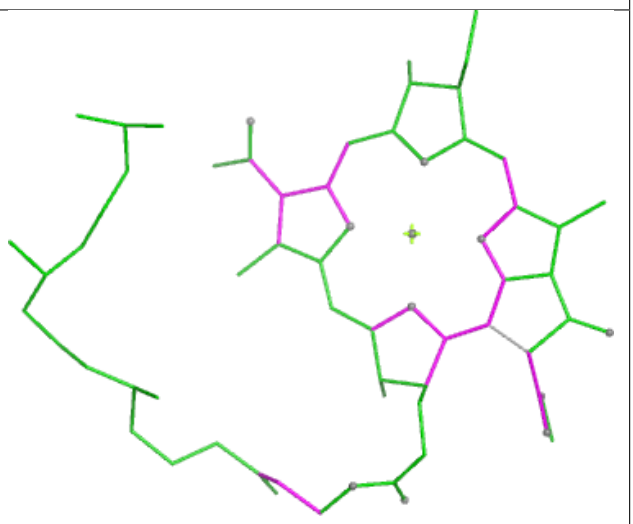


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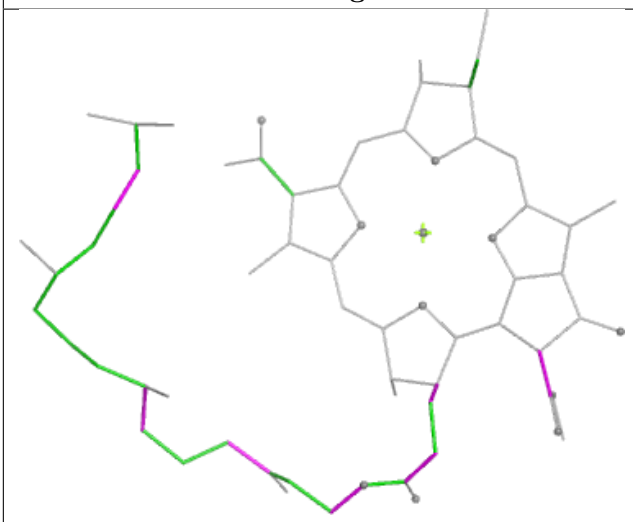
Ligand BCL BG 102



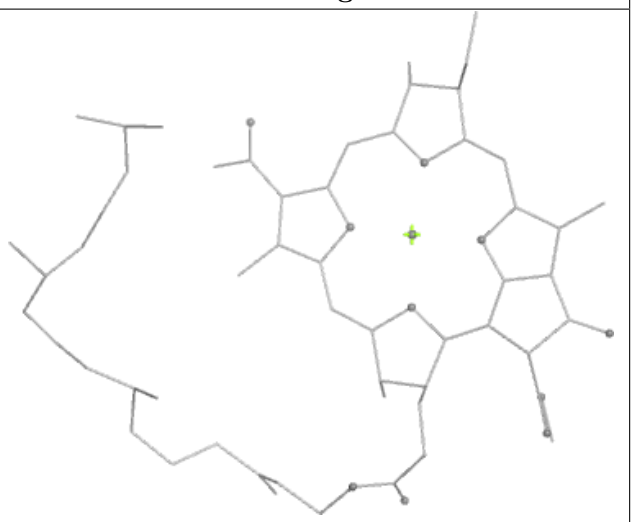
Bond lengths



Bond angles

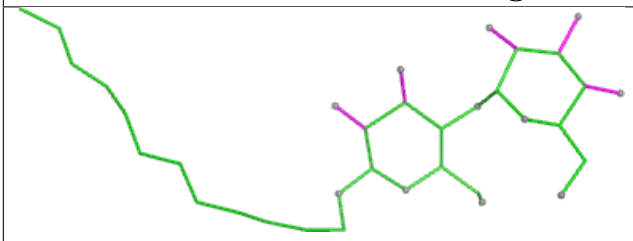


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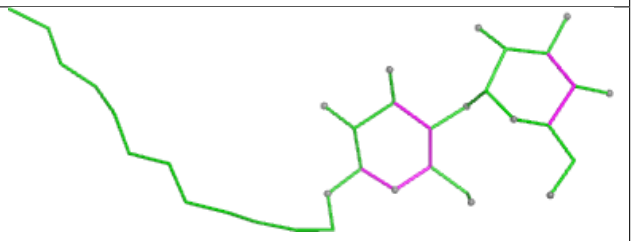


Rings

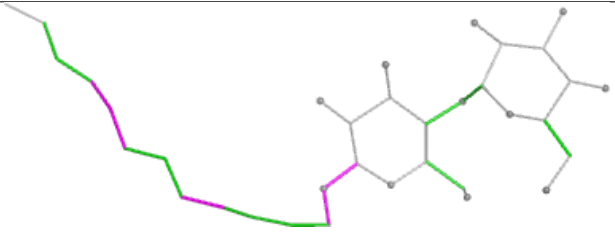
Ligand LMT BH 101



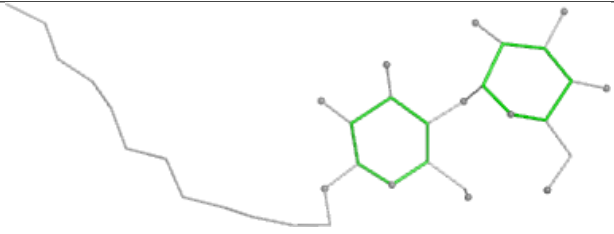
Bond lengths



Bond angles

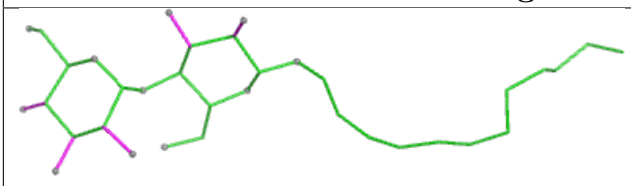


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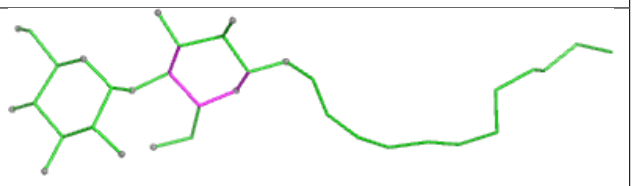


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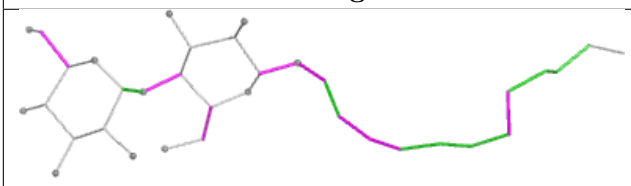
Ligand LMT M 401



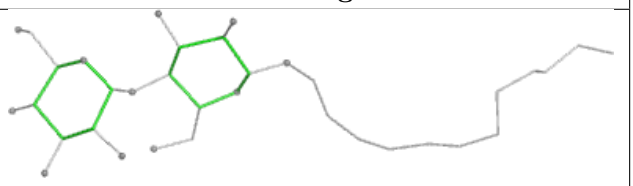
Bond lengths



Bond angles

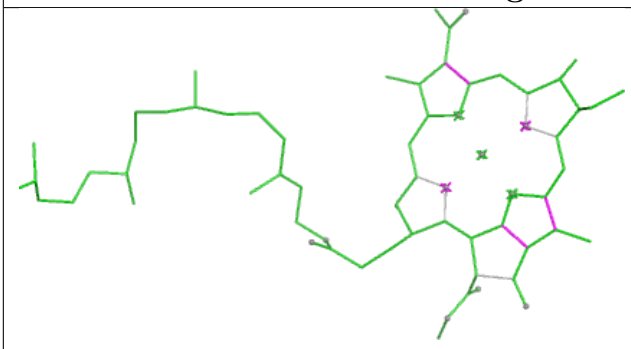


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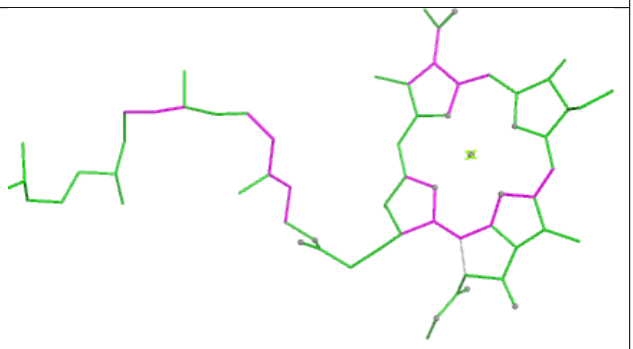


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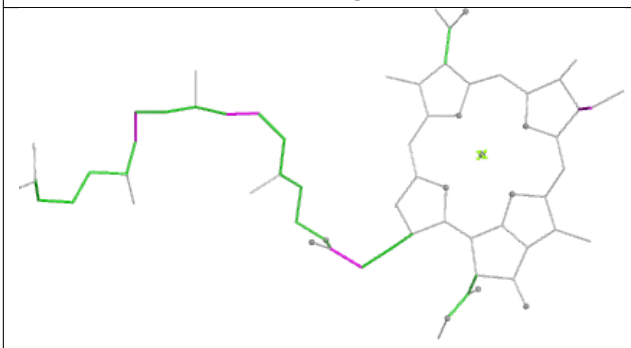
Ligand BCL Bh 1205



Bond lengths



Bond angles

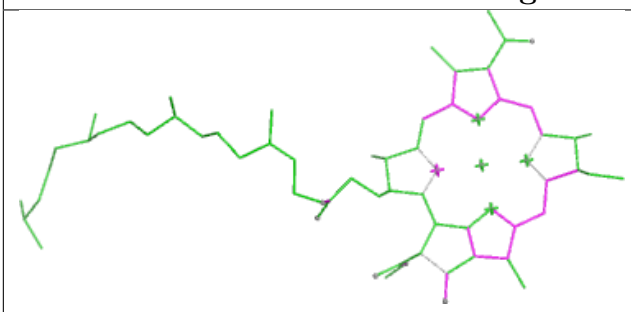


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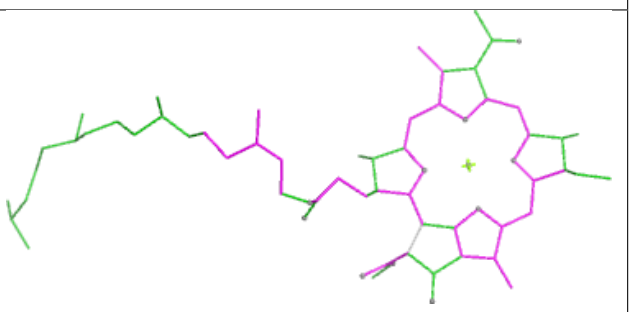


Rings

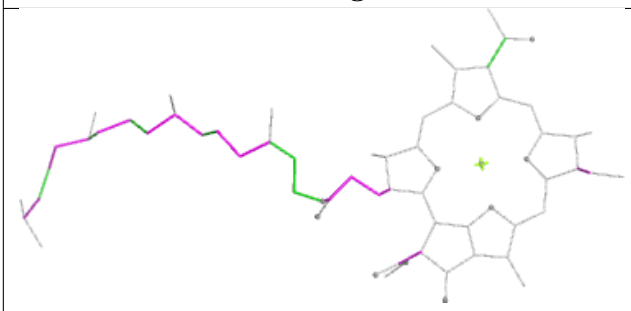
Ligand BCL Al 101



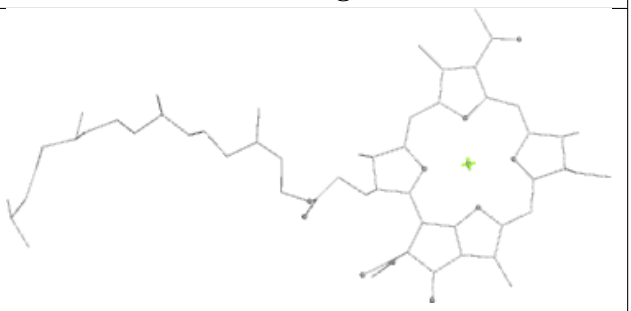
Bond lengths



Bond angles

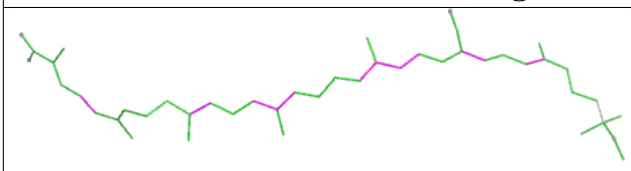


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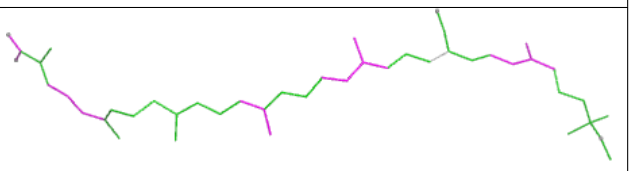


Rings

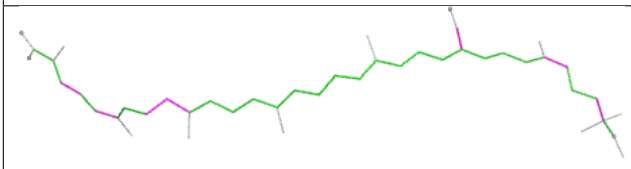
Ligand V7N Bf 1202



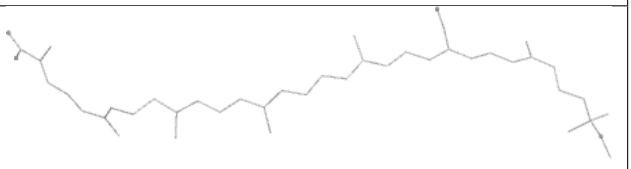
Bond lengths



Bond angles

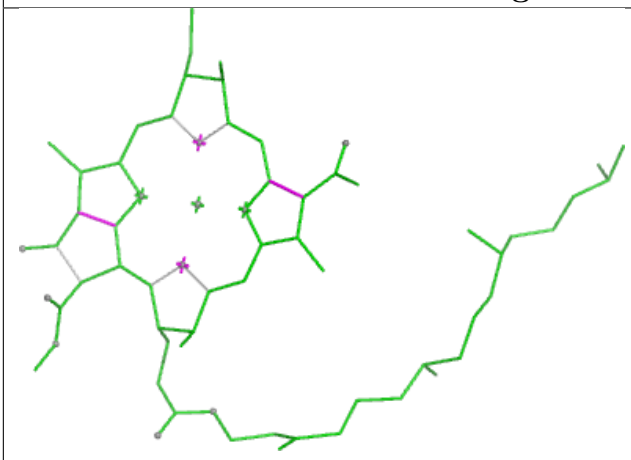


Torsions

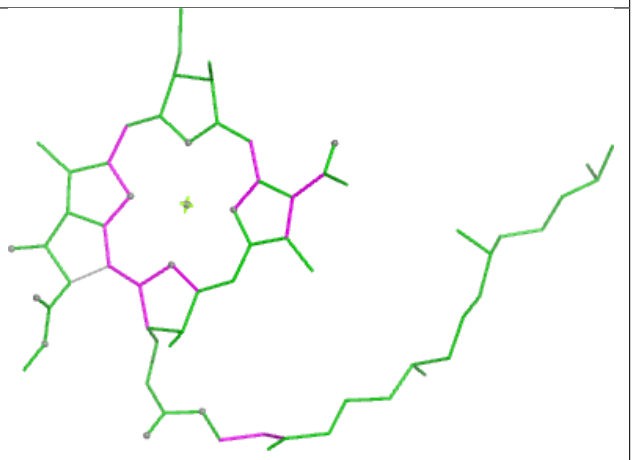


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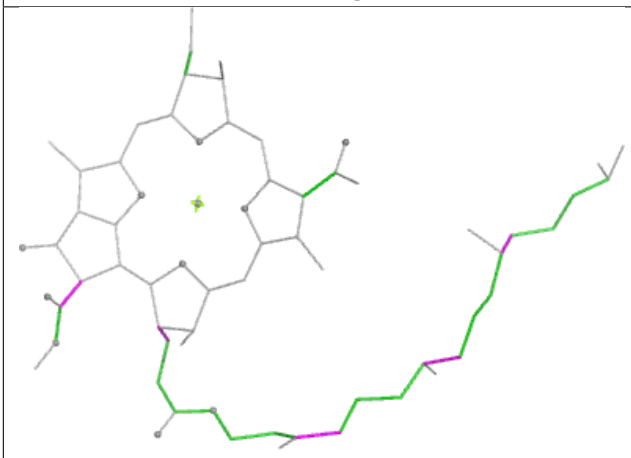
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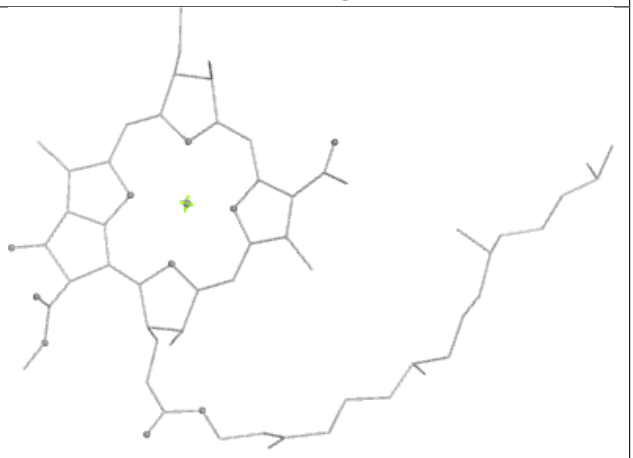
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Bond angles

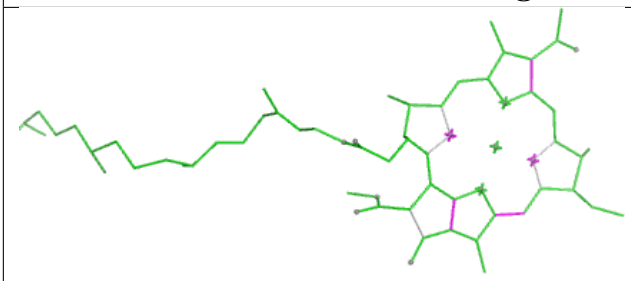


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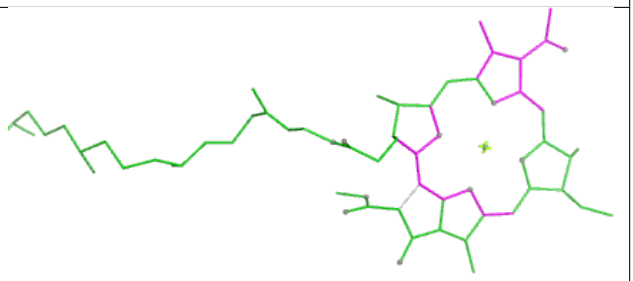


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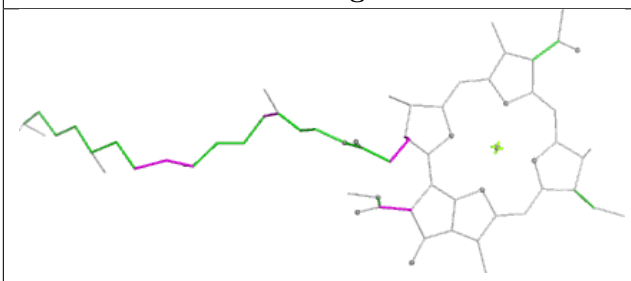
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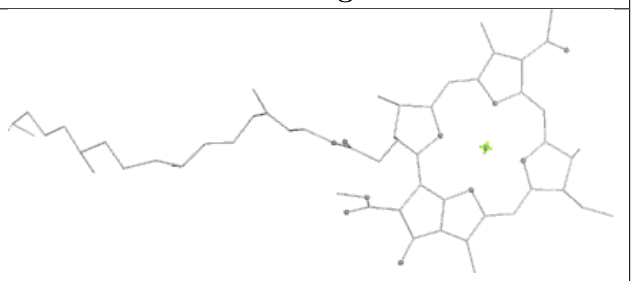
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Bond angles

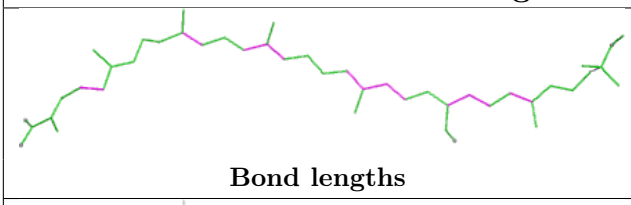


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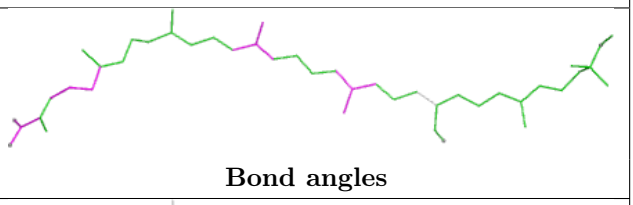


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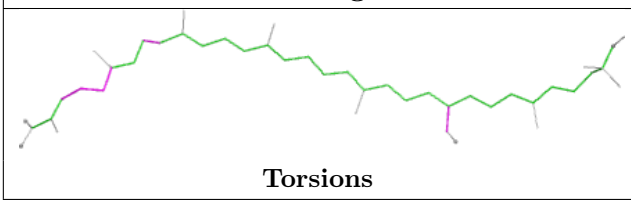
Ligand V7N BT 101



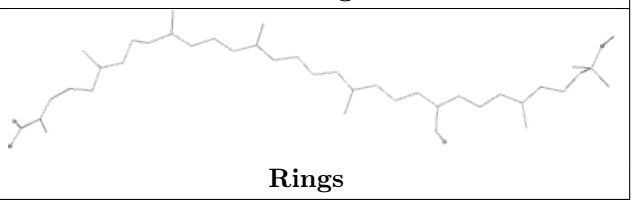
Bond lengths



Bond angles

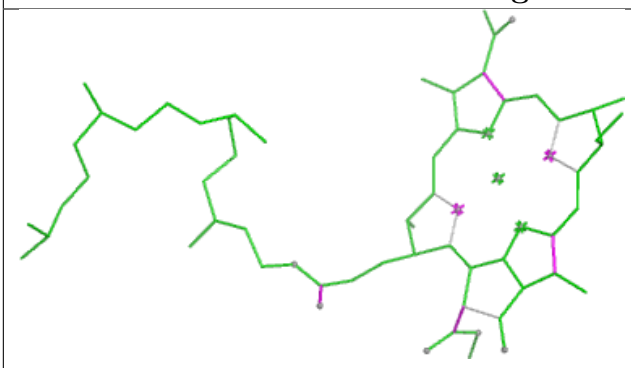


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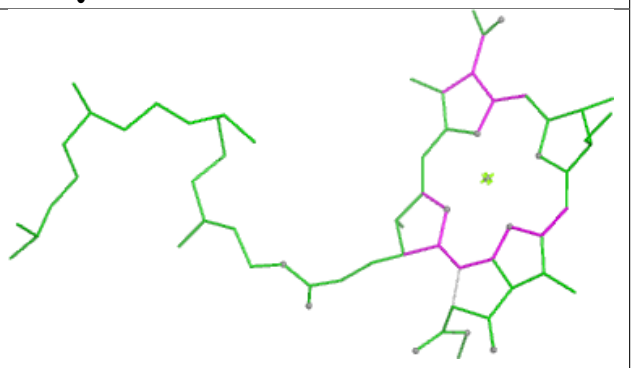


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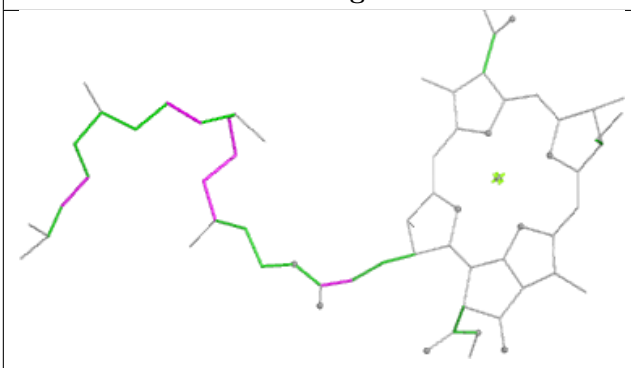
Ligand BCL AQ 102



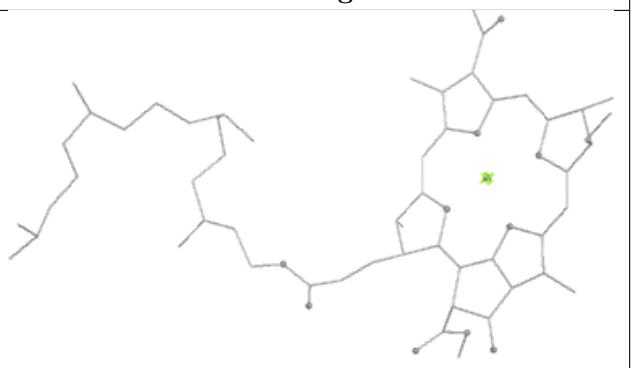
Bond lengths



Bond angles

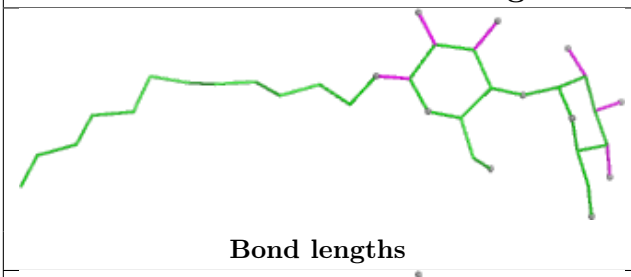


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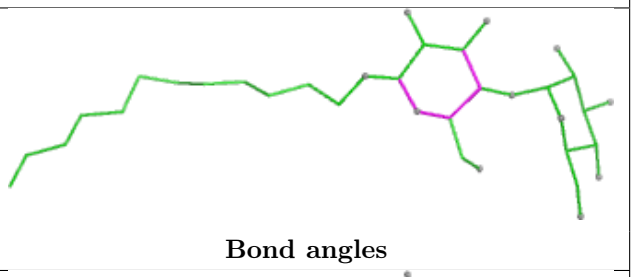


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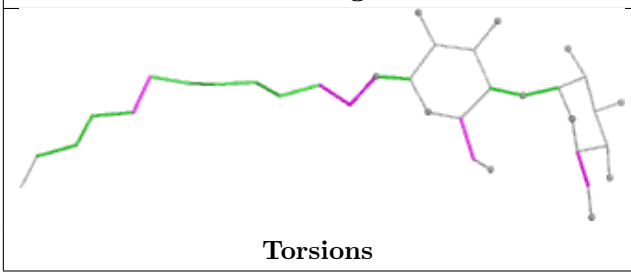
Ligand LMT BG 103



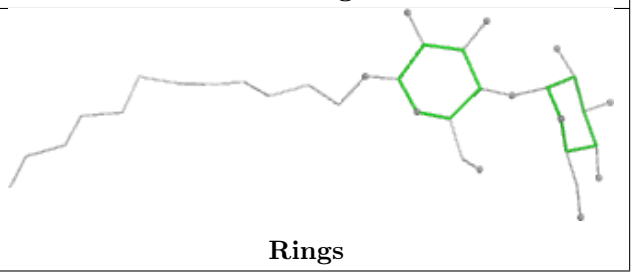
Bond lengths



Bond angles

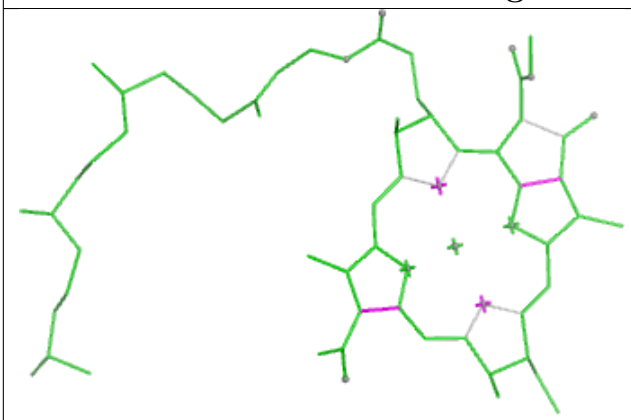


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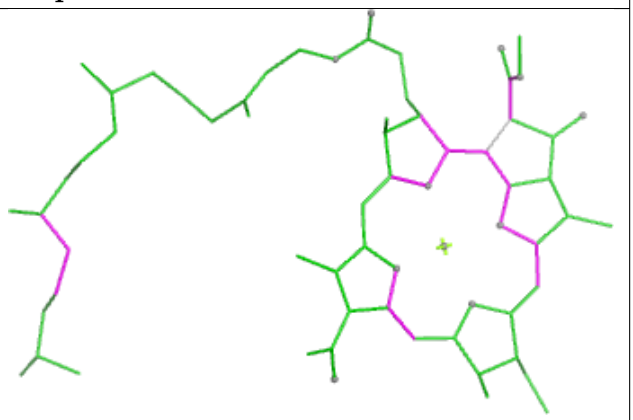


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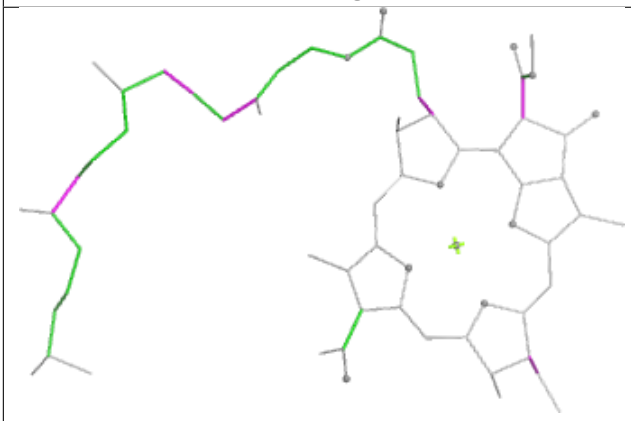
Ligand BCL Bp 1204



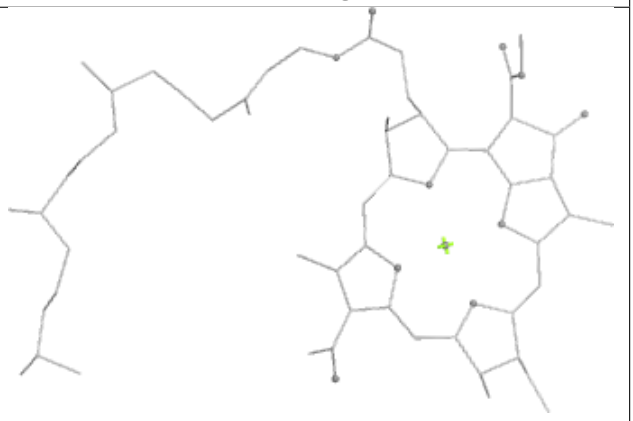
Bond lengths



Bond angles

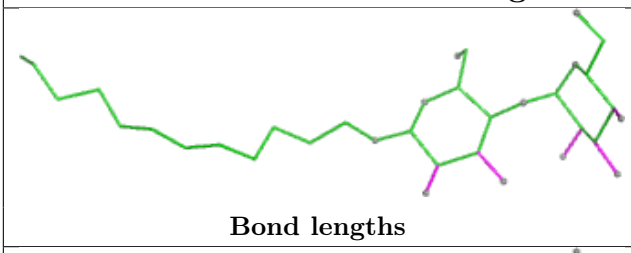


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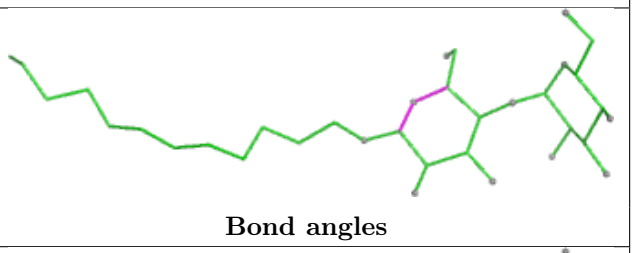


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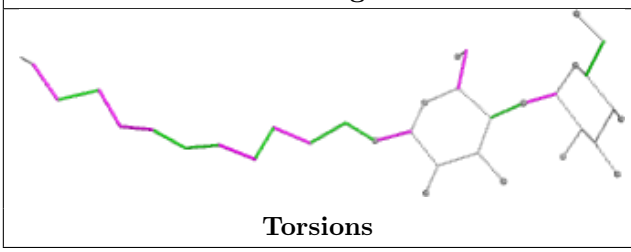
Ligand LMT BC 102



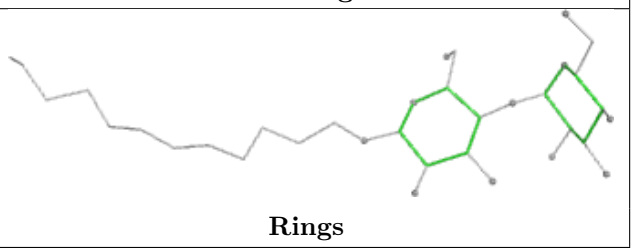
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Bond angles

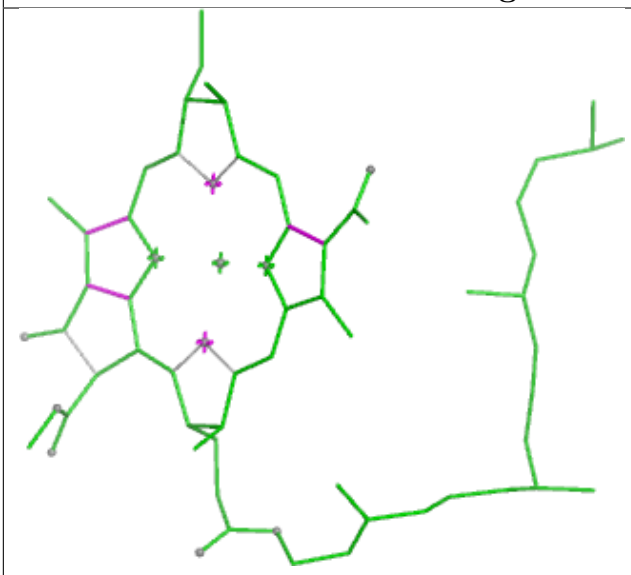


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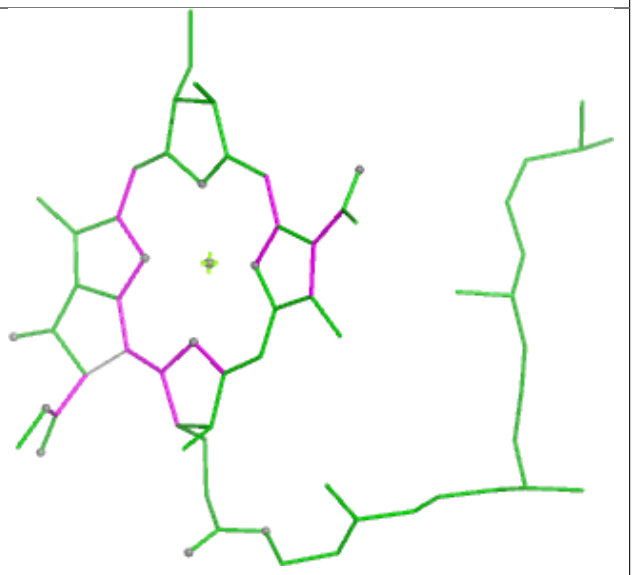


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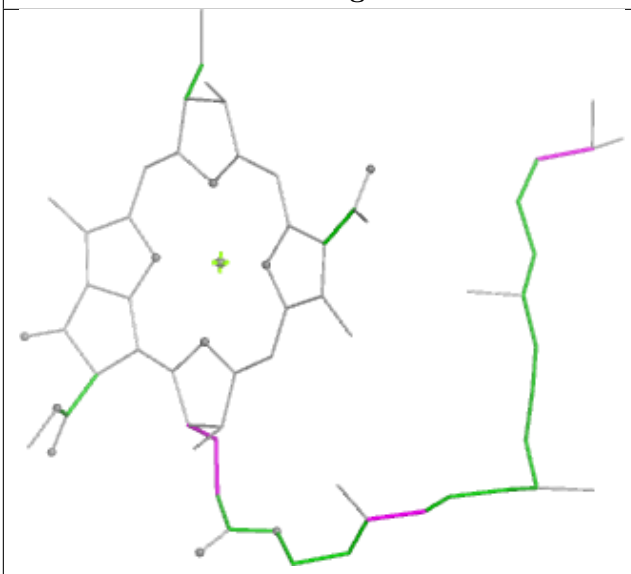
Ligand BCL AW 1204



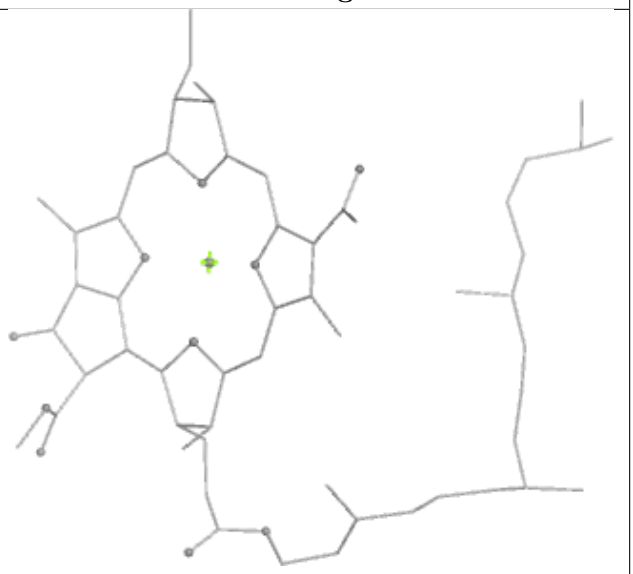
Bond lengths



Bond angles

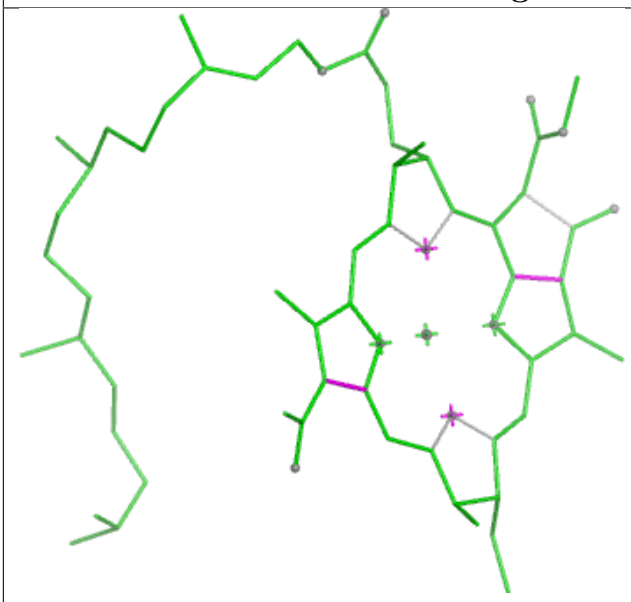


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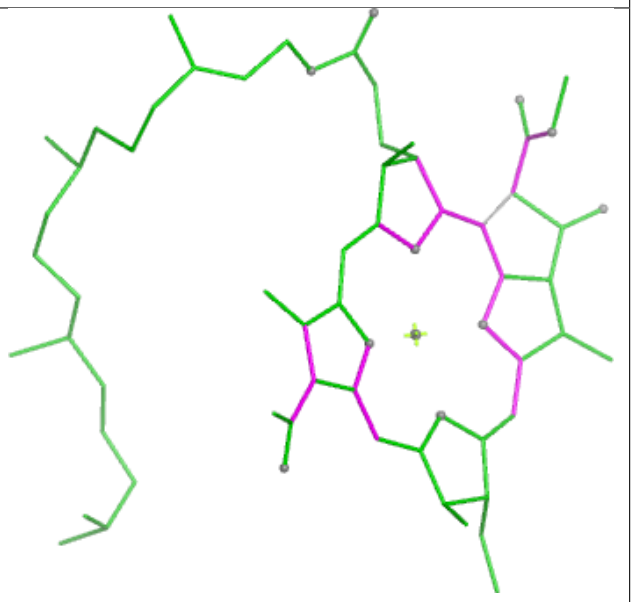


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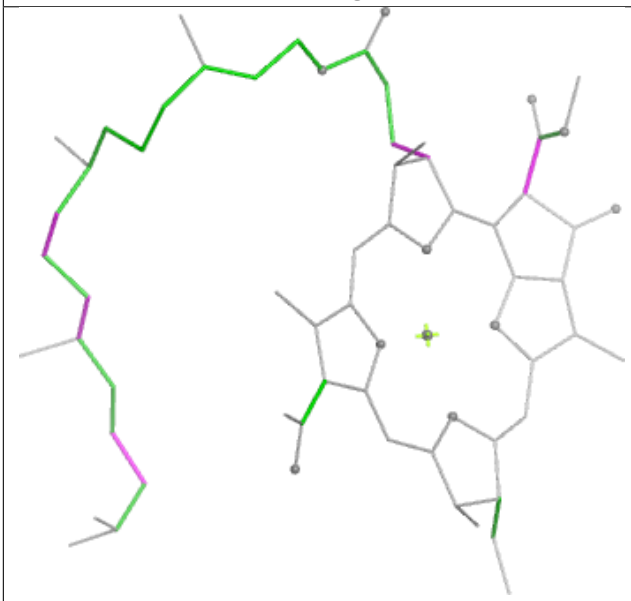
Ligand BCL BN 101



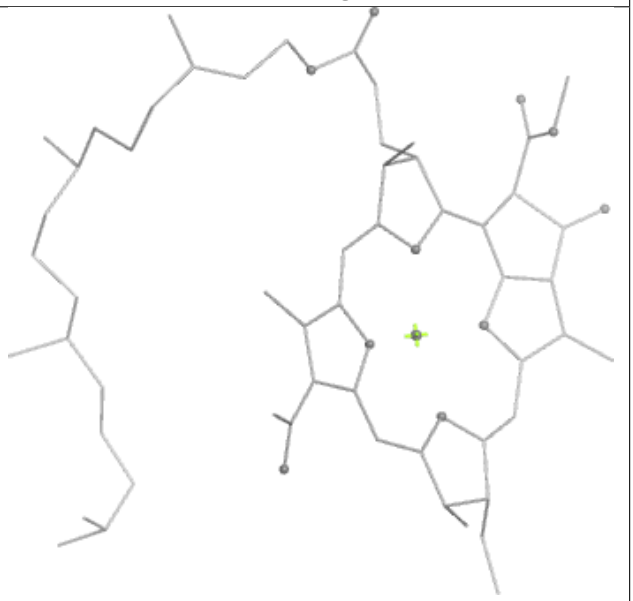
Bond lengths



Bond angles

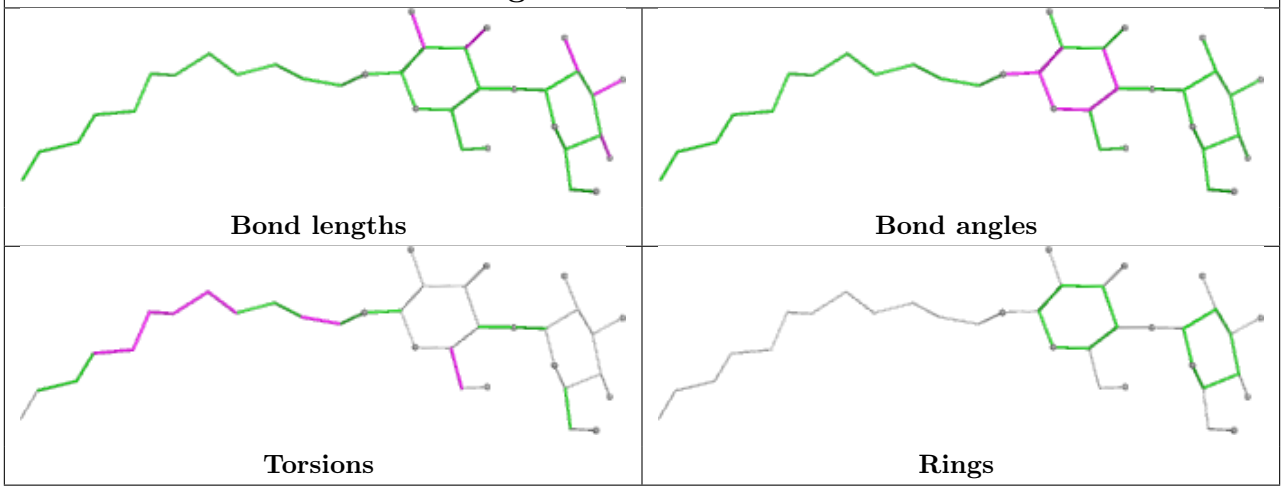


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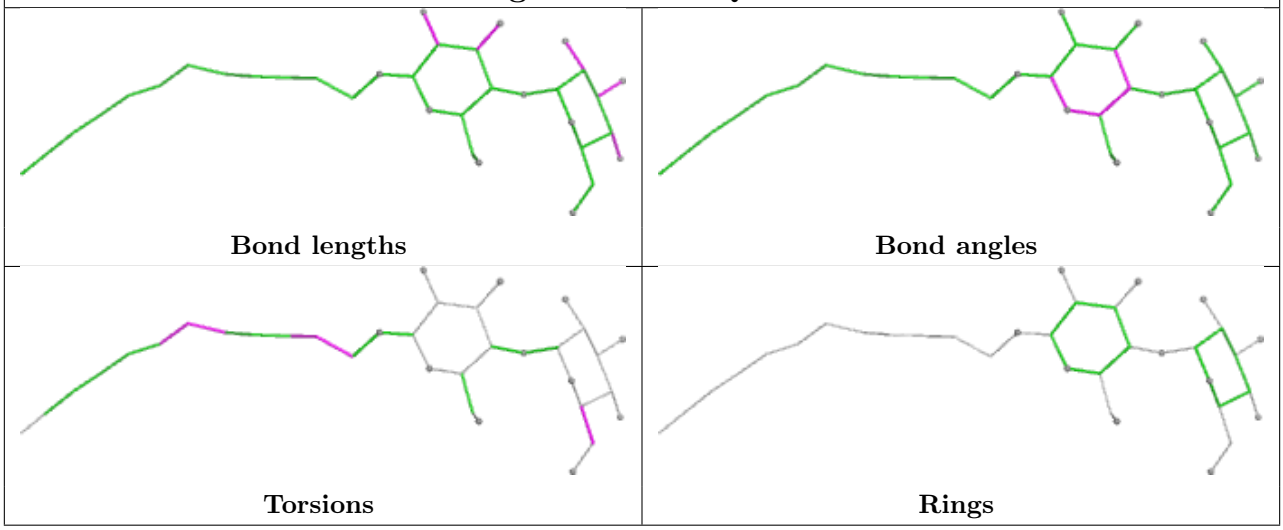


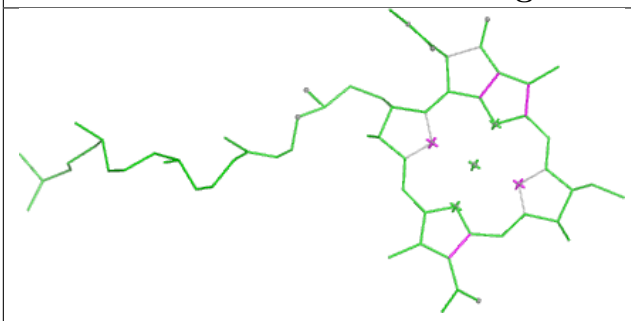
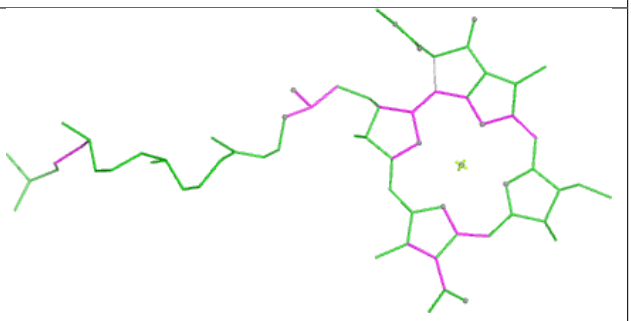
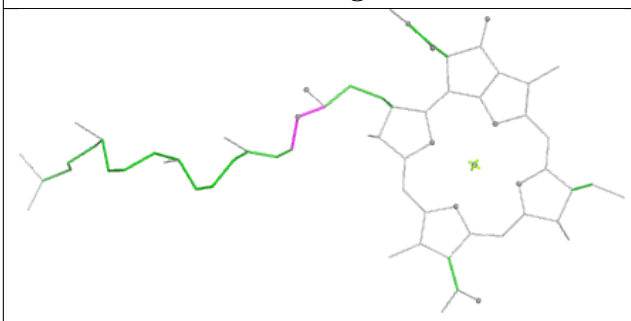
Rings

Ligand LMT Bf 1203

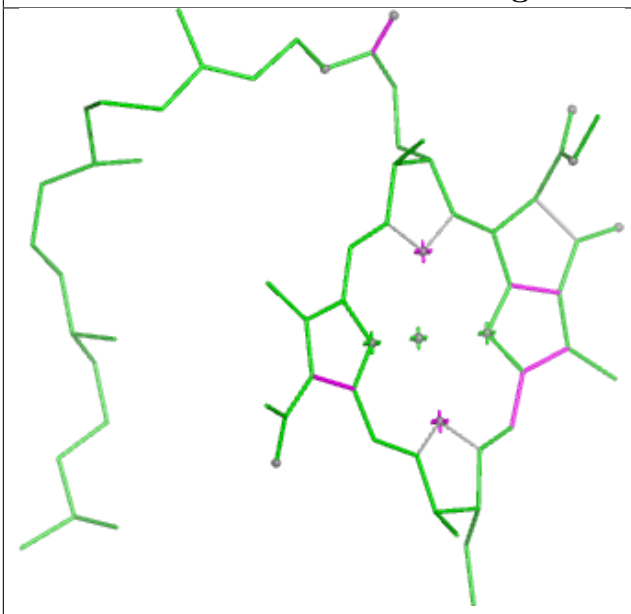


Ligand LMT BQ 102

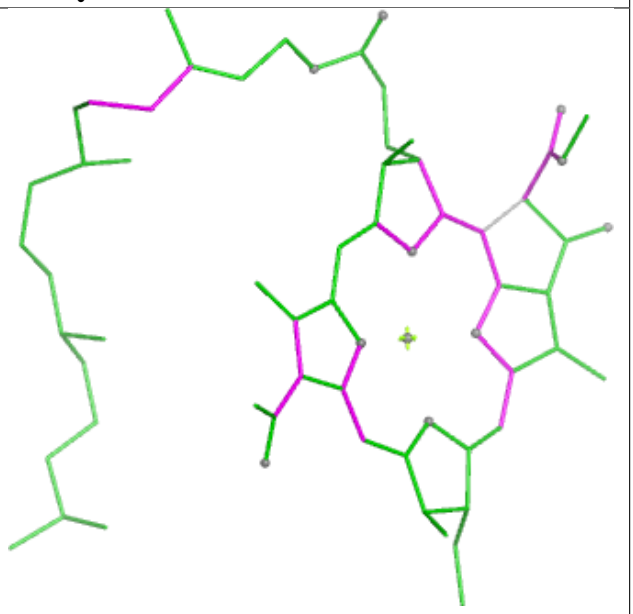


Ligand BCL Bk 103	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

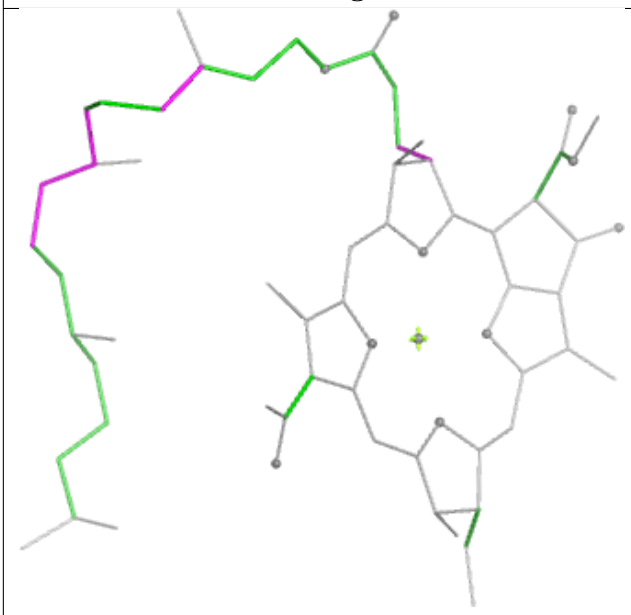
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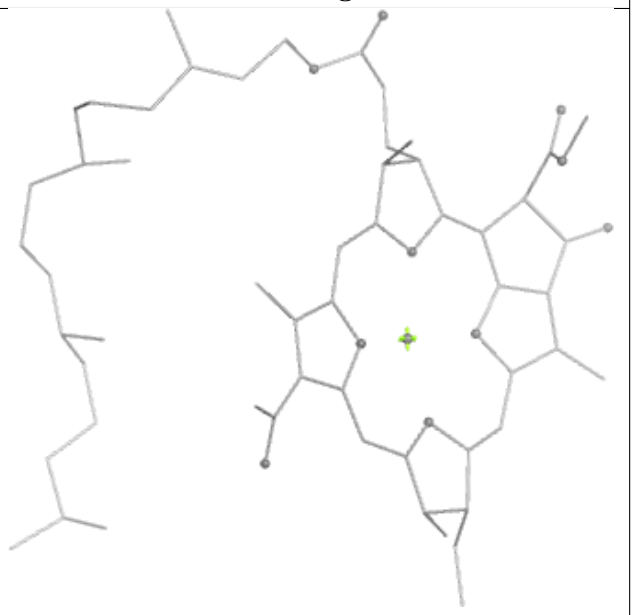
Bond lengths



Bond angles

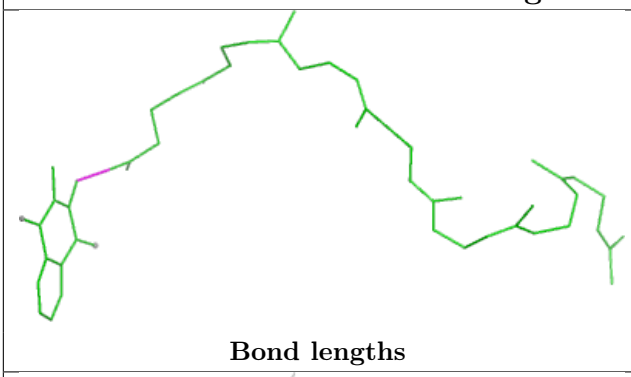


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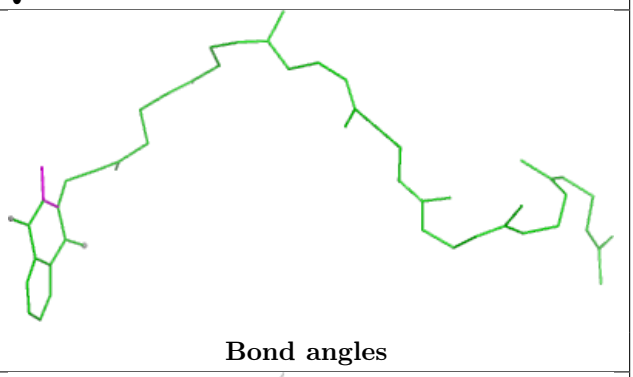


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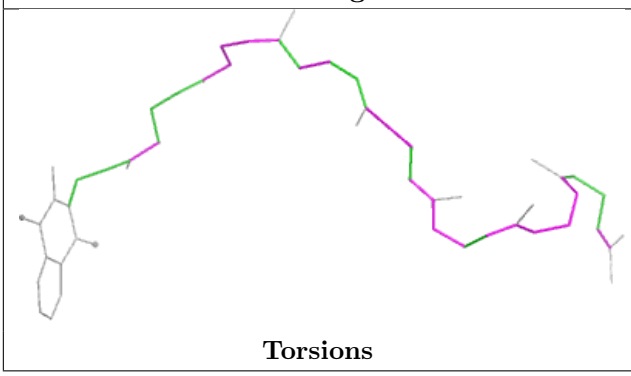
Ligand MQ8 L 305



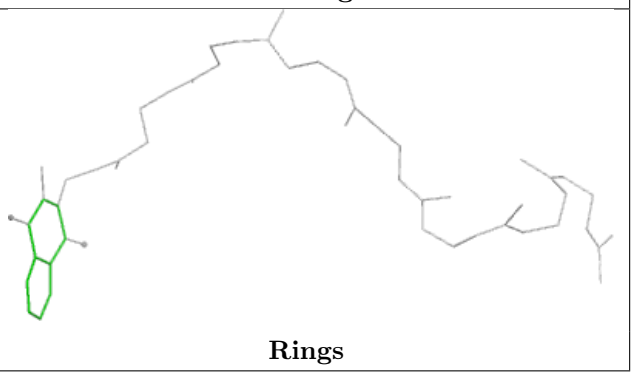
Bond lengths



Bond angles

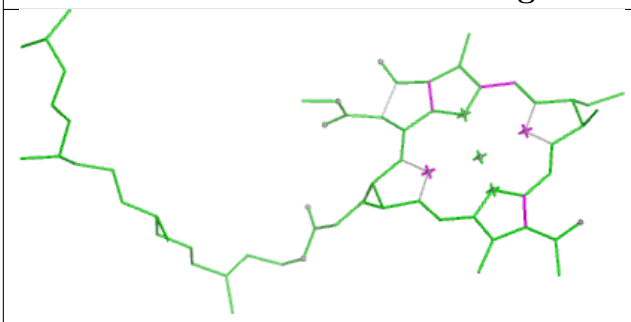


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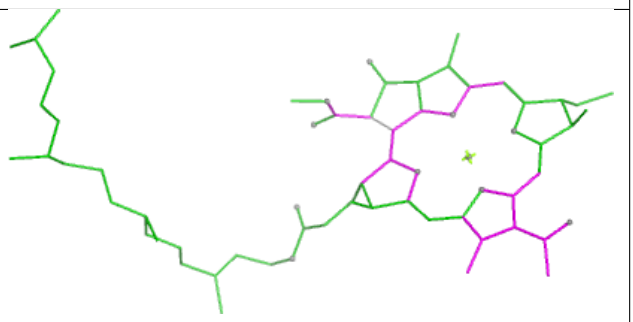


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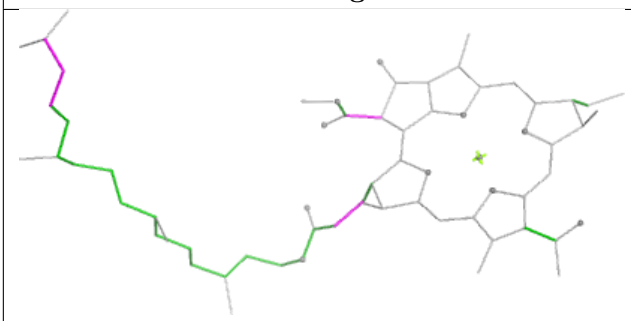
Ligand BCL AI 101



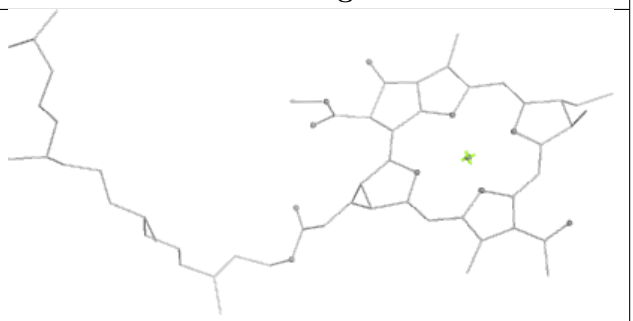
Bond lengths



Bond angles

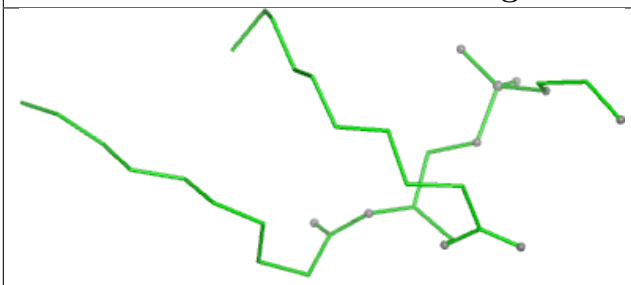


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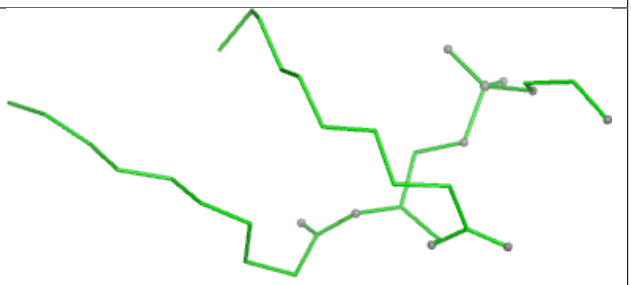


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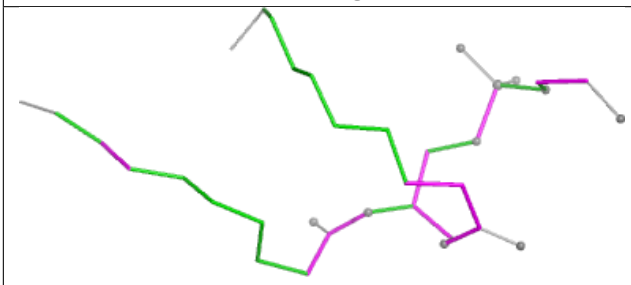
Ligand PEX AA 1101



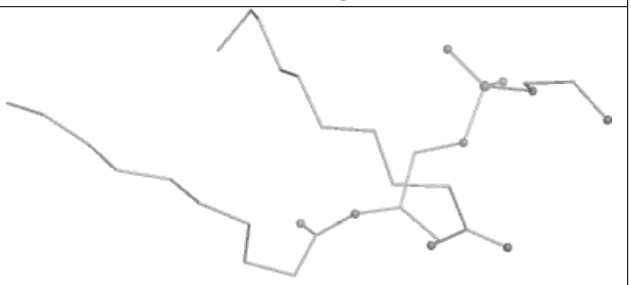
Bond lengths



Bond angles

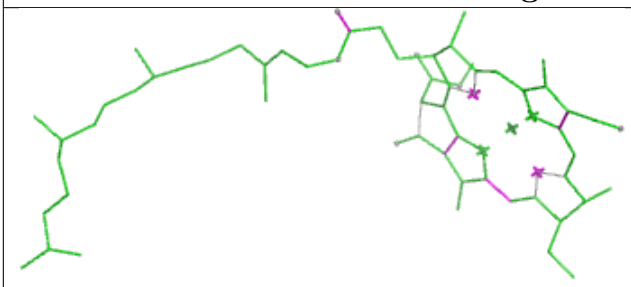


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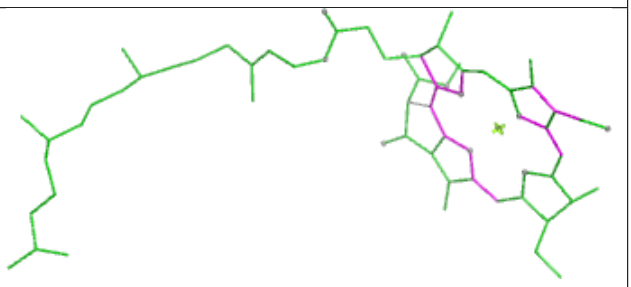


Rings

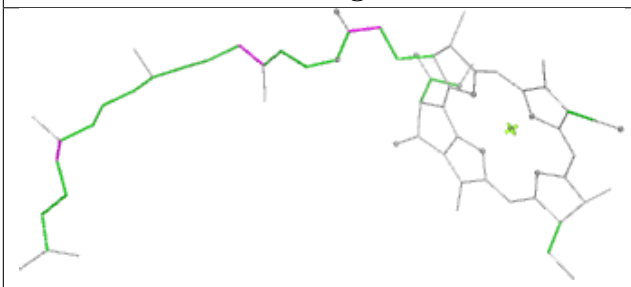
Ligand BCL M 405



Bond lengths



Bond angles

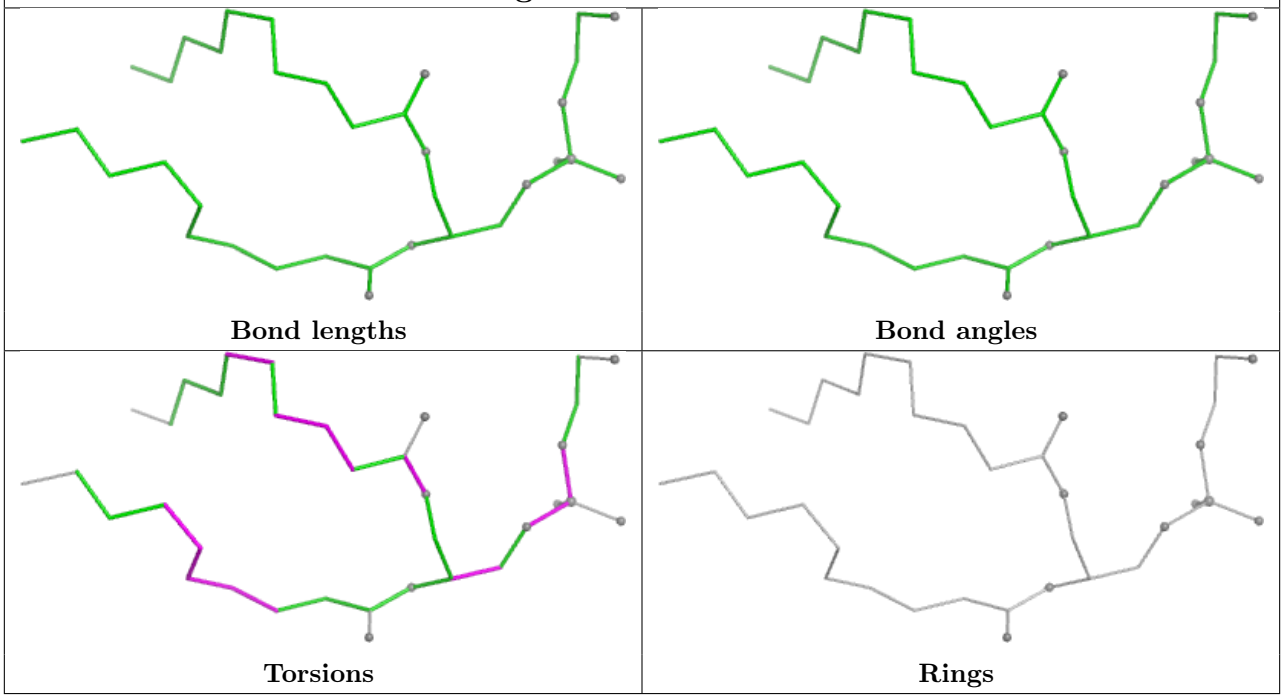


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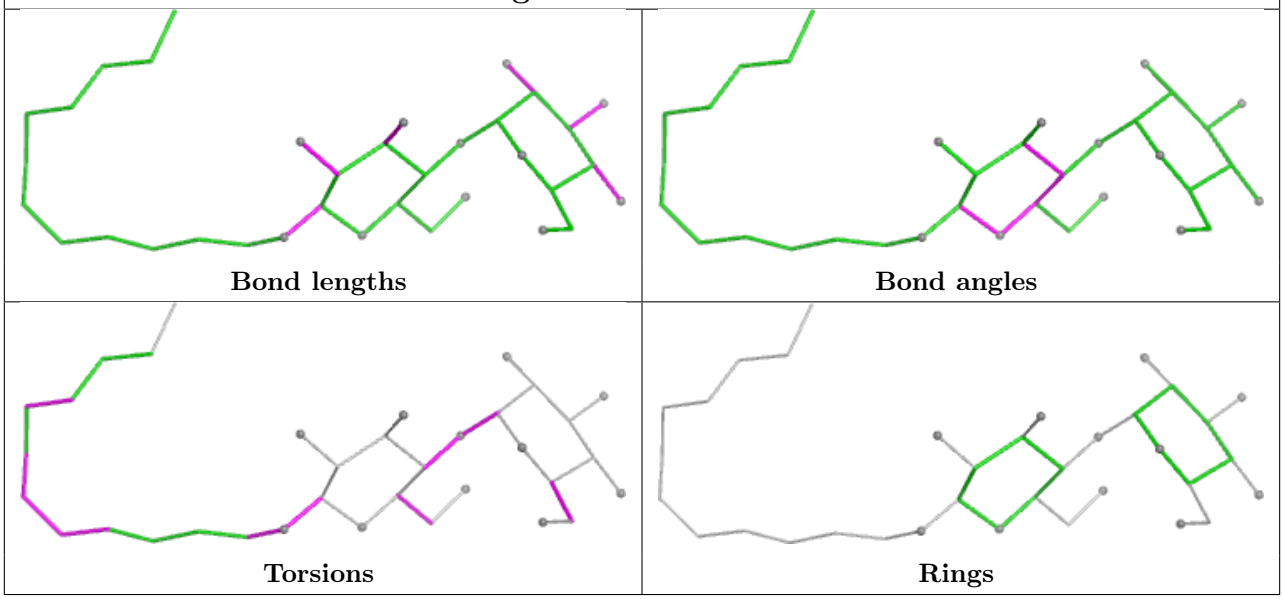


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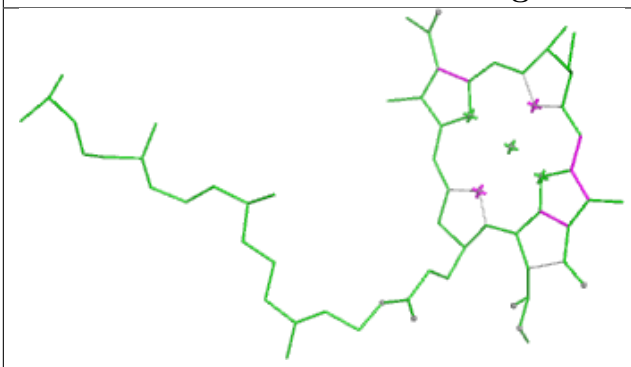
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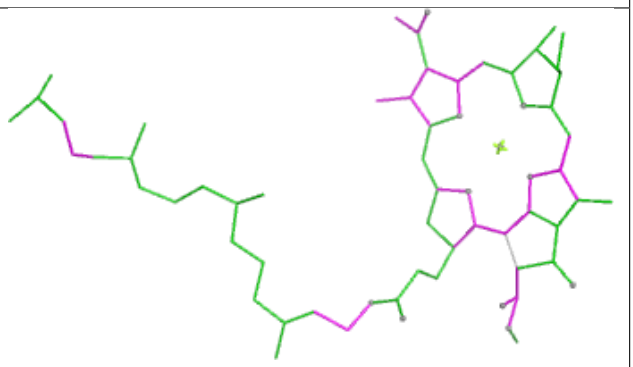
Ligand LMT Ad 102



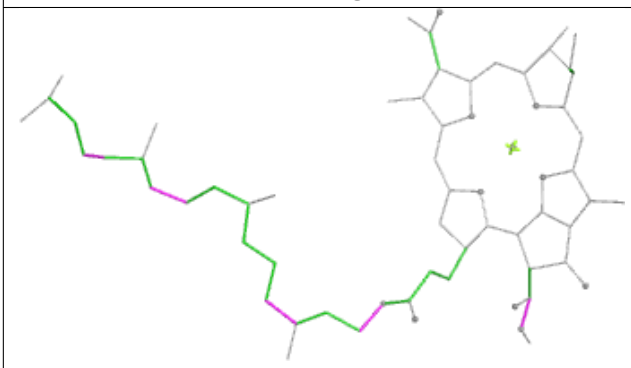
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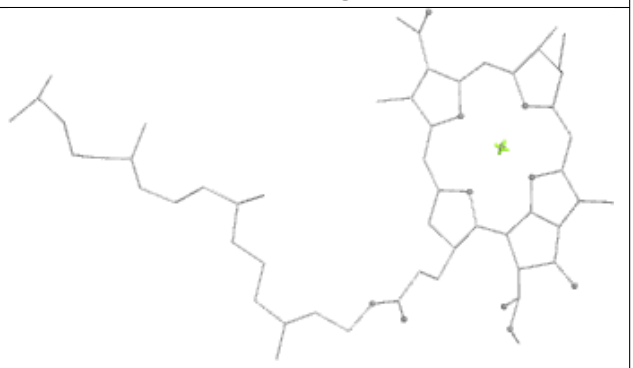
Bond lengths



Bond angles

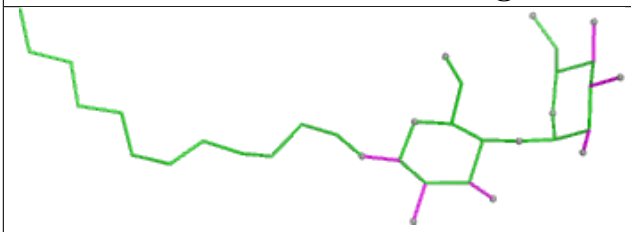


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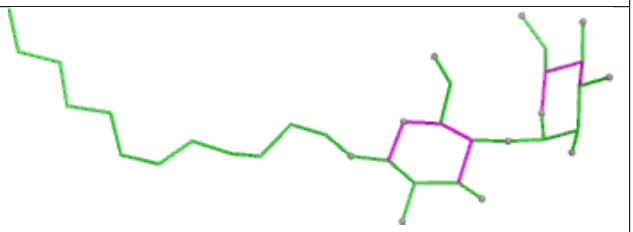


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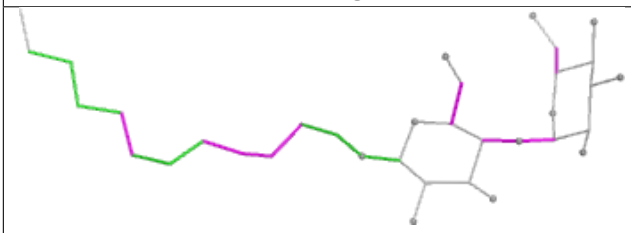
Ligand LMT AW 1201



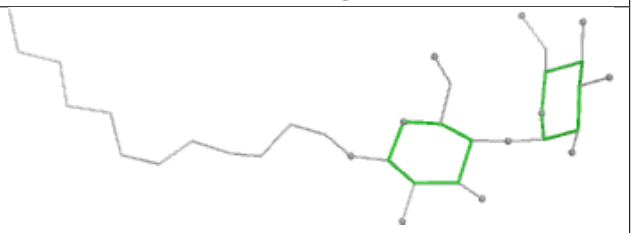
Bond lengths



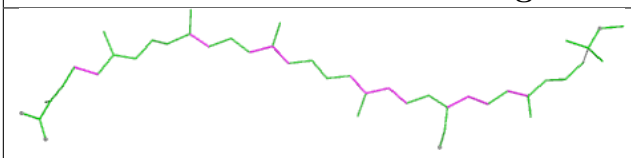
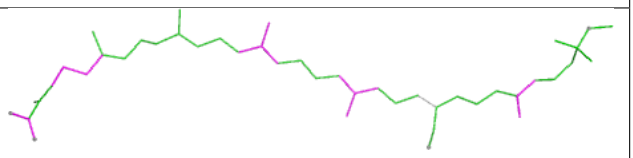
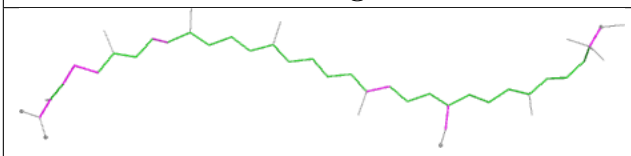
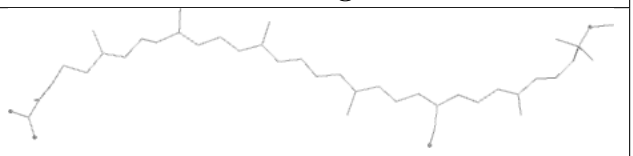
Bond angles

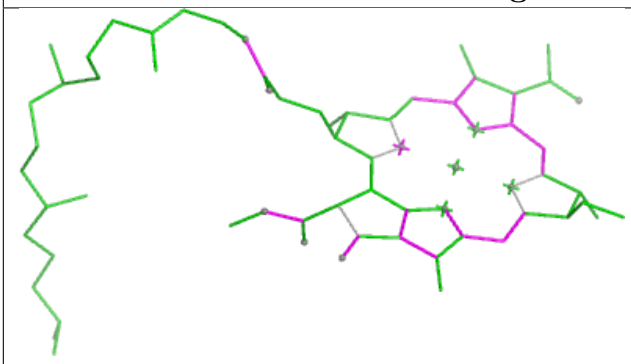
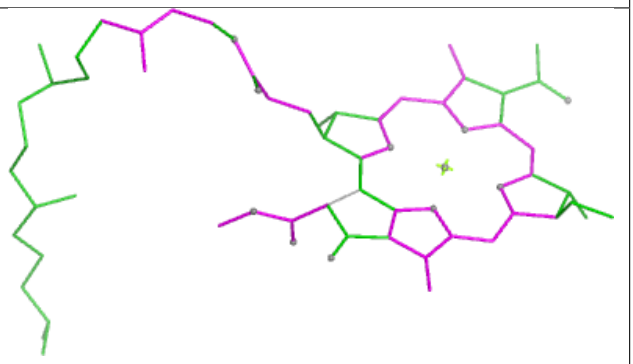
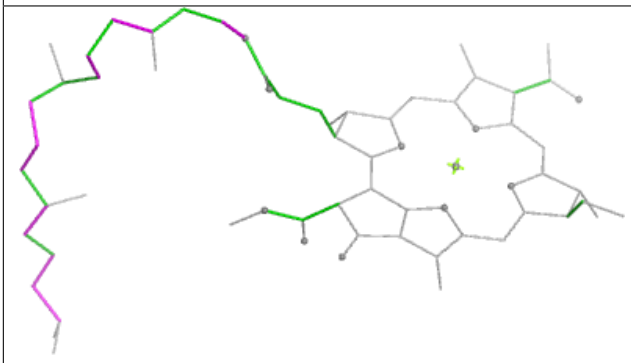
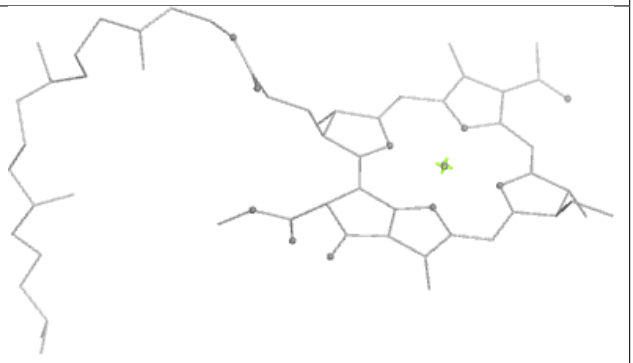


Torsions

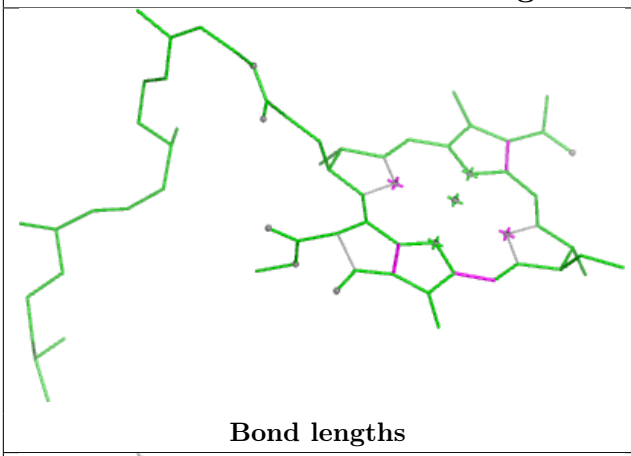


Rings

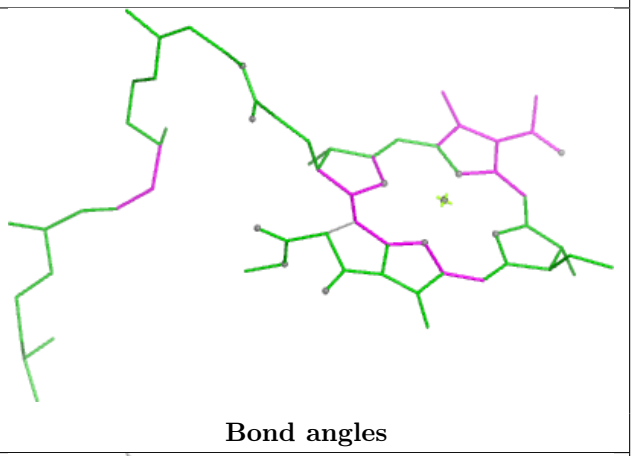
Ligand V7N Bn 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL Am 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

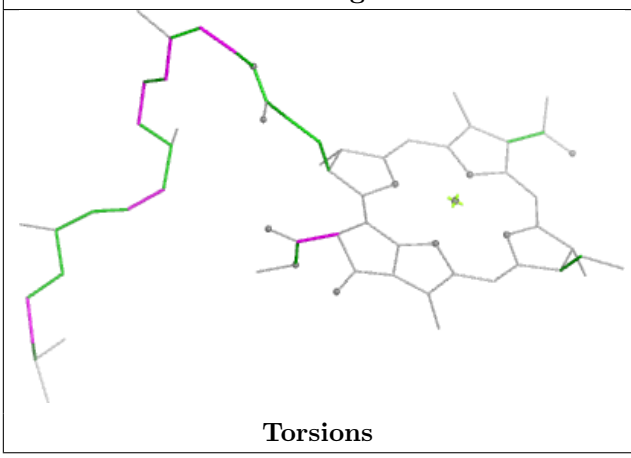
Ligand BCL Ac 101



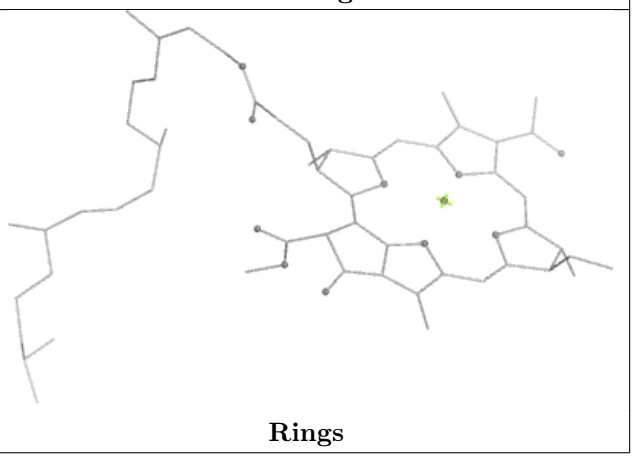
Bond lengths



Bond angles

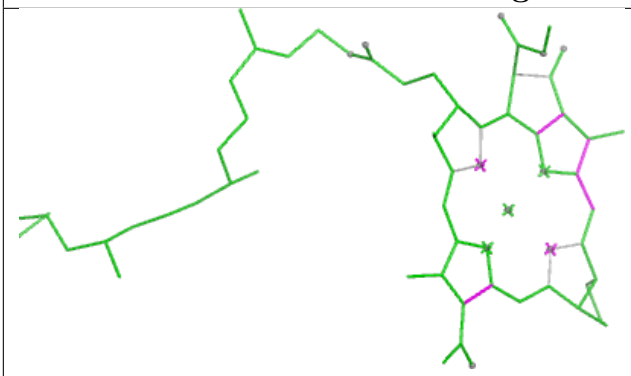


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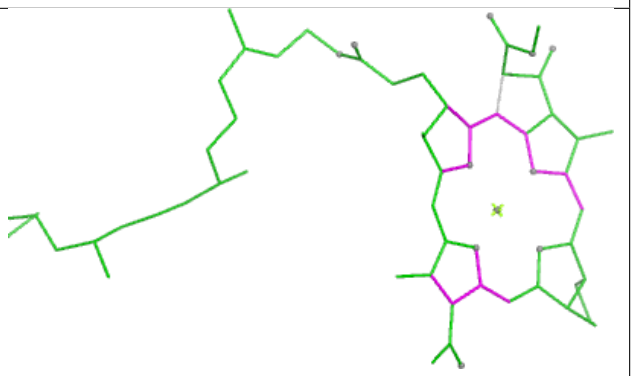


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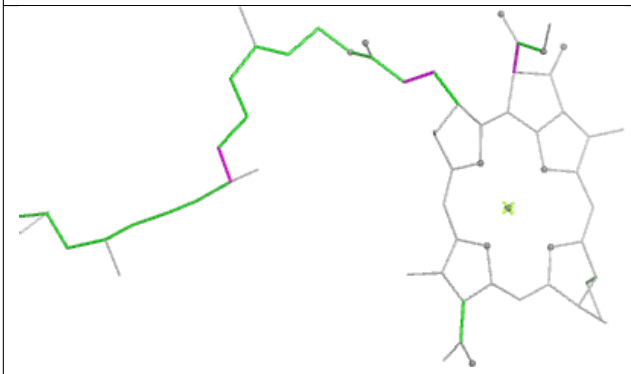
Ligand BCL AC 101



Bond lengths



Bond angles

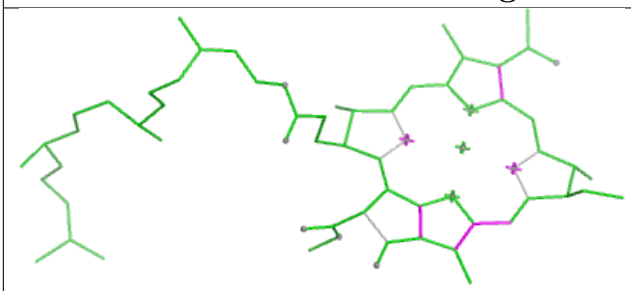


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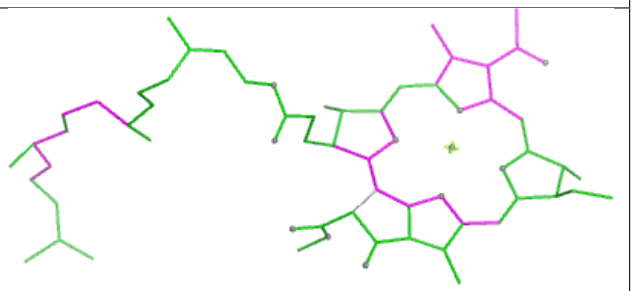


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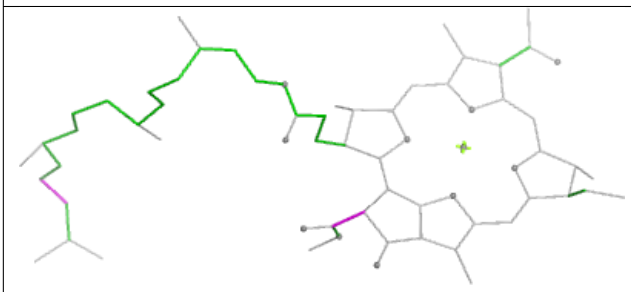
Ligand BCL AW 1202



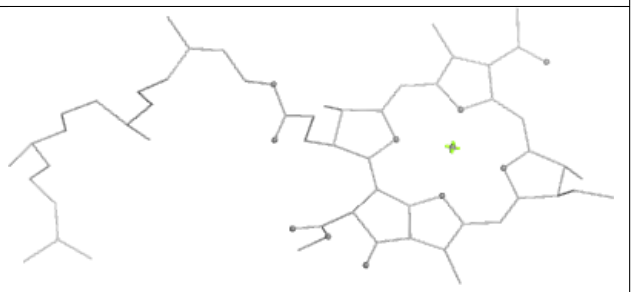
Bond lengths



Bond angles

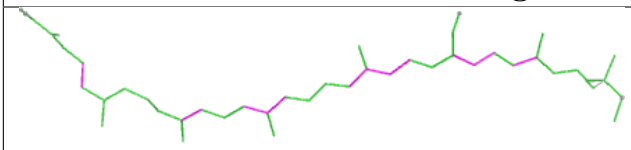


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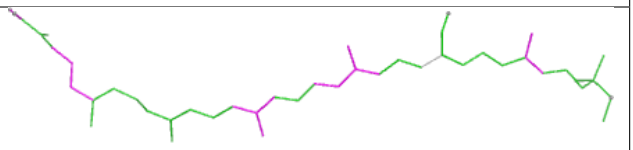


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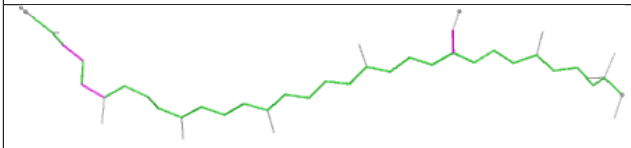
Ligand V7N BN 102



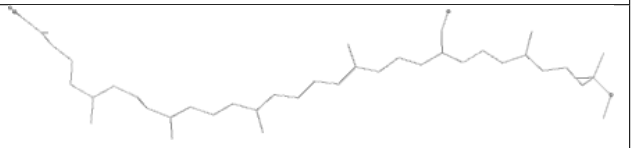
Bond lengths



Bond angles

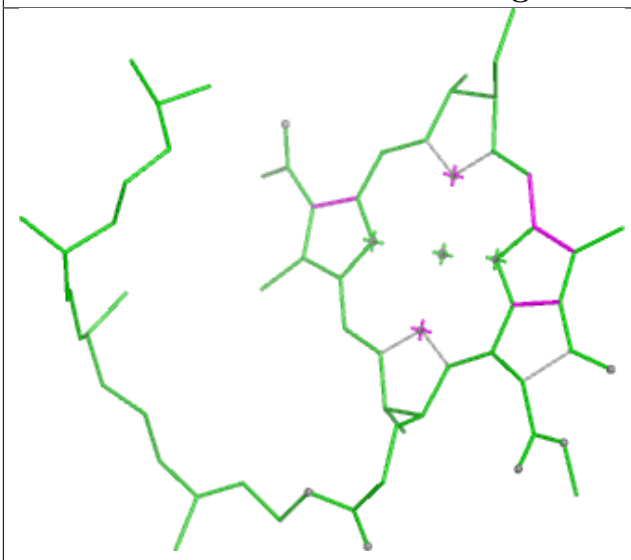


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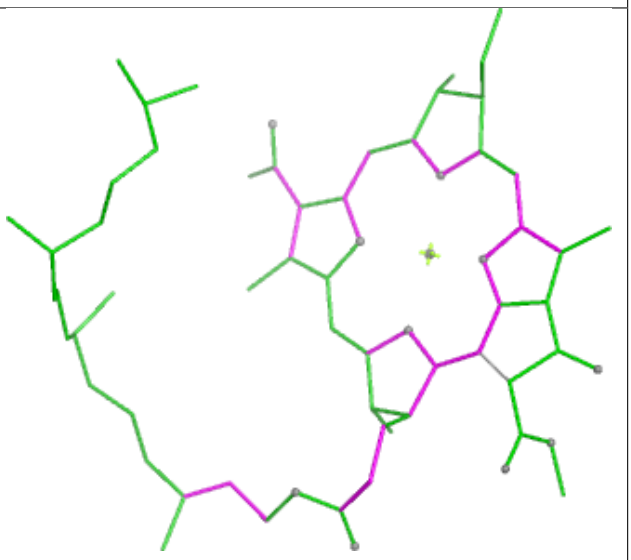


Rings

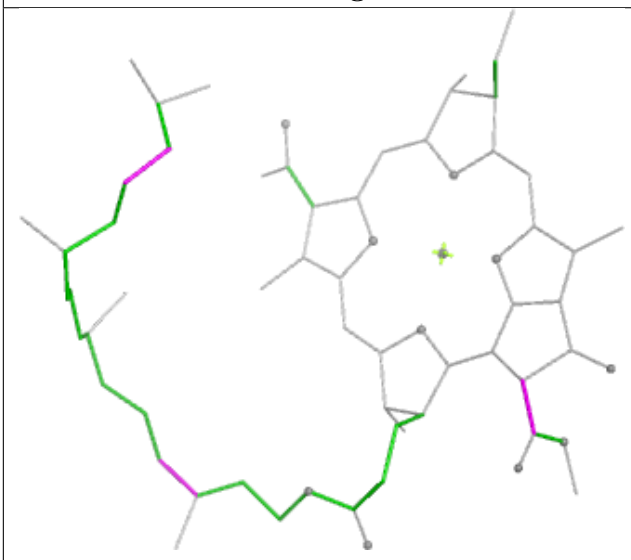
Ligand BCL BA 103



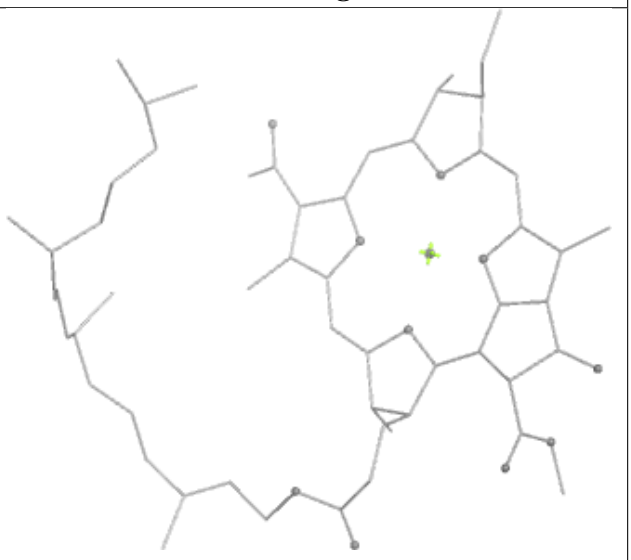
Bond lengths



Bond angles

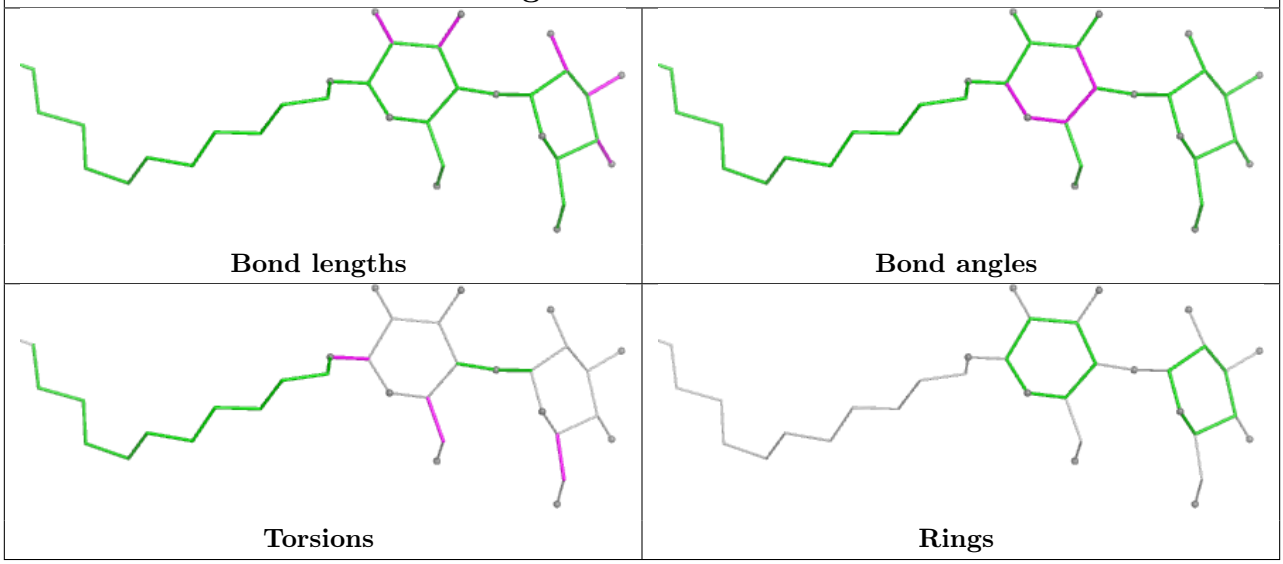


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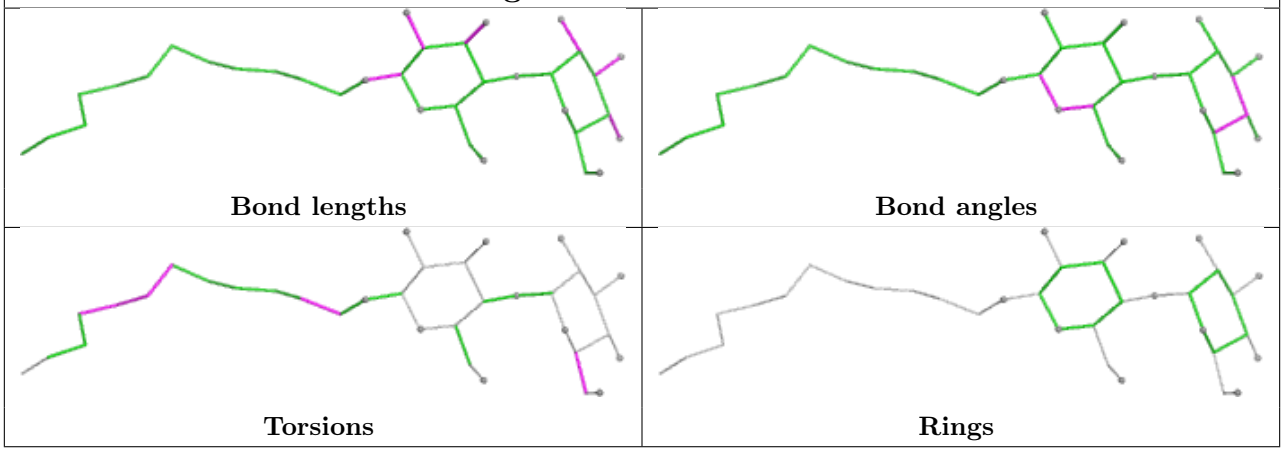


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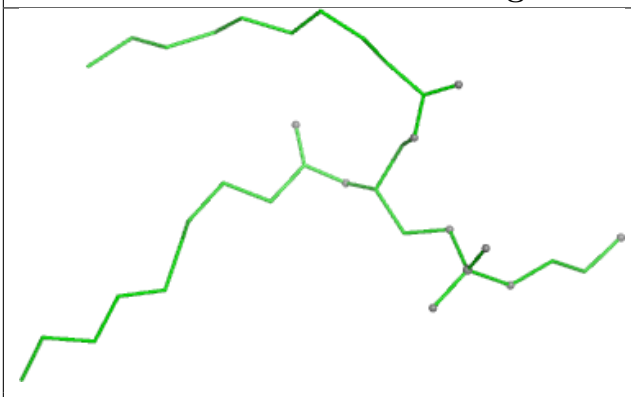
Ligand LMT C 401



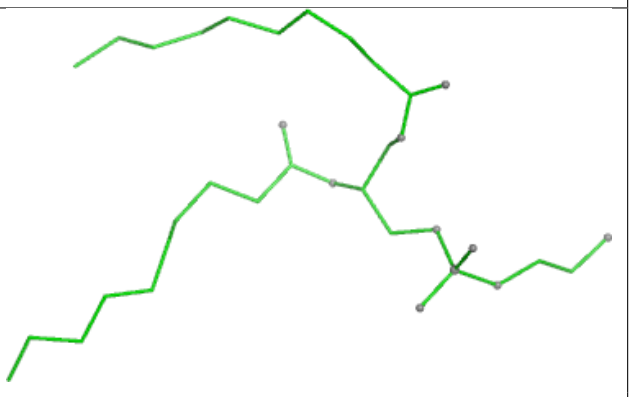
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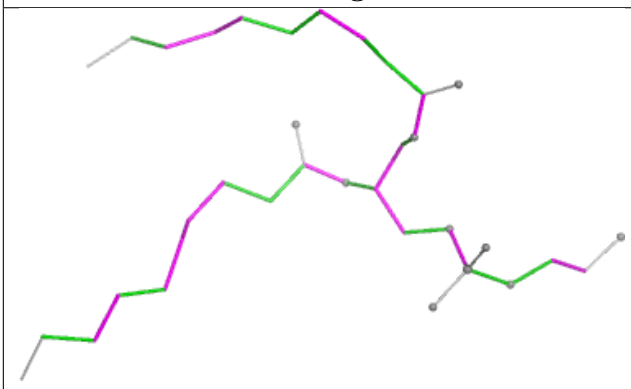
Ligand PEX Be 1104



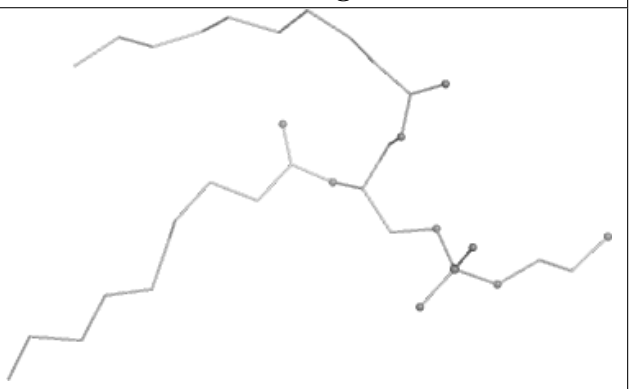
Bond lengths



Bond angles

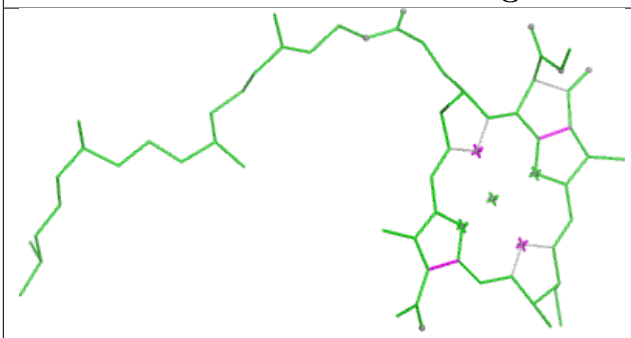


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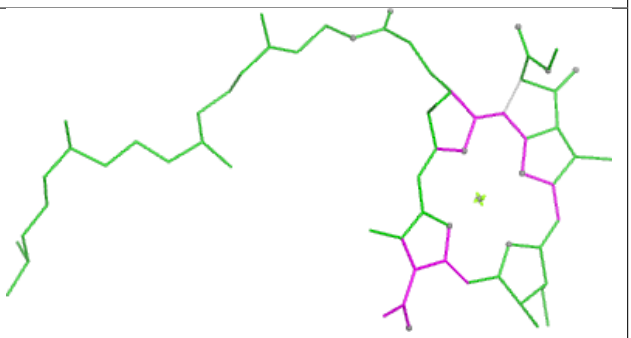


Rings

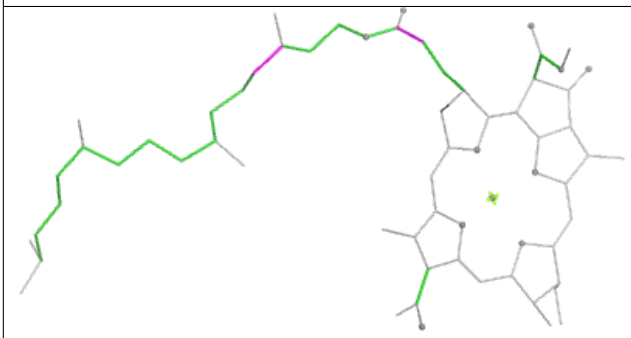
Ligand BCL AD 1102



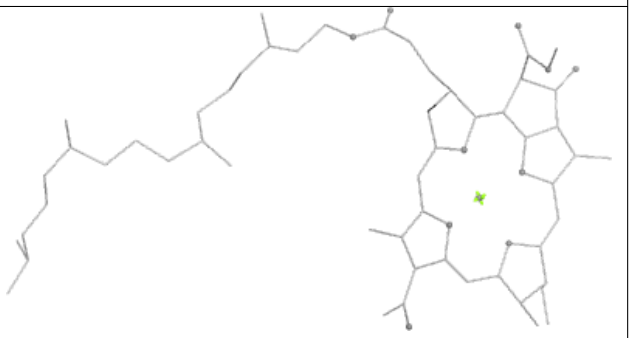
Bond lengths



Bond angles

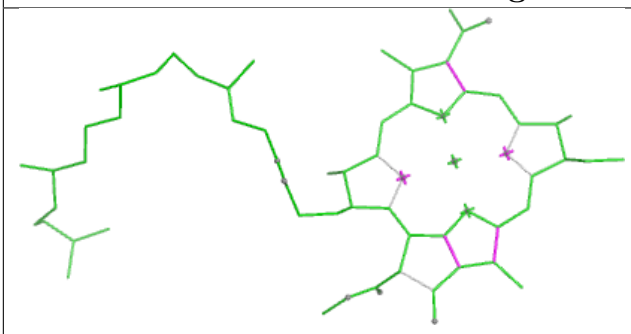


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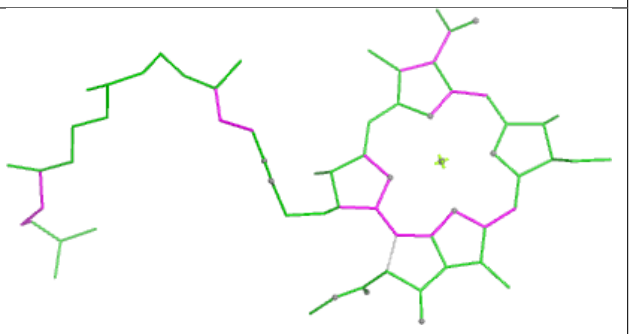


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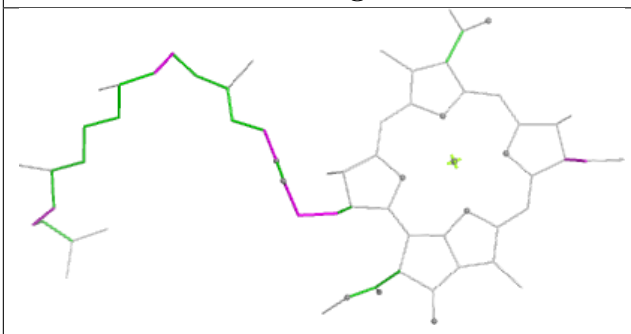
Ligand BCL Bc 1204



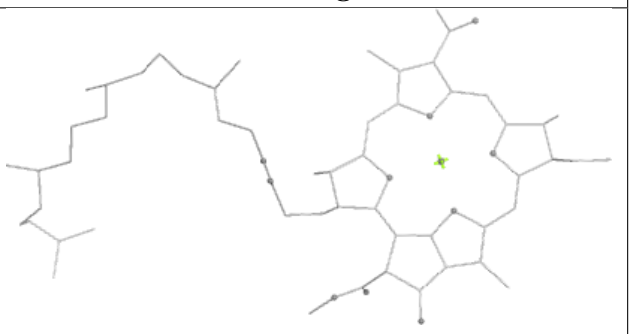
Bond lengths



Bond angles

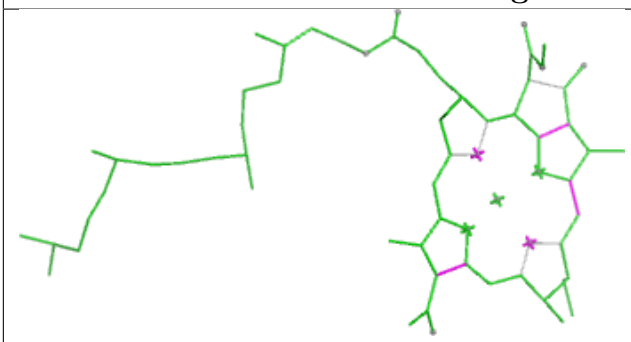


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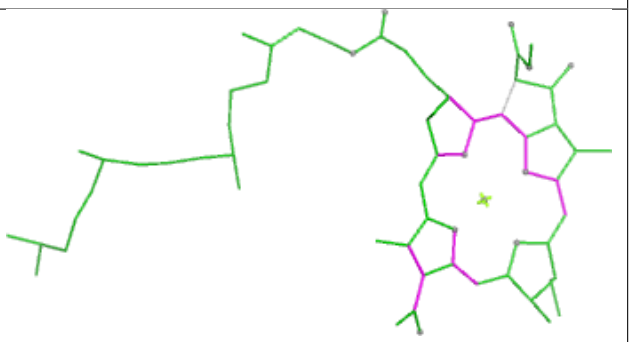


Rings

Ligand BCL AG 101



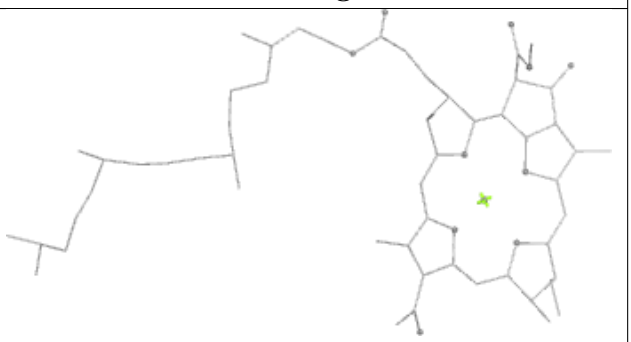
Bond lengths



Bond angles

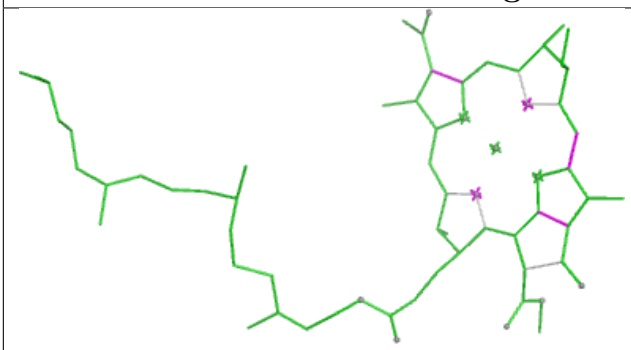


Torsions

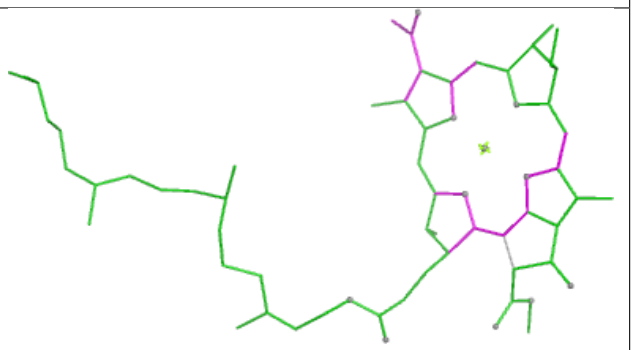


Rings

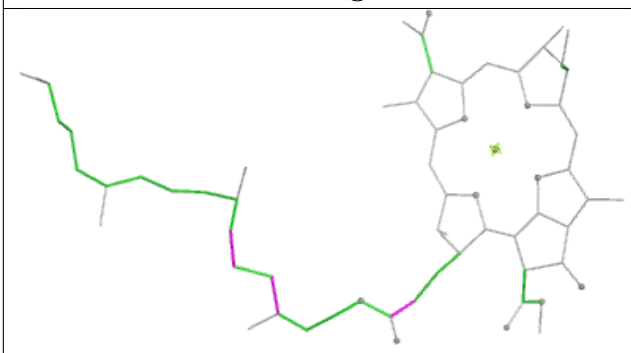
Ligand BCL AP 1102



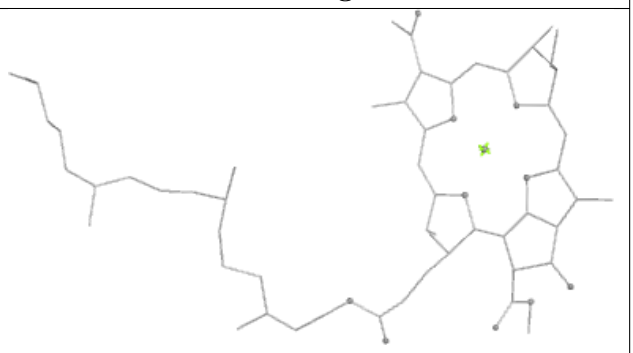
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Bond angles

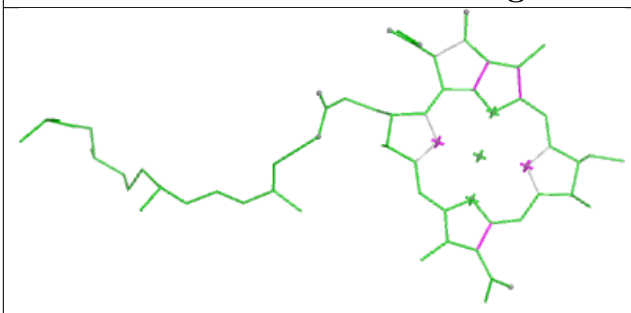


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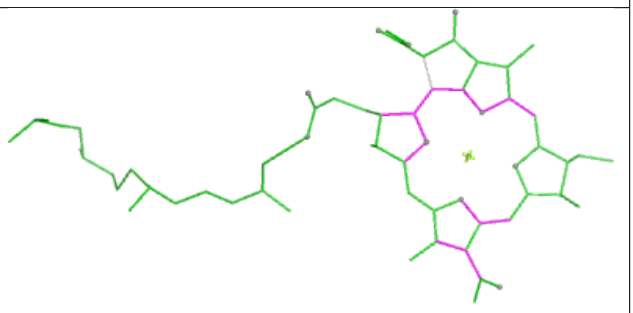


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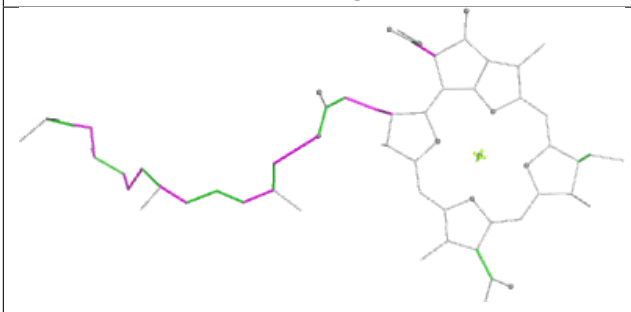
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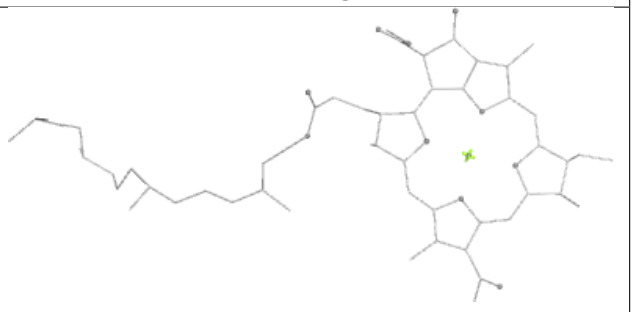
Bond lengths



Bond angles

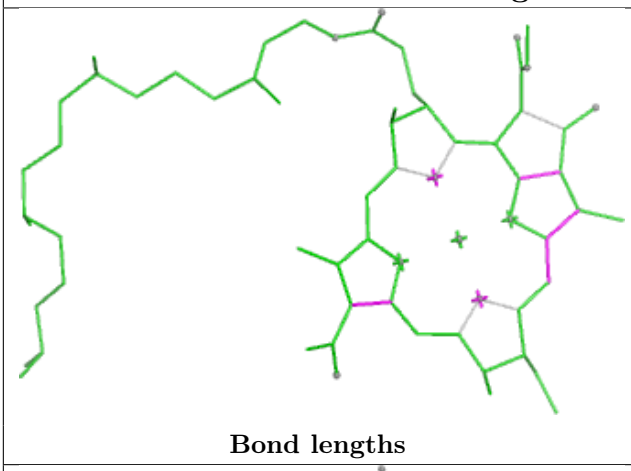


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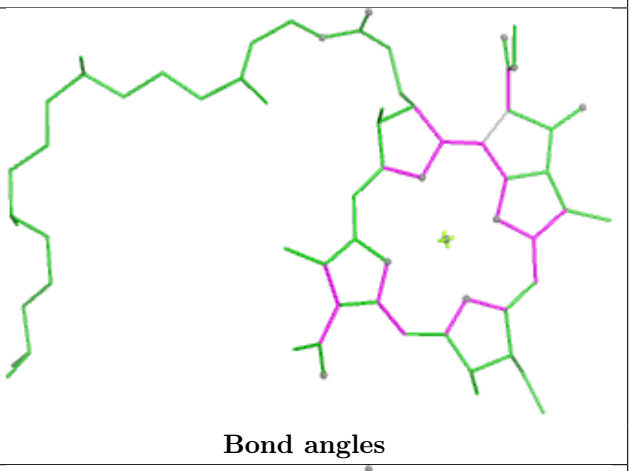


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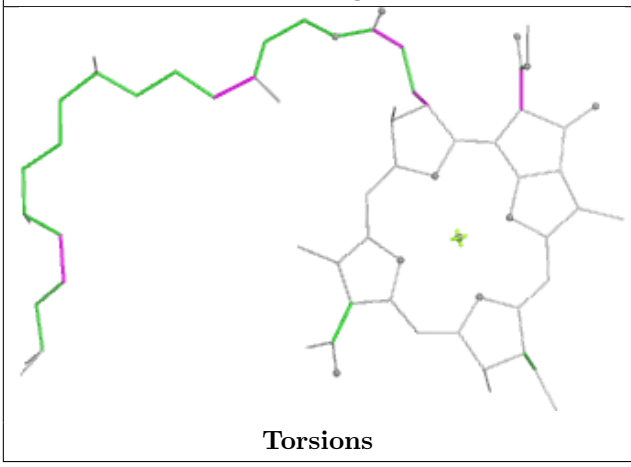
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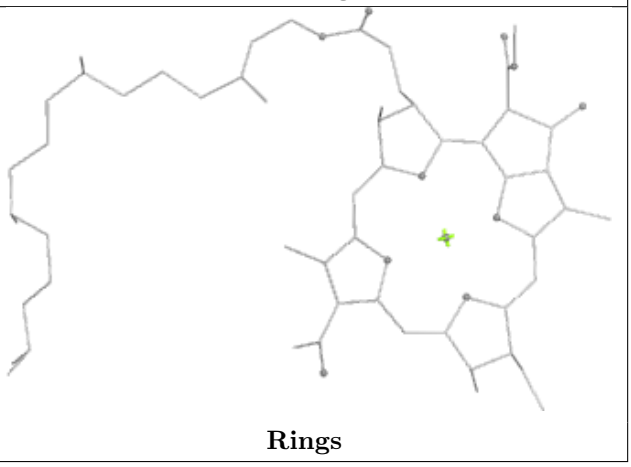
Bond lengths



Bond angles

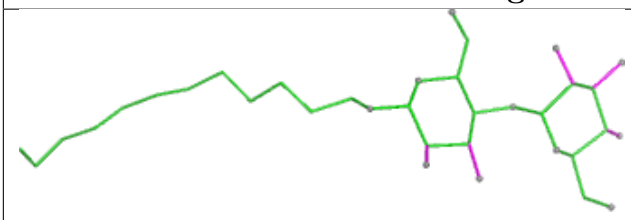


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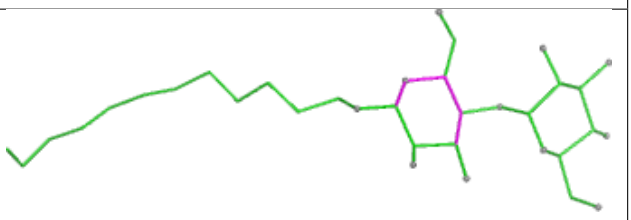


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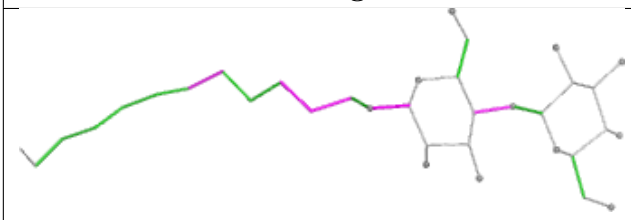
Ligand LMT BK 101



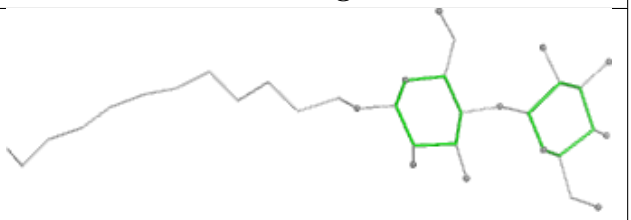
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Bond angles

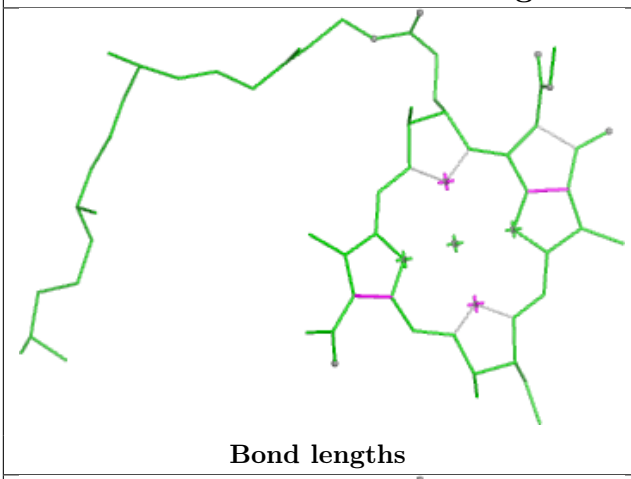


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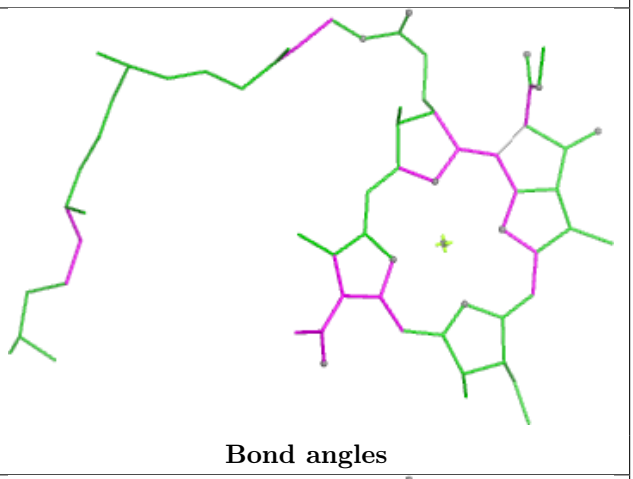


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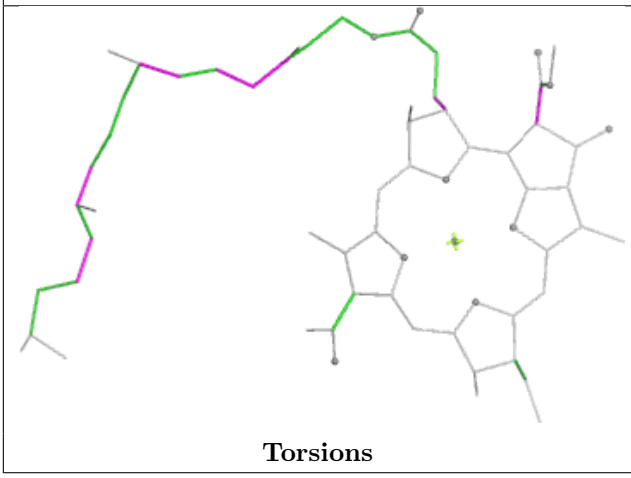
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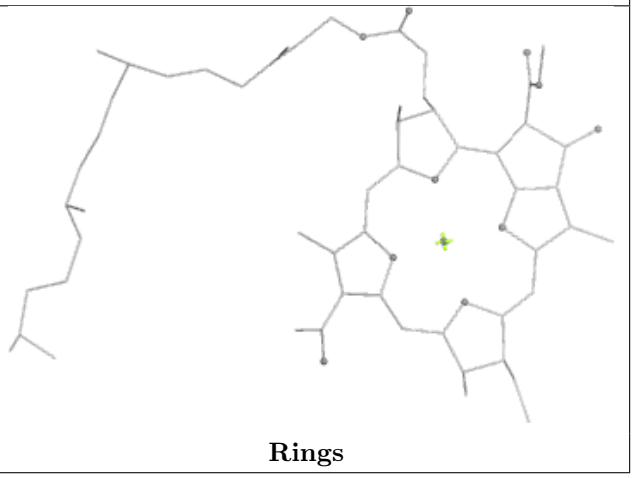
Bond lengths



Bond angles

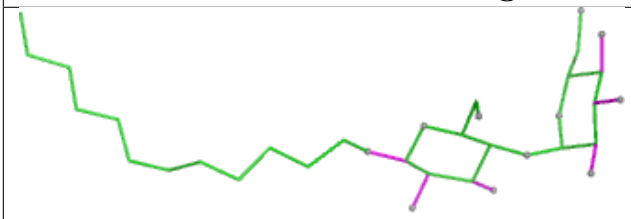


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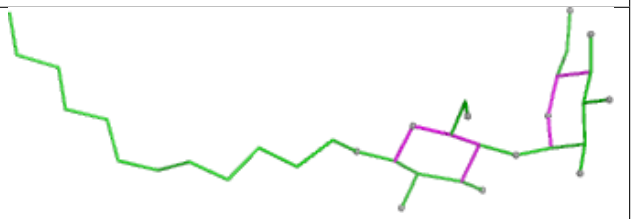


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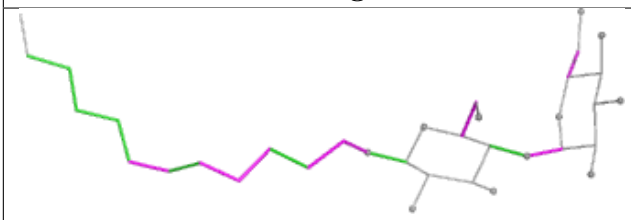
Ligand LMT AX 1201



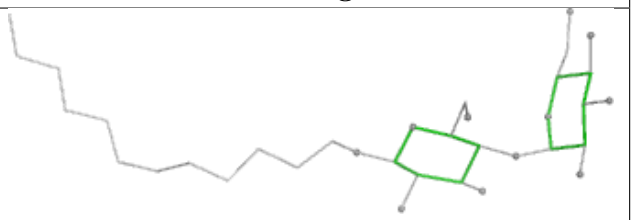
Bond lengths



Bond angles

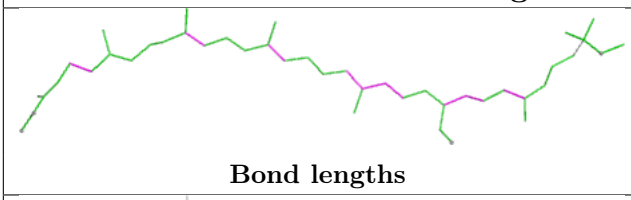


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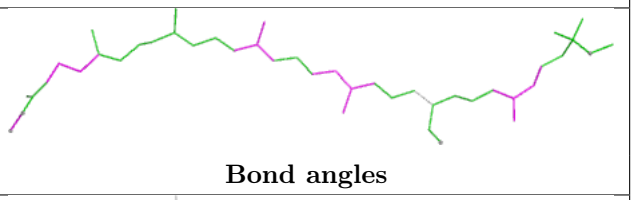


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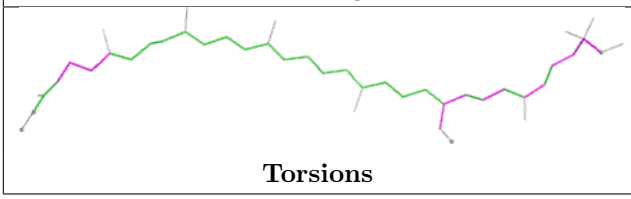
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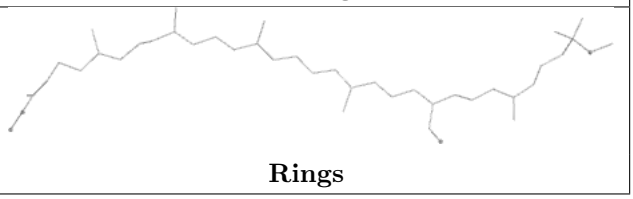
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Bond angles

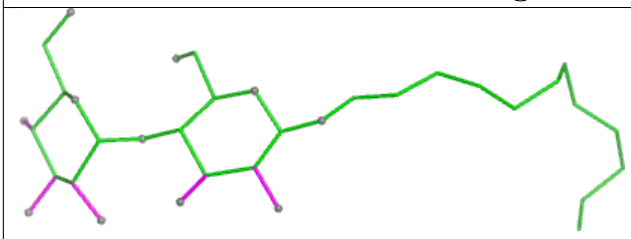


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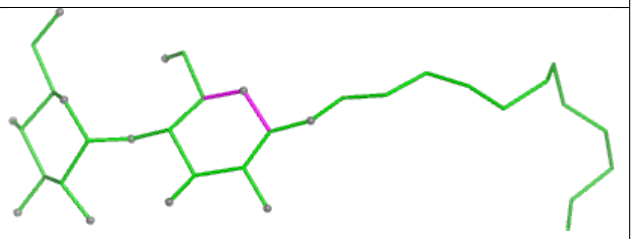


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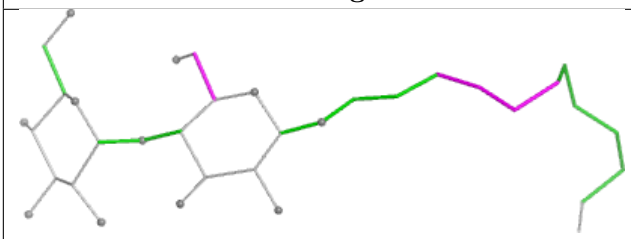
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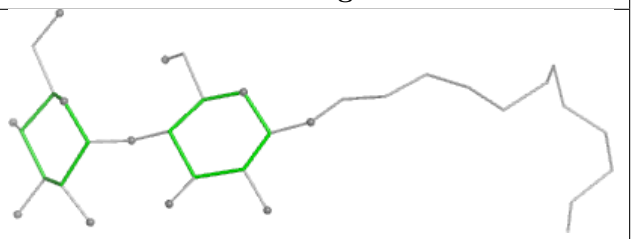
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Bond angles

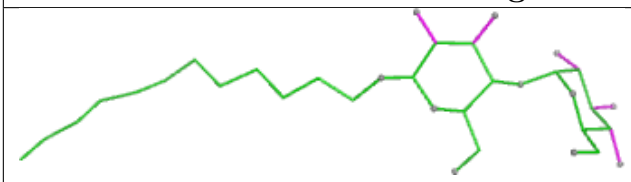


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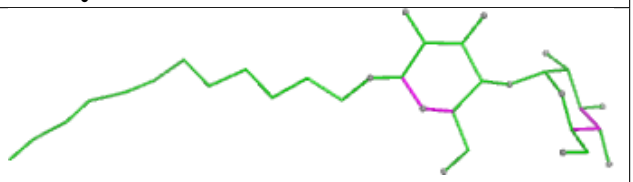


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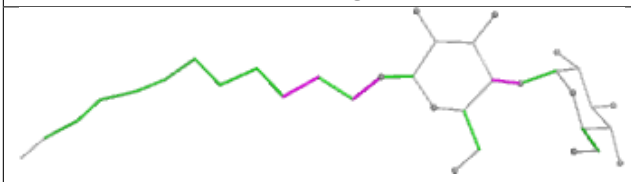
Ligand LMT BQ 101



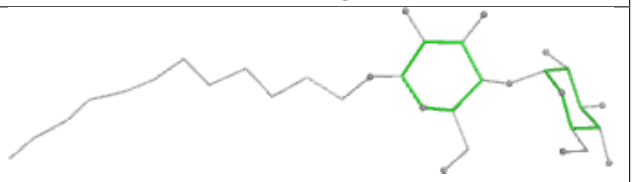
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Bond angles

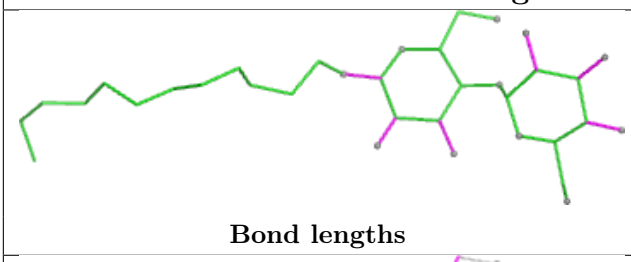


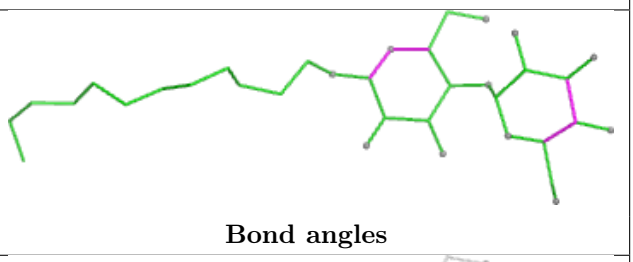
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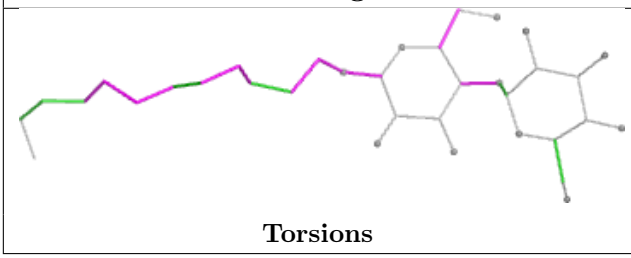


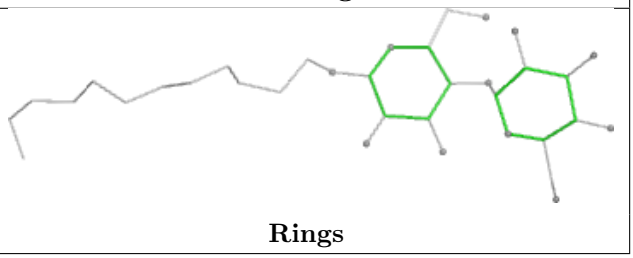
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Ligand LMT BS 102

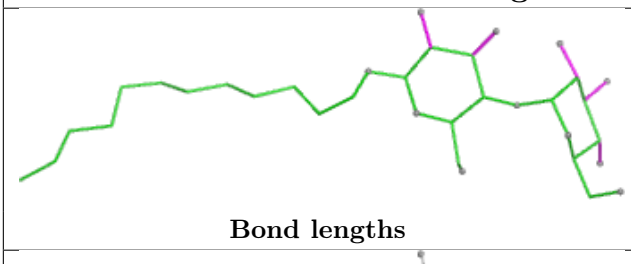

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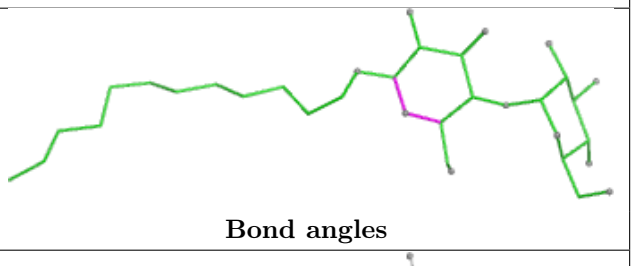

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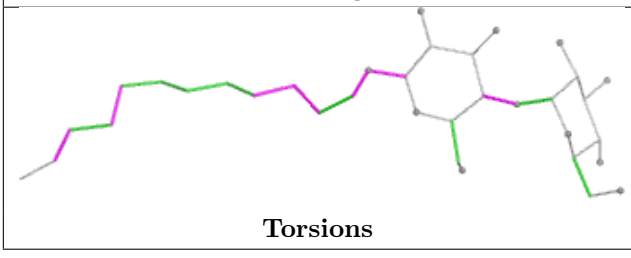

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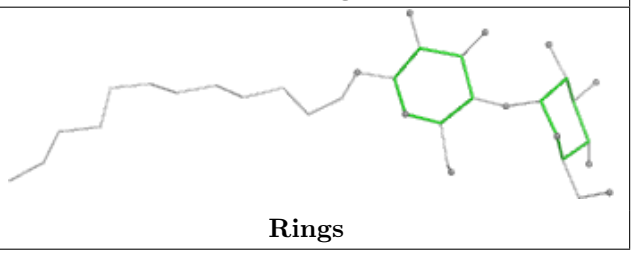

Rings

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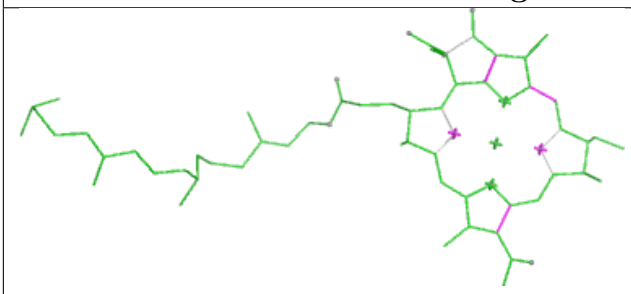

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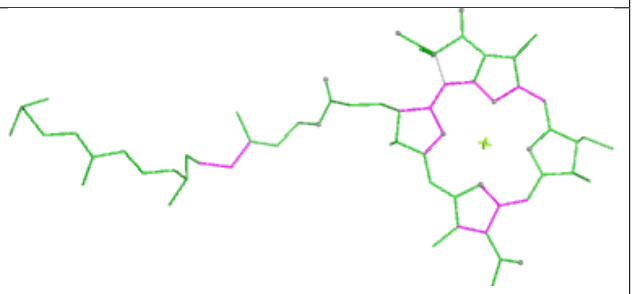

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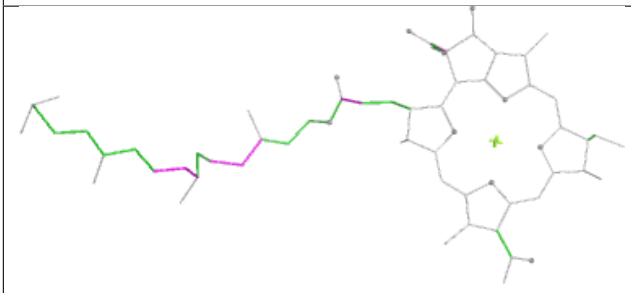

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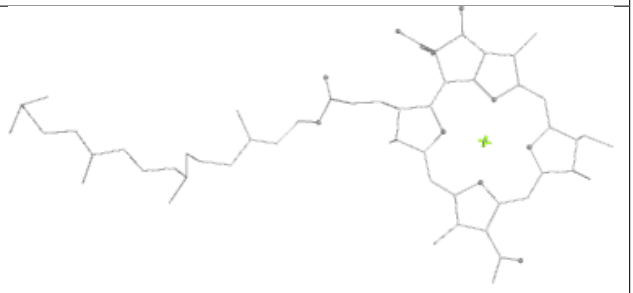

Rings

Ligand BCL AH 101

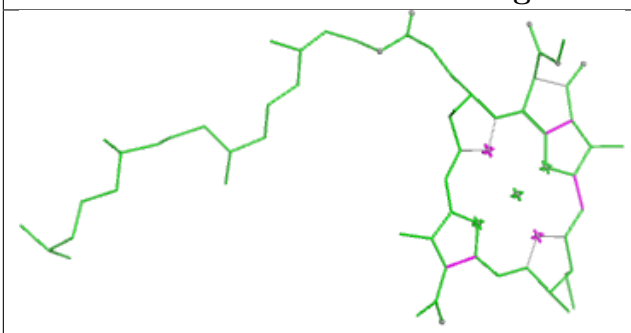

Bond lengths


Bond angles

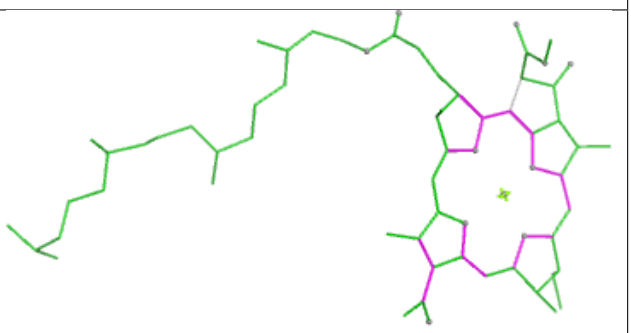

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Rings

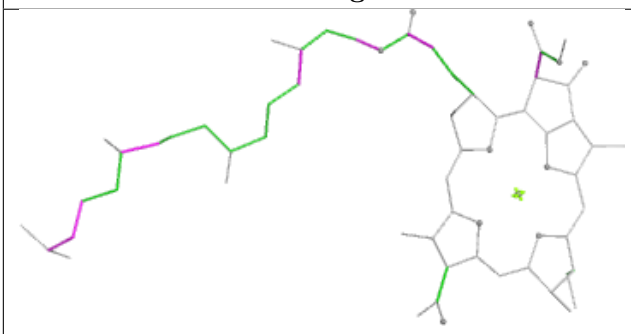
Ligand BCL AF 102



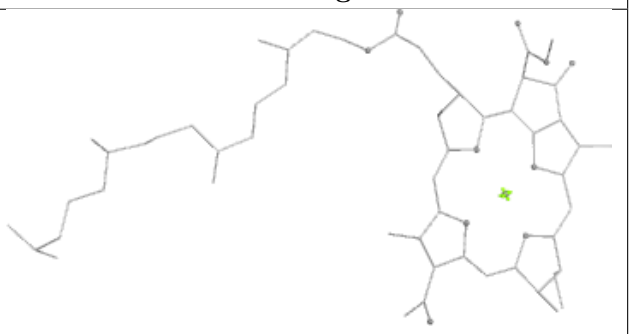
Bond lengths



Bond angles

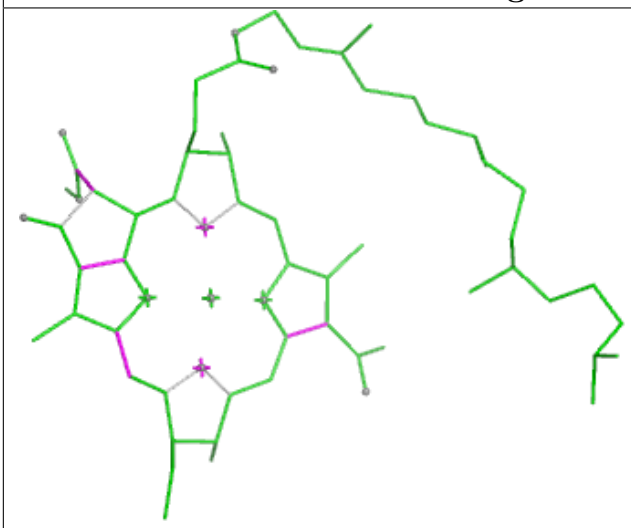


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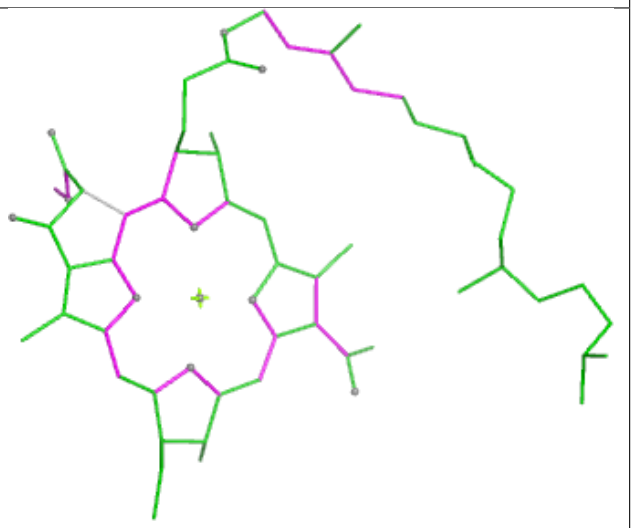


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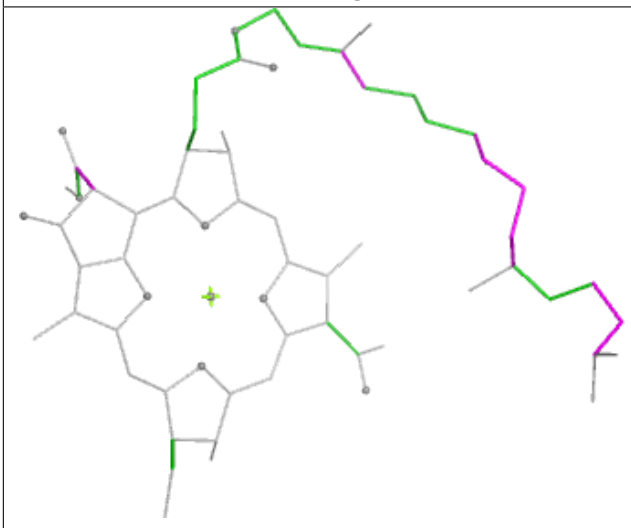
Ligand BCL AM 102



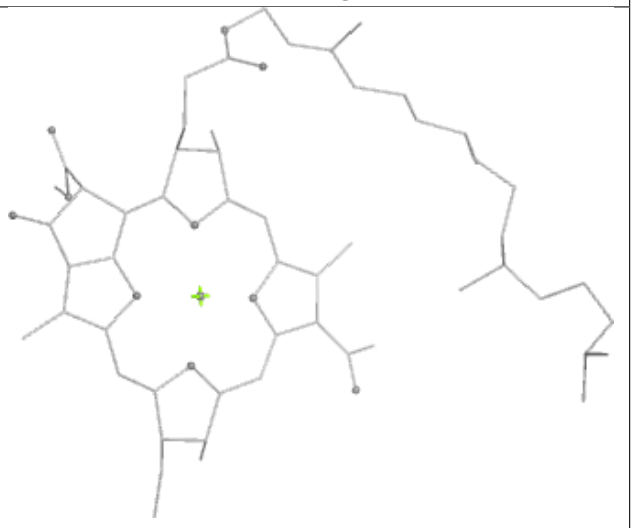
Bond lengths



Bond angles

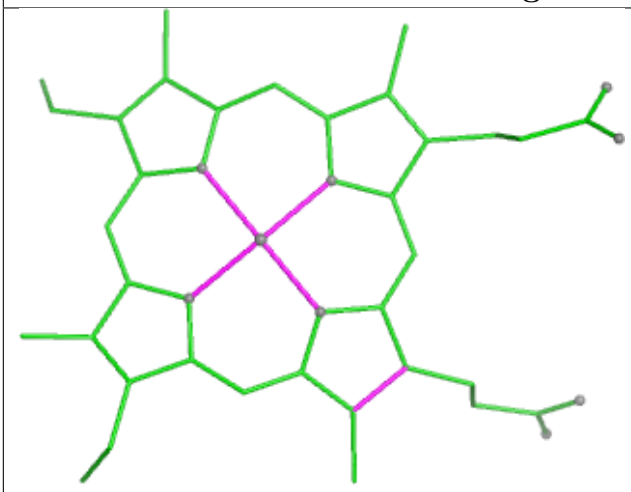


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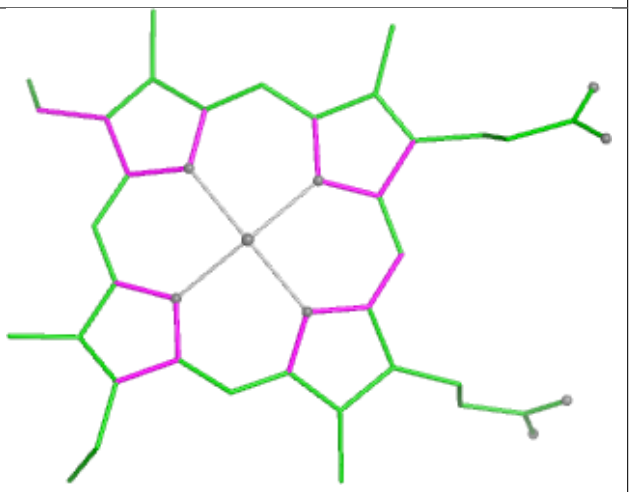


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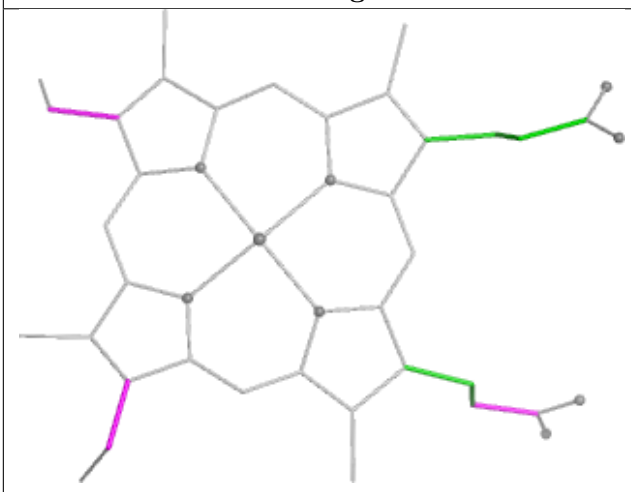
Ligand HEC C 404



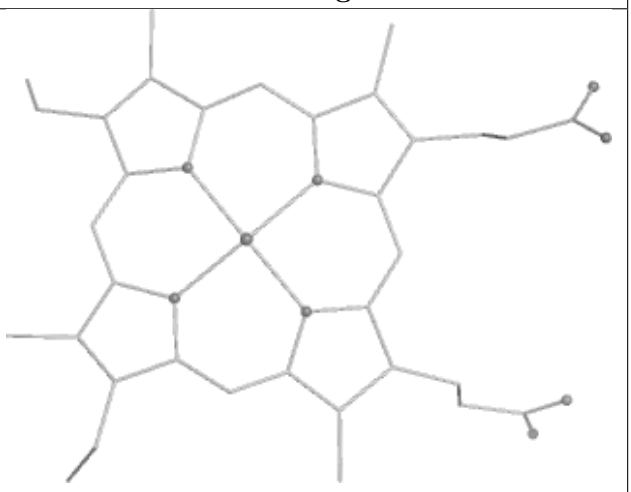
Bond lengths



Bond angles

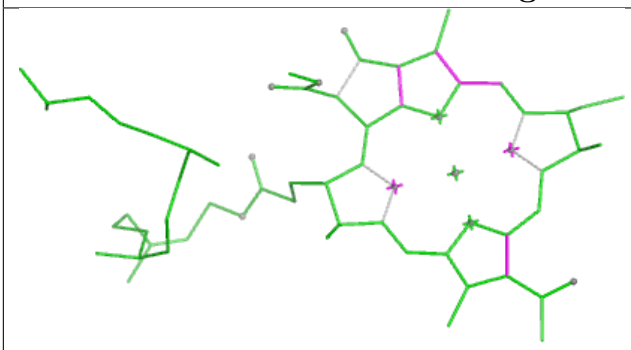


Torsions

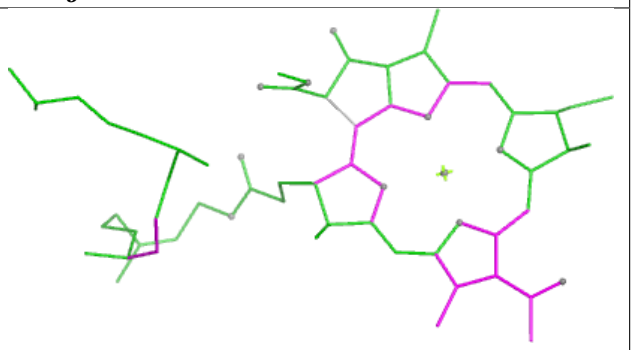


Rings

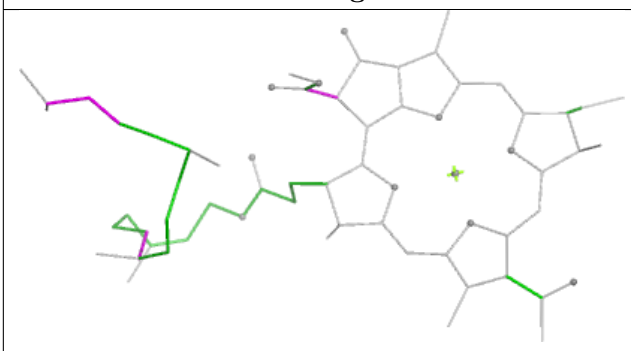
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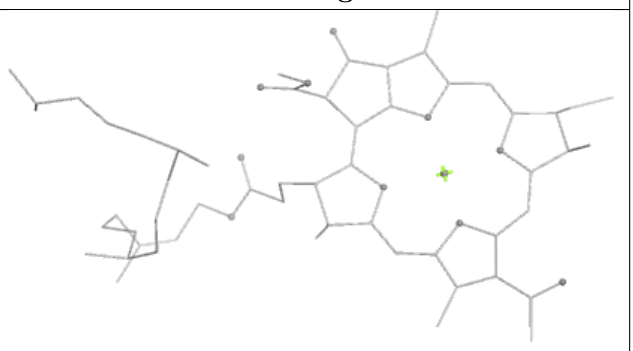
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Bond angles

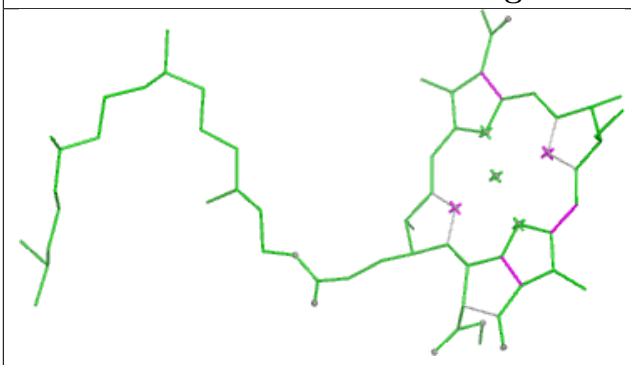


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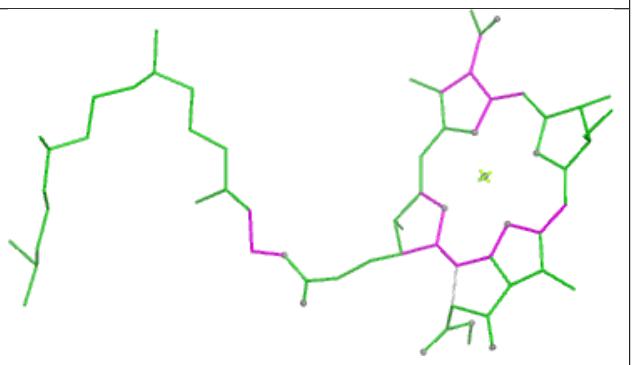


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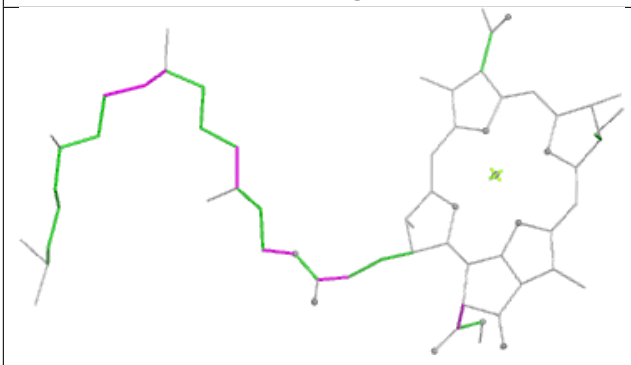
Ligand BCL AT 1103



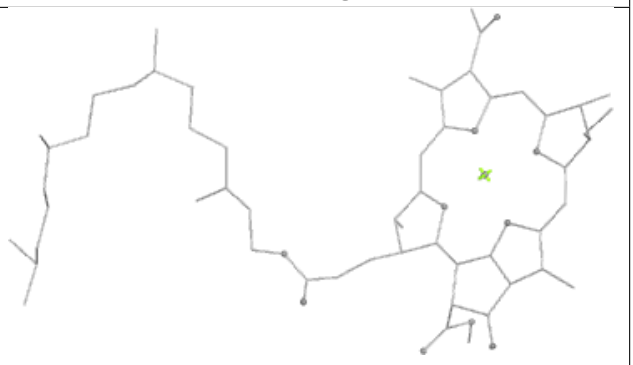
Bond lengths



Bond angles

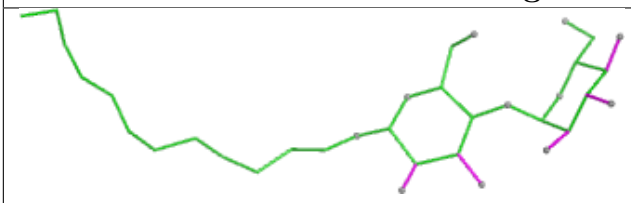


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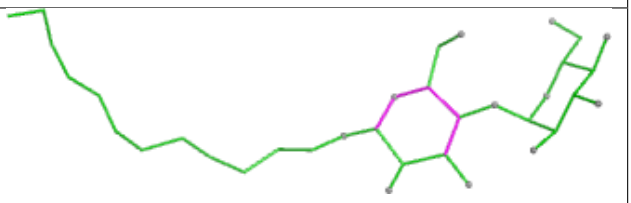


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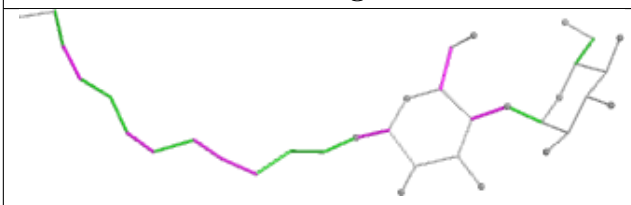
Ligand LMT L 304



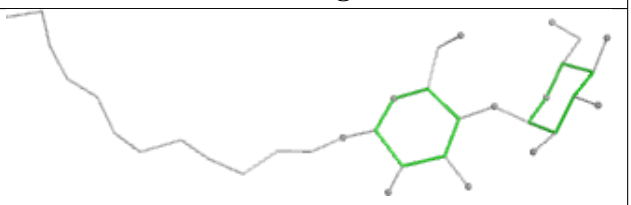
Bond lengths



Bond angles

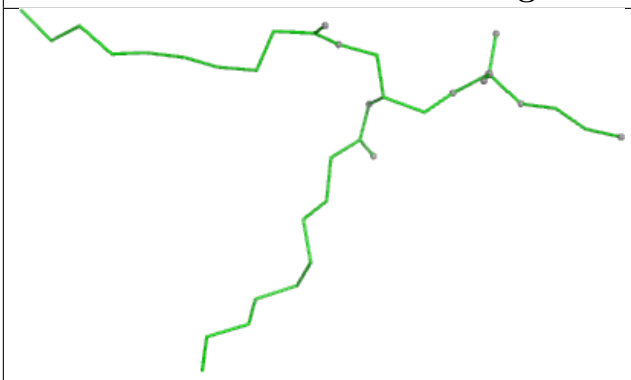


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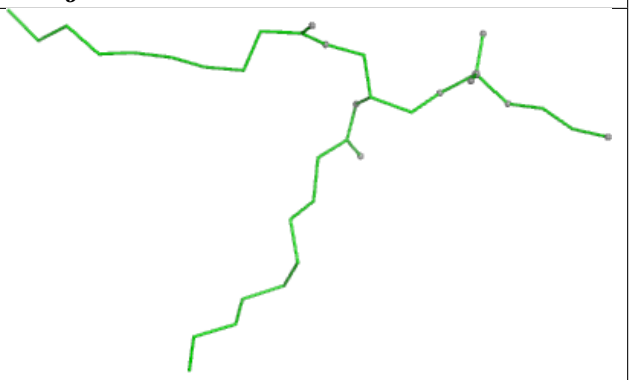


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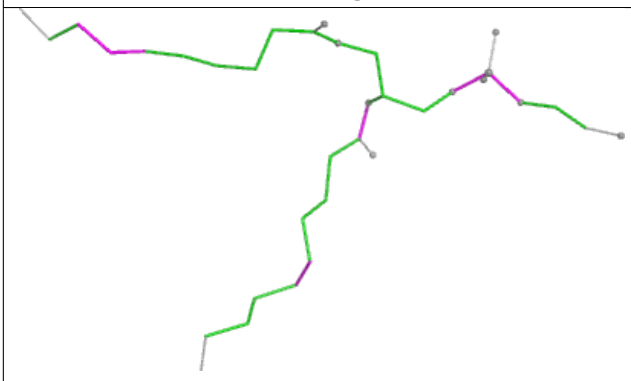
Ligand PEX Aj 103



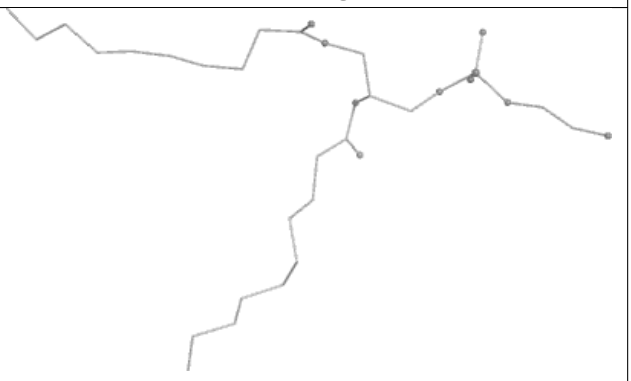
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Bond angles

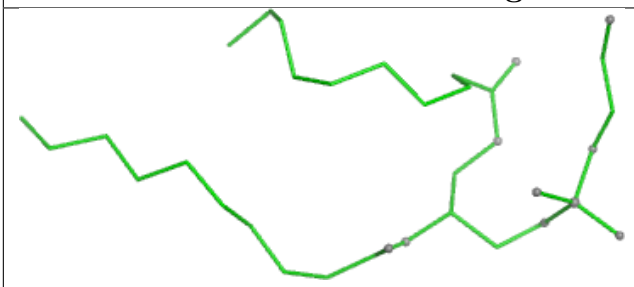


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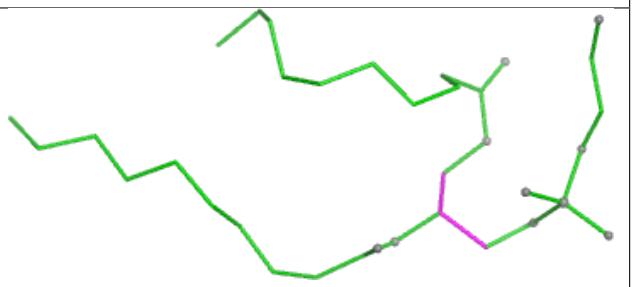


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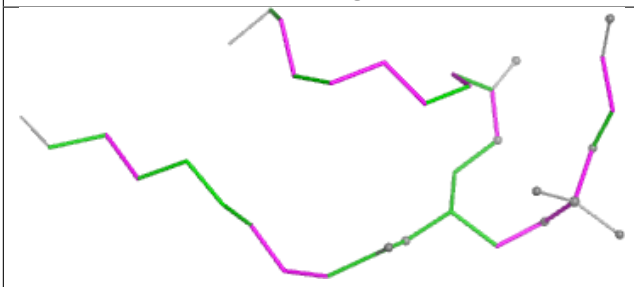
Ligand PEX Bh 1203



Bond lengths



Bond angles

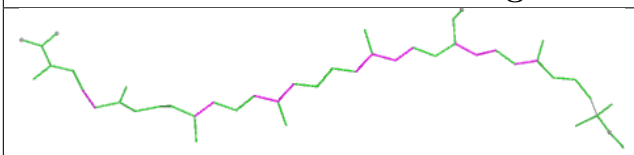


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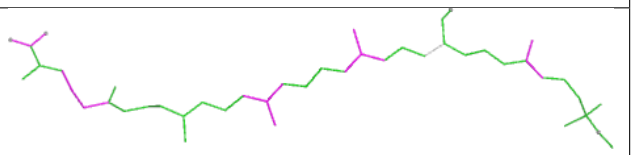


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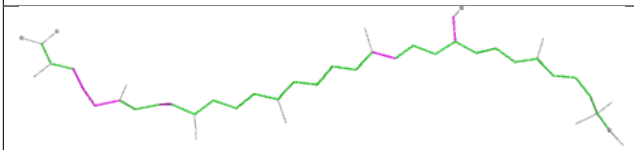
Ligand V7N Bh 1202



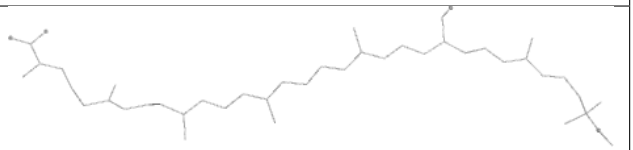
Bond lengths



Bond angles

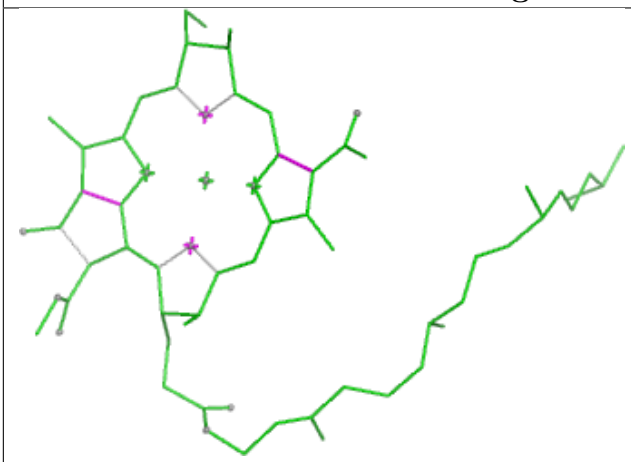


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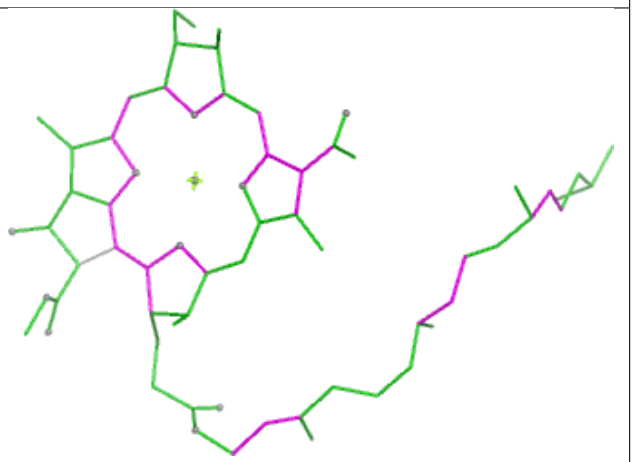


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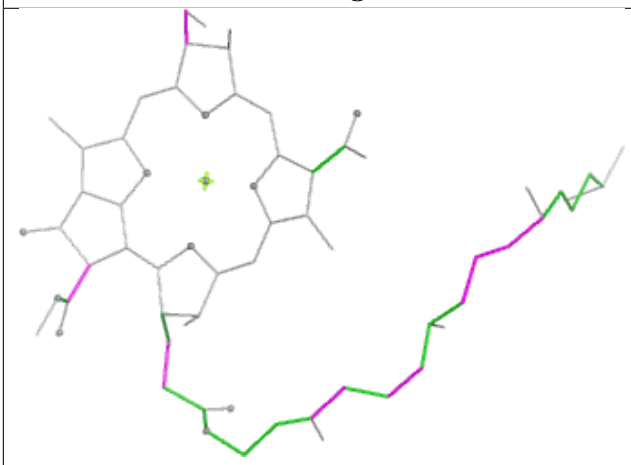
Ligand BCL BX 102



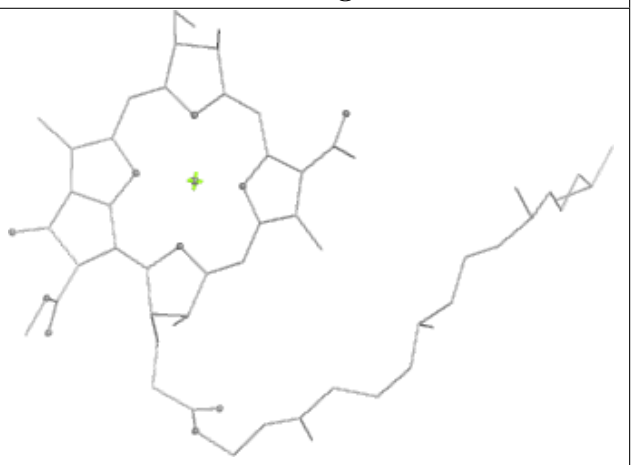
Bond lengths



Bond angles

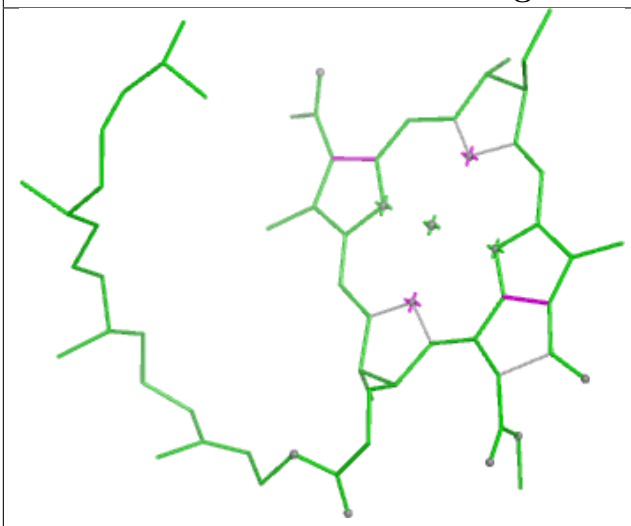


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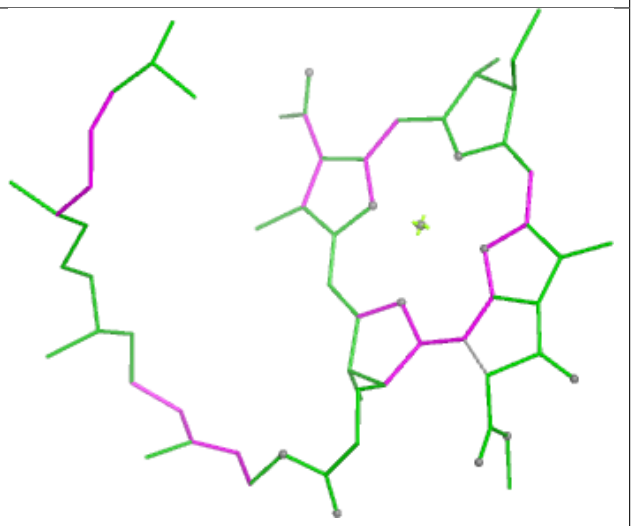


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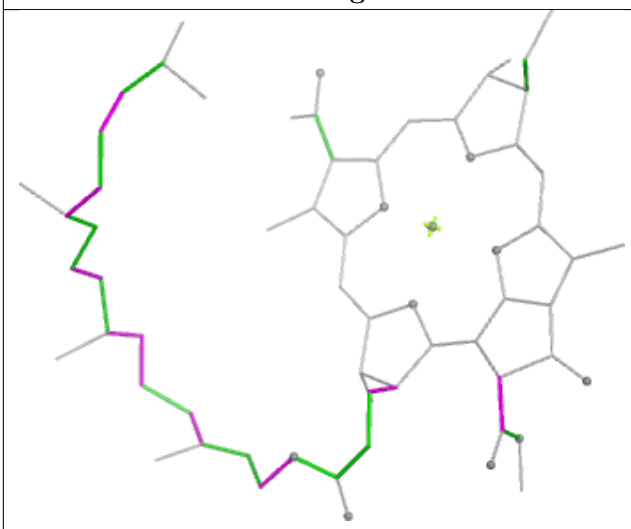
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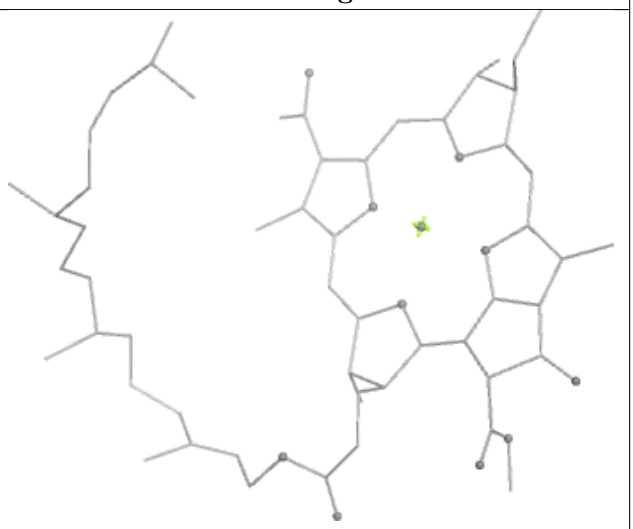
Bond lengths



Bond angles

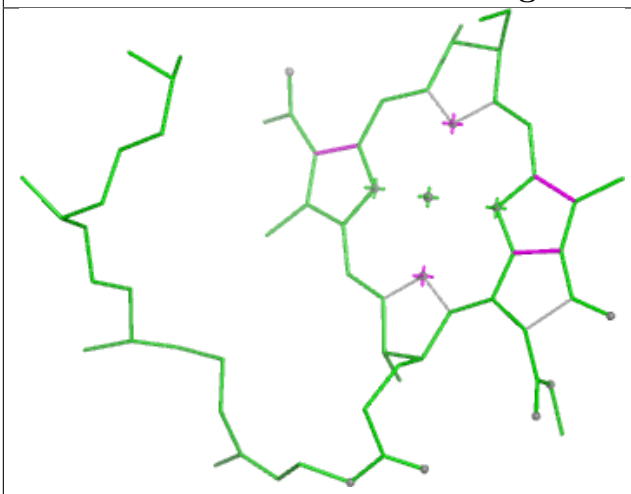


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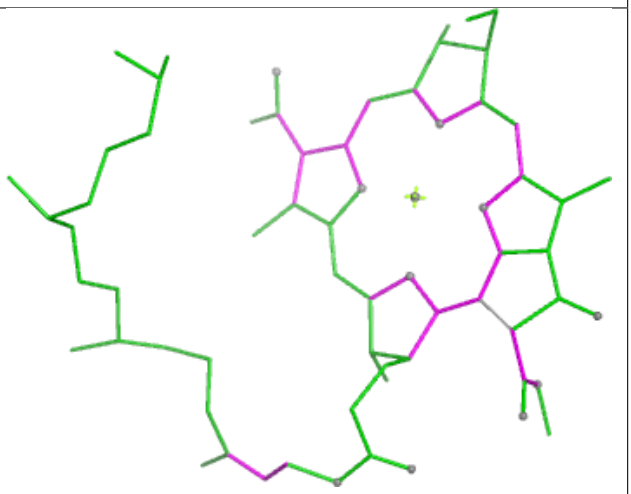


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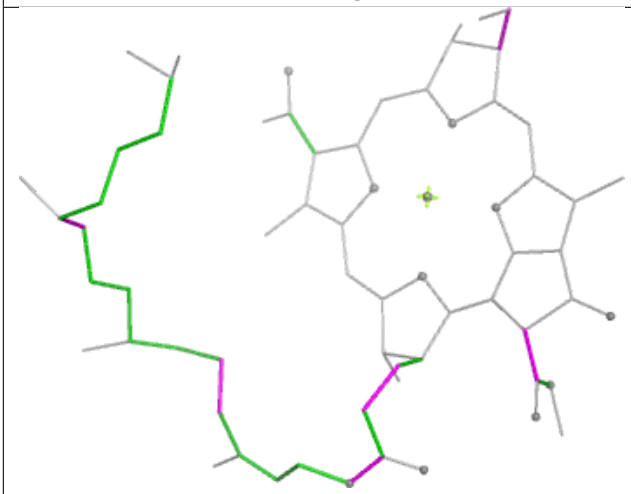
Ligand BCL BI 102



Bond lengths



Bond angles

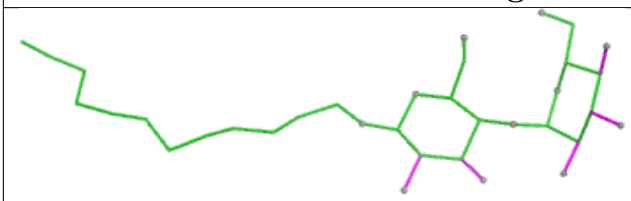


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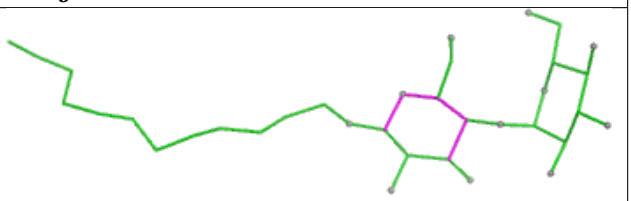


Rings

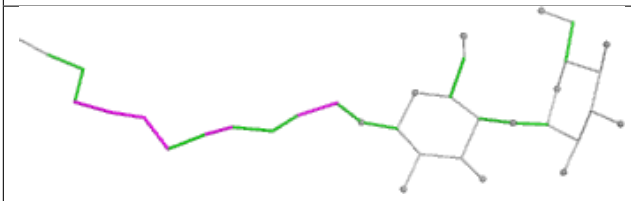
Ligand LMT Bj 1201



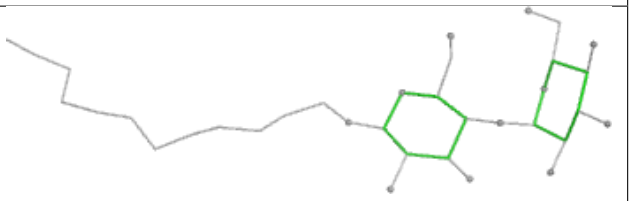
Bond lengths



Bond angles

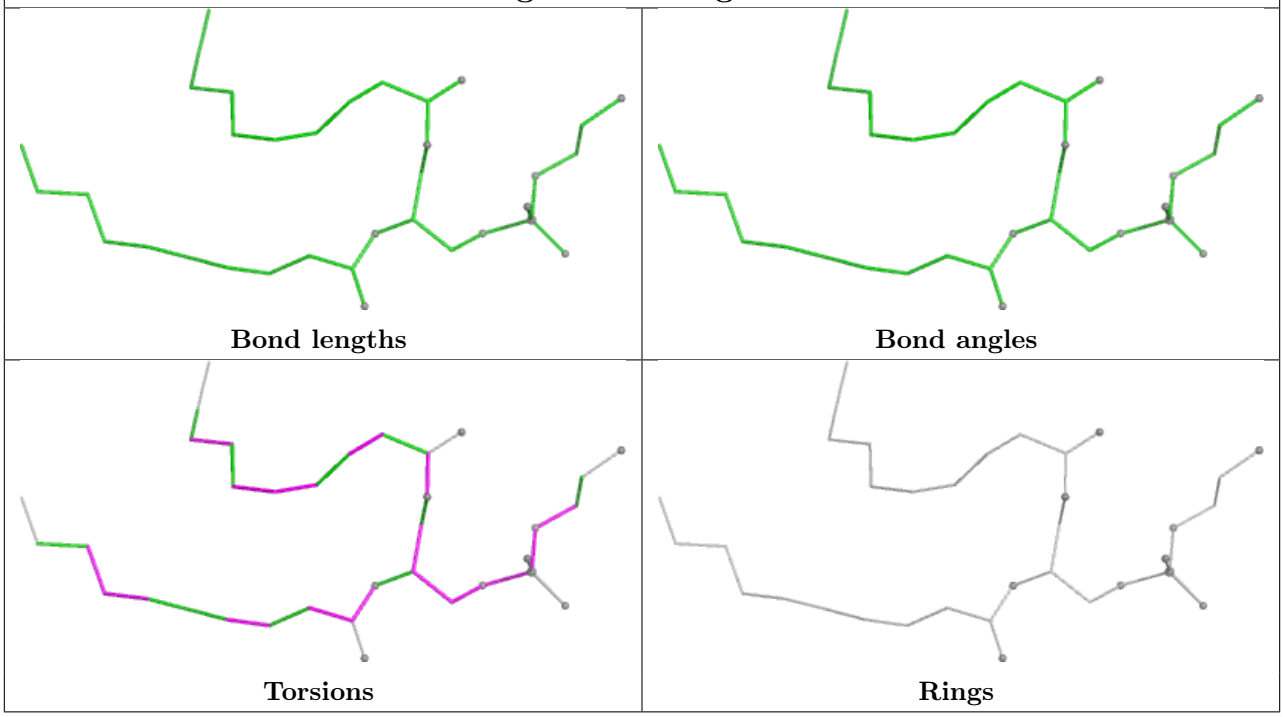


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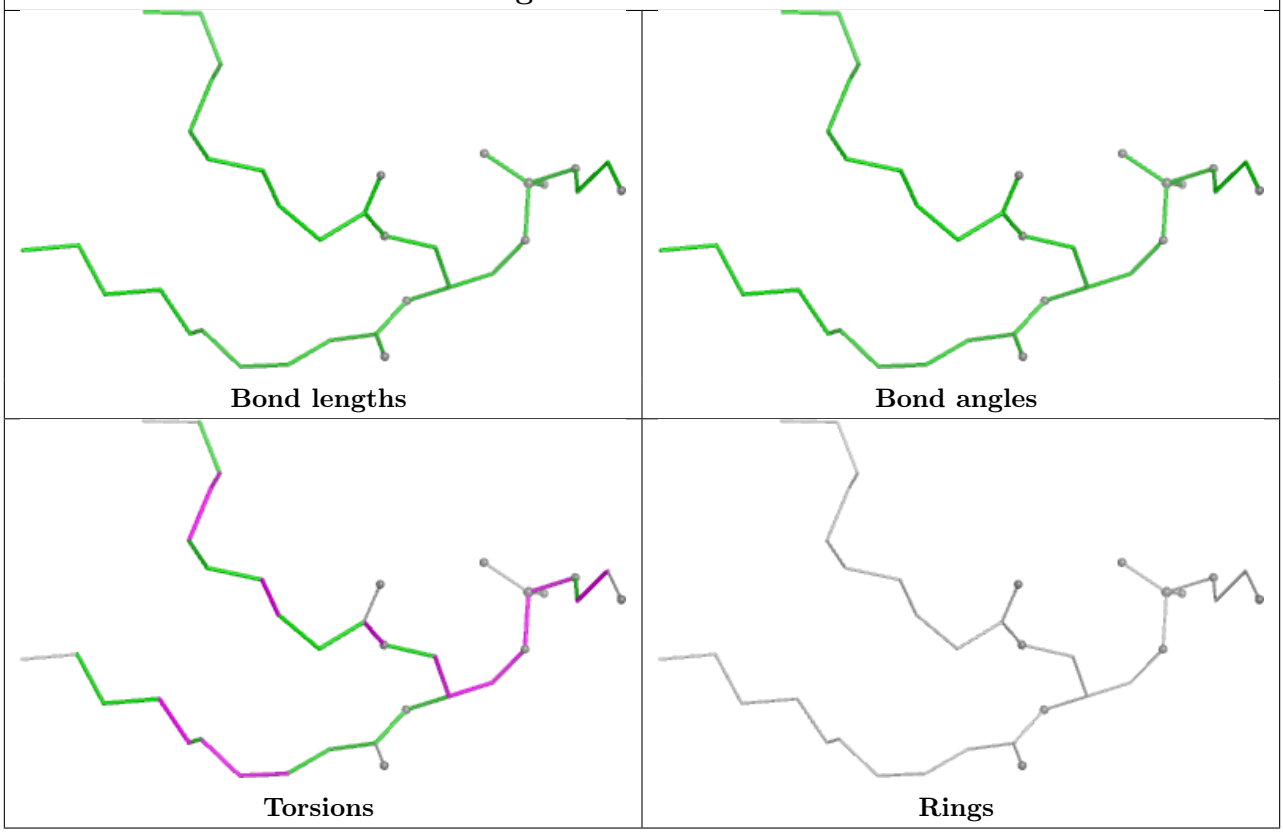


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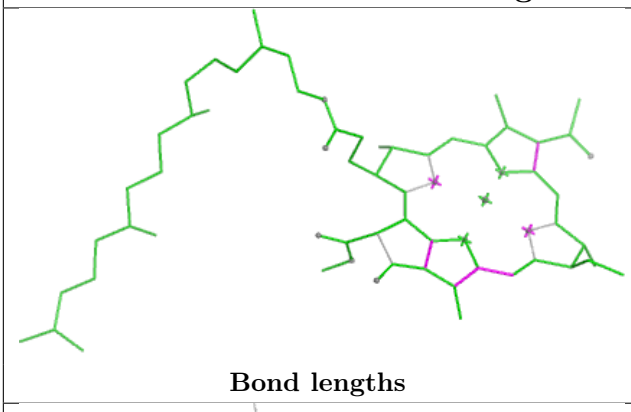
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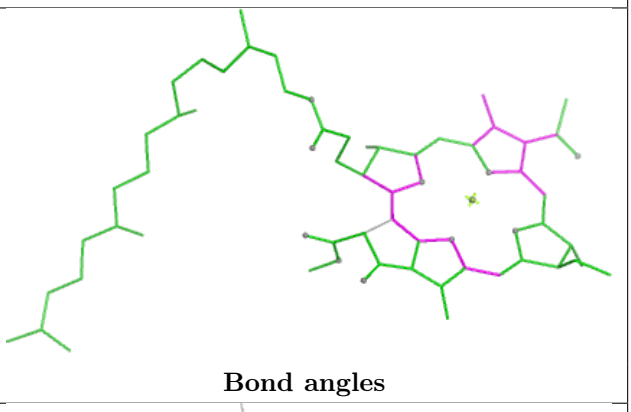
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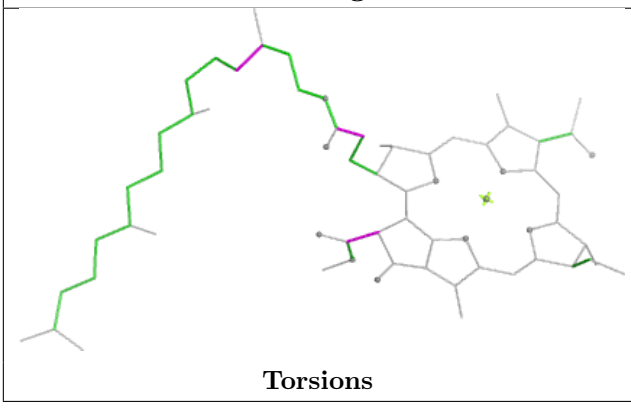
Ligand BCL Ad 101



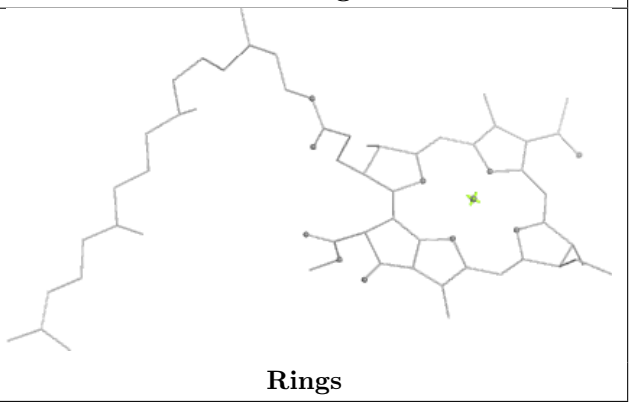
Bond lengths



Bond angles

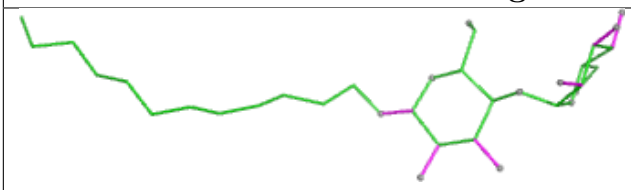


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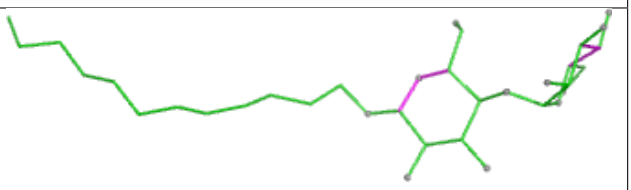


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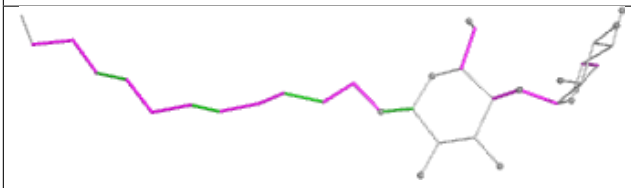
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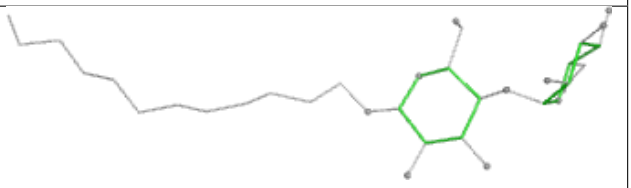
Bond lengths



Bond angles

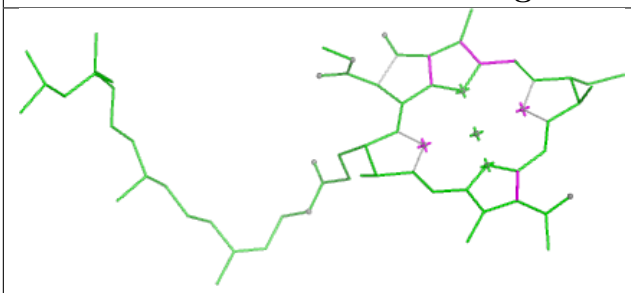


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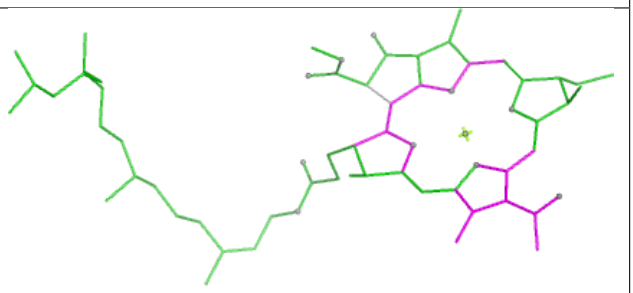


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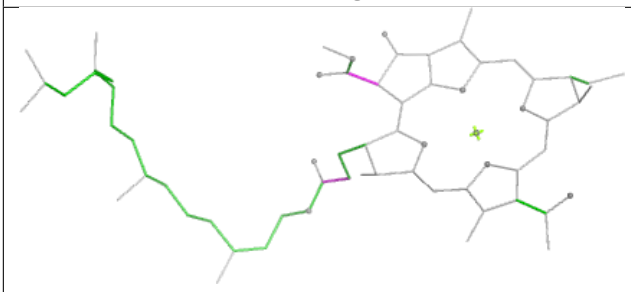
Ligand BCL Ah 101



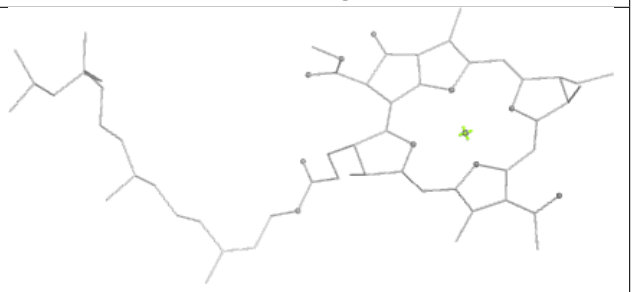
Bond lengths



Bond angles

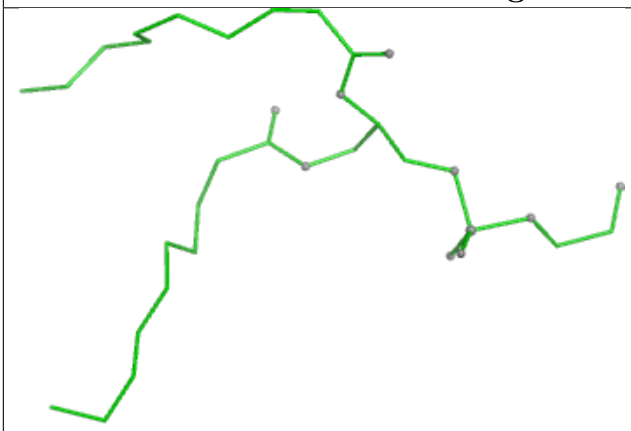


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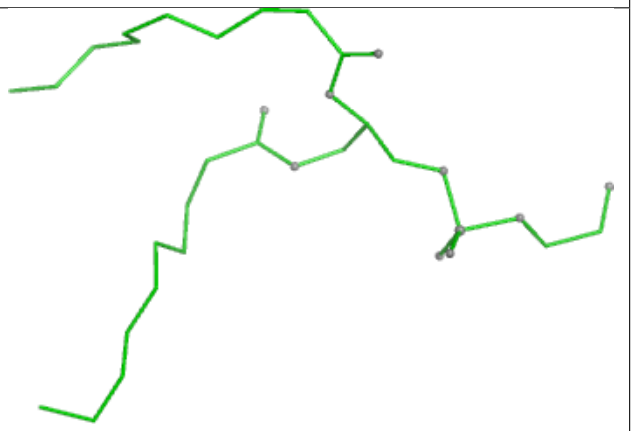


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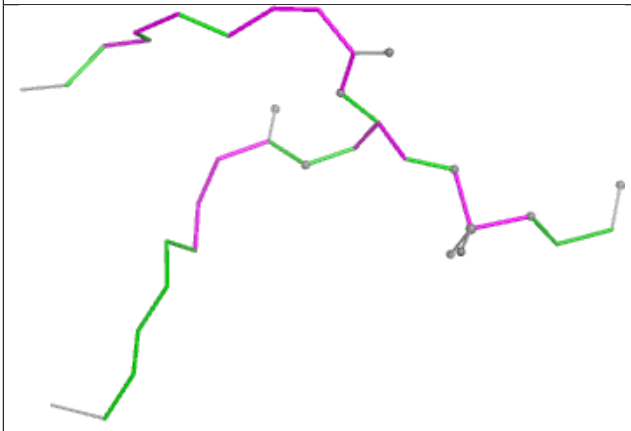
Ligand PEX Bc 1203



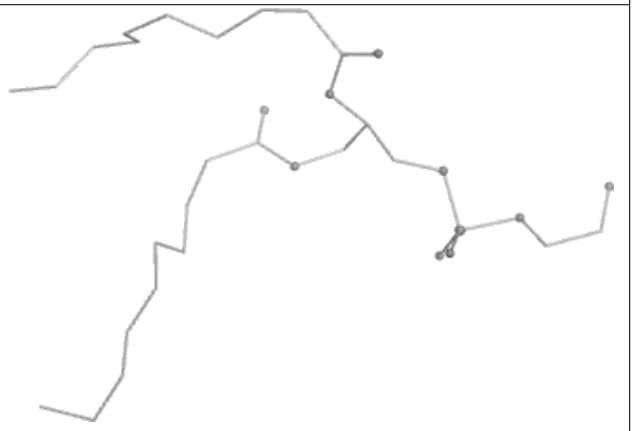
Bond lengths



Bond angles

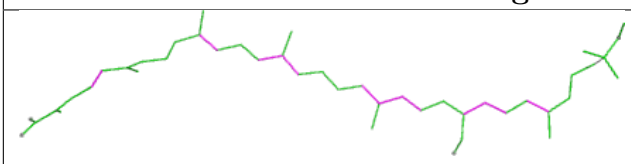


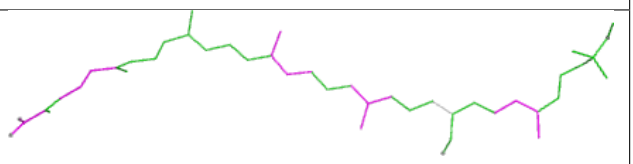
Torsions

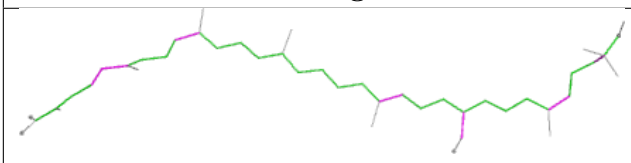


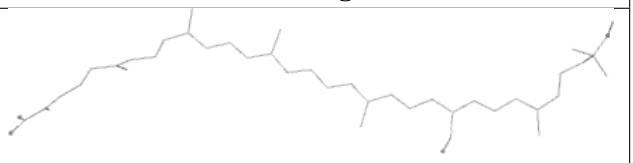
Rings

Ligand V7N BV 101

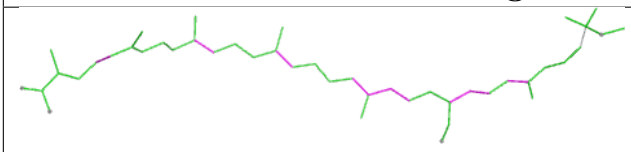

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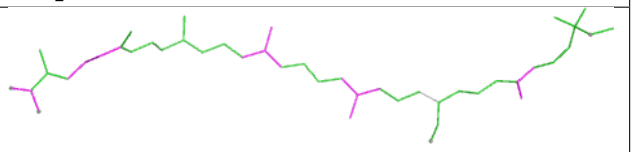

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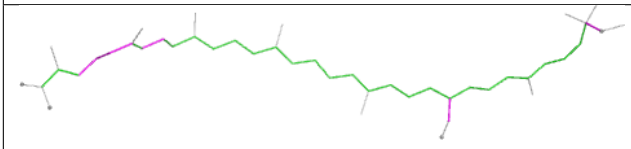

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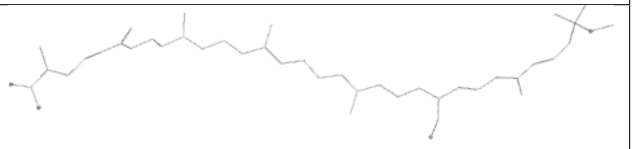

Rings

Ligand V7N Bp 1202

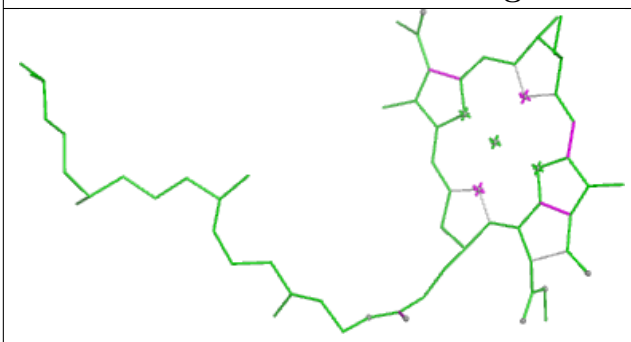

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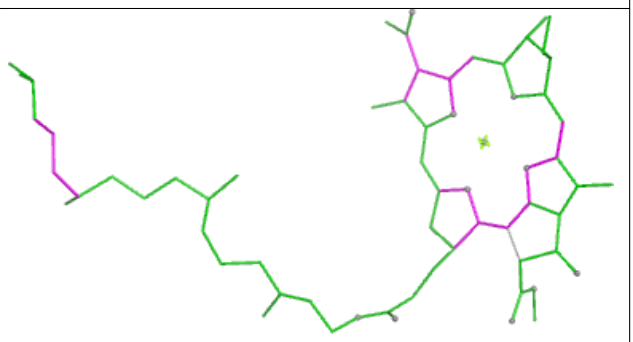

Bond angles

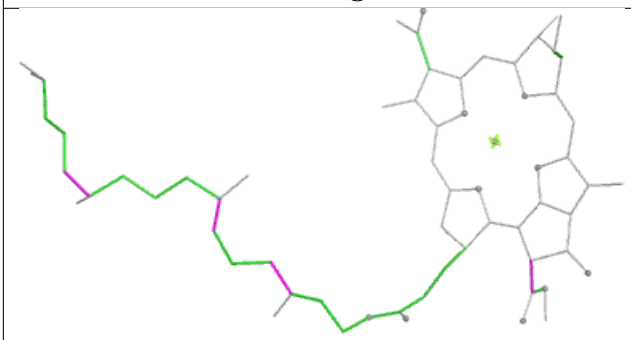

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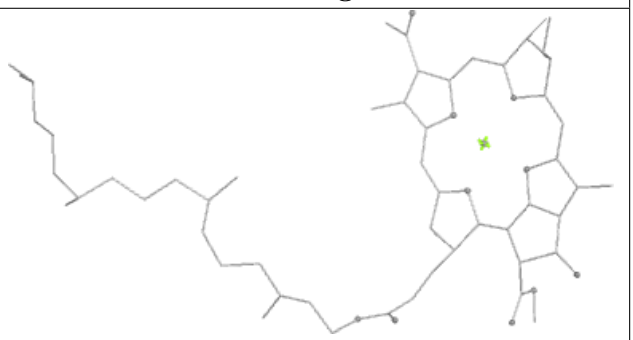

Rings

Ligand BCL AV 1001

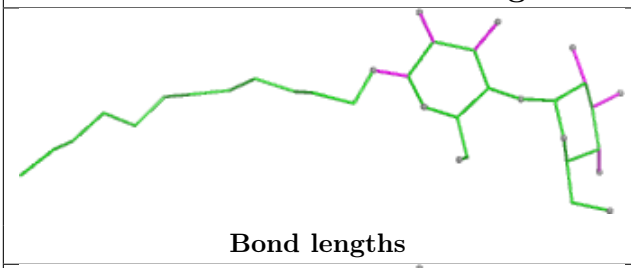

Bond lengths


Bond angles

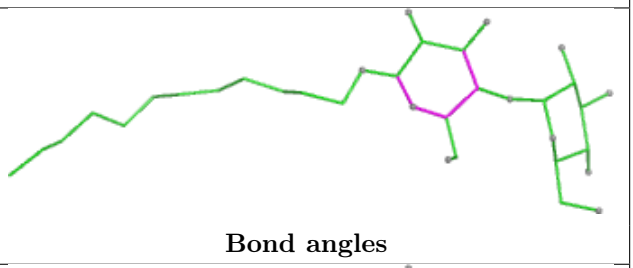

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Rings

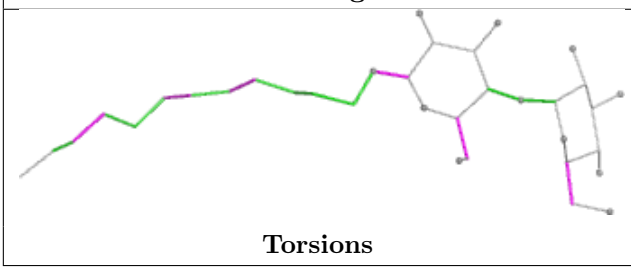
Ligand LMT BO 101



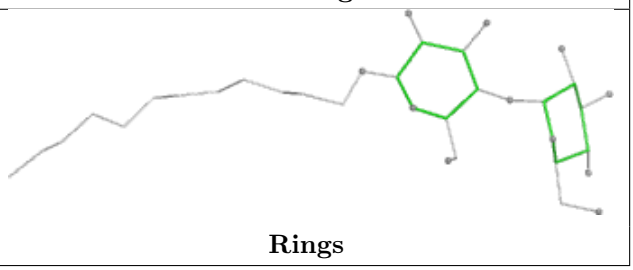
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Bond angles

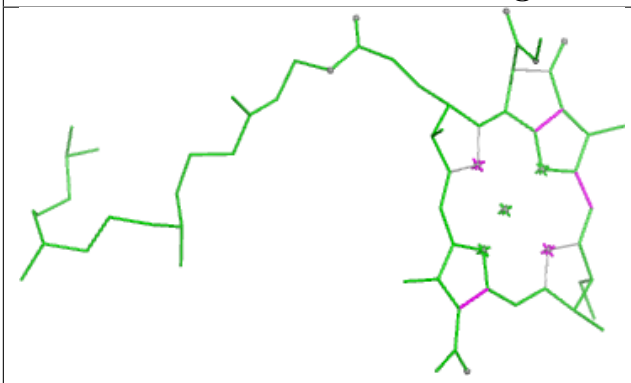


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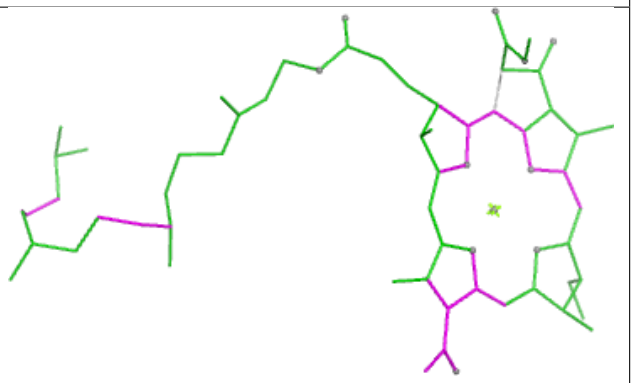


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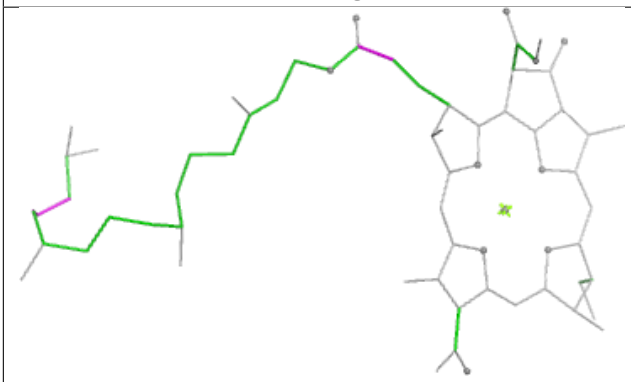
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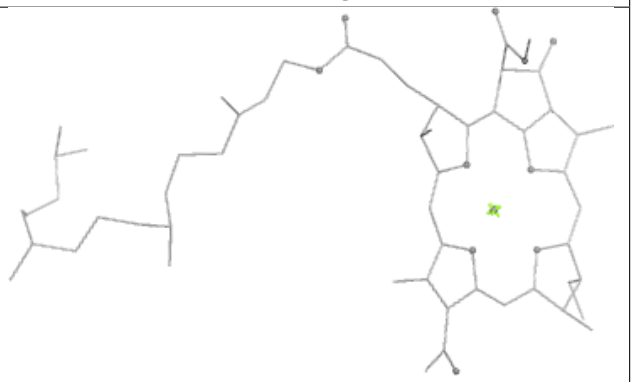
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Bond angles

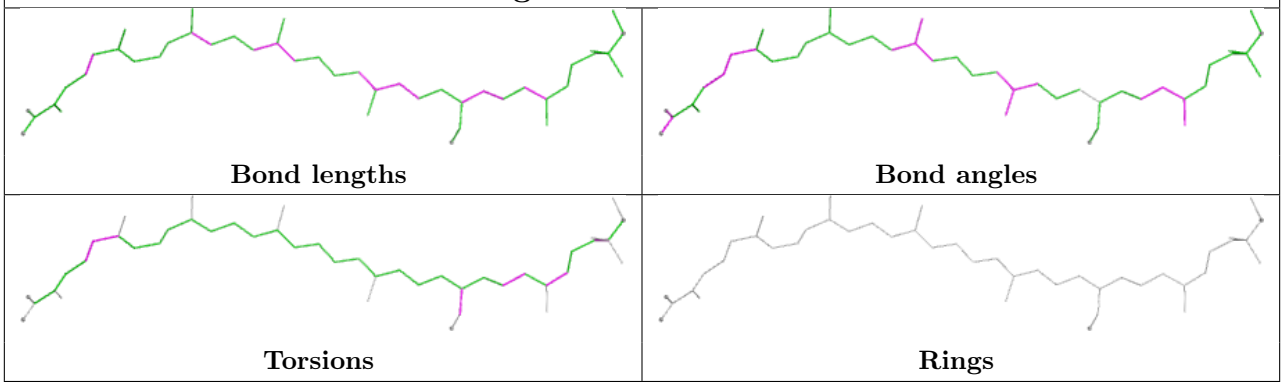


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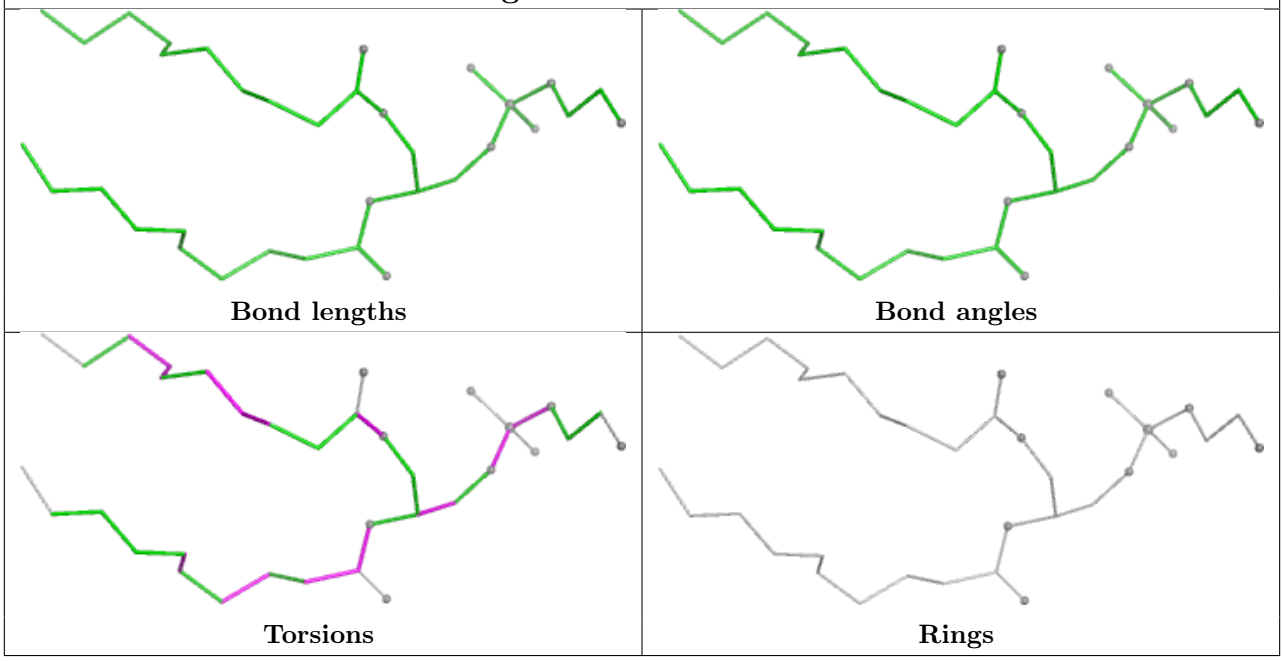


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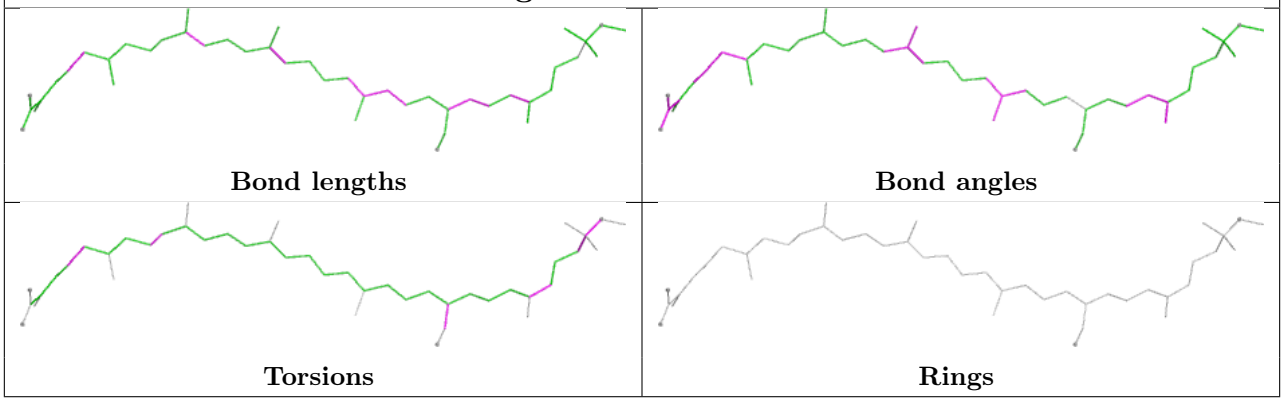
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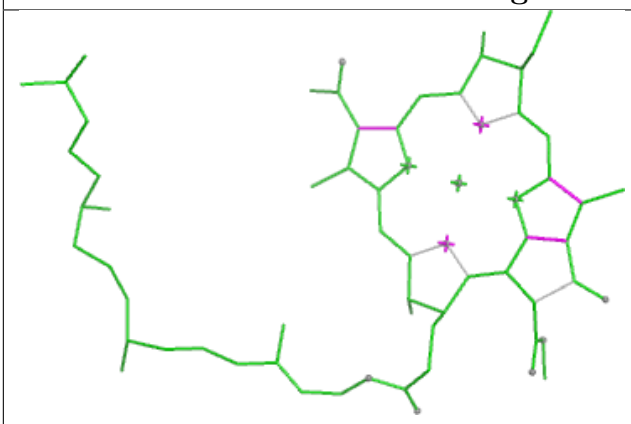
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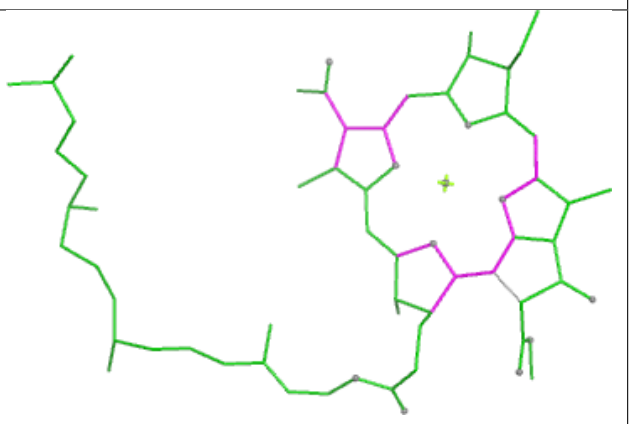
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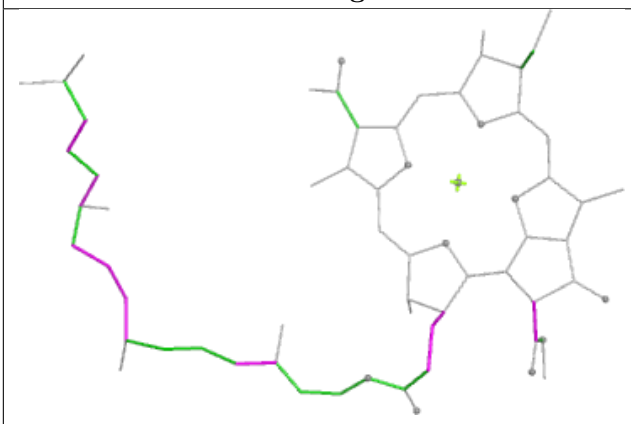
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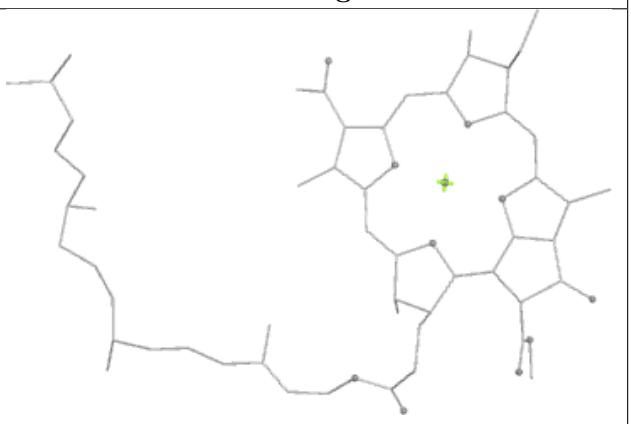
Bond lengths



Bond angles

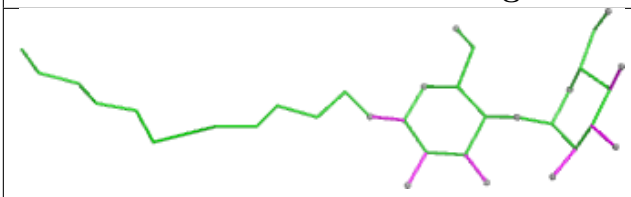


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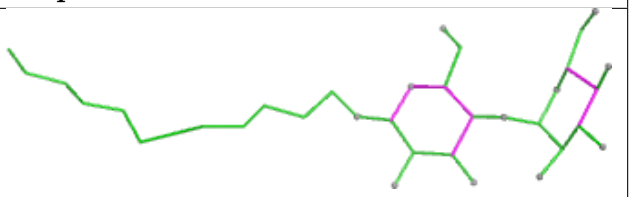


Rings

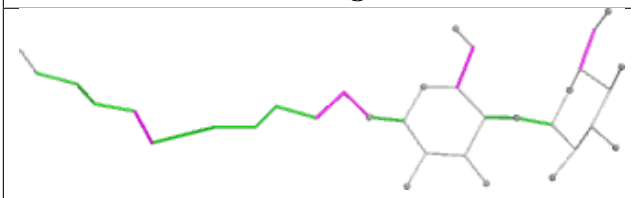
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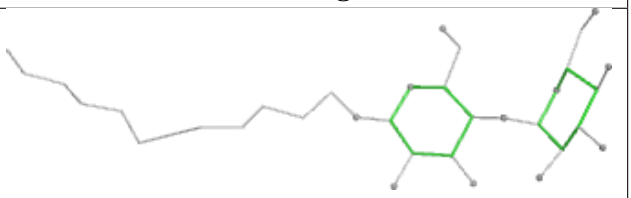
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Bond angles

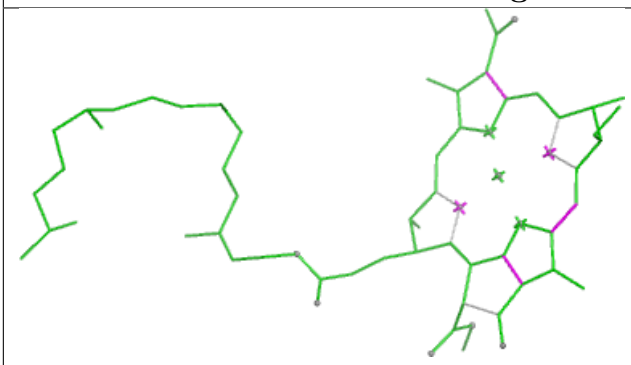


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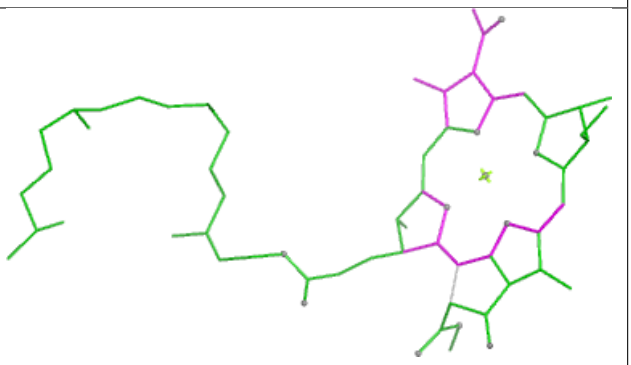


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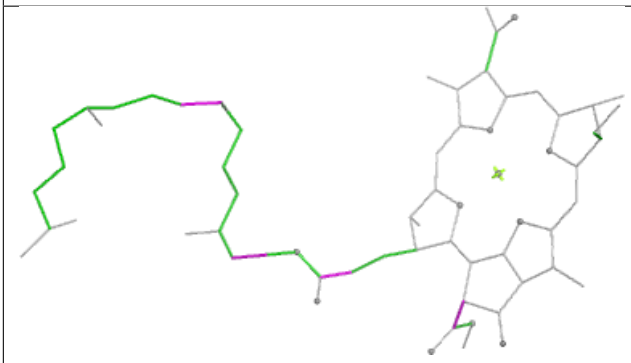
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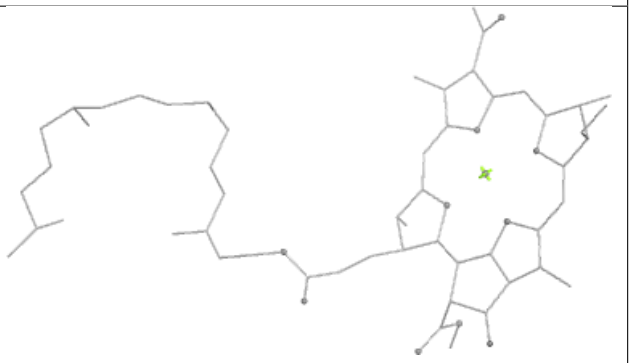
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Bond angles

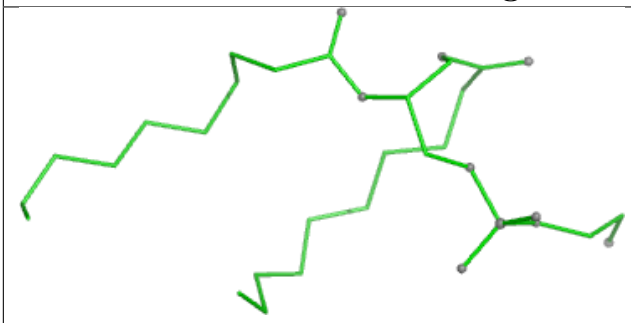


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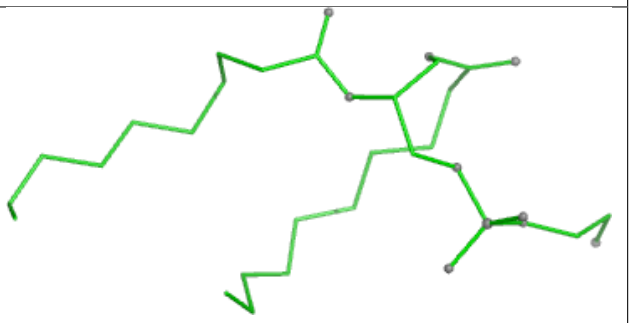


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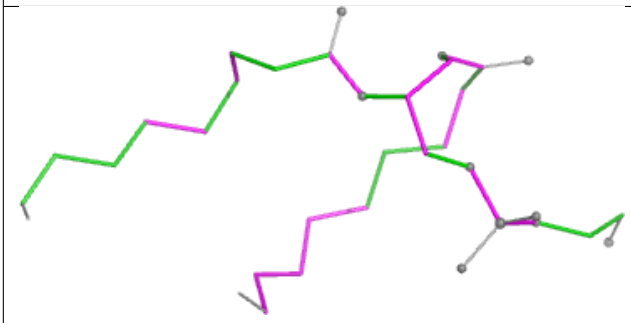
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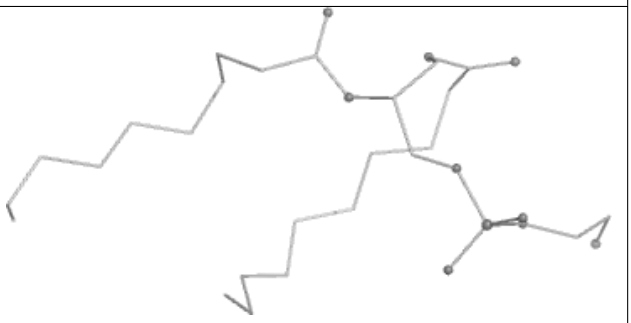
Bond lengths



Bond angles

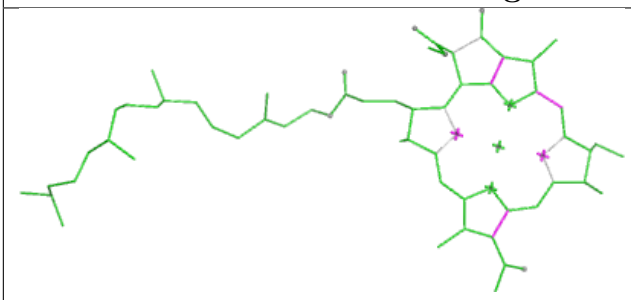


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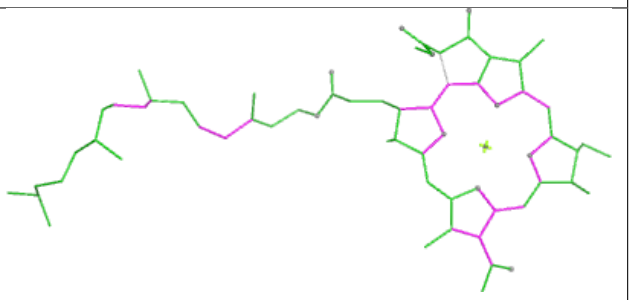


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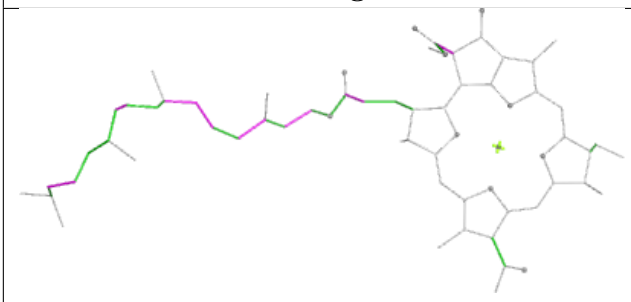
Ligand BCL AE 1102



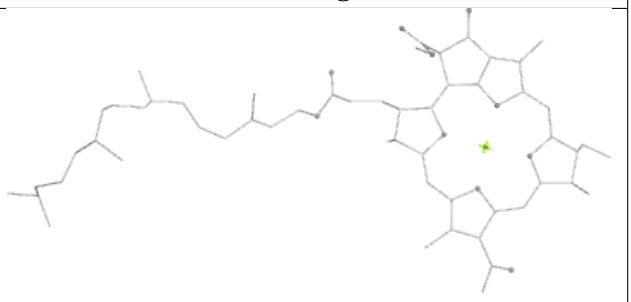
Bond lengths



Bond angles

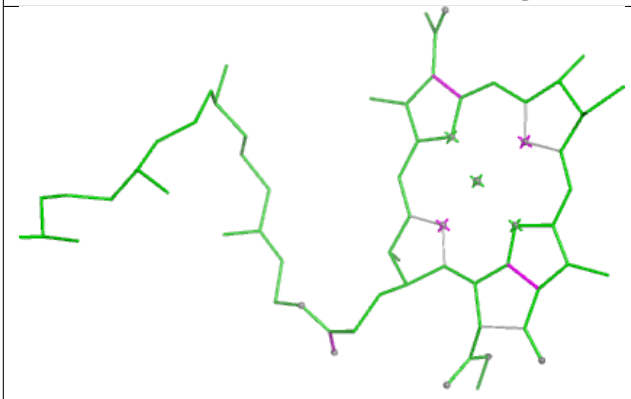


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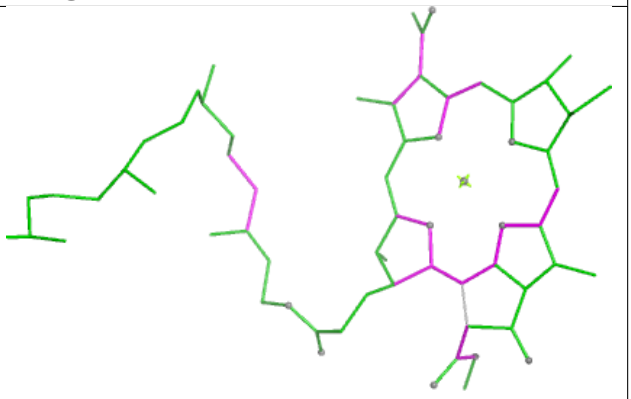


Rings

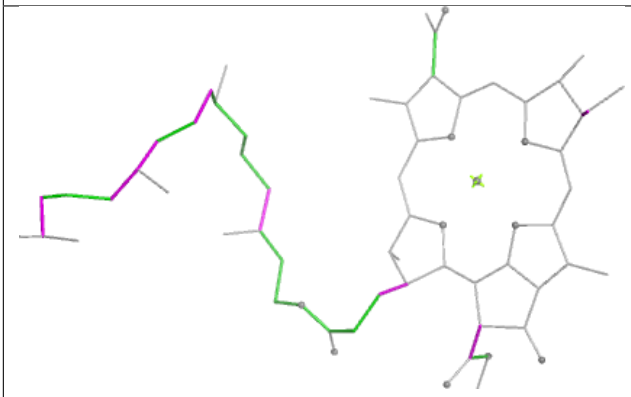
Ligand BCL Bg 103



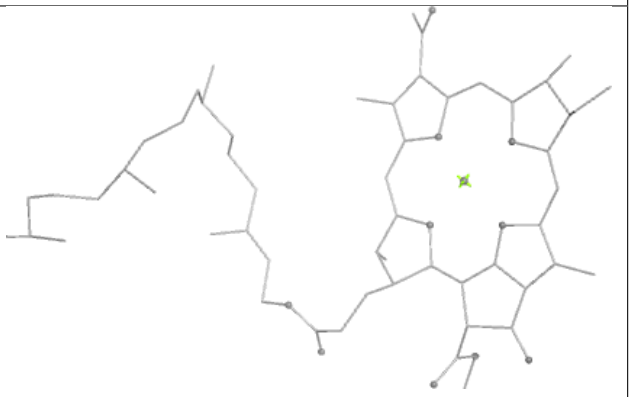
Bond lengths



Bond angles

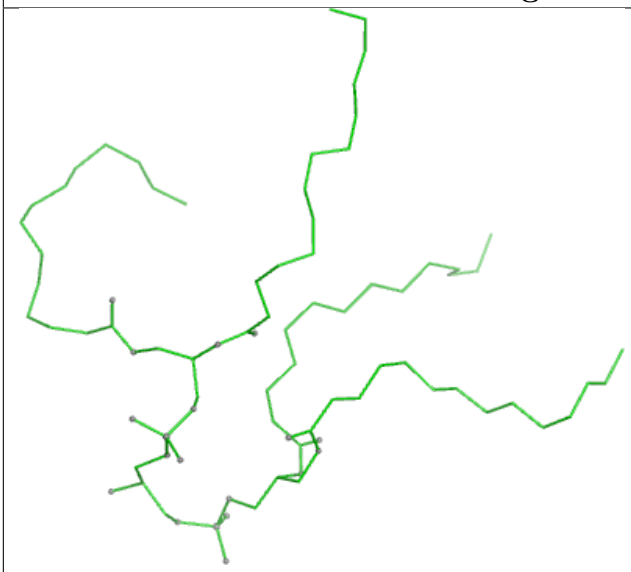


Torsions



Rings

Ligand CD4 M 403



Bond lengths



Bond angles

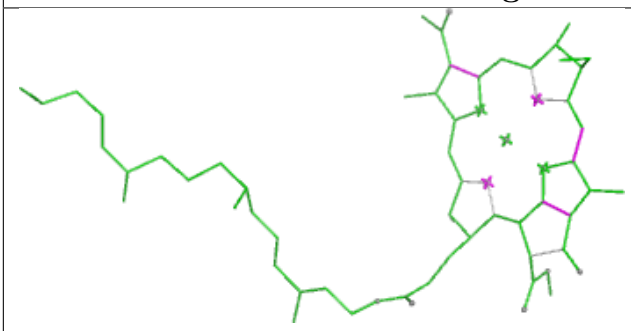


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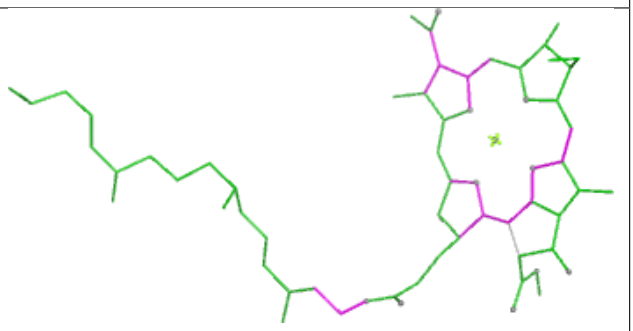


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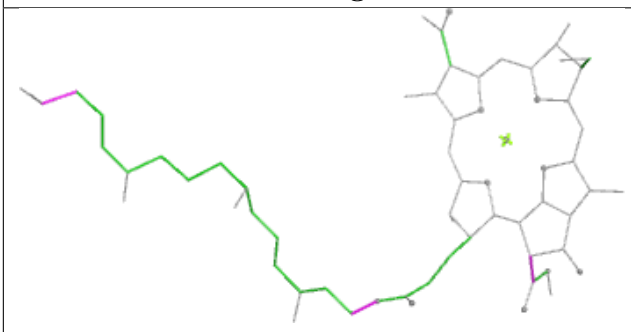
Ligand BCL AU 1001



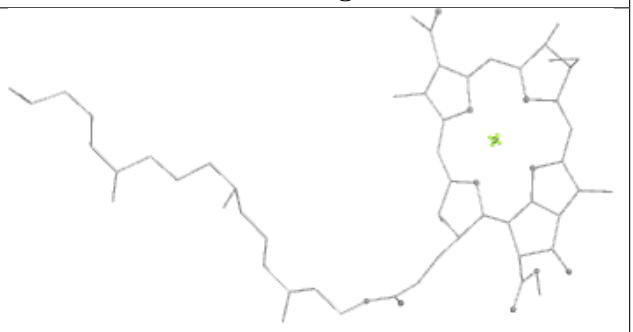
Bond lengths



Bond angles

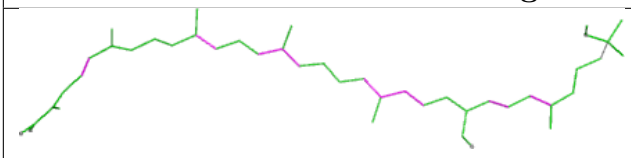


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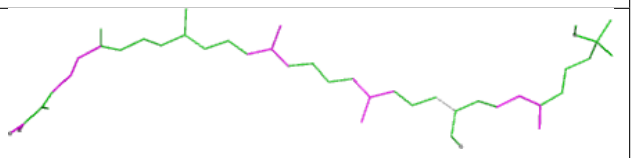


Rings

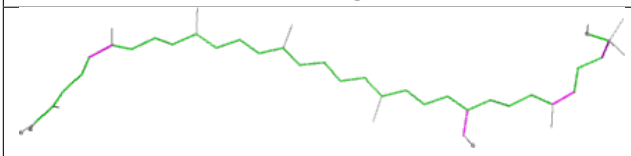
Ligand V7N Bi 101



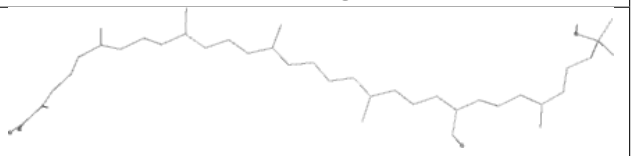
Bond lengths



Bond angles

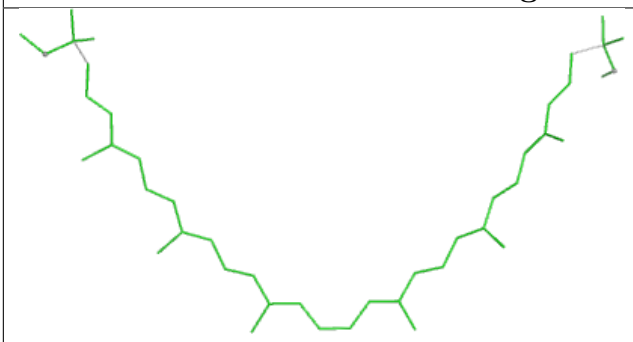


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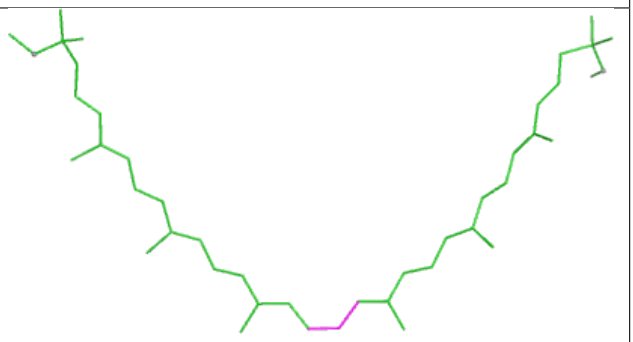


Rings

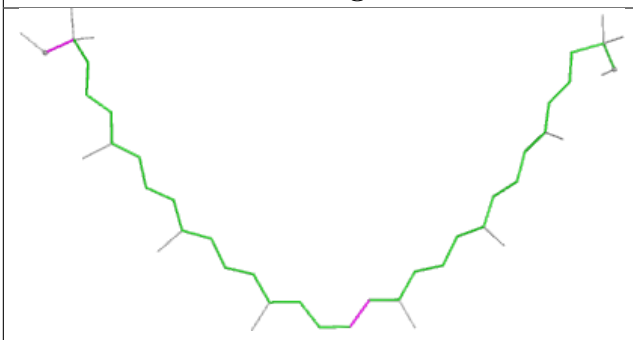
Ligand CRT M 407



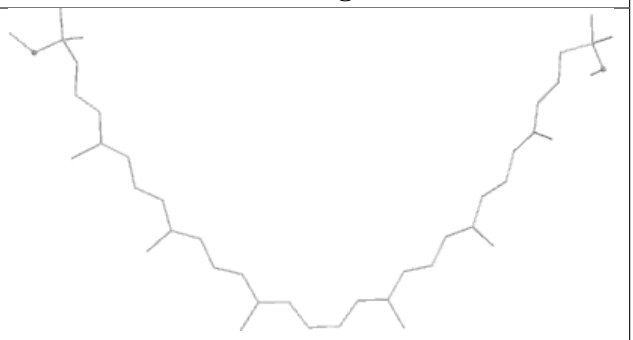
Bond lengths



Bond angles

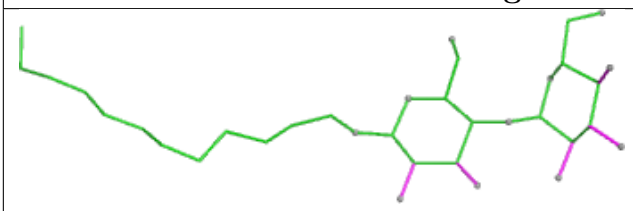


Torsions

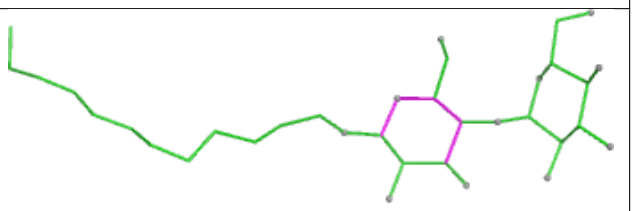


Rings

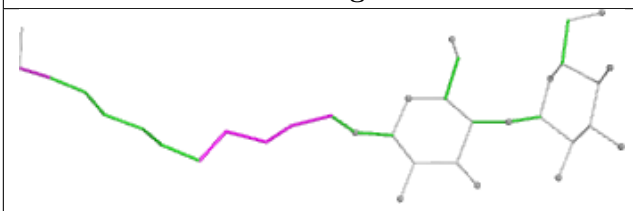
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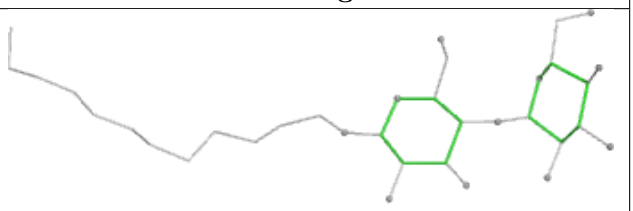
Bond lengths



Bond angles

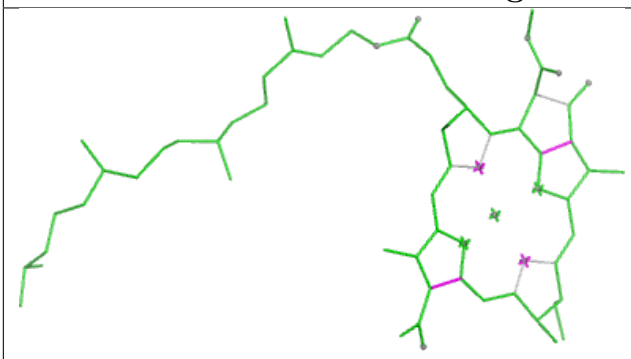


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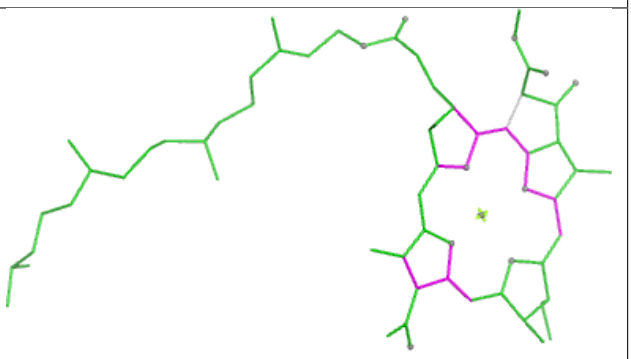


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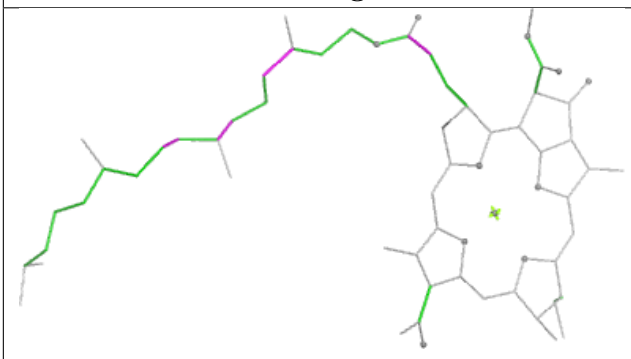
Ligand BCL AJ 1102



Bond lengths



Bond angles

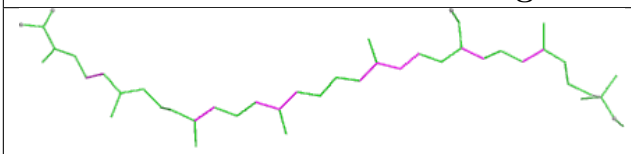


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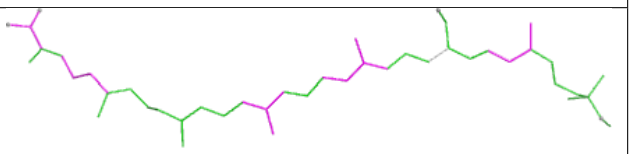


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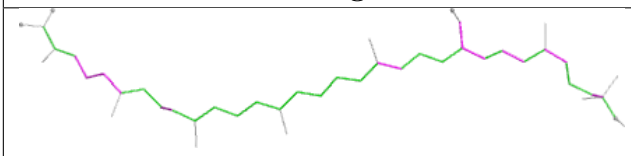
Ligand V7N BJ 101



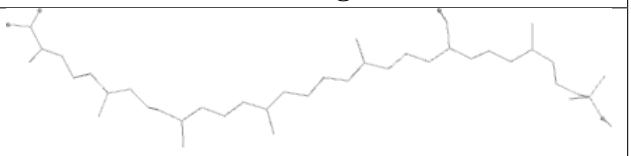
Bond lengths



Bond angles

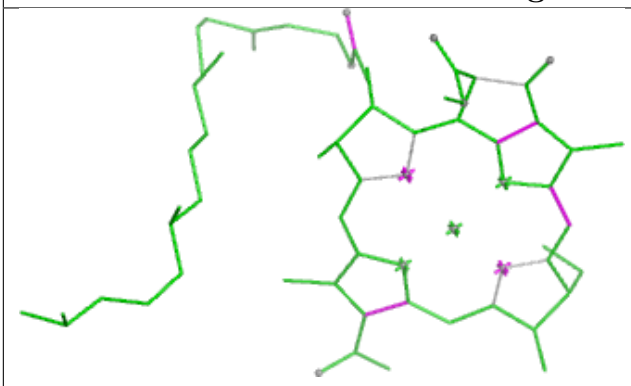


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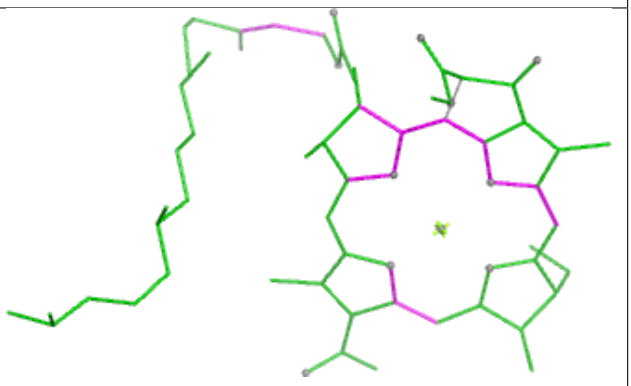


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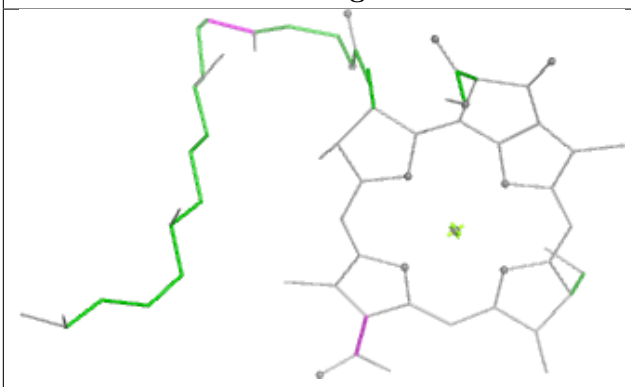
Ligand BCL L 302



Bond lengths



Bond angles

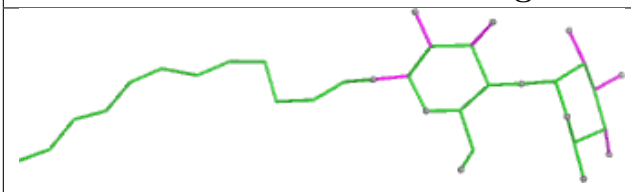


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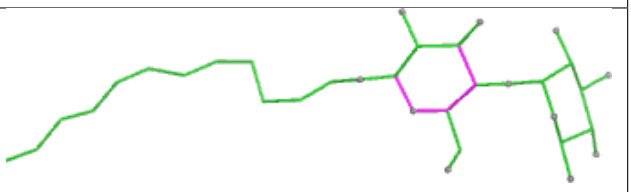


Rings

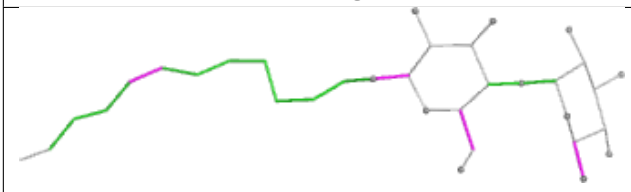
Ligand LMT BI 103



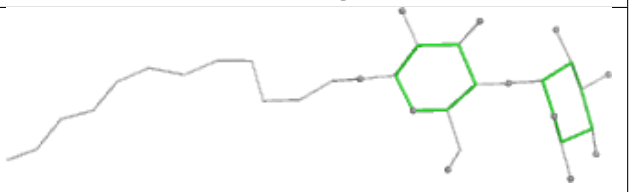
Bond lengths



Bond angles

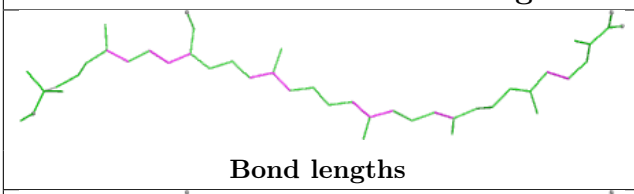


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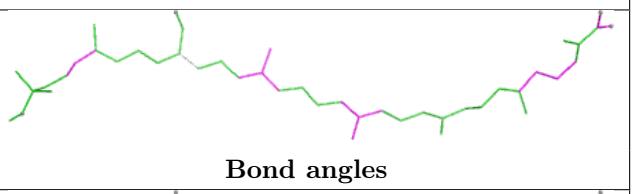


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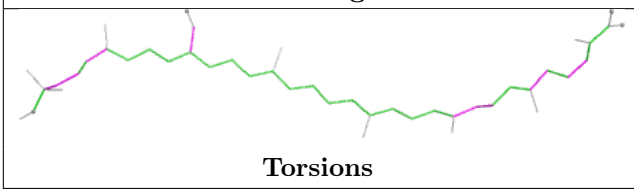
Ligand V7N BS 103



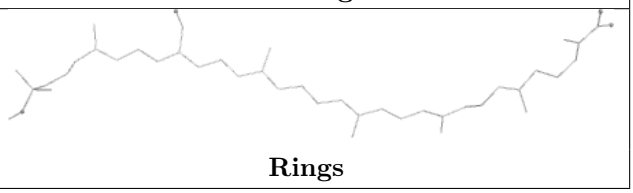
Bond lengths



Bond angles

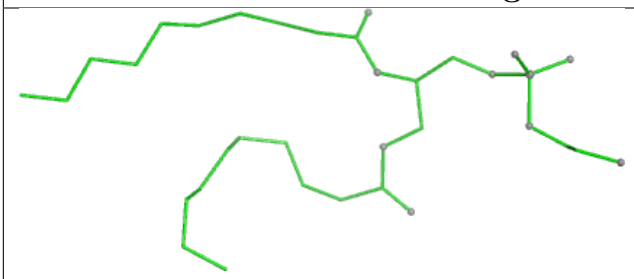


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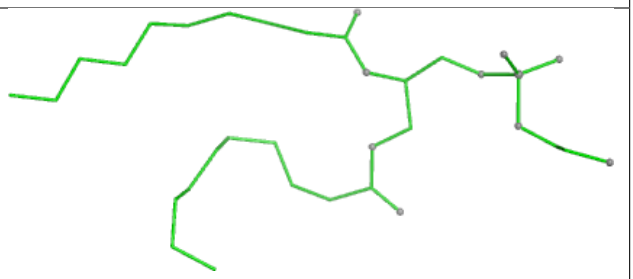


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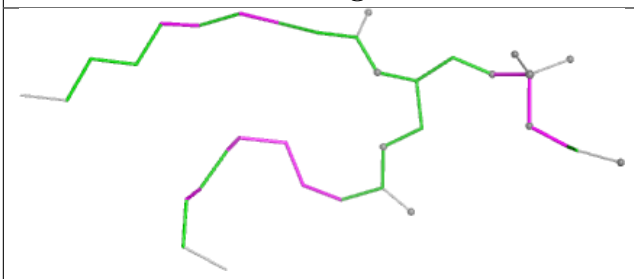
Ligand PEX AT 1101



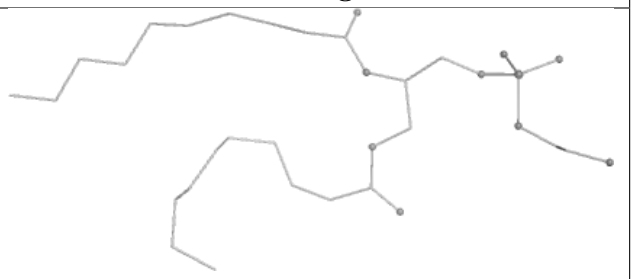
Bond lengths



Bond angles

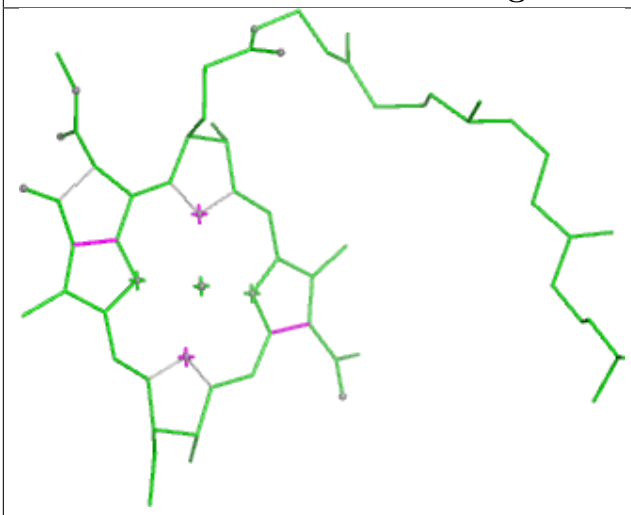


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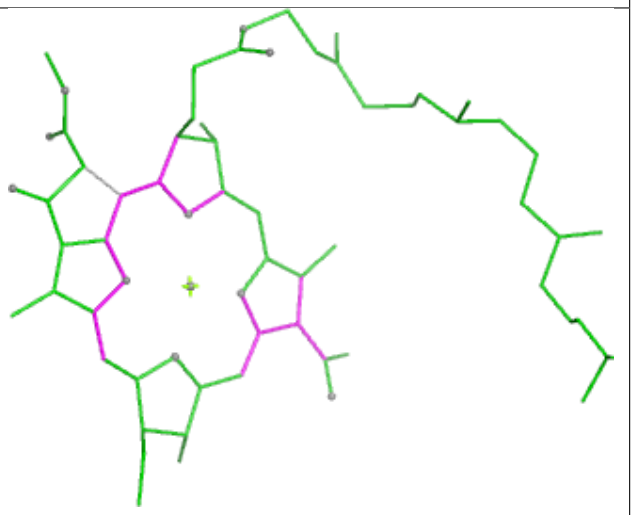


Rings

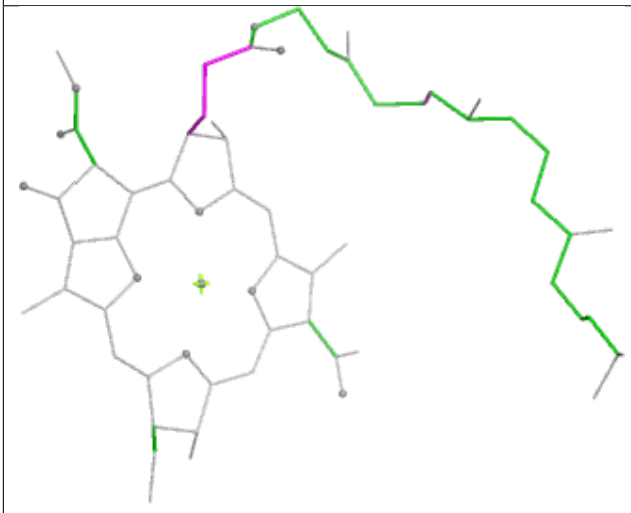
Ligand BCL Be 1105



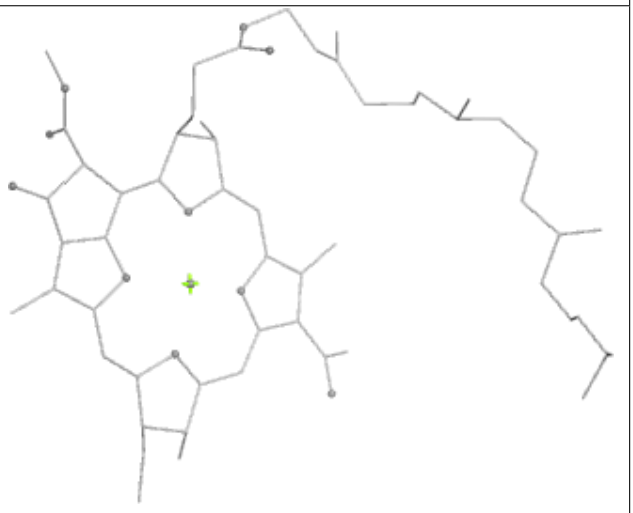
Bond lengths



Bond angles

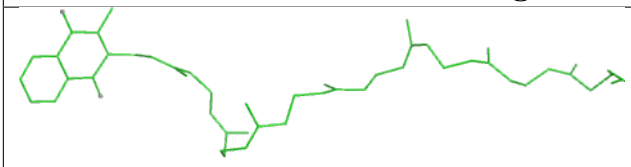


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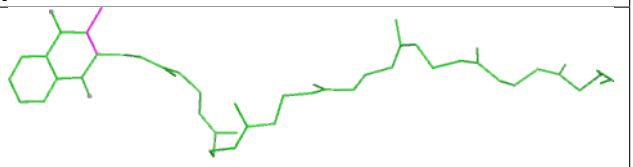


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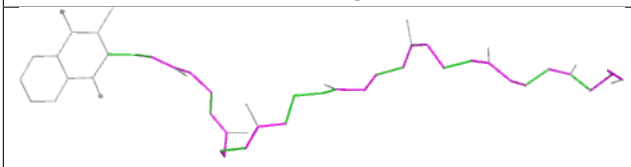
Ligand MQ8 Ad 103



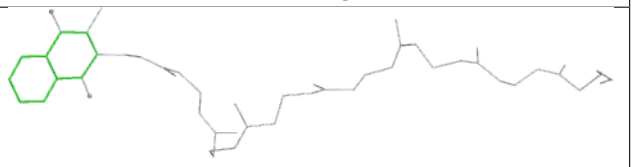
Bond lengths



Bond angles

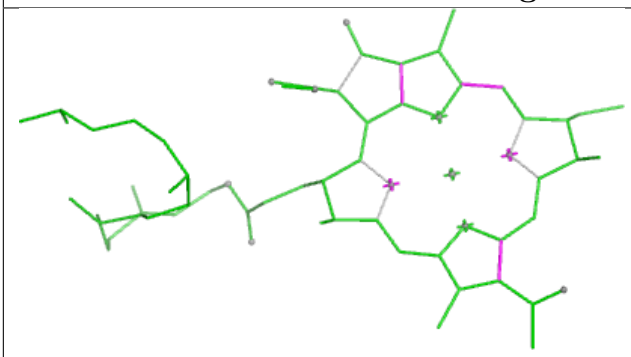


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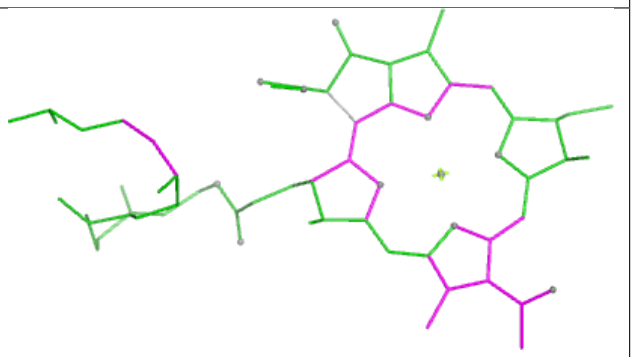


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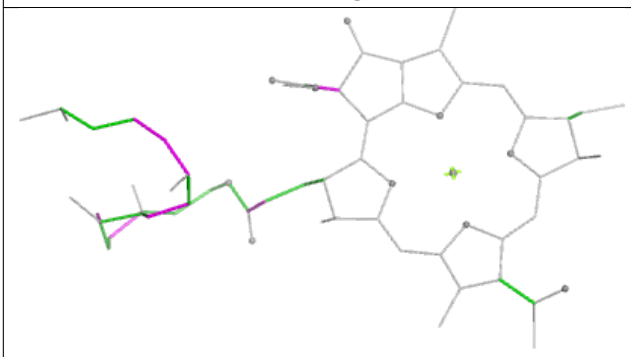
Ligand BCL Ai 101



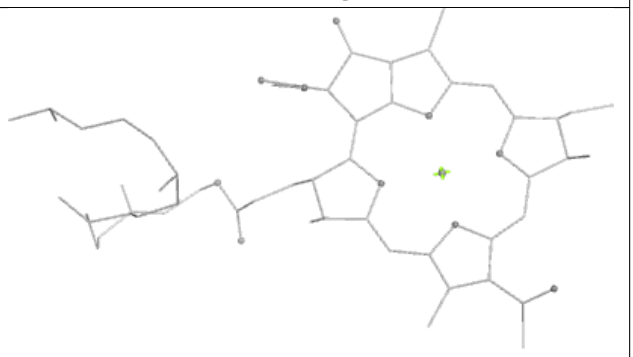
Bond lengths



Bond angles

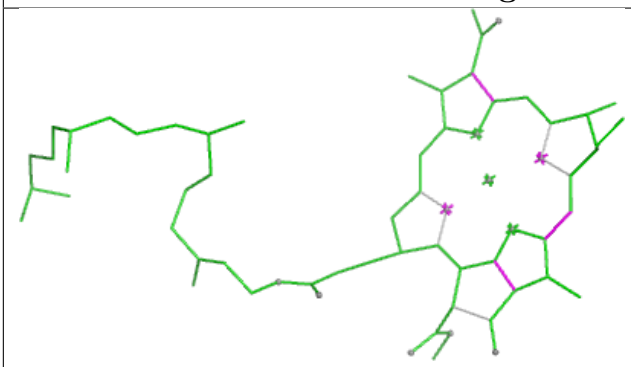


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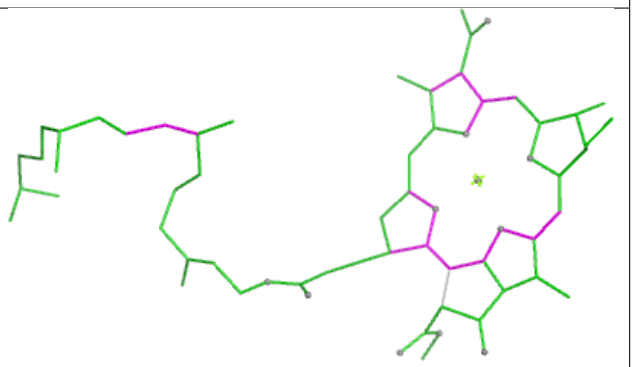


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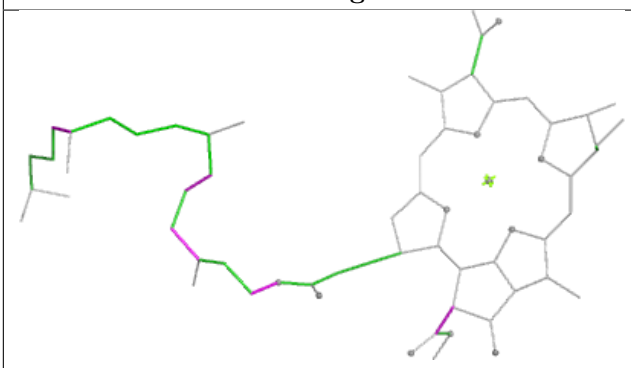
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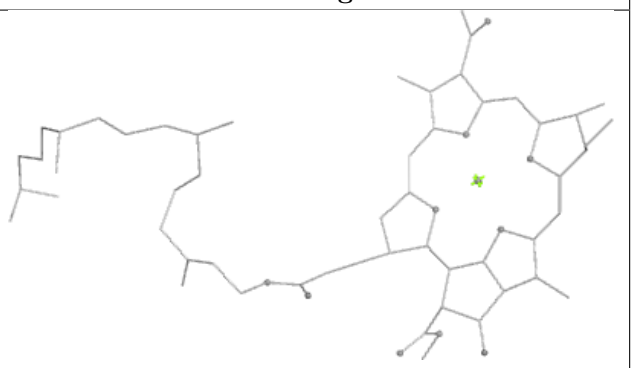
Bond lengths



Bond angles

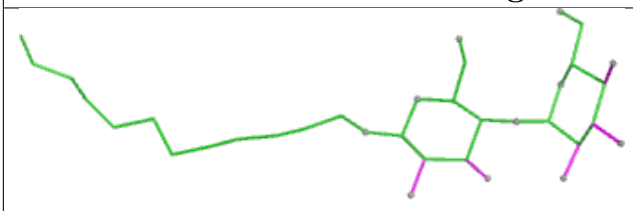


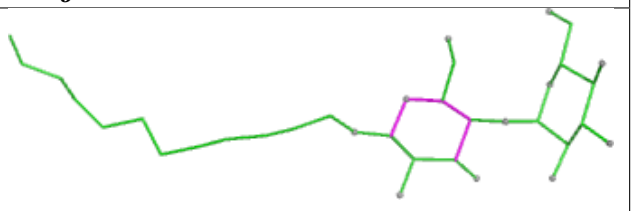
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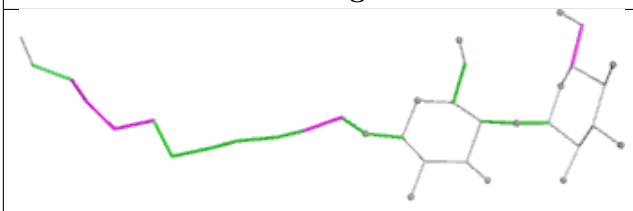


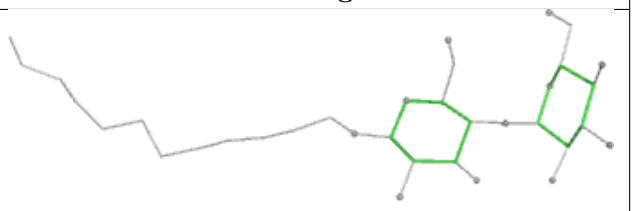
Rings

Ligand LMT Bj 1203

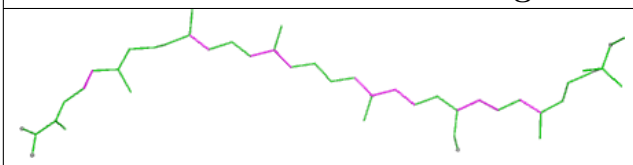

Bond lengths

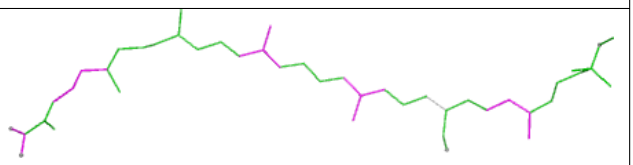

Bond angles

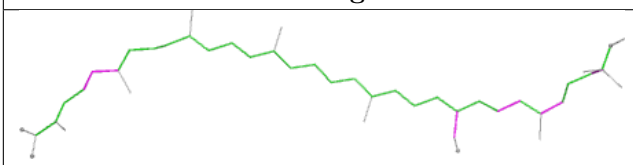

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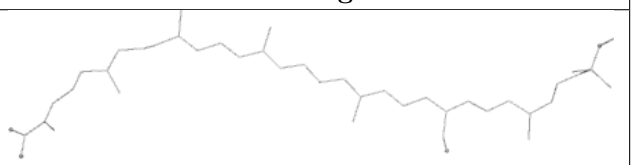

Rings

Ligand V7N BF 103

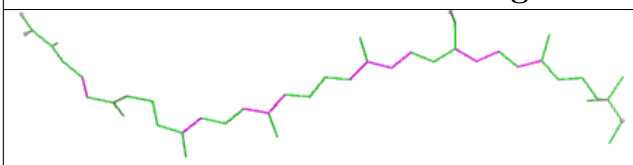

Bond lengths

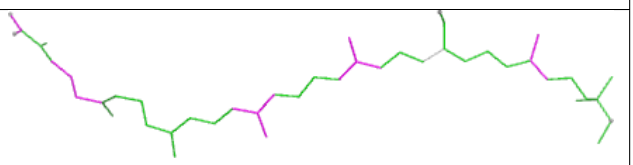

Bond angles

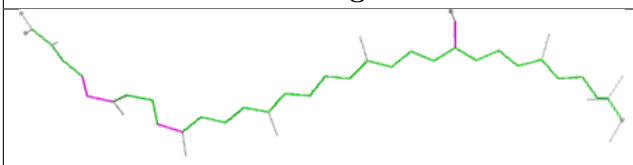

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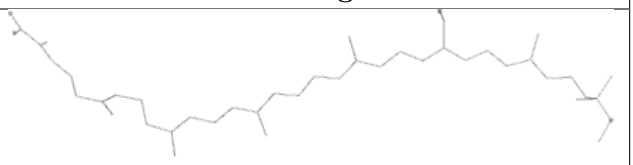

Rings

Ligand V7N BK 104

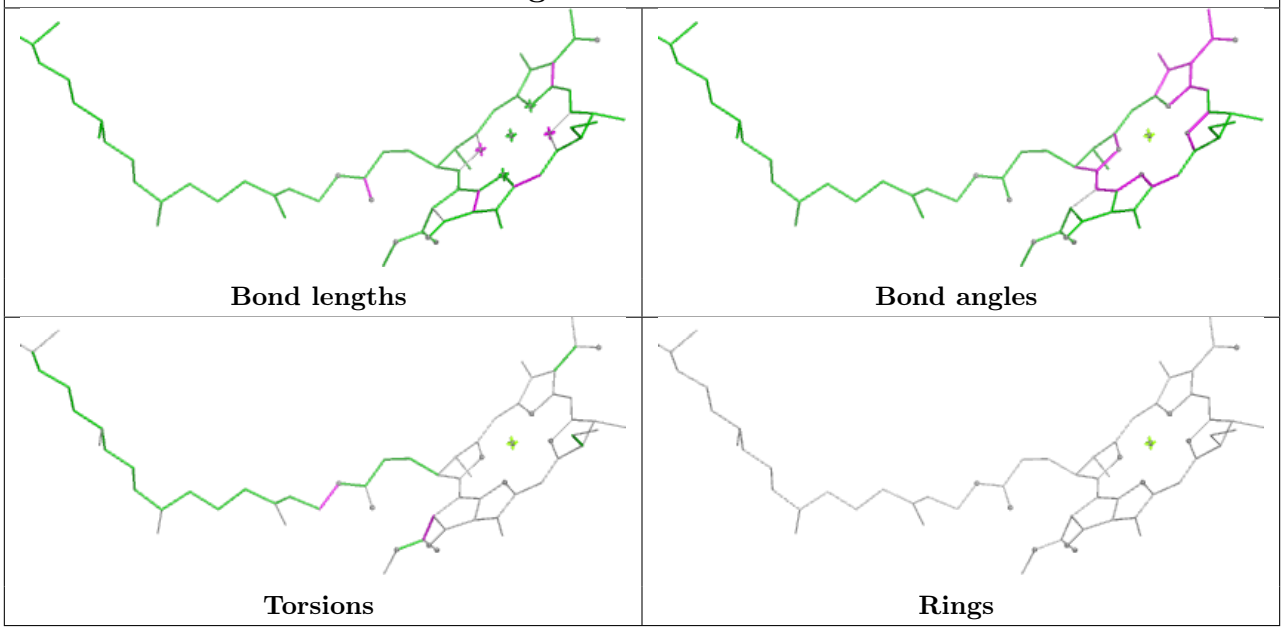

Bond lengths


Bond angles

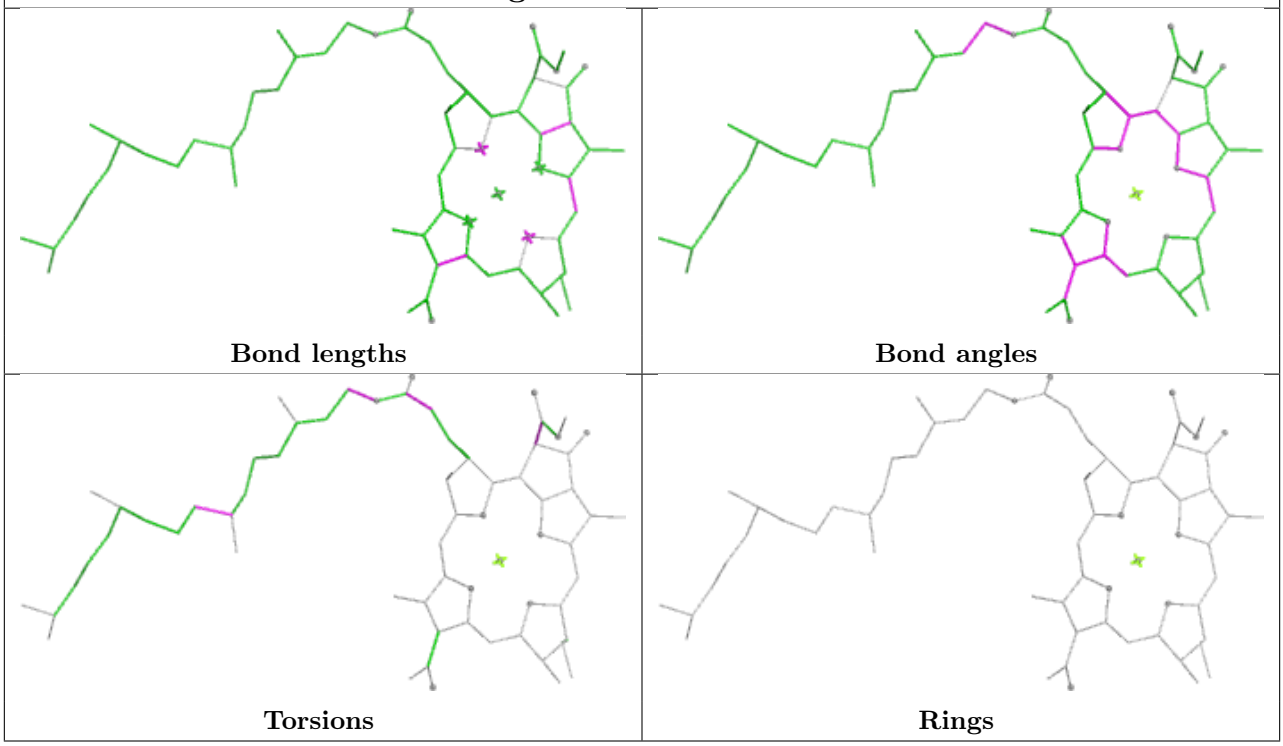

Torsions


Rings

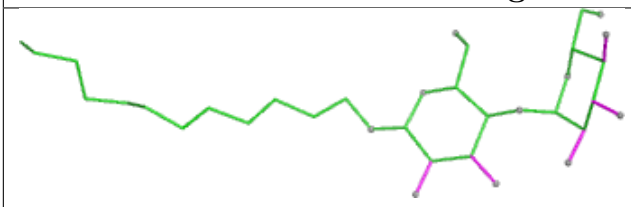
Ligand BCL L 301



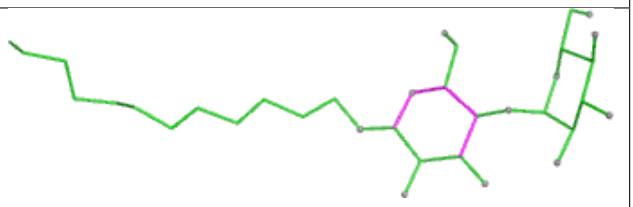
Ligand BCL AM 101



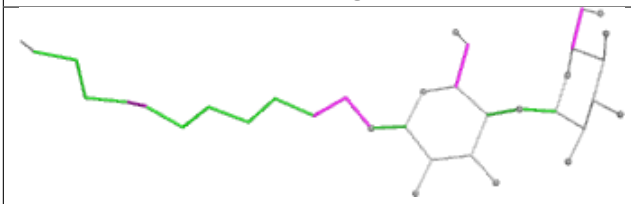
Ligand LMT BR 102



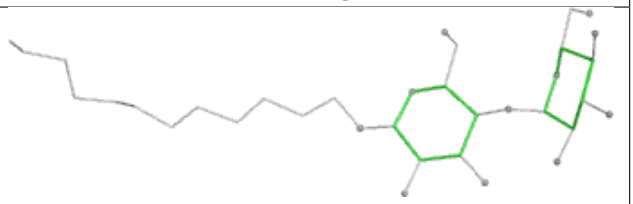
Bond lengths



Bond angles

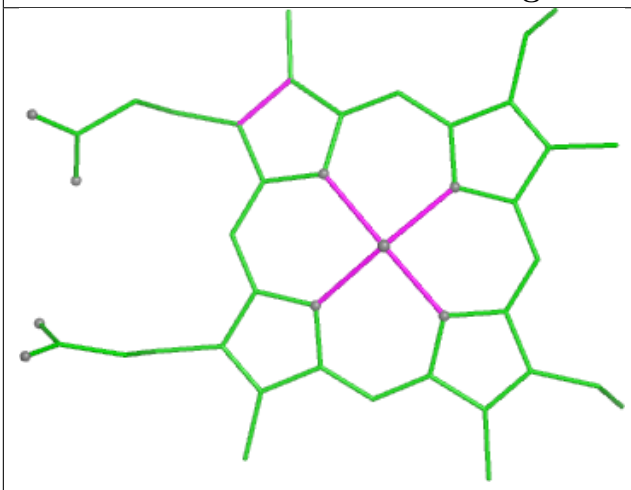


Torsions

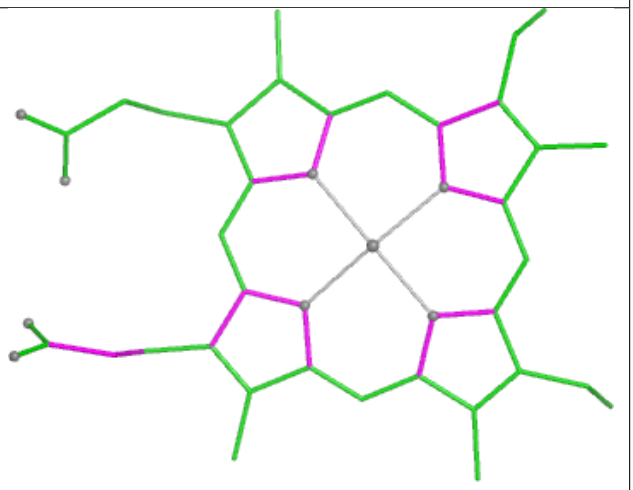


Rings

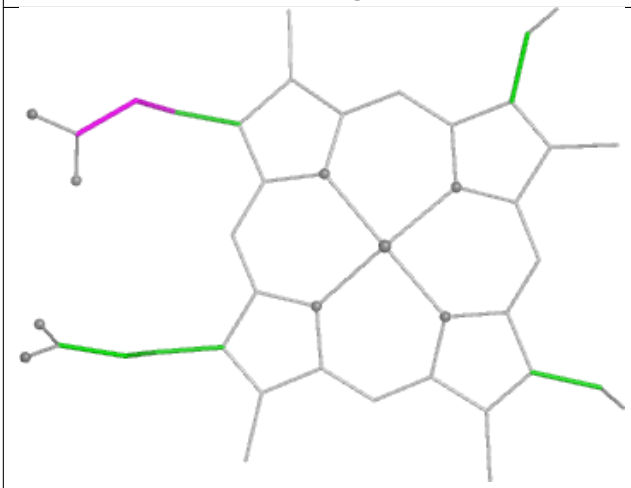
Ligand HEC C 403



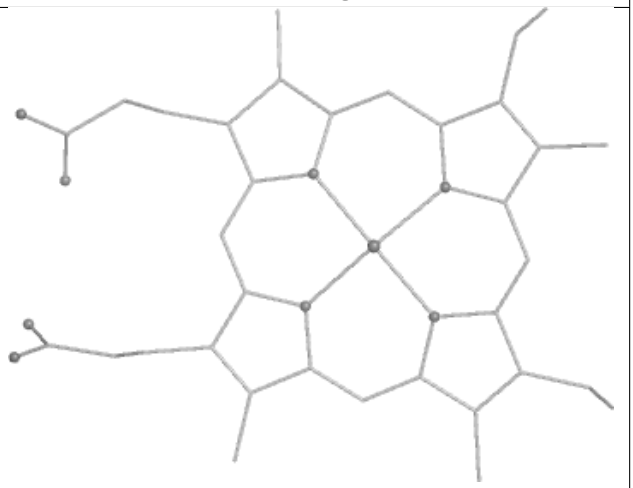
Bond lengths



Bond angles

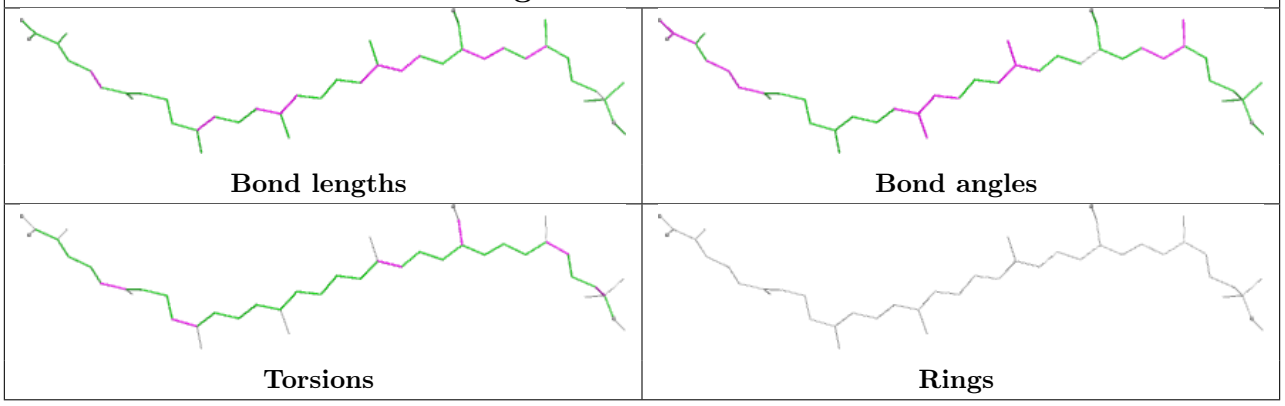


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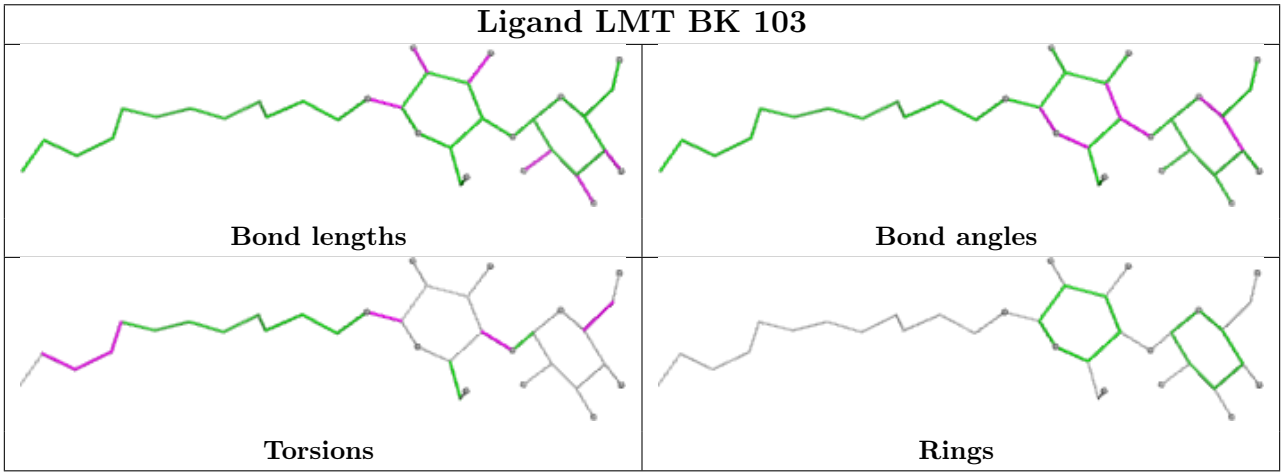


Rings

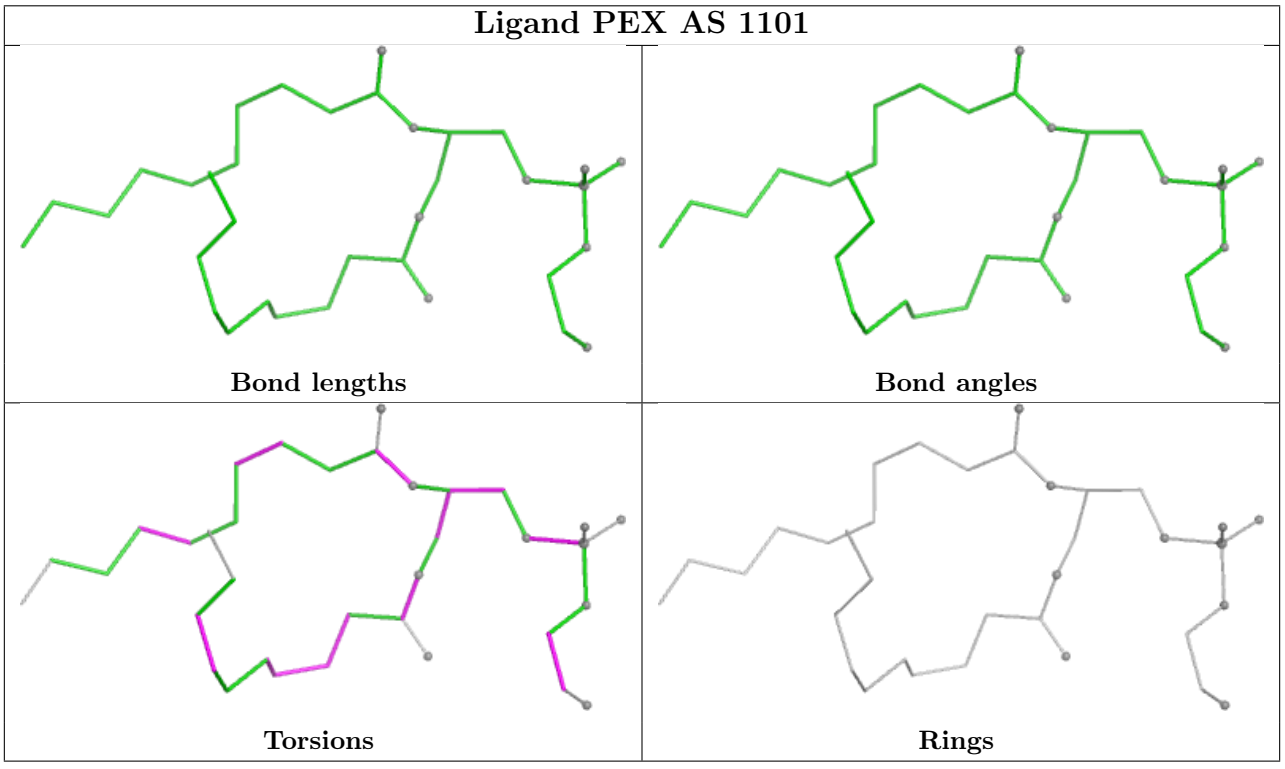
Ligand V7N BP 102



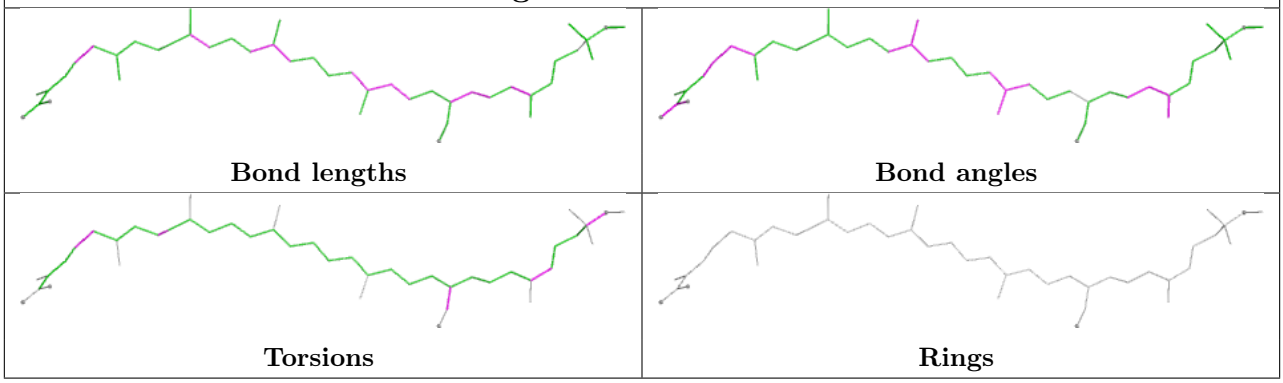
Ligand LMT BK 103



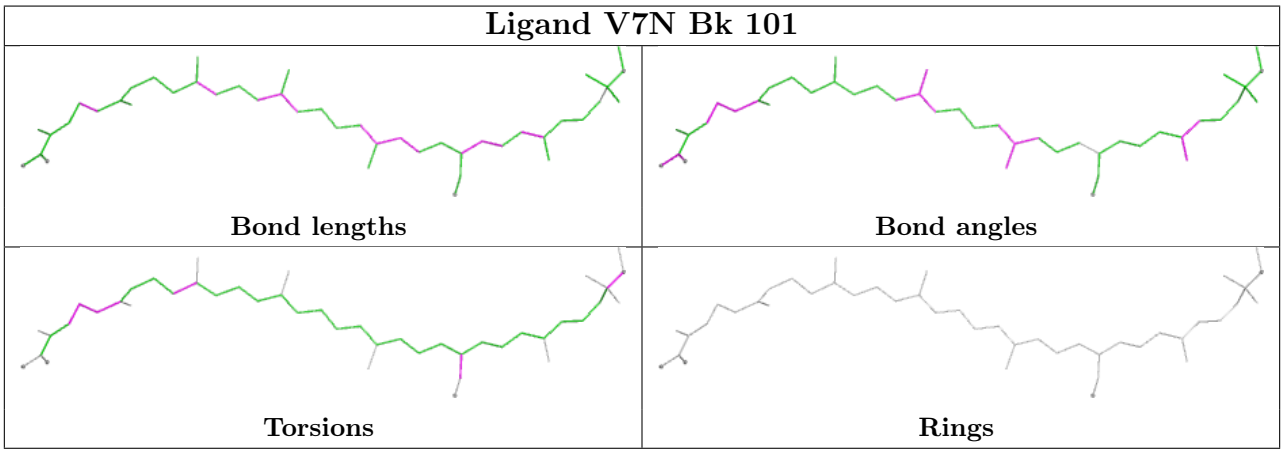
Ligand PEX AS 1101



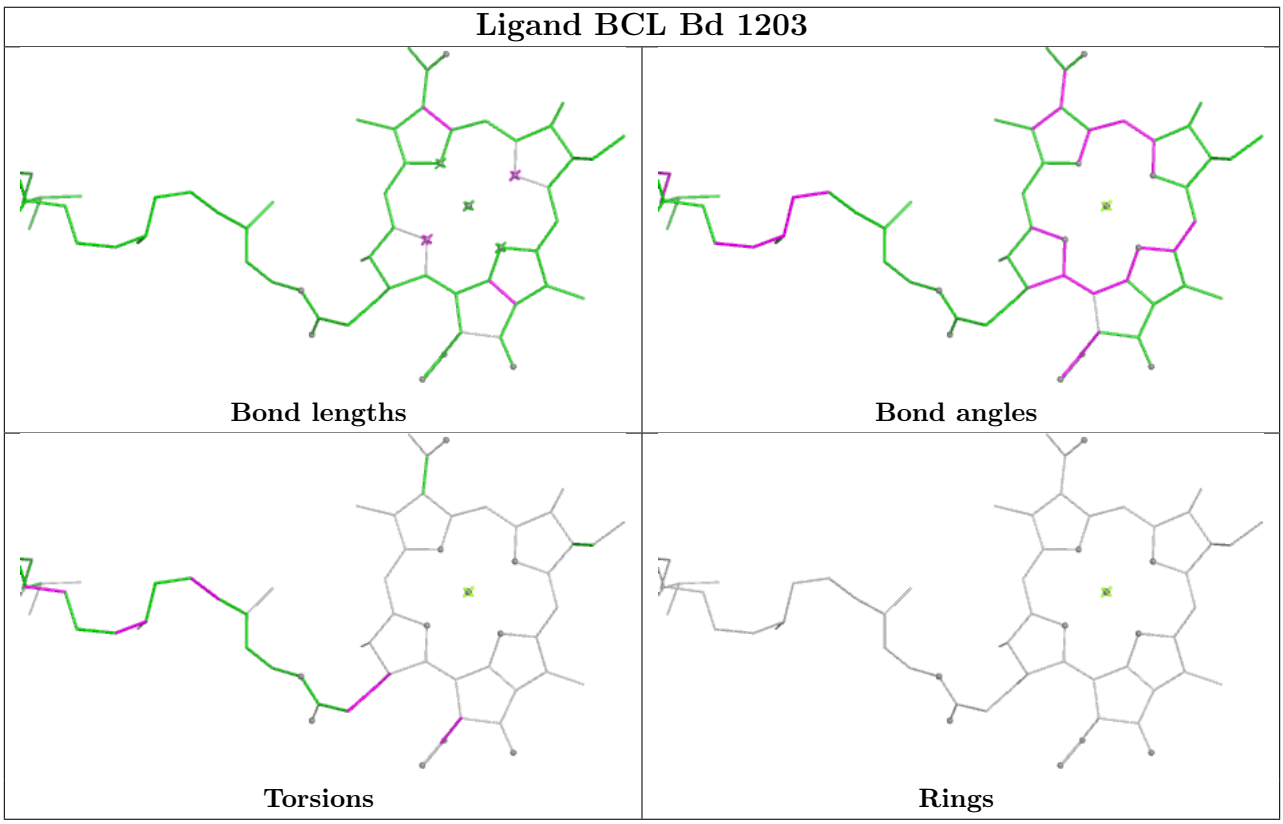
Ligand V7N Bl 1202



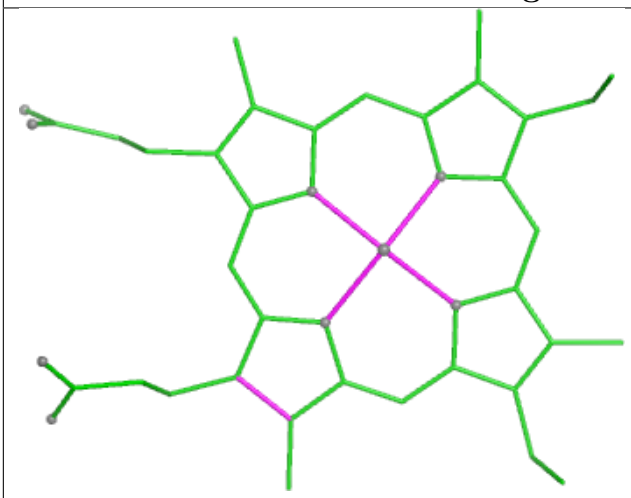
Ligand V7N Bk 101



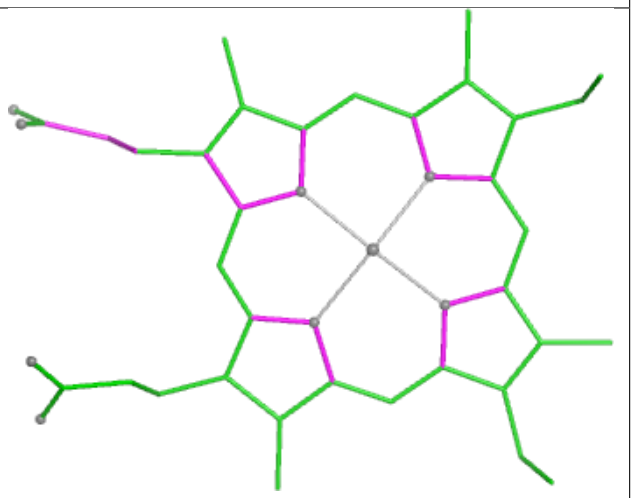
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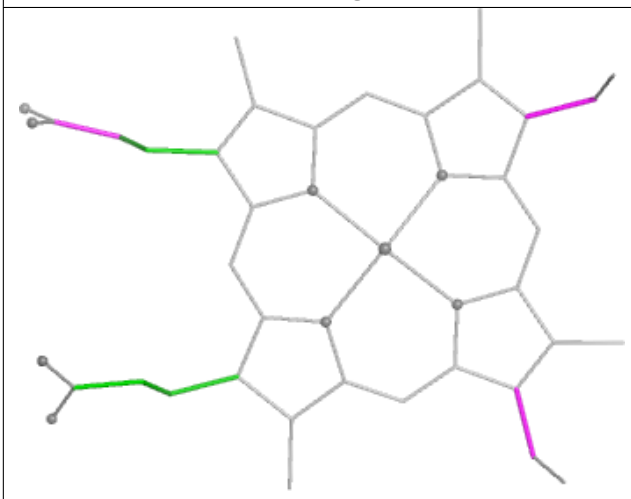
Ligand HEC C 405



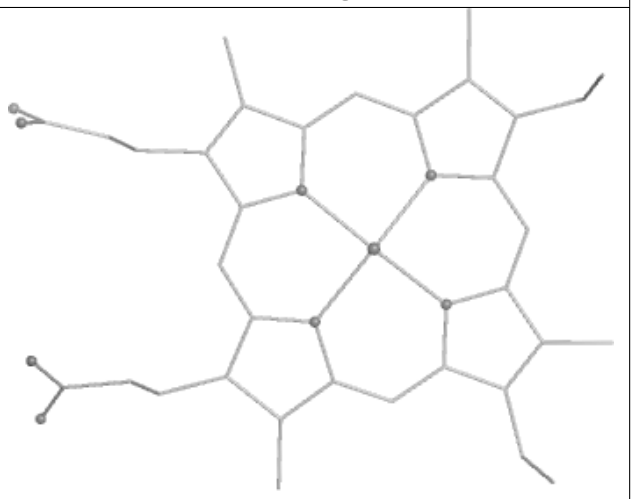
Bond lengths



Bond angles

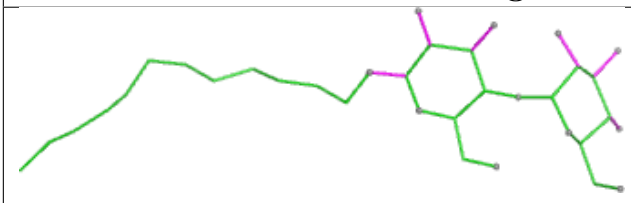


Torsions

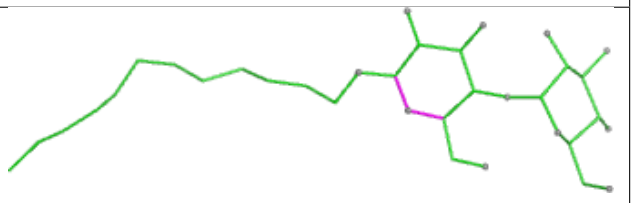


Rings

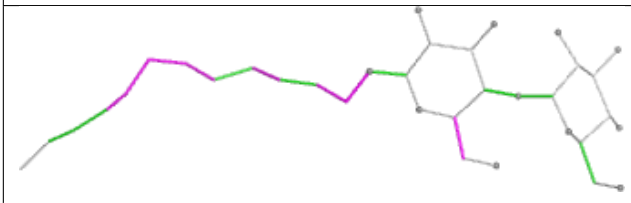
Ligand LMT Bf 1201



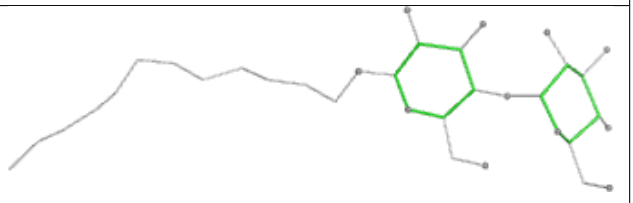
Bond lengths



Bond angles

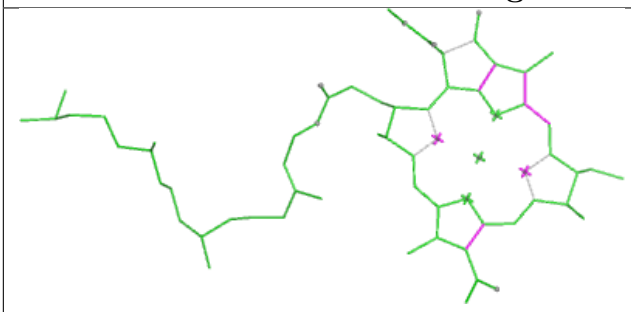


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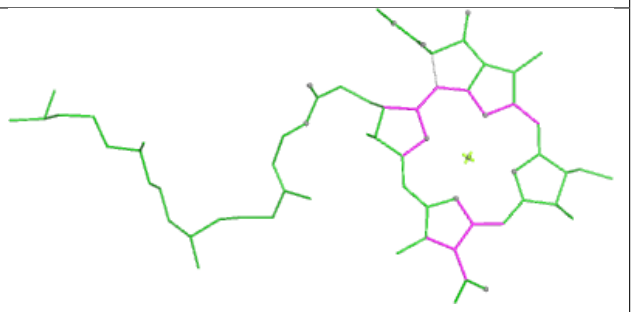


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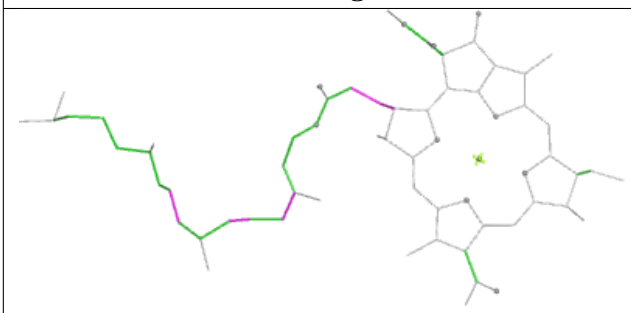
Ligand BCL Bb 1203



Bond lengths



Bond angles

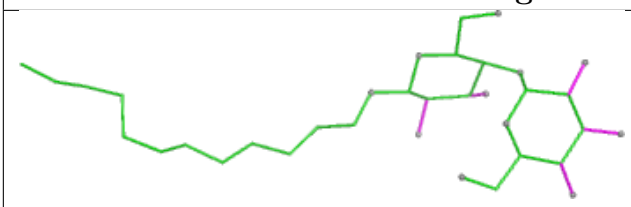


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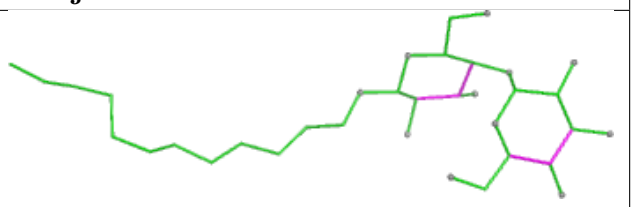


Rings

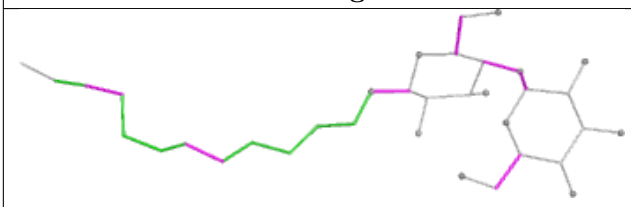
Ligand LMT Aj 102



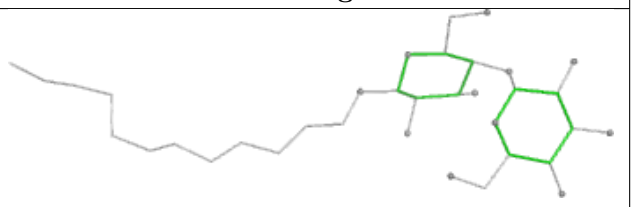
Bond lengths



Bond angles

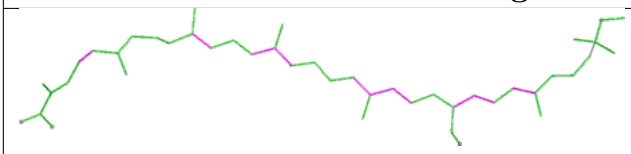


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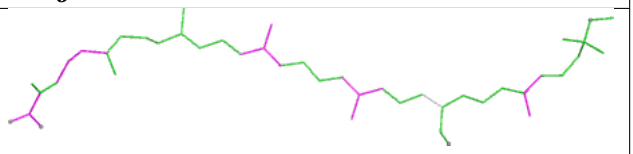


Rings

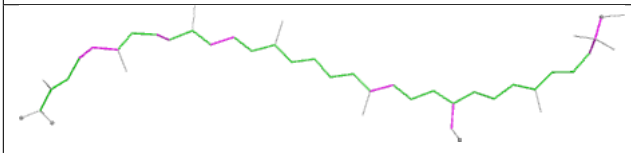
Ligand V7N Bj 1202



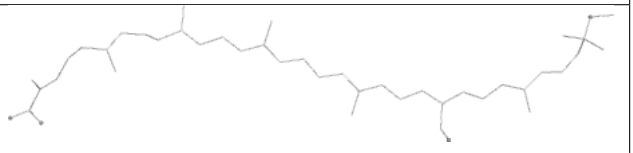
Bond lengths



Bond angles

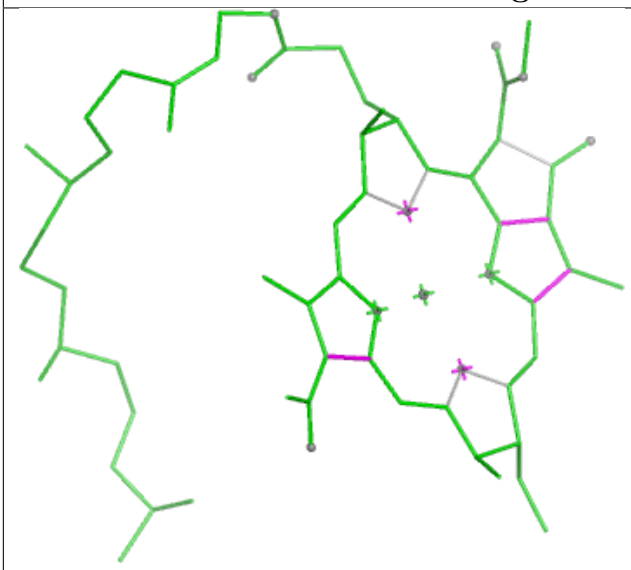


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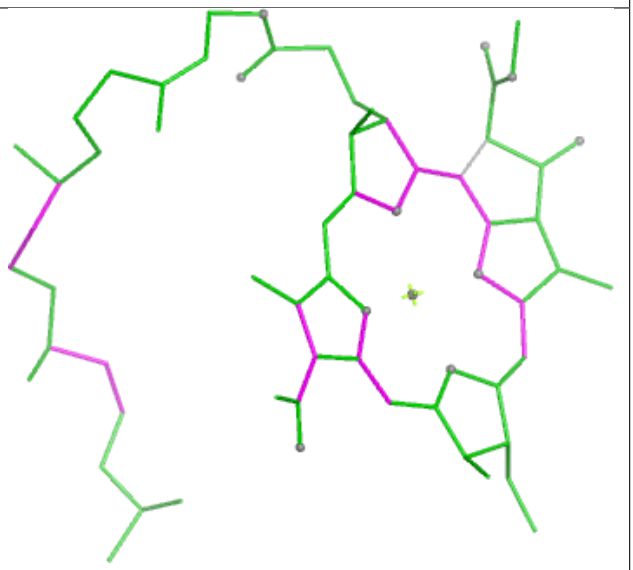


Rings

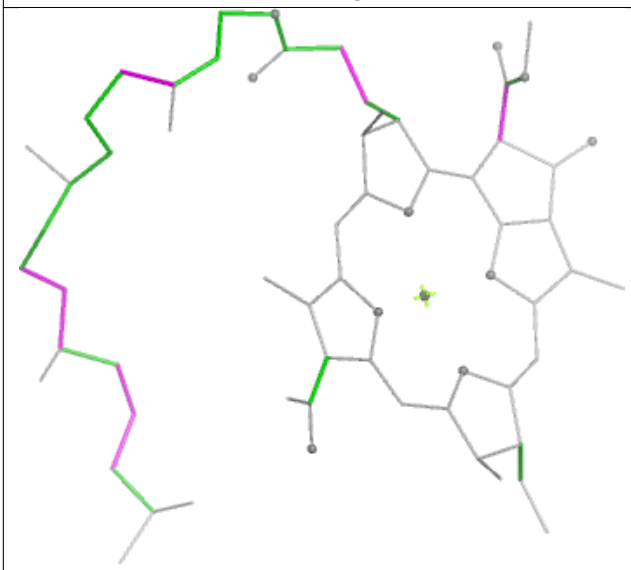
Ligand BCL BO 103



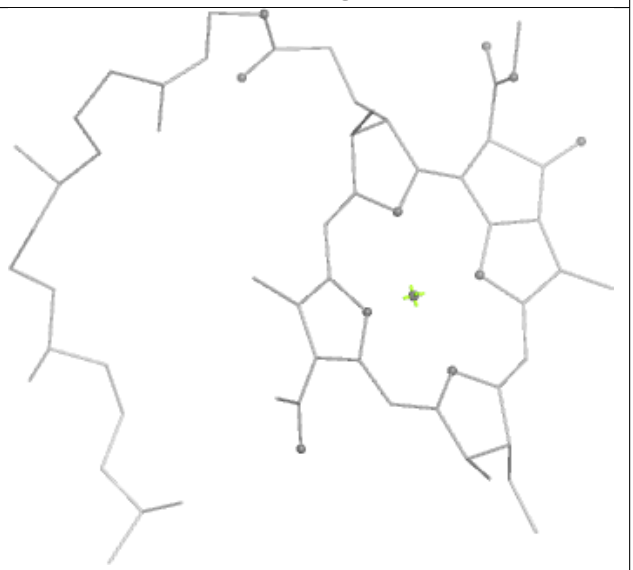
Bond lengths



Bond angles

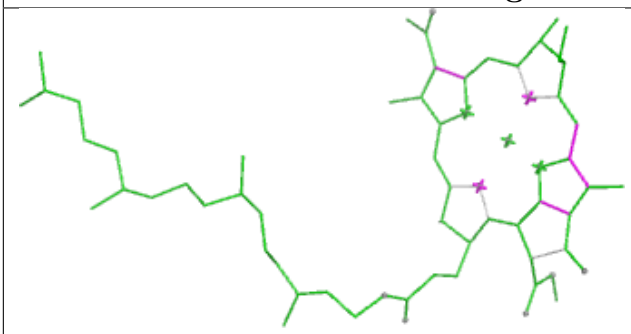


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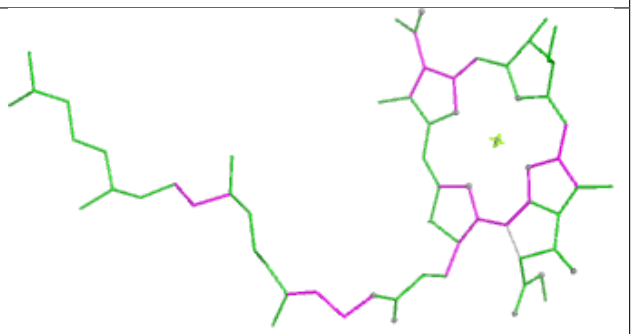


Rings

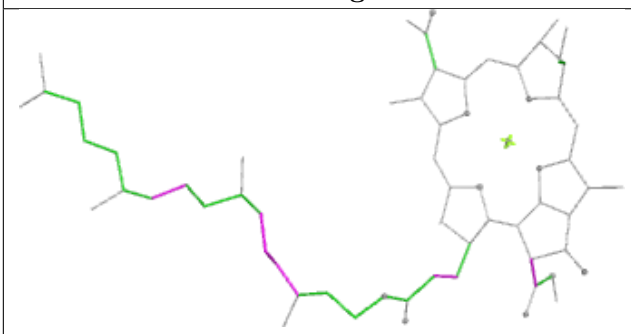
Ligand BCL AS 1102



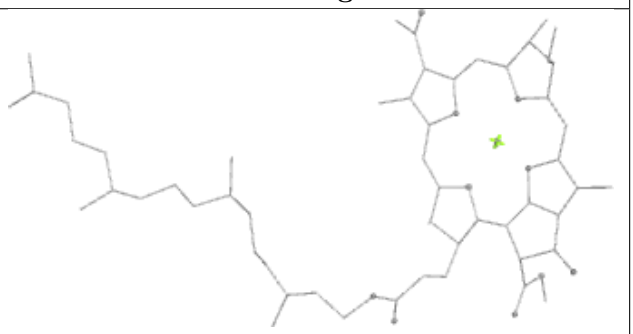
Bond lengths



Bond angles

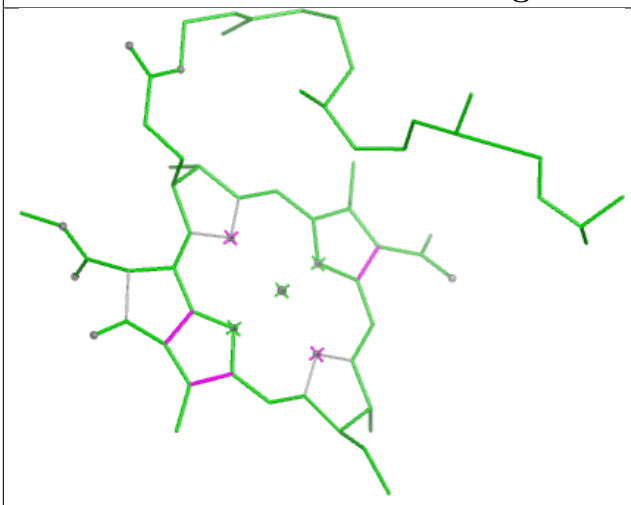


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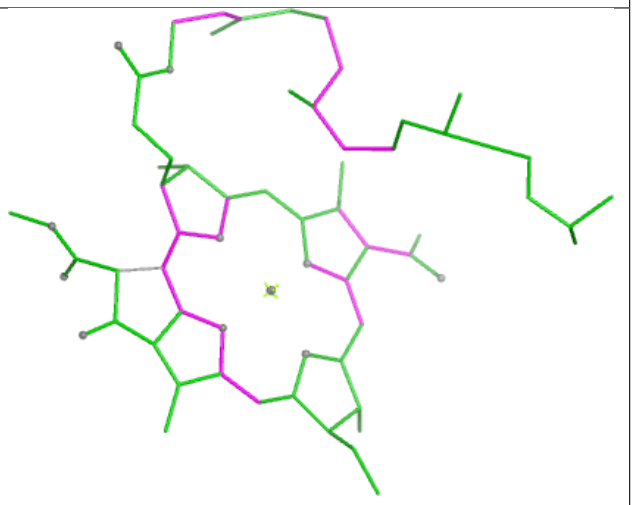


Rings

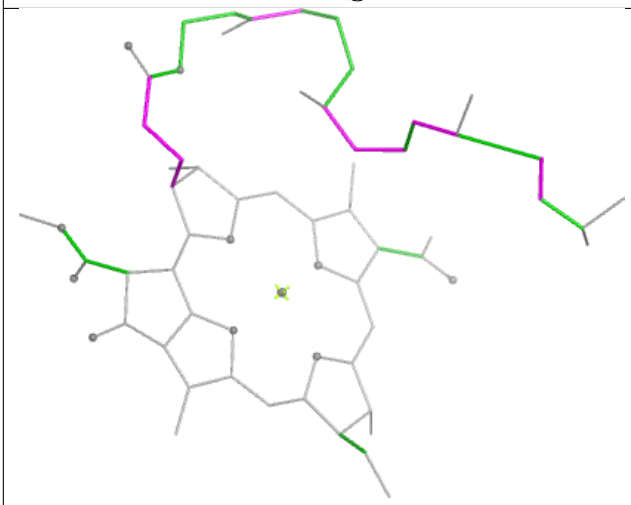
Ligand BCL BC 101



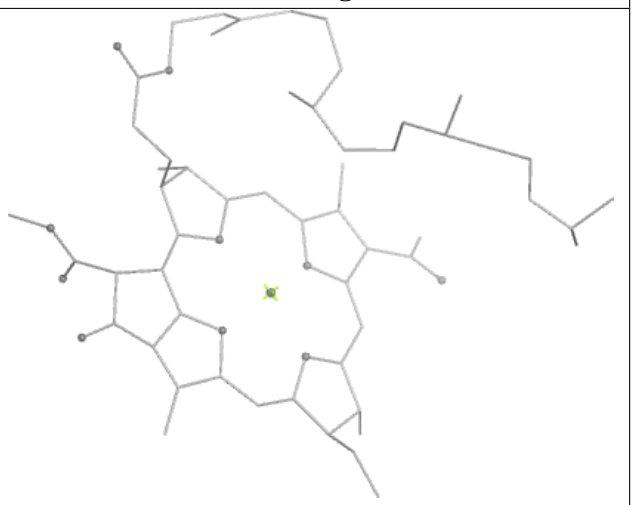
Bond lengths



Bond angles

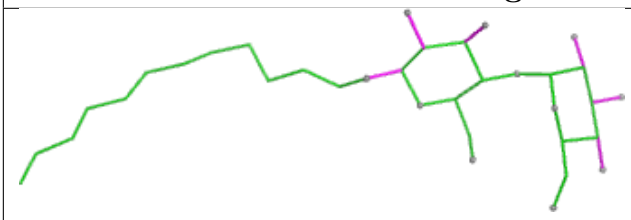


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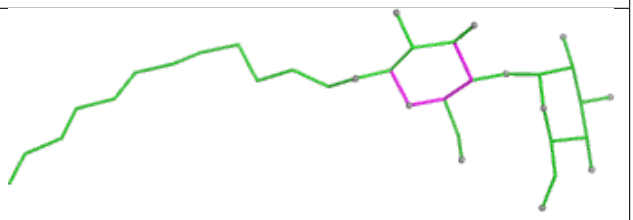


Rings

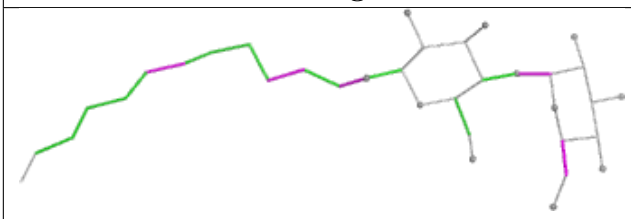
Ligand LMT Bc 1201



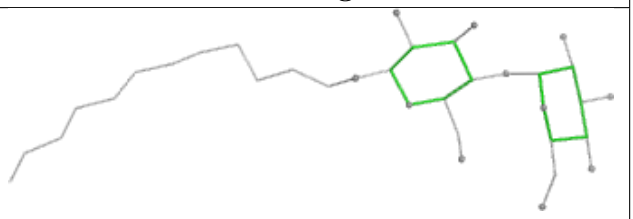
Bond lengths



Bond angles

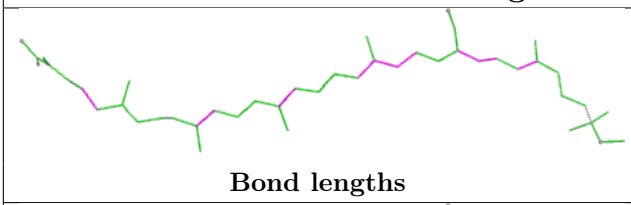


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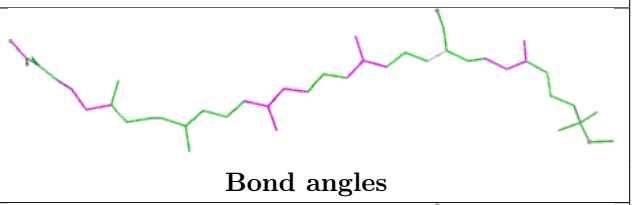


Rings

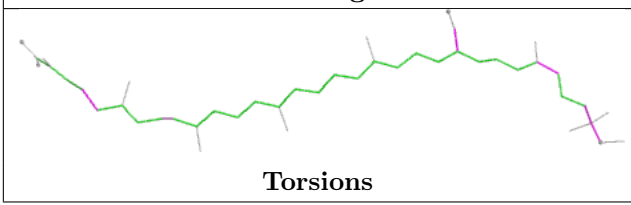
Ligand V7N Be 1103



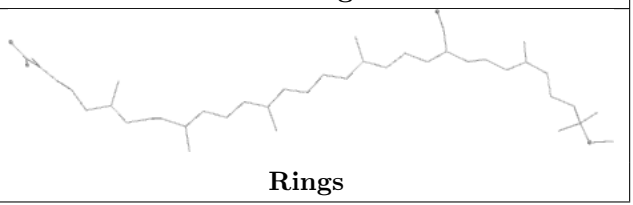
Bond lengths



Bond angles

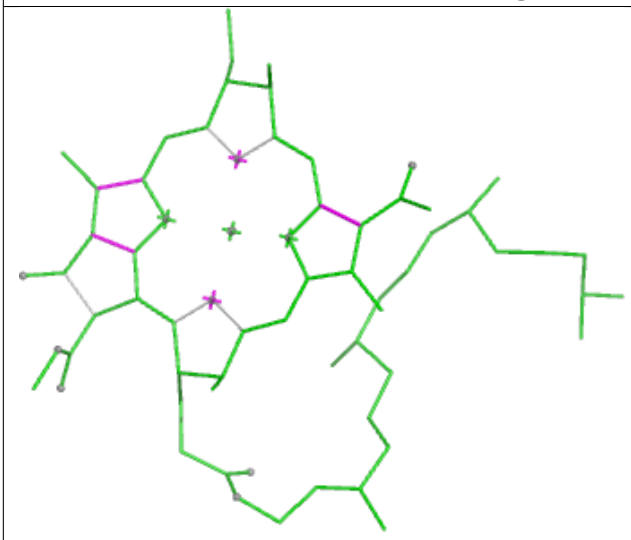


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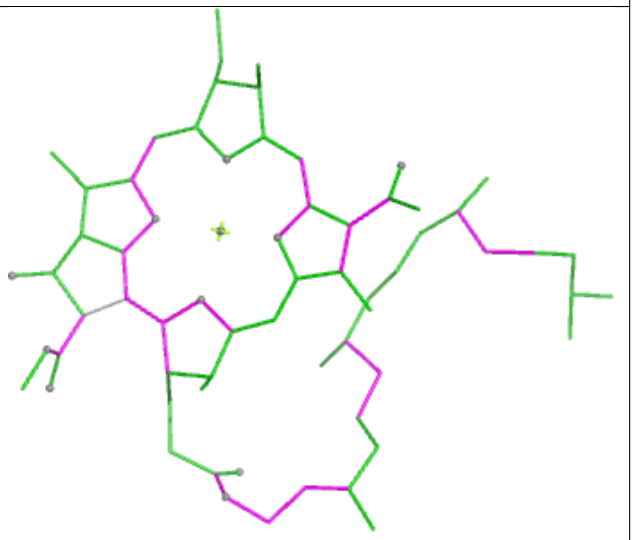


Rings

Ligand BCL BB 101



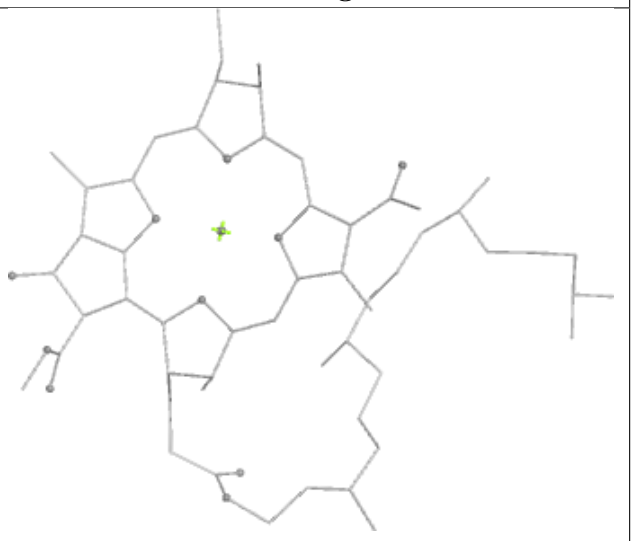
Bond lengths



Bond angles

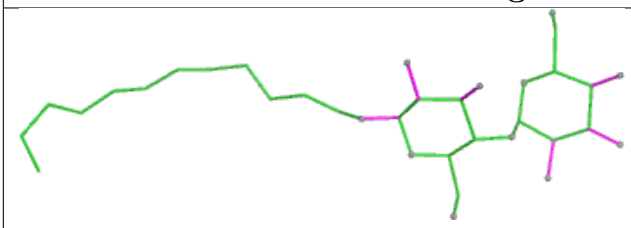


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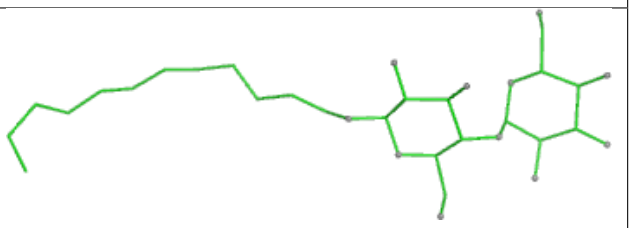


Rings

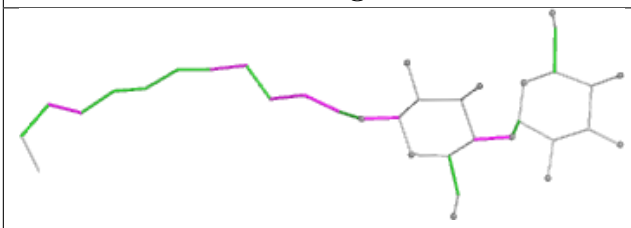
Ligand LMT BO 104



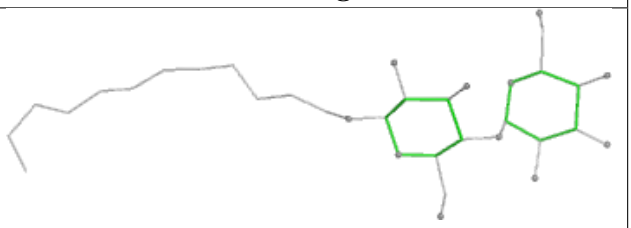
Bond lengths



Bond angles

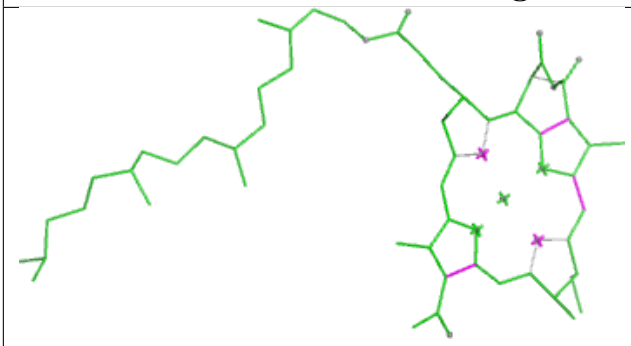


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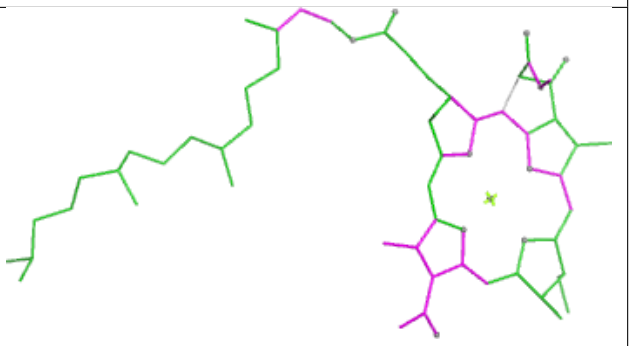


Rings

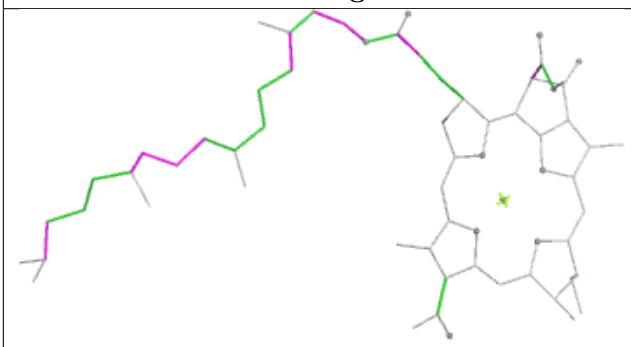
Ligand BCL AO 101



Bond lengths



Bond angles

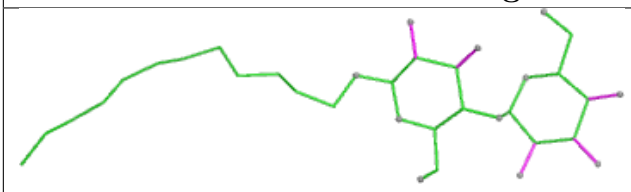


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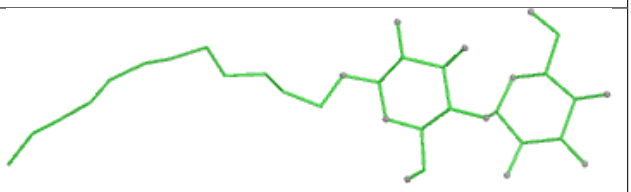


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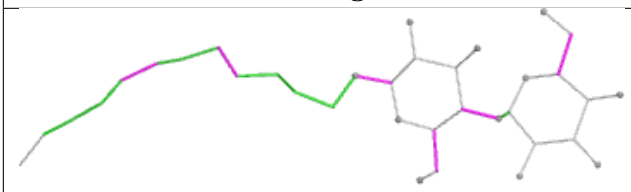
Ligand LMT Bd 1201



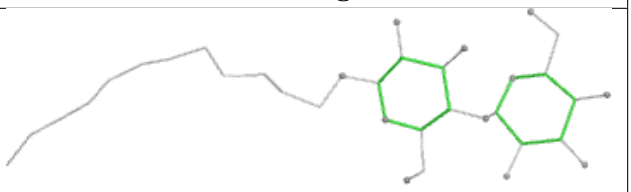
Bond lengths



Bond angles

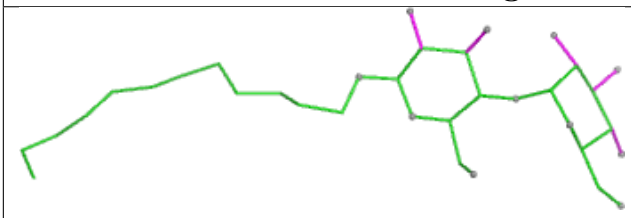


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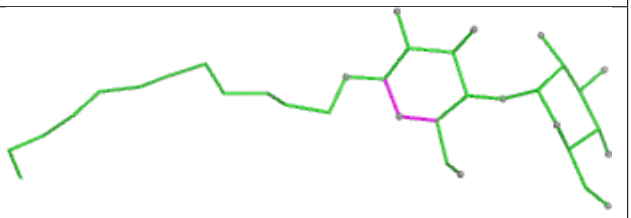


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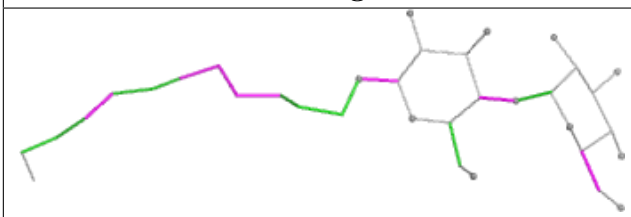
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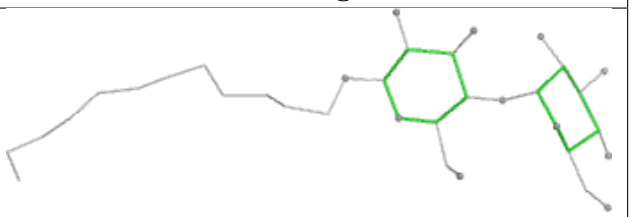
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Bond angles

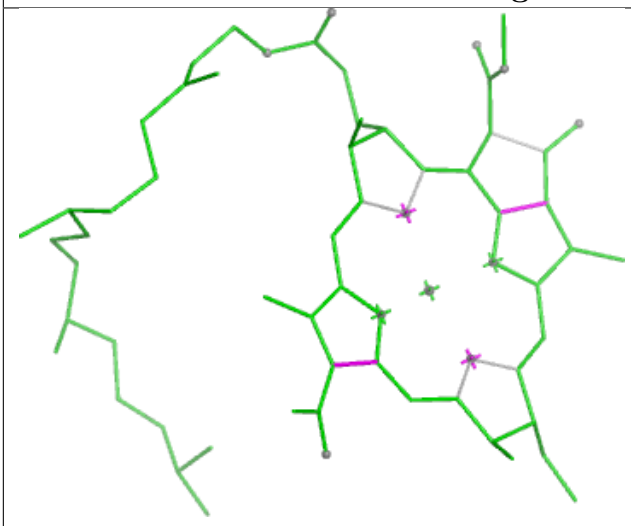


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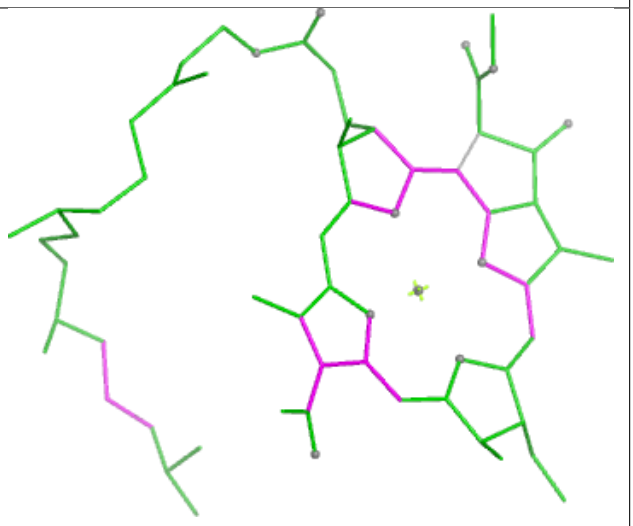


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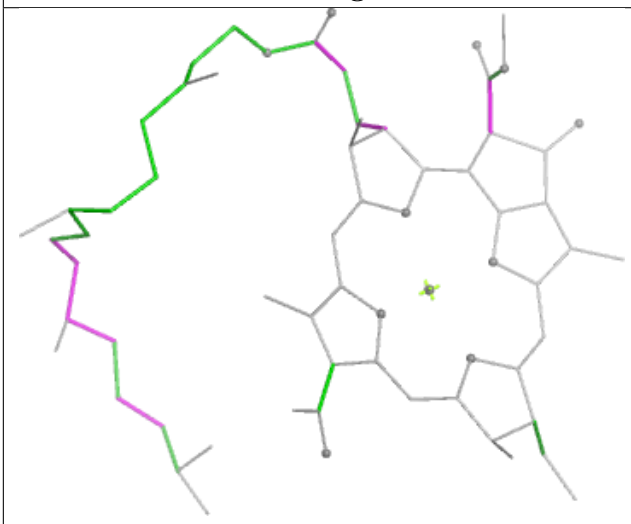
Ligand BCL BU 102



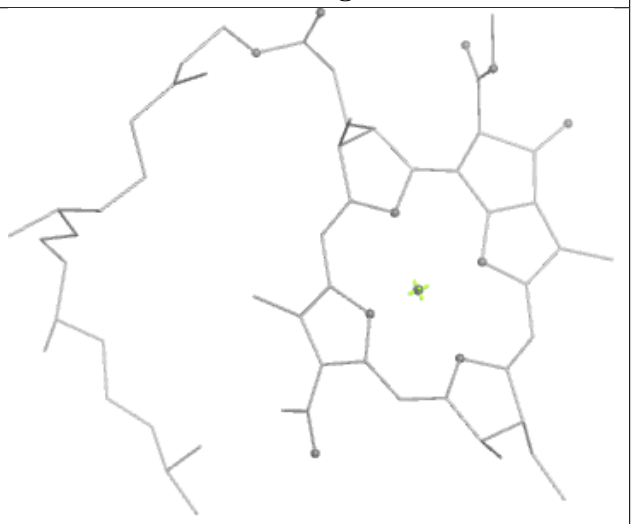
Bond lengths



Bond angles

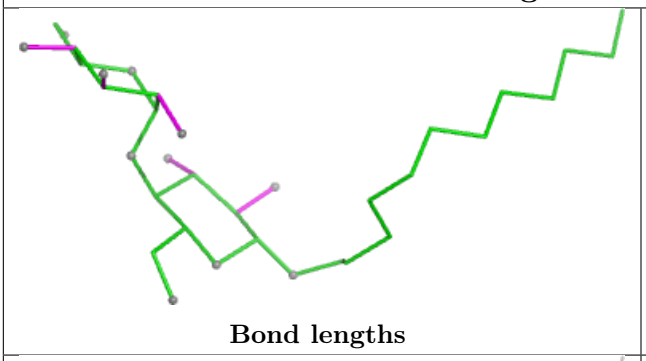


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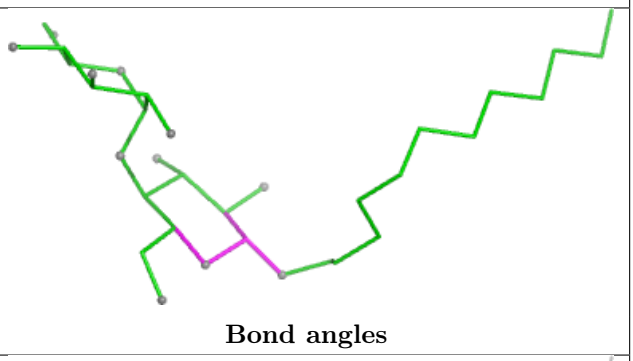


Rings

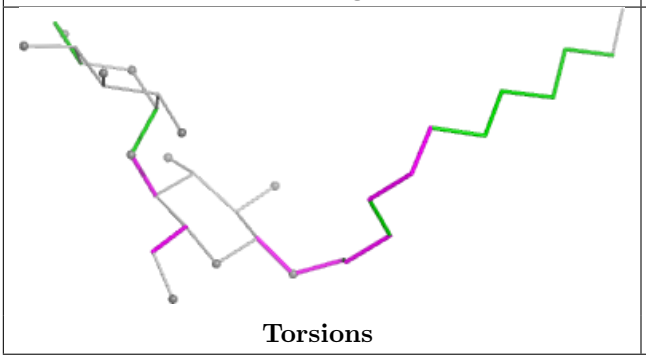
Ligand LMT K 201



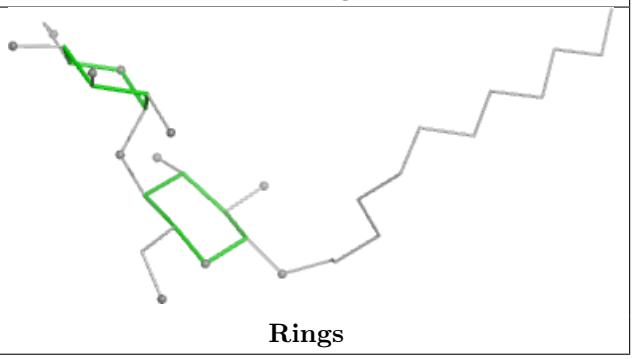
Bond lengths



Bond angles

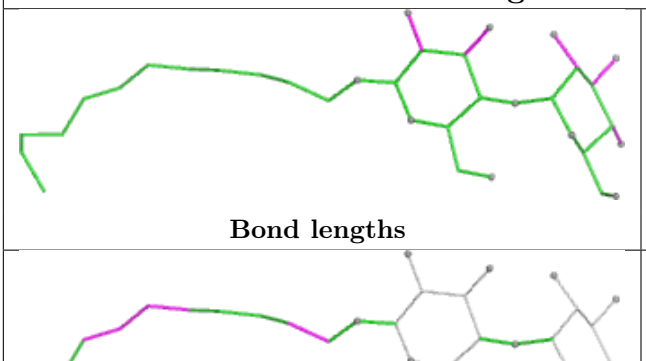


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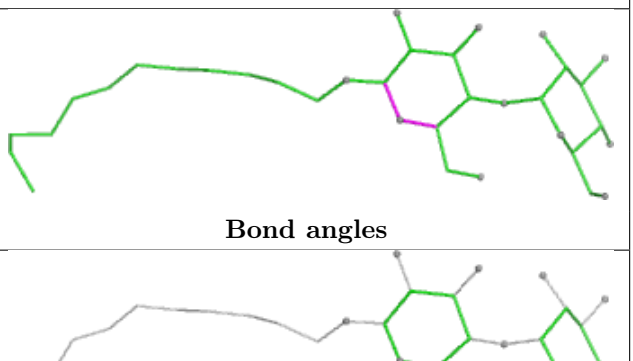


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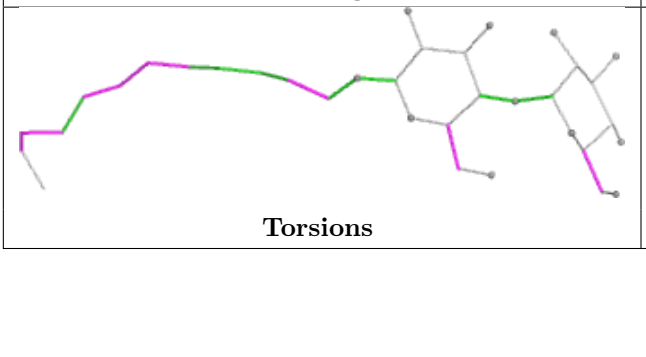
Ligand LMT BH 103



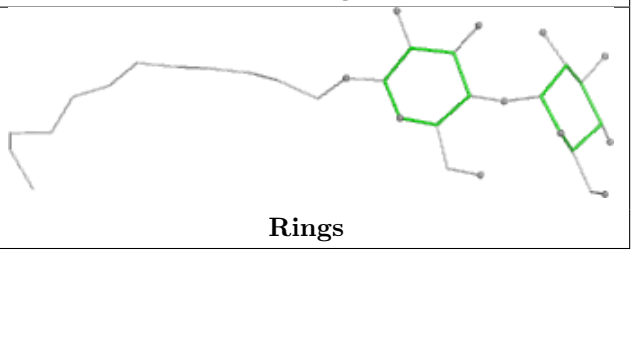
Bond lengths



Bond angles

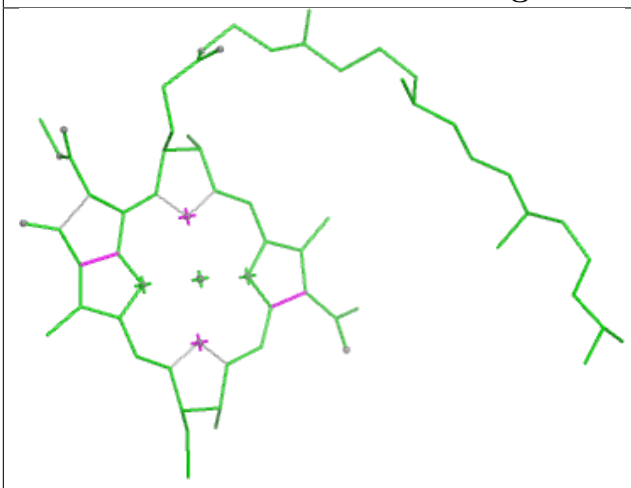


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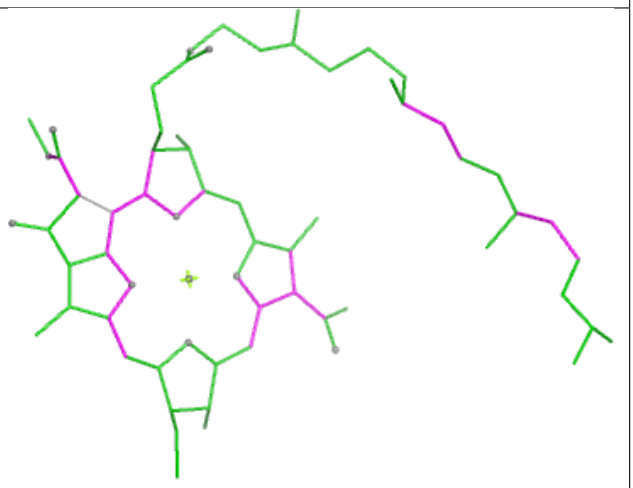


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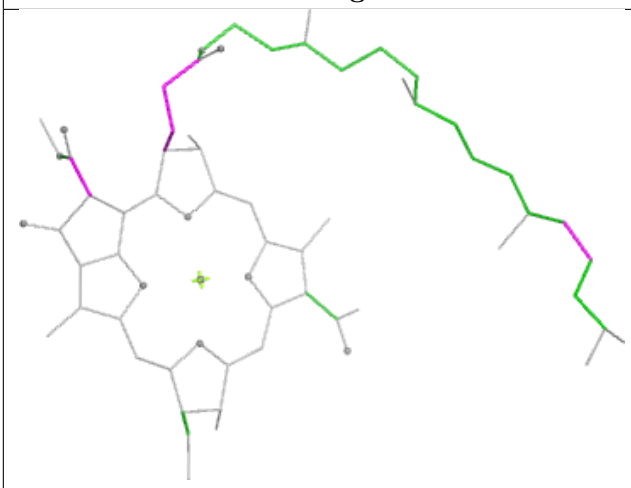
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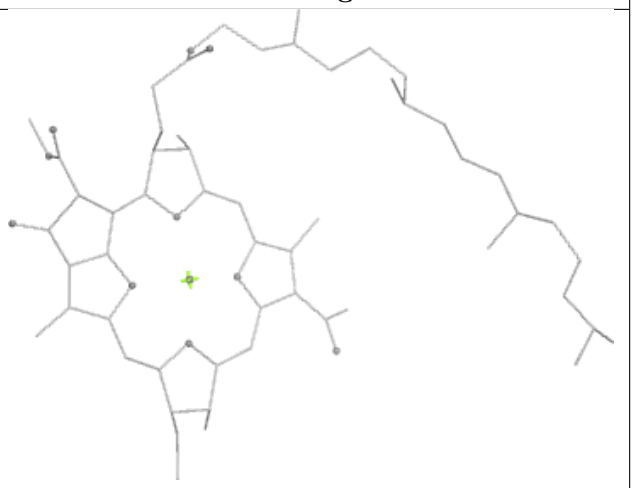
Bond lengths



Bond angles

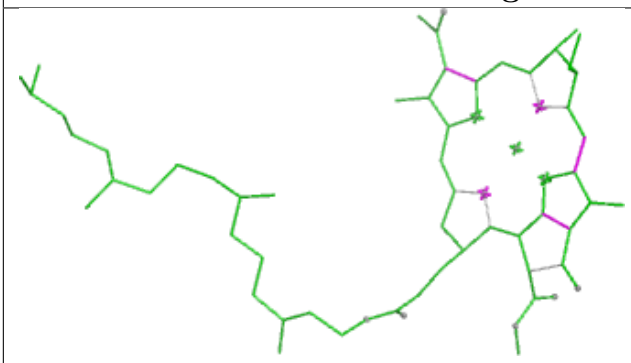


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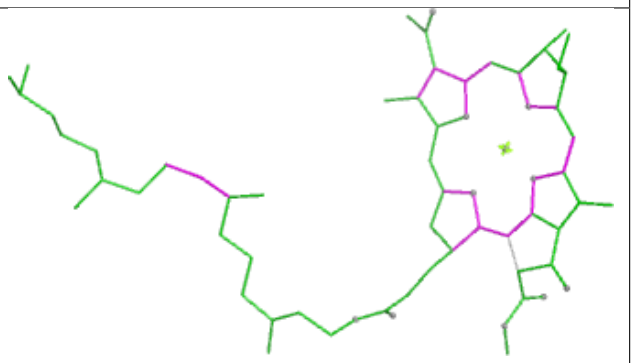


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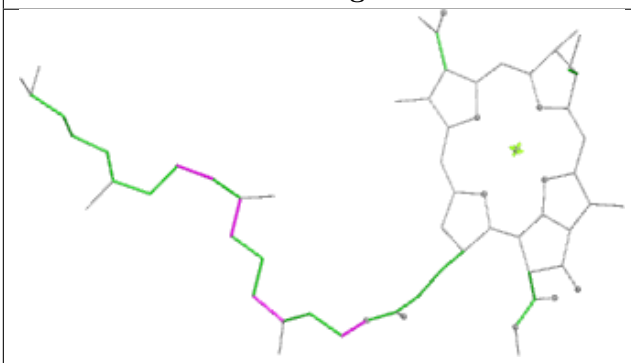
Ligand BCL AX 1202



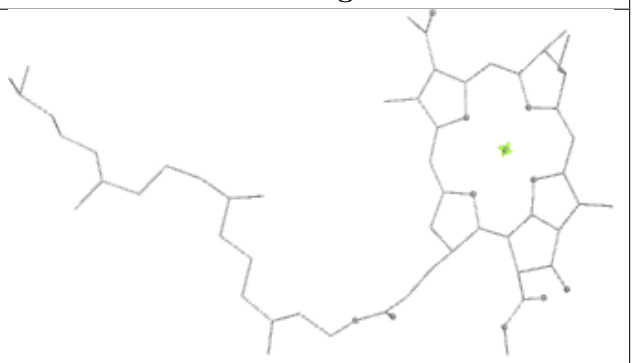
Bond lengths



Bond angles



Torsions



Rings

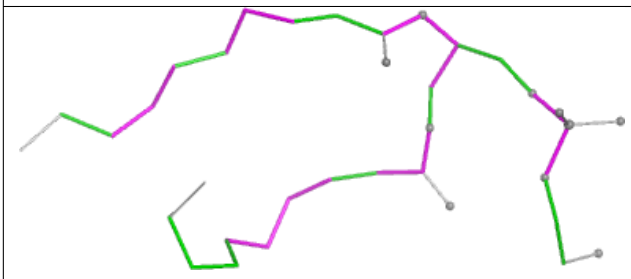
Ligand PEX AJ 1101



Bond lengths



Bond angles

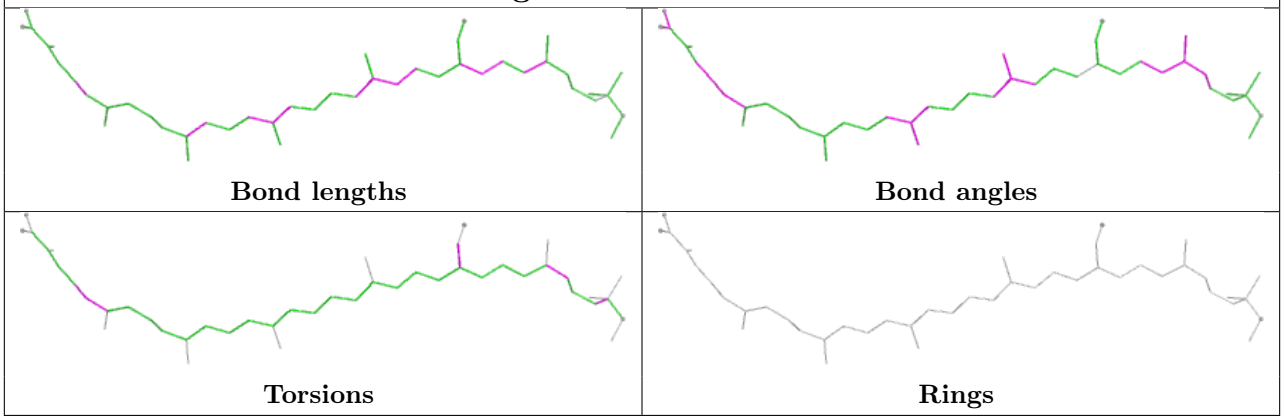


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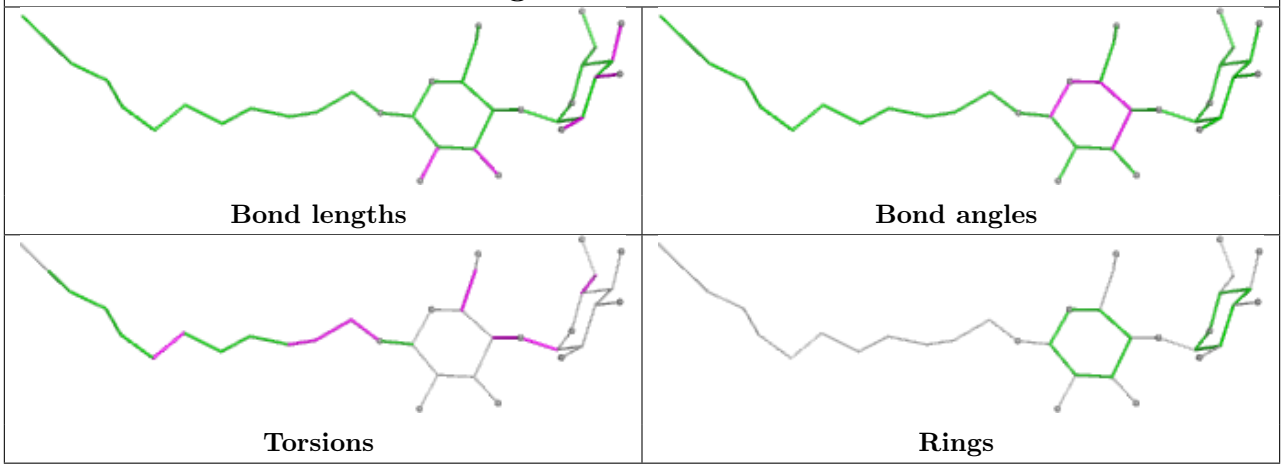


Rings

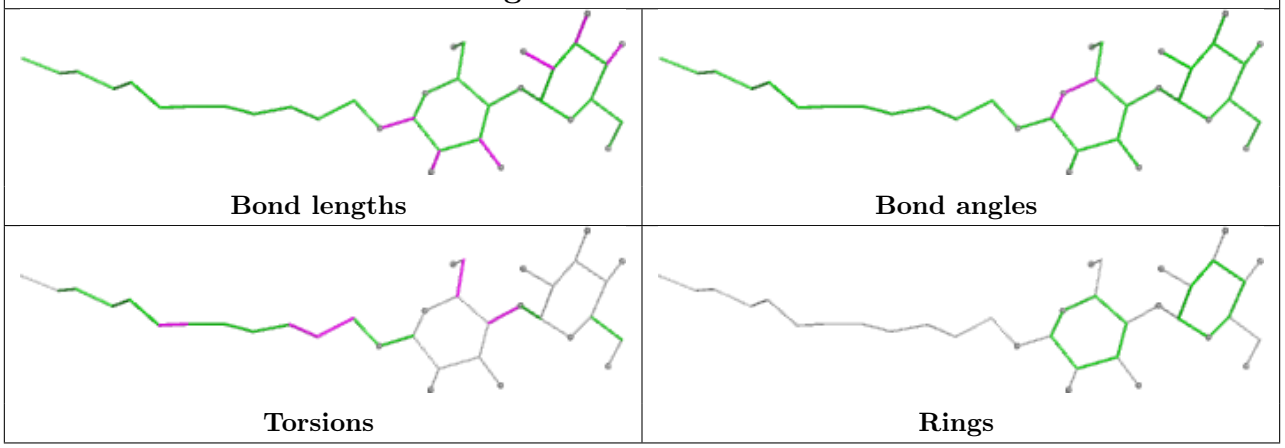
Ligand V7N BR 103



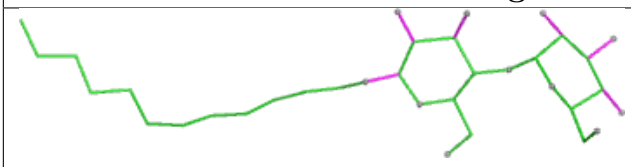
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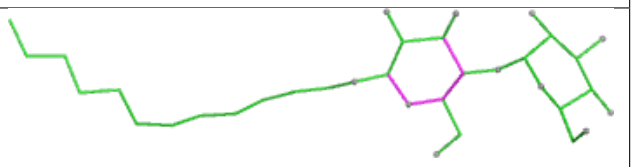


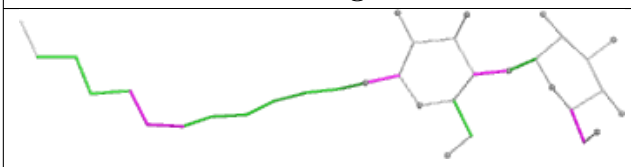
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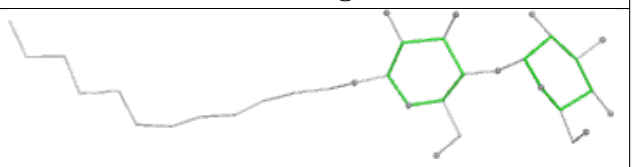


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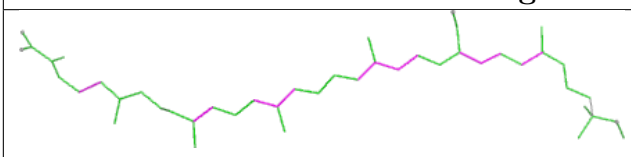

Bond lengths

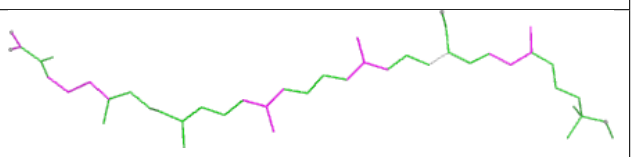

Bond angles

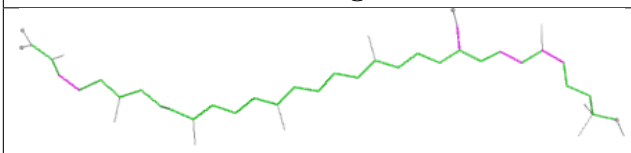

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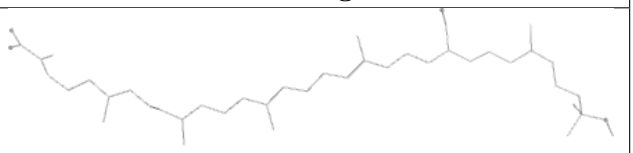

Rings

Ligand V7N BI 101

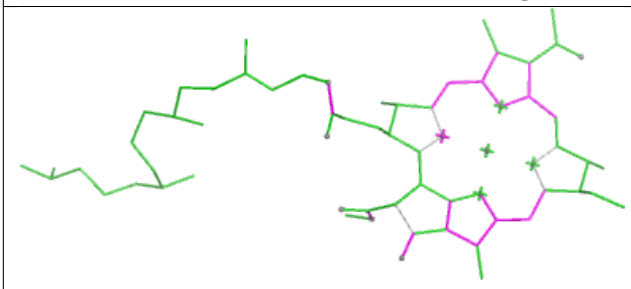

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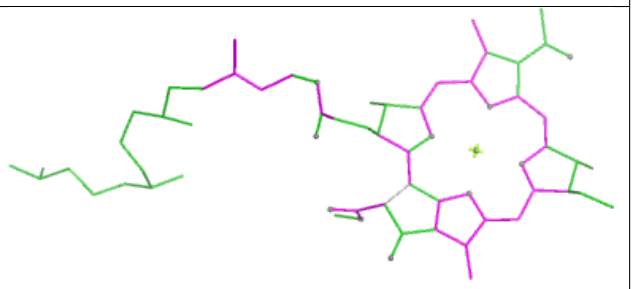

Bond angles

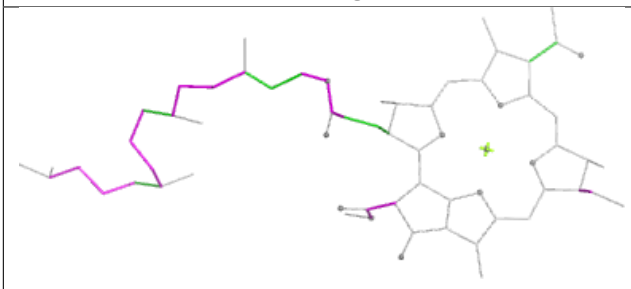

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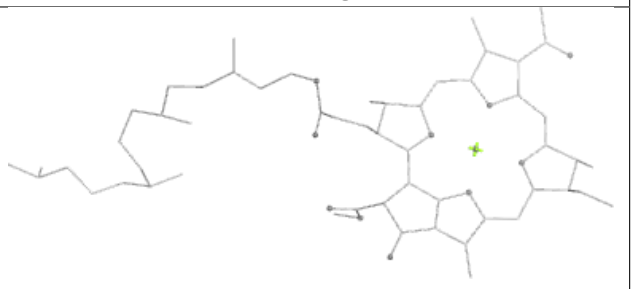

Rings

Ligand BCL Ao 101

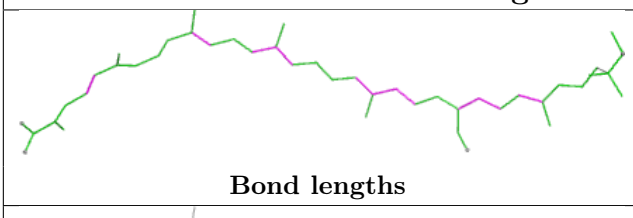

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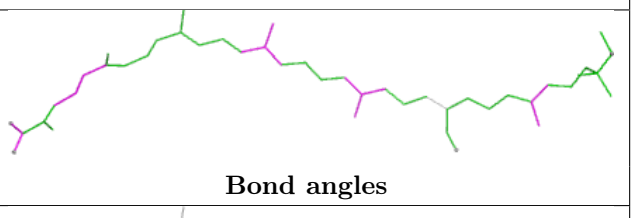

Bond angles

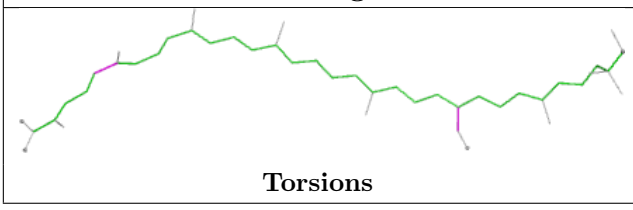

Torsions


Rings

Ligand V7N BU 104

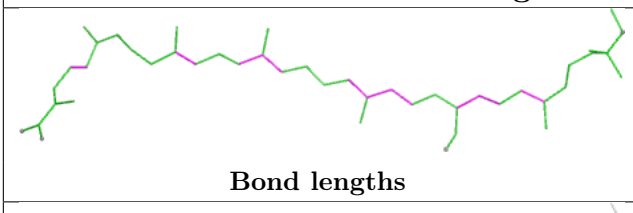

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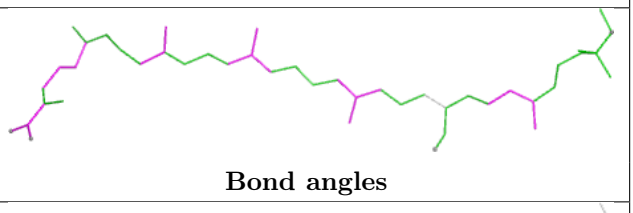

Bond angles

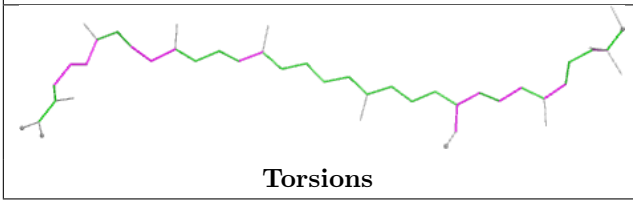

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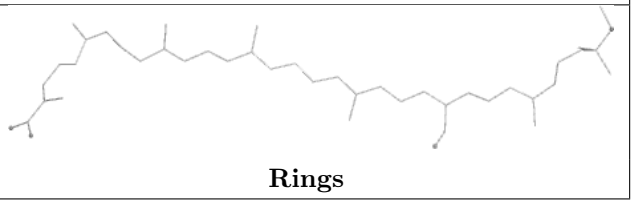

Rings

Ligand V7N AF 101

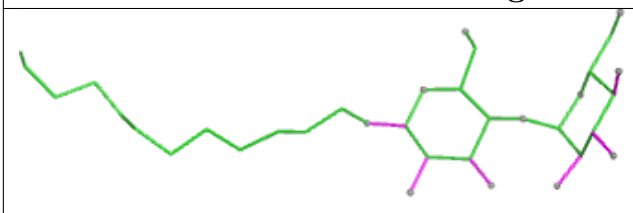

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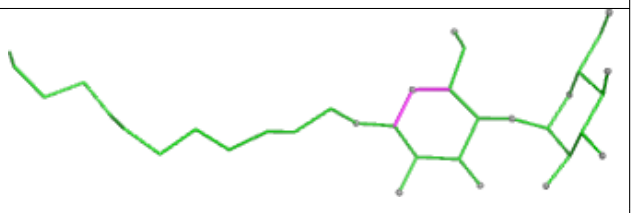

Bond angles

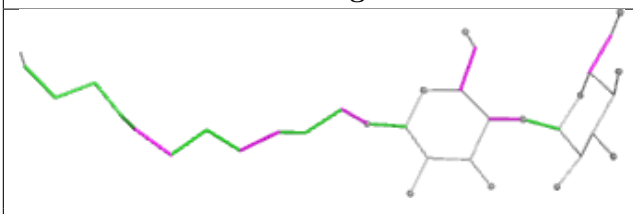

Torsions

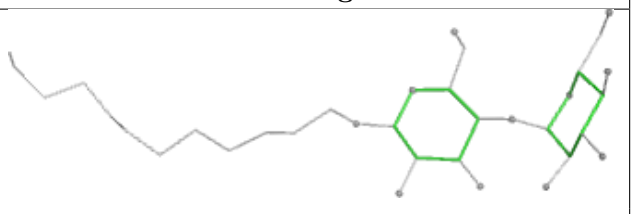

Rings

Ligand LMT Bl 1201


Bond lengths


Bond angles


Torsions


Rings

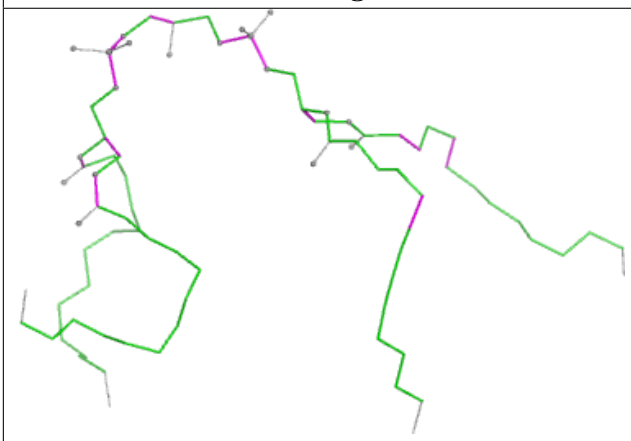
Ligand CD4 Af 102



Bond lengths



Bond angles

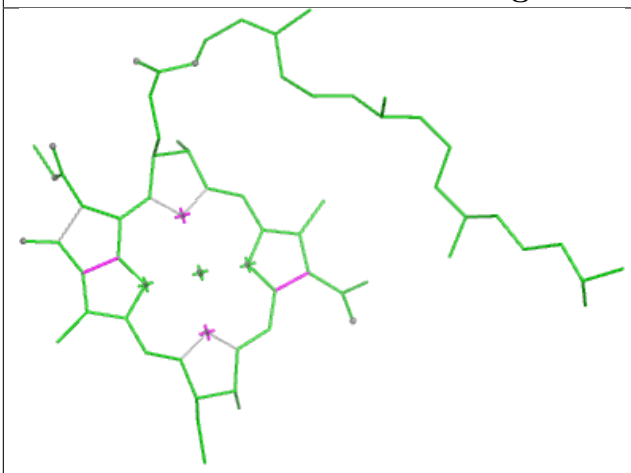


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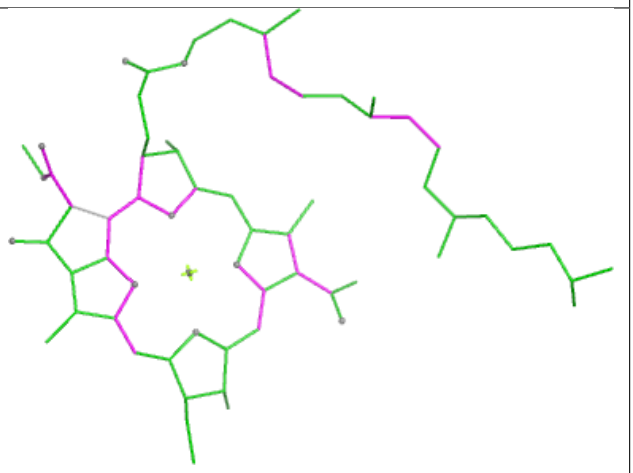


Rings

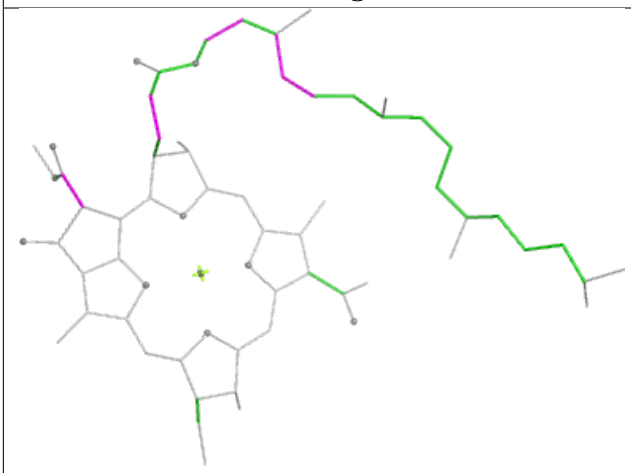
Ligand BCL BD 101



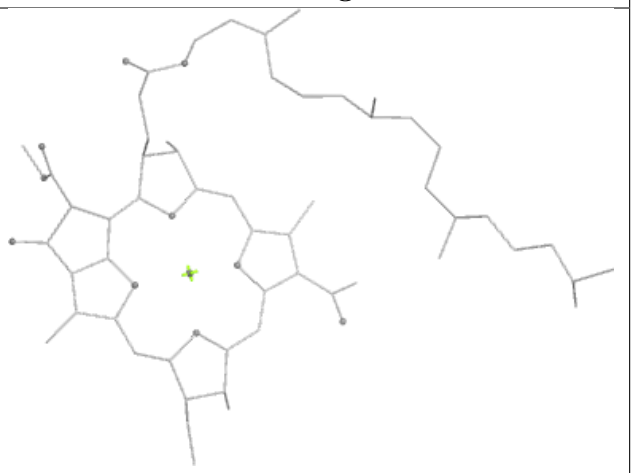
Bond lengths



Bond angles

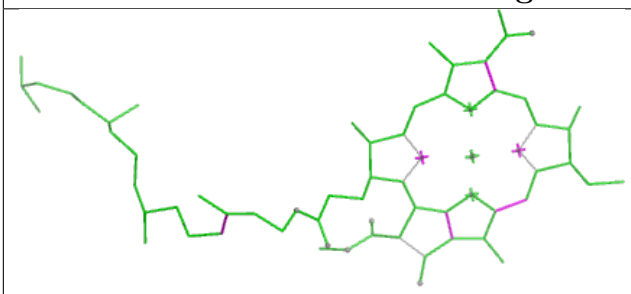


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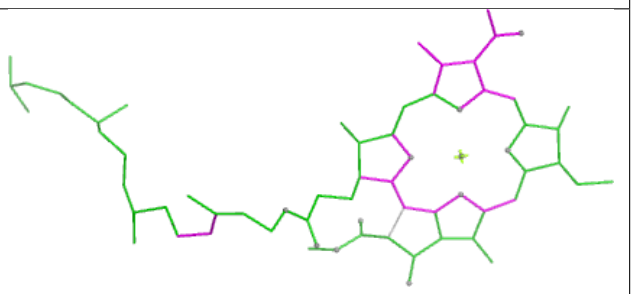


Rings

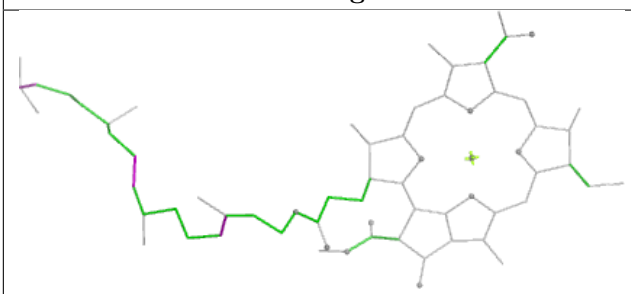
Ligand BCL Aa 102



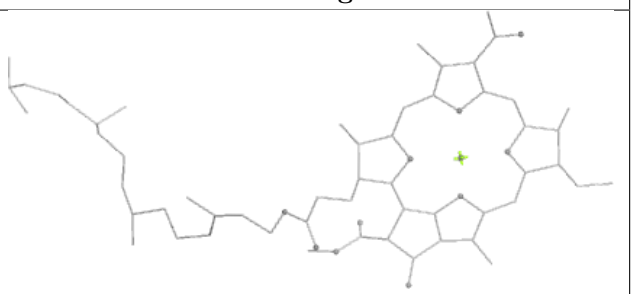
Bond lengths



Bond angles

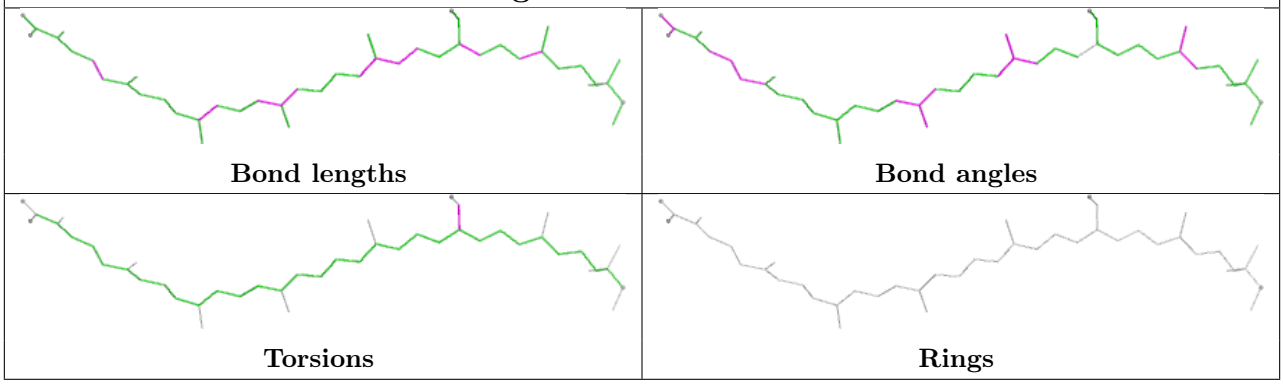


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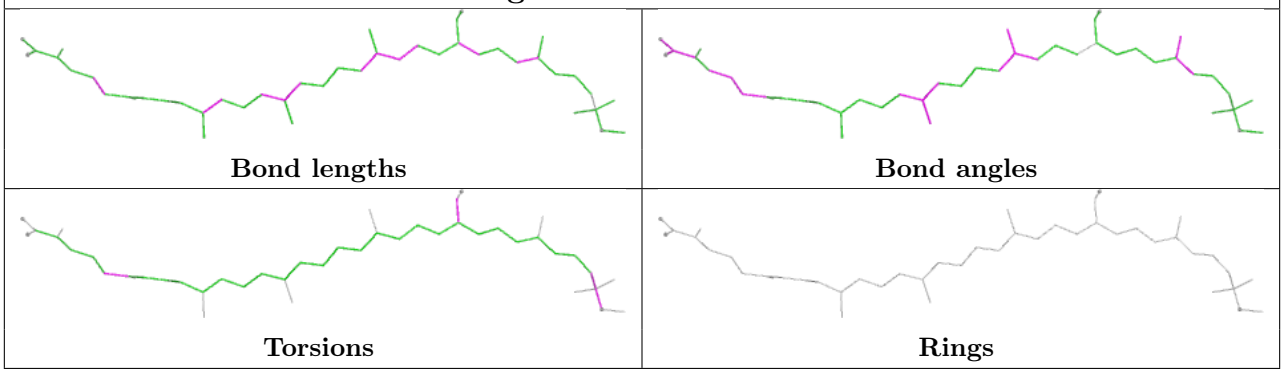


Rings

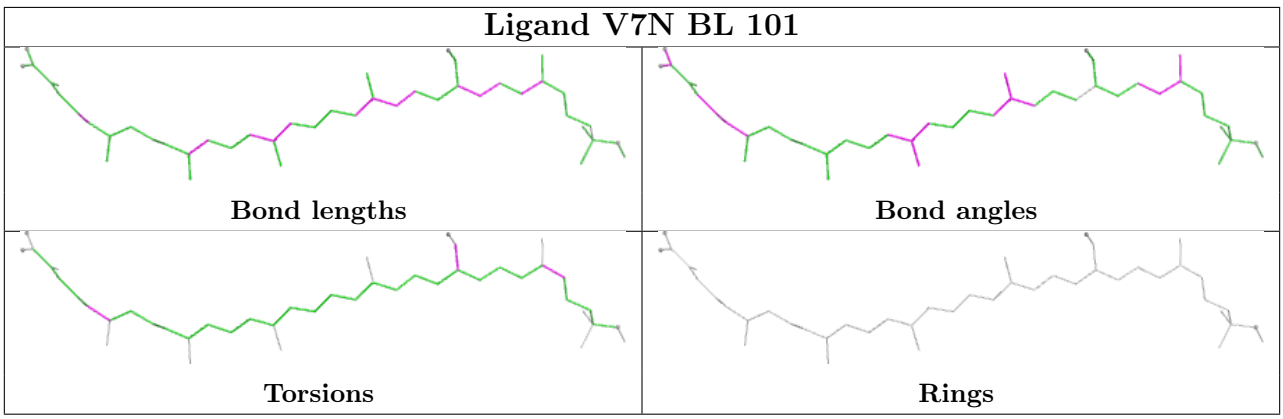
Ligand V7N BH 102



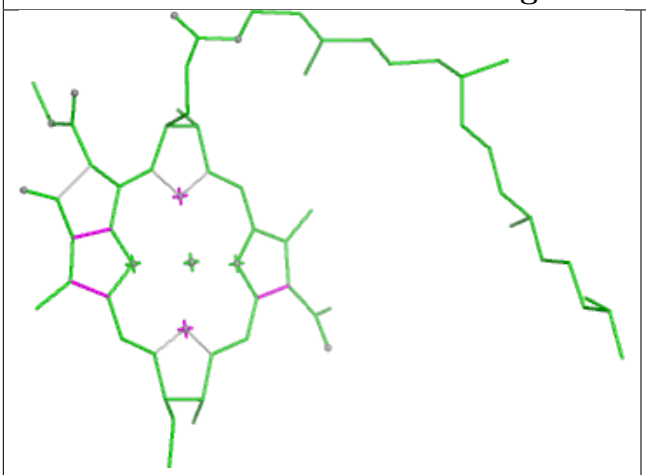
Ligand V7N Bd 1202



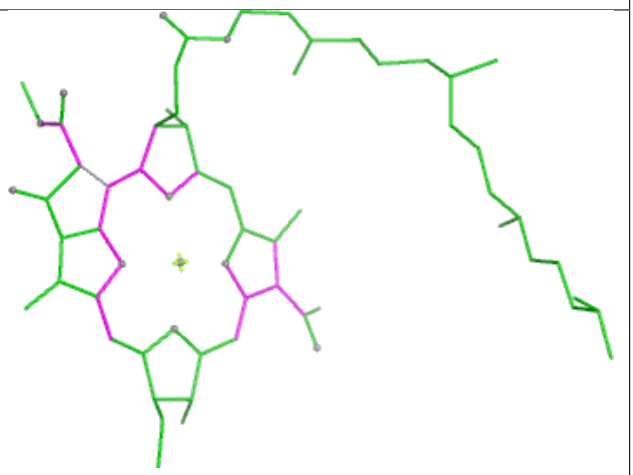
Ligand V7N BL 101



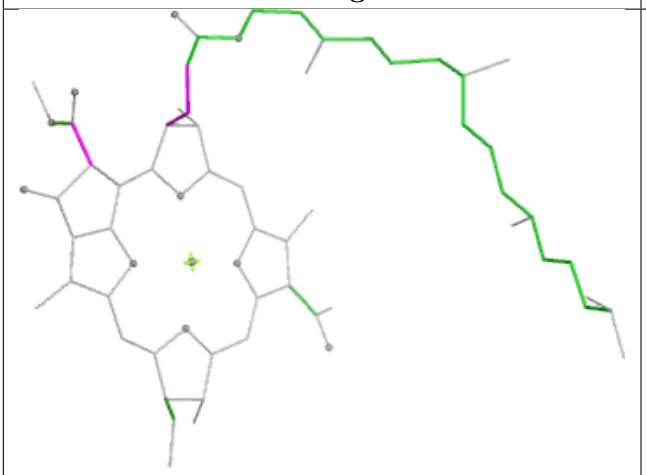
Ligand BCL Bi 102



Bond lengths



Bond angles

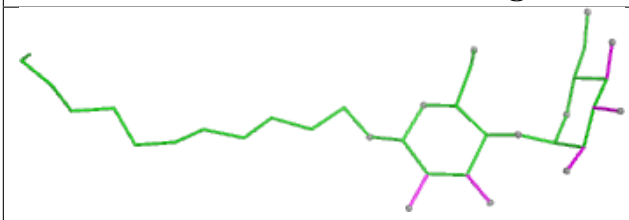


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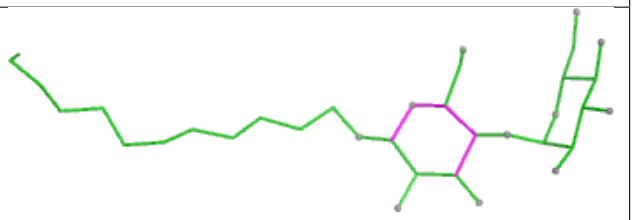


Rings

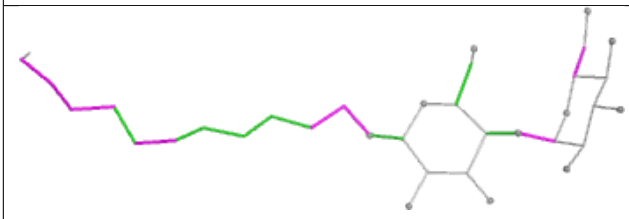
Ligand LMT BA 104



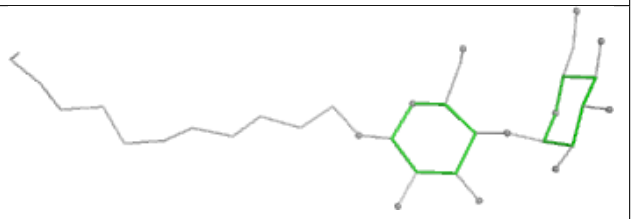
Bond lengths



Bond angles

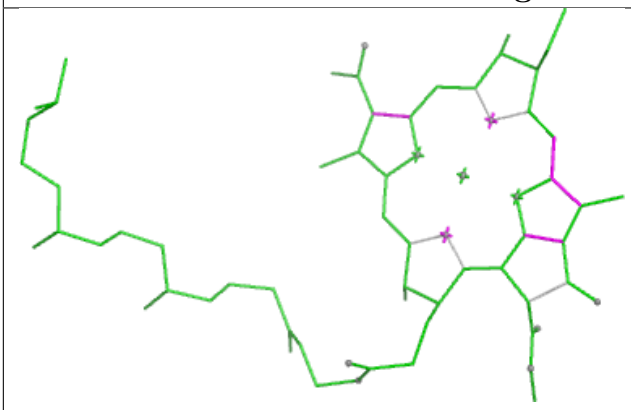


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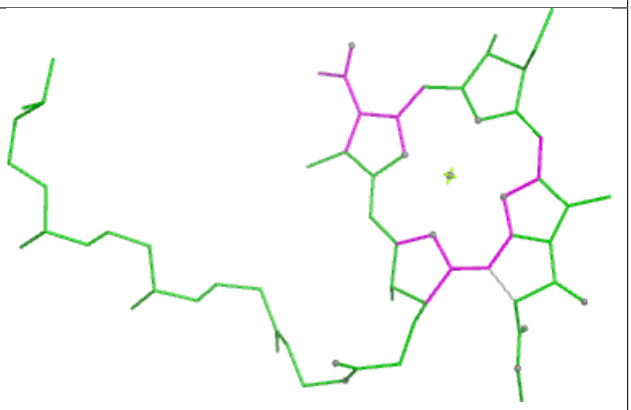


Rings

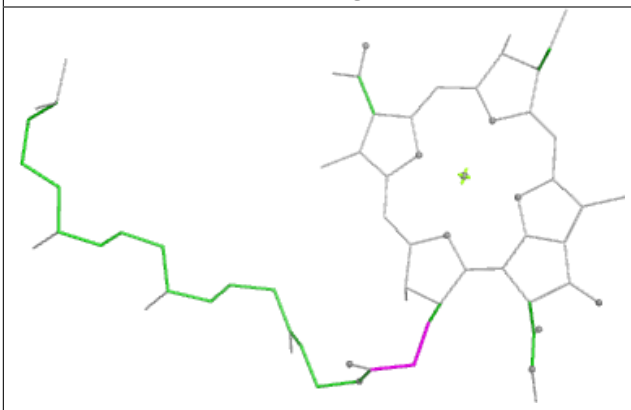
Ligand BCL BL 102



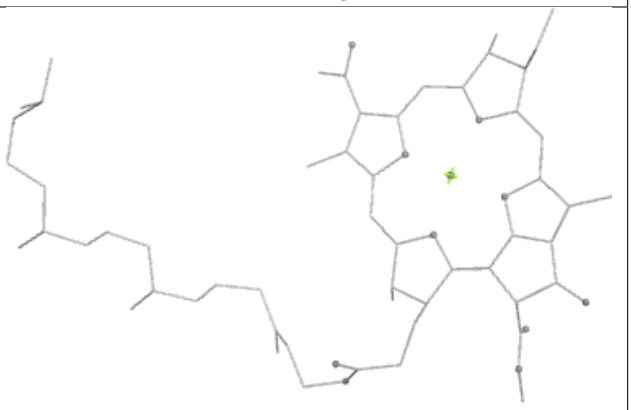
Bond lengths



Bond angles

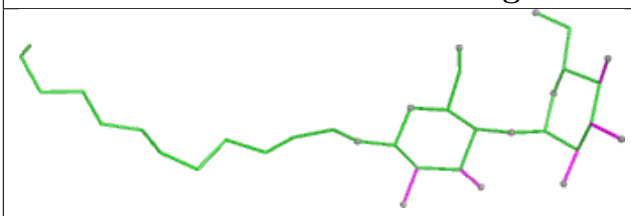


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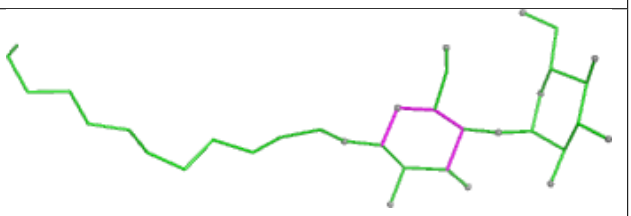


Rings

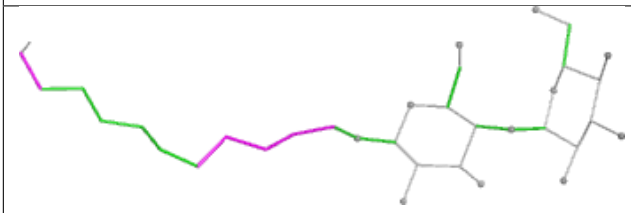
Ligand LMT Bh 1204



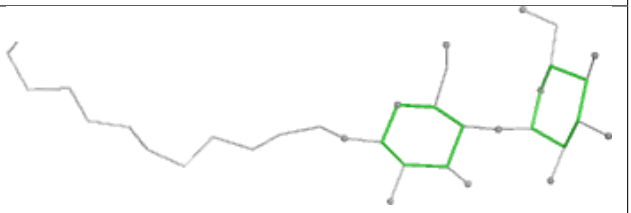
Bond lengths



Bond angles

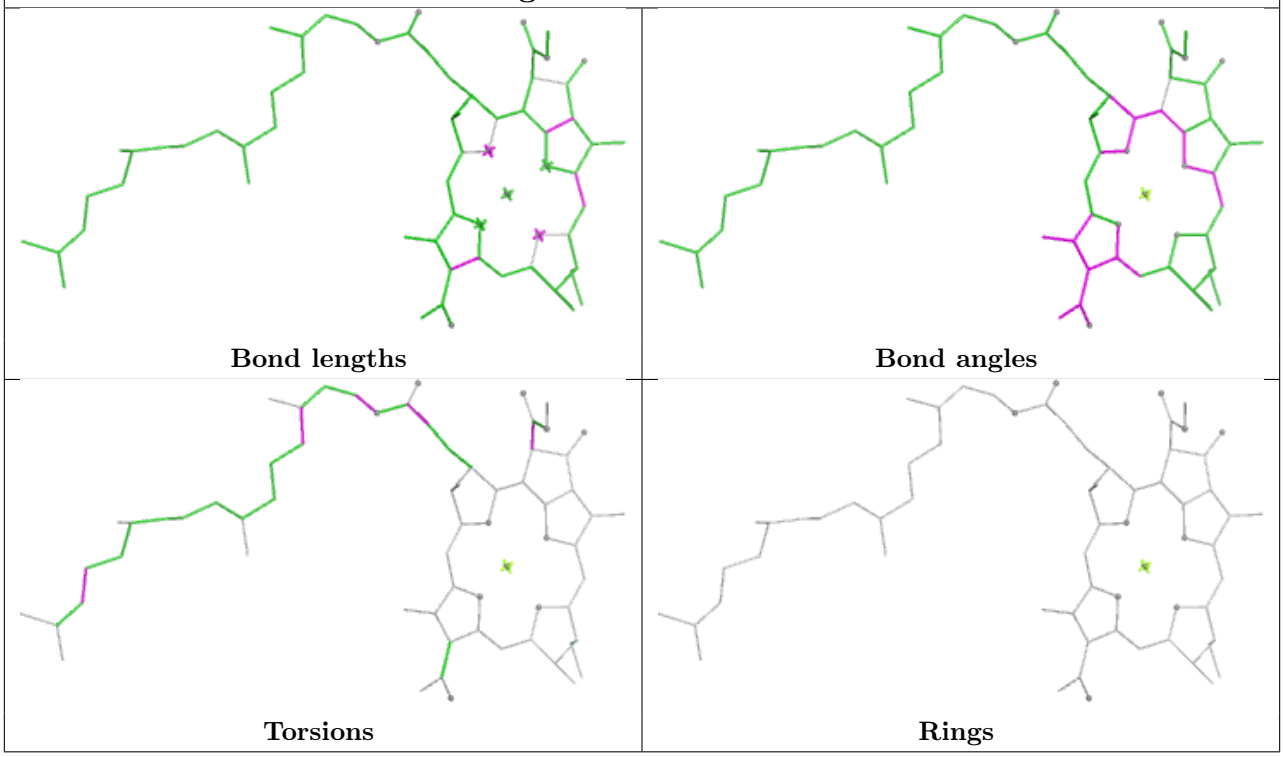


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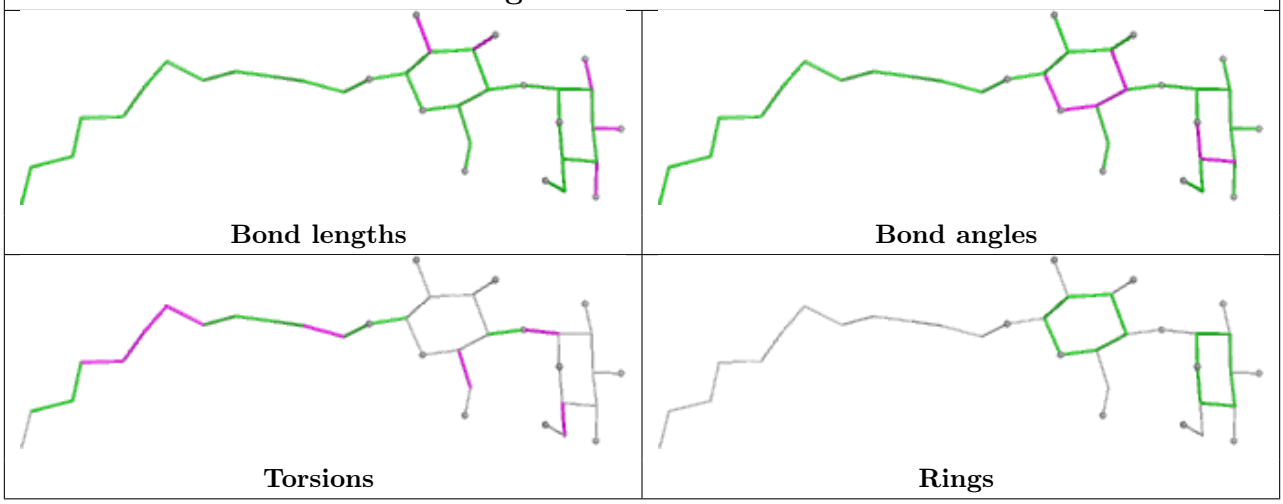


Rings

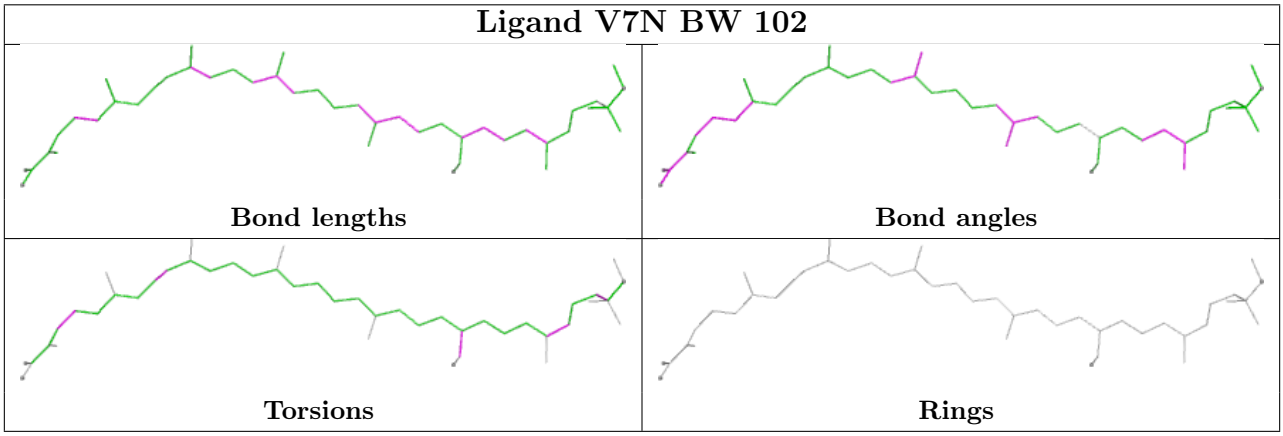
Ligand BCL AI 102



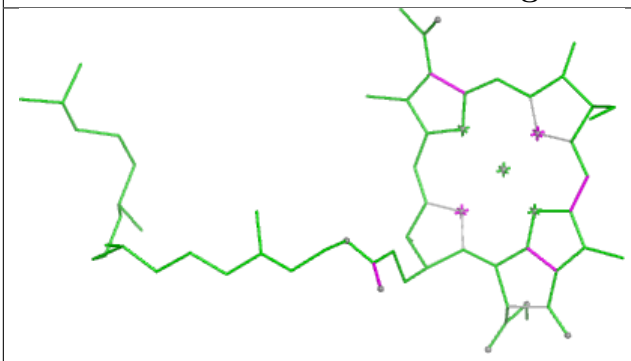
Ligand LMT Be 1102



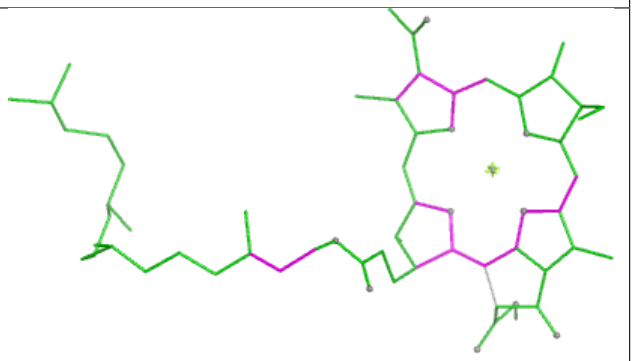
Ligand V7N BW 102



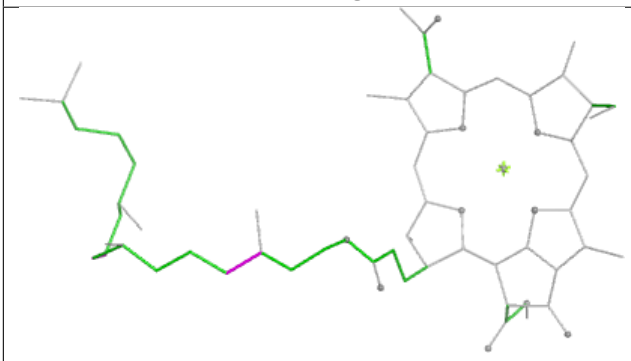
Ligand BCL M 404



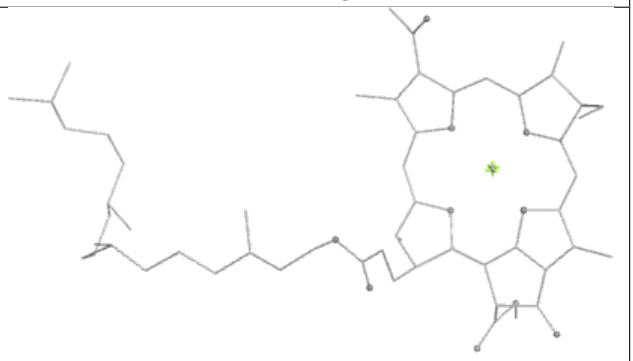
Bond lengths



Bond angles

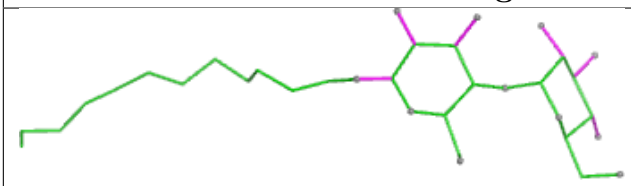


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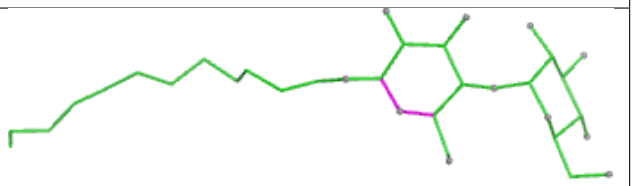


Rings

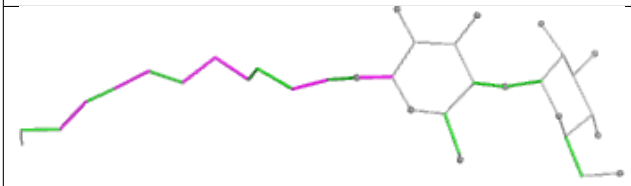
Ligand LMT BM 1001



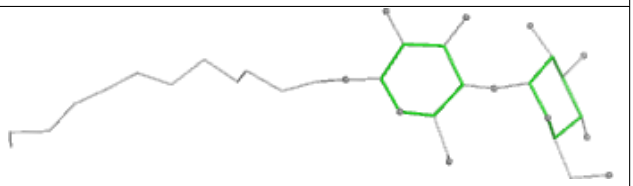
Bond lengths



Bond angles



Torsions

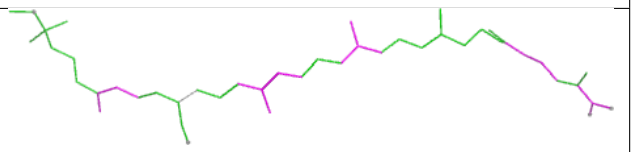


Rings

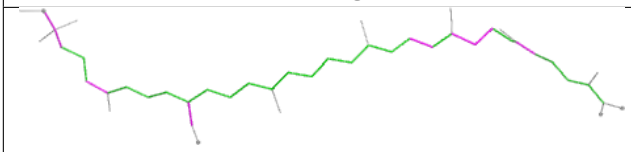
Ligand V7N Aa 101



Bond lengths



Bond angles

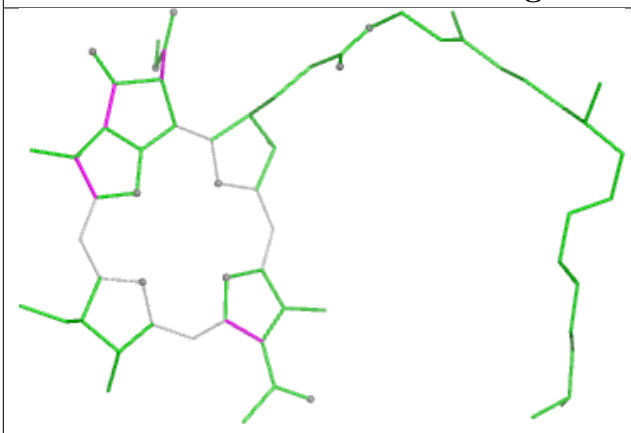


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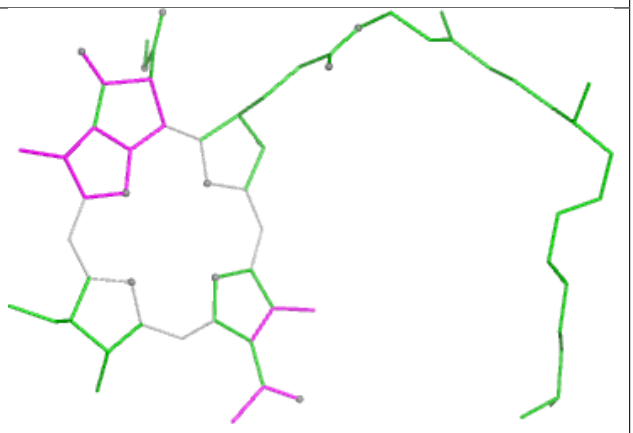


Rings

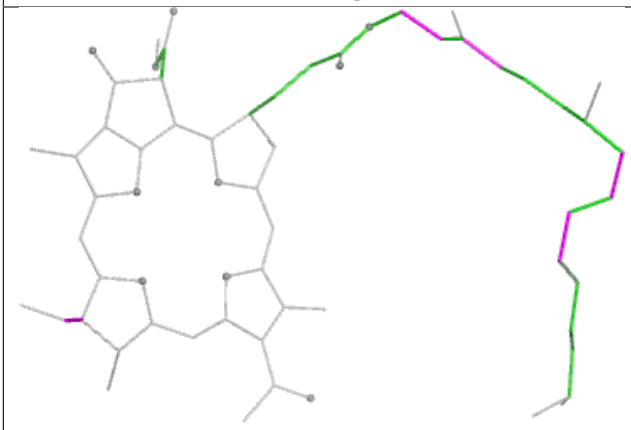
Ligand BPH L 303



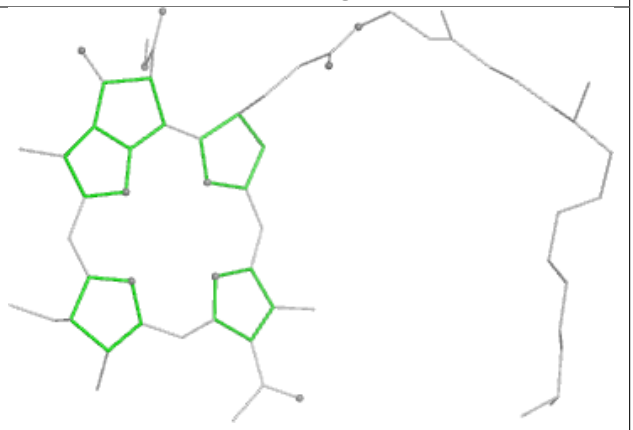
Bond lengths



Bond angles

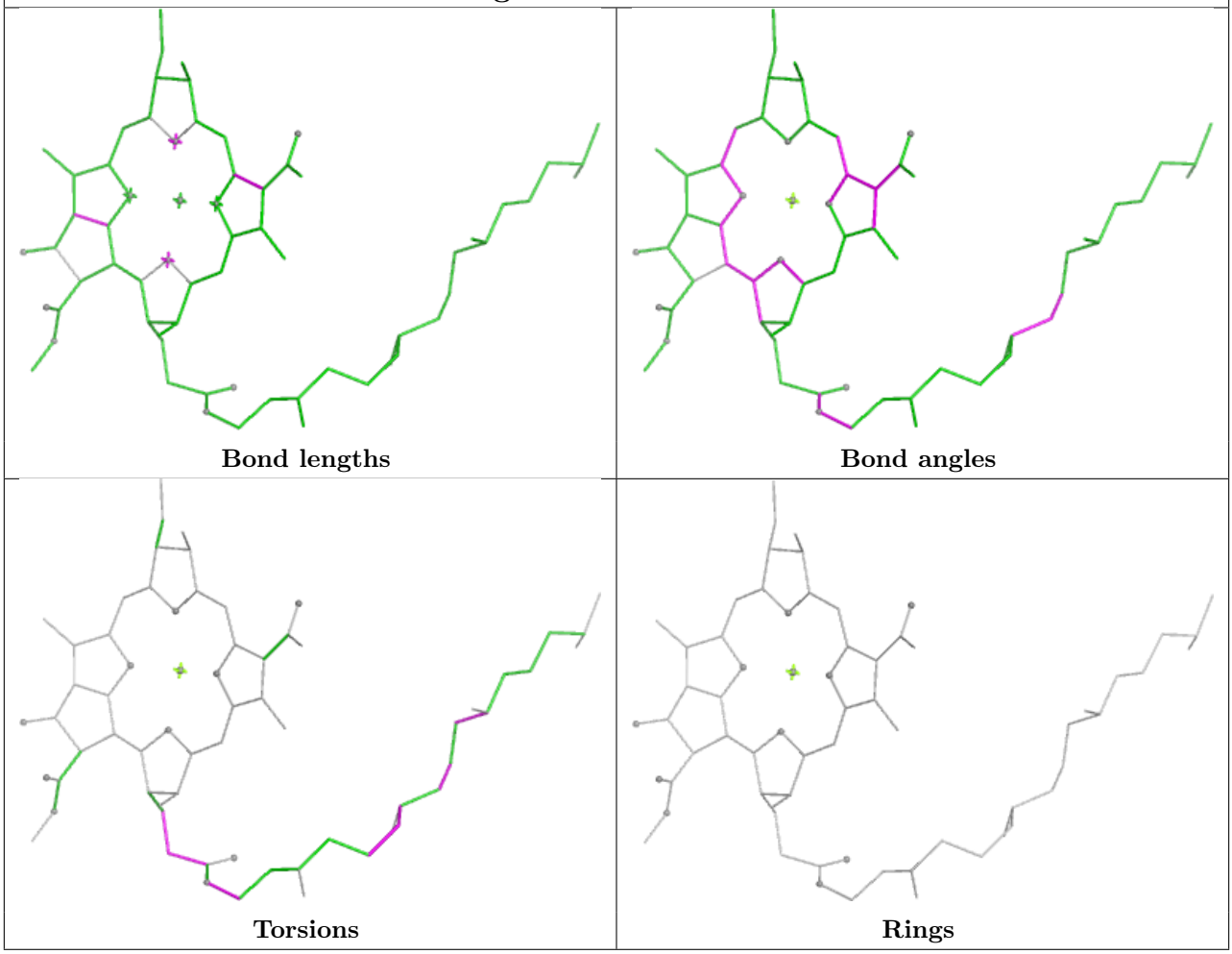


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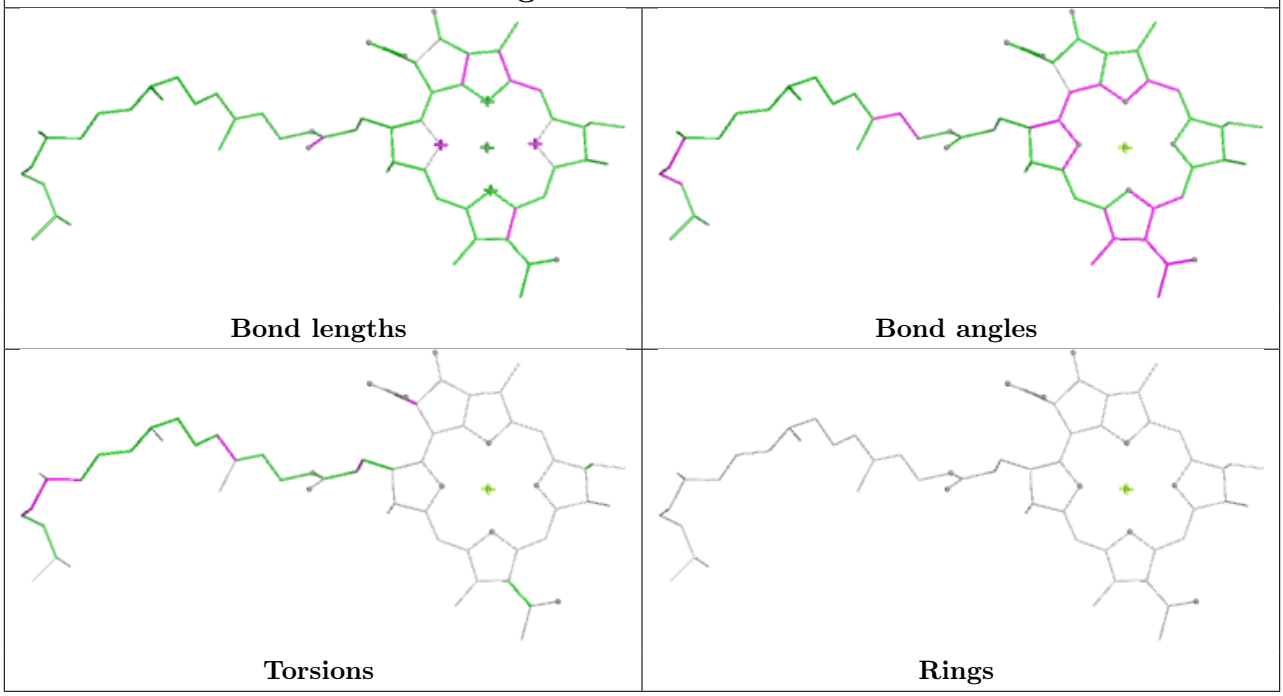


Rings

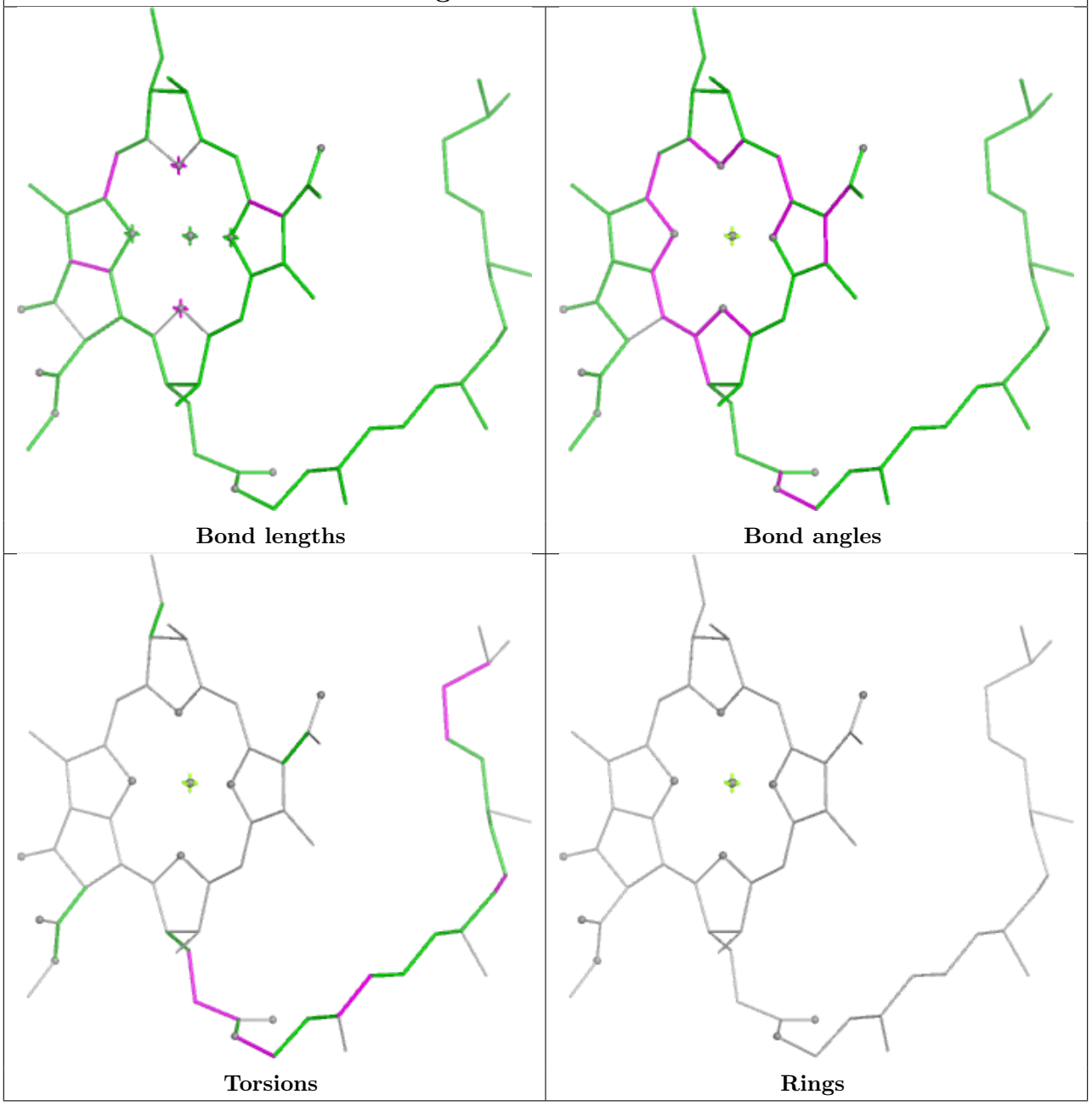
Ligand BCL BP 101



Ligand BCL Ae 101



Ligand BCL BV 102



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

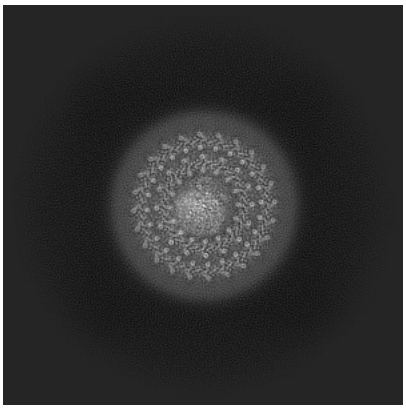
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-51760. These allow visual inspection of the internal detail of the map and identification of artifacts.

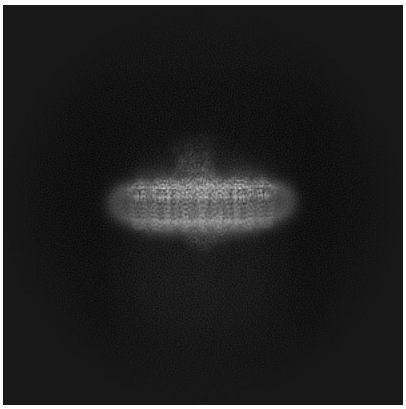
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

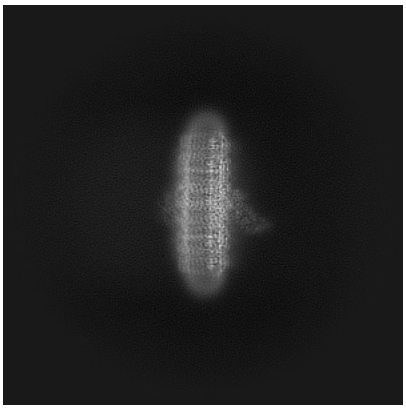
6.1.1 Primary map



X

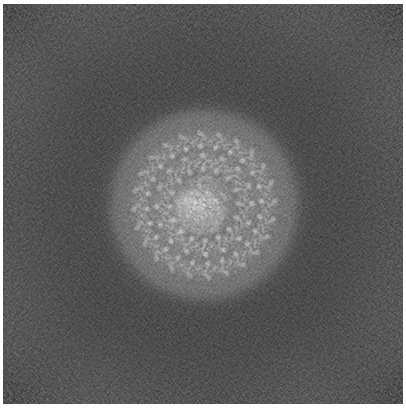


Y

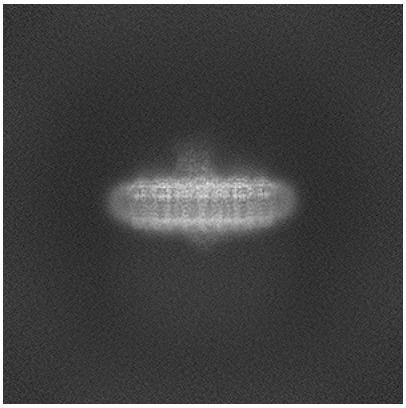


Z

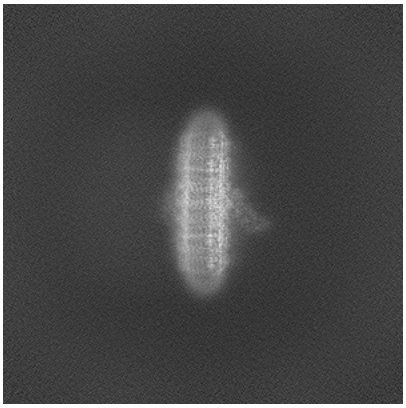
6.1.2 Raw map



X



Y

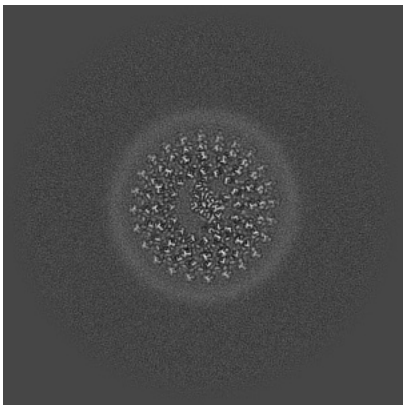


Z

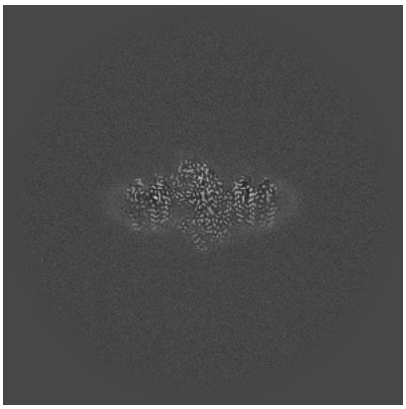
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

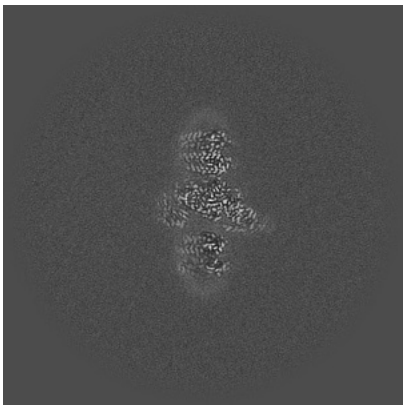
6.2.1 Primary map



X Index: 300

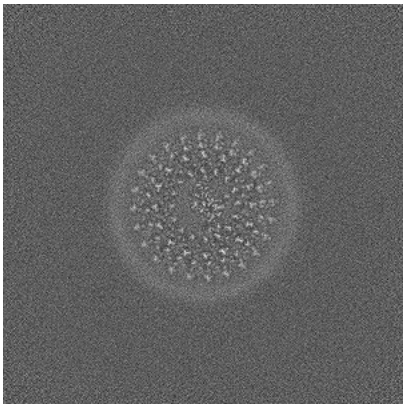


Y Index: 300

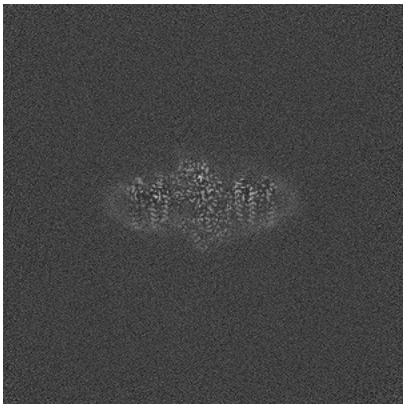


Z Index: 300

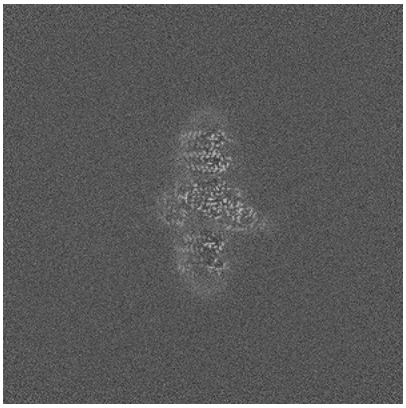
6.2.2 Raw map



X Index: 300



Y Index: 300

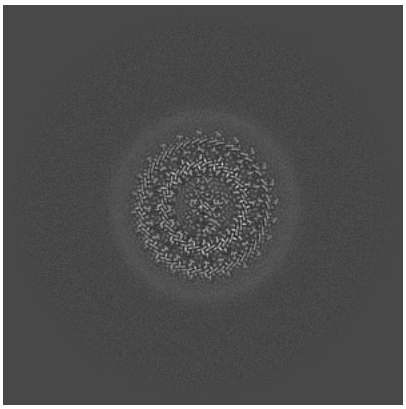


Z Index: 300

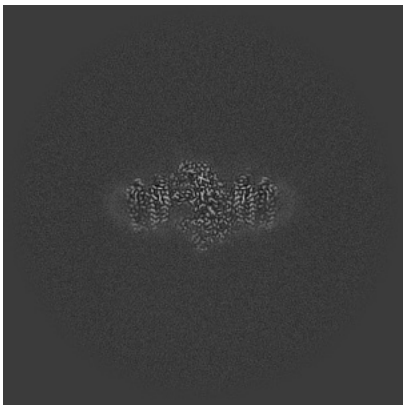
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

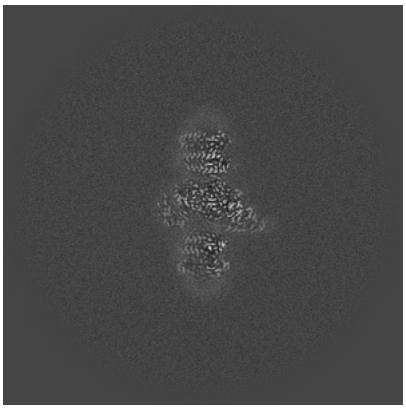
6.3.1 Primary map



X Index: 311

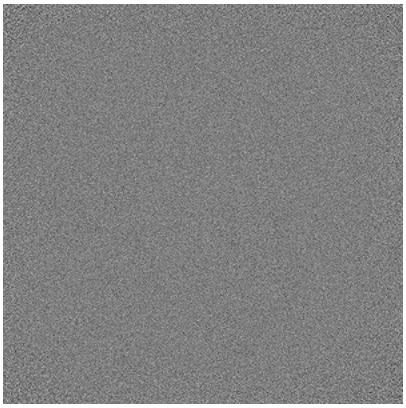


Y Index: 301

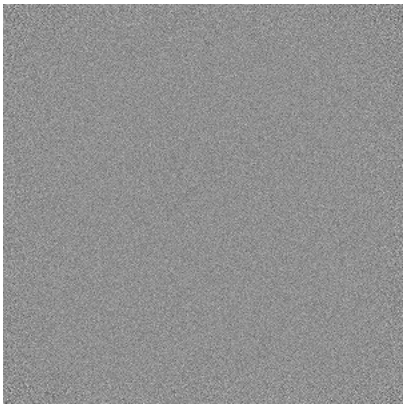


Z Index: 299

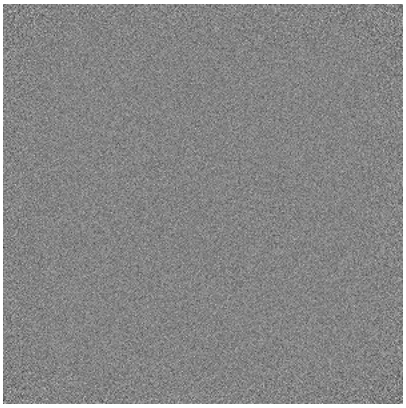
6.3.2 Raw map



X Index: 0



Y Index: 0

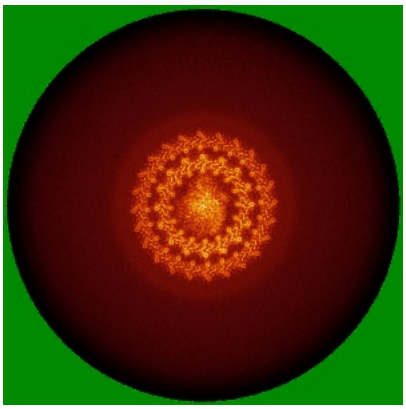


Z Index: 599

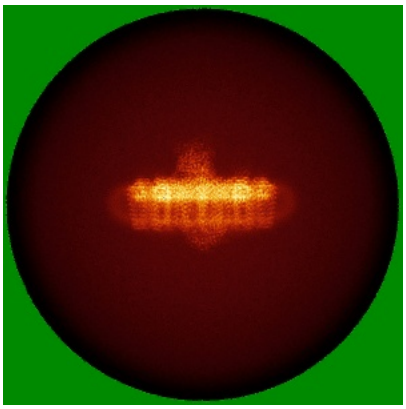
The images above show the largest variance slices of the map in three orthogonal directions.

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

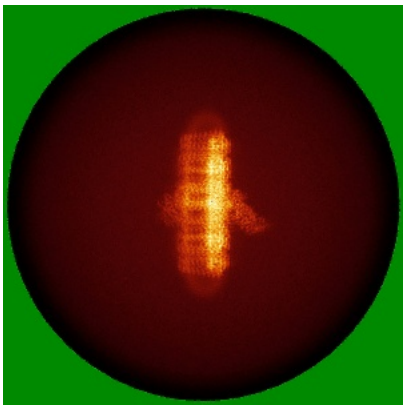
6.4.1 Primary map



X

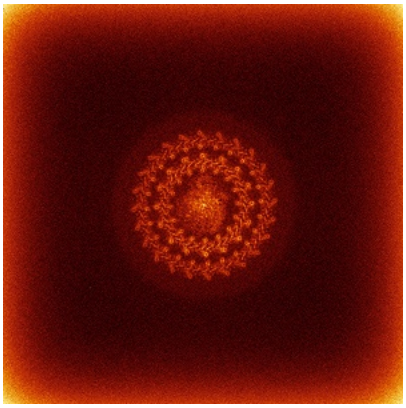


Y

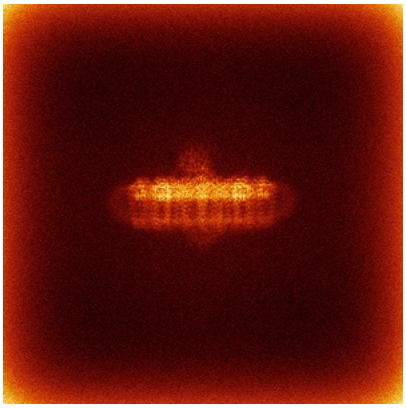


Z

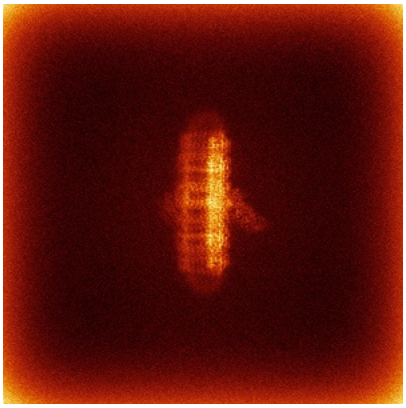
6.4.2 Raw map



X



Y

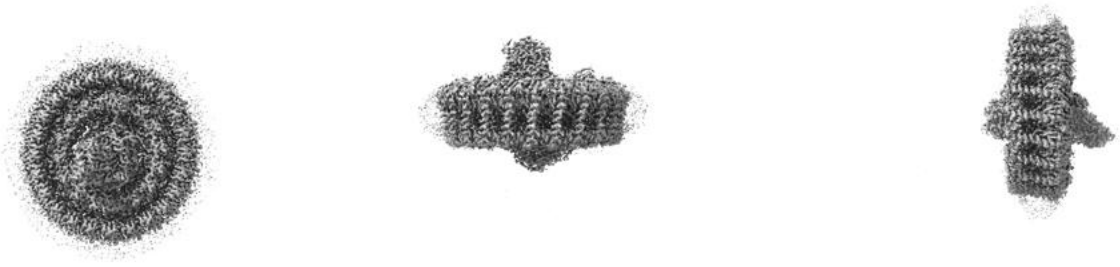


Z

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 0.0687. 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.

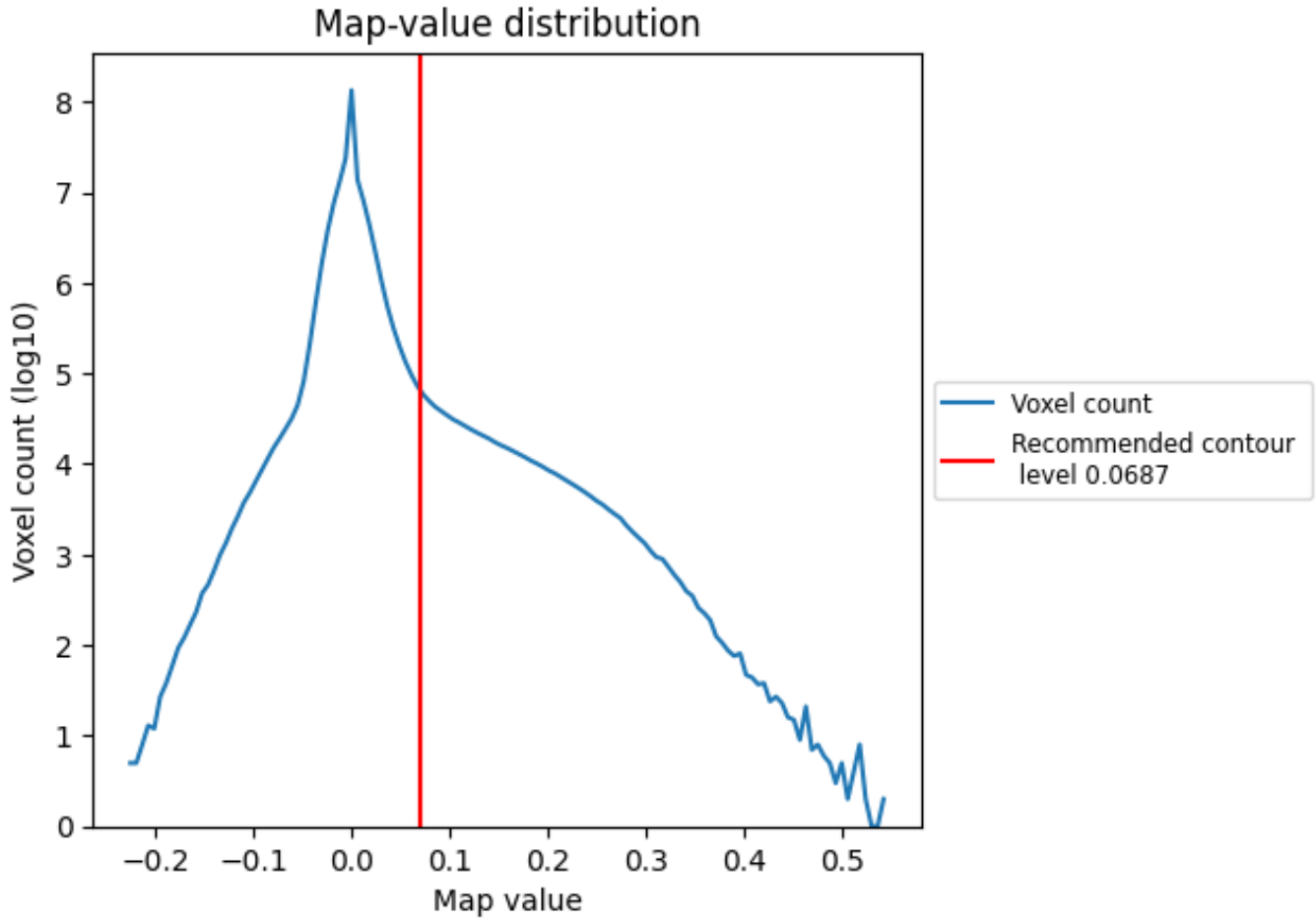
6.6 Mask visualisation (i)

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

7 Map analysis

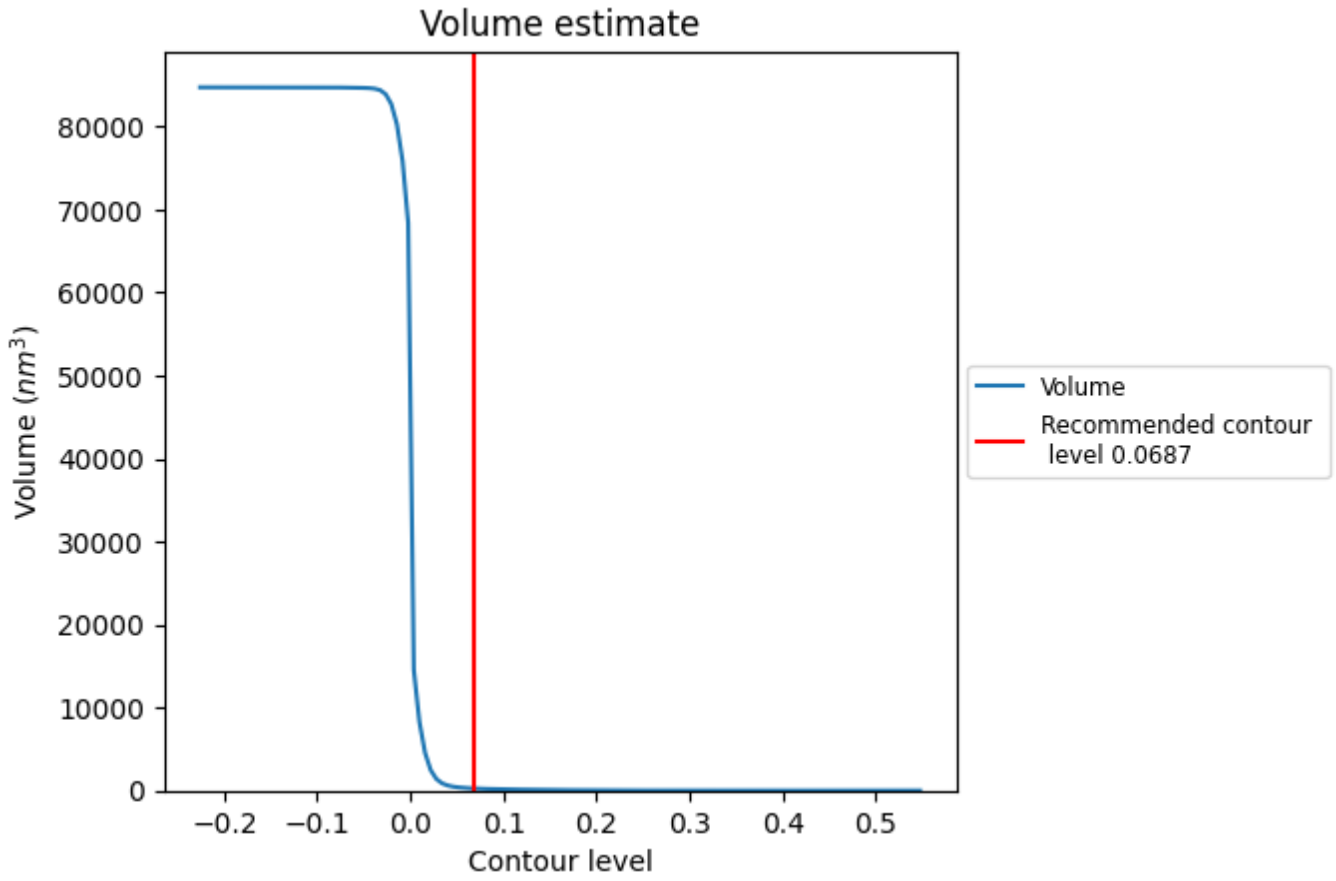
This section contains the results of statistical analysis of the map.

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.

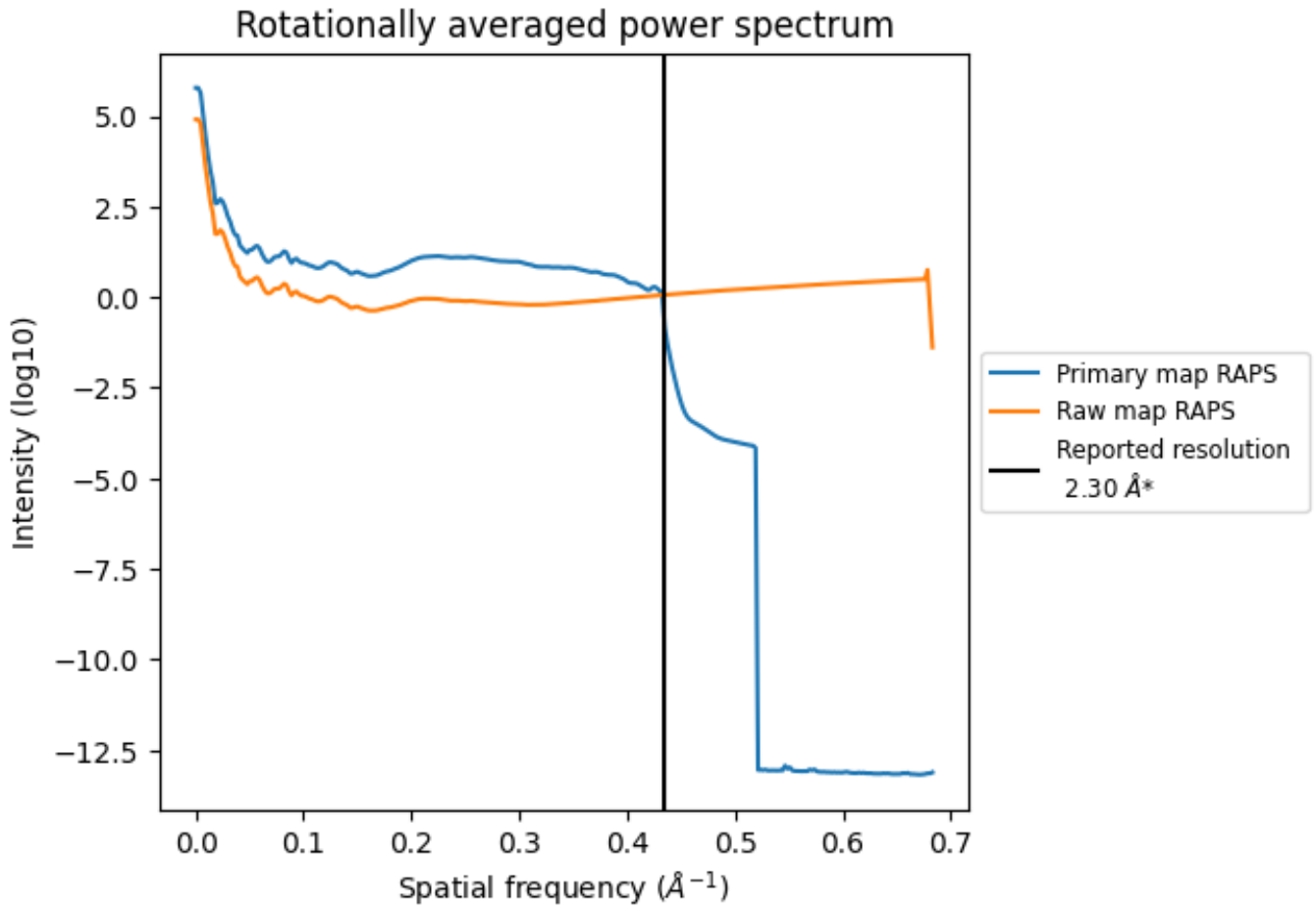
7.2 Volume estimate



The volume at the recommended contour level is 251 nm^3; this corresponds to an approximate mass of 227 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)

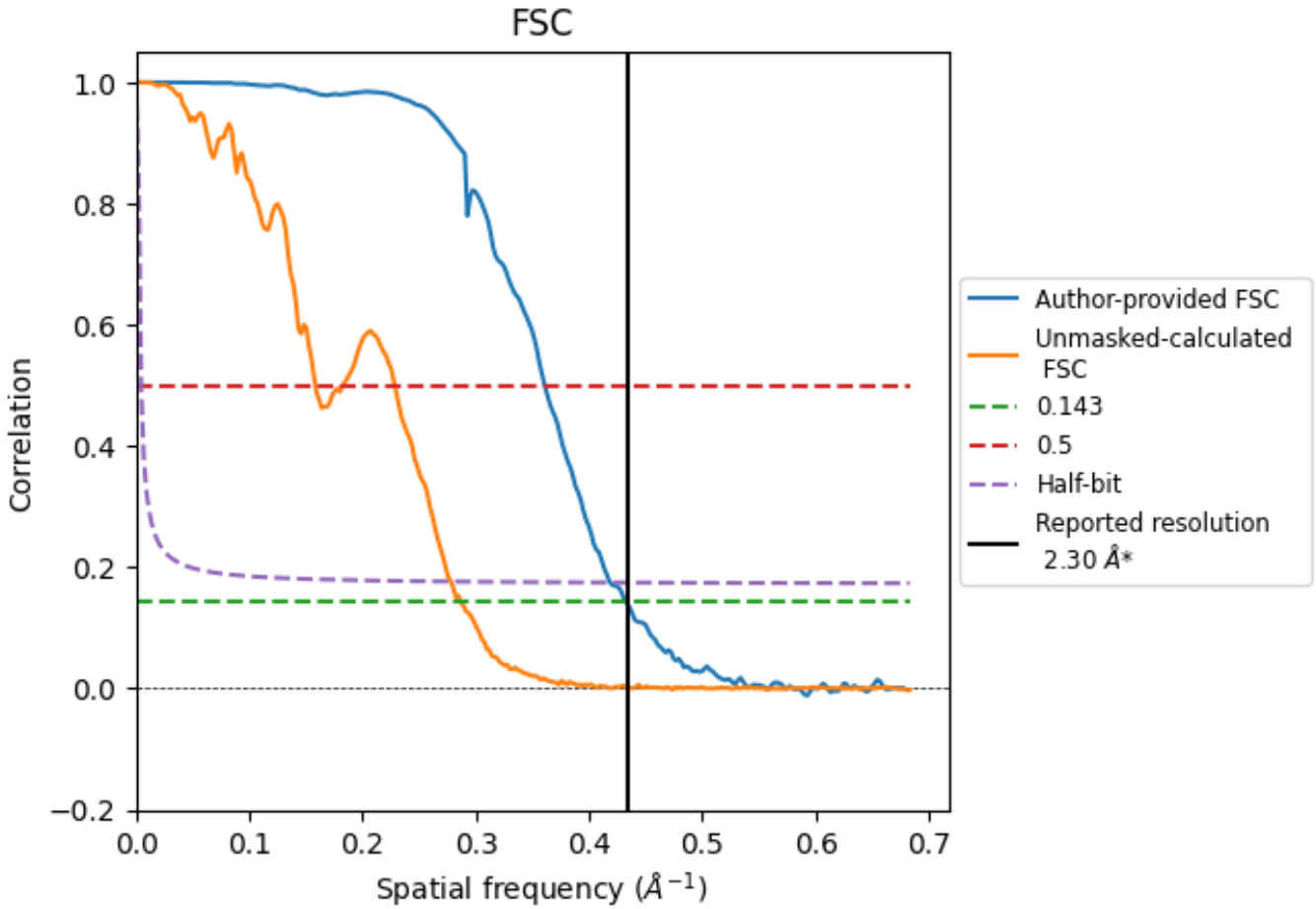


*Reported resolution corresponds to spatial frequency of 0.435 $Å^{-1}$

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 0.435 Å^{-1}

8.2 Resolution estimates (i)

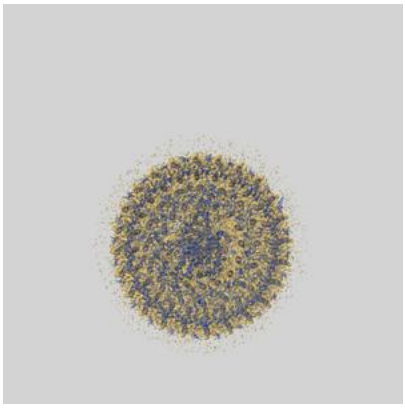
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.30	-	-
Author-provided FSC curve	2.31	2.77	2.39
Unmasked-calculated*	3.49	6.32	3.60

*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 3.49 differs from the reported value 2.3 by more than 10 %

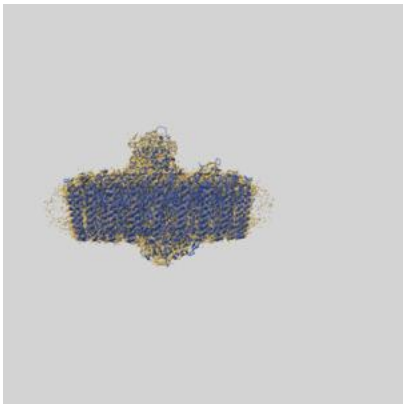
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-51760 and PDB model 9H19. Per-residue inclusion information can be found in section 3 on page 27.

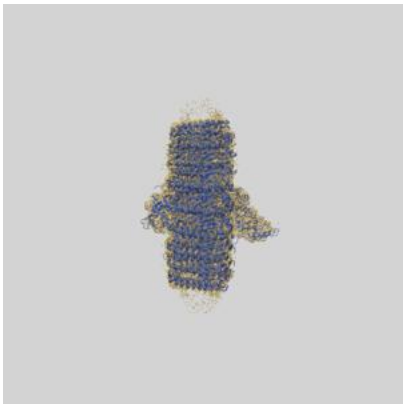
9.1 Map-model overlay



X



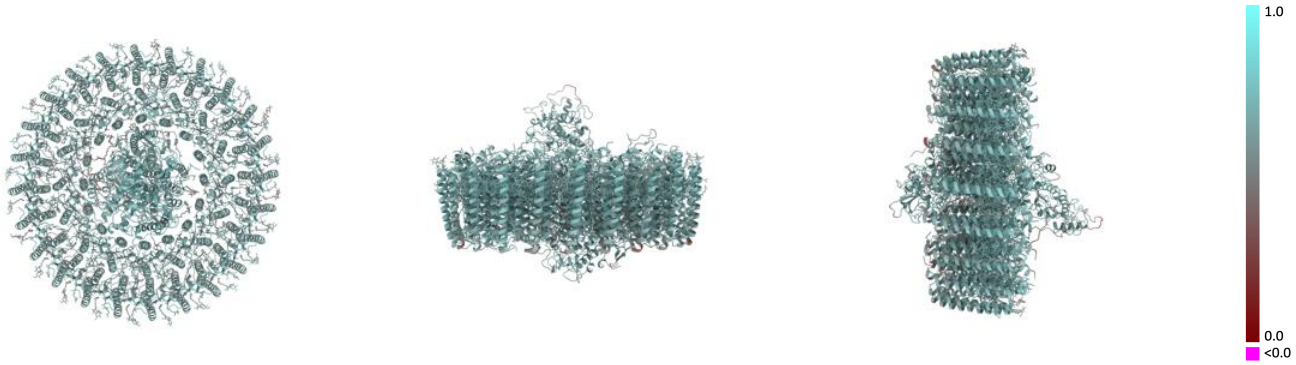
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0687 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.

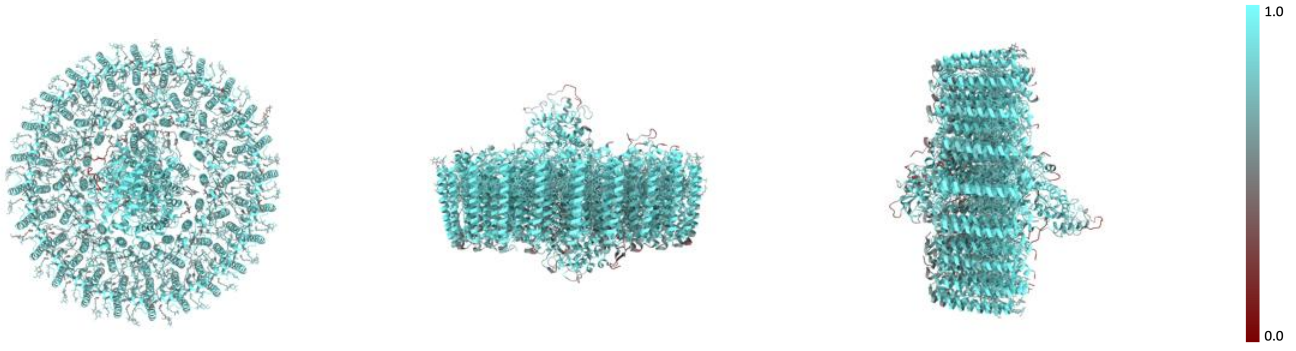
9.2 Q-score mapped to coordinate model (i)



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.

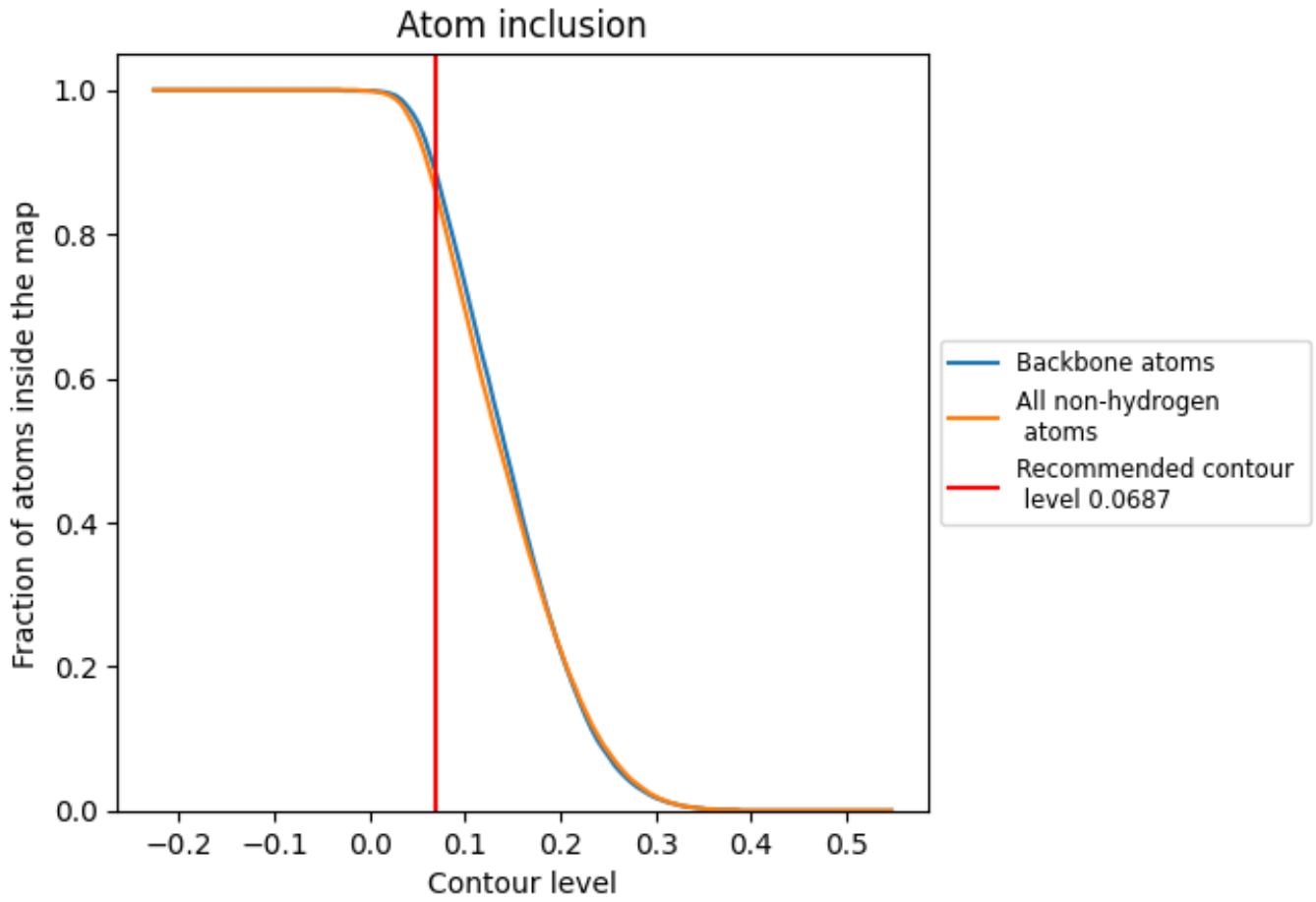
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0687).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 86% 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 (0.0687) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8630	0.6400
AA	0.9230	0.6540
AB	0.8400	0.6280
AC	0.9150	0.6520
AD	0.9100	0.6460
AE	0.8320	0.6320
AF	0.8840	0.6390
AG	0.8880	0.6450
AH	0.8370	0.6310
AI	0.8410	0.6360
AJ	0.8870	0.6450
AK	0.8210	0.6220
AL	0.8860	0.6360
AM	0.8680	0.6290
AN	0.8430	0.6310
AO	0.8850	0.6440
AP	0.8960	0.6410
AQ	0.8110	0.6200
AR	0.8650	0.6390
AS	0.8590	0.6270
AT	0.7960	0.6160
AU	0.8630	0.6340
AV	0.9210	0.6460
AW	0.8110	0.6230
AX	0.9080	0.6480
Aa	0.7400	0.5820
Ab	0.8950	0.6480
Ac	0.9160	0.6550
Ad	0.8350	0.6300
Ae	0.8930	0.6580
Af	0.8440	0.6320
Ag	0.9050	0.6450
Ah	0.9180	0.6580
Ai	0.8550	0.6320
Aj	0.8510	0.6370



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Chain	Atom inclusion	Q-score
Ak	0.9510	0.6740
Al	0.9370	0.6650
Am	0.9420	0.6700
An	0.9370	0.6630
Ao	0.8830	0.6450
Ap	0.8980	0.6350
BA	0.8520	0.6330
BB	0.8130	0.6180
BC	0.8810	0.6380
BD	0.8830	0.6490
BE	0.8120	0.6020
BF	0.8580	0.6280
BG	0.8540	0.6270
BH	0.8000	0.5960
BI	0.8620	0.6290
BJ	0.8930	0.6440
BK	0.7670	0.6010
BL	0.8560	0.6320
BM	0.8740	0.6290
BN	0.8610	0.6280
BO	0.8340	0.6240
BP	0.8510	0.6350
BQ	0.8010	0.6050
BR	0.8480	0.6300
BS	0.8410	0.6030
BT	0.7680	0.5560
BU	0.8060	0.5860
BV	0.8350	0.6220
BW	0.8190	0.6160
BX	0.8670	0.6400
Ba	0.8120	0.6140
Bb	0.8480	0.6360
Bc	0.8570	0.6410
Bd	0.8810	0.6520
Be	0.8650	0.6430
Bf	0.8750	0.6510
Bg	0.8590	0.6410
Bh	0.8450	0.6360
Bi	0.7950	0.6150
Bj	0.8450	0.6470
Bk	0.8860	0.6590
Bl	0.8970	0.6660

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Chain	Atom inclusion	Q-score
Bm	0.8810	0.6500
Bn	0.8790	0.6500
Bo	0.8420	0.6360
Bp	0.8480	0.6400
C	0.8740	0.6460
H	0.7870	0.6460
K	0.7460	0.6060
L	0.9510	0.6890
M	0.9380	0.6800
S	0.8520	0.6610